



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2024 – 01:48 PM JST

PDB ID : 8KC3
EMDB ID : EMD-37091
Title : Cryo-EM structure of human C-terminally bound ATG9A-ATG2A-WIPI4 complex
Authors : Wang, Y.; Stjepanovic, G.
Deposited on : 2023-08-05
Resolution : 7.00 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:

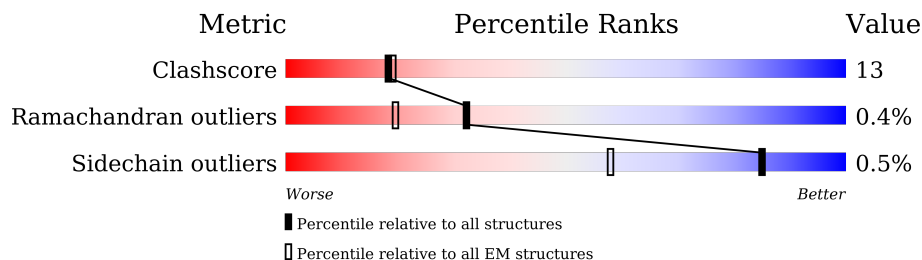
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

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 7.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	839	
1	B	839	
1	C	839	
2	D	360	
3	E	1938	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15687 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 Autophagy-related protein 9A.

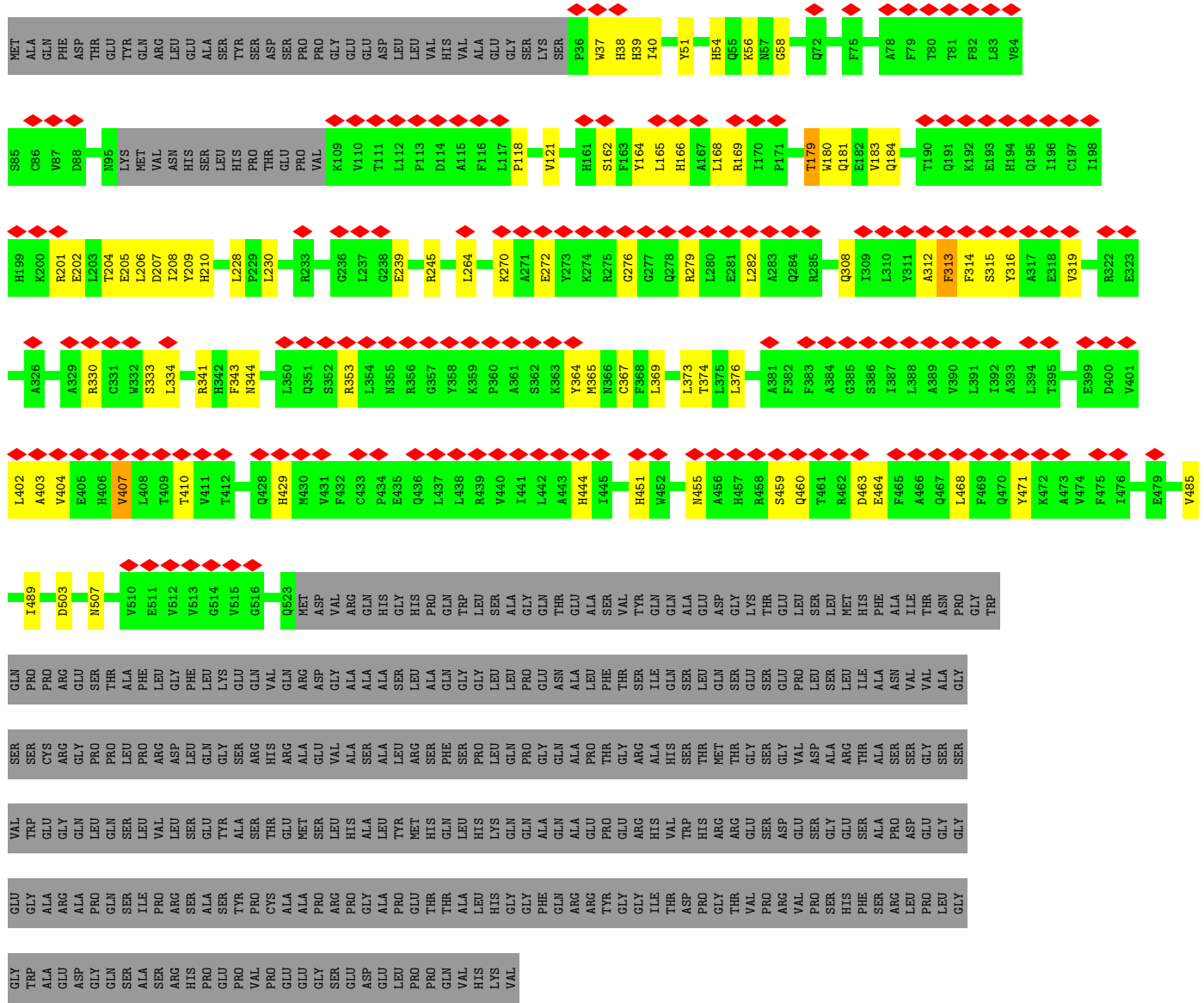
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	475	Total	C	N	O	S	0	0
			2998	1891	559	543	5		
1	B	475	Total	C	N	O	S	0	0
			2926	1843	548	532	3		
1	C	475	Total	C	N	O	S	0	0
			2936	1858	538	535	5		

- Molecule 2 is a protein called WD repeat domain phosphoinositide-interacting protein 4.

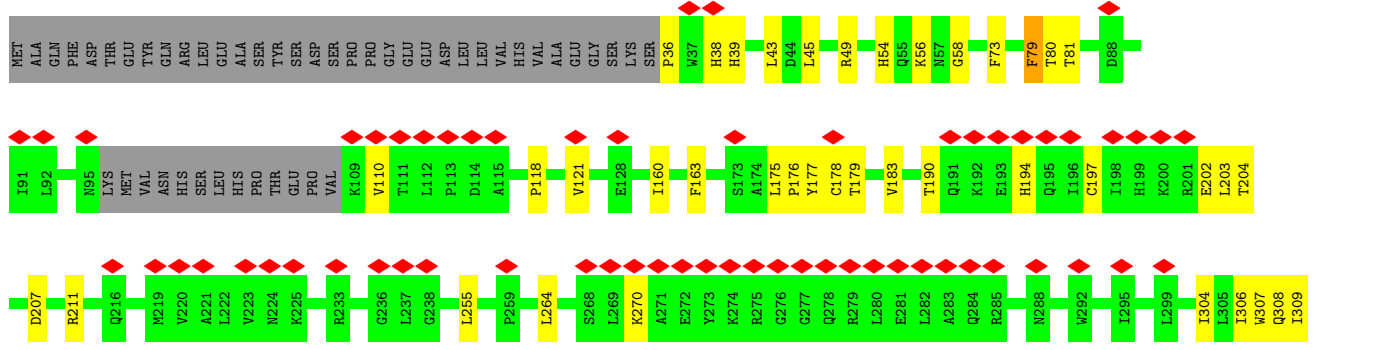
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	360	Total	C	N	O	0	0
			1777	1057	360	360		

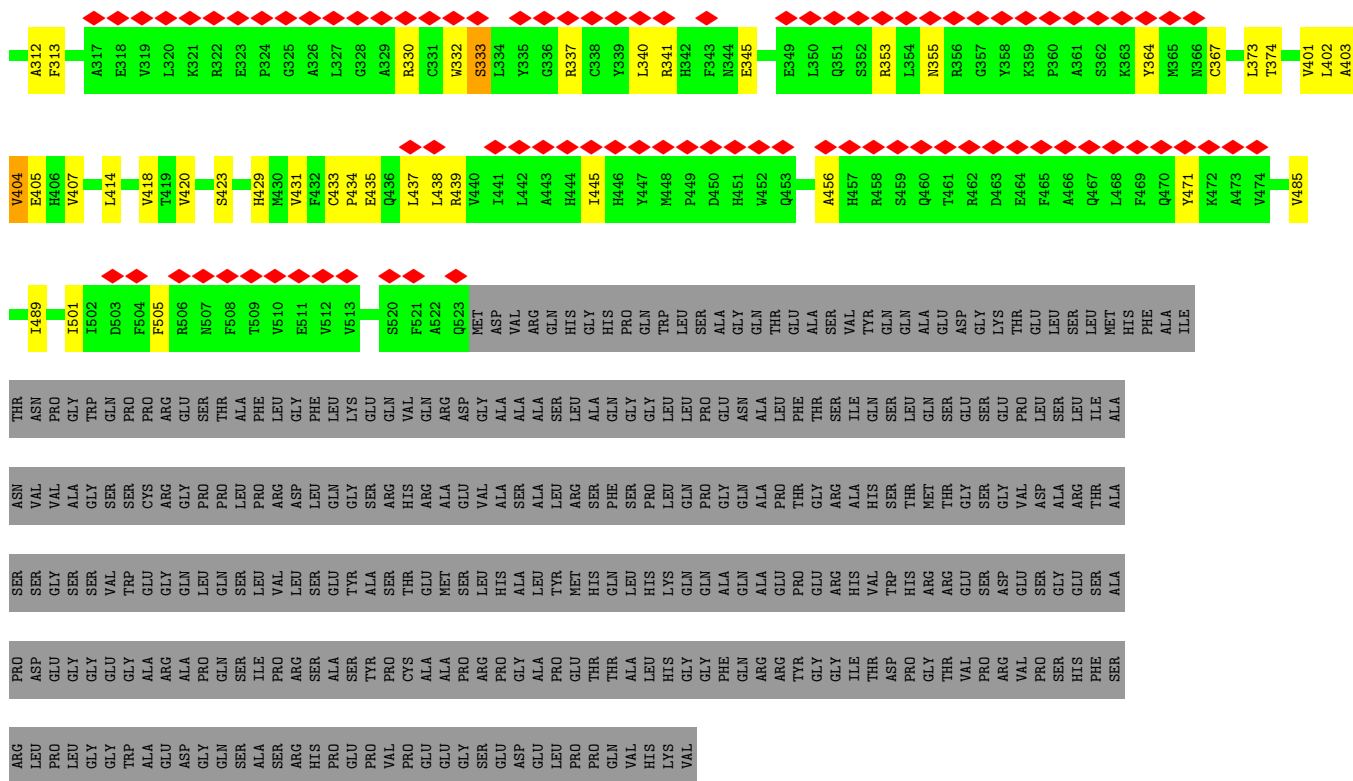
- Molecule 3 is a protein called Autophagy-related protein 2 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	830	Total	C	N	O	S	0	0
			5050	3121	934	980	15		

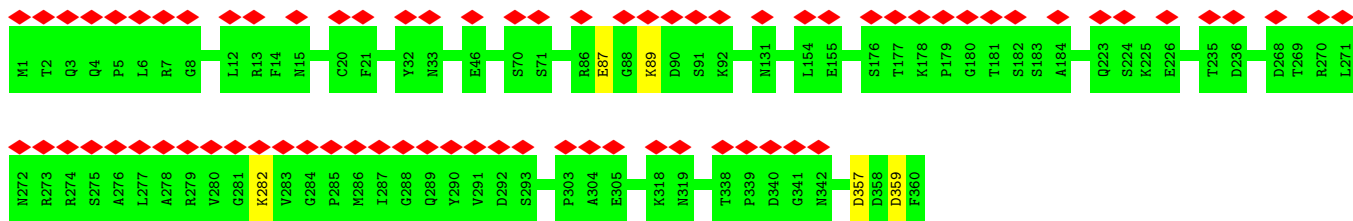


• Molecule 1: Autophagy-related protein 9A

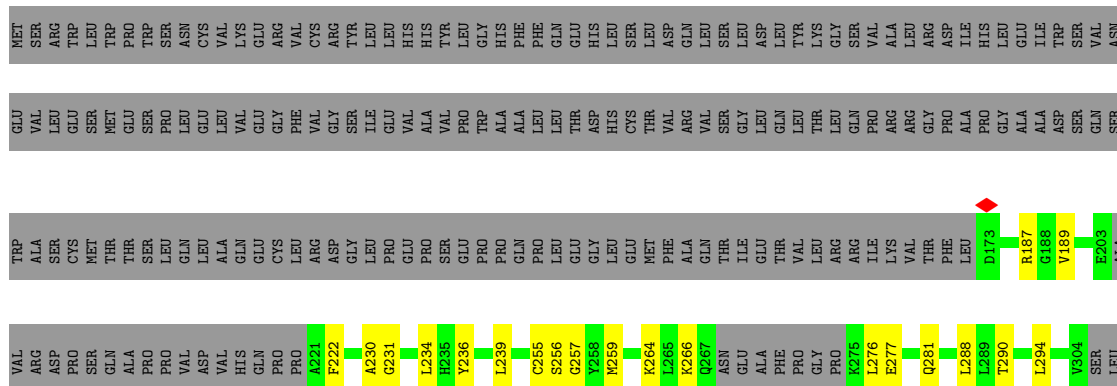
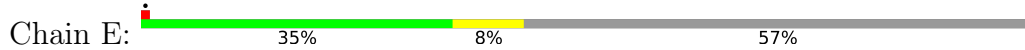




• Molecule 2: WD repeat domain phosphoinositide-interacting protein 4



• Molecule 3: Autophagy-related protein 2 homolog A



HIS	S1555	L1558	V1565	ALA	PRO	THR	THR	THR	GLY	GLY	GLN	GLU	ALA	PRO	GLY	GLY	GLY	ASN	LEU	GLY	GLY	PRO	PRO	GLU	C1576	C1577	L1578	S1581	R1586	L1587	F1596	D1599	V1604	I1608	S1614	GLU	THR	SER	ALA	GLU	ALA	ARG	PRO	PRO	ARG	ALA	GLN	PRO	SER	SER	PRO	LEU	GLU	GLY	GLN	ASN	CYS	S1705	L1709	K1710	R1711	GLY	VAL	GLU																					
THR	THR	GLY	SER	GLN	GLU	ALA	PRO	GLY	GLY	GLY	ASN	HIS	SER	PRO	SER	PRO	PRO	ASP	GLN	GLN	GLN	PRO	THR	PHE	R1665	T1670	S1671	E1672	V1673	W1676	L1677	D1678	TYR	HIS	GLY	GLY	LYS	HIS	VAL	THR	THR	MET	ASP	GLN	VAL	VAL	GLY	GLY	ARG	TRP	LEU	LEU	PRO	PRO	ILE	ILE	GLU	THR	TYR	ARG	LYS	ASP	ARG	TYR	GLY	ARG	LEU	LEU	ARG	MET	ARG	GLY	GLN	LEU	LEU	GLN	ASN	CYS	S1705	L1709	K1710	R1711	GLY	VAL	GLU
SER	SER	THR	ALA	SER	ALA	ILE	ARG	LYS	ASN	GLN	LEU	PRO	ARG	LEU	LEU	VAL	GLN	ALA	ILE	VAL	GLY	GLY	VAL	PRO	MET	HIS	SER	VAL	VAL	VAL	GLN	ASP	LEU	PHE	GLY	GLY	PHE	ARG	ASP	LEU	LEU	TRP	LEU	LEU	SER	SER	LEU	LEU	ILE	ILE	GLU	ASP	LYS	ARG	TYR	ARG	LYS	ASP	ALA	ARG	GLY	ARG	LEU	LEU	ARG	MET	ARG	GLY	GLN	LEU	LEU	GLN	ASN	CYS	S1705	L1709	K1710	R1711	GLY	VAL	GLU				
VAL	ALA	LYS	ALA	TYR	ASP	THR	VAL	VAL	ARG	GLY	GLY	ILE	LEU	ASP	ASP	THR	ALA	GLN	THR	ILE	CYS	ASP	VAL	VAL	ALA	GLU	ASP	SER	THR	VAL	ARG	GLY	HIS	GLU	GLN	LYS	GLY	LEU	THR	GLY	VAL	VAL	GLY	GLY	VAL	ILE	ILE	ARG	GLN	LEU	PRO	PRO	THR	VAL	VAL	LYS	PRO	PRO	LEU	LEU	ILE	LEU	ALA	ALA	THR	GLU	ALA	THR	SER	SER															
LEU	LEU	GLY	MET	ASN	GLN	ILE	PRO	ASP	ALA	HIS	LYS	ASP	HIS	ALA	LEU	LYS	TRP	ARG	SER	ASP	SER	ALA	GLN	ASP	ALA	GLN	ASP	ALA	GLY	HIS	GLU	GLN	LYS	GLY	LEU	THR	GLY	VAL	VAL	GLY	GLY	VAL	ILE	ILE	ARG	GLN	LEU	PRO	PRO	THR	VAL	VAL	LYS	PRO	PRO	LEU	LEU	ILE	LEU	ALA	ALA	THR	GLU	ALA	THR	SER	SER																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65.17	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.843	Depositor
Minimum map value	-0.351	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/3061	0.63	3/4225 (0.1%)
1	B	0.48	0/2983	0.63	2/4119 (0.0%)
1	C	0.50	0/3005	0.65	3/4157 (0.1%)
2	D	0.35	0/1776	0.73	0/2471
3	E	0.26	0/5077	0.56	1/6963 (0.0%)
All	All	0.42	0/15902	0.63	9/21935 (0.0%)

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	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	LEU	N-CA-C	7.26	130.61	111.00
1	B	367	CYS	N-CA-C	7.04	130.00	111.00
1	A	404	VAL	N-CA-C	-7.03	92.02	111.00
1	A	465	PHE	N-CA-C	-5.61	95.86	111.00
1	C	404	VAL	N-CA-C	-5.57	95.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	308	GLN	Mainchain

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Mol	Chain	Res	Type	Group
2	D	359	ASP	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	2998	0	2145	91	0
1	B	2926	0	2016	59	0
1	C	2936	0	1987	88	0
2	D	1777	0	789	2	0
3	E	5050	0	3675	108	0
All	All	15687	0	10612	338	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 13.

The worst 5 of 338 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:C:340:LEU:HD22	1:C:445:ILE:CG2	1.67	1.23
1:C:364:TYR:CE1	1:C:438:LEU:HD21	1.83	1.12
1:A:368:PHE:CZ	1:A:433:CYS:HB3	1.92	1.04
1:A:438:LEU:HD12	1:A:456:ALA:HB1	1.43	0.97
1:A:438:LEU:HD12	1:A:456:ALA:CB	1.95	0.97

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	471/839 (56%)	436 (93%)	34 (7%)	1 (0%)	44	78
1	B	471/839 (56%)	431 (92%)	38 (8%)	2 (0%)	30	68
1	C	471/839 (56%)	432 (92%)	37 (8%)	2 (0%)	30	68
2	D	358/360 (99%)	345 (96%)	11 (3%)	2 (1%)	22	60
3	E	776/1938 (40%)	681 (88%)	92 (12%)	3 (0%)	30	68
All	All	2547/4815 (53%)	2325 (91%)	212 (8%)	10 (0%)	32	68

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	282	LYS
3	E	673	LEU
1	B	407	VAL
1	B	179	THR
3	E	602	ARG

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	165/717 (23%)	164 (99%)	1 (1%)	84	88
1	B	142/717 (20%)	140 (99%)	2 (1%)	62	75
1	C	147/717 (20%)	146 (99%)	1 (1%)	81	87
3	E	304/1662 (18%)	304 (100%)	0	100	100
All	All	758/3813 (20%)	754 (100%)	4 (0%)	85	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	PHE
1	B	313	PHE
1	B	341	ARG

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Mol	Chain	Res	Type
1	C	79	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	ASN
1	B	366	ASN
3	E	802	GLN
1	C	342	HIS
1	C	406	HIS

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](#)

There are no ligands in this entry.

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.

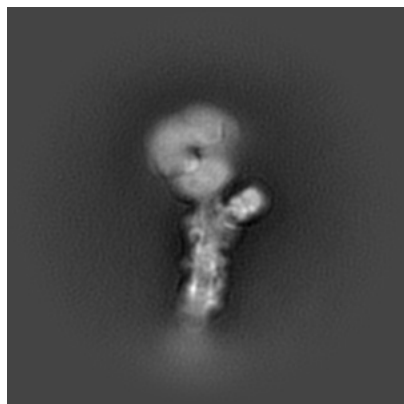
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37091. These allow visual inspection of the internal detail of the map and identification of artifacts.

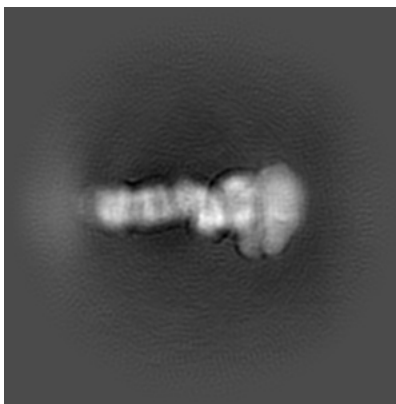
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

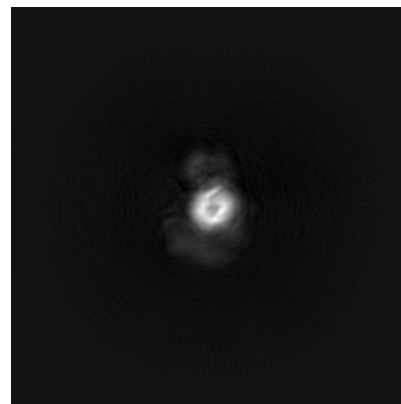
6.1.1 Primary map



X

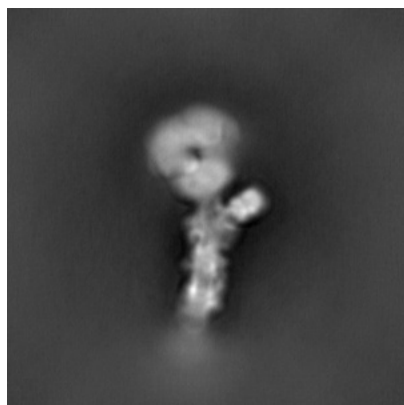


Y

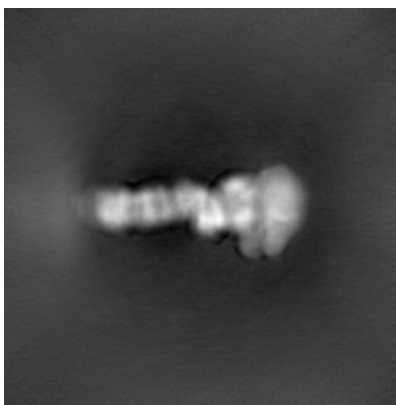


Z

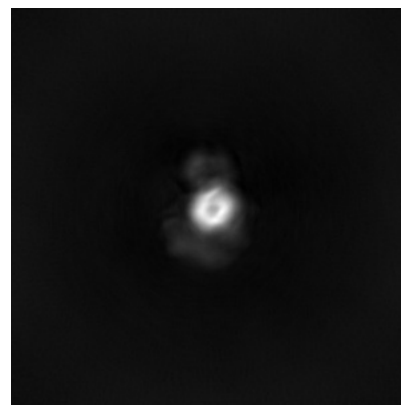
6.1.2 Raw map



X



Y



Z

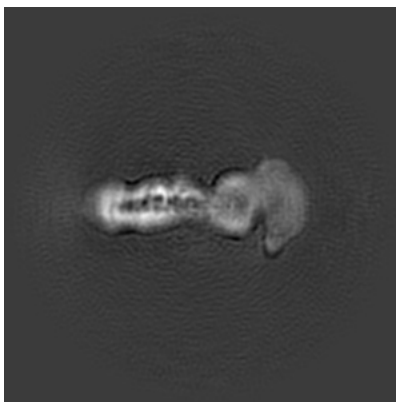
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

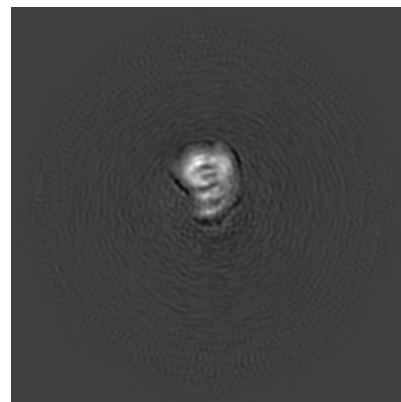
6.2.1 Primary map



X Index: 300



Y Index: 300

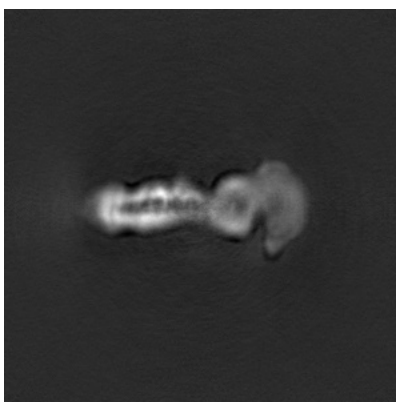


Z Index: 300

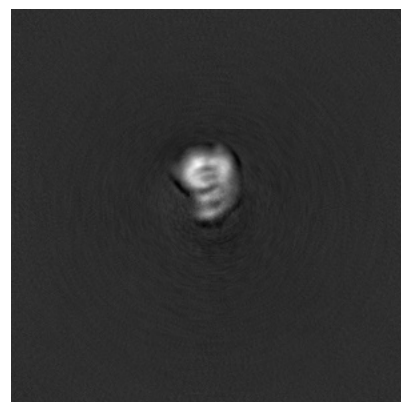
6.2.2 Raw map



X Index: 300



Y Index: 300

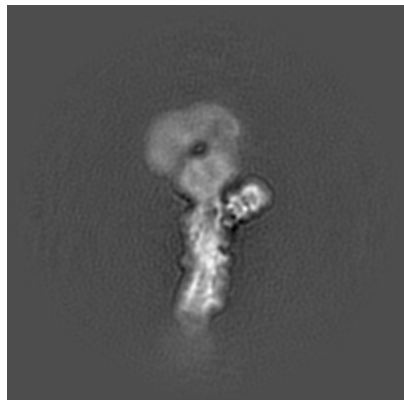


Z Index: 300

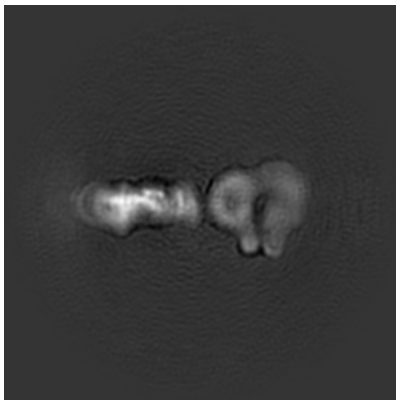
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

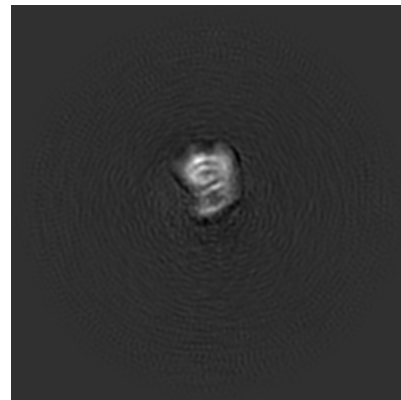
6.3.1 Primary map



X Index: 289

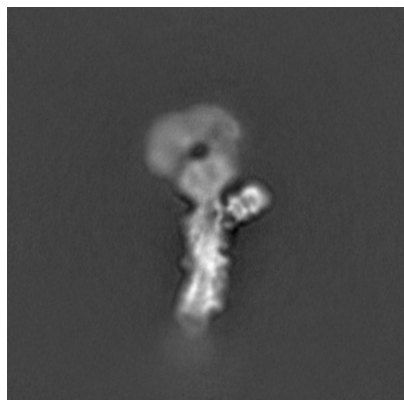


Y Index: 281

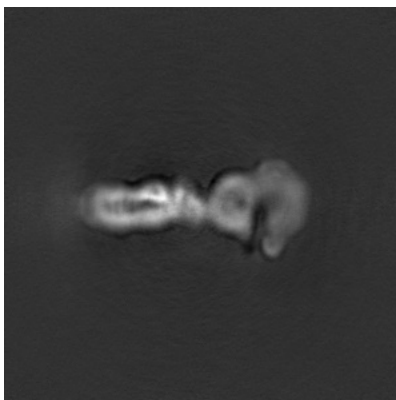


Z Index: 296

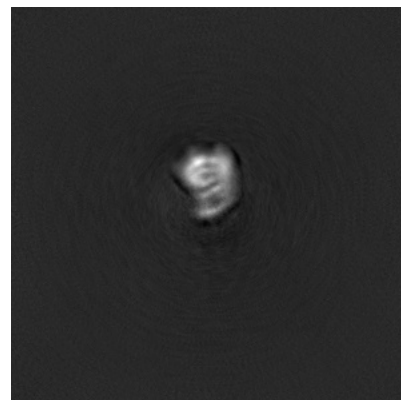
6.3.2 Raw map



X Index: 289



Y Index: 291



Z Index: 297

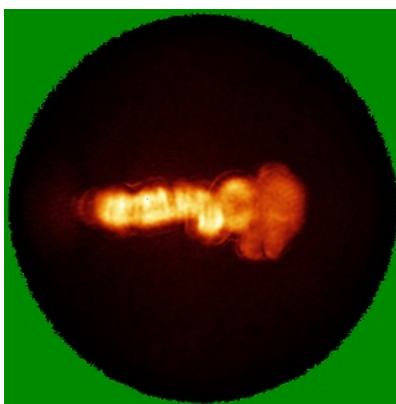
The images above show the largest variance slices of the map in three orthogonal directions.

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

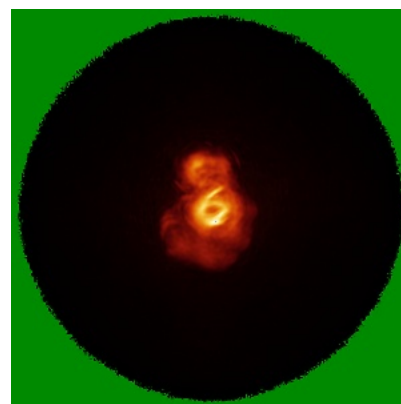
6.4.1 Primary map



X

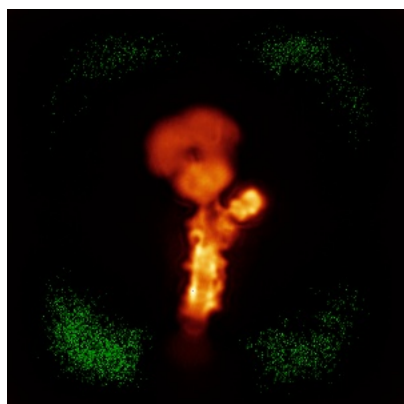


Y

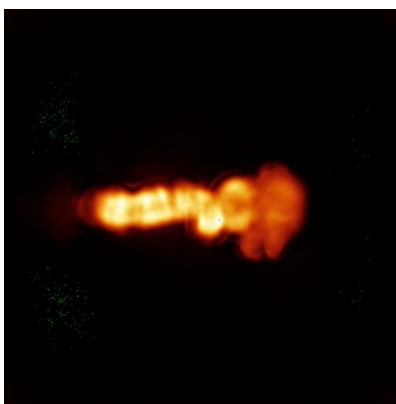


Z

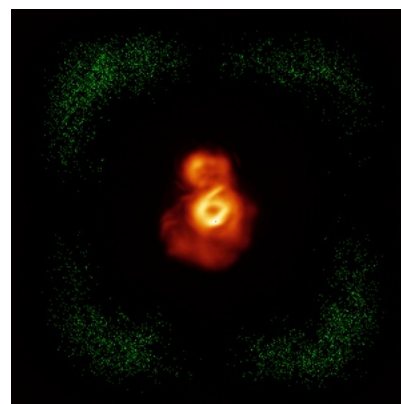
6.4.2 Raw map



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 0.11. 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.

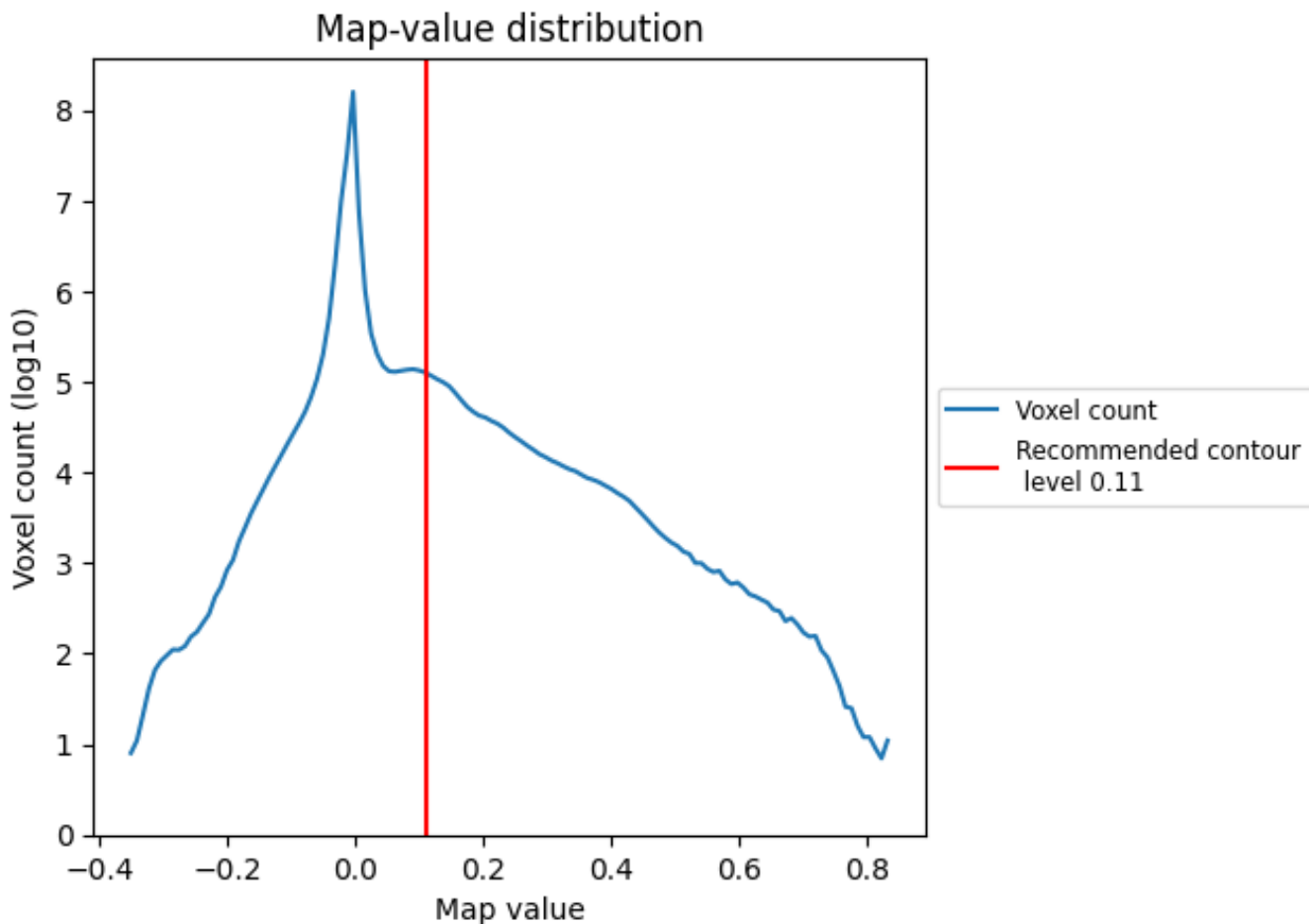
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

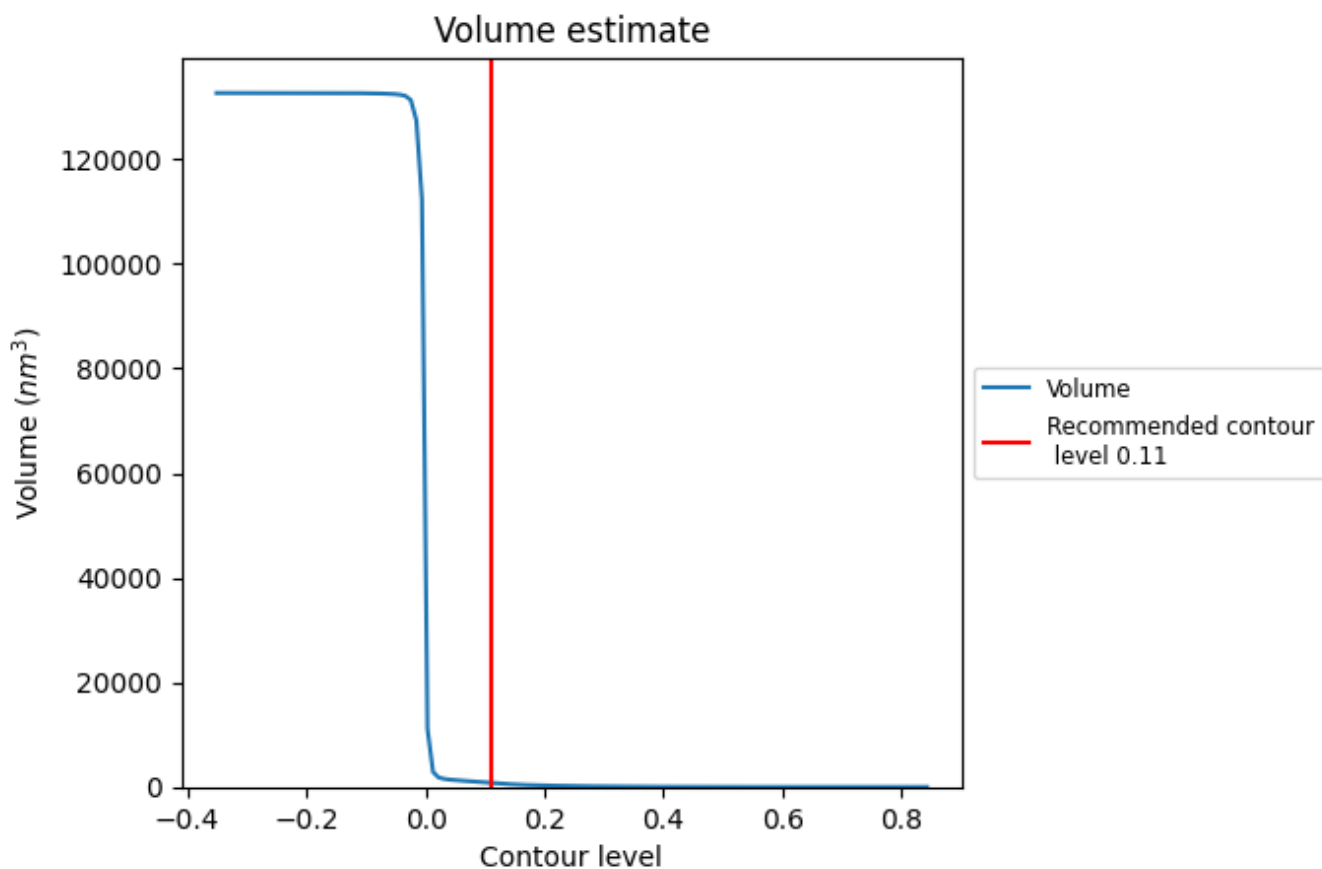
This section contains the results of statistical analysis of the map.

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.

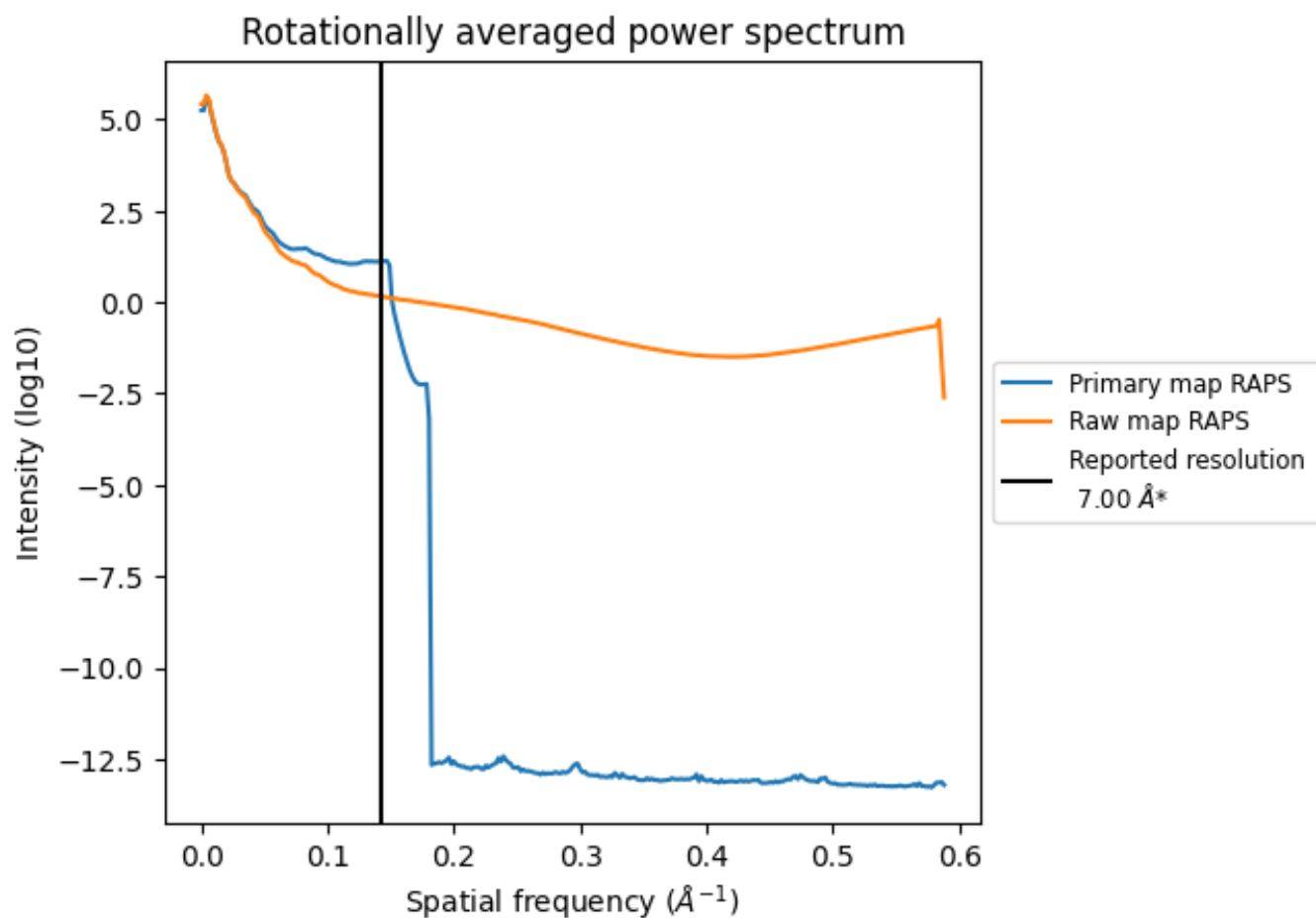
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 775 nm^3 ; this corresponds to an approximate mass of 700 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](#)

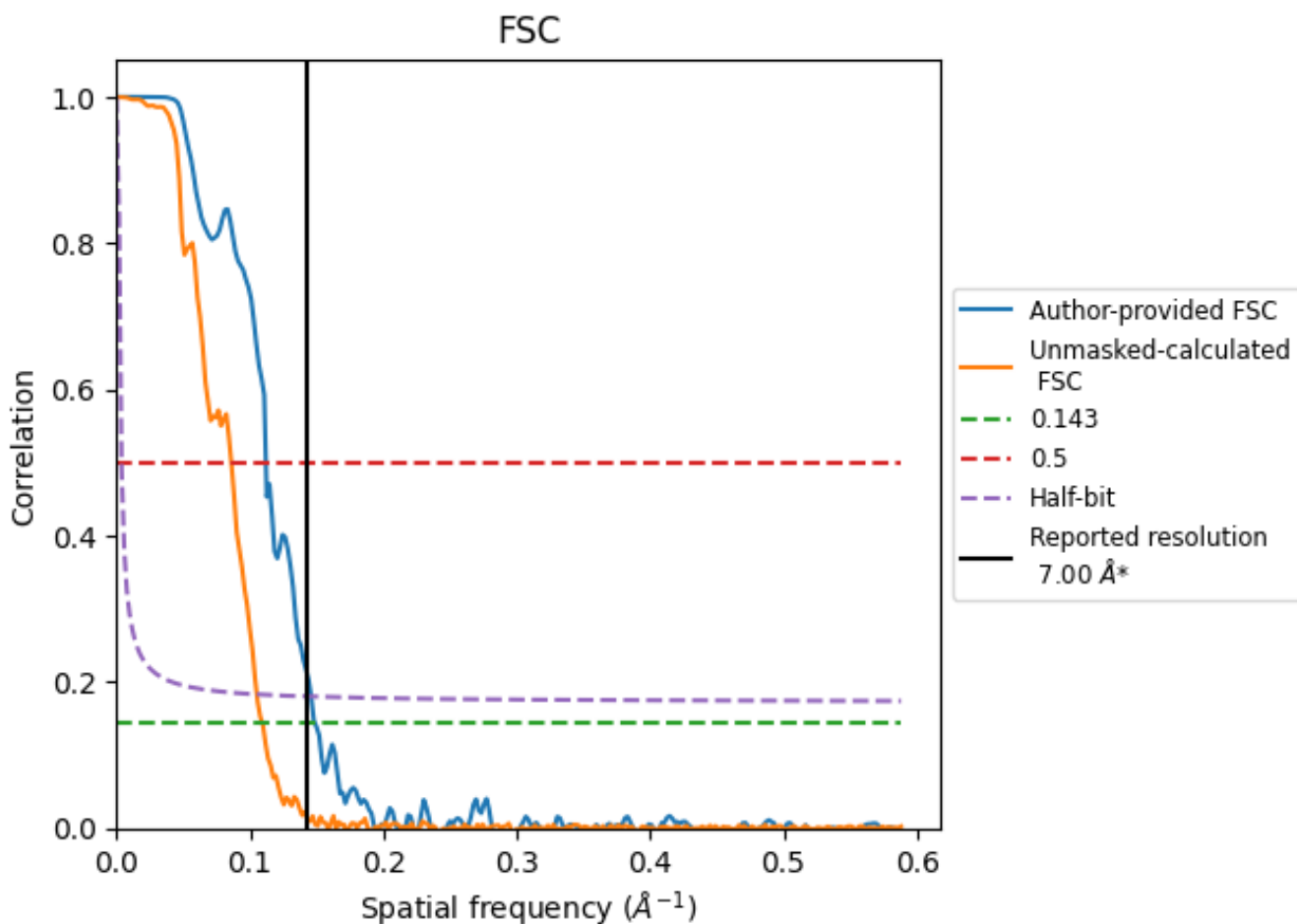


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 Å⁻¹

8.2 Resolution estimates [i](#)

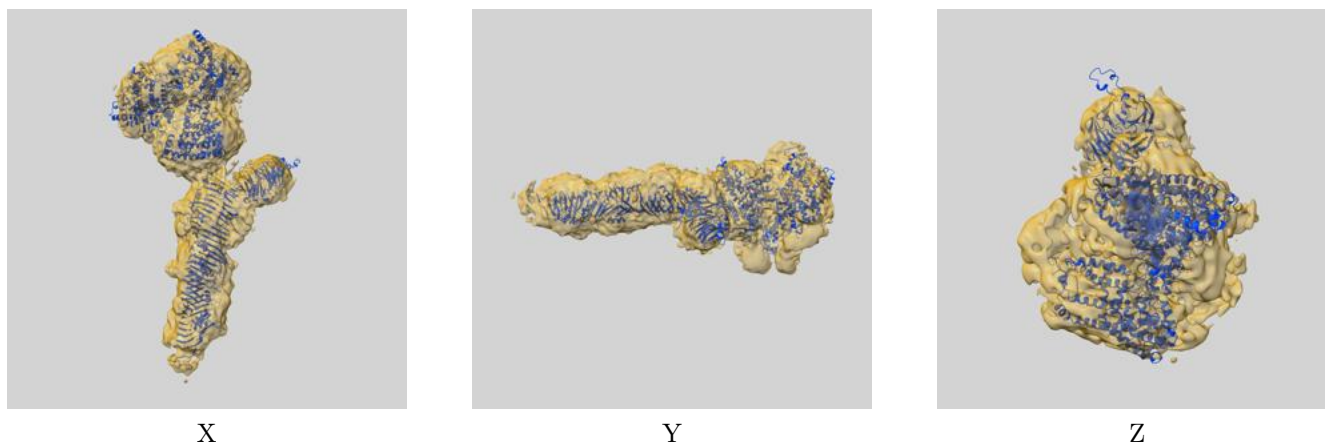
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	6.72	8.92	6.85
Unmasked-calculated*	9.14	11.61	9.50

*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 9.14 differs from the reported value 7.0 by more than 10 %

9 Map-model fit [i](#)

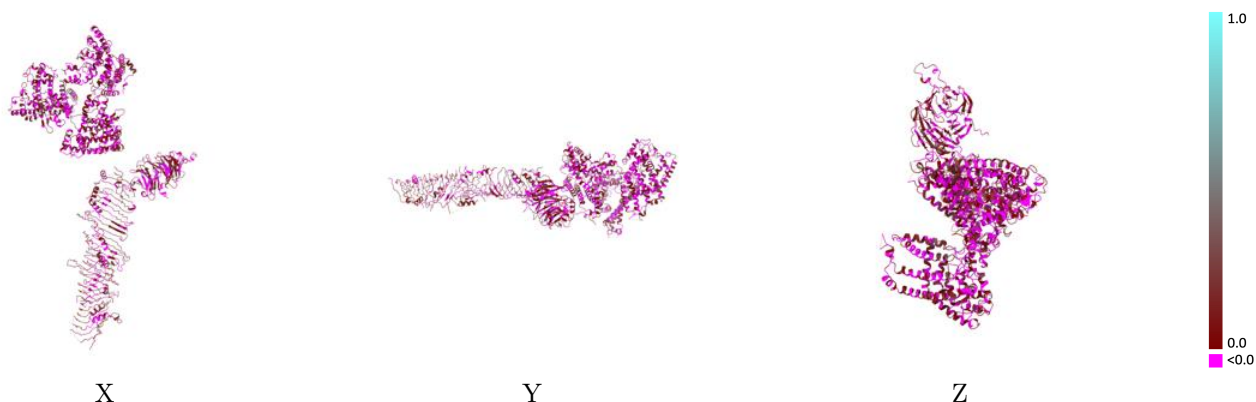
This section contains information regarding the fit between EMDB map EMD-37091 and PDB model 8KC3. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



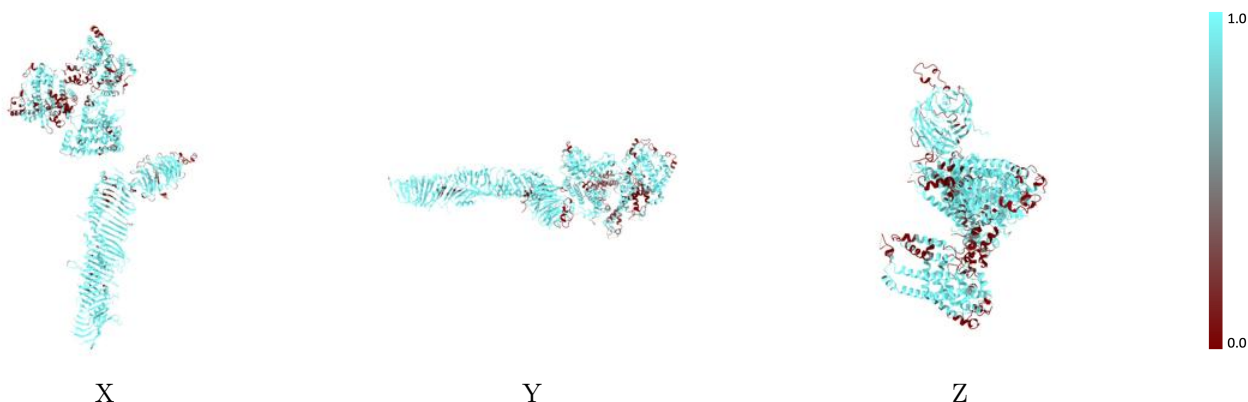
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



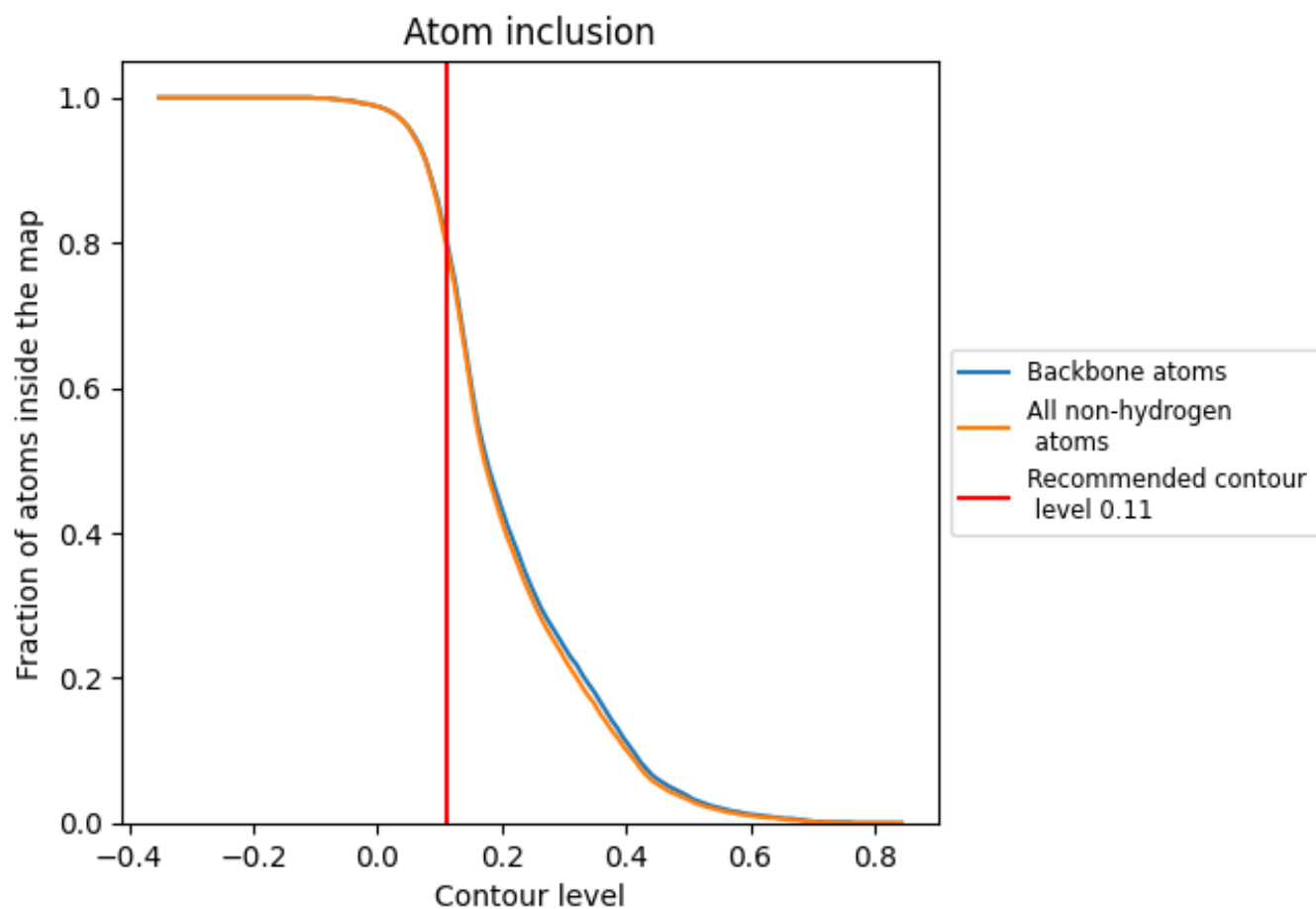
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).













9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.0450
A	 0.8590	 0.0300
B	 0.6190	 0.0140
C	 0.6610	 0.0170
D	 0.7980	 0.0440
E	 0.9500	 0.0880

