



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 8C06 / pdb_00008c06
EMDB ID : EMD-16355
Title : Structure of Dimeric HECT E3 Ubiquitin Ligase UBR5
Authors : Hehl, L.A.; Prabu, J.R.; Schulman, B.A.
Deposited on : 2022-12-16
Resolution : 2.70 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
MolProbity : 4-5-2 with Phenix2.0
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

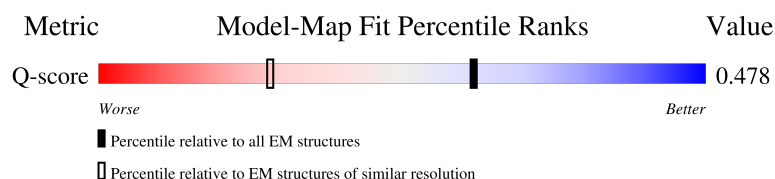
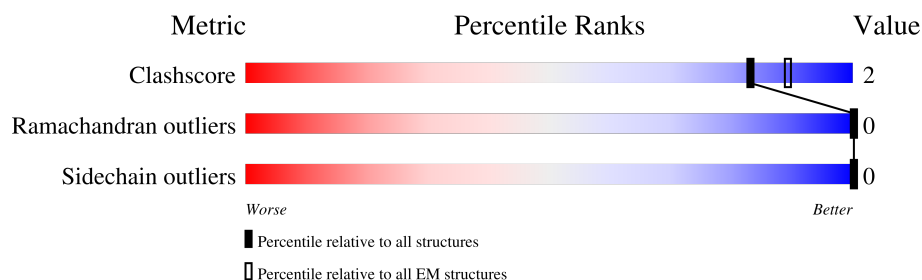
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



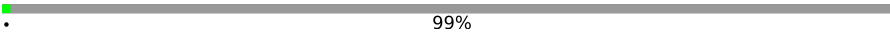
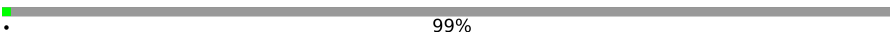
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	2806	10% 31% 67%
1	B	2806	7% 23% 75%
1	D	2806	11% 31% 67%
1	E	2806	7% 23% 75%

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Mol	Chain	Length	Quality of chain
1	F	2806	 99%
1	G	2806	 99%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25324 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 E3 ubiquitin-protein ligase UBR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	925	Total	C	N	O	S	0	0
			7080	4480	1226	1317	57		
1	B	694	Total	C	N	O	S	0	0
			5353	3407	941	974	31		
1	D	925	Total	C	N	O	S	0	0
			7080	4480	1226	1317	57		
1	E	694	Total	C	N	O	S	0	0
			5353	3407	941	974	31		
1	F	30	Total	C	N	O	S	0	0
			226	135	46	44	1		
1	G	30	Total	C	N	O	S	0	0
			226	135	46	44	1		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O95071
A	-5	SER	-	expression tag	UNP O95071
A	-4	GLY	-	expression tag	UNP O95071
A	-3	SER	-	expression tag	UNP O95071
A	-2	GLY	-	expression tag	UNP O95071
A	-1	ALA	-	expression tag	UNP O95071
A	0	PRO	-	expression tag	UNP O95071
A	503	ARG	LYS	engineered mutation	UNP O95071
A	710	ASP	LEU	engineered mutation	UNP O95071
B	-6	GLY	-	expression tag	UNP O95071
B	-5	SER	-	expression tag	UNP O95071
B	-4	GLY	-	expression tag	UNP O95071
B	-3	SER	-	expression tag	UNP O95071
B	-2	GLY	-	expression tag	UNP O95071
B	-1	ALA	-	expression tag	UNP O95071
B	0	PRO	-	expression tag	UNP O95071
B	503	ARG	LYS	engineered mutation	UNP O95071
B	710	ASP	LEU	engineered mutation	UNP O95071

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP O95071
D	-5	SER	-	expression tag	UNP O95071
D	-4	GLY	-	expression tag	UNP O95071
D	-3	SER	-	expression tag	UNP O95071
D	-2	GLY	-	expression tag	UNP O95071
D	-1	ALA	-	expression tag	UNP O95071
D	0	PRO	-	expression tag	UNP O95071
D	503	ARG	LYS	engineered mutation	UNP O95071
D	710	ASP	LEU	engineered mutation	UNP O95071
E	-6	GLY	-	expression tag	UNP O95071
E	-5	SER	-	expression tag	UNP O95071
E	-4	GLY	-	expression tag	UNP O95071
E	-3	SER	-	expression tag	UNP O95071
E	-2	GLY	-	expression tag	UNP O95071
E	-1	ALA	-	expression tag	UNP O95071
E	0	PRO	-	expression tag	UNP O95071
E	503	ARG	LYS	engineered mutation	UNP O95071
E	710	ASP	LEU	engineered mutation	UNP O95071
F	-6	GLY	-	expression tag	UNP O95071
F	-5	SER	-	expression tag	UNP O95071
F	-4	GLY	-	expression tag	UNP O95071
F	-3	SER	-	expression tag	UNP O95071
F	-2	GLY	-	expression tag	UNP O95071
F	-1	ALA	-	expression tag	UNP O95071
F	0	PRO	-	expression tag	UNP O95071
F	503	ARG	LYS	engineered mutation	UNP O95071
F	710	ASP	LEU	engineered mutation	UNP O95071
G	-6	GLY	-	expression tag	UNP O95071
G	-5	SER	-	expression tag	UNP O95071
G	-4	GLY	-	expression tag	UNP O95071
G	-3	SER	-	expression tag	UNP O95071
G	-2	GLY	-	expression tag	UNP O95071
G	-1	ALA	-	expression tag	UNP O95071
G	0	PRO	-	expression tag	UNP O95071
G	503	ARG	LYS	engineered mutation	UNP O95071
G	710	ASP	LEU	engineered mutation	UNP O95071

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	A	3	Total Zn 3 3	0

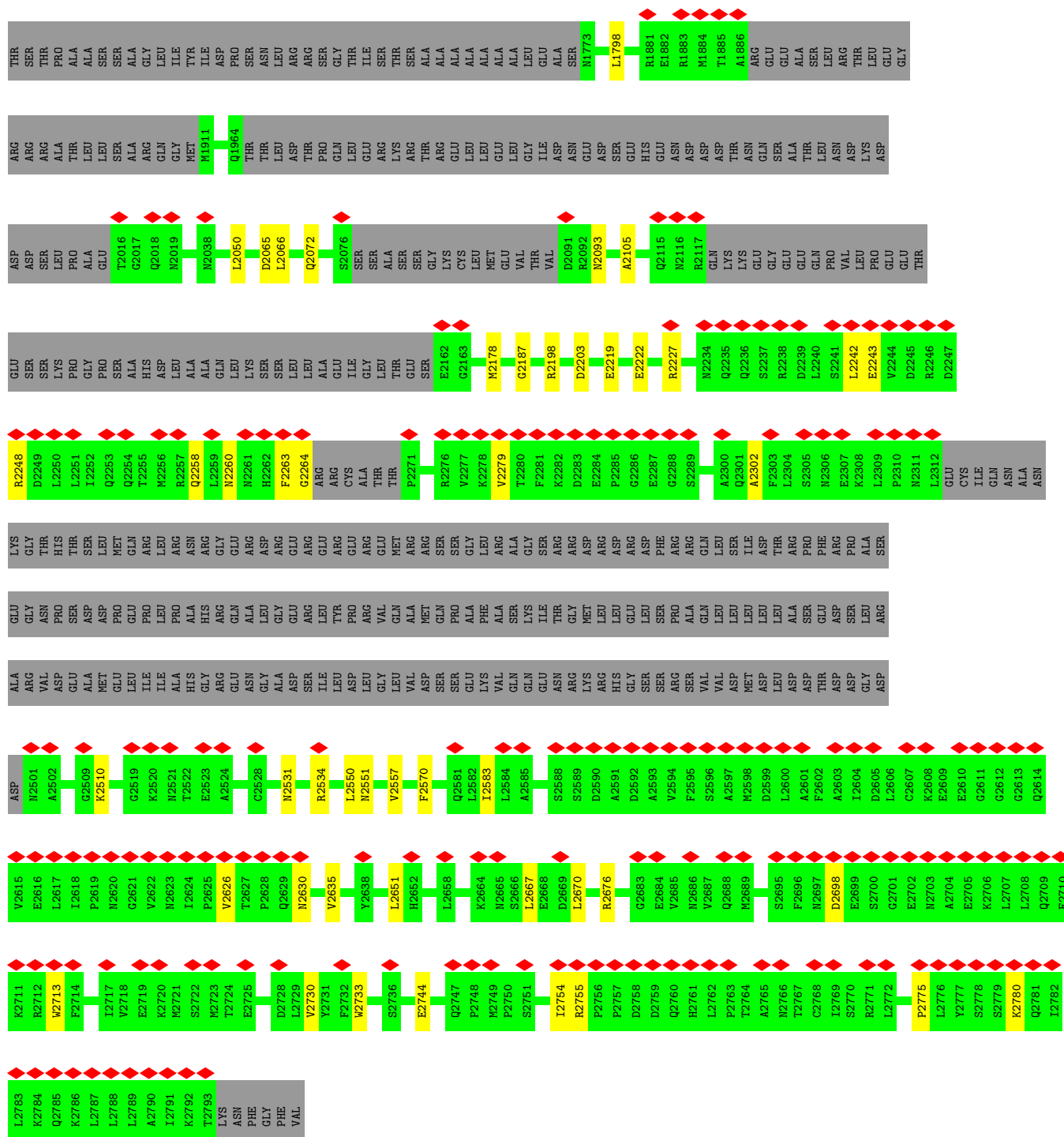
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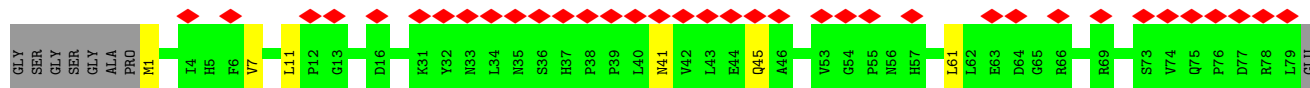
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	D	3	3	3	0







• Molecule 1: E3 ubiquitin-protein ligase UBR5





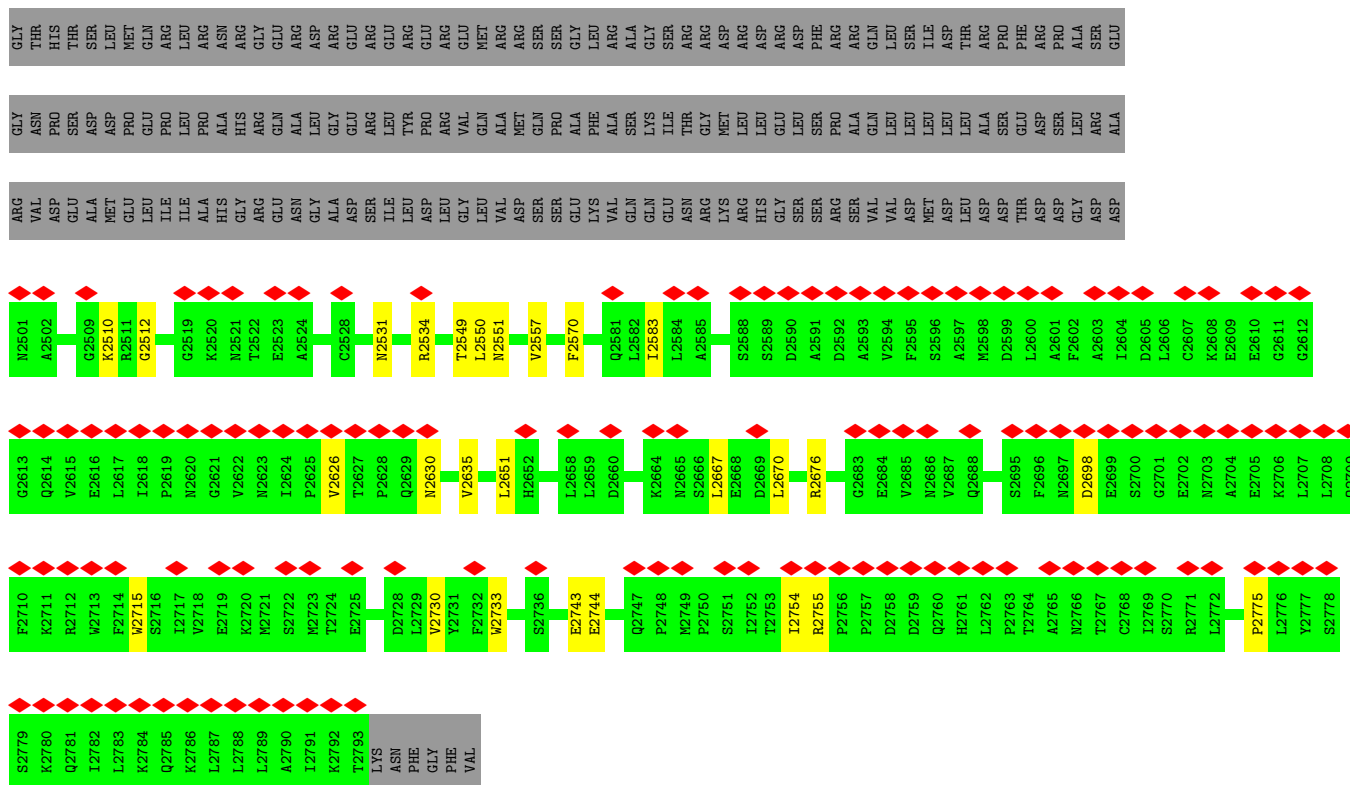


LEU
LEU
ALA
ILE
LYS
THR
LYS
ASN
PHE
GLY
PHE
VAL

- Molecule 1: E3 ubiquitin-protein ligase UBR5

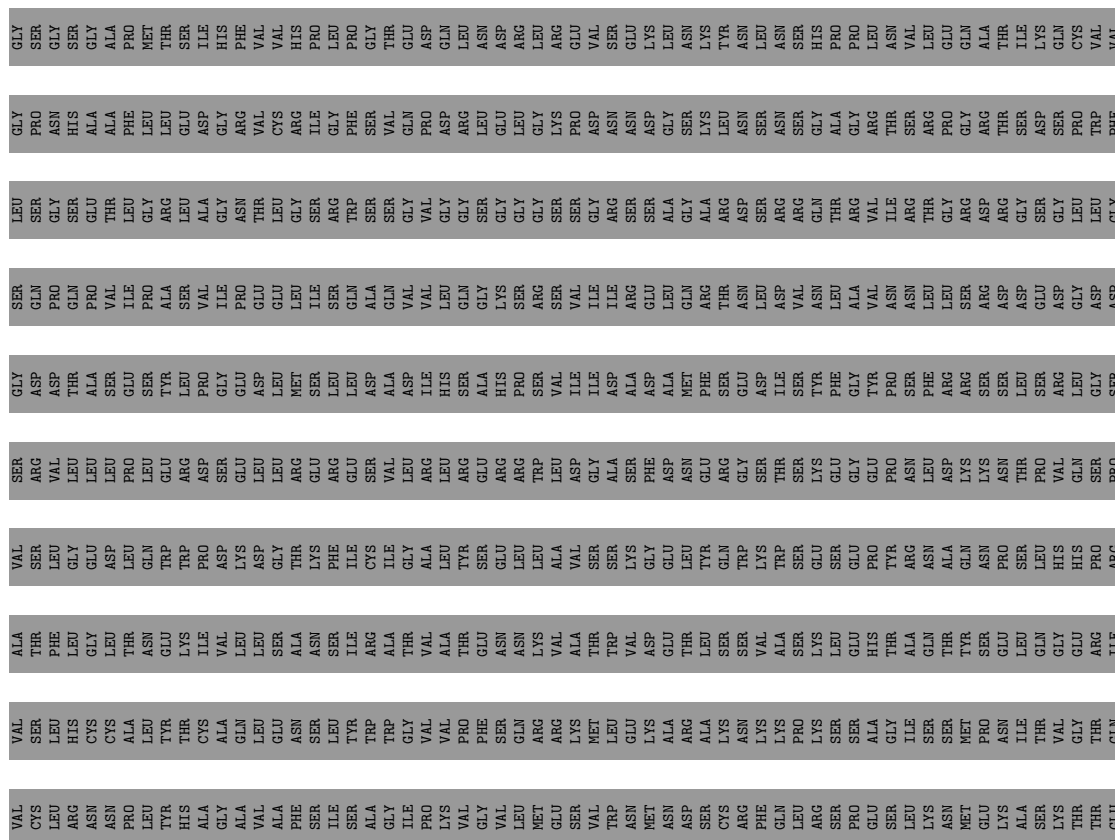
[illegible]





- Molecule 1: E3 ubiquitin-protein ligase UBR5

Chain F: 99%





- Molecule 1: E3 ubiquitin-protein ligase UBR5





ALA	GLU	VAL	ALA	ARG
ASN	LYS	VAL	SER	LEU
THR	LEU	ALA	GLN	ASN
CYS	LEU	GLU	SER	CYS
ILE	GLN	GLN	SER	PHE
SER	PHE	PRO	ASP	ARG
ARG	LYS	LEU	ALA	ASN
LEU	ARG	HIS	ASP	ILE
TRP	TRP	ALA	ALA	GLY
PHE	PHE	MET	VAL	ARG
PRO	TRP	ARG	PHE	ILE
LEU	SER	LYS	SER	LEU
THR	ILE	GLY	ALA	GLY
SER	VAL	LEU	MET	LEU
SER	GLU	LEU	ASP	CYS
SER	LYS	ASP	LEU	LEU
GLN	MET	VAL	ALA	LEU
ILE	SER	LEU	PHE	GLN
LEU	MET	PRO	ALA	ASN
THR	THR	LYS	ILE	GLU
GLN	ARG	ASN	ASP	LEU
LYS	GLU	SER	LEU	CYS
LEU	GLN	LEU	CYS	PRO
LEU	ASP	GLU	LYS	ILE
LEU	LEU	ASP	GLU	THR
ALA	VAL	LEU	GLU	LEU
ILE	TYR	THR	GLY	ASN
LYS	PHE	GLU	GLY	ARG
THR	TRP	GLU	GLY	HIS
LYS	THR	ASP	GLN	VAL
ASN	SER	PHE	VAL	ILE
PHE	SER	ARG	GLU	LYS
PHE	PRO	LEU	LEU	VAL
VAL	LEU	VAL	PRO	LEU
	PRO	ASN	ASN	GLY
	ALA	GLY	ARG	GLY
	SER	CYS	VAL	LYS
	GLU	GLY	ASN	VAL
	GLU	GLU	ILE	ASN
	GLY	VAL	PRO	TRP
	PHE	ASN	VAL	HIS
	GLN	VAL	THR	ASP
	PRO	GLN	PRO	PHE
	MET	MET	GLN	ALA
	PRO	LEU	ASN	PHE
	SER	ILE	VAL	PHE
	THR	SER	TYR	ASP
	ILE	PHE	GLU	PRO
	ARG	SER	VAL	MET
	PRO	PHE	TYR	GLN
	PRO	ASN	LYS	GLY
	ASP	ASP	TYR	SER
	ASP	GLU	ALA	GLU
	GLN	SER	GLU	ARG
	HIS	GLY	HIS	GLN
	LEU	GLU	ARG	LEU
	PRO	ASN	MET	ILE
	THR	ALA	TYR	LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	226919	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 ($e^-/\text{\AA}^2$)	67.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0101	Depositor
Map size (Å)	326.86078, 326.86078, 326.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8511999, 0.8511999, 0.8511999	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

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	0.18	0/7223	0.43	0/9821
1	B	0.17	0/5476	0.43	0/7439
1	D	0.18	0/7223	0.43	0/9821
1	E	0.17	0/5476	0.43	0/7439
1	F	0.20	0/230	0.64	0/312
1	G	0.20	0/230	0.64	0/312
All	All	0.18	0/25858	0.43	0/35144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7080	0	6948	32	0
1	B	5353	0	5187	29	0
1	D	7080	0	6948	27	0
1	E	5353	0	5187	32	0
1	F	226	0	207	5	0
1	G	226	0	207	3	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
All	All	25324	0	24684	118	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 2.

The worst 5 of 118 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:D:1211:CYS:O	1:D:1215:CYS:HB2	1.77	0.84
1:A:1211:CYS:O	1:A:1215:CYS:HB2	1.77	0.82
1:E:2531:ASN:OD1	1:E:2534:ARG:NH2	2.33	0.61
1:B:2531:ASN:OD1	1:B:2534:ARG:NH2	2.33	0.60
1:A:804:ALA:HB2	1:A:846:MET:HG3	1.82	0.60

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	909/2806 (32%)	860 (95%)	49 (5%)	0	100	100
1	B	680/2806 (24%)	643 (95%)	37 (5%)	0	100	100
1	D	909/2806 (32%)	859 (94%)	50 (6%)	0	100	100
1	E	680/2806 (24%)	643 (95%)	37 (5%)	0	100	100
1	F	28/2806 (1%)	25 (89%)	3 (11%)	0	100	100
1	G	28/2806 (1%)	25 (89%)	3 (11%)	0	100	100
All	All	3234/16836 (19%)	3055 (94%)	179 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	766/2422 (32%)	766 (100%)	0	100	100
1	B	564/2422 (23%)	564 (100%)	0	100	100
1	D	766/2422 (32%)	766 (100%)	0	100	100
1	E	564/2422 (23%)	564 (100%)	0	100	100
1	F	22/2422 (1%)	22 (100%)	0	100	100
1	G	22/2422 (1%)	22 (100%)	0	100	100
All	All	2704/14532 (19%)	2704 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	879	HIS
1	E	1812	GLN
1	G	1715	GLN
1	D	1411	ASN
1	E	1852	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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

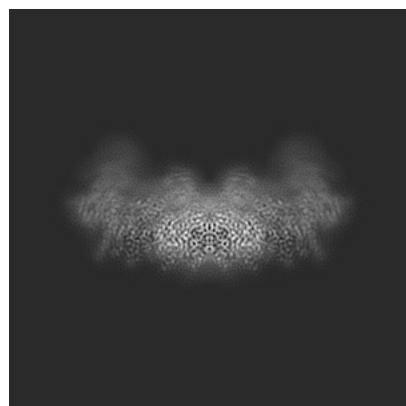
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16355. These allow visual inspection of the internal detail of the map and identification of artifacts.

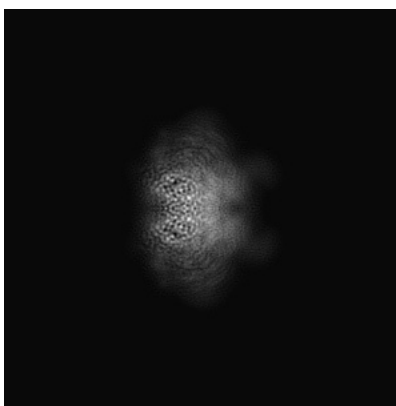
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

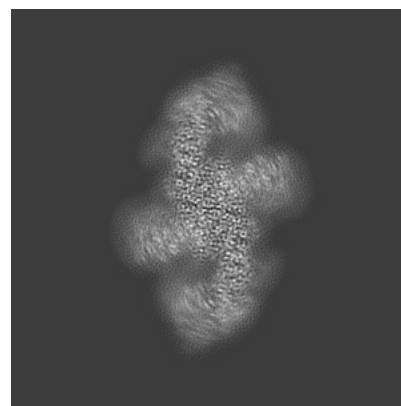
6.1.1 Primary map



X

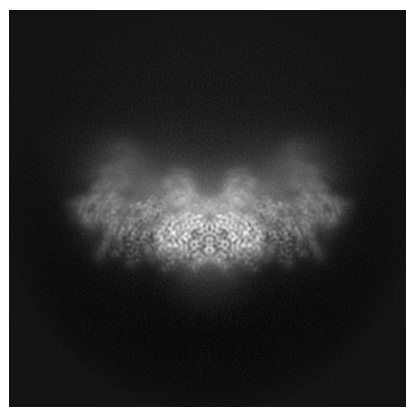


Y

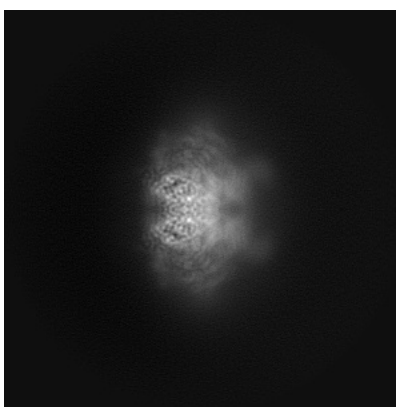


Z

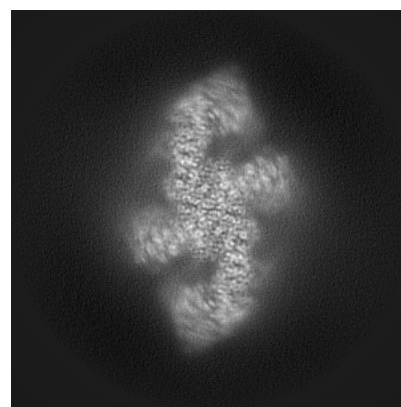
6.1.2 Raw map



X



Y

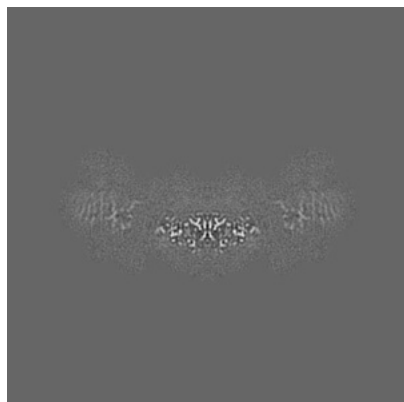


Z

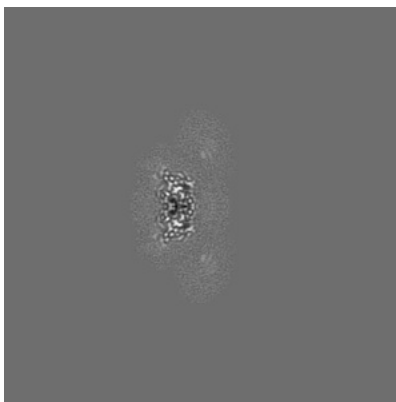
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

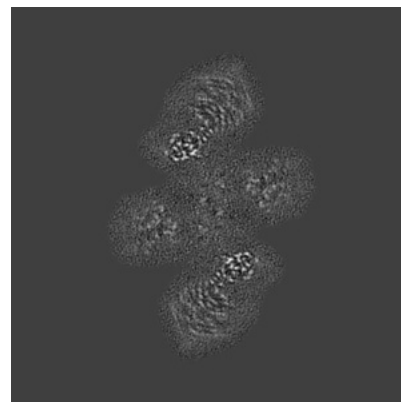
6.2.1 Primary map



X Index: 192

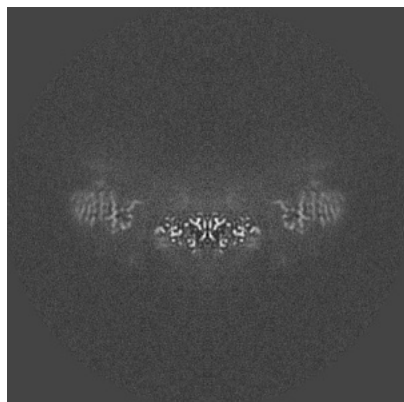


Y Index: 192

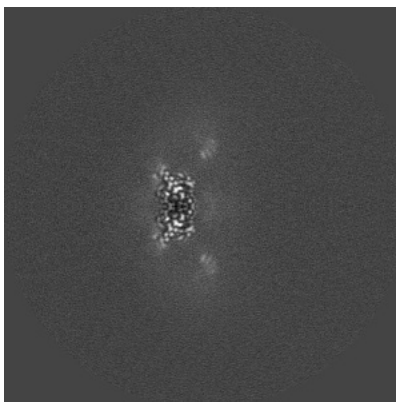


Z Index: 192

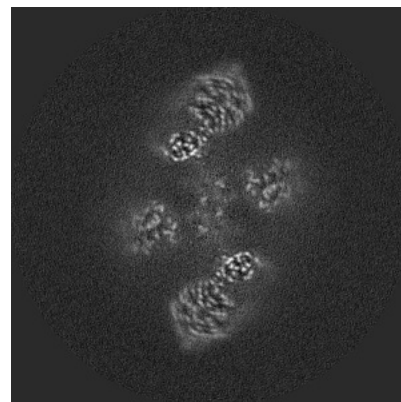
6.2.2 Raw map



X Index: 192



Y Index: 192

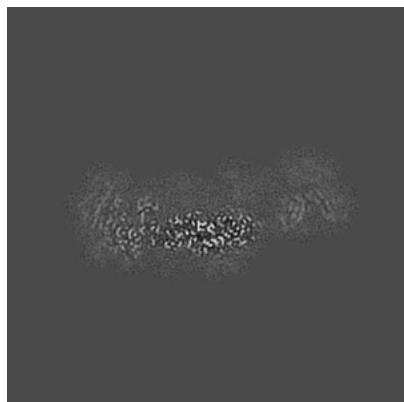


Z Index: 192

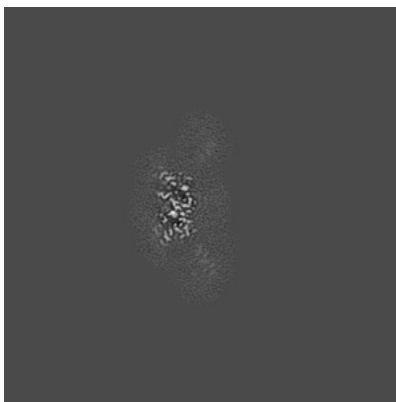
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

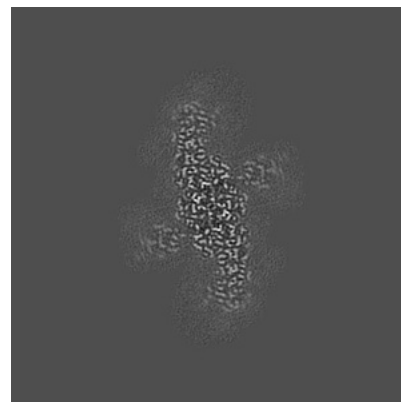
6.3.1 Primary map



X Index: 204

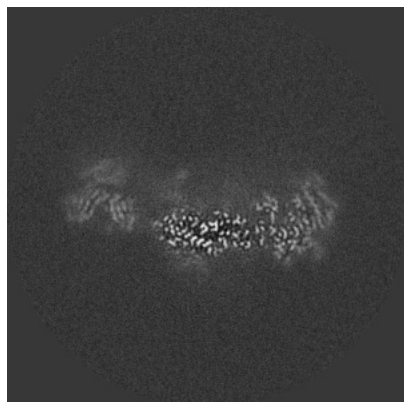


Y Index: 190

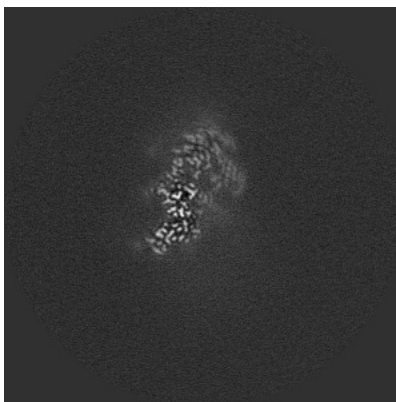


Z Index: 170

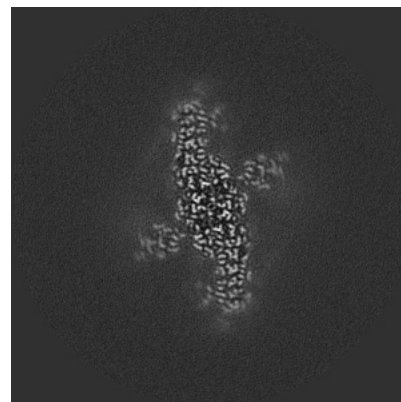
6.3.2 Raw map



X Index: 180



Y Index: 214

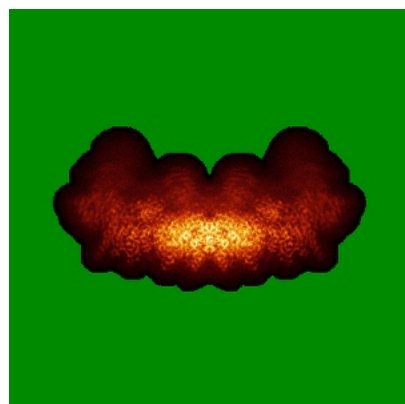


Z Index: 170

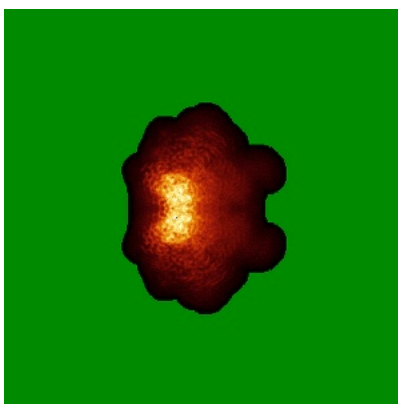
The images above show the largest variance slices of the map in three orthogonal directions.

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

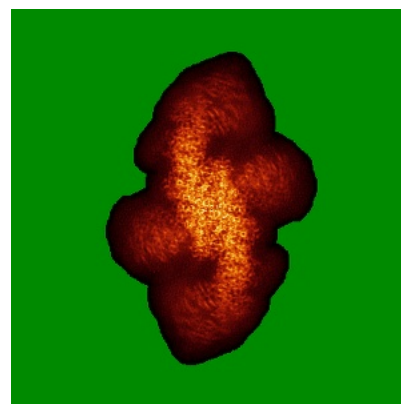
6.4.1 Primary map



X

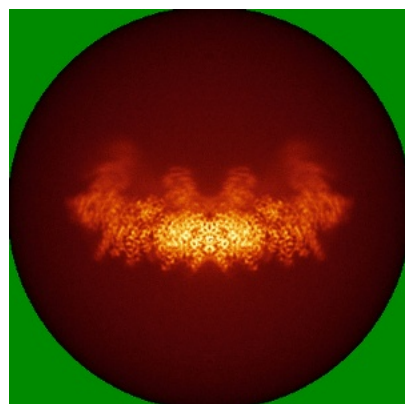


Y

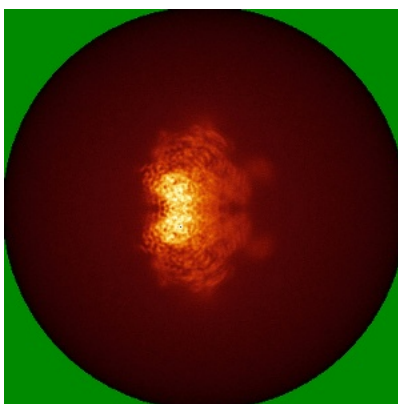


Z

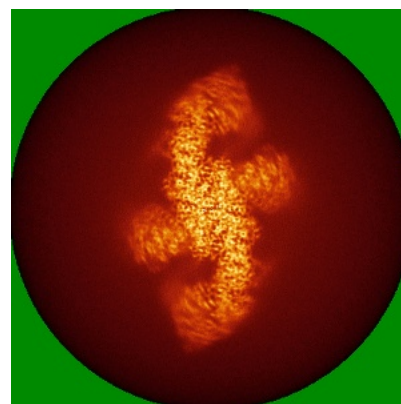
6.4.2 Raw map



X



Y

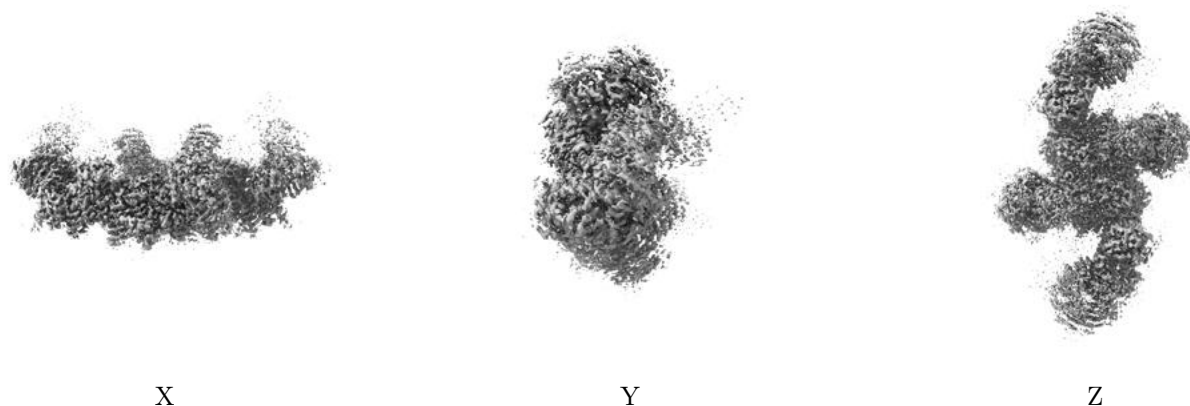


Z

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.

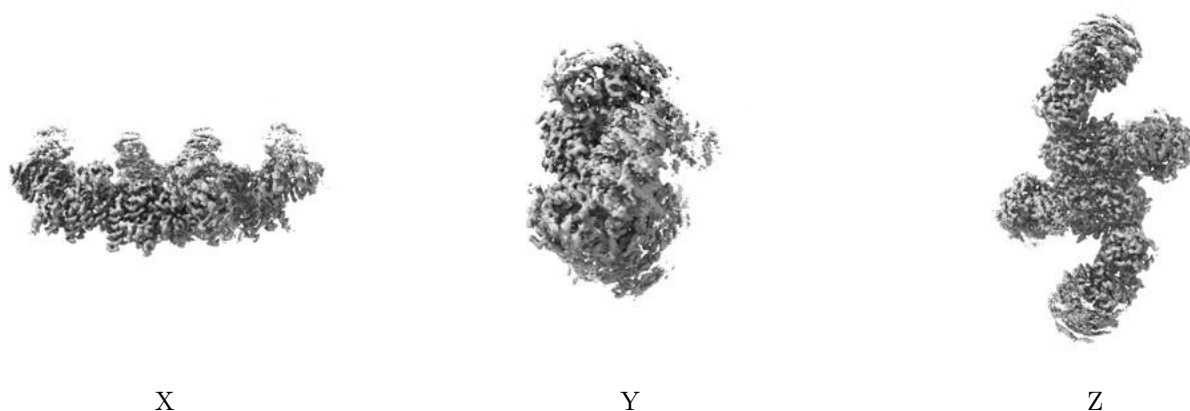
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0101. 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.

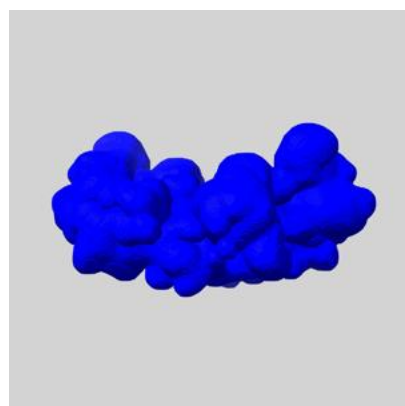
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

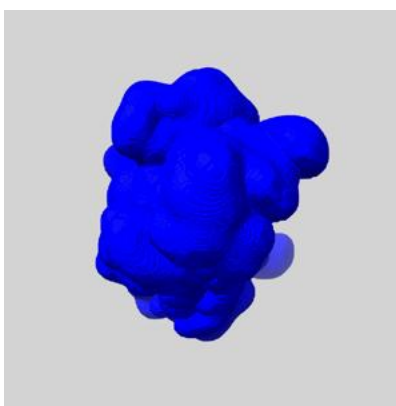
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

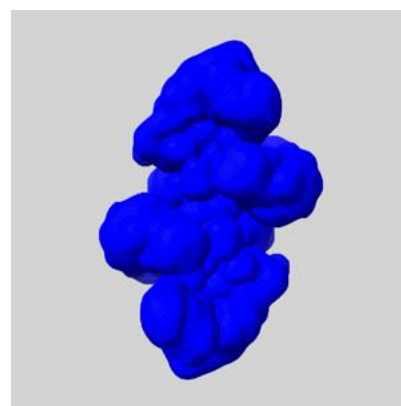
6.6.1 emd_16355_msk_1.map [i](#)



X



Y

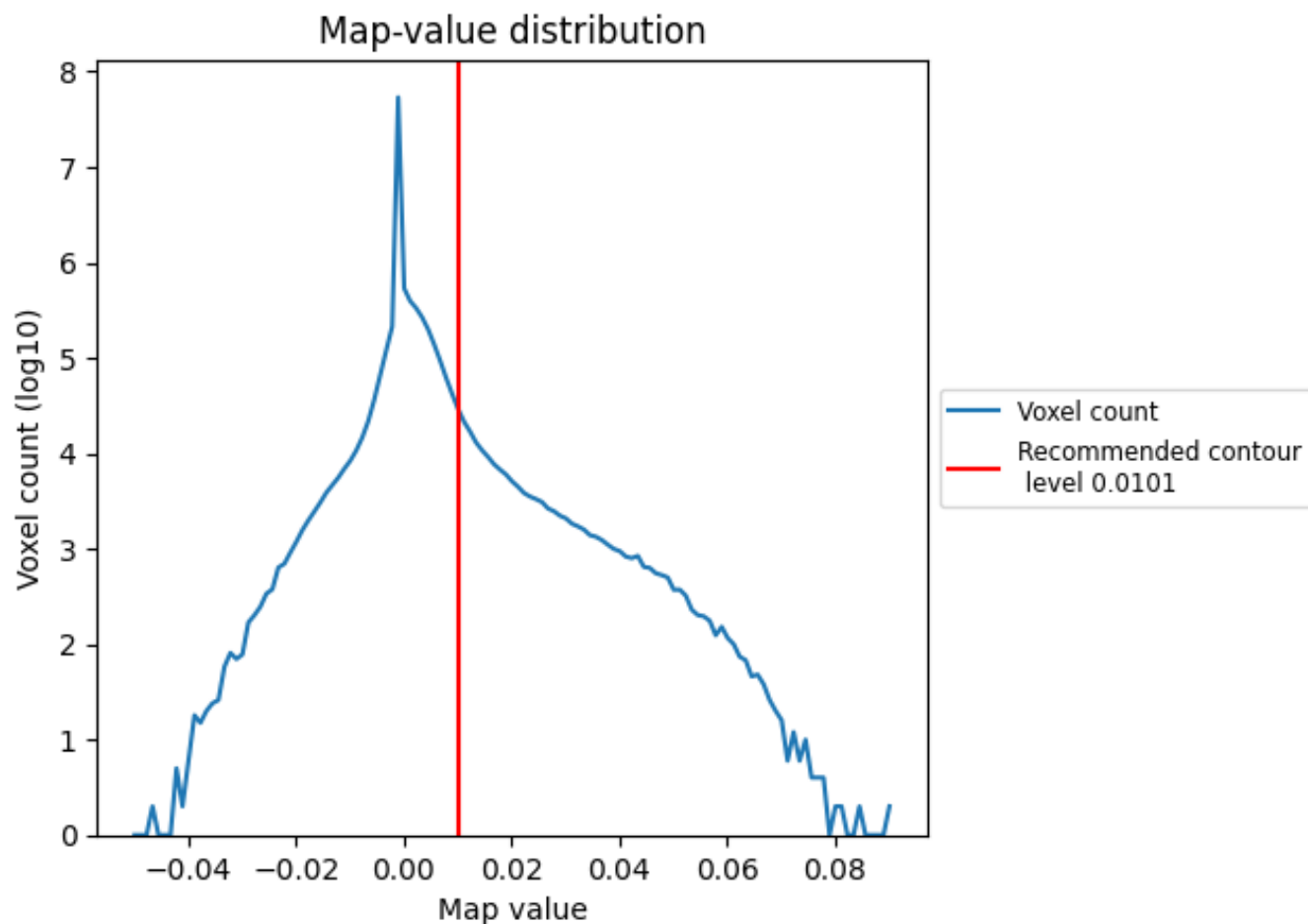


Z

7 Map analysis [i](#)

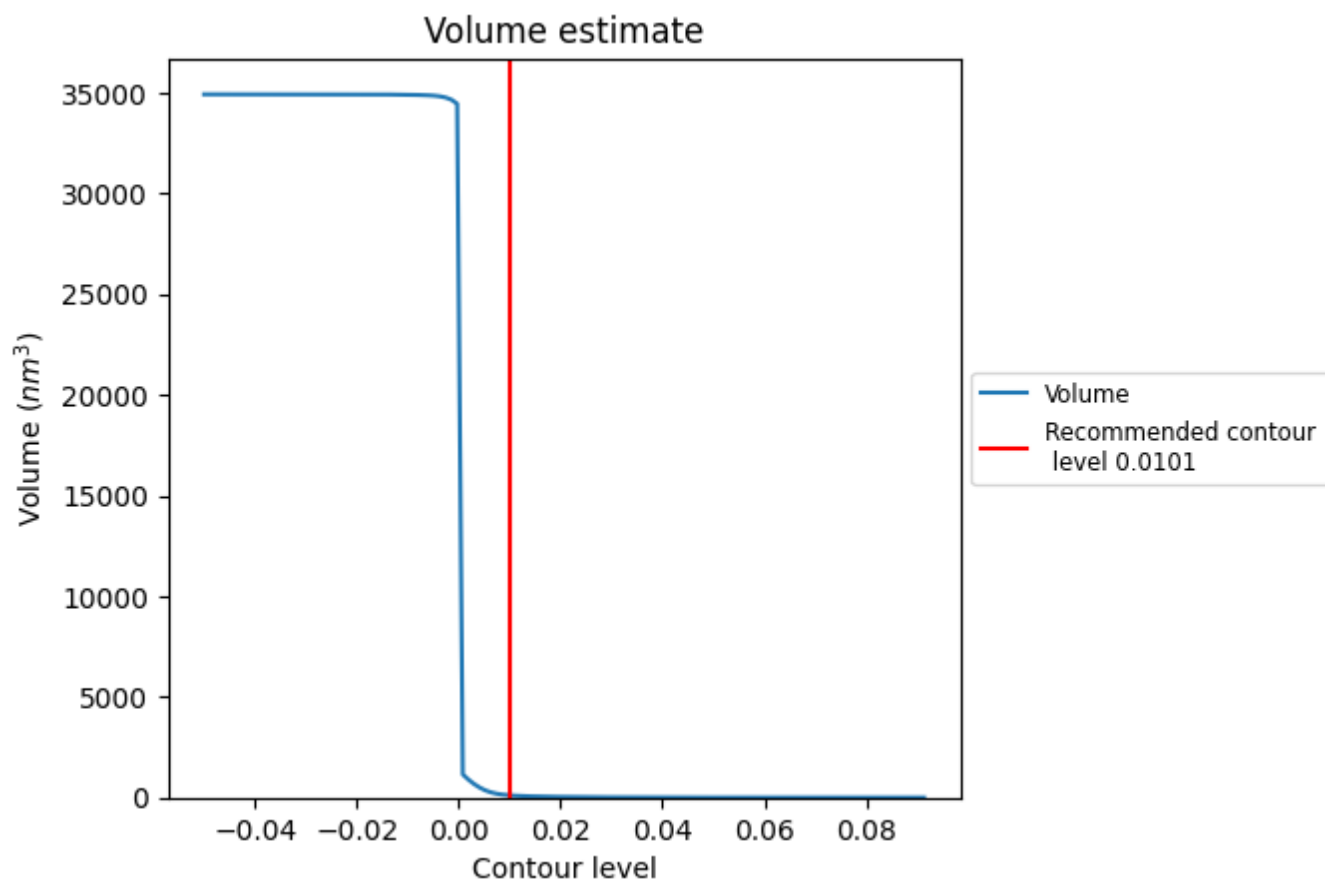
This section contains the results of statistical analysis of the map.

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.

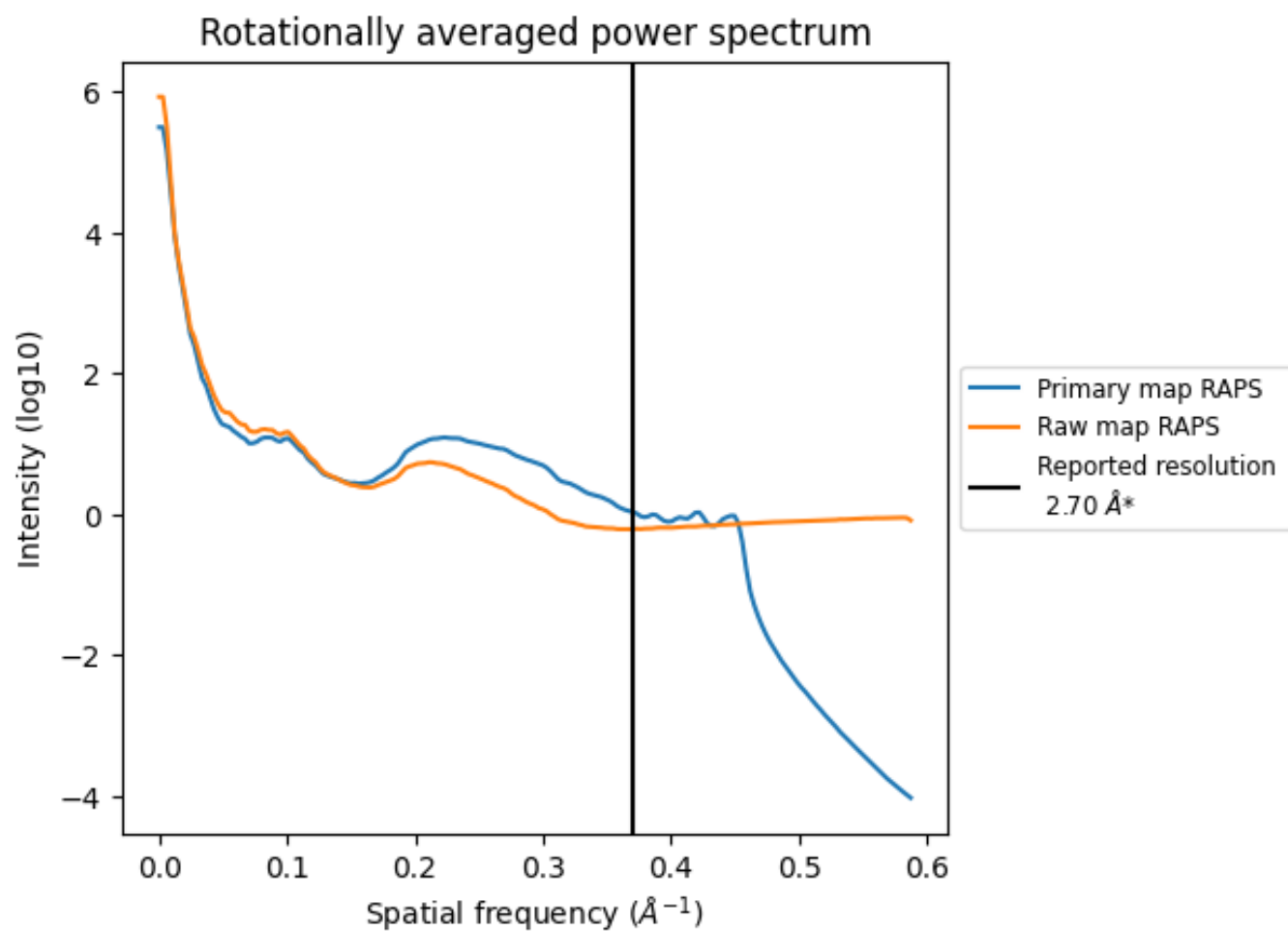
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ

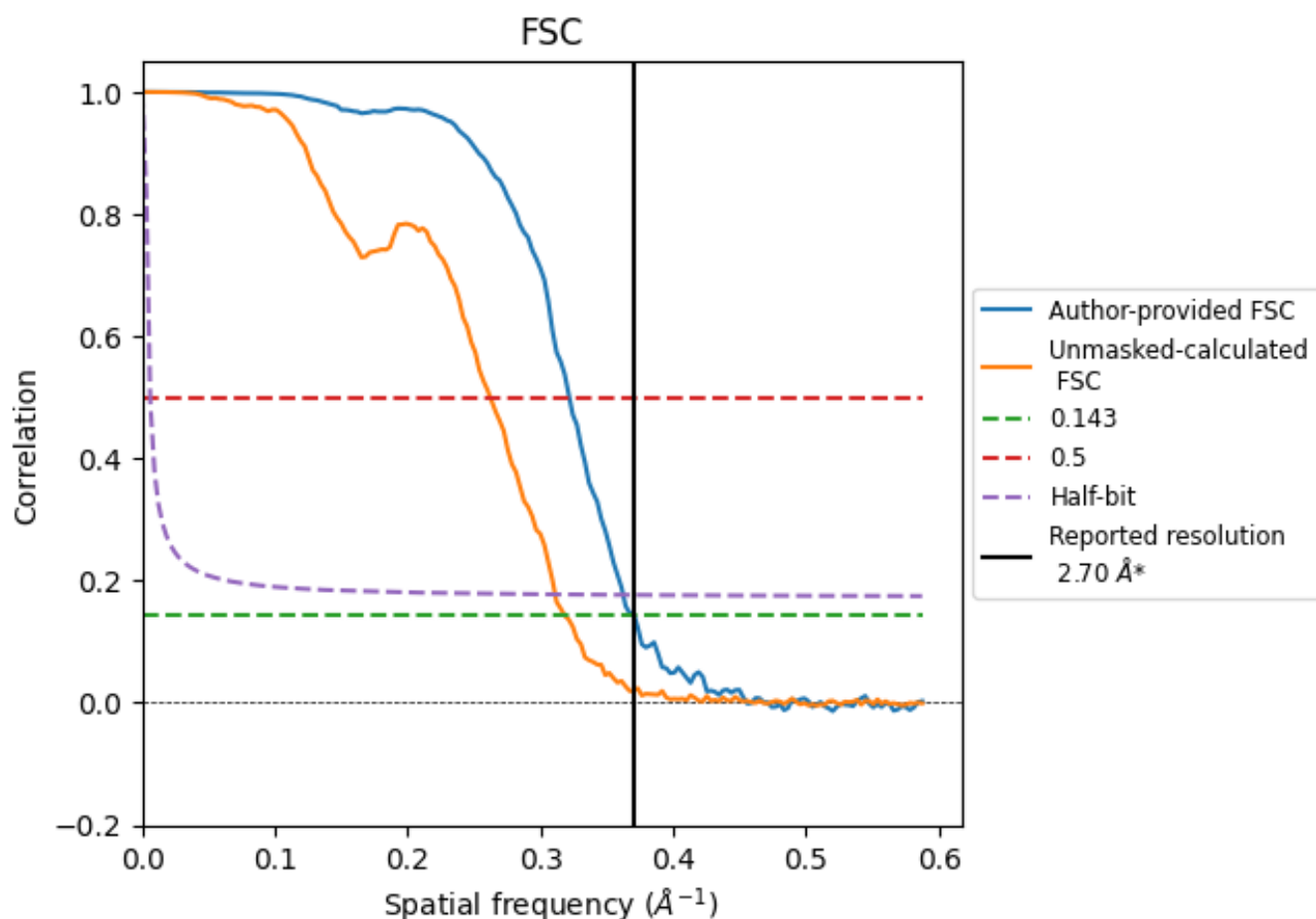


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

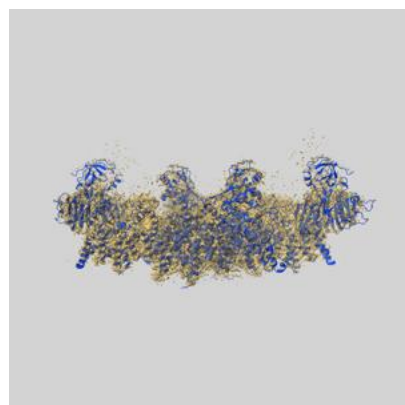
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.11	2.76
Unmasked-calculated*	3.14	3.82	3.22

*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 3.14 differs from the reported value 2.7 by more than 10 %

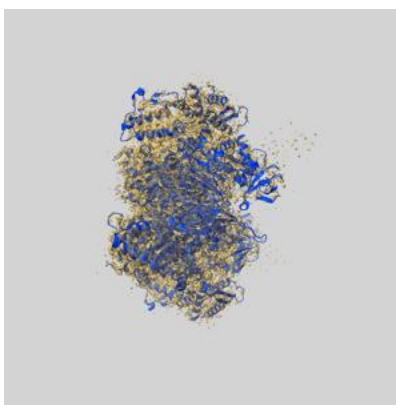
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16355 and PDB model 8C06. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

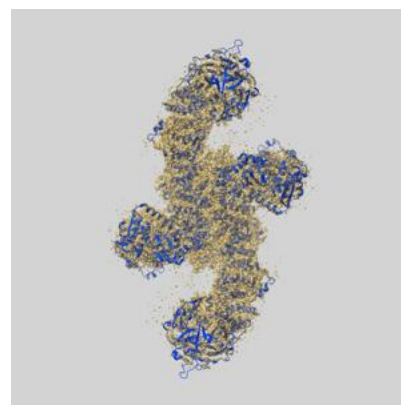
9.1 Map-model overlay [i](#)



X



Y



Z

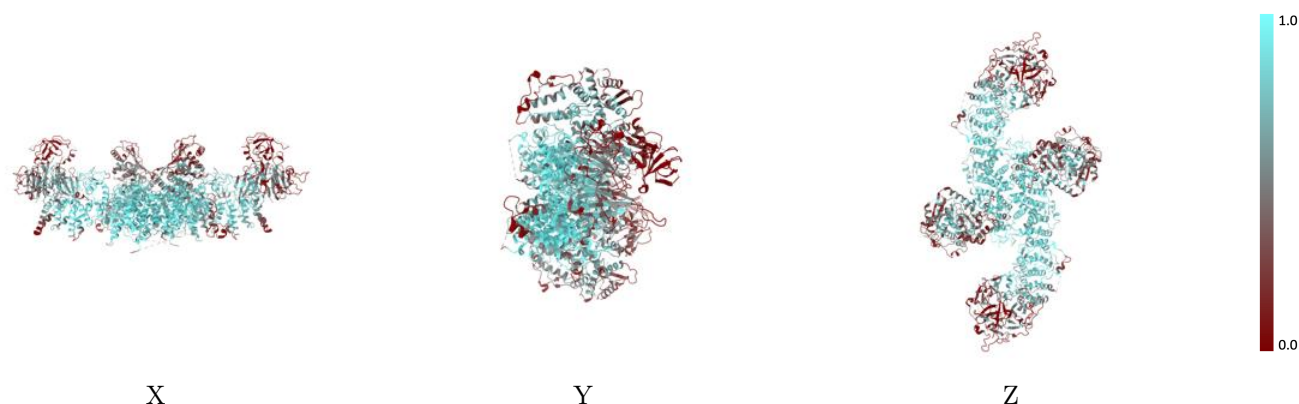
The images above show the 3D surface view of the map at the recommended contour level 0.0101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



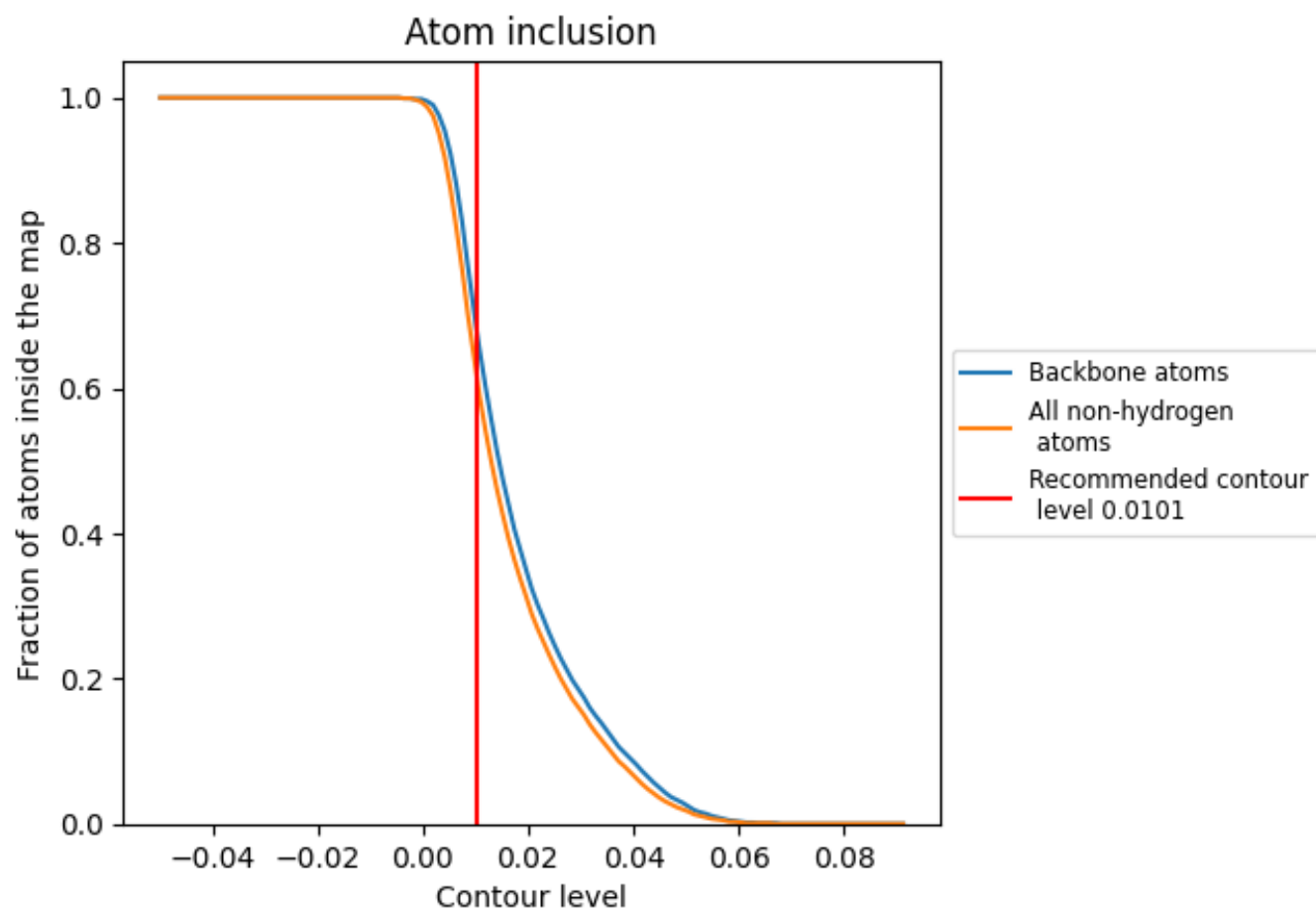
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0101).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 62% 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 (0.0101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.4780
A	0.6070	0.4650
B	0.6460	0.4990
D	0.6060	0.4640
E	0.6470	0.4970
F	0.5390	0.4430
G	0.5340	0.4410

1.0

0.0

<0.0