WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Jun 13, 2022 – 04:19 pm BST

PDB ID	:	7ZBN
EMDB ID	:	EMD-14587
Title	:	Cryo-EM structure of the human GS-GN complex in the inhibited state
Authors	:	Marr, L.; Zeqiraj, E.
Deposited on	:	2022-03-23
Resolution	:	2.62 Å(reported)

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 2.62 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▊ Percentile relative to all structures

▯ Percentile relative to all EM structures
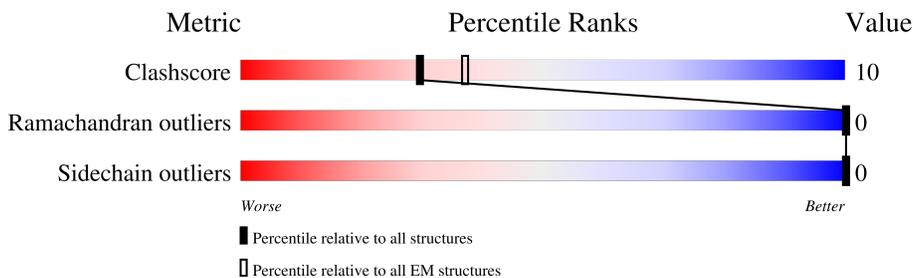
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	737	10% 67% 17% 16%
1	C	737	10% 66% 18% 16%
2	B	737	10% 64% 20% 16%
2	D	737	10% 63% 21% 16%
3	E	333	8% 8% • 90%
3	F	333	9% 8% • 90%
3	G	333	8% 8% • 90%
3	H	333	9% 8% • 90%

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2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 41588 atoms, of which 20466 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 Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	617	Total 9830	C 3202	H 4842	N 858	O 903	S 25	0	0
1	C	617	Total 9830	C 3202	H 4842	N 858	O 903	S 25	0	0

- Molecule 2 is a protein called Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	B	621	Total 9896	C 3218	H 4879	N 862	O 911	P 1	S 25	0	0
2	D	621	Total 9896	C 3218	H 4879	N 862	O 911	P 1	S 25	0	0

- Molecule 3 is a protein called Isoform GN-1 of Glycogenin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	33	Total 534	C 170	H 256	N 49	O 58	S 1	0	0
3	F	33	Total 534	C 170	H 256	N 49	O 58	S 1	0	0
3	G	33	Total 534	C 170	H 256	N 49	O 58	S 1	0	0
3	H	33	Total 534	C 170	H 256	N 49	O 58	S 1	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	THR	conflict	UNP P46976
E	195	PHE	TYR	conflict	UNP P46976
F	2	ALA	THR	conflict	UNP P46976
F	195	PHE	TYR	conflict	UNP P46976
G	2	ALA	THR	conflict	UNP P46976

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Chain	Residue	Modelled	Actual	Comment	Reference
G	195	PHE	TYR	conflict	UNP P46976
H	2	ALA	THR	conflict	UNP P46976
H	195	PHE	TYR	conflict	UNP P46976

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glycogen [starch] synthase, muscle

- Molecule 1: Glycogen [starch] synthase, muscle

• Molecule 2: Glycogen [starch] synthase, muscle

Chain B:

• Molecule 2: Glycogen [starch] synthase, muscle

Chain D:

10%

63% 21% 16%

• Molecule 3: Isoform GN-1 of Glycogenin-1

Chain E:

8%

8% 90%

• Molecule 3: Isoform GN-1 of Glycogenin-1

9%

Chain F: 8%   •   90%

• Molecule 3: Isoform GN-1 of Glycogenin-1

8%

Chain G: 8%   •   90%

S301 E302 E303 R304 K305 E306 R307 W308 E309 Q310 G311 Q312 A313 D314 Y315 M316 G317 A318 D319 S320 F321 D322 N323 I324 K325 R326 K327 L328 D329 T330 Y331 L332 GLN

• Molecule 3: Isoform GN-1 of Glycogenin-1

9%

Chain H:

8% . 90%

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

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

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

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

THR HIS PRO GLU PHE LEU ILE LEU TRP TRP ASN ILE PHE THR THR ASN VAL LEU PRO LEU LEU GLN GLN PHE GLY LEU VAL LYS ASP THR CYS SER TYR VAL ASN VAL GLU ASP VAL SER GLY ALA ILE SER HIS LEU SER LEU GLY GLU ILE PRO ALA MET ALA GLN PRO PHE VAL ♦ S300

S301 E302 E303 R304 K305 E306 R307 W308 E309 Q310 G311 Q312 A313 D314 Y315 M316 G317 A318 D319 S320 F321 D322 N323 I324 K325 R326 K327 L328 D329 T330 Y331 L332 GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	739232	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 $(e^-/\text{Å}^2)$	34.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.313	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	204.48, 204.48, 204.48	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.34	0/5121	0.51	0/6942
1	C	0.34	0/5121	0.51	0/6942
2	B	0.34	0/5140	0.51	0/6968
2	D	0.35	0/5140	0.51	0/6968
3	E	0.24	0/282	0.48	0/375
3	F	0.24	0/282	0.49	0/375
3	G	0.24	0/282	0.48	0/375
3	H	0.25	0/282	0.49	0/375
All	All	0.34	0/21650	0.51	0/29320

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 ⓘ

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	4988	4842	4854	99	0
1	C	4988	4842	4854	105	0
2	B	5017	4879	4878	111	0
2	D	5017	4879	4878	116	0
3	E	278	256	256	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	278	256	256	3	0
3	G	278	256	256	4	0
3	H	278	256	256	3	0
All	All	21122	20466	20488	421	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 10.

The worst 5 of 421 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)
2:D:497:VAL:HG12	2:D:524:ILE:HD13	1.64	0.79
2:B:497:VAL:HG12	2:B:524:ILE:HD13	1.64	0.79
2:D:379:THR:HG22	2:D:488:LEU:HD11	1.68	0.76
1:A:259:SER:HG	1:A:262:THR:HG1	1.33	0.75
1:C:259:SER:HG	1:C:262:THR:HG1	1.34	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	611/737 (83%)	592 (97%)	19 (3%)	0	100	100
1	C	611/737 (83%)	592 (97%)	19 (3%)	0	100	100
2	B	614/737 (83%)	598 (97%)	16 (3%)	0	100	100
2	D	614/737 (83%)	599 (98%)	15 (2%)	0	100	100
3	E	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
3	F	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
3	G	31/333 (9%)	29 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	31/333 (9%)	29 (94%)	2 (6%)	0	100	100
All	All	2574/4280 (60%)	2497 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	529/638 (83%)	529 (100%)	0	100	100
1	C	529/638 (83%)	529 (100%)	0	100	100
2	B	531/637 (83%)	531 (100%)	0	100	100
2	D	531/637 (83%)	531 (100%)	0	100	100
3	E	29/294 (10%)	29 (100%)	0	100	100
3	F	29/294 (10%)	29 (100%)	0	100	100
3	G	29/294 (10%)	29 (100%)	0	100	100
3	H	29/294 (10%)	29 (100%)	0	100	100
All	All	2236/3726 (60%)	2236 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	417	ASN
1	C	417	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	SEP	D	641	2	8,9,10	1.36	1 (12%)	8,12,14	1.56	2 (25%)
2	SEP	B	641	2	8,9,10	1.37	1 (12%)	8,12,14	1.55	2 (25%)

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
2	SEP	D	641	2	-	0/5/8/10	-
2	SEP	B	641	2	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	641	SEP	P-O1P	3.02	1.60	1.50
2	D	641	SEP	P-O1P	3.01	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	641	SEP	OG-CB-CA	3.07	111.14	108.14
2	D	641	SEP	OG-CB-CA	3.03	111.09	108.14
2	D	641	SEP	P-OG-CB	-2.12	112.45	118.30
2	B	641	SEP	P-OG-CB	-2.10	112.50	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	641	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	641	SEP	1	0
2	B	641	SEP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

This section contains visualisations of the EMDB entry EMD-14587. 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 ⓘ
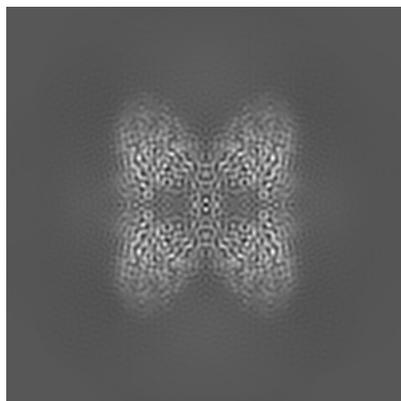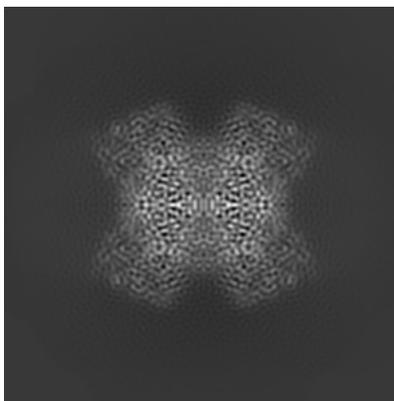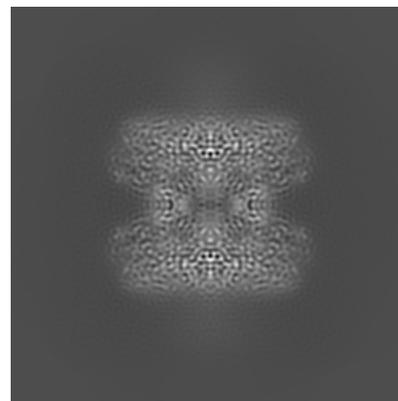
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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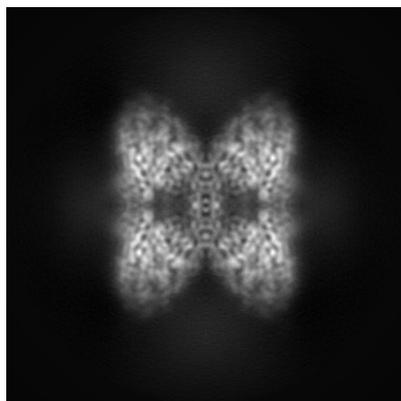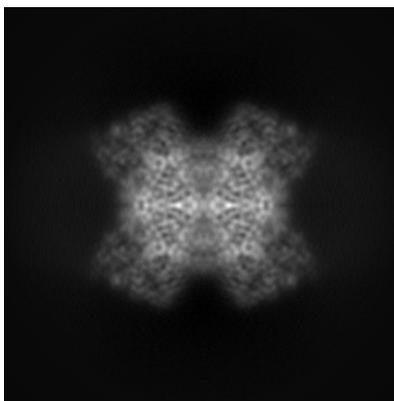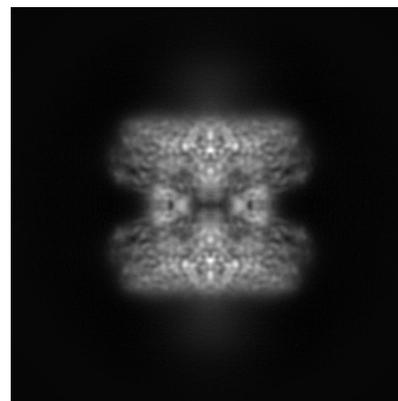
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
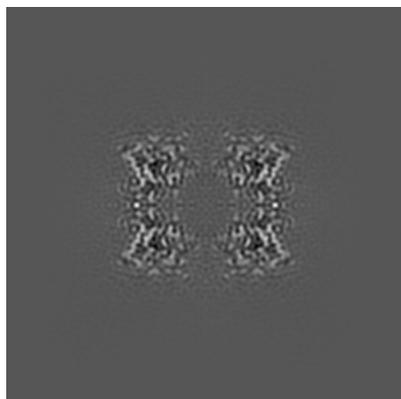
6.2.1 Primary map
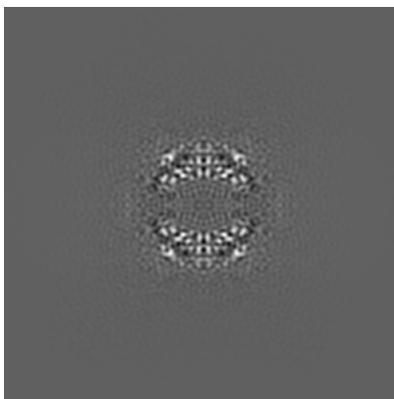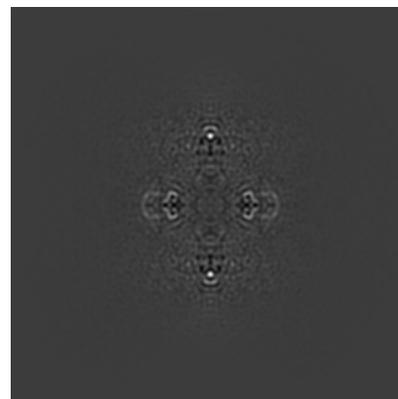
| X Index: 144 | Y Index: 144 | Z Index: 144 |

6.2.2 Raw map
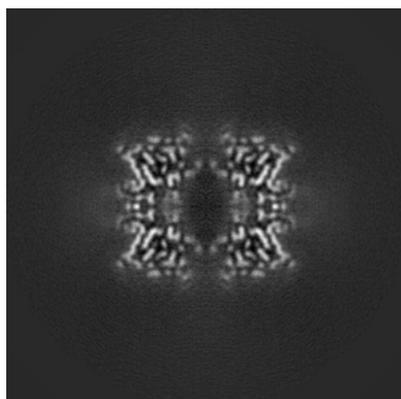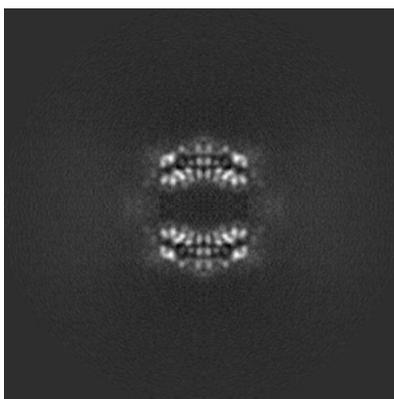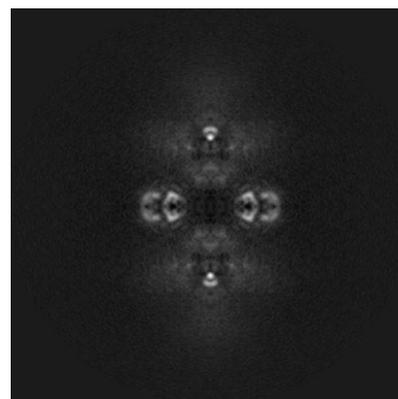
| X Index: 144 | Y Index: 144 | Z Index: 144 |

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

6.3 Largest variance slices ⓘ
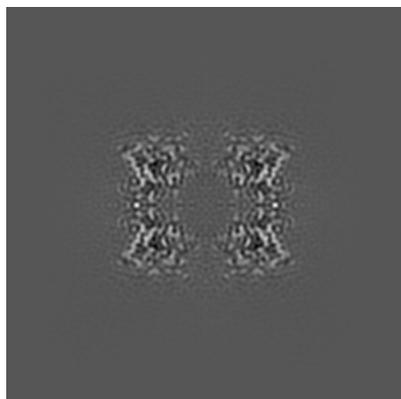
6.3.1 Primary map
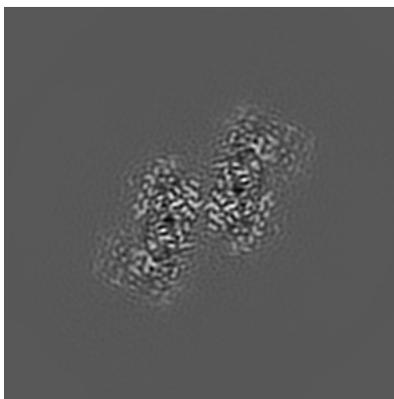
X Index: 144	Y Index: 184	Z Index: 115
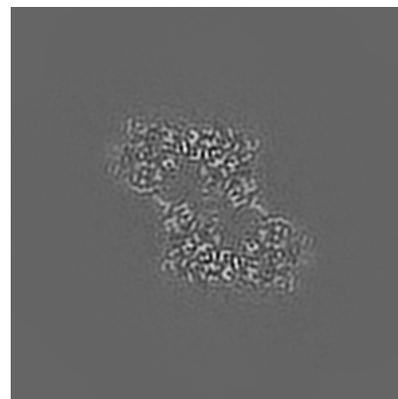
6.3.2 Raw map
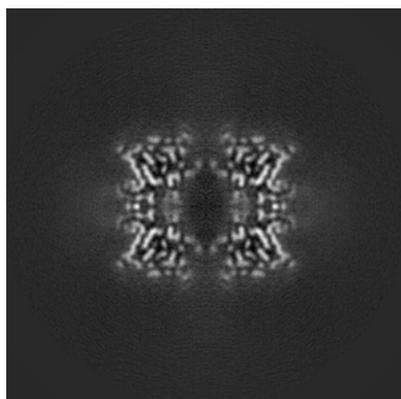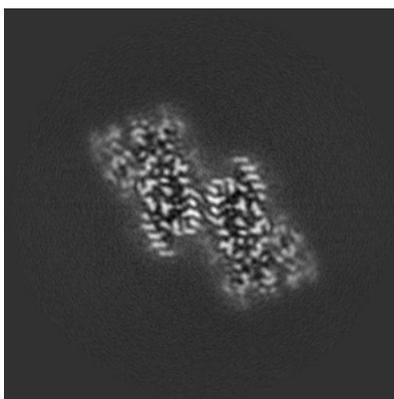
X Index: 144	Y Index: 100	Z Index: 115
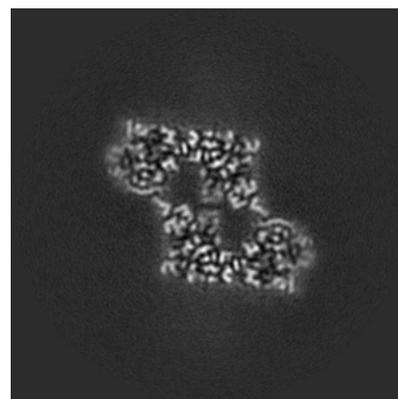
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X   Y   Z
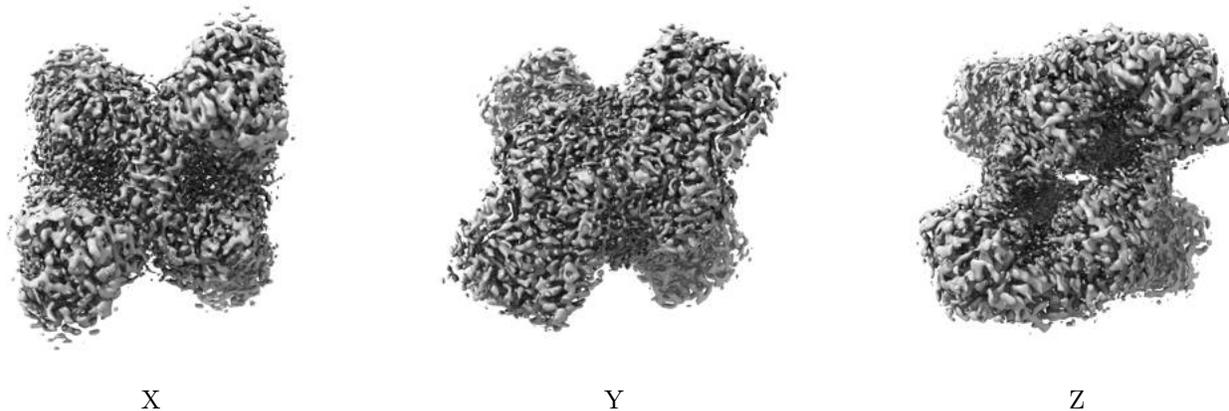
The images above show the 3D surface view of the map at the recommended contour level 0.025.
These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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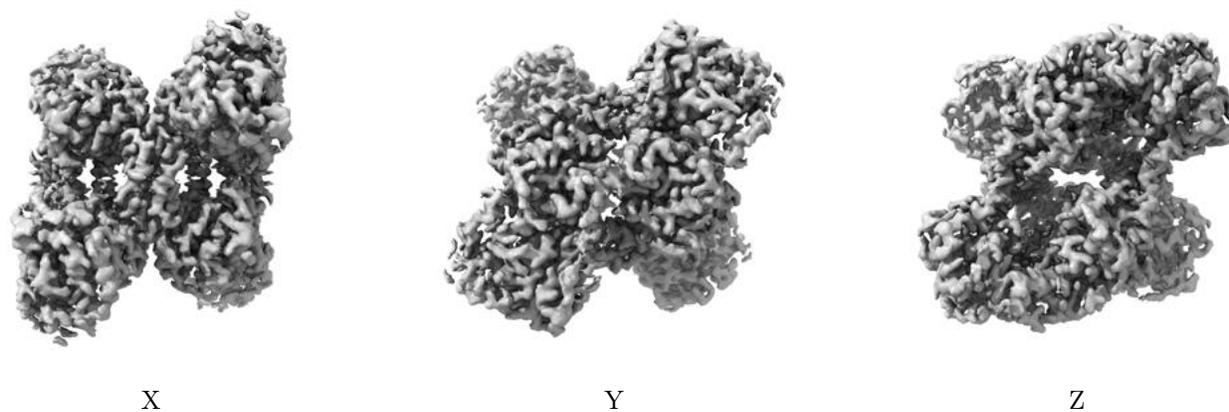
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

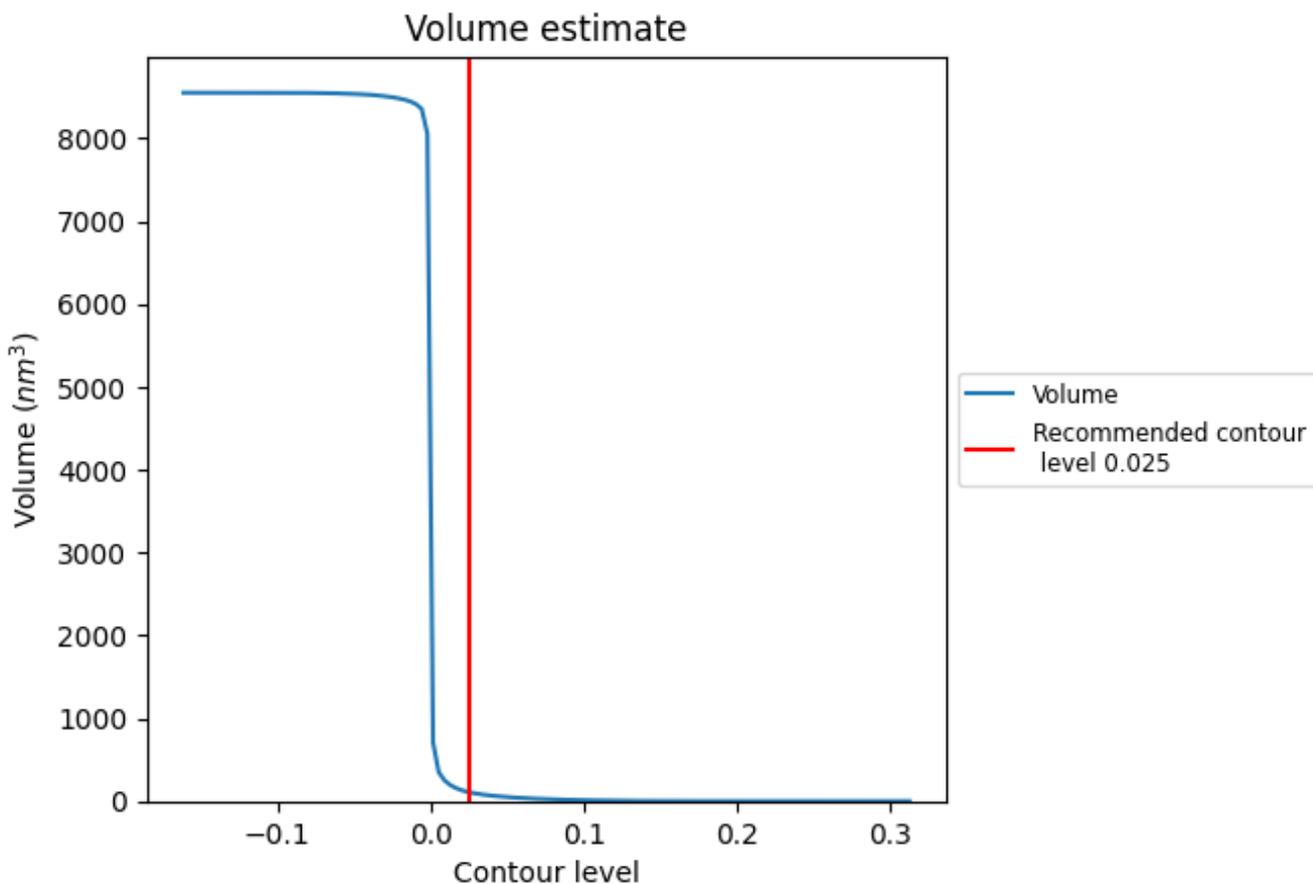### 6.5.1 emd_14587_msk_1.map ⓘ
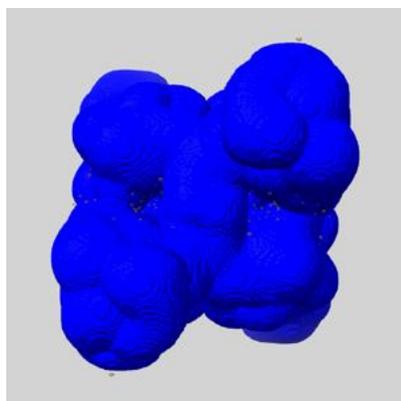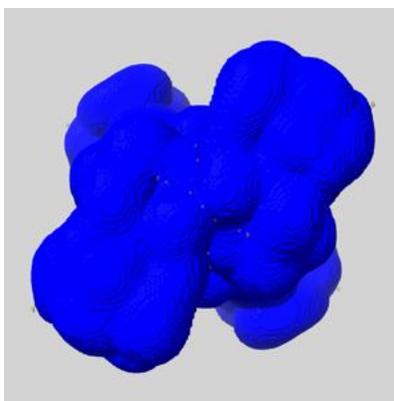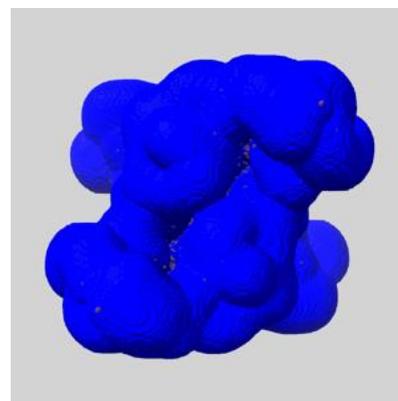
X Y Z

7 Map analysis (i)

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

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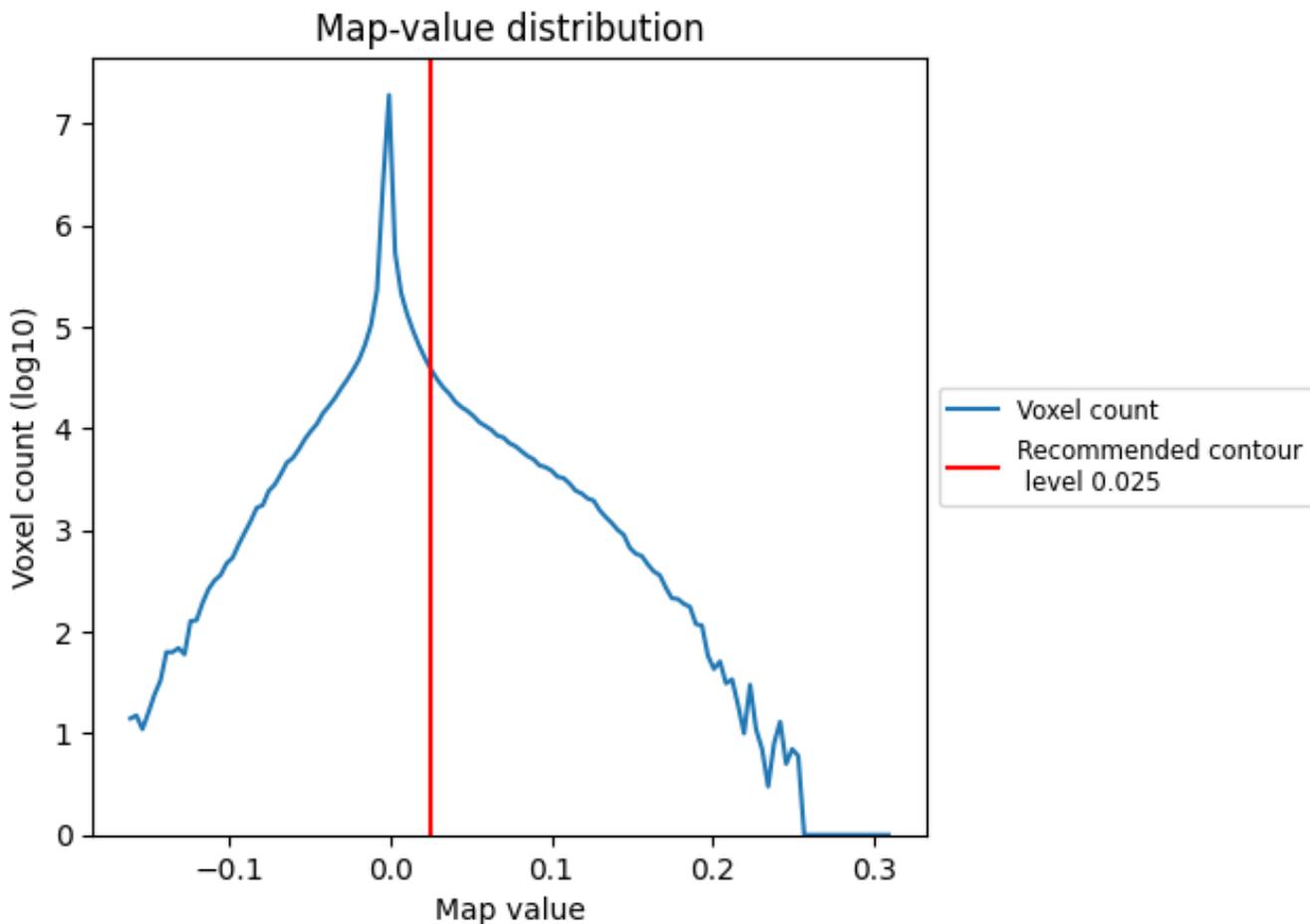
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ

The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 99 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 ⓘ
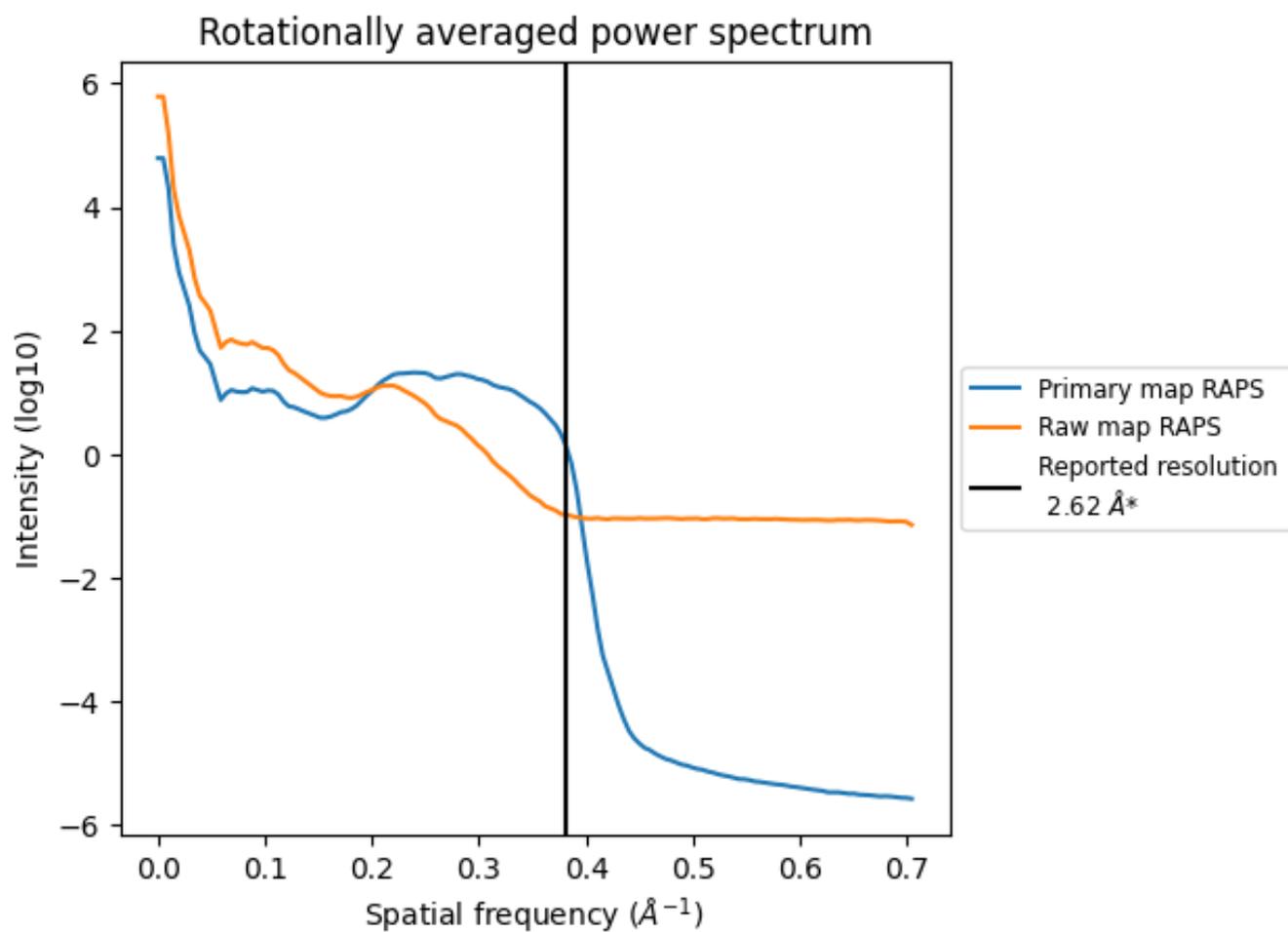
*Reported resolution corresponds to spatial frequency of 0.382 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ
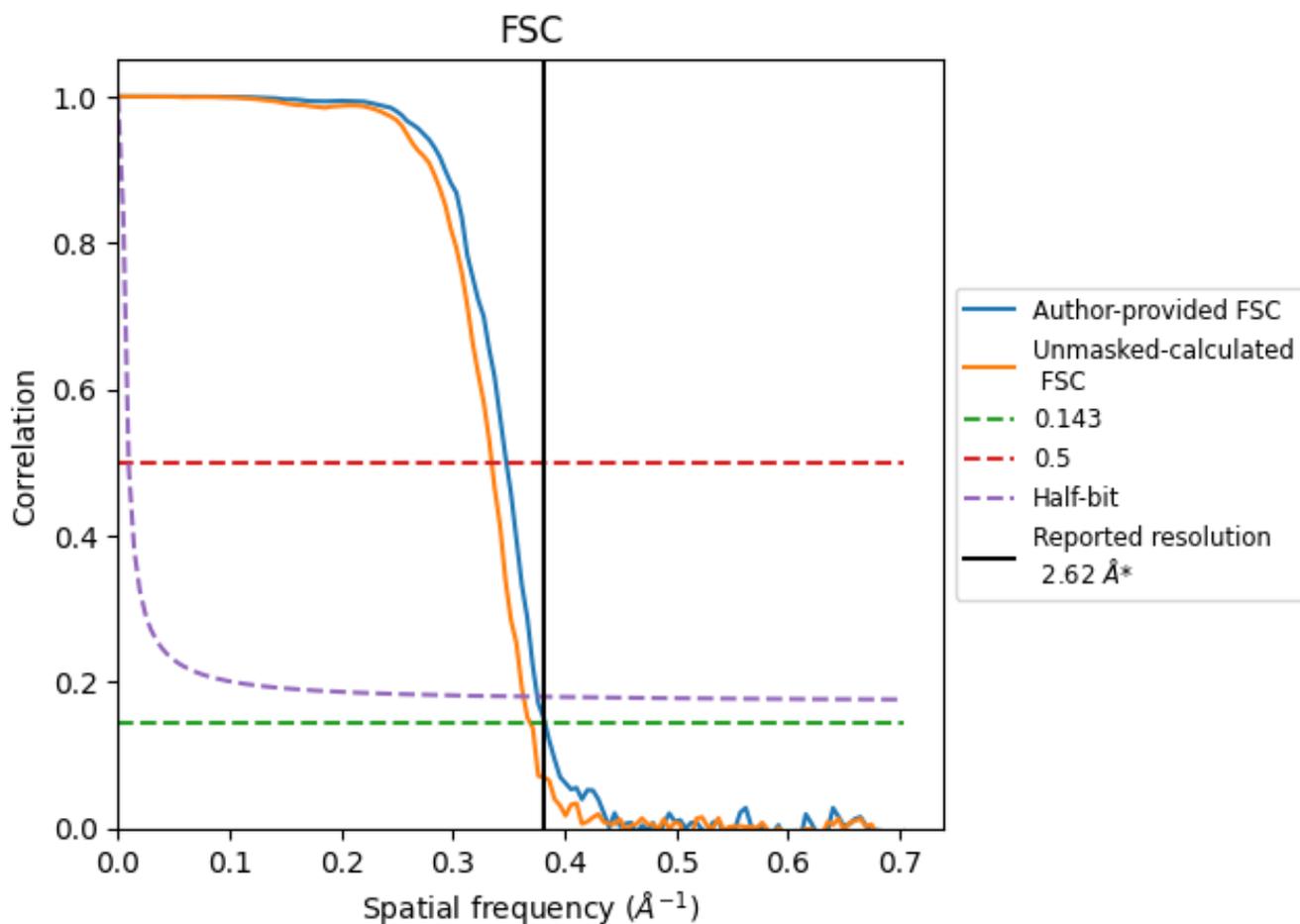
*Reported resolution corresponds to spatial frequency of 0.382 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.61	2.87	2.66
Unmasked-calculated*	2.71	2.99	2.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14587 and PDB model 7ZBN. Per-residue inclusion information can be found in section 3 on page 5.

9.1   Map-model overlay ⓘ

<div align="center">X   Y   Z</div>
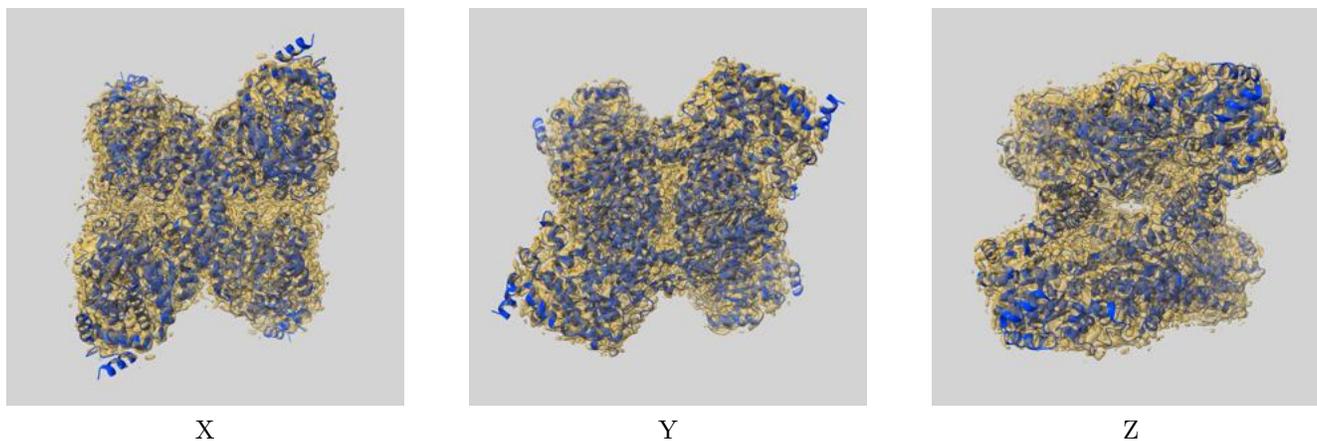
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion ⓘ
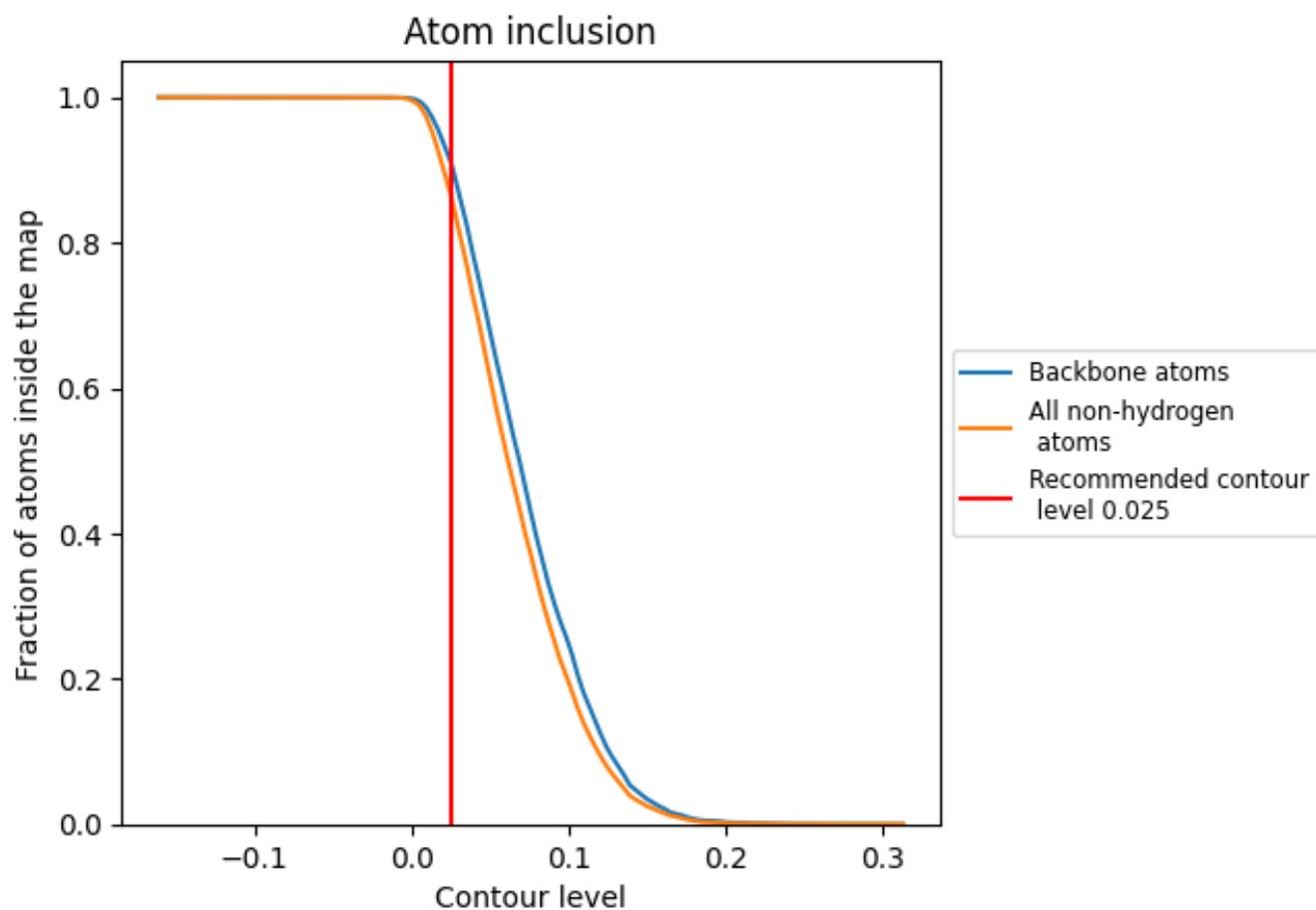
At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.