



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 01:01 pm GMT

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)

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.39

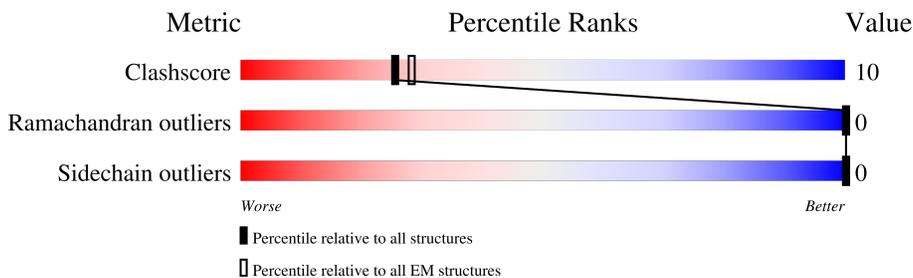
1 Overall quality at a glance

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	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	737	 67% 17% 16%
1	C	737	 66% 18% 16%
2	B	737	 64% 20% 16%
2	D	737	 63% 21% 16%
3	E	333	 6% 8% 8% 90%
3	F	333	 6% 8% 8% 90%
3	G	333	 6% 8% 8% 90%
3	H	333	 6% 8% 8% 90%

2 Entry composition [i](#)

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
			Total	C	H	N	O	S		
1	A	617	9830	3202	4842	858	903	25	0	0
1	C	617	9830	3202	4842	858	903	25	0	0

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

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

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

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

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

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

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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 [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	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 [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	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 [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	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 [i](#)

There are no RNA molecules in this entry.

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

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	B	641	2	8,9,10	1.37	1 (12%)	8,12,14	1.55	2 (25%)
2	SEP	D	641	2	8,9,10	1.36	1 (12%)	8,12,14	1.56	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	B	641	2	-	1/5/8/10	-
2	SEP	D	641	2	-	0/5/8/10	-

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(°)	Ideal(°)
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	B	641	SEP	1	0
2	D	641	SEP	1	0

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.

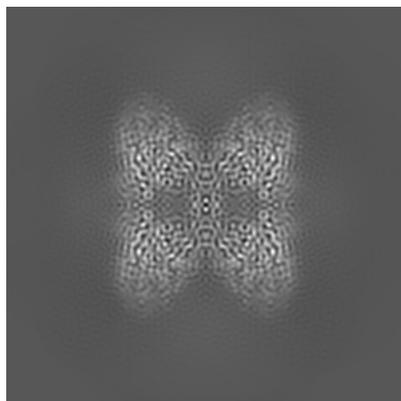
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14587. These allow visual inspection of the internal detail of the map and identification of artifacts.

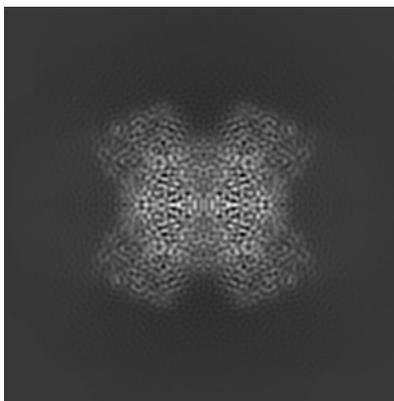
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

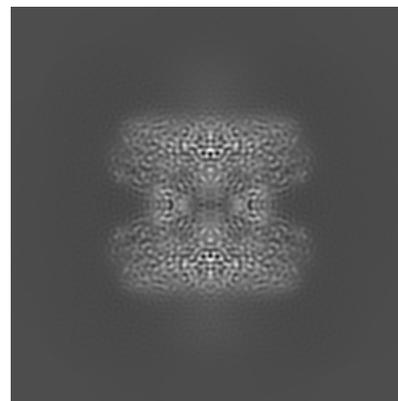
6.1.1 Primary map



X

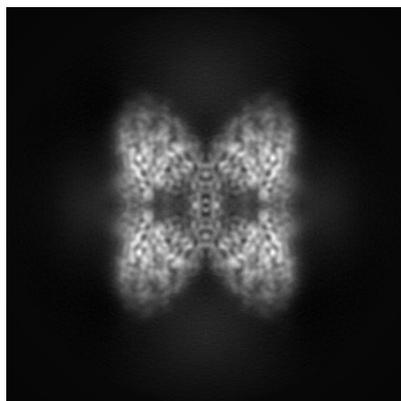


Y

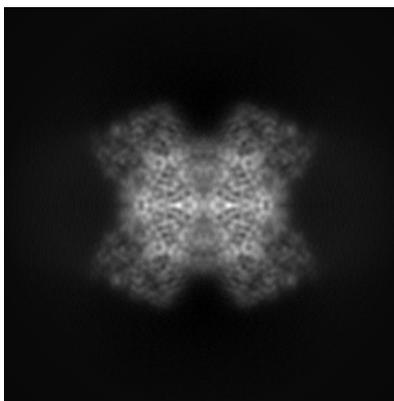


Z

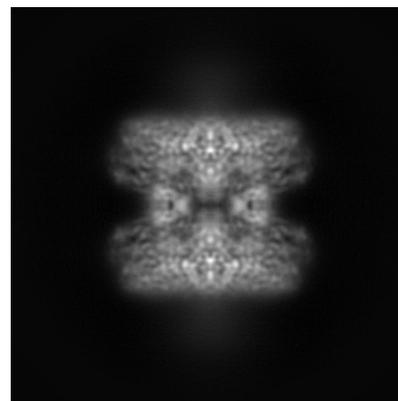
6.1.2 Raw map



X



Y

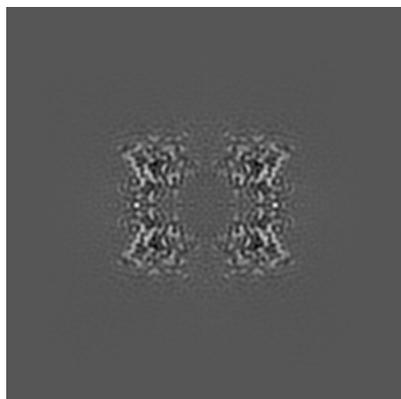


Z

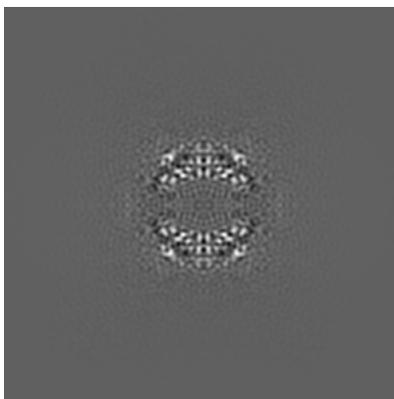
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

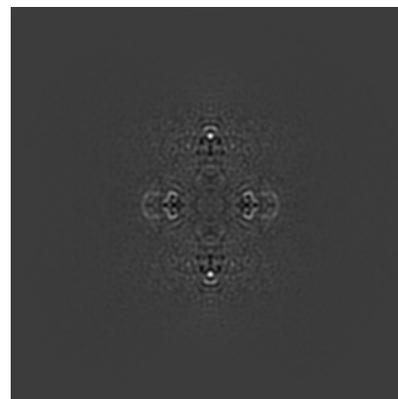
6.2.1 Primary map



X Index: 144

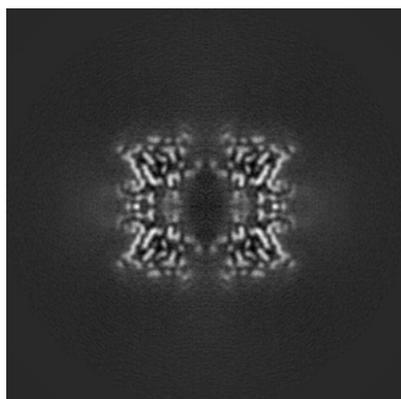


Y Index: 144

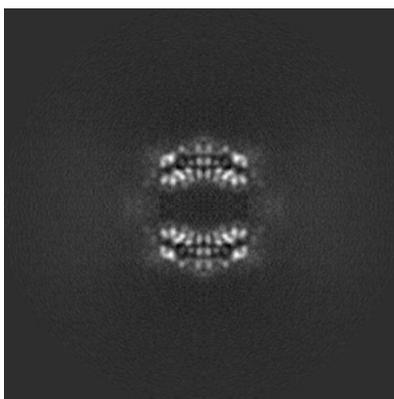


Z Index: 144

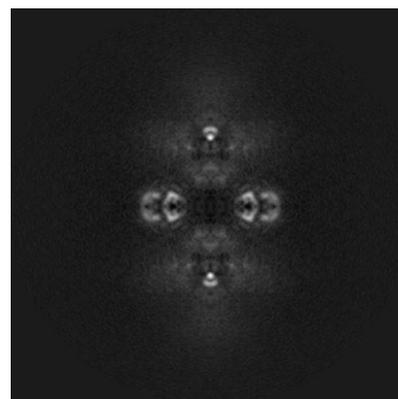
6.2.2 Raw map



X Index: 144



Y Index: 144

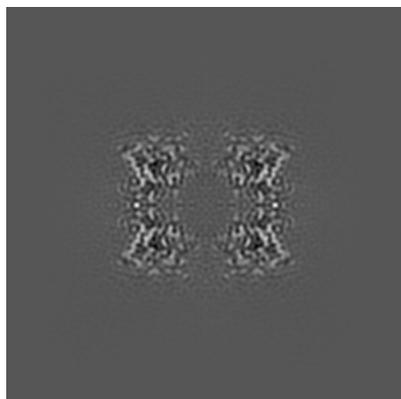


Z Index: 144

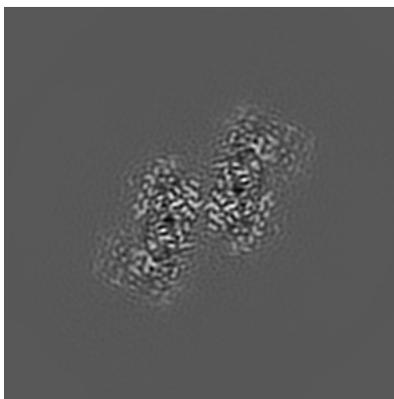
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

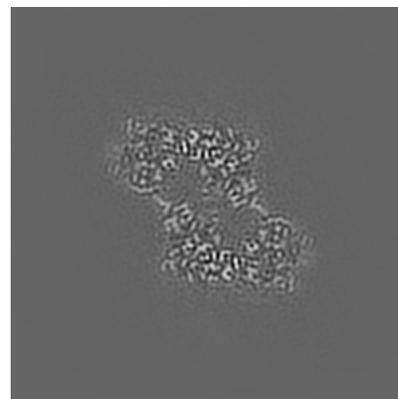
6.3.1 Primary map



X Index: 144

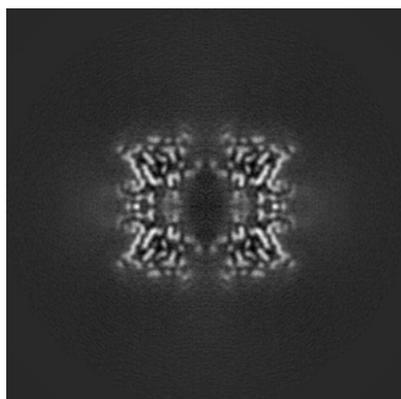


Y Index: 184

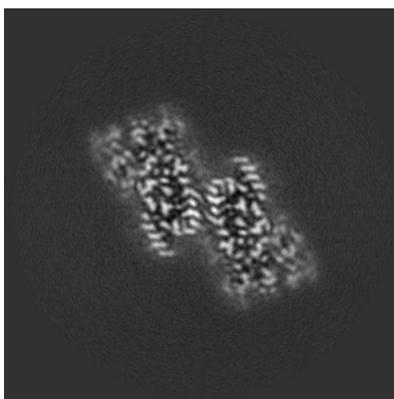


Z Index: 115

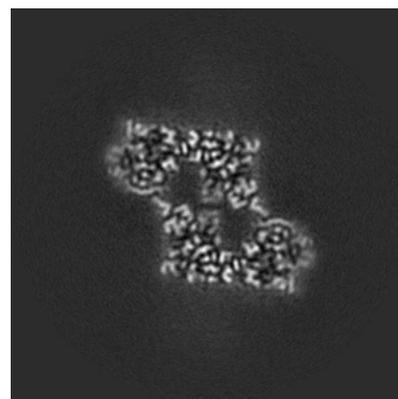
6.3.2 Raw map



X Index: 144



Y Index: 100

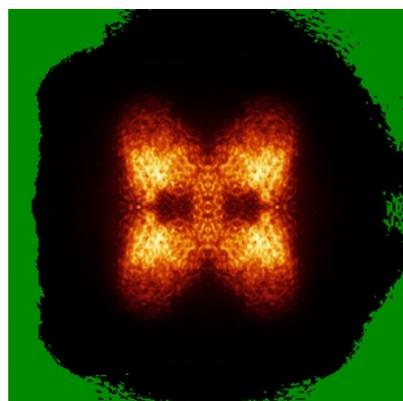


Z Index: 115

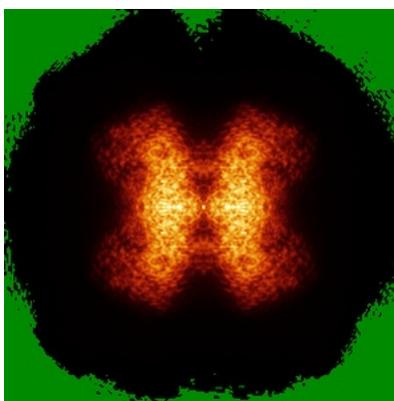
The images above show the largest variance slices of the map in three orthogonal directions.

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

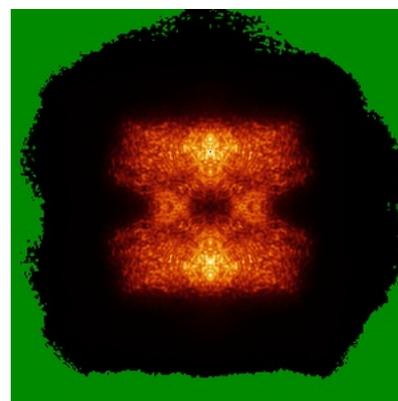
6.4.1 Primary map



X

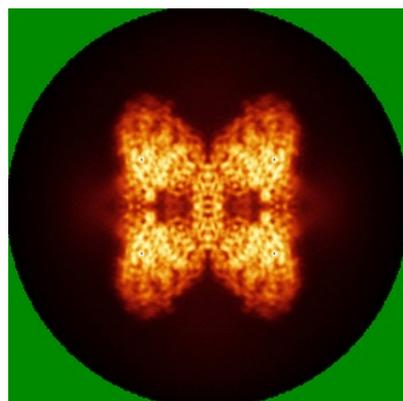


Y

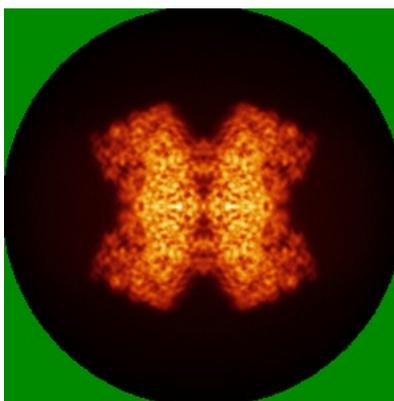


Z

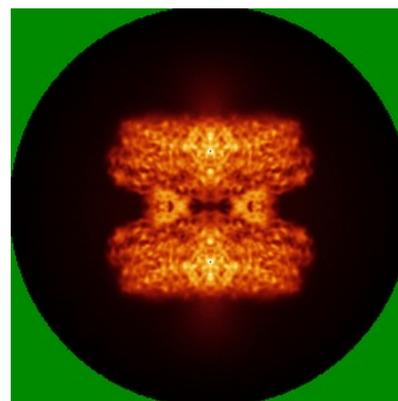
6.4.2 Raw map



X



Y

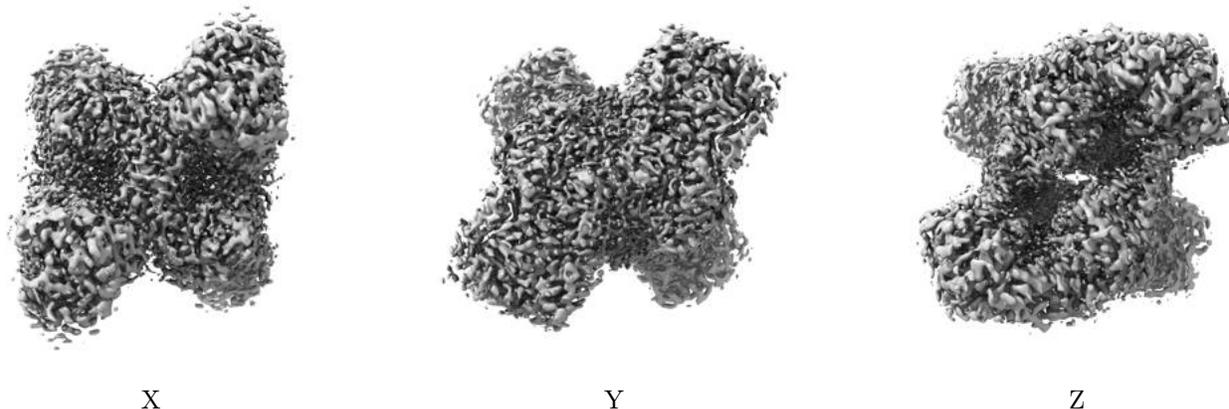


Z

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.

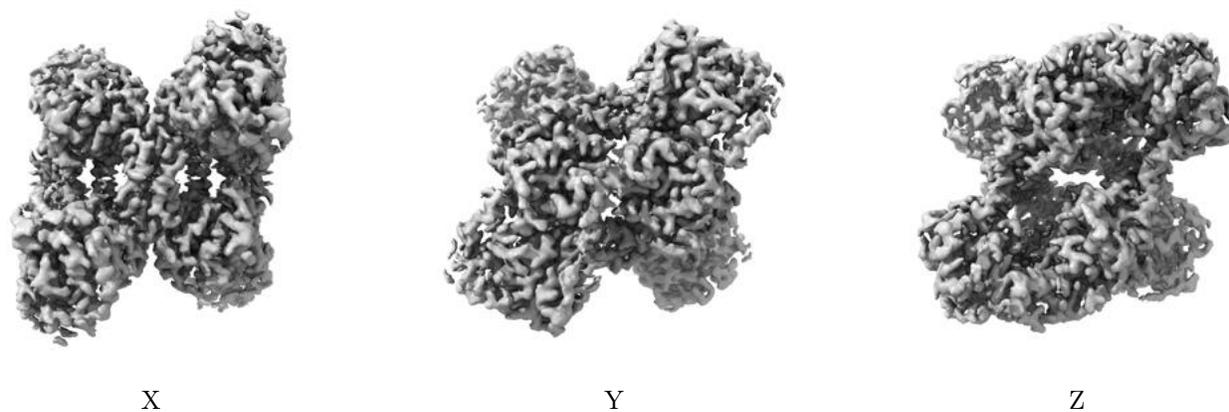
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

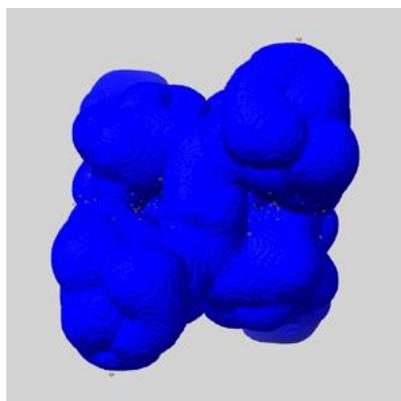
6.6 Mask visualisation [i](#)

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

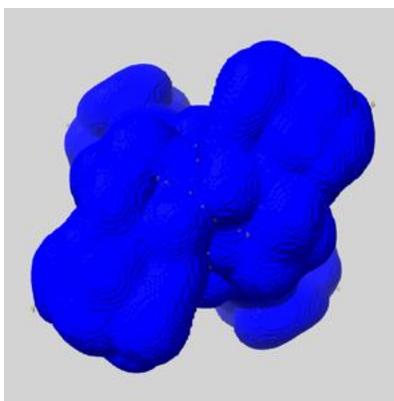
A mask typically either:

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

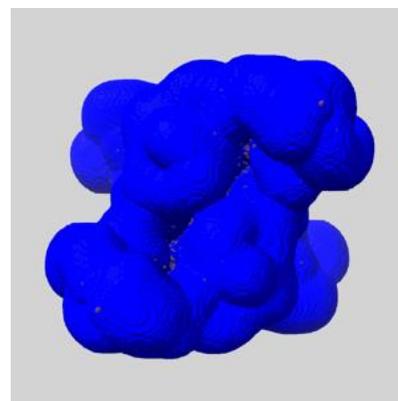
6.6.1 emd_14587_msk_1.map [i](#)



X



Y

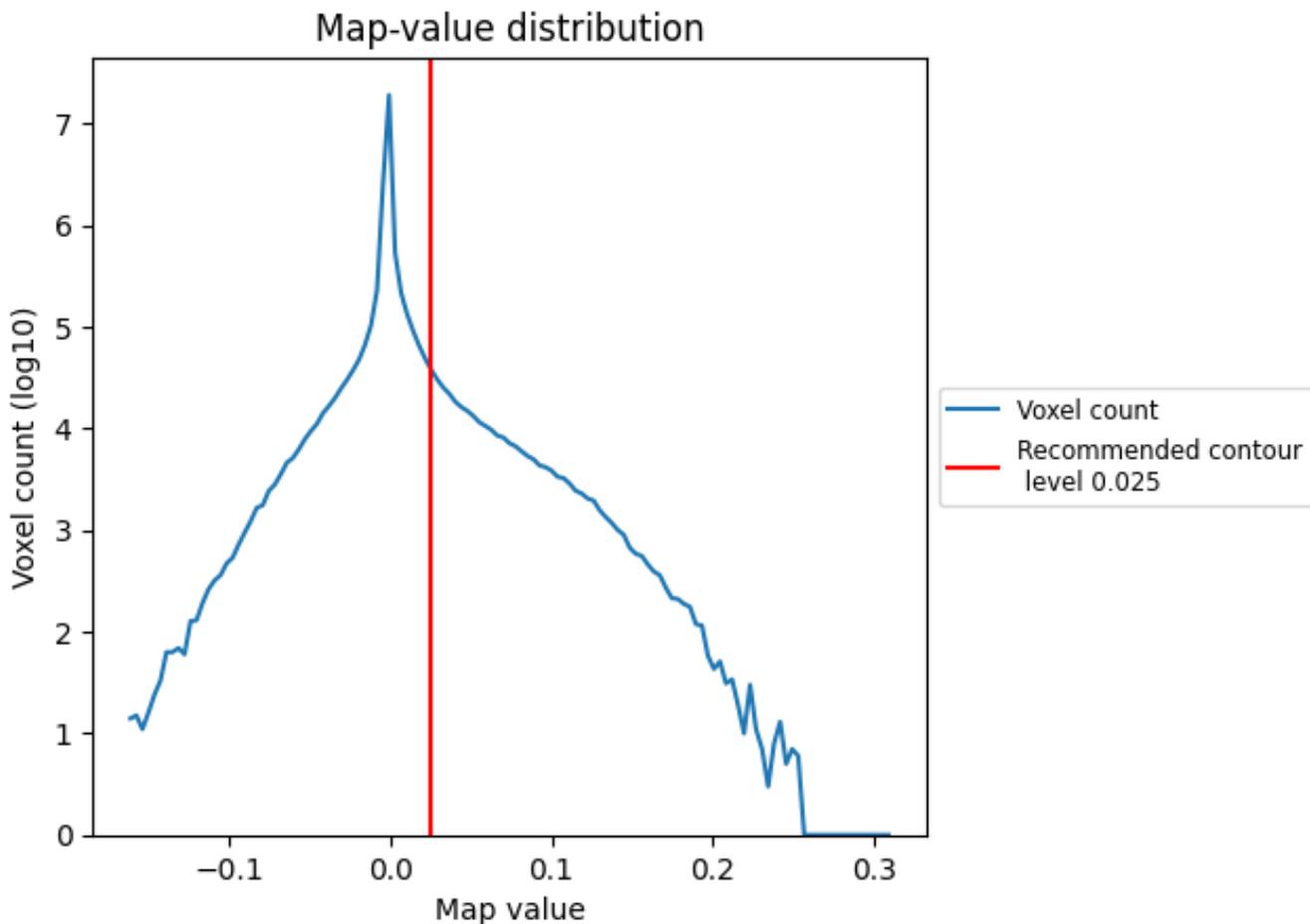


Z

7 Map analysis [i](#)

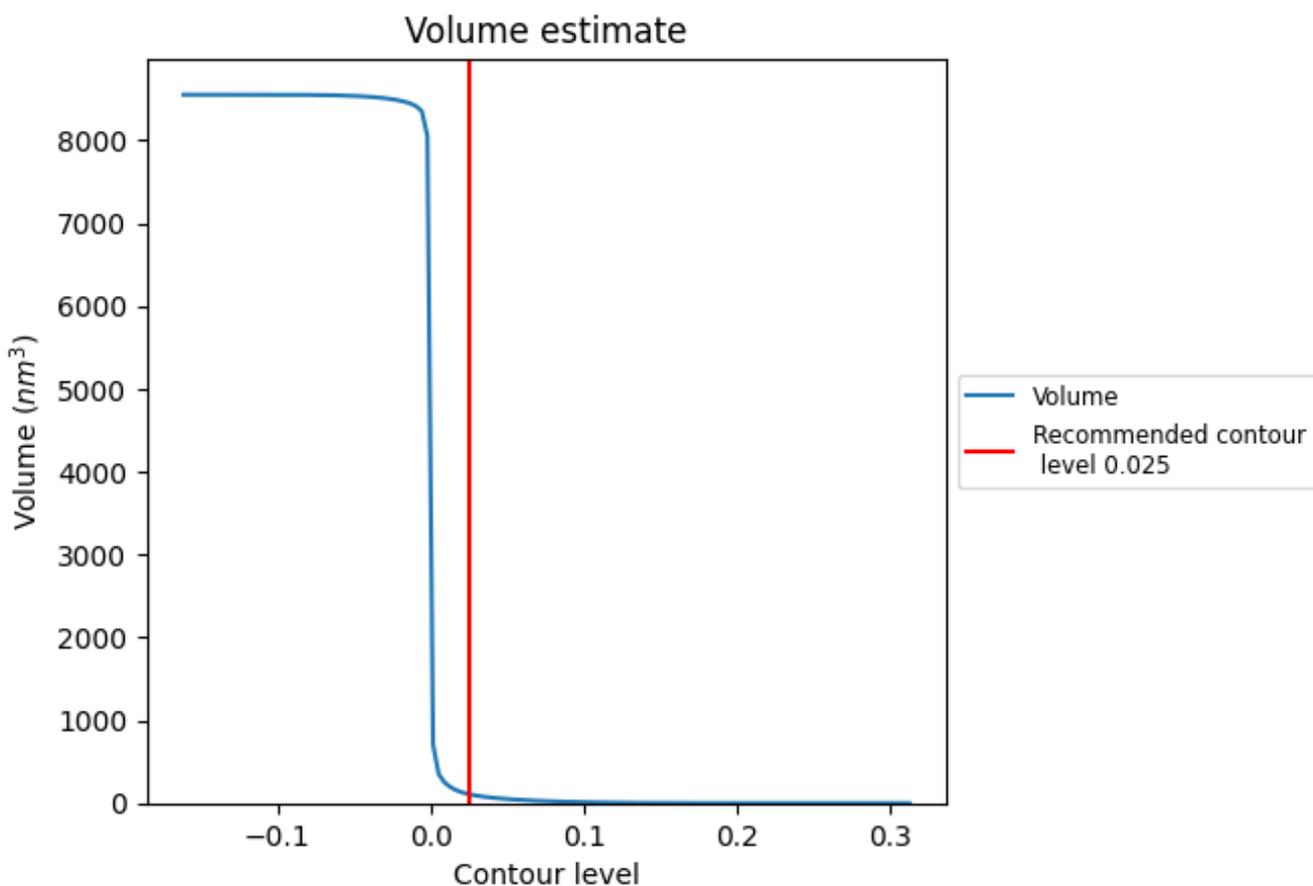
This section contains the results of statistical analysis of the map.

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.

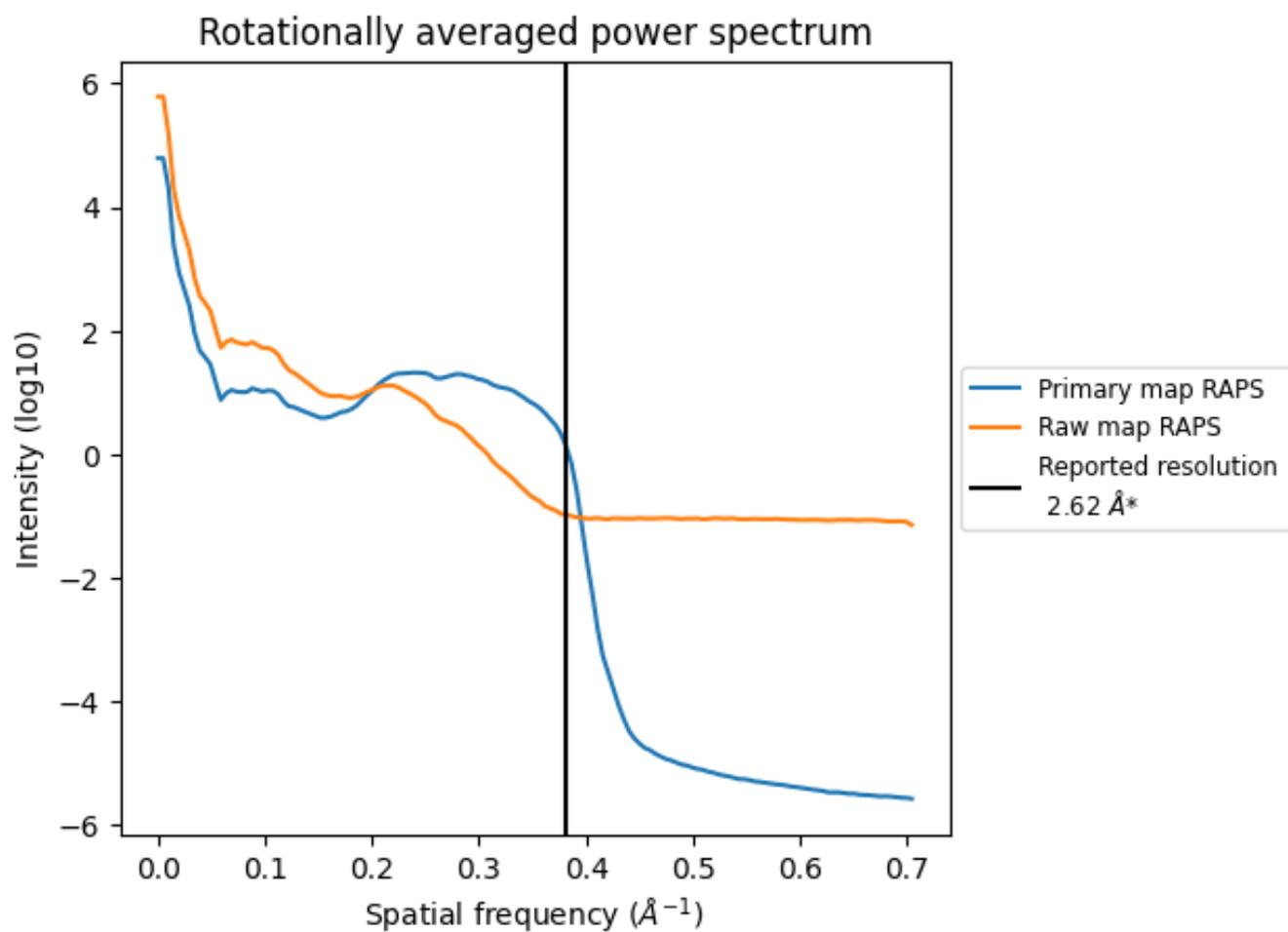
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 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 [i](#)

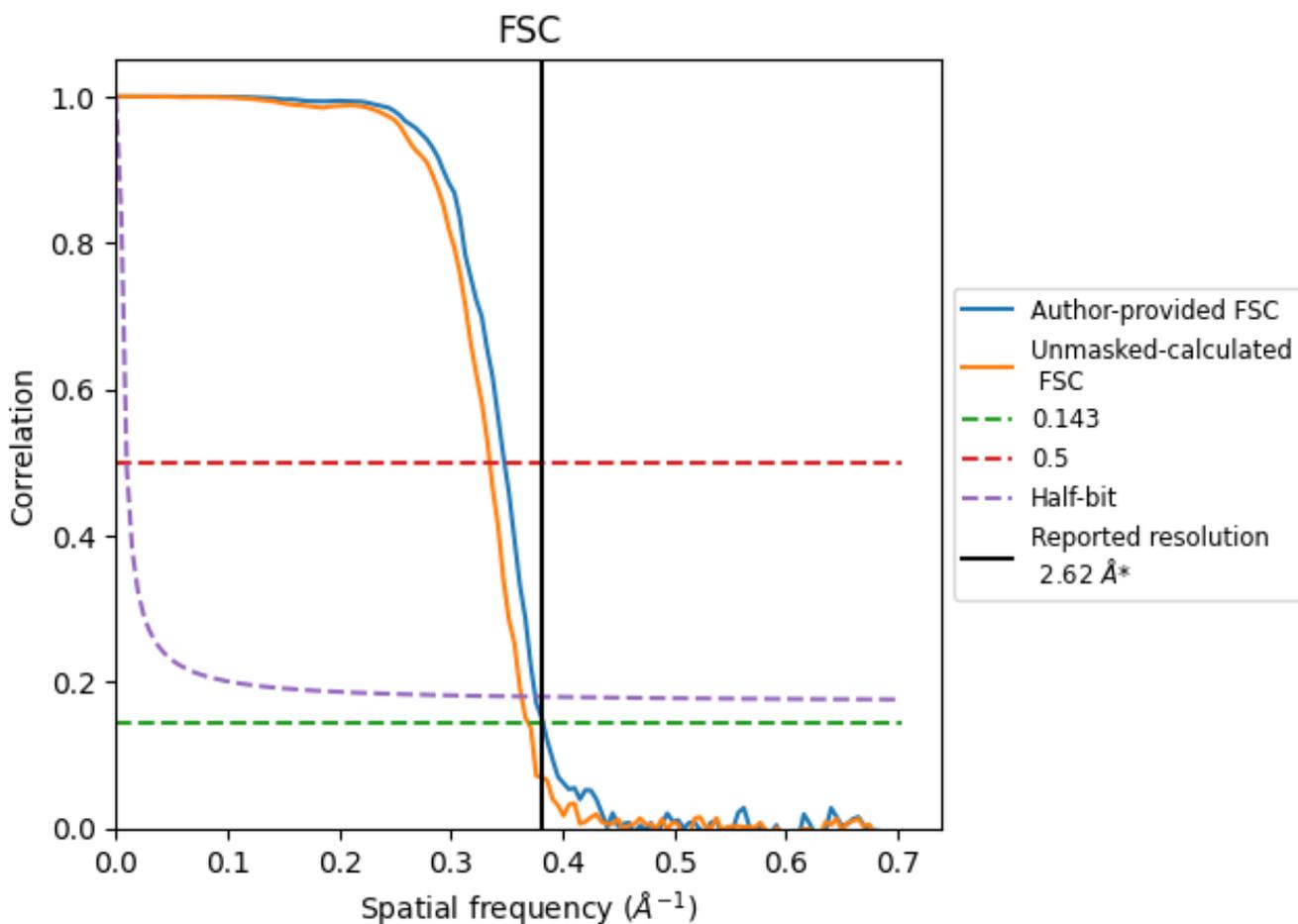


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 Å⁻¹

8.2 Resolution estimates [i](#)

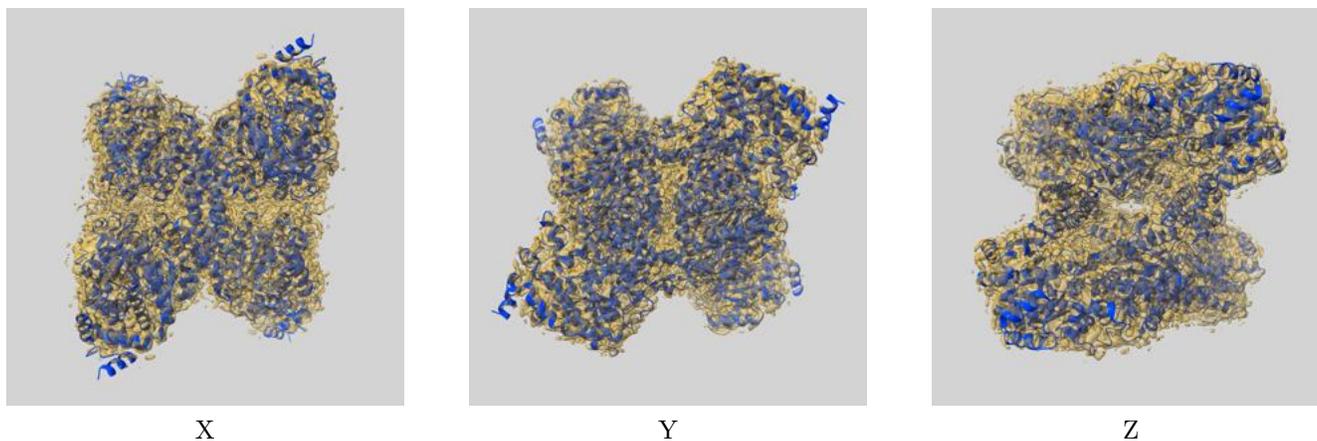
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.61	2.87	2.66
Unmasked-calculated*	2.71	2.99	2.75

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

9 Map-model fit [i](#)

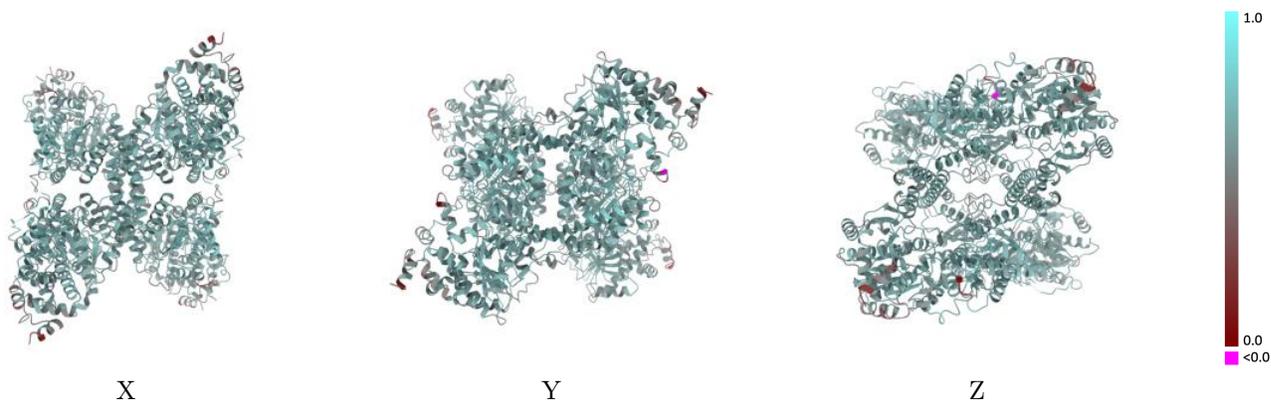
This section contains information regarding the fit between EMDB map EMD-14587 and PDB model 7ZBN. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



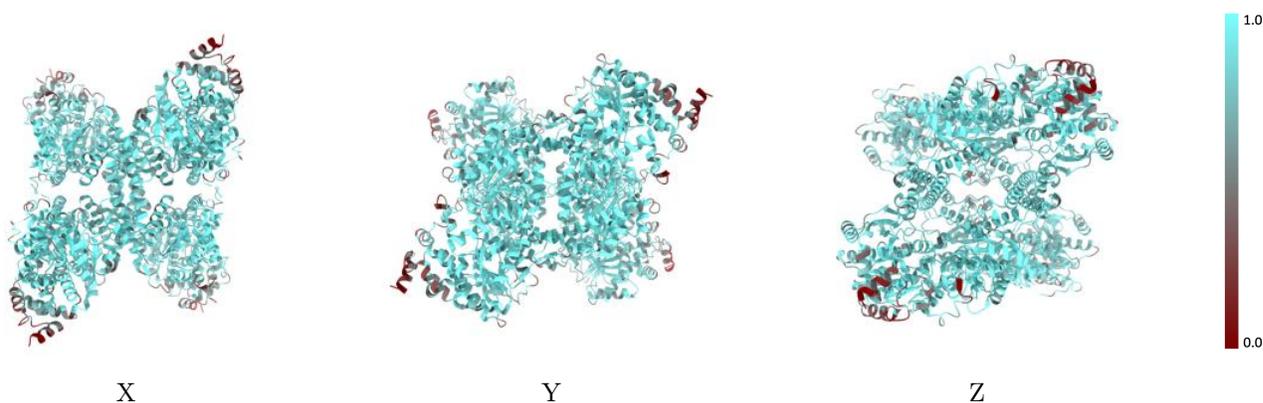
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



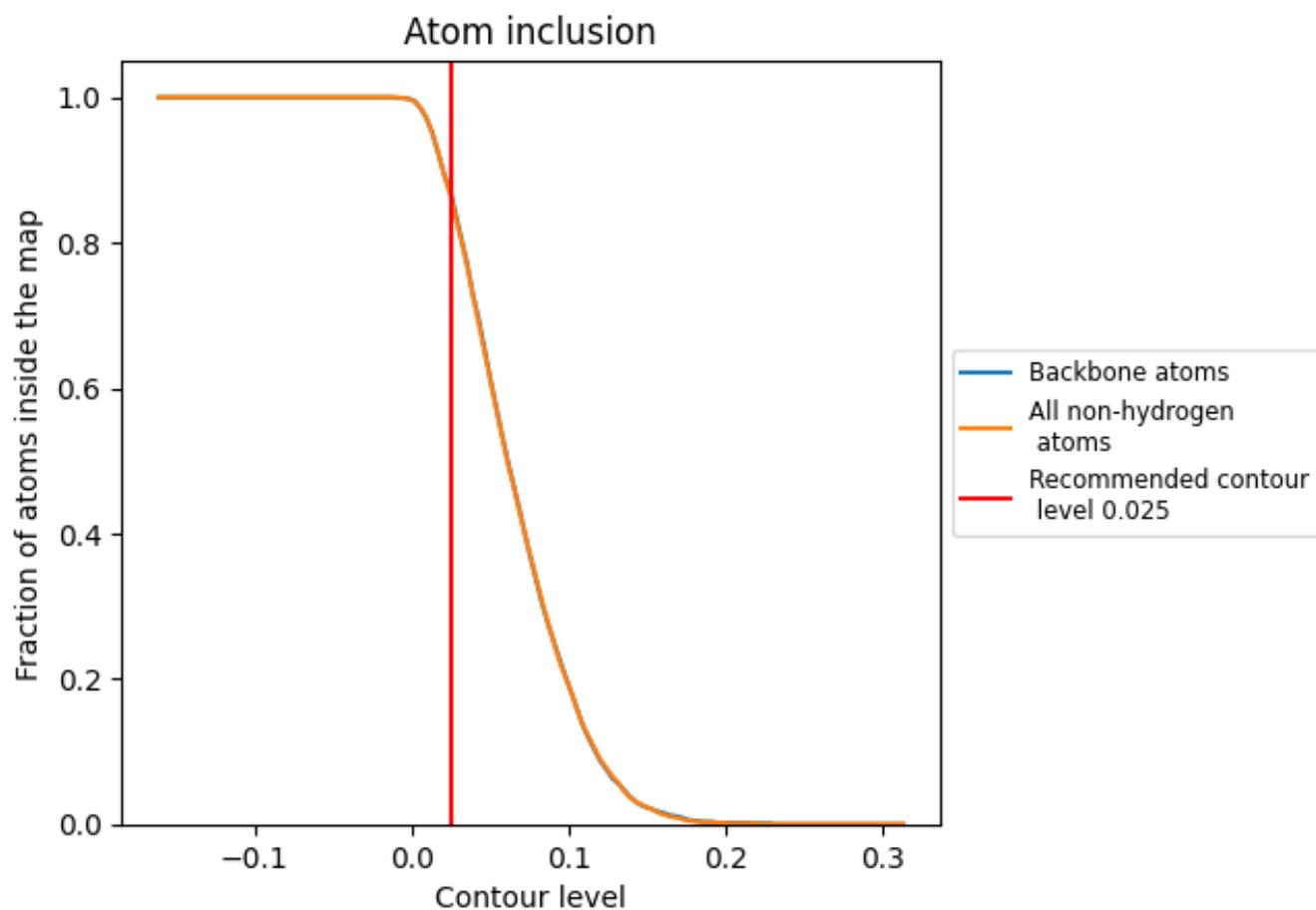
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.6200
A	 0.8910	 0.6290
B	 0.8890	 0.6280
C	 0.8920	 0.6300
D	 0.8910	 0.6290
E	 0.3720	 0.4620
F	 0.3680	 0.4690
G	 0.3720	 0.4700
H	 0.3640	 0.4720

