



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 10:59 am BST

PDB ID : 7Q0B
EMDB ID : EMD-13743
Title : Human GYS1-GYG1 complex inhibited state
Authors : McCorvie, T.J.; Shrestha, L.; Froese, D.S.; Ferreira, I.M.; Yue, W.W.
Deposited on : 2021-10-14
Resolution : 3.00 Å(reported)
Based on initial model : 4QLB

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

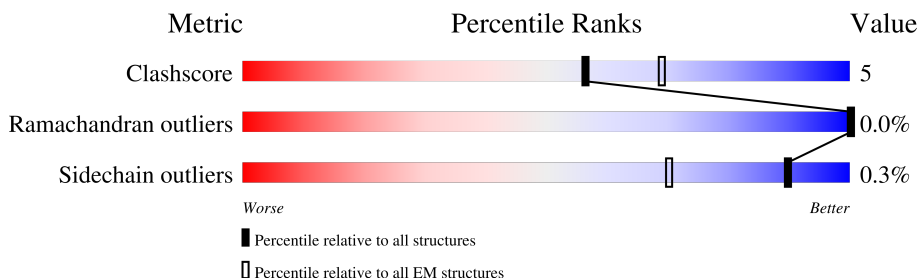
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	737	
1	D	737	
2	B	737	
2	C	737	
3	E	350	
3	F	350	
3	G	350	
3	H	350	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21168 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 Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	620	Total	C	N	O	S	0	0
			5002	3209	858	910	25		
1	D	620	Total	C	N	O	S	0	0
			5002	3209	858	910	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	623	Total	C	N	O	P S	0	0
			5026	3222	861	917	1 25		
2	C	623	Total	C	N	O	P S	0	0
			5026	3222	861	917	1 25		

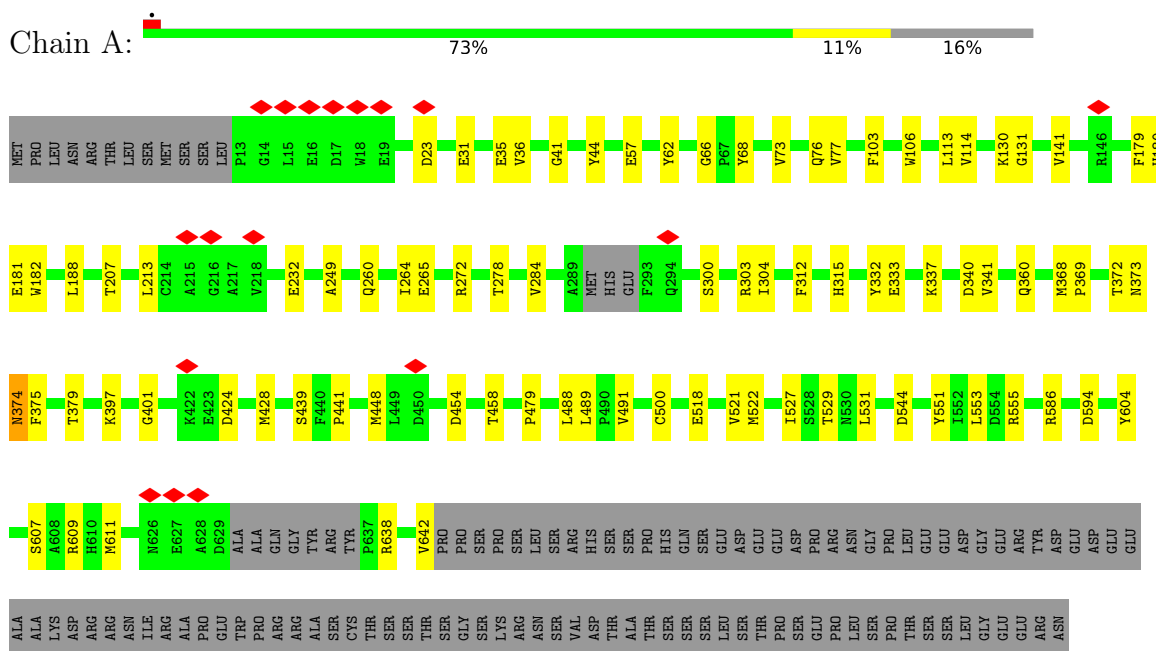
- Molecule 3 is a protein called Glycogenin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	33	Total	C	N	O	S	0	0
			278	170	49	58	1		
3	F	33	Total	C	N	O	S	0	0
			278	170	49	58	1		
3	G	33	Total	C	N	O	S	0	0
			278	170	49	58	1		
3	H	33	Total	C	N	O	S	0	0
			278	170	49	58	1		

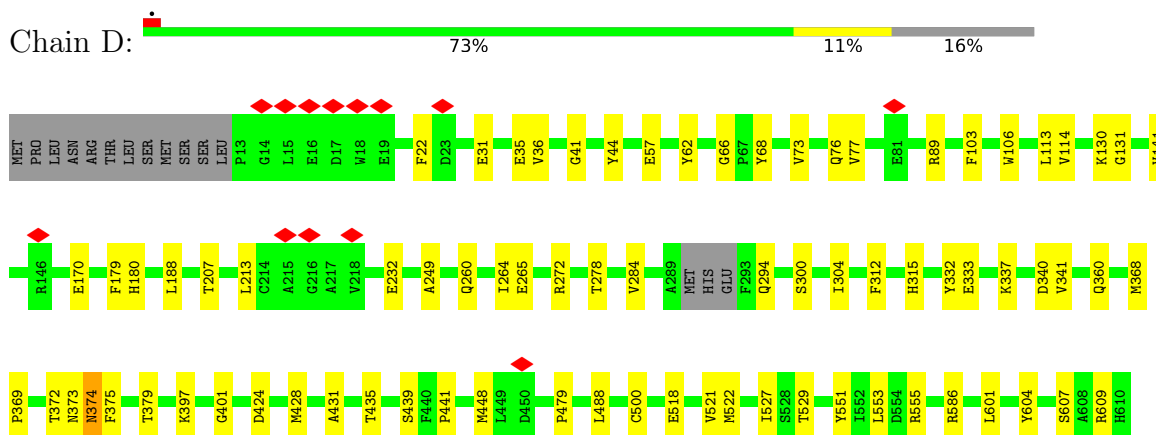
3 Residue-property plots

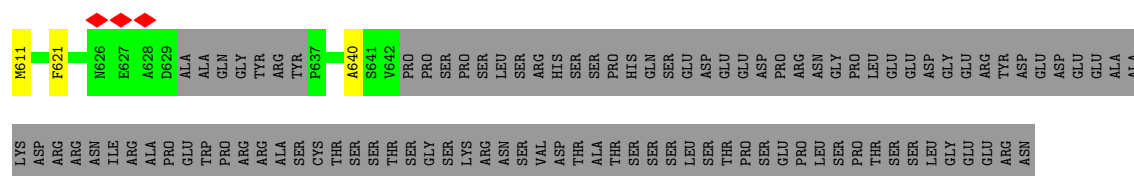
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



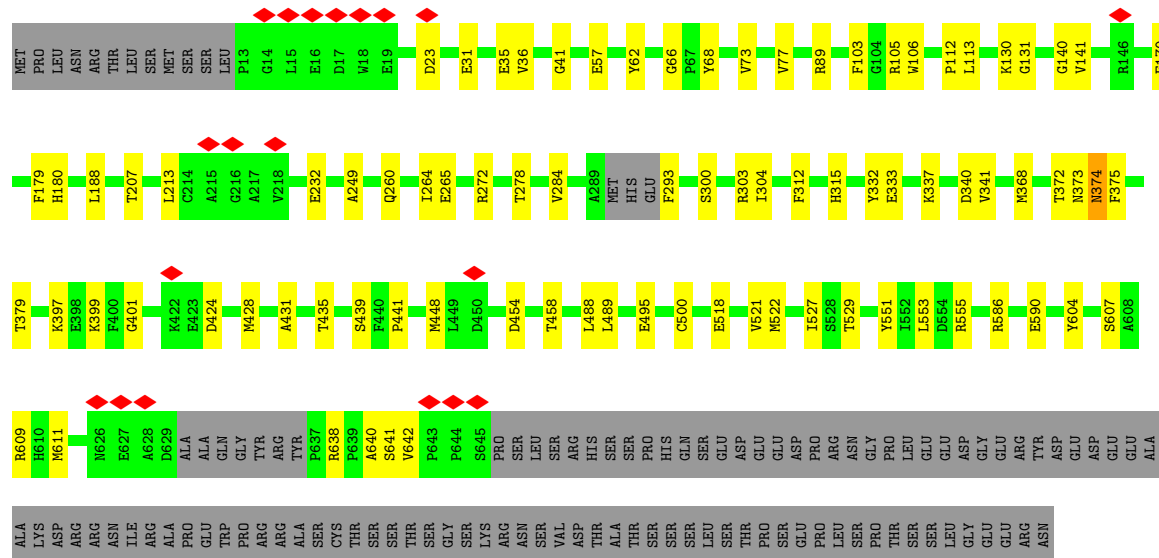
- Molecule 1: Glycogen [starch] synthase, muscle





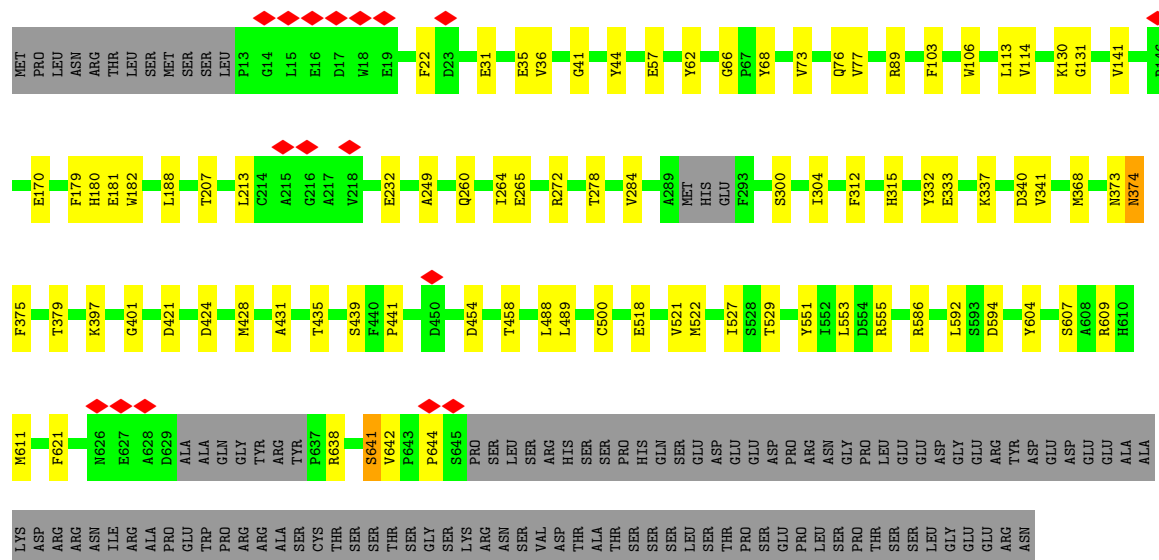
• Molecule 2: Glycogen [starch] synthase, muscle

Chain B: 73% 12% 15%



• Molecule 2: Glycogen [starch] synthase, muscle

Chain C: 73% 11% 15%



• Molecule 3: Glycogenin-1

SER	HIS	THR	LYS	SER	VAL	MET
HIS	PRO	HIS	HIS	ALA	ASP	THR
LEU	LEU	PRO	LEU	ALA	VAL	ASP
SER	GLU	GLU	PRO	PRO	LEU	GLN
LEU	LEU	PHE	PHE	ASP	SER	GLN
GLY	LEU	ILE	ILE	PRO	SER	PHE
GLU	ILE	ILE	TYR	GLY	GLY	VAL
ILE	LEU	ASN	ASN	TRP	ASP	THR
PRO	PRO	LEU	LEU	PRO	ASP	THR
ALA	TRP	SER	SER	ASP	ALA	THR
MET	ILE	SER	SER	CYS	HIS	ASN
ALA	ILE	ILE	ILE	PHE	LEU	ASN
GLN	PHE	PHE	SER	ASN	THR	ASP
PRO	THR	THR	ILE	SER	GLY	TYR
PHE	THR	THR	TYR	GLY	MET	ALA
VAL	ASN	VAL	SER	VAL	LYS	ALA
S317		LEU	TYR	PHE	ARG	LYS
S318	◆	LEU	PRO	VAL	GLU	GLY
E319	◆	LEU	ALA	GLN	PRO	ALA
E320		LEU	PHE	PRO	LEU	VAL
R321		LEU	PHE	SER	GLY	LEU
K322		GLN	LYS	VAL	THR	SER
E323		PHE	PHE	GLU	LEU	GLY
R324	◆	GLY	GLY	THR	THR	SER
		LEU	ALA	TYR	LYS	SER
M333	◆	VAL	SER	ASN	LEU	LEU
		LYS	ALA	GLN	HIS	LYS
D339	◆	ASP	LYS	LEU	CYS	GLN
N340		THR	VAL	LEU	TRP	ARG
		CYS	VAL	SER	THR	ARG
R343		TYR	PHE	ALA	LEU	THR
		ASN	GLY	GLU	THR	ARG
L349		VAL	ARG	GLN	TYR	LEU
GLN		LEU	VAL	GLY	ASP	VAL
		SER	LYS	ASP	ALA	GLN
		SER	TYR	GLN	VAL	PRO
		ASP	THR	THR	THR	THR
		ASP	PRO	GLY	VAL	ALA
		LEU	TRP	ILE	LEU	ALA
		LEU	ASN	LEU	VAL	MET
		SER	LYS	ASN	ARG	ARG
		CYS	THR	THR	LEU	LYS
		GLY	LYS	PHE	ALA	VAL
		PHE	VAL	PHE	ASN	VAL
		THR	SER	THR	ILE	GLU
		GLU	SER	SER	ASP	GLY
		ASP	GLU	TRP	LEU	VAL
		VAL	THR	ALA	PHE	THR
		THR	HIS	THR	ASP	PHE
		VAL	ASP	ASP	VAL	ASP
		GLY	PRO	THR	ARG	GLU
		THR	ASN	ILE	VAL	VAL
		ILE	MET	ARG	LEU	THR

Chain F:  7% 91%

[illegible]

Chain G:  7% 91%

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	113271	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	347.52, 347.52, 347.52	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.086, 1.086, 1.086	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	0.28	0/5135	0.49	0/6962
1	D	0.28	0/5135	0.49	0/6962
2	B	0.28	0/5150	0.49	0/6983
2	C	0.28	0/5150	0.49	0/6983
3	E	0.24	0/282	0.50	0/375
3	F	0.24	0/282	0.50	0/375
3	G	0.24	0/282	0.50	0/375
3	H	0.24	0/282	0.49	0/375
All	All	0.28	0/21698	0.49	0/29390

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	5002	0	4867	48	0
1	D	5002	0	4867	45	0
2	B	5026	0	4884	51	0
2	C	5026	0	4885	48	0
3	E	278	0	256	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	278	0	256	5	0
3	G	278	0	256	4	0
3	H	278	0	256	3	0
All	All	21168	0	20527	196	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 5.

The worst 5 of 196 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:B:341:VAL:HG21	2:B:555:ARG:HH12	1.58	0.69
2:C:31:GLU:OE2	2:C:180:HIS:NE2	2.25	0.68
2:B:31:GLU:OE2	2:B:180:HIS:NE2	2.26	0.68
1:D:31:GLU:OE2	1:D:180:HIS:NE2	2.25	0.68
1:A:31:GLU:OE2	1:A:180:HIS:NE2	2.26	0.67

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	614/737 (83%)	593 (97%)	21 (3%)	0	100	100
1	D	614/737 (83%)	594 (97%)	20 (3%)	0	100	100
2	B	616/737 (84%)	592 (96%)	23 (4%)	1 (0%)	44	77
2	C	616/737 (84%)	592 (96%)	24 (4%)	0	100	100
3	E	31/350 (9%)	30 (97%)	1 (3%)	0	100	100
3	F	31/350 (9%)	30 (97%)	1 (3%)	0	100	100
3	G	31/350 (9%)	30 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	31/350 (9%)	30 (97%)	1 (3%)	0	100	100
All	All	2584/4348 (59%)	2491 (96%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	640	ALA

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	533/638 (84%)	531 (100%)	2 (0%)	89	95
1	D	533/638 (84%)	531 (100%)	2 (0%)	89	95
2	B	535/637 (84%)	534 (100%)	1 (0%)	92	97
2	C	535/637 (84%)	534 (100%)	1 (0%)	92	97
3	E	29/310 (9%)	29 (100%)	0	100	100
3	F	29/310 (9%)	29 (100%)	0	100	100
3	G	29/310 (9%)	29 (100%)	0	100	100
3	H	29/310 (9%)	29 (100%)	0	100	100
All	All	2252/3790 (59%)	2246 (100%)	6 (0%)	90	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	374	ASN
1	D	360	GLN
1	D	374	ASN
1	A	374	ASN
1	A	360	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	B	641	2	8,9,10	1.44	1 (12%)	8,12,14	1.57	2 (25%)
2	SEP	C	641	2	8,9,10	1.44	1 (12%)	8,12,14	1.75	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	-	2/5/8/10	-
2	SEP	C	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	C	641	SEP	P-O1P	3.18	1.60	1.50
2	B	641	SEP	P-O1P	3.12	1.60	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	641	SEP	OG-CB-CA	3.64	111.69	108.14
2	B	641	SEP	OG-CB-CA	2.87	110.94	108.14
2	C	641	SEP	P-OG-CB	-2.63	111.06	118.30
2	B	641	SEP	P-OG-CB	-2.61	111.12	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	641	SEP	N-CA-CB-OG
2	C	641	SEP	CB-OG-P-O1P
2	B	641	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	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.

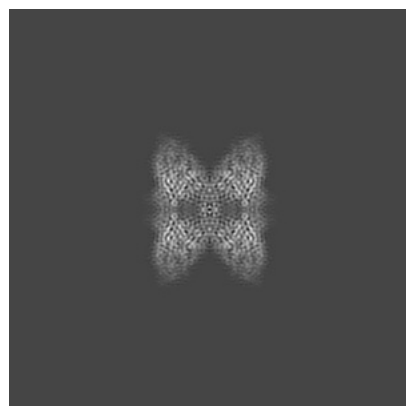
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13743. These allow visual inspection of the internal detail of the map and identification of artifacts.

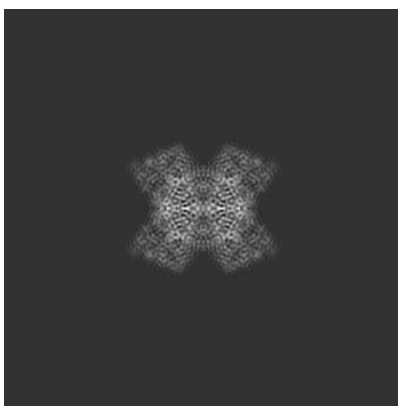
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

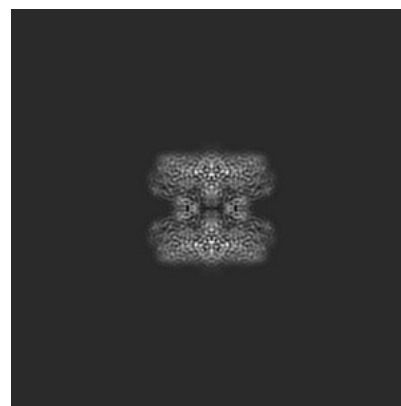
6.1.1 Primary map



X

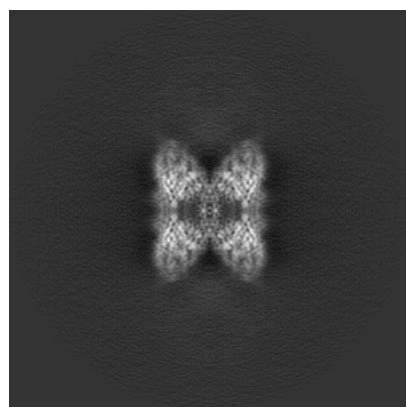


Y

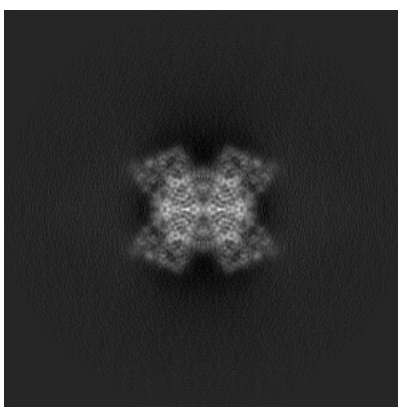


Z

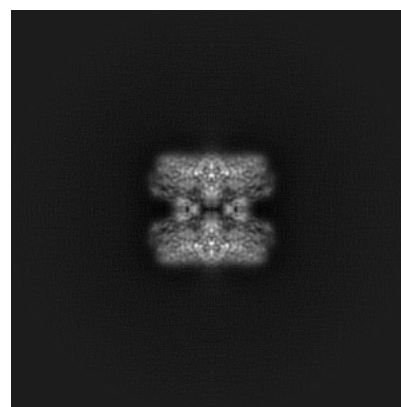
6.1.2 Raw map



X



Y

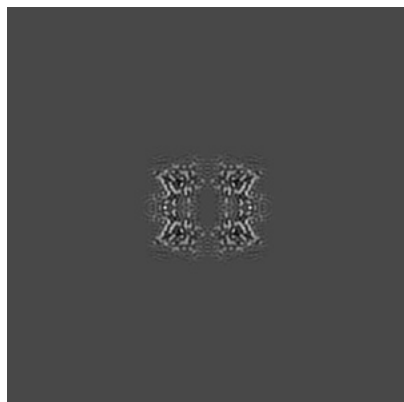


Z

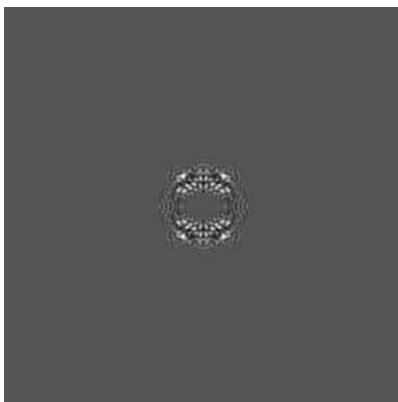
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

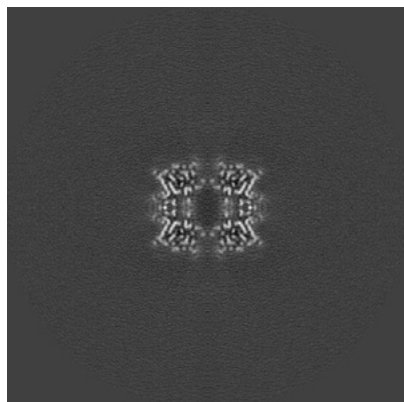


Y Index: 160

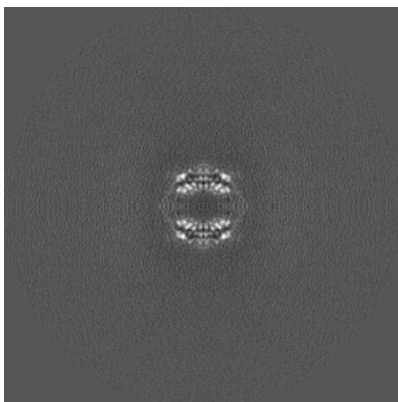


Z Index: 160

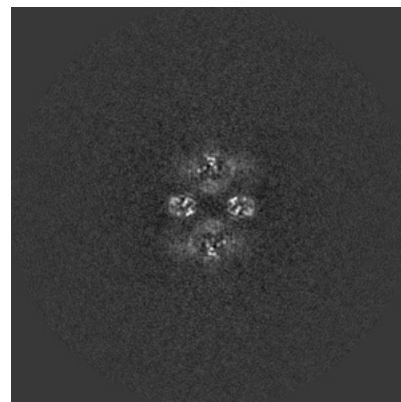
6.2.2 Raw map



X Index: 160



Y Index: 160

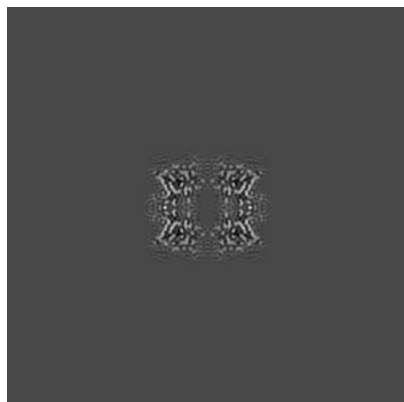


Z Index: 160

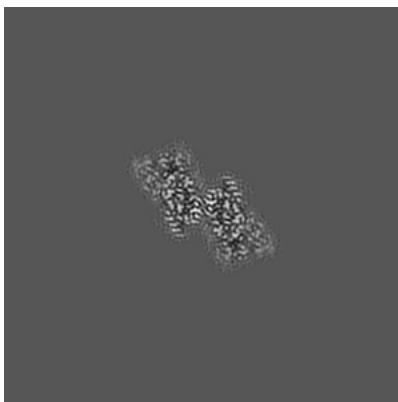
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

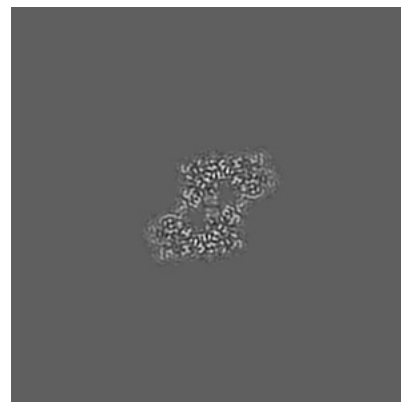
6.3.1 Primary map



X Index: 160

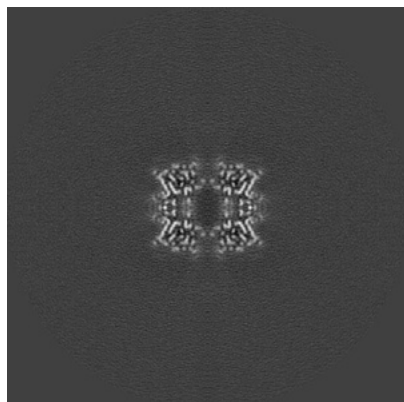


Y Index: 130

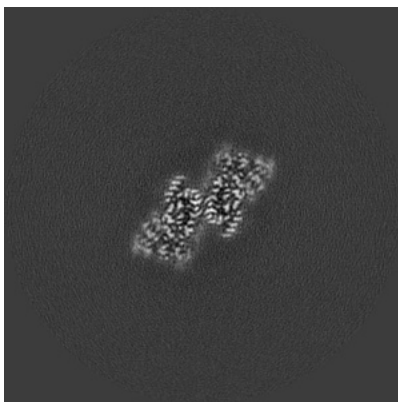


Z Index: 179

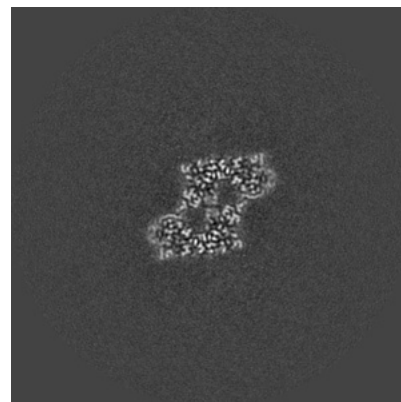
6.3.2 Raw map



X Index: 160



Y Index: 190

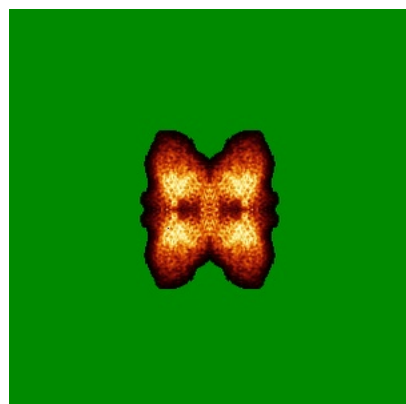


Z Index: 179

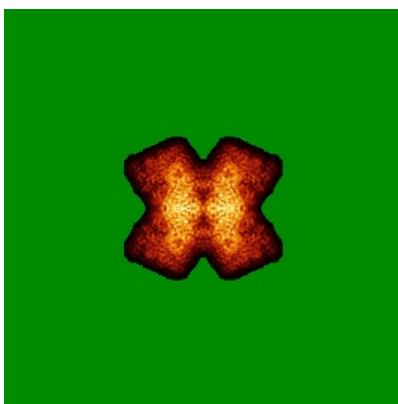
The images above show the largest variance slices of the map in three orthogonal directions.

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

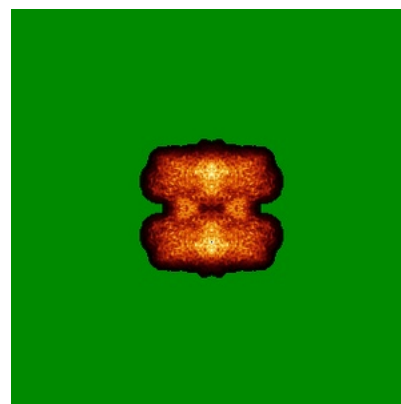
6.4.1 Primary map



X

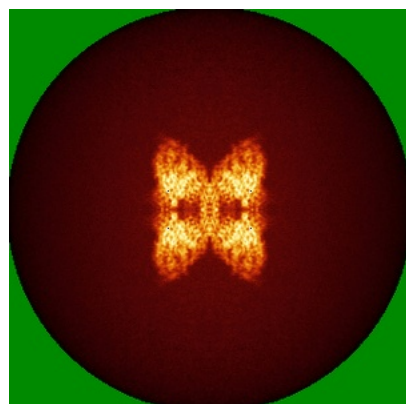


Y

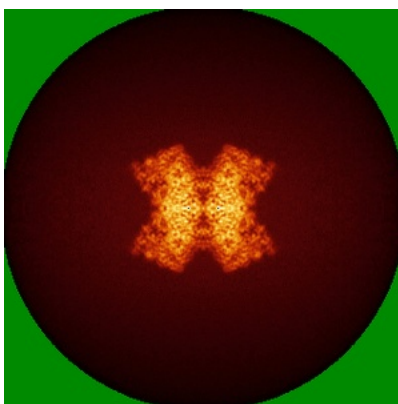


Z

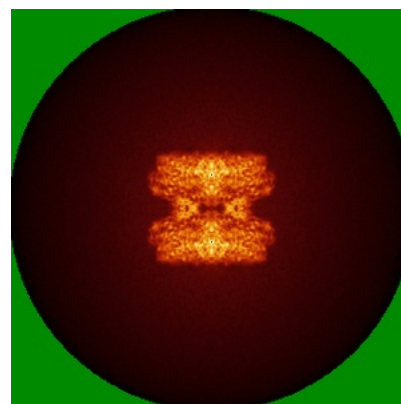
6.4.2 Raw map



X



Y

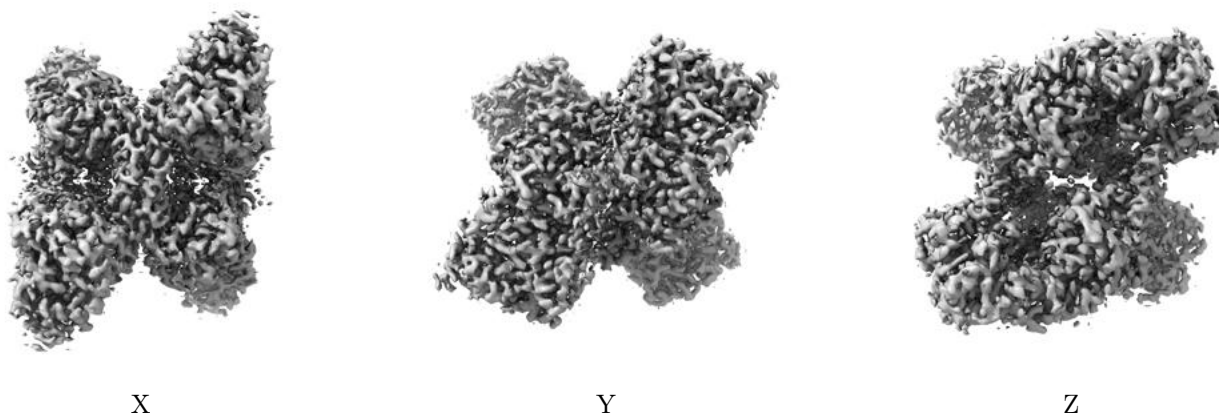


Z

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.

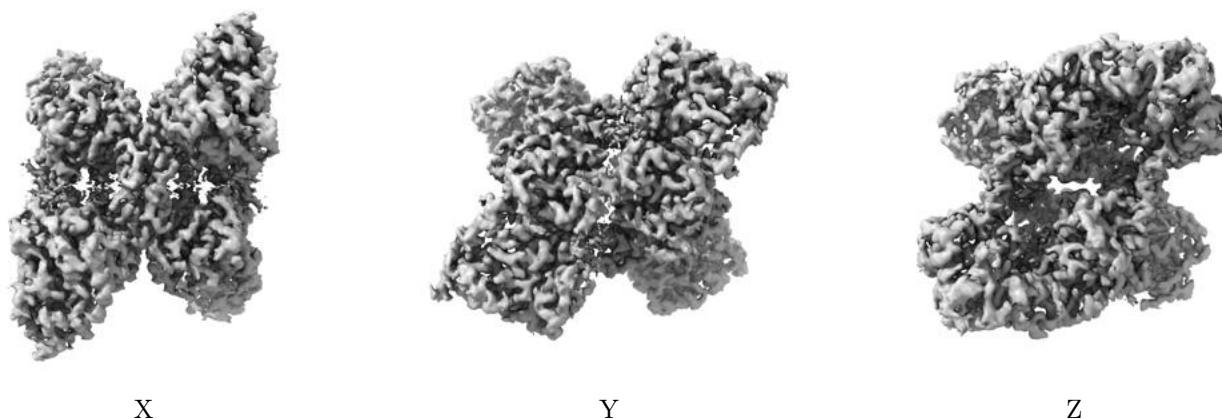
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. 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.

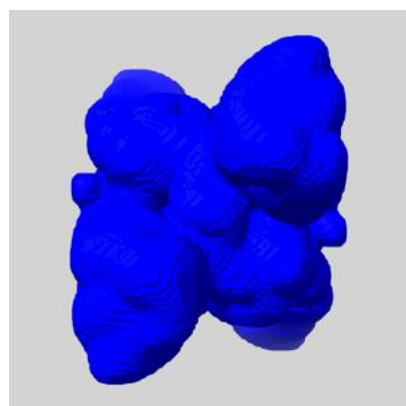
6.6 Mask visualisation [i](#)

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

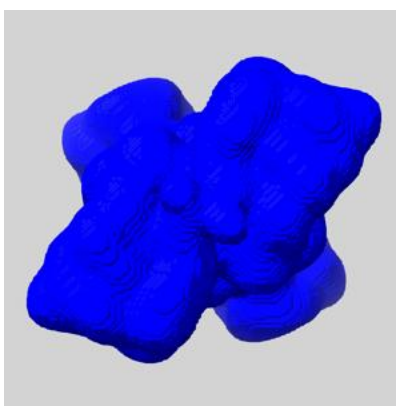
A mask typically either:

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

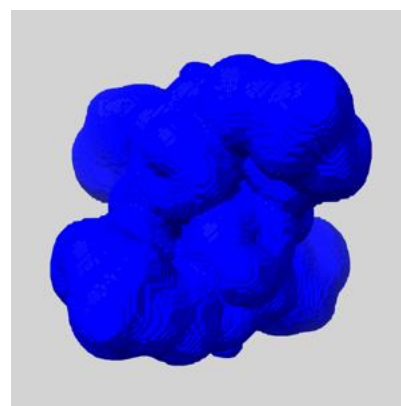
6.6.1 emd_13743_msk_1.map [i](#)



X



Y

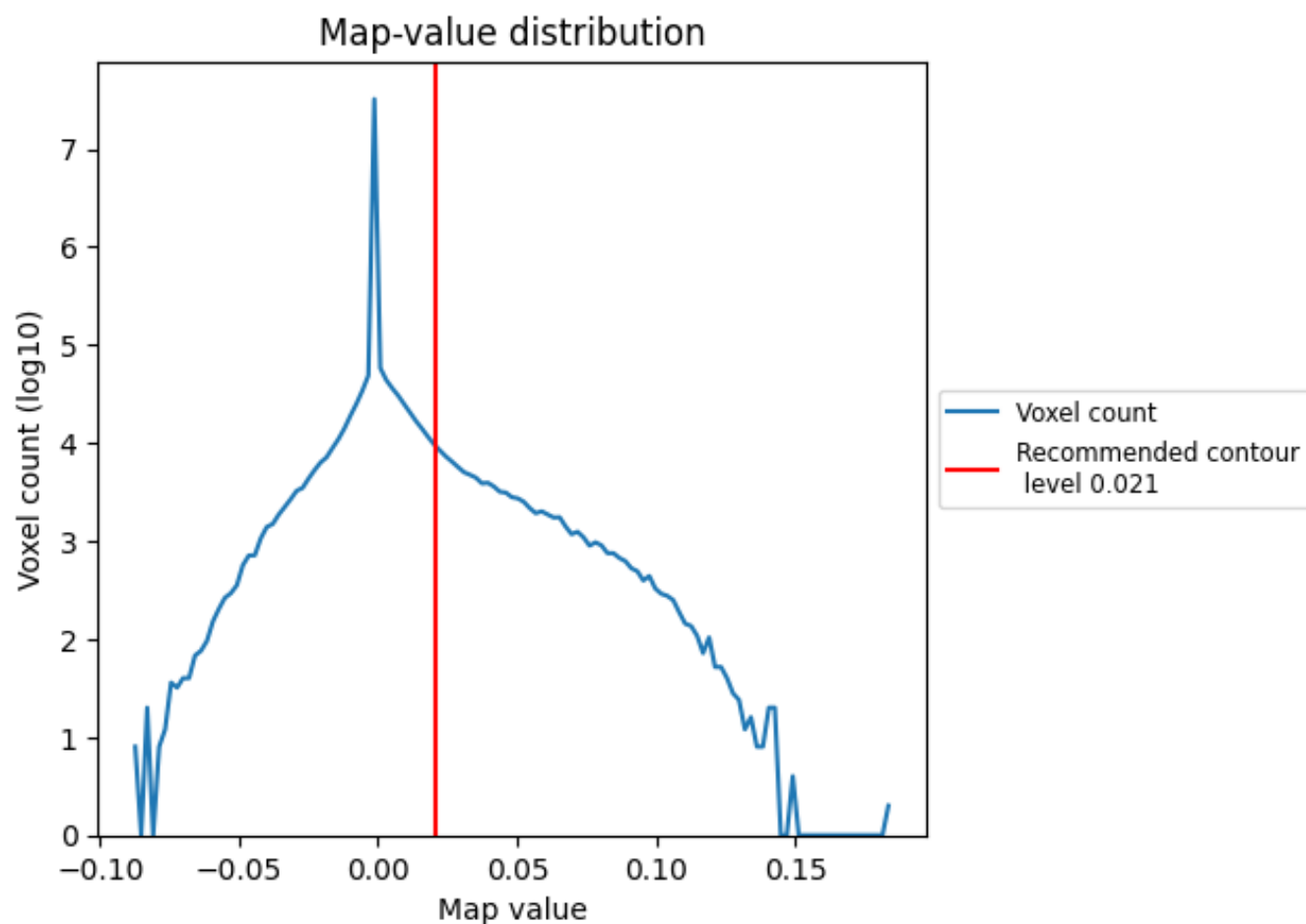


Z

7 Map analysis [i](#)

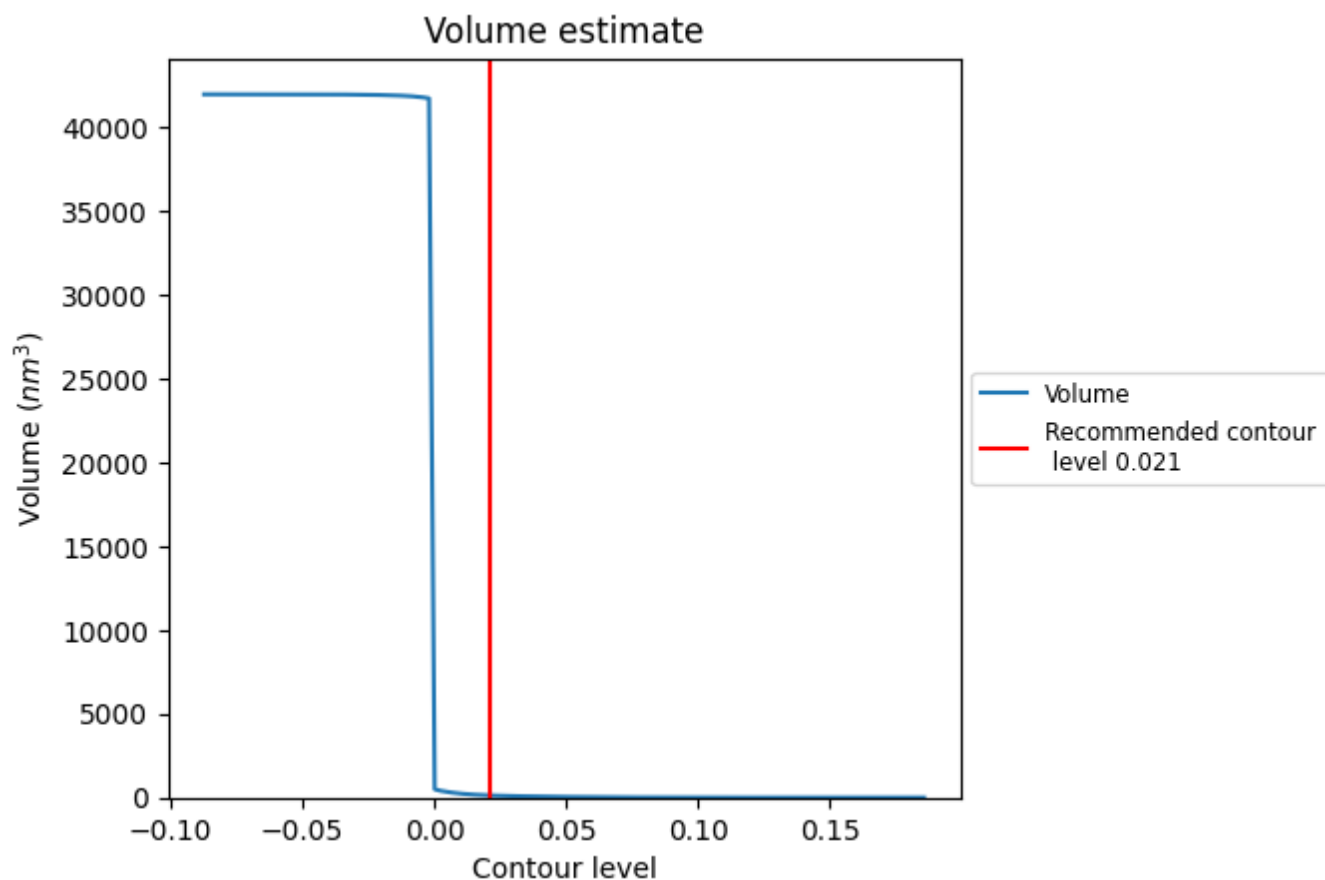
This section contains the results of statistical analysis of the map.

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.

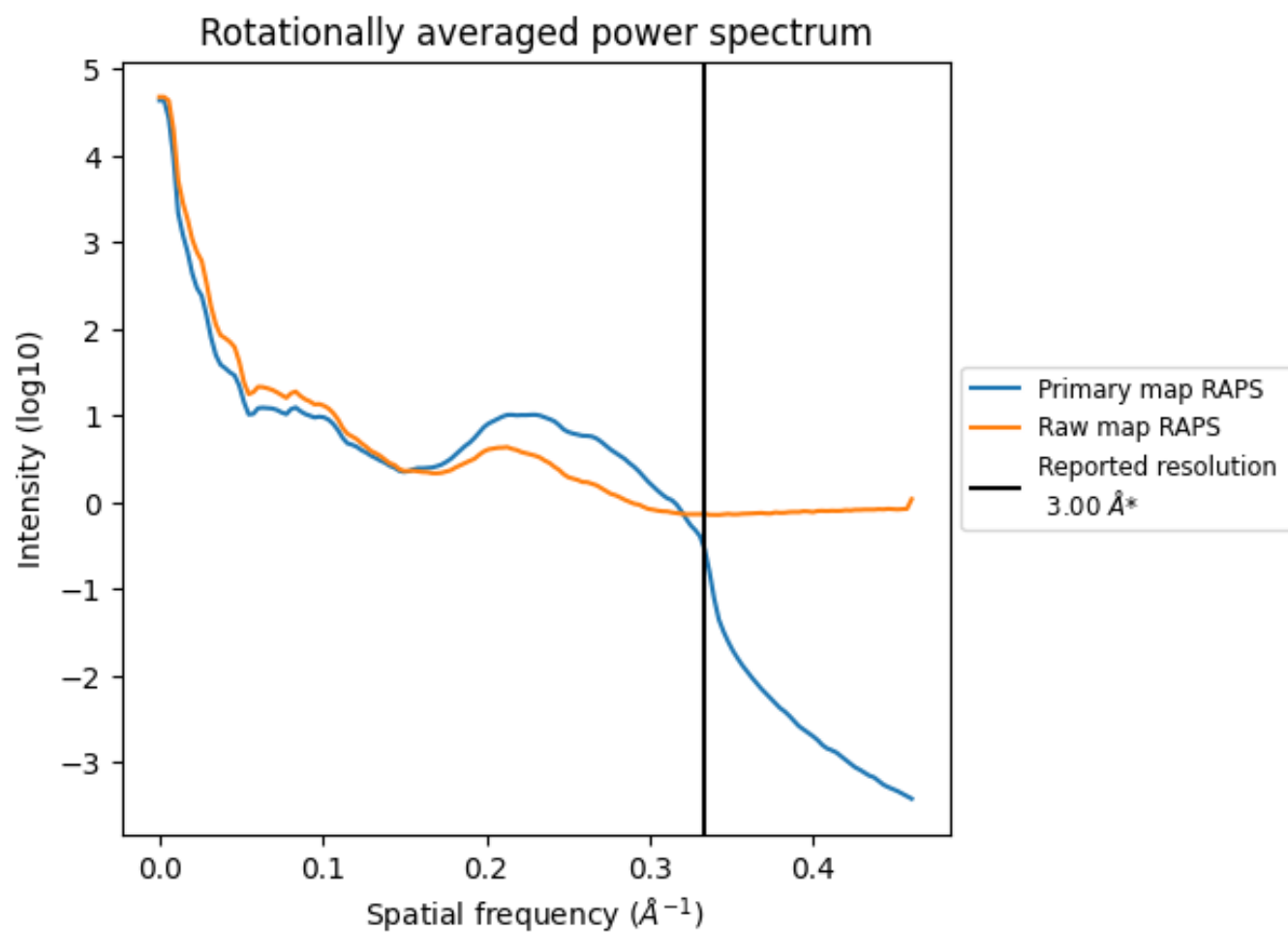
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 ⓘ

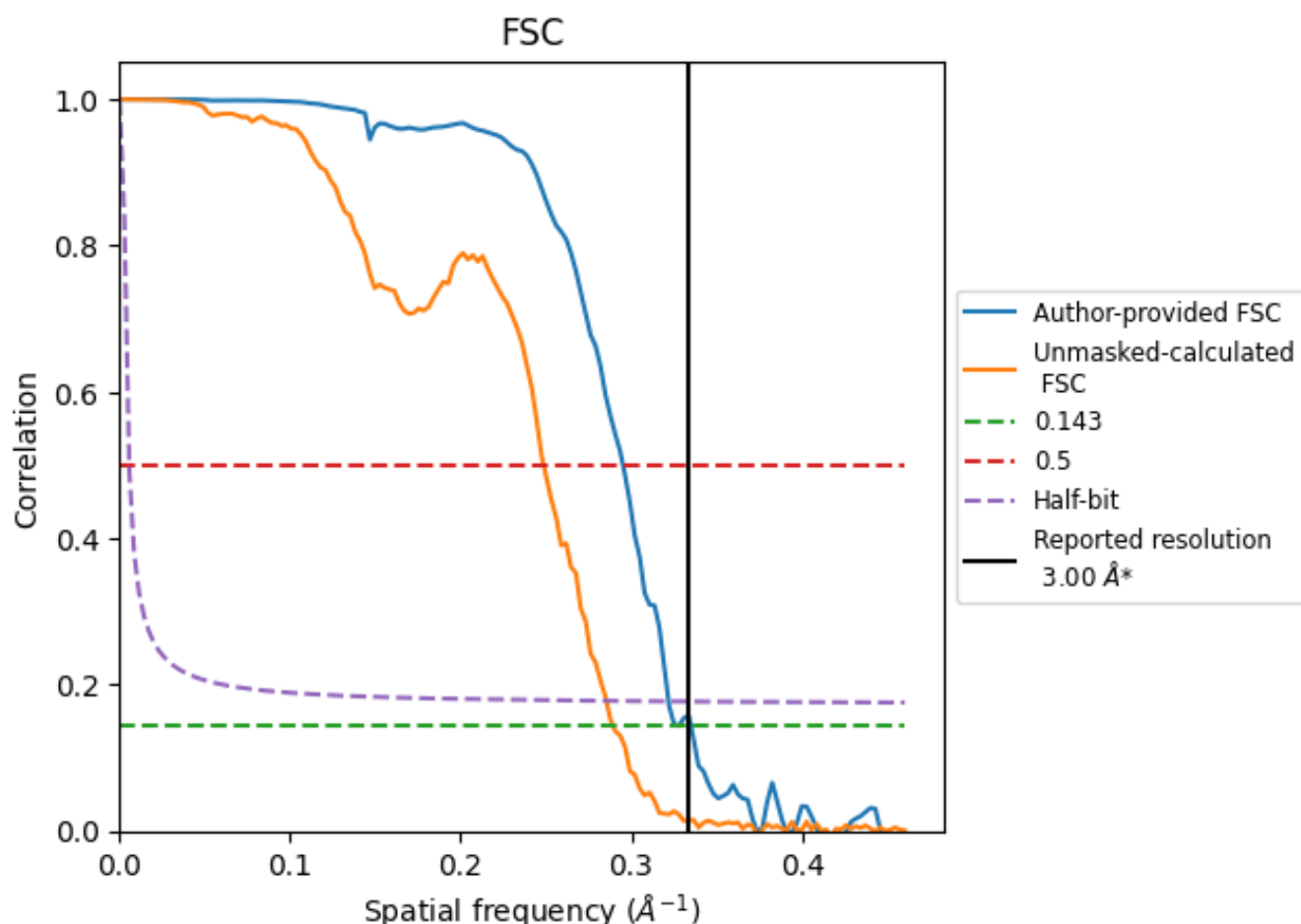


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

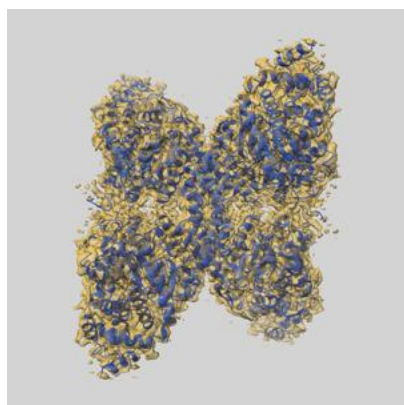
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.00
Author-provided FSC curve	2.99	3.39	3.11	-
Unmasked-calculated*	3.46	4.02	3.50	-

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

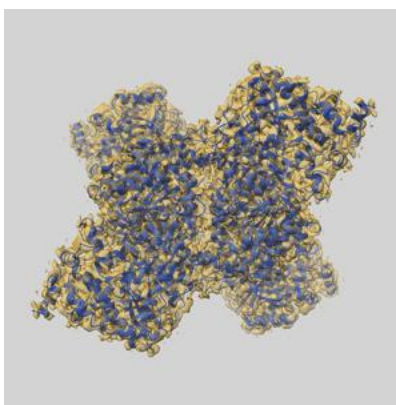
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13743 and PDB model 7Q0B. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

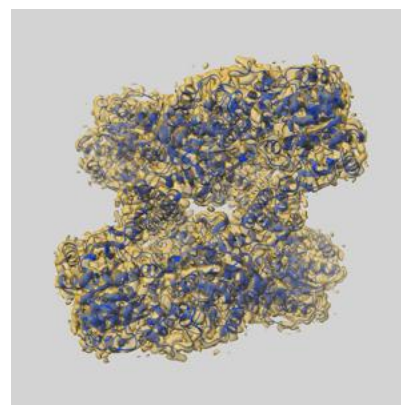
9.1 Map-model overlay [i](#)



X



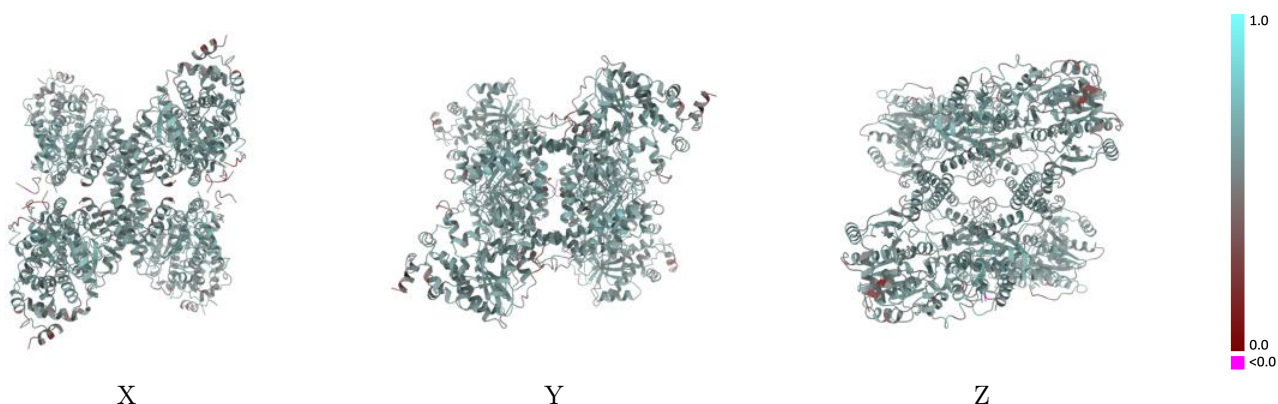
Y



Z

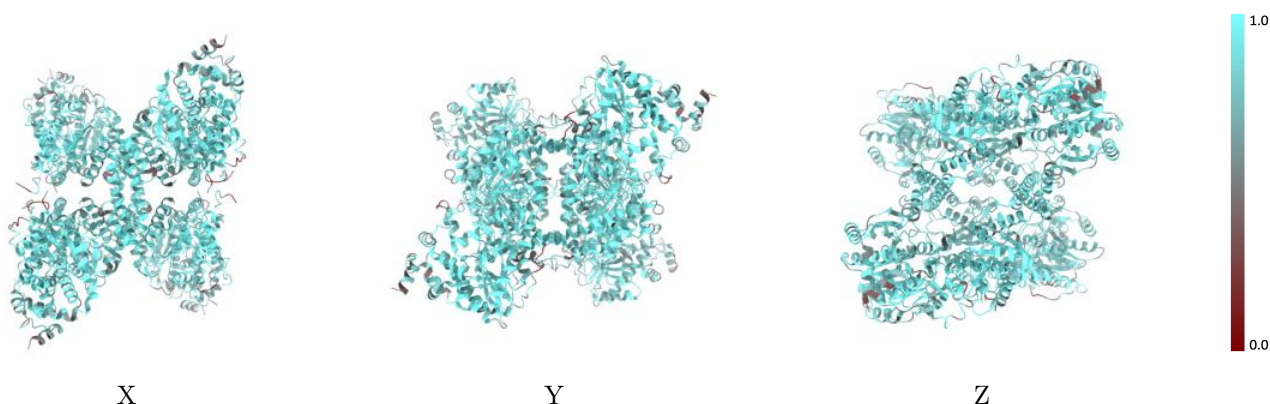
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



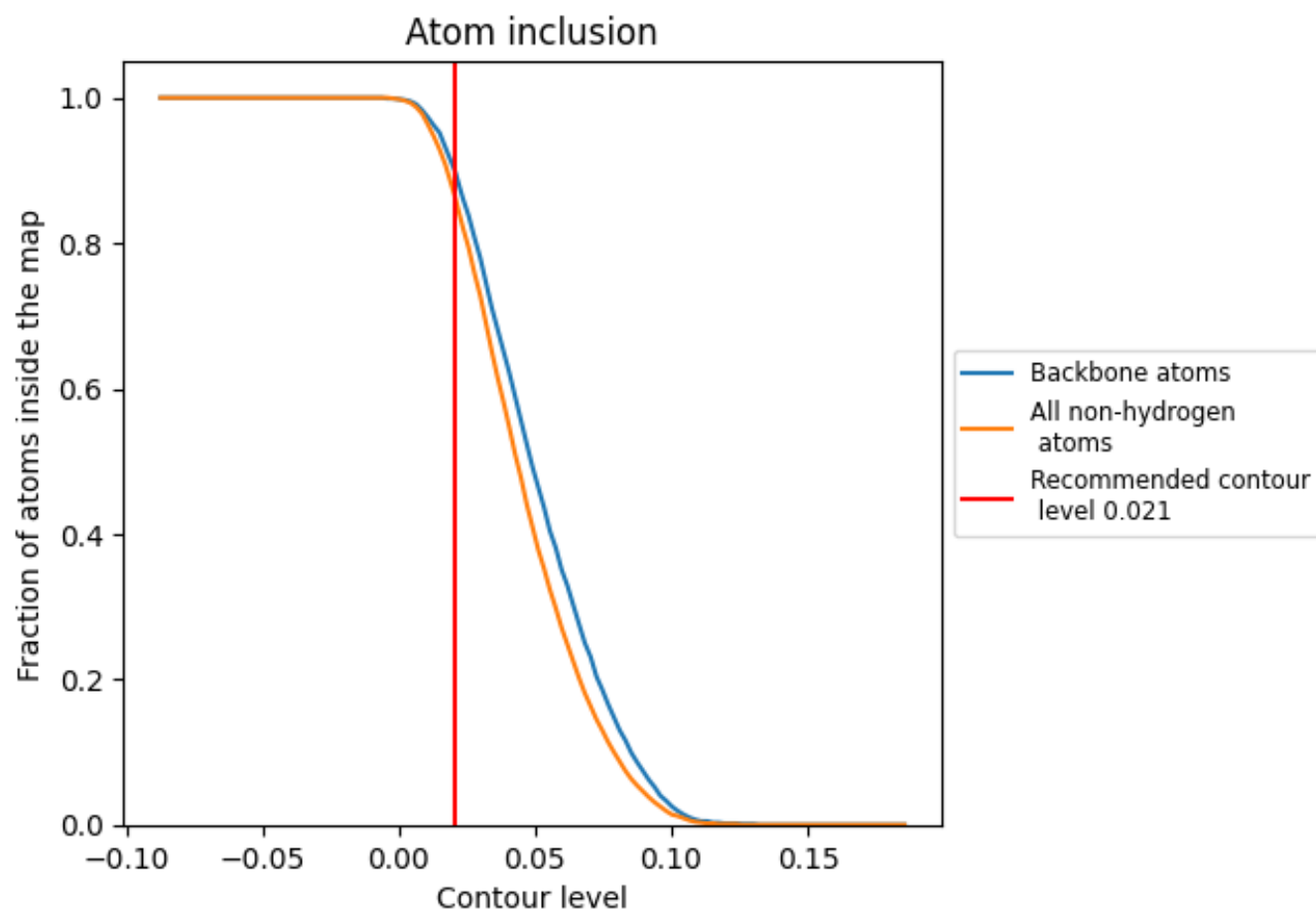
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8600</div>	<div><div></div>0.5690</div>
A	<div><div></div>0.8720</div>	<div><div></div>0.5750</div>
B	<div><div></div>0.8660</div>	<div><div></div>0.5720</div>
C	<div><div></div>0.8700</div>	<div><div></div>0.5740</div>
D	<div><div></div>0.8690</div>	<div><div></div>0.5730</div>
E	<div><div></div>0.6840</div>	<div><div></div>0.4920</div>
F	<div><div></div>0.6880</div>	<div><div></div>0.4860</div>
G	<div><div></div>0.6840</div>	<div><div></div>0.4940</div>
H	<div><div></div>0.6840</div>	<div><div></div>0.4920</div>

1.0

0.0

<0.0