



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 09:06 AM UTC

PDB ID : 9E1T / pdb_00009e1t
EMDB ID : EMD-47420
Title : CryoEM structure of LARGE1 bound to UDP-GlcA
Authors : Joseph, S.; Spellmon, N.; Campbell, K.P.
Deposited on : 2024-10-21
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

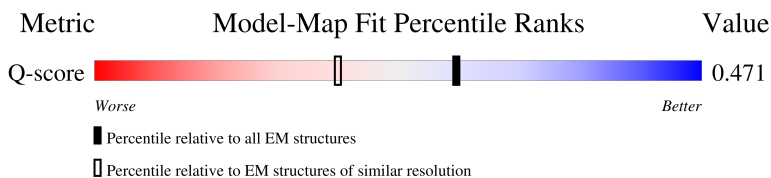
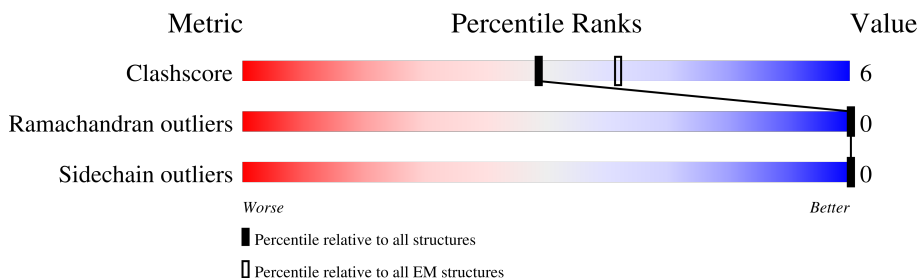
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	770	
1	B	770	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10056 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 Xylosyl- and glucuronyltransferase LARGE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4990	3233	841	888	28		
1	B	602	Total	C	N	O	S	0	0
			4990	3233	841	888	28		

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O95461
A	-6	SER	-	expression tag	UNP O95461
A	-5	ALA	-	expression tag	UNP O95461
A	-4	LEU	-	expression tag	UNP O95461
A	-3	LEU	-	expression tag	UNP O95461
A	-2	ILE	-	expression tag	UNP O95461
A	-1	LEU	-	expression tag	UNP O95461
A	0	ALA	-	expression tag	UNP O95461
A	1	LEU	-	expression tag	UNP O95461
A	2	VAL	-	expression tag	UNP O95461
A	3	GLY	-	expression tag	UNP O95461
A	4	ALA	-	expression tag	UNP O95461
A	5	ALA	-	expression tag	UNP O95461
A	6	VAL	-	expression tag	UNP O95461
A	7	ALA	-	expression tag	UNP O95461
A	8	ASP	-	expression tag	UNP O95461
A	9	TYR	-	expression tag	UNP O95461
A	10	LYS	-	expression tag	UNP O95461
A	11	ASP	-	expression tag	UNP O95461
A	12	HIS	-	expression tag	UNP O95461
A	13	ASP	-	expression tag	UNP O95461
A	14	GLY	-	expression tag	UNP O95461
A	15	ASP	-	expression tag	UNP O95461
A	16	TYR	-	expression tag	UNP O95461
A	17	LYS	-	expression tag	UNP O95461
A	18	ASP	-	expression tag	UNP O95461

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP O95461
A	20	ASP	-	expression tag	UNP O95461
A	21	ILE	-	expression tag	UNP O95461
A	22	ASP	-	expression tag	UNP O95461
A	23	TYR	-	expression tag	UNP O95461
A	24	LYS	-	expression tag	UNP O95461
A	25	ASP	-	expression tag	UNP O95461
A	26	ASP	-	expression tag	UNP O95461
A	27	ASP	-	expression tag	UNP O95461
A	28	ASP	-	expression tag	UNP O95461
A	29	LYS	-	expression tag	UNP O95461
A	30	LEU	-	expression tag	UNP O95461
A	31	ALA	-	expression tag	UNP O95461
A	32	ALA	-	expression tag	UNP O95461
A	33	ALA	-	expression tag	UNP O95461
A	757	HIS	-	expression tag	UNP O95461
A	758	HIS	-	expression tag	UNP O95461
A	759	HIS	-	expression tag	UNP O95461
A	760	HIS	-	expression tag	UNP O95461
A	761	HIS	-	expression tag	UNP O95461
A	762	HIS	-	expression tag	UNP O95461
B	-7	MET	-	initiating methionine	UNP O95461
B	-6	SER	-	expression tag	UNP O95461
B	-5	ALA	-	expression tag	UNP O95461
B	-4	LEU	-	expression tag	UNP O95461
B	-3	LEU	-	expression tag	UNP O95461
B	-2	ILE	-	expression tag	UNP O95461
B	-1	LEU	-	expression tag	UNP O95461
B	0	ALA	-	expression tag	UNP O95461
B	1	LEU	-	expression tag	UNP O95461
B	2	VAL	-	expression tag	UNP O95461
B	3	GLY	-	expression tag	UNP O95461
B	4	ALA	-	expression tag	UNP O95461
B	5	ALA	-	expression tag	UNP O95461
B	6	VAL	-	expression tag	UNP O95461
B	7	ALA	-	expression tag	UNP O95461
B	8	ASP	-	expression tag	UNP O95461
B	9	TYR	-	expression tag	UNP O95461
B	10	LYS	-	expression tag	UNP O95461
B	11	ASP	-	expression tag	UNP O95461
B	12	HIS	-	expression tag	UNP O95461
B	13	ASP	-	expression tag	UNP O95461

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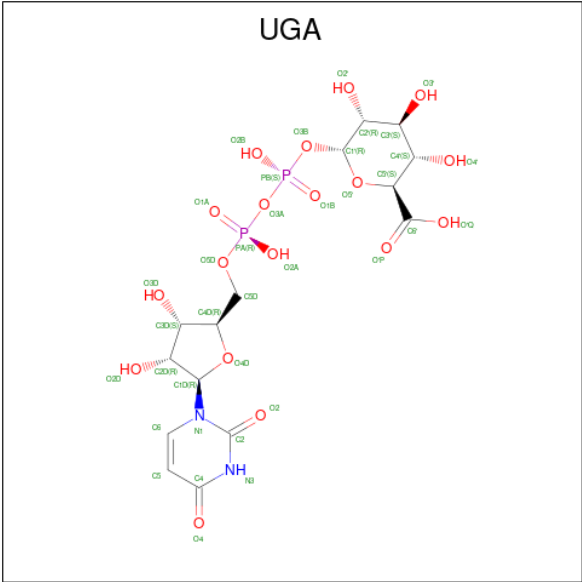
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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	expression tag	UNP O95461
B	15	ASP	-	expression tag	UNP O95461
B	16	TYR	-	expression tag	UNP O95461
B	17	LYS	-	expression tag	UNP O95461
B	18	ASP	-	expression tag	UNP O95461
B	19	HIS	-	expression tag	UNP O95461
B	20	ASP	-	expression tag	UNP O95461
B	21	ILE	-	expression tag	UNP O95461
B	22	ASP	-	expression tag	UNP O95461
B	23	TYR	-	expression tag	UNP O95461
B	24	LYS	-	expression tag	UNP O95461
B	25	ASP	-	expression tag	UNP O95461
B	26	ASP	-	expression tag	UNP O95461
B	27	ASP	-	expression tag	UNP O95461
B	28	ASP	-	expression tag	UNP O95461
B	29	LYS	-	expression tag	UNP O95461
B	30	LEU	-	expression tag	UNP O95461
B	31	ALA	-	expression tag	UNP O95461
B	32	ALA	-	expression tag	UNP O95461
B	33	ALA	-	expression tag	UNP O95461
B	757	HIS	-	expression tag	UNP O95461
B	758	HIS	-	expression tag	UNP O95461
B	759	HIS	-	expression tag	UNP O95461
B	760	HIS	-	expression tag	UNP O95461
B	761	HIS	-	expression tag	UNP O95461
B	762	HIS	-	expression tag	UNP O95461

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mn	0
			1	1	
2	B	1	Total	Mn	0
			1	1	

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (CCD ID: UGA) (formula: C₁₅H₂₂N₂O₁₈P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			37	15	2	18	2	
3	B	1	Total	C	N	O	P	0
			37	15	2	18	2	

ARG	ASN	L222	L324	R398	N544	S719
TYR	LEU	H223	H325	R399	L545	N720
THR	ARG		G326	L400	L546	K721
ALA	ALA		H327	Y401	R547	K723
SER	GLY	L235	L328	T403	M551	Y723
GLN	ILE	E236	S329	L402	I554	R724
ARG	VAL	R237	T330	E406	M559	I725
GLU	ALA	V238	S331	Y407	S562	C726
GLU	GLY	T239			D563	L727
ASN	ASN	V240			F566	K728
GLU	SER		D334	L411	A586	
LEU	SER	Q265	Q335	R414	K590	E732
GLU	GLU	E271	D336		R601	E733
VAL	CYS	N272	I337	F417	Y602	F734
ARG	GLY		F338	Q418	L604	Q735
ARG	GLN		N339	S421	M616	
MET	PRO	D275	A340	E422	L617	G743
GLU	VAL	V276	V341	A423	D618	F744
VAL	VAL	Y277	T342	D424	R626	
GLU	GLU	L278	R343		E658	Y749
GLU	K134	G279	L348	E428	R655	L750
GLU	C135	ASN	V349	Q431	D671	T751
ASN	E136	LEU	Y350	F439	F674	A752
ARG		TRP	N357	D440	F677	GLU
ALA	S150	LYS	Q359	L442	K681	ASN
LEU	R151	ASN	L360	R448	I685	SER
ARG	D152	HIS	S361	R455	F677	HIS
ARG	V153	ARG	D362	F467	K681	HIS
GLN	V154	ARG	H363	A468	I686	HIS
LEU		P287	T364	D470	D689	HIS
SER	K158	W288	R365	D473	E694	
LEU	M166		S366	V474	M703	
GLN	L172	G292	E367		A709	
GLY	L182	R293	Q368		P710	
ARG	L185	G294	R371		S711	
PRO	L189	Y295	S374		I714	
SER		N296			F717	
HIS	D202	I300	I379		R718	
ARG	E203	L301	H380			
GLY	L204	L302	W381			
ASN	L205	L303	H382			
HIS	S206	D305	S383			
SER	K209	K306	P384			
TYR	W210	L307	LYS			
SER	T211	R308	LEU			
MET	P212	K309	ARG			
GLU	W213	H310	VAL			
GLY	H214	R311	LYS			
THR	H215	E313	ASN			
GLY	Y216	W315	LYS			
ASP		R316	VAL			
SER		R317	ASN			
GLU		L318	LYS			
		A320	HIS			
		R322	VAL			
		E323	E395			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	347589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0078	Depositor
Map size (Å)	211.712, 211.712, 211.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/5126	0.24	0/6952
1	B	0.12	0/5126	0.24	0/6952
All	All	0.12	0/10252	0.24	0/13904

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	4990	0	4911	61	0
1	B	4990	0	4911	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	19	0	0
3	B	37	0	19	0	0
All	All	10056	0	9860	115	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 6.

The worst 5 of 115 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:A:717:PHE:HB3	1:A:723:TYR:CG	2.26	0.71
1:A:547:ARG:NH2	1:A:681:LYS:HE2	2.06	0.70
1:B:717:PHE:HB3	1:B:723:TYR:CG	2.28	0.68
1:B:547:ARG:NH2	1:B:681:LYS:HE2	2.12	0.65
1:A:403:THR:HG23	1:B:411:LEU:HD22	1.80	0.64

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	596/770 (77%)	580 (97%)	16 (3%)	0	100	100
1	B	596/770 (77%)	579 (97%)	17 (3%)	0	100	100
All	All	1192/1540 (77%)	1159 (97%)	33 (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	540/683 (79%)	540 (100%)	0	100	100
1	B	540/683 (79%)	540 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1080/1366 (79%)	1080 (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 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	166	ASN
1	B	359	GLN
1	B	553	HIS
1	B	426	ASN
1	A	426	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	UGA	A	802	2	38,39,39	0.69	1 (2%)	56,60,60	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UGA	B	802	2	38,39,39	0.71	1 (2%)	56,60,60	0.64	0

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
3	UGA	A	802	2	-	11/25/61/61	0/3/3/3
3	UGA	B	802	2	-	12/25/61/61	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	UGA	O'Q-C6'	-3.11	1.20	1.30
3	A	802	UGA	O'Q-C6'	-2.97	1.21	1.30

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

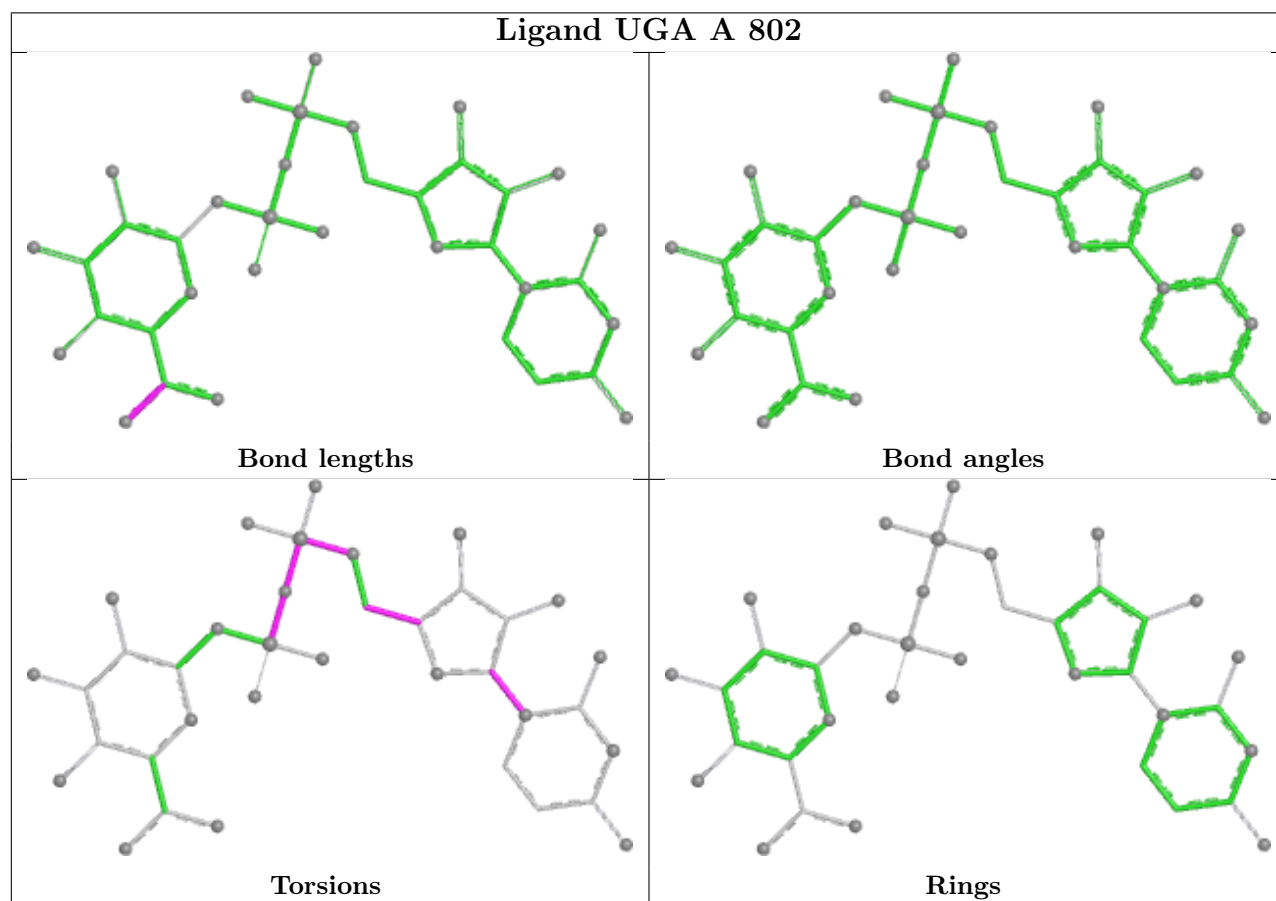
Mol	Chain	Res	Type	Atoms
3	A	802	UGA	PB-O3A-PA-O5D
3	A	802	UGA	C5D-O5D-PA-O3A
3	A	802	UGA	C5D-O5D-PA-O1A
3	A	802	UGA	C5D-O5D-PA-O2A
3	A	802	UGA	O4D-C1D-N1-C6

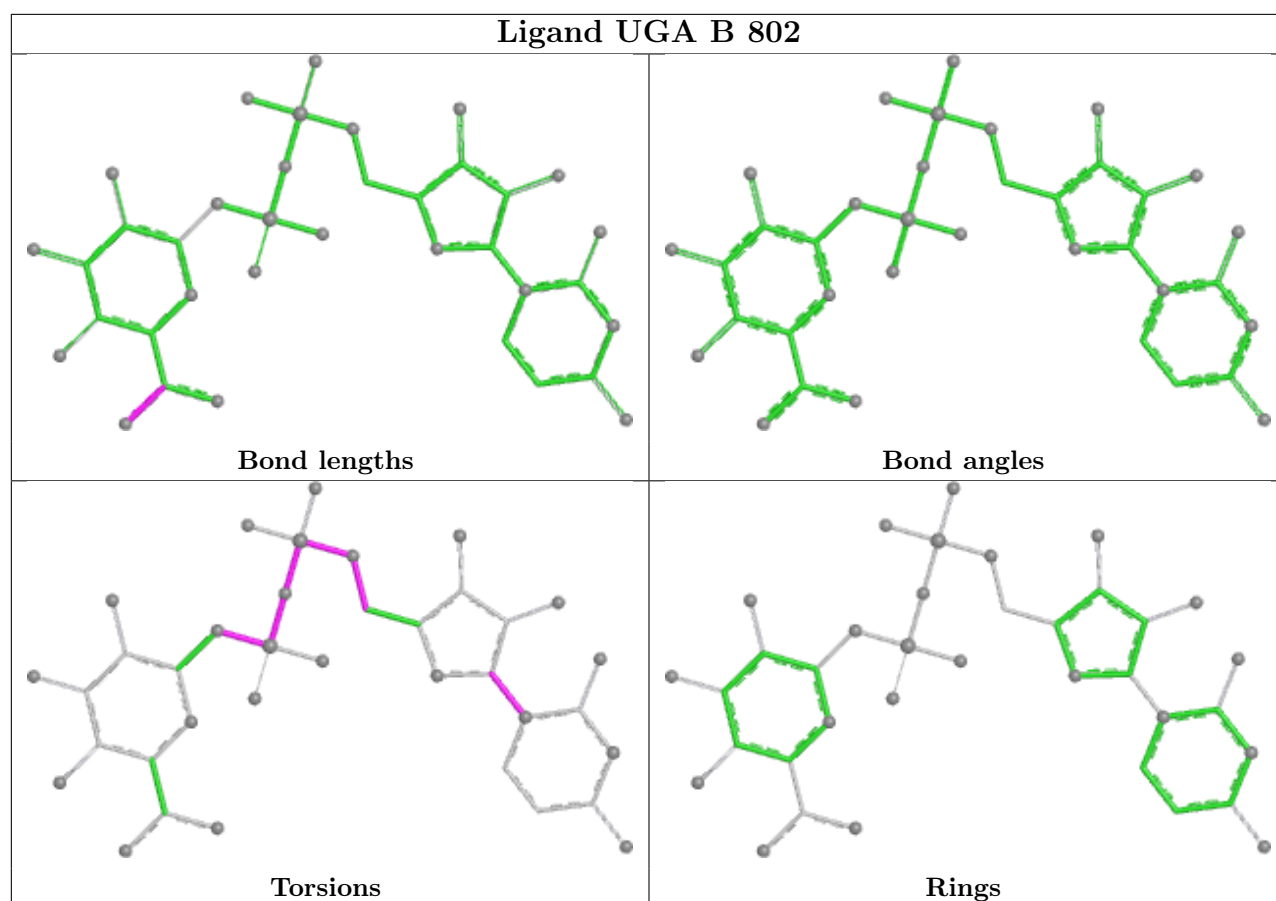
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

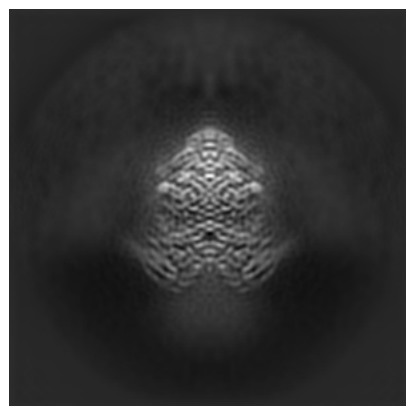
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47420. These allow visual inspection of the internal detail of the map and identification of artifacts.

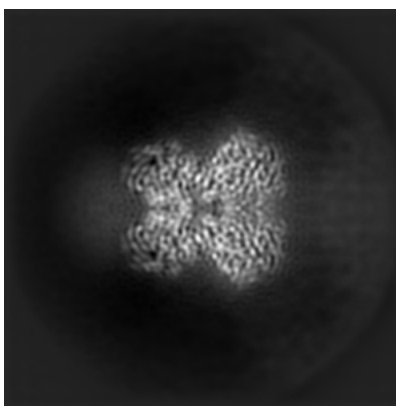
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

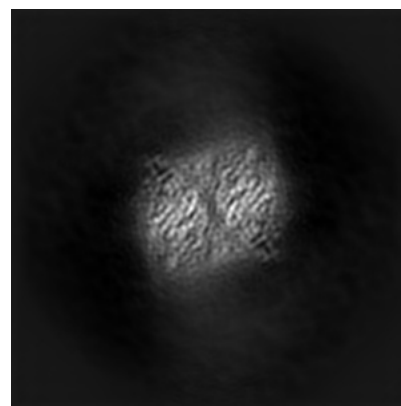
6.1.1 Primary map



X

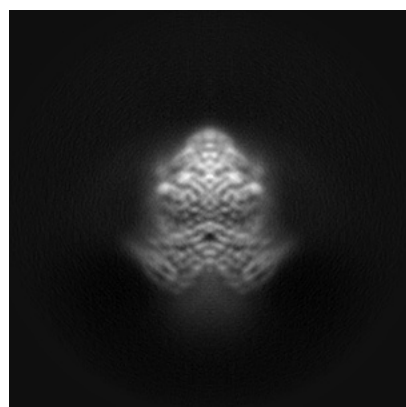


Y

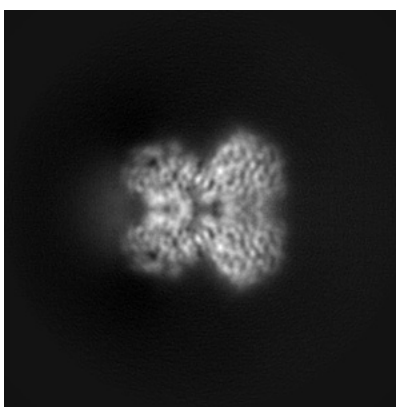


Z

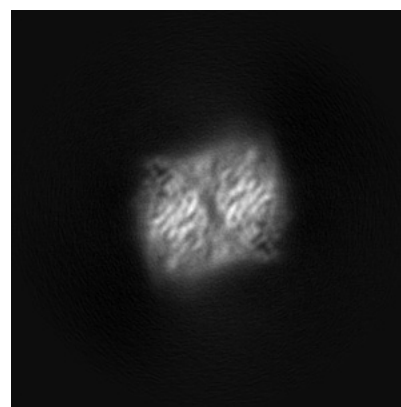
6.1.2 Raw map



X



Y

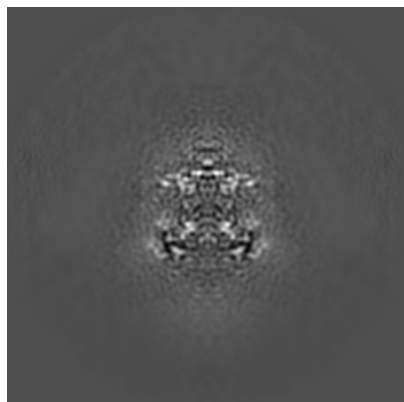


Z

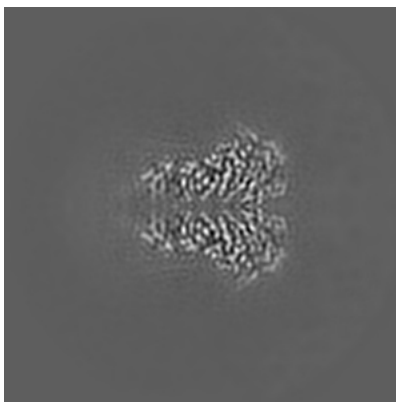
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

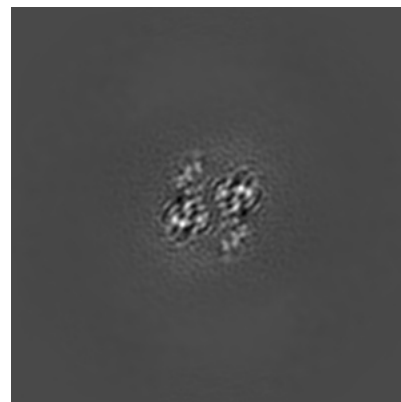
6.2.1 Primary map



X Index: 128

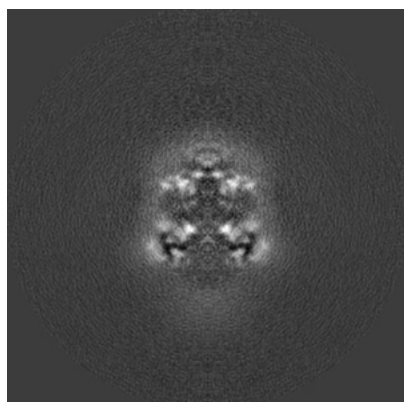


Y Index: 128

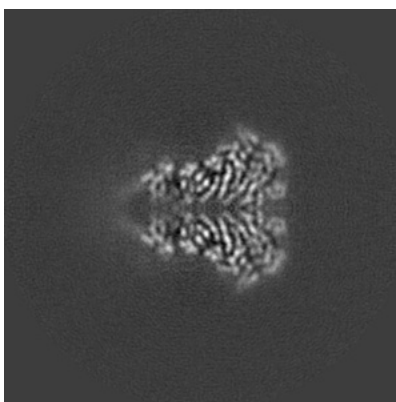


Z Index: 128

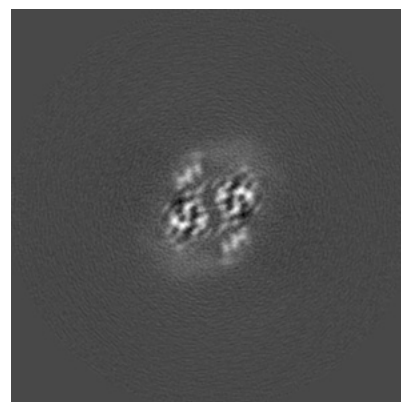
6.2.2 Raw map



X Index: 128



Y Index: 128

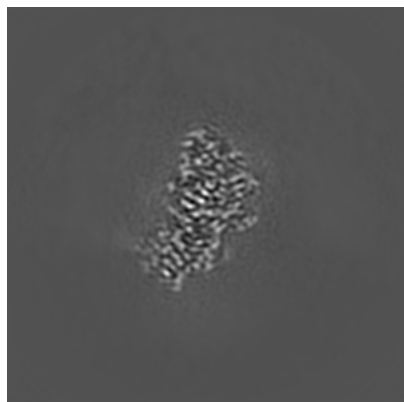


Z Index: 128

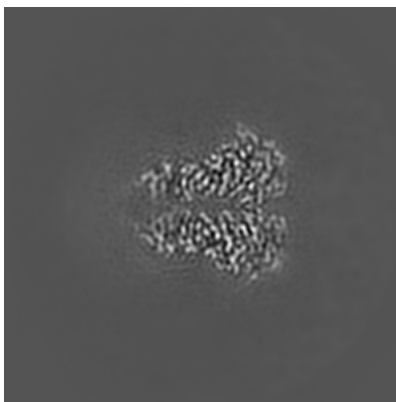
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

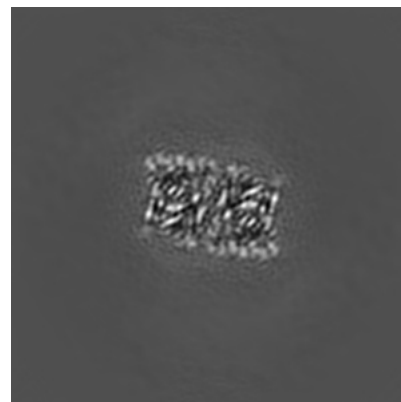
6.3.1 Primary map



X Index: 109

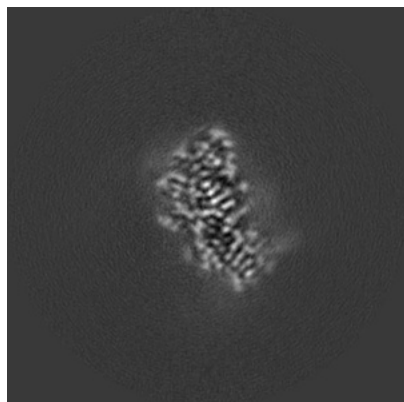


Y Index: 127

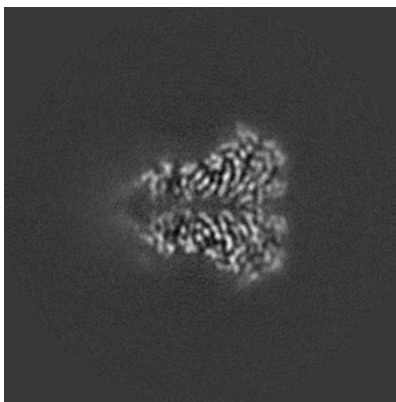


Z Index: 143

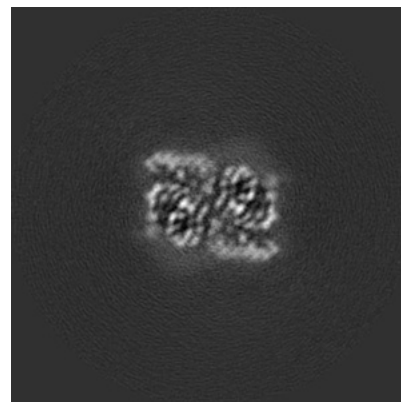
6.3.2 Raw map



X Index: 147



Y Index: 127

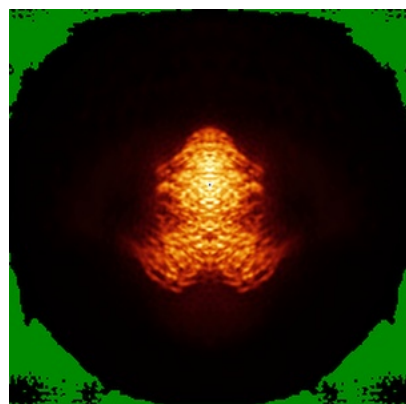


Z Index: 141

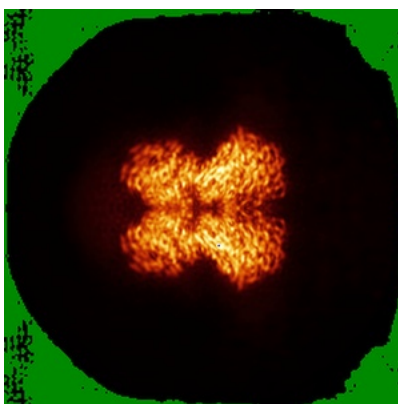
The images above show the largest variance slices of the map in three orthogonal directions.

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

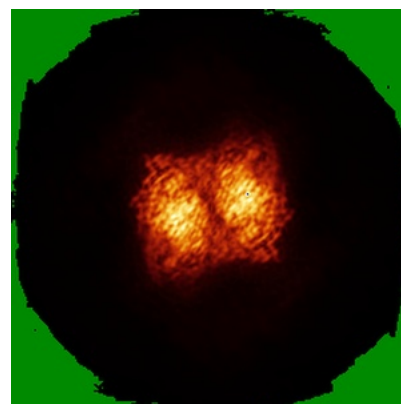
6.4.1 Primary map



X

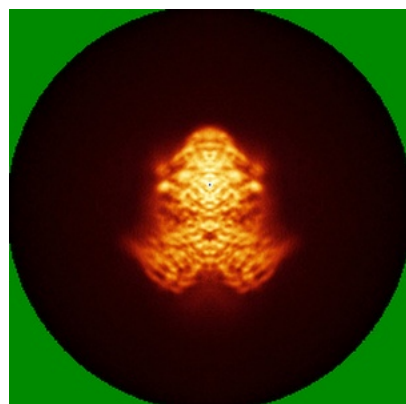


Y

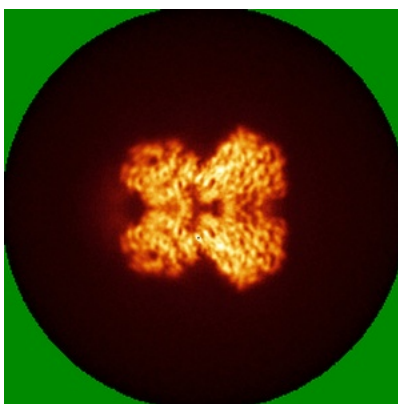


Z

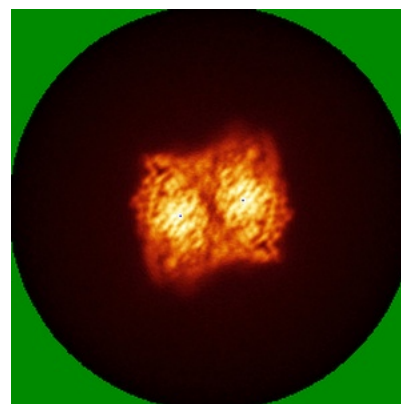
6.4.2 Raw map



X



Y

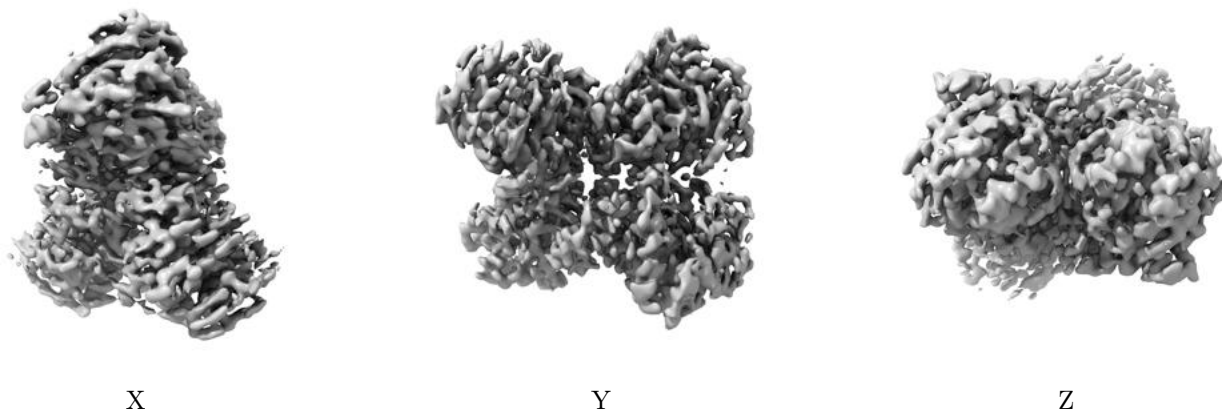


Z

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.

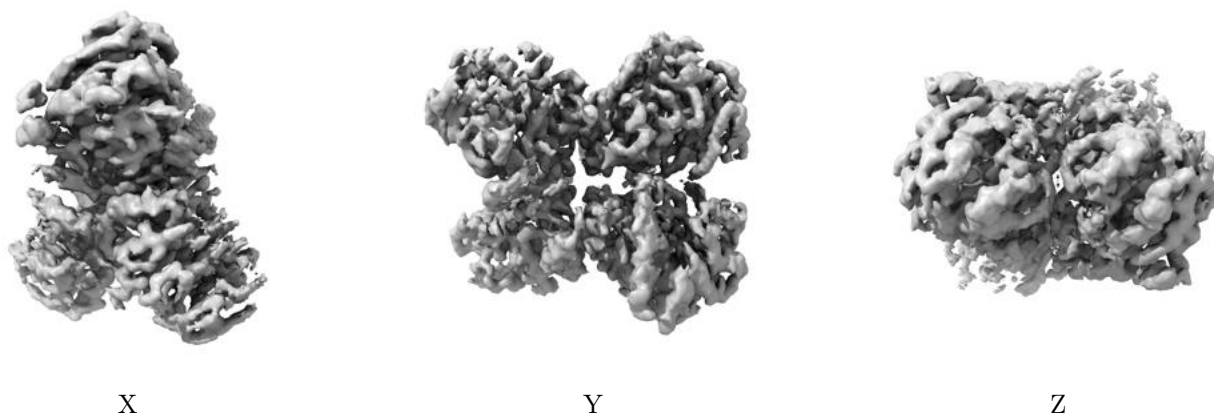
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0078. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

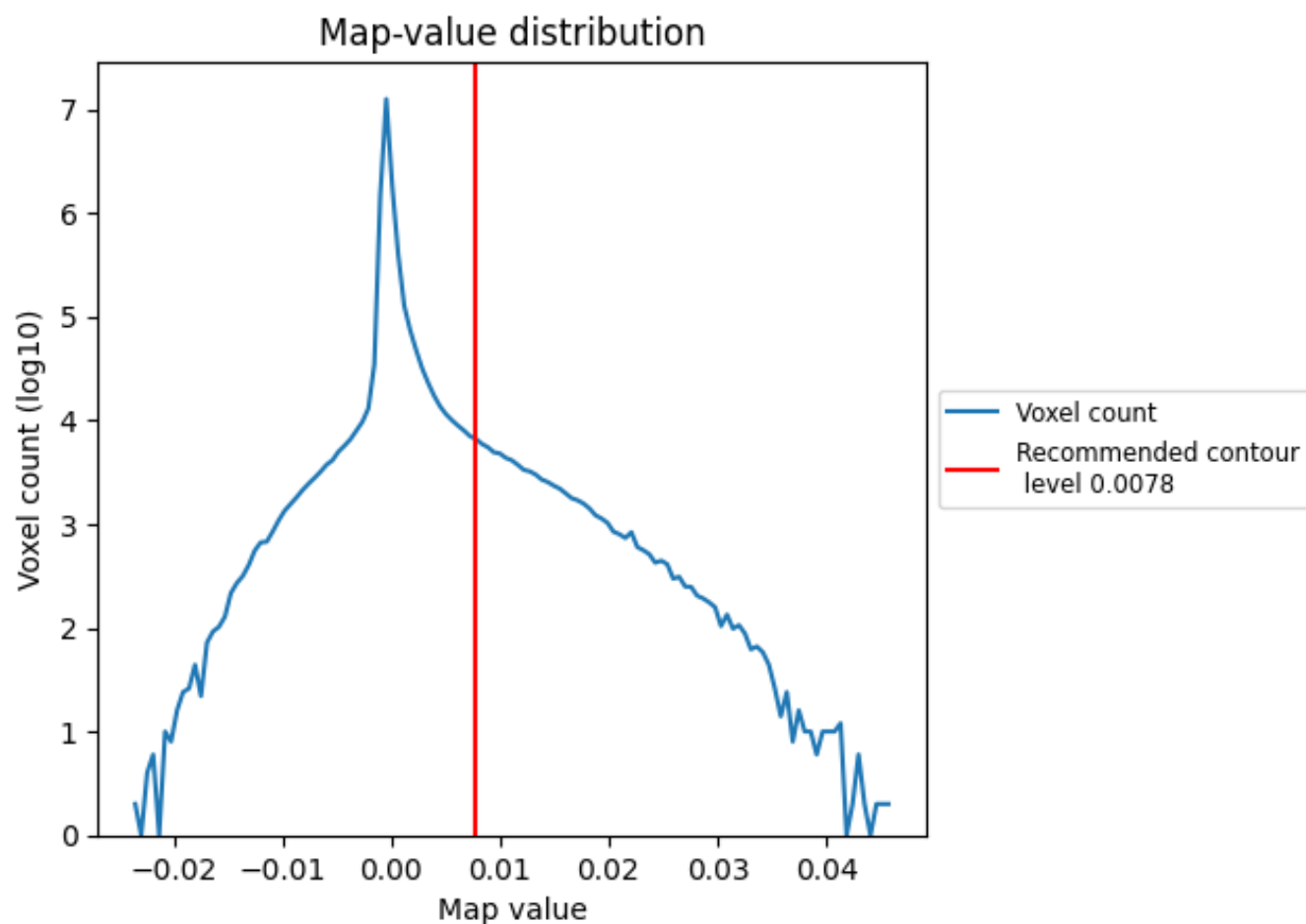
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

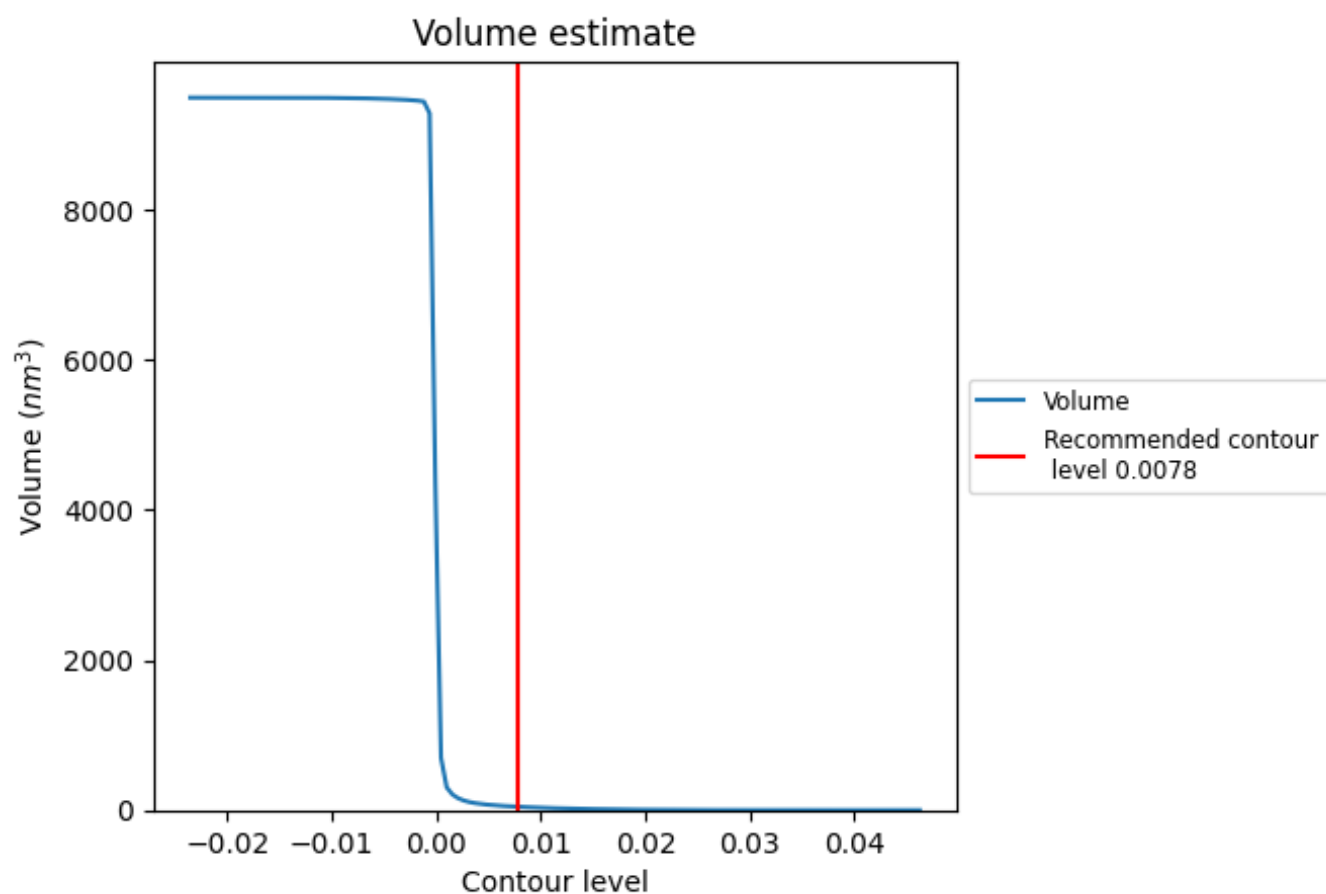
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

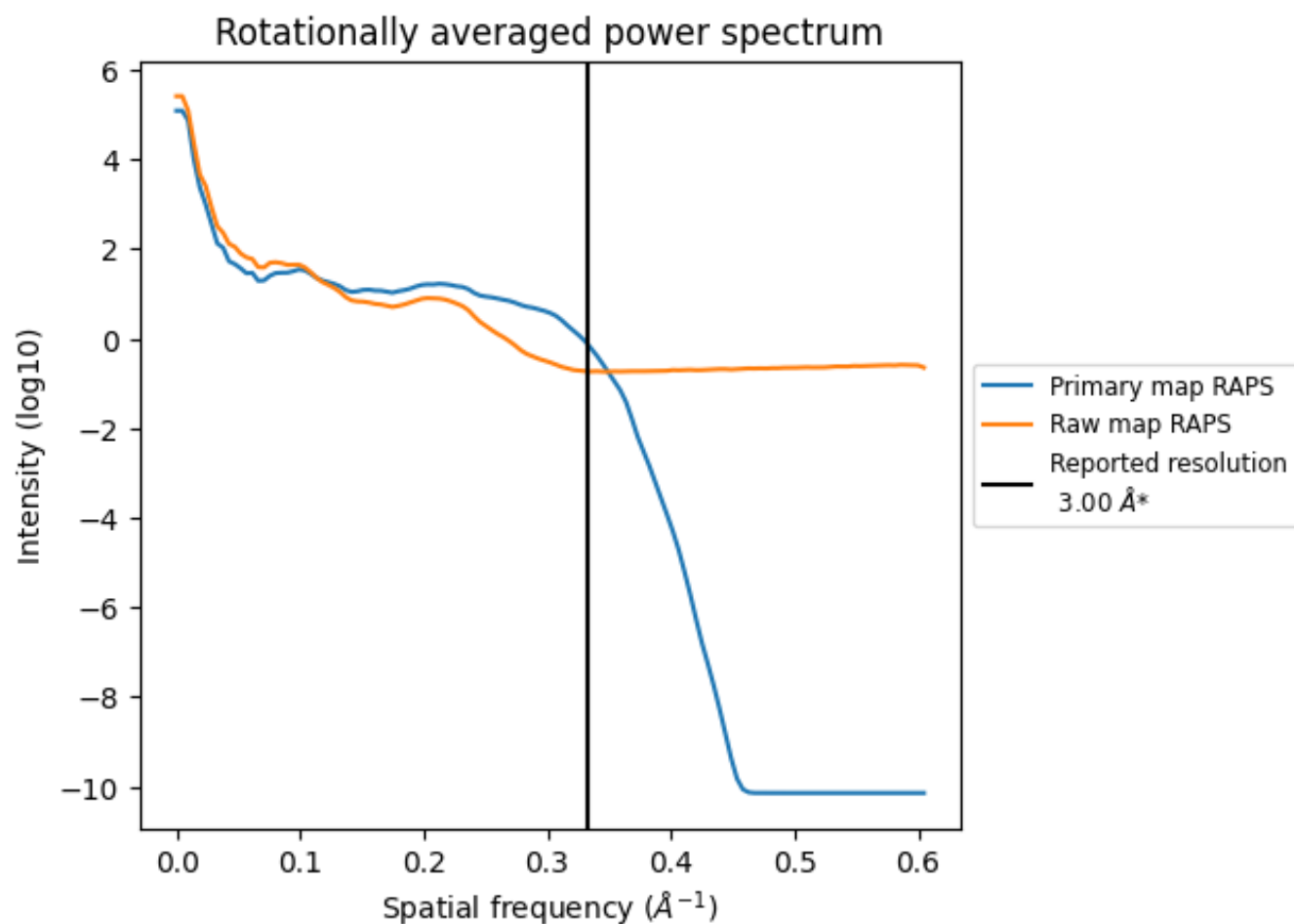
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 41 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 ⓘ

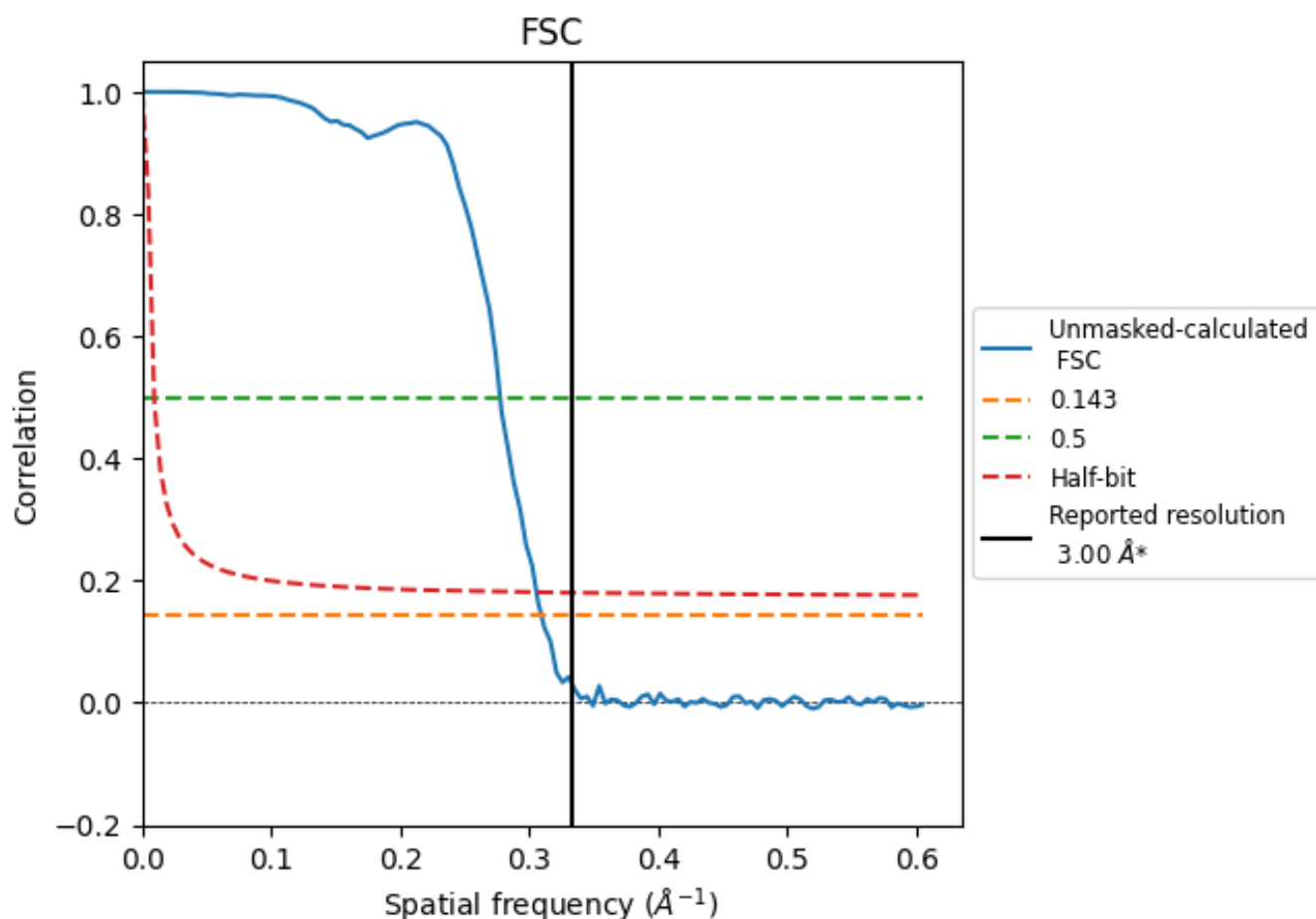


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

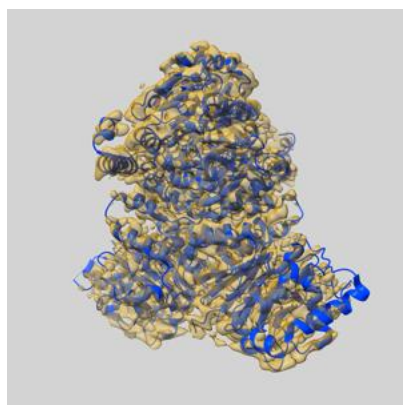
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.60	3.27

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

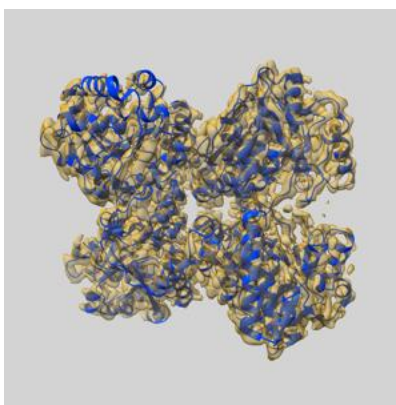
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47420 and PDB model 9E1T. Per-residue inclusion information can be found in section [3](#) on page [7](#).

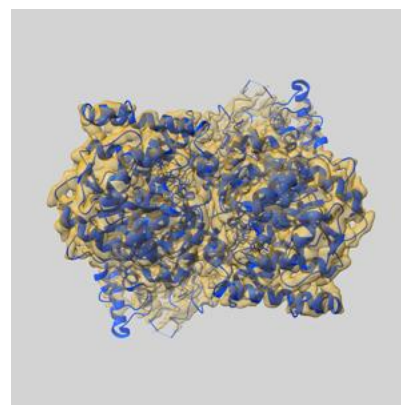
9.1 Map-model overlay [i](#)



X



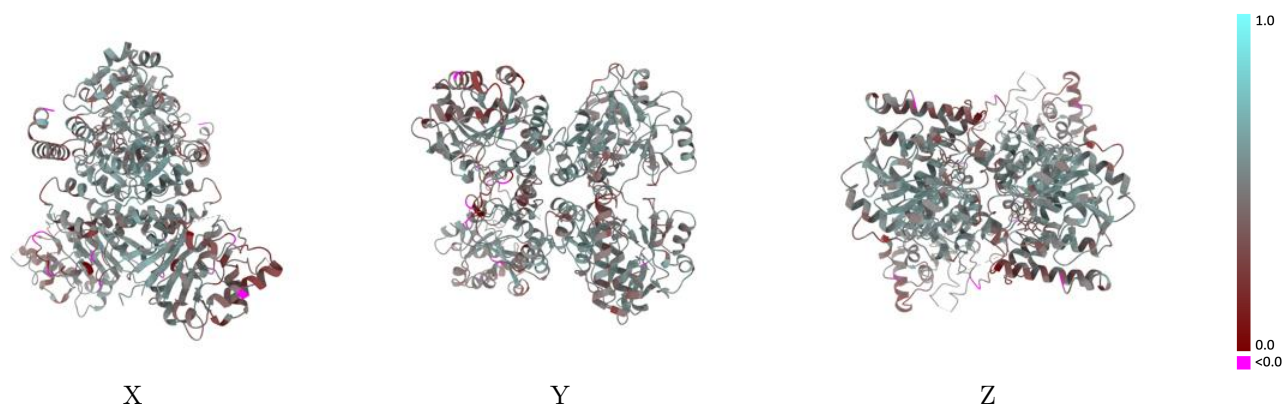
Y



Z

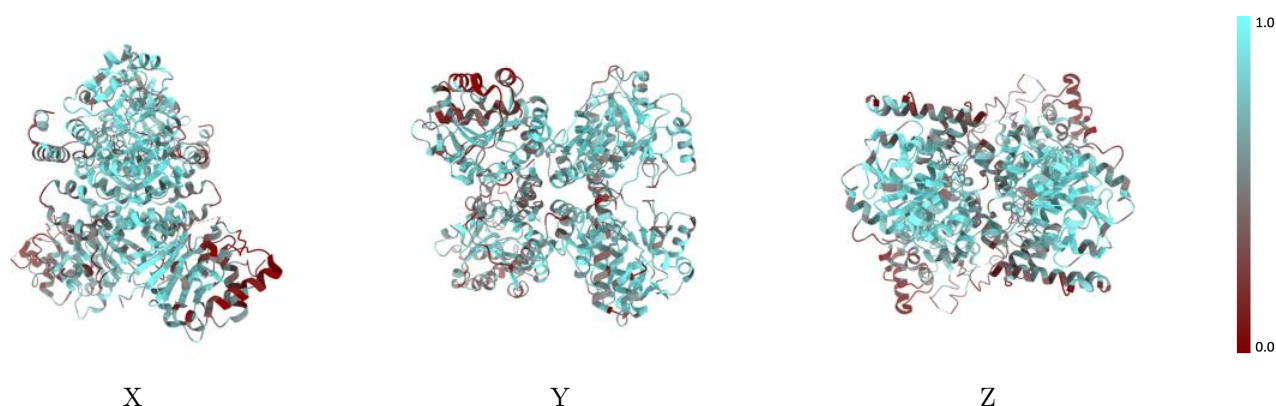
The images above show the 3D surface view of the map at the recommended contour level 0.0078 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



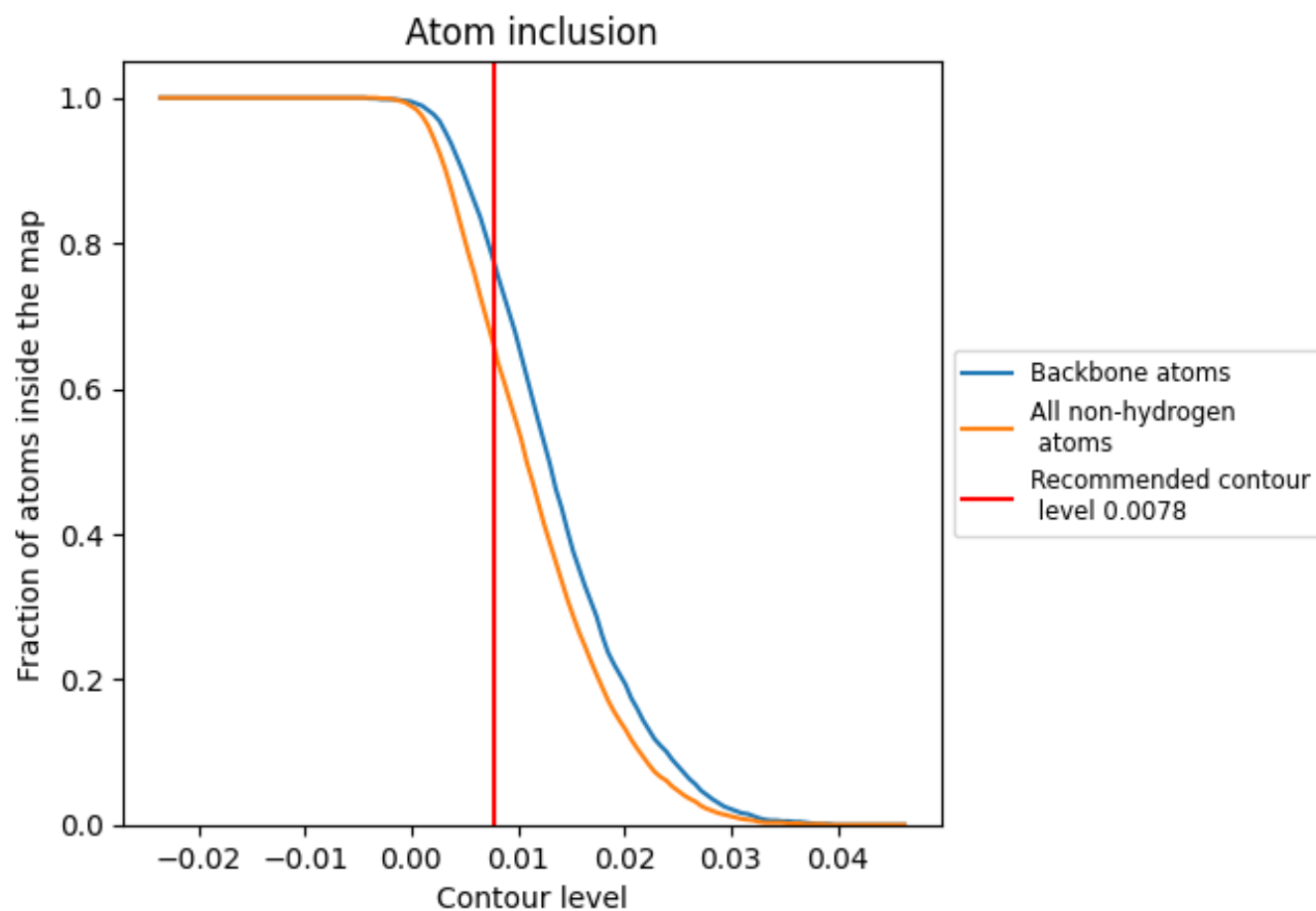
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0078).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% 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 (0.0078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4710
A	0.6530	0.4730
B	0.6590	0.4700

