



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 12:21 AM EST

PDB ID : 7ZZ1
EMDB ID : EMD-15031
Title : Cryo-EM structure of "CT react" conformation of Lactococcus lactis pyruvate carboxylase with acetyl-CoA
Authors : Lopez-Alonso, J.P.; Lazaro, M.; Gil, D.; Choi, P.H.; Tong, L.; Valle, M.
Deposited on : 2022-05-25
Resolution : 2.27 Å(reported)
Based on initial model : 5VYW

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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.40

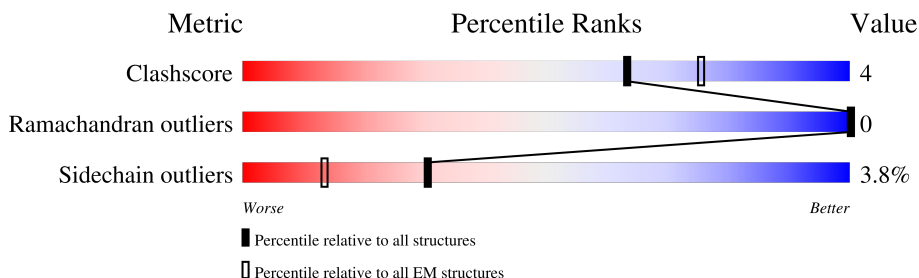
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.27 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	1143	
1	B	1143	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4958 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	541	Total	C	N	O	S	0	0
			4301	2736	731	815	19		
1	B	77	Total	C	N	O	S	0	0
			576	360	96	116	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A2A9IR05
A	-4	PRO	-	expression tag	UNP A0A2A9IR05
A	-3	ARG	-	expression tag	UNP A0A2A9IR05
A	-2	GLY	-	expression tag	UNP A0A2A9IR05
A	-1	SER	-	expression tag	UNP A0A2A9IR05
A	0	HIS	-	expression tag	UNP A0A2A9IR05
A	1055	ALA	THR	conflict	UNP A0A2A9IR05
B	-5	VAL	-	expression tag	UNP A0A2A9IR05
B	-4	PRO	-	expression tag	UNP A0A2A9IR05
B	-3	ARG	-	expression tag	UNP A0A2A9IR05
B	-2	GLY	-	expression tag	UNP A0A2A9IR05
B	-1	SER	-	expression tag	UNP A0A2A9IR05
B	0	HIS	-	expression tag	UNP A0A2A9IR05
B	1055	ALA	THR	conflict	UNP A0A2A9IR05

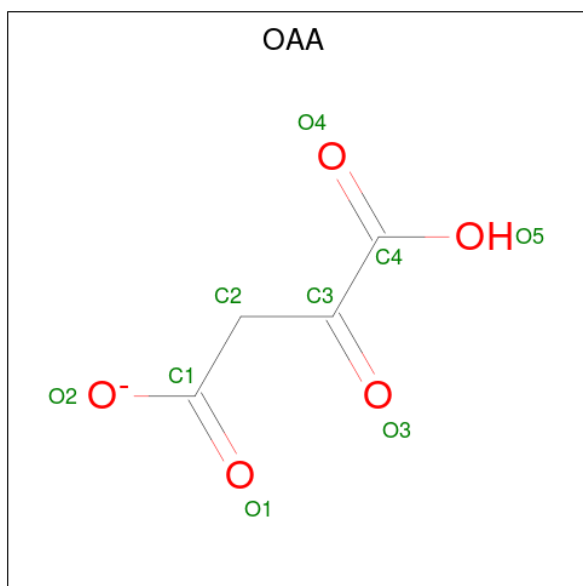
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

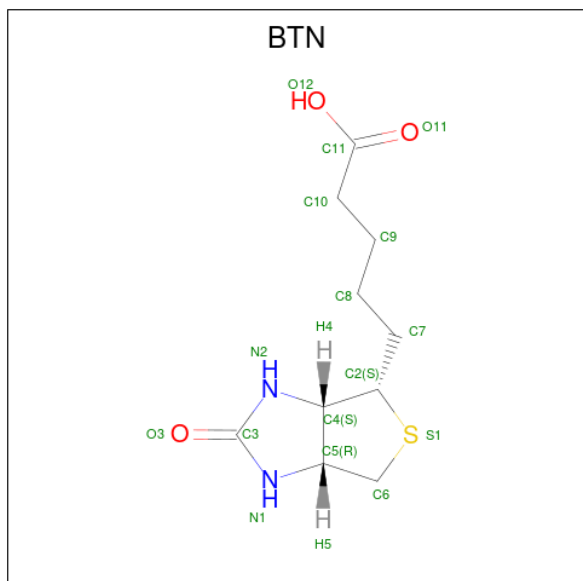
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mn	0
			1	1	

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			9	4	5	

- Molecule 5 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).

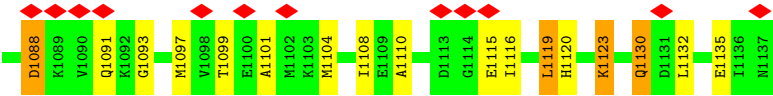


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	S	0
			15	10	2	2	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	55	Total	O	0
			55	55	

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128599	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.647	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.138	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: OAA, KCX, BTN, MN, MG

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	0.31	0/4383	0.50	0/5933
1	B	0.40	0/580	0.83	2/782 (0.3%)
All	All	0.32	0/4963	0.55	2/6715 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1119	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	1130	GLN	CA-CB-CG	5.47	125.44	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	702	VAL	Mainchain

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	4301	0	4244	30	0
1	B	576	0	592	9	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	9	0	2	0	0
5	B	15	0	15	1	0
6	A	55	0	0	0	0
All	All	4958	0	4853	39	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 4.

The worst 5 of 39 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:B:1097:MET:HB3	1:B:1108:ILE:HD11	1.76	0.67
1:B:1070:GLN:HG3	1:B:1135:GLU:HG2	1.77	0.66
1:B:1088:ASP:OD1	1:B:1088:ASP:N	2.29	0.63
1:A:972:TYR:HB3	1:A:975:VAL:HB	1.81	0.62
1:A:840:VAL:HG22	1:A:882:GLN:HE21	1.67	0.58

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	538/1143 (47%)	528 (98%)	10 (2%)	0	100	100
1	B	75/1143 (7%)	69 (92%)	6 (8%)	0	100	100
All	All	613/2286 (27%)	597 (97%)	16 (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	459/954 (48%)	448 (98%)	11 (2%)	44	59
1	B	63/954 (7%)	54 (86%)	9 (14%)	2	2
All	All	522/1908 (27%)	502 (96%)	20 (4%)	30	40

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1088	ASP
1	B	1115	GLU
1	B	1130	GLN
1	B	1123	LYS
1	A	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	749	GLN
1	A	882	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	KCX	A	703	3,1	10,11,12	0.84	0	6,12,14	1.59	1 (16%)

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
1	KCX	A	703	3,1	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	KCX	OQ1-CX-NZ	-3.64	119.39	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
5	BTN	B	1201	1	15,16,17	3.37	2 (13%)	20,21,23	1.71	4 (20%)
4	OAA	A	1203	-	8,8,8	2.17	3 (37%)	8,10,10	1.53	1 (12%)

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
5	BTN	B	1201	1	-	2/6/27/28	0/2/2/2
4	OAA	A	1203	-	-	6/8/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1201	BTN	C2-S1	-9.54	1.67	1.82
5	B	1201	BTN	O3-C3	8.49	1.41	1.23
4	A	1203	OAA	O3-C3	3.94	1.31	1.23
4	A	1203	OAA	O4-C4	3.45	1.31	1.22
4	A	1203	OAA	O1-C1	2.79	1.31	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	BTN	C4-C2-S1	5.34	111.10	105.03
5	B	1201	BTN	C5-C6-S1	2.74	109.84	106.06
4	A	1203	OAA	O4-C4-C3	-2.34	118.90	121.81
5	B	1201	BTN	C2-C4-N2	-2.16	111.05	113.34
5	B	1201	BTN	C6-C5-N1	-2.01	110.60	113.18

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	OAA	C2-C3-C4-O5
5	B	1201	BTN	S1-C2-C7-C8
5	B	1201	BTN	C4-C2-C7-C8
4	A	1203	OAA	C1-C2-C3-O3

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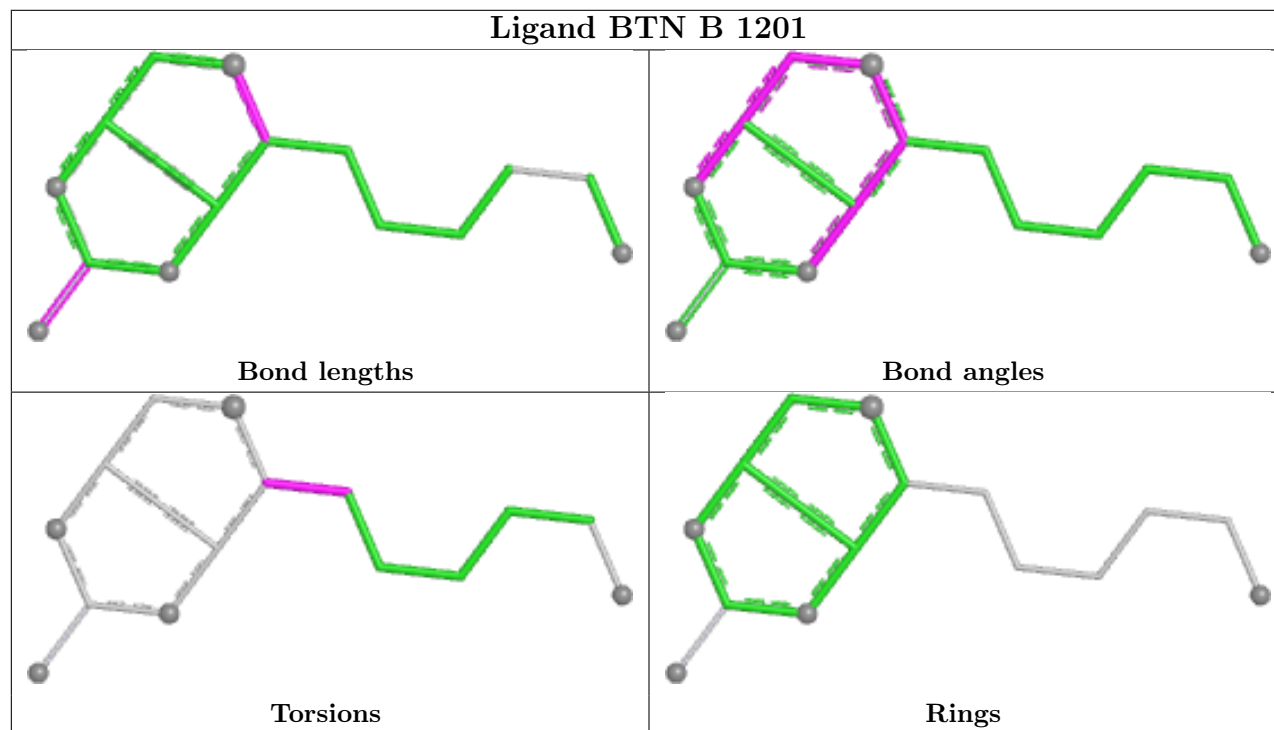
Mol	Chain	Res	Type	Atoms
4	A	1203	OAA	O3-C3-C4-O4

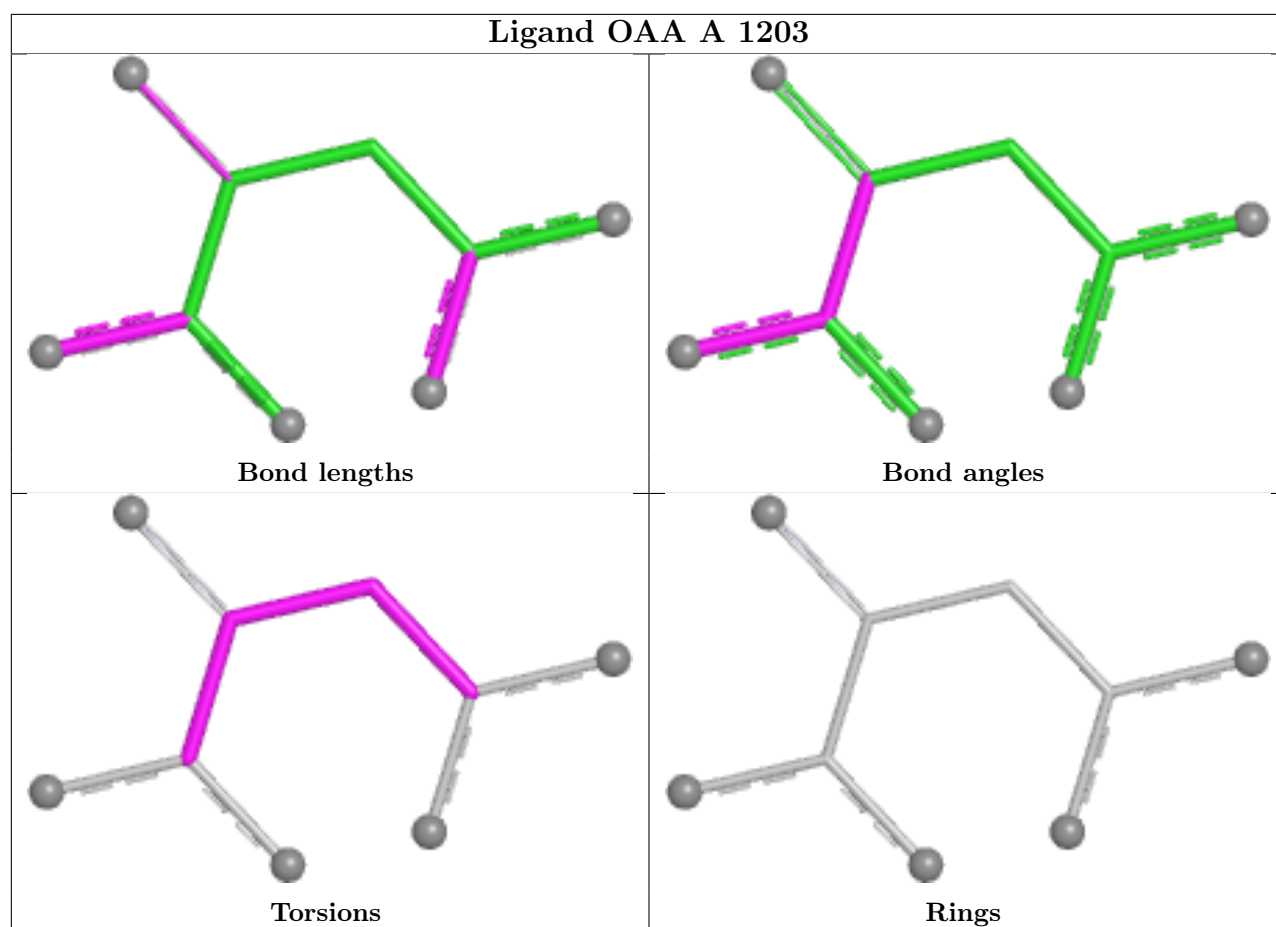
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	BTN	1	0

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.

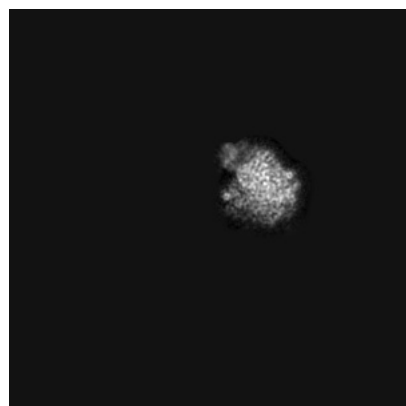
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15031. These allow visual inspection of the internal detail of the map and identification of artifacts.

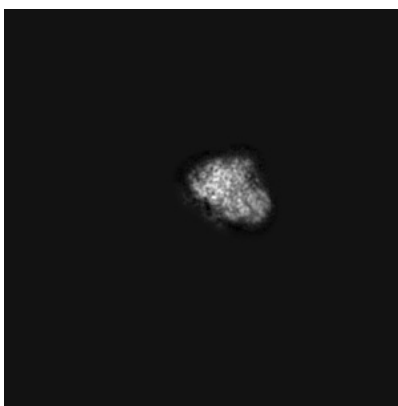
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

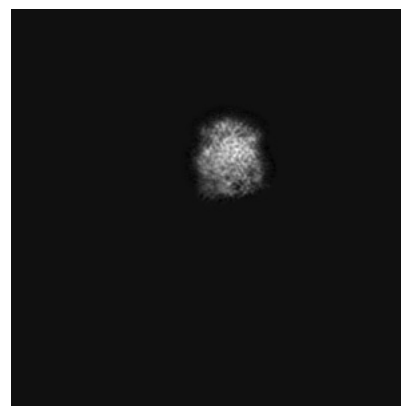
6.1.1 Primary map



X

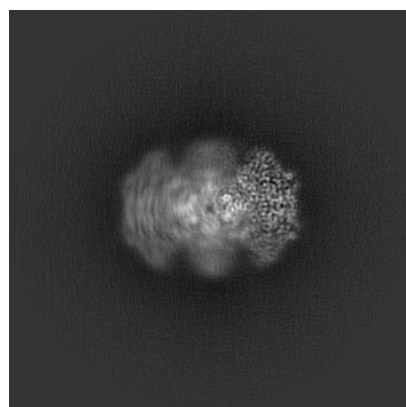


Y

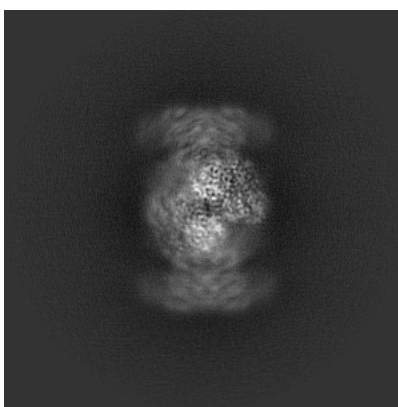


Z

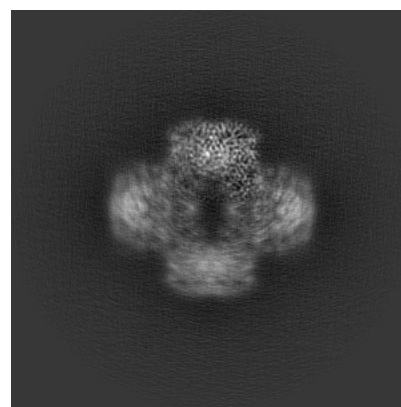
6.1.2 Raw map



X



Y

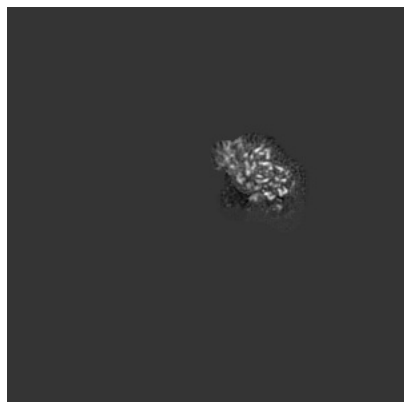


Z

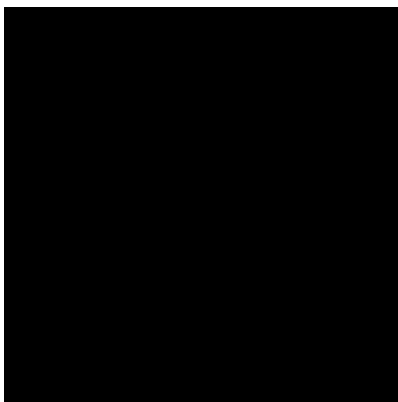
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

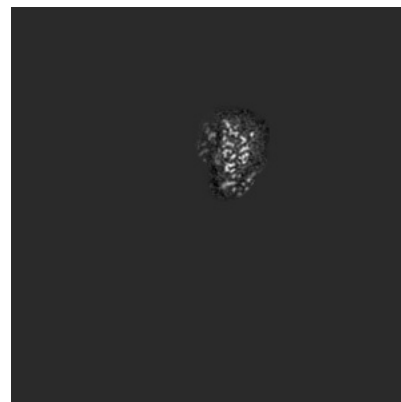
6.2.1 Primary map



X Index: 150

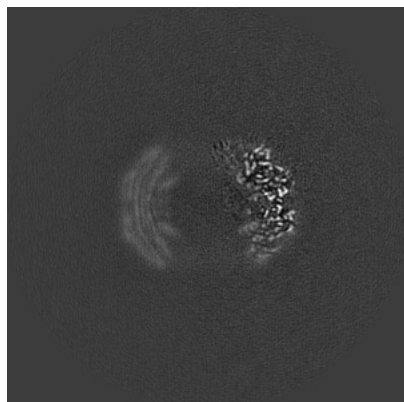


Y Index: 150

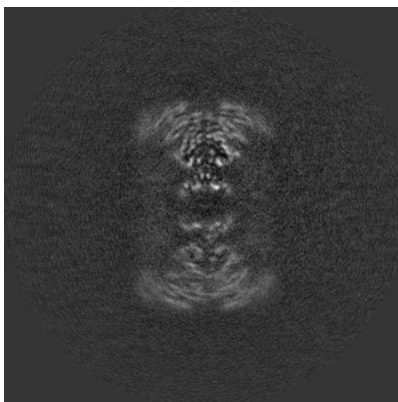


Z Index: 150

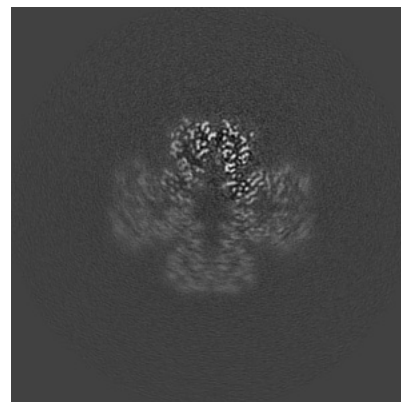
6.2.2 Raw map



X Index: 150



Y Index: 150

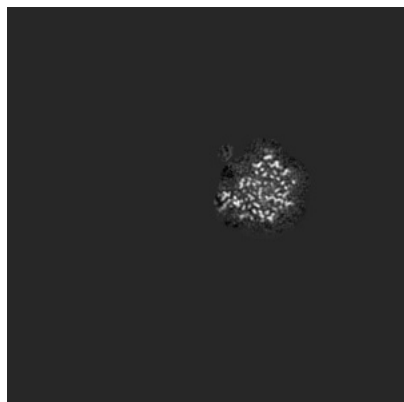


Z Index: 150

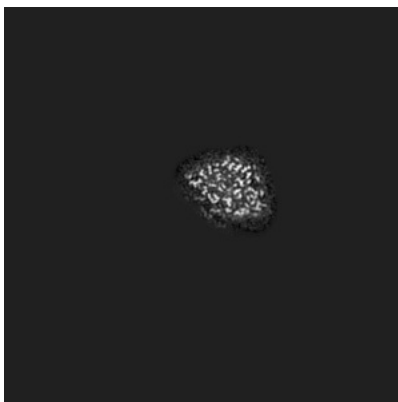
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

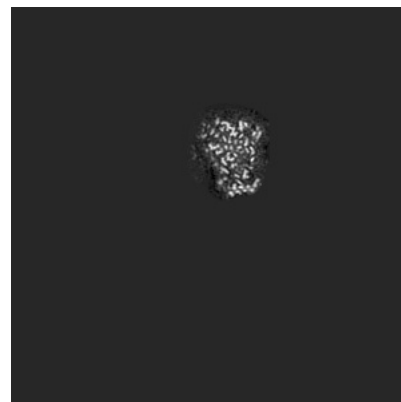
6.3.1 Primary map



X Index: 167

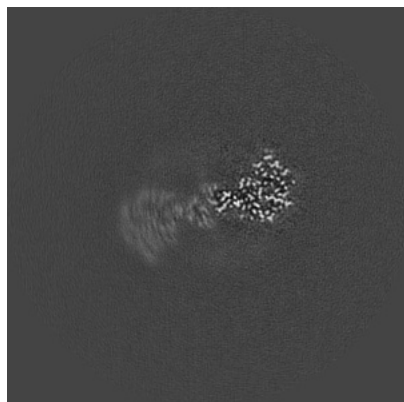


Y Index: 191

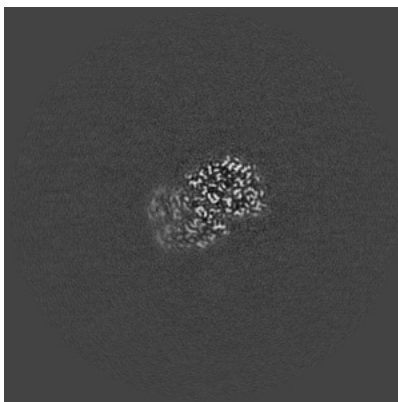


Z Index: 159

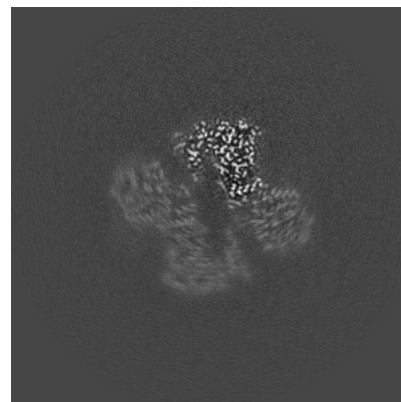
6.3.2 Raw map



X Index: 167



Y Index: 191

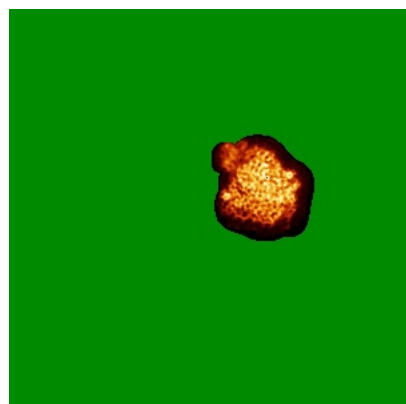


Z Index: 158

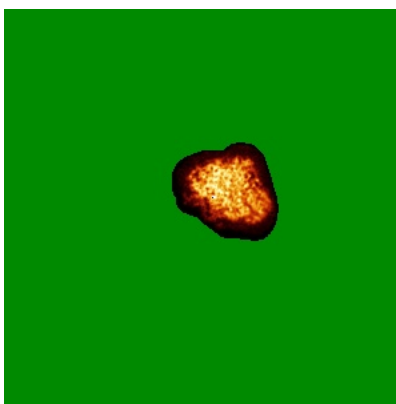
The images above show the largest variance slices of the map in three orthogonal directions.

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

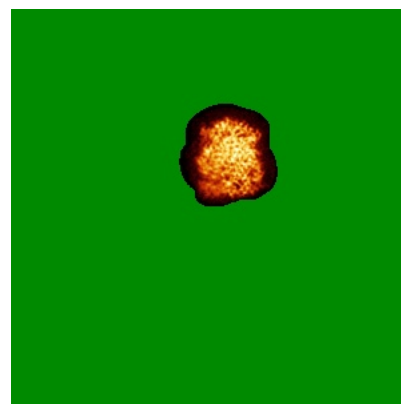
6.4.1 Primary map



X

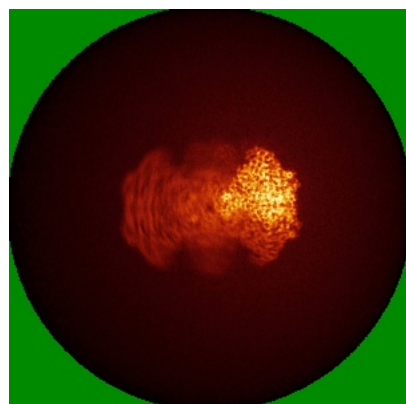


Y

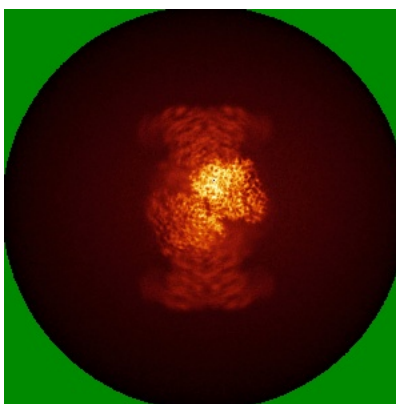


Z

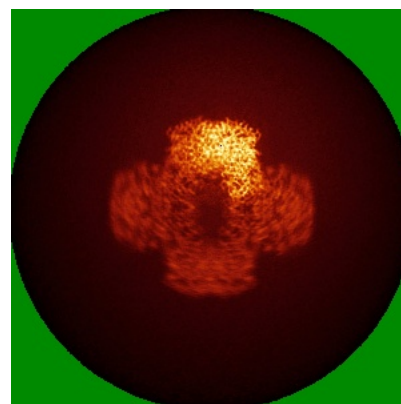
6.4.2 Raw map



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.

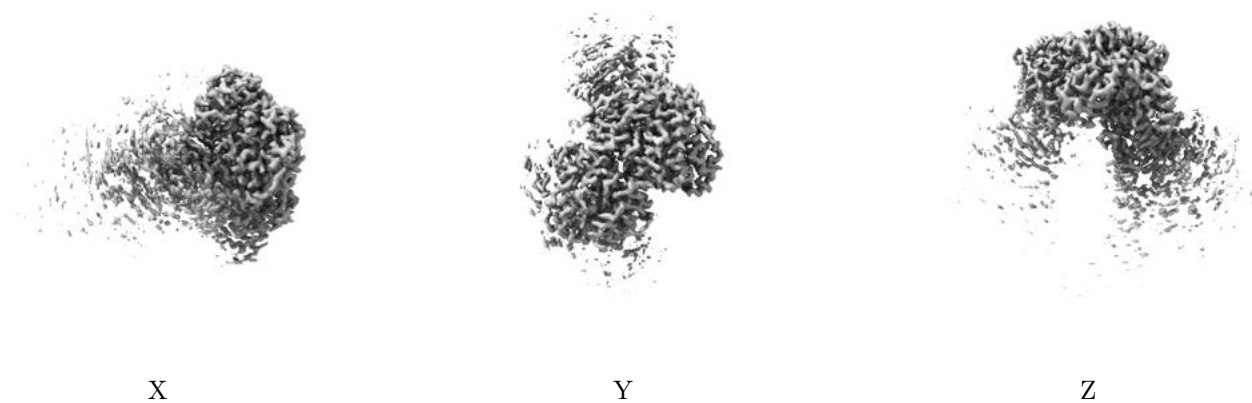
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.138. 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.

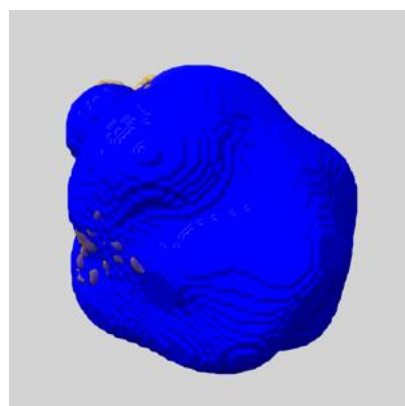
6.6 Mask visualisation [i](#)

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

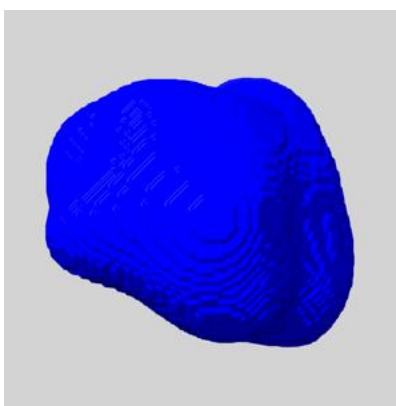
A mask typically either:

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

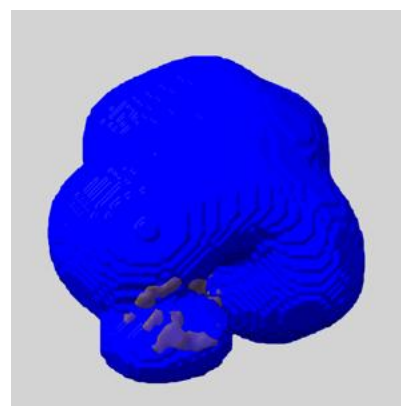
6.6.1 emd_15031_msk_1.map [i](#)



X



Y

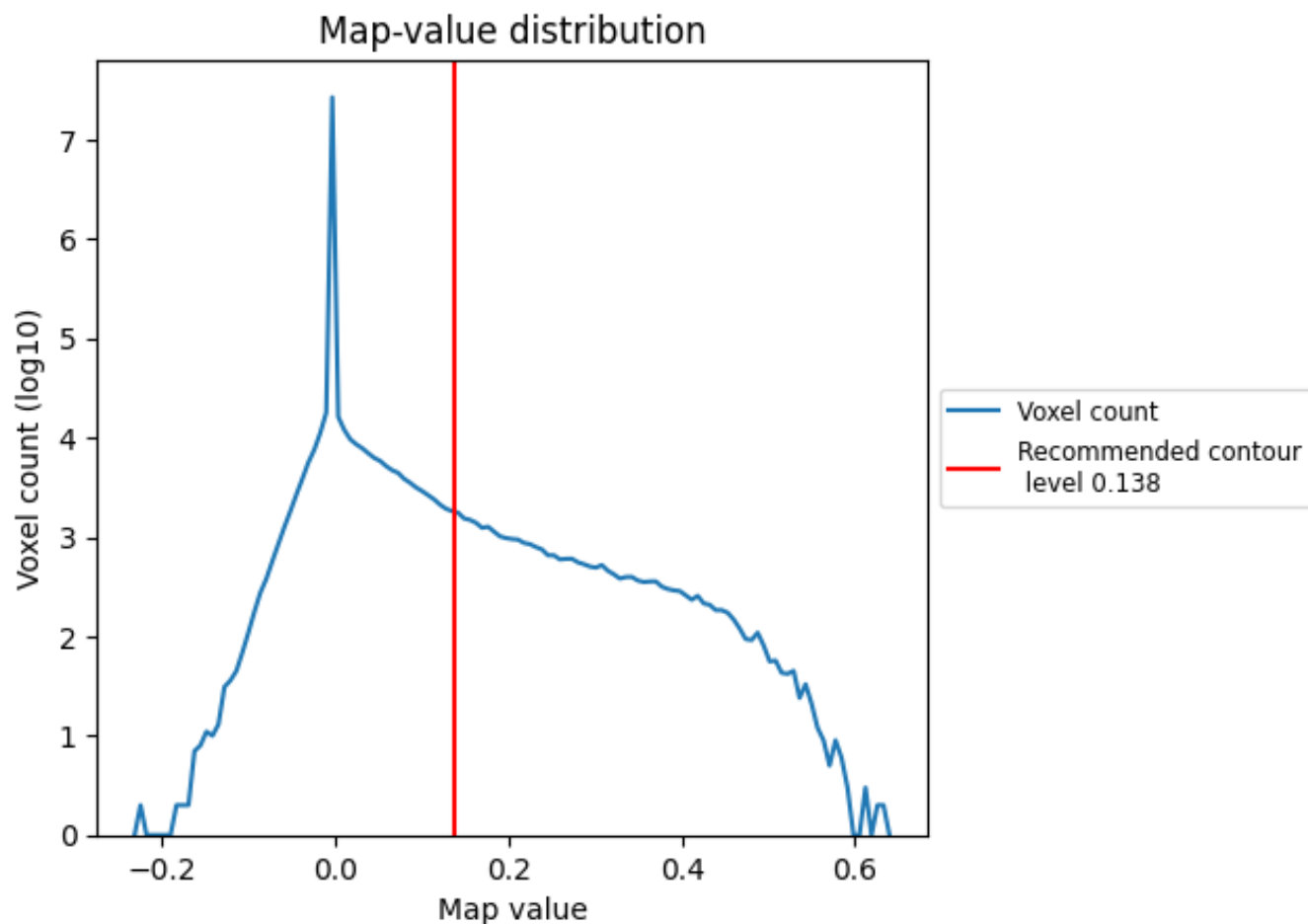


Z

7 Map analysis [i](#)

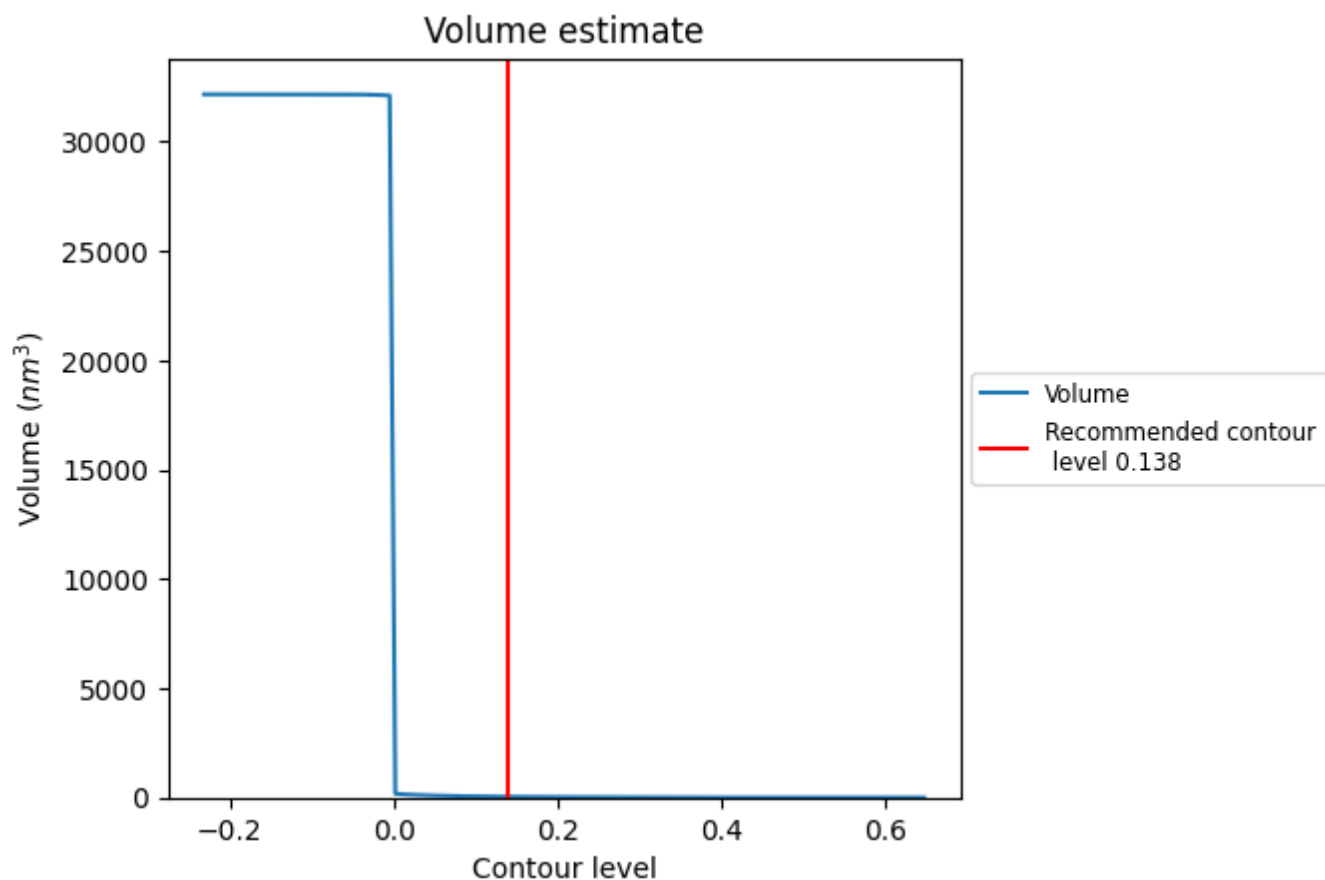
This section contains the results of statistical analysis of the map.

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.

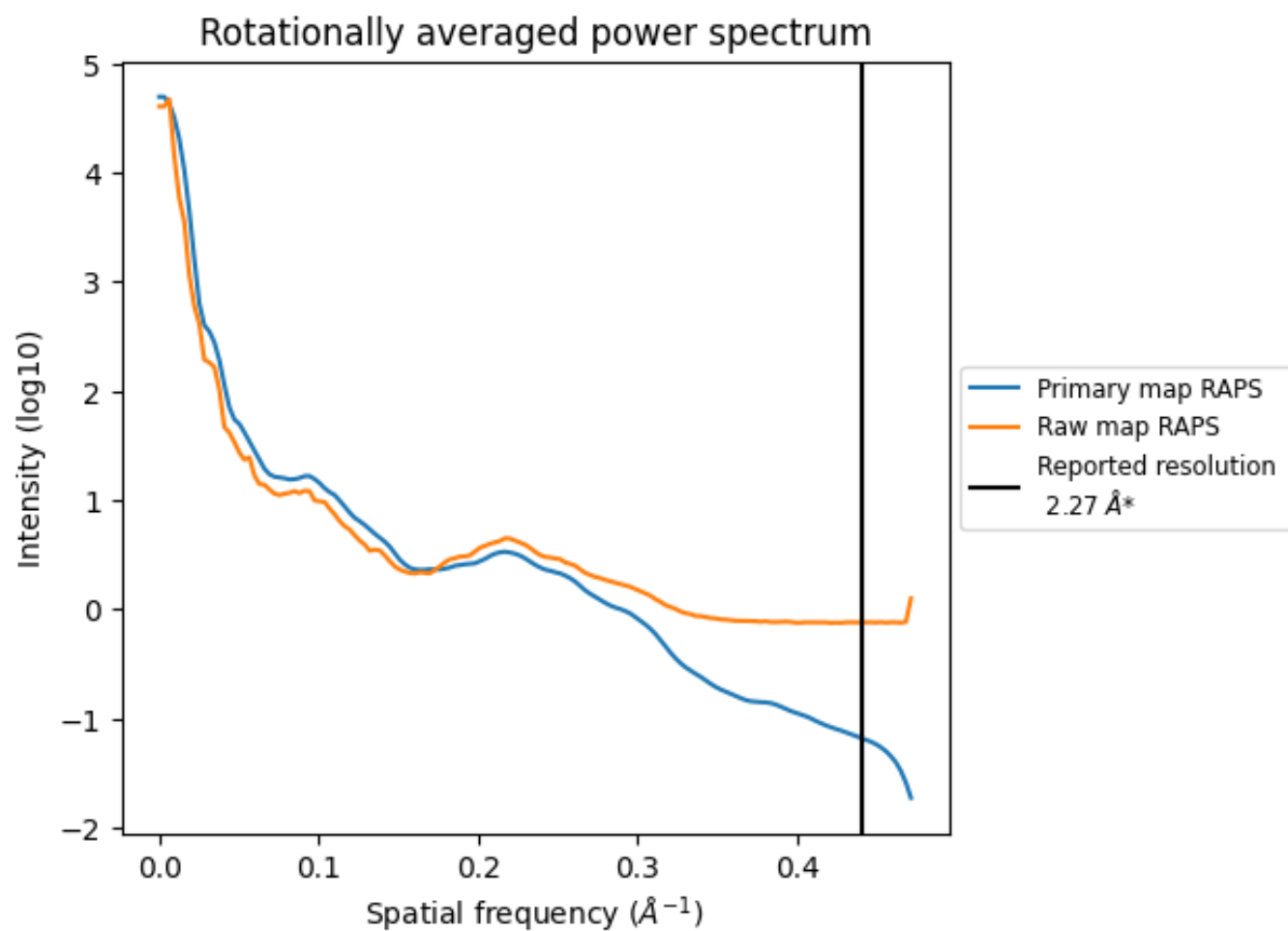
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 37 nm^3 ; this corresponds to an approximate mass of 34 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 ⓘ

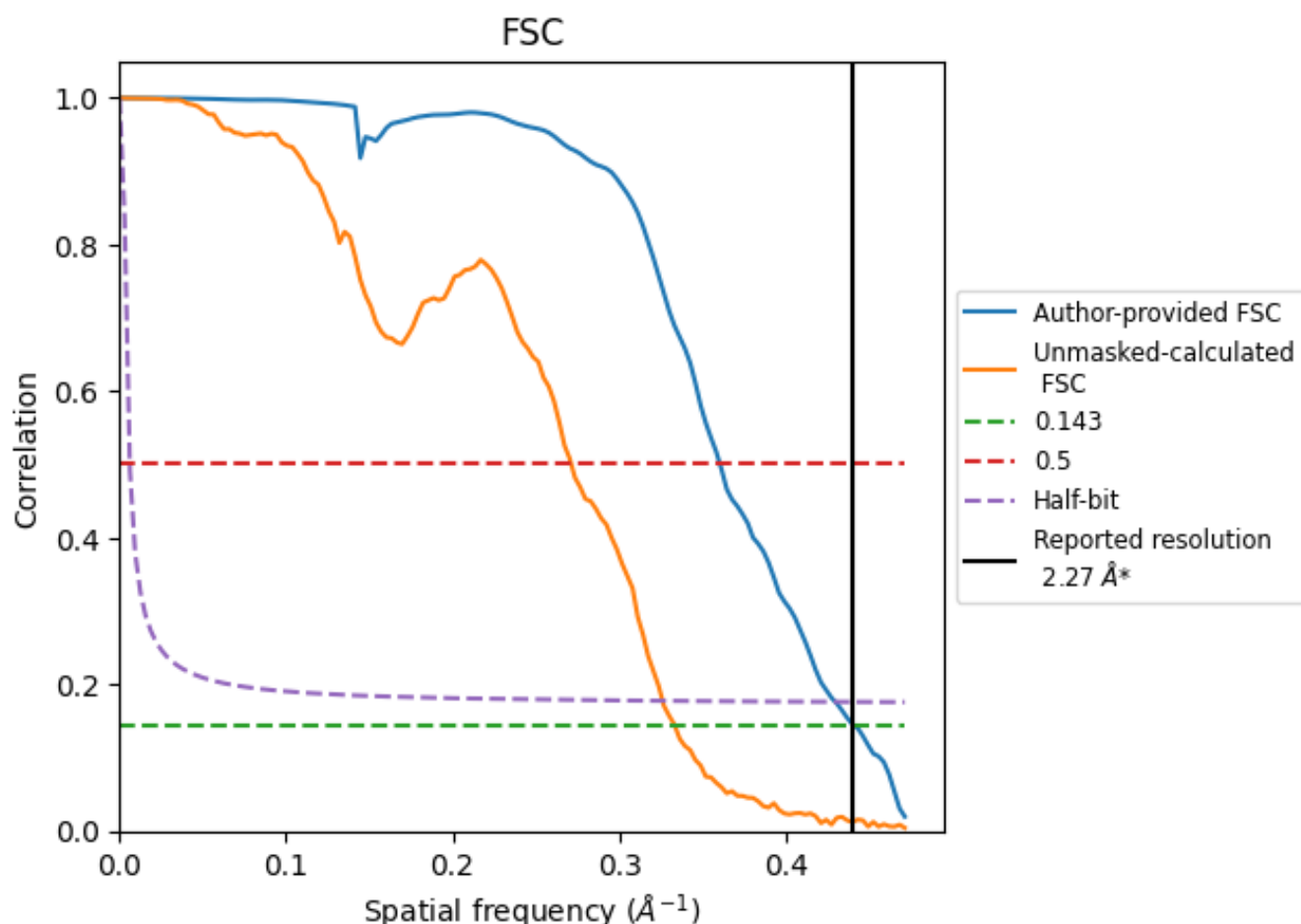


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

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 0.441 \AA^{-1}

8.2 Resolution estimates [i](#)

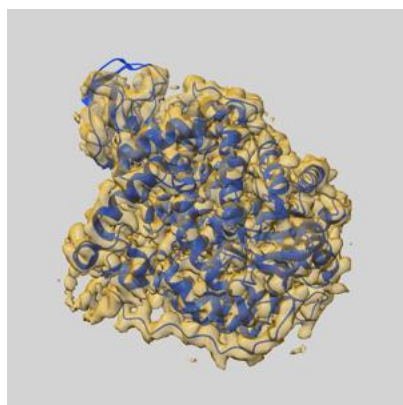
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.77	2.33
Unmasked-calculated*	3.00	3.68	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.27 by more than 10 %

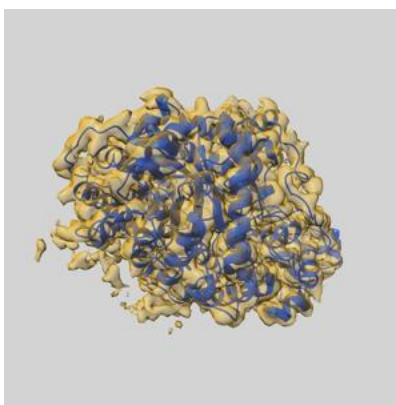
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15031 and PDB model 7ZZ1. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

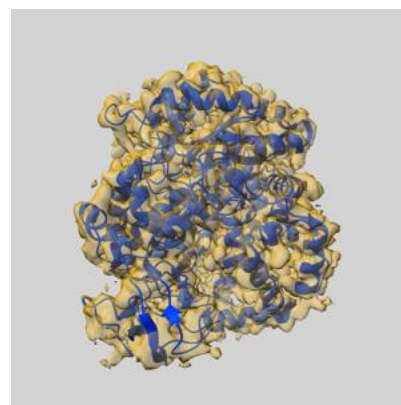
9.1 Map-model overlay [i](#)



X



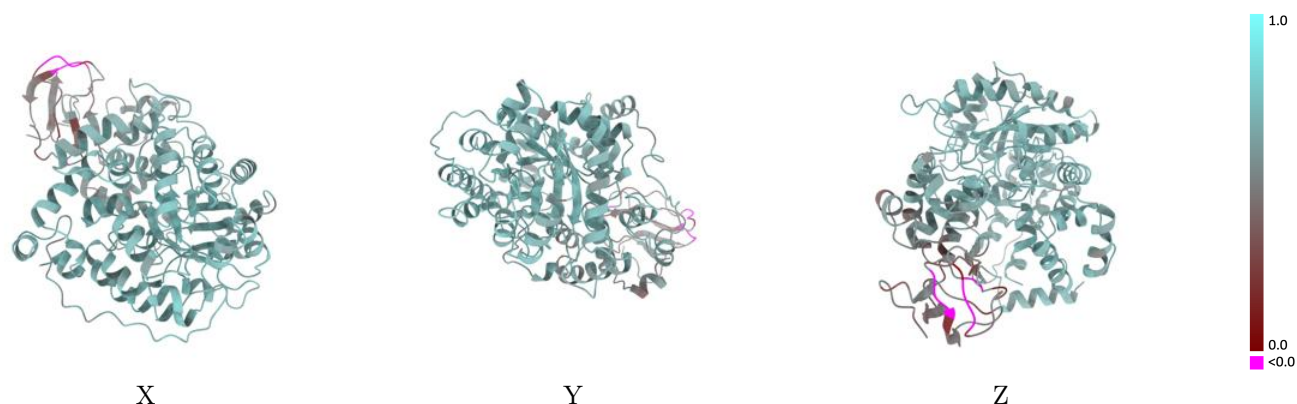
Y



Z

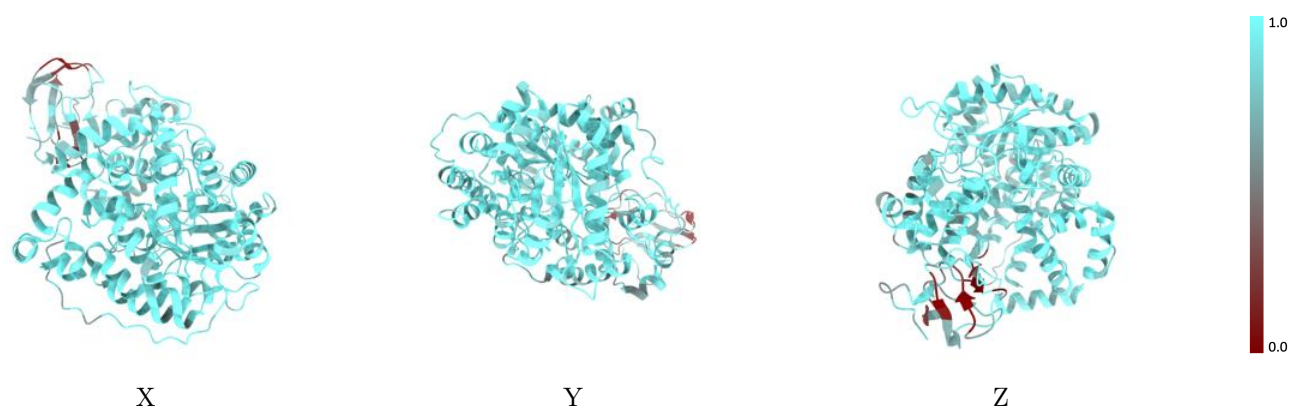
The images above show the 3D surface view of the map at the recommended contour level 0.138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



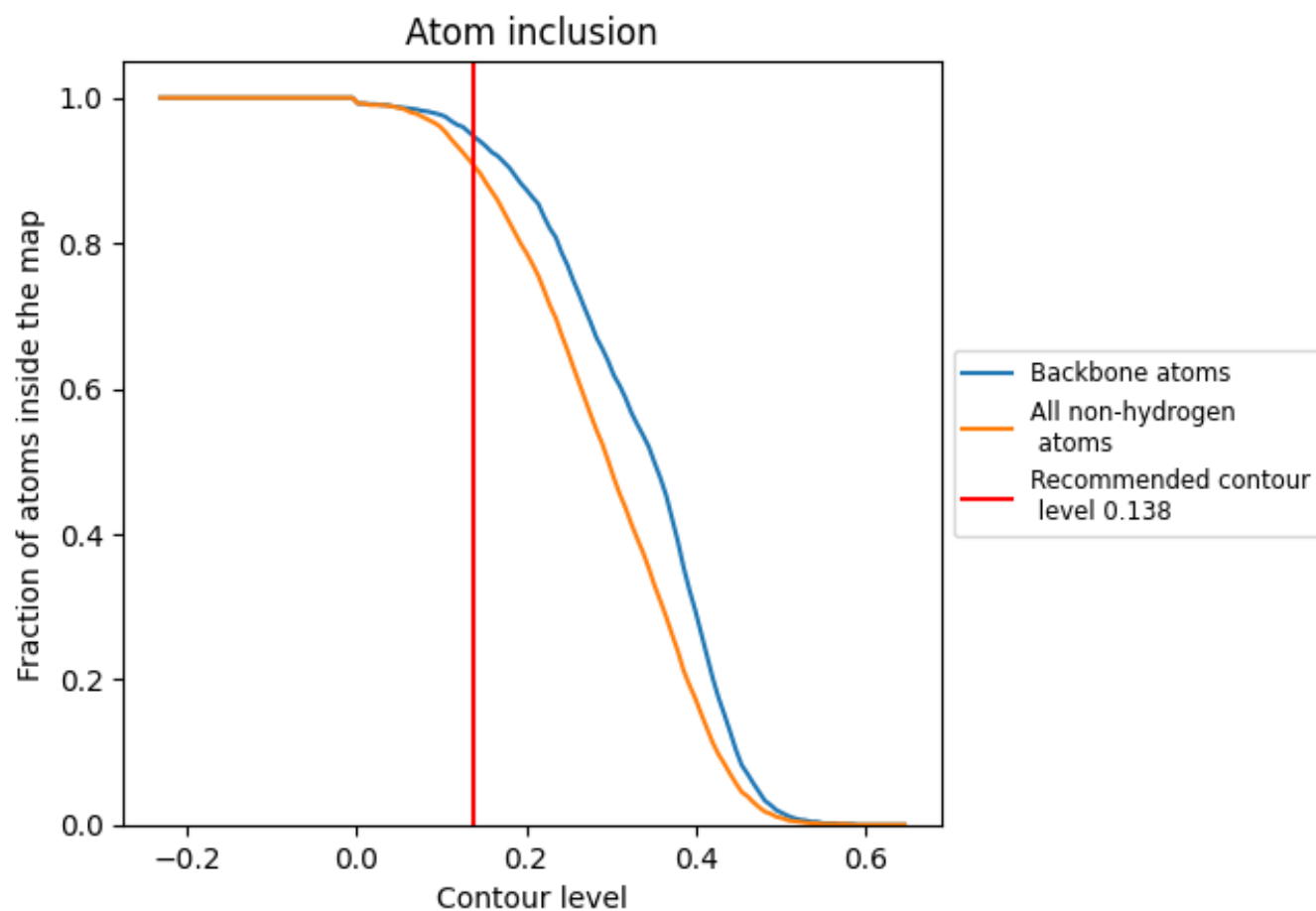
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.138).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9070	<div></div> 0.6170
A	<div></div> 0.9430	<div></div> 0.6480
B	<div></div> 0.6470	<div></div> 0.3890

