



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:43 AM UTC

PDB ID : 7ZZ6 / pdb_00007zz6
EMDB ID : EMD-15036
Title : Cryo-EM structure of "CT-CT dimer" 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 : 2.15 Å(reported)
Based on initial model : 5VYW

This is a Full wwPDB EM Validation 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
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

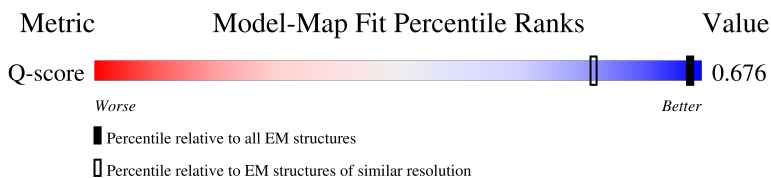
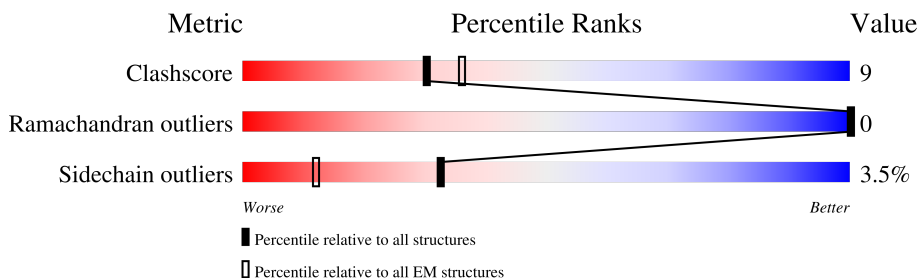
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.15 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	2551 (1.66 - 2.65)

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	 34% 10% 56%
1	D	1143	 34% 10% 55%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PYR	A	1203	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8257 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	D	509	Total	C	N	O	S	0	0
			4047	2574	685	770	18		
1	A	508	Total	C	N	O	S	0	0
			4037	2568	682	769	18		

There are 14 discrepancies between the modelled and reference sequences:

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

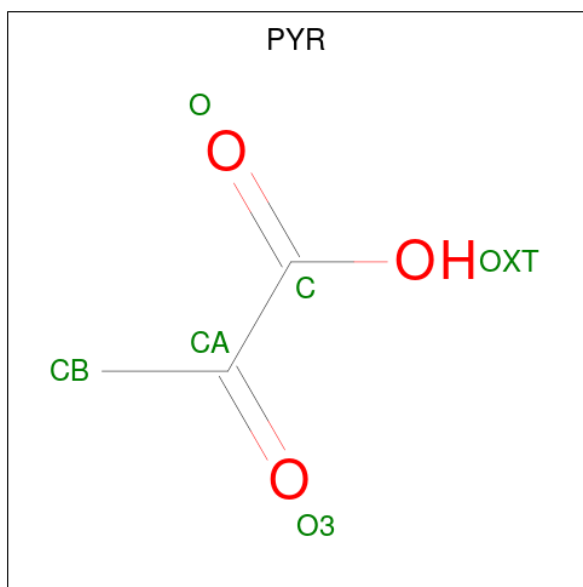
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



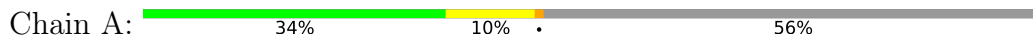
Mol	Chain	Residues	Atoms			AltConf
4	D	1	Total	C	O	0
			6	3	3	
4	A	1	Total	C	O	0
			6	3	3	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	D	99	Total	O	0
			99	99	
5	A	58	Total	O	0
			58	58	

ASP	LEU	LEU	ILE	GLU	ILE	ASN	ILE	GLY	ALA	THR	PRO	GLY	SER	VAL	LEU	GLU	ILE	LEU	VAL	LYS	GLY	ALA	GLY	ASP	LYS	VAL	GLN	LYS	GLY	GLN	ALA	LEU	MET	VAL	THR	GLU	THR	THR	GLY	MET	LYS	MET	GLY	THR	PRO	PHE	ASP	GLY	GLU	ILE	ILE	VAL	ASP	LEU	HIS	VAL	VAL	LYS	GLY	GLU	GLN	THR	GLN
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- Molecule 1: Pyruvate carboxylase

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1369092	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	0.849	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/4111	0.37	0/5565
1	D	0.24	0/4122	0.38	0/5580
All	All	0.24	0/8233	0.37	0/11145

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	4037	0	3980	79	0
1	D	4047	0	3987	72	0
2	A	1	0	0	1	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	0	0	0
4	D	6	0	0	0	0
5	A	58	0	0	1	0
5	D	99	0	0	0	0
All	All	8257	0	7967	144	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 9.

All (144) 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:D:532:LEU:HD22	1:D:549:MET:HG2	1.68	0.76
1:A:840:VAL:HG23	1:A:842:LEU:HD23	1.71	0.71
1:D:819:GLU:OE2	1:A:797:HIS:NE2	2.24	0.68
1:A:894:GLY:HA2	1:A:897:LEU:HD12	1.74	0.68
1:A:753:ASP:OD2	2:A:1201:MG:MG	1.38	0.66
1:A:753:ASP:OD2	5:A:1301:HOH:O	2.14	0.65
1:D:797:HIS:NE2	1:A:819:GLU:OE2	2.25	0.64
1:D:683:GLN:NE2	1:D:687:ASP:OD1	2.30	0.64
1:D:679:LYS:NZ	1:D:861:GLY:O	2.30	0.64
1:D:952:ASP:OD1	1:D:956:LYS:NZ	2.30	0.63
1:D:858:MET:HE3	1:D:858:MET:HA	1.80	0.63
1:D:885:LEU:HD12	1:D:889:ASP:HB3	1.80	0.62
1:A:679:LYS:NZ	1:A:861:GLY:O	2.27	0.62
1:D:825:MET:HG2	1:D:853:TYR:CE1	2.34	0.61
1:A:885:LEU:HD12	1:A:889:ASP:HB3	1.83	0.60
1:A:683:GLN:NE2	1:A:687:ASP:OD1	2.34	0.59
1:D:637:ARG:HA	1:D:663:GLU:HB3	1.84	0.59
1:A:664:ALA:HB1	1:A:692:LEU:HD22	1.82	0.59
1:A:852:MET:HE2	1:A:852:MET:HA	1.85	0.59
1:D:730:HIS:NE2	1:D:756:ASP:OD1	2.32	0.58
1:A:663:GLU:HG3	1:A:699:ILE:HB	1.85	0.58
1:A:972:TYR:HB3	1:A:975:VAL:HB	1.86	0.58
1:A:532:LEU:O	1:A:536:HIS:NE2	2.36	0.57
1:D:791:ASN:O	1:D:795:ILE:HG12	2.06	0.56
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.34	0.56
1:D:664:ALA:HB1	1:D:692:LEU:HD22	1.85	0.56
1:D:501:LYS:NZ	1:D:509:GLU:OE2	2.38	0.56
1:D:886:THR:OG1	1:D:887:GLU:N	2.38	0.56
1:A:823:HIS:ND1	1:A:823:HIS:O	2.39	0.56
1:D:950:LYS:NZ	1:D:960:GLU:OE2	2.39	0.56
1:D:974:GLN:NE2	1:D:978:ASP:OD1	2.39	0.56
1:A:791:ASN:O	1:A:795:ILE:HG12	2.06	0.56
1:A:609:ASN:N	1:A:609:ASN:OD1	2.39	0.56
1:D:894:GLY:HA2	1:D:897:LEU:HD23	1.88	0.55
1:D:498:GLU:OE1	1:D:500:LYS:NZ	2.39	0.55
1:A:950:LYS:NZ	1:A:960:GLU:OE2	2.36	0.55
1:A:656:ARG:NH1	1:A:696:GLY:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:773:SER:OG	1:A:737:SER:O	2.24	0.54
1:A:974:GLN:NE2	1:A:978:ASP:OD1	2.39	0.54
1:D:606:ARG:HB2	1:D:609:ASN:O	2.08	0.53
1:A:586:TRP:CD2	1:A:964:HIS:HB2	2.43	0.53
1:A:878:LEU:HD12	1:A:881:ILE:HD11	1.90	0.53
1:A:886:THR:OG1	1:A:887:GLU:N	2.41	0.53
1:A:637:ARG:HA	1:A:663:GLU:HB3	1.91	0.52
1:A:825:MET:HE1	1:A:850:LYS:HG2	1.91	0.52
1:A:846:PHE:HA	1:A:849:ILE:HB	1.92	0.52
1:D:593:ARG:NH1	1:D:599:THR:O	2.33	0.52
1:D:586:TRP:CD2	1:D:964:HIS:HB2	2.44	0.52
1:A:663:GLU:HG2	1:A:701:ALA:HB2	1.91	0.52
1:D:557:ASP:HB2	1:D:596:MET:HG2	1.91	0.52
1:D:822:MET:SD	1:A:790:LYS:NZ	2.83	0.52
1:D:823:HIS:ND1	1:D:823:HIS:O	2.42	0.52
1:D:846:PHE:HA	1:D:849:ILE:HB	1.92	0.51
1:D:568:MET:O	1:D:568:MET:HE2	2.11	0.51
1:A:645:LEU:HD13	1:A:692:LEU:HD23	1.93	0.51
1:D:532:LEU:O	1:D:536:HIS:NE2	2.43	0.51
1:A:623:GLU:OE2	1:A:626:ARG:NH2	2.42	0.50
1:D:972:TYR:HB3	1:D:975:VAL:HB	1.92	0.50
1:A:771:MET:O	1:A:774:ILE:HG22	2.11	0.50
1:A:923:GLN:O	1:A:927:VAL:HG22	2.12	0.50
1:A:682:ILE:HG12	1:A:720:GLU:HG3	1.94	0.50
1:D:866:VAL:O	1:D:869:SER:N	2.45	0.49
1:A:845:ARG:HB2	1:A:848:GLU:HG2	1.93	0.49
1:D:929:ASP:N	1:D:929:ASP:OD1	2.45	0.49
1:A:852:MET:HG2	1:A:881:ILE:HG23	1.93	0.49
1:A:706:ALA:HB3	1:A:708:LEU:HG	1.94	0.49
1:D:943:LYS:HD2	1:D:944:VAL:H	1.78	0.48
1:A:866:VAL:O	1:A:869:SER:N	2.46	0.48
1:D:586:TRP:CE2	1:D:964:HIS:HB2	2.49	0.48
1:D:921:LYS:O	1:D:925:ILE:HG12	2.14	0.48
1:D:575:ASP:OD1	1:D:579:ARG:NH1	2.41	0.47
1:D:922:LEU:O	1:D:926:ILE:HG12	2.14	0.47
1:D:663:GLU:HG2	1:D:701:ALA:HB2	1.96	0.47
1:D:771:MET:O	1:D:774:ILE:HG22	2.13	0.47
1:A:533:ARG:HG2	1:A:573:THR:HG21	1.96	0.47
1:D:889:ASP:O	1:D:893:ARG:HB3	2.15	0.47
1:A:640:ASP:OD1	1:A:647:GLN:NE2	2.48	0.47
1:D:645:LEU:HD13	1:D:692:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LYS:HD2	1:A:944:VAL:H	1.80	0.46
1:D:600:MET:HG2	1:D:634:ASP:HB2	1.97	0.46
1:D:546:LEU:HD13	1:D:588:ARG:HG3	1.97	0.46
1:D:499:LYS:HB3	1:D:499:LYS:HE3	1.68	0.46
1:D:737:SER:O	1:A:773:SER:OG	2.32	0.46
1:A:593:ARG:NH1	1:A:599:THR:O	2.37	0.46
1:A:908:ARG:HD2	1:A:931:ALA:O	2.16	0.45
1:D:583:GLU:HB3	1:D:990:THR:HB	1.98	0.45
1:D:842:LEU:HD11	1:D:845:ARG:HH11	1.81	0.45
1:A:894:GLY:O	1:A:928:LYS:NZ	2.49	0.45
1:D:845:ARG:HD2	1:D:848:GLU:OE2	2.17	0.45
1:D:564:PHE:O	1:D:600:MET:HE2	2.17	0.45
1:A:546:LEU:HD13	1:A:588:ARG:HG3	1.98	0.45
1:D:852:MET:HG2	1:D:881:ILE:HG23	1.99	0.44
1:A:534:ASP:OD2	1:A:732:HIS:HE1	2.00	0.44
1:D:682:ILE:HG12	1:D:720:GLU:HG3	1.99	0.44
1:D:687:ASP:O	1:D:691:GLU:HG3	2.17	0.44
1:D:908:ARG:HG2	1:D:927:VAL:HG11	1.99	0.44
1:D:533:ARG:HG2	1:D:573:THR:HG21	2.00	0.44
1:D:967:ILE:HA	1:D:967:ILE:HD13	1.73	0.44
1:A:568:MET:O	1:A:568:MET:HE2	2.18	0.44
1:A:872:VAL:HG13	1:A:903:VAL:HA	1.98	0.44
1:D:706:ALA:HB3	1:D:708:LEU:HG	2.00	0.43
1:A:678:PRO:O	1:A:681:ASN:ND2	2.46	0.43
1:D:761:SER:OG	1:D:800:GLU:HB2	2.19	0.43
1:D:982:MET:HE2	1:D:982:MET:HA	2.00	0.43
1:D:774:ILE:HD12	1:D:774:ILE:HA	1.83	0.43
1:A:714:ALA:HB2	1:A:743:THR:HG23	2.01	0.42
1:A:894:GLY:HA2	1:A:897:LEU:CD1	2.44	0.42
1:D:853:TYR:CE1	1:D:865:LYS:HD2	2.55	0.42
1:A:679:LYS:HE2	1:A:915:VAL:HG13	2.02	0.42
1:A:852:MET:HE2	1:A:855:LYS:HZ2	1.84	0.42
1:A:680:TYR:OH	1:A:862:ASP:O	2.32	0.42
1:D:663:GLU:HG3	1:D:699:ILE:HB	2.00	0.42
1:D:825:MET:HE2	1:D:830:TYR:CD2	2.54	0.42
1:A:827:GLY:O	1:A:831:THR:HG23	2.20	0.42
1:A:823:HIS:O	1:A:823:HIS:CG	2.73	0.42
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.50	0.41
1:D:500:LYS:HD2	1:D:561:PRO:HG2	2.02	0.41
1:A:586:TRP:CE2	1:A:964:HIS:HB2	2.55	0.41
1:D:760:ALA:O	1:A:815:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:823:HIS:CD2	1:D:850:LYS:HD2	2.55	0.41
1:A:935:ASP:CG	1:A:940:HIS:HE2	2.28	0.41
1:A:767:SER:OG	1:A:768:GLN:N	2.54	0.41
1:A:807:ALA:N	1:A:808:PRO:HD2	2.36	0.41
1:A:845:ARG:NE	1:A:848:GLU:OE1	2.34	0.41
1:A:878:LEU:HD12	1:A:878:LEU:HA	1.91	0.41
1:A:500:LYS:HB3	1:A:500:LYS:HE3	1.80	0.41
1:A:564:PHE:O	1:A:600:MET:HE2	2.21	0.41
1:A:610:ALA:HB3	1:A:971:MET:SD	2.61	0.41
1:A:890:VAL:O	1:A:894:GLY:HA3	2.21	0.41
1:A:908:ARG:HG2	1:A:927:VAL:HG12	2.03	0.41
1:A:908:ARG:HD3	1:A:930:LYS:HB3	2.03	0.41
1:A:557:ASP:HB2	1:A:596:MET:HG2	2.02	0.40
1:D:534:ASP:OD2	1:D:732:HIS:HE1	2.04	0.40
1:D:807:ALA:N	1:D:808:PRO:HD2	2.37	0.40
1:A:709:LEU:HG	1:A:714:ALA:HB2	2.04	0.40
1:D:714:ALA:HB2	1:D:743:THR:HG23	2.04	0.40
1:A:568:MET:SD	1:A:569:TRP:HB2	2.62	0.40
1:D:552:ILE:HB	1:D:798:TYR:CE1	2.56	0.40
1:D:859:MET:SD	1:D:887:GLU:HG3	2.62	0.40
1:A:967:ILE:HD13	1:A:967:ILE:HA	1.73	0.40
1:D:790:LYS:NZ	1:A:822:MET:SD	2.95	0.40
1:A:608:SER:HB2	1:A:615:ASN:ND2	2.37	0.40
1:A:618:ASP:O	1:A:622:GLU:HG3	2.22	0.40
1:A:708:LEU:HD11	1:A:824:GLU:HB3	2.04	0.40

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	505/1143 (44%)	489 (97%)	16 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	506/1143 (44%)	492 (97%)	14 (3%)	0	100	100
All	All	1011/2286 (44%)	981 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/954 (45%)	417 (97%)	13 (3%)	36	38
1	D	431/954 (45%)	414 (96%)	17 (4%)	28	28
All	All	861/1908 (45%)	831 (96%)	30 (4%)	32	32

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	494	LEU
1	D	500	LYS
1	D	569	TRP
1	D	609	ASN
1	D	705	MET
1	D	736	THR
1	D	757	VAL
1	D	770	SER
1	D	814	THR
1	D	825	MET
1	D	849	ILE
1	D	883	ASN
1	D	886	THR
1	D	928	LYS
1	D	934	THR
1	D	948	THR
1	D	967	ILE
1	A	542	THR

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Mol	Chain	Res	Type
1	A	569	TRP
1	A	609	ASN
1	A	705	MET
1	A	770	SER
1	A	849	ILE
1	A	886	THR
1	A	915	VAL
1	A	934	THR
1	A	948	THR
1	A	955	GLN
1	A	967	ILE
1	A	993	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	496	ASN
1	D	615	ASN
1	D	653	GLN
1	D	780	HIS
1	D	836	GLN
1	D	940	HIS
1	D	955	GLN
1	A	836	GLN
1	A	882	GLN
1	A	895	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	703	1,3	10,11,12	0.89	0	6,12,14	1.53	1 (16%)
1	KCX	D	703	1,3	10,11,12	0.86	0	6,12,14	1.37	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	1,3	-	0/9/10/12	-
1	KCX	D	703	1,3	-	0/9/10/12	-

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	A	703	KCX	OQ1-CX-NZ	-3.26	119.96	124.92
1	D	703	KCX	OQ1-CX-NZ	-2.99	120.37	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 6 ligands modelled in this entry, 4 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
4	PYR	D	1203	-	5,5,5	2.98	3 (60%)	3,6,6	1.76	1 (33%)
4	PYR	A	1203	-	5,5,5	3.02	3 (60%)	3,6,6	1.63	1 (33%)

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
4	PYR	D	1203	-	-	1/4/4/4	-
4	PYR	A	1203	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	PYR	CA-C	-4.53	1.39	1.54
4	D	1203	PYR	CA-C	-4.41	1.39	1.54
4	A	1203	PYR	O3-CA	3.59	1.31	1.23
4	D	1203	PYR	O3-CA	3.54	1.31	1.23
4	D	1203	PYR	O-C	3.52	1.31	1.22
4	A	1203	PYR	O-C	3.49	1.31	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1203	PYR	OXT-C-CA	2.49	120.49	113.59
4	A	1203	PYR	OXT-C-CA	2.29	119.95	113.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1203	PYR	OXT-C-CA-CB
4	A	1203	PYR	O-C-CA-CB
4	A	1203	PYR	OXT-C-CA-CB
4	A	1203	PYR	OXT-C-CA-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

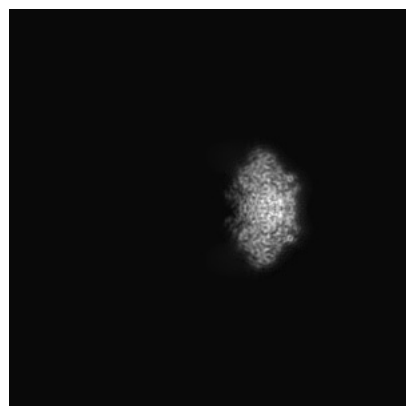
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15036. These allow visual inspection of the internal detail of the map and identification of artifacts.

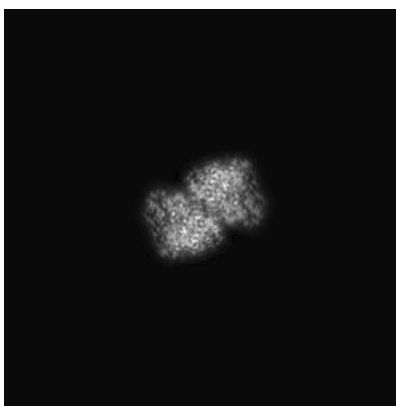
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

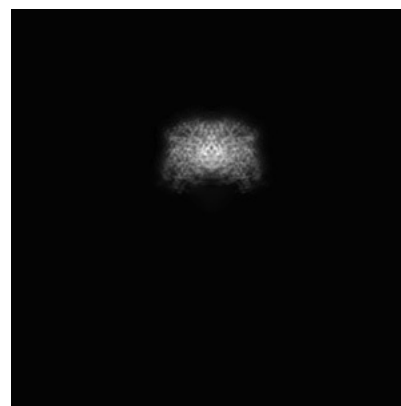
6.1.1 Primary map



X

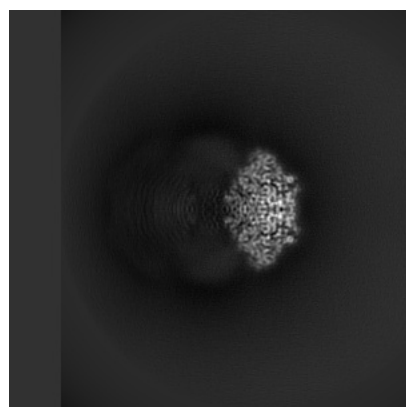


Y

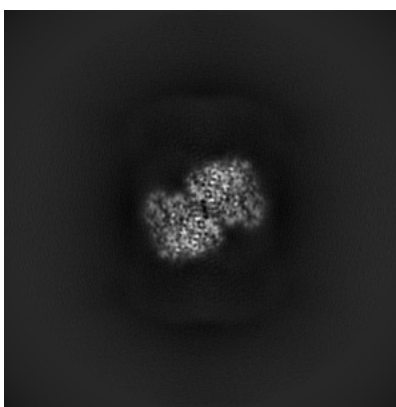


Z

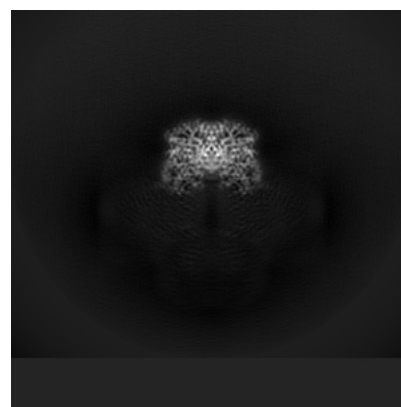
6.1.2 Raw map



X



Y

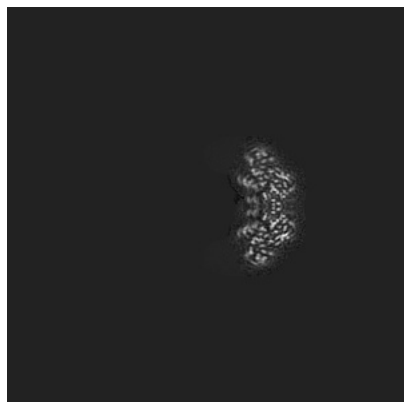


Z

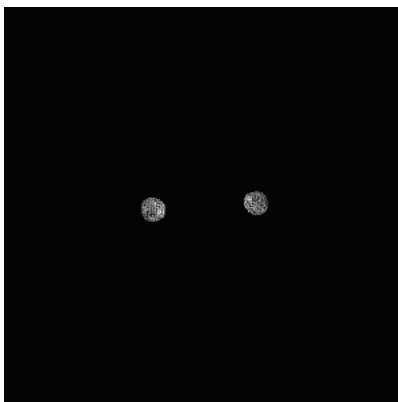
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

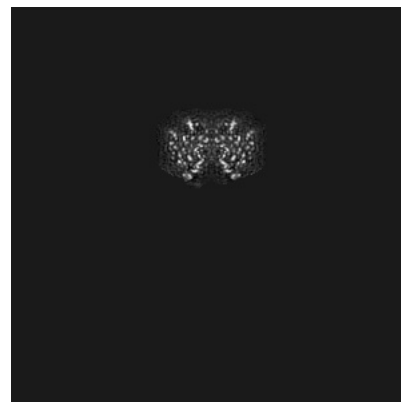
6.2.1 Primary map



X Index: 150

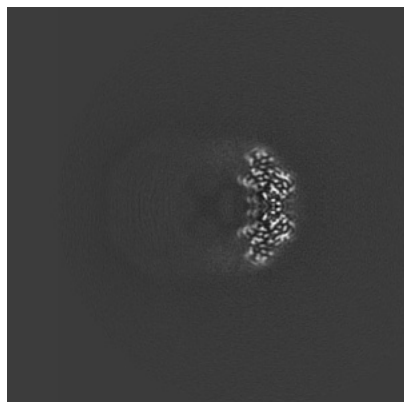


Y Index: 150

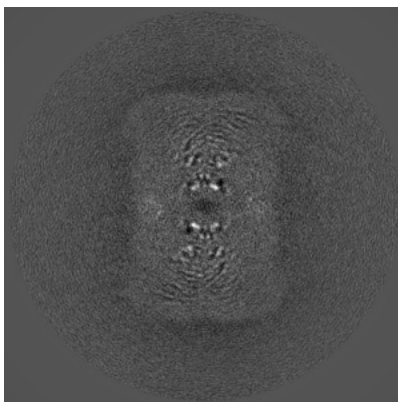


Z Index: 150

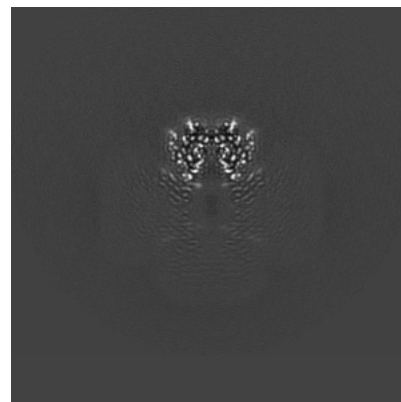
6.2.2 Raw map



X Index: 150



Y Index: 150

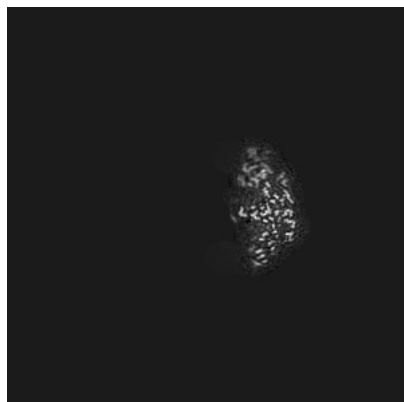


Z Index: 150

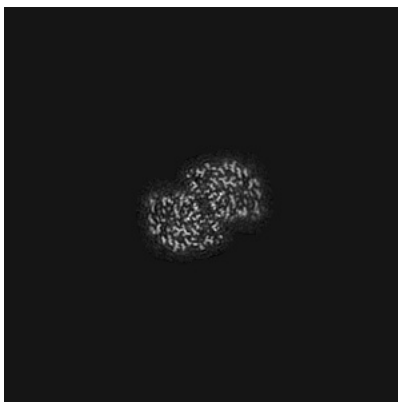
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 143

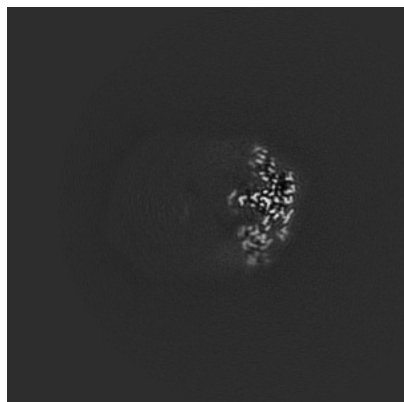


Y Index: 194

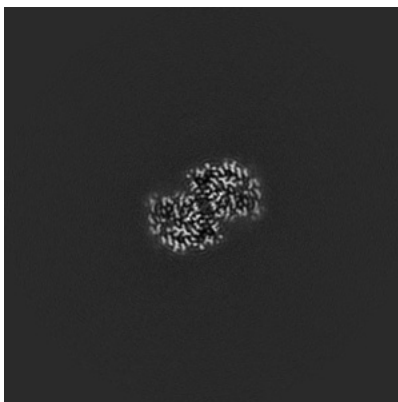


Z Index: 144

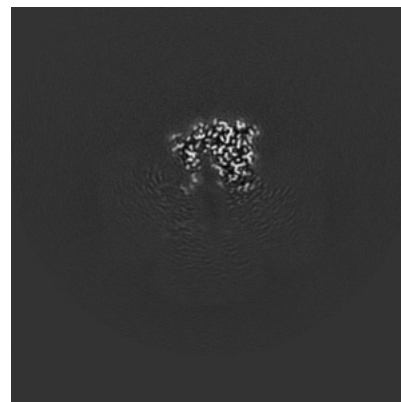
6.3.2 Raw map



X Index: 157



Y Index: 194

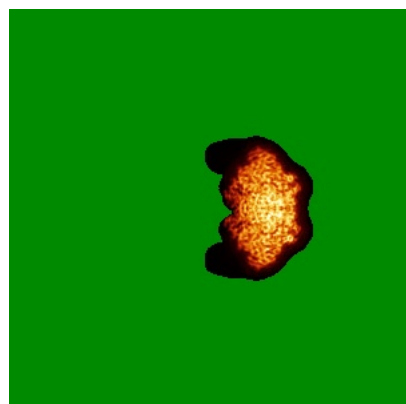


Z Index: 156

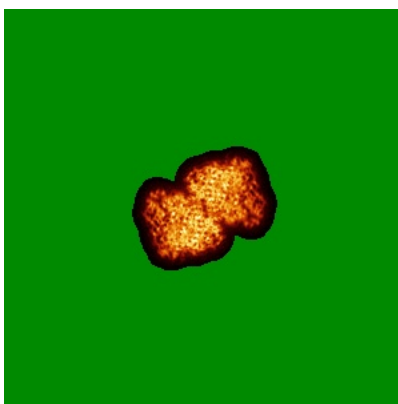
The images above show the largest variance slices of the map in three orthogonal directions.

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

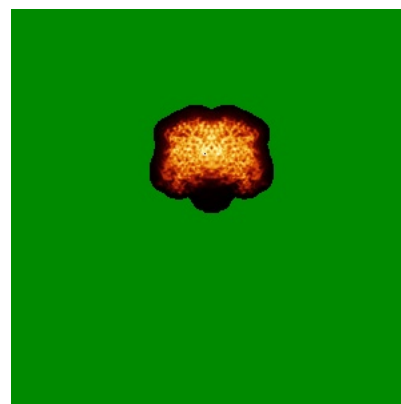
6.4.1 Primary map



X

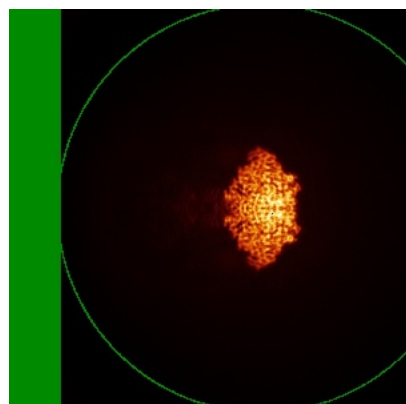


Y

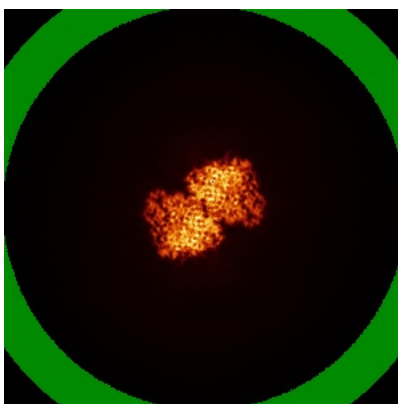


Z

6.4.2 Raw map



X



Y

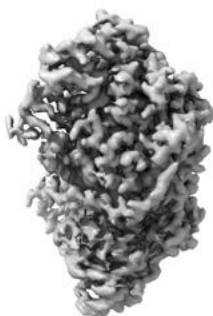


Z

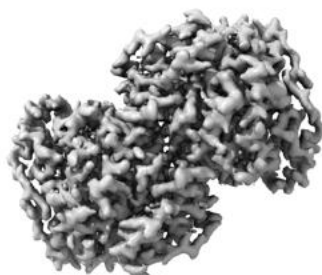
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

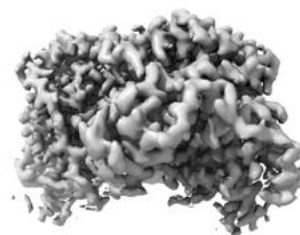
6.5.1 Primary map



X



Y



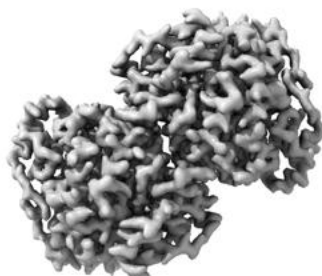
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

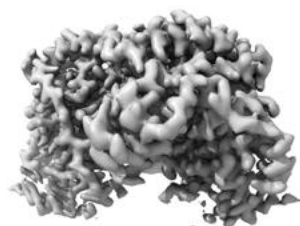
6.5.2 Raw map



X



Y



Z

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

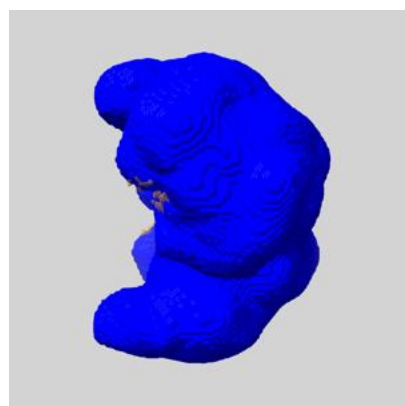
6.6 Mask visualisation [i](#)

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

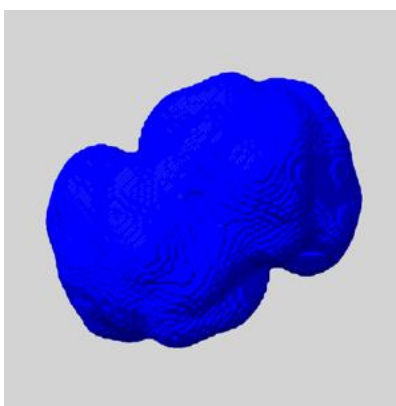
A mask typically either:

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

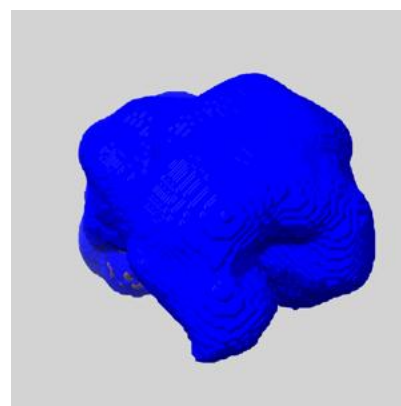
6.6.1 emd_15036_msk_1.map [i](#)



X



Y

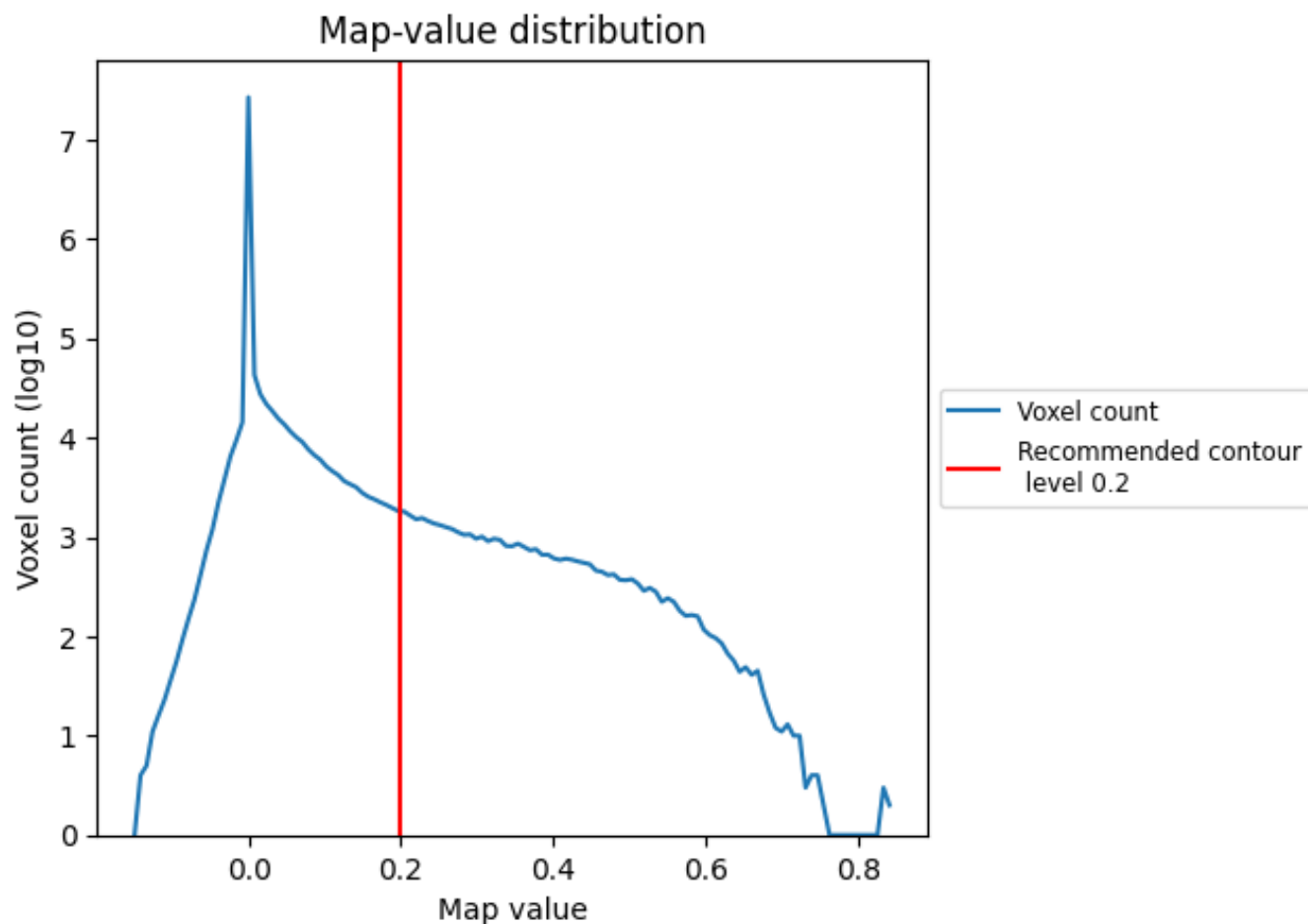


Z

7 Map analysis [i](#)

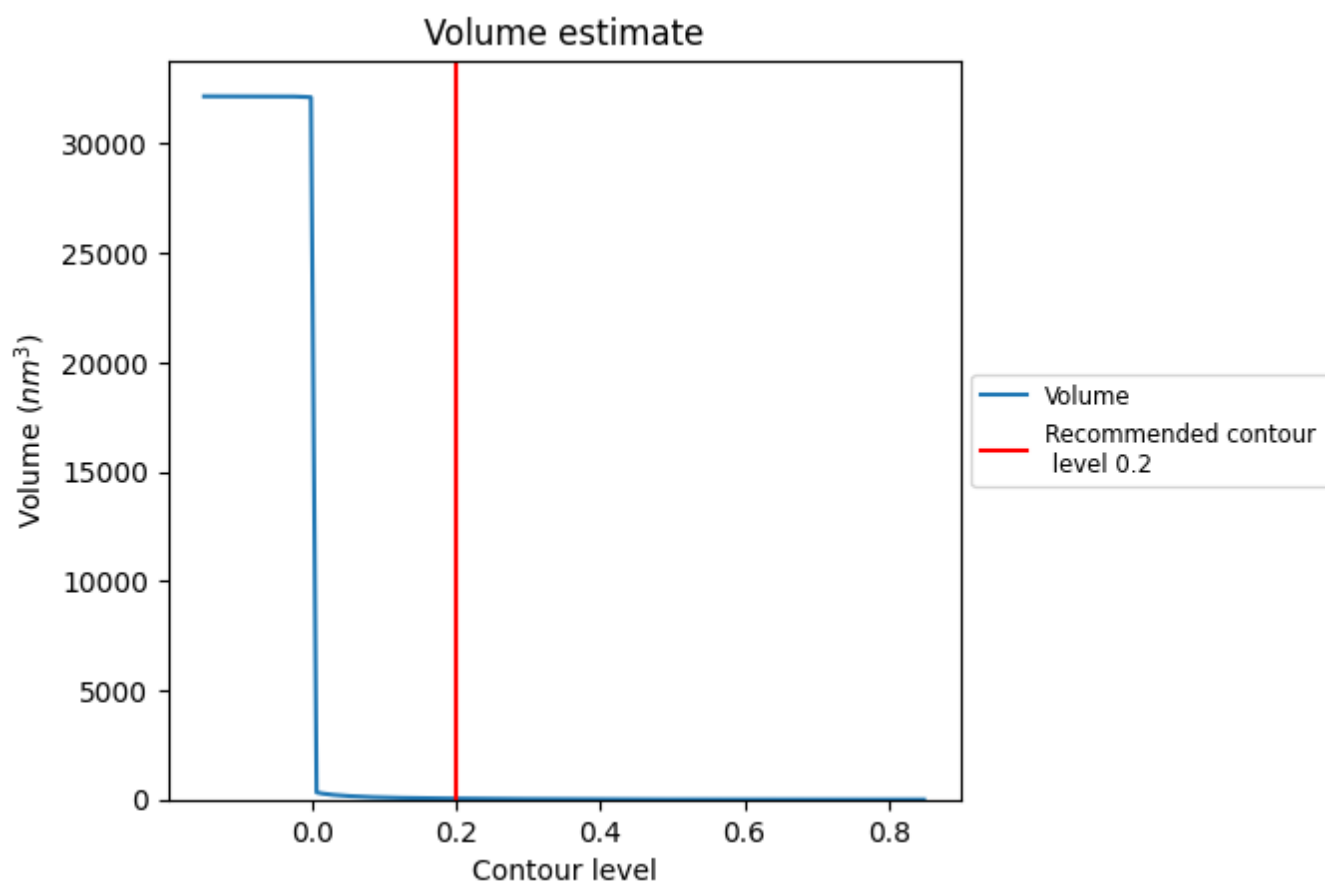
This section contains the results of statistical analysis of the map.

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.

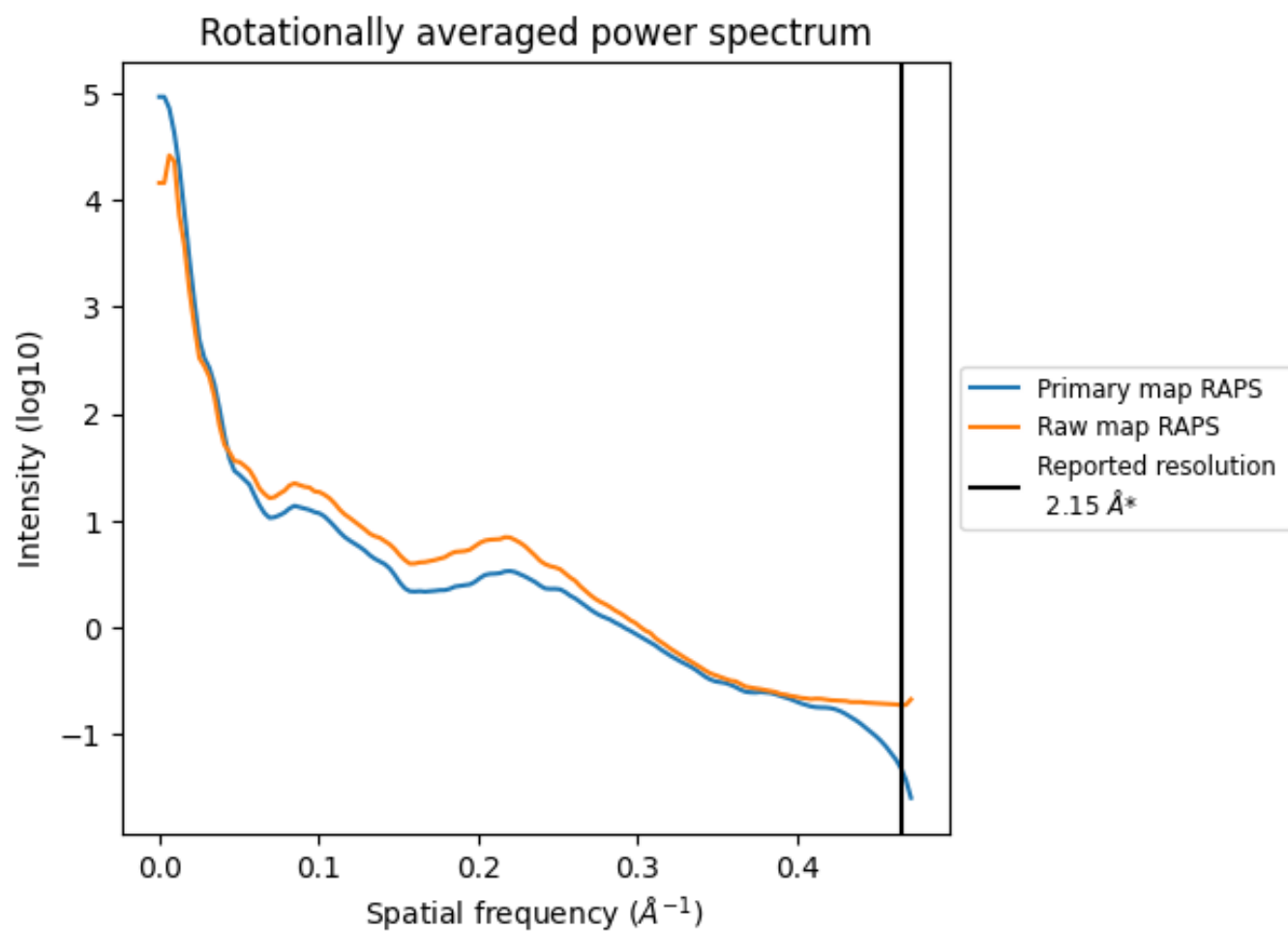
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 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 ⓘ

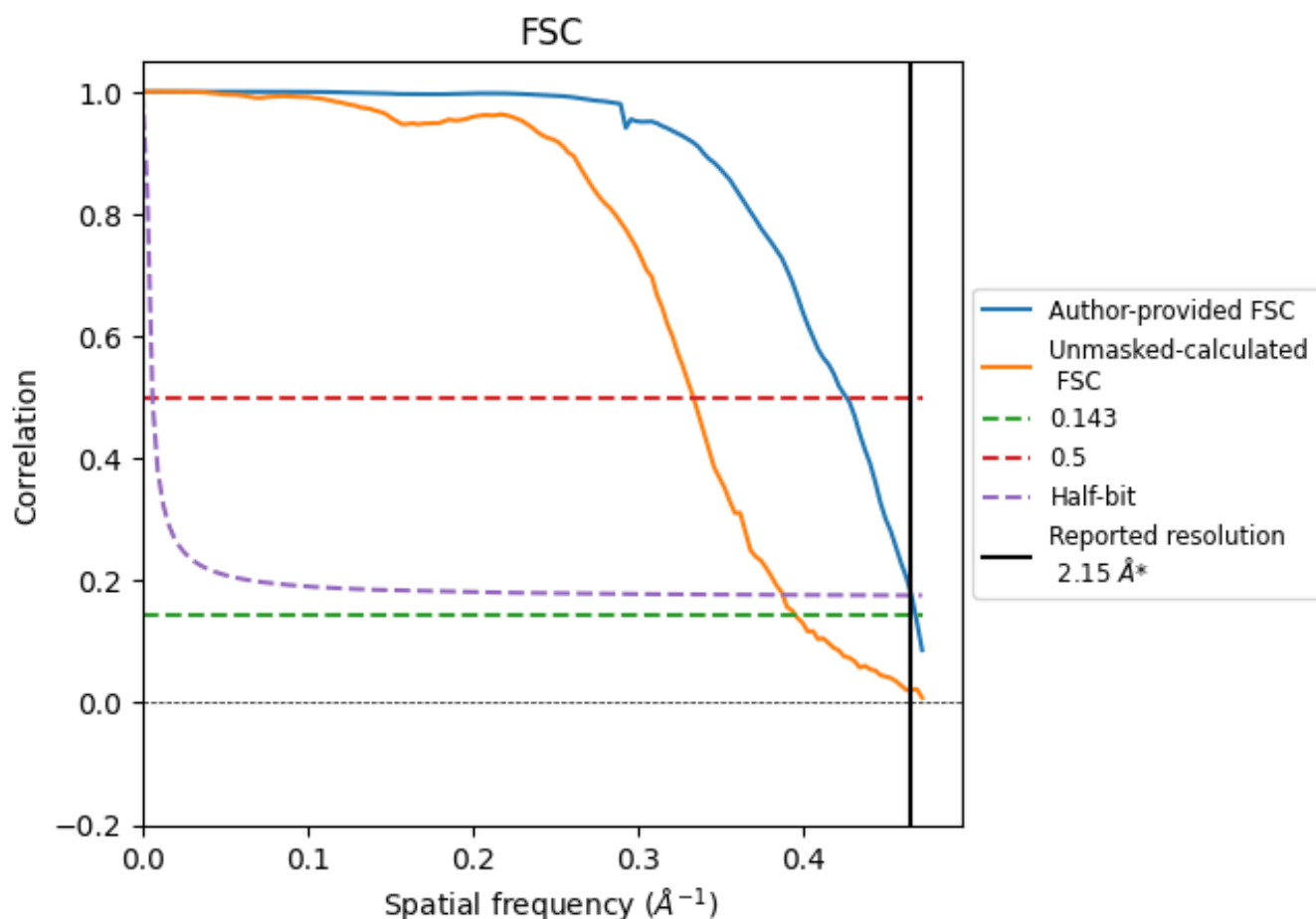


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 Å⁻¹

8.2 Resolution estimates [i](#)

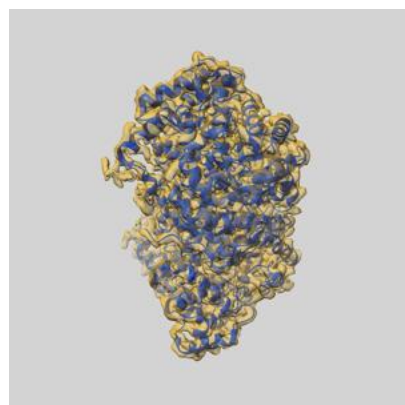
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.14	2.35	2.15
Unmasked-calculated*	2.53	3.00	2.58

*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 2.53 differs from the reported value 2.15 by more than 10 %

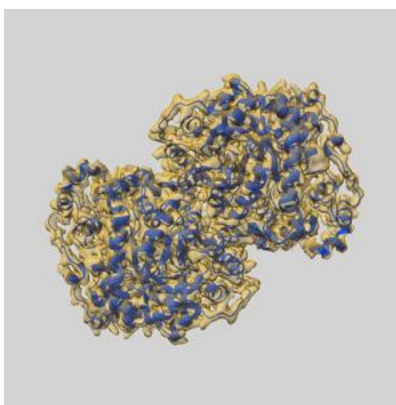
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15036 and PDB model 7ZZ6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

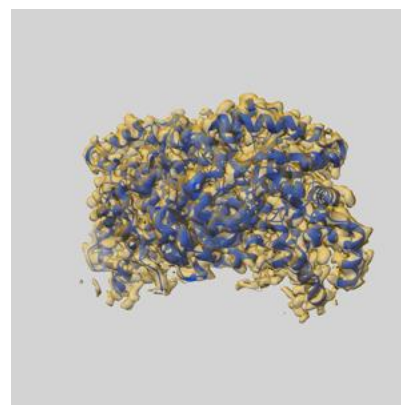
9.1 Map-model overlay [i](#)



X



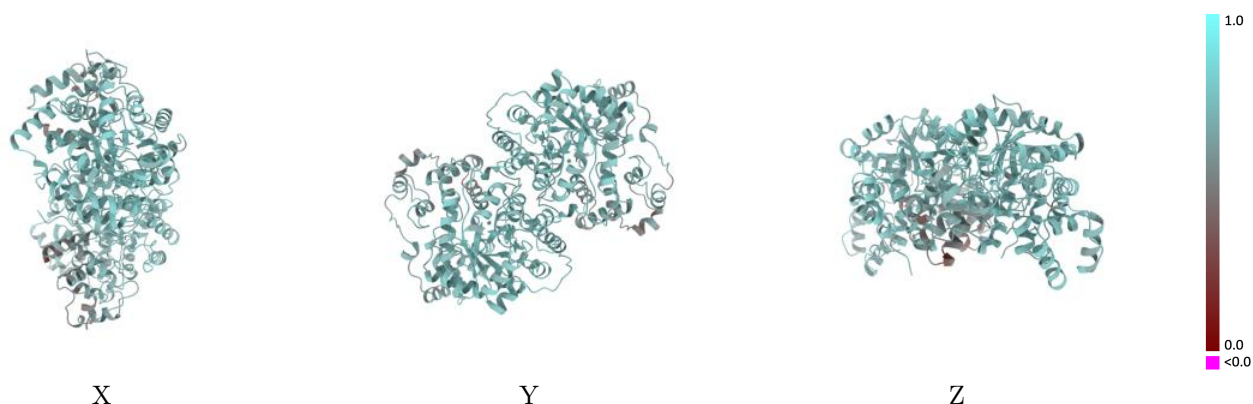
Y



Z

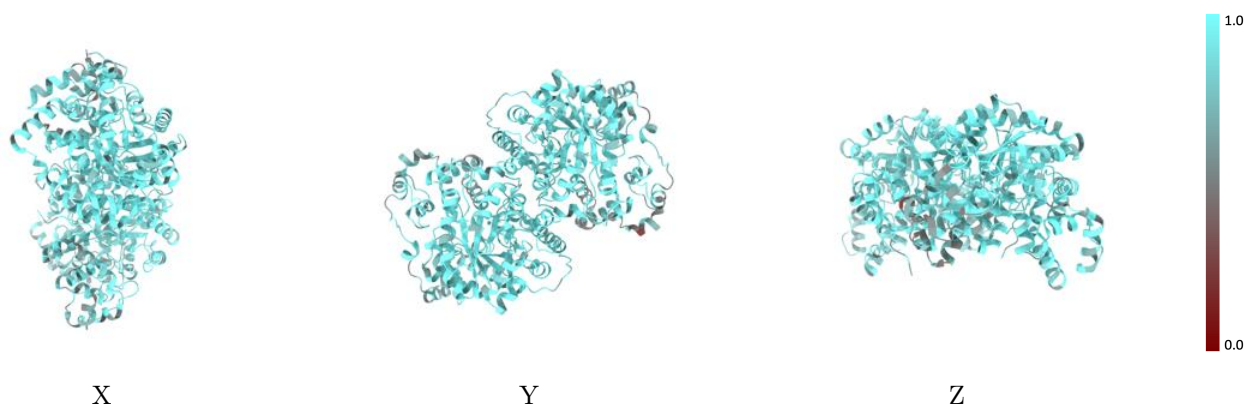
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



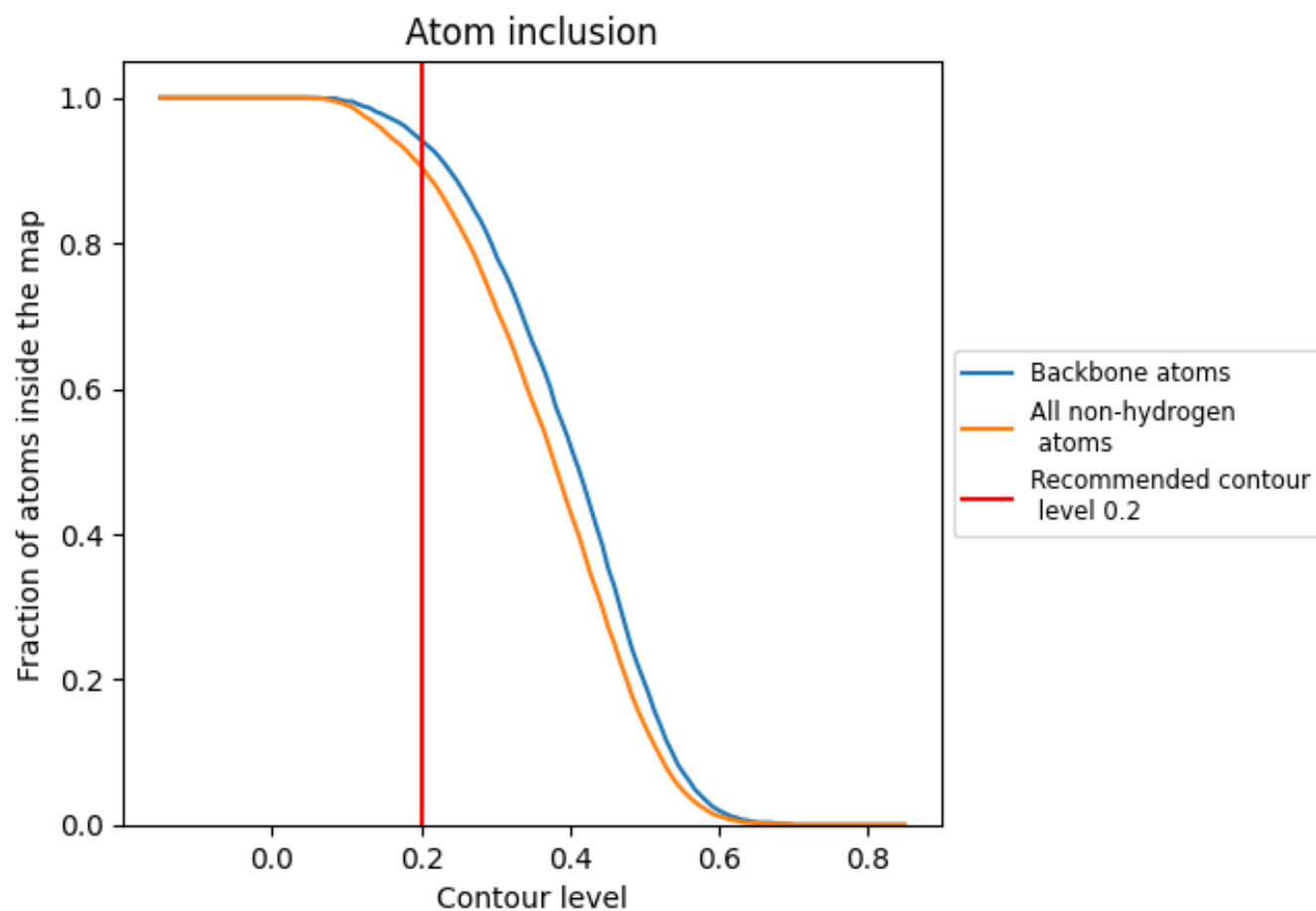
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.6760
A	0.9010	0.6730
D	0.9150	0.6780

