



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:09 PM UTC

PDB ID : 9CTM / pdb_00009ctm
EMDB ID : EMD-45911
Title : Condensing region of EcPKS2 - acetylated dataset
Authors : Schubert, H.L.; Hill, C.P.
Deposited on : 2024-07-25
Resolution : 2.92 Å(reported)
Based on initial model : .

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

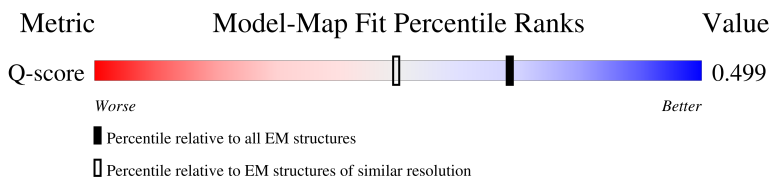
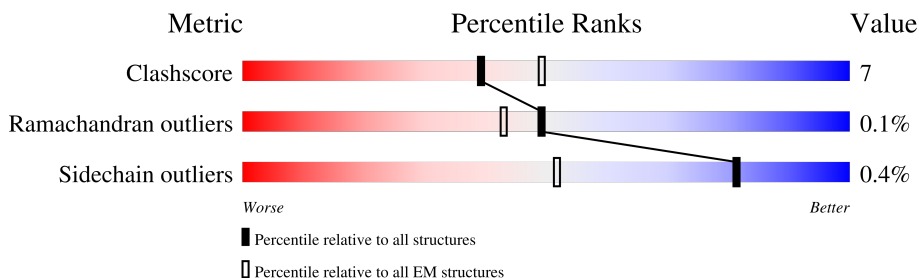
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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	2287	
1	B	2287	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26266 atoms, of which 13032 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 Polyketide synthase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	862	Total	C	H	N	O	S	0	0
			13133	4180	6516	1121	1267	49		
1	B	862	Total	C	H	N	O	S	0	0
			13133	4180	6516	1121	1267	49		

- Molecule 1: Polyketide synthase 2



S188	T189	D195	R199	I210	L225	M229	T236	D241	E242	S243	G250	E251	V267	T300	C334	D343	I347	I350	K351	H356	S361	K366	S369	I370	M373	R376	N388	I391	D396	L399	D409	I413	T422					
ALA	GLI	GLI	ALA	SER	SER	GLM	GLM	ASP	ASP	ALA	P16	P17	K18	A31	L35	E41	N51	M58	V59	R64	R65	M104	L105	V117	V137	S138	M139	D143	T144	M147	K148	D152	D153	V158	H163	Y166	T185	A186



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106739	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.148	Depositor
Minimum map value	-1.278	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.266	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: SCY

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	0.10	0/6755	0.25	0/9152
1	B	0.11	0/6755	0.29	0/9152
All	All	0.10	0/13510	0.27	0/18304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6617	6516	6515	87	0
1	B	6617	6516	6516	108	0
All	All	13234	13032	13031	189	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 7.

All (189) 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:573:ILE:HB	1:B:635:ILE:HD11	1.62	0.82
1:A:589:ASP:OD2	1:A:620:ARG:NH2	2.15	0.80
1:B:195:ASP:OD1	1:B:199:ARG:NH1	2.19	0.76
1:B:330:THR:HG21	1:B:391:ILE:HG23	1.69	0.75
1:A:195:ASP:OD1	1:A:199:ARG:NH1	2.20	0.74
1:A:330:THR:HG21	1:A:391:ILE:HG23	1.72	0.71
1:A:292:GLU:OE1	1:B:18:LYS:NZ	2.23	0.70
1:A:144:THR:OG1	1:B:144:THR:OG1	2.08	0.68
1:A:685:PHE:CE2	1:A:689:LEU:HD11	2.31	0.65
1:A:484:THR:O	1:A:492:ARG:NH1	2.30	0.65
1:A:770:GLU:N	1:A:770:GLU:OE1	2.31	0.64
1:B:484:THR:O	1:B:492:ARG:NH1	2.31	0.63
1:A:649:LEU:HD22	1:A:694:VAL:HG11	1.80	0.63
1:A:649:LEU:CD2	1:A:694:VAL:HG11	2.29	0.62
1:A:368:LYS:O	1:A:372:THR:HG23	2.00	0.61
1:B:770:GLU:N	1:B:770:GLU:OE1	2.33	0.61
1:B:535:MET:HE1	1:B:544:ILE:HG21	1.82	0.61
1:B:635:ILE:O	1:B:635:ILE:HG22	2.01	0.60
1:B:648:GLU:HB2	1:B:695:THR:HG22	1.83	0.60
1:A:685:PHE:CZ	1:A:689:LEU:HD11	2.36	0.60
1:B:675:ILE:HD12	1:B:675:ILE:O	2.02	0.60
1:A:225:LEU:HD21	1:B:158:VAL:HG13	1.83	0.60
1:B:682:MET:HE3	1:B:686:MET:SD	2.42	0.59
1:A:351:LYS:NZ	1:A:361:SER:OG	2.35	0.59
1:B:376:ARG:NH2	1:B:409:ASP:O	2.34	0.59
1:A:235:SER:OG	1:A:236:THR:N	2.36	0.58
1:B:558:LEU:HD11	1:B:582:ALA:HB2	1.84	0.58
1:B:675:ILE:CD1	1:B:682:MET:HE1	2.33	0.58
1:B:185:THR:HG22	1:B:423:THR:HG21	1.85	0.58
1:A:639:VAL:CG1	1:A:704:ILE:HD12	2.34	0.57
1:B:819:PHE:CZ	1:B:823:LEU:HD11	2.39	0.57
1:A:376:ARG:NH2	1:A:409:ASP:O	2.36	0.57
1:A:674:THR:O	1:A:674:THR:HG22	2.03	0.57
1:A:31:ALA:HB1	1:A:267:VAL:HG13	1.86	0.57
1:B:581:ASN:HD21	1:B:606:LEU:HD11	1.68	0.57
1:A:203:MET:HE2	1:A:205:VAL:HG22	1.85	0.57
1:A:453:ARG:NH1	1:A:488:SER:O	2.37	0.57
1:A:210:ILE:HG22	1:A:210:ILE:O	2.05	0.56
1:B:210:ILE:HG22	1:B:210:ILE:O	2.06	0.56
1:B:330:THR:HG23	1:B:399:LEU:CD1	2.36	0.56
1:B:31:ALA:HB1	1:B:267:VAL:HG13	1.87	0.55
1:B:65:ARG:NH2	1:B:251:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:HG21	1:B:236:THR:HG22	1.88	0.55
1:B:645:ALA:HB3	1:B:675:ILE:HD11	1.88	0.55
1:B:695:THR:O	1:B:695:THR:HG23	2.07	0.54
1:B:373:MET:HE3	1:B:413:ILE:HD12	1.88	0.54
1:B:703:ASN:OD1	1:B:703:ASN:O	2.24	0.54
1:B:643:LYS:C	1:B:682:MET:HE2	2.31	0.54
1:A:372:THR:HG22	1:A:379:PRO:HD3	1.90	0.54
1:A:761:ASN:OD1	1:A:762:LEU:N	2.41	0.54
1:A:372:THR:HG22	1:A:379:PRO:CD	2.38	0.54
1:B:139:ASN:O	1:B:163:HIS:NE2	2.39	0.53
1:A:535:MET:HE1	1:A:544:ILE:HG21	1.90	0.53
1:B:594:MET:HE1	1:B:823:LEU:HD13	1.90	0.53
1:A:59:VAL:HG21	1:A:236:THR:HG22	1.91	0.53
1:A:147:MET:HE2	1:B:225:LEU:HD13	1.91	0.52
1:A:669:SER:HB2	1:A:793:VAL:HG13	1.91	0.52
1:A:250:GLY:N	1:A:356:HIS:O	2.42	0.52
1:A:191:LEU:HD12	1:A:417:SER:HB2	1.92	0.52
1:B:650:THR:OG1	1:B:653:GLU:OE1	2.25	0.52
1:B:532:ARG:NH2	1:B:563:MET:O	2.43	0.52
1:B:117:VAL:HG11	1:B:857:VAL:HG21	1.92	0.52
1:B:581:ASN:ND2	1:B:627:ALA:HB1	2.25	0.52
1:A:89:GLU:OE2	1:A:89:GLU:N	2.36	0.52
1:A:191:LEU:HD12	1:A:417:SER:CB	2.40	0.52
1:A:350:ILE:HD12	1:A:368:LYS:HB2	1.92	0.51
1:A:117:VAL:HG11	1:A:857:VAL:HG21	1.92	0.51
1:A:148:LYS:NZ	1:A:876:GLU:O	2.43	0.51
1:A:855:SER:O	1:A:859:GLU:HG2	2.11	0.51
1:B:241:ASP:OD2	1:B:243:SER:OG	2.29	0.51
1:A:649:LEU:HD12	1:A:653:GLU:HB3	1.93	0.51
1:A:803:THR:HG21	1:A:829:HIS:CD2	2.45	0.51
1:B:153:ASP:C	1:B:153:ASP:OD1	2.53	0.51
1:B:573:ILE:HD12	1:B:635:ILE:HG12	1.92	0.51
1:A:798:LEU:HD12	1:A:804:ILE:HD11	1.93	0.51
1:A:241:ASP:OD2	1:A:243:SER:OG	2.29	0.51
1:A:521:SER:O	1:A:584:GLN:NE2	2.43	0.50
1:B:105:LEU:HD13	1:B:166:TYR:HA	1.93	0.50
1:B:761:ASN:OD1	1:B:762:LEU:N	2.45	0.50
1:B:638:GLU:OE1	1:B:638:GLU:N	2.42	0.50
1:B:819:PHE:CE2	1:B:823:LEU:HD11	2.46	0.50
1:A:594:MET:HG3	1:A:838:LEU:HD21	1.93	0.50
1:A:187:SCY:HE2	1:A:187:SCY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG13	1:B:225:LEU:HD21	1.94	0.50
1:B:343:ASP:N	1:B:343:ASP:OD1	2.44	0.49
1:B:148:LYS:NZ	1:B:876:GLU:O	2.45	0.49
1:A:277:ASN:OD1	1:A:277:ASN:C	2.55	0.49
1:B:581:ASN:O	1:B:585:LEU:HG	2.13	0.49
1:B:350:ILE:HD12	1:B:368:LYS:HB2	1.94	0.49
1:B:441:ALA:O	1:B:442:SER:OG	2.11	0.49
1:A:639:VAL:HG13	1:A:704:ILE:HD12	1.95	0.49
1:B:740:ILE:O	1:B:745:TRP:NE1	2.44	0.49
1:A:343:ASP:OD1	1:A:343:ASP:N	2.43	0.48
1:B:669:SER:HB3	1:B:793:VAL:HG13	1.95	0.48
1:B:250:GLY:N	1:B:356:HIS:O	2.46	0.48
1:B:675:ILE:HD12	1:B:682:MET:HE1	1.93	0.48
1:A:639:VAL:HG11	1:A:704:ILE:HD12	1.96	0.48
1:B:351:LYS:NZ	1:B:361:SER:OG	2.37	0.48
1:A:662:VAL:HG12	1:A:675:ILE:HD11	1.96	0.47
1:B:186:ALA:O	1:B:189:THR:OG1	2.23	0.47
1:B:574:MET:HB3	1:B:575:PRO:HD3	1.96	0.47
1:B:330:THR:O	1:B:334:CYS:SG	2.66	0.47
1:B:388:ASN:HB3	1:B:391:ILE:HD12	1.96	0.47
1:B:551:LEU:HD22	1:B:624:ILE:HD11	1.95	0.47
1:A:225:LEU:C	1:A:225:LEU:HD23	2.40	0.47
1:A:650:THR:HG22	1:A:651:TRP:N	2.30	0.47
1:B:443:ASP:N	1:B:443:ASP:OD1	2.47	0.47
1:B:559:MET:O	1:B:559:MET:HE3	2.14	0.47
1:B:740:ILE:HG22	1:B:744:ARG:HB2	1.97	0.47
1:B:686:MET:HB3	1:B:696:VAL:HG11	1.97	0.46
1:B:675:ILE:HD12	1:B:675:ILE:C	2.40	0.46
1:A:647:VAL:HG12	1:A:696:VAL:HG13	1.96	0.46
1:B:187:SCY:O	1:B:188:SER:CB	2.64	0.46
1:B:551:LEU:HD13	1:B:624:ILE:HG13	1.98	0.46
1:B:794:ILE:O	1:B:798:LEU:HD22	2.15	0.46
1:B:347:ILE:CG2	1:B:399:LEU:HD22	2.46	0.45
1:A:590:LEU:CD2	1:A:838:LEU:HD22	2.47	0.45
1:B:104:MET:HE1	1:B:137:VAL:HG23	1.98	0.45
1:B:396:ASP:OD2	1:B:396:ASP:N	2.49	0.45
1:A:675:ILE:HG12	1:A:685:PHE:HE2	1.81	0.45
1:A:342:LYS:HD2	1:A:342:LYS:H	1.82	0.45
1:A:458:LEU:HD23	1:A:506:ILE:HG23	1.98	0.45
1:B:505:GLU:OE2	1:B:507:GLN:NE2	2.50	0.45
1:A:699:VAL:O	1:A:699:VAL:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:TRP:CZ3	1:B:664:ALA:HB1	2.52	0.44
1:A:155:ALA:HB1	1:B:229:MET:HG2	2.00	0.44
1:B:41:GLU:OE2	1:B:64:ARG:NH2	2.49	0.44
1:B:423:THR:O	1:B:423:THR:HG23	2.16	0.44
1:B:668:ASN:HB3	1:B:793:VAL:HG11	1.99	0.44
1:B:685:PHE:CZ	1:B:689:LEU:HD11	2.53	0.44
1:A:105:LEU:HD13	1:A:166:TYR:HA	1.99	0.44
1:A:647:VAL:CG1	1:A:696:VAL:HG13	2.48	0.44
1:A:436:ALA:N	1:A:847:SER:OG	2.51	0.44
1:A:645:ALA:CB	1:A:686:MET:SD	3.06	0.44
1:B:647:VAL:HG12	1:B:696:VAL:HG13	1.99	0.44
1:B:152:ASP:O	1:B:153:ASP:CG	2.62	0.43
1:A:41:GLU:OE2	1:A:64:ARG:NH2	2.51	0.43
1:A:605:SER:O	1:A:606:LEU:HB3	2.18	0.43
1:A:699:VAL:O	1:A:699:VAL:CG1	2.67	0.43
1:B:558:LEU:HD11	1:B:582:ALA:CB	2.47	0.43
1:B:649:LEU:HB2	1:B:654:ALA:HB2	1.99	0.43
1:B:689:LEU:O	1:B:692:GLN:O	2.37	0.43
1:A:455:GLU:HG3	1:A:506:ILE:HG21	2.01	0.43
1:A:647:VAL:CG1	1:A:689:LEU:HD13	2.49	0.43
1:A:663:VAL:O	1:A:675:ILE:HD12	2.19	0.43
1:B:794:ILE:HG23	1:B:798:LEU:CD2	2.49	0.43
1:B:436:ALA:N	1:B:847:SER:OG	2.52	0.43
1:B:594:MET:CG	1:B:838:LEU:HD21	2.49	0.43
1:B:649:LEU:HD11	1:B:689:LEU:HD21	2.00	0.43
1:B:369:VAL:O	1:B:373:MET:N	2.52	0.42
1:A:198:GLU:OE1	1:A:199:ARG:NH2	2.52	0.42
1:B:590:LEU:CD2	1:B:838:LEU:HD22	2.49	0.42
1:B:635:ILE:O	1:B:635:ILE:CG2	2.67	0.42
1:A:703:ASN:O	1:A:704:ILE:HD13	2.20	0.42
1:A:831:VAL:HG23	1:A:831:VAL:O	2.18	0.42
1:A:594:MET:HE1	1:A:823:LEU:HD13	2.01	0.42
1:A:663:VAL:C	1:A:675:ILE:HD12	2.45	0.42
1:A:594:MET:HE3	1:A:835:PRO:HA	2.01	0.42
1:A:682:MET:O	1:A:686:MET:HE2	2.19	0.42
1:B:559:MET:HE3	1:B:559:MET:C	2.45	0.42
1:A:577:PHE:CD2	1:A:606:LEU:HD22	2.55	0.42
1:B:458:LEU:HD23	1:B:506:ILE:HG23	2.02	0.42
1:A:748:PRO:O	1:A:751:GLN:HG2	2.20	0.41
1:B:649:LEU:HB3	1:B:653:GLU:HB3	2.02	0.41
1:A:646:ALA:HA	1:A:673:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:VAL:HG12	1:B:664:ALA:H	1.85	0.41
1:B:644:MET:HA	1:B:675:ILE:O	2.20	0.41
1:B:594:MET:O	1:B:834:ASN:N	2.52	0.41
1:A:758:GLN:N	1:A:758:GLN:OE1	2.53	0.41
1:B:594:MET:SD	1:B:823:LEU:HD13	2.61	0.41
1:A:298:MET:HA	1:A:301:ILE:HG22	2.02	0.41
1:B:143:ASP:O	1:B:147:MET:HG2	2.21	0.41
1:B:605:SER:O	1:B:606:LEU:HB3	2.20	0.41
1:A:373:MET:HE2	1:A:431:SER:HA	2.03	0.41
1:A:651:TRP:CZ3	1:A:664:ALA:HB1	2.56	0.41
1:A:713:GLU:HB3	1:A:714:PRO:HD3	2.03	0.41
1:B:35:LEU:HD22	1:B:370:ILE:HG21	2.03	0.41
1:B:535:MET:SD	1:B:563:MET:HE1	2.61	0.41
1:B:682:MET:O	1:B:683:THR:C	2.63	0.41
1:A:558:LEU:HD21	1:A:582:ALA:CB	2.51	0.41
1:B:713:GLU:HB3	1:B:714:PRO:HD3	2.02	0.41
1:B:794:ILE:HG23	1:B:798:LEU:HD21	2.02	0.41
1:A:647:VAL:HG11	1:A:689:LEU:HD13	2.04	0.40
1:B:552:SER:N	1:B:553:PRO:HD2	2.37	0.40
1:A:649:LEU:HD12	1:A:653:GLU:CB	2.51	0.40
1:B:51:ASN:CB	1:B:58:MET:HE3	2.51	0.40
1:B:824:GLY:O	1:B:828:SER:OG	2.36	0.40
1:B:831:VAL:O	1:B:831:VAL:HG23	2.21	0.40
1:B:577:PHE:O	1:B:581:ASN:ND2	2.55	0.40

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	859/2287 (38%)	829 (96%)	29 (3%)	1 (0%)	48 76

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	859/2287 (38%)	826 (96%)	33 (4%)	0	100	100
All	All	1718/4574 (38%)	1655 (96%)	62 (4%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA

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	718/1929 (37%)	717 (100%)	1 (0%)	88	97
1	B	718/1929 (37%)	713 (99%)	5 (1%)	76	91
All	All	1436/3858 (37%)	1430 (100%)	6 (0%)	81	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	695	THR
1	B	153	ASP
1	B	225	LEU
1	B	373	MET
1	B	637	CYS
1	B	663	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	498	ASN
1	A	829	HIS
1	B	364	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	498	ASN
1	B	581	ASN
1	B	758	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SCY	A	187	1	7,8,9	0.85	0	4,9,11	0.69	0
1	SCY	B	187	1	7,8,9	0.90	0	4,9,11	0.74	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
1	SCY	A	187	1	-	2/5/7/9	-
1	SCY	B	187	1	-	4/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	187	SCY	OCD-CD-SG-CB
1	A	187	SCY	CE-CD-SG-CB
1	B	187	SCY	N-CA-CB-SG
1	B	187	SCY	C-CA-CB-SG
1	B	187	SCY	OCD-CD-SG-CB
1	B	187	SCY	CE-CD-SG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	187	SCY	1	0
1	B	187	SCY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

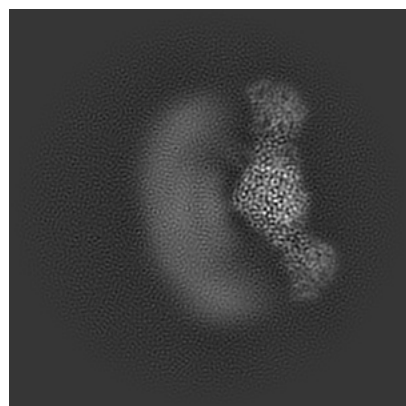
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45911. These allow visual inspection of the internal detail of the map and identification of artifacts.

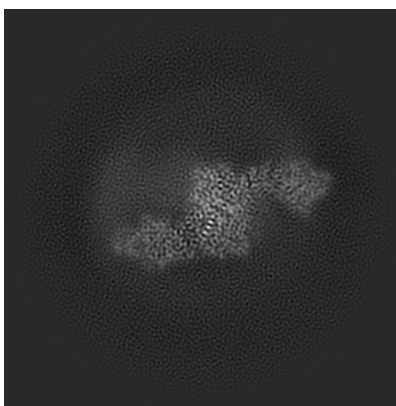
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

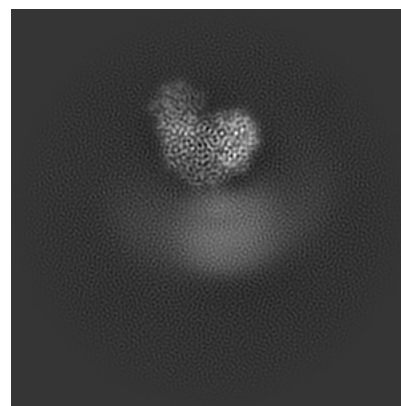
6.1.1 Primary map



X

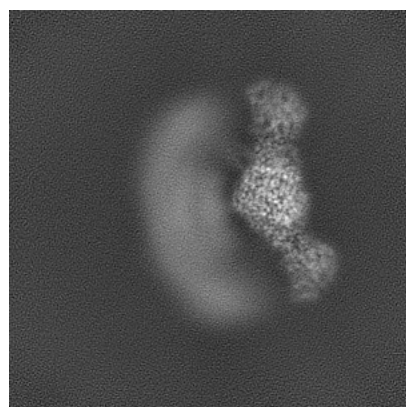


Y

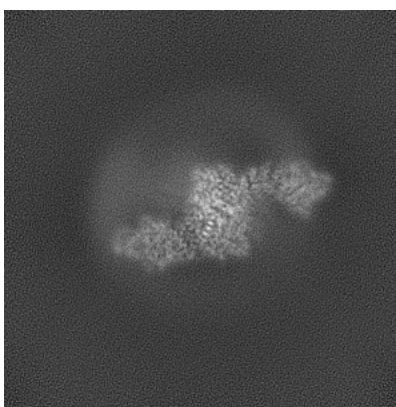


Z

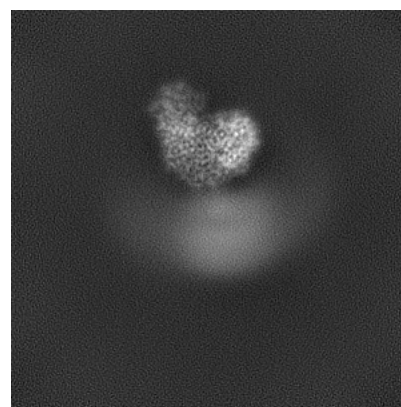
6.1.2 Raw map



X



Y

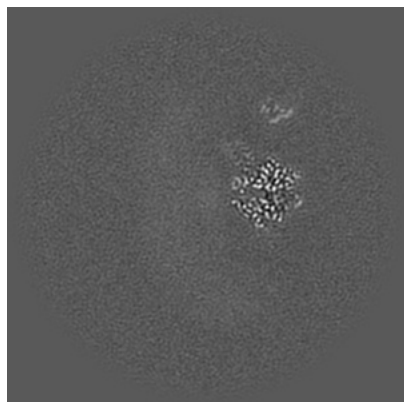


Z

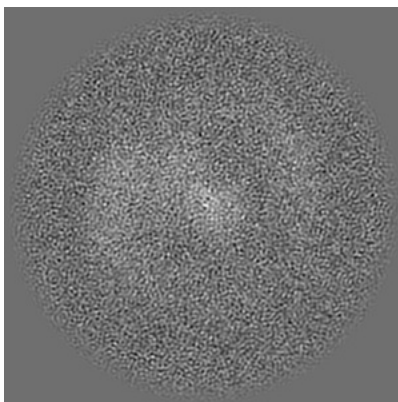
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

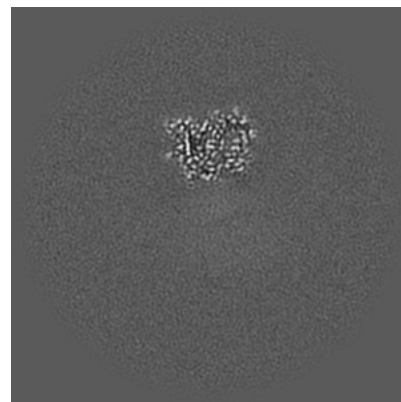
6.2.1 Primary map



X Index: 150

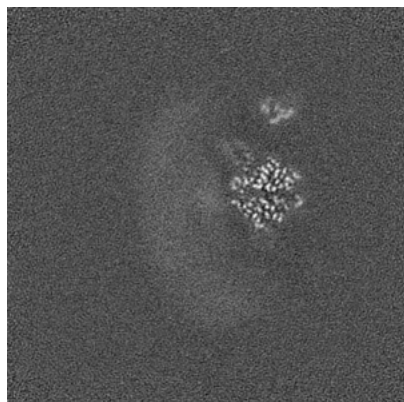


Y Index: 150

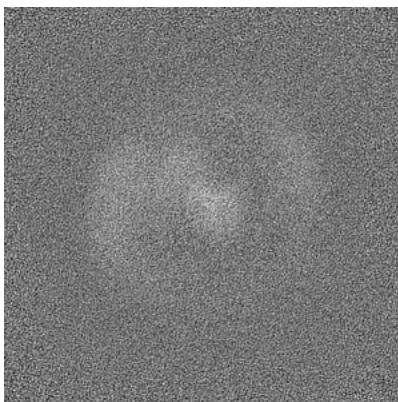


Z Index: 150

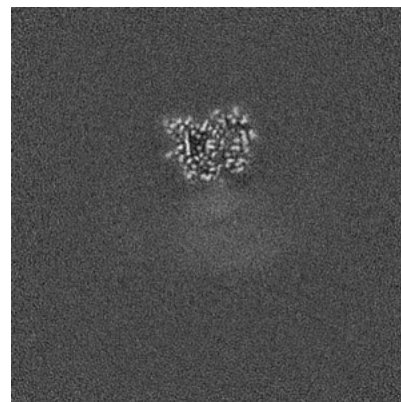
6.2.2 Raw map



X Index: 150



Y Index: 150

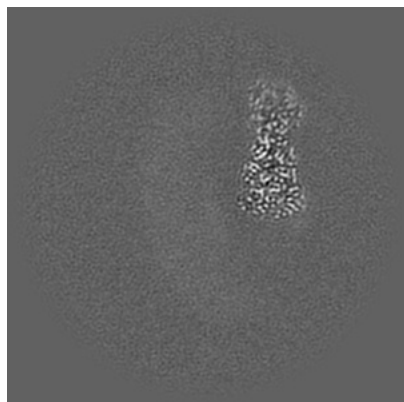


Z Index: 150

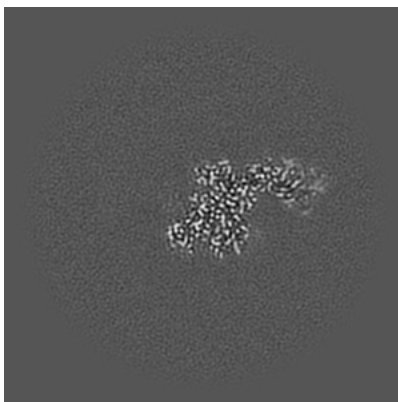
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

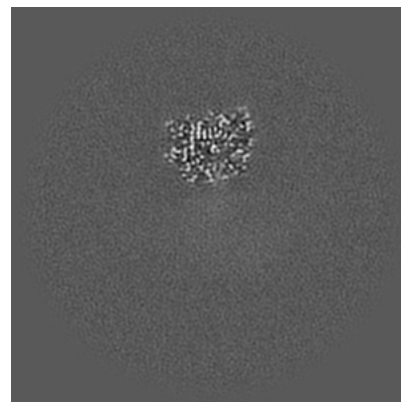
6.3.1 Primary map



X Index: 167

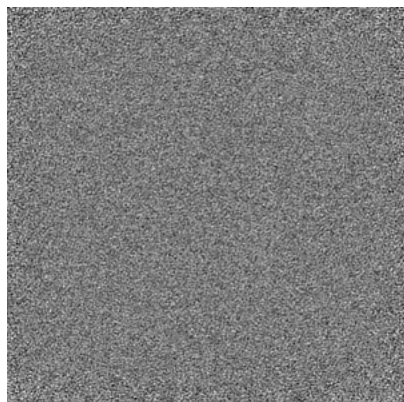


Y Index: 199

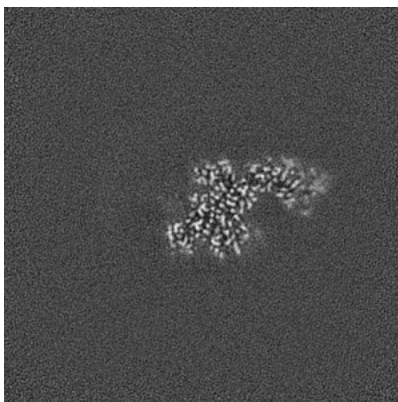


Z Index: 153

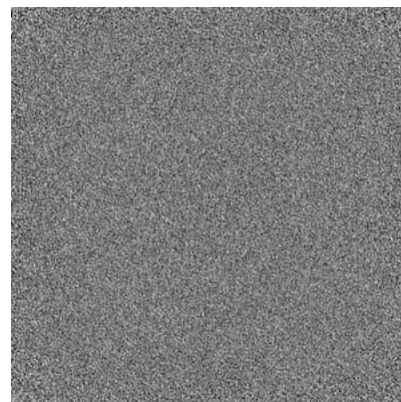
6.3.2 Raw map



X Index: 0



Y Index: 199

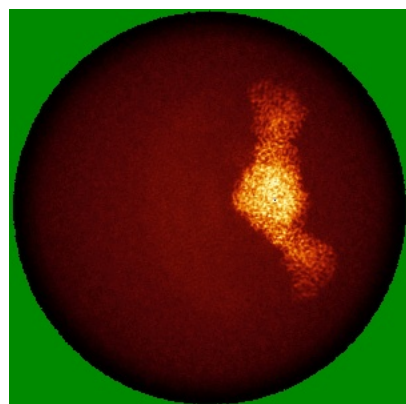


Z Index: 0

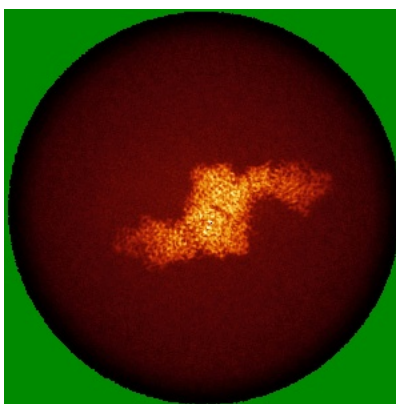
The images above show the largest variance slices of the map in three orthogonal directions.

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

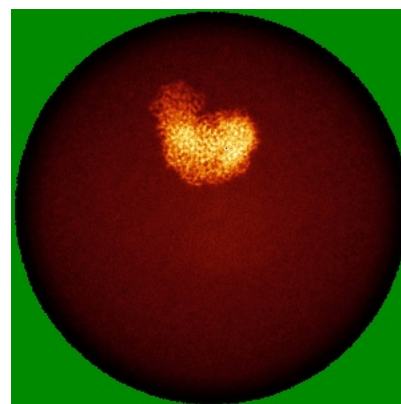
6.4.1 Primary map



X

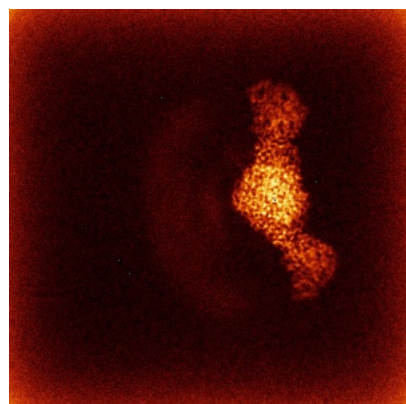


Y

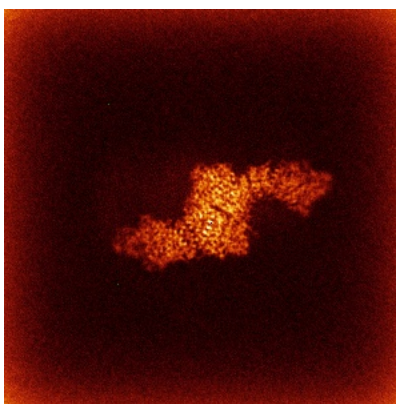


Z

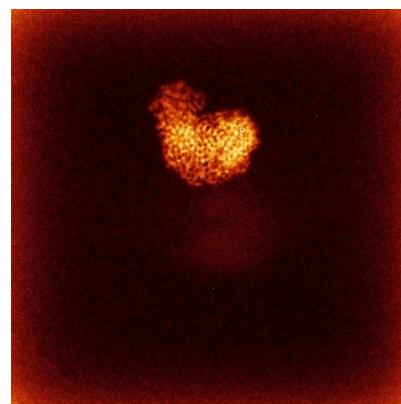
6.4.2 Raw map



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](#)

This section was not generated.

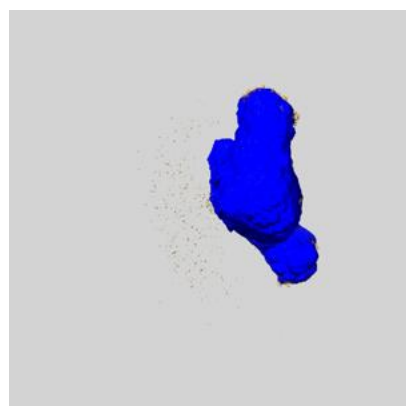
6.6 Mask visualisation [i](#)

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

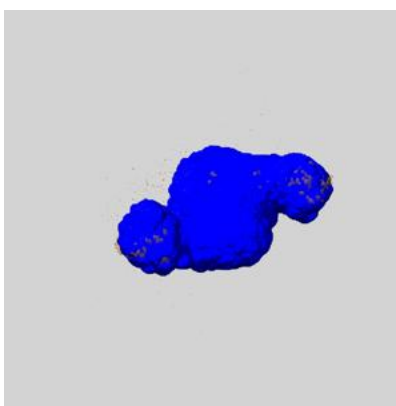
A mask typically either:

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

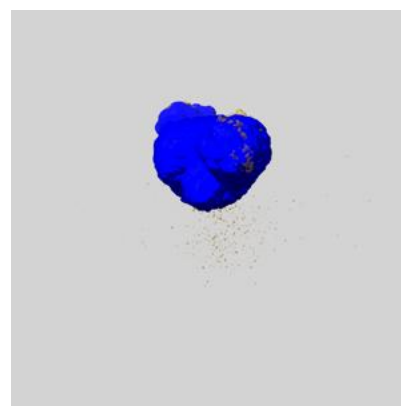
6.6.1 emd_45911_msk_1.map [i](#)



X



Y

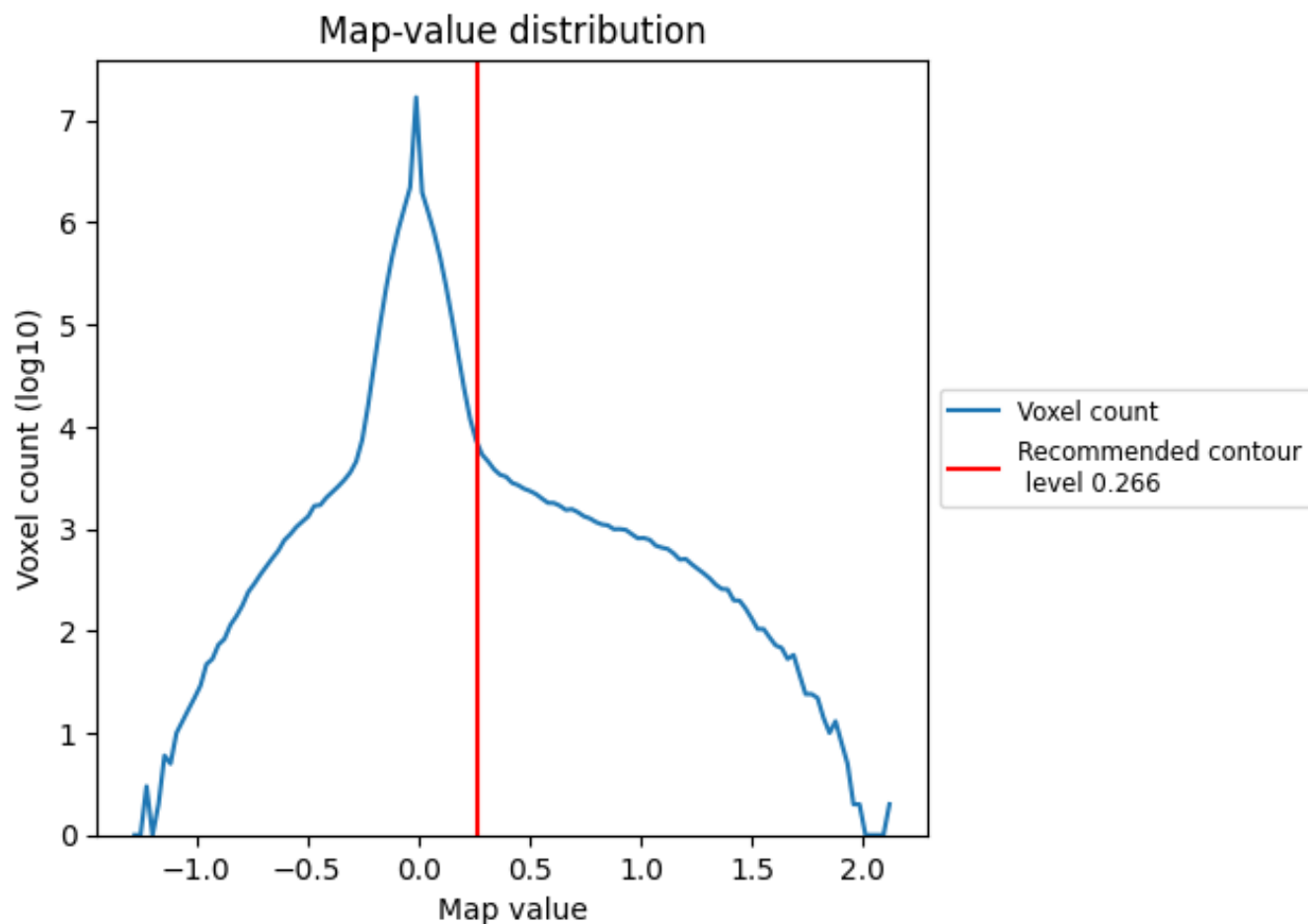


Z

7 Map analysis [i](#)

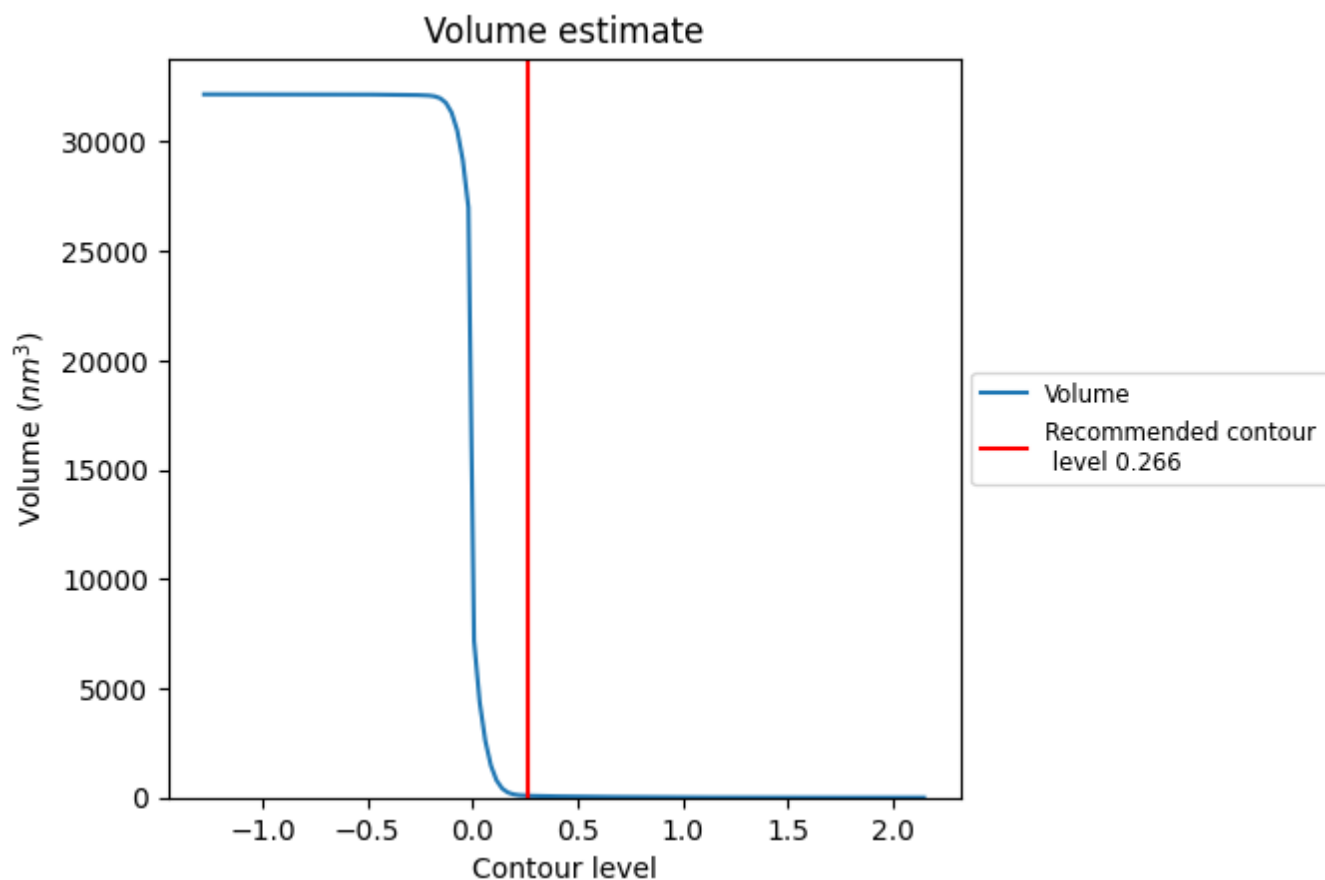
This section contains the results of statistical analysis of the map.

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.

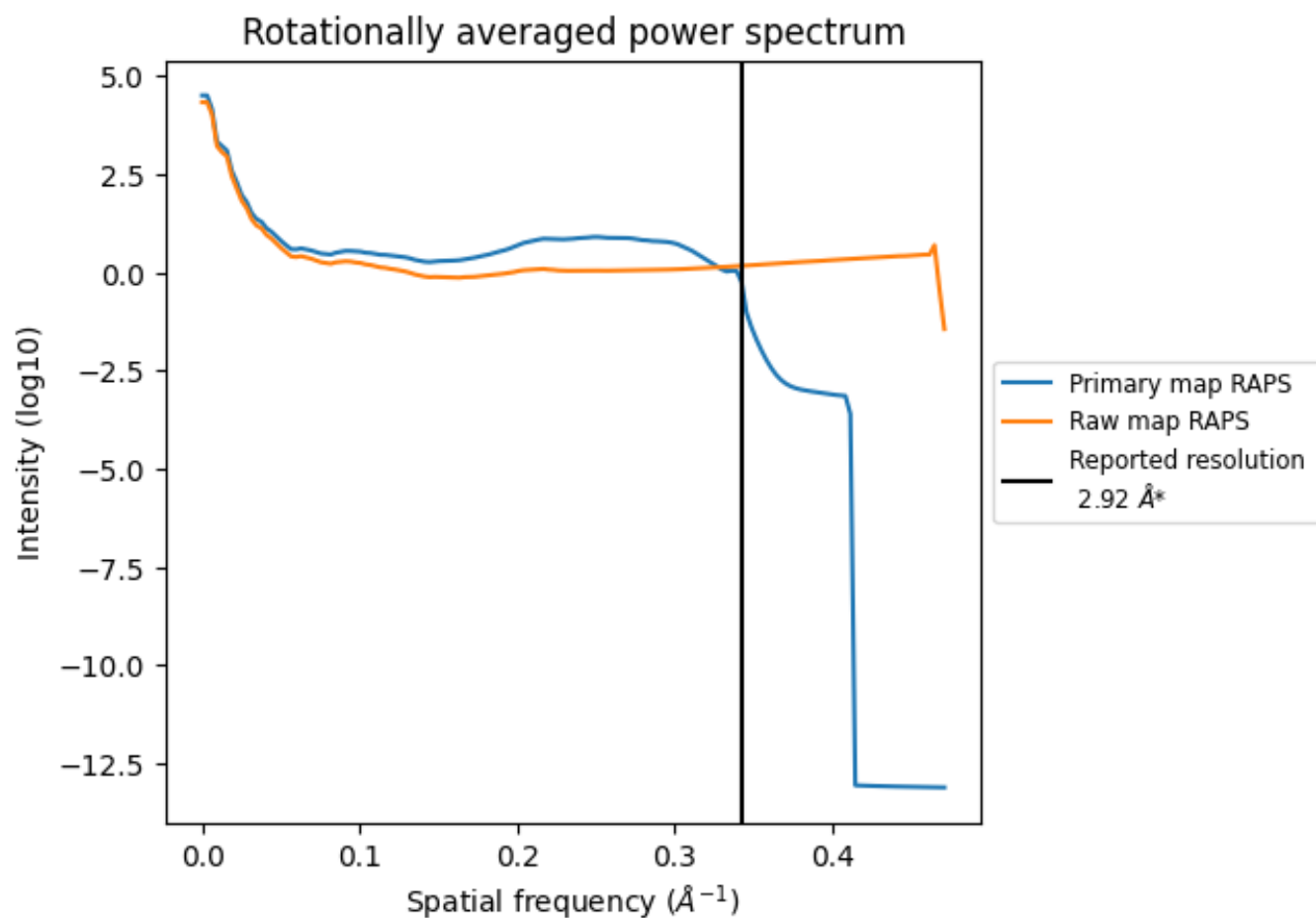
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 83 nm³; this corresponds to an approximate mass of 75 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 ⓘ

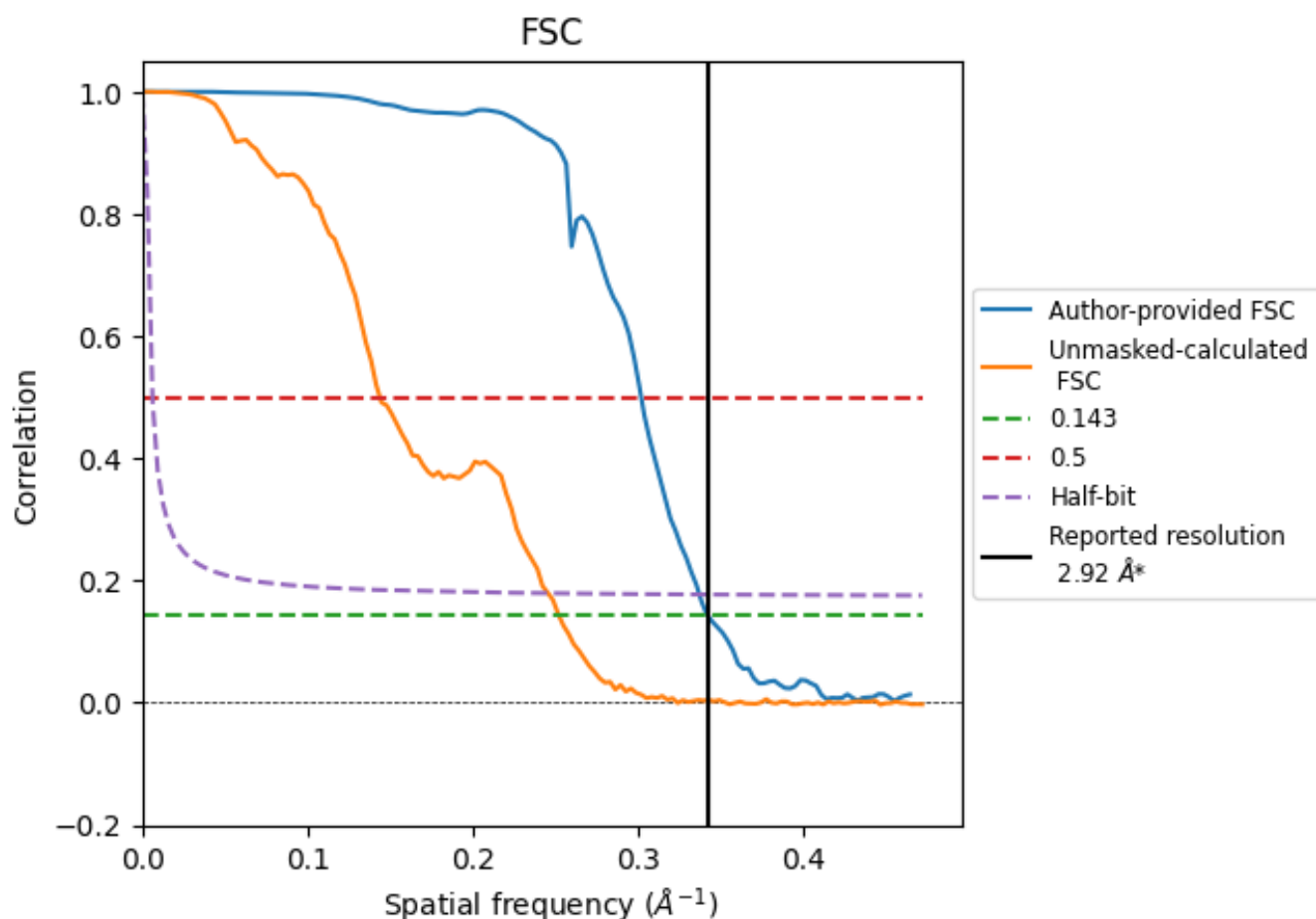


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.31	2.97
Unmasked-calculated*	3.97	6.96	4.07

*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 3.97 differs from the reported value 2.92 by more than 10 %

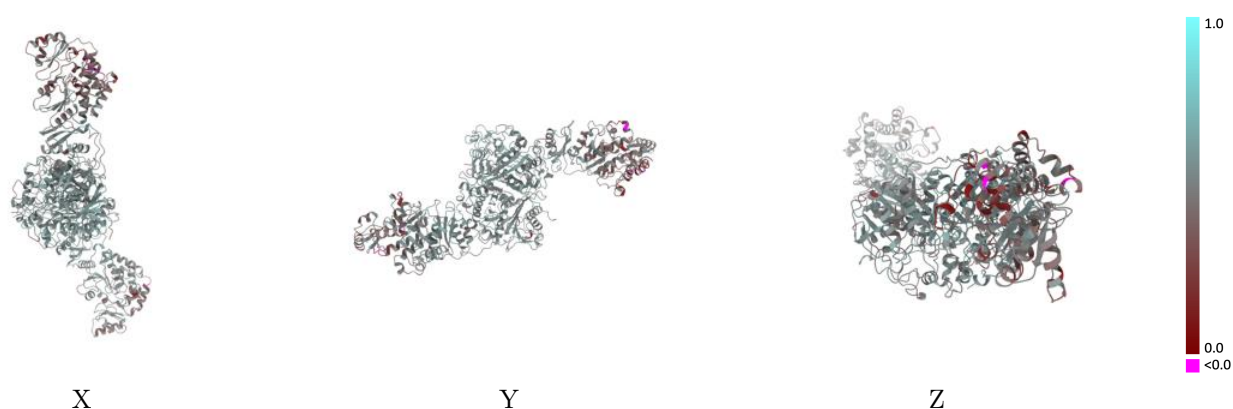
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45911 and PDB model 9CTM. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

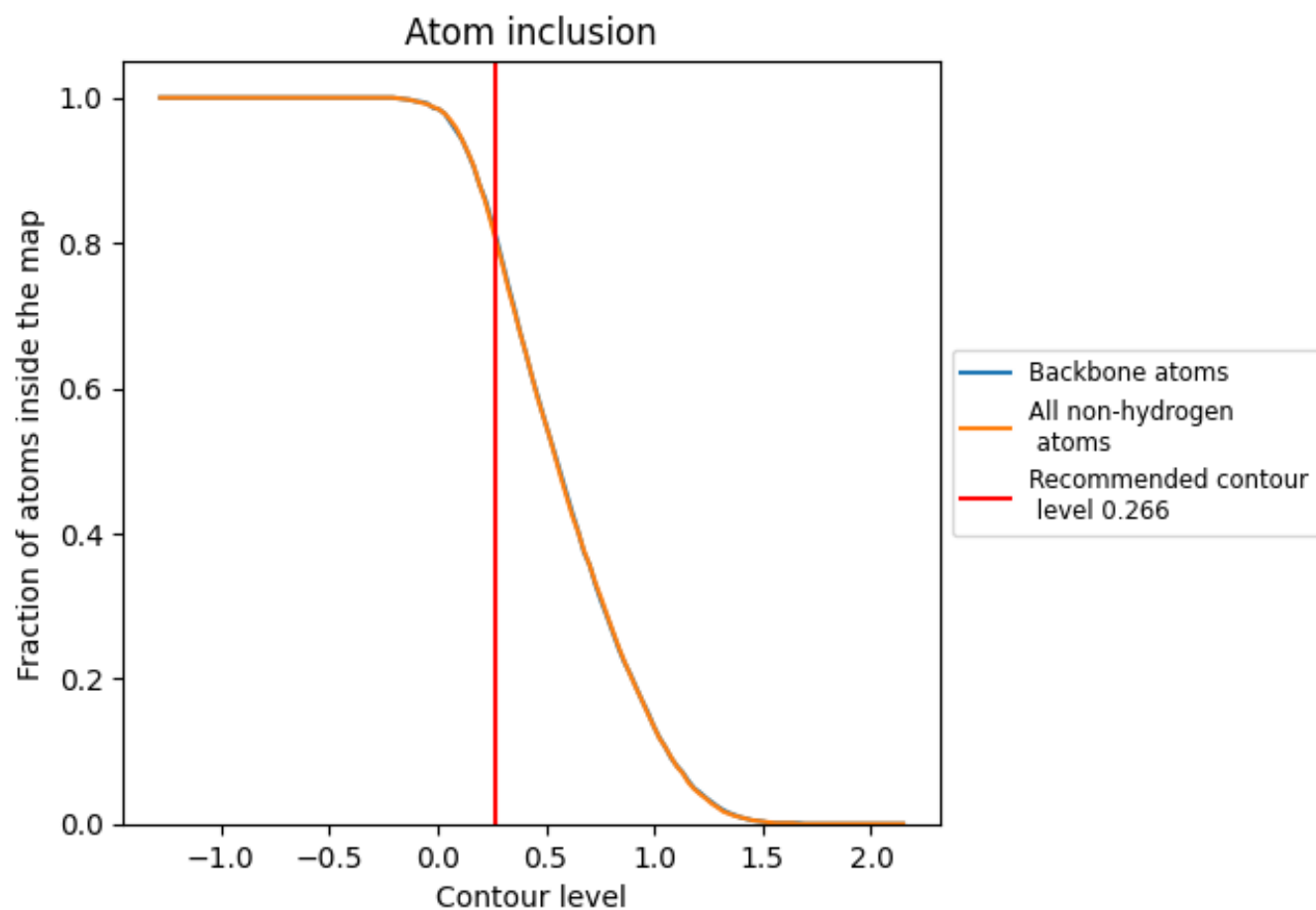


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4990
A	0.8180	0.5050
B	0.8000	0.4920

