



Full wwPDB EM Validation Report ⓘ

Nov 17, 2025 – 12:21 PM JST

PDB ID : 9V4O / pdb_00009v4o
EMDB ID : EMD-64781
Title : Cryo-EM structure of A. thaliana MET1 with bound SAH
Authors : Zhang, Z.; Liu, Y.; Li, W.; Du, J.
Deposited on : 2025-05-24
Resolution : 2.92 Å(reported)

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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

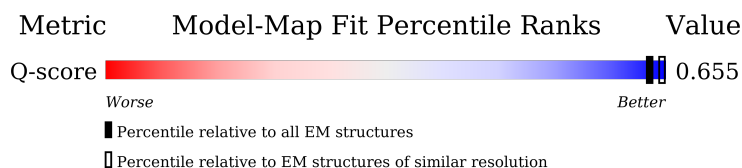
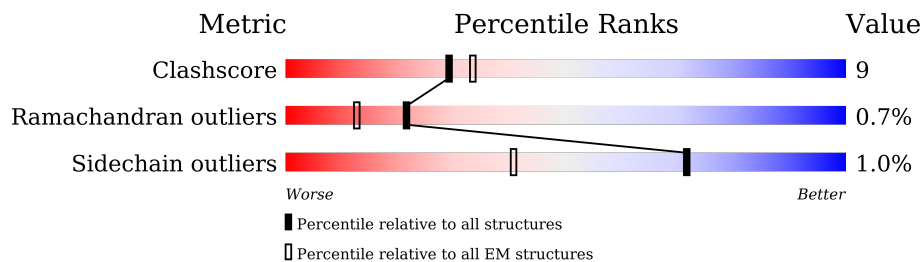
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	1574	<div> <div style="width: 55%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 32%; background-color: grey;"></div> </div> <div>55% 12% • 32%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8498 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 DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1064	Total	C	N	O	S	0	0
			8471	5405	1456	1565	45		

There are 40 discrepancies between the modelled and reference sequences:

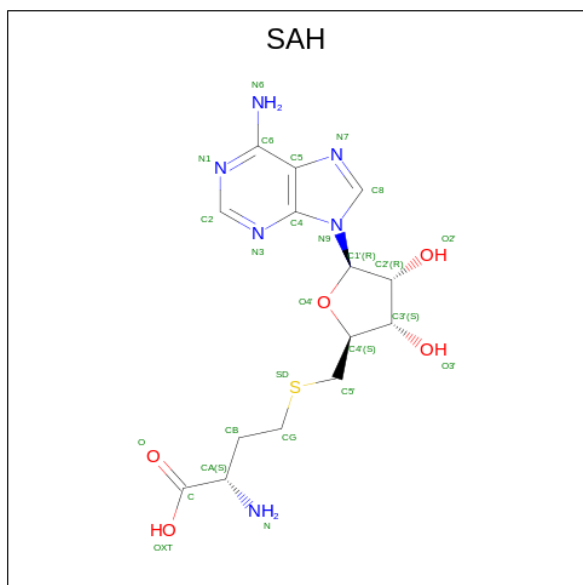
Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP P34881
A	-38	SER	-	expression tag	UNP P34881
A	-37	TYR	-	expression tag	UNP P34881
A	-36	TYR	-	expression tag	UNP P34881
A	-35	HIS	-	expression tag	UNP P34881
A	-34	HIS	-	expression tag	UNP P34881
A	-33	HIS	-	expression tag	UNP P34881
A	-32	HIS	-	expression tag	UNP P34881
A	-31	HIS	-	expression tag	UNP P34881
A	-30	HIS	-	expression tag	UNP P34881
A	-29	HIS	-	expression tag	UNP P34881
A	-28	HIS	-	expression tag	UNP P34881
A	-27	HIS	-	expression tag	UNP P34881
A	-26	HIS	-	expression tag	UNP P34881
A	-25	ASP	-	expression tag	UNP P34881
A	-24	TYR	-	expression tag	UNP P34881
A	-23	ASP	-	expression tag	UNP P34881
A	-22	ILE	-	expression tag	UNP P34881
A	-21	ASP	-	expression tag	UNP P34881
A	-20	TYR	-	expression tag	UNP P34881
A	-19	LYS	-	expression tag	UNP P34881
A	-18	ASP	-	expression tag	UNP P34881
A	-17	ASP	-	expression tag	UNP P34881
A	-16	ASP	-	expression tag	UNP P34881
A	-15	ASP	-	expression tag	UNP P34881
A	-14	LYS	-	expression tag	UNP P34881
A	-13	PRO	-	expression tag	UNP P34881

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	THR	-	expression tag	UNP P34881
A	-11	THR	-	expression tag	UNP P34881
A	-10	GLU	-	expression tag	UNP P34881
A	-9	ASN	-	expression tag	UNP P34881
A	-8	LEU	-	expression tag	UNP P34881
A	-7	TYR	-	expression tag	UNP P34881
A	-6	PHE	-	expression tag	UNP P34881
A	-5	GLN	-	expression tag	UNP P34881
A	-4	GLY	-	expression tag	UNP P34881
A	-3	ALA	-	expression tag	UNP P34881
A	-2	MET	-	expression tag	UNP P34881
A	-1	GLY	-	expression tag	UNP P34881
A	0	SER	-	expression tag	UNP P34881

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

K1521	A1289	LVS	S966
K1527	M1303	I1091	F967
LYS		R1092	
SER			Y975
PRO	F1306	I1098	E983
GLN	G1307	F1099	
HTS	V1308	A1100	D989
GLN			1990
PRO	S1326	D1116	
			D998
	P1332	I1121	
	F1333	E1122	K1016
		Y1123	
	P1346		Y1025
	K1360	V1142	
	E1361	M1153	F1033
			C1034
	I1371	Q1159	F1037
	L1389	Q1199	P1049
	N1390	G1200	A1050
		F1201	N1051
	R1393	S1202	M1052
		G1203	K1053
	W1405	M1204	P1054
		ASN	K1055
	P1425	ARG	F1056
	F1426	PHE	S1057
	C1427	ASN	
	L1428	GLN	K1060
	P1429	SER	ASP
	N1430	SER	ASP
	T1431	W1212	THR
	A1432	S1213	LEU
	E1433	K1214	LEU
	R1434	V1215	ARG
			LYS
	W1438	E1218	LYS
		M1219	LYS
	L1441		GLY
	Y1442	S1225	LYS
	G1443		GLY
		D1228	VAL
	P1452		GLU
			SER
	Q1459	R1233	GLU
	P1460	Y1234	ILE
		F1235	GLU
			SER
	M1466	E1261	GLU
			ILE
	R1479	Y1264	VAL
		Q1265	LYS
	R1483		PRO
		G1277	VAL
	N1496		GLU
			PRO
	H1499	R1282	PRO
		K1283	
		R1284	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	629218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	19.216	Depositor
Minimum map value	-0.183	Depositor
Average map value	-0.052	Depositor
Map value standard deviation	0.459	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: ZN, SAH

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	0.30	0/8672	0.53	0/11724

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	8471	0	8397	153	0
2	A	26	0	19	3	0
3	A	1	0	0	0	0
All	All	8498	0	8416	153	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 (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:LEU:HD21	1:A:901:LYS:HA	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:HG22	1:A:431:ASP:H	1.49	0.77
1:A:406:ILE:HG21	1:A:423:ILE:HD12	1.72	0.72
1:A:466:ILE:HG12	1:A:476:ILE:HG12	1.72	0.72
1:A:1346:PRO:HB3	1:A:1360:LYS:HE3	1.74	0.70
1:A:805:LEU:HD12	1:A:808:ILE:HD11	1.72	0.69
1:A:361:PRO:HB3	1:A:404:ARG:HD2	1.74	0.68
1:A:1099:PHE:O	2:A:1601:SAH:HG2	1.94	0.67
1:A:1428:LEU:HG	1:A:1438:TRP:CE3	2.29	0.67
1:A:708:ARG:NH2	1:A:808:ILE:O	2.22	0.66
1:A:1371:ILE:HG21	1:A:1483:ARG:HE	1.61	0.66
1:A:1091:ILE:HD11	1:A:1521:LYS:HG3	1.78	0.65
1:A:896:LYS:HB2	1:A:905:PHE:HB2	1.79	0.64
1:A:1049:PRO:HB2	1:A:1051:ASN:HD22	1.63	0.63
1:A:406:ILE:HD13	1:A:423:ILE:HD11	1.81	0.63
1:A:1204:MET:HA	1:A:1213:SER:HB2	1.80	0.62
1:A:1452:PRO:HG3	1:A:1466:MET:HE2	1.81	0.61
1:A:1219:MET:HA	1:A:1219:MET:HE3	1.82	0.61
1:A:630:THR:HG23	1:A:1225:SER:HB3	1.82	0.61
1:A:370:GLU:HB2	1:A:457:PHE:HD2	1.65	0.60
1:A:519:SER:O	1:A:520:ARG:C	2.42	0.60
1:A:1428:LEU:HD13	1:A:1428:LEU:H	1.67	0.60
1:A:1204:MET:N	1:A:1214:LYS:H	1.97	0.60
1:A:1052:MET:C	1:A:1053:LYS:HD3	2.26	0.59
1:A:440:ASN:ND2	1:A:472:ASP:OD2	2.36	0.58
1:A:524:LEU:HD11	1:A:532:ARG:HH21	1.69	0.58
1:A:348:LYS:HD3	1:A:595:TRP:CH2	2.39	0.57
1:A:1496:ASN:OD1	1:A:1499:HIS:ND1	2.37	0.57
1:A:1203:GLY:C	1:A:1214:LYS:HB3	2.30	0.57
1:A:525:SER:H	1:A:528:ASP:HB2	1.68	0.57
1:A:1235:PHE:HB3	1:A:1289:ALA:HB3	1.85	0.57
1:A:1052:MET:HG2	1:A:1053:LYS:N	2.19	0.57
1:A:745:LEU:HD11	1:A:801:MET:HE2	1.88	0.56
1:A:1055:LYS:O	1:A:1057:SER:N	2.38	0.56
1:A:1426:PHE:HD2	1:A:1428:LEU:HD12	1.69	0.56
1:A:1204:MET:H	1:A:1214:LYS:H	1.53	0.55
1:A:358:TYR:OH	1:A:409:GLU:OE1	2.20	0.55
1:A:520:ARG:HE	1:A:523:ARG:HH22	1.55	0.55
1:A:630:THR:HG22	1:A:1153:MET:HE1	1.90	0.54
1:A:396:TRP:CZ2	1:A:487:LEU:HD23	2.43	0.54
1:A:430:THR:HG22	1:A:431:ASP:N	2.22	0.54
1:A:353:GLU:OE1	1:A:590:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:PRO:C	1:A:1431:THR:N	2.62	0.53
1:A:732:VAL:HG21	1:A:808:ILE:HD12	1.91	0.53
1:A:577:CYS:HB2	1:A:580:VAL:HG23	1.91	0.52
1:A:937:SER:HB2	1:A:1466:MET:HE1	1.91	0.52
1:A:1092:ARG:HD3	1:A:1116:ASP:HB3	1.90	0.52
1:A:388:LEU:HB3	1:A:483:ALA:HA	1.90	0.52
1:A:1199:GLN:HE21	1:A:1218:GLU:HG2	1.74	0.52
1:A:1433:GLU:O	1:A:1434:ARG:HB2	2.08	0.52
1:A:1443:GLY:HA3	1:A:1466:MET:HG3	1.91	0.52
1:A:898:ASN:H	1:A:904:PHE:HA	1.75	0.52
1:A:1428:LEU:N	1:A:1429:PRO:CD	2.73	0.51
1:A:901:LYS:HB2	1:A:901:LYS:NZ	2.25	0.51
1:A:1429:PRO:O	1:A:1430:ASN:C	2.54	0.50
1:A:821:TRP:HH2	1:A:1264:TYR:CE1	2.28	0.50
1:A:879:PHE:HZ	1:A:884:LYS:HD3	1.76	0.50
1:A:511:ILE:HA	1:A:514:PHE:CE1	2.47	0.50
1:A:1203:GLY:CA	1:A:1215:VAL:HG23	2.41	0.50
1:A:1303:MET:HA	1:A:1332:PRO:HD2	1.93	0.49
1:A:1390:ASN:ND2	1:A:1460:PRO:O	2.46	0.49
1:A:520:ARG:HE	1:A:523:ARG:NH2	2.10	0.48
1:A:347:ILE:HG23	1:A:592:HIS:HB2	1.95	0.48
1:A:575:LYS:HB2	1:A:576:ARG:HH11	1.78	0.48
1:A:567:ALA:HA	1:A:575:LYS:HE3	1.94	0.48
1:A:826:ARG:NH2	1:A:1228:ASP:OD2	2.46	0.48
1:A:1051:ASN:ND2	1:A:1052:MET:SD	2.87	0.48
1:A:900:SER:O	1:A:901:LYS:HG3	2.14	0.48
1:A:897:LEU:HA	1:A:904:PHE:CB	2.44	0.47
1:A:767:ASP:O	1:A:768:HIS:CG	2.66	0.47
1:A:1099:PHE:HB3	2:A:1601:SAH:H5'2	1.95	0.47
1:A:574:VAL:O	1:A:575:LYS:HD2	2.14	0.47
1:A:419:ILE:HG22	1:A:421:VAL:H	1.79	0.47
1:A:821:TRP:CH2	1:A:1264:TYR:CE1	3.03	0.47
1:A:406:ILE:HD13	1:A:423:ILE:CD1	2.45	0.47
1:A:459:SER:OG	1:A:460:GLN:N	2.49	0.46
1:A:1303:MET:HE2	1:A:1333:PHE:HE2	1.80	0.46
1:A:1052:MET:O	1:A:1053:LYS:HD3	2.15	0.46
1:A:600:LYS:HG2	1:A:601:LYS:H	1.81	0.46
1:A:767:ASP:CG	1:A:768:HIS:H	2.24	0.46
1:A:1049:PRO:C	1:A:1051:ASN:N	2.70	0.46
1:A:1428:LEU:HG	1:A:1438:TRP:CD2	2.50	0.46
1:A:478:ILE:HG23	1:A:487:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:PHE:CZ	1:A:884:LYS:HD3	2.51	0.45
1:A:620:SER:OG	1:A:621:LYS:N	2.47	0.45
1:A:1034:CYS:HB3	1:A:1056:PHE:CZ	2.52	0.45
1:A:527:ALA:O	1:A:531:LYS:HG2	2.17	0.45
1:A:983:GLU:H	1:A:983:GLU:CD	2.24	0.45
1:A:1430:ASN:O	1:A:1431:THR:C	2.60	0.45
1:A:1201:PHE:HZ	1:A:1218:GLU:HG3	1.82	0.45
1:A:1426:PHE:CD2	1:A:1438:TRP:HE3	2.35	0.45
1:A:807:ASP:O	1:A:807:ASP:OD1	2.35	0.44
1:A:896:LYS:HE3	1:A:905:PHE:CB	2.47	0.44
1:A:1405:TRP:CE2	1:A:1426:PHE:CE2	3.05	0.44
1:A:439:LEU:HB2	1:A:472:ASP:HA	1.98	0.44
1:A:490:PRO:HG3	1:A:498:TRP:CD1	2.53	0.44
1:A:975:TYR:OH	1:A:998:ASP:OD2	2.25	0.44
1:A:1308:VAL:O	1:A:1326:SER:OG	2.30	0.44
1:A:1459:GLN:HA	1:A:1460:PRO:HD3	1.84	0.44
1:A:1098:ILE:HG12	1:A:1121:ILE:HD12	1.99	0.44
1:A:1265:GLN:O	1:A:1289:ALA:HA	2.18	0.44
1:A:575:LYS:HB2	1:A:576:ARG:NH1	2.33	0.43
1:A:520:ARG:O	1:A:521:VAL:C	2.61	0.43
1:A:1052:MET:HE2	1:A:1053:LYS:HA	2.01	0.43
1:A:744:THR:HA	1:A:755:ALA:O	2.18	0.43
1:A:599:LYS:HD2	1:A:599:LYS:HA	1.84	0.43
1:A:396:TRP:CH2	1:A:487:LEU:HD23	2.54	0.43
1:A:826:ARG:O	1:A:830:ILE:HG12	2.18	0.43
1:A:1100:ALA:O	2:A:1601:SAH:HA	2.19	0.43
1:A:1426:PHE:CZ	1:A:1441:LEU:HD12	2.53	0.43
1:A:641:TYR:HB3	1:A:1212:TRP:HB2	2.01	0.43
1:A:897:LEU:HD12	1:A:967:PHE:CD2	2.54	0.43
1:A:430:THR:CG2	1:A:431:ASP:H	2.26	0.43
1:A:1122:GLU:O	1:A:1142:VAL:HA	2.18	0.43
1:A:360:LEU:HD22	1:A:1428:LEU:HB2	2.00	0.42
1:A:1303:MET:HE2	1:A:1333:PHE:CE2	2.54	0.42
1:A:773:HIS:CE1	1:A:800:CYS:HB3	2.54	0.42
1:A:353:GLU:O	1:A:553:ARG:NH2	2.52	0.42
1:A:1282:ARG:HH21	1:A:1284:ARG:NH2	2.16	0.42
1:A:406:ILE:CG1	1:A:410:LEU:HD12	2.49	0.42
1:A:1233:ARG:HH21	1:A:1527:LYS:HZ2	1.67	0.42
1:A:382:GLU:H	1:A:382:GLU:CD	2.26	0.42
1:A:646:PRO:O	1:A:1204:MET:SD	2.78	0.42
1:A:749:ASP:N	1:A:749:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:LYS:HD3	1:A:1033:PHE:CE2	2.55	0.42
1:A:1025:TYR:OH	1:A:1277:GLY:O	2.31	0.42
1:A:920:ASN:OD1	1:A:921:PRO:HD2	2.19	0.42
1:A:712:TRP:HZ3	1:A:762:MET:HE3	1.85	0.41
1:A:393:LEU:HD23	1:A:427:GLY:HA3	2.02	0.41
1:A:720:THR:HG22	1:A:721:SER:N	2.35	0.41
1:A:439:LEU:HA	1:A:439:LEU:HD23	1.70	0.41
1:A:1479:ARG:O	1:A:1483:ARG:HG3	2.20	0.41
1:A:903:GLY:HA2	1:A:911:TYR:O	2.20	0.41
1:A:1201:PHE:HE1	1:A:1215:VAL:HG22	1.85	0.41
1:A:393:LEU:HD11	1:A:485:TYR:CD2	2.56	0.41
1:A:521:VAL:HG21	1:A:573:ASN:O	2.21	0.41
1:A:583:LEU:HD12	1:A:583:LEU:HA	1.92	0.41
1:A:607:LEU:HD12	1:A:607:LEU:HA	1.89	0.41
1:A:1037:PHE:CD2	1:A:1049:PRO:HD3	2.56	0.41
1:A:1054:PRO:HG2	1:A:1056:PHE:CE1	2.56	0.41
1:A:1303:MET:HG2	1:A:1332:PRO:HG2	2.03	0.41
1:A:516:ARG:HD3	1:A:571:ASP:OD2	2.21	0.40
1:A:898:ASN:O	1:A:899:VAL:C	2.64	0.40
1:A:1306:PHE:HD2	1:A:1308:VAL:HG23	1.86	0.40
1:A:1371:ILE:HD13	1:A:1371:ILE:HA	1.92	0.40
1:A:1389:LEU:O	1:A:1393:ARG:HG3	2.21	0.40
1:A:636:ILE:HD11	1:A:1261:GLU:HG2	2.03	0.40
1:A:720:THR:HG22	1:A:721:SER:H	1.87	0.40
1:A:989:ASP:OD1	1:A:990:ILE:N	2.54	0.40
1:A:1159:GLN:H	1:A:1159:GLN:HG2	1.69	0.40
1:A:1199:GLN:HG2	1:A:1218:GLU:HG2	2.03	0.40
1:A:1360:LYS:HG3	1:A:1361:GLU:HG3	2.03	0.40
1:A:1429:PRO:O	1:A:1431:THR:N	2.54	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	1050/1574 (67%)	950 (90%)	93 (9%)	7 (1%)	19	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1425	PRO
1	A	1431	THR
1	A	899	VAL
1	A	1201	PHE
1	A	1433	GLU
1	A	1202	SER
1	A	1428	LEU

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	921/1367 (67%)	912 (99%)	9 (1%)	73	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	901	LYS
1	A	1051	ASN
1	A	1052	MET
1	A	1121	ILE
1	A	1123	TYR
1	A	1199	GLN
1	A	1201	PHE
1	A	1204	MET
1	A	1428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	997	GLN
1	A	1051	ASN
1	A	1199	GLN
1	A	1501	HIS
1	A	1503	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	SAH	A	1601	-	24,28,28	1.49	4 (16%)	25,40,40	1.97	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	1601	-	-	2/11/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	SAH	OXT-C	-4.54	1.15	1.30
2	A	1601	SAH	C2'-C1'	-2.44	1.50	1.53
2	A	1601	SAH	CA-N	-2.08	1.38	1.48
2	A	1601	SAH	CG-SD	-2.05	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	SAH	N3-C2-N1	-4.41	121.78	128.68
2	A	1601	SAH	CB-CG-SD	-3.98	104.38	113.31
2	A	1601	SAH	CB-CA-C	3.92	119.64	110.30
2	A	1601	SAH	C1'-N9-C4	-2.84	121.65	126.64
2	A	1601	SAH	C4-C5-N7	-2.80	106.48	109.40
2	A	1601	SAH	C3'-C2'-C1'	2.51	104.75	100.98
2	A	1601	SAH	OXT-C-O	-2.03	119.48	124.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	SAH	OXT-C-CA-CB
2	A	1601	SAH	O-C-CA-CB

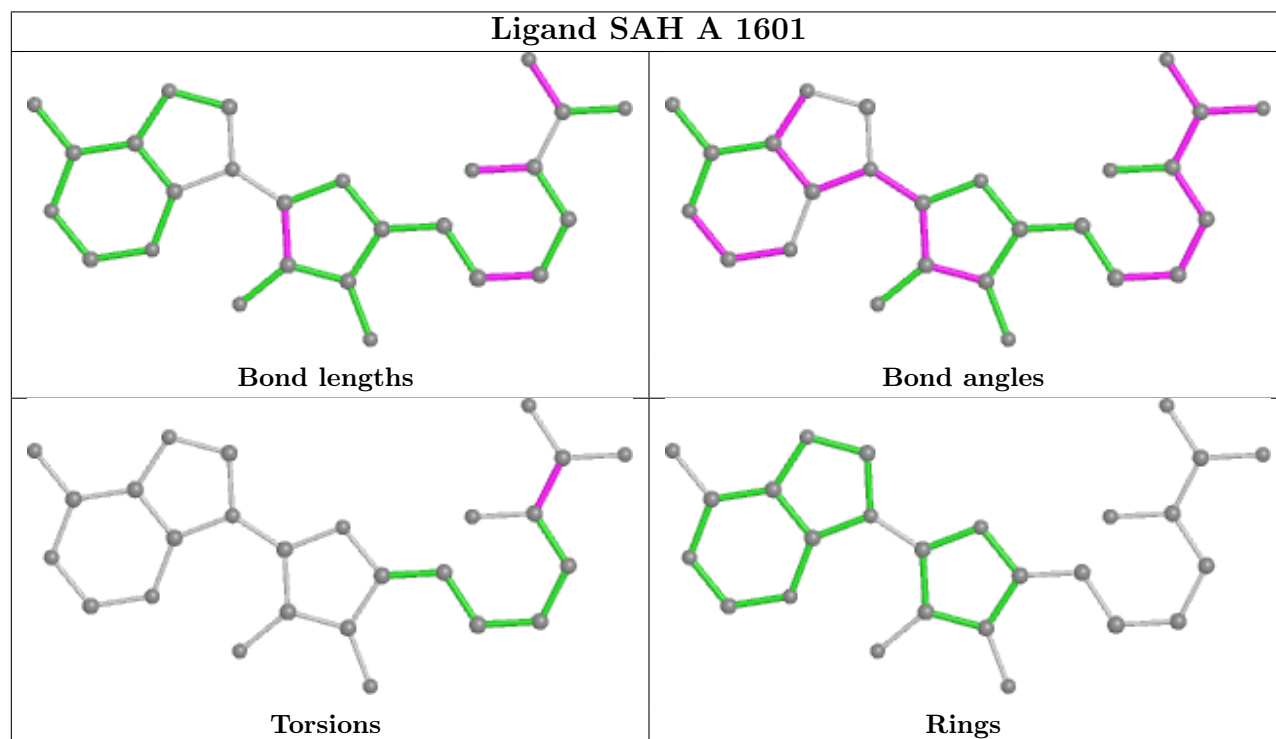
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	SAH	3	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.

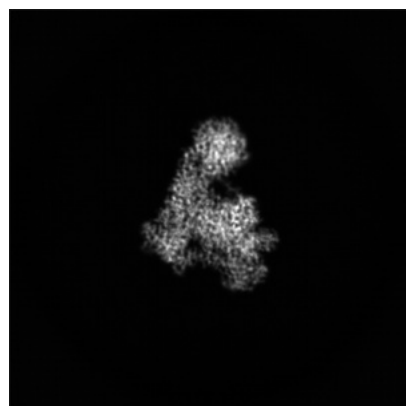
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64781. These allow visual inspection of the internal detail of the map and identification of artifacts.

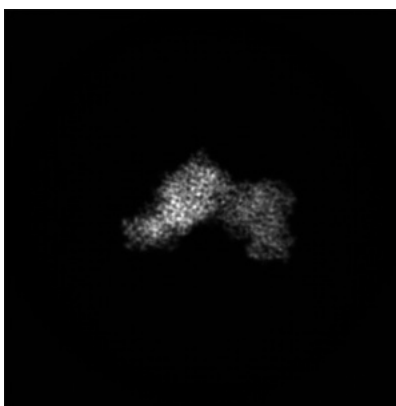
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

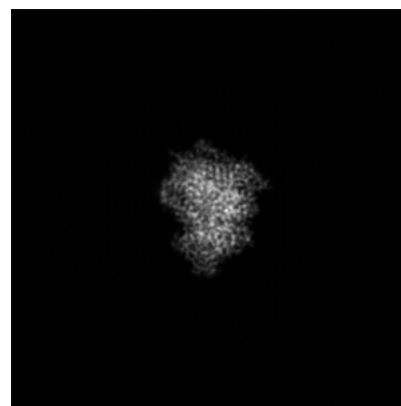
6.1.1 Primary map



X

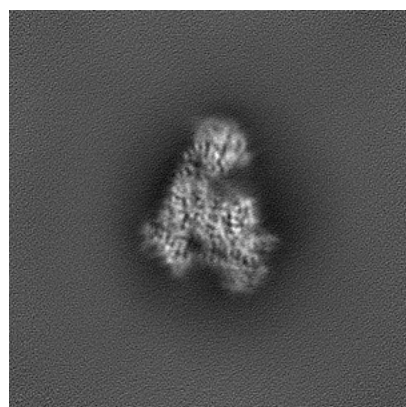


Y

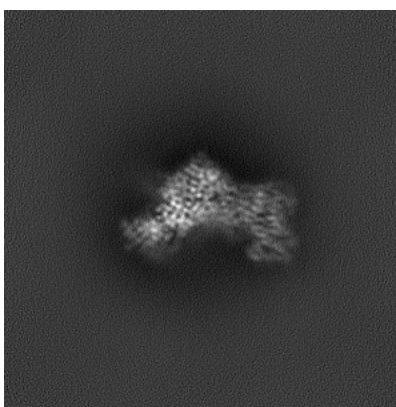


Z

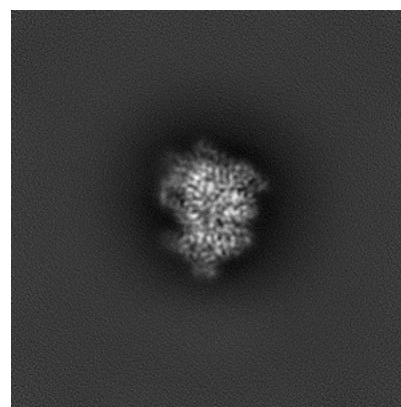
6.1.2 Raw map



X



Y

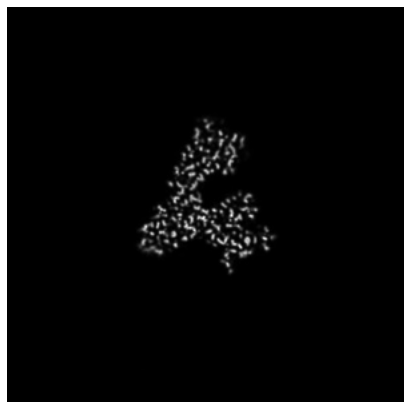


Z

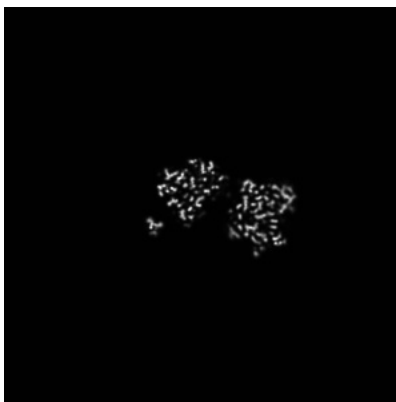
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

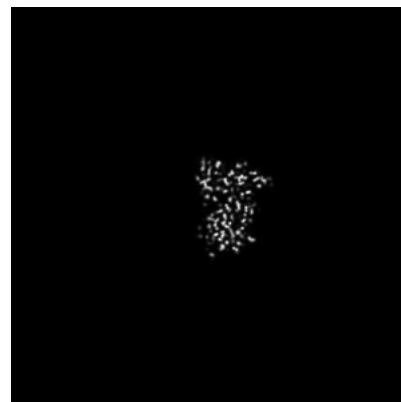
6.2.1 Primary map



X Index: 160

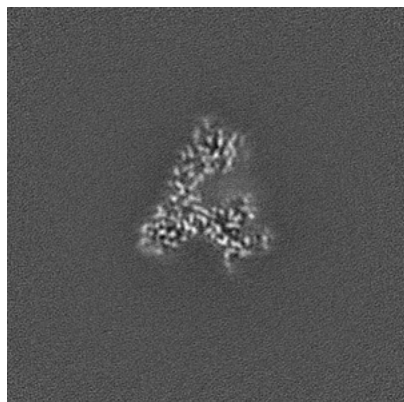


Y Index: 160

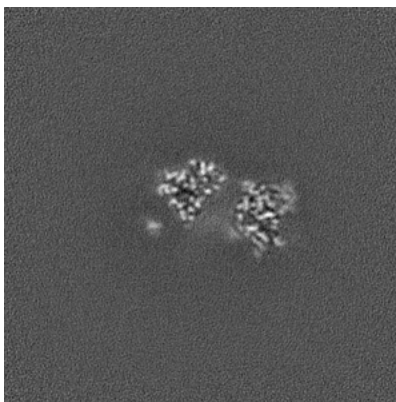


Z Index: 160

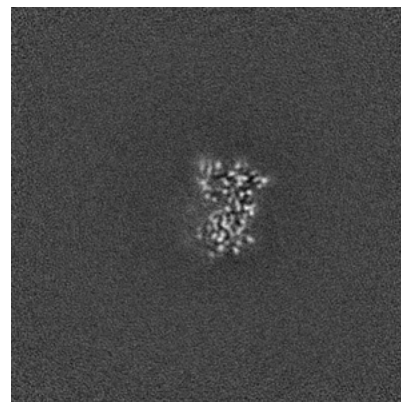
6.2.2 Raw map



X Index: 160



Y Index: 160

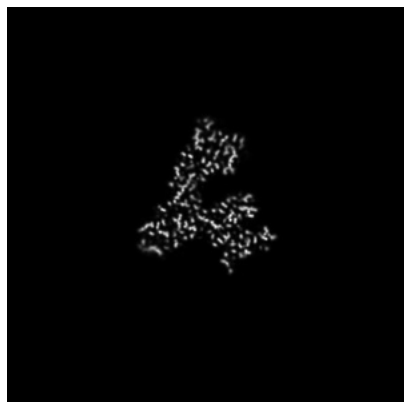


Z Index: 160

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

6.3 Largest variance slices [i](#)

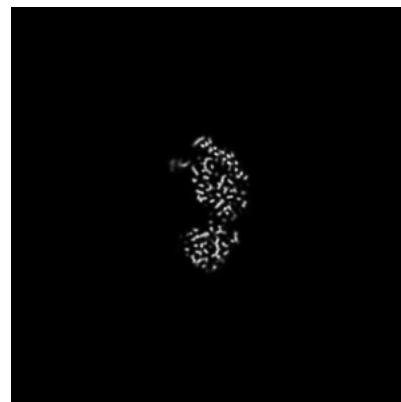
6.3.1 Primary map



X Index: 159

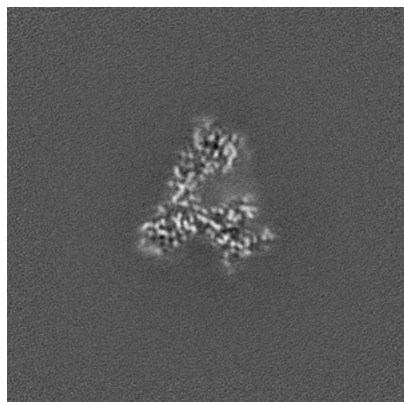


Y Index: 180

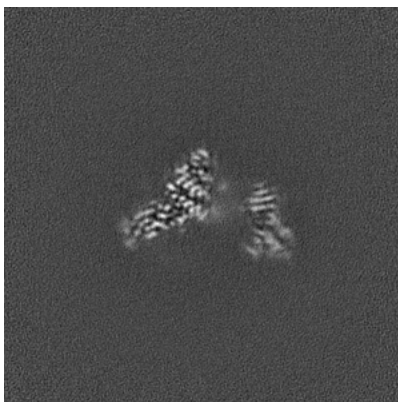


Z Index: 135

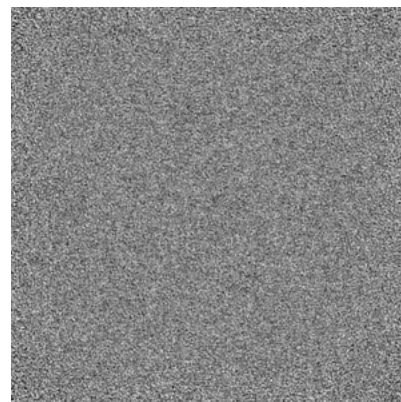
6.3.2 Raw map



X Index: 159



Y Index: 180

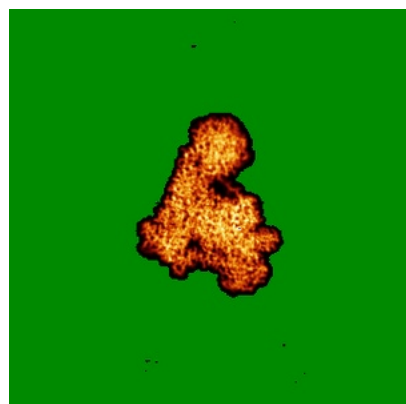


Z Index: 319

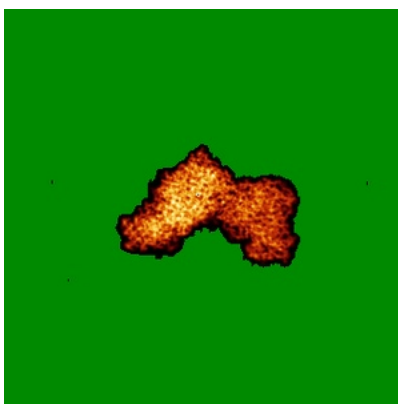
The images above show the largest variance slices of the map in three orthogonal directions.

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

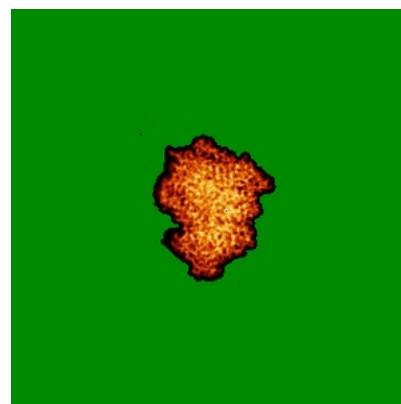
6.4.1 Primary map



X

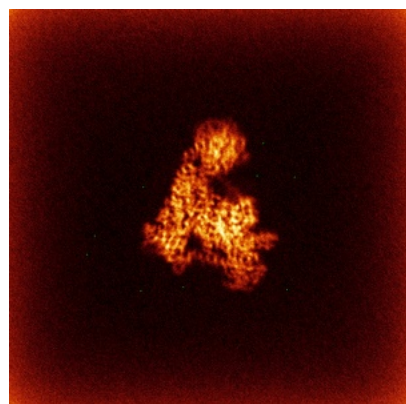


Y

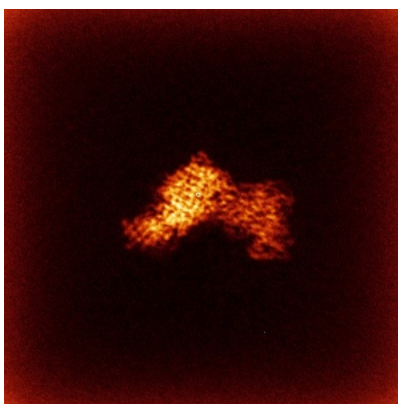


Z

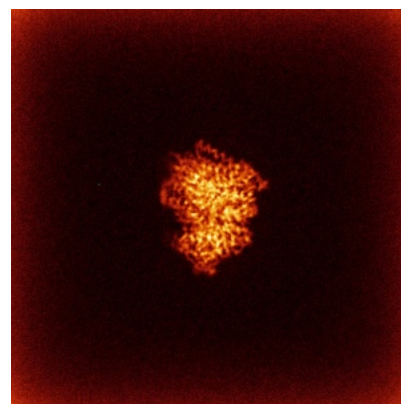
6.4.2 Raw map



X



Y

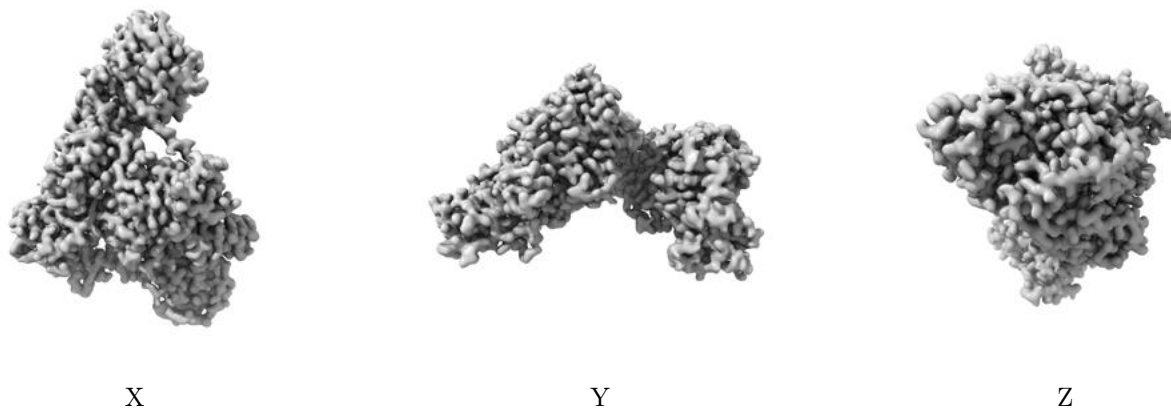


Z

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.

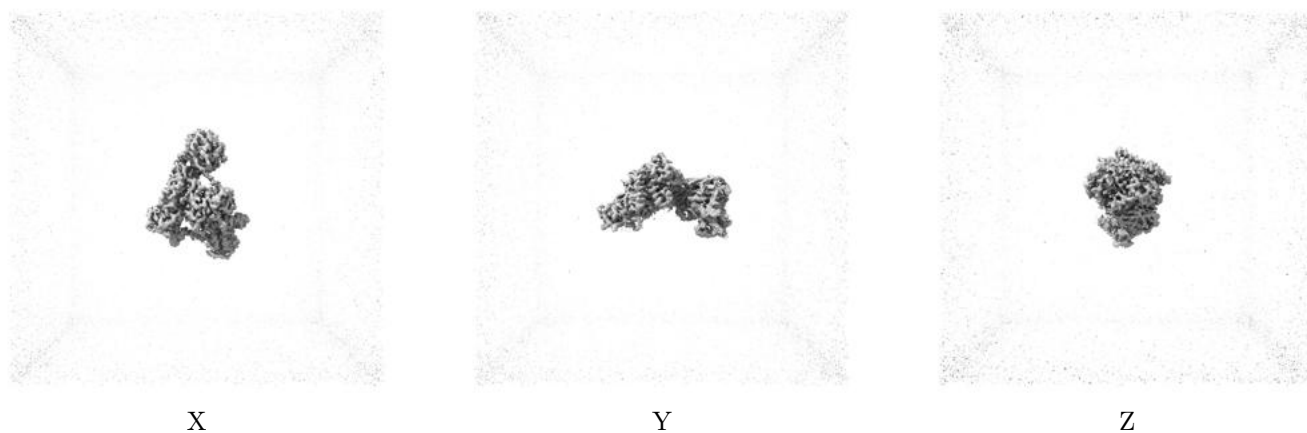
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

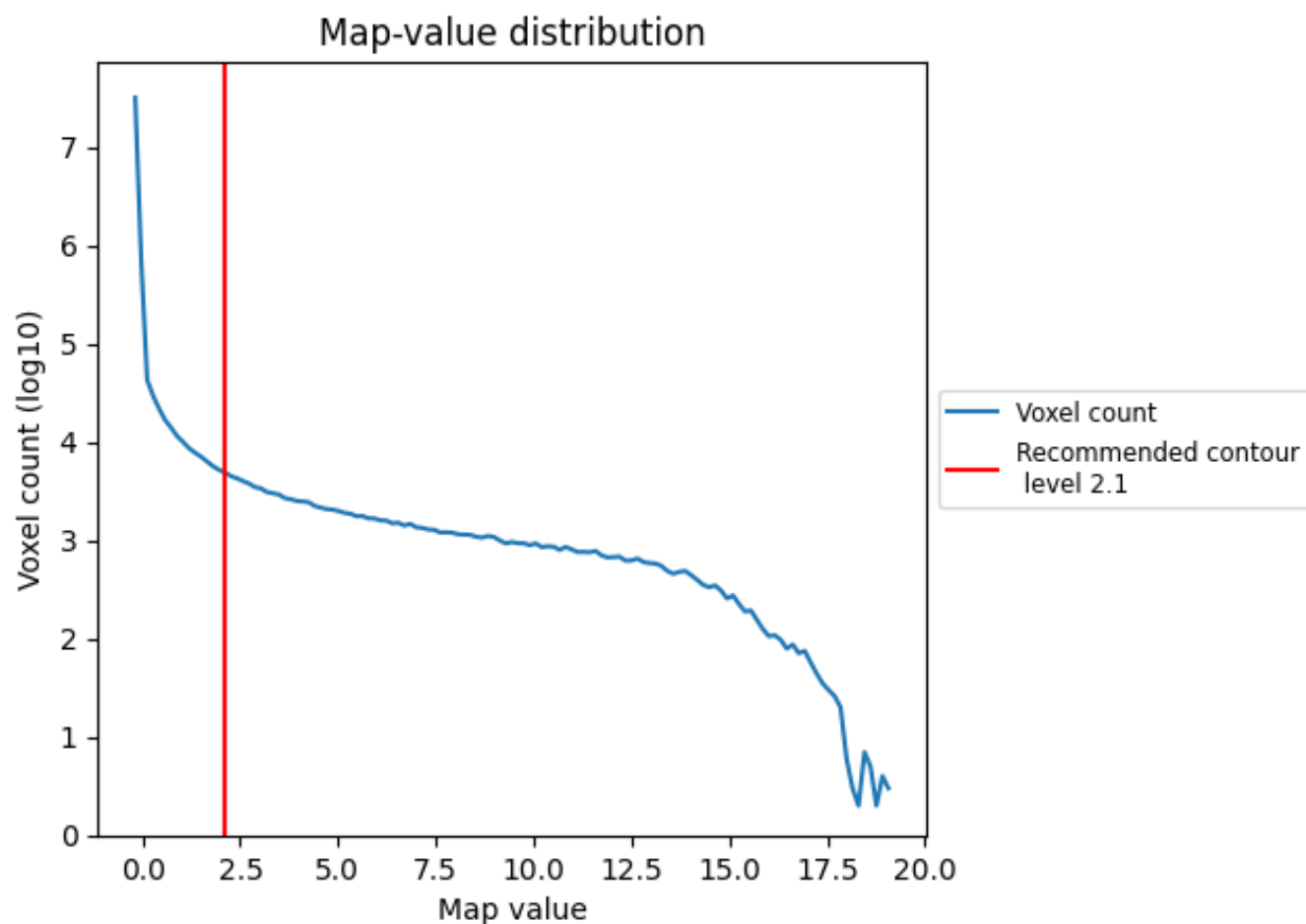
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

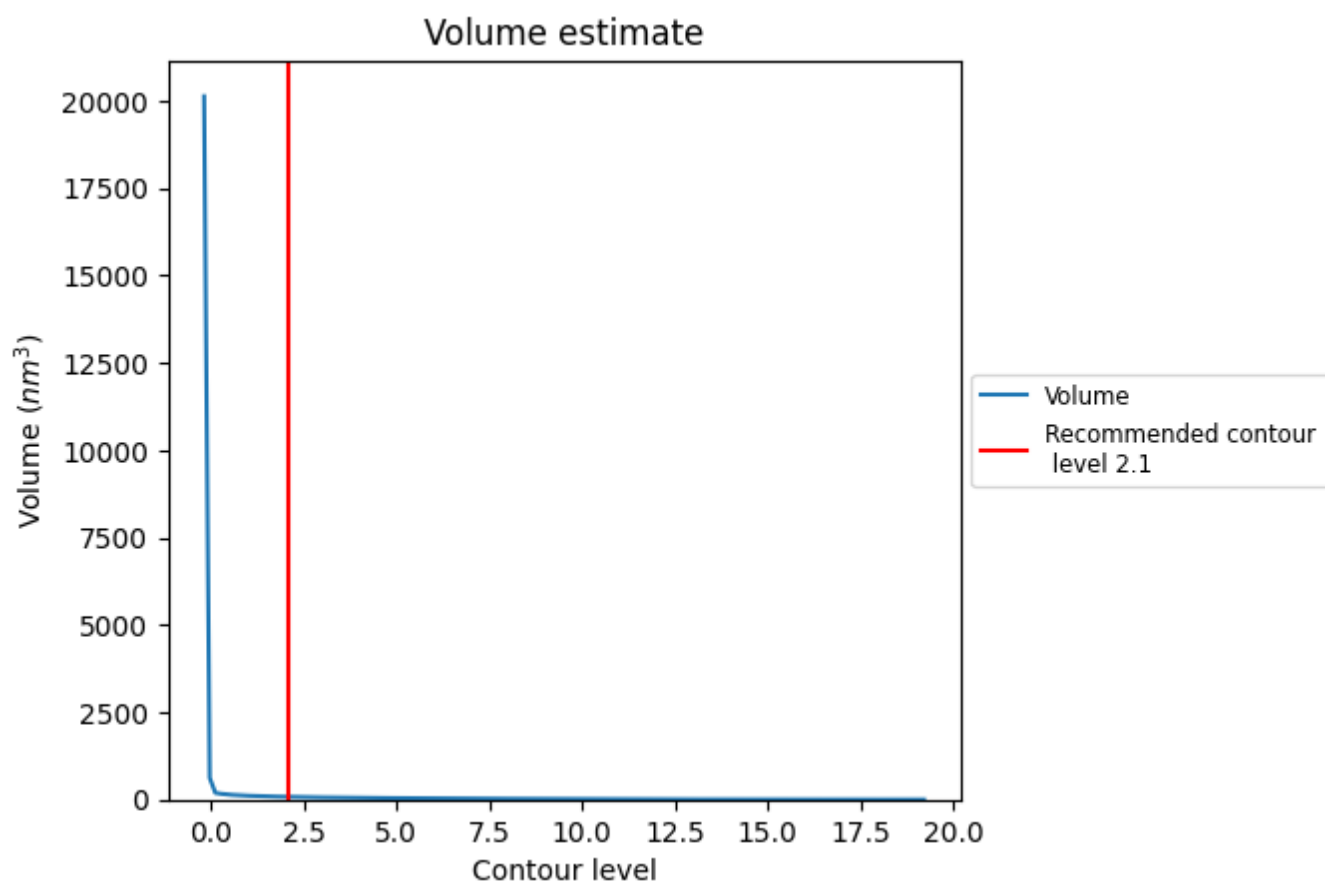
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

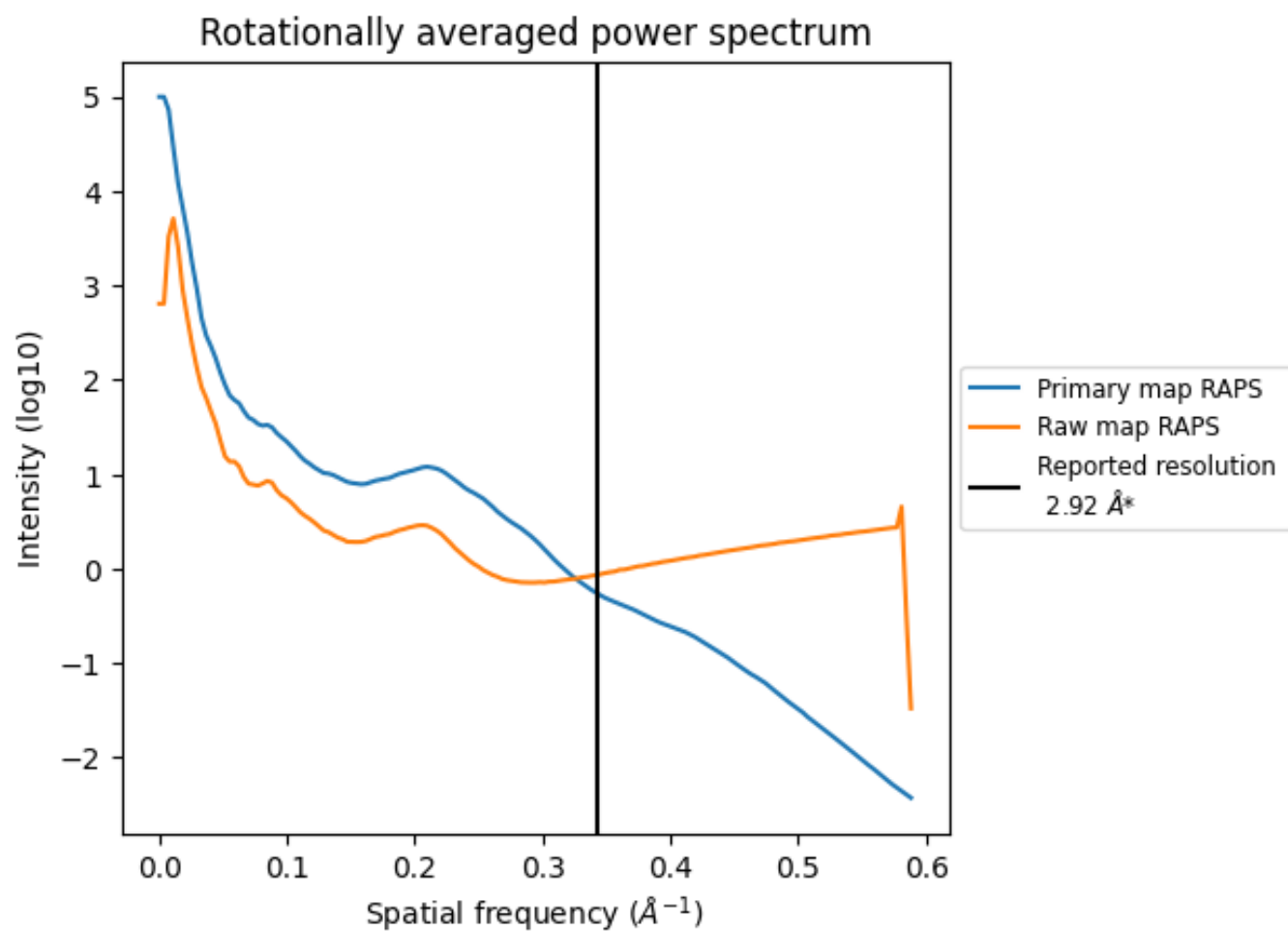
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 69 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 ⓘ

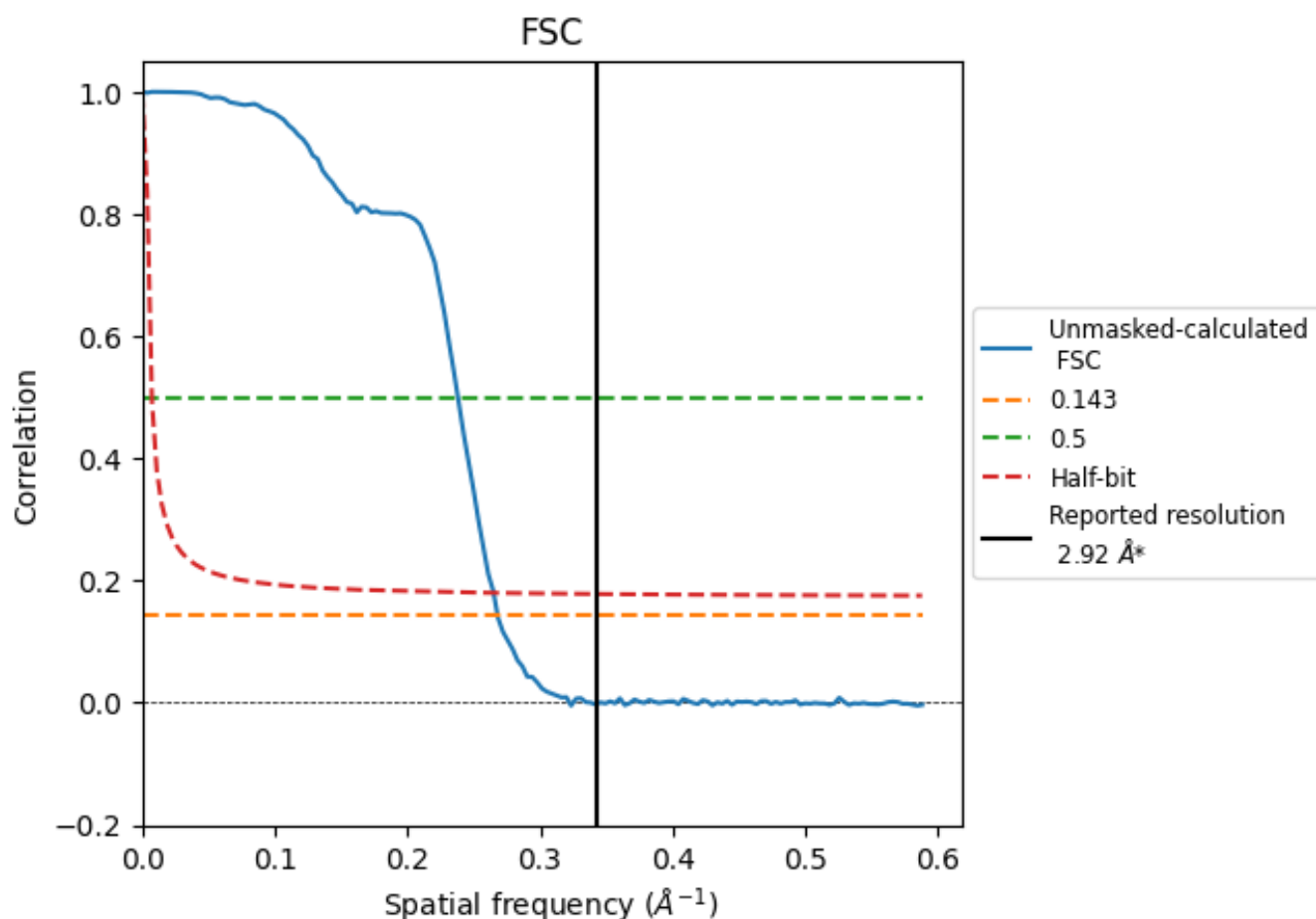


*Reported resolution corresponds to spatial frequency of 0.342 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

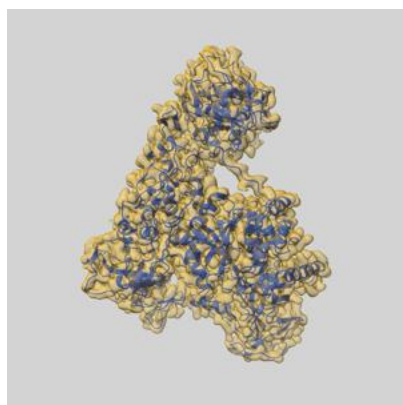
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.20	3.77

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

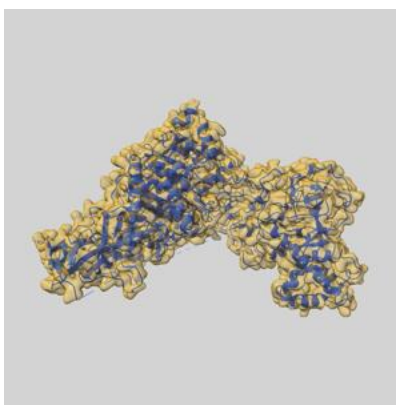
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64781 and PDB model 9V4O. Per-residue inclusion information can be found in section [3](#) on page [5](#).

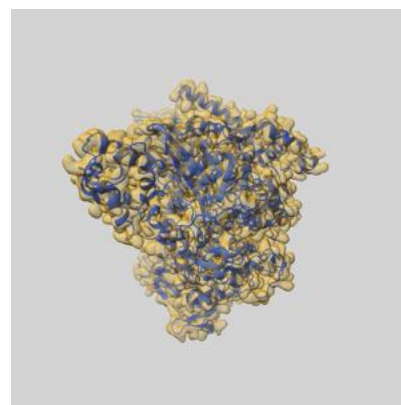
9.1 Map-model overlay [i](#)



X



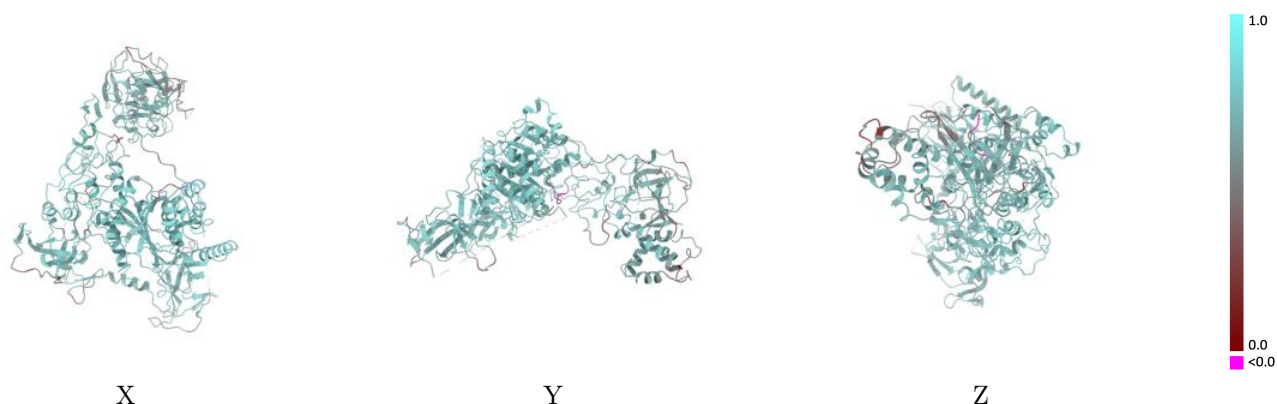
Y



Z

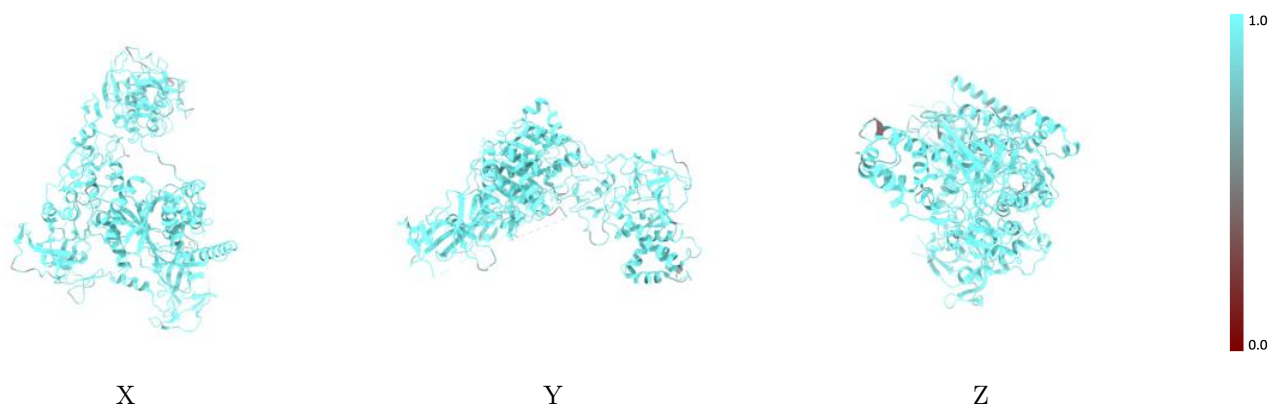
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



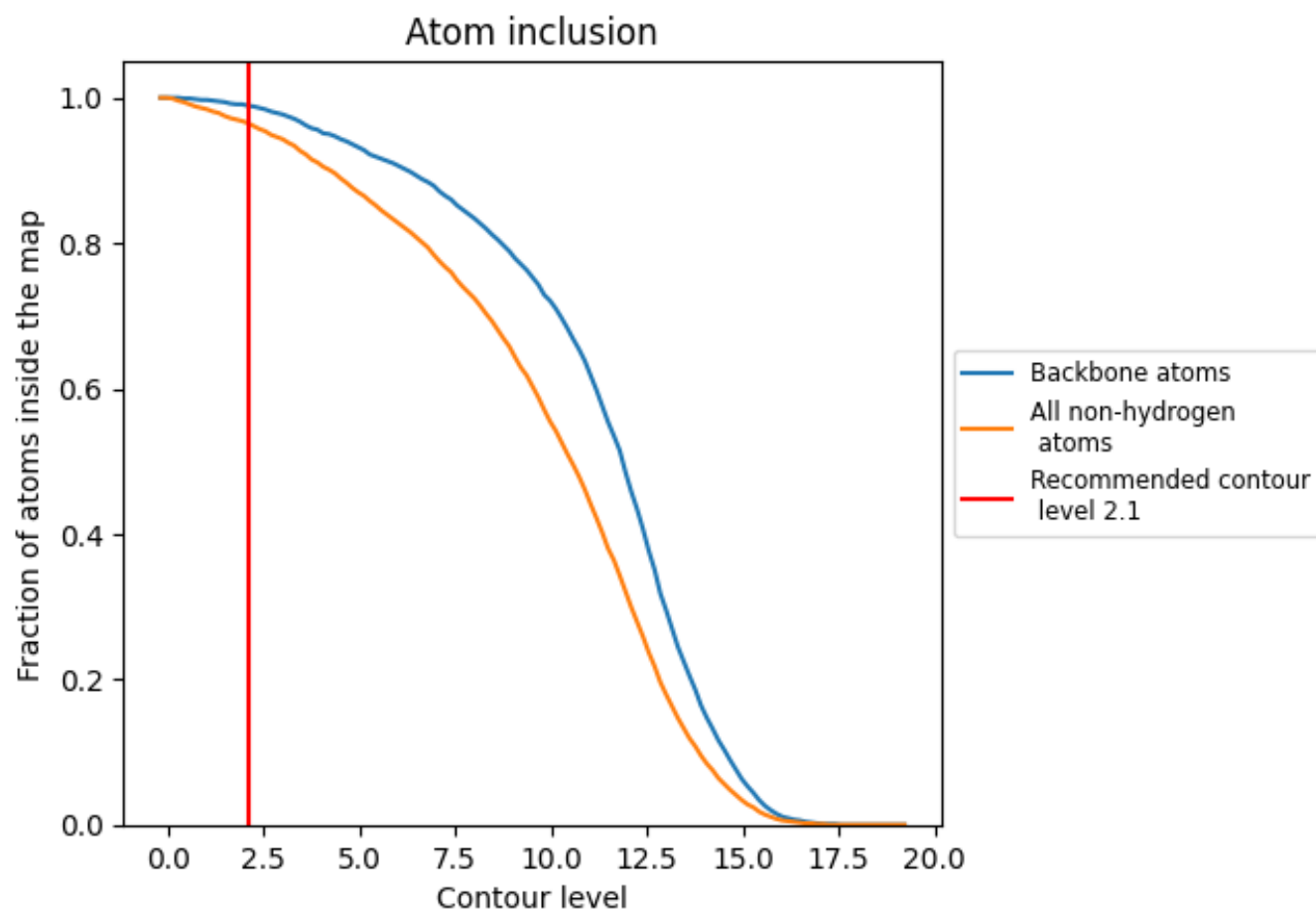
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9650	<div><div></div></div> 0.6550
A	<div><div></div></div> 0.9650	<div><div></div></div> 0.6550

