



Full wwPDB EM Validation Report ⓘ

Jul 7, 2025 – 05:20 PM JST

PDB ID : 9KWB / pdb_00009kwb
EMDB ID : EMD-62606
Title : Cas12a-PCPS-dark
Authors : Zhang, M.F.
Deposited on : 2024-12-05
Resolution : 2.60 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

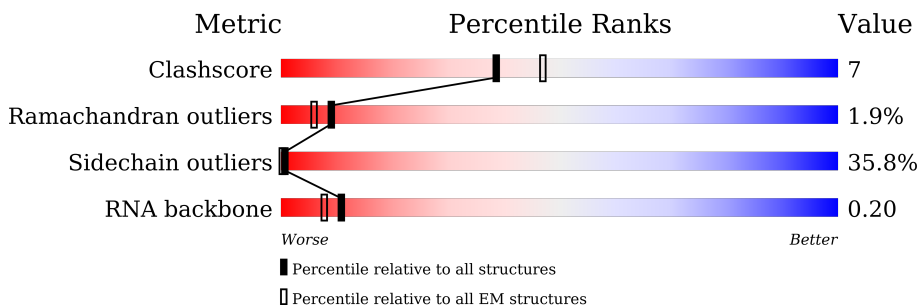
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1225	 57% 31% 10% ..
2	B	27	 56% 37% 7%
3	C	7	 57% 43%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10514 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 LbCas12a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1209	Total	C	N	O	S	0	0
			9793	6301	1598	1866	28		

- Molecule 2 is a RNA chain called RNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	27	Total	C	N	O	P	0	0
			575	257	98	193	27		

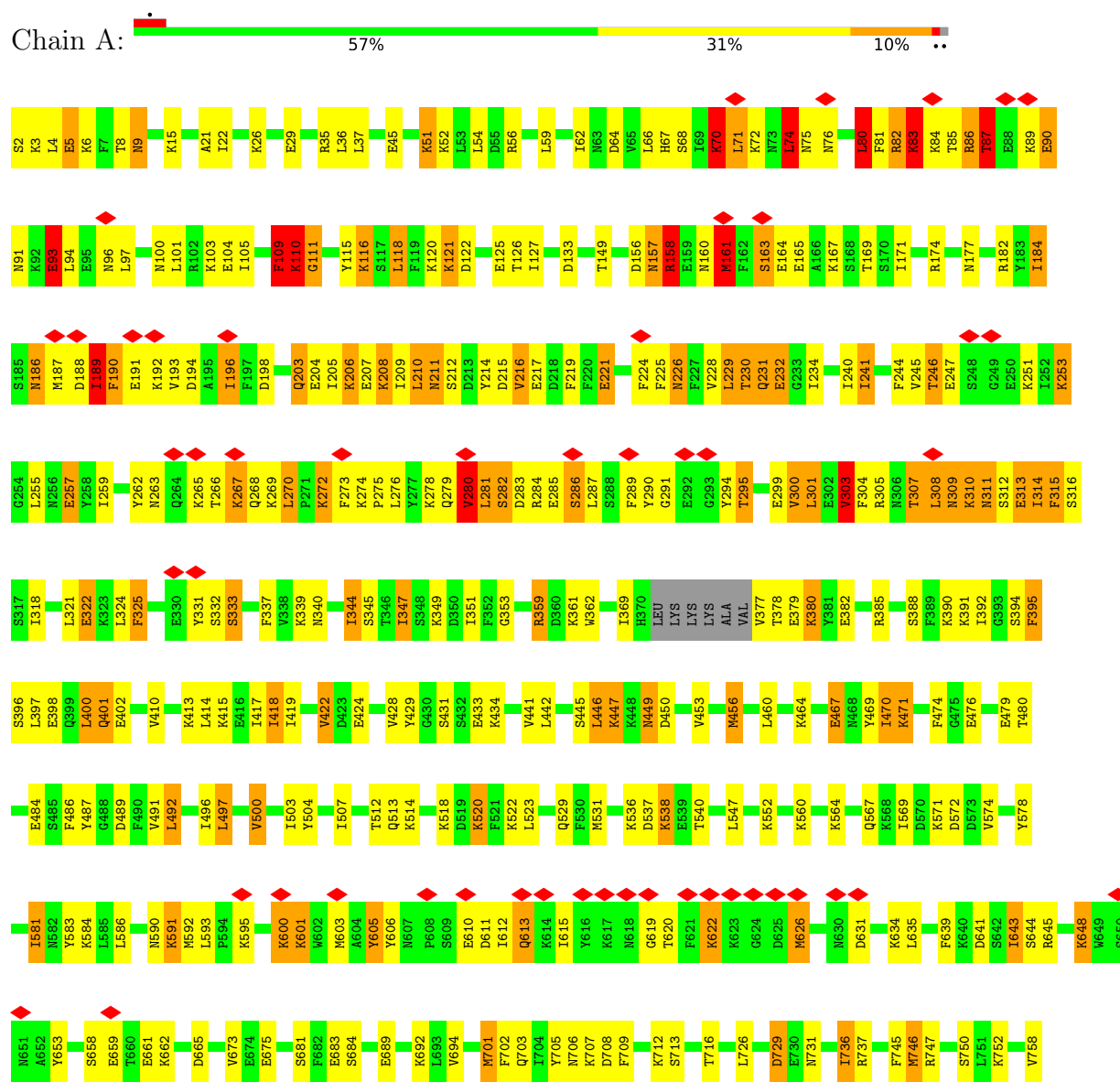
- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*AP*AP*CP*CP*CP*C)-3').

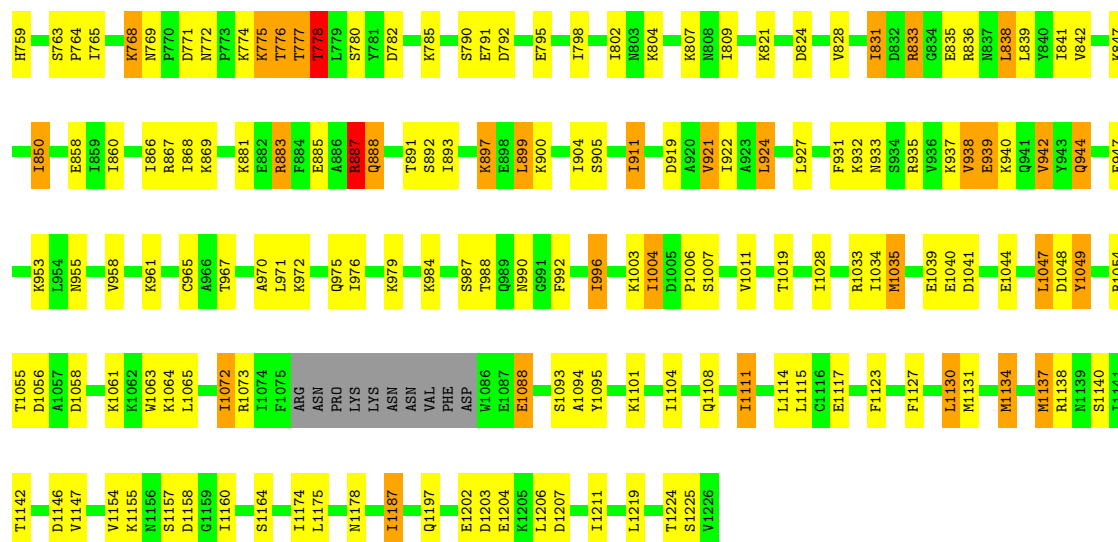
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	7	Total	C	N	O	P	0	0
			146	66	27	46	7		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: LbCas12a





• Molecule 2: RNA (27-MER)



• Molecule 3: RNA (5'-R(P*AP*AP*AP*CP*CP*CP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.886	Depositor
Minimum map value	-0.602	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	291.84, 291.84, 291.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.57, 0.57, 0.57	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.75	0/10003	0.98	59/13489 (0.4%)
2	B	0.41	0/642	0.79	1/998 (0.1%)
3	C	0.32	0/162	0.71	0/249
All	All	0.73	0/10807	0.97	60/14736 (0.4%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SER	N-CA-C	-11.48	101.54	114.62
1	A	216	VAL	N-CA-C	-10.06	103.67	113.53
1	A	290	TYR	N-CA-C	-9.74	101.39	113.38
1	A	161	MET	N-CA-C	-9.18	100.87	112.90
1	A	315	PHE	N-CA-C	-7.69	102.98	111.36
2	B	14	A	C2'-C3'-O3'	7.57	120.86	109.50
1	A	241	ILE	N-CA-C	-7.53	103.51	110.82
1	A	955	ASN	N-CA-C	-7.51	102.77	112.23
1	A	885	GLU	N-CA-C	-7.09	100.50	110.50
1	A	109	PHE	N-CA-C	7.04	121.97	113.23
1	A	775	LYS	N-CA-C	-6.88	98.71	109.72
1	A	446	LEU	N-CA-C	-6.87	102.79	113.02
1	A	992	PHE	N-CA-C	-6.75	105.08	113.38
1	A	643	ILE	N-CA-C	-6.69	103.70	111.00
1	A	919	ASP	N-CA-C	-6.64	102.23	111.52
1	A	705	TYR	N-CA-C	6.63	120.33	109.06
1	A	164	GLU	N-CA-C	-6.55	102.42	110.61
1	A	1127	PHE	N-CA-C	-6.53	104.25	111.36
1	A	1225	SER	N-CA-C	-6.47	104.42	112.90
1	A	990	ASN	N-CA-C	-6.36	105.28	114.12
1	A	768	LYS	N-CA-C	6.33	121.00	113.28
1	A	157	ASN	N-CA-C	-6.24	106.63	114.56
1	A	74	LEU	N-CA-C	-6.22	104.19	110.97
1	A	83	LYS	N-CA-C	-6.22	103.81	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	6.19	119.30	109.65
1	A	80	LEU	N-CA-C	-6.13	103.23	111.87
1	A	270	LEU	N-CA-C	-6.06	102.41	109.93
1	A	486	PHE	N-CA-C	-6.05	103.43	111.96
1	A	883	ARG	N-CA-C	-6.02	106.06	113.41
1	A	64	ASP	N-CA-C	-5.90	105.67	114.64
1	A	76	ASN	N-CA-C	-5.84	106.02	113.02
1	A	1095	TYR	N-CA-C	-5.81	104.86	111.14
1	A	211	ASN	N-CA-C	-5.74	105.77	112.89
1	A	615	ILE	N-CA-C	-5.71	104.95	110.72
1	A	267	LYS	N-CA-C	5.68	118.12	111.02
1	A	333	SER	N-CA-C	-5.68	105.08	112.23
1	A	217	GLU	CB-CA-C	-5.67	109.04	115.79
1	A	247	GLU	N-CA-C	-5.62	106.41	113.72
1	A	706	ASN	N-CA-C	-5.57	100.85	109.14
1	A	158	ARG	N-CA-C	-5.56	106.50	113.28
1	A	70	LYS	N-CA-C	-5.53	99.02	110.80
1	A	110	LYS	N-CA-C	5.52	118.08	110.35
1	A	777	THR	N-CA-C	5.52	120.38	113.43
1	A	1147	VAL	N-CA-C	5.40	115.41	107.15
1	A	189	ILE	N-CA-C	5.39	120.55	109.34
1	A	881	LYS	N-CA-C	-5.37	105.09	111.69
1	A	118	LEU	N-CA-C	-5.31	106.75	113.43
1	A	838	LEU	N-CA-C	-5.29	105.42	111.14
1	A	1048	ASP	N-CA-C	-5.27	99.82	108.41
1	A	709	PHE	N-CA-C	-5.19	106.34	113.30
1	A	93	GLU	N-CA-C	-5.15	105.36	111.69
1	A	5	GLU	N-CA-C	5.13	117.61	111.71
1	A	790	SER	N-CA-C	-5.12	106.44	113.30
1	A	309	ASN	N-CA-C	-5.10	107.01	113.18
1	A	192	LYS	N-CA-C	-5.05	106.97	113.23
1	A	447	LYS	N-CA-C	-5.05	105.82	112.94
1	A	970	ALA	N-CA-C	5.03	118.18	111.75
1	A	295	THR	N-CA-C	-5.02	108.42	114.75
1	A	1004	ILE	N-CA-C	-5.00	100.59	108.90
1	A	759	HIS	N-CA-C	-5.00	97.82	108.93

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	9793	0	9475	145	0
2	B	575	0	287	3	0
3	C	146	0	78	0	0
All	All	10514	0	9840	145	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 (145) 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:190:PHE:HB3	1:A:221:GLU:HG2	1.65	0.79
1:A:74:LEU:HD11	1:A:100:ASN:HA	1.65	0.78
1:A:244:PHE:CE2	1:A:246:THR:HG23	2.22	0.74
1:A:189:ILE:H	1:A:221:GLU:HB3	1.53	0.72
1:A:244:PHE:CZ	1:A:246:THR:HG23	2.26	0.71
1:A:746:MET:HE1	1:A:792:ASP:HB3	1.75	0.67
1:A:244:PHE:CE2	1:A:246:THR:CG2	2.80	0.65
1:A:938:VAL:HG12	1:A:942:VAL:HB	1.79	0.65
1:A:831:ILE:HD11	1:A:839:LEU:HD22	1.80	0.64
1:A:303:VAL:HG12	1:A:308:LEU:HB2	1.78	0.64
1:A:253:LYS:HB3	1:A:257:GLU:HB2	1.79	0.63
1:A:90:GLU:HA	1:A:93:GLU:HB3	1.81	0.62
1:A:86:ARG:HB2	1:A:93:GLU:HG3	1.82	0.61
1:A:606:TYR:HE2	1:A:641:ASP:HB3	1.64	0.61
1:A:887:ARG:O	1:A:887:ARG:HG2	2.00	0.60
1:A:110:LYS:O	1:A:111:GLY:C	2.45	0.60
1:A:303:VAL:HG13	1:A:307:THR:HB	1.83	0.60
1:A:203:GLN:HA	1:A:206:LYS:HE3	1.84	0.59
1:A:500:VAL:HA	1:A:503:ILE:HD12	1.84	0.59
1:A:156:ASP:HA	1:A:160:ASN:HD22	1.67	0.58
1:A:547:LEU:HD22	1:A:578:TYR:HB3	1.85	0.58
1:A:924:LEU:HD22	1:A:947:GLU:HG2	1.86	0.58
1:A:887:ARG:O	1:A:887:ARG:CG	2.54	0.56
1:A:351:ILE:HA	1:A:413:LYS:HG2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD22	1:A:523:LEU:HD22	1.88	0.55
1:A:842:VAL:HG13	1:A:850:ILE:HG23	1.89	0.53
1:A:593:LEU:HD23	1:A:639:PHE:HB3	1.91	0.53
1:A:228:VAL:HG22	1:A:232:GLU:HB2	1.90	0.52
1:A:899:LEU:HD23	2:B:10:A:H5'	1.92	0.52
1:A:467:GLU:HB2	1:A:497:LEU:HD22	1.91	0.52
1:A:1058:ASP:HB3	1:A:1061:LYS:HD3	1.92	0.52
1:A:382:GLU:HG2	1:A:385:ARG:HH11	1.74	0.52
1:A:1203:ASP:HA	1:A:1206:LEU:HG	1.92	0.50
1:A:460:LEU:HB3	1:A:504:TYR:HD1	1.76	0.50
1:A:764:PRO:HA	1:A:778:THR:HG22	1.94	0.50
1:A:263:ASN:HA	1:A:268:GLN:H	1.78	0.49
1:A:569:ILE:HD12	1:A:689:GLU:HB3	1.94	0.49
1:A:620:THR:HA	1:A:626:MET:HB2	1.94	0.49
1:A:1063:TRP:HE3	1:A:1154:VAL:HG11	1.78	0.49
1:A:900:LYS:HB3	1:A:942:VAL:HG11	1.95	0.49
1:A:314:ILE:HD12	1:A:496:ILE:HB	1.94	0.48
1:A:51:LYS:HB2	1:A:51:LYS:HE2	1.54	0.48
1:A:460:LEU:HB3	1:A:504:TYR:CD1	2.49	0.48
1:A:189:ILE:O	1:A:193:VAL:HG23	2.14	0.48
1:A:610:GLU:HA	1:A:613:GLN:HB2	1.96	0.48
1:A:4:LEU:HD23	1:A:976:ILE:HG21	1.95	0.47
1:A:807:LYS:HD3	1:A:807:LYS:HA	1.71	0.47
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.74	0.47
1:A:337:PHE:HB3	1:A:394:SER:HB2	1.97	0.47
1:A:1072:ILE:HD13	1:A:1088:GLU:HG2	1.95	0.47
1:A:1137:MET:HE3	1:A:1137:MET:HB3	1.58	0.47
1:A:311:ASN:HA	1:A:314:ILE:HD13	1.96	0.47
1:A:769:ASN:HB3	1:A:772:ASN:HB2	1.97	0.47
1:A:208:LYS:HA	1:A:208:LYS:HD3	1.56	0.46
1:A:453:VAL:HA	1:A:456:MET:HE2	1.96	0.46
1:A:538:LYS:HB3	1:A:538:LYS:HE3	1.24	0.46
1:A:726:LEU:HA	1:A:729:ASP:HB2	1.98	0.46
1:A:518:LYS:HA	1:A:747:ARG:HD2	1.96	0.46
1:A:380:LYS:HA	1:A:380:LYS:HD2	1.80	0.46
1:A:1111:ILE:HG12	1:A:1114:LEU:HB2	1.98	0.46
1:A:359:ARG:HE	1:A:359:ARG:HB3	1.34	0.45
1:A:456:MET:HE2	1:A:456:MET:HB2	1.76	0.45
1:A:82:ARG:HA	1:A:86:ARG:HH12	1.81	0.45
1:A:362:TRP:HH2	1:A:388:SER:HB2	1.80	0.45
1:A:600:LYS:H	1:A:600:LYS:HG3	1.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HB	1:A:469:TYR:HE2	1.81	0.45
1:A:86:ARG:HB3	1:A:87:THR:H	1.61	0.45
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.81	0.45
1:A:1049:TYR:O	1:A:1055:THR:HG21	2.17	0.45
1:A:1094:ALA:HB3	1:A:1130:LEU:HD21	1.99	0.45
1:A:272:LYS:H	1:A:272:LYS:HG3	1.36	0.45
1:A:1134:MET:HE3	1:A:1134:MET:HB3	1.61	0.45
1:A:619:GLY:HA2	1:A:622:LYS:HG3	1.99	0.44
1:A:244:PHE:HE2	1:A:246:THR:HG22	1.82	0.44
1:A:897:LYS:HB2	1:A:897:LYS:HE2	1.52	0.44
1:A:927:LEU:HD12	1:A:944:GLN:HG3	2.00	0.44
1:A:883:ARG:HG2	1:A:888:GLN:HA	2.00	0.44
1:A:70:LYS:HA	1:A:70:LYS:HD2	1.66	0.44
1:A:83:LYS:H	1:A:86:ARG:HH22	1.66	0.43
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.73	0.43
1:A:601:LYS:HB3	1:A:601:LYS:HE3	1.42	0.43
1:A:244:PHE:CZ	1:A:246:THR:CG2	2.98	0.43
1:A:285:GLU:HB3	1:A:286:SER:H	1.64	0.43
1:A:605:TYR:HD1	1:A:605:TYR:HA	1.71	0.43
1:A:648:LYS:HA	1:A:648:LYS:HD2	1.49	0.43
1:A:996:ILE:HD11	1:A:1187:ILE:HG23	1.99	0.43
1:A:1028:ILE:HG23	1:A:1034:ILE:HD12	2.00	0.43
1:A:401:GLN:HG2	1:A:410:VAL:HB	1.99	0.43
1:A:347:ILE:HD12	1:A:347:ILE:HA	1.58	0.43
1:A:391:LYS:HE2	1:A:391:LYS:HB2	1.61	0.43
1:A:414:LEU:HA	1:A:417:ILE:HD12	2.01	0.43
1:A:418:ILE:O	1:A:422:VAL:HG23	2.19	0.43
1:A:833:ARG:H	1:A:833:ARG:HG2	1.54	0.43
1:A:15:LYS:HG2	2:B:23:G:H5"	2.01	0.43
1:A:158:ARG:HA	1:A:158:ARG:HD3	1.56	0.43
1:A:1206:LEU:HA	1:A:1206:LEU:HD23	1.70	0.43
1:A:21:ALA:HB1	1:A:702:PHE:HB3	2.01	0.42
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.62	0.42
1:A:325:PHE:HD1	1:A:325:PHE:HA	1.70	0.42
1:A:190:PHE:HB3	1:A:221:GLU:CG	2.44	0.42
1:A:1047:LEU:HD23	1:A:1063:TRP:HB2	2.01	0.42
1:A:1115:LEU:HD22	1:A:1123:PHE:HZ	1.84	0.42
1:A:340:ASN:HA	1:A:344:ILE:HG13	2.02	0.42
1:A:520:LYS:HB2	1:A:745:PHE:HB3	2.01	0.42
1:A:785:LYS:HB2	2:B:3:A:H5"	2.00	0.42
1:A:86:ARG:O	1:A:87:THR:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HB2	1:A:121:LYS:HE2	1.27	0.42
1:A:591:LYS:HE2	1:A:591:LYS:HB2	1.25	0.42
1:A:116:LYS:HD3	1:A:116:LYS:HA	1.26	0.42
1:A:210:LEU:H	1:A:210:LEU:HG	1.61	0.42
1:A:471:LYS:HB2	1:A:471:LYS:HE3	1.74	0.42
1:A:196:ILE:H	1:A:196:ILE:HG13	1.30	0.42
1:A:449:ASN:HD22	1:A:449:ASN:HA	1.55	0.42
1:A:470:ILE:HA	1:A:470:ILE:HD12	1.77	0.42
1:A:694:VAL:HG21	1:A:701:MET:HE2	2.01	0.42
1:A:279:GLN:O	1:A:280:VAL:C	2.63	0.42
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.74	0.42
1:A:161:MET:HE3	1:A:169:THR:HB	2.02	0.41
1:A:231:GLN:HG2	1:A:234:ILE:HG13	2.02	0.41
1:A:1035:MET:HE2	1:A:1035:MET:HB2	1.58	0.41
1:A:828:VAL:HG13	1:A:921:VAL:HG12	2.02	0.41
1:A:80:LEU:H	1:A:80:LEU:HG	1.68	0.41
1:A:253:LYS:H	1:A:253:LYS:HG2	1.42	0.41
1:A:189:ILE:N	1:A:221:GLU:HB3	2.29	0.41
1:A:1219:LEU:HD23	1:A:1219:LEU:HA	1.82	0.41
1:A:226:ASN:HD22	1:A:226:ASN:HA	1.64	0.41
1:A:186:ASN:C	1:A:221:GLU:HG3	2.46	0.41
1:A:581:ILE:HD13	1:A:583:TYR:HB2	2.03	0.41
1:A:736:ILE:HG13	1:A:971:LEU:HD23	2.02	0.41
1:A:274:LYS:HA	1:A:275:PRO:HD3	1.91	0.41
1:A:839:LEU:HD21	1:A:938:VAL:HG21	2.02	0.41
1:A:312:SER:HA	1:A:315:PHE:CD2	2.56	0.41
1:A:841:ILE:HD11	1:A:911:ILE:HD11	2.03	0.41
1:A:121:LYS:H	1:A:121:LYS:HG3	1.49	0.41
1:A:838:LEU:HD23	1:A:937:LYS:HA	2.02	0.41
1:A:395:PHE:HD1	1:A:395:PHE:HA	1.74	0.40
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.94	0.40
1:A:474:PHE:HA	1:A:487:TYR:HE1	1.85	0.40
1:A:868:ILE:HD13	1:A:868:ILE:HA	1.93	0.40
1:A:939:GLU:H	1:A:939:GLU:HG3	1.56	0.40
1:A:1006:PRO:HB2	1:A:1175:LEU:HD22	2.02	0.40
1:A:109:PHE:O	1:A:110:LYS:C	2.64	0.40
1:A:310:LYS:HA	1:A:313:GLU:HB2	2.03	0.40
1:A:322:GLU:O	1:A:325:PHE:HB2	2.20	0.40
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.91	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	1203/1225 (98%)	1051 (87%)	129 (11%)	23 (2%)	6	13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	VAL
1	A	887	ARG
1	A	87	THR
1	A	163	SER
1	A	281	LEU
1	A	291	GLY
1	A	300	VAL
1	A	303	VAL
1	A	353	GLY
1	A	778	THR
1	A	229	LEU
1	A	230	THR
1	A	776	THR
1	A	167	LYS
1	A	188	ASP
1	A	282	SER
1	A	286	SER
1	A	71	LEU
1	A	177	ASN
1	A	246	THR
1	A	933	ASN
1	A	111	GLY
1	A	209	ILE

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	1046/1112 (94%)	672 (64%)	374 (36%)	0 0

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LYS
1	A	5	GLU
1	A	6	LYS
1	A	8	THR
1	A	9	ASN
1	A	22	ILE
1	A	26	LYS
1	A	29	GLU
1	A	35	ARG
1	A	36	LEU
1	A	45	GLU
1	A	51	LYS
1	A	52	LYS
1	A	54	LEU
1	A	56	ARG
1	A	59	LEU
1	A	62	ILE
1	A	66	LEU
1	A	67	HIS
1	A	70	LYS
1	A	71	LEU
1	A	72	LYS
1	A	74	LEU
1	A	75	ASN
1	A	80	LEU
1	A	81	PHE
1	A	82	ARG
1	A	83	LYS
1	A	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	85	THR
1	A	86	ARG
1	A	87	THR
1	A	89	LYS
1	A	90	GLU
1	A	91	ASN
1	A	93	GLU
1	A	94	LEU
1	A	96	ASN
1	A	97	LEU
1	A	101	LEU
1	A	103	LYS
1	A	104	GLU
1	A	105	ILE
1	A	109	PHE
1	A	110	LYS
1	A	115	TYR
1	A	116	LYS
1	A	118	LEU
1	A	120	LYS
1	A	121	LYS
1	A	122	ASP
1	A	125	GLU
1	A	126	THR
1	A	127	ILE
1	A	133	ASP
1	A	149	THR
1	A	157	ASN
1	A	158	ARG
1	A	161	MET
1	A	163	SER
1	A	165	GLU
1	A	171	ILE
1	A	174	ARG
1	A	182	ARG
1	A	184	ILE
1	A	186	ASN
1	A	187	MET
1	A	189	ILE
1	A	190	PHE
1	A	191	GLU
1	A	194	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	ILE
1	A	198	ASP
1	A	203	GLN
1	A	204	GLU
1	A	205	ILE
1	A	206	LYS
1	A	207	GLU
1	A	208	LYS
1	A	210	LEU
1	A	211	ASN
1	A	212	SER
1	A	214	TYR
1	A	215	ASP
1	A	216	VAL
1	A	219	PHE
1	A	221	GLU
1	A	225	PHE
1	A	226	ASN
1	A	229	LEU
1	A	230	THR
1	A	231	GLN
1	A	232	GLU
1	A	240	ILE
1	A	241	ILE
1	A	245	VAL
1	A	251	LYS
1	A	253	LYS
1	A	255	LEU
1	A	257	GLU
1	A	259	ILE
1	A	262	TYR
1	A	265	LYS
1	A	266	THR
1	A	267	LYS
1	A	269	LYS
1	A	270	LEU
1	A	272	LYS
1	A	273	PHE
1	A	276	LEU
1	A	278	LYS
1	A	280	VAL
1	A	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	282	SER
1	A	283	ASP
1	A	284	ARG
1	A	287	LEU
1	A	289	PHE
1	A	294	TYR
1	A	295	THR
1	A	299	GLU
1	A	300	VAL
1	A	301	LEU
1	A	303	VAL
1	A	304	PHE
1	A	305	ARG
1	A	307	THR
1	A	308	LEU
1	A	309	ASN
1	A	310	LYS
1	A	311	ASN
1	A	313	GLU
1	A	314	ILE
1	A	316	SER
1	A	318	ILE
1	A	321	LEU
1	A	322	GLU
1	A	324	LEU
1	A	325	PHE
1	A	331	TYR
1	A	332	SER
1	A	333	SER
1	A	339	LYS
1	A	344	ILE
1	A	345	SER
1	A	347	ILE
1	A	349	LYS
1	A	359	ARG
1	A	361	LYS
1	A	369	ILE
1	A	377	VAL
1	A	378	THR
1	A	379	GLU
1	A	380	LYS
1	A	390	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	392	ILE
1	A	395	PHE
1	A	396	SER
1	A	398	GLU
1	A	400	LEU
1	A	401	GLN
1	A	402	GLU
1	A	415	LYS
1	A	418	ILE
1	A	419	ILE
1	A	422	VAL
1	A	424	GLU
1	A	428	VAL
1	A	429	TYR
1	A	431	SER
1	A	433	GLU
1	A	434	LYS
1	A	441	VAL
1	A	442	LEU
1	A	445	SER
1	A	446	LEU
1	A	447	LYS
1	A	449	ASN
1	A	450	ASP
1	A	456	MET
1	A	464	LYS
1	A	467	GLU
1	A	470	ILE
1	A	471	LYS
1	A	476	GLU
1	A	479	GLU
1	A	480	THR
1	A	484	GLU
1	A	489	ASP
1	A	491	VAL
1	A	492	LEU
1	A	497	LEU
1	A	500	VAL
1	A	507	ILE
1	A	512	THR
1	A	513	GLN
1	A	514	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	LYS
1	A	522	LYS
1	A	529	GLN
1	A	531	MET
1	A	536	LYS
1	A	537	ASP
1	A	538	LYS
1	A	540	THR
1	A	552	LYS
1	A	560	LYS
1	A	564	LYS
1	A	567	GLN
1	A	571	LYS
1	A	572	ASP
1	A	574	VAL
1	A	581	ILE
1	A	584	LYS
1	A	586	LEU
1	A	590	ASN
1	A	591	LYS
1	A	592	MET
1	A	595	LYS
1	A	600	LYS
1	A	601	LYS
1	A	603	MET
1	A	605	TYR
1	A	611	ASP
1	A	612	ILE
1	A	613	GLN
1	A	622	LYS
1	A	626	MET
1	A	631	ASP
1	A	634	LYS
1	A	635	LEU
1	A	643	ILE
1	A	644	SER
1	A	645	ARG
1	A	648	LYS
1	A	653	TYR
1	A	658	SER
1	A	659	GLU
1	A	661	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	662	LYS
1	A	665	ASP
1	A	673	VAL
1	A	675	GLU
1	A	681	SER
1	A	683	GLU
1	A	684	SER
1	A	692	LYS
1	A	701	MET
1	A	703	GLN
1	A	707	LYS
1	A	708	ASP
1	A	712	LYS
1	A	713	SER
1	A	716	THR
1	A	729	ASP
1	A	731	ASN
1	A	736	ILE
1	A	737	ARG
1	A	746	MET
1	A	750	SER
1	A	752	LYS
1	A	758	VAL
1	A	763	SER
1	A	765	ILE
1	A	768	LYS
1	A	771	ASP
1	A	774	LYS
1	A	775	LYS
1	A	776	THR
1	A	777	THR
1	A	778	THR
1	A	780	SER
1	A	782	ASP
1	A	791	GLU
1	A	795	GLU
1	A	798	ILE
1	A	802	ILE
1	A	804	LYS
1	A	809	ILE
1	A	821	LYS
1	A	824	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	831	ILE
1	A	833	ARG
1	A	835	GLU
1	A	836	ARG
1	A	847	LYS
1	A	850	ILE
1	A	858	GLU
1	A	860	ILE
1	A	866	ILE
1	A	867	ARG
1	A	869	LYS
1	A	887	ARG
1	A	888	GLN
1	A	891	THR
1	A	892	SER
1	A	893	ILE
1	A	897	LYS
1	A	899	LEU
1	A	904	ILE
1	A	905	SER
1	A	911	ILE
1	A	921	VAL
1	A	922	ILE
1	A	924	LEU
1	A	931	PHE
1	A	932	LYS
1	A	935	ARG
1	A	938	VAL
1	A	939	GLU
1	A	940	LYS
1	A	942	VAL
1	A	944	GLN
1	A	953	LYS
1	A	958	VAL
1	A	961	LYS
1	A	965	CYS
1	A	967	THR
1	A	972	LYS
1	A	975	GLN
1	A	979	LYS
1	A	984	LYS
1	A	987	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	988	THR
1	A	996	ILE
1	A	1003	LYS
1	A	1004	ILE
1	A	1007	SER
1	A	1011	VAL
1	A	1019	THR
1	A	1033	ARG
1	A	1035	MET
1	A	1039	GLU
1	A	1040	GLU
1	A	1041	ASP
1	A	1044	GLU
1	A	1047	LEU
1	A	1049	TYR
1	A	1054	ARG
1	A	1056	ASP
1	A	1064	LYS
1	A	1065	LEU
1	A	1072	ILE
1	A	1073	ARG
1	A	1088	GLU
1	A	1093	SER
1	A	1101	LYS
1	A	1104	ILE
1	A	1108	GLN
1	A	1111	ILE
1	A	1117	GLU
1	A	1130	LEU
1	A	1131	MET
1	A	1134	MET
1	A	1137	MET
1	A	1138	ARG
1	A	1140	SER
1	A	1142	THR
1	A	1146	ASP
1	A	1155	LYS
1	A	1157	SER
1	A	1158	ASP
1	A	1160	ILE
1	A	1164	SER
1	A	1174	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1178	ASN
1	A	1187	ILE
1	A	1197	GLN
1	A	1202	GLU
1	A	1204	GLU
1	A	1207	ASP
1	A	1211	ILE
1	A	1224	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	30	ASN
1	A	33	ASN
1	A	75	ASN
1	A	91	ASN
1	A	96	ASN
1	A	112	ASN
1	A	142	ASN
1	A	145	ASN
1	A	160	ASN
1	A	226	ASN
1	A	279	GLN
1	A	401	GLN
1	A	449	ASN
1	A	502	HIS
1	A	513	GLN
1	A	529	GLN
1	A	630	ASN
1	A	703	GLN
1	A	759	HIS
1	A	767	ASN
1	A	772	ASN
1	A	888	GLN
1	A	895	ASN
1	A	928	ASN
1	A	933	ASN
1	A	944	GLN
1	A	955	ASN
1	A	990	ASN
1	A	1100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1105	ASN
1	A	1136	GLN
1	A	1170	GLN
1	A	1172	ASN
1	A	1197	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	26/27 (96%)	9 (34%)	3 (11%)
3	C	6/7 (85%)	3 (50%)	0
All	All	32/34 (94%)	12 (37%)	3 (9%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	U
2	B	15	G
2	B	16	U
2	B	17	G
2	B	23	G
2	B	24	G
2	B	26	G
2	B	28	U
2	B	29	U
3	C	32	A
3	C	33	A
3	C	34	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	14	A
2	B	23	G
2	B	28	U

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

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](#)

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.

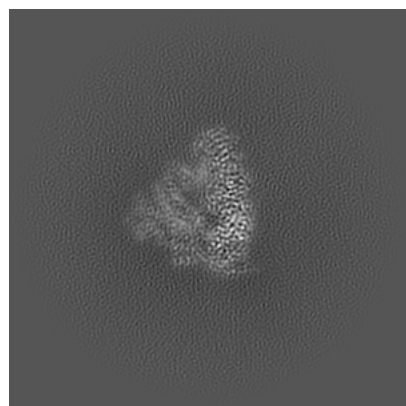
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62606. These allow visual inspection of the internal detail of the map and identification of artifacts.

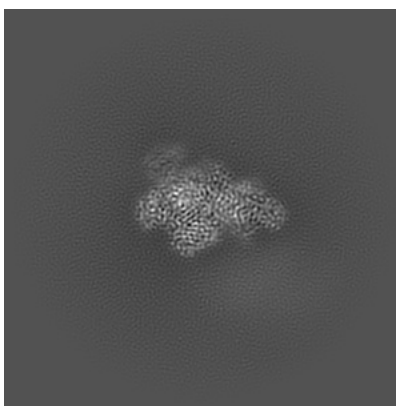
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

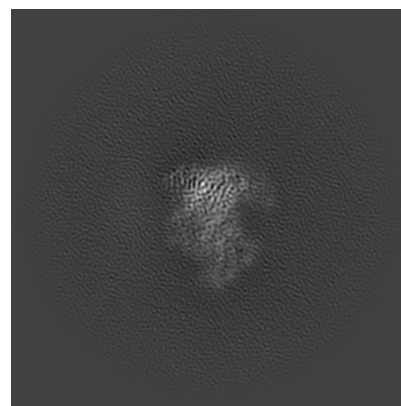
6.1.1 Primary map



X

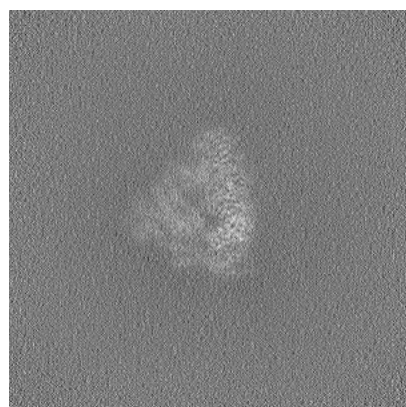


Y

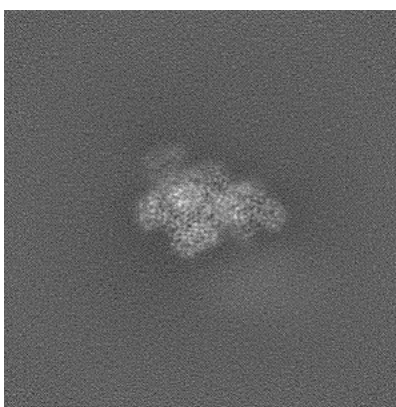


Z

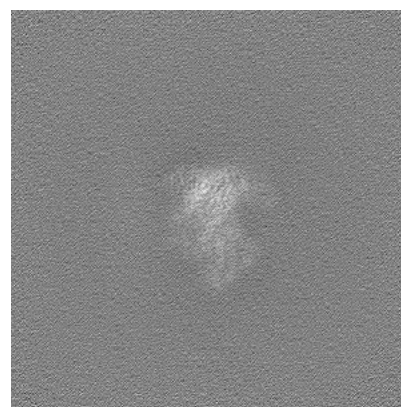
6.1.2 Raw map



X



Y

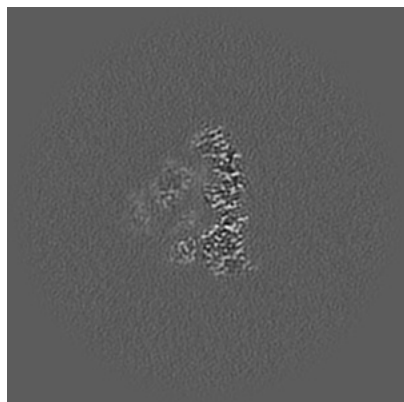


Z

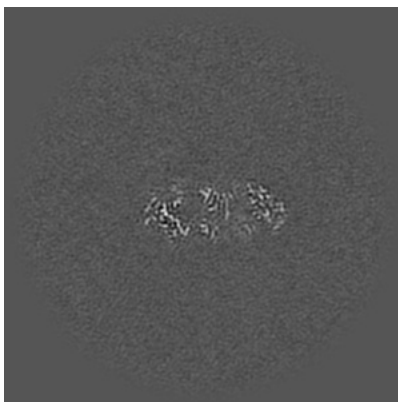
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

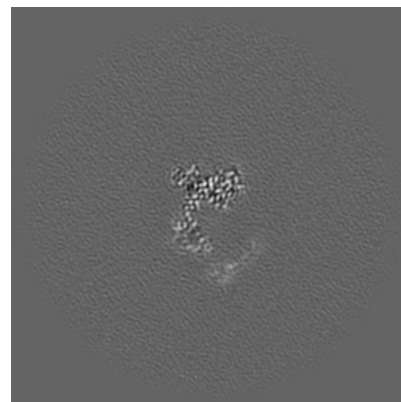
6.2.1 Primary map



X Index: 256

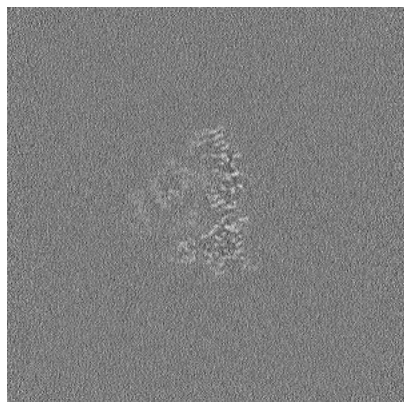


Y Index: 256

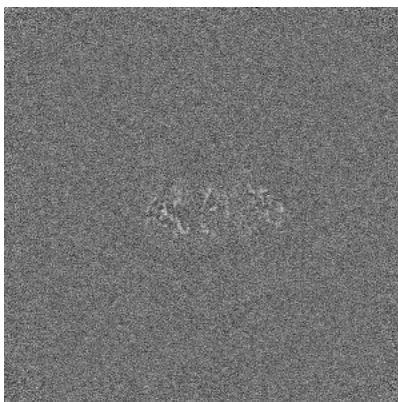


Z Index: 256

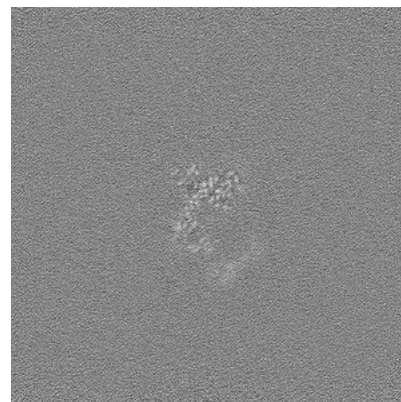
6.2.2 Raw map



X Index: 256



Y Index: 256

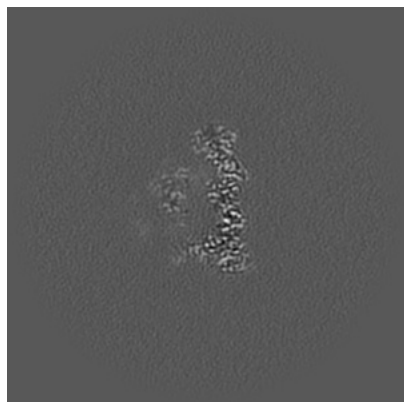


Z Index: 256

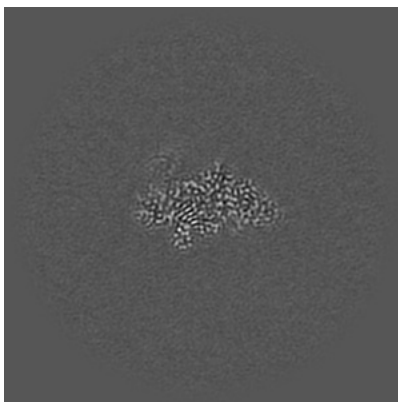
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

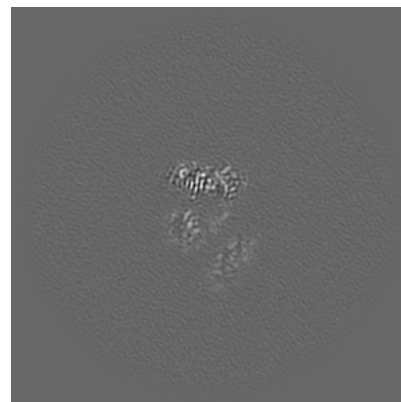
6.3.1 Primary map



X Index: 247

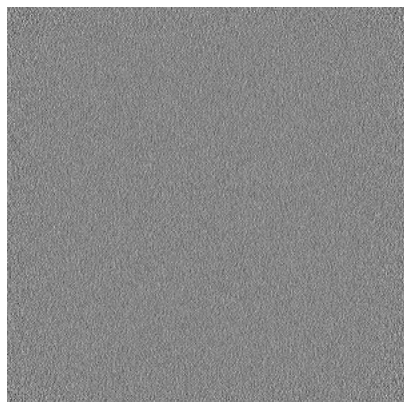


Y Index: 279

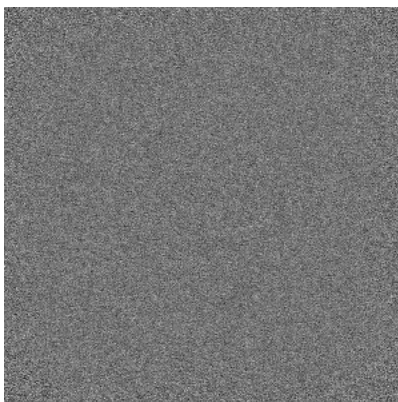


Z Index: 244

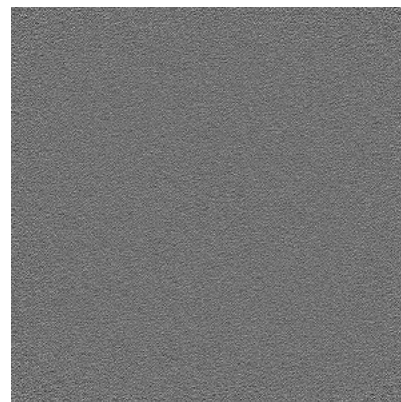
6.3.2 Raw map



X Index: 0



Y Index: 0

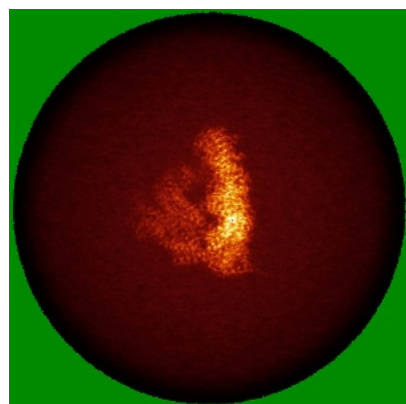


Z Index: 0

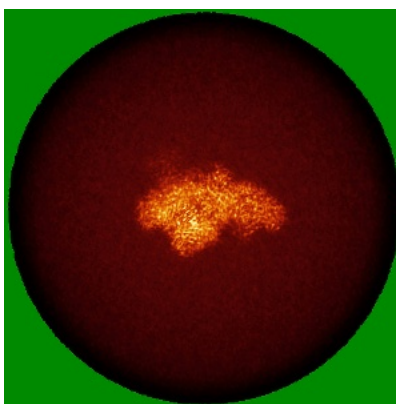
The images above show the largest variance slices of the map in three orthogonal directions.

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

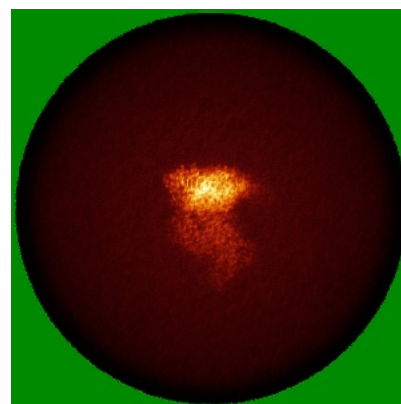
6.4.1 Primary map



X

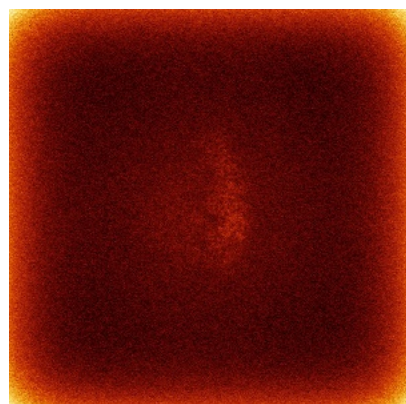


Y

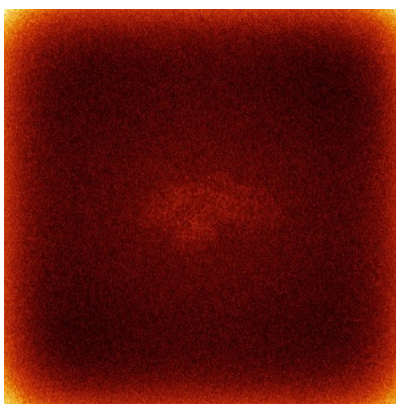


Z

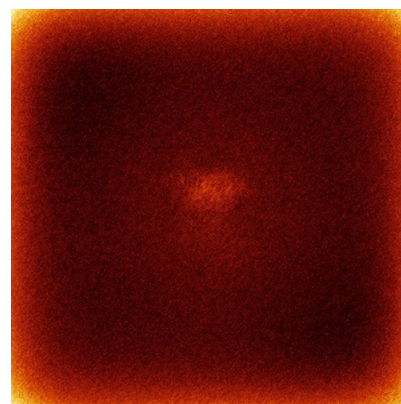
6.4.2 Raw map



X



Y

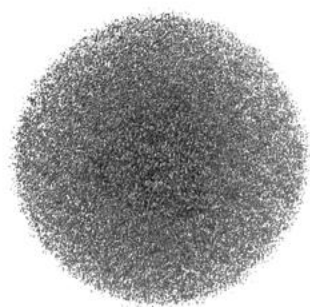


Z

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](#)

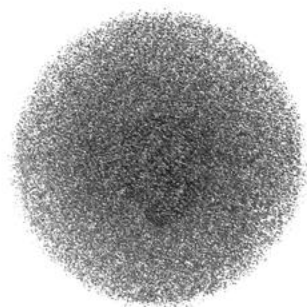
6.5.1 Primary map



X



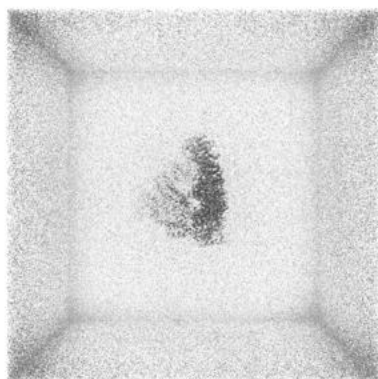
Y



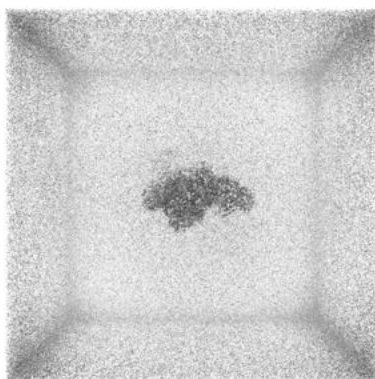
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

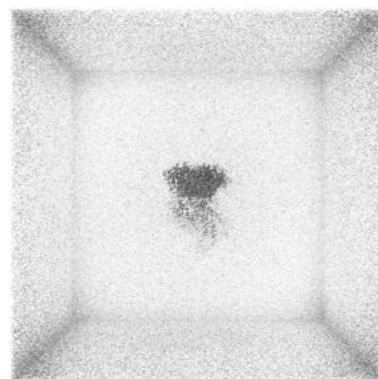
6.5.2 Raw map



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.

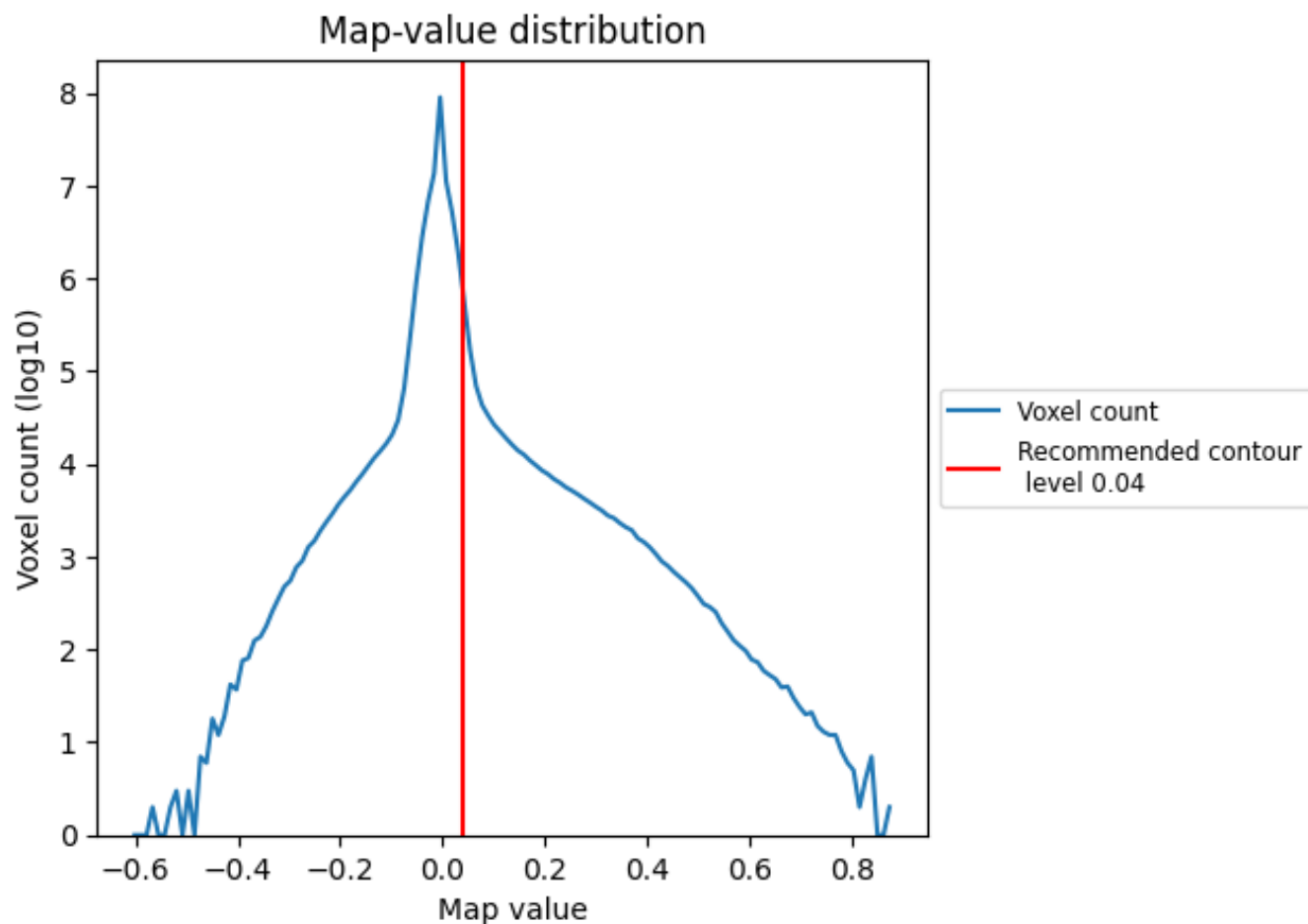
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

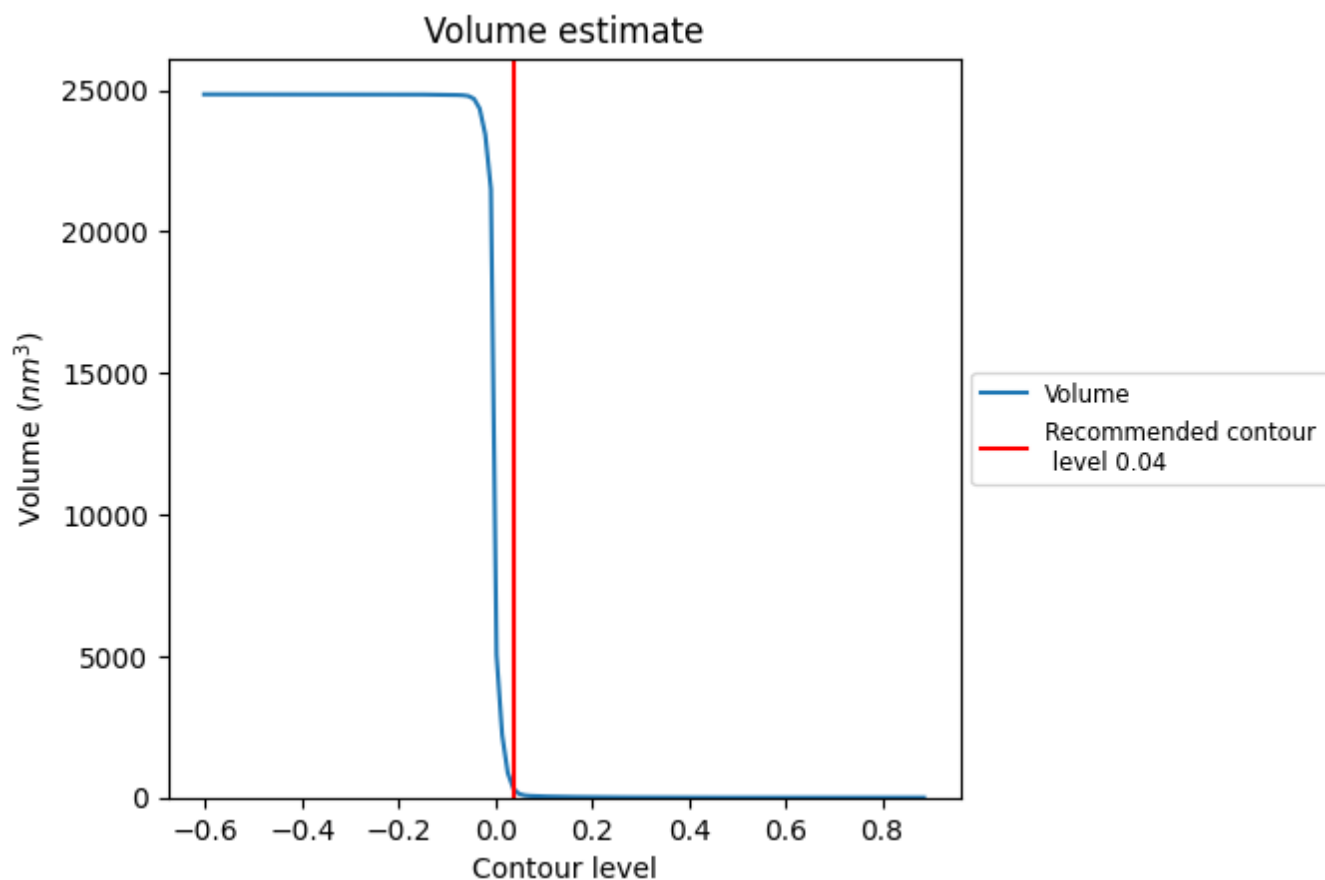
This section contains the results of statistical analysis of the map.

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.

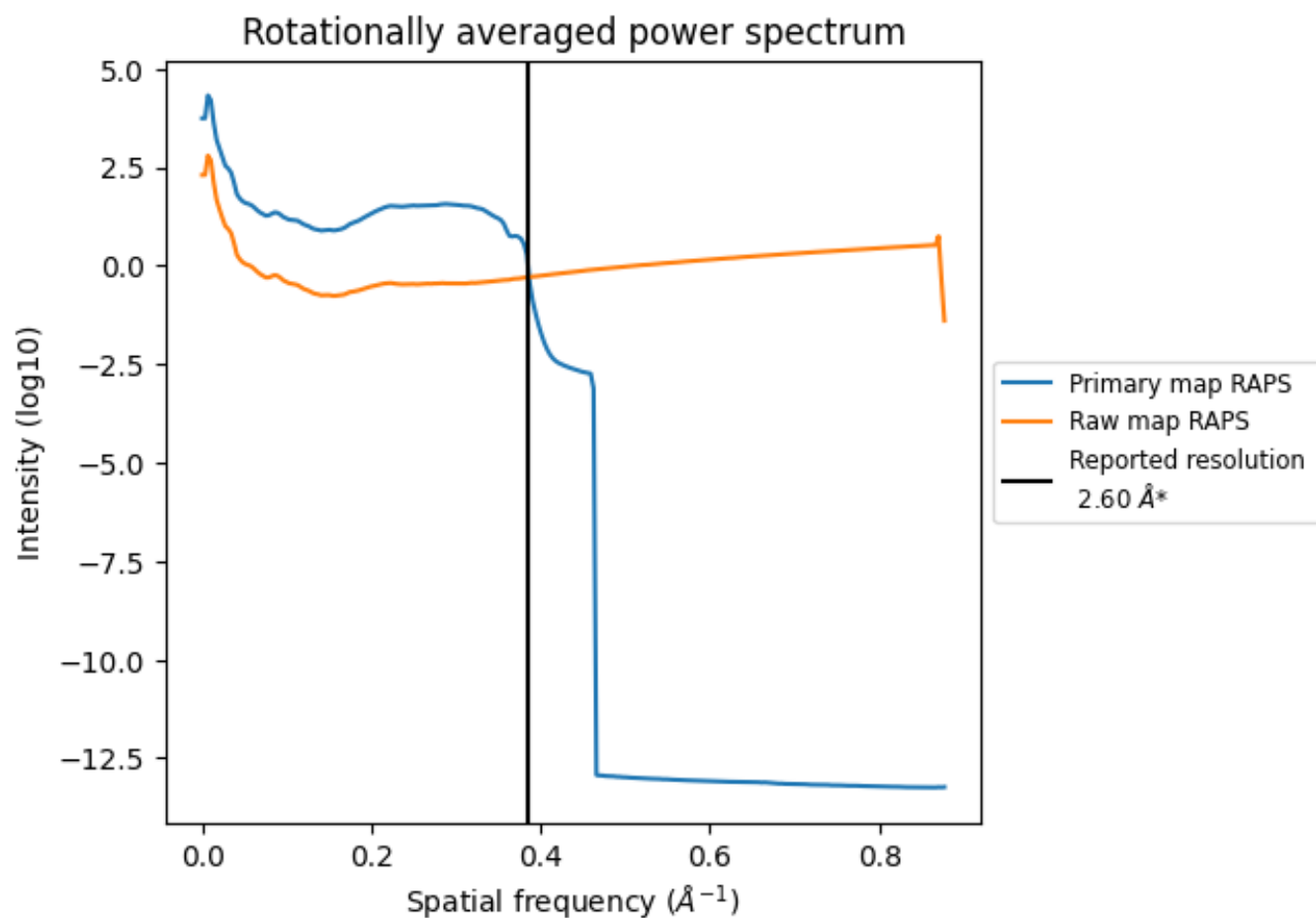
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm^3 ; this corresponds to an approximate mass of 243 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 ⓘ

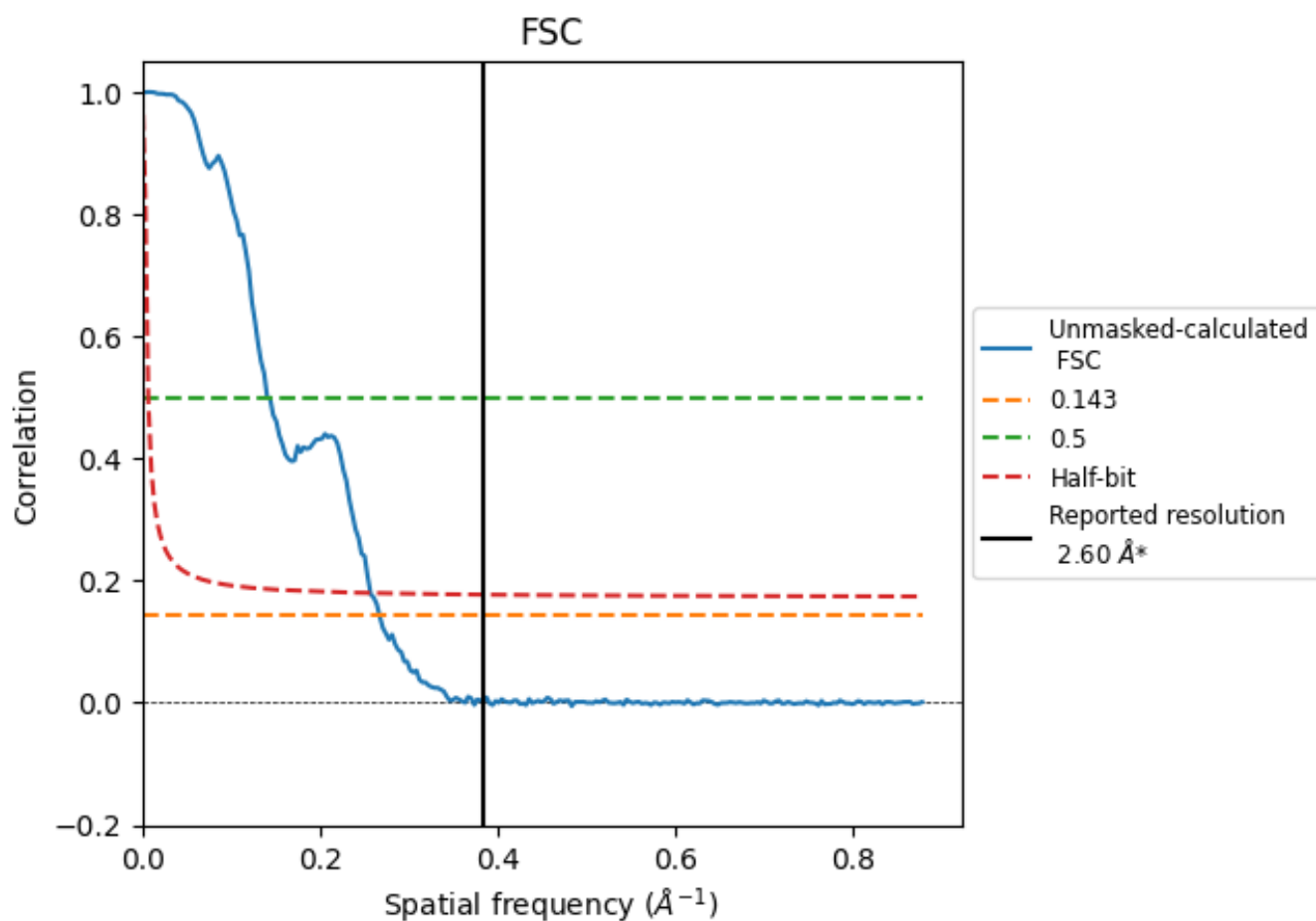


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

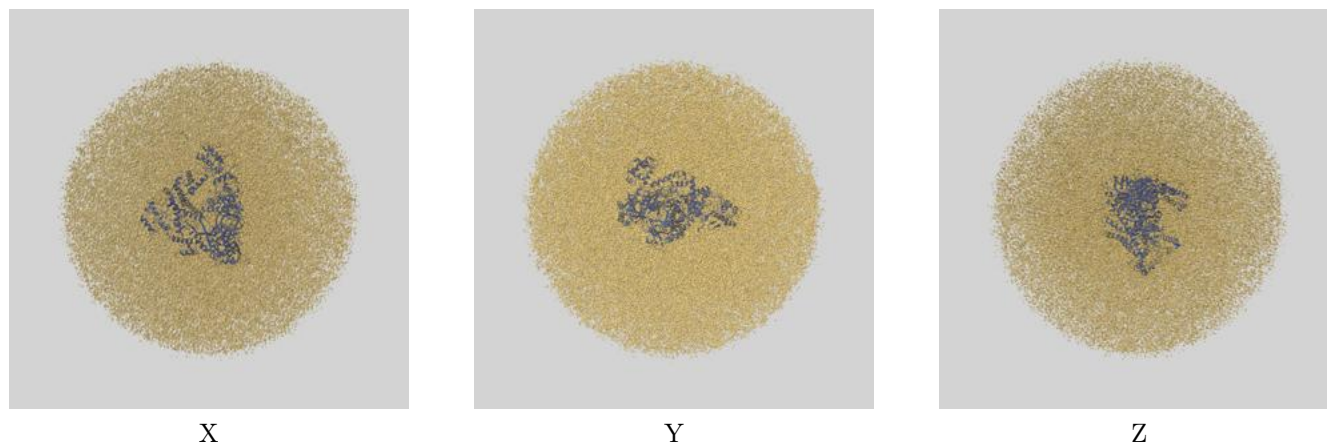
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	7.09	3.89

*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 3.75 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

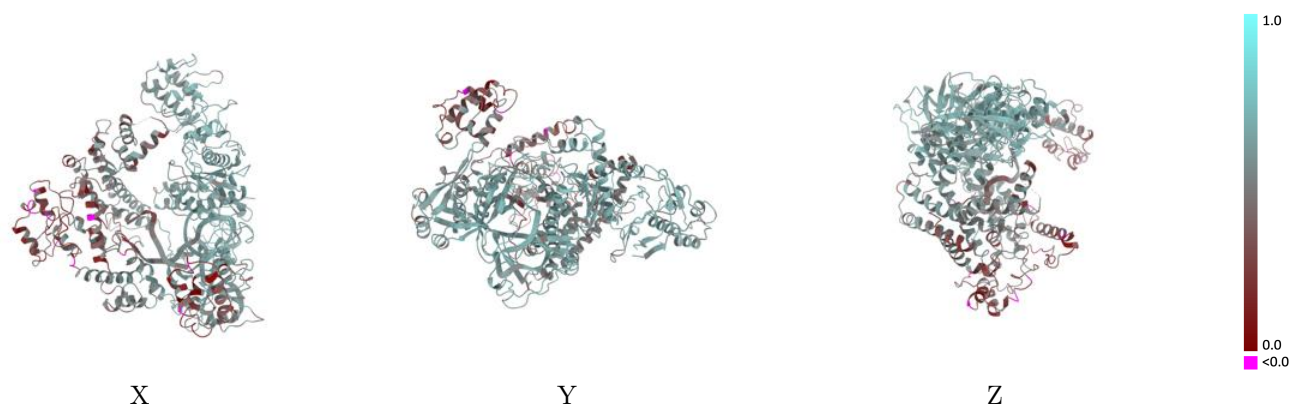
This section contains information regarding the fit between EMDB map EMD-62606 and PDB model 9KWB. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



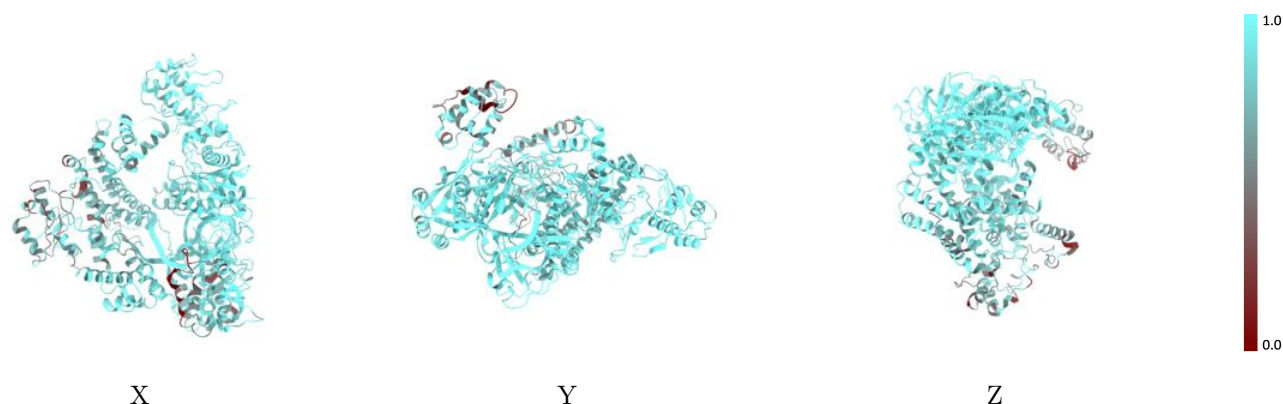
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



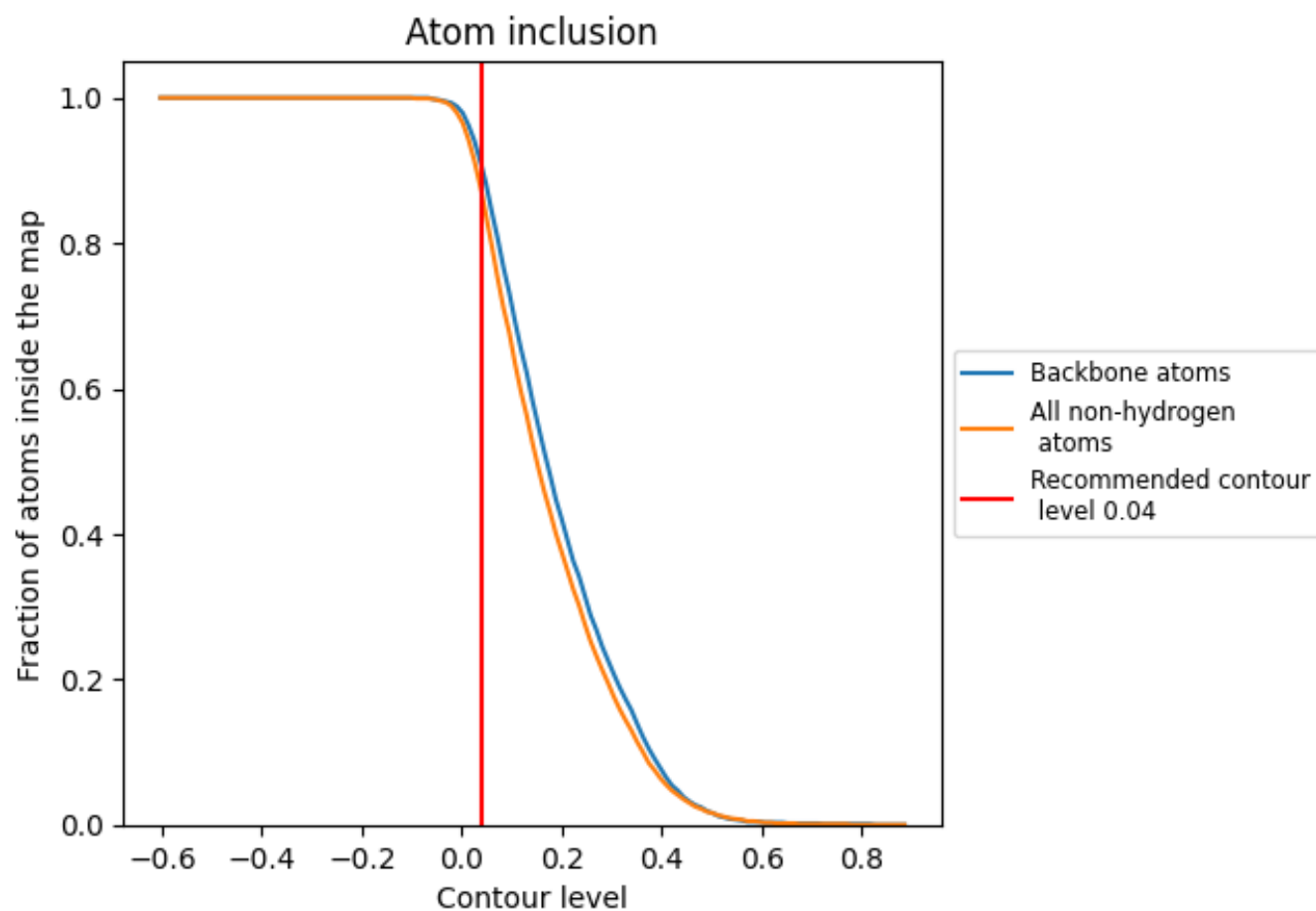
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8700	<div></div> 0.5080
A	<div></div> 0.8640	<div></div> 0.5060
B	<div></div> 0.9600	<div></div> 0.5760
C	<div></div> 0.8970	<div></div> 0.4120

