



Full wwPDB EM Validation Report ⓘ

Jun 16, 2026 – 06:26 PM EDT

PDB ID : 10MK / pdb_000010mk
EMDB ID : EMD-75288
Title : SemiClosed Mtb-EC: Cryo-EM structure of Mtb RNAP elongation complex (substrate loading mimic) with a semiclosed active site (closed TL, open RH-FL)
Authors : Dhingra, Y.; Darst, S.A.
Deposited on : 2026-01-27
Resolution : 3.30 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:

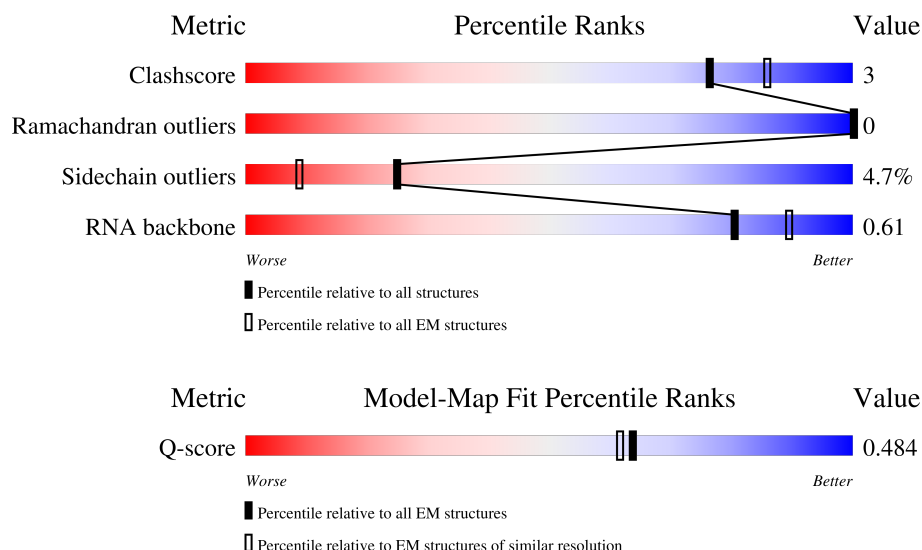
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	347	
1	B	347	
2	E	110	

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Mol	Chain	Length	Quality of chain
3	P	54	<div><div></div><div>43%19%39%</div></div>
4	R	20	<div><div></div><div>45%5%50%</div></div>
5	C	1178	<div><div></div><div>83%10%7%</div></div>
6	D	1318	<div><div></div><div>86%10% . .</div></div>
7	Q	54	<div><div></div><div>37%13%50%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24981 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1720	1083	297	337	3		
1	B	237	Total	C	N	O	S	0	0
			1769	1117	301	348	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	82	Total	C	N	O	0	0
			645	412	107	126		

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	33	Total	C	N	O	P	0	0
			665	315	117	200	33		

- Molecule 4 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	10	Total	C	N	O	P	0	0
			221	98	45	68	10		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1095	Total	C	N	O	S	0	0
			8485	5310	1490	1646	39		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1278	Total	C	N	O	S	0	0
			9981	6252	1814	1873	42		

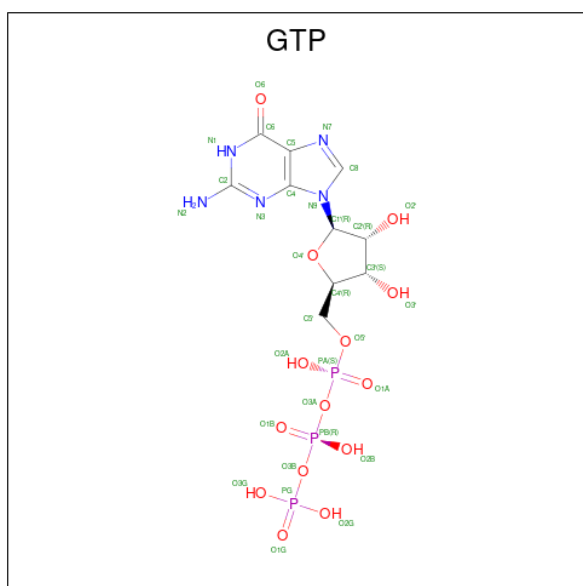
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P9WGY7
D	0	ALA	-	expression tag	UNP P9WGY7

- Molecule 7 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	27	Total	C	N	O	P	0	0
			555	261	105	162	27		

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total 2	Mg 2	0

- Molecule 11 is water.

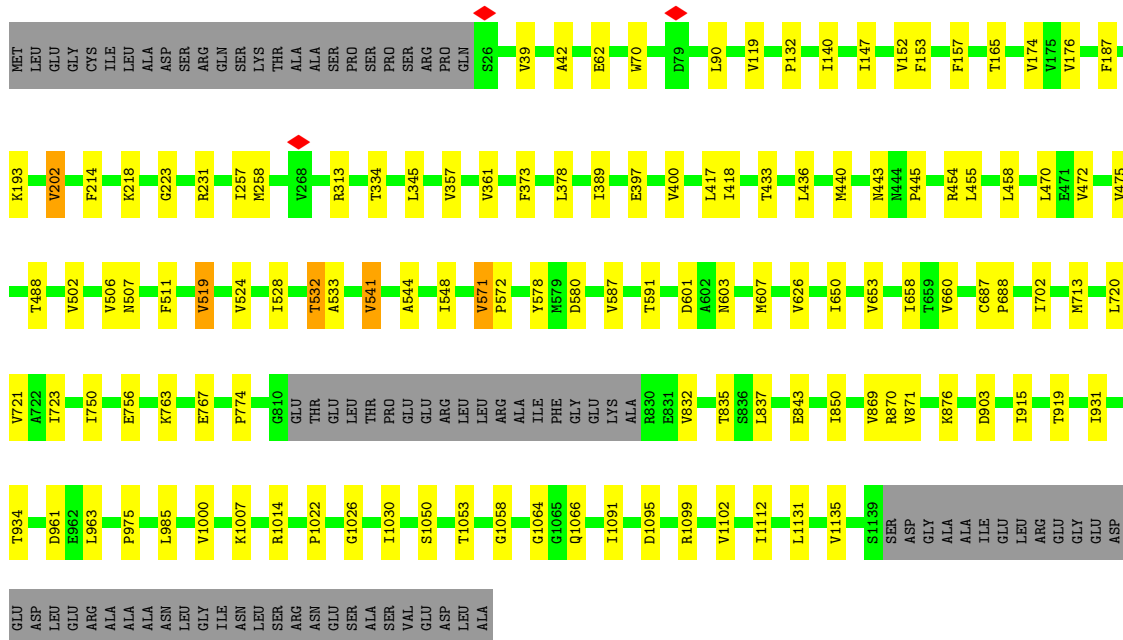
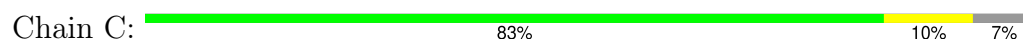
Mol	Chain	Residues	Atoms		AltConf
11	A	79	Total 79	O 79	0
11	B	61	Total 61	O 61	0
11	E	33	Total 33	O 33	0
11	P	28	Total 28	O 28	0
11	R	10	Total 10	O 10	0
11	C	301	Total 301	O 301	0
11	D	370	Total 370	O 370	0
11	Q	22	Total 22	O 22	0



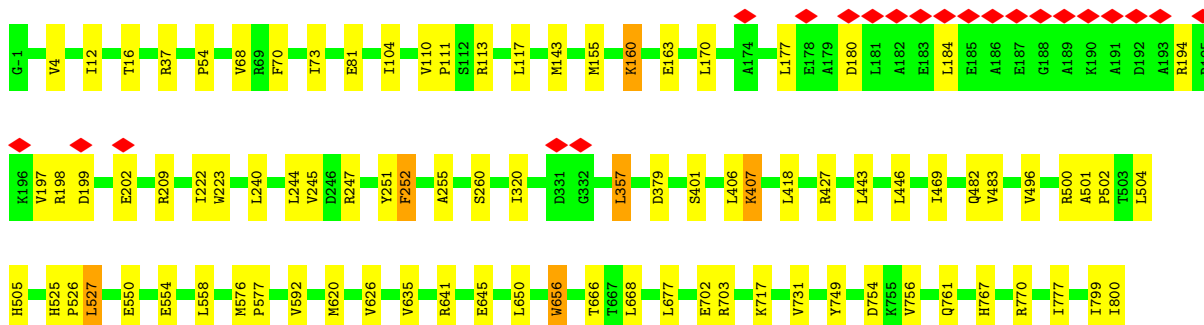
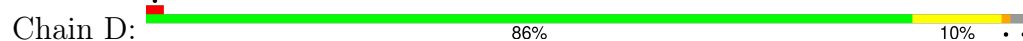
• Molecule 4: RNA

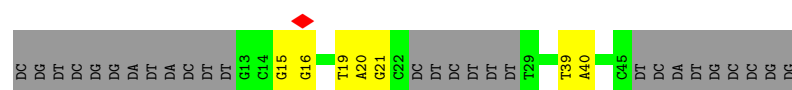


• Molecule 5: DNA-directed RNA polymerase subunit beta



• Molecule 6: DNA-directed RNA polymerase subunit beta'





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54790	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 ($e^-/\text{\AA}^2$)	50.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	325.248, 325.248, 325.248	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84699994, 0.84699994, 0.84699994	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: MG, GTP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/1746	0.35	0/2375
1	B	0.20	0/1796	0.35	0/2447
2	E	0.22	0/658	0.34	0/896
3	P	0.27	0/742	0.38	0/1140
4	R	0.29	0/248	0.41	0/386
5	C	0.25	0/8641	0.35	0/11716
6	D	0.23	0/10148	0.34	0/13718
7	Q	0.18	0/621	0.29	0/954
All	All	0.24	0/24600	0.35	0/33632

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	1720	0	1764	14	0
1	B	1769	0	1798	20	0
2	E	645	0	642	2	0
3	P	665	0	370	6	0
4	R	221	0	108	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	8485	0	8415	47	0
6	D	9981	0	10062	59	0
7	Q	555	0	303	4	0
8	D	32	0	12	0	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	A	79	0	0	0	0
11	B	61	0	0	0	0
11	C	301	0	0	0	0
11	D	370	0	0	1	0
11	E	33	0	0	0	0
11	P	28	0	0	0	0
11	Q	22	0	0	0	0
11	R	10	0	0	0	0
All	All	24981	0	23474	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.73	0.70
1:A:213:LYS:HG2	1:B:223:ARG:HG3	1.74	0.70
5:C:756:GLU:HB3	5:C:870:ARG:HG3	1.74	0.68
5:C:1091:ILE:HD12	5:C:1102:VAL:HG21	1.74	0.68
5:C:152:VAL:HG11	5:C:418:ILE:HD12	1.77	0.65
1:A:191:LYS:HE2	1:A:193:ILE:HD11	1.78	0.65
5:C:42:ALA:HB2	5:C:975:PRO:HG2	1.78	0.65
1:B:97:LEU:HB2	1:B:110:ILE:HG22	1.78	0.65
6:D:501:ALA:HB3	6:D:502:PRO:HD3	1.77	0.64
7:Q:20:DA:H2''	7:Q:21:DG:H5''	1.78	0.64
6:D:184:LEU:HD13	6:D:194:ARG:HG2	1.80	0.63
1:B:7:PRO:HA	1:B:25:PRO:HD2	1.80	0.63
1:B:183:VAL:HA	1:B:187:THR:HG22	1.80	0.62
5:C:62:GLU:HG3	5:C:70:TRP:HB2	1.83	0.60
6:D:1056:GLU:HB3	6:D:1063:LYS:HB3	1.84	0.59
5:C:919:THR:HG23	6:D:731:VAL:HG23	1.85	0.59
6:D:1080:ILE:HG21	6:D:1112:MET:HE3	1.84	0.59
3:P:14:DT:H2'	3:P:15:DA:C8	2.38	0.58
5:C:571:VAL:HG22	5:C:572:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:981:ARG:HD3	6:D:986:GLY:HA2	1.86	0.57
6:D:1054:ARG:HB2	6:D:1065:THR:HG23	1.85	0.57
6:D:749:TYR:HD2	6:D:777:ILE:HG23	1.68	0.57
6:D:827:PRO:HG3	6:D:858:LYS:HB2	1.86	0.57
6:D:952:LEU:HD22	6:D:957:ILE:HD11	1.87	0.56
6:D:170:LEU:HD21	6:D:209:ARG:HE	1.70	0.56
1:B:107:ALA:HB2	1:B:123:MET:HE2	1.87	0.56
5:C:165:THR:HG21	5:C:440:MET:HE2	1.87	0.55
1:A:93:VAL:HG21	1:A:116:VAL:HG21	1.88	0.55
6:D:70:PHE:HB3	6:D:73:ILE:HD11	1.89	0.55
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.89	0.54
6:D:240:LEU:O	6:D:244:LEU:HG	2.08	0.54
6:D:849:TYR:O	6:D:853:THR:HG23	2.07	0.54
5:C:650:ILE:HD13	5:C:660:VAL:HG22	1.90	0.54
6:D:184:LEU:HD11	6:D:197:VAL:HG21	1.89	0.53
6:D:500:ARG:HG2	6:D:501:ALA:H	1.73	0.52
1:A:225:LEU:HD21	1:B:9:LEU:HD23	1.91	0.52
5:C:1058:GLY:H	5:C:1064:GLY:HA3	1.75	0.52
6:D:504:LEU:HB3	6:D:1005:GLU:HG3	1.92	0.51
5:C:1007:LYS:HB3	5:C:1022:PRO:HB2	1.93	0.51
1:B:14:LEU:HD12	1:B:18:ARG:HH11	1.75	0.51
6:D:823:LEU:HD23	6:D:835:PRO:HB3	1.93	0.51
1:B:24:GLU:HB3	1:B:25:PRO:HD3	1.93	0.50
5:C:174:VAL:HG23	5:C:440:MET:HG3	1.93	0.50
5:C:1050:SER:HB3	5:C:1053:THR:O	2.12	0.50
6:D:1062:TYR:HE2	6:D:1082:LYS:HA	1.76	0.50
1:A:18:ARG:HG3	1:A:197:GLU:HB2	1.94	0.49
5:C:1135:VAL:HG22	6:D:12:ILE:HG13	1.94	0.49
6:D:110:VAL:HB	6:D:111:PRO:HD3	1.94	0.49
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.95	0.49
1:B:93:VAL:HG21	1:B:116:VAL:HG21	1.93	0.49
6:D:851:ILE:O	6:D:854:HIS:HB2	2.12	0.49
6:D:756:VAL:HG12	6:D:770:ARG:HG3	1.93	0.49
1:A:15:THR:HG23	1:A:17:ASN:H	1.78	0.49
1:B:3:ILE:HG21	1:B:234:ILE:HG22	1.94	0.49
5:C:721:VAL:HG23	5:C:915:ILE:HG23	1.94	0.49
6:D:525:HIS:CE1	6:D:527:LEU:HB2	2.47	0.49
7:Q:15:DG:H2"	7:Q:16:DG:C8	2.48	0.49
5:C:140:ILE:HG12	5:C:147:ILE:HG12	1.94	0.49
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.95	0.48
5:C:774:PRO:HG3	5:C:832:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:39:DT:H2''	7:Q:40:DA:C8	2.48	0.48
1:A:26:LEU:HD11	1:A:34:LEU:HD23	1.96	0.48
5:C:157:PHE:CE1	5:C:389:ILE:HD11	2.48	0.47
5:C:507:ASN:HD21	5:C:511:PHE:HB2	1.79	0.47
5:C:541:VAL:HG12	5:C:578:TYR:HB2	1.96	0.47
5:C:544:ALA:HB2	5:C:580:ASP:HB2	1.97	0.47
5:C:132:PRO:HB3	5:C:153:PHE:HE1	1.80	0.47
5:C:750:ILE:HG12	5:C:876:LYS:HG2	1.97	0.46
6:D:767:HIS:CE1	6:D:770:ARG:HH22	2.33	0.46
6:D:255:ALA:HB3	6:D:260:SER:HB3	1.96	0.46
6:D:641:ARG:HG3	6:D:656:TRP:CD1	2.49	0.46
5:C:378:LEU:HD11	5:C:455:LEU:HD22	1.97	0.46
5:C:532:THR:HG22	5:C:533:ALA:H	1.80	0.46
5:C:1102:VAL:HG22	5:C:1112:ILE:HG23	1.96	0.46
6:D:576:MET:HG2	6:D:577:PRO:HD2	1.96	0.46
5:C:658:ILE:HD11	5:C:688:PRO:HB3	1.98	0.46
6:D:922:ALA:HB2	6:D:981:ARG:HE	1.81	0.46
5:C:223:GLY:HA3	5:C:231:ARG:HH21	1.81	0.46
6:D:155:MET:SD	6:D:223:TRP:HB2	2.56	0.46
6:D:645:GLU:H	6:D:645:GLU:HG2	1.57	0.45
2:E:39:PRO:HG2	2:E:42:GLU:HG3	1.98	0.45
7:Q:19:DT:H2''	7:Q:20:DA:C8	2.52	0.45
3:P:21:DC:H2'	3:P:22:DG:C8	2.52	0.45
5:C:397:GLU:HA	5:C:400:VAL:HG12	1.97	0.45
6:D:885:ILE:HD13	6:D:1260:ALA:HB2	1.99	0.44
5:C:470:LEU:HD11	6:D:866:ARG:HH12	1.82	0.44
6:D:222:ILE:HG21	6:D:247:ARG:HD3	1.99	0.44
1:A:213:LYS:HE2	1:A:213:LYS:HB3	1.76	0.44
5:C:903:ASP:HB2	5:C:1014:ARG:HG3	1.98	0.44
5:C:961:ASP:C	5:C:963:LEU:H	2.23	0.44
6:D:104:ILE:HD12	6:D:379:ASP:HB3	1.98	0.44
5:C:850:ILE:HG22	5:C:871:VAL:HG22	2.00	0.44
6:D:54:PRO:HG3	6:D:81:GLU:O	2.18	0.44
3:P:15:DA:H2'	3:P:16:DT:H71	2.00	0.44
1:B:24:GLU:HA	1:B:191:LYS:HG3	2.00	0.43
1:B:167:ILE:HG23	6:D:620:MET:HE1	2.00	0.43
6:D:1046:ILE:HG22	6:D:1110:GLN:HA	1.99	0.43
5:C:470:LEU:HD11	6:D:866:ARG:NH1	2.33	0.43
6:D:525:HIS:NE2	6:D:717:LYS:HE2	2.34	0.43
5:C:1095:ASP:O	5:C:1099:ARG:HG3	2.19	0.43
3:P:22:DG:H2'	3:P:23:DC:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:985:LEU:HD23	5:C:985:LEU:HA	1.84	0.43
2:E:82:LEU:HD11	6:D:1274:PRO:HB3	2.01	0.42
5:C:187:PHE:CD2	5:C:202:VAL:HB	2.54	0.42
1:B:15:THR:HG22	1:B:16:ASP:H	1.84	0.42
6:D:143:MET:HG2	6:D:251:TYR:HE1	1.84	0.42
1:A:64:THR:O	1:A:73:VAL:HG12	2.19	0.42
6:D:702:GLU:HG3	6:D:703:ARG:HG3	2.00	0.42
6:D:800:ILE:HD13	6:D:800:ILE:HA	1.93	0.42
5:C:502:VAL:HG23	5:C:587:VAL:O	2.20	0.42
6:D:160:LYS:HA	6:D:163:GLU:HG2	2.02	0.42
1:B:6:ARG:NH1	1:B:237:SER:HA	2.35	0.42
1:B:92:PRO:HA	1:B:140:VAL:O	2.20	0.42
5:C:400:VAL:HG23	5:C:417:LEU:HB3	2.02	0.42
6:D:1256:LYS:HG2	6:D:1257:LEU:H	1.84	0.42
6:D:576:MET:HB3	6:D:576:MET:HE2	1.80	0.42
5:C:445:PRO:HB2	5:C:713:MET:HE1	2.01	0.42
6:D:1254:ILE:HD11	6:D:1256:LYS:HE3	2.01	0.42
5:C:720:LEU:HD12	5:C:1026:GLY:O	2.20	0.42
5:C:202:VAL:HG13	5:C:214:PHE:HB2	2.02	0.41
6:D:199:ASP:O	6:D:202:GLU:HG3	2.20	0.41
5:C:519:VAL:HG12	5:C:524:VAL:HG13	2.02	0.41
5:C:607:MET:HE2	5:C:607:MET:HB3	1.85	0.41
6:D:180:ASP:HB2	6:D:198:ARG:HH22	1.84	0.41
6:D:550:GLU:O	6:D:554:GLU:HG3	2.20	0.41
5:C:571:VAL:HG13	5:C:572:PRO:O	2.21	0.41
6:D:407:LYS:HE3	6:D:407:LYS:HB2	1.59	0.41
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.89	0.41
6:D:113:ARG:HD3	6:D:1238:ILE:HD12	2.03	0.41
1:A:81:LYS:HB2	1:A:81:LYS:HE3	1.92	0.41
3:P:18:DC:H2"	3:P:19:DG:C8	2.55	0.41
6:D:1053:VAL:HG12	6:D:1103:ASP:O	2.20	0.41
1:A:170:PRO:O	1:A:199:LYS:HG2	2.21	0.41
1:A:218:LEU:HA	1:A:218:LEU:HD23	1.88	0.41
5:C:931:ILE:O	5:C:934:THR:HB	2.21	0.41
6:D:446:LEU:HB2	11:D:1767:HOH:O	2.20	0.41
6:D:1061:PHE:HA	6:D:1080:ILE:O	2.20	0.41
6:D:357:LEU:HD12	6:D:357:LEU:HA	1.91	0.41
5:C:157:PHE:HE1	5:C:389:ILE:HD11	1.85	0.40
6:D:245:VAL:HA	6:D:252:PHE:CE2	2.56	0.40
1:B:2:LEU:HD13	1:B:2:LEU:HA	1.95	0.40
3:P:34:DT:H2"	3:P:35:DA:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:H	1:B:205:ARG:HD3	1.87	0.40
6:D:525:HIS:CD2	6:D:526:PRO:HD2	2.56	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	224/347 (65%)	215 (96%)	9 (4%)	0	100	100
1	B	235/347 (68%)	226 (96%)	9 (4%)	0	100	100
2	E	80/110 (73%)	75 (94%)	5 (6%)	0	100	100
5	C	1091/1178 (93%)	1043 (96%)	48 (4%)	0	100	100
6	D	1274/1318 (97%)	1223 (96%)	51 (4%)	0	100	100
All	All	2904/3300 (88%)	2782 (96%)	122 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/297 (65%)	190 (98%)	4 (2%)	47	67
1	B	196/297 (66%)	190 (97%)	6 (3%)	35	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	69/90 (77%)	65 (94%)	4 (6%)	18	47
5	C	928/998 (93%)	880 (95%)	48 (5%)	21	49
6	D	1056/1095 (96%)	1003 (95%)	53 (5%)	22	50
All	All	2443/2777 (88%)	2328 (95%)	115 (5%)	25	52

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	43	LEU
1	A	106	THR
1	A	138	LEU
1	B	56	ILE
1	B	64	THR
1	B	111	VAL
1	B	138	LEU
1	B	150	VAL
1	B	205	ARG
2	E	31	THR
2	E	36	THR
2	E	92	LEU
2	E	103	LEU
5	C	39	VAL
5	C	90	LEU
5	C	119	VAL
5	C	176	VAL
5	C	193	LYS
5	C	202	VAL
5	C	218	LYS
5	C	257	ILE
5	C	258	MET
5	C	313	ARG
5	C	334	THR
5	C	345	LEU
5	C	357	VAL
5	C	361	VAL
5	C	373	PHE
5	C	433	THR
5	C	436	LEU
5	C	443	ASN
5	C	454	ARG

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Mol	Chain	Res	Type
5	C	458	LEU
5	C	472	VAL
5	C	475	VAL
5	C	488	THR
5	C	506	VAL
5	C	519	VAL
5	C	528	ILE
5	C	532	THR
5	C	541	VAL
5	C	548	ILE
5	C	571	VAL
5	C	591	THR
5	C	601	ASP
5	C	603	ASN
5	C	626	VAL
5	C	653	VAL
5	C	687	CYS
5	C	702	ILE
5	C	723	ILE
5	C	763	LYS
5	C	767	GLU
5	C	835	THR
5	C	837	LEU
5	C	843	GLU
5	C	869	VAL
5	C	1000	VAL
5	C	1030	ILE
5	C	1066	GLN
5	C	1131	LEU
6	D	4	VAL
6	D	16	THR
6	D	37	ARG
6	D	68	VAL
6	D	117	LEU
6	D	160	LYS
6	D	177	LEU
6	D	252	PHE
6	D	320	ILE
6	D	357	LEU
6	D	401	SER
6	D	406	LEU
6	D	407	LYS

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Mol	Chain	Res	Type
6	D	418	LEU
6	D	427	ARG
6	D	443	LEU
6	D	469	ILE
6	D	482	GLN
6	D	483	VAL
6	D	496	VAL
6	D	505	HIS
6	D	527	LEU
6	D	558	LEU
6	D	592	VAL
6	D	626	VAL
6	D	635	VAL
6	D	650	LEU
6	D	656	TRP
6	D	666	THR
6	D	668	LEU
6	D	677	LEU
6	D	754	ASP
6	D	761	GLN
6	D	799	ILE
6	D	821	LYS
6	D	863	THR
6	D	867	THR
6	D	909	THR
6	D	911	ILE
6	D	965	VAL
6	D	968	CYS
6	D	1028	LEU
6	D	1060	ARG
6	D	1065	THR
6	D	1088	VAL
6	D	1097	ARG
6	D	1111	LEU
6	D	1121	VAL
6	D	1128	ARG
6	D	1173	THR
6	D	1211	THR
6	D	1217	THR
6	D	1264	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	ASN
2	E	106	HIS
5	C	388	GLN
5	C	443	ASN
5	C	444	ASN
5	C	612	GLN
5	C	718	ASN
5	C	751	HIS
5	C	866	ASN
5	C	1034	HIS
6	D	267	ASN
6	D	351	ASN
6	D	416	ASN
6	D	439	HIS
6	D	510	GLN
6	D	523	GLN
6	D	761	GLN
6	D	766	ASN
6	D	1160	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	8/20 (40%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	18	G

There are no RNA pucker outliers to report.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are 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
8	GTP	D	1401	-	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)

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
8	GTP	D	1401	-	-	4/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1401	GTP	C5-N7	-2.04	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1401	GTP	C5-C4-N3	-4.88	120.63	128.39
8	D	1401	GTP	C2-N3-C4	4.64	120.28	112.30
8	D	1401	GTP	C2-N1-C6	-3.10	119.49	125.11
8	D	1401	GTP	N9-C4-N3	2.84	131.63	125.95
8	D	1401	GTP	N9-C8-N7	-2.72	108.35	113.40
8	D	1401	GTP	C5-C6-N1	2.60	119.86	113.25
8	D	1401	GTP	C8-N7-C5	2.52	108.75	104.26
8	D	1401	GTP	O6-C6-C5	-2.39	120.22	126.53
8	D	1401	GTP	C2'-C1'-N9	-2.10	107.41	113.25

There are no chirality outliers.

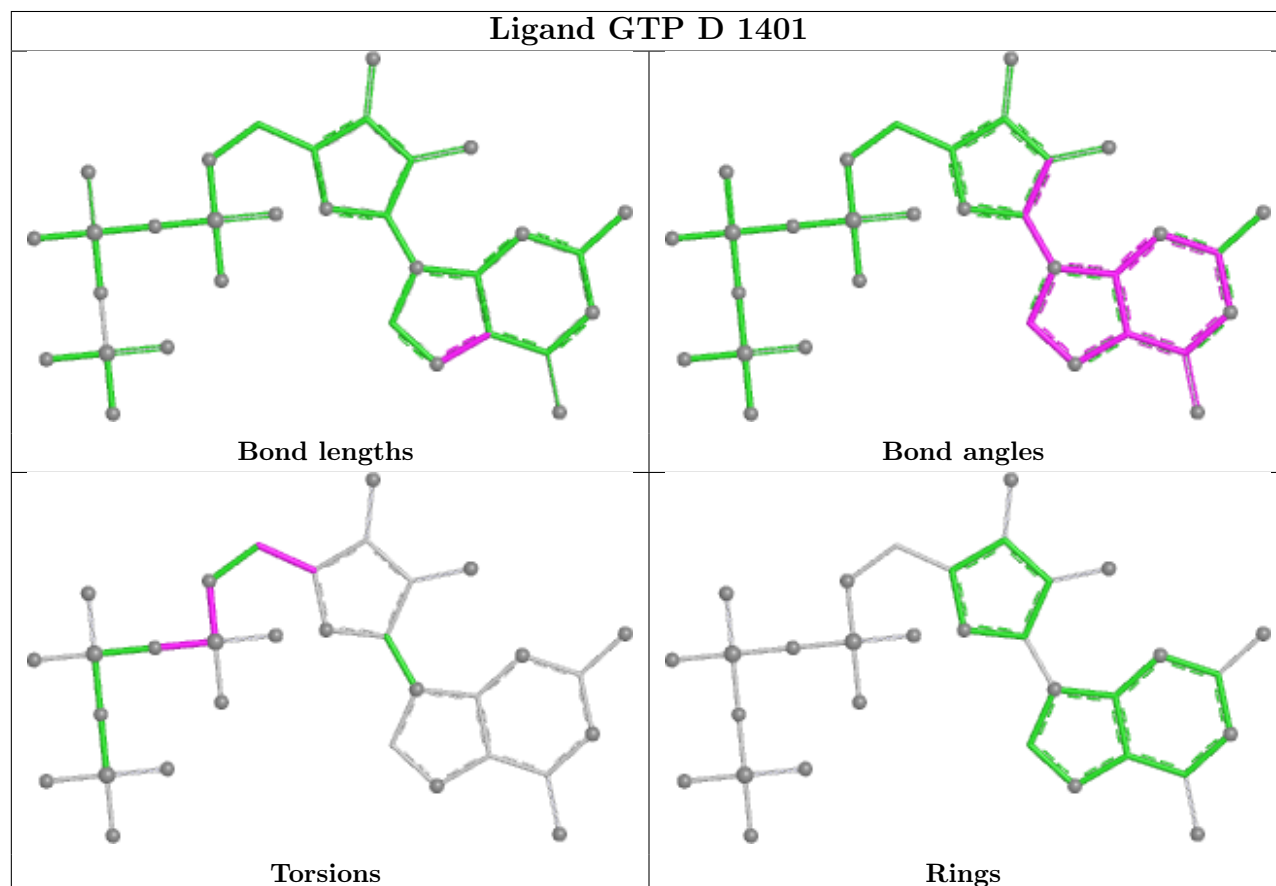
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	1401	GTP	C5'-O5'-PA-O1A
8	D	1401	GTP	PB-O3A-PA-O1A
8	D	1401	GTP	C3'-C4'-C5'-O5'
8	D	1401	GTP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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.

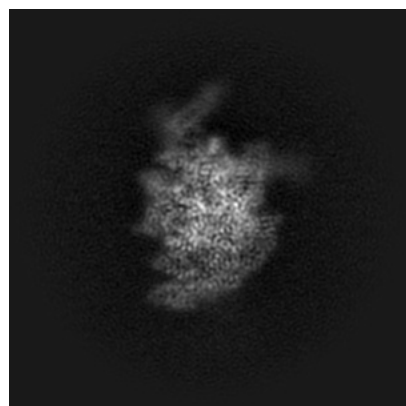
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75288. These allow visual inspection of the internal detail of the map and identification of artifacts.

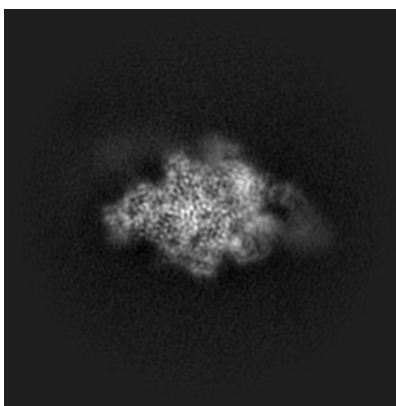
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

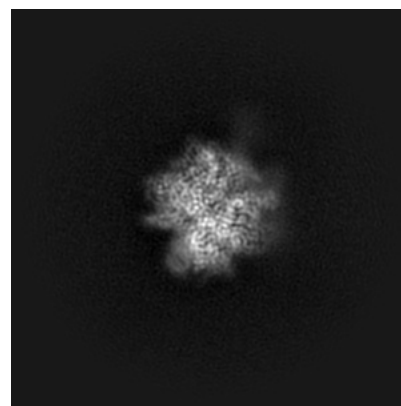
6.1.1 Primary map



X

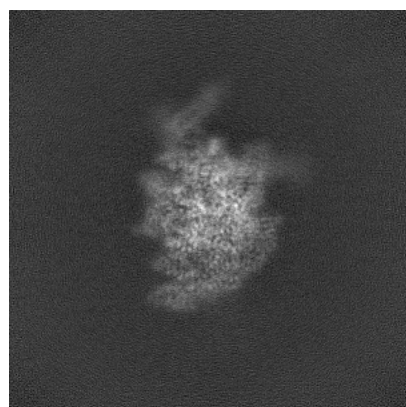


Y

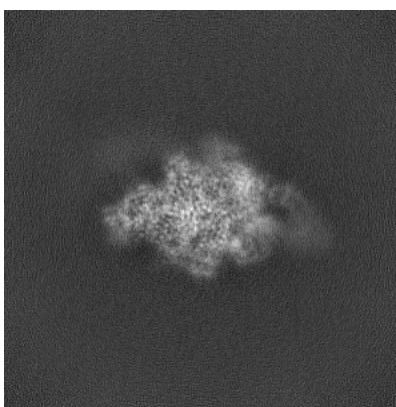


Z

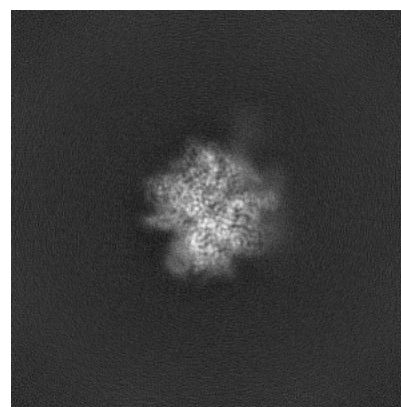
6.1.2 Raw map



X



Y

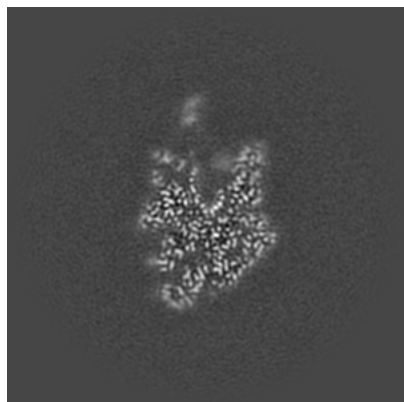


Z

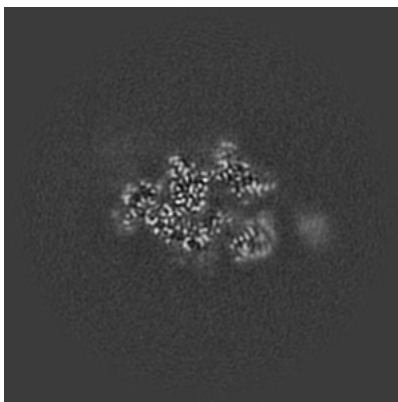
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

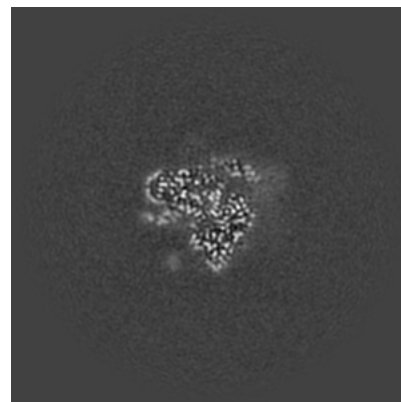
6.2.1 Primary map



X Index: 192

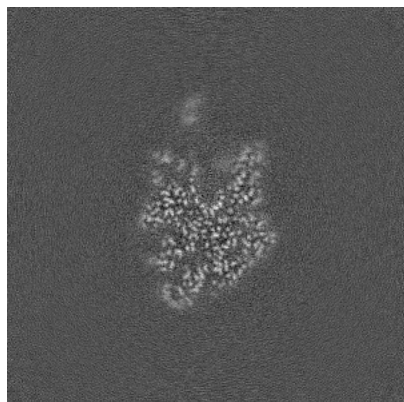


Y Index: 192

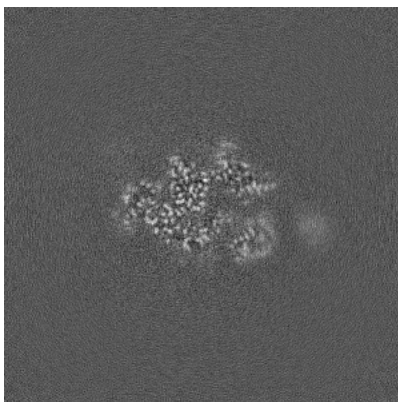


Z Index: 192

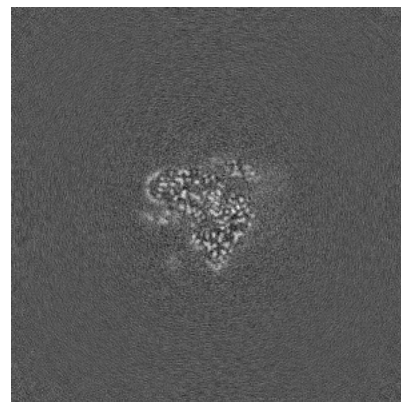
6.2.2 Raw map



X Index: 192



Y Index: 192

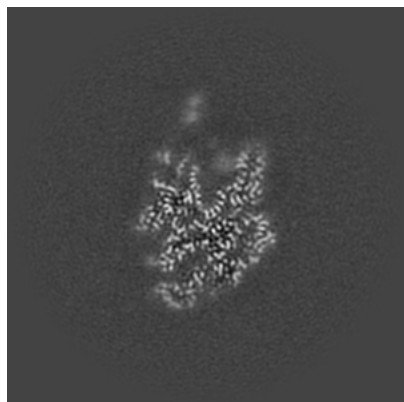


Z Index: 192

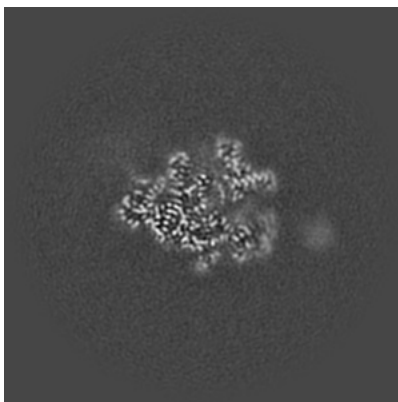
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

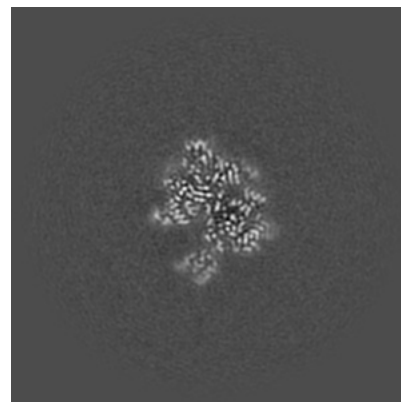
6.3.1 Primary map



X Index: 190

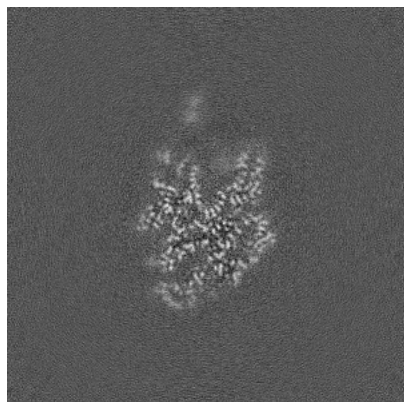


Y Index: 199

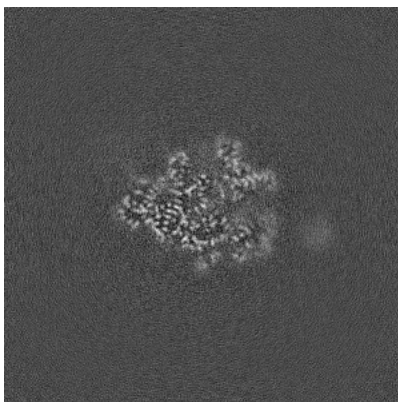


Z Index: 172

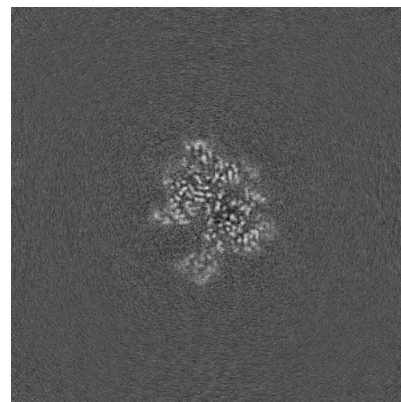
6.3.2 Raw map



X Index: 190



Y Index: 199

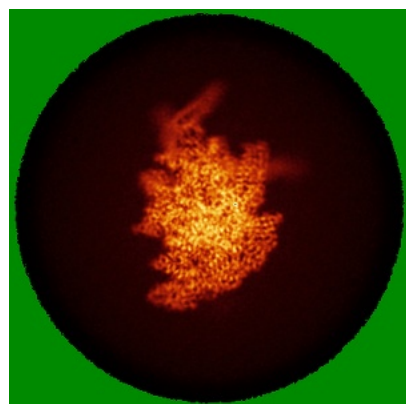


Z Index: 172

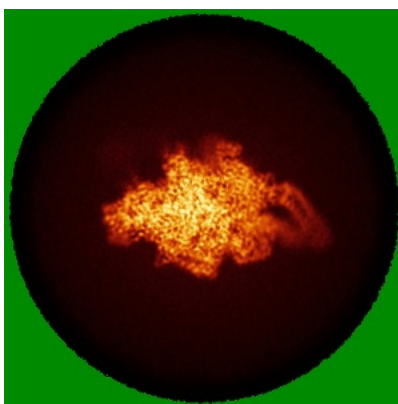
The images above show the largest variance slices of the map in three orthogonal directions.

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

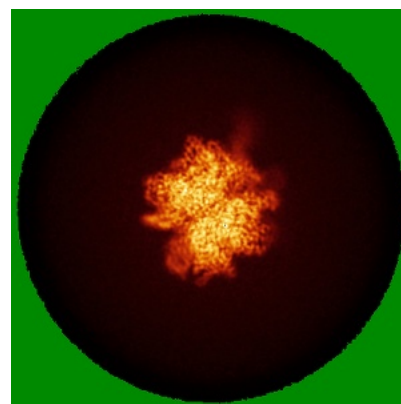
6.4.1 Primary map



X

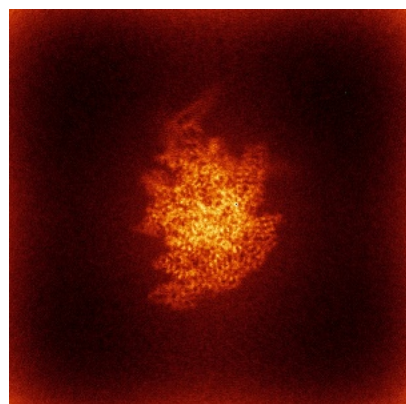


Y

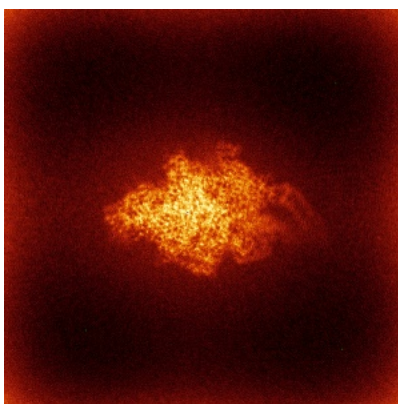


Z

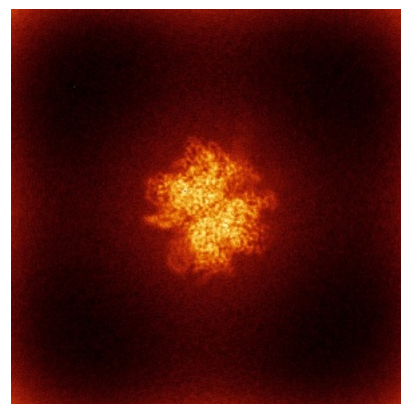
6.4.2 Raw map



X



Y



Z

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

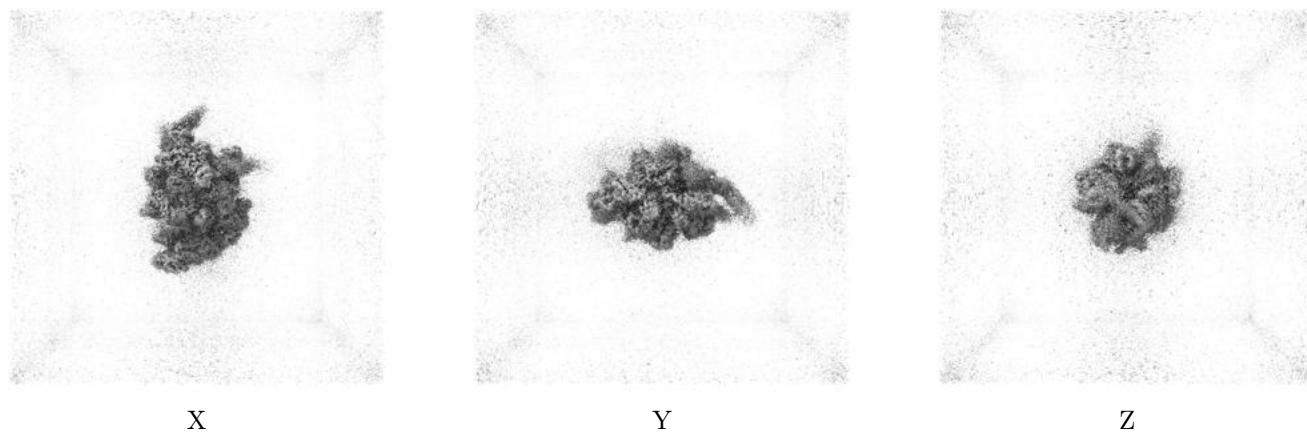
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

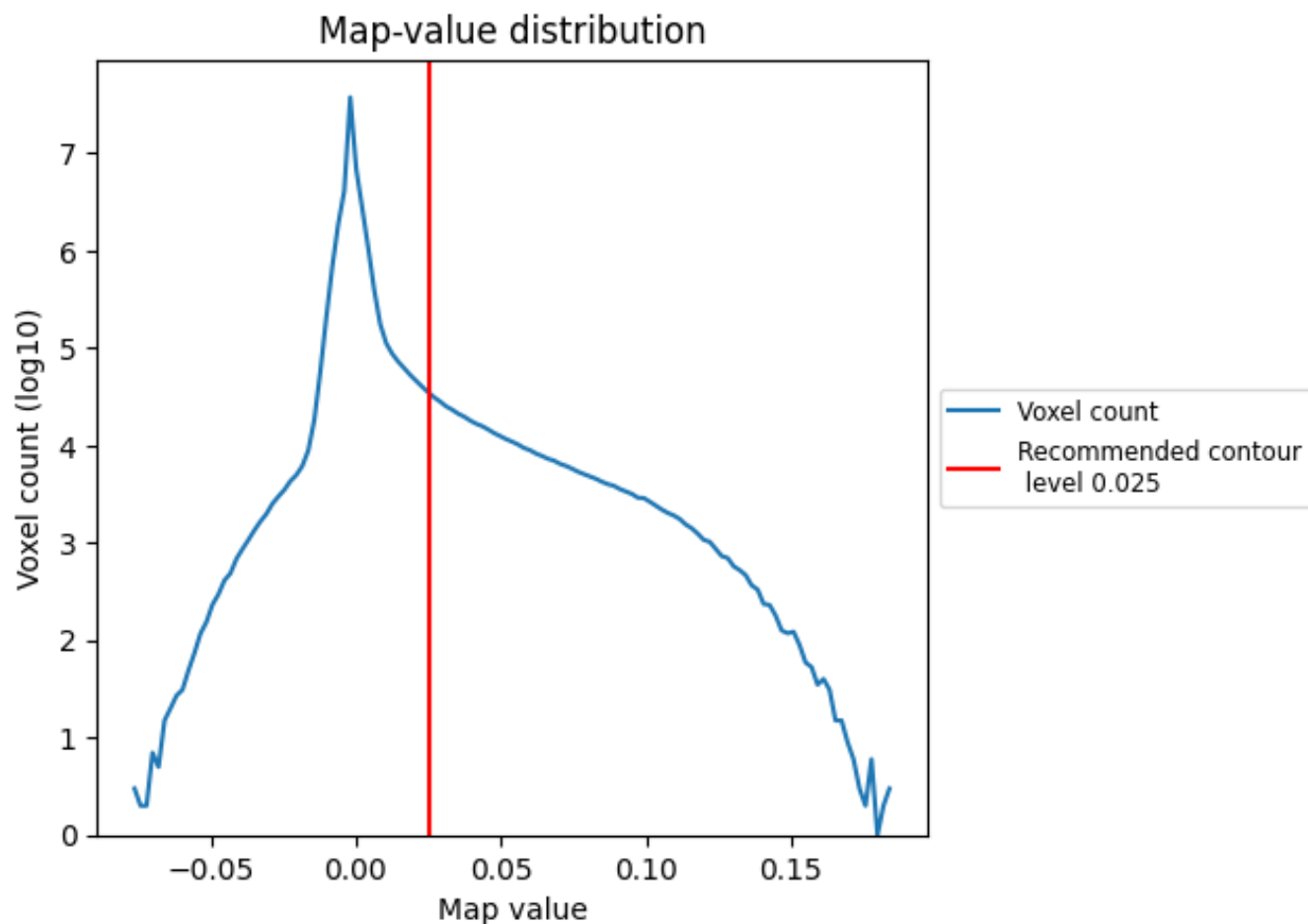
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

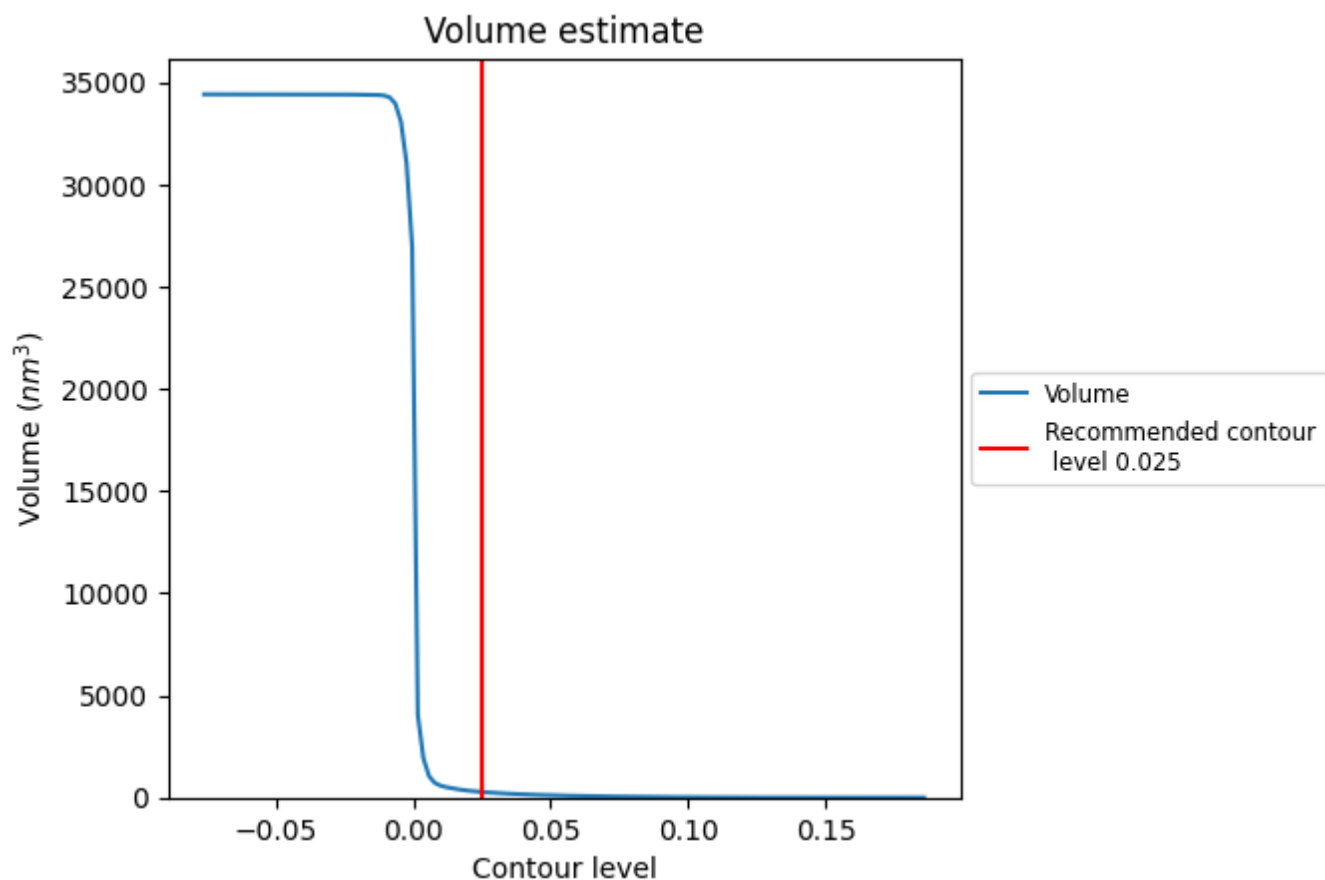
This section contains the results of statistical analysis of the map.

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.

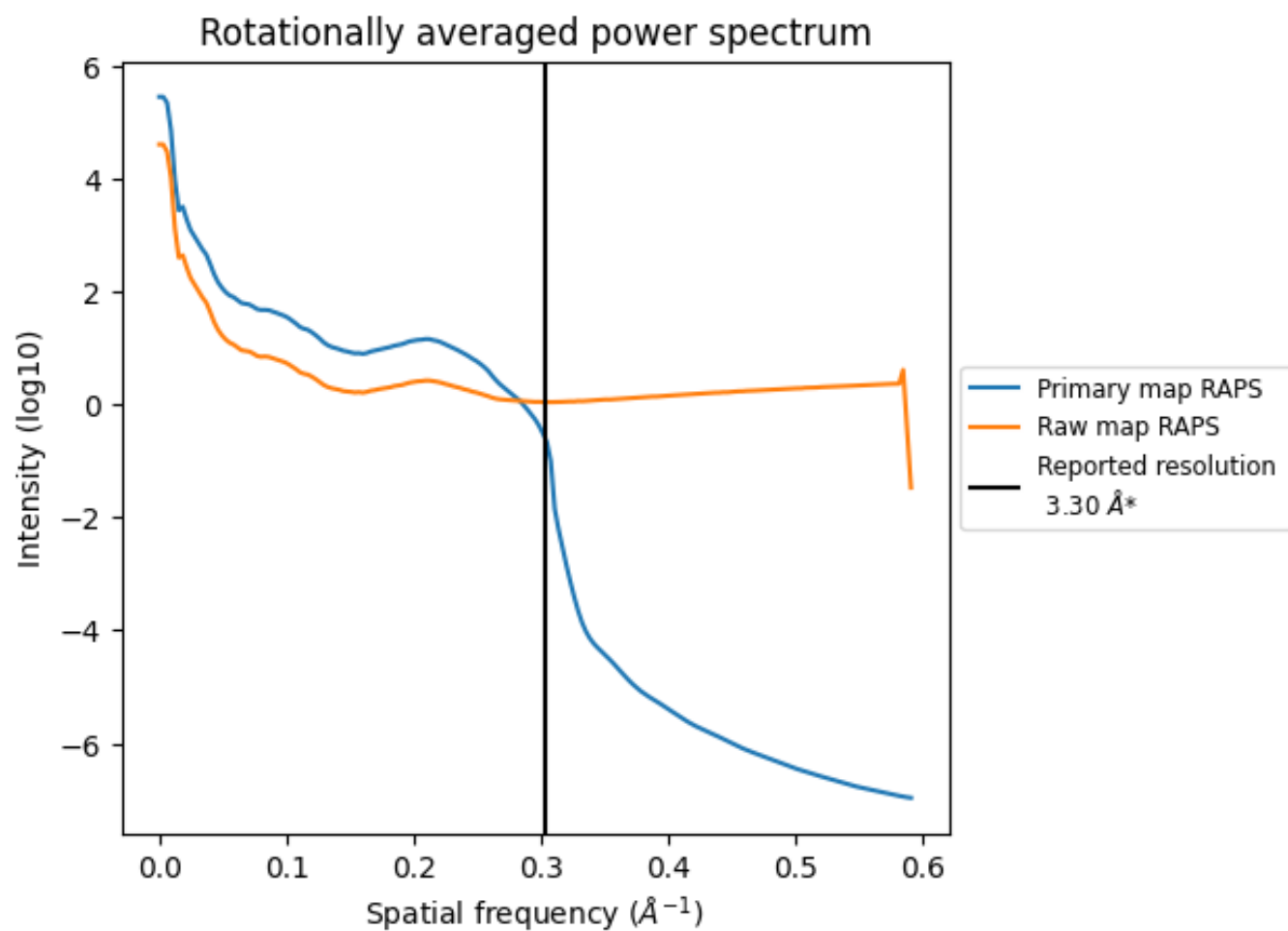
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm³; this corresponds to an approximate mass of 246 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 ⓘ

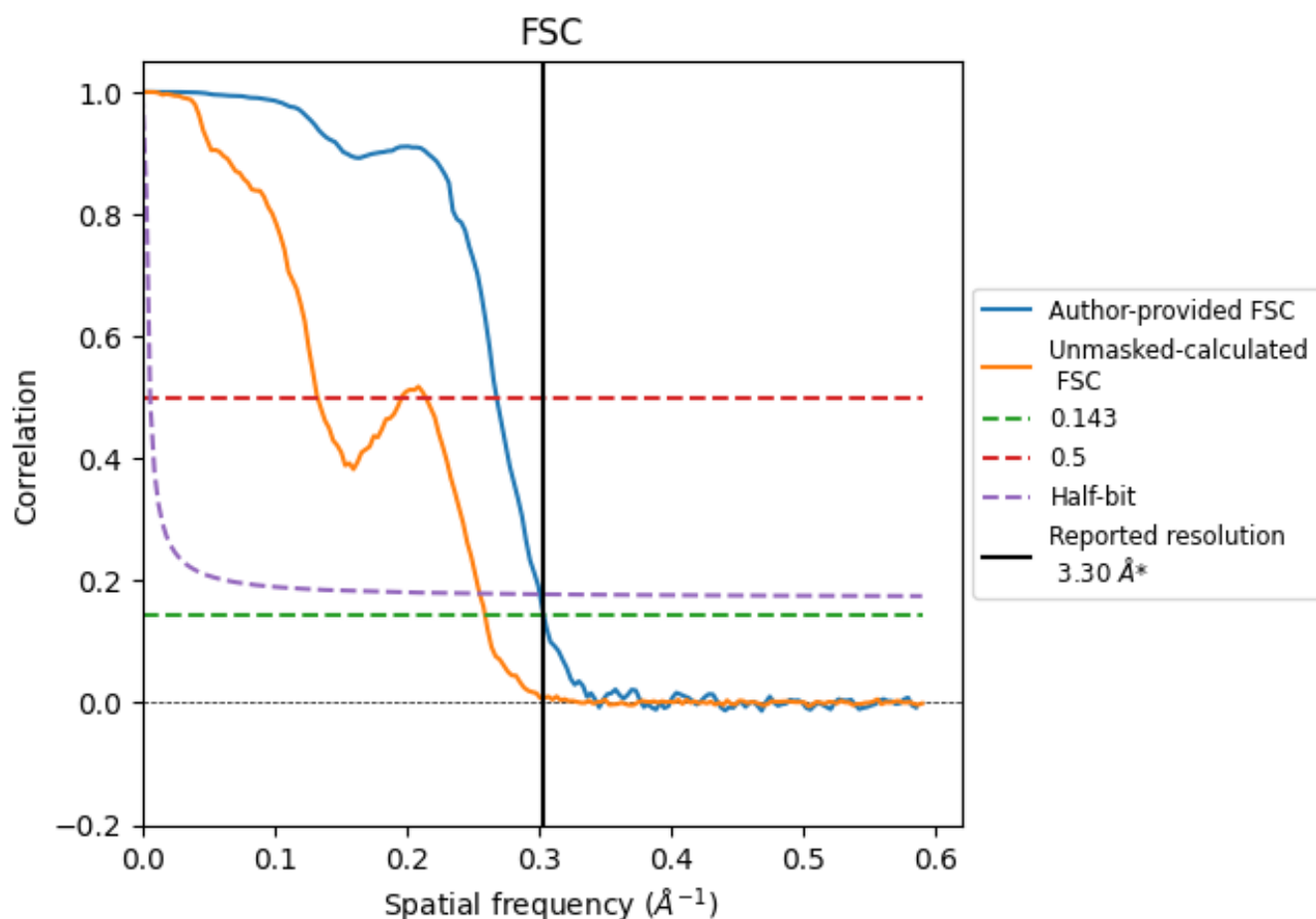


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

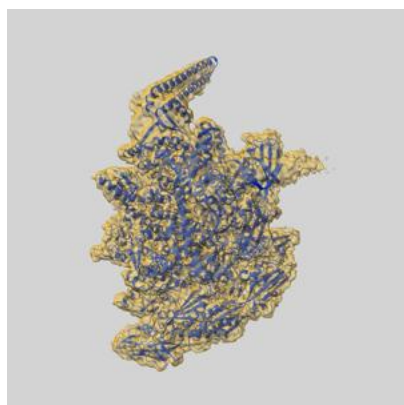
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.73	3.32
Unmasked-calculated*	3.85	7.54	3.92

*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 3.85 differs from the reported value 3.3 by more than 10 %

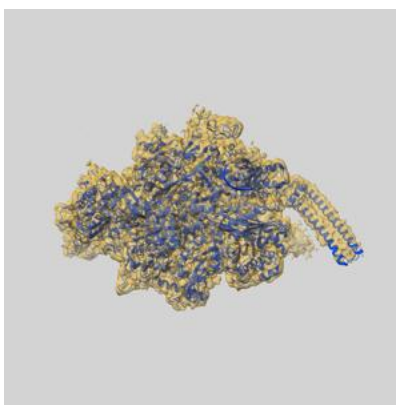
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75288 and PDB model 10MK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

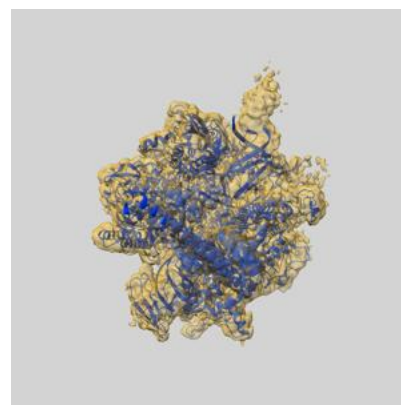
9.1 Map-model overlay [i](#)



X



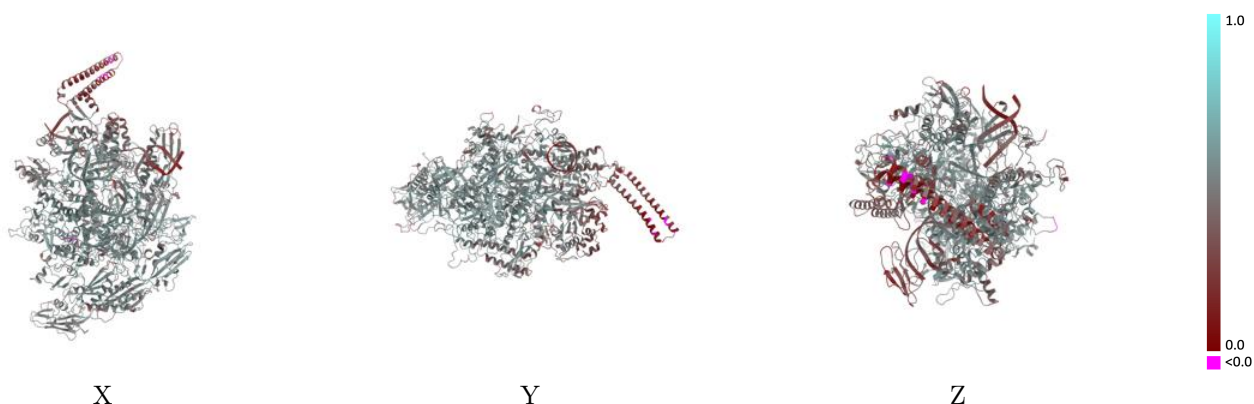
Y



Z

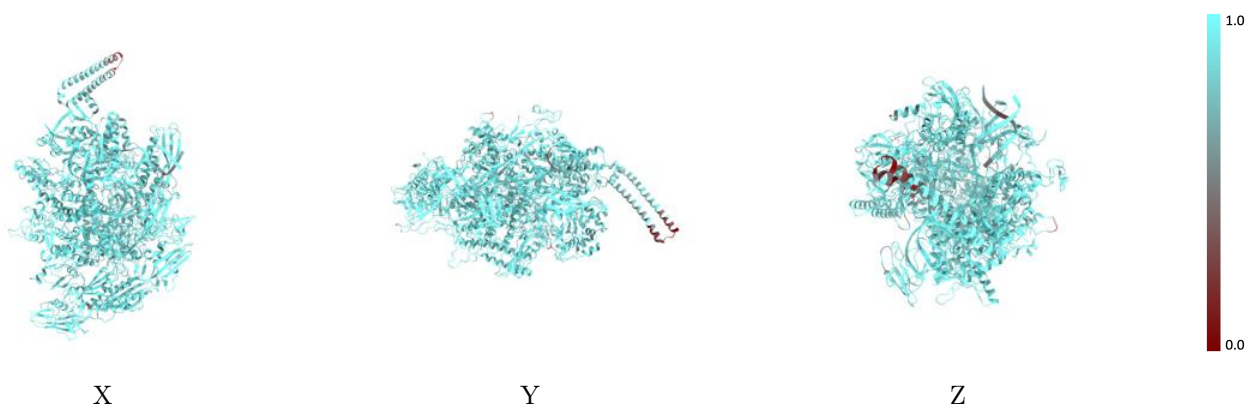
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



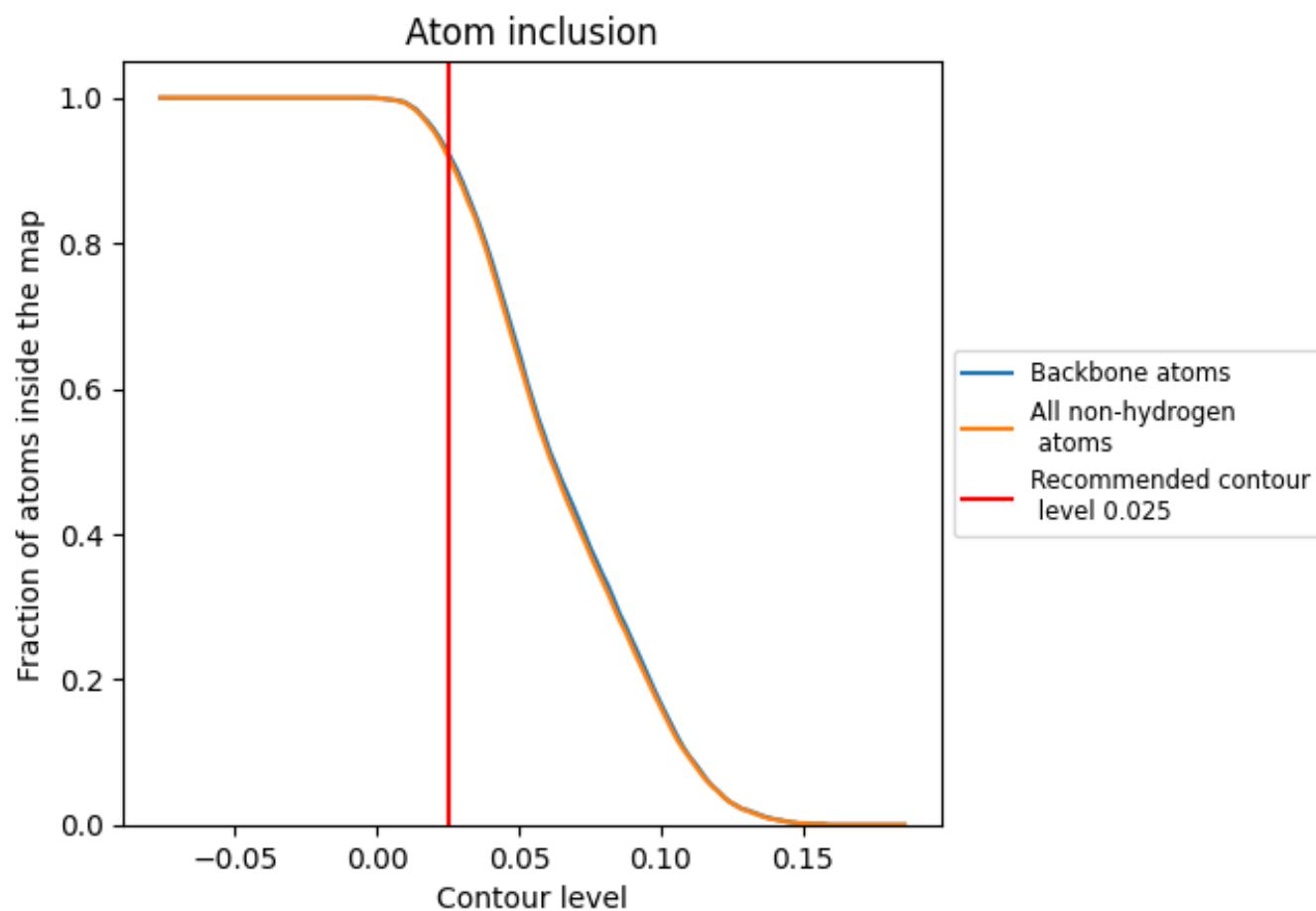
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9200</div>	<div><div></div>0.4840</div>
A	<div><div></div>0.9410</div>	<div><div></div>0.5150</div>
B	<div><div></div>0.9240</div>	<div><div></div>0.4890</div>
C	<div><div></div>0.9330</div>	<div><div></div>0.5030</div>
D	<div><div></div>0.9150</div>	<div><div></div>0.4700</div>
E	<div><div></div>0.9190</div>	<div><div></div>0.4950</div>
P	<div><div></div>0.9820</div>	<div><div></div>0.4180</div>
Q	<div><div></div>0.8340</div>	<div><div></div>0.3620</div>
R	<div><div></div>0.9680</div>	<div><div></div>0.5300</div>

1.0

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