Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 05:26 AM EDT

PDB ID	:	9OWR / pdb_00009owr
EMDB ID	:	EMD-70941
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in 5 mM Ca2+
Deposited on	:	2025-06-02
Resolution	:	2.96 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

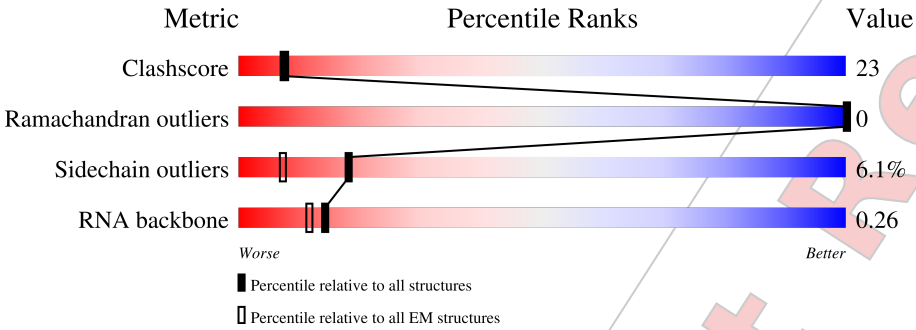
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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 <=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	417	6% 23% 51% 25%
2	B	116	65% 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9927 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 RNA chain called RNase P RNA component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	U	C	conflict	GB 143442
A	417	C	G	conflict	GB 143442

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

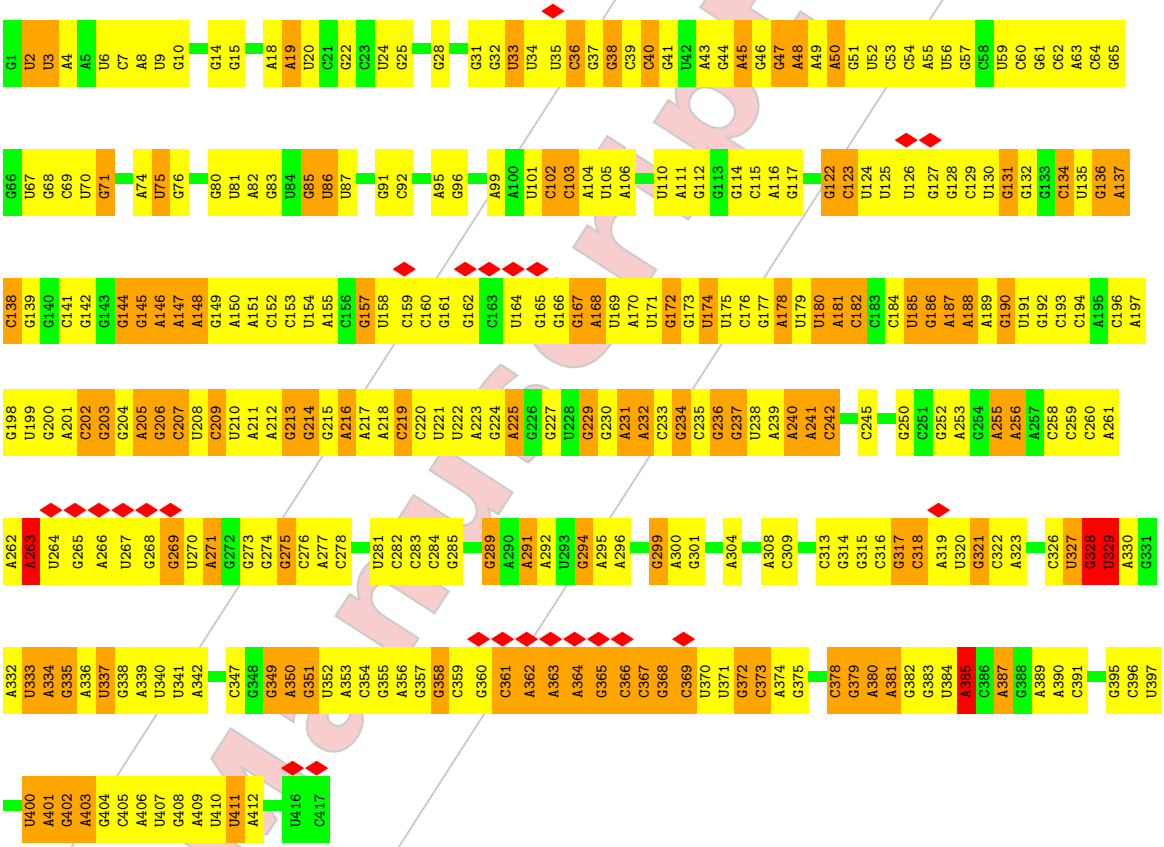
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	18	18	18	0

3 Residue-property plots (i)

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.

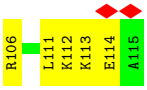
- Molecule 1: RNase P RNA component

Chain A:



- Molecule 2: Ribonuclease P protein component

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	615963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.472	Depositor
Minimum map value	-0.153	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0519	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.59	0/10038	0.91	13/15661 (0.1%)
2	B	0.34	0/962	0.64	1/1281 (0.1%)
All	All	0.58	0/11000	0.89	14/16942 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	U	O3'-P-O5'	-9.40	89.90	104.00
1	A	299	G	O3'-P-O5'	-7.17	93.25	104.00
1	A	328	G	O3'-P-O5'	-6.42	94.38	104.00
1	A	329	U	C1'-C2'-O2'	-6.26	102.41	111.80
1	A	387	A	O3'-P-O5'	-5.81	95.29	104.00
1	A	385	A	C4'-C3'-C2'	-5.72	96.88	102.60
1	A	139	G	O3'-P-O5'	-5.71	95.44	104.00
1	A	263	A	C2'-C3'-O3'	-5.53	105.41	113.70
2	B	4	LYS	N-CA-C	-5.41	105.03	111.03
1	A	289	G	C4'-C3'-C2'	-5.38	97.22	102.60
1	A	44	G	C4'-C3'-C2'	-5.36	97.25	102.60
1	A	333	U	O3'-P-O5'	-5.32	96.02	104.00
1	A	263	A	P-O3'-C3'	5.14	127.91	120.20
1	A	385	A	O4'-C4'-C3'	-5.09	98.91	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	6	ARG	Sidechain

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	8962	0	4509	287	0
2	B	947	0	1008	29	0
3	A	18	0	0	0	0
All	All	9927	0	5517	312	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 23.

All (312) 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:364:A:C4	1:A:365:G:H1'	1.96	1.01
1:A:148:A:N6	1:A:177:G:N3	2.19	0.90
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.89
1:A:148:A:H61	1:A:177:G:H1'	1.44	0.83
1:A:230:G:H21	1:A:231:A:H2'	1.45	0.82
1:A:172:G:H5"	1:A:216:A:H61	1.42	0.82
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.82
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.80
1:A:378:C:H3'	1:A:379:G:C8	2.18	0.79
1:A:378:C:H3'	1:A:379:G:H8	1.50	0.77
1:A:154:U:H2'	1:A:155:A:C8	2.21	0.76
1:A:379:G:C8	1:A:379:G:OP2	2.41	0.73
1:A:207:C:H2'	1:A:208:U:C6	2.24	0.72
1:A:322:C:H2'	1:A:323:A:C8	2.25	0.71
1:A:230:G:N2	1:A:231:A:H2'	2.06	0.70
1:A:47:G:H1	1:A:385:A:H62	1.37	0.69
1:A:206:G:N1	1:A:232:A:O2'	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.69
1:A:385:A:H1'	1:A:401:A:C8	2.28	0.68
2:B:7:ILE:HA	2:B:42:ARG:HH21	1.58	0.68
1:A:382:G:H2'	1:A:383:G:O4'	1.94	0.68
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
1:A:148:A:H61	1:A:177:G:C1'	2.08	0.66
1:A:31:G:N2	1:A:32:G:N2	2.43	0.66
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.65
1:A:185:U:H2'	1:A:186:G:C8	2.32	0.65
2:B:0:GLY:HA2	2:B:65:ARG:HB3	1.79	0.65
1:A:45:A:H62	2:B:62:ARG:NH2	1.96	0.64
1:A:138:C:H4'	1:A:138:C:OP2	1.94	0.64
1:A:161:G:H3'	1:A:162:G:H8	1.62	0.64
1:A:187:A:N3	1:A:245:C:O2'	2.28	0.64
1:A:122:G:H3'	1:A:123:C:H5"	1.78	0.64
1:A:130:U:H2'	1:A:131:G:C8	2.34	0.63
1:A:380:A:H3'	1:A:381:A:H8	1.63	0.63
1:A:45:A:H62	2:B:62:ARG:HH22	1.46	0.63
1:A:157:G:H1	1:A:169:U:H3	1.46	0.63
1:A:206:G:H1'	1:A:207:C:H5	1.62	0.63
2:B:56:VAL:O	2:B:60:ILE:HG12	1.98	0.63
1:A:241:A:H2'	1:A:242:C:C6	2.35	0.62
1:A:154:U:H2'	1:A:155:A:H8	1.62	0.62
1:A:155:A:H1'	1:A:217:A:N3	2.15	0.61
1:A:379:G:H8	1:A:379:G:OP2	1.83	0.61
1:A:130:U:H2'	1:A:131:G:H8	1.65	0.61
1:A:177:G:C8	1:A:178:A:H2'	2.36	0.60
2:B:89:ALA:HA	2:B:92:MET:SD	2.42	0.60
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.60
1:A:374:A:H2'	1:A:375:G:C8	2.37	0.59
1:A:147:A:H2'	1:A:148:A:O4'	2.03	0.59
1:A:186:G:N2	1:A:188:A:H3'	2.16	0.59
1:A:364:A:OP1	1:A:365:G:N7	2.35	0.59
1:A:216:A:H2'	1:A:217:A:C8	2.38	0.59
1:A:136:G:O2'	1:A:137:A:N7	2.36	0.58
1:A:379:G:H8	1:A:379:G:P	2.25	0.58
1:A:186:G:N1	1:A:189:A:OP2	2.35	0.58
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:373:C:H2'	1:A:374:A:C8	2.39	0.58
1:A:407:U:H2'	1:A:408:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:A:H1'	1:A:240:A:N1	2.19	0.58
1:A:220:C:H2'	1:A:221:U:C6	2.38	0.58
1:A:159:C:H2'	1:A:160:C:C6	2.39	0.57
1:A:147:A:H3'	1:A:148:A:H8	1.69	0.57
1:A:60:C:H2'	1:A:61:G:H8	1.68	0.57
1:A:208:U:H3	1:A:225:A:H61	1.52	0.57
1:A:252:G:C2'	1:A:253:A:H5'	2.35	0.57
1:A:31:G:C2	1:A:32:G:C2	2.93	0.56
1:A:32:G:H2'	1:A:33:U:H5'	1.88	0.56
1:A:364:A:H3'	1:A:364:A:OP2	2.05	0.56
2:B:106:ARG:HB2	2:B:113:LYS:HA	1.88	0.56
1:A:381:A:C2	1:A:382:G:H1'	2.41	0.56
1:A:63:A:H2'	1:A:64:C:O4'	2.06	0.56
1:A:411:U:H2'	1:A:412:A:C8	2.40	0.56
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.56
1:A:147:A:O2'	1:A:148:A:H5'	2.06	0.56
1:A:194:C:N4	1:A:202:C:OP2	2.37	0.55
1:A:115:C:H2'	1:A:116:A:H8	1.72	0.55
1:A:31:G:N2	1:A:37:G:C4	2.75	0.55
1:A:181:A:H2'	1:A:182:C:O4'	2.06	0.55
1:A:381:A:H2'	1:A:382:G:O4'	2.07	0.55
1:A:198:G:H22	1:A:200:G:H3'	1.71	0.55
1:A:241:A:H2'	1:A:242:C:H6	1.71	0.55
1:A:161:G:H3'	1:A:162:G:C8	2.42	0.55
1:A:207:C:H2'	1:A:208:U:H6	1.72	0.55
1:A:255:A:OP1	1:A:256:A:O2'	2.25	0.55
1:A:198:G:N2	1:A:200:G:H3'	2.21	0.54
1:A:338:G:H2'	1:A:339:A:H8	1.73	0.54
1:A:123:C:H4'	1:A:123:C:OP1	2.08	0.54
1:A:338:G:H2'	1:A:339:A:C8	2.43	0.54
1:A:59:U:H2'	1:A:60:C:C6	2.42	0.54
1:A:166:G:H2'	1:A:167:G:C8	2.43	0.54
1:A:315:G:H2'	1:A:316:C:C6	2.43	0.54
1:A:161:G:N2	1:A:164:U:H3'	2.23	0.54
1:A:187:A:O2'	1:A:188:A:C8	2.61	0.54
1:A:64:C:O2'	1:A:82:A:N1	2.29	0.54
1:A:186:G:H22	1:A:189:A:P	2.31	0.53
1:A:205:A:H2'	1:A:205:A:N3	2.23	0.53
1:A:339:A:O2'	1:A:340:U:H5'	2.08	0.53
1:A:385:A:H8	1:A:400:U:HO2'	1.52	0.53
1:A:190:G:H2'	1:A:191:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:A:H2	1:A:270:U:O2	1.92	0.53
1:A:172:G:H4'	1:A:217:A:N1	2.24	0.53
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.53
1:A:60:C:H2'	1:A:61:G:C8	2.43	0.52
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.52
2:B:79:LYS:HD2	2:B:81:TYR:HE1	1.74	0.52
2:B:56:VAL:HA	2:B:59:ARG:HH12	1.75	0.52
1:A:176:C:H2'	1:A:177:G:O4'	2.08	0.52
1:A:268:G:H2'	1:A:269:G:C8	2.45	0.52
2:B:17:PHE:HE1	2:B:82:VAL:HG11	1.75	0.52
2:B:112:LYS:HG3	2:B:114:GLU:HG2	1.92	0.52
1:A:381:A:C6	1:A:382:G:C4	2.98	0.52
1:A:178:A:C8	1:A:180:U:C5	2.98	0.51
1:A:153:C:H2'	1:A:154:U:C6	2.46	0.51
1:A:349:G:N2	1:A:350:A:H62	2.08	0.51
1:A:316:C:H2'	1:A:317:G:N7	2.26	0.51
1:A:181:A:C2	1:A:182:C:H1'	2.45	0.51
1:A:222:U:H2'	1:A:223:A:C8	2.45	0.51
1:A:350:A:C5	1:A:380:A:H1'	2.46	0.51
1:A:3:U:H2'	1:A:4:A:C8	2.45	0.50
1:A:230:G:N3	1:A:230:G:H2'	2.26	0.50
1:A:215:G:N2	1:A:217:A:H3'	2.26	0.50
1:A:252:G:H2'	1:A:253:A:H5'	1.94	0.50
2:B:99:LYS:O	2:B:102:ILE:HG13	2.12	0.50
1:A:199:U:H2'	1:A:200:G:O4'	2.12	0.50
1:A:203:G:C4	1:A:205:A:H1'	2.46	0.50
1:A:18:A:H2'	1:A:19:A:C8	2.47	0.50
1:A:208:U:H3	1:A:225:A:N6	2.09	0.50
1:A:174:U:H2'	1:A:175:U:C6	2.46	0.50
1:A:116:A:H2'	1:A:117:G:H8	1.76	0.50
1:A:165:G:H3'	1:A:166:G:H8	1.77	0.50
1:A:322:C:H2'	1:A:323:A:H8	1.74	0.50
1:A:379:G:H21	1:A:380:A:H8	1.57	0.50
1:A:261:A:H2	1:A:271:A:N7	2.10	0.50
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.50
1:A:75:U:H3	1:A:291:A:H1'	1.77	0.49
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.49
1:A:2:U:H2'	1:A:3:U:C6	2.46	0.49
1:A:383:G:H2'	1:A:384:U:O4'	2.11	0.49
1:A:124:U:H2'	1:A:125:U:O4'	2.13	0.49
1:A:138:C:H5"	1:A:138:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.49
2:B:74:GLU:HB3	2:B:111:LEU:HD11	1.94	0.49
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.49
1:A:175:U:H2'	1:A:176:C:C6	2.48	0.49
1:A:319:A:H1'	1:A:320:U:C5	2.47	0.49
1:A:378:C:C3'	1:A:379:G:H8	2.21	0.49
1:A:92:C:OP2	1:A:138:C:H5'	2.13	0.49
2:B:44:GLY:HA3	2:B:82:VAL:HG22	1.95	0.49
1:A:161:G:H22	1:A:164:U:H3'	1.78	0.48
1:A:334:A:O4'	1:A:335:G:N2	2.46	0.48
1:A:378:C:H2'	1:A:379:G:H1'	1.95	0.48
1:A:141:C:O2	1:A:241:A:N6	2.46	0.48
1:A:327:U:H2'	1:A:328:G:C8	2.49	0.48
1:A:230:G:H2'	1:A:231:A:C8	2.49	0.48
1:A:380:A:C6	1:A:381:A:C5	3.01	0.48
2:B:24:ALA:HB2	2:B:29:VAL:HG22	1.96	0.48
1:A:147:A:C4	1:A:148:A:C8	3.02	0.48
1:A:38:G:H2'	1:A:39:C:H6	1.79	0.48
1:A:55:A:H2'	1:A:56:U:C6	2.49	0.48
1:A:274:G:H2'	1:A:275:G:O4'	2.14	0.48
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.48
1:A:95:A:H2'	1:A:96:G:C8	2.49	0.47
1:A:327:U:H2'	1:A:328:G:H8	1.79	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
1:A:177:G:H2'	1:A:178:A:C8	2.50	0.47
1:A:196:C:H2'	1:A:197:A:O4'	2.15	0.47
1:A:295:A:O2'	1:A:296:A:H5'	2.13	0.47
1:A:378:C:C3'	1:A:379:G:C8	2.94	0.47
1:A:262:A:H3'	1:A:263:A:C8	2.49	0.47
1:A:70:U:H2'	1:A:71:G:O4'	2.14	0.47
1:A:236:G:H2'	1:A:237:G:H8	1.79	0.47
1:A:31:G:C2	1:A:32:G:N1	2.83	0.47
1:A:45:A:C8	1:A:45:A:H5'	2.50	0.47
1:A:224:G:H2'	1:A:225:A:O4'	2.14	0.47
1:A:379:G:H2'	1:A:380:A:H5"	1.97	0.47
1:A:159:C:H2'	1:A:160:C:H6	1.78	0.46
1:A:169:U:H2'	1:A:170:A:C8	2.49	0.46
1:A:230:G:C5	1:A:231:A:C6	3.04	0.46
1:A:380:A:H3'	1:A:381:A:C8	2.47	0.46
1:A:114:G:H2'	1:A:115:C:C6	2.50	0.46
1:A:71:G:H1'	1:A:295:A:H2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:U:H2'	1:A:341:U:O4'	2.16	0.46
1:A:315:G:H2'	1:A:316:C:H6	1.81	0.46
1:A:85:G:H1'	1:A:86:U:C4	2.50	0.46
1:A:95:A:H2'	1:A:96:G:H8	1.79	0.46
1:A:102:C:H2'	1:A:103:C:C6	2.51	0.46
1:A:110:U:H2'	1:A:111:A:C8	2.50	0.46
1:A:207:C:H2'	1:A:208:U:O4'	2.16	0.46
1:A:37:G:N1	1:A:38:G:C5	2.84	0.45
1:A:116:A:H2'	1:A:117:G:C8	2.50	0.45
1:A:14:G:C2'	1:A:401:A:H61	2.29	0.45
1:A:135:U:H2'	1:A:136:G:O4'	2.14	0.45
1:A:214:G:H1	1:A:219:C:H42	1.63	0.45
1:A:38:G:H2'	1:A:39:C:C6	2.51	0.45
1:A:24:U:H5"	2:B:3:LYS:HE2	1.99	0.45
1:A:110:U:H2'	1:A:111:A:H8	1.81	0.45
1:A:178:A:C4	1:A:180:U:C4	3.05	0.45
1:A:222:U:H2'	1:A:223:A:H8	1.81	0.45
1:A:350:A:H3'	1:A:351:G:O4'	2.17	0.45
2:B:111:LEU:HD12	2:B:111:LEU:HA	1.86	0.45
1:A:284:C:H2'	1:A:285:G:O4'	2.17	0.45
1:A:167:G:H2'	1:A:168:A:C8	2.52	0.44
1:A:144:G:C2	1:A:145:G:H1'	2.52	0.44
1:A:201:A:C4	1:A:231:A:H2	2.35	0.44
1:A:201:A:H4'	1:A:202:C:H6	1.82	0.44
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.44
1:A:9:U:H2'	1:A:10:G:H8	1.82	0.44
1:A:277:A:H61	1:A:391:C:H4'	1.81	0.44
1:A:337:U:H3'	1:A:338:G:H5'	1.99	0.44
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.44
2:B:56:VAL:HA	2:B:59:ARG:NH1	2.32	0.44
1:A:165:G:H3'	1:A:166:G:C8	2.52	0.44
1:A:172:G:H5"	1:A:216:A:N6	2.22	0.44
1:A:230:G:C2	1:A:231:A:C4	3.06	0.44
1:A:352:U:H2'	1:A:353:A:C8	2.53	0.44
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.44
1:A:115:C:H2'	1:A:116:A:C8	2.51	0.44
1:A:206:G:H1'	1:A:207:C:C5	2.48	0.44
1:A:220:C:H2'	1:A:221:U:H6	1.79	0.44
2:B:37:GLU:CD	2:B:37:GLU:H	2.26	0.44
1:A:335:G:OP2	2:B:8:LYS:NZ	2.49	0.43
1:A:407:U:H2'	1:A:408:G:H8	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:HB3	2:B:88:PRO:HG2	2.00	0.43
2:B:1:MET:HE3	2:B:1:MET:HB3	1.54	0.43
1:A:134:C:H2'	1:A:135:U:C6	2.53	0.43
1:A:214:G:H2'	1:A:215:G:C8	2.53	0.43
1:A:396:C:H2'	1:A:397:U:C6	2.53	0.43
1:A:114:G:H2'	1:A:115:C:H6	1.83	0.43
1:A:198:G:O2'	1:A:227:G:N2	2.51	0.43
1:A:402:G:C2'	1:A:403:A:H5'	2.48	0.43
1:A:56:U:H2'	1:A:57:G:H8	1.83	0.43
2:B:4:LYS:HE2	2:B:4:LYS:HB2	1.75	0.43
2:B:72:LYS:HE3	2:B:72:LYS:HB3	1.67	0.43
1:A:197:A:N1	1:A:232:A:N6	2.66	0.43
1:A:363:A:O2'	1:A:364:A:O4'	2.33	0.43
1:A:59:U:HO2'	1:A:258:C:HO2'	1.65	0.43
1:A:82:A:H3'	1:A:83:G:H8	1.83	0.43
1:A:85:G:H2'	1:A:87:U:C4	2.53	0.43
1:A:281:U:H2'	1:A:282:C:H6	1.83	0.43
1:A:358:G:H1	1:A:366:C:H42	1.66	0.43
1:A:146:A:N7	1:A:180:U:C4	2.87	0.42
1:A:36:C:H6	1:A:36:C:P	2.42	0.42
1:A:37:G:C2	1:A:38:G:C8	3.07	0.42
1:A:48:A:N1	1:A:50:A:H1'	2.34	0.42
1:A:321:G:C2	1:A:322:C:C2	3.08	0.42
2:B:105:LEU:HD23	2:B:105:LEU:HA	1.85	0.42
1:A:334:A:H4'	1:A:335:G:OP1	2.19	0.42
1:A:405:C:C2	1:A:406:A:C8	3.08	0.42
1:A:31:G:N1	1:A:37:G:C5	2.87	0.42
1:A:38:G:C6	1:A:39:C:C4	3.07	0.42
1:A:71:G:O2'	1:A:294:G:N2	2.52	0.42
1:A:104:A:H2'	1:A:105:U:O4'	2.20	0.42
1:A:206:G:H1	1:A:232:A:HO2'	1.58	0.42
1:A:213:G:H2'	1:A:214:G:C8	2.55	0.42
1:A:221:U:H2'	1:A:222:U:C6	2.55	0.42
1:A:123:C:H2'	1:A:124:U:O4'	2.19	0.42
1:A:269:G:H3'	1:A:270:U:H6	1.84	0.42
1:A:308:A:H2'	1:A:309:C:C6	2.54	0.42
1:A:355:G:H2'	1:A:356:A:C8	2.54	0.42
1:A:364:A:H3'	1:A:364:A:P	2.60	0.42
1:A:404:G:C6	1:A:405:C:C4	3.08	0.42
1:A:137:A:H1'	1:A:240:A:H61	1.83	0.42
1:A:62:C:H2'	1:A:63:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:G:N3	1:A:230:G:N2	2.68	0.42
1:A:31:G:N2	1:A:32:G:H22	2.17	0.42
1:A:172:G:OP1	1:A:216:A:N6	2.53	0.42
1:A:317:G:O6	1:A:321:G:C2	2.73	0.42
1:A:7:C:H2'	1:A:8:A:H8	1.85	0.42
1:A:208:U:H2'	1:A:209:C:O4'	2.20	0.42
1:A:317:G:C5	1:A:318:C:N3	2.87	0.42
1:A:349:G:H22	1:A:350:A:H62	1.65	0.41
1:A:363:A:C2'	1:A:364:A:C1'	2.93	0.41
1:A:380:A:C4	1:A:381:A:C8	3.08	0.41
1:A:39:C:H2'	1:A:40:C:C6	2.55	0.41
1:A:353:A:H3'	1:A:354:C:C6	2.55	0.41
2:B:27:GLN:HA	2:B:86:ARG:HB2	2.01	0.41
1:A:316:C:H2'	1:A:317:G:C8	2.54	0.41
1:A:379:G:C3'	1:A:380:A:H5"	2.51	0.41
1:A:14:G:H2'	1:A:385:A:N1	2.36	0.41
1:A:111:A:H2'	1:A:112:G:C8	2.55	0.41
1:A:283:C:H2'	1:A:284:C:C6	2.55	0.41
1:A:356:A:H3'	1:A:357:G:C8	2.56	0.41
2:B:67:CYS:SG	2:B:98:LYS:HA	2.60	0.41
1:A:144:G:H8	1:A:144:G:H5"	1.86	0.41
1:A:223:A:H2'	1:A:224:G:C8	2.55	0.41
1:A:239:A:H5'	1:A:240:A:OP1	2.20	0.41
1:A:263:A:OP2	1:A:263:A:H8	2.03	0.41
1:A:36:C:H2'	1:A:37:G:H8	1.83	0.41
1:A:218:A:H3'	1:A:219:C:C6	2.55	0.41
2:B:2:LYS:HE2	2:B:2:LYS:HB3	1.55	0.41
1:A:178:A:C5	1:A:180:U:C5	3.08	0.41
1:A:33:U:H4'	1:A:34:U:O4'	2.20	0.41
1:A:59:U:H2'	1:A:60:C:H6	1.86	0.41
1:A:82:A:H3'	1:A:83:G:C8	2.56	0.41
1:A:158:U:H2'	1:A:159:C:O4'	2.20	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.85	0.41
1:A:230:G:N3	1:A:230:G:C2'	2.84	0.41
1:A:270:U:C2'	1:A:271:A:H5"	2.51	0.41
1:A:329:U:H5"	1:A:329:U:H6	1.86	0.41
2:B:75:VAL:HG13	2:B:81:TYR:HE2	1.86	0.41
1:A:262:A:H8	1:A:262:A:O5'	2.03	0.40
1:A:300:A:H2'	1:A:301:G:H5'	2.02	0.40
1:A:19:A:H2'	1:A:20:U:C6	2.56	0.40
1:A:144:G:C6	1:A:145:G:C4	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:G:C6	1:A:43:A:C2	3.10	0.40
1:A:234:G:N3	1:A:234:G:C2'	2.84	0.40
1:A:320:U:H2'	1:A:321:G:O4'	2.22	0.40
1:A:7:C:H2'	1:A:8:A:C8	2.56	0.40
1:A:85:G:H4'	1:A:86:U:C6	2.57	0.40
1:A:148:A:N1	1:A:177:G:O2'	2.52	0.40
1:A:230:G:C4	1:A:231:A:C5	3.10	0.40
1:A:369:C:H2'	1:A:370:U:O4'	2.22	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
2	B	114/116 (98%)	104 (91%)	10 (9%)	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
2	B	99/99 (100%)	93 (94%)	6 (6%)	15 36

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

Mol	Chain	Res	Type
2	B	1	MET
2	B	2	LYS
2	B	4	LYS
2	B	9	LYS
2	B	27	GLN
2	B	72	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	14	GLN
2	B	27	GLN
2	B	38	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	178 (42%)	16 (3%)

All (178) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	U
1	A	6	U
1	A	15	G
1	A	19	A
1	A	22	G
1	A	28	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	G
1	A	40	C
1	A	41	G
1	A	45	A
1	A	46	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A

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Mol	Chain	Res	Type
1	A	51	G
1	A	52	U
1	A	53	C
1	A	54	C
1	A	65	G
1	A	67	U
1	A	68	G
1	A	69	C
1	A	71	G
1	A	74	A
1	A	75	U
1	A	76	G
1	A	80	G
1	A	81	U
1	A	85	G
1	A	86	U
1	A	99	A
1	A	101	U
1	A	102	C
1	A	103	C
1	A	106	A
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	129	C
1	A	131	G
1	A	132	G
1	A	134	C
1	A	136	G
1	A	137	A
1	A	138	C
1	A	142	G
1	A	144	G
1	A	145	G
1	A	146	A
1	A	147	A
1	A	148	A
1	A	149	G
1	A	150	A
1	A	151	A

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Mol	Chain	Res	Type
1	A	152	C
1	A	157	G
1	A	167	G
1	A	168	A
1	A	171	U
1	A	172	G
1	A	173	G
1	A	174	U
1	A	178	A
1	A	179	U
1	A	180	U
1	A	181	A
1	A	182	C
1	A	184	C
1	A	185	U
1	A	186	G
1	A	187	A
1	A	188	A
1	A	190	G
1	A	192	G
1	A	193	C
1	A	202	C
1	A	203	G
1	A	204	G
1	A	205	A
1	A	206	G
1	A	207	C
1	A	209	C
1	A	210	U
1	A	212	A
1	A	213	G
1	A	214	G
1	A	216	A
1	A	219	C
1	A	225	A
1	A	229	G
1	A	231	A
1	A	232	A
1	A	233	C
1	A	234	G
1	A	235	C
1	A	236	G

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Mol	Chain	Res	Type
1	A	237	G
1	A	238	U
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	255	A
1	A	256	A
1	A	259	C
1	A	260	C
1	A	263	A
1	A	264	U
1	A	265	G
1	A	266	A
1	A	267	U
1	A	269	G
1	A	271	A
1	A	273	G
1	A	275	G
1	A	278	C
1	A	289	G
1	A	291	A
1	A	292	A
1	A	294	G
1	A	299	G
1	A	304	A
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	326	C
1	A	328	G
1	A	329	U
1	A	330	A
1	A	332	A
1	A	333	U
1	A	334	A
1	A	335	G
1	A	336	A
1	A	337	U
1	A	342	A

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Mol	Chain	Res	Type
1	A	347	C
1	A	349	G
1	A	350	A
1	A	351	G
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	378	C
1	A	379	G
1	A	380	A
1	A	381	A
1	A	385	A
1	A	387	A
1	A	389	A
1	A	390	A
1	A	395	G
1	A	400	U
1	A	401	A
1	A	402	G
1	A	403	A
1	A	409	A
1	A	410	U
1	A	411	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	52	U
1	A	67	U
1	A	75	U
1	A	91	G

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Mol	Chain	Res	Type
1	A	126	U
1	A	204	G
1	A	211	A
1	A	232	A
1	A	235	C
1	A	263	A
1	A	276	C
1	A	333	U
1	A	363	A
1	A	365	G
1	A	389	A

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 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

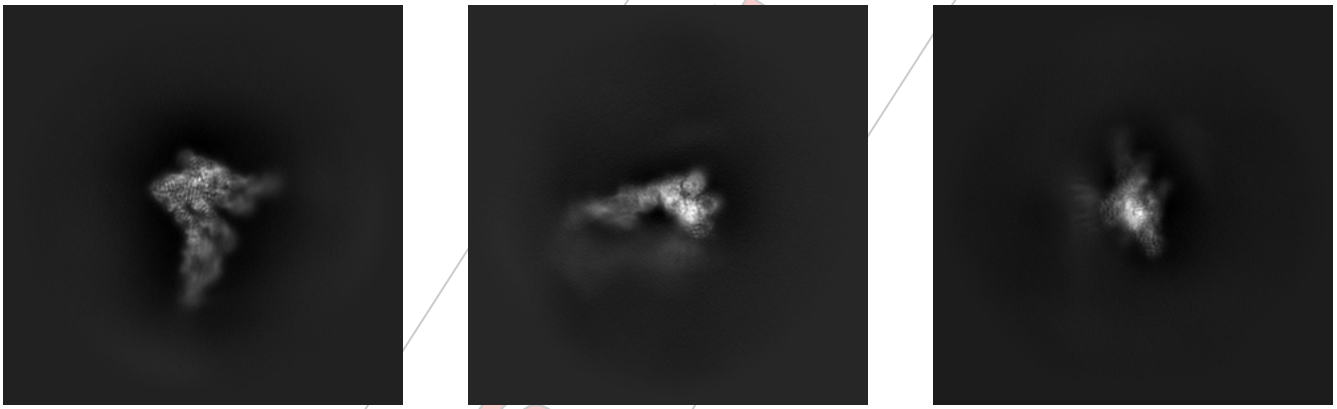
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70941. 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.

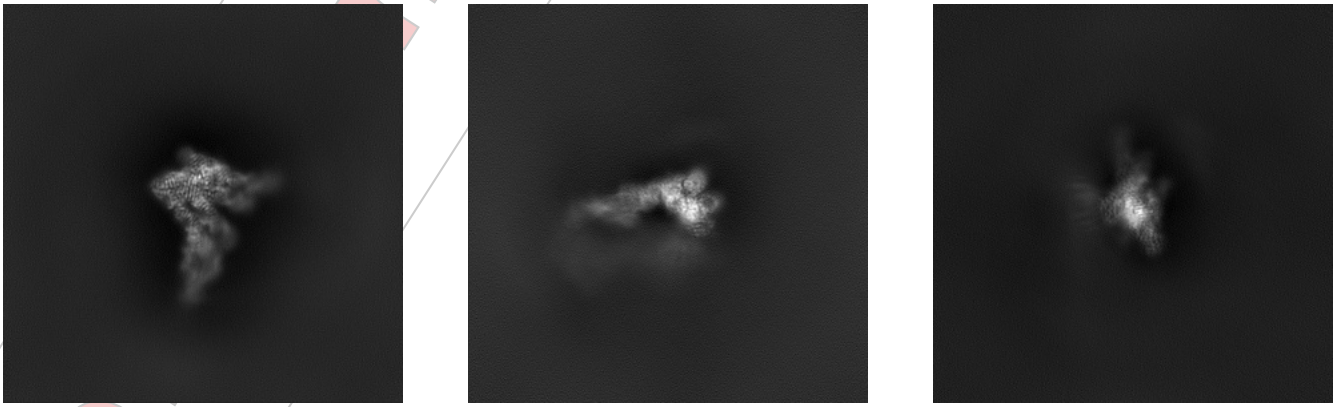
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

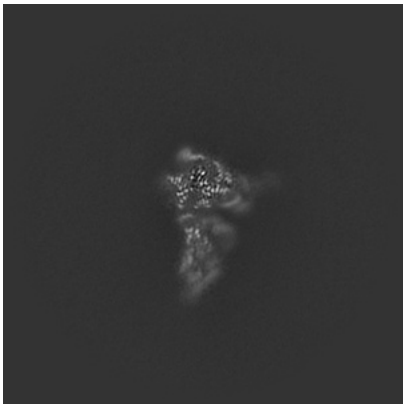


X Y Z

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

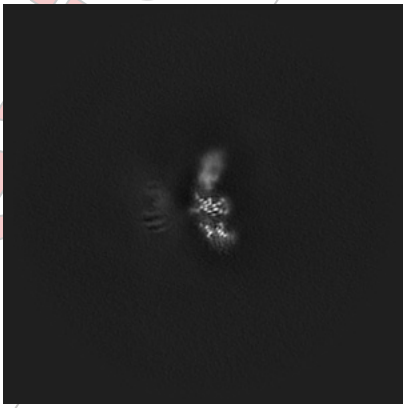
6.2 Central slices (i)

6.2.1 Primary map



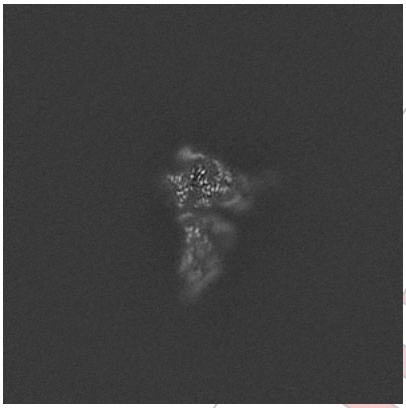
X Index: 200

Y Index: 200

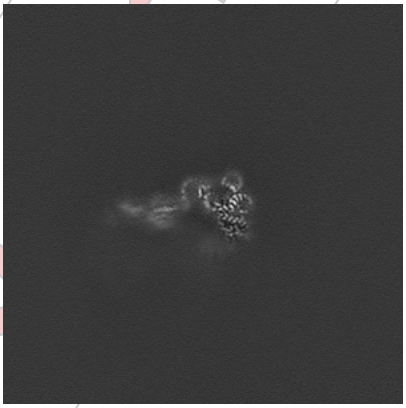


Z Index: 200

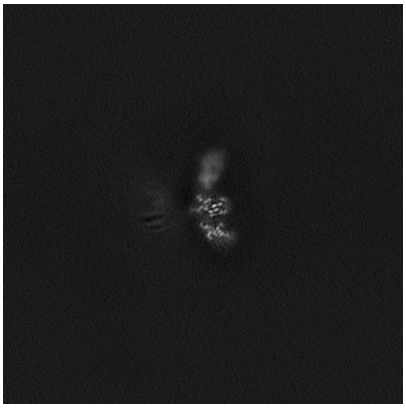
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

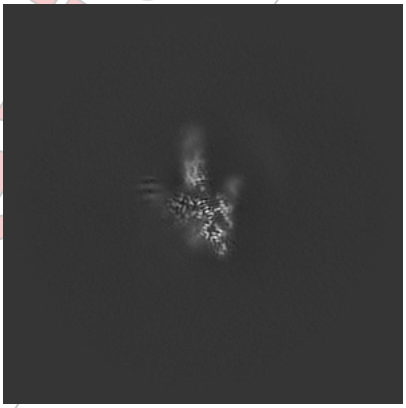
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

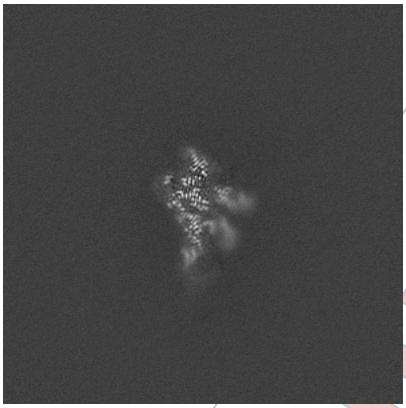
X Index: 207

Y Index: 192



Z Index: 222

6.3.2 Raw map



X Index: 207

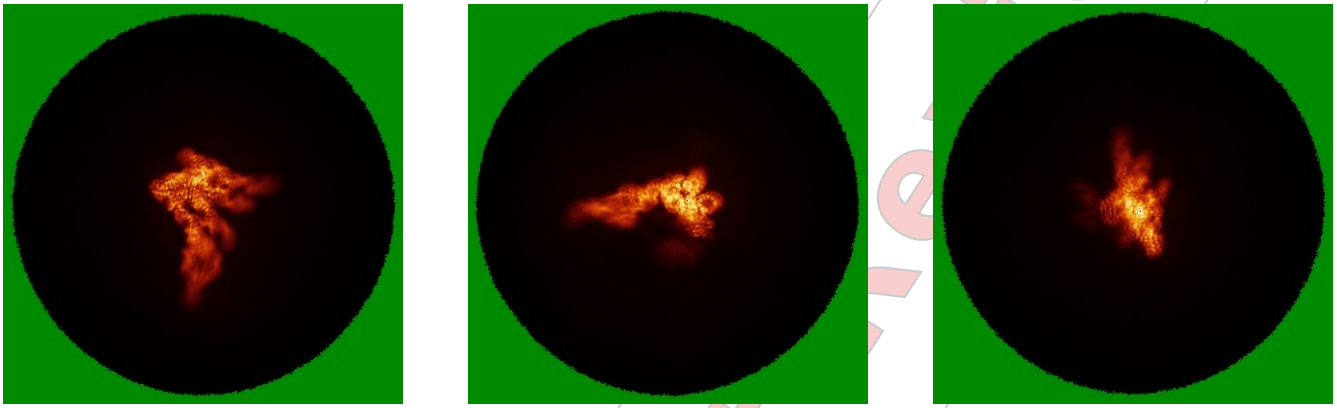
Y Index: 192

Z Index: 223

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

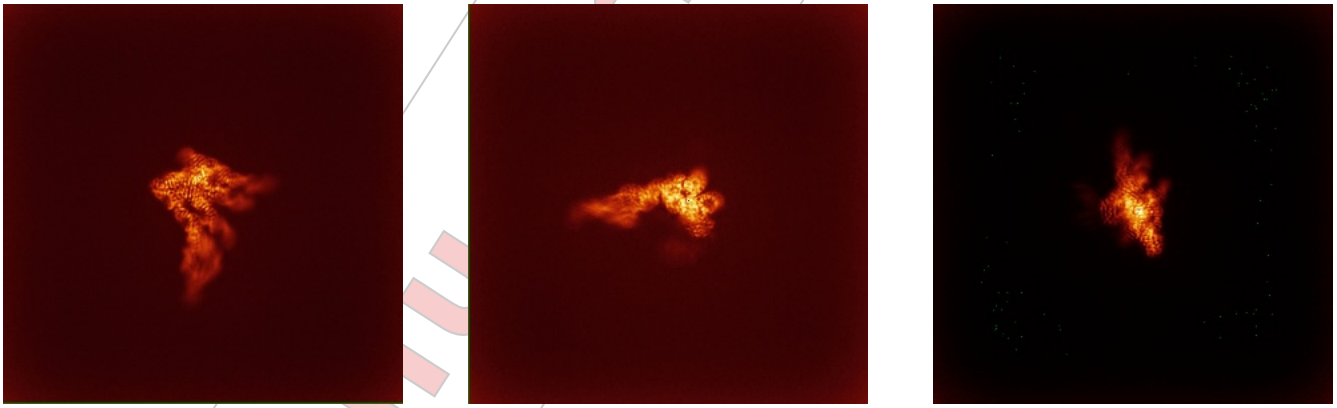
6.4 Orthogonal standard-deviation projections (False-color)

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 0.0519. 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.

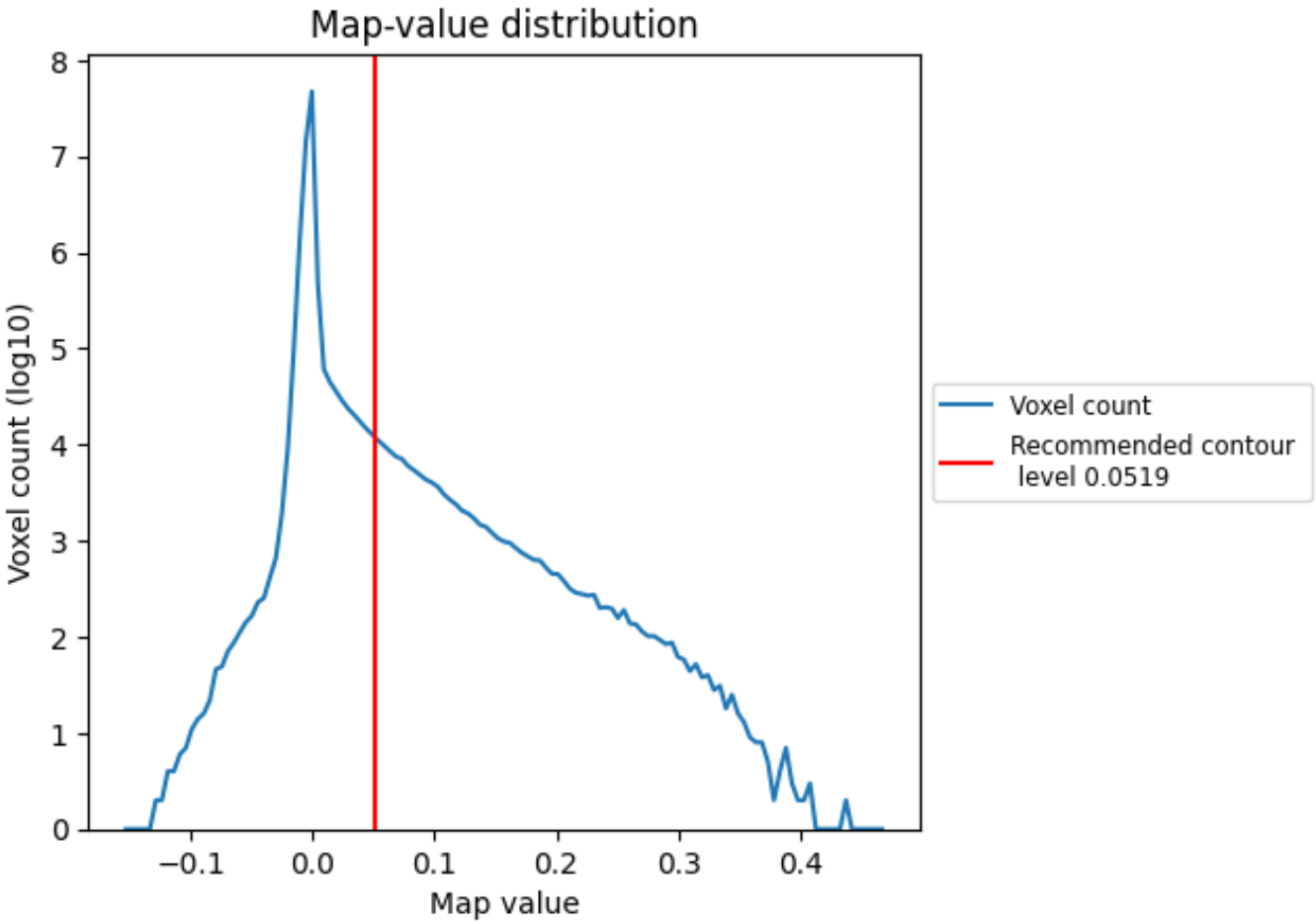
6.6 Mask visualisation (i)

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

7 Map analysis

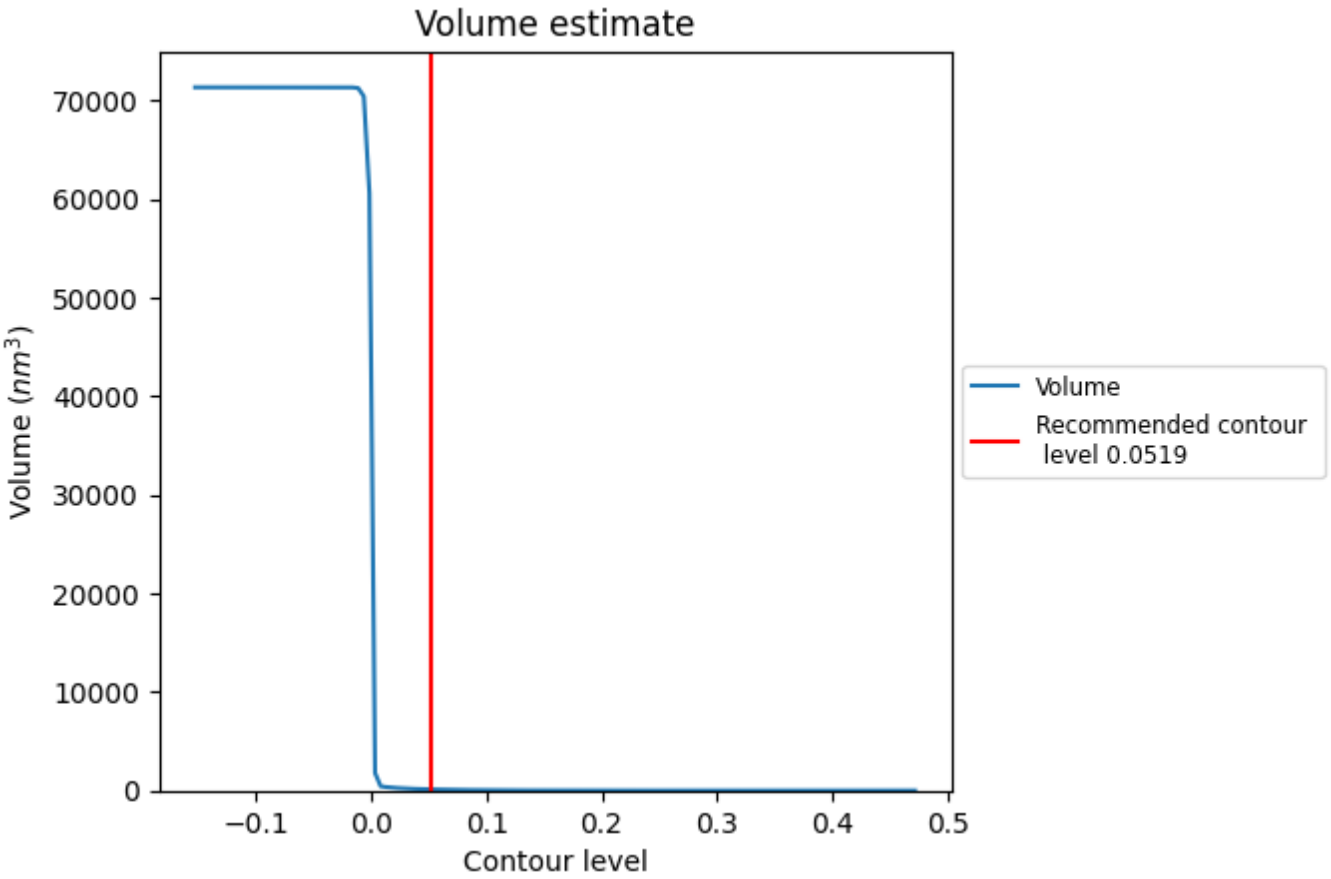
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

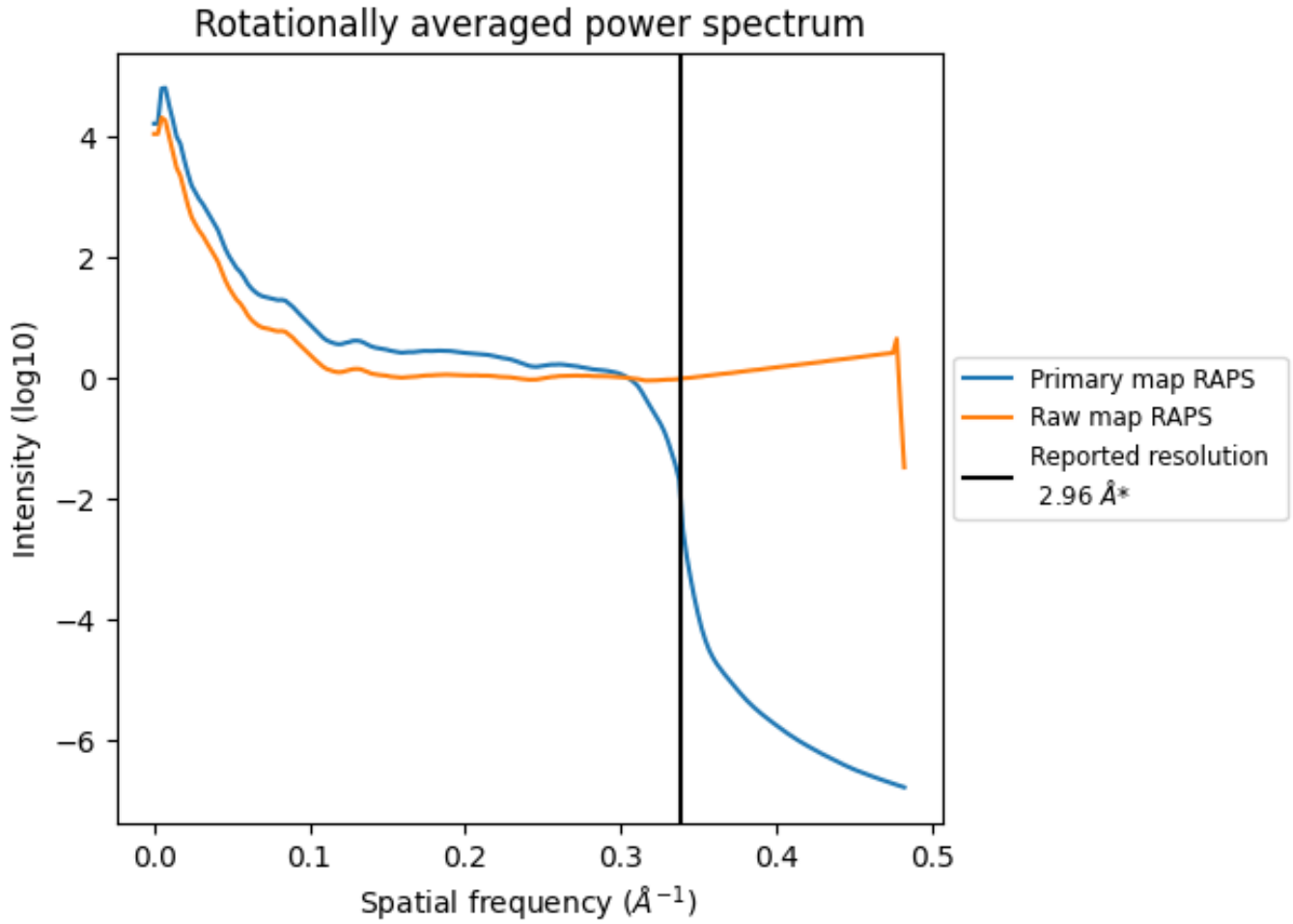
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 108 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 (i)

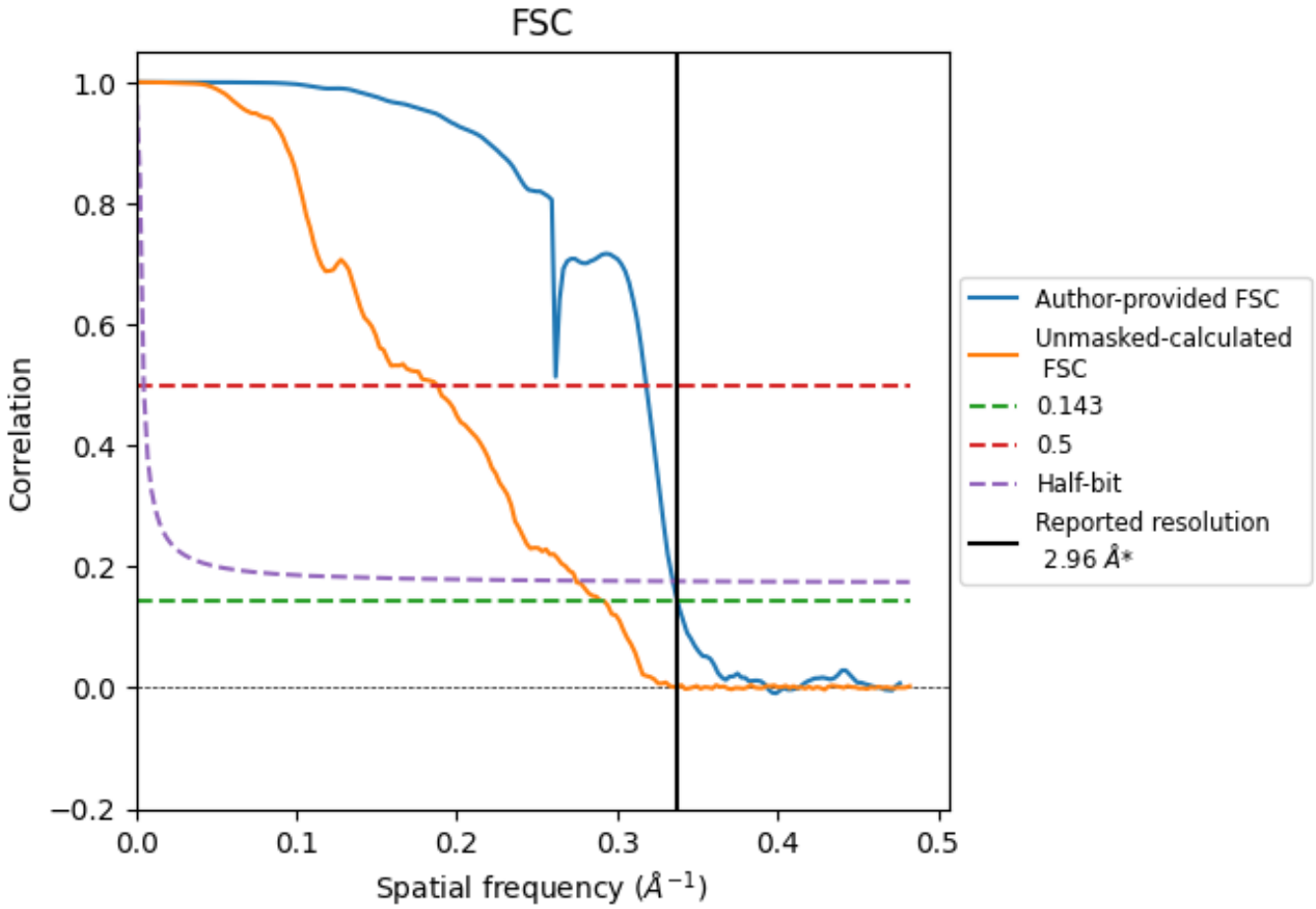


*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

8.2 Resolution estimates (i)

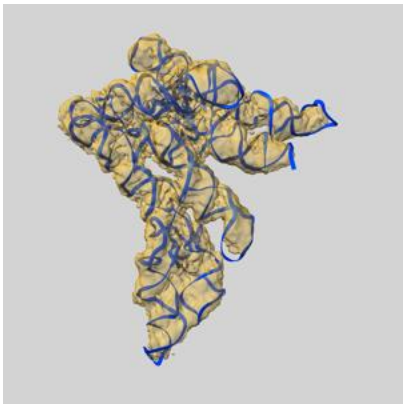
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.14	2.99
Unmasked-calculated*	3.43	5.33	3.64

*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 3.43 differs from the reported value 2.96 by more than 10 %

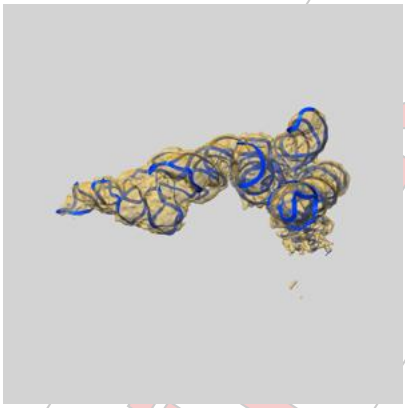
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70941 and PDB model 9OWR. Per-residue inclusion information can be found in section 3 on page 4.

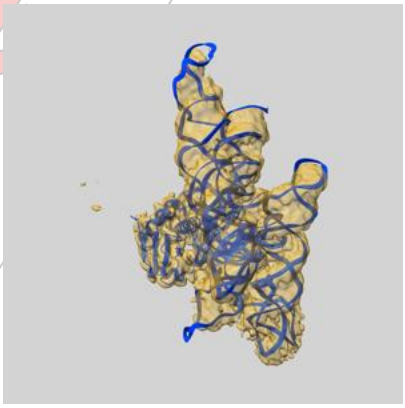
9.1 Map-model overlay



X



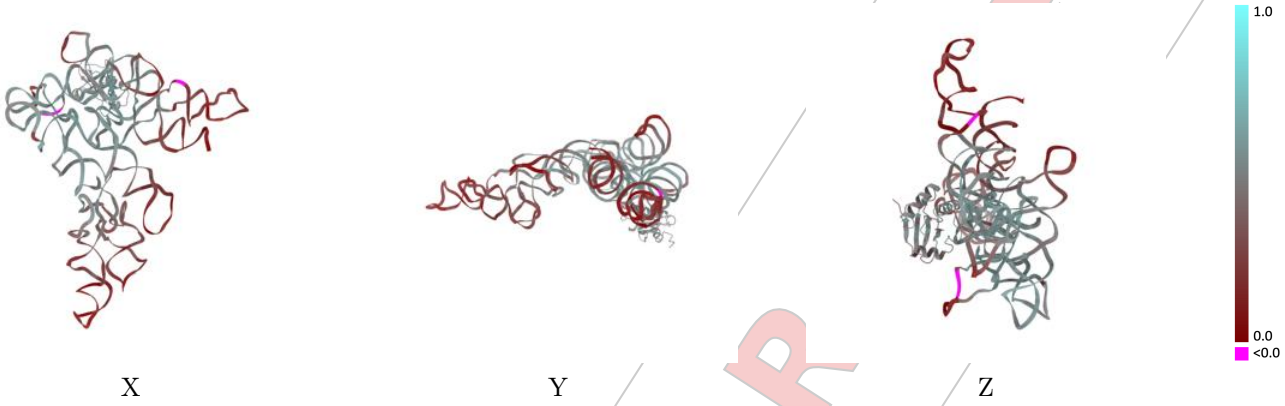
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0519 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.

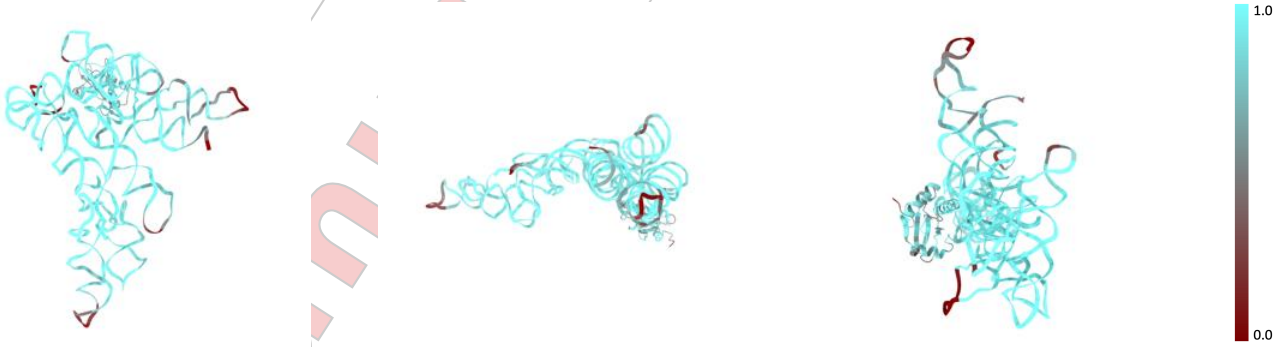
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

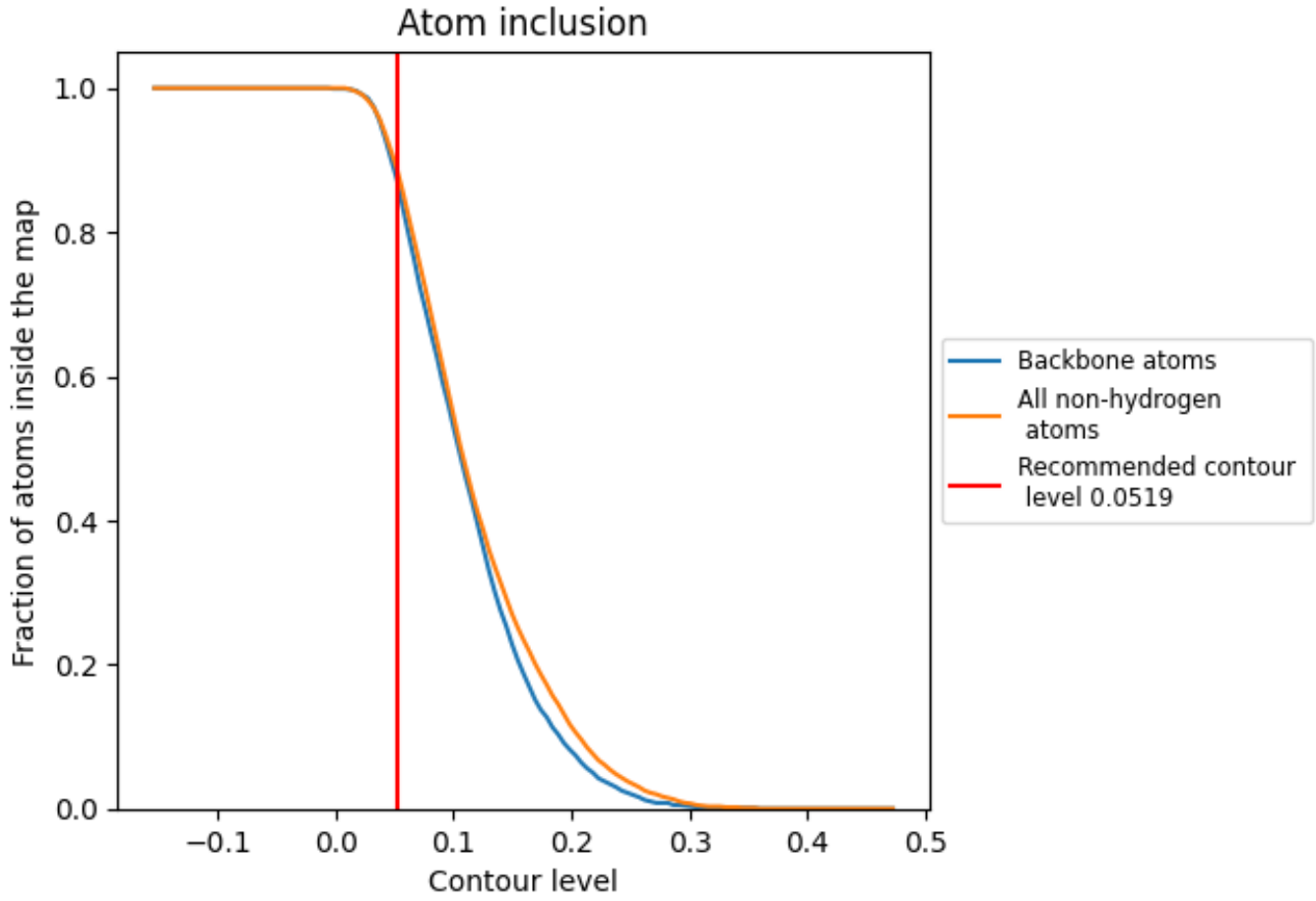
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0519).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.3970
A	0.8990	0.3870
B	0.7940	0.4950

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 11:53 AM EDT

PDB ID	:	9OWS / pdb_00009ows
EMDB ID	:	EMD-70942
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in 5 mM Mg2+
Deposited on	:	2025-06-02
Resolution	:	2.87 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

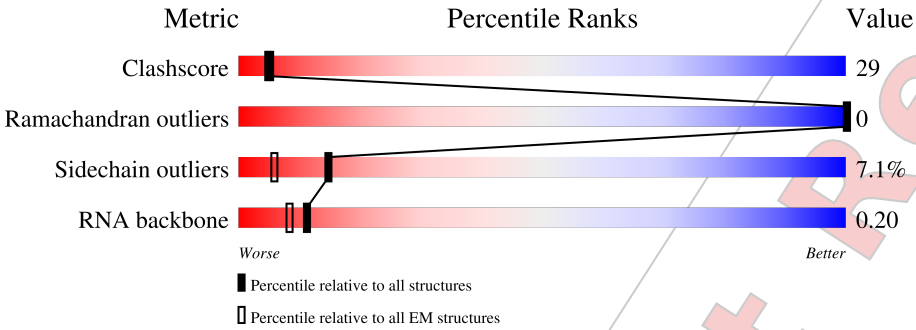
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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 <=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	417	17% 49% 33%
2	B	116	65% 30%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9931 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

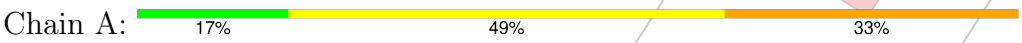
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	22	22	22	0

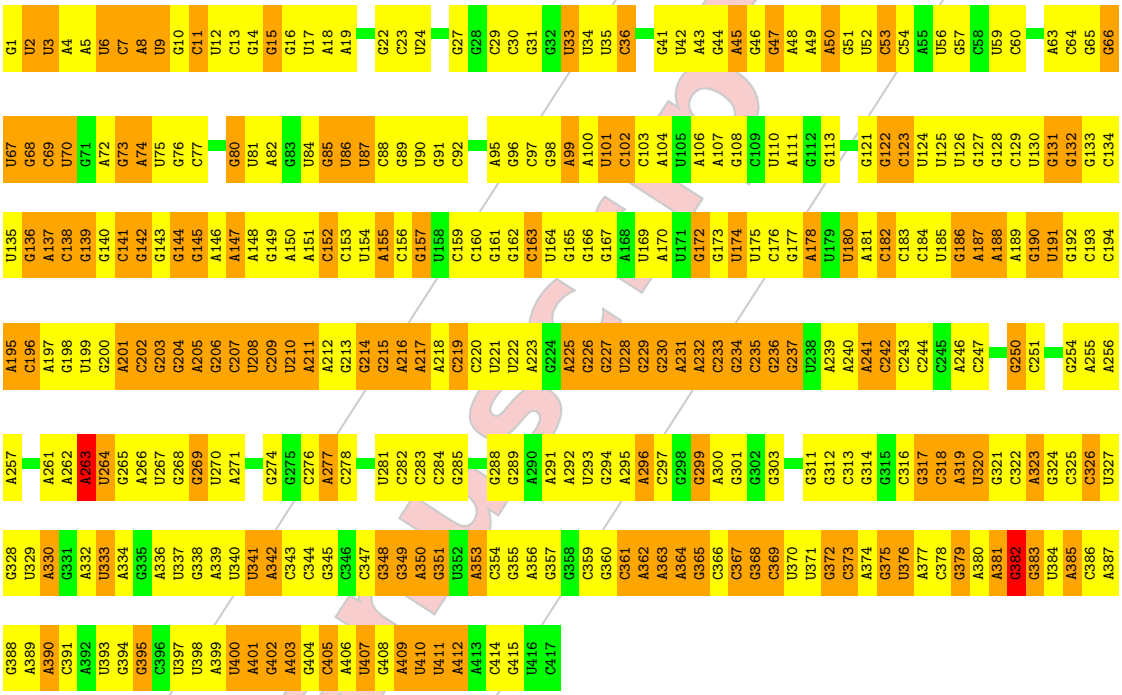
3 Residue-property plots (i)

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: RNase P RNA (417-MER)

Chain A:





- Molecule 2: Ribonuclease P protein component

Chain B:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	998359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.086	Depositor
Minimum map value	-0.313	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.66	0/10038	0.98	11/15661 (0.1%)
2	B	0.41	0/962	0.71	1/1281 (0.1%)
All	All	0.64	0/11000	0.96	12/16942 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	G	O3'-P-O5'	-7.99	92.01	104.00
1	A	14	G	O3'-P-O5'	-6.69	93.97	104.00
1	A	277	A	C2'-C3'-O3'	-6.54	99.69	109.50
2	B	4	LYS	N-CA-C	-5.44	104.99	111.03
1	A	263	A	P-O3'-C3'	5.41	128.31	120.20
1	A	44	G	C4'-C3'-C2'	-5.33	97.27	102.60
1	A	333	U	C2'-C3'-O3'	-5.28	105.78	113.70
1	A	382	G	O3'-P-O5'	-5.12	96.32	104.00
1	A	274	G	C4'-C3'-C2'	-5.10	97.50	102.60
1	A	263	A	C4'-C3'-O3'	5.09	120.64	113.00
1	A	348	G	C2'-C3'-O3'	-5.08	106.08	113.70
1	A	250	G	C4'-C3'-O3'	-5.08	105.39	113.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	6	ARG	Sidechain

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	8962	0	4510	378	0
2	B	947	0	1008	31	0
3	A	22	0	0	1	0
All	All	9931	0	5518	406	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 29.

All (406) 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:161:G:H3'	1:A:162:G:C8	1.51	1.46
1:A:161:G:H3'	1:A:162:G:N7	1.26	1.43
1:A:162:G:O3'	1:A:163:C:C5	1.85	1.30
1:A:161:G:C3'	1:A:162:G:C8	2.17	1.27
1:A:154:U:H2'	1:A:155:A:C8	1.78	1.16
1:A:162:G:O3'	1:A:163:C:H5	1.27	1.04
1:A:162:G:O3'	1:A:163:C:C6	2.14	0.99
1:A:163:C:C6	1:A:163:C:P	2.57	0.97
1:A:161:G:C3'	1:A:162:G:N7	2.22	0.97
1:A:349:G:H1	1:A:378:C:H42	1.11	0.91
1:A:163:C:P	1:A:163:C:H6	1.93	0.90
1:A:162:G:C8	1:A:162:G:O5'	2.25	0.90
1:A:164:U:C4	1:A:165:G:C5	2.62	0.87
1:A:72:A:H2'	1:A:73:G:C8	2.09	0.87
1:A:371:U:H5"	1:A:372:G:H5'	1.57	0.86
1:A:154:U:H2'	1:A:155:A:H8	1.37	0.86
1:A:157:G:H1	1:A:169:U:H3	1.23	0.85
1:A:164:U:O4	1:A:165:G:C6	2.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:U:H2'	1:A:181:A:H8	1.39	0.85
1:A:161:G:C3'	1:A:162:G:H8	1.87	0.83
1:A:217:A:H2'	1:A:218:A:C8	2.13	0.82
1:A:161:G:C2'	1:A:162:G:C8	2.63	0.82
1:A:164:U:C4	1:A:165:G:C6	2.67	0.82
1:A:293:U:OP2	3:A:511:MG:MG	1.25	0.77
1:A:349:G:H1'	1:A:350:A:C8	2.19	0.77
1:A:165:G:H3'	1:A:166:G:H8	1.49	0.77
1:A:47:G:H1	1:A:385:A:H62	1.31	0.76
1:A:348:G:H3'	1:A:349:G:H8	1.50	0.76
1:A:162:G:C8	1:A:162:G:P	2.79	0.75
1:A:142:G:C5	1:A:189:A:C2	2.75	0.75
1:A:367:C:H2'	1:A:368:G:C8	2.22	0.74
1:A:199:U:O2	1:A:206:G:H4'	1.87	0.74
1:A:393:U:H2'	1:A:394:G:C8	2.21	0.74
1:A:380:A:H2'	1:A:381:A:C8	2.21	0.74
1:A:162:G:O2'	1:A:164:U:C6	2.40	0.74
1:A:184:C:H2'	1:A:185:U:C6	2.25	0.71
1:A:206:G:H1'	1:A:207:C:C5	2.26	0.70
1:A:165:G:H3'	1:A:166:G:C8	2.27	0.70
1:A:348:G:H2'	1:A:381:A:H61	1.56	0.70
1:A:17:U:H3	1:A:342:A:H61	1.37	0.69
1:A:385:A:H8	1:A:400:U:HO2'	1.41	0.69
1:A:222:U:H2'	1:A:223:A:H8	1.58	0.69
1:A:161:G:H2'	1:A:162:G:C8	2.27	0.69
1:A:164:U:H2'	1:A:165:G:O4'	1.92	0.69
1:A:172:G:H4'	1:A:217:A:H61	1.57	0.69
1:A:181:A:H3'	1:A:182:C:H6	1.57	0.69
1:A:213:G:H3'	1:A:214:G:H8	1.57	0.68
1:A:161:G:H22	1:A:164:U:H3'	1.58	0.68
1:A:155:A:C1'	1:A:217:A:H1'	2.23	0.68
1:A:348:G:H3'	1:A:349:G:C8	2.28	0.68
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.67
1:A:89:G:H2'	1:A:90:U:C6	2.28	0.67
1:A:162:G:H1'	1:A:164:U:C6	2.30	0.67
1:A:203:G:C4	1:A:205:A:H1'	2.30	0.67
1:A:162:G:O5'	1:A:162:G:H8	1.76	0.66
1:A:241:A:H2'	1:A:242:C:C6	2.29	0.66
1:A:164:U:O4	1:A:165:G:O6	2.13	0.66
1:A:155:A:H1'	1:A:217:A:H1'	1.76	0.66
1:A:190:G:H2'	1:A:191:U:O4'	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:A:H2'	1:A:147:A:O4'	1.97	0.65
1:A:122:G:H3'	1:A:123:C:H5"	1.78	0.65
2:B:0:GLY:HA2	2:B:65:ARG:HB3	1.79	0.65
1:A:162:G:O4'	1:A:164:U:C5	2.49	0.65
1:A:180:U:H2'	1:A:181:A:C8	2.27	0.65
1:A:162:G:C1'	1:A:164:U:C5	2.80	0.64
1:A:230:G:H21	1:A:231:A:H2'	1.62	0.64
1:A:66:G:H2'	1:A:67:U:O2	1.97	0.64
1:A:162:G:H8	1:A:162:G:P	2.19	0.64
1:A:349:G:H1'	1:A:350:A:H8	1.62	0.64
1:A:222:U:H2'	1:A:223:A:C8	2.32	0.64
1:A:161:G:N2	1:A:165:G:C8	2.66	0.64
1:A:186:G:H8	1:A:186:G:H5"	1.62	0.64
1:A:349:G:H1	1:A:378:C:N4	1.90	0.64
1:A:45:A:H62	2:B:62:ARG:HH22	1.47	0.63
1:A:110:U:H2'	1:A:111:A:C8	2.33	0.63
1:A:206:G:H1'	1:A:207:C:H5	1.61	0.63
1:A:221:U:H2'	1:A:222:U:C6	2.33	0.63
1:A:69:C:H2'	1:A:70:U:C6	2.33	0.63
1:A:67:U:H4'	1:A:68:G:OP1	1.99	0.63
1:A:141:C:H3'	1:A:142:G:H5"	1.80	0.62
1:A:379:G:N2	1:A:380:A:H62	1.98	0.62
2:B:6:ARG:HD2	2:B:8:LYS:HD3	1.81	0.62
1:A:163:C:C5	1:A:163:C:P	2.88	0.62
2:B:56:VAL:O	2:B:60:ILE:HG12	1.98	0.62
1:A:59:U:H2'	1:A:60:C:C6	2.34	0.62
1:A:45:A:H62	2:B:62:ARG:NH2	1.96	0.62
1:A:130:U:H2'	1:A:131:G:C8	2.35	0.62
1:A:163:C:C6	1:A:163:C:OP1	2.51	0.62
1:A:15:G:N2	1:A:345:G:H1'	2.15	0.61
1:A:56:U:O2	1:A:100:A:H2	1.83	0.61
1:A:199:U:H2'	1:A:200:G:O4'	2.01	0.61
1:A:164:U:N3	1:A:165:G:C5	2.69	0.61
1:A:7:C:H2'	1:A:8:A:C8	2.36	0.61
1:A:380:A:C2	1:A:381:A:C5	2.89	0.60
1:A:9:U:H2'	1:A:10:G:C8	2.37	0.60
1:A:161:G:N2	1:A:164:U:C6	2.69	0.60
1:A:194:C:H5"	1:A:195:A:H5'	1.83	0.60
1:A:226:G:H3'	1:A:227:G:H8	1.67	0.59
2:B:89:ALA:HA	2:B:92:MET:SD	2.42	0.59
1:A:409:A:H3'	1:A:410:U:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:U:H2'	1:A:131:G:H8	1.68	0.59
1:A:181:A:H3'	1:A:182:C:C6	2.36	0.59
1:A:348:G:C2'	1:A:381:A:H61	2.15	0.59
2:B:3:LYS:HD3	2:B:8:LYS:HE2	1.85	0.59
1:A:99:A:H2'	1:A:100:A:C8	2.38	0.58
1:A:380:A:H2'	1:A:381:A:H8	1.66	0.58
1:A:68:G:C8	1:A:68:G:H5"	2.39	0.58
1:A:181:A:C2	1:A:182:C:H1'	2.39	0.58
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.58
1:A:88:C:H2'	1:A:89:G:C8	2.38	0.58
1:A:59:U:H2'	1:A:60:C:H6	1.67	0.58
1:A:200:G:C6	1:A:232:A:C5	2.92	0.58
1:A:162:G:O4'	1:A:164:U:H5	1.86	0.58
1:A:2:U:H2'	1:A:3:U:C6	2.39	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.57
1:A:210:U:H3	1:A:223:A:H61	1.51	0.57
1:A:230:G:N2	1:A:231:A:H2'	2.19	0.57
1:A:206:G:H1	1:A:232:A:HO2'	1.50	0.57
1:A:16:G:N2	1:A:344:C:H1'	2.19	0.57
1:A:161:G:O3'	1:A:162:G:H8	1.87	0.57
1:A:166:G:C3'	1:A:167:G:H8	2.17	0.57
1:A:136:G:O3'	1:A:137:A:H2'	2.03	0.57
1:A:96:G:H3'	1:A:97:C:H6	1.69	0.57
1:A:385:A:H1'	1:A:401:A:C8	2.39	0.57
1:A:166:G:C8	1:A:166:G:H5"	2.39	0.57
1:A:88:C:H2'	1:A:89:G:H8	1.70	0.56
1:A:186:G:N1	1:A:189:A:OP2	2.33	0.56
1:A:123:C:H4'	1:A:123:C:OP1	2.06	0.56
1:A:162:G:H1'	1:A:164:U:C5	2.40	0.56
1:A:200:G:N2	1:A:232:A:H1'	2.21	0.56
1:A:330:A:H2	1:A:390:A:C2	2.23	0.56
1:A:382:G:C8	1:A:382:G:H5"	2.39	0.56
1:A:64:C:O2'	1:A:82:A:N1	2.28	0.56
1:A:164:U:C5	1:A:165:G:N7	2.74	0.55
1:A:374:A:H2'	1:A:375:G:C8	2.41	0.55
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.55
1:A:139:G:N3	1:A:188:A:H2	2.04	0.55
1:A:162:G:C1'	1:A:164:U:C6	2.88	0.55
1:A:162:G:H1'	1:A:164:U:H6	1.71	0.55
1:A:56:U:H1'	1:A:99:A:N1	2.22	0.55
1:A:174:U:H2'	1:A:175:U:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:G:H1	1:A:320:U:H3	1.54	0.55
2:B:106:ARG:HB2	2:B:113:LYS:HA	1.87	0.55
1:A:246:A:H2'	1:A:247:C:C6	2.42	0.55
1:A:11:C:H2'	1:A:12:U:C6	2.42	0.54
1:A:57:G:H4'	1:A:101:U:O4	2.07	0.54
1:A:182:C:H2'	1:A:183:C:H6	1.72	0.54
1:A:338:G:H2'	1:A:339:A:C8	2.42	0.54
1:A:206:G:N3	1:A:207:C:N4	2.55	0.54
1:A:72:A:H2'	1:A:73:G:H8	1.71	0.54
1:A:161:G:O3'	1:A:162:G:C8	2.61	0.54
1:A:204:G:N3	1:A:204:G:H2'	2.21	0.54
1:A:85:G:H4'	1:A:86:U:C4	2.42	0.54
1:A:56:U:O2	1:A:100:A:C2	2.61	0.54
1:A:338:G:H2'	1:A:339:A:H8	1.72	0.54
1:A:386:C:O2'	1:A:399:A:N3	2.37	0.53
1:A:215:G:N2	1:A:217:A:H3'	2.23	0.53
1:A:56:U:O2'	1:A:100:A:N1	2.37	0.53
1:A:195:A:OP2	1:A:197:A:N6	2.40	0.53
1:A:198:G:H4'	1:A:228:U:H4'	1.90	0.53
1:A:8:A:C6	1:A:9:U:C4	2.97	0.53
1:A:208:U:H2'	1:A:209:C:C6	2.44	0.53
1:A:411:U:H2'	1:A:412:A:C8	2.43	0.53
1:A:199:U:H5	1:A:227:G:H22	1.56	0.53
1:A:215:G:H22	1:A:217:A:H3'	1.73	0.53
1:A:110:U:H2'	1:A:111:A:H8	1.74	0.53
1:A:182:C:H2'	1:A:183:C:C6	2.44	0.53
1:A:213:G:H3'	1:A:214:G:C8	2.42	0.53
1:A:339:A:H2'	1:A:340:U:H6	1.75	0.53
1:A:73:G:H22	1:A:291:A:H2'	1.74	0.52
1:A:198:G:C4'	1:A:228:U:H4'	2.38	0.52
1:A:217:A:C2	1:A:218:A:C4	2.97	0.52
1:A:45:A:C2	1:A:388:G:H2'	2.44	0.52
1:A:53:C:H2'	1:A:54:C:C6	2.44	0.52
1:A:268:G:H2'	1:A:269:G:C8	2.45	0.52
1:A:163:C:H6	1:A:163:C:O5'	1.92	0.52
1:A:217:A:H2'	1:A:218:A:H8	1.73	0.52
1:A:101:U:H4'	1:A:102:C:OP1	2.09	0.52
1:A:356:A:H3'	1:A:357:G:H8	1.74	0.52
2:B:56:VAL:HA	2:B:59:ARG:HH12	1.75	0.52
1:A:360:G:O2'	1:A:364:A:N6	2.42	0.52
1:A:407:U:H2'	1:A:408:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:C:H2'	1:A:197:A:C8	2.45	0.51
1:A:269:G:H3'	1:A:270:U:H6	1.74	0.51
1:A:135:U:O2'	1:A:136:G:H5'	2.10	0.51
2:B:112:LYS:HG3	2:B:114:GLU:HG2	1.92	0.51
1:A:203:G:C5	1:A:205:A:H1'	2.44	0.51
2:B:79:LYS:HD2	2:B:81:TYR:HE1	1.74	0.51
2:B:7:ILE:HA	2:B:42:ARG:HH21	1.75	0.51
1:A:162:G:C3'	1:A:163:C:C5	2.90	0.51
1:A:380:A:C2	1:A:381:A:C4	2.99	0.51
1:A:144:G:C6	1:A:145:G:C4	2.99	0.51
1:A:339:A:H2'	1:A:340:U:C6	2.45	0.51
1:A:154:U:O2'	1:A:155:A:H5'	2.11	0.50
1:A:164:U:C4	1:A:165:G:N7	2.79	0.50
1:A:206:G:N1	1:A:232:A:O2'	2.44	0.50
1:A:229:G:N3	1:A:230:G:N2	2.60	0.50
1:A:76:G:H2'	1:A:77:C:O4'	2.11	0.50
1:A:188:A:O2'	1:A:244:C:O2'	2.22	0.50
2:B:17:PHE:HE1	2:B:82:VAL:HG11	1.75	0.50
1:A:87:U:H2'	1:A:88:C:C6	2.47	0.50
1:A:198:G:O3'	1:A:227:G:N2	2.44	0.50
1:A:201:A:C2	1:A:232:A:C4	2.99	0.50
1:A:409:A:H3'	1:A:410:U:H6	1.76	0.50
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.50
1:A:155:A:H1'	1:A:217:A:N3	2.26	0.50
1:A:166:G:H3'	1:A:167:G:C8	2.47	0.50
1:A:261:A:H2'	1:A:262:A:C8	2.46	0.50
1:A:296:A:H2'	1:A:297:C:O4'	2.11	0.50
2:B:99:LYS:O	2:B:102:ILE:HG13	2.12	0.50
1:A:289:G:O2'	1:A:296:A:N6	2.45	0.50
1:A:142:G:C6	1:A:189:A:C2	2.99	0.50
1:A:196:C:H2'	1:A:197:A:O4'	2.12	0.50
1:A:8:A:H3'	1:A:9:U:H6	1.77	0.49
1:A:143:G:C6	1:A:144:G:N7	2.81	0.49
1:A:269:G:H3'	1:A:270:U:C6	2.47	0.49
1:A:341:U:H5"	1:A:341:U:H6	1.77	0.49
1:A:66:G:H2'	1:A:67:U:C2	2.47	0.49
1:A:322:C:H2'	1:A:323:A:C8	2.47	0.49
1:A:96:G:H3'	1:A:97:C:C6	2.48	0.49
1:A:176:C:H2'	1:A:177:G:O4'	2.12	0.49
1:A:201:A:N6	1:A:230:G:H1	2.11	0.49
1:A:218:A:C4	1:A:219:C:H1'	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:U:H2'	1:A:125:U:O4'	2.12	0.49
1:A:410:U:H2'	1:A:411:U:C6	2.47	0.49
1:A:414:C:H2'	1:A:415:G:C8	2.47	0.49
1:A:54:C:C2	1:A:395:G:C2	3.01	0.49
1:A:162:G:C3'	1:A:163:C:H5	2.22	0.49
1:A:371:U:H4'	1:A:373:C:H5	1.77	0.49
1:A:407:U:H2'	1:A:408:G:C8	2.47	0.49
2:B:44:GLY:HA3	2:B:82:VAL:HG22	1.95	0.49
1:A:85:G:H2'	1:A:87:U:C4	2.47	0.49
1:A:175:U:H2'	1:A:176:C:C6	2.48	0.48
1:A:177:G:C8	1:A:178:A:H2'	2.47	0.48
2:B:74:GLU:HB3	2:B:111:LEU:HD11	1.94	0.48
1:A:209:C:C2	1:A:225:A:C2	3.01	0.48
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.48
1:A:381:A:C2	1:A:382:G:H1'	2.48	0.48
1:A:162:G:C1'	1:A:164:U:H5	2.26	0.48
1:A:166:G:H2'	1:A:167:G:C8	2.48	0.48
1:A:236:G:H8	1:A:236:G:H5"	1.78	0.48
1:A:155:A:N3	1:A:216:A:C2	2.82	0.48
1:A:186:G:H5"	1:A:186:G:C8	2.46	0.48
2:B:24:ALA:HB2	2:B:29:VAL:HG22	1.96	0.48
1:A:17:U:H2'	1:A:18:A:C8	2.48	0.48
1:A:211:A:C6	1:A:223:A:C6	3.02	0.48
1:A:201:A:C4	1:A:231:A:H2	2.31	0.47
1:A:164:U:H2'	1:A:165:G:C8	2.49	0.47
1:A:183:C:H2'	1:A:184:C:C6	2.49	0.47
1:A:54:C:H1'	1:A:395:G:N2	2.29	0.47
1:A:142:G:C4	1:A:189:A:C2	3.02	0.47
1:A:221:U:H2'	1:A:222:U:H6	1.75	0.47
2:B:7:ILE:HG23	2:B:42:ARG:NH2	2.30	0.47
1:A:153:C:H2'	1:A:154:U:C6	2.49	0.47
2:B:4:LYS:C	2:B:6:ARG:H	2.22	0.47
1:A:195:A:H2'	1:A:195:A:N3	2.29	0.47
1:A:201:A:N6	1:A:230:G:H22	2.12	0.47
1:A:45:A:C8	1:A:45:A:H5'	2.50	0.47
1:A:195:A:H3'	1:A:196:C:H6	1.80	0.47
1:A:228:U:H2'	1:A:229:G:C4	2.50	0.47
1:A:294:G:H2'	1:A:295:A:C8	2.49	0.47
1:A:380:A:O2'	1:A:381:A:H5'	2.15	0.47
1:A:199:U:C4	1:A:200:G:C5	3.02	0.47
1:A:341:U:C4	1:A:342:A:N7	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:G:H2'	1:A:381:A:N6	2.29	0.47
1:A:53:C:H2'	1:A:54:C:H6	1.79	0.47
1:A:185:U:H2'	1:A:186:G:C8	2.50	0.46
1:A:17:U:H3	1:A:342:A:N6	2.10	0.46
1:A:241:A:H2'	1:A:242:C:H6	1.79	0.46
1:A:186:G:N2	1:A:188:A:H3'	2.31	0.46
1:A:208:U:H2'	1:A:209:C:H6	1.81	0.46
1:A:218:A:C5	1:A:219:C:H1'	2.50	0.46
1:A:347:C:C2	1:A:383:G:C2	3.04	0.46
1:A:385:A:H8	1:A:400:U:O2'	1.97	0.46
2:B:1:MET:HB3	2:B:1:MET:HE3	1.54	0.46
1:A:8:A:C4	1:A:408:G:N2	2.84	0.46
1:A:24:U:H5"	2:B:3:LYS:HE2	1.98	0.46
1:A:408:G:C6	1:A:409:A:C5	3.04	0.46
1:A:144:G:C6	1:A:145:G:C5	3.04	0.46
1:A:144:G:C2	1:A:145:G:H1'	2.51	0.46
1:A:232:A:H4'	1:A:233:C:H6	1.81	0.46
1:A:350:A:H2'	1:A:351:G:C8	2.51	0.46
1:A:210:U:H3'	1:A:211:A:H8	1.80	0.46
1:A:234:G:O2'	1:A:235:C:O5'	2.27	0.46
1:A:152:C:H2'	1:A:153:C:C6	2.51	0.46
1:A:226:G:H4'	1:A:226:G:OP1	2.16	0.46
1:A:349:G:C8	1:A:380:A:N6	2.84	0.46
1:A:200:G:N1	1:A:232:A:C4	2.85	0.45
1:A:155:A:H2'	1:A:156:C:O4'	2.16	0.45
1:A:215:G:O2'	1:A:218:A:N6	2.49	0.45
1:A:166:G:C3'	1:A:167:G:C8	2.99	0.45
1:A:213:G:C2	1:A:221:U:C2	3.04	0.45
1:A:8:A:H3'	1:A:9:U:C6	2.52	0.45
1:A:23:C:O2	1:A:336:A:O2'	2.33	0.45
1:A:84:U:O3'	1:A:86:U:O4	2.35	0.45
1:A:198:G:H2'	1:A:200:G:N7	2.32	0.45
1:A:284:C:H2'	1:A:285:G:O4'	2.17	0.45
1:A:8:A:C2	1:A:408:G:C2	3.05	0.45
1:A:162:G:O2'	1:A:163:C:C6	2.70	0.45
1:A:336:A:H2'	1:A:337:U:C6	2.51	0.45
1:A:198:G:N2	1:A:201:A:OP2	2.47	0.45
1:A:42:U:H2'	1:A:43:A:C8	2.52	0.45
2:B:56:VAL:HA	2:B:59:ARG:NH1	2.32	0.45
1:A:143:G:N2	1:A:184:C:H1'	2.32	0.45
1:A:47:G:H1	1:A:385:A:N6	2.07	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:A:H8	1:A:74:A:H5"	1.81	0.44
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.44
1:A:397:U:H2'	1:A:398:U:O4'	2.16	0.44
2:B:105:LEU:HD23	2:B:105:LEU:HA	1.85	0.44
2:B:4:LYS:HE2	2:B:4:LYS:HB2	1.75	0.44
1:A:159:C:H2'	1:A:160:C:C6	2.52	0.44
1:A:187:A:H2'	1:A:188:A:C8	2.52	0.44
1:A:206:G:C2	1:A:207:C:N4	2.85	0.44
1:A:406:A:C6	1:A:407:U:C4	3.06	0.44
1:A:87:U:H2'	1:A:88:C:H6	1.82	0.44
1:A:200:G:N2	1:A:206:G:C2	2.85	0.44
1:A:17:U:H2'	1:A:18:A:H8	1.82	0.44
1:A:189:A:H3'	1:A:190:G:H5'	2.00	0.44
1:A:207:C:H2'	1:A:208:U:H6	1.82	0.44
2:B:37:GLU:CD	2:B:37:GLU:H	2.26	0.44
1:A:138:C:OP1	1:A:138:C:H4'	2.14	0.44
1:A:197:A:H3'	1:A:198:G:H8	1.83	0.44
1:A:242:C:H2'	1:A:243:C:O4'	2.18	0.44
1:A:98:G:C2'	1:A:107:A:H61	2.31	0.43
1:A:207:C:C2'	1:A:208:U:H5'	2.48	0.43
2:B:72:LYS:HE3	2:B:72:LYS:HB3	1.67	0.43
1:A:197:A:C6	1:A:198:G:C4	3.06	0.43
1:A:197:A:C2	1:A:198:G:H1'	2.53	0.43
1:A:210:U:C3'	1:A:211:A:H8	2.31	0.43
1:A:227:G:N3	1:A:227:G:H2'	2.33	0.43
2:B:2:LYS:HB3	2:B:2:LYS:HE2	1.55	0.43
1:A:166:G:H3'	1:A:167:G:H8	1.80	0.43
1:A:216:A:C2	1:A:217:A:C4	3.06	0.43
1:A:219:C:O5'	1:A:219:C:H6	2.01	0.43
1:A:376:U:H2'	1:A:377:A:C8	2.54	0.43
1:A:1:G:N2	1:A:415:G:H1'	2.33	0.43
1:A:187:A:O5'	1:A:187:A:H8	2.01	0.43
1:A:210:U:H3	1:A:223:A:N6	2.14	0.43
1:A:281:U:H2'	1:A:282:C:H6	1.83	0.43
1:A:348:G:H21	1:A:381:A:H62	1.64	0.43
1:A:190:G:C2	1:A:191:U:C2	3.07	0.43
1:A:207:C:H2'	1:A:208:U:C6	2.54	0.43
1:A:343:C:H2'	1:A:344:C:O4'	2.19	0.43
1:A:356:A:H3'	1:A:357:G:C8	2.53	0.43
1:A:382:G:C2	1:A:383:G:H1'	2.53	0.43
1:A:11:C:H2'	1:A:12:U:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:U:H2'	1:A:136:G:O4'	2.19	0.43
1:A:353:A:H3'	1:A:354:C:C6	2.54	0.43
1:A:326:C:H2'	1:A:327:U:C6	2.53	0.43
2:B:27:GLN:HB3	2:B:88:PRO:HG2	2.00	0.43
1:A:207:C:O2'	1:A:208:U:H5'	2.19	0.42
1:A:144:G:C5	1:A:145:G:C8	3.06	0.42
1:A:225:A:H2'	1:A:225:A:N3	2.34	0.42
1:A:403:A:H2'	1:A:404:G:O4'	2.19	0.42
1:A:85:G:H4'	1:A:86:U:C5	2.54	0.42
1:A:95:A:H2'	1:A:96:G:O4'	2.18	0.42
1:A:189:A:O2'	1:A:190:G:OP1	2.31	0.42
1:A:236:G:H2'	1:A:237:G:H8	1.84	0.42
1:A:405:C:C2	1:A:406:A:C8	3.07	0.42
1:A:300:A:H2'	1:A:301:G:H5'	2.02	0.42
1:A:393:U:H2'	1:A:394:G:H8	1.80	0.42
1:A:36:C:H6	1:A:36:C:P	2.42	0.42
1:A:197:A:C2'	1:A:198:G:H5'	2.50	0.42
1:A:232:A:H4'	1:A:233:C:C6	2.54	0.42
2:B:27:GLN:HA	2:B:86:ARG:HB2	2.02	0.42
1:A:318:C:H2'	1:A:319:A:N3	2.35	0.42
1:A:198:G:H4'	1:A:228:U:C5'	2.50	0.42
1:A:50:A:H5'	1:A:388:G:H5"	2.01	0.41
1:A:200:G:C6	1:A:232:A:C4	3.08	0.41
2:B:67:CYS:SG	2:B:98:LYS:HA	2.60	0.41
1:A:33:U:H4'	1:A:34:U:O4'	2.20	0.41
1:A:156:C:H42	1:A:170:A:H61	1.67	0.41
1:A:194:C:N4	1:A:202:C:OP2	2.53	0.41
1:A:198:G:C4	1:A:200:G:OP2	2.74	0.41
1:A:123:C:H2'	1:A:124:U:O4'	2.20	0.41
1:A:137:A:O2'	1:A:138:C:P	2.79	0.41
1:A:141:C:H3'	1:A:142:G:C5'	2.47	0.41
1:A:283:C:H2'	1:A:284:C:C6	2.55	0.41
1:A:373:C:H2'	1:A:374:A:C8	2.55	0.41
1:A:142:G:C6	1:A:189:A:H2	2.38	0.41
1:A:263:A:H4'	1:A:264:U:OP1	2.20	0.41
1:A:63:A:N6	1:A:80:G:O6	2.54	0.41
1:A:407:U:C2	1:A:408:G:C8	3.09	0.41
1:A:10:G:H2'	1:A:11:C:C6	2.56	0.41
1:A:216:A:H2'	1:A:217:A:C8	2.56	0.41
1:A:323:A:H2'	1:A:324:G:O4'	2.20	0.41
2:B:112:LYS:HA	2:B:112:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:G:H1	1:A:130:U:H3	1.68	0.41
1:A:122:G:C2	1:A:123:C:H1'	2.55	0.41
1:A:201:A:N6	1:A:229:G:H1'	2.36	0.41
1:A:380:A:N1	1:A:381:A:C6	2.88	0.41
1:A:6:U:H2'	1:A:7:C:O4'	2.21	0.41
1:A:220:C:H2'	1:A:221:U:H6	1.86	0.41
1:A:376:U:H2'	1:A:377:A:H8	1.85	0.41
1:A:401:A:H2'	1:A:402:G:O4'	2.21	0.41
1:A:155:A:O2'	1:A:217:A:H1'	2.20	0.40
1:A:8:A:C5	1:A:9:U:C5	3.09	0.40
1:A:23:C:H2'	1:A:24:U:C6	2.57	0.40
1:A:196:C:C4	1:A:197:A:C5	3.09	0.40
1:A:211:A:C2	1:A:223:A:C4	3.09	0.40
1:A:230:G:H2'	1:A:230:G:N3	2.36	0.40
1:A:132:G:H3'	1:A:133:G:H8	1.87	0.40
1:A:354:C:H2'	1:A:355:G:C8	2.57	0.40
1:A:354:C:H2'	1:A:355:G:O4'	2.22	0.40
1:A:364:A:C4	1:A:365:G:H1'	2.57	0.40
1:A:369:C:H2'	1:A:370:U:O4'	2.22	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	
2	B	114/116 (98%)	106 (93%)	8 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	99/99 (100%)	92 (93%)	7 (7%)	12 33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET
2	B	2	LYS
2	B	4	LYS
2	B	9	LYS
2	B	11	GLU
2	B	27	GLN
2	B	72	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	14	GLN
2	B	27	GLN
2	B	38	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	209 (50%)	24 (5%)

All (209) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	U
1	A	4	A
1	A	5	A

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Mol	Chain	Res	Type
1	A	6	U
1	A	7	C
1	A	8	A
1	A	9	U
1	A	11	C
1	A	13	C
1	A	15	G
1	A	19	A
1	A	22	G
1	A	27	G
1	A	29	C
1	A	30	C
1	A	31	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	41	G
1	A	45	A
1	A	46	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	53	C
1	A	65	G
1	A	66	G
1	A	67	U
1	A	68	G
1	A	69	C
1	A	70	U
1	A	73	G
1	A	74	A
1	A	75	U
1	A	80	G
1	A	81	U
1	A	85	G
1	A	86	U
1	A	87	U
1	A	91	G
1	A	92	C
1	A	99	A

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Mol	Chain	Res	Type
1	A	101	U
1	A	102	C
1	A	103	C
1	A	104	A
1	A	106	A
1	A	108	G
1	A	113	G
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	129	C
1	A	131	G
1	A	132	G
1	A	134	C
1	A	136	G
1	A	137	A
1	A	138	C
1	A	139	G
1	A	140	G
1	A	141	C
1	A	142	G
1	A	144	G
1	A	145	G
1	A	147	A
1	A	148	A
1	A	149	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	155	A
1	A	157	G
1	A	163	C
1	A	172	G
1	A	173	G
1	A	174	U
1	A	178	A
1	A	180	U
1	A	182	C
1	A	186	G
1	A	187	A

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Mol	Chain	Res	Type
1	A	188	A
1	A	190	G
1	A	191	U
1	A	192	G
1	A	193	C
1	A	195	A
1	A	196	C
1	A	201	A
1	A	202	C
1	A	203	G
1	A	204	G
1	A	205	A
1	A	206	G
1	A	207	C
1	A	208	U
1	A	209	C
1	A	210	U
1	A	211	A
1	A	212	A
1	A	214	G
1	A	215	G
1	A	216	A
1	A	217	A
1	A	219	C
1	A	225	A
1	A	226	G
1	A	227	G
1	A	228	U
1	A	229	G
1	A	230	G
1	A	231	A
1	A	232	A
1	A	233	C
1	A	234	G
1	A	235	C
1	A	236	G
1	A	237	G
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G

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Mol	Chain	Res	Type
1	A	251	C
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	263	A
1	A	264	U
1	A	265	G
1	A	266	A
1	A	267	U
1	A	269	G
1	A	271	A
1	A	277	A
1	A	278	C
1	A	288	G
1	A	292	A
1	A	296	A
1	A	299	G
1	A	303	G
1	A	311	G
1	A	312	G
1	A	313	C
1	A	314	G
1	A	316	C
1	A	317	G
1	A	318	C
1	A	319	A
1	A	320	U
1	A	321	G
1	A	323	A
1	A	325	C
1	A	326	C
1	A	328	G
1	A	329	U
1	A	330	A
1	A	332	A
1	A	333	U
1	A	334	A
1	A	341	U
1	A	342	A
1	A	349	G
1	A	350	A

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Mol	Chain	Res	Type
1	A	351	G
1	A	353	A
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	385	A
1	A	387	A
1	A	389	A
1	A	390	A
1	A	391	C
1	A	395	G
1	A	400	U
1	A	401	A
1	A	402	G
1	A	403	A
1	A	405	C
1	A	407	U
1	A	409	A
1	A	410	U
1	A	411	U
1	A	412	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	52	U

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Mol	Chain	Res	Type
1	A	66	G
1	A	67	U
1	A	68	G
1	A	91	G
1	A	126	U
1	A	136	G
1	A	137	A
1	A	186	G
1	A	187	A
1	A	201	A
1	A	204	G
1	A	216	A
1	A	232	A
1	A	235	C
1	A	236	G
1	A	254	G
1	A	263	A
1	A	276	C
1	A	277	A
1	A	329	U
1	A	363	A
1	A	382	G
1	A	389	A

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 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

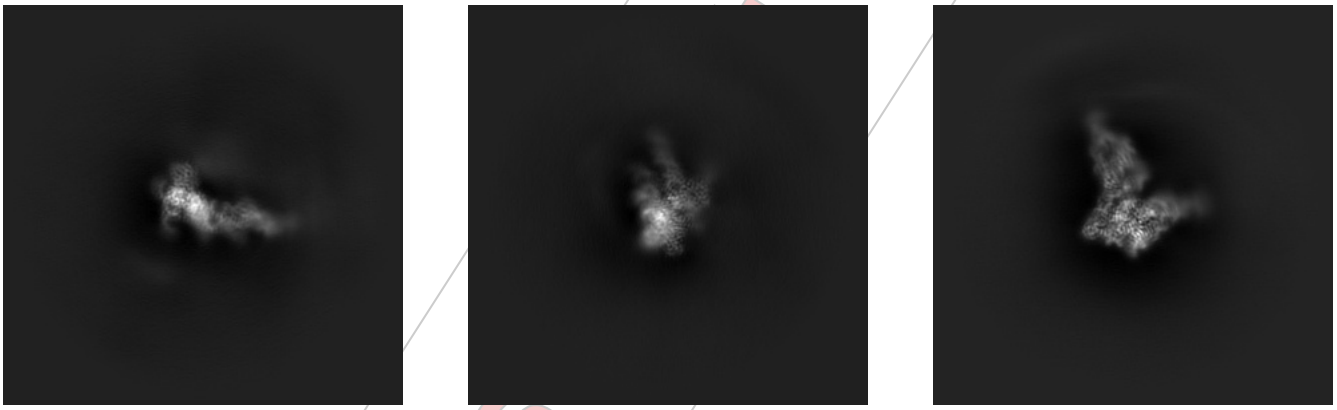
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70942. 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.

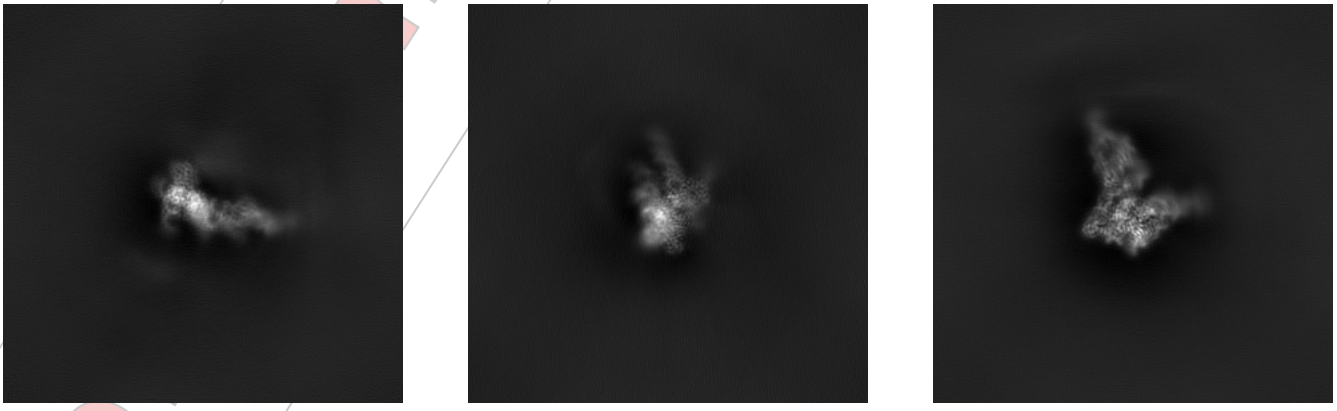
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

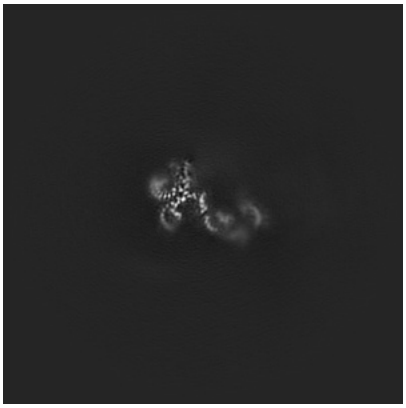


X Y Z

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

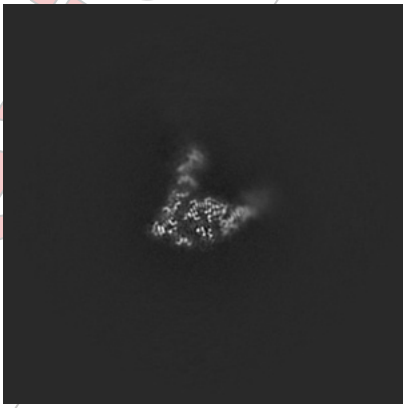
6.2 Central slices (i)

6.2.1 Primary map



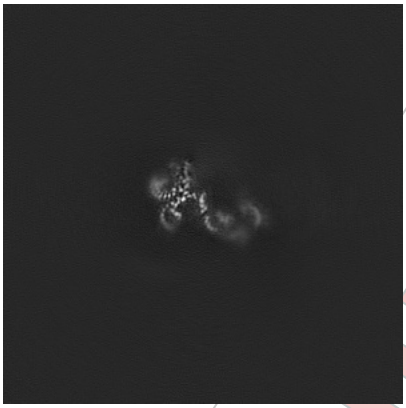
X Index: 200

Y Index: 200



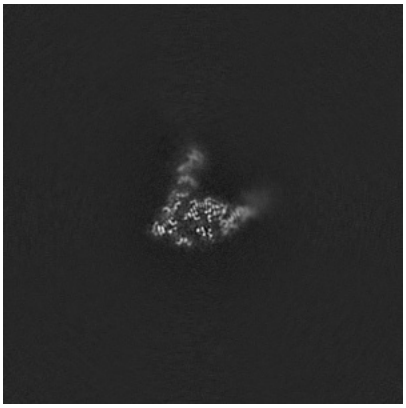
Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

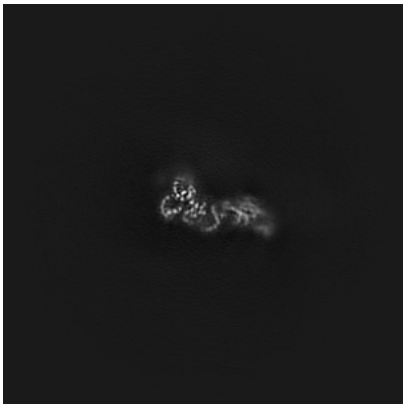


Z Index: 200

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

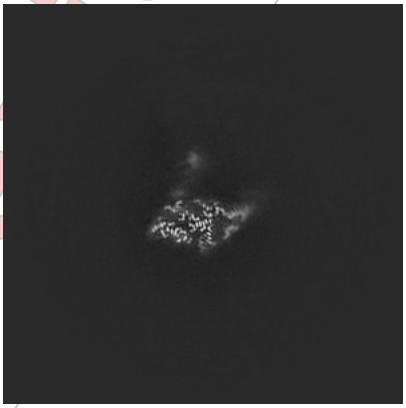
6.3 Largest variance slices (i)

6.3.1 Primary map



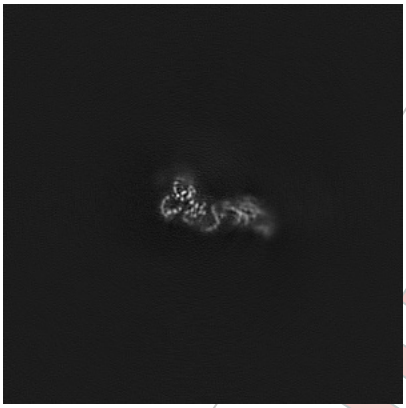
X Index: 187

Y Index: 175



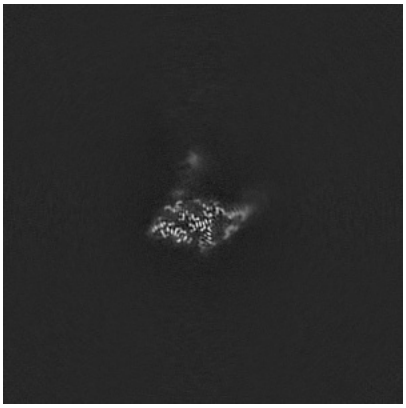
Z Index: 205

6.3.2 Raw map



X Index: 187

Y Index: 173

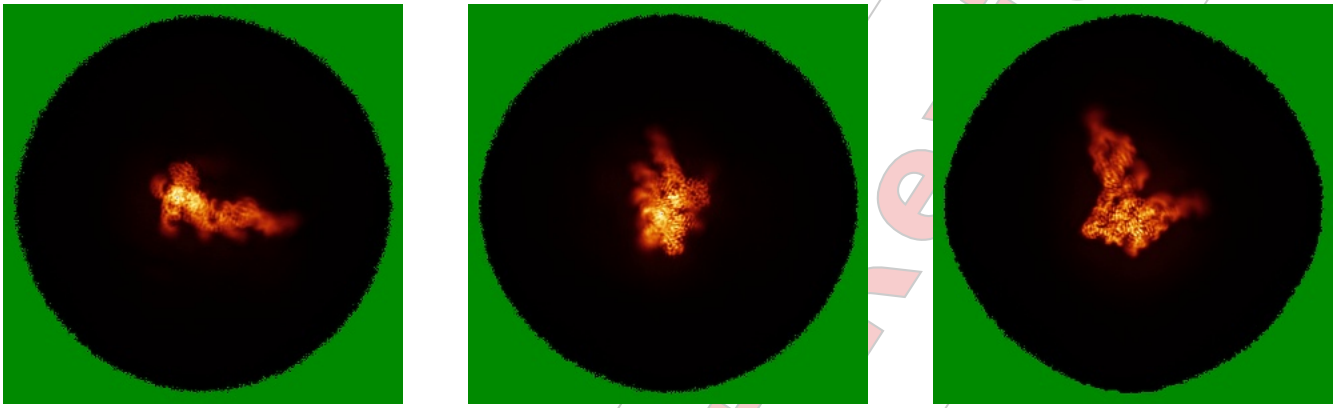


Z Index: 205

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

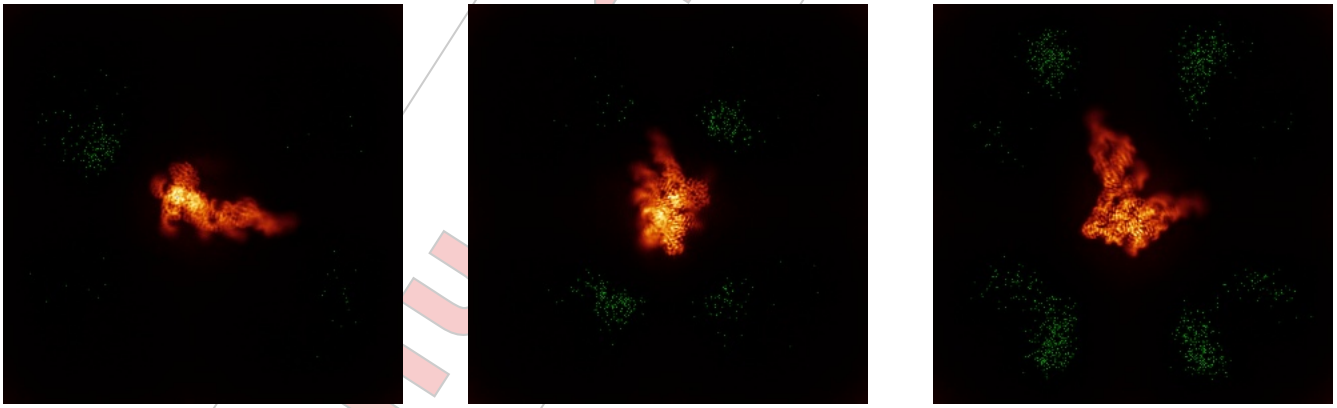
6.4 Orthogonal standard-deviation projections (False-color)

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 0.03. 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.

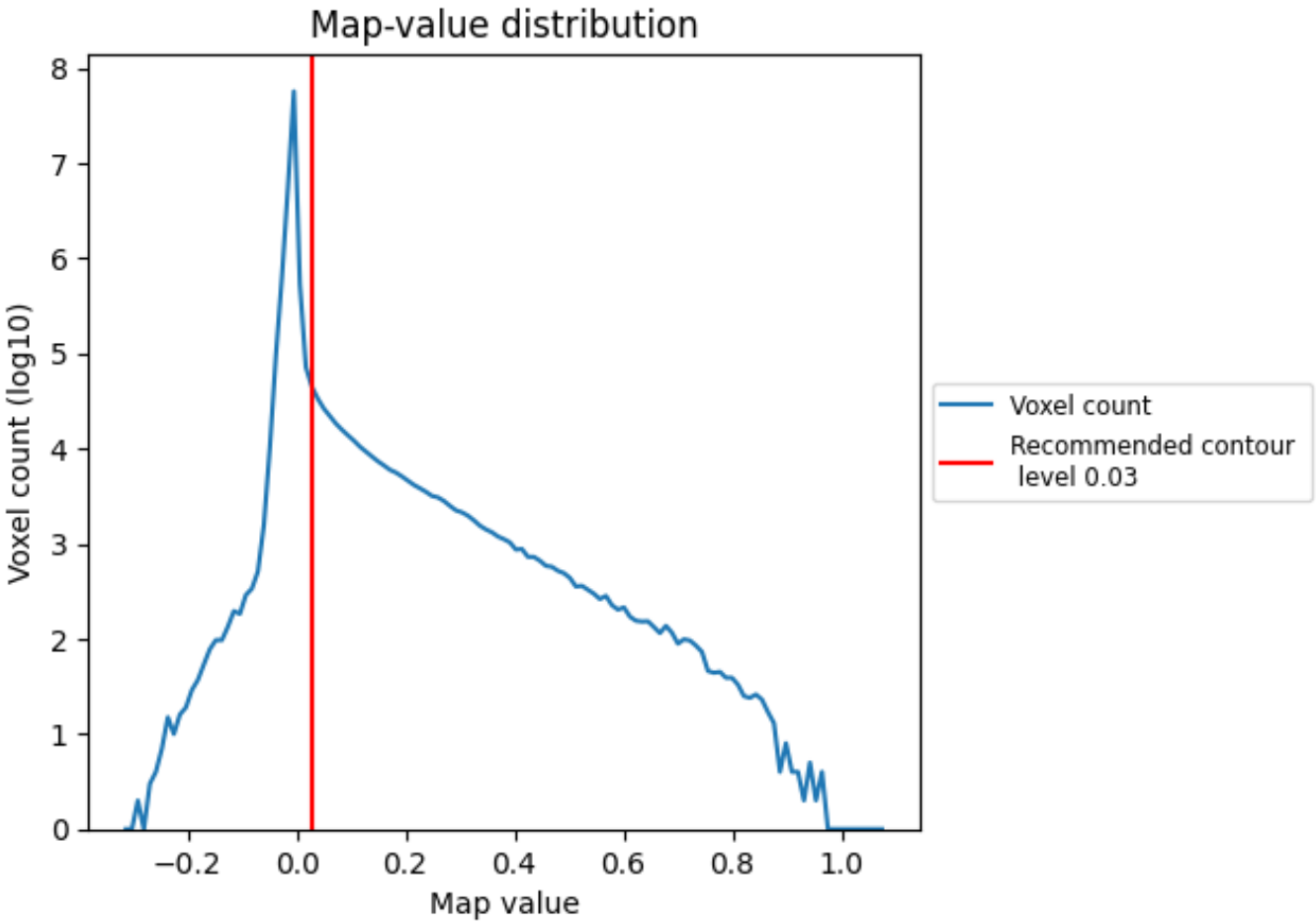
6.6 Mask visualisation (i)

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

7 Map analysis

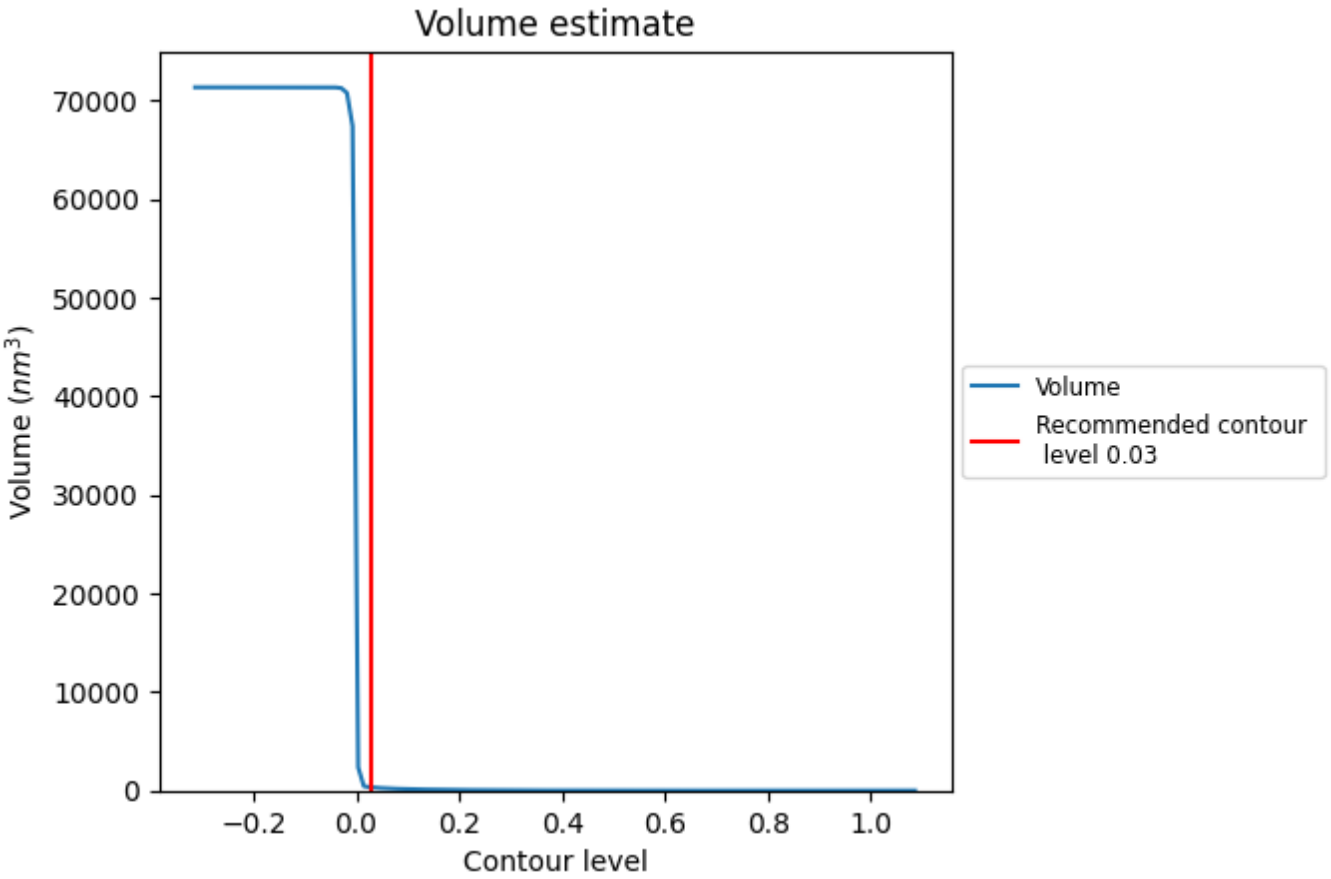
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

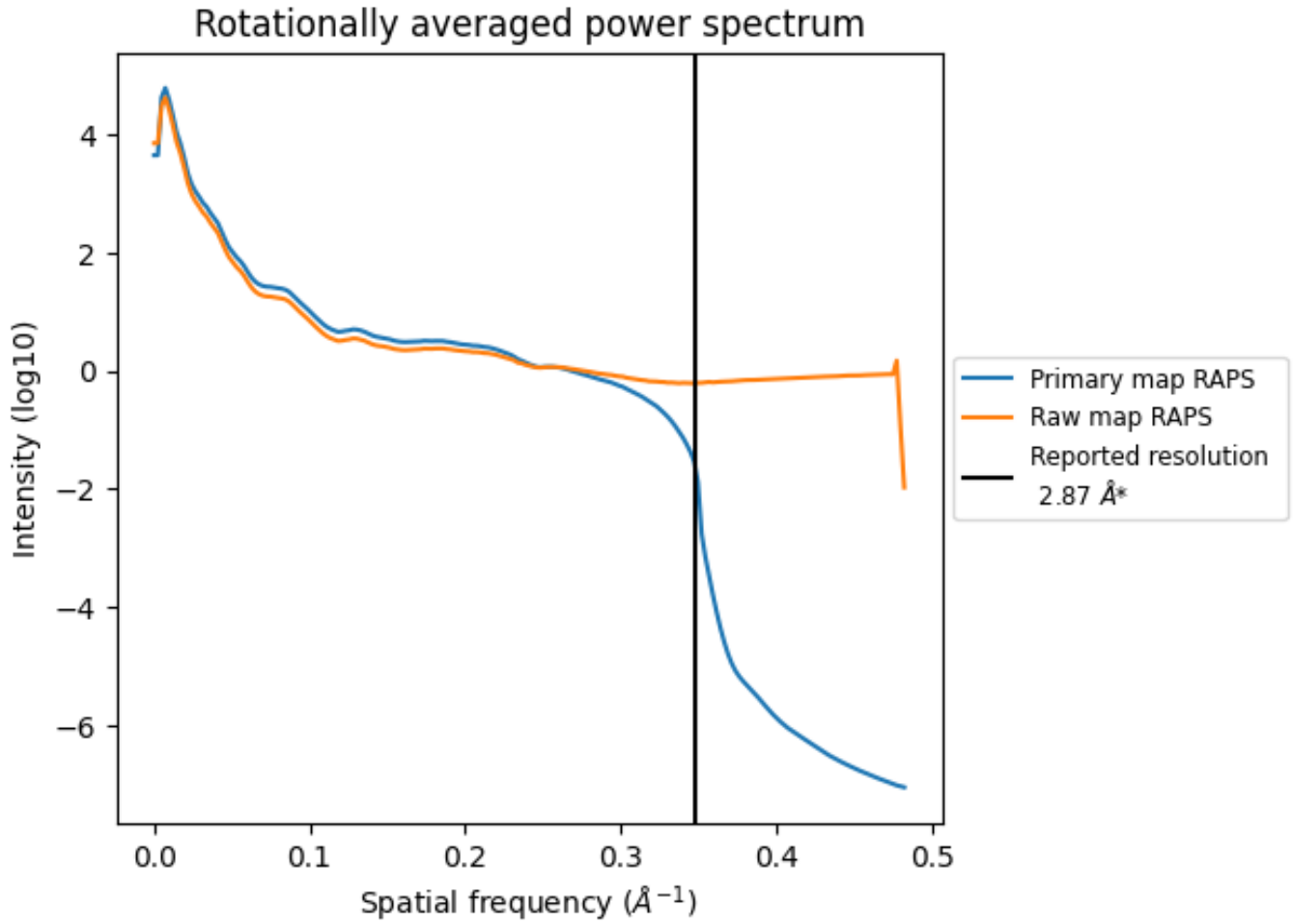
7.2 Volume estimate (i)



The volume at the recommended contour level is 327 nm^3; this corresponds to an approximate mass of 295 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 (i)

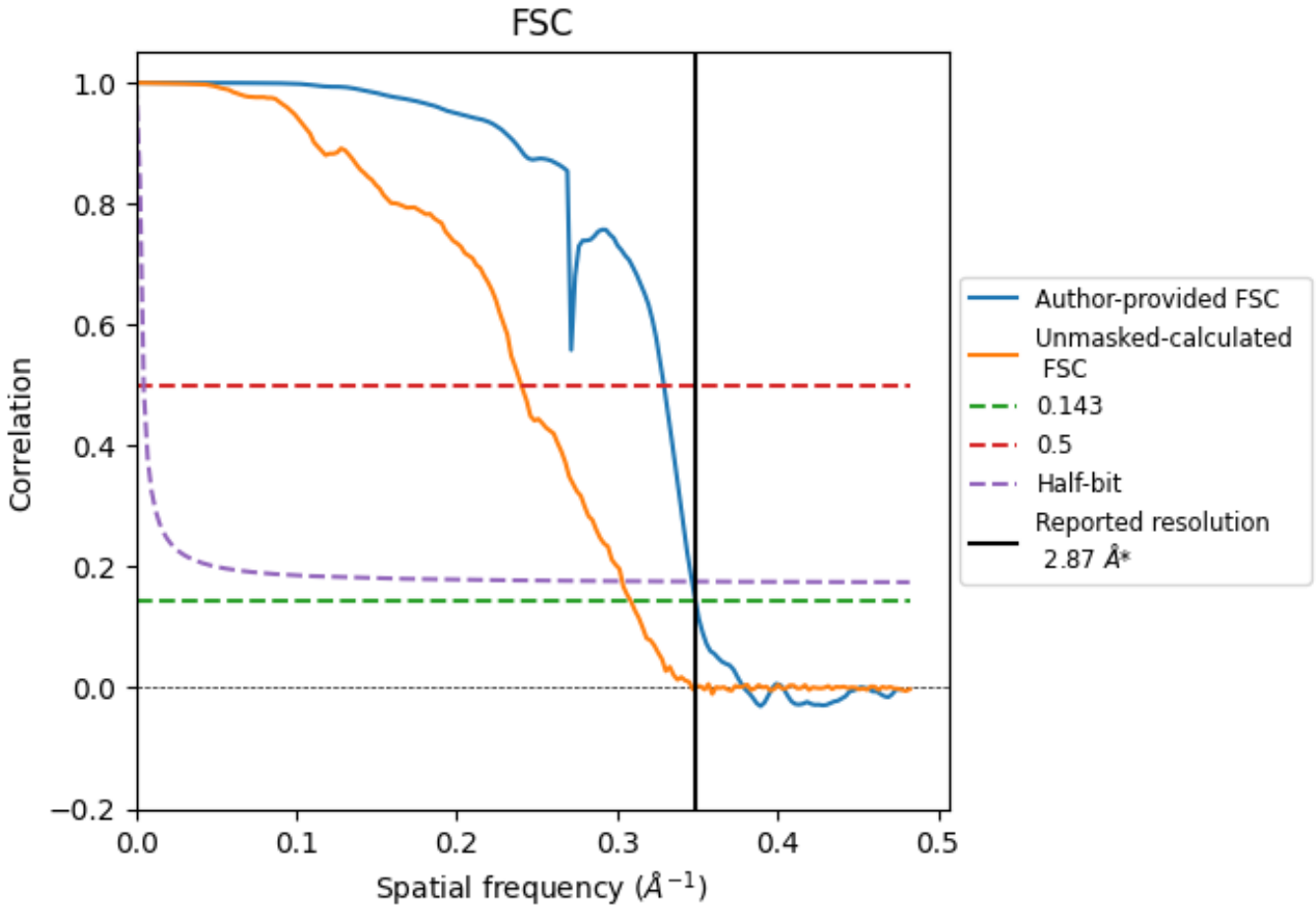


*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

8.2 Resolution estimates (i)

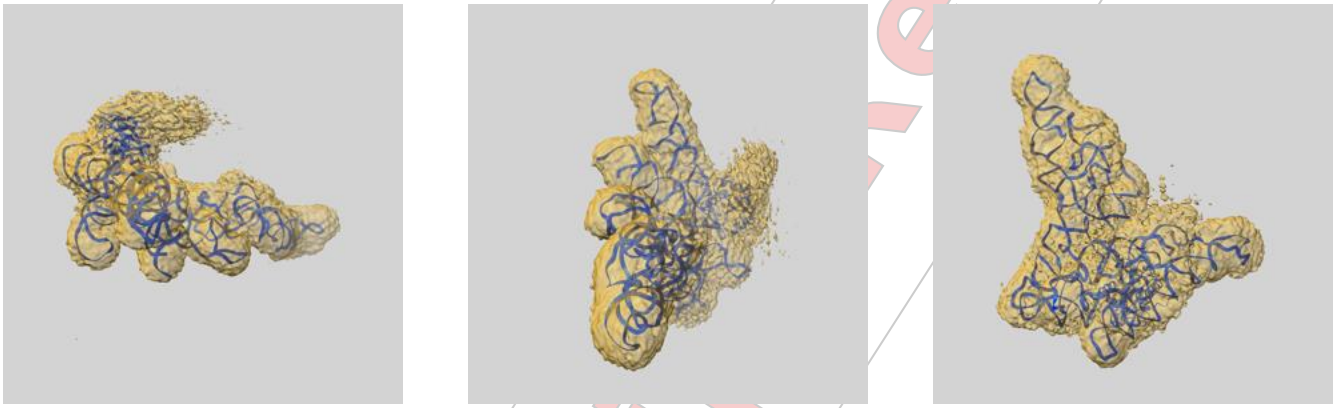
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.04	2.88
Unmasked-calculated*	3.24	4.16	3.30

*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 3.24 differs from the reported value 2.87 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70942 and PDB model 9OWS. Per-residue inclusion information can be found in section 3 on page 4.

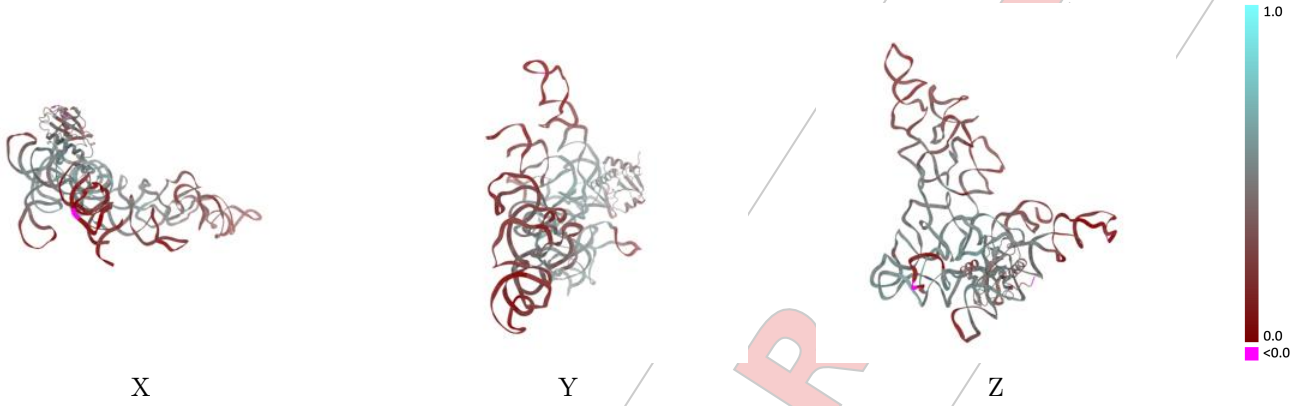
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

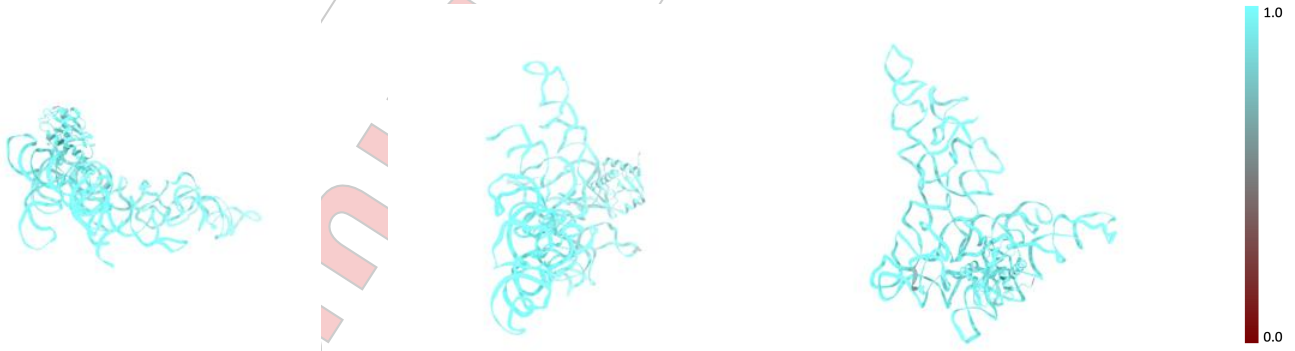
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

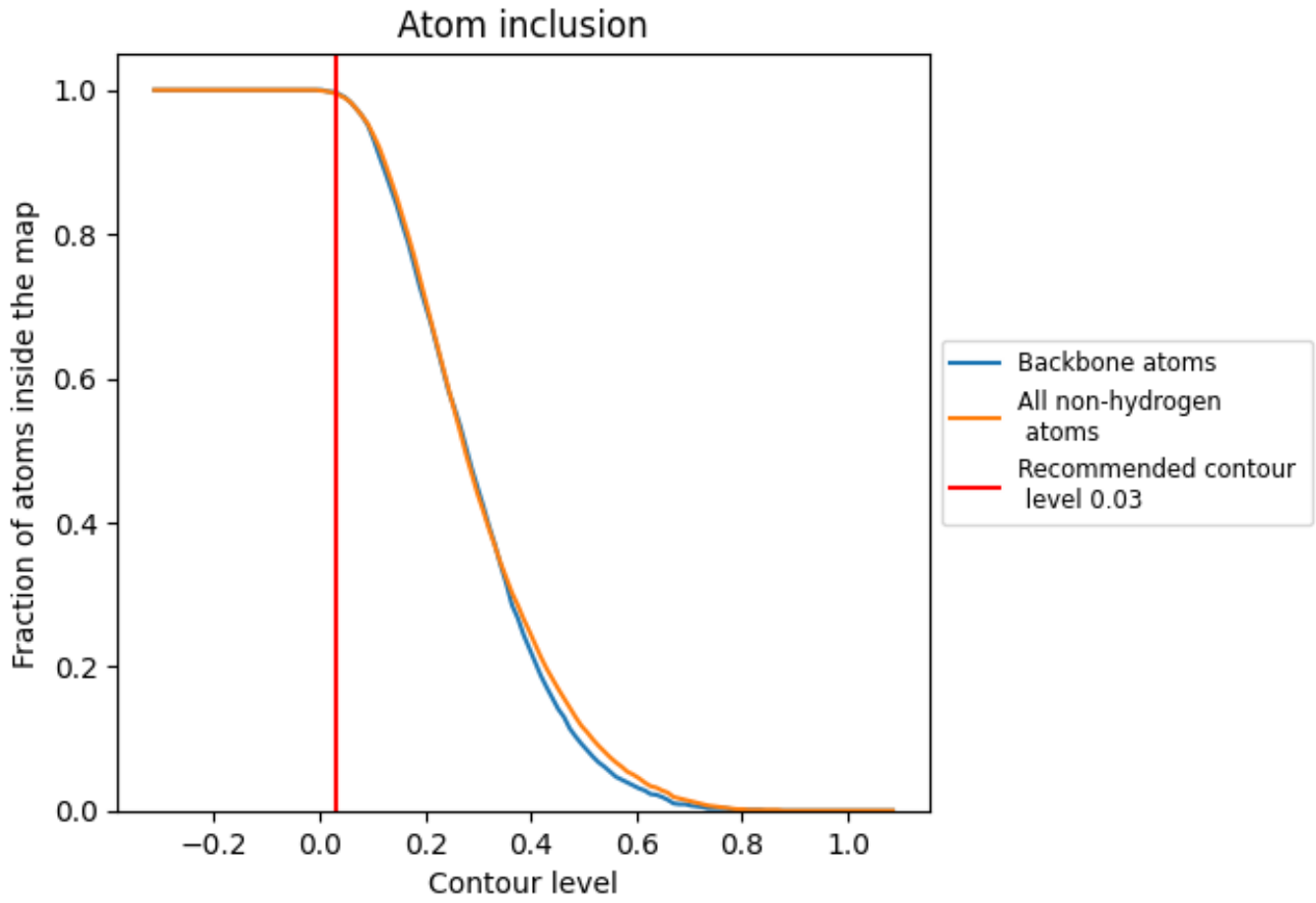
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9950	0.3940
A	0.9980	0.3900
B	0.9660	0.4320

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 02:46 PM EDT

PDB ID	:	9OWT / pdb_00009owt
EMDB ID	:	EMD-70943
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with precursor tRNA in 5 mM Ca2+
Deposited on	:	2025-06-02
Resolution	:	2.82 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

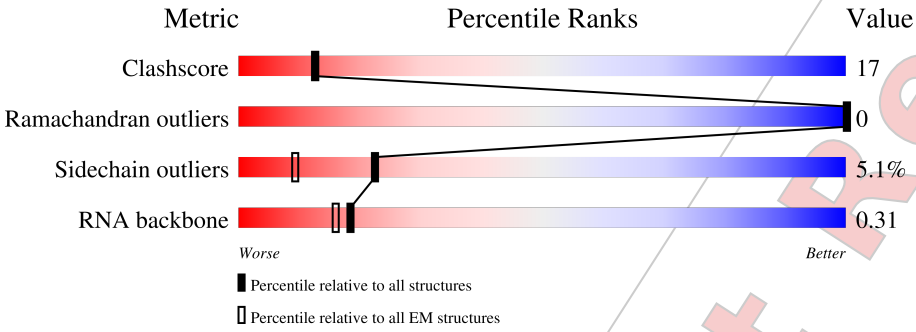
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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 <=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	417	32% 46% 22%
2	B	116	74% 22% •
3	C	92	29% 48% 20% •
3	E	92	• 5% • 90%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12015 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor tRNA (89-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	89	1889	842	326	632	89	0	0
			Total	C	N	O	P		
3	E	9	188	84	29	66	9	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

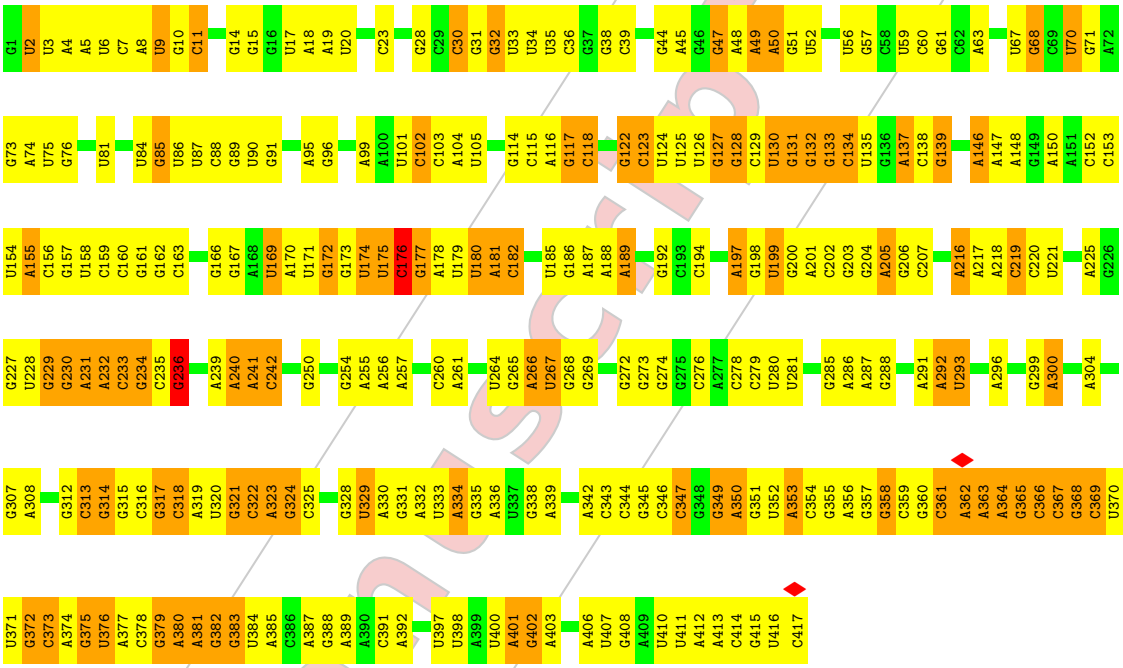
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	28	28	28	0
			Total	Ca	
4	C	1	1	1	0

3 Residue-property plots (i)

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: RNase P RNA (417-MER)

Chain A:

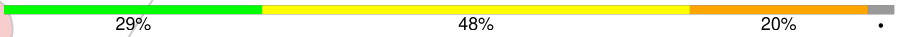


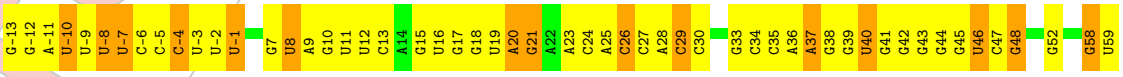
- Molecule 2: Ribonuclease P protein component

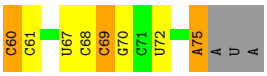
Chain B:

- Molecule 3: precursor tRNA (89-MER)

Chain C:

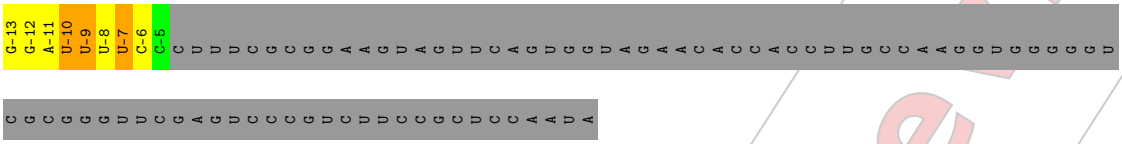






• Molecule 3: precursor tRNA (89-MER)

Chain E: 5% 90%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.52	0/10038	0.82	5/15661 (0.0%)
2	B	0.39	0/962	0.57	0/1281
3	C	0.53	0/2107	0.81	3/3281 (0.1%)
3	E	0.43	0/208	0.61	0/321
All	All	0.51	0/13315	0.80	8/20544 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	G	C4'-C3'-C2'	-5.82	96.78	102.60
3	C	69	C	C4'-C3'-C2'	-5.68	96.92	102.60
3	C	69	C	O3'-P-O5'	-5.62	95.57	104.00
3	C	46	U	C2'-C3'-O3'	5.56	117.83	109.50
1	A	176	C	C2'-C3'-O3'	5.28	121.63	113.70
1	A	240	A	C4'-C3'-C2'	-5.13	97.47	102.60
1	A	139	G	O3'-P-O5'	-5.12	96.31	104.00
1	A	84	U	O3'-P-O5'	-5.10	96.35	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8962	0	4509	229	0
2	B	947	0	1008	23	0
3	C	1889	0	957	40	0
3	E	188	0	96	8	0
4	A	28	0	0	0	0
4	C	1	0	0	0	0
All	All	12015	0	6570	288	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 17.

All (288) 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:364:A:C4	1:A:365:G:H1'	1.96	1.01
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.89
1:A:349:G:H21	1:A:350:A:H62	1.24	0.85
3:C:8:U:H5'	3:C:48:G:H5'	1.55	0.85
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.81
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.81
1:A:234:G:H2'	1:A:236:G:H5'	1.63	0.79
1:A:378:C:H3'	1:A:379:G:C8	2.19	0.77
1:A:45:A:H62	2:B:62:ARG:NH2	1.84	0.75
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.74
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.73
3:C:-11:A:H2	3:E:-7:U:H3	1.35	0.73
2:B:63:TYR:HB3	2:B:97:VAL:HG11	1.72	0.70
3:E:-13:G:H2'	3:E:-12:G:O4'	1.91	0.70
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.68
1:A:349:G:H22	1:A:379:G:H1'	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:G:H1	1:A:385:A:H62	1.39	0.68
1:A:9:U:H2'	1:A:10:G:H8	1.57	0.68
1:A:203:G:C5	1:A:205:A:H1'	2.29	0.68
1:A:50:A:C8	1:A:50:A:H5"	2.29	0.68
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.67
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.67
1:A:180:U:H2'	1:A:181:A:H8	1.59	0.66
1:A:378:C:H3'	1:A:379:G:H8	1.59	0.66
1:A:350:A:H1'	1:A:380:A:C2	2.31	0.66
1:A:349:G:N2	1:A:350:A:H62	1.93	0.65
1:A:349:G:N2	1:A:379:G:H1'	2.10	0.65
1:A:18:A:H2'	1:A:19:A:H8	1.62	0.65
1:A:374:A:H2'	1:A:375:G:C8	2.32	0.65
1:A:161:G:H3'	1:A:162:G:H8	1.62	0.64
1:A:146:A:H4'	1:A:146:A:OP1	1.97	0.63
1:A:172:G:H1'	1:A:217:A:H61	1.63	0.63
3:C:-7:U:H2'	3:C:-6:C:C6	2.33	0.63
1:A:102:C:H2'	1:A:103:C:O4'	1.99	0.63
1:A:181:A:C2	1:A:182:C:H1'	2.33	0.63
3:C:27:C:H2'	3:C:28:A:C8	2.35	0.62
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.62
1:A:45:A:H62	2:B:62:ARG:HH22	1.47	0.62
1:A:160:C:H3'	1:A:161:G:H8	1.64	0.61
2:B:56:VAL:O	2:B:60:ILE:HG13	1.99	0.61
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.61
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.60
1:A:350:A:H1'	1:A:380:A:N1	2.17	0.59
1:A:379:G:H4'	1:A:380:A:H8	1.66	0.59
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.59
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.84	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
1:A:379:G:H4'	1:A:380:A:C8	2.37	0.59
1:A:137:A:C8	1:A:137:A:H5"	2.38	0.59
1:A:364:A:OP1	1:A:365:G:N7	2.35	0.58
1:A:137:A:H5"	1:A:137:A:H8	1.67	0.58
1:A:3:U:H2'	1:A:4:A:H8	1.67	0.58
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.58
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.57
1:A:32:G:H22	1:A:34:U:H1'	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-11:A:H2'	3:C:-10:U:C6	2.40	0.57
3:C:38:G:H2'	3:C:39:G:C8	2.40	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:307:G:H2'	1:A:308:A:H8	1.70	0.57
2:B:22:SER:HG	3:C:-4:C:H5	1.50	0.57
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.56
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:14:G:H2'	1:A:385:A:N1	2.21	0.56
1:A:133:G:O2'	1:A:134:C:H5'	2.06	0.56
1:A:85:G:O2'	1:A:87:U:O4	2.24	0.56
1:A:308:A:N1	1:A:329:U:H5	2.04	0.56
3:C:26:C:H2'	3:C:27:C:C6	2.41	0.56
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.56
3:C:-9:U:H3	3:E:-9:U:H3	1.54	0.56
1:A:154:U:H2'	1:A:155:A:C4	2.40	0.55
1:A:315:G:H2'	1:A:316:C:C6	2.40	0.55
1:A:364:A:H3'	1:A:364:A:OP2	2.05	0.55
1:A:412:A:H2'	1:A:413:A:C8	2.42	0.55
3:E:-7:U:H2'	3:E:-6:C:C6	2.42	0.55
1:A:10:G:H2'	1:A:11:C:H6	1.70	0.55
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.55
1:A:49:A:N1	1:A:387:A:O2'	2.37	0.55
1:A:5:A:H2'	1:A:6:U:C6	2.42	0.55
1:A:59:U:H2'	1:A:60:C:C6	2.42	0.54
2:B:92:MET:HB3	2:B:97:VAL:HG23	1.88	0.54
1:A:241:A:H2'	1:A:242:C:C6	2.42	0.54
1:A:85:G:H4'	1:A:85:G:OP1	2.08	0.54
1:A:229:G:H5'	1:A:230:G:OP2	2.08	0.54
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.54
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.54
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.53
1:A:5:A:H2'	1:A:6:U:H6	1.72	0.53
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.53
3:C:8:U:H5'	3:C:48:G:C5'	2.35	0.53
1:A:160:C:H3'	1:A:161:G:C8	2.43	0.53
1:A:197:A:H2	1:A:229:G:H1'	1.74	0.53
1:A:264:U:H2'	1:A:265:G:O4'	2.09	0.53
1:A:349:G:O6	1:A:379:G:N2	2.42	0.52
1:A:166:G:H2'	1:A:167:G:C8	2.44	0.52
3:C:40:U:H2'	3:C:41:G:C8	2.44	0.52
1:A:216:A:O2'	1:A:217:A:H8	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.52
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.51
3:C:-8:U:C2	3:C:-7:U:C5	2.99	0.51
1:A:219:C:H2'	1:A:220:C:H6	1.76	0.51
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.51
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.50
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.50
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.50
1:A:267:U:C2	3:C:75:A:C2	2.99	0.50
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.50
1:A:180:U:H2'	1:A:181:A:C8	2.45	0.50
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.50
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.50
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.50
1:A:307:G:H2'	1:A:308:A:C8	2.47	0.50
3:C:29:C:H2'	3:C:30:C:C6	2.47	0.50
1:A:186:G:N1	1:A:189:A:OP2	2.35	0.50
1:A:161:G:H3'	1:A:162:G:C8	2.45	0.50
1:A:373:C:H2'	1:A:374:A:C8	2.47	0.50
1:A:181:A:H2'	1:A:182:C:O4'	2.12	0.49
1:A:349:G:H4'	1:A:350:A:H5'	1.94	0.49
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.49
1:A:85:G:H1'	1:A:86:U:H5	1.77	0.49
1:A:344:C:H2'	1:A:345:G:C8	2.47	0.49
3:E:-10:U:H2'	3:E:-9:U:C6	2.47	0.49
1:A:317:G:N1	1:A:321:G:C2	2.79	0.49
3:C:-7:U:H2'	3:C:-6:C:H6	1.78	0.49
1:A:19:A:H2'	1:A:20:U:C6	2.48	0.48
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.48
1:A:280:U:H2'	1:A:281:U:C6	2.49	0.48
1:A:401:A:H2'	1:A:402:G:O4'	2.13	0.48
1:A:178:A:OP1	1:A:180:U:H1'	2.14	0.48
1:A:347:C:H1'	1:A:383:G:N2	2.29	0.48
1:A:23:C:O2	1:A:336:A:O2'	2.28	0.48
1:A:230:G:C5'	1:A:230:G:H8	2.26	0.48
1:A:280:U:H2'	1:A:281:U:H6	1.79	0.48
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.48
1:A:268:G:H2'	1:A:269:G:H8	1.79	0.48
1:A:385:A:H1'	1:A:401:A:C8	2.49	0.48
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.47
1:A:230:G:H8	1:A:230:G:H5'	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:A:H2'	1:A:228:U:O2'	2.15	0.47
1:A:216:A:HO2'	1:A:217:A:H8	1.62	0.47
1:A:335:G:C8	1:A:335:G:H3'	2.49	0.47
1:A:180:U:O2'	1:A:181:A:H5'	2.13	0.47
3:C:41:G:H2'	3:C:42:G:C8	2.49	0.47
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.47
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.47
1:A:176:C:H2'	1:A:177:G:C8	2.49	0.47
3:C:-9:U:O2'	3:C:-8:U:H5'	2.14	0.47
1:A:155:A:H2'	1:A:156:C:C6	2.50	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
1:A:411:U:H2'	1:A:412:A:C8	2.48	0.47
2:B:112:LYS:O	2:B:113:LYS:C	2.58	0.47
3:C:-8:U:HO2'	3:C:-7:U:H6	1.62	0.47
1:A:175:U:H2'	1:A:176:C:O4'	2.15	0.47
1:A:233:C:H4'	1:A:234:G:O5'	2.15	0.47
3:C:60:C:H2'	3:C:61:C:H6	1.80	0.47
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.80	0.47
3:C:27:C:H2'	3:C:28:A:H8	1.80	0.47
1:A:198:G:N2	1:A:200:G:H3'	2.30	0.46
1:A:376:U:H2'	1:A:377:A:C8	2.49	0.46
3:C:24:C:H2'	3:C:25:A:C8	2.51	0.46
1:A:338:G:H2'	1:A:339:A:H8	1.80	0.46
1:A:371:U:H4'	1:A:373:C:H5	1.79	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.46
2:B:111:LEU:C	2:B:113:LYS:N	2.72	0.46
1:A:352:U:H2'	1:A:353:A:C8	2.51	0.46
1:A:229:G:N2	1:A:231:A:H3'	2.29	0.46
1:A:285:G:O2'	1:A:300:A:N6	2.49	0.46
1:A:350:A:C1'	1:A:380:A:N1	2.78	0.46
1:A:50:A:C8	1:A:50:A:C5'	2.99	0.46
1:A:147:A:H2'	1:A:148:A:C8	2.51	0.46
1:A:292:A:H2'	1:A:293:U:C6	2.51	0.46
1:A:101:U:OP2	1:A:279:C:H4'	2.17	0.45
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.45
1:A:268:G:C2	3:C:75:A:C2	3.04	0.45
3:C:-13:G:C4	3:C:-12:G:C8	3.05	0.45
3:C:37:A:H2'	3:C:38:G:C8	2.51	0.45
1:A:331:G:H4'	1:A:332:A:H5'	1.98	0.45
1:A:154:U:H4'	1:A:218:A:H4'	1.99	0.45
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:A:H2'	1:A:380:A:N3	2.32	0.45
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.45
1:A:60:C:H2'	1:A:61:G:H8	1.82	0.45
2:B:86:ARG:HH22	3:E:-13:G:H21	1.64	0.45
2:B:111:LEU:C	2:B:113:LYS:H	2.25	0.45
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.45
2:B:49:LYS:HG3	3:C:-1:U:O5'	2.17	0.45
1:A:292:A:H2'	1:A:293:U:H6	1.82	0.44
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.44
1:A:68:G:N3	1:A:68:G:H2'	2.31	0.44
2:B:99:LYS:HD3	2:B:99:LYS:O	2.17	0.44
1:A:17:U:H2'	1:A:18:A:H8	1.82	0.44
1:A:114:G:H2'	1:A:115:C:C6	2.52	0.44
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.44
3:C:-9:U:H2'	3:C:-8:U:C6	2.53	0.44
3:E:-9:U:H2'	3:E:-8:U:H6	1.83	0.44
1:A:363:A:O2'	1:A:364:A:O4'	2.33	0.44
1:A:219:C:H2'	1:A:220:C:C6	2.52	0.44
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.44
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.44
1:A:414:C:H2'	1:A:415:G:C8	2.53	0.44
3:C:-10:U:C2	3:C:-9:U:C5	3.06	0.44
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.43
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.43
1:A:123:C:H2'	1:A:124:U:O4'	2.18	0.43
3:E:-9:U:H2'	3:E:-8:U:C6	2.53	0.43
1:A:166:G:H2'	1:A:167:G:H8	1.83	0.43
1:A:350:A:C8	1:A:380:A:C6	3.06	0.43
1:A:355:G:H2'	1:A:356:A:C8	2.54	0.43
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.43
2:B:11:GLU:O	2:B:15:GLU:HG3	2.19	0.43
1:A:14:G:C2'	1:A:401:A:H61	2.31	0.43
1:A:217:A:H2'	1:A:218:A:O4'	2.18	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:382:G:H2'	1:A:383:G:O4'	2.18	0.43
1:A:169:U:H2'	1:A:170:A:C8	2.54	0.43
1:A:358:G:H1	1:A:366:C:H42	1.66	0.43
2:B:98:LYS:O	2:B:102:ILE:HD13	2.19	0.43
3:C:16:U:H5	3:C:58:G:O6	2.02	0.43
3:C:34:C:H2'	3:C:35:C:H6	1.83	0.43
1:A:50:A:N3	1:A:50:A:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:U:H2'	1:A:60:C:H6	1.84	0.42
1:A:134:C:H2'	1:A:135:U:C6	2.55	0.42
3:C:16:U:C5	3:C:58:G:O6	2.72	0.42
1:A:343:C:H2'	1:A:344:C:C6	2.54	0.42
1:A:354:C:H2'	1:A:355:G:O4'	2.19	0.42
1:A:132:G:H3'	1:A:133:G:H8	1.83	0.42
1:A:220:C:H2'	1:A:221:U:H6	1.85	0.42
1:A:313:C:H2'	1:A:314:G:C8	2.54	0.42
3:C:-10:U:H2'	3:C:-9:U:C6	2.55	0.42
1:A:334:A:H62	2:B:10:ASN:HD22	1.68	0.42
1:A:17:U:H2'	1:A:18:A:C8	2.55	0.42
1:A:89:G:H2'	1:A:90:U:C6	2.54	0.42
1:A:128:G:H2'	1:A:129:C:H6	1.82	0.42
1:A:324:G:H2'	1:A:325:C:H6	1.84	0.42
1:A:335:G:C8	1:A:335:G:C3'	3.03	0.42
1:A:349:G:N2	1:A:378:C:C2	2.88	0.42
3:C:42:G:H2'	3:C:43:G:C8	2.55	0.42
1:A:174:U:H2'	1:A:175:U:C6	2.54	0.42
1:A:186:G:N2	1:A:188:A:H3'	2.34	0.42
1:A:95:A:H2'	1:A:96:G:C8	2.55	0.42
1:A:115:C:H2'	1:A:116:A:H8	1.85	0.42
3:C:21:G:H8	3:C:21:G:OP2	2.03	0.42
3:C:35:C:H2'	3:C:36:A:O4'	2.20	0.42
1:A:260:C:H2'	1:A:261:A:O4'	2.20	0.42
1:A:308:A:N1	1:A:329:U:C5	2.88	0.42
1:A:344:C:H2'	1:A:345:G:H8	1.85	0.42
1:A:56:U:H2'	1:A:57:G:H8	1.85	0.41
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.41
2:B:73:GLU:OE1	2:B:73:GLU:N	2.52	0.41
1:A:19:A:H2'	1:A:20:U:H6	1.85	0.41
1:A:102:C:O5'	1:A:102:C:H6	2.03	0.41
1:A:117:G:H3'	1:A:118:C:H6	1.86	0.41
1:A:95:A:H2'	1:A:96:G:H8	1.85	0.41
1:A:267:U:C4	3:C:75:A:C4	3.08	0.41
1:A:279:C:H2'	1:A:280:U:C6	2.55	0.41
1:A:287:A:H3'	1:A:288:G:H8	1.86	0.41
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.41
1:A:334:A:H62	2:B:10:ASN:ND2	2.17	0.41
1:A:9:U:C2	1:A:10:G:C8	3.09	0.41
1:A:227:G:O2'	1:A:228:U:H5'	2.19	0.41
1:A:335:G:H3'	1:A:335:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:C:O2'	1:A:230:G:O6	2.38	0.41
1:A:220:C:H2'	1:A:221:U:C6	2.56	0.41
1:A:229:G:N1	1:A:232:A:OP2	2.54	0.41
1:A:352:U:H2'	1:A:353:A:H8	1.86	0.41
1:A:356:A:H3'	1:A:357:G:C8	2.56	0.41
3:C:67:U:H2'	3:C:68:C:O4'	2.20	0.41
1:A:38:G:H2'	1:A:39:C:C6	2.55	0.41
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.41
1:A:364:A:H3'	1:A:364:A:P	2.60	0.41
1:A:350:A:C4	1:A:380:A:C5	3.09	0.41
3:C:-9:U:C2	3:C:-8:U:C5	3.09	0.41
1:A:2:U:H2'	1:A:3:U:H6	1.84	0.41
1:A:180:U:C2'	1:A:181:A:H5'	2.51	0.41
1:A:199:U:O2	1:A:199:U:O4'	2.38	0.41
1:A:350:A:C4	1:A:380:A:C4	3.09	0.41
1:A:380:A:C2	1:A:381:A:N9	2.89	0.41
1:A:89:G:H2'	1:A:90:U:H6	1.86	0.41
1:A:286:A:N6	1:A:299:G:H1'	2.36	0.40
1:A:397:U:H2'	1:A:398:U:C6	2.56	0.40
3:C:-13:G:H3'	3:C:-12:G:H8	1.87	0.40
1:A:353:A:H2'	1:A:354:C:O4'	2.21	0.40
3:C:8:U:O2	3:C:20:A:H2	2.04	0.40
3:C:60:C:H2'	3:C:61:C:C6	2.56	0.40
1:A:266:A:N3	1:A:266:A:H2'	2.36	0.40
1:A:369:C:H2'	1:A:370:U:O4'	2.22	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	
2	B	114/116 (98%)	110 (96%)	4 (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
2	B	99/99 (100%)	94 (95%)	5 (5%)	20 49

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	71	LEU
2	B	92	MET
2	B	97	VAL
2	B	105	LEU
2	B	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	164 (39%)	16 (3%)
3	C	88/92 (95%)	38 (43%)	4 (4%)
3	E	8/92 (8%)	4 (50%)	0
All	All	512/601 (85%)	206 (40%)	20 (3%)

All (206) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U

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Mol	Chain	Res	Type
1	A	11	C
1	A	15	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	44	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	63	A
1	A	67	U
1	A	68	G
1	A	70	U
1	A	74	A
1	A	75	U
1	A	76	G
1	A	81	U
1	A	85	G
1	A	88	C
1	A	91	G
1	A	99	A
1	A	102	C
1	A	104	A
1	A	105	U
1	A	117	G
1	A	118	C
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	133	G
1	A	134	C

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Mol	Chain	Res	Type
1	A	137	A
1	A	138	C
1	A	139	G
1	A	146	A
1	A	150	A
1	A	152	C
1	A	153	C
1	A	155	A
1	A	157	G
1	A	158	U
1	A	159	C
1	A	163	C
1	A	169	U
1	A	171	U
1	A	172	G
1	A	173	G
1	A	174	U
1	A	175	U
1	A	177	G
1	A	179	U
1	A	180	U
1	A	181	A
1	A	182	C
1	A	185	U
1	A	187	A
1	A	189	A
1	A	192	G
1	A	197	A
1	A	199	U
1	A	202	C
1	A	204	G
1	A	205	A
1	A	206	G
1	A	207	C
1	A	216	A
1	A	219	C
1	A	225	A
1	A	229	G
1	A	230	G
1	A	231	A
1	A	232	A
1	A	233	C

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Mol	Chain	Res	Type
1	A	234	G
1	A	235	C
1	A	236	G
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	266	A
1	A	267	U
1	A	272	G
1	A	273	G
1	A	274	G
1	A	276	C
1	A	278	C
1	A	291	A
1	A	292	A
1	A	293	U
1	A	296	A
1	A	300	A
1	A	304	A
1	A	312	G
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	342	A
1	A	346	C
1	A	347	C

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Mol	Chain	Res	Type
1	A	349	G
1	A	350	A
1	A	351	G
1	A	353	A
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	389	A
1	A	391	C
1	A	392	A
1	A	400	U
1	A	401	A
1	A	402	G
1	A	403	A
1	A	406	A
1	A	407	U
1	A	408	G
1	A	410	U
3	C	-10	U
3	C	-8	U
3	C	-7	U
3	C	-5	C
3	C	-4	C
3	C	-3	U

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Mol	Chain	Res	Type
3	C	-2	U
3	C	-1	U
3	C	8	U
3	C	9	A
3	C	10	G
3	C	11	U
3	C	12	U
3	C	13	C
3	C	15	G
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	21	G
3	C	23	A
3	C	26	C
3	C	29	C
3	C	33	G
3	C	37	A
3	C	40	U
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	52	G
3	C	58	G
3	C	59	U
3	C	60	C
3	C	70	G
3	C	72	U
3	C	75	A
3	E	-11	A
3	E	-10	U
3	E	-9	U
3	E	-7	U

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	50	A
1	A	67	U

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Mol	Chain	Res	Type
1	A	75	U
1	A	122	G
1	A	126	U
1	A	137	A
1	A	176	C
1	A	201	A
1	A	204	G
1	A	232	A
1	A	235	C
1	A	240	A
1	A	292	A
1	A	349	G
1	A	363	A
1	A	365	G
3	C	7	G
3	C	46	U
3	C	59	U
3	C	69	C

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 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

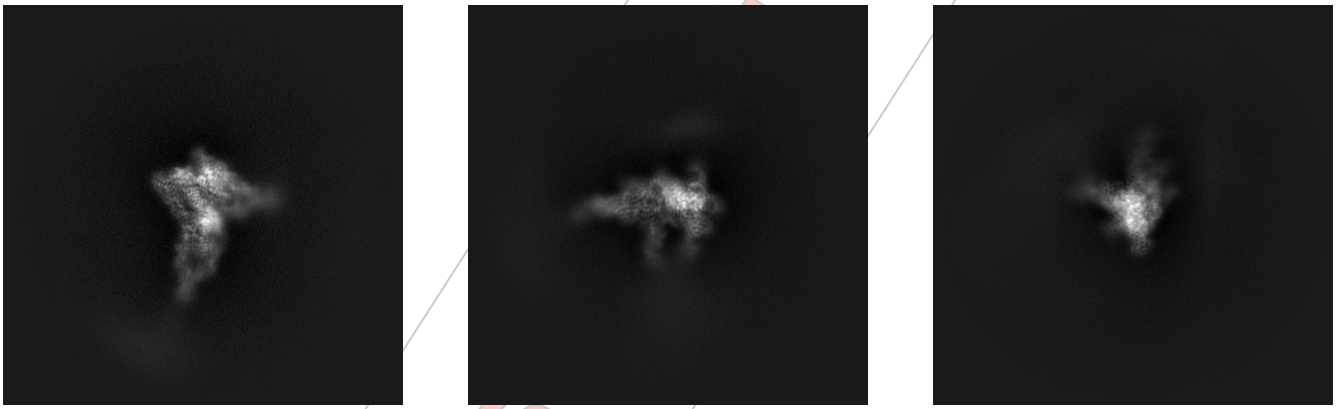
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70943. 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.

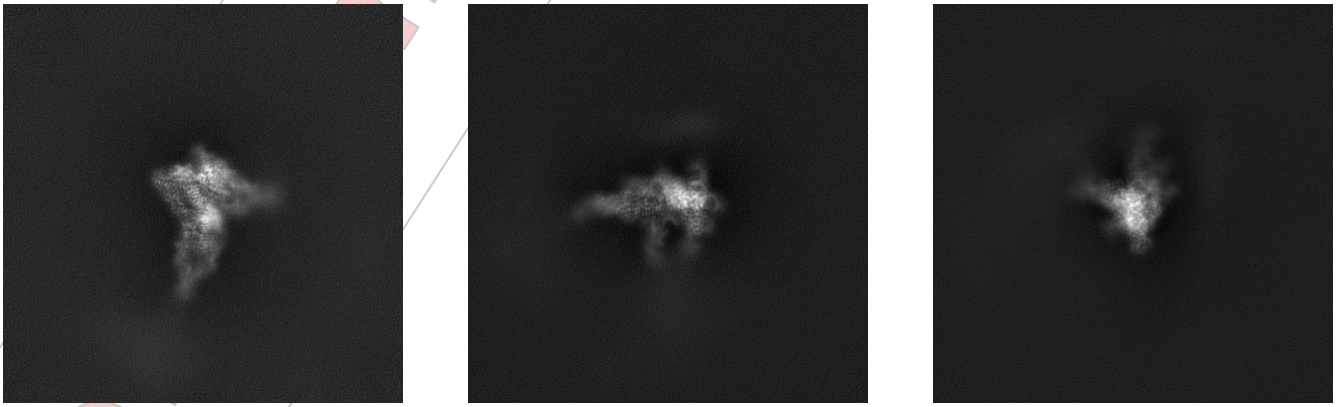
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

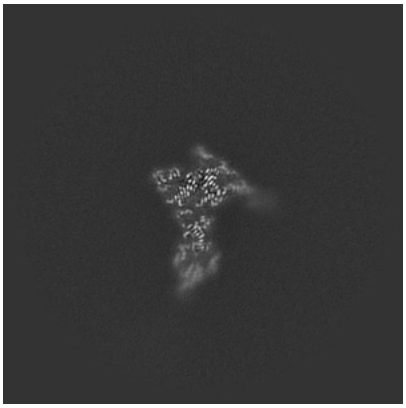


X Y Z

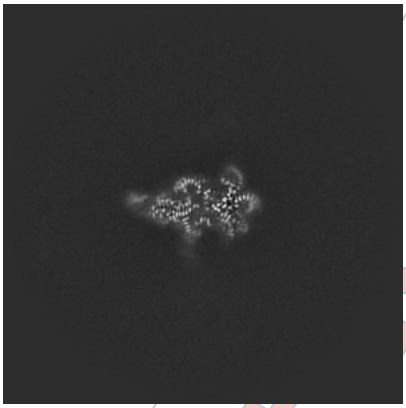
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

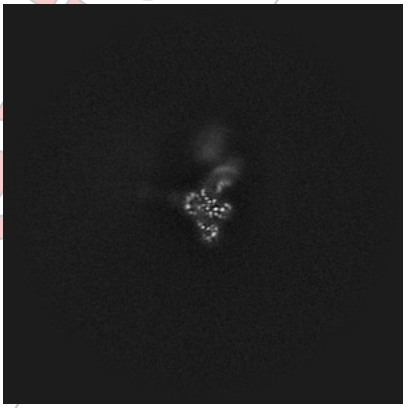
6.2.1 Primary map



X Index: 200

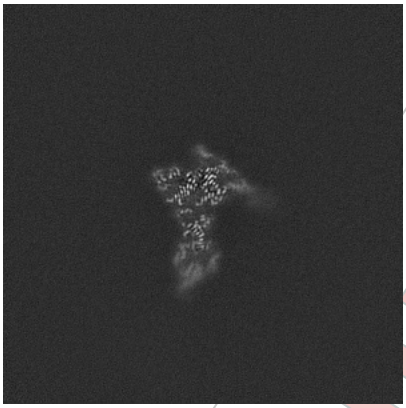


Y Index: 200

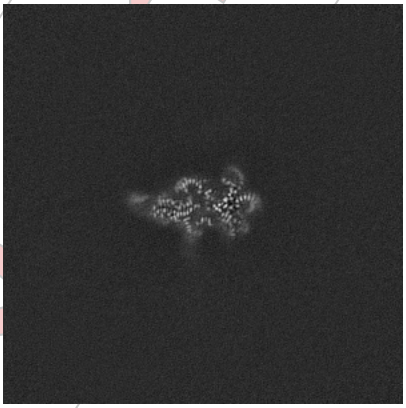


Z Index: 200

6.2.2 Raw map



X Index: 200



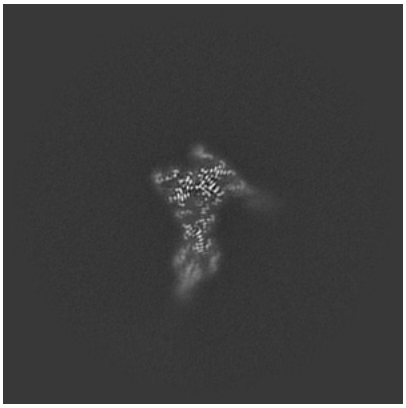
Y Index: 200

Z Index: 200

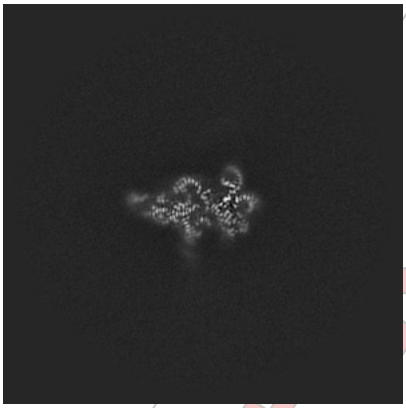
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



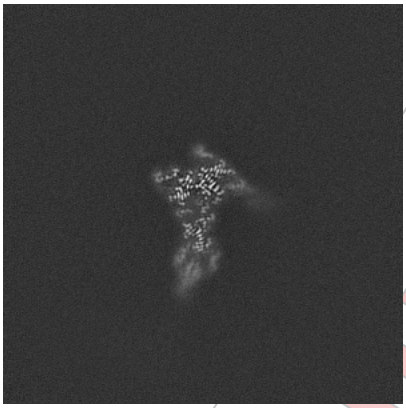
X Index: 198



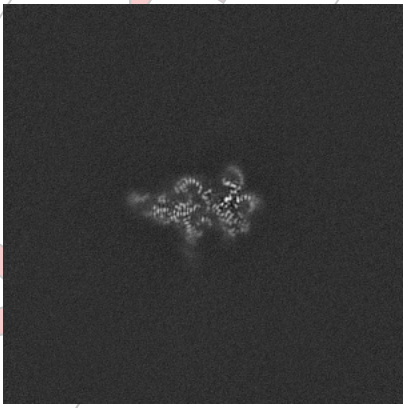
Y Index: 201

Z Index: 227

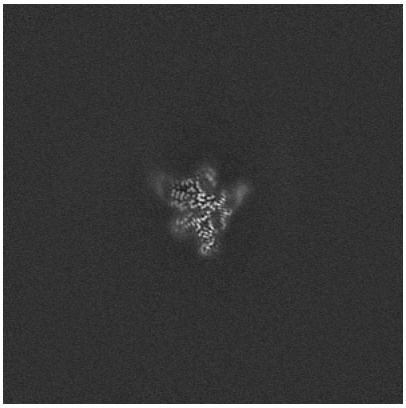
6.3.2 Raw map



X Index: 198



Y Index: 201

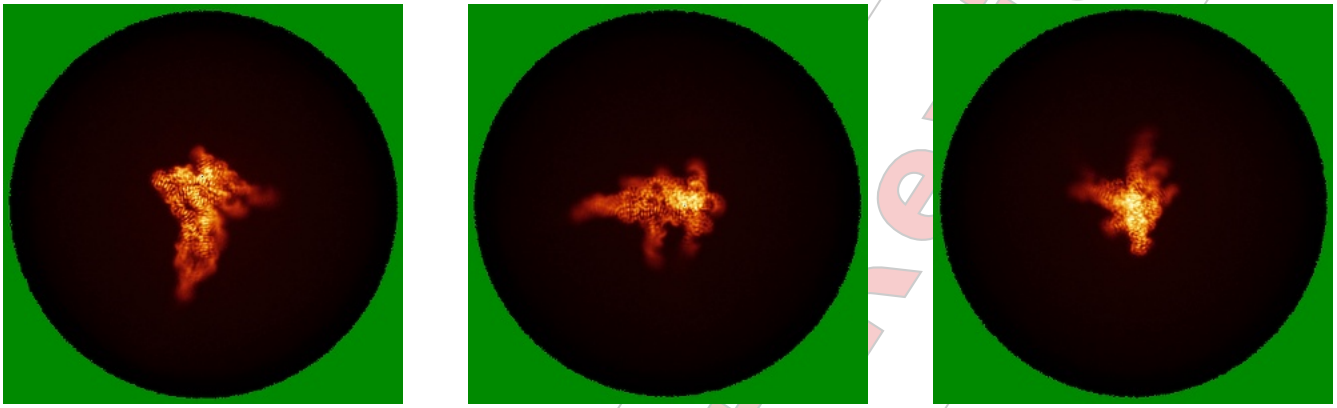


Z Index: 228

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

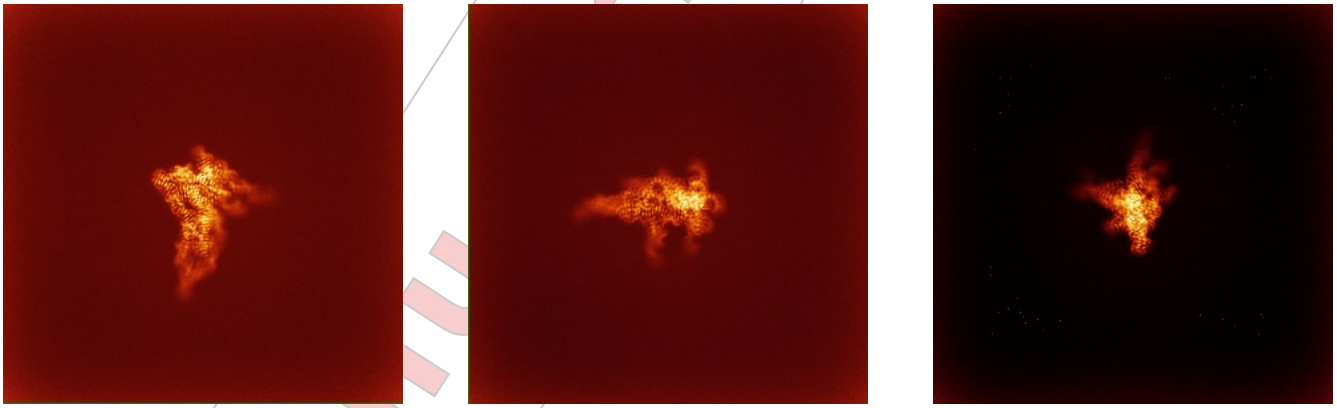
6.4 Orthogonal standard-deviation projections (False-color)

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 0.026. 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.

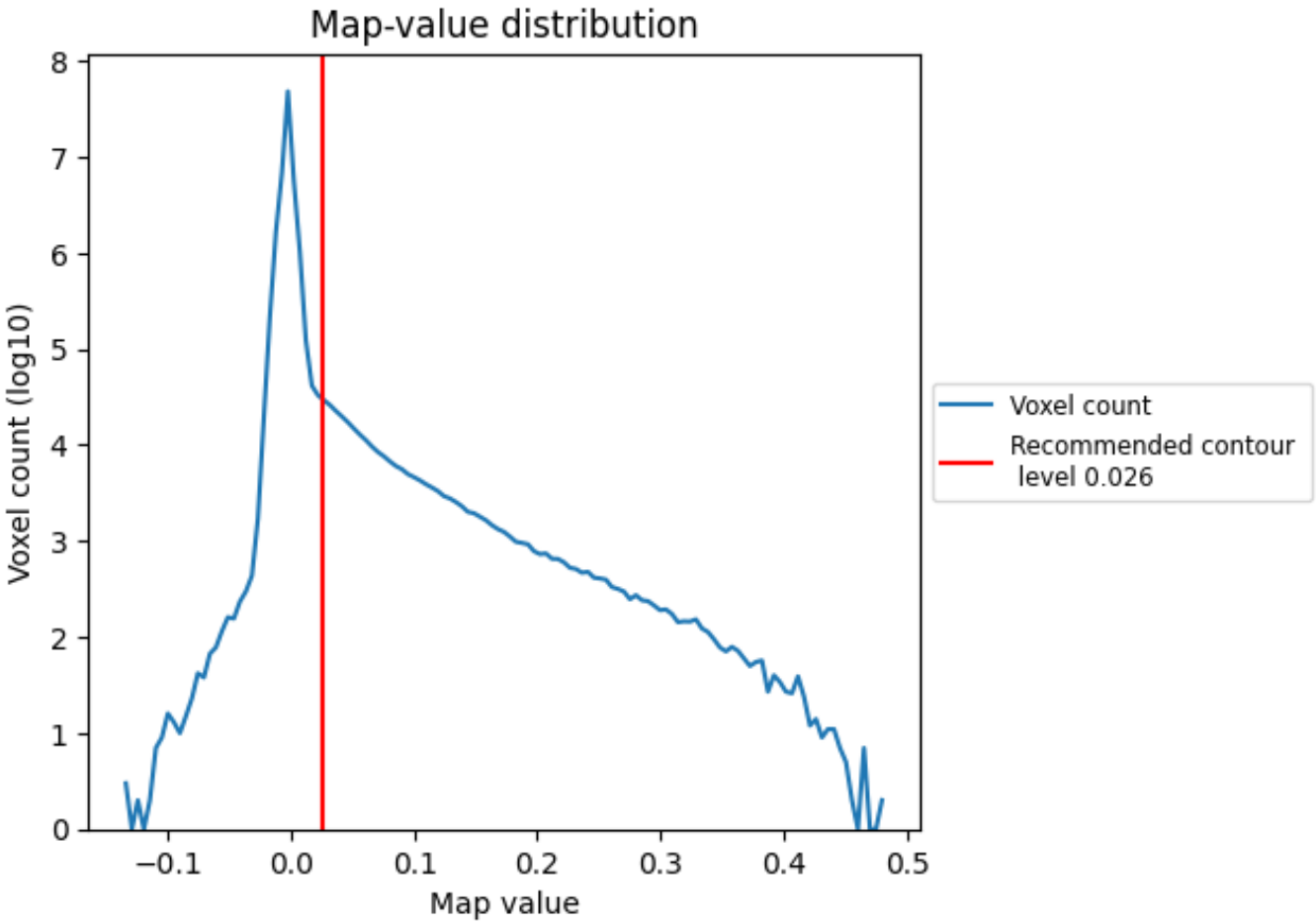
6.6 Mask visualisation (i)

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

7 Map analysis

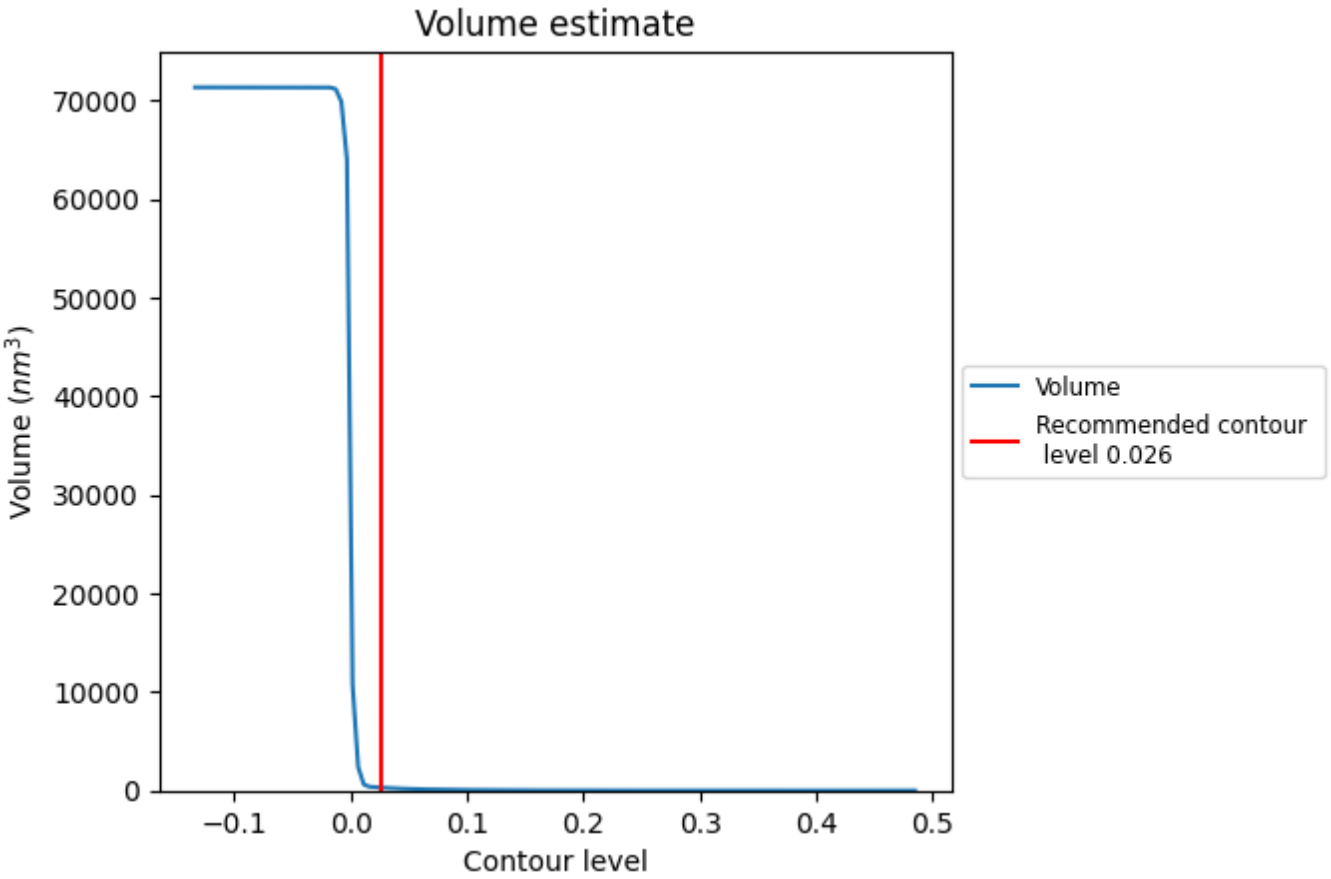
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

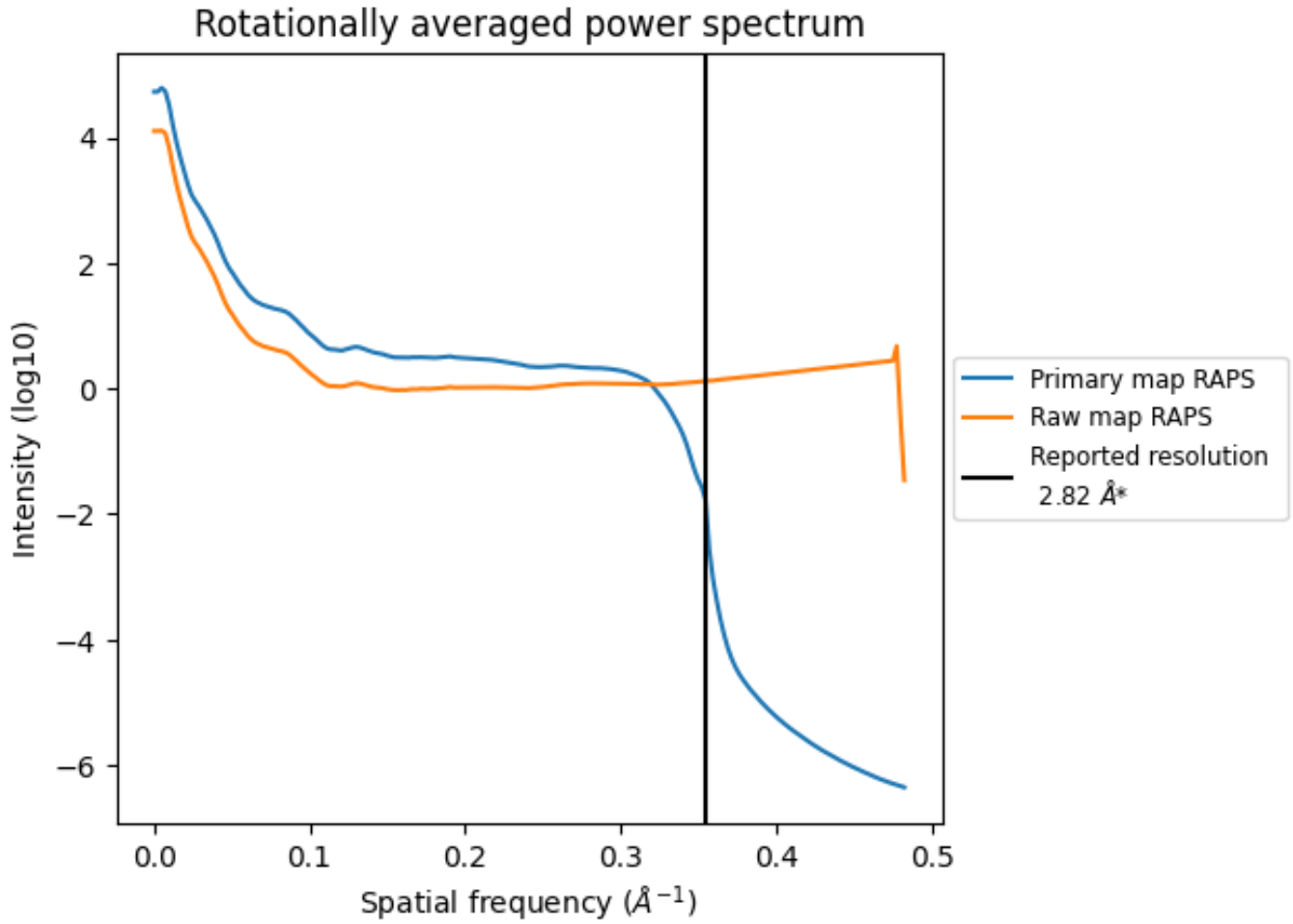
7.2 Volume estimate



The volume at the recommended contour level is 297 nm^3; this corresponds to an approximate mass of 269 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 (i)

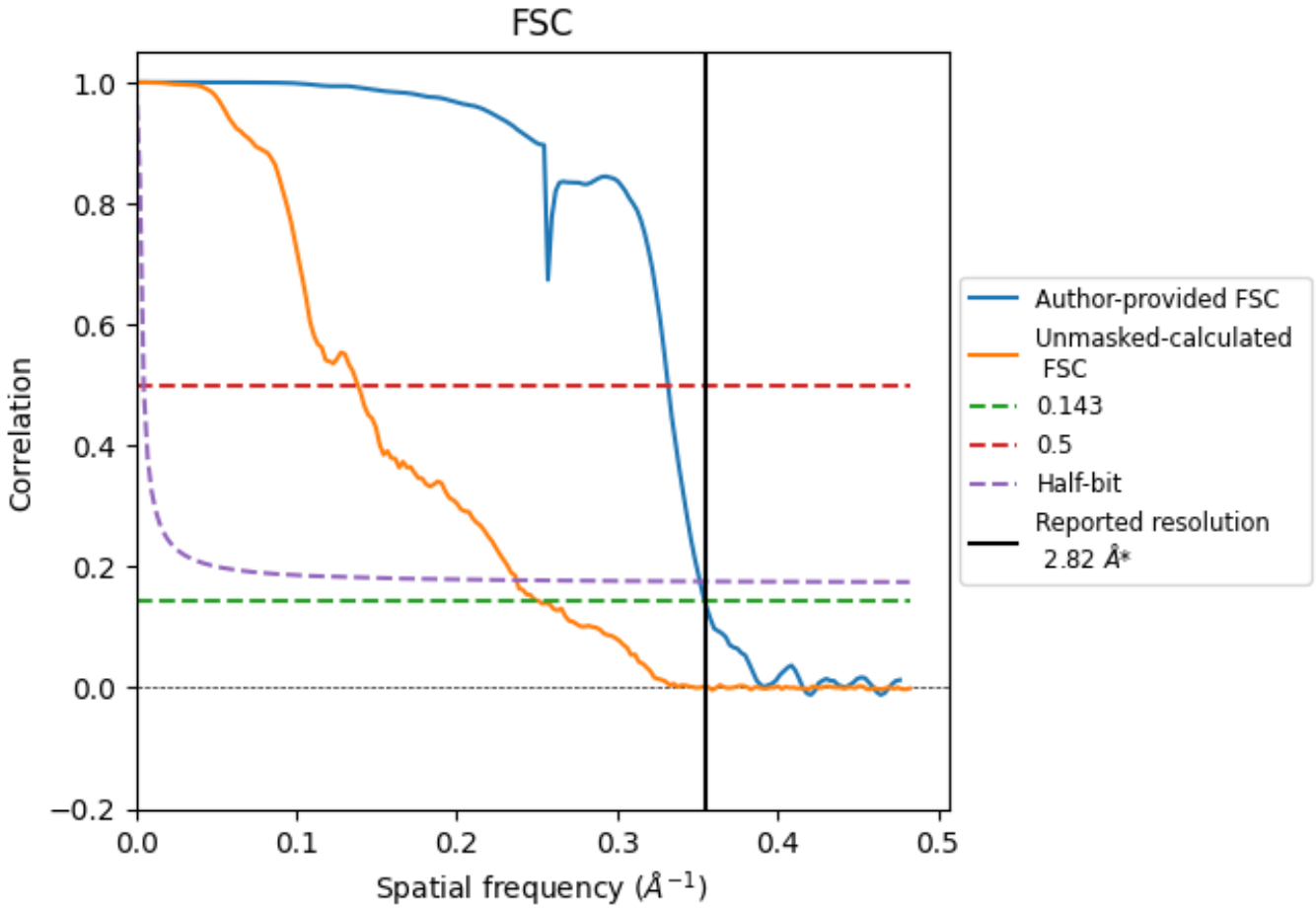


*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8.2 Resolution estimates (i)

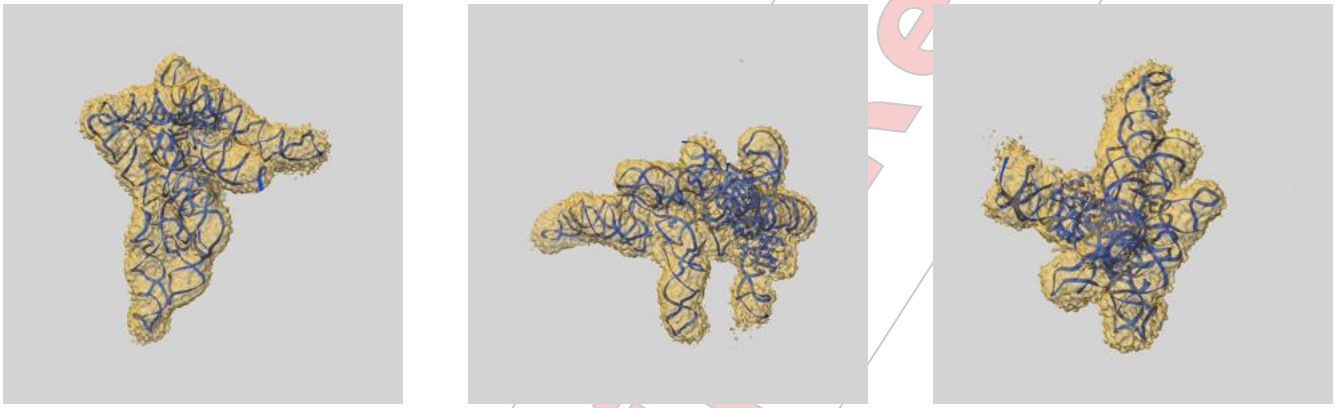
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.01	2.84
Unmasked-calculated*	3.98	7.24	4.22

*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 3.98 differs from the reported value 2.82 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70943 and PDB model 9OWT. Per-residue inclusion information can be found in section 3 on page 4.

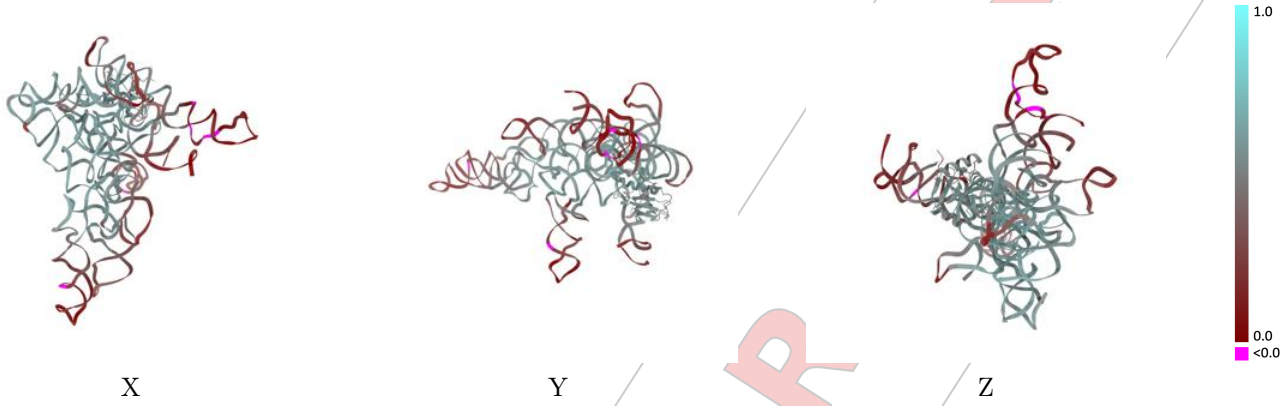
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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)



X Y Z

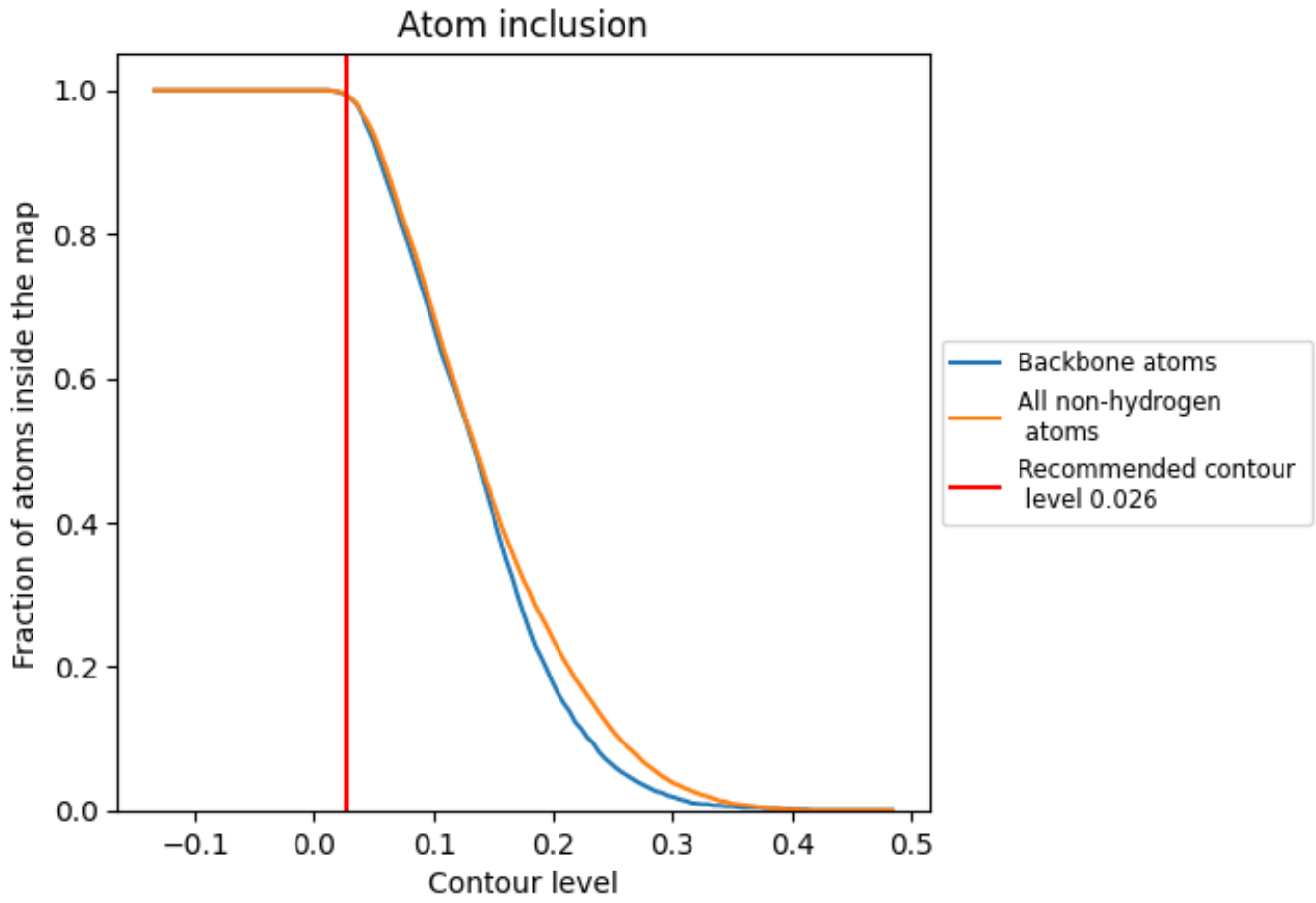
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.4460
A	0.9950	0.4450
B	0.9940	0.5350
C	0.9970	0.4210
E	0.9470	0.2980

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 04:10 PM EDT

PDB ID	:	9OWU / pdb_00009owu
EMDB ID	:	EMD-70944
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with precursor tRNA in 1 mM Ca2+
Deposited on	:	2025-06-02
Resolution	:	2.93 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

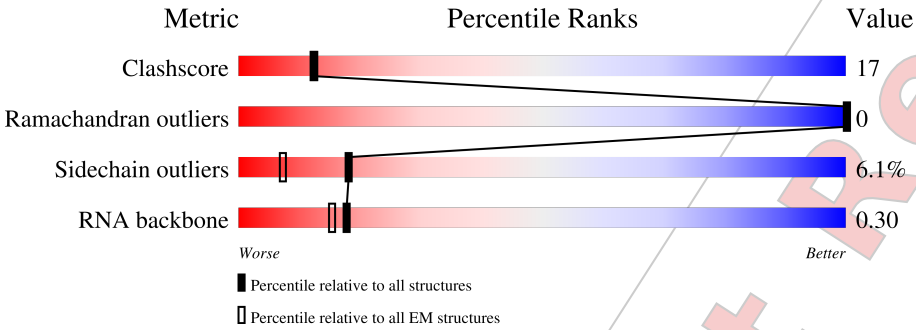
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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 <=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	417	32% 43% 24%
2	B	116	74% 22%
3	C	92	24% 47% 26%
3	E	92	90%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12011 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor tRNA (89-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	89	1889	842	326	632	89	0	0
			Total	C	N	O	P		
3	E	9	188	84	29	66	9	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

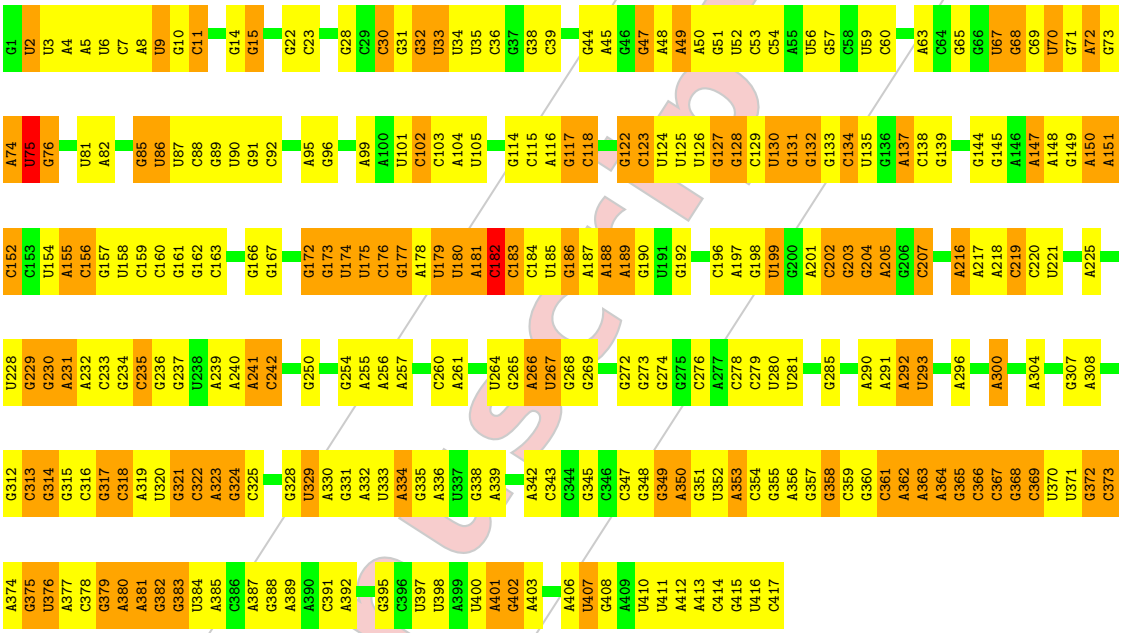
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	25	25	25	0

3 Residue-property plots (i)

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.

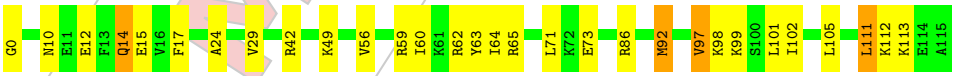
• Molecule 1: RNase P RNA (417-MER)

Chain A:



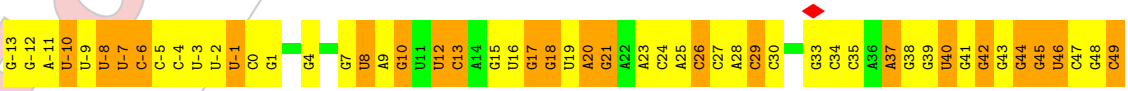
• Molecule 2: Ribonuclease P protein component

Chain B:

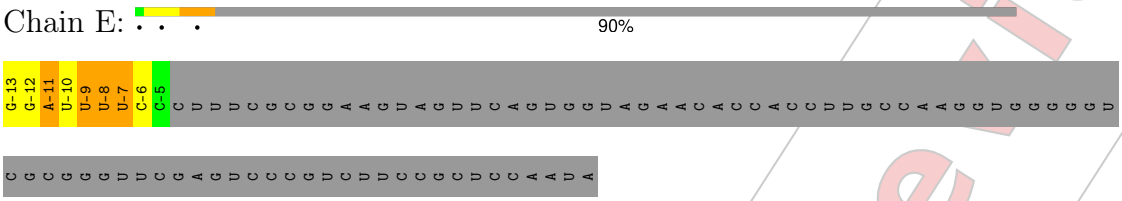


• Molecule 3: precursor tRNA (89-MER)

Chain C:



• Molecule 3: precursor tRNA (89-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229735	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.54	0/10038	0.87	7/15661 (0.0%)
2	B	0.45	0/962	0.66	0/1281
3	C	0.59	0/2107	0.91	3/3281 (0.1%)
3	E	0.58	0/208	0.87	0/321
All	All	0.54	0/13315	0.87	10/20544 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	U	C2'-C3'-O3'	6.57	119.36	109.50
1	A	230	G	O3'-P-O5'	5.93	112.90	104.00
1	A	182	C	C4'-C3'-C2'	-5.86	96.75	102.60
3	C	69	C	C4'-C3'-C2'	-5.67	96.93	102.60
3	C	69	C	O3'-P-O5'	-5.62	95.57	104.00
3	C	46	U	C2'-C3'-O3'	5.57	117.86	109.50
1	A	137	A	O3'-P-O5'	-5.33	96.01	104.00
1	A	75	U	C1'-C2'-O2'	-5.15	104.08	111.80
1	A	230	G	C4'-C3'-C2'	-5.14	97.46	102.60
1	A	69	C	O3'-P-O5'	5.03	111.54	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8962	0	4511	225	0
2	B	947	0	1008	23	0
3	C	1889	0	957	42	0
3	E	188	0	96	9	0
4	A	25	0	0	0	0
All	All	12011	0	6572	288	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 17.

All (288) 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:148:A:H2'	1:A:149:G:O4'	1.43	1.17
1:A:364:A:C4	1:A:365:G:H1'	1.96	1.00
1:A:371:U:H5"	1:A:372:G:H5'	1.56	0.86
1:A:85:G:H1'	1:A:86:U:H5	1.40	0.84
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.83
1:A:174:U:H2'	1:A:175:U:C6	2.20	0.77
1:A:378:C:H3'	1:A:379:G:C8	2.19	0.77
1:A:367:C:H2'	1:A:368:G:C8	2.20	0.76
1:A:203:G:C5	1:A:205:A:H1'	2.21	0.76
1:A:45:A:H62	2:B:62:ARG:NH2	1.83	0.76
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.76
3:C:-11:A:H2	3:E:-7:U:H3	1.34	0.73
1:A:147:A:H2'	1:A:148:A:C8	2.22	0.73
1:A:349:G:H22	1:A:379:G:H1'	1.55	0.72
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.72
2:B:63:TYR:HB3	2:B:97:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:U:H2'	1:A:10:G:H8	1.57	0.69
1:A:47:G:H1	1:A:385:A:H62	1.39	0.69
1:A:14:G:C2'	1:A:401:A:H61	2.06	0.69
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.69
1:A:349:G:H21	1:A:350:A:H62	1.39	0.68
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.68
1:A:378:C:H3'	1:A:379:G:H8	1.59	0.67
3:C:17:G:O2'	3:C:56:G:N2	2.27	0.67
1:A:174:U:H2'	1:A:175:U:H6	1.60	0.67
1:A:180:U:H2'	1:A:181:A:H8	1.59	0.66
3:C:-7:U:H2'	3:C:-6:C:O4'	1.95	0.66
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.65
1:A:199:U:H1'	1:A:207:C:O5'	1.98	0.64
1:A:349:G:N2	1:A:379:G:H1'	2.12	0.64
1:A:72:A:H2'	1:A:73:G:C8	2.33	0.63
1:A:161:G:H3'	1:A:162:G:H8	1.63	0.63
1:A:149:G:H2'	1:A:150:A:C8	2.33	0.63
1:A:197:A:C2	1:A:229:G:H1'	2.33	0.63
2:B:56:VAL:O	2:B:60:ILE:HG13	1.99	0.62
3:C:27:C:H2'	3:C:28:A:C8	2.34	0.62
1:A:85:G:H1'	1:A:86:U:C5	2.29	0.62
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.62
1:A:173:G:O2'	1:A:174:U:H5'	2.00	0.61
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.61
1:A:197:A:H2	1:A:229:G:H1'	1.66	0.61
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.61
1:A:154:U:H2'	1:A:155:A:C4	2.35	0.61
1:A:45:A:H62	2:B:62:ARG:HH22	1.46	0.61
1:A:241:A:H2'	1:A:242:C:C6	2.36	0.61
2:B:14:GLN:O	2:B:15:GLU:C	2.44	0.61
1:A:160:C:H3'	1:A:161:G:H8	1.67	0.60
1:A:148:A:H2'	1:A:149:G:C4'	2.32	0.60
1:A:379:G:H4'	1:A:380:A:C8	2.37	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
1:A:229:G:H2'	1:A:231:A:N7	2.17	0.59
1:A:379:G:H4'	1:A:380:A:H8	1.66	0.59
1:A:32:G:H22	1:A:34:U:H1'	1.68	0.59
3:C:10:G:N1	3:C:24:C:O2	2.36	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:3:U:H2'	1:A:4:A:H8	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.58
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.84	0.57
3:C:40:U:H2'	3:C:41:G:C8	2.39	0.57
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.57
1:A:364:A:H3'	1:A:364:A:OP2	2.05	0.56
3:C:38:G:H2'	3:C:39:G:C8	2.40	0.56
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.56
1:A:315:G:H2'	1:A:316:C:C6	2.40	0.56
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.56
3:C:26:C:H2'	3:C:27:C:C6	2.41	0.56
1:A:10:G:H2'	1:A:11:C:H6	1.70	0.56
1:A:374:A:H2'	1:A:375:G:C8	2.41	0.56
1:A:364:A:OP1	1:A:365:G:N7	2.35	0.55
1:A:186:G:H8	1:A:186:G:H5"	1.70	0.55
1:A:412:A:H2'	1:A:413:A:C8	2.41	0.55
2:B:92:MET:HB3	2:B:97:VAL:HG23	1.88	0.55
3:C:-11:A:H2'	3:C:-10:U:C6	2.40	0.55
3:C:43:G:H3'	3:C:44:G:H2'	1.89	0.55
3:E:-7:U:H2'	3:E:-6:C:C6	2.42	0.55
1:A:5:A:H2'	1:A:6:U:C6	2.42	0.55
1:A:308:A:N1	1:A:329:U:H5	2.04	0.55
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.55
1:A:186:G:H5"	1:A:186:G:C8	2.41	0.54
1:A:102:C:H2'	1:A:103:C:O4'	2.08	0.54
1:A:307:G:H2'	1:A:308:A:H8	1.70	0.54
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.54
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.54
1:A:186:G:N2	1:A:188:A:H3'	2.23	0.53
1:A:264:U:H2'	1:A:265:G:O4'	2.09	0.53
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.53
1:A:5:A:H2'	1:A:6:U:H6	1.72	0.53
3:C:-9:U:H3	3:E:-9:U:H3	1.56	0.53
1:A:147:A:H2'	1:A:148:A:H8	1.71	0.53
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.52
1:A:166:G:H2'	1:A:167:G:C8	2.45	0.52
1:A:198:G:N2	1:A:201:A:OP2	2.42	0.52
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.52
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:G:H2'	3:C:42:G:C8	2.45	0.52
1:A:216:A:O2'	1:A:217:A:H8	1.93	0.52
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.51
1:A:267:U:C2	3:C:75:A:C2	2.99	0.51
1:A:197:A:H2'	1:A:228:U:O2'	2.10	0.51
1:A:14:G:C1'	1:A:401:A:H61	2.24	0.51
1:A:219:C:H2'	1:A:220:C:H6	1.76	0.51
1:A:347:C:H2'	1:A:348:G:O4'	2.10	0.51
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.51
3:C:12:U:H2'	3:C:13:C:O4'	2.11	0.51
3:C:-8:U:C2	3:C:-7:U:C5	2.99	0.51
1:A:148:A:C4	1:A:149:G:H1'	2.46	0.50
1:A:376:U:H2'	1:A:377:A:C8	2.45	0.50
3:E:-9:U:H2'	3:E:-8:U:H6	1.76	0.50
1:A:14:G:H1'	1:A:401:A:H61	1.77	0.50
1:A:85:G:O2'	1:A:87:U:O4	2.28	0.50
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.50
3:C:8:U:O2	3:C:20:A:H2	1.94	0.50
1:A:182:C:H2'	1:A:183:C:H6	1.76	0.50
3:C:44:G:H4'	3:C:45:G:O5'	2.12	0.50
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.50
1:A:356:A:H3'	1:A:357:G:H8	1.76	0.50
1:A:317:G:N1	1:A:321:G:C2	2.79	0.49
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.49
3:C:42:G:H2'	3:C:43:G:C8	2.47	0.49
1:A:23:C:O2	1:A:336:A:O2'	2.28	0.49
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.49
1:A:228:U:H2'	1:A:229:G:O4'	2.12	0.49
1:A:236:G:H2'	1:A:237:G:O4'	2.12	0.49
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.49
1:A:307:G:H2'	1:A:308:A:C8	2.46	0.49
1:A:348:G:N2	1:A:380:A:N7	2.61	0.49
1:A:49:A:N1	1:A:387:A:O2'	2.42	0.49
1:A:371:U:H4'	1:A:373:C:H5	1.78	0.49
3:C:29:C:H2'	3:C:30:C:C6	2.47	0.49
1:A:161:G:H3'	1:A:162:G:C8	2.45	0.49
3:C:10:G:N3	3:C:10:G:H2'	2.26	0.49
1:A:15:G:N2	1:A:345:G:H1'	2.28	0.49
1:A:202:C:H5'	1:A:203:G:C8	2.48	0.49
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.48
1:A:160:C:H3'	1:A:161:G:C8	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:U:H2'	1:A:353:A:C8	2.49	0.48
1:A:178:A:OP1	1:A:180:U:H1'	2.14	0.48
1:A:180:U:O2'	1:A:181:A:H5'	2.13	0.48
1:A:186:G:N1	1:A:189:A:OP2	2.39	0.48
1:A:280:U:H2'	1:A:281:U:C6	2.49	0.48
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.48
3:E:-8:U:C4	3:E:-7:U:C4	3.02	0.48
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.48
1:A:280:U:H2'	1:A:281:U:H6	1.79	0.48
1:A:149:G:N2	1:A:177:G:H1'	2.28	0.48
1:A:385:A:H1'	1:A:401:A:C8	2.49	0.48
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.47
3:C:-9:U:O2'	3:C:-8:U:H5'	2.14	0.47
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.47
1:A:411:U:H2'	1:A:412:A:C8	2.49	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
1:A:132:G:H3'	1:A:133:G:H8	1.79	0.47
1:A:357:G:H22	1:A:367:C:H42	1.61	0.47
3:E:-8:U:C6	3:E:-8:U:H5"	2.49	0.47
1:A:229:G:H5"	1:A:229:G:H8	1.79	0.47
1:A:268:G:H2'	1:A:269:G:H8	1.79	0.47
1:A:176:C:H2'	1:A:177:G:C8	2.50	0.47
1:A:401:A:H2'	1:A:402:G:O4'	2.13	0.47
2:B:111:LEU:C	2:B:113:LYS:N	2.72	0.47
3:E:-9:U:H2'	3:E:-8:U:C6	2.49	0.47
1:A:335:G:C8	1:A:335:G:H3'	2.50	0.47
2:B:112:LYS:O	2:B:113:LYS:C	2.58	0.47
1:A:180:U:H2'	1:A:181:A:C8	2.45	0.46
1:A:172:G:C4	1:A:173:G:C8	3.03	0.46
1:A:349:G:N2	1:A:350:A:H62	2.09	0.46
3:C:27:C:H2'	3:C:28:A:H8	1.80	0.46
3:C:24:C:H2'	3:C:25:A:C8	2.51	0.46
1:A:14:G:H2'	1:A:385:A:N1	2.30	0.46
1:A:59:U:H2'	1:A:60:C:C6	2.51	0.46
1:A:71:G:O2'	1:A:73:G:N7	2.41	0.46
1:A:285:G:O2'	1:A:300:A:N6	2.49	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.46
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.46
2:B:101:LEU:HD12	2:B:101:LEU:HA	1.81	0.46
1:A:173:G:H2'	1:A:174:U:H6	1.81	0.46
1:A:71:G:N1	1:A:74:A:OP2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:A:H2'	1:A:343:C:O4'	2.16	0.46
3:C:37:A:H2'	3:C:38:G:C8	2.51	0.46
1:A:184:C:H2'	1:A:185:U:C6	2.51	0.45
1:A:292:A:H2'	1:A:293:U:C6	2.51	0.45
1:A:268:G:C2	3:C:75:A:C2	3.04	0.45
1:A:338:G:H2'	1:A:339:A:H8	1.80	0.45
3:C:-13:G:C4	3:C:-12:G:C8	3.05	0.45
3:C:-8:U:HO2'	3:C:-7:U:H6	1.64	0.45
1:A:348:G:H3'	1:A:349:G:H8	1.81	0.45
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.45
1:A:219:C:H2'	1:A:220:C:C6	2.52	0.45
1:A:67:U:H4'	1:A:68:G:OP1	2.17	0.45
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.45
2:B:99:LYS:HD3	2:B:99:LYS:O	2.17	0.44
3:C:43:G:H3'	3:C:44:G:C2'	2.47	0.44
1:A:380:A:H2'	1:A:380:A:N3	2.32	0.44
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.44
1:A:292:A:H2'	1:A:293:U:H6	1.82	0.44
2:B:111:LEU:C	2:B:113:LYS:H	2.25	0.44
3:C:-9:U:H2'	3:C:-8:U:C6	2.53	0.44
1:A:101:U:OP2	1:A:279:C:H4'	2.17	0.44
1:A:155:A:H2'	1:A:156:C:C6	2.53	0.44
1:A:175:U:H2'	1:A:176:C:H6	1.82	0.44
1:A:175:U:H2'	1:A:176:C:C6	2.53	0.44
2:B:14:GLN:O	2:B:17:PHE:N	2.51	0.44
1:A:114:G:H2'	1:A:115:C:C6	2.52	0.44
1:A:331:G:H4'	1:A:332:A:H5'	1.99	0.44
1:A:382:G:H2'	1:A:383:G:O4'	2.18	0.44
1:A:182:C:H2'	1:A:183:C:C6	2.52	0.44
1:A:217:A:H2'	1:A:218:A:O4'	2.18	0.44
1:A:358:G:H1	1:A:366:C:H42	1.66	0.44
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.43
3:C:-10:U:C2	3:C:-9:U:C5	3.06	0.43
1:A:151:A:H2'	1:A:152:C:O4'	2.18	0.43
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.43
3:C:34:C:H2'	3:C:35:C:H6	1.83	0.43
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.43
1:A:414:C:H2'	1:A:415:G:C8	2.53	0.43
1:A:204:G:N1	1:A:235:C:N3	2.67	0.43
1:A:123:C:H2'	1:A:124:U:O4'	2.18	0.43
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LYS:O	2:B:102:ILE:HD13	2.19	0.43
3:C:18:G:C5	3:C:56:G:N2	2.86	0.43
1:A:313:C:H2'	1:A:314:G:C8	2.54	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:369:C:H2'	1:A:370:U:O4'	2.19	0.43
3:E:-12:G:H2'	3:E:-11:A:O4'	2.19	0.43
1:A:128:G:H2'	1:A:129:C:H6	1.82	0.42
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.42
1:A:95:A:H2'	1:A:96:G:H8	1.85	0.42
1:A:355:G:H2'	1:A:356:A:C8	2.53	0.42
1:A:348:G:H1'	1:A:382:G:N2	2.34	0.42
2:B:86:ARG:HH12	3:E:-13:G:H1'	1.84	0.42
1:A:95:A:H2'	1:A:96:G:C8	2.55	0.42
1:A:38:G:H2'	1:A:39:C:C6	2.55	0.42
1:A:56:U:H2'	1:A:57:G:H8	1.85	0.42
1:A:334:A:H62	2:B:10:ASN:ND2	2.17	0.42
1:A:363:A:C2'	1:A:364:A:C1'	2.93	0.42
1:A:179:U:H1'	1:A:203:G:H5'	2.02	0.42
1:A:354:C:H2'	1:A:355:G:O4'	2.19	0.42
2:B:73:GLU:N	2:B:73:GLU:OE1	2.52	0.42
1:A:115:C:H2'	1:A:116:A:H8	1.85	0.42
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.42
1:A:10:G:C6	1:A:406:A:N1	2.88	0.42
1:A:81:U:H1'	1:A:82:A:N7	2.35	0.42
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.42
1:A:260:C:H2'	1:A:261:A:O4'	2.20	0.42
1:A:324:G:H2'	1:A:325:C:H6	1.84	0.42
3:C:-10:U:H2'	3:C:-9:U:C6	2.55	0.42
1:A:75:U:O2'	1:A:76:G:P	2.78	0.41
1:A:216:A:HO2'	1:A:217:A:H8	1.67	0.41
1:A:267:U:C4	3:C:75:A:C4	3.08	0.41
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.41
1:A:335:G:C8	1:A:335:G:C3'	3.03	0.41
1:A:364:A:H3'	1:A:364:A:P	2.60	0.41
3:C:29:C:H2'	3:C:30:C:H6	1.85	0.41
1:A:117:G:H3'	1:A:118:C:H6	1.85	0.41
1:A:134:C:H2'	1:A:135:U:C6	2.56	0.41
1:A:189:A:N3	1:A:189:A:H2'	2.34	0.41
1:A:279:C:H2'	1:A:280:U:C6	2.55	0.41
3:C:21:G:OP2	3:C:21:G:H8	2.03	0.41
3:C:67:U:H2'	3:C:68:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.41
1:A:144:G:C6	1:A:145:G:C4	3.09	0.41
1:A:220:C:H2'	1:A:221:U:H6	1.85	0.41
1:A:266:A:N3	1:A:266:A:H2'	2.36	0.41
1:A:334:A:H62	2:B:10:ASN:HD22	1.68	0.41
1:A:406:A:H2'	1:A:407:U:O4'	2.20	0.41
3:C:-9:U:C2	3:C:-8:U:C5	3.09	0.41
1:A:180:U:C2'	1:A:181:A:H5'	2.51	0.41
2:B:49:LYS:HG3	3:C:-1:U:O5'	2.20	0.41
1:A:54:C:C2	1:A:395:G:C2	3.09	0.41
1:A:102:C:O5'	1:A:102:C:H6	2.03	0.41
1:A:174:U:H5"	1:A:220:C:OP1	2.21	0.41
1:A:220:C:H2'	1:A:221:U:C6	2.56	0.41
1:A:352:U:H2'	1:A:353:A:H8	1.84	0.41
1:A:353:A:H2'	1:A:354:C:O4'	2.21	0.41
1:A:397:U:H2'	1:A:398:U:C6	2.56	0.41
3:C:43:G:H3'	3:C:44:G:H3'	2.02	0.41
1:A:71:G:N2	1:A:73:G:H3'	2.36	0.41
1:A:335:G:H3'	1:A:335:G:H8	1.85	0.41
1:A:373:C:H2'	1:A:374:A:C8	2.56	0.41
1:A:380:A:C2	1:A:381:A:N9	2.89	0.40
3:C:49:C:H2'	3:C:50:G:C8	2.56	0.40
3:C:13:C:H42	3:C:21:G:H1	1.69	0.40
1:A:32:G:H3'	1:A:33:U:C6	2.57	0.40
1:A:150:A:H3'	1:A:151:A:H8	1.85	0.40
1:A:241:A:H2'	1:A:242:C:H6	1.84	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
2	B	114/116 (98%)	109 (96%)	5 (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
2	B	99/99 (100%)	93 (94%)	6 (6%)	15 35

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

Mol	Chain	Res	Type
2	B	14	GLN
2	B	71	LEU
2	B	92	MET
2	B	97	VAL
2	B	105	LEU
2	B	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN
2	B	66	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	168 (40%)	15 (3%)
3	C	88/92 (95%)	47 (53%)	7 (7%)
3	E	8/92 (8%)	5 (62%)	0
All	All	512/601 (85%)	220 (42%)	22 (4%)

All (220) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U
1	A	11	C
1	A	15	G
1	A	22	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	44	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	53	C
1	A	63	A
1	A	65	G
1	A	67	U
1	A	68	G
1	A	70	U
1	A	72	A
1	A	74	A
1	A	75	U
1	A	76	G
1	A	85	G
1	A	86	U
1	A	88	C
1	A	89	G
1	A	90	U
1	A	91	G
1	A	92	C
1	A	99	A
1	A	102	C
1	A	104	A
1	A	105	U
1	A	117	G
1	A	118	C
1	A	122	G

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Mol	Chain	Res	Type
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	134	C
1	A	137	A
1	A	138	C
1	A	139	G
1	A	147	A
1	A	150	A
1	A	151	A
1	A	152	C
1	A	155	A
1	A	156	C
1	A	157	G
1	A	158	U
1	A	159	C
1	A	163	C
1	A	172	G
1	A	173	G
1	A	174	U
1	A	175	U
1	A	177	G
1	A	179	U
1	A	180	U
1	A	181	A
1	A	182	C
1	A	183	C
1	A	186	G
1	A	187	A
1	A	188	A
1	A	189	A
1	A	190	G
1	A	192	G
1	A	196	C
1	A	199	U
1	A	202	C
1	A	203	G
1	A	204	G

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Mol	Chain	Res	Type
1	A	205	A
1	A	207	C
1	A	216	A
1	A	219	C
1	A	225	A
1	A	229	G
1	A	230	G
1	A	231	A
1	A	232	A
1	A	233	C
1	A	234	G
1	A	235	C
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	266	A
1	A	267	U
1	A	272	G
1	A	273	G
1	A	274	G
1	A	276	C
1	A	278	C
1	A	290	A
1	A	291	A
1	A	292	A
1	A	293	U
1	A	296	A
1	A	300	A
1	A	304	A
1	A	312	G
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C

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Mol	Chain	Res	Type
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	349	G
1	A	350	A
1	A	351	G
1	A	353	A
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	389	A
1	A	391	C
1	A	392	A
1	A	400	U
1	A	401	A
1	A	402	G
1	A	403	A
1	A	407	U
1	A	408	G
1	A	410	U

Continued on next page...

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Mol	Chain	Res	Type
3	C	-10	U
3	C	-8	U
3	C	-7	U
3	C	-6	C
3	C	-5	C
3	C	-4	C
3	C	-3	U
3	C	-2	U
3	C	-1	U
3	C	0	C
3	C	1	G
3	C	4	G
3	C	7	G
3	C	8	U
3	C	9	A
3	C	10	G
3	C	12	U
3	C	13	C
3	C	15	G
3	C	16	U
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	21	G
3	C	23	A
3	C	26	C
3	C	29	C
3	C	33	G
3	C	37	A
3	C	40	U
3	C	42	G
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	49	C
3	C	51	G
3	C	52	G
3	C	53	U
3	C	58	G

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Mol	Chain	Res	Type
3	C	59	U
3	C	60	C
3	C	70	G
3	C	72	U
3	C	75	A
3	E	-11	A
3	E	-10	U
3	E	-9	U
3	E	-8	U
3	E	-7	U

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	52	U
1	A	75	U
1	A	122	G
1	A	126	U
1	A	138	C
1	A	176	C
1	A	182	C
1	A	187	A
1	A	230	G
1	A	232	A
1	A	240	A
1	A	292	A
1	A	349	G
1	A	363	A
1	A	365	G
3	C	-4	C
3	C	-2	U
3	C	7	G
3	C	44	G
3	C	46	U
3	C	59	U
3	C	69	C

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 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

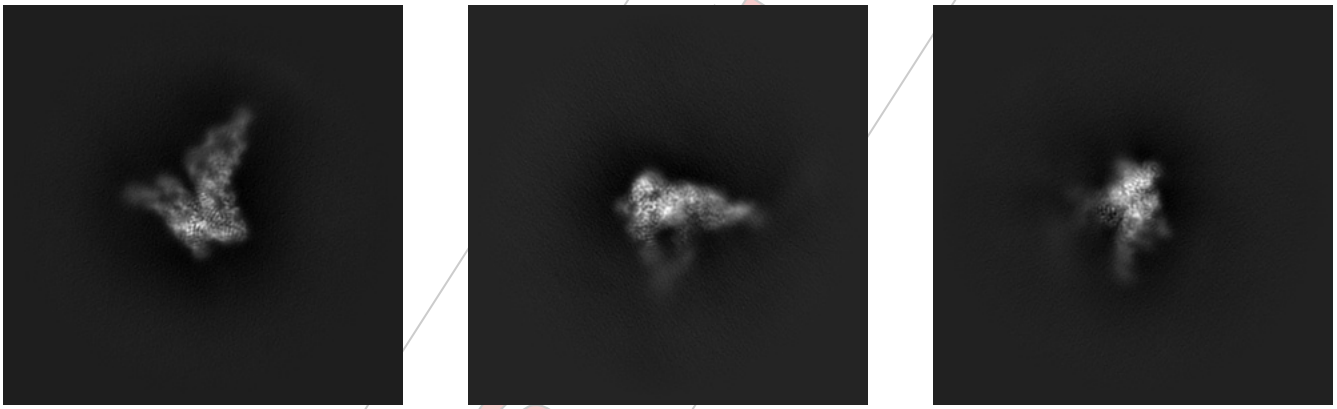
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70944. 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.

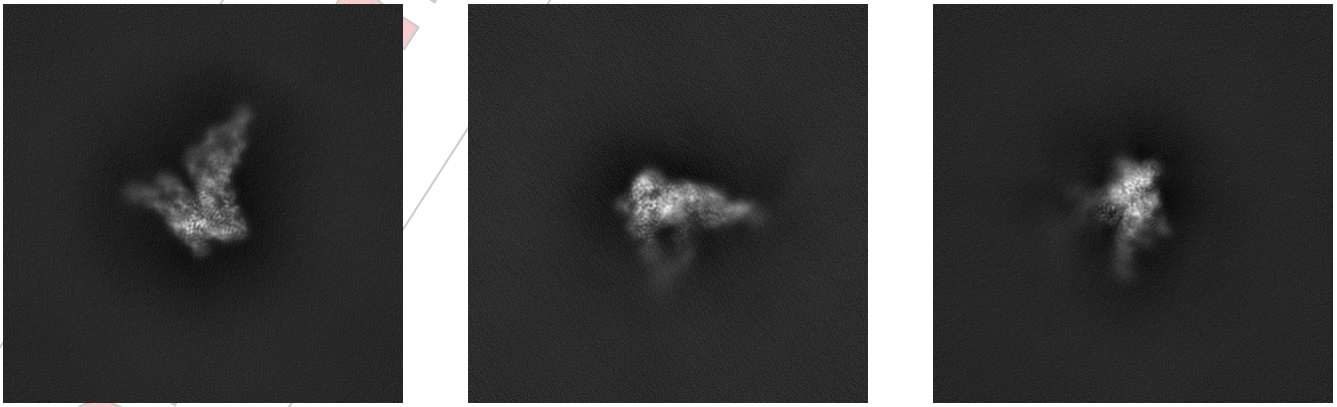
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

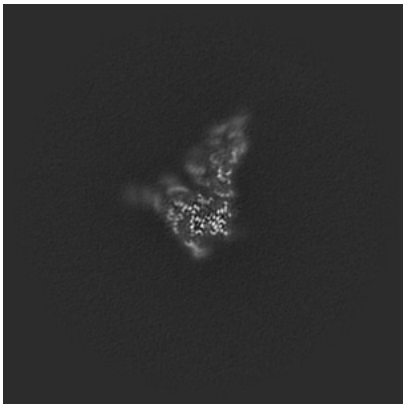


X Y Z

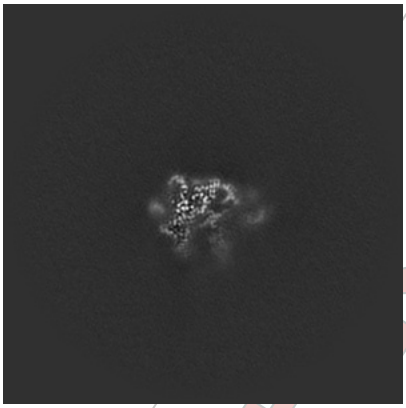
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



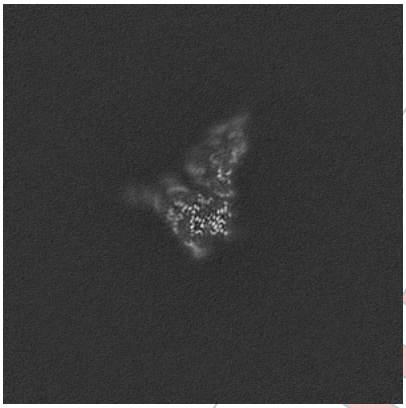
X Index: 200



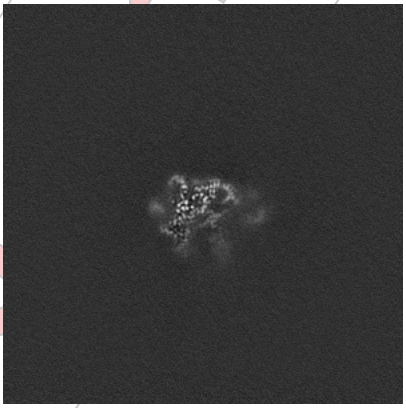
Y Index: 200

Z Index: 200

6.2.2 Raw map



X Index: 200



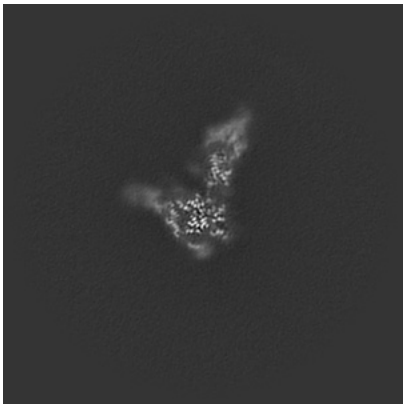
Y Index: 200

Z Index: 200

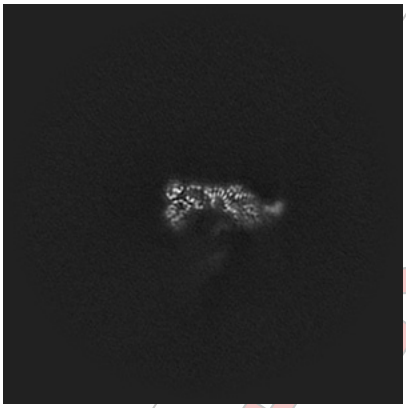
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

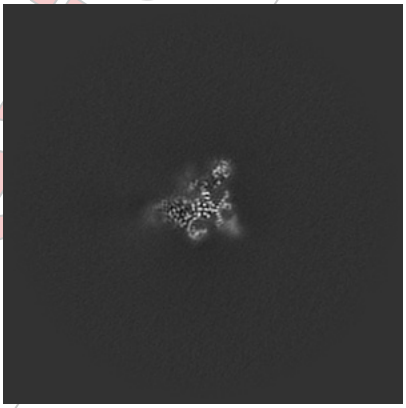
6.3.1 Primary map



X Index: 195

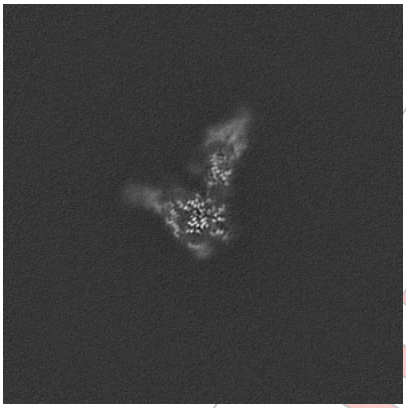


Y Index: 220

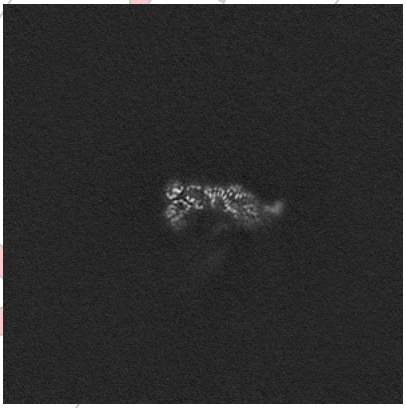


Z Index: 179

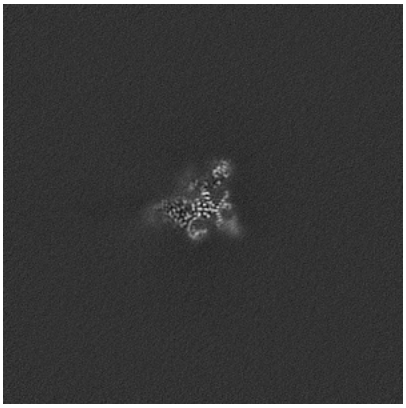
6.3.2 Raw map



X Index: 195



Y Index: 220



Z Index: 179

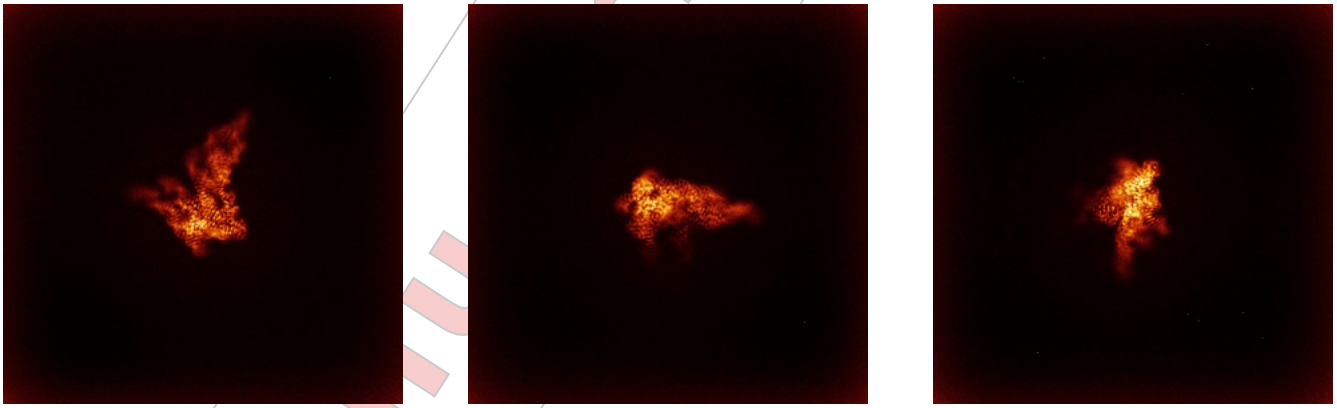
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

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 0.014. 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.

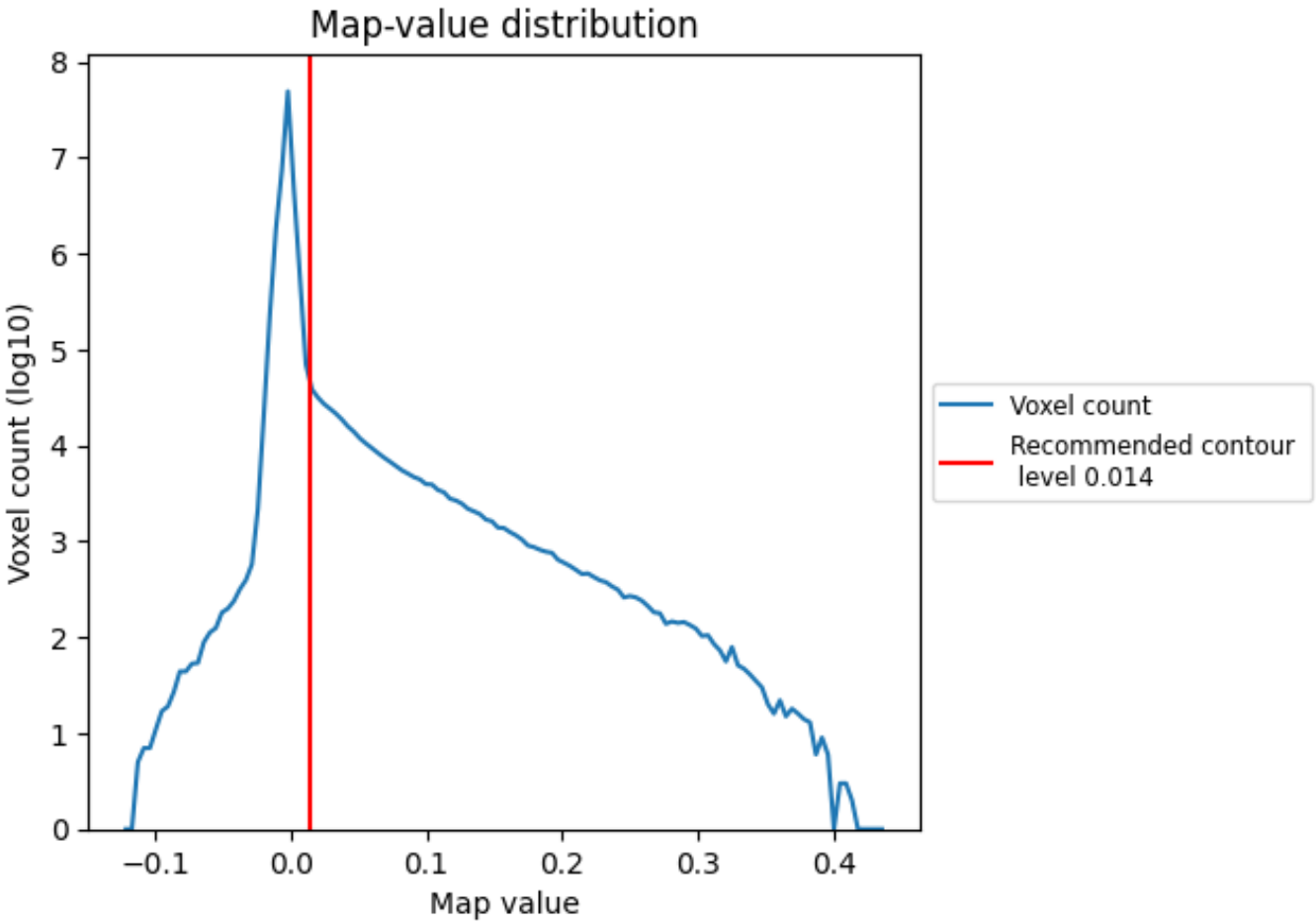
6.6 Mask visualisation (i)

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

7 Map analysis

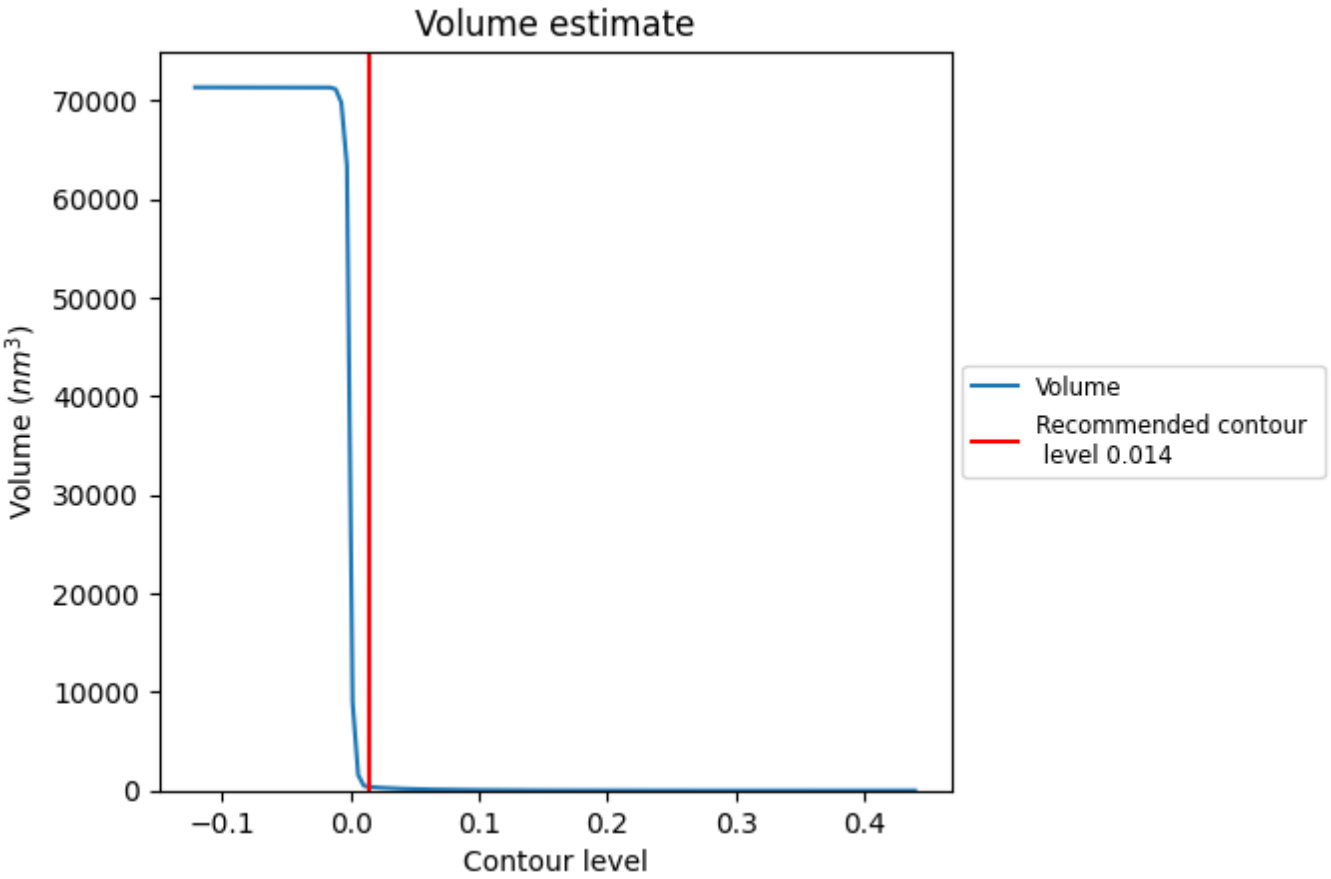
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

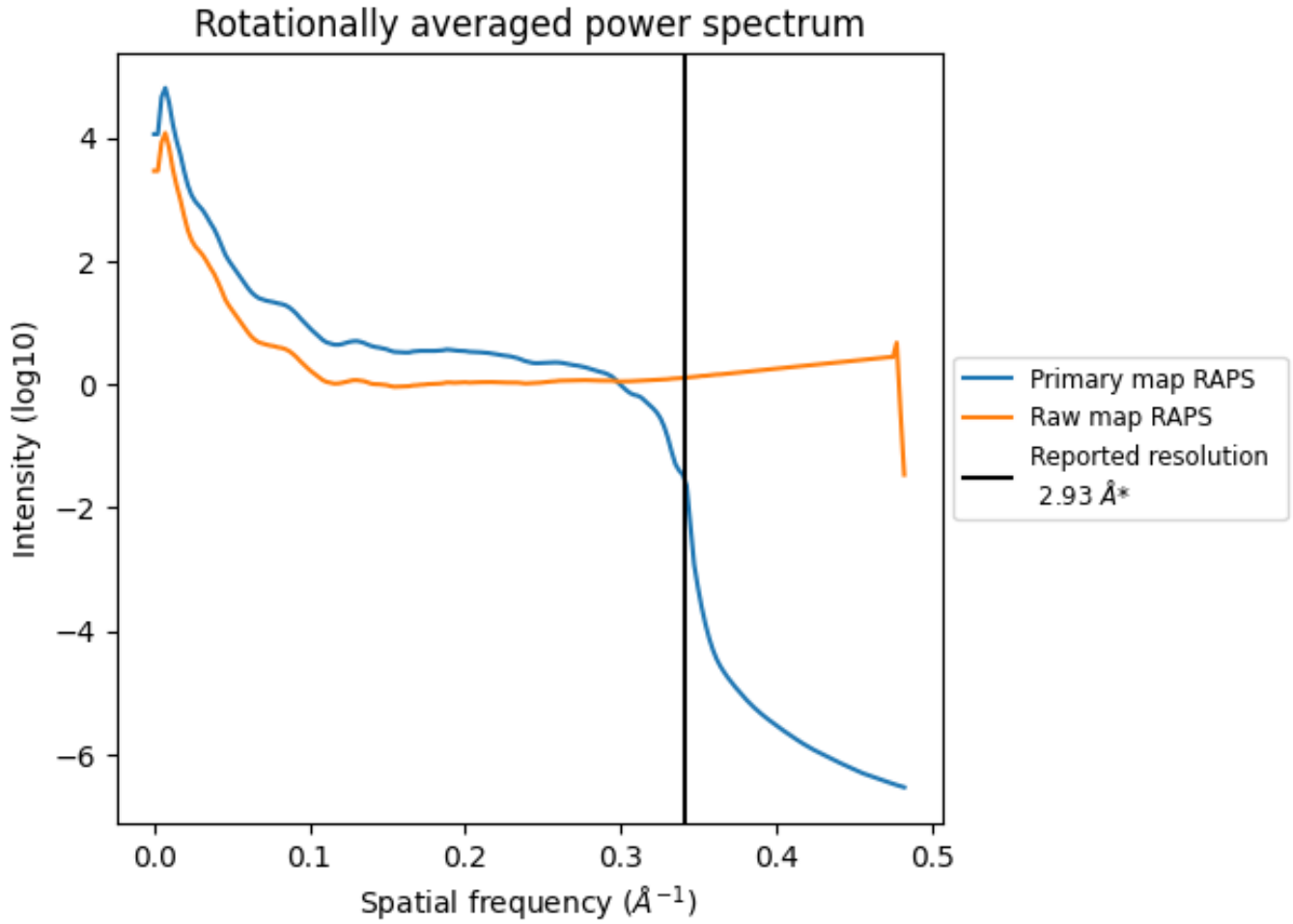
7.2 Volume estimate



The volume at the recommended contour level is 386 nm^3; this corresponds to an approximate mass of 349 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 (i)

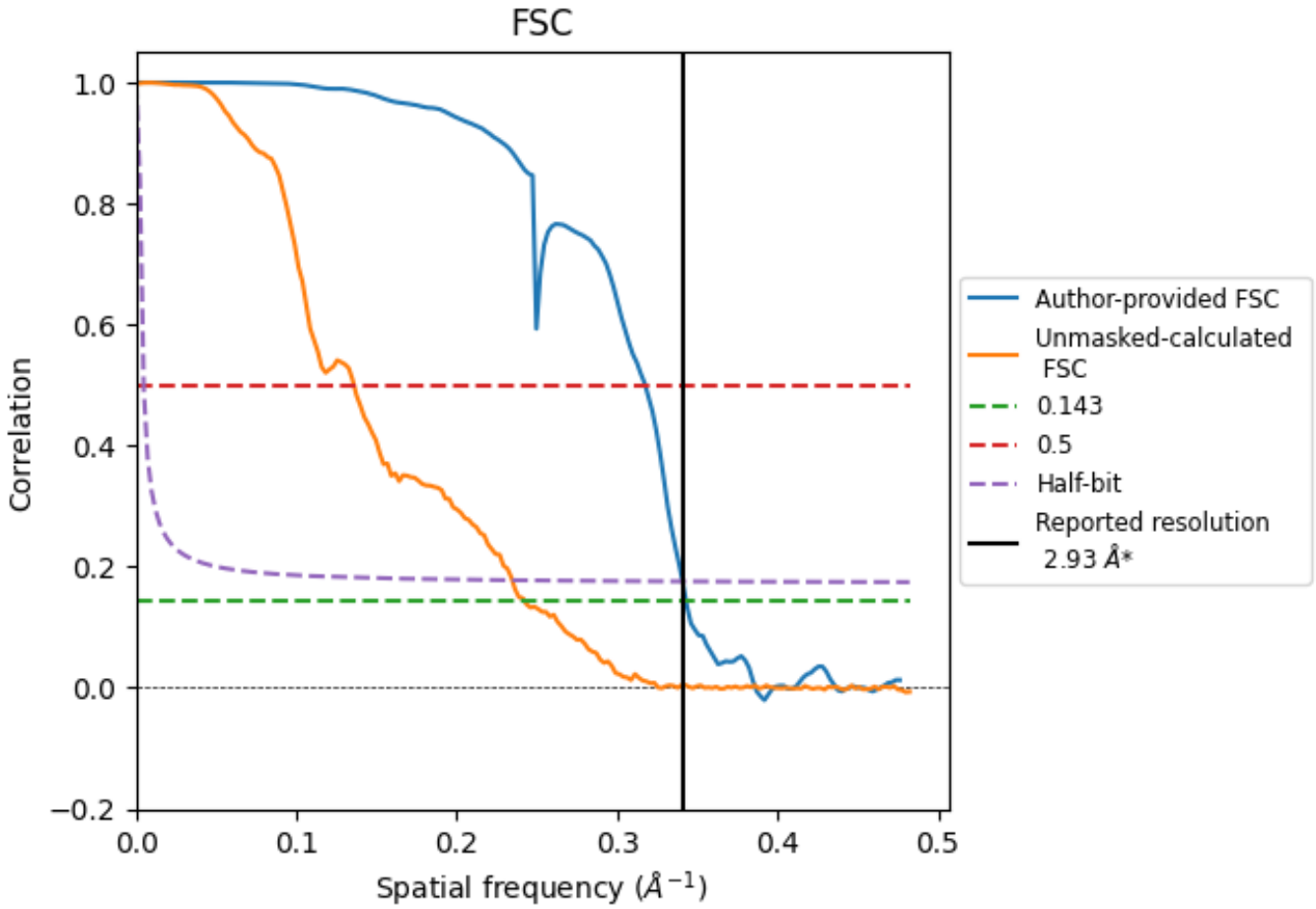


*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

8.2 Resolution estimates (i)

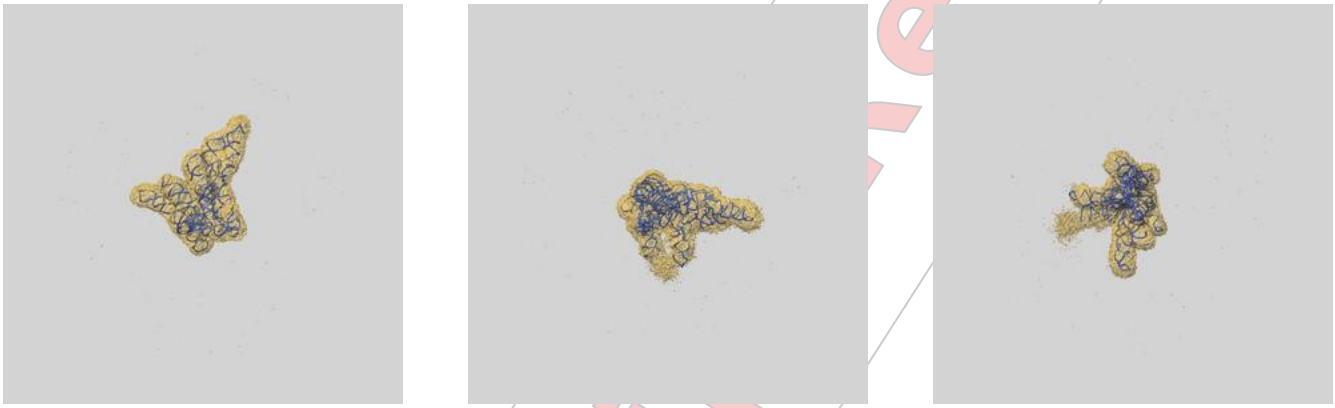
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.15	2.94
Unmasked-calculated*	4.13	7.36	4.26

*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 4.13 differs from the reported value 2.93 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70944 and PDB model 9OWU. Per-residue inclusion information can be found in section 3 on page 4.

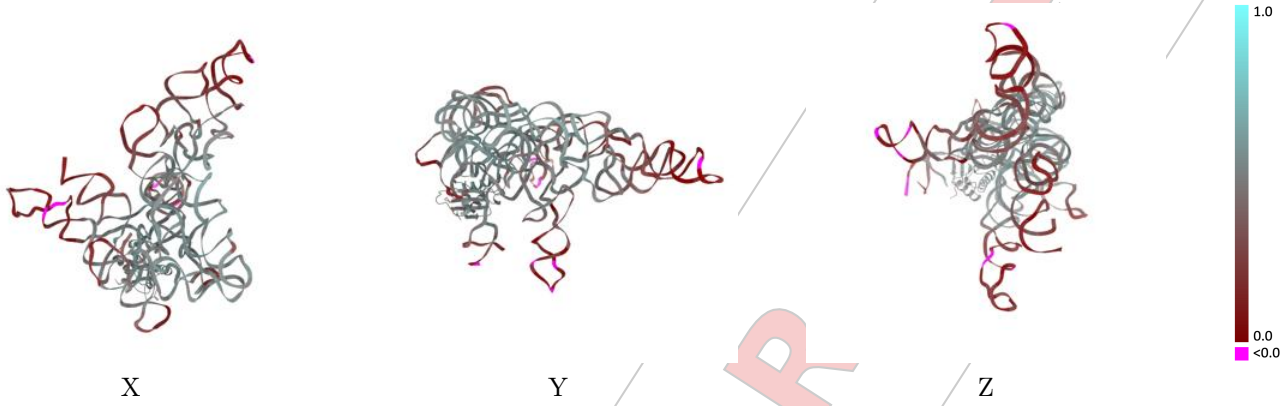
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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)



X Y Z

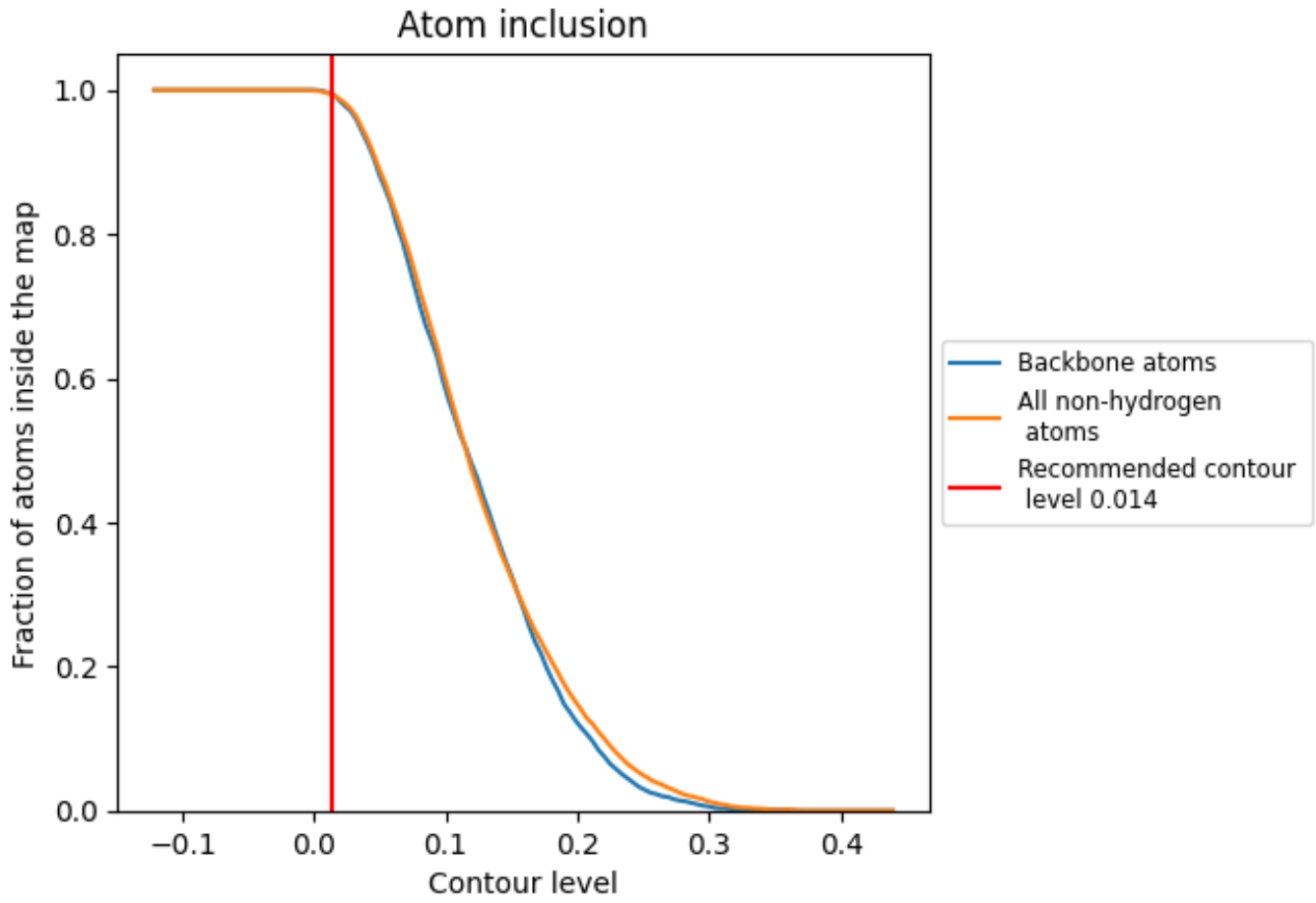
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.4020
A	1.0000	0.4040
B	0.9960	0.4990
C	0.9680	0.3590
E	0.9520	0.2500

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 04:23 PM EDT

PDB ID	:	9OWV / pdb_00009owv
EMDB ID	:	EMD-70945
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with mature tRNA in 5 mM Ca2+
Deposited on	:	2025-06-02
Resolution	:	3.02 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

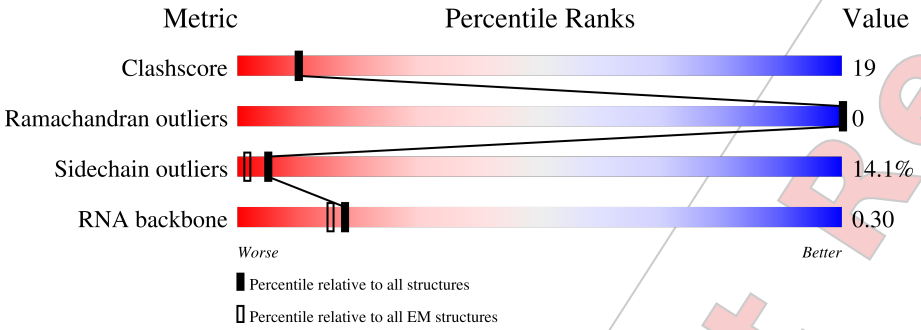
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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 <=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	417	29% 44% 26%
2	C	78	42% 45% 9%
3	B	116	60% 29% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11537 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a RNA chain called mature tRNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C	75	1601	713	285	528	75	0	0

- Molecule 3 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

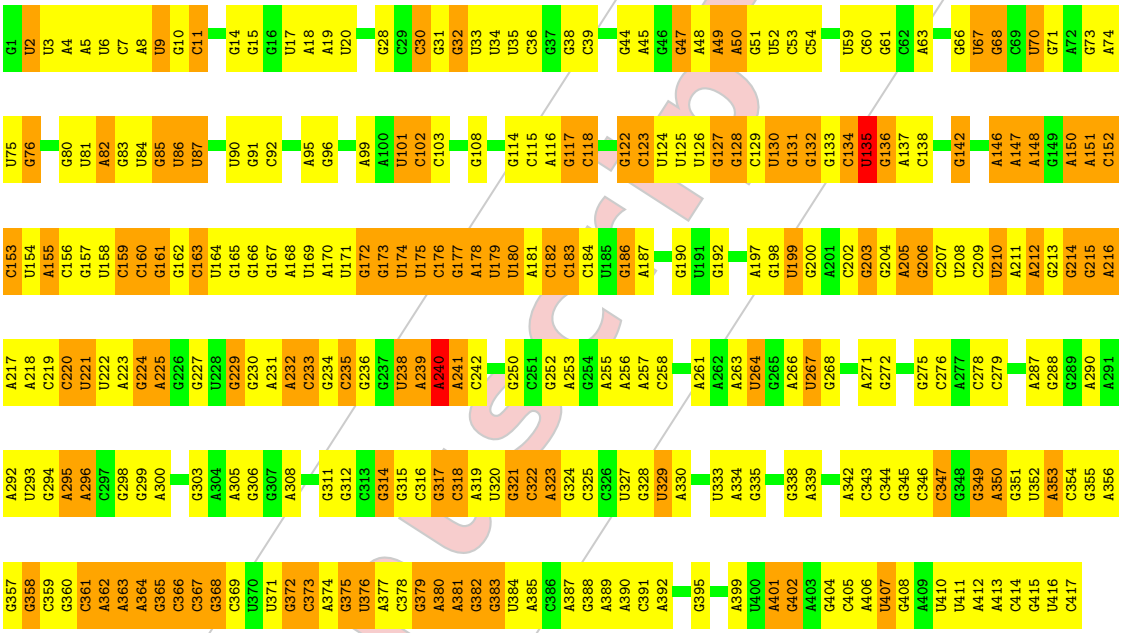
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	24	24	24	0
4	C	3	Total	Ca	0
			3	3	

3 Residue-property plots (i)

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.

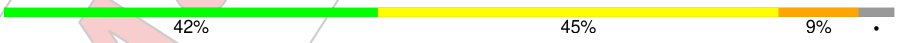
- Molecule 1: RNase P RNA (417-MER)

Chain A:



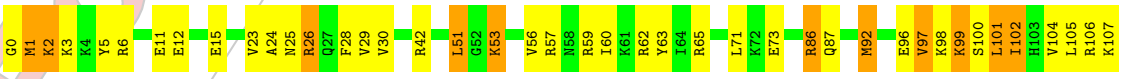
- Molecule 2: mature tRNA (75-MER)

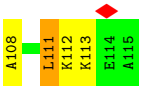
Chain C:



- Molecule 3: Ribonuclease P protein component

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.515	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.55	0/10038	0.89	7/15661 (0.0%)
2	C	0.45	0/1788	0.68	1/2786 (0.0%)
3	B	0.54	0/962	0.84	0/1281
All	All	0.54	0/12788	0.86	8/19728 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	A	C2'-C3'-O3'	-7.05	103.13	113.70
2	C	63	G	O3'-P-O5'	-6.88	93.68	104.00
1	A	49	A	O3'-P-O5'	-6.45	94.33	104.00
1	A	108	G	O3'-P-O5'	-5.96	95.07	104.00
1	A	258	C	C1'-C2'-O2'	-5.62	99.98	108.40
1	A	84	U	O3'-P-O5'	-5.48	95.78	104.00
1	A	135	U	O3'-P-O5'	5.37	112.05	104.00
1	A	328	G	O3'-P-O5'	-5.07	96.40	104.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	106	ARG	Sidechain
3	B	26	ARG	Sidechain
3	B	59	ARG	Sidechain
3	B	86	ARG	Sidechain

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	8962	0	4510	262	0
2	C	1601	0	810	23	0
3	B	947	0	1008	35	0
4	A	24	0	0	0	0
4	C	3	0	0	0	0
All	All	11537	0	6328	311	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 19.

All (311) 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:364:A:C4	1:A:365:G:H1'	1.96	1.01
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.87
1:A:349:G:H21	1:A:350:A:H62	1.24	0.85
1:A:135:U:H3'	1:A:136:G:H5"	1.60	0.83
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.82
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.81
1:A:222:U:H2'	1:A:223:A:H8	1.48	0.78
1:A:378:C:H3'	1:A:379:G:C8	2.19	0.78
1:A:174:U:H2'	1:A:175:U:C6	2.20	0.77
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.76
1:A:219:C:H2'	1:A:220:C:C6	2.20	0.75
1:A:160:C:H1'	1:A:167:G:H22	1.50	0.74
1:A:222:U:H2'	1:A:223:A:C8	2.22	0.74
1:A:219:C:H2'	1:A:220:C:H6	1.53	0.73
1:A:215:G:H1'	1:A:218:A:N6	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.73
1:A:180:U:H2'	1:A:181:A:H8	1.55	0.71
3:B:63:TYR:HB3	3:B:97:VAL:HG11	1.72	0.71
1:A:9:U:H2'	1:A:10:G:H8	1.57	0.70
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.69
1:A:45:A:H62	3:B:62:ARG:NH2	1.90	0.69
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
3:B:0:GLY:HA3	3:B:65:ARG:HB3	1.75	0.68
1:A:349:G:H22	1:A:379:G:H1'	1.58	0.68
1:A:234:G:H3'	1:A:235:C:H4'	1.76	0.68
2:C:27:C:H2'	2:C:28:A:C8	2.30	0.67
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.66
1:A:378:C:H3'	1:A:379:G:H8	1.59	0.66
2:C:27:C:H2'	2:C:28:A:H8	1.60	0.66
1:A:350:A:H1'	1:A:380:A:C2	2.31	0.65
1:A:174:U:H2'	1:A:175:U:H6	1.60	0.65
1:A:349:G:N2	1:A:379:G:H1'	2.10	0.65
3:B:30:VAL:HG21	3:B:105:LEU:HD12	1.79	0.65
1:A:374:A:H2'	1:A:375:G:C8	2.32	0.65
1:A:18:A:H2'	1:A:19:A:H8	1.62	0.65
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.65
3:B:51:LEU:HD11	3:B:86:ARG:O	1.97	0.65
1:A:349:G:N2	1:A:350:A:H62	1.93	0.63
1:A:147:A:H8	1:A:178:A:H62	1.45	0.63
1:A:314:G:H22	1:A:323:A:H2	1.43	0.62
3:B:56:VAL:O	3:B:60:ILE:HG13	1.99	0.61
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.61
1:A:174:U:H5"	1:A:220:C:P	2.40	0.61
1:A:167:G:H2'	1:A:168:A:C8	2.36	0.61
1:A:173:G:O2'	1:A:174:U:H5'	2.00	0.60
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.60
1:A:238:U:H4'	2:C:54:U:H5"	1.82	0.60
1:A:232:A:H1'	1:A:233:C:H5	1.67	0.60
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.60
1:A:350:A:H1'	1:A:380:A:N1	2.17	0.60
3:B:12:GLU:HG2	3:B:42:ARG:HH22	1.67	0.59
1:A:3:U:H2'	1:A:4:A:H8	1.67	0.59
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.59
1:A:165:G:H2'	1:A:166:G:C8	2.37	0.59
1:A:148:A:N6	1:A:177:G:H1'	2.17	0.59
1:A:379:G:H4'	1:A:380:A:H8	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:G:H22	1:A:34:U:H1'	1.68	0.58
1:A:147:A:H8	1:A:178:A:N6	2.01	0.58
1:A:379:G:H4'	1:A:380:A:C8	2.37	0.58
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.19	0.58
1:A:148:A:N6	1:A:177:G:O2'	2.36	0.57
1:A:10:G:H2'	1:A:11:C:H6	1.70	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:315:G:H2'	1:A:316:C:C6	2.40	0.57
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.56
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.56
1:A:215:G:O3'	1:A:216:A:H8	1.88	0.56
1:A:364:A:OP1	1:A:365:G:N7	2.36	0.56
3:B:23:VAL:HG21	3:B:108:ALA:HA	1.87	0.56
1:A:199:U:C5	1:A:206:G:H1'	2.41	0.56
1:A:14:G:H2'	1:A:385:A:N1	2.21	0.56
1:A:45:A:H62	3:B:62:ARG:HH22	1.54	0.56
1:A:152:C:O2	1:A:173:G:N1	2.37	0.56
2:C:14:A:H3'	2:C:15:G:H8	1.70	0.56
1:A:199:U:H5	1:A:206:G:H1'	1.71	0.56
3:B:92:MET:HB3	3:B:97:VAL:HG23	1.88	0.56
1:A:364:A:H3'	1:A:364:A:OP2	2.05	0.55
2:C:26:C:H1'	2:C:43:G:H22	1.72	0.55
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.55
1:A:47:G:H1	1:A:385:A:H62	1.55	0.55
1:A:5:A:H2'	1:A:6:U:H6	1.72	0.55
1:A:59:U:H2'	1:A:60:C:C6	2.42	0.55
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.55
1:A:85:G:O2'	1:A:87:U:O4	2.23	0.55
1:A:221:U:H2'	1:A:222:U:C6	2.42	0.54
1:A:287:A:H2'	1:A:288:G:O4'	2.08	0.54
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.54
1:A:212:A:H2'	1:A:213:G:O4'	2.07	0.54
2:C:28:A:H2'	2:C:29:C:O4'	2.06	0.54
1:A:215:G:H2'	1:A:216:A:O2'	2.06	0.54
1:A:412:A:H2'	1:A:413:A:C8	2.41	0.54
3:B:23:VAL:HG11	3:B:107:LYS:O	2.07	0.54
1:A:5:A:H2'	1:A:6:U:C6	2.42	0.54
1:A:214:G:H3'	1:A:215:G:H8	1.72	0.54
1:A:220:C:H2'	1:A:221:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.53
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.53
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.52
1:A:170:A:C2	1:A:171:U:H1'	2.44	0.52
1:A:349:G:O6	1:A:379:G:N2	2.42	0.52
1:A:387:A:OP1	3:B:53:LYS:HD3	2.10	0.52
1:A:290:A:C2	1:A:295:A:C5	2.98	0.52
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.52
1:A:85:G:H1'	1:A:86:U:H5	1.75	0.52
1:A:168:A:H2'	1:A:169:U:C6	2.44	0.52
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.52
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.51
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.51
3:B:23:VAL:HB	3:B:108:ALA:HB2	1.92	0.51
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.51
1:A:54:C:C2	1:A:395:G:C2	2.98	0.51
1:A:155:A:N6	1:A:168:A:N7	2.58	0.51
1:A:240:A:H2	2:C:52:G:N3	2.09	0.51
2:C:37:A:H2'	2:C:38:G:C8	2.46	0.51
1:A:147:A:H5"	1:A:177:G:H22	1.75	0.51
1:A:401:A:H2'	1:A:402:G:O4'	2.11	0.51
1:A:174:U:C5'	1:A:220:C:H5'	2.41	0.51
1:A:183:C:H2'	1:A:184:C:C6	2.46	0.51
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.51
2:C:26:C:H1'	2:C:43:G:N2	2.26	0.51
1:A:317:G:N1	1:A:321:G:C2	2.79	0.50
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.50
1:A:142:G:H4'	1:A:142:G:OP1	2.10	0.50
1:A:153:C:H2'	1:A:154:U:C2	2.46	0.50
1:A:186:G:H8	1:A:186:G:H5"	1.77	0.50
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.50
1:A:156:C:N4	1:A:169:U:O4	2.44	0.50
1:A:373:C:H2'	1:A:374:A:C8	2.47	0.50
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.50
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.50
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.50
1:A:344:C:H2'	1:A:345:G:C8	2.47	0.50
1:A:349:G:H4'	1:A:350:A:H5'	1.94	0.50
1:A:388:G:OP2	3:B:53:LYS:HB2	2.12	0.49
1:A:161:G:H4'	1:A:163:C:C5	2.48	0.49
1:A:203:G:C5	1:A:205:A:H1'	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:U:H2'	1:A:222:U:H6	1.77	0.49
1:A:216:A:O2'	1:A:217:A:H8	1.96	0.49
1:A:182:C:H2'	1:A:183:C:C6	2.48	0.48
2:C:42:G:H2'	2:C:43:G:C8	2.48	0.48
1:A:150:A:H2'	1:A:151:A:C8	2.48	0.48
1:A:169:U:H2'	1:A:170:A:H8	1.78	0.48
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.48
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.48
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.48
1:A:132:G:H3'	1:A:133:G:H8	1.79	0.48
3:B:23:VAL:HG11	3:B:107:LYS:C	2.38	0.48
1:A:171:U:O2	1:A:216:A:N6	2.46	0.48
1:A:174:U:H5"	1:A:219:C:O3'	2.13	0.48
2:C:69:C:H2'	2:C:70:G:C8	2.48	0.48
1:A:19:A:H2'	1:A:20:U:C6	2.48	0.48
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.48
1:A:82:A:H2'	1:A:83:G:O4'	2.13	0.48
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.48
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.48
1:A:411:U:H2'	1:A:412:A:C8	2.48	0.48
2:C:26:C:H2'	2:C:27:C:C6	2.49	0.48
1:A:71:G:H1'	1:A:295:A:H2	1.78	0.48
1:A:371:U:H4'	1:A:373:C:H5	1.79	0.48
1:A:177:G:H3'	1:A:178:A:C8	2.49	0.47
1:A:347:C:H1'	1:A:383:G:N2	2.29	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
3:B:96:GLU:O	3:B:99:LYS:N	2.47	0.47
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.47
1:A:172:G:C4	1:A:173:G:C8	3.03	0.47
2:C:14:A:H3'	2:C:15:G:C8	2.50	0.47
3:B:112:LYS:O	3:B:113:LYS:C	2.58	0.47
1:A:176:C:H2'	1:A:177:G:C8	2.50	0.47
1:A:376:U:H2'	1:A:377:A:C8	2.49	0.47
1:A:267:U:C2	2:C:75:A:C2	3.02	0.47
1:A:293:U:H2'	1:A:294:G:O4'	2.15	0.47
1:A:350:A:C1'	1:A:380:A:N1	2.78	0.47
1:A:153:C:HO2'	1:A:218:A:HO2'	1.57	0.46
1:A:181:A:H3'	1:A:182:C:C6	2.50	0.46
1:A:352:U:H2'	1:A:353:A:C8	2.51	0.46
1:A:210:U:H2'	1:A:211:A:O4'	2.16	0.46
3:B:111:LEU:C	3:B:113:LYS:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:A:H1'	1:A:216:A:C2	2.51	0.46
1:A:151:A:H2'	1:A:152:C:O4'	2.16	0.46
1:A:308:A:N1	1:A:329:U:H5	2.14	0.46
1:A:220:C:C2	1:A:221:U:C5	3.04	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.45
1:A:338:G:H2'	1:A:339:A:H8	1.80	0.45
3:B:53:LYS:O	3:B:57:ARG:HG3	2.16	0.45
1:A:268:G:C6	2:C:75:A:N1	2.84	0.45
3:B:24:ALA:HB2	3:B:29:VAL:HG13	1.98	0.45
1:A:148:A:H62	1:A:177:G:H1'	1.82	0.45
1:A:76:G:N3	1:A:296:A:H2	2.15	0.45
1:A:151:A:C2	1:A:152:C:H1'	2.51	0.45
3:B:25:ASN:CG	3:B:104:VAL:HB	2.41	0.45
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.45
1:A:50:A:N3	1:A:50:A:H2'	2.31	0.45
1:A:199:U:H3	1:A:227:G:N2	2.15	0.45
1:A:404:G:H2'	1:A:405:C:O4'	2.17	0.45
1:A:87:U:H6	1:A:87:U:O5'	2.00	0.45
1:A:239:A:H4'	1:A:241:A:C5'	2.47	0.45
2:C:21:G:H2'	2:C:22:A:C8	2.52	0.45
3:B:111:LEU:C	3:B:113:LYS:H	2.25	0.45
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.44
3:B:100:SER:O	3:B:101:LEU:C	2.59	0.44
3:B:2:LYS:HE3	3:B:2:LYS:HB3	1.38	0.44
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.44
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.44
3:B:28:PHE:HB2	3:B:104:VAL:HG11	2.00	0.44
1:A:181:A:H3'	1:A:182:C:H6	1.83	0.44
2:C:34:C:H2'	2:C:35:C:H6	1.82	0.44
1:A:102:C:H2'	1:A:103:C:O4'	2.18	0.44
1:A:175:U:H2'	1:A:176:C:H6	1.82	0.44
1:A:60:C:H2'	1:A:61:G:H8	1.82	0.44
1:A:128:G:H2'	1:A:129:C:H6	1.82	0.44
1:A:173:G:H2'	1:A:174:U:H6	1.82	0.44
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.44
2:C:29:C:H2'	2:C:30:C:C6	2.51	0.44
1:A:114:G:H2'	1:A:115:C:C6	2.52	0.44
1:A:175:U:H2'	1:A:176:C:C6	2.53	0.44
1:A:350:A:C8	1:A:380:A:C6	3.06	0.44
2:C:21:G:H2'	2:C:22:A:H8	1.83	0.44
1:A:134:C:H2'	1:A:135:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:A:H2'	1:A:380:A:N3	2.32	0.44
1:A:382:G:H2'	1:A:383:G:O4'	2.18	0.44
3:B:12:GLU:HG2	3:B:42:ARG:NH2	2.32	0.44
1:A:101:U:OP2	1:A:279:C:H4'	2.17	0.43
1:A:358:G:H1	1:A:366:C:H42	1.66	0.43
1:A:17:U:H2'	1:A:18:A:H8	1.82	0.43
1:A:152:C:H2'	1:A:153:C:O4'	2.18	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.43
1:A:173:G:O2'	1:A:219:C:O2'	2.26	0.43
1:A:177:G:H2'	1:A:178:A:N7	2.34	0.43
1:A:355:G:H2'	1:A:356:A:C8	2.54	0.43
3:B:11:GLU:O	3:B:15:GLU:HG3	2.19	0.43
1:A:154:U:H2'	1:A:155:A:C4	2.54	0.43
1:A:354:C:H2'	1:A:355:G:O4'	2.19	0.43
1:A:68:G:N3	1:A:68:G:H2'	2.34	0.43
3:B:51:LEU:HD13	3:B:51:LEU:HA	1.67	0.43
3:B:73:GLU:OE1	3:B:73:GLU:N	2.52	0.43
1:A:166:G:H2'	1:A:167:G:C8	2.54	0.43
1:A:214:G:N2	1:A:218:A:H61	2.17	0.43
1:A:171:U:C2	1:A:172:G:C8	3.07	0.43
1:A:200:G:C6	1:A:232:A:C5	3.07	0.43
3:B:1:MET:HB3	3:B:1:MET:HE3	1.68	0.42
1:A:224:G:H3'	1:A:225:A:H5"	2.01	0.42
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.42
3:B:3:LYS:C	3:B:5:TYR:N	2.78	0.42
1:A:216:A:O2'	1:A:217:A:OP2	2.33	0.42
1:A:252:G:H2'	1:A:253:A:O4'	2.20	0.42
1:A:95:A:H2'	1:A:96:G:C8	2.55	0.42
1:A:239:A:H4'	1:A:241:A:H5"	2.01	0.42
1:A:343:C:H2'	1:A:344:C:C6	2.54	0.42
1:A:349:G:N2	1:A:378:C:C2	2.88	0.42
1:A:406:A:H2'	1:A:407:U:O4'	2.20	0.42
3:B:53:LYS:H	3:B:53:LYS:HG2	1.54	0.42
1:A:17:U:H2'	1:A:18:A:C8	2.55	0.42
1:A:123:C:H2'	1:A:124:U:O4'	2.19	0.42
1:A:146:A:OP1	1:A:146:A:H4'	2.19	0.42
1:A:199:U:H5	1:A:206:G:N3	2.18	0.42
1:A:344:C:H2'	1:A:345:G:H8	1.85	0.42
2:C:9:A:H5'	2:C:45:G:H21	1.85	0.42
1:A:180:U:O2'	1:A:181:A:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:A:O5'	1:A:263:A:H8	2.02	0.42
1:A:298:G:O2'	1:A:299:G:H5'	2.20	0.42
1:A:363:A:O2'	1:A:364:A:O4'	2.32	0.42
1:A:208:U:H2'	1:A:209:C:O4'	2.20	0.42
1:A:311:G:C8	1:A:311:G:H5"	2.54	0.42
1:A:95:A:H2'	1:A:96:G:H8	1.85	0.41
1:A:133:G:C2'	1:A:134:C:H5'	2.50	0.41
1:A:363:A:C2'	1:A:364:A:C1'	2.93	0.41
1:A:10:G:C6	1:A:406:A:N1	2.88	0.41
1:A:19:A:H2'	1:A:20:U:H6	1.85	0.41
1:A:38:G:H2'	1:A:39:C:C6	2.55	0.41
1:A:147:A:N6	1:A:177:G:O2'	2.53	0.41
1:A:209:C:H2'	1:A:210:U:C6	2.55	0.41
1:A:215:G:O2'	1:A:217:A:N7	2.52	0.41
1:A:239:A:H5'	1:A:241:A:H5"	2.00	0.41
1:A:59:U:H2'	1:A:60:C:H6	1.84	0.41
1:A:171:U:H2'	1:A:172:G:C8	2.56	0.41
1:A:229:G:N2	1:A:231:A:H3'	2.35	0.41
2:C:39:G:H2'	2:C:40:U:C6	2.55	0.41
1:A:153:C:O2'	1:A:218:A:O2'	2.29	0.41
1:A:220:C:H2'	1:A:221:U:H6	1.83	0.41
1:A:364:A:H3'	1:A:364:A:P	2.60	0.41
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.41
1:A:350:A:C4	1:A:380:A:C5	3.09	0.41
1:A:14:G:C2'	1:A:401:A:H61	2.33	0.41
1:A:151:A:C2	1:A:175:U:C2	3.09	0.41
1:A:350:A:C4	1:A:380:A:C4	3.09	0.41
1:A:414:C:H2'	1:A:415:G:C8	2.53	0.41
1:A:102:C:H2'	1:A:103:C:C6	2.56	0.41
1:A:311:G:H5"	1:A:311:G:H8	1.85	0.41
1:A:263:A:H2'	1:A:264:U:O4'	2.21	0.41
1:A:160:C:C2'	1:A:166:G:H1	2.34	0.41
3:B:111:LEU:HA	3:B:111:LEU:HD22	1.80	0.41
1:A:267:U:C4	2:C:75:A:C4	3.09	0.41
1:A:67:U:H1'	1:A:68:G:C8	2.57	0.40
1:A:117:G:H3'	1:A:118:C:H6	1.86	0.40
1:A:179:U:H1'	1:A:203:G:H5'	2.04	0.40
1:A:215:G:N2	1:A:217:A:H3'	2.36	0.40
1:A:363:A:C8	1:A:363:A:C5'	3.03	0.40
1:A:9:U:C2	1:A:10:G:C8	3.09	0.40
1:A:102:C:H2'	1:A:103:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:A:O5'	1:A:218:A:H8	2.05	0.40
1:A:272:G:C8	1:A:272:G:H5"	2.57	0.40
1:A:363:A:H2'	1:A:364:A:C5	2.56	0.40
2:C:35:C:H2'	2:C:36:A:O4'	2.20	0.40
1:A:353:A:H2'	1:A:354:C:O4'	2.21	0.40
3:B:3:LYS:O	3:B:6:ARG:N	2.43	0.40
1:A:158:U:H2'	1:A:159:C:C6	2.57	0.40
1:A:377:A:H3'	1:A:378:C:H6	1.86	0.40
3:B:101:LEU:O	3:B:102:ILE:C	2.65	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
3	B	114/116 (98%)	106 (93%)	8 (7%)	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
3	B	99/99 (100%)	85 (86%)	14 (14%)	3 12

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	1	MET
3	B	2	LYS
3	B	26	ARG
3	B	51	LEU
3	B	53	LYS
3	B	71	LEU
3	B	87	GLN
3	B	92	MET
3	B	97	VAL
3	B	98	LYS
3	B	99	LYS
3	B	101	LEU
3	B	102	ILE
3	B	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	10	ASN
3	B	14	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	183 (43%)	21 (5%)
2	C	74/78 (94%)	22 (29%)	2 (2%)
All	All	490/495 (98%)	205 (41%)	23 (4%)

All (205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U
1	A	11	C
1	A	15	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U

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Mol	Chain	Res	Type
1	A	35	U
1	A	36	C
1	A	44	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	53	C
1	A	63	A
1	A	66	G
1	A	67	U
1	A	68	G
1	A	70	U
1	A	74	A
1	A	75	U
1	A	76	G
1	A	80	G
1	A	81	U
1	A	82	A
1	A	85	G
1	A	86	U
1	A	87	U
1	A	90	U
1	A	91	G
1	A	92	C
1	A	99	A
1	A	101	U
1	A	102	C
1	A	117	G
1	A	118	C
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	134	C
1	A	135	U

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Mol	Chain	Res	Type
1	A	136	G
1	A	137	A
1	A	138	C
1	A	142	G
1	A	146	A
1	A	147	A
1	A	148	A
1	A	150	A
1	A	151	A
1	A	152	C
1	A	153	C
1	A	155	A
1	A	157	G
1	A	159	C
1	A	160	C
1	A	161	G
1	A	162	G
1	A	163	C
1	A	164	U
1	A	172	G
1	A	173	G
1	A	174	U
1	A	175	U
1	A	177	G
1	A	178	A
1	A	179	U
1	A	180	U
1	A	182	C
1	A	183	C
1	A	186	G
1	A	187	A
1	A	190	G
1	A	192	G
1	A	197	A
1	A	198	G
1	A	199	U
1	A	202	C
1	A	203	G
1	A	204	G
1	A	205	A
1	A	207	C
1	A	210	U

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Mol	Chain	Res	Type
1	A	212	A
1	A	214	G
1	A	215	G
1	A	216	A
1	A	220	C
1	A	221	U
1	A	224	G
1	A	225	A
1	A	229	G
1	A	230	G
1	A	232	A
1	A	233	C
1	A	235	C
1	A	236	G
1	A	238	U
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	261	A
1	A	264	U
1	A	266	A
1	A	267	U
1	A	271	A
1	A	275	G
1	A	276	C
1	A	278	C
1	A	292	A
1	A	295	A
1	A	296	A
1	A	300	A
1	A	303	G
1	A	305	A
1	A	306	G
1	A	312	G
1	A	314	G
1	A	317	G
1	A	318	C

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Mol	Chain	Res	Type
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	325	C
1	A	327	U
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	335	G
1	A	342	A
1	A	346	C
1	A	347	C
1	A	349	G
1	A	350	A
1	A	351	G
1	A	353	A
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	389	A
1	A	390	A
1	A	391	C

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Mol	Chain	Res	Type
1	A	392	A
1	A	399	A
1	A	401	A
1	A	402	G
1	A	407	U
1	A	408	G
1	A	410	U
2	C	4	G
2	C	10	G
2	C	11	U
2	C	12	U
2	C	13	C
2	C	14	A
2	C	16	U
2	C	17	G
2	C	18	G
2	C	20	A
2	C	23	A
2	C	26	C
2	C	27	C
2	C	33	G
2	C	37	A
2	C	44	G
2	C	45	G
2	C	46	U
2	C	47	C
2	C	58	G
2	C	59	U
2	C	75	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	50	A
1	A	52	U
1	A	67	U
1	A	75	U
1	A	85	G
1	A	91	G
1	A	101	U
1	A	122	G
1	A	126	U

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Mol	Chain	Res	Type
1	A	136	G
1	A	176	C
1	A	206	G
1	A	232	A
1	A	233	C
1	A	255	A
1	A	271	A
1	A	334	A
1	A	349	G
1	A	363	A
1	A	365	G
1	A	389	A
2	C	15	G
2	C	46	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 27 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

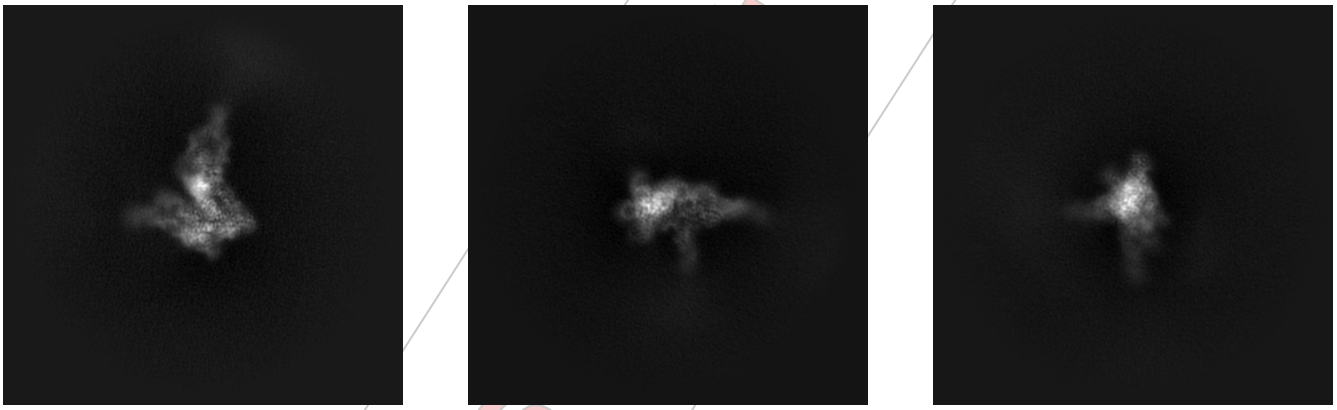
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70945. 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.

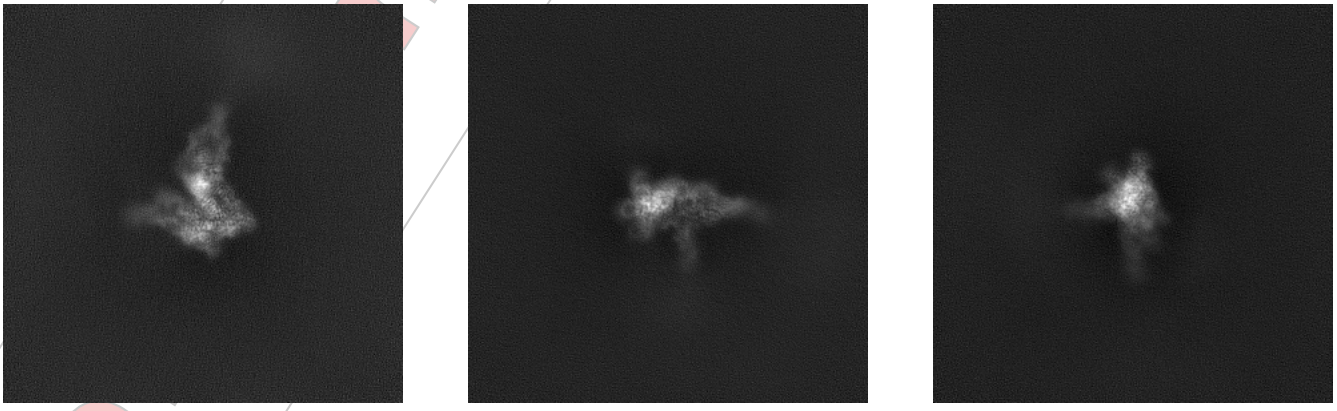
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

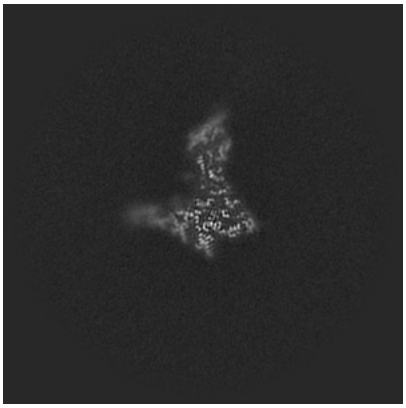


X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map

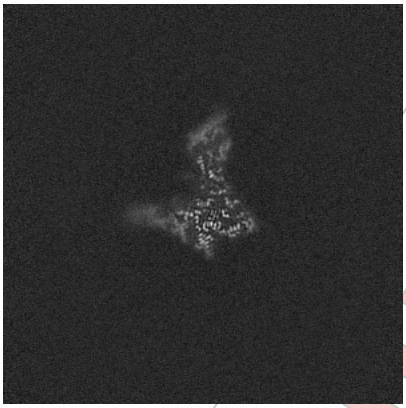


X Index: 200

Y Index: 200

Z Index: 200

6.2.2 Raw map



X Index: 200

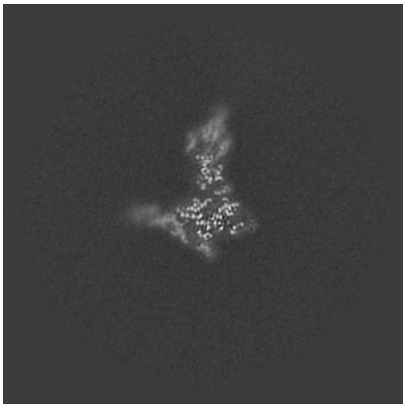
Y Index: 200

Z Index: 200

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

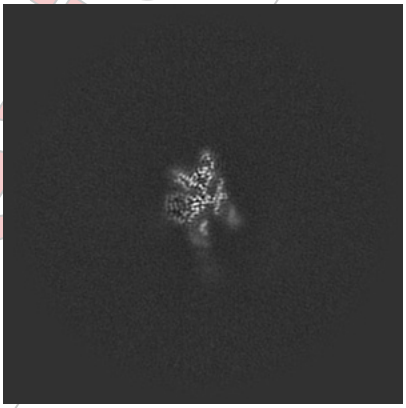
6.3 Largest variance slices (i)

6.3.1 Primary map



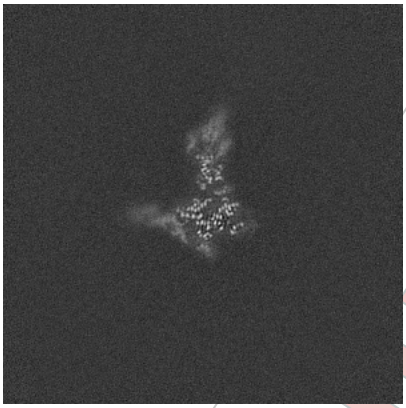
X Index: 197

Y Index: 199

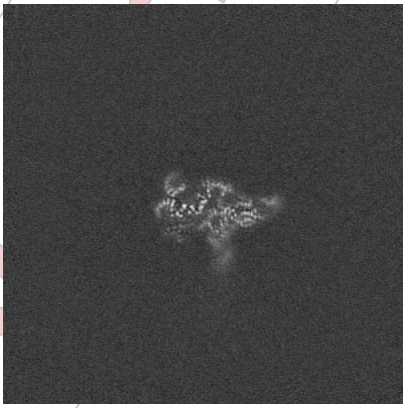


Z Index: 175

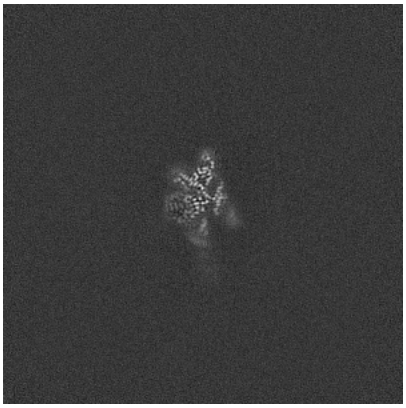
6.3.2 Raw map



X Index: 197



Y Index: 198

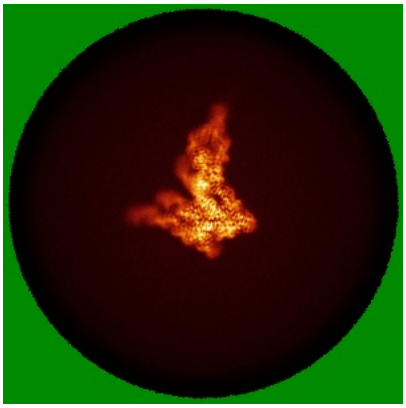


Z Index: 176

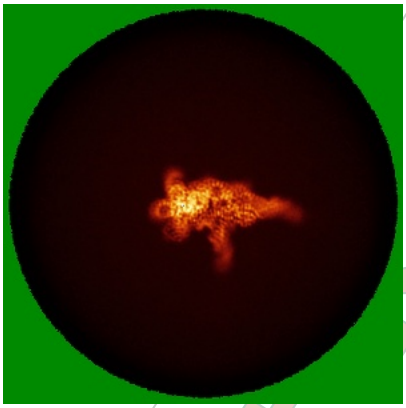
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

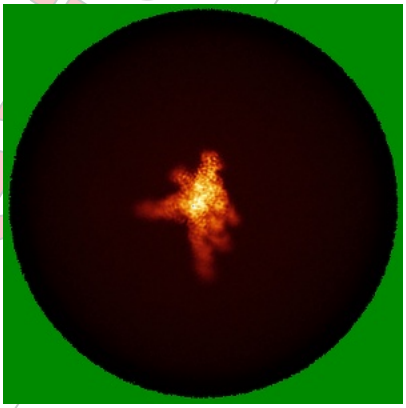
6.4.1 Primary map



X

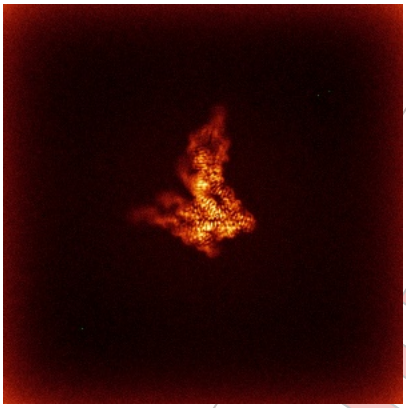


Y

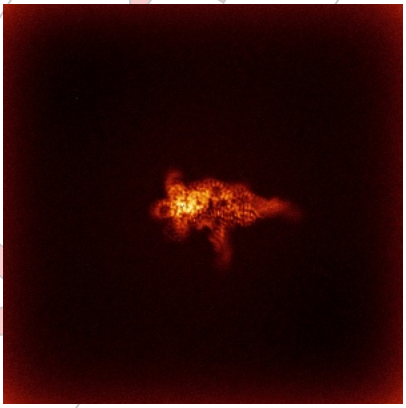


Z

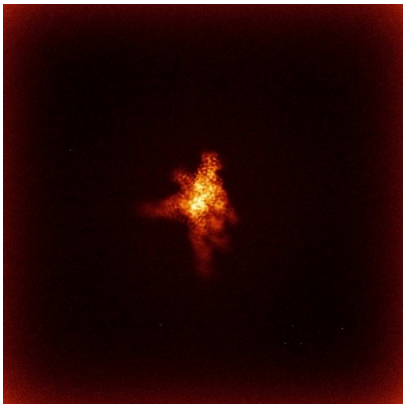
6.4.2 Raw map



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 0.03. 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.

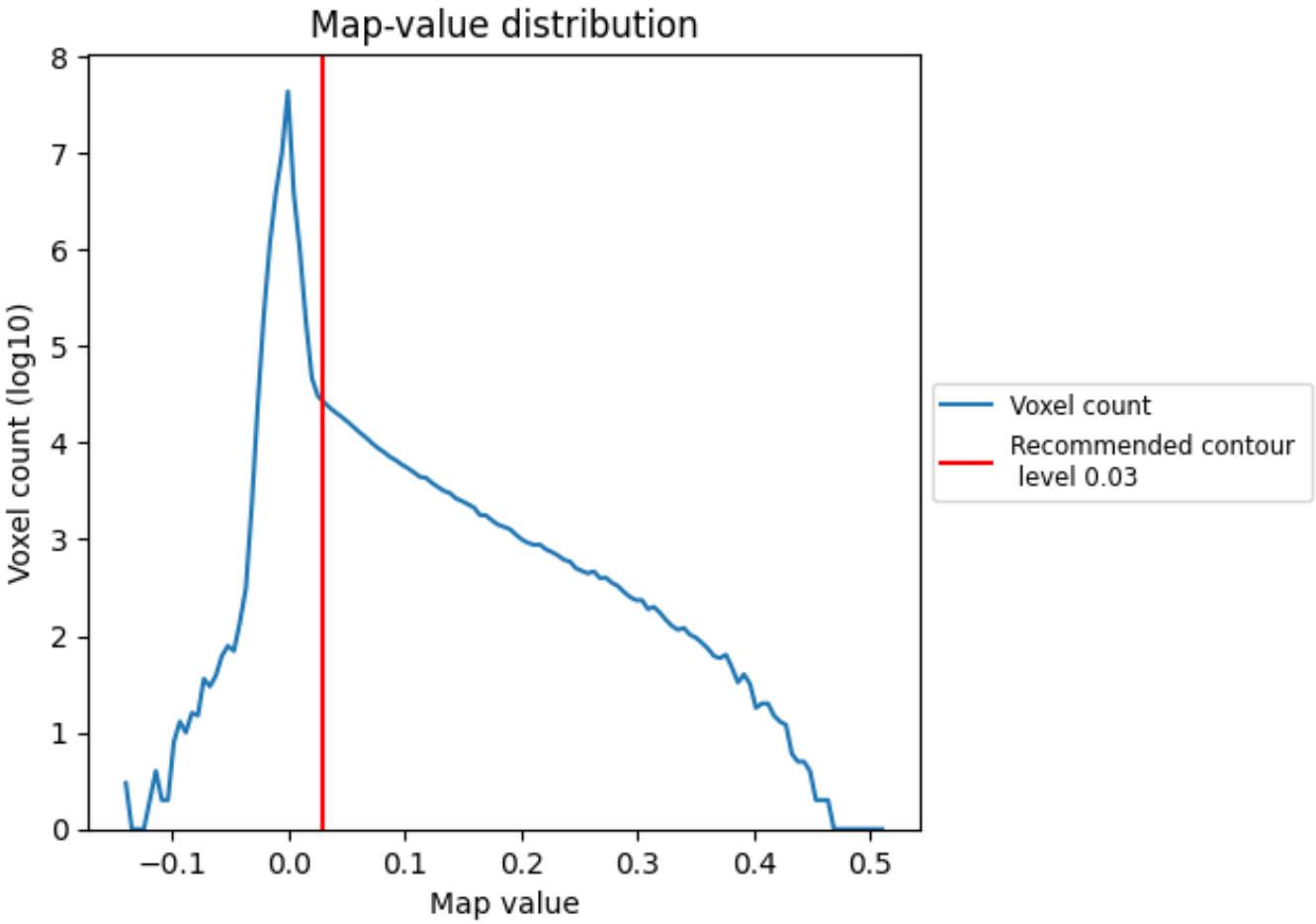
6.6 Mask visualisation (i)

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

7 Map analysis

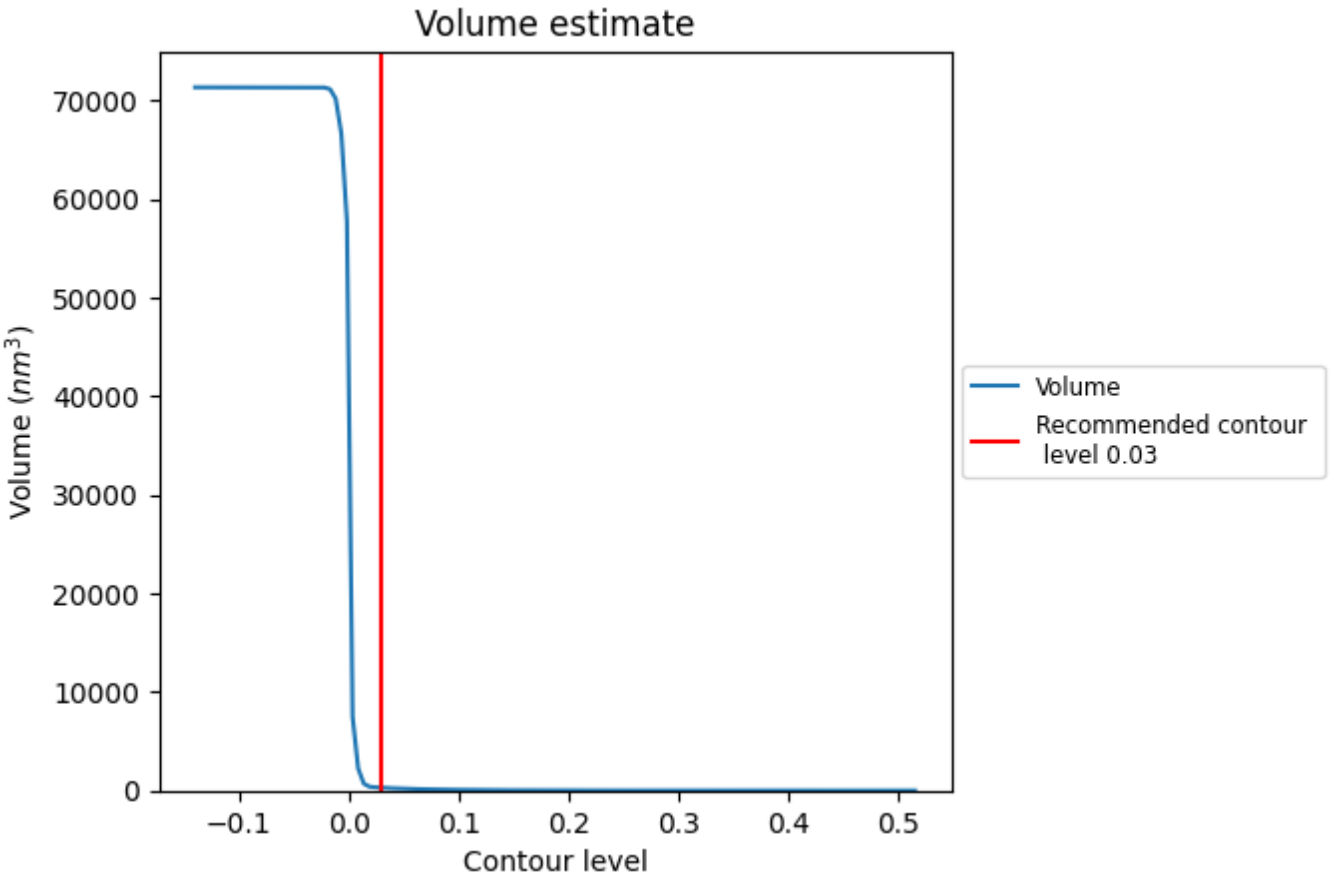
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

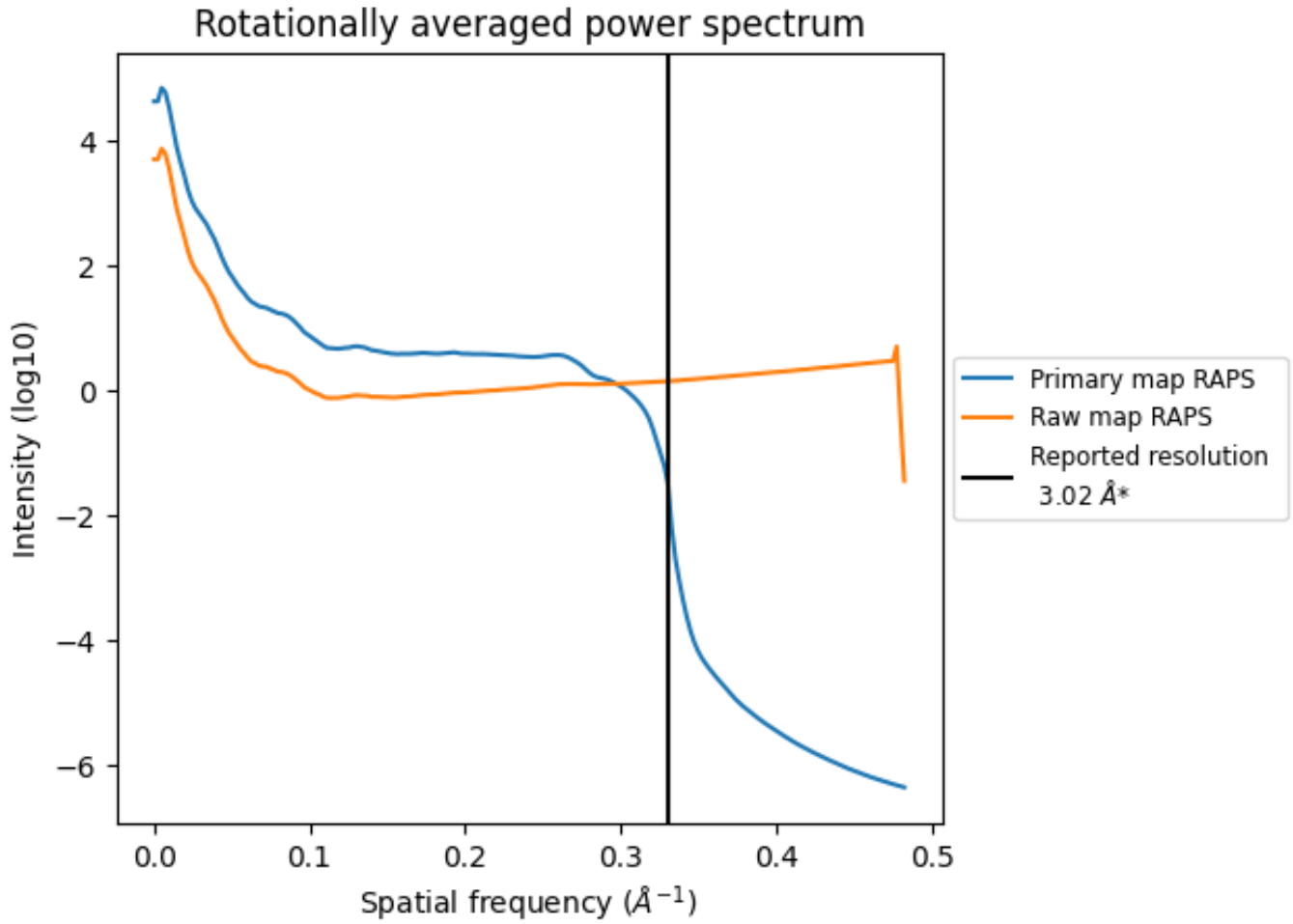
7.2 Volume estimate (i)



The volume at the recommended contour level is 288 nm^3; this corresponds to an approximate mass of 260 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 (i)

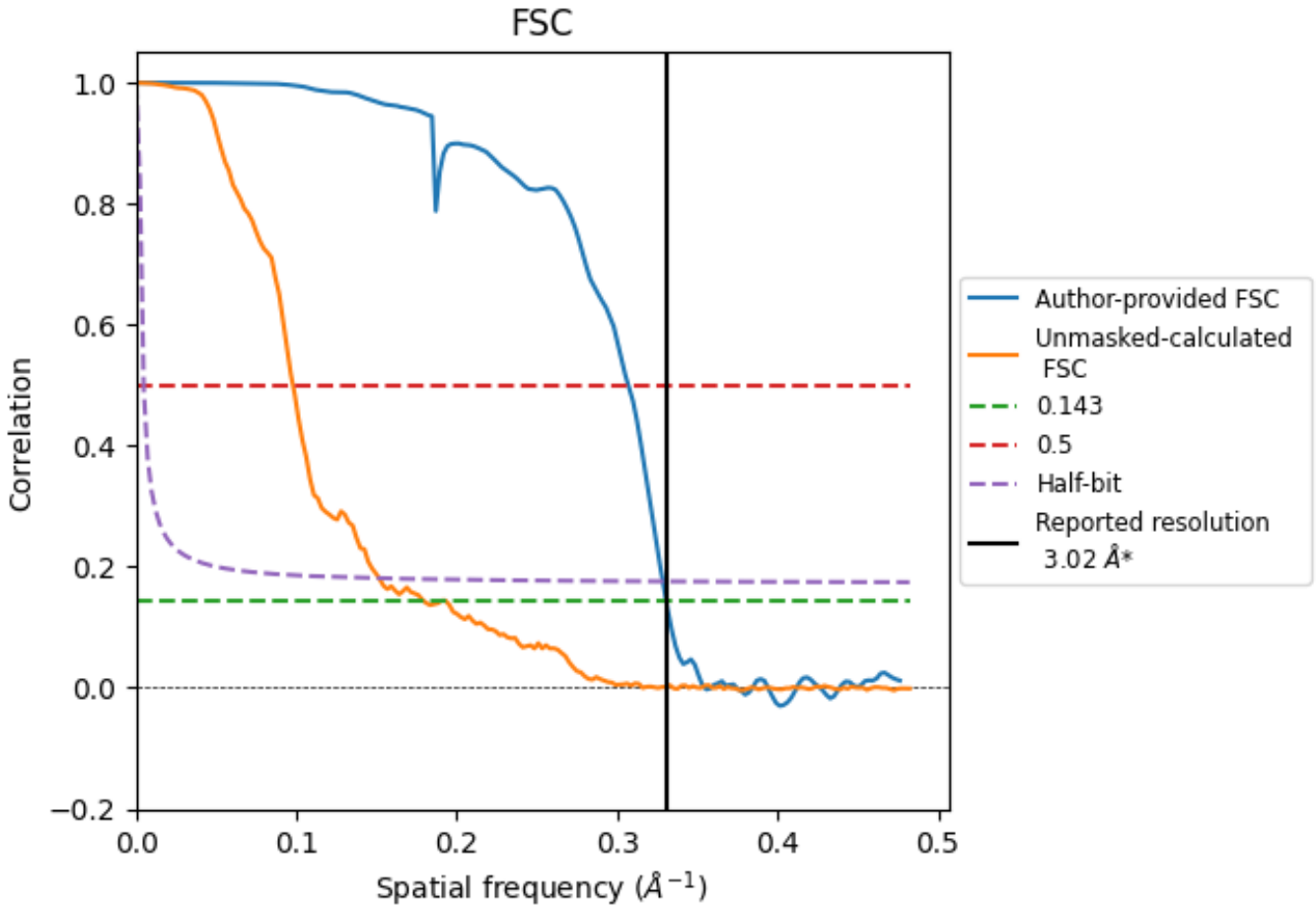


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates (i)

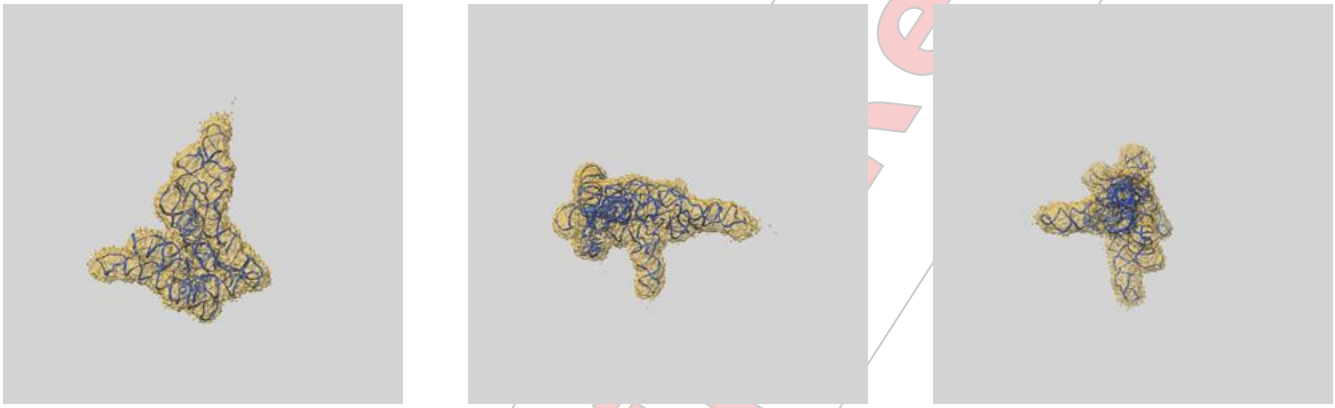
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.26	3.04
Unmasked-calculated*	5.56	10.22	6.60

*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 5.56 differs from the reported value 3.02 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70945 and PDB model 9OWV. Per-residue inclusion information can be found in section 3 on page 4.

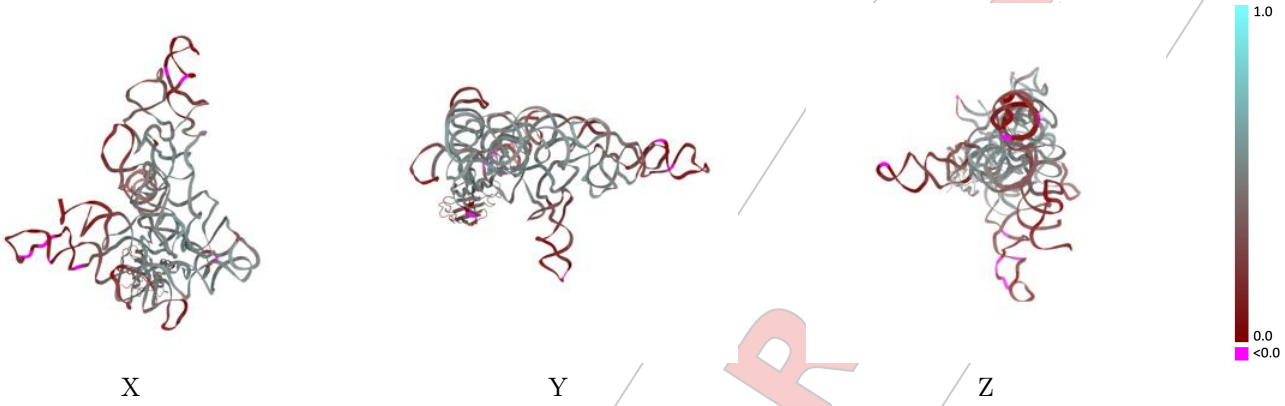
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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



X Y Z

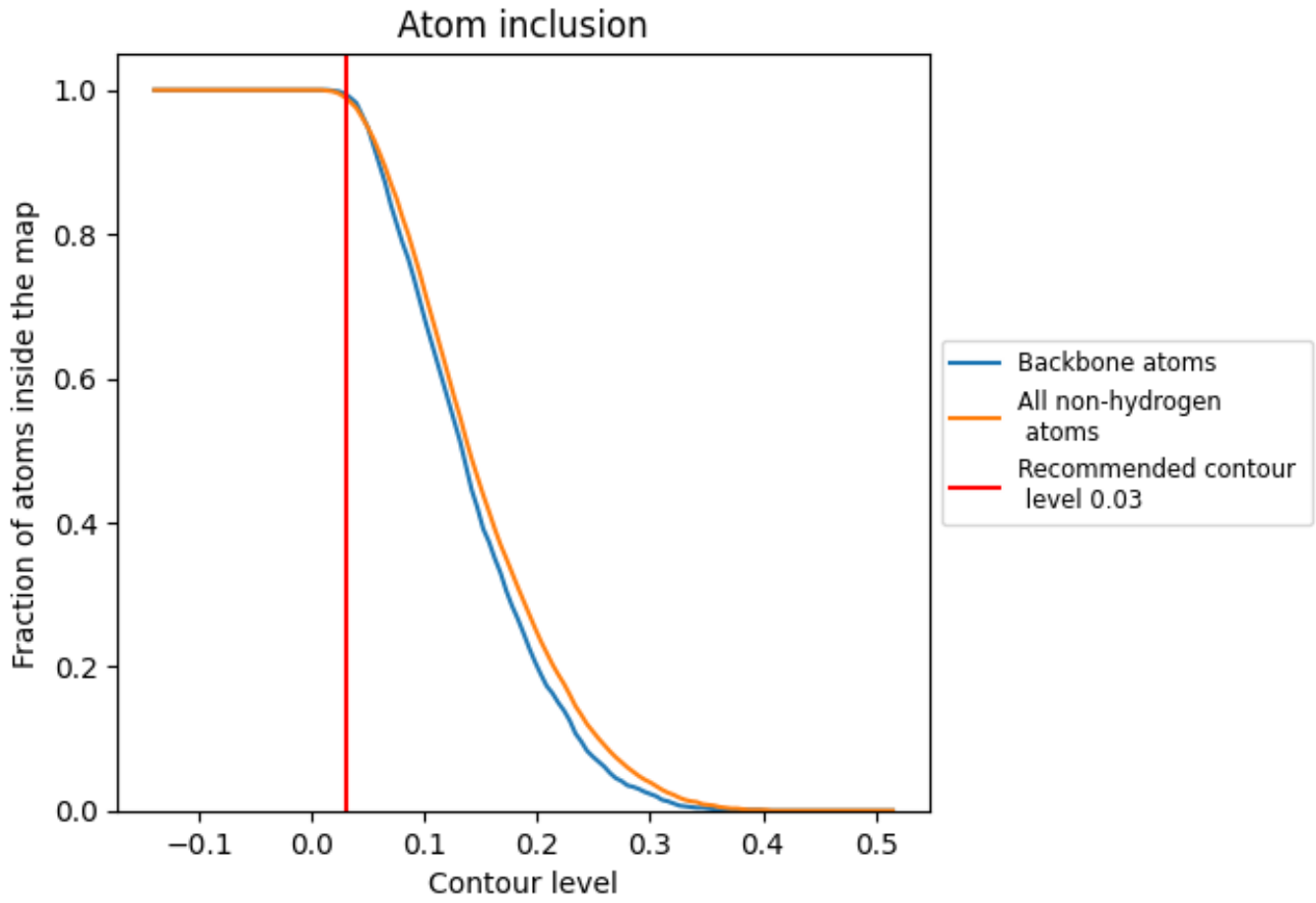
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9890	0.3890
A	0.9950	0.3940
B	0.9160	0.4000
C	0.9980	0.3590

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 04:29 PM EDT

PDB ID	:	9OWW / pdb_00009oww
EMDB ID	:	EMD-70946
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with the precursor tRNA with non-complementary 5' leader
Deposited on	:	2025-06-02
Resolution	:	2.83 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

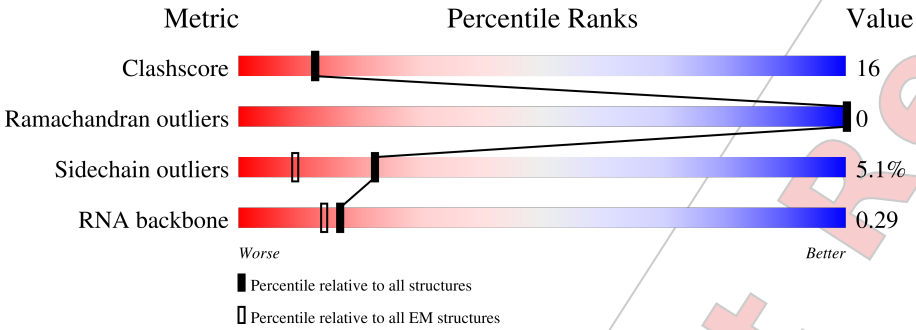
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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 <=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	417	33% 43% 24% •
2	B	116	74% 22% •
3	C	92	26% 42% 21% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11703 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor tRNA (89-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	83	1765	787	309	586	83	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

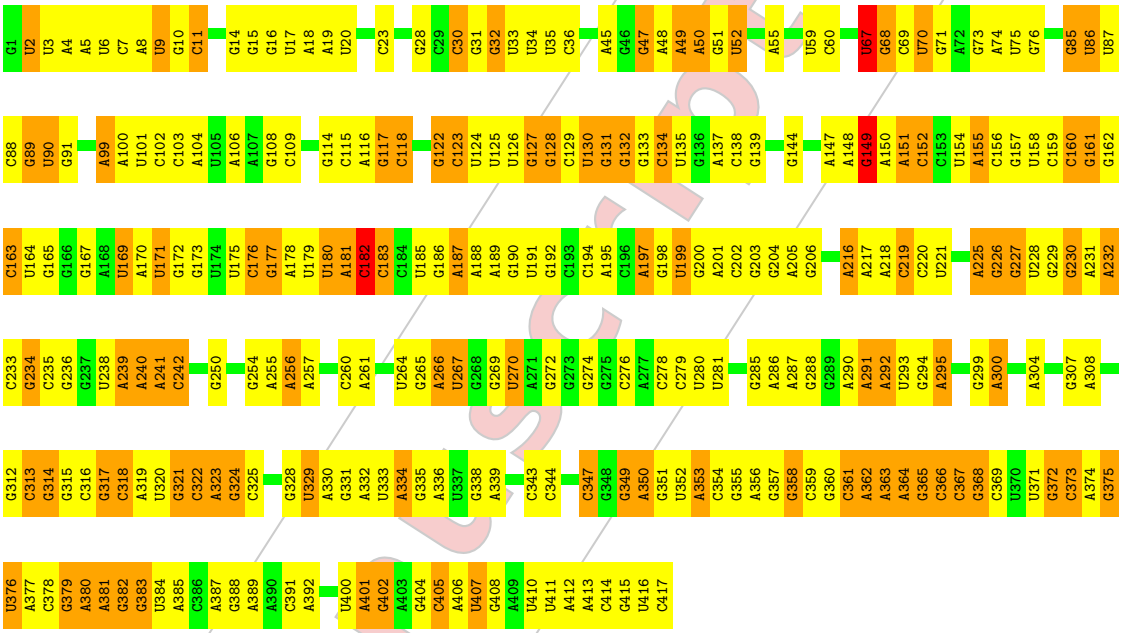
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	29	29	29	0

3 Residue-property plots (i)

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: RNase P RNA (417-MER)

Chain A:

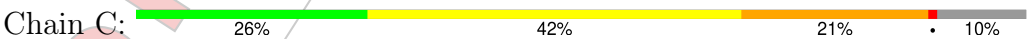


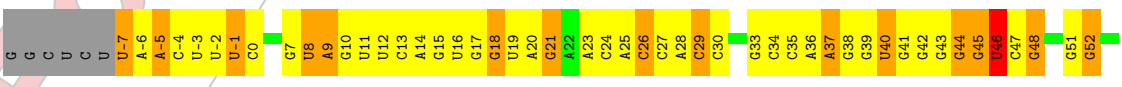
• Molecule 2: Ribonuclease P protein component

Chain B:

• Molecule 3: precursor tRNA (89-MER)

Chain C:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.53	0/10038	0.84	6/15661 (0.0%)
2	B	0.40	0/962	0.57	0/1281
3	C	0.58	0/1970	0.89	1/3068 (0.0%)
All	All	0.53	0/12970	0.83	7/20010 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	C	O3'-P-O5'	-5.94	95.09	104.00
1	A	182	C	C4'-C3'-C2'	-5.89	96.71	102.60
1	A	149	G	O3'-P-O5'	-5.70	95.44	104.00
3	C	46	U	C2'-C3'-O3'	5.54	117.82	109.50
1	A	67	U	O3'-P-O5'	-5.41	95.88	104.00
1	A	69	C	O3'-P-O5'	5.35	112.02	104.00
1	A	240	A	C4'-C3'-C2'	-5.04	97.56	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8962	0	4510	224	0
2	B	947	0	1008	27	0
3	C	1765	0	894	46	0
4	A	29	0	0	1	0
All	All	11703	0	6412	283	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 16.

All (283) 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:364:A:C4	1:A:365:G:H1'	1.96	1.01
3:C:43:G:H3'	3:C:44:G:H3'	1.49	0.93
1:A:226:G:C2'	1:A:227:G:H5'	2.00	0.92
1:A:226:G:O2'	1:A:227:G:H5'	1.70	0.90
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.88
3:C:8:U:H5'	3:C:48:G:H5'	1.55	0.88
1:A:349:G:H21	1:A:350:A:H62	1.24	0.83
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.80
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.79
1:A:378:C:H3'	1:A:379:G:C8	2.19	0.77
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.77
1:A:45:A:H62	2:B:62:ARG:NH2	1.84	0.77
2:B:86:ARG:NH2	3:C:-5:A:H4'	2.01	0.75
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.73
1:A:225:A:C2'	1:A:226:G:H5'	2.18	0.73
1:A:9:U:H2'	1:A:10:G:C8	2.24	0.72
1:A:47:G:H1	1:A:385:A:H62	1.39	0.71
2:B:63:TYR:HB3	2:B:97:VAL:HG11	1.72	0.70
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:U:H2'	1:A:10:G:H8	1.58	0.69
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.69
1:A:349:G:H22	1:A:379:G:H1'	1.58	0.68
1:A:180:U:H2'	1:A:181:A:H8	1.58	0.67
1:A:216:A:HO2'	1:A:217:A:H8	1.41	0.67
1:A:350:A:H1'	1:A:380:A:C2	2.30	0.67
1:A:169:U:H2'	1:A:170:A:H8	1.59	0.66
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.66
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.66
1:A:349:G:N2	1:A:350:A:H62	1.93	0.66
1:A:349:G:N2	1:A:379:G:H1'	2.10	0.66
1:A:378:C:H3'	1:A:379:G:H8	1.59	0.66
3:C:40:U:H2'	3:C:41:G:H8	1.61	0.66
1:A:50:A:C8	1:A:50:A:H5"	2.31	0.66
1:A:374:A:H2'	1:A:375:G:C8	2.32	0.64
1:A:230:G:O6	4:A:529:CA:CA	1.75	0.64
1:A:18:A:H2'	1:A:19:A:H8	1.62	0.64
1:A:45:A:H62	2:B:62:ARG:HH22	1.47	0.63
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.63
1:A:203:G:C5	1:A:205:A:H1'	2.34	0.62
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.62
3:C:27:C:H2'	3:C:28:A:C8	2.35	0.61
2:B:56:VAL:O	2:B:60:ILE:HG13	2.00	0.61
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.61
1:A:225:A:H2'	1:A:226:G:H5'	1.82	0.60
2:B:26:ARG:CZ	3:C:-7:U:H3'	2.31	0.60
2:B:49:LYS:HD2	3:C:-1:U:H5'	1.82	0.60
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.60
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.60
1:A:266:A:H2'	1:A:267:U:H5'	1.84	0.60
1:A:350:A:H1'	1:A:380:A:N1	2.17	0.59
2:B:86:ARG:HH21	3:C:-5:A:H4'	1.66	0.59
1:A:3:U:H2'	1:A:4:A:H8	1.68	0.59
1:A:379:G:H4'	1:A:380:A:H8	1.66	0.59
1:A:229:G:N2	1:A:231:A:H3'	2.17	0.59
1:A:32:G:H22	1:A:34:U:H1'	1.67	0.59
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
1:A:226:G:H2'	1:A:227:G:H5'	1.82	0.59
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.84	0.59
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:G:H2'	1:A:11:C:C6	2.37	0.58
1:A:379:G:H4'	1:A:380:A:C8	2.37	0.58
1:A:14:G:H2'	1:A:385:A:N1	2.19	0.58
1:A:364:A:OP1	1:A:365:G:N7	2.35	0.58
1:A:360:G:H22	1:A:363:A:H5"	1.68	0.57
3:C:40:U:H2'	3:C:41:G:C8	2.38	0.57
3:C:38:G:H2'	3:C:39:G:C8	2.40	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:67:U:H4'	1:A:68:G:OP1	2.06	0.56
1:A:199:U:H5	1:A:206:G:H1'	1.70	0.56
1:A:315:G:H2'	1:A:316:C:C6	2.40	0.56
1:A:308:A:N1	1:A:329:U:H5	2.04	0.56
1:A:364:A:H3'	1:A:364:A:OP2	2.05	0.56
1:A:229:G:H22	1:A:232:A:P	2.28	0.56
2:B:92:MET:HB3	2:B:97:VAL:HG23	1.88	0.56
3:C:26:C:H2'	3:C:27:C:C6	2.41	0.56
1:A:412:A:H2'	1:A:413:A:C8	2.42	0.55
1:A:5:A:H2'	1:A:6:U:C6	2.41	0.55
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.55
1:A:8:A:C2'	1:A:9:U:H5'	2.36	0.55
1:A:307:G:H2'	1:A:308:A:H8	1.70	0.55
1:A:5:A:H2'	1:A:6:U:H6	1.71	0.55
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.55
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.55
1:A:144:G:H1	1:A:182:C:H42	1.55	0.54
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.54
2:B:26:ARG:NH2	3:C:-7:U:H3'	2.21	0.54
1:A:59:U:H2'	1:A:60:C:C6	2.42	0.54
1:A:154:U:H2'	1:A:155:A:C4	2.42	0.54
1:A:186:G:H8	1:A:186:G:H5"	1.73	0.54
1:A:85:G:O2'	1:A:87:U:O4	2.26	0.54
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.53
3:C:42:G:H2'	3:C:43:G:C8	2.43	0.53
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.53
1:A:199:U:C5	1:A:206:G:H1'	2.43	0.53
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.53
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.52
1:A:264:U:H2'	1:A:265:G:O4'	2.09	0.52
1:A:99:A:H2'	1:A:100:A:C8	2.44	0.52
1:A:349:G:O6	1:A:379:G:N2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.52
3:C:8:U:H5'	3:C:48:G:C5'	2.35	0.52
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.52
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.51
1:A:10:G:H2'	1:A:11:C:H6	1.74	0.51
1:A:49:A:N1	1:A:387:A:O2'	2.37	0.51
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.51
1:A:216:A:O2'	1:A:217:A:H8	1.93	0.51
1:A:23:C:O2	1:A:336:A:O2'	2.28	0.51
3:C:43:G:C3'	3:C:44:G:H3'	2.33	0.51
3:C:42:G:C3'	3:C:43:G:H8	2.23	0.51
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.51
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.50
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.50
1:A:307:G:H2'	1:A:308:A:C8	2.46	0.50
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.50
1:A:317:G:N1	1:A:321:G:C2	2.80	0.50
3:C:-5:A:N3	3:C:-5:A:H2'	2.25	0.50
1:A:219:C:H2'	1:A:220:C:H6	1.76	0.49
3:C:29:C:H2'	3:C:30:C:C6	2.47	0.49
1:A:161:G:H4'	1:A:163:C:C5	2.48	0.49
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.49
1:A:266:A:C2'	1:A:267:U:H5'	2.43	0.49
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.49
1:A:241:A:H2'	1:A:242:C:C6	2.47	0.49
1:A:385:A:H8	1:A:400:U:HO2'	1.61	0.49
3:C:43:G:H3'	3:C:44:G:C3'	2.34	0.49
1:A:373:C:H2'	1:A:374:A:C8	2.47	0.49
1:A:89:G:H2'	1:A:90:U:C6	2.48	0.48
1:A:280:U:H2'	1:A:281:U:C6	2.48	0.48
1:A:180:U:O2'	1:A:181:A:H5'	2.13	0.48
1:A:19:A:H2'	1:A:20:U:C6	2.48	0.48
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.48
1:A:52:U:H5	3:C:65:C:H41	1.62	0.48
1:A:148:A:H3'	1:A:149:G:H8	1.77	0.48
1:A:186:G:N2	1:A:188:A:H3'	2.28	0.48
1:A:132:G:H3'	1:A:133:G:H8	1.79	0.48
1:A:349:G:H4'	1:A:350:A:H5'	1.94	0.48
1:A:178:A:OP1	1:A:180:U:H1'	2.14	0.47
1:A:371:U:H4'	1:A:373:C:H5	1.79	0.47
1:A:169:U:H2'	1:A:170:A:C8	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:G:C8	1:A:335:G:H3'	2.50	0.47
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.47
1:A:160:C:O2	1:A:167:G:N1	2.47	0.47
1:A:176:C:H2'	1:A:177:G:C8	2.50	0.47
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.47
1:A:411:U:H2'	1:A:412:A:C8	2.49	0.47
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.47
1:A:347:C:H1'	1:A:383:G:N2	2.29	0.47
1:A:338:G:H2'	1:A:339:A:H8	1.80	0.47
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.47
1:A:71:G:H1'	1:A:291:A:H61	1.80	0.47
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.47
1:A:198:G:N2	1:A:200:G:H3'	2.30	0.46
1:A:350:A:C1'	1:A:380:A:N1	2.78	0.46
1:A:352:U:H2'	1:A:353:A:C8	2.51	0.46
3:C:27:C:H2'	3:C:28:A:H8	1.80	0.46
3:C:60:C:H2'	3:C:61:C:H6	1.80	0.46
1:A:280:U:H2'	1:A:281:U:H6	1.79	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.46
1:A:194:C:H5"	1:A:195:A:O4'	2.16	0.46
2:B:112:LYS:O	2:B:113:LYS:C	2.58	0.46
3:C:24:C:H2'	3:C:25:A:C8	2.51	0.46
1:A:195:A:H1'	3:C:18:G:C5	2.50	0.46
1:A:376:U:H2'	1:A:377:A:C8	2.49	0.46
3:C:25:A:H2	3:C:43:G:H22	1.64	0.46
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.45
1:A:285:G:O2'	1:A:300:A:N6	2.49	0.45
3:C:14:A:C2	3:C:21:G:H1'	2.51	0.45
3:C:37:A:H2'	3:C:38:G:C8	2.51	0.45
1:A:234:G:H2'	1:A:236:G:H5'	1.98	0.45
2:B:111:LEU:C	2:B:113:LYS:N	2.72	0.45
1:A:103:C:H3'	1:A:104:A:H8	1.82	0.45
1:A:180:U:H2'	1:A:181:A:C8	2.45	0.45
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.45
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.45
1:A:86:U:H2'	1:A:87:U:O4'	2.17	0.45
1:A:267:U:C2	3:C:75:A:C2	3.05	0.45
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.45
2:B:111:LEU:HD22	2:B:111:LEU:HA	1.80	0.44
1:A:219:C:H2'	1:A:220:C:C6	2.52	0.44
1:A:331:G:H4'	1:A:332:A:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:G:C2’	1:A:270:U:H5’	2.47	0.44
1:A:363:A:O2’	1:A:364:A:O4’	2.33	0.44
3:C:34:C:H2’	3:C:35:C:H6	1.83	0.44
1:A:364:A:H2’	1:A:365:G:O4’	2.18	0.44
1:A:32:G:N2	1:A:34:U:H1’	2.32	0.44
1:A:380:A:H2’	1:A:380:A:N3	2.32	0.44
1:A:17:U:H2’	1:A:18:A:H8	1.82	0.44
1:A:365:G:N3	1:A:365:G:H2’	2.33	0.44
1:A:114:G:H2’	1:A:115:C:C6	2.52	0.44
2:B:99:LYS:HD3	2:B:99:LYS:O	2.17	0.44
1:A:147:A:H2’	1:A:148:A:C8	2.53	0.43
1:A:197:A:H2’	1:A:228:U:O2’	2.18	0.43
1:A:217:A:H2’	1:A:218:A:O4’	2.19	0.43
1:A:225:A:C3’	1:A:226:G:H5’	2.48	0.43
1:A:355:G:H2’	1:A:356:A:C8	2.53	0.43
1:A:350:A:C8	1:A:380:A:C6	3.06	0.43
2:B:11:GLU:O	2:B:15:GLU:HG3	2.19	0.43
3:C:45:G:O2’	3:C:46:U:O4’	2.37	0.43
1:A:382:G:H2’	1:A:383:G:O4’	2.18	0.43
1:A:414:C:H2’	1:A:415:G:C8	2.53	0.43
3:C:-5:A:N3	3:C:-5:A:H5”	2.33	0.43
1:A:123:C:H2’	1:A:124:U:O4’	2.18	0.43
1:A:294:G:H2’	1:A:295:A:C8	2.53	0.43
2:B:111:LEU:C	2:B:113:LYS:H	2.25	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:128:G:H2’	1:A:129:C:H6	1.83	0.43
2:B:49:LYS:CD	3:C:-1:U:H5’	2.48	0.43
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.80	0.43
1:A:313:C:H2’	1:A:314:G:C8	2.54	0.43
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.43
1:A:324:G:H2’	1:A:325:C:H6	1.85	0.42
3:C:16:U:H5	3:C:58:G:O6	2.02	0.42
3:C:16:U:C5	3:C:58:G:O6	2.72	0.42
1:A:17:U:H2’	1:A:18:A:C8	2.55	0.42
1:A:89:G:H2’	1:A:90:U:H6	1.85	0.42
1:A:186:G:H5”	1:A:186:G:C8	2.51	0.42
1:A:358:G:H1	1:A:366:C:H42	1.66	0.42
1:A:363:A:C2’	1:A:364:A:C1’	2.93	0.42
1:A:220:C:H2’	1:A:221:U:H6	1.85	0.42
1:A:334:A:H62	2:B:10:ASN:ND2	2.17	0.42
1:A:200:G:N3	1:A:205:A:H2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.42
1:A:85:G:H4'	1:A:85:G:OP1	2.19	0.42
2:B:73:GLU:N	2:B:73:GLU:OE1	2.52	0.42
3:C:65:C:H2'	3:C:66:U:C6	2.55	0.42
1:A:8:A:H2'	1:A:9:U:H5'	2.02	0.42
1:A:265:G:H4'	1:A:267:U:O2	2.19	0.42
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.42
2:B:98:LYS:O	2:B:102:ILE:HD13	2.19	0.42
3:C:-6:A:N3	3:C:-6:A:H2'	2.35	0.42
1:A:199:U:O2	1:A:199:U:O4'	2.38	0.42
1:A:279:C:H2'	1:A:280:U:C6	2.55	0.42
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.42
1:A:364:A:H3'	1:A:364:A:P	2.60	0.42
3:C:51:G:N2	3:C:52:G:H1'	2.35	0.42
1:A:354:C:H2'	1:A:355:G:O4'	2.19	0.41
1:A:349:G:N2	1:A:378:C:C2	2.88	0.41
1:A:406:A:H2'	1:A:407:U:O4'	2.20	0.41
1:A:117:G:H3'	1:A:118:C:H6	1.86	0.41
1:A:239:A:H4'	1:A:241:A:H5'	2.02	0.41
1:A:287:A:H3'	1:A:288:G:H8	1.86	0.41
1:A:335:G:C8	1:A:335:G:C3'	3.03	0.41
3:C:40:U:C2	3:C:41:G:C8	3.08	0.41
3:C:42:G:C3'	3:C:43:G:C8	3.03	0.41
1:A:134:C:H2'	1:A:135:U:C6	2.55	0.41
1:A:182:C:C2'	1:A:183:C:H5'	2.50	0.41
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.41
1:A:335:G:H3'	1:A:335:G:H8	1.85	0.41
1:A:144:G:H1	1:A:182:C:N4	2.19	0.41
1:A:260:C:H2'	1:A:261:A:O4'	2.20	0.41
1:A:334:A:H62	2:B:10:ASN:HD22	1.68	0.41
1:A:350:A:C4	1:A:380:A:C4	3.09	0.41
1:A:186:G:N1	1:A:189:A:OP2	2.47	0.41
1:A:353:A:H2'	1:A:354:C:O4'	2.21	0.41
1:A:220:C:H2'	1:A:221:U:C6	2.56	0.41
1:A:256:A:H62	3:C:0:C:N4	2.19	0.41
1:A:115:C:H2'	1:A:116:A:H8	1.85	0.41
1:A:151:A:H2'	1:A:152:C:O4'	2.21	0.41
1:A:187:A:H2'	1:A:188:A:C8	2.56	0.41
1:A:266:A:H2'	1:A:266:A:N3	2.36	0.41
1:A:292:A:C5	1:A:293:U:C5	3.08	0.41
1:A:377:A:H3'	1:A:378:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:A:C2	1:A:381:A:N9	2.89	0.41
3:C:35:C:H2'	3:C:36:A:O4'	2.20	0.41
3:C:42:G:H3'	3:C:43:G:H8	1.85	0.41
3:C:60:C:H2'	3:C:61:C:C6	2.56	0.41
1:A:286:A:N6	1:A:299:G:H1'	2.36	0.41
1:A:2:U:H2'	1:A:3:U:H6	1.84	0.40
1:A:16:G:N2	1:A:344:C:H1'	2.36	0.40
1:A:180:U:C2'	1:A:181:A:H5'	2.51	0.40
1:A:350:A:C4	1:A:380:A:C5	3.09	0.40
1:A:356:A:H3'	1:A:357:G:C8	2.56	0.40
1:A:401:A:H2'	1:A:402:G:O4'	2.20	0.40
3:C:9:A:N3	3:C:44:G:H1'	2.35	0.40
1:A:385:A:C8	1:A:400:U:O2'	2.74	0.40
3:C:29:C:H2'	3:C:30:C:H6	1.85	0.40
1:A:170:A:H3'	1:A:171:U:H6	1.86	0.40
1:A:352:U:H2'	1:A:353:A:H8	1.86	0.40
1:A:8:A:O2'	1:A:9:U:H5'	2.21	0.40
3:C:72:U:H2'	3:C:73:C:O4'	2.21	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	
2	B	114/116 (98%)	110 (96%)	4 (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
2	B	99/99 (100%)	94 (95%)	5 (5%)	20 40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	71	LEU
2	B	92	MET
2	B	97	VAL
2	B	105	LEU
2	B	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	168 (40%)	16 (3%)
3	C	83/92 (90%)	35 (42%)	6 (7%)
All	All	499/509 (98%)	203 (40%)	22 (4%)

All (203) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U
1	A	11	C
1	A	15	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U

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Mol	Chain	Res	Type
1	A	36	C
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	55	A
1	A	67	U
1	A	68	G
1	A	70	U
1	A	74	A
1	A	75	U
1	A	76	G
1	A	85	G
1	A	86	U
1	A	88	C
1	A	89	G
1	A	90	U
1	A	91	G
1	A	99	A
1	A	101	U
1	A	102	C
1	A	106	A
1	A	108	G
1	A	109	C
1	A	117	G
1	A	118	C
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	134	C
1	A	137	A
1	A	138	C
1	A	139	G
1	A	149	G
1	A	150	A

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Mol	Chain	Res	Type
1	A	151	A
1	A	152	C
1	A	155	A
1	A	156	C
1	A	157	G
1	A	158	U
1	A	159	C
1	A	160	C
1	A	161	G
1	A	162	G
1	A	163	C
1	A	164	U
1	A	165	G
1	A	169	U
1	A	171	U
1	A	172	G
1	A	173	G
1	A	175	U
1	A	177	G
1	A	179	U
1	A	180	U
1	A	181	A
1	A	182	C
1	A	183	C
1	A	185	U
1	A	187	A
1	A	190	G
1	A	191	U
1	A	192	G
1	A	197	A
1	A	199	U
1	A	202	C
1	A	204	G
1	A	216	A
1	A	219	C
1	A	225	A
1	A	226	G
1	A	227	G
1	A	230	G
1	A	232	A
1	A	233	C
1	A	234	G

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Mol	Chain	Res	Type
1	A	235	C
1	A	238	U
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	266	A
1	A	267	U
1	A	270	U
1	A	272	G
1	A	274	G
1	A	276	C
1	A	278	C
1	A	290	A
1	A	291	A
1	A	292	A
1	A	295	A
1	A	300	A
1	A	304	A
1	A	312	G
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	343	C
1	A	347	C
1	A	349	G
1	A	350	A

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Mol	Chain	Res	Type
1	A	351	G
1	A	353	A
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	389	A
1	A	391	C
1	A	392	A
1	A	401	A
1	A	402	G
1	A	404	G
1	A	405	C
1	A	407	U
1	A	408	G
1	A	410	U
3	C	-5	A
3	C	-4	C
3	C	-3	U
3	C	-2	U
3	C	-1	U
3	C	8	U
3	C	9	A
3	C	10	G
3	C	11	U

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Mol	Chain	Res	Type
3	C	12	U
3	C	13	C
3	C	15	G
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	21	G
3	C	23	A
3	C	26	C
3	C	29	C
3	C	33	G
3	C	37	A
3	C	40	U
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	52	G
3	C	58	G
3	C	59	U
3	C	60	C
3	C	63	G
3	C	72	U
3	C	75	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	50	A
1	A	67	U
1	A	75	U
1	A	101	U
1	A	122	G
1	A	126	U
1	A	137	A
1	A	176	C
1	A	182	C
1	A	201	A
1	A	232	A
1	A	233	C

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Mol	Chain	Res	Type
1	A	240	A
1	A	349	G
1	A	363	A
1	A	365	G
3	C	-7	U
3	C	-4	C
3	C	7	G
3	C	18	G
3	C	46	U
3	C	59	U

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 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

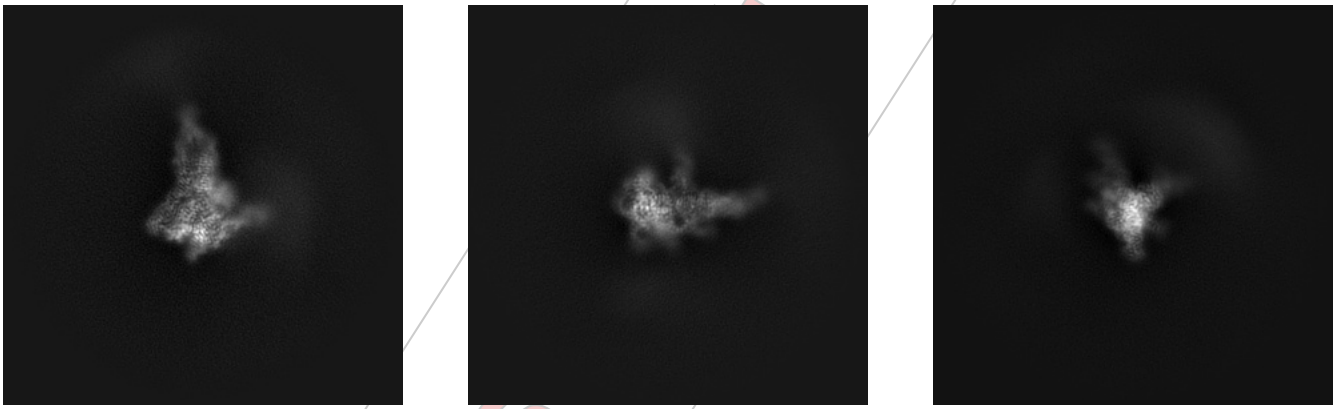
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70946. 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.

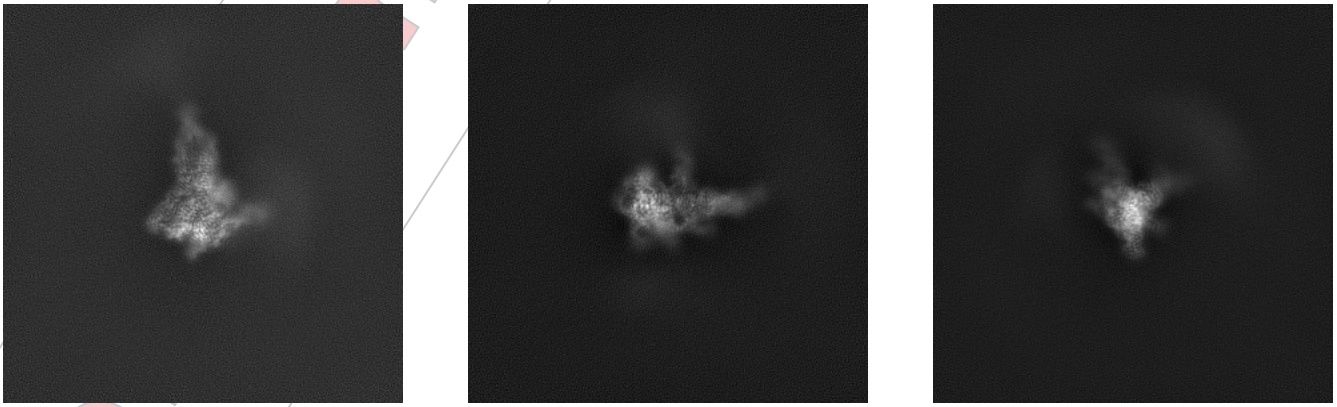
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

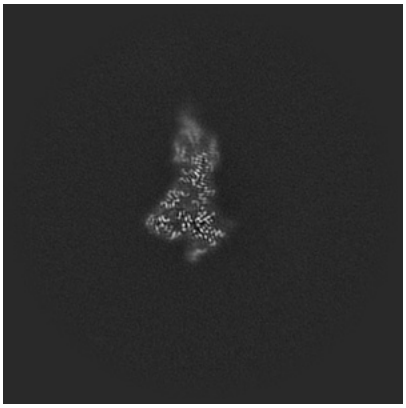


X Y Z

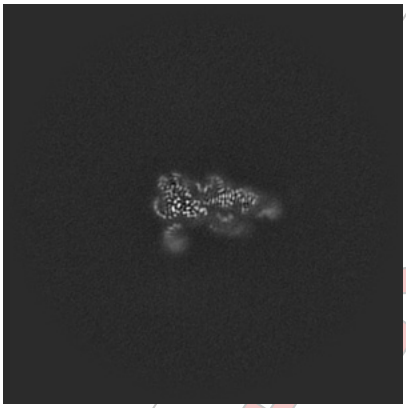
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



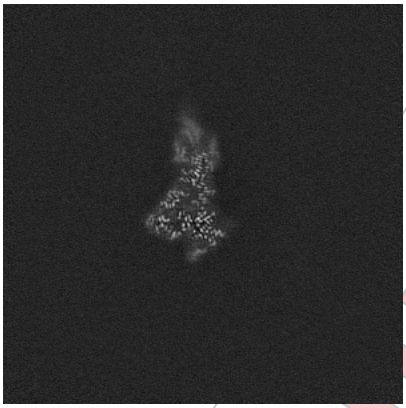
X Index: 200



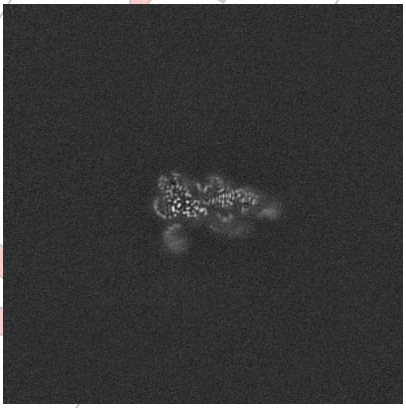
Y Index: 200

Z Index: 200

6.2.2 Raw map



X Index: 200



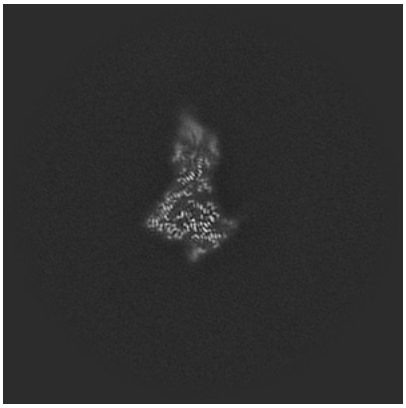
Y Index: 200

Z Index: 200

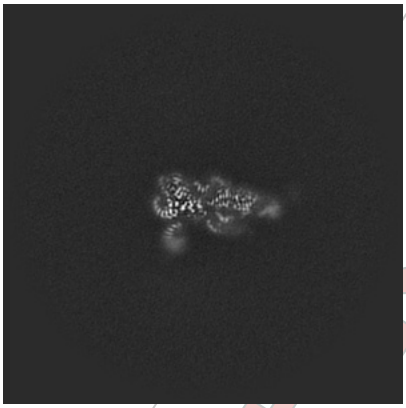
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



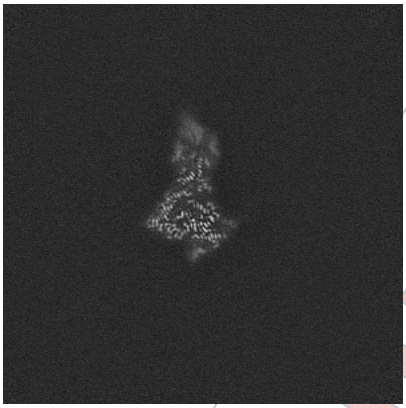
X Index: 197



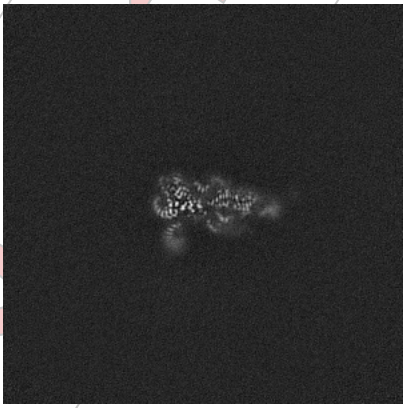
Y Index: 198

Z Index: 173

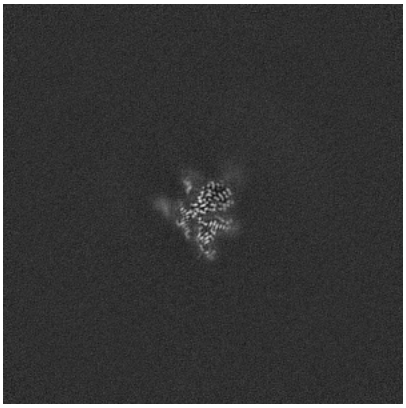
6.3.2 Raw map



X Index: 197



Y Index: 198

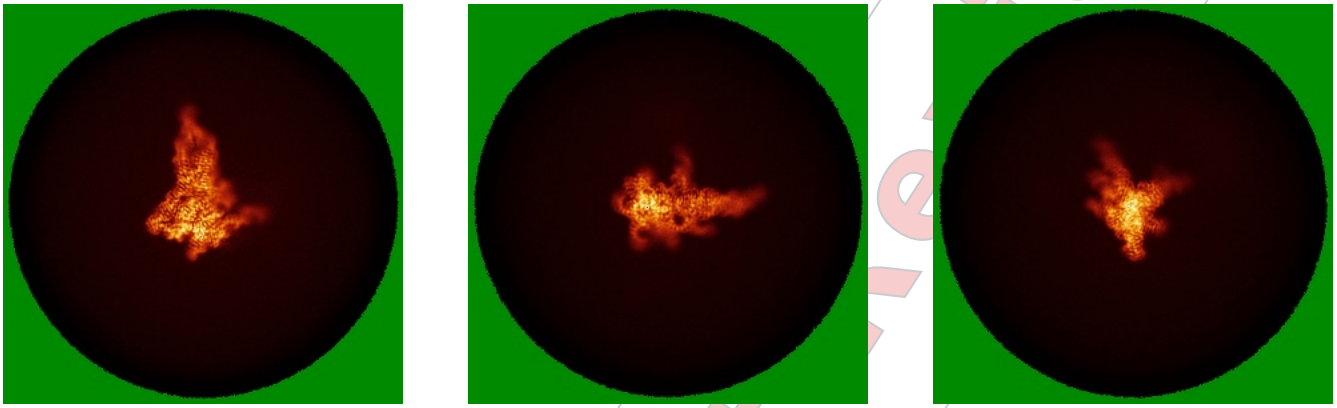


Z Index: 173

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

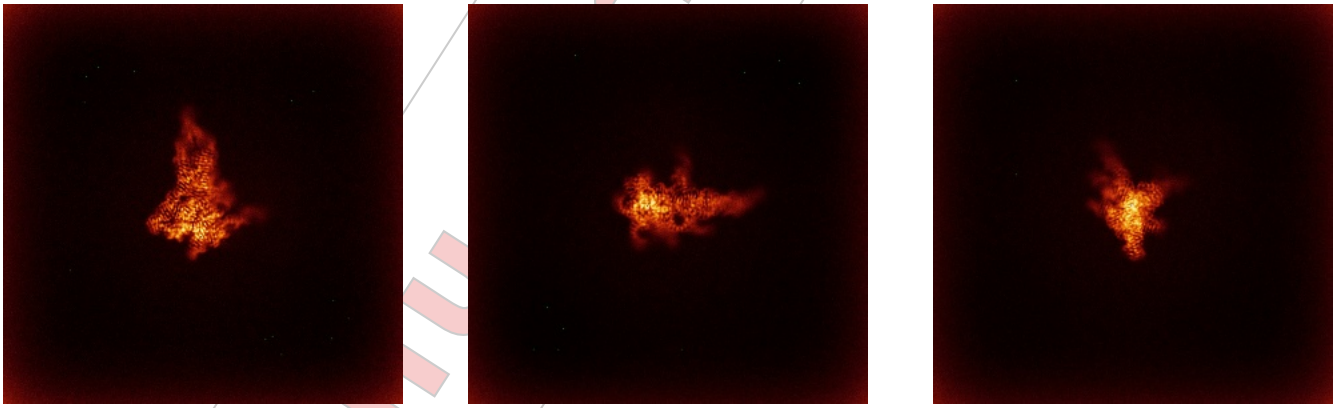
6.4 Orthogonal standard-deviation projections (False-color)

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 0.03. 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.

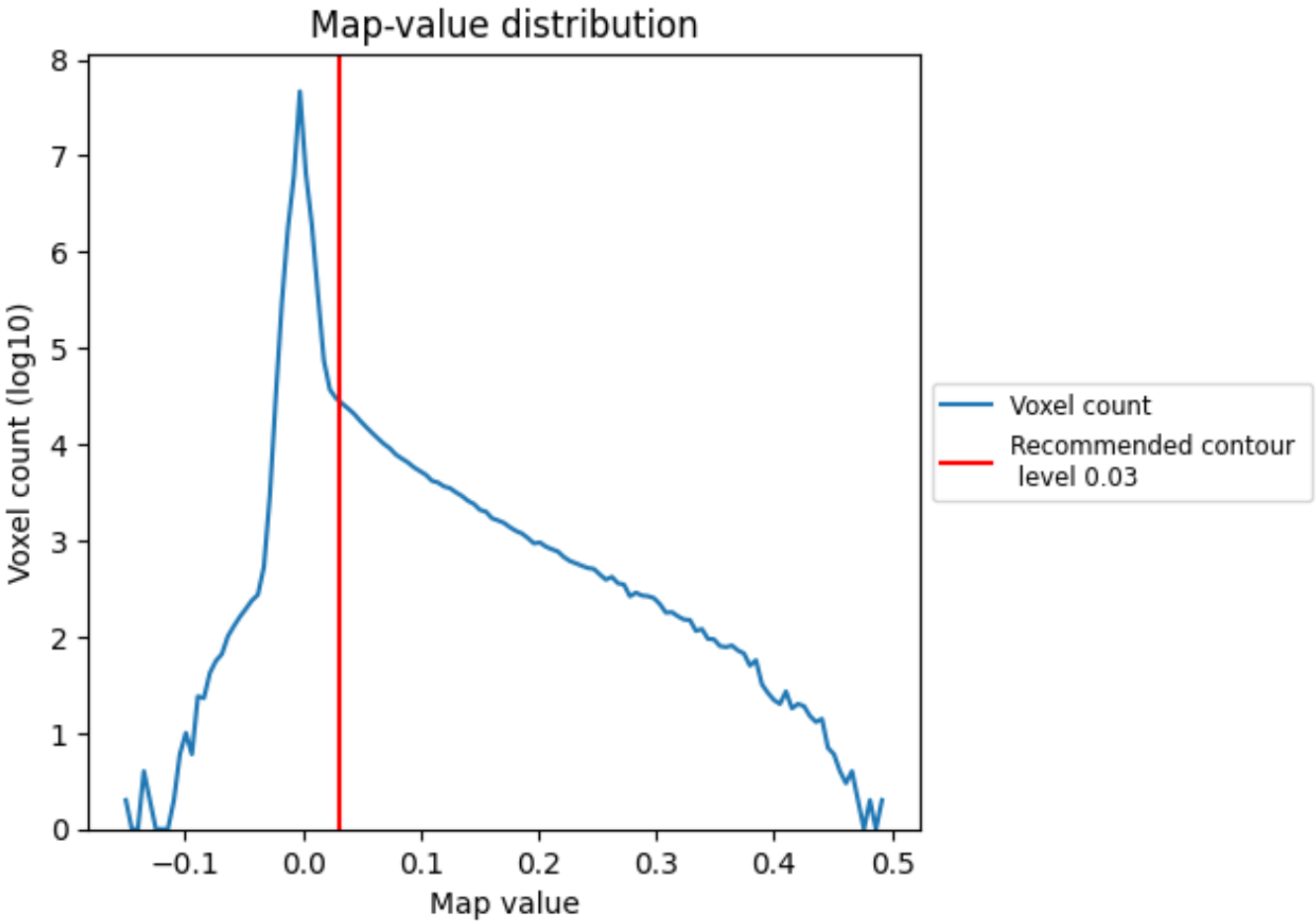
6.6 Mask visualisation (i)

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

7 Map analysis

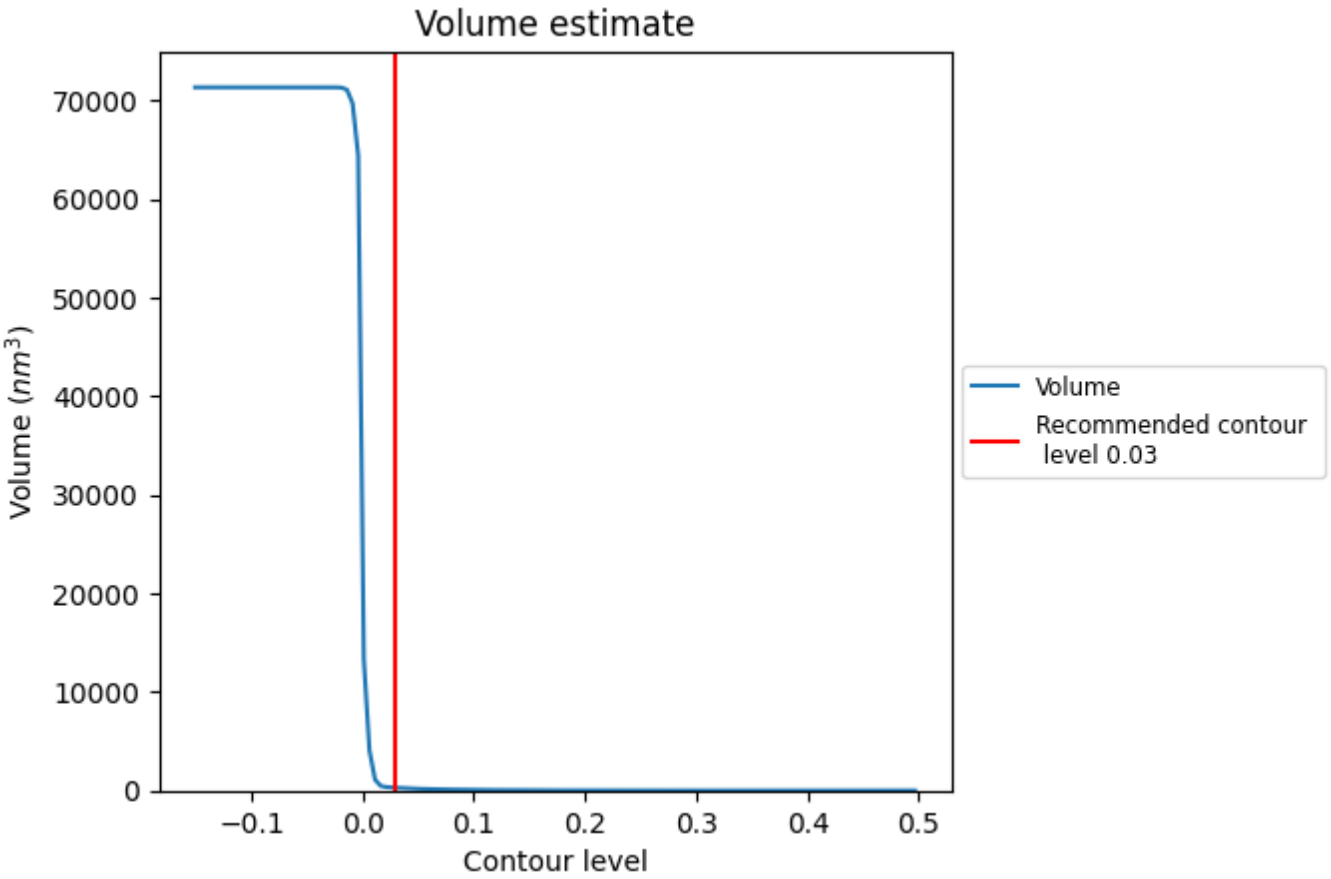
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

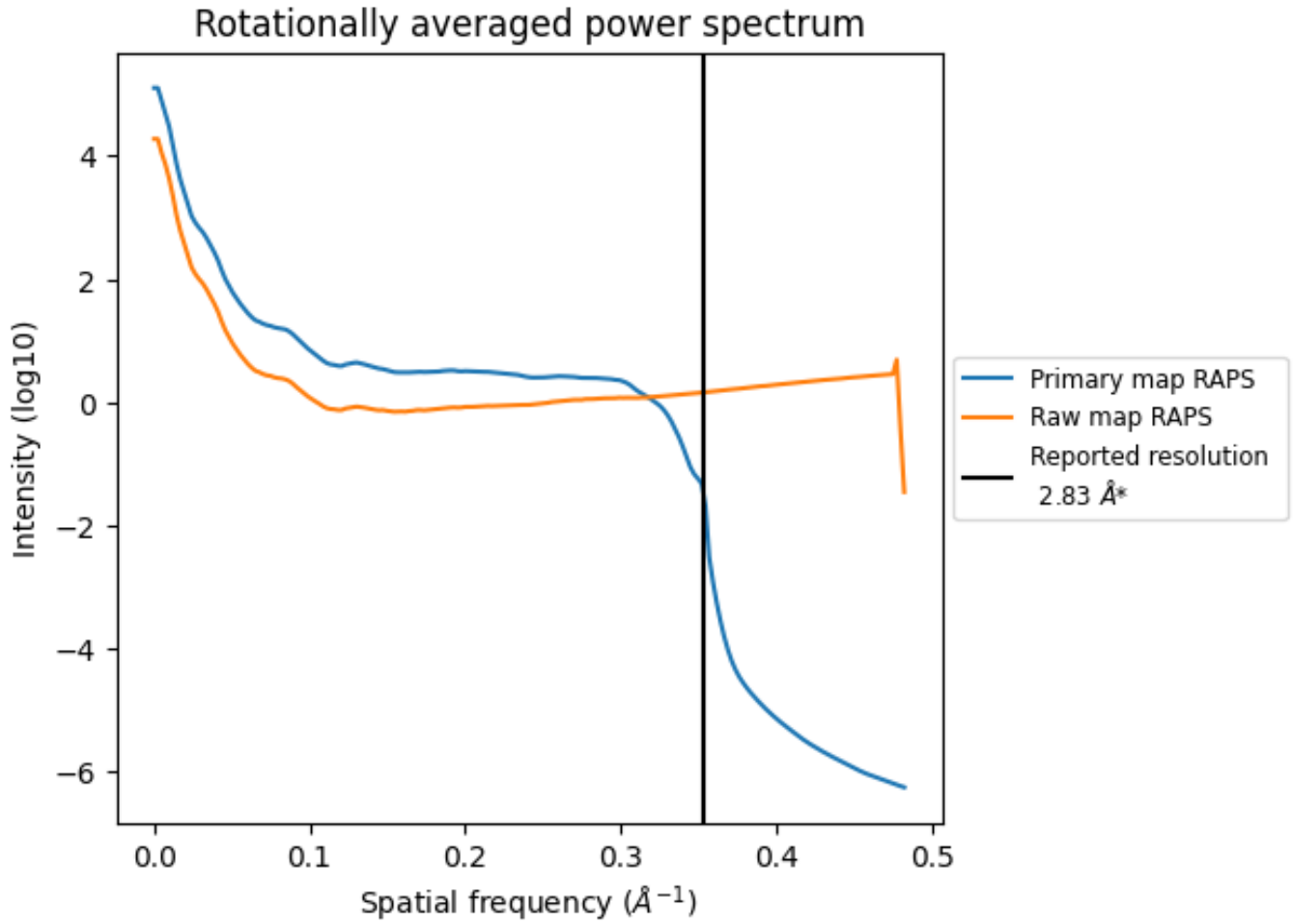
7.2 Volume estimate (i)



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 259 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 (i)

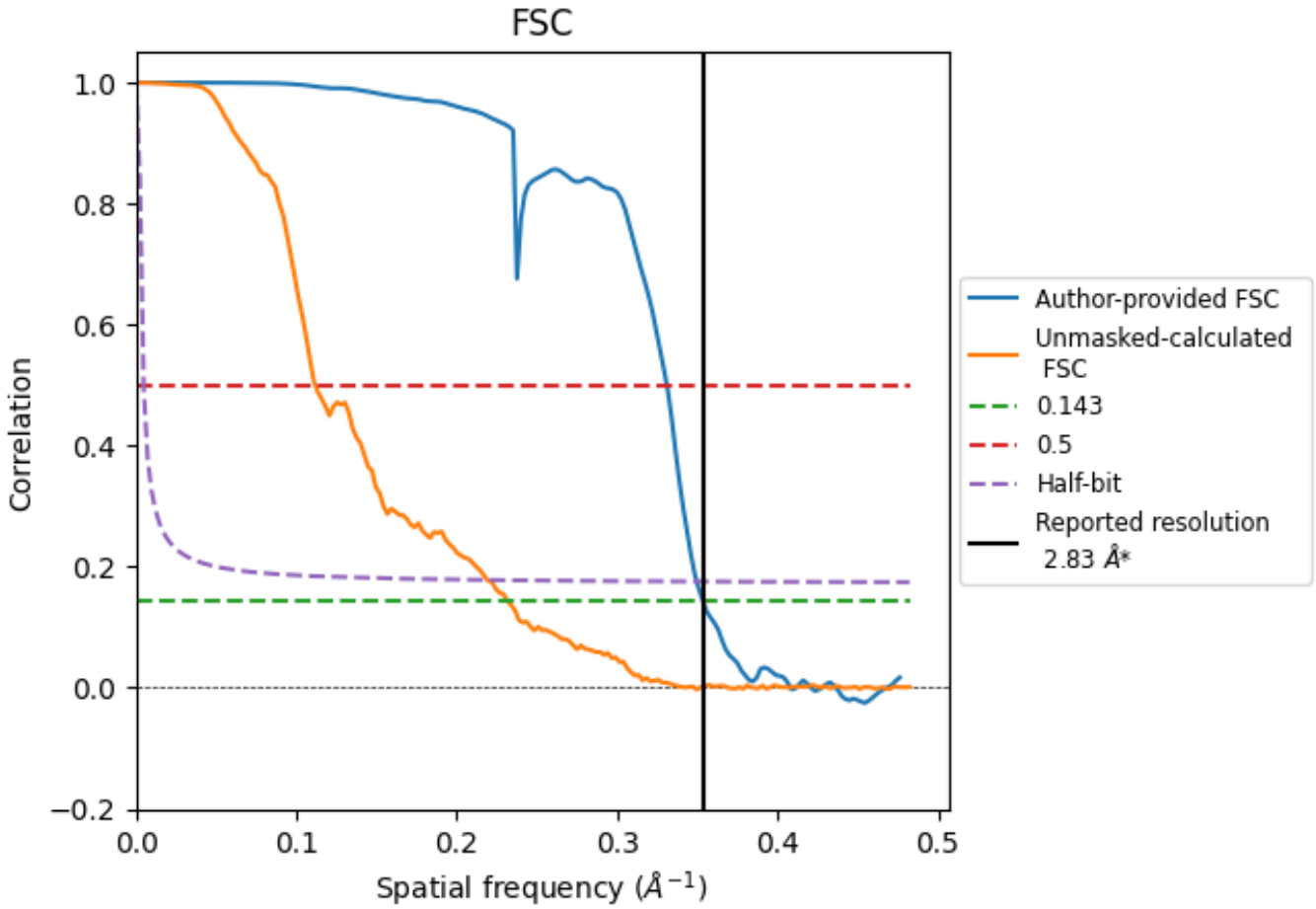


*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

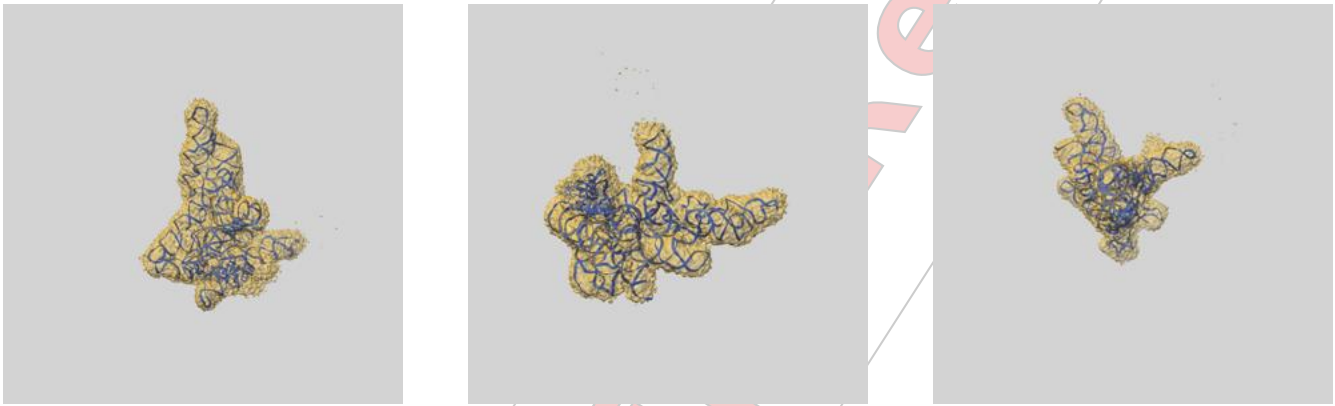
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.02	2.86
Unmasked-calculated*	4.32	8.95	4.57

*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 4.32 differs from the reported value 2.83 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70946 and PDB model 9OWW. Per-residue inclusion information can be found in section 3 on page 4.

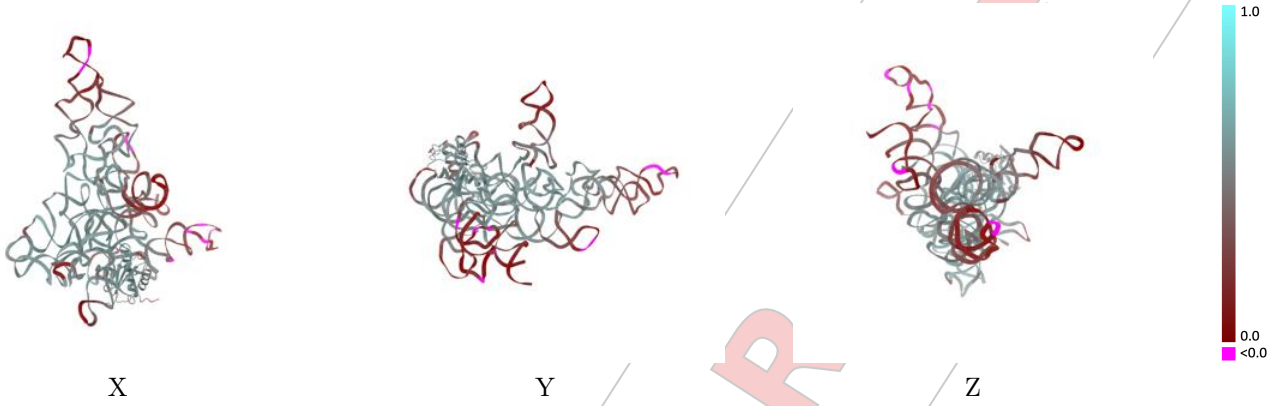
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

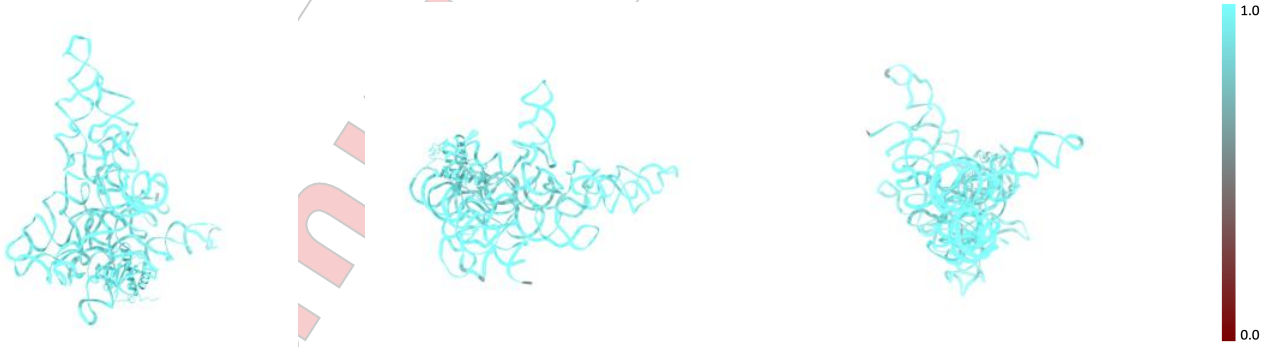
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

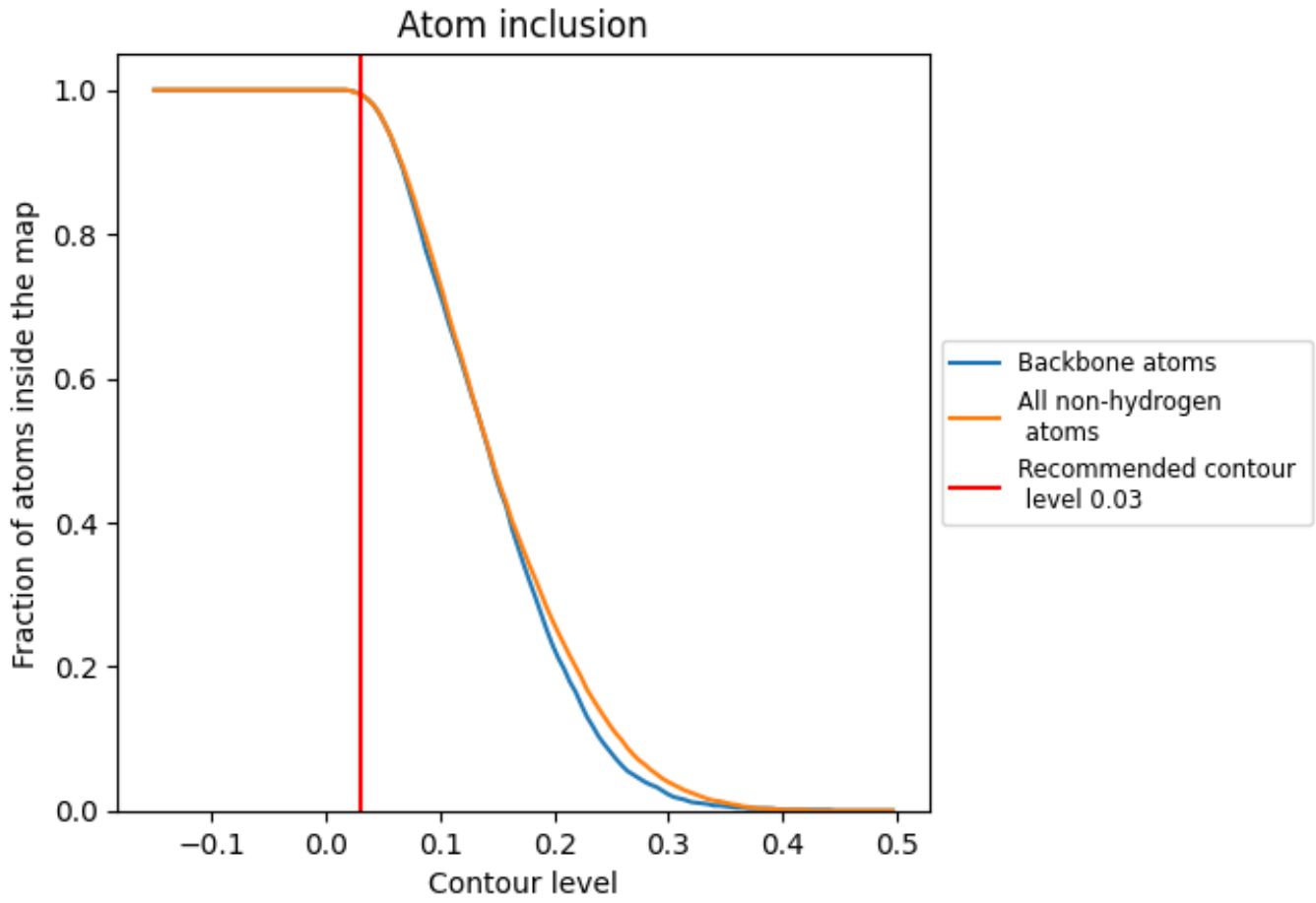
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.4370
A	0.9950	0.4290
B	0.9890	0.5200
C	0.9950	0.4310

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 04:41 PM EDT

PDB ID	:	9OWX / pdb_00009owx
EMDB ID	:	EMD-70947
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with the precursor tRNA with loop-back 5' leader (sub-conformation 1 of tRNA anticodon arm tilted)
Deposited on	:	2025-06-02
Resolution	:	2.70 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

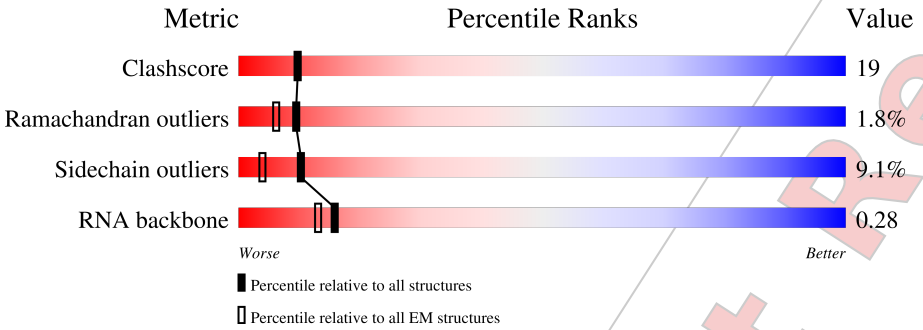
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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 <=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	417	30% 45% 23%
2	B	116	71% 23%
3	C	111	26% 44% 26%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12229 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor RNA (108-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	108	2293	1022	397	766	108	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

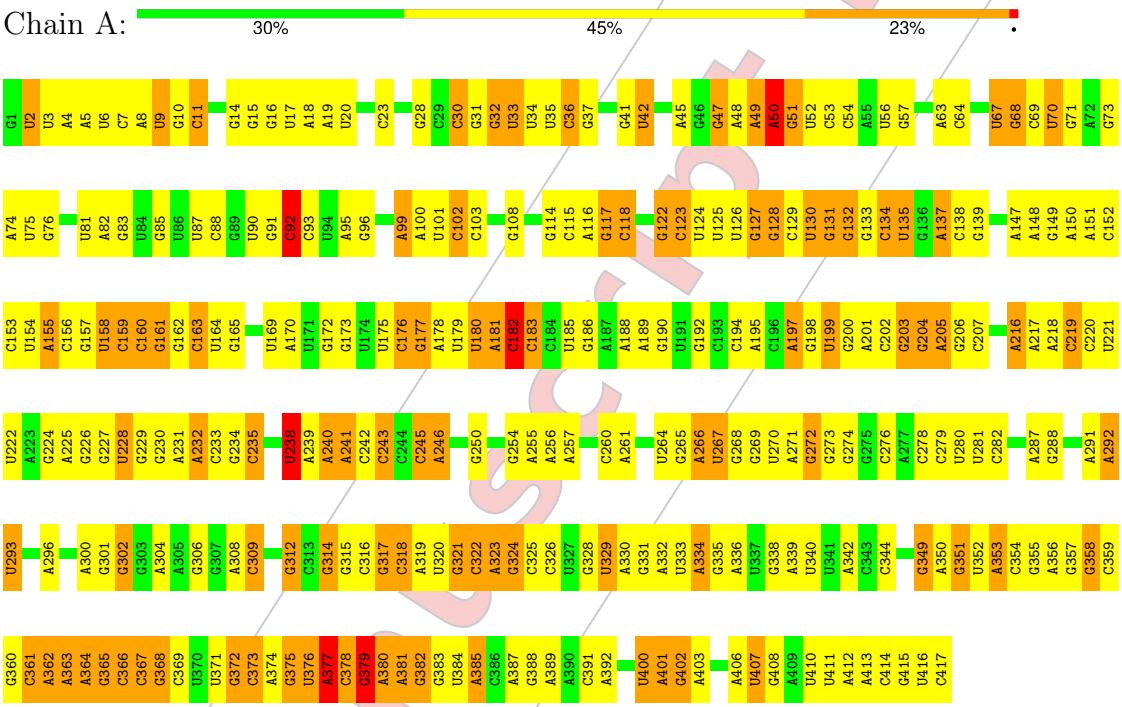
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	26	26	26	0
4	C	1	Total	Ca	0
			1	1	

3 Residue-property plots (i)

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.

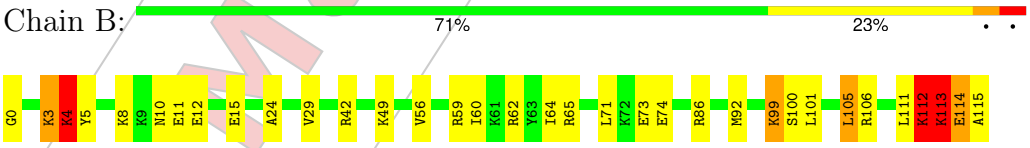
• Molecule 1: RNase P RNA (417-MER)

Chain A:



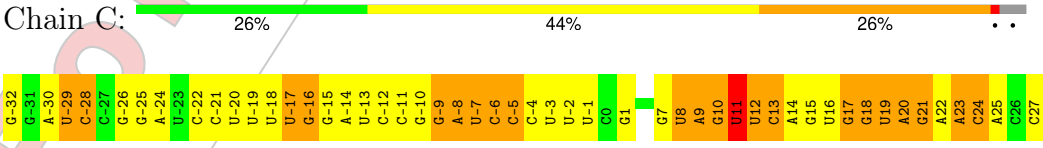
• Molecule 2: Ribonuclease P protein component

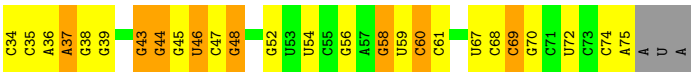
Chain B:



• Molecule 3: precursor RNA (108-MER)

Chain C:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	508154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.537	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.55	0/10038	0.90	10/15661 (0.1%)
2	B	0.57	1/962 (0.1%)	0.73	1/1281 (0.1%)
3	C	0.73	1/2558 (0.0%)	0.91	5/3984 (0.1%)
All	All	0.59	2/13558 (0.0%)	0.89	16/20926 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	11	U	O3'-P	24.79	1.98	1.61
2	B	100	SER	CA-CB	-6.89	1.42	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	11	U	O3'-P-O5'	10.03	119.05	104.00
1	A	377	A	C4'-C3'-C2'	-6.51	96.09	102.60
3	C	46	U	C2'-C3'-O3'	6.20	118.79	109.50
3	C	-5	C	O3'-P-O5'	-6.16	94.76	104.00
1	A	182	C	C4'-C3'-C2'	-5.91	96.69	102.60
1	A	379	G	O3'-P-O5'	-5.86	95.22	104.00
1	A	92	C	O3'-P-O5'	-5.82	95.27	104.00
3	C	69	C	C4'-C3'-C2'	-5.70	96.90	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	U	O3'-P-O5'	-5.62	95.57	104.00
3	C	69	C	O3'-P-O5'	-5.61	95.59	104.00
1	A	176	C	C2'-C3'-O3'	5.54	122.01	113.70
1	A	50	A	O3'-P-O5'	-5.26	96.10	104.00
1	A	238	U	O3'-P-O5'	-5.26	96.11	104.00
1	A	50	A	C4'-C3'-O3'	-5.17	105.24	113.00
1	A	240	A	C4'-C3'-C2'	-5.09	97.51	102.60
2	B	4	LYS	N-CA-C	-5.07	105.94	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8962	0	4510	275	0
2	B	947	0	1008	32	0
3	C	2293	0	1162	51	0
4	A	26	0	0	1	0
4	C	1	0	0	0	0
All	All	12229	0	6680	344	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 19.

All (344) 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:158:U:H3'	1:A:159:C:C6	1.40	1.55
1:A:158:U:C3'	1:A:159:C:C6	2.17	1.28
3:C:11:U:O3'	3:C:12:U:P	1.98	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:U:O3'	1:A:159:C:O4'	1.57	1.19
2:B:86:ARG:HH12	3:C:-32:G:H1'	1.21	1.05
1:A:364:A:C4	1:A:365:G:H1'	1.96	0.99
2:B:105:LEU:HB3	2:B:111:LEU:HG	1.51	0.92
1:A:378:C:H3'	1:A:379:G:H8	1.35	0.92
1:A:158:U:C3'	1:A:159:C:H6	1.63	0.92
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.90
1:A:350:A:H1'	1:A:380:A:C2	2.10	0.85
1:A:363:A:H2'	1:A:364:A:C4	2.12	0.83
1:A:158:U:H2'	1:A:159:C:C1'	2.09	0.82
2:B:106:ARG:HH11	2:B:113:LYS:HA	1.44	0.82
1:A:158:U:H2'	1:A:159:C:H1'	1.62	0.82
1:A:378:C:H3'	1:A:379:G:C8	2.14	0.82
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.81
1:A:314:G:H1	1:A:323:A:H61	1.30	0.80
1:A:315:G:H2'	1:A:316:C:C6	2.16	0.80
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.78
2:B:86:ARG:NH1	3:C:-32:G:H1'	1.99	0.77
1:A:159:C:H3'	1:A:160:C:C5	2.19	0.76
1:A:352:U:H3	1:A:377:A:H2	1.34	0.76
1:A:158:U:H2'	1:A:159:C:N1	2.01	0.75
1:A:45:A:H62	2:B:62:ARG:NH2	1.84	0.75
3:C:-10:G:H3'	3:C:-9:G:H8	1.51	0.74
1:A:14:G:H2'	1:A:385:A:N1	2.03	0.74
1:A:158:U:C2'	1:A:159:C:C1'	2.66	0.73
1:A:158:U:H3'	1:A:159:C:H6	0.94	0.73
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.73
1:A:50:A:C8	1:A:50:A:H5"	2.23	0.72
1:A:158:U:H3'	1:A:159:C:C5	2.17	0.72
1:A:350:A:H3'	1:A:351:G:C8	2.24	0.72
1:A:350:A:H3'	1:A:351:G:H8	1.56	0.71
1:A:216:A:HO2'	1:A:217:A:H8	1.39	0.70
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.68
1:A:158:U:C2'	1:A:159:C:H1'	2.23	0.68
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
1:A:349:G:H1	1:A:379:G:H1'	1.58	0.68
1:A:180:U:H2'	1:A:181:A:H8	1.59	0.68
1:A:159:C:H3'	1:A:160:C:C6	2.29	0.68
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.68
1:A:9:U:H2'	1:A:10:G:H8	1.57	0.67
3:C:23:A:H3'	3:C:24:C:H6	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:U:C2'	1:A:159:C:C6	2.77	0.67
1:A:67:U:H3	1:A:69:C:H41	1.43	0.66
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.66
1:A:308:A:N1	1:A:329:U:H5	1.95	0.65
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.65
1:A:379:G:H5"	1:A:380:A:OP1	1.96	0.65
2:B:112:LYS:O	2:B:114:GLU:N	2.31	0.64
1:A:374:A:H2'	1:A:375:G:C8	2.32	0.64
1:A:18:A:H2'	1:A:19:A:H8	1.62	0.64
3:C:11:U:C3'	3:C:12:U:P	2.86	0.64
1:A:272:G:H5"	1:A:272:G:H8	1.62	0.64
3:C:-10:G:H3'	3:C:-9:G:C8	2.33	0.64
1:A:102:C:H2'	1:A:103:C:O4'	1.99	0.63
2:B:56:VAL:O	2:B:60:ILE:HG13	2.00	0.62
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.62
1:A:160:C:O4'	1:A:160:C:OP2	2.04	0.61
1:A:308:A:N1	1:A:329:U:C5	2.69	0.61
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.61
1:A:314:G:H1	1:A:323:A:N6	1.99	0.61
1:A:45:A:H62	2:B:62:ARG:HH22	1.47	0.61
1:A:82:A:OP2	4:A:526:CA:CA	1.78	0.61
1:A:203:G:C5	1:A:205:A:H1'	2.36	0.61
3:C:-7:U:H2'	3:C:-6:C:C6	2.35	0.61
1:A:350:A:H1'	1:A:380:A:N1	2.15	0.60
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.84	0.60
2:B:113:LYS:C	2:B:115:ALA:H	2.08	0.60
1:A:360:G:H22	1:A:363:A:H5"	1.67	0.59
1:A:161:G:H4'	1:A:163:C:H5	1.65	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.59
1:A:350:A:H1'	1:A:380:A:C6	2.37	0.59
1:A:385:A:H8	1:A:400:U:HO2'	1.47	0.59
2:B:4:LYS:HD3	2:B:5:TYR:HE1	1.68	0.58
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.58
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.58
1:A:147:A:H61	1:A:177:G:H2'	1.68	0.58
3:C:-17:U:H3'	3:C:-16:G:H8	1.68	0.58
1:A:158:U:O3'	1:A:159:C:H6	1.87	0.58
1:A:159:C:H2'	1:A:159:C:O2	2.03	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:158:U:C3'	1:A:159:C:O4'	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:G:C5	1:A:316:C:C4	2.91	0.58
1:A:16:G:N2	1:A:344:C:H1'	2.19	0.57
2:B:112:LYS:O	2:B:113:LYS:C	2.47	0.57
1:A:32:G:H22	1:A:34:U:H1'	1.68	0.57
1:A:272:G:H5"	1:A:272:G:C8	2.40	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:350:A:C2	1:A:380:A:H1'	2.39	0.57
2:B:74:GLU:OE1	2:B:111:LEU:HD22	2.05	0.56
1:A:3:U:H2'	1:A:4:A:H8	1.68	0.56
1:A:10:G:H2'	1:A:11:C:H6	1.70	0.56
1:A:148:A:H61	1:A:177:G:H1'	1.71	0.56
1:A:308:A:C2	1:A:329:U:H5	2.23	0.56
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:315:G:H2'	1:A:316:C:H6	1.67	0.56
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.56
1:A:241:A:H2'	1:A:242:C:C6	2.41	0.56
2:B:4:LYS:HD3	2:B:5:TYR:CE1	2.40	0.56
1:A:380:A:C6	1:A:381:A:C5	2.94	0.56
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.56
1:A:385:A:H1'	1:A:401:A:C8	2.41	0.56
1:A:16:G:C2	1:A:344:C:C2	2.94	0.56
1:A:158:U:C2'	1:A:159:C:N1	2.69	0.56
1:A:364:A:H3'	1:A:364:A:OP2	2.06	0.56
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.56
1:A:412:A:H2'	1:A:413:A:C8	2.42	0.55
1:A:5:A:H2'	1:A:6:U:C6	2.41	0.55
3:C:-15:G:H2'	3:C:-14:A:H8	1.70	0.55
3:C:27:C:H2'	3:C:28:A:C8	2.41	0.55
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.55
1:A:5:A:H2'	1:A:6:U:H6	1.71	0.55
1:A:364:A:OP1	1:A:365:G:N7	2.36	0.54
1:A:99:A:H2'	1:A:100:A:C8	2.41	0.54
3:C:10:G:N3	3:C:10:G:H2'	2.23	0.54
1:A:197:A:H2'	1:A:228:U:O2'	2.06	0.54
2:B:106:ARG:HH11	2:B:113:LYS:CA	2.16	0.54
1:A:161:G:H4'	1:A:163:C:C5	2.42	0.54
1:A:381:A:C2	1:A:382:G:H1'	2.42	0.54
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.54
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.54
1:A:218:A:C5	1:A:219:C:H1'	2.43	0.53
1:A:36:C:H2'	1:A:37:G:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-8:A:H2'	3:C:-7:U:O4'	2.08	0.53
3:C:15:G:H2'	3:C:58:G:H1	1.74	0.53
1:A:14:G:H2'	1:A:385:A:C6	2.44	0.53
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.53
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.53
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.53
1:A:154:U:H2'	1:A:155:A:C5	2.44	0.52
1:A:159:C:H3'	1:A:160:C:C4	2.44	0.52
1:A:264:U:H2'	1:A:265:G:O4'	2.09	0.52
1:A:216:A:O2'	1:A:217:A:H8	1.93	0.52
3:C:8:U:H5'	3:C:48:G:H5'	1.91	0.52
3:C:9:A:C2	3:C:44:G:H1'	2.44	0.52
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.52
1:A:229:G:N2	1:A:231:A:H3'	2.25	0.52
1:A:154:U:H2'	1:A:155:A:C4	2.45	0.52
1:A:49:A:N1	1:A:387:A:O2'	2.37	0.51
1:A:134:C:H2'	1:A:135:U:C6	2.45	0.51
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.51
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.51
1:A:158:U:O3'	1:A:159:C:C6	2.62	0.51
1:A:64:C:O2'	1:A:82:A:N1	2.42	0.51
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.51
1:A:169:U:H2'	1:A:170:A:H8	1.76	0.51
1:A:147:A:N6	1:A:177:G:H2'	2.26	0.51
3:C:-13:U:H2'	3:C:-12:C:C6	2.46	0.50
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.50
1:A:317:G:N1	1:A:321:G:C2	2.79	0.50
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.50
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.50
1:A:373:C:H2'	1:A:374:A:C8	2.47	0.50
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.50
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.50
3:C:-22:C:H2'	3:C:-21:C:C6	2.47	0.50
1:A:350:A:H1'	1:A:380:A:C4	2.46	0.50
3:C:8:U:O2	3:C:20:A:H2	1.95	0.49
1:A:180:U:H2'	1:A:181:A:C8	2.45	0.49
1:A:92:C:H2'	1:A:93:C:C6	2.47	0.49
1:A:158:U:C3'	1:A:159:C:C1'	2.90	0.49
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.49
1:A:147:A:H2'	1:A:148:A:C8	2.48	0.49
1:A:169:U:H2'	1:A:170:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.49
3:C:-30:A:H2'	3:C:-29:U:O4'	2.12	0.49
1:A:377:A:C2	1:A:378:C:H1'	2.48	0.49
1:A:267:U:C2	3:C:75:A:C2	3.01	0.49
1:A:19:A:H2'	1:A:20:U:C6	2.48	0.48
1:A:401:A:H2'	1:A:402:G:O4'	2.13	0.48
3:C:24:C:H2'	3:C:25:A:O4'	2.13	0.48
1:A:23:C:O2	1:A:336:A:O2'	2.28	0.48
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.48
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.48
3:C:-29:U:H2'	3:C:-28:C:O4'	2.13	0.48
1:A:354:C:H2'	1:A:355:G:C8	2.49	0.48
1:A:280:U:H2'	1:A:281:U:C6	2.48	0.48
3:C:12:U:H2'	3:C:13:C:O4'	2.14	0.48
1:A:132:G:H3'	1:A:133:G:H8	1.79	0.48
1:A:301:G:C2'	1:A:302:G:H5'	2.43	0.48
3:C:23:A:H3'	3:C:24:C:C6	2.46	0.48
3:C:17:G:O6	3:C:54:U:H1'	2.14	0.48
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.48
1:A:180:U:O2'	1:A:181:A:H5'	2.13	0.48
1:A:378:C:H2'	1:A:379:G:O4'	2.13	0.48
1:A:280:U:H2'	1:A:281:U:H6	1.79	0.47
1:A:349:G:N2	1:A:380:A:C8	2.82	0.47
1:A:411:U:H2'	1:A:412:A:C8	2.48	0.47
1:A:268:G:O6	3:C:75:A:N6	2.47	0.47
3:C:21:G:H2'	3:C:22:A:C8	2.49	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.47
1:A:137:A:H8	1:A:137:A:H5"	1.79	0.47
1:A:335:G:C8	1:A:335:G:H3'	2.49	0.47
1:A:47:G:H1	1:A:385:A:H62	1.63	0.47
1:A:338:G:H2'	1:A:339:A:H8	1.80	0.47
2:B:105:LEU:CB	2:B:111:LEU:HG	2.34	0.47
1:A:371:U:H4'	1:A:373:C:H5	1.79	0.47
1:A:160:C:O4'	1:A:160:C:P	2.72	0.46
1:A:363:A:O2'	1:A:364:A:O4'	2.33	0.46
2:B:111:LEU:O	2:B:113:LYS:N	2.46	0.46
3:C:25:A:H2	3:C:43:G:H22	1.63	0.46
1:A:36:C:H2'	1:A:37:G:H8	1.80	0.46
1:A:50:A:H3'	1:A:51:G:H8	1.80	0.46
1:A:158:U:H2'	1:A:159:C:C6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:A:H2'	3:C:38:G:C8	2.51	0.46
1:A:198:G:N2	1:A:200:G:H3'	2.31	0.46
3:C:38:G:H2'	3:C:39:G:C8	2.51	0.46
1:A:158:U:C3'	1:A:159:C:N1	2.75	0.46
1:A:186:G:N1	1:A:189:A:OP2	2.41	0.46
1:A:137:A:H5"	1:A:137:A:C8	2.51	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.46
1:A:292:A:H2'	1:A:293:U:C6	2.51	0.45
1:A:315:G:C6	1:A:316:C:C4	3.03	0.45
1:A:352:U:H2'	1:A:353:A:C8	2.51	0.45
1:A:376:U:H3'	1:A:377:A:H8	1.82	0.45
3:C:-20:U:H2'	3:C:-19:U:O4'	2.16	0.45
1:A:68:G:N3	1:A:68:G:H2'	2.31	0.45
1:A:268:G:C6	3:C:75:A:N1	2.85	0.45
3:C:-13:U:H2'	3:C:-12:C:H6	1.79	0.45
3:C:11:U:H3	3:C:23:A:H61	1.64	0.45
3:C:60:C:H2'	3:C:61:C:H6	1.80	0.45
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.45
1:A:292:A:H2'	1:A:293:U:H6	1.82	0.45
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.45
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.45
1:A:114:G:H2'	1:A:115:C:C6	2.52	0.45
1:A:158:U:O3'	1:A:159:C:C1'	2.61	0.45
1:A:350:A:C1'	1:A:380:A:C6	2.99	0.45
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.45
3:C:19:U:H6	3:C:19:U:H2'	1.66	0.45
1:A:339:A:H2'	1:A:340:U:C6	2.53	0.44
1:A:350:A:H1'	1:A:380:A:C5	2.52	0.44
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.44
1:A:17:U:H2'	1:A:18:A:H8	1.82	0.44
1:A:331:G:H4'	1:A:332:A:H5'	1.98	0.44
2:B:3:LYS:HB3	2:B:8:LYS:HE3	1.99	0.44
1:A:14:G:C2'	1:A:401:A:H61	2.31	0.44
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.44
1:A:358:G:H1	1:A:366:C:H42	1.66	0.44
1:A:242:C:H2'	1:A:243:C:O4'	2.18	0.44
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.44
1:A:82:A:H2'	1:A:83:G:O4'	2.17	0.43
1:A:238:U:H4'	3:C:54:U:H5"	2.00	0.43
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.80	0.43
1:A:67:U:H3	1:A:69:C:N4	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:G:C2	1:A:326:C:C2	3.07	0.43
1:A:376:U:H2'	1:A:377:A:C8	2.53	0.43
1:A:18:A:C6	1:A:342:A:N1	2.86	0.43
1:A:217:A:H2'	1:A:218:A:O4'	2.18	0.43
1:A:355:G:H2'	1:A:356:A:C8	2.54	0.43
3:C:34:C:H2'	3:C:35:C:H6	1.83	0.43
1:A:204:G:N1	1:A:235:C:N3	2.67	0.43
1:A:123:C:H2'	1:A:124:U:O4'	2.19	0.43
1:A:160:C:OP2	1:A:160:C:C4'	2.65	0.43
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.43
1:A:159:C:O4'	1:A:159:C:P	2.72	0.43
1:A:186:G:N2	1:A:188:A:H3'	2.33	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
2:B:73:GLU:N	2:B:73:GLU:OE1	2.52	0.43
1:A:383:G:H2'	1:A:383:G:N3	2.34	0.43
1:A:50:A:N3	1:A:50:A:H2'	2.34	0.43
1:A:349:G:N1	1:A:379:G:H1'	2.31	0.43
1:A:63:A:H2'	1:A:64:C:O4'	2.19	0.43
1:A:235:C:H6	1:A:235:C:H2'	1.69	0.43
1:A:156:C:H1'	1:A:216:A:C2	2.54	0.43
1:A:200:G:C6	1:A:232:A:C5	3.07	0.43
1:A:324:G:H2'	1:A:325:C:H6	1.84	0.43
1:A:380:A:C2	1:A:381:A:C4	3.07	0.43
2:B:49:LYS:HG3	3:C:-1:U:O5'	2.19	0.43
1:A:375:G:C4	1:A:376:U:H1'	2.54	0.42
3:C:-22:C:H2'	3:C:-21:C:H6	1.83	0.42
1:A:95:A:H2'	1:A:96:G:C8	2.55	0.42
1:A:308:A:H2'	1:A:309:C:O4'	2.19	0.42
1:A:364:A:H3'	1:A:364:A:P	2.60	0.42
1:A:406:A:H2'	1:A:407:U:O4'	2.20	0.42
1:A:414:C:H2'	1:A:415:G:C8	2.53	0.42
2:B:11:GLU:O	2:B:15:GLU:HG3	2.19	0.42
1:A:17:U:H2'	1:A:18:A:C8	2.55	0.42
1:A:95:A:H2'	1:A:96:G:H8	1.85	0.42
1:A:128:G:H2'	1:A:129:C:H6	1.82	0.42
1:A:260:C:H2'	1:A:261:A:O4'	2.20	0.42
1:A:349:G:N2	1:A:350:A:N7	2.68	0.42
3:C:-11:C:C2	3:C:-10:G:C8	3.08	0.42
1:A:335:G:C8	1:A:335:G:C3'	3.03	0.42
1:A:199:U:H5	1:A:206:G:H1'	1.84	0.42
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:G:H3'	1:A:335:G:H8	1.85	0.42
3:C:35:C:H2'	3:C:36:A:O4'	2.20	0.42
1:A:155:A:H2'	1:A:156:C:C6	2.55	0.42
1:A:334:A:H62	2:B:10:ASN:ND2	2.17	0.42
1:A:380:A:H3'	1:A:381:A:H8	1.85	0.42
1:A:92:C:H2'	1:A:93:C:H6	1.85	0.41
1:A:354:C:H2'	1:A:355:G:O4'	2.19	0.41
1:A:381:A:H5"	1:A:382:G:H8	1.85	0.41
3:C:18:G:H5'	3:C:56:G:N2	2.34	0.41
1:A:10:G:C6	1:A:406:A:N1	2.88	0.41
1:A:115:C:H2'	1:A:116:A:H8	1.85	0.41
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.41
2:B:49:LYS:HD2	3:C:-1:U:H5'	2.02	0.41
3:C:27:C:H2'	3:C:28:A:H8	1.85	0.41
1:A:279:C:H2'	1:A:280:U:C6	2.55	0.41
1:A:353:A:H2'	1:A:354:C:O4'	2.21	0.41
1:A:9:U:C2	1:A:10:G:C8	3.09	0.41
1:A:41:G:H2'	1:A:42:U:O4'	2.20	0.41
1:A:157:G:H2'	1:A:158:U:O4'	2.20	0.41
1:A:221:U:H2'	1:A:222:U:C6	2.55	0.41
1:A:245:C:H2'	1:A:246:A:C8	2.55	0.41
1:A:334:A:H62	2:B:10:ASN:HD22	1.68	0.41
1:A:377:A:C6	1:A:378:C:H1'	2.55	0.41
1:A:45:A:H2	1:A:388:G:H2'	1.82	0.41
1:A:56:U:H2'	1:A:57:G:H8	1.85	0.41
1:A:148:A:H3'	1:A:149:G:H8	1.86	0.41
1:A:266:A:N3	1:A:266:A:H2'	2.36	0.41
1:A:381:A:H5"	1:A:382:G:C8	2.56	0.41
3:C:18:G:N2	3:C:56:G:H1'	2.36	0.41
1:A:133:G:C2'	1:A:134:C:H5'	2.50	0.41
1:A:182:C:C2'	1:A:183:C:H5'	2.50	0.41
1:A:315:G:C2	1:A:323:A:C2	3.08	0.41
2:B:113:LYS:C	2:B:115:ALA:N	2.74	0.41
1:A:148:A:N6	1:A:177:G:H1'	2.33	0.41
1:A:180:U:C2'	1:A:181:A:H5'	2.51	0.41
1:A:199:U:O2	1:A:199:U:O4'	2.38	0.41
1:A:281:U:H2'	1:A:282:C:H6	1.86	0.41
1:A:351:G:H2'	1:A:352:U:C6	2.56	0.41
1:A:356:A:H3'	1:A:357:G:C8	2.56	0.41
2:B:99:LYS:HB2	2:B:99:LYS:HE3	1.71	0.41
3:C:67:U:H2'	3:C:68:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:A:H1'	3:C:18:G:N7	2.36	0.40
1:A:287:A:H3'	1:A:288:G:H8	1.85	0.40
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.40
3:C:10:G:H3'	3:C:11:U:C6	2.56	0.40
1:A:19:A:H2'	1:A:20:U:H6	1.85	0.40
1:A:159:C:H5"	1:A:160:C:N4	2.36	0.40
1:A:350:A:C5	1:A:380:A:C8	3.09	0.40
1:A:352:U:H2'	1:A:353:A:H8	1.86	0.40
1:A:117:G:H3'	1:A:118:C:H6	1.86	0.40
1:A:32:G:H3'	1:A:33:U:C6	2.57	0.40
1:A:268:G:C6	3:C:75:A:C6	3.10	0.40
1:A:357:G:H22	1:A:367:C:H42	1.70	0.40
2:B:101:LEU:HD12	2:B:101:LEU:HA	1.81	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
2	B	114/116 (98%)	109 (96%)	3 (3%)	2 (2%)	7 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	113	LYS
2	B	112	LYS

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
2	B	99/99 (100%)	90 (91%)	9 (9%)	7 19

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

Mol	Chain	Res	Type
2	B	3	LYS
2	B	4	LYS
2	B	71	LEU
2	B	92	MET
2	B	99	LYS
2	B	105	LEU
2	B	112	LYS
2	B	113	LYS
2	B	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN
2	B	87	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	177 (42%)	19 (4%)
3	C	107/111 (96%)	49 (45%)	9 (8%)
All	All	523/528 (99%)	226 (43%)	28 (5%)

All (226) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U
1	A	11	C
1	A	15	G

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Mol	Chain	Res	Type
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	42	U
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	53	C
1	A	54	C
1	A	67	U
1	A	68	G
1	A	70	U
1	A	74	A
1	A	75	U
1	A	76	G
1	A	85	G
1	A	87	U
1	A	88	C
1	A	90	U
1	A	91	G
1	A	92	C
1	A	99	A
1	A	101	U
1	A	102	C
1	A	108	G
1	A	117	G
1	A	118	C
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	134	C

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Mol	Chain	Res	Type
1	A	135	U
1	A	137	A
1	A	138	C
1	A	139	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	153	C
1	A	155	A
1	A	158	U
1	A	159	C
1	A	160	C
1	A	161	G
1	A	162	G
1	A	163	C
1	A	164	U
1	A	165	G
1	A	172	G
1	A	173	G
1	A	175	U
1	A	176	C
1	A	177	G
1	A	178	A
1	A	179	U
1	A	180	U
1	A	181	A
1	A	182	C
1	A	183	C
1	A	185	U
1	A	190	G
1	A	192	G
1	A	194	C
1	A	197	A
1	A	199	U
1	A	202	C
1	A	203	G
1	A	204	G
1	A	205	A
1	A	207	C
1	A	216	A
1	A	219	C
1	A	220	C

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Mol	Chain	Res	Type
1	A	224	G
1	A	225	A
1	A	226	G
1	A	227	G
1	A	228	U
1	A	230	G
1	A	233	C
1	A	234	G
1	A	235	C
1	A	238	U
1	A	239	A
1	A	240	A
1	A	241	A
1	A	243	C
1	A	245	C
1	A	246	A
1	A	250	G
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	266	A
1	A	267	U
1	A	269	G
1	A	270	U
1	A	271	A
1	A	272	G
1	A	273	G
1	A	274	G
1	A	276	C
1	A	278	C
1	A	291	A
1	A	292	A
1	A	293	U
1	A	296	A
1	A	300	A
1	A	302	G
1	A	304	A
1	A	306	G
1	A	309	C
1	A	312	G
1	A	314	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	349	G
1	A	351	G
1	A	353	A
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	377	A
1	A	378	C
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	384	U
1	A	385	A
1	A	389	A
1	A	391	C
1	A	392	A
1	A	400	U
1	A	401	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	402	G
1	A	403	A
1	A	407	U
1	A	408	G
1	A	410	U
3	C	-29	U
3	C	-28	C
3	C	-26	G
3	C	-25	G
3	C	-24	A
3	C	-18	U
3	C	-17	U
3	C	-16	G
3	C	-9	G
3	C	-8	A
3	C	-7	U
3	C	-6	C
3	C	-5	C
3	C	-4	C
3	C	-3	U
3	C	-2	U
3	C	1	G
3	C	7	G
3	C	8	U
3	C	9	A
3	C	10	G
3	C	11	U
3	C	12	U
3	C	13	C
3	C	14	A
3	C	16	U
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	21	G
3	C	23	A
3	C	24	C
3	C	29	C
3	C	33	G
3	C	37	A
3	C	43	G

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Mol	Chain	Res	Type
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	52	G
3	C	58	G
3	C	59	U
3	C	60	C
3	C	70	G
3	C	72	U
3	C	74	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	50	A
1	A	52	U
1	A	67	U
1	A	75	U
1	A	122	G
1	A	126	U
1	A	137	A
1	A	158	U
1	A	176	C
1	A	182	C
1	A	201	A
1	A	232	A
1	A	240	A
1	A	271	A
1	A	272	G
1	A	292	A
1	A	363	A
1	A	365	G
1	A	377	A
3	C	-26	G
3	C	-18	U
3	C	-4	C
3	C	7	G
3	C	18	G
3	C	19	U
3	C	46	U

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Mol	Chain	Res	Type
3	C	59	U
3	C	69	C

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 27 ligands modelled in this entry, 27 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	11:U	O3'	12:U	P	1.98

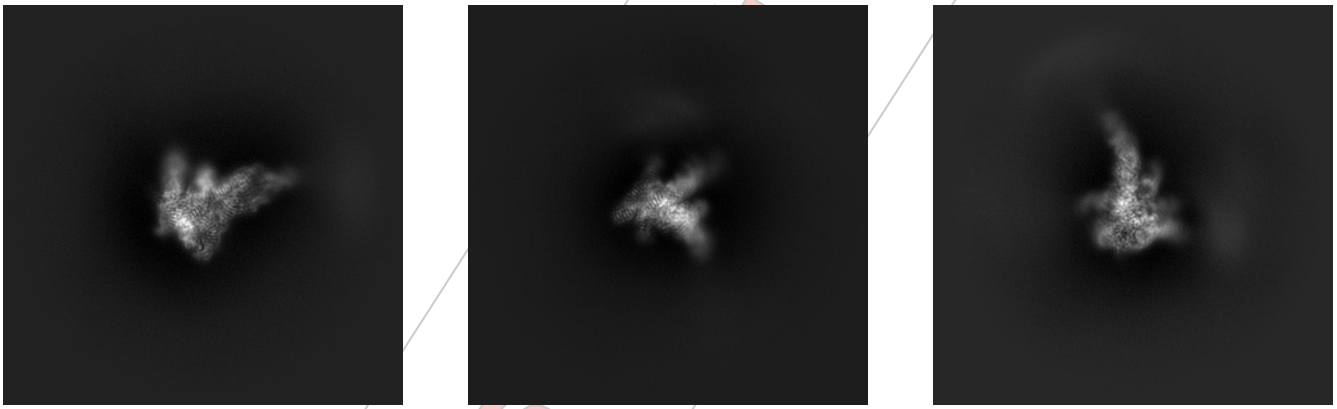
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70947. 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.

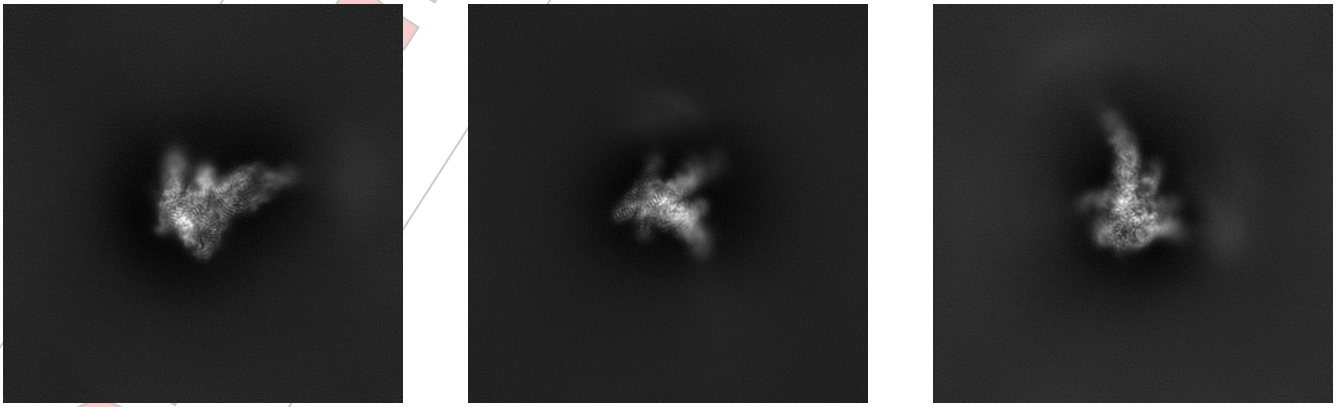
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

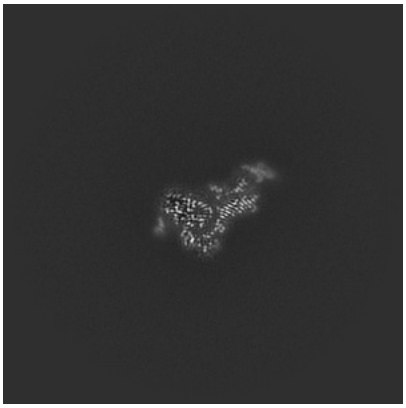


X Y Z

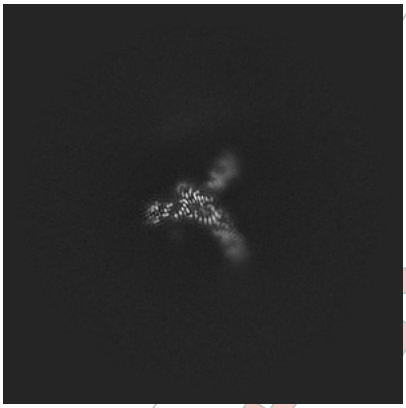
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

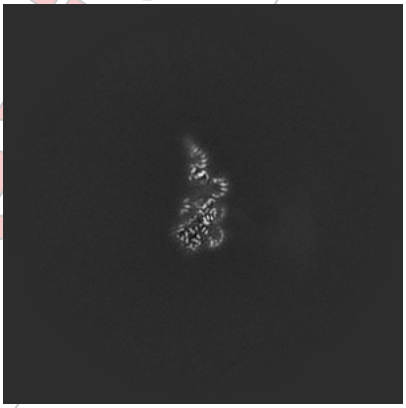
6.2.1 Primary map



X Index: 200

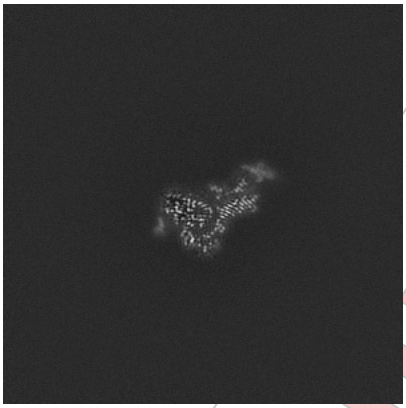


Y Index: 200

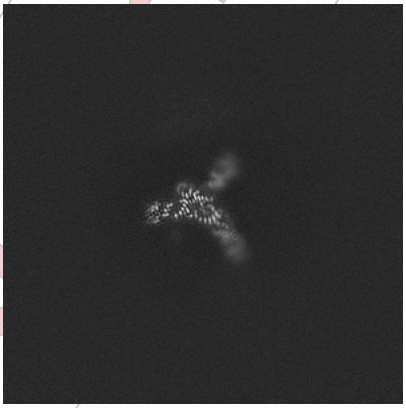


Z Index: 200

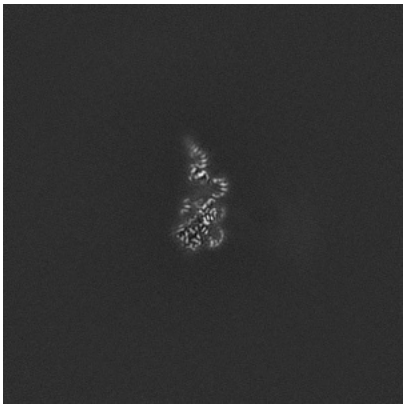
6.2.2 Raw map



X Index: 200



Y Index: 200

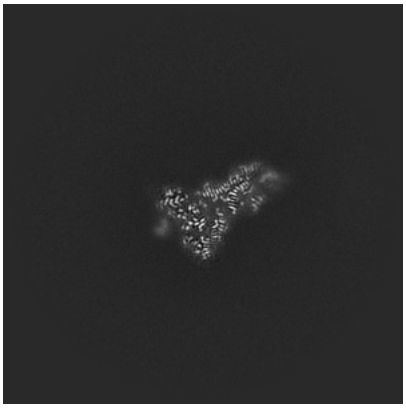


Z Index: 200

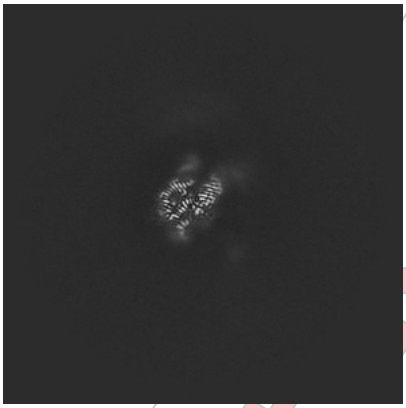
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

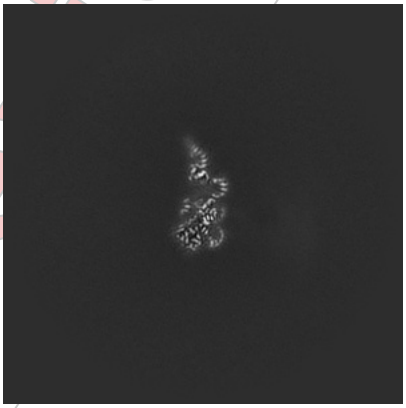
6.3.1 Primary map



X Index: 194

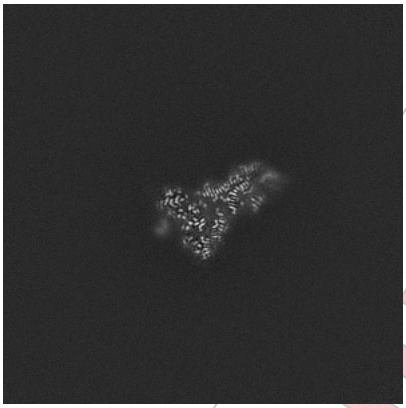


Y Index: 186

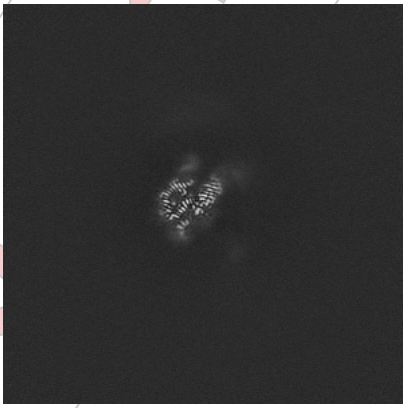


Z Index: 200

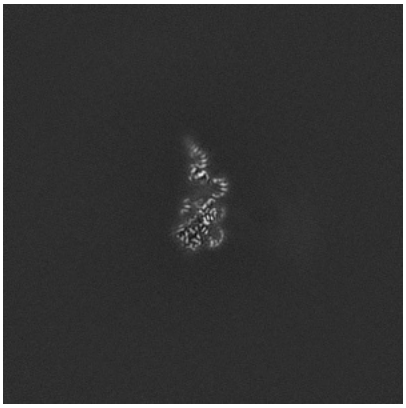
6.3.2 Raw map



X Index: 194



Y Index: 186

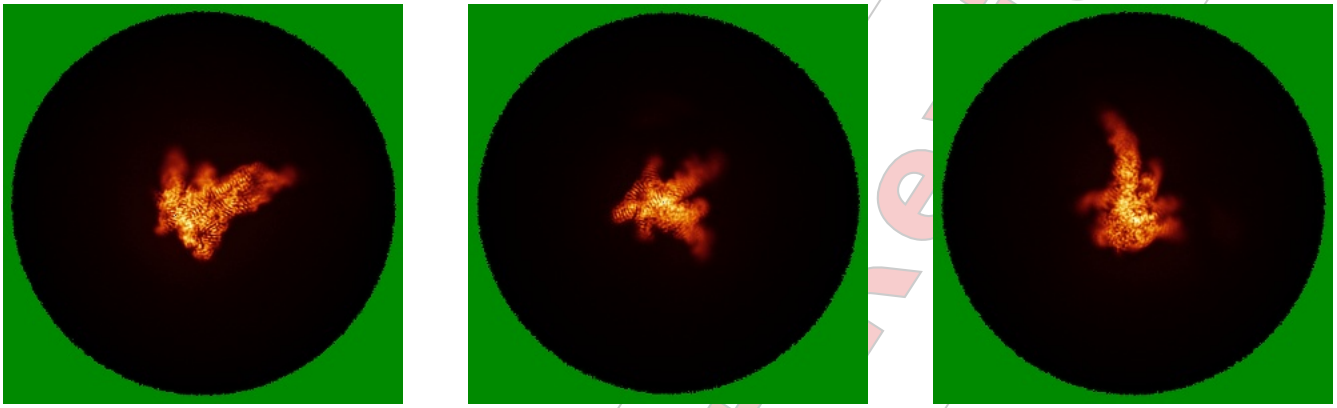


Z Index: 200

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

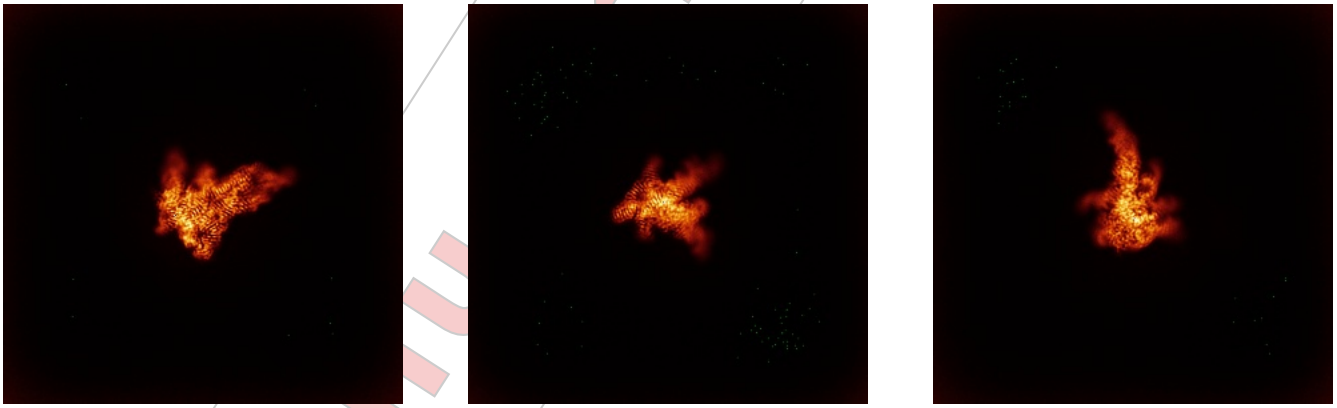
6.4 Orthogonal standard-deviation projections (False-color)

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.

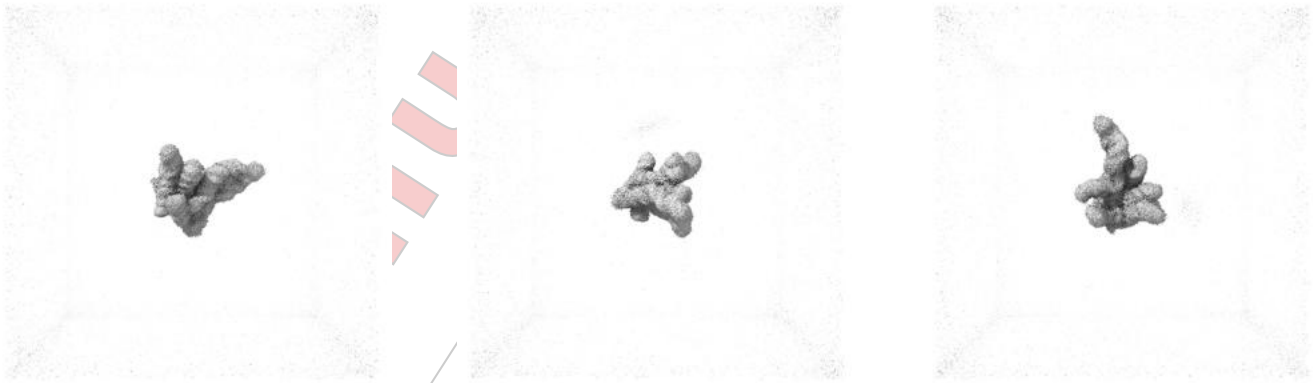
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

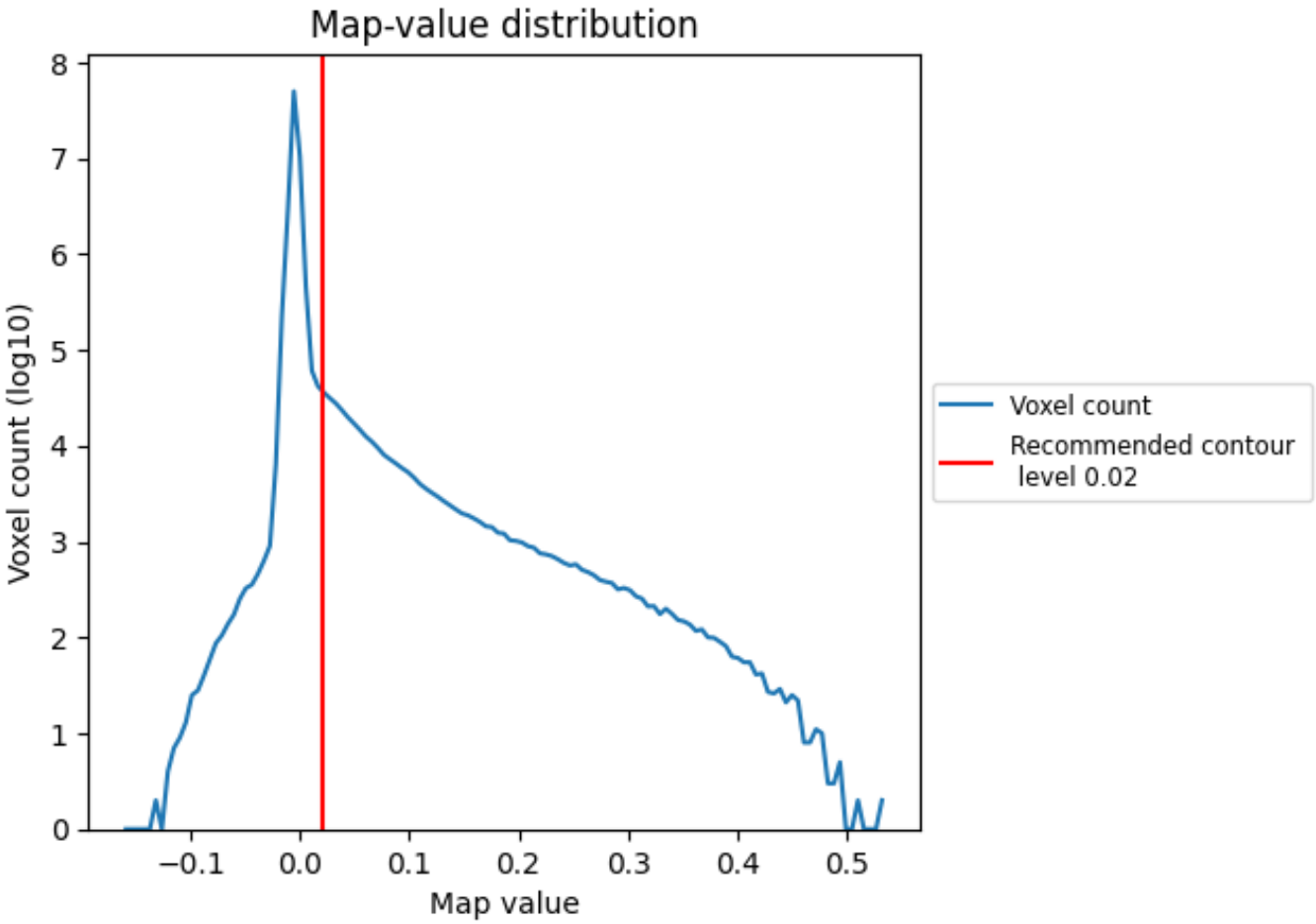
6.6 Mask visualisation (i)

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

7 Map analysis

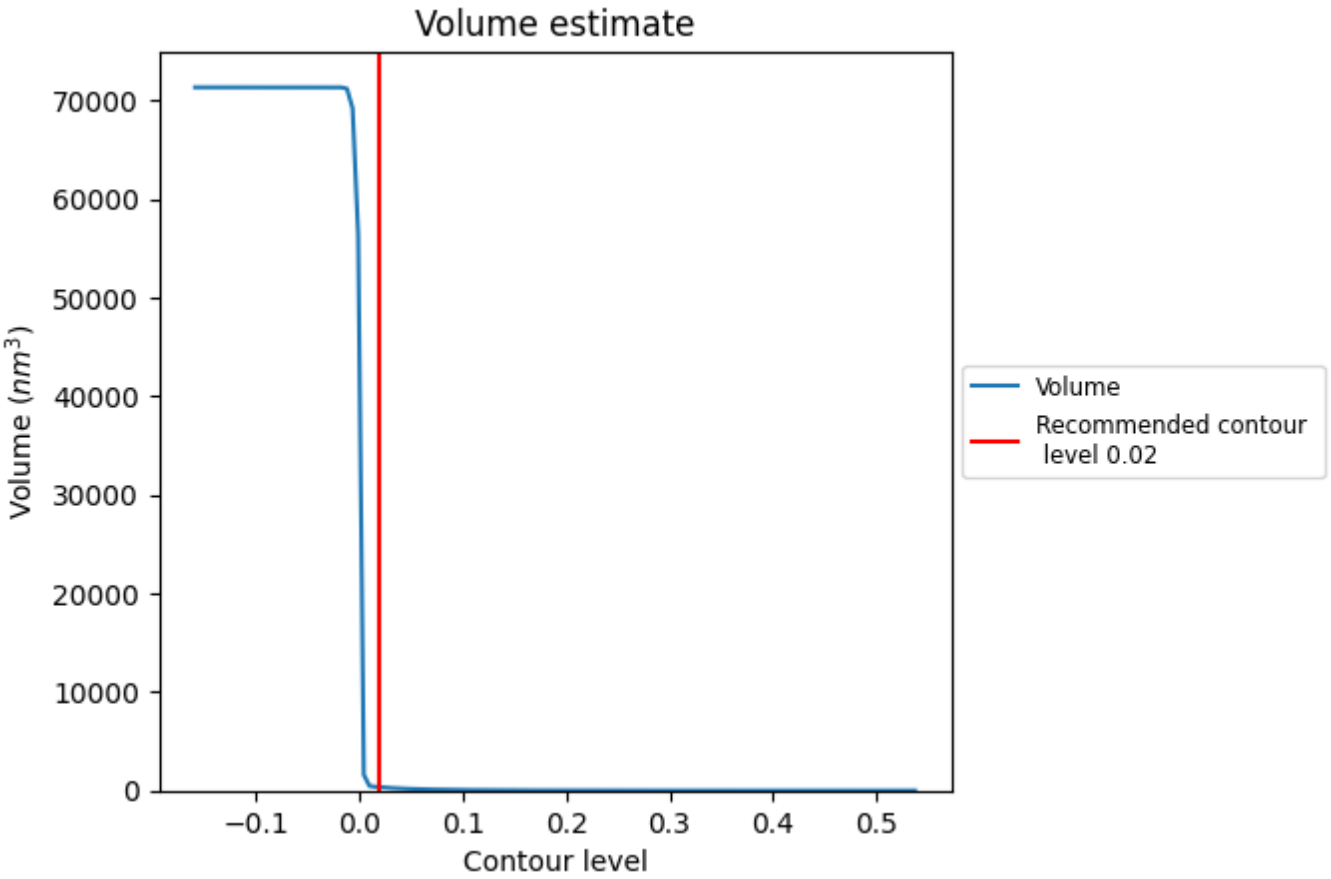
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

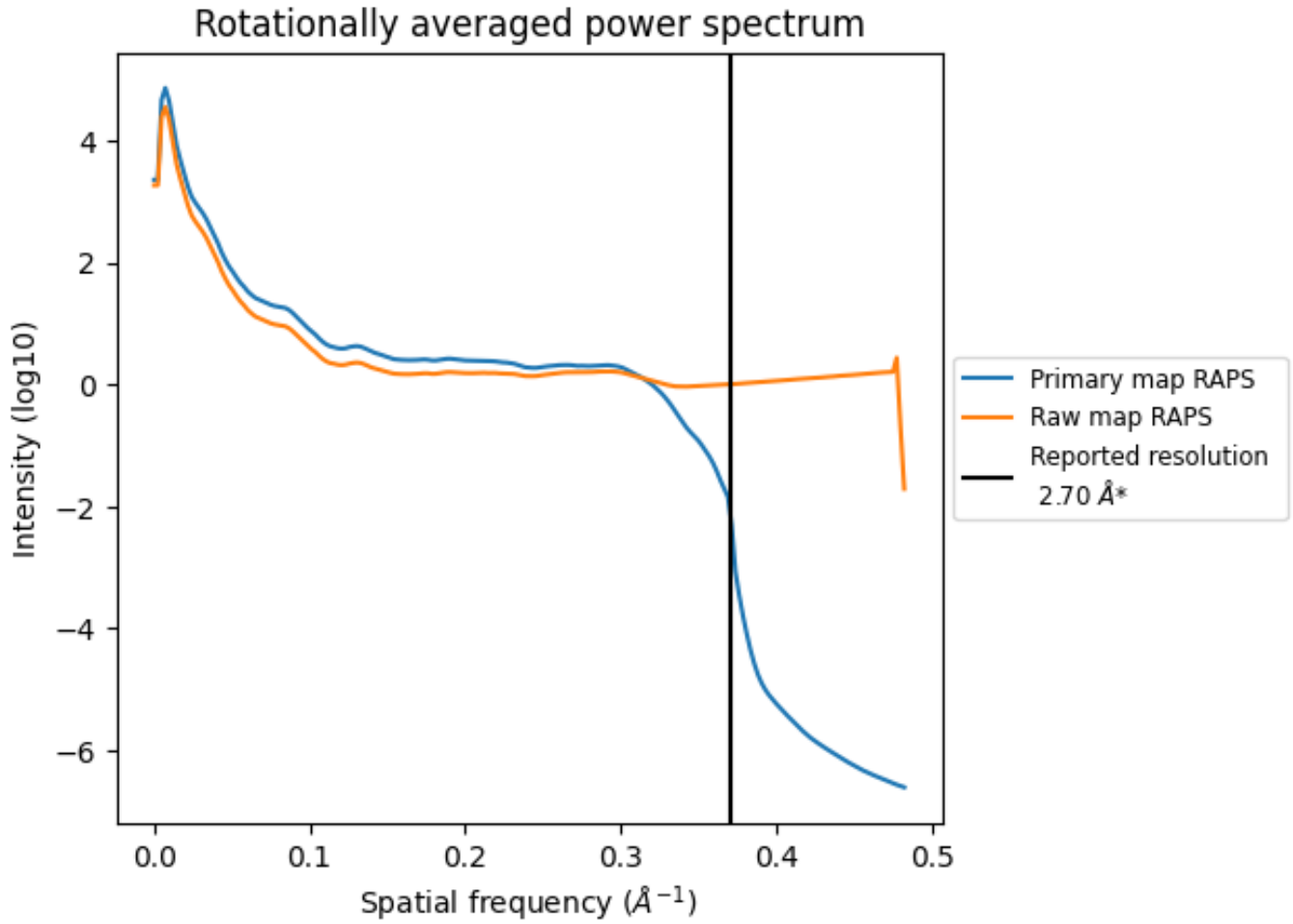
7.2 Volume estimate (i)



The volume at the recommended contour level is 340 nm^3; this corresponds to an approximate mass of 307 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 (i)

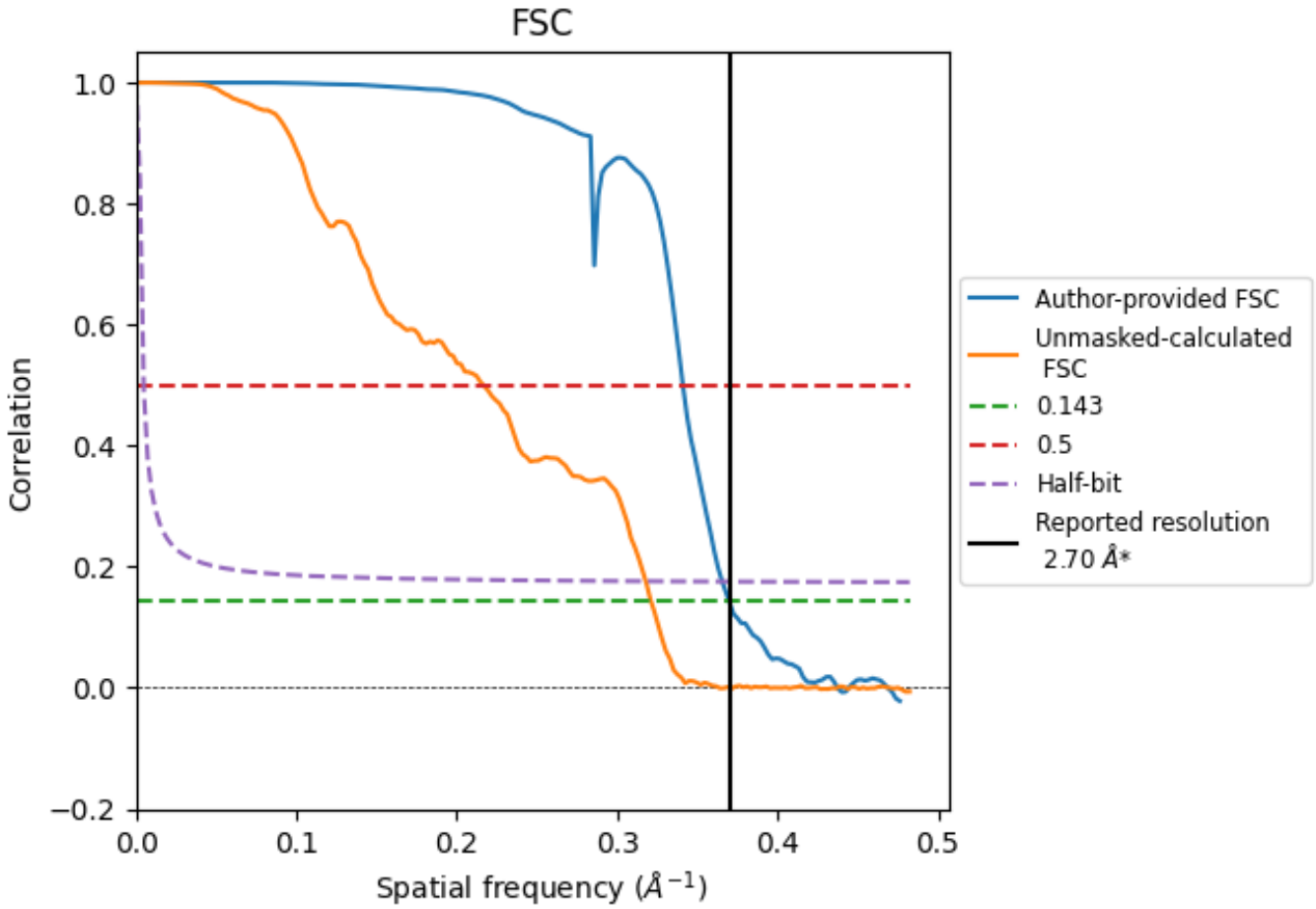


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

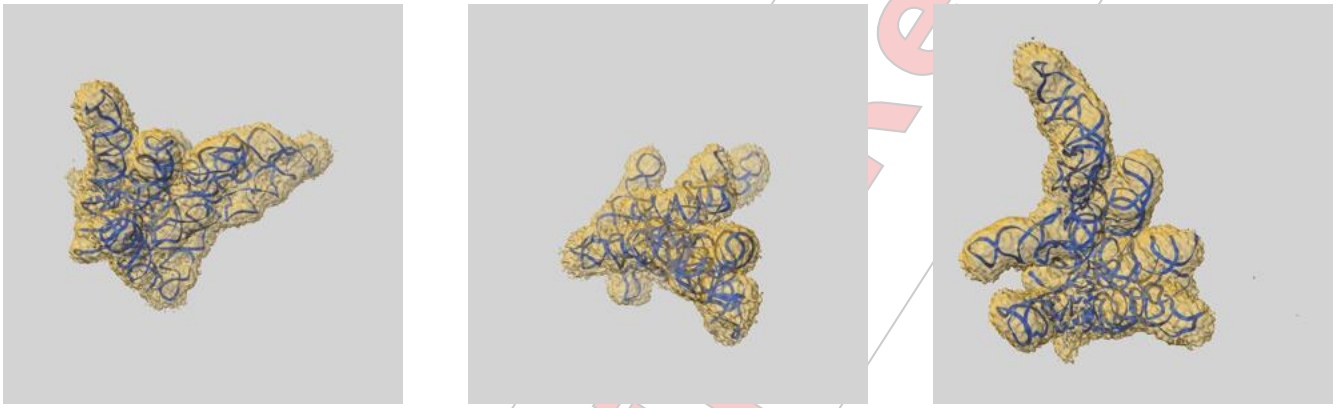
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	2.93	2.74
Unmasked-calculated*	3.12	4.62	3.15

*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 3.12 differs from the reported value 2.7 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70947 and PDB model 9OWX. Per-residue inclusion information can be found in section 3 on page 4.

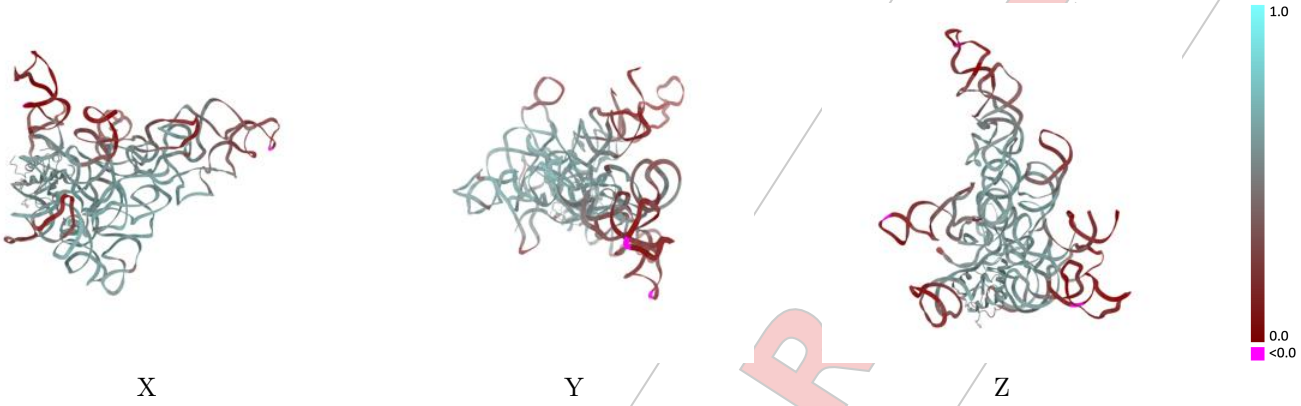
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

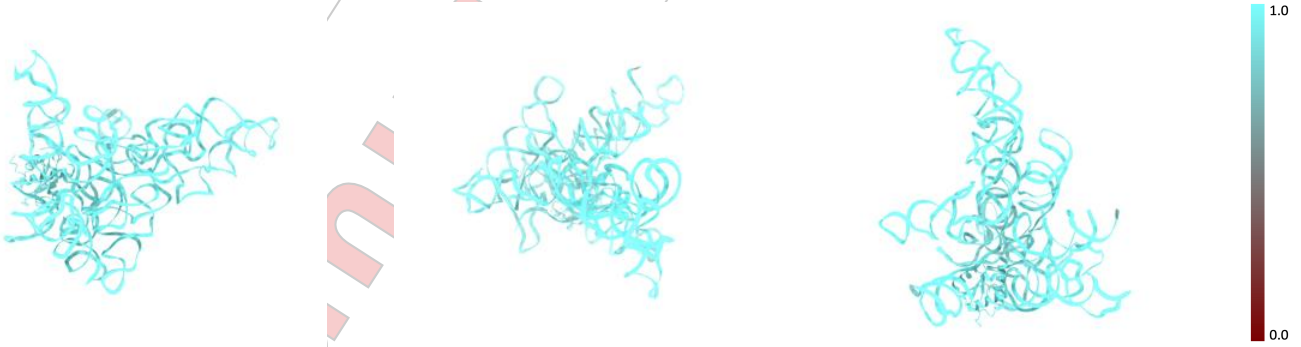
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

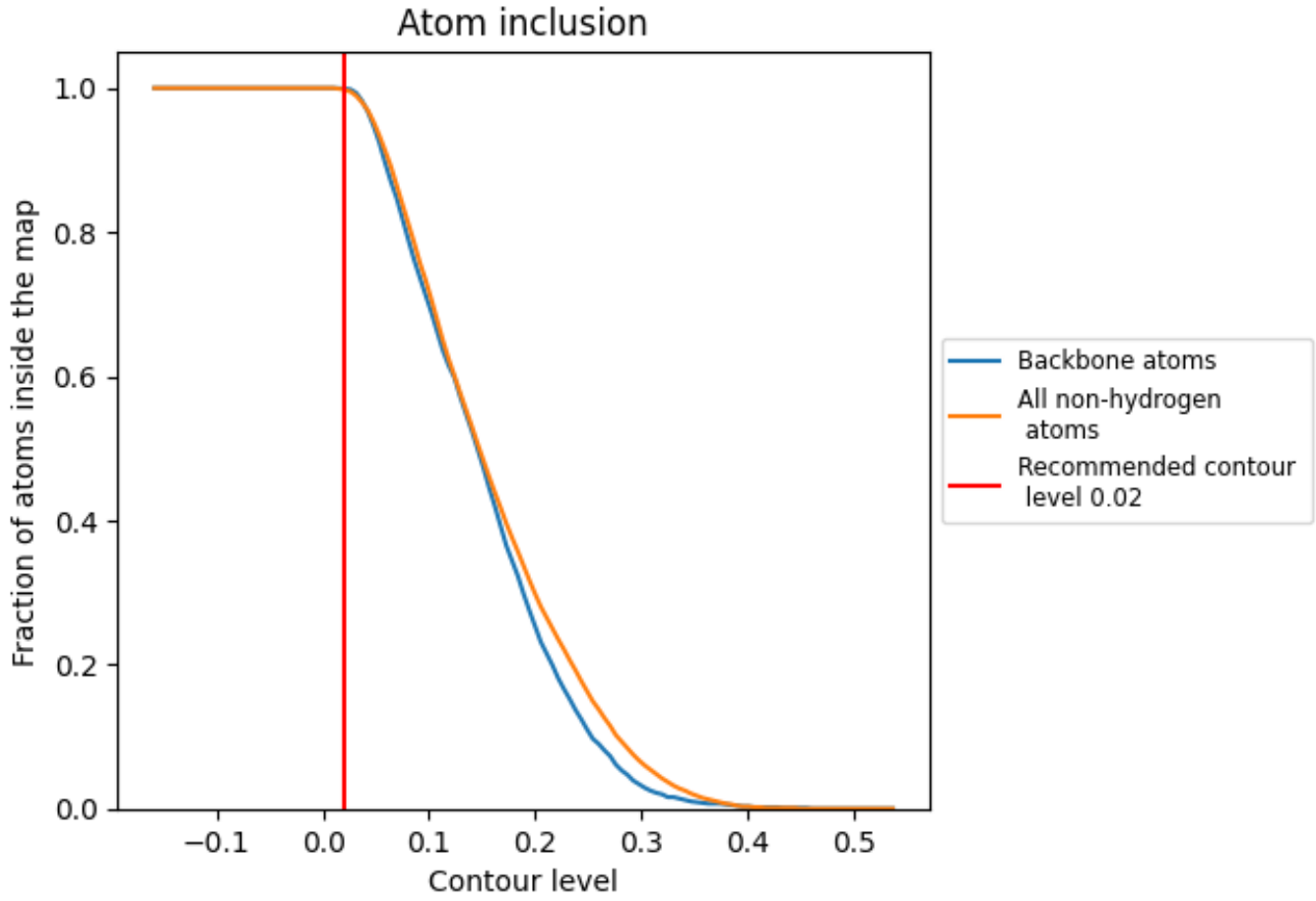
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9980	0.4660
A	0.9990	0.4690
B	0.9980	0.5510
C	0.9950	0.4210

Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 04:14 PM EDT

PDB ID	:	9OWY / pdb_00009owy
EMDB ID	:	EMD-70948
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme in complex with the precursor tRNA with loop-back 5' leader (sub-conformation 2 of tRNA anticodon arm tilted)
Deposited on	:	2025-06-02
Resolution	:	2.69 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

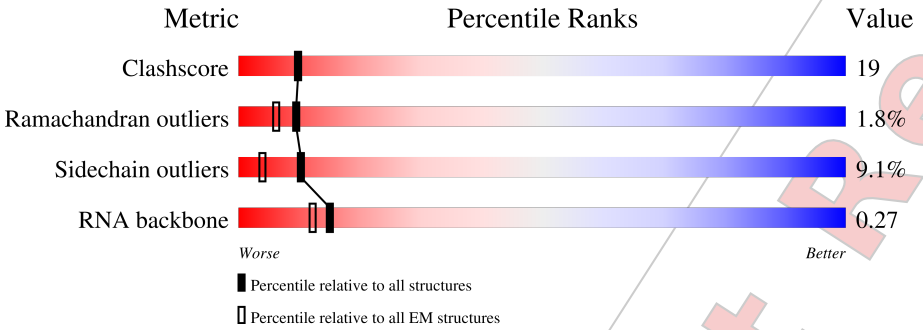
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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 <=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	417	28% 46% 25%
2	B	116	72% 22% • •
3	C	111	28% 47% 22% • •

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12231 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 RNA chain called RNase P RNA (417-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8962	3996	1660	2889	417	0	0

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor tRNA (108-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	108	2293	1022	397	766	108	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

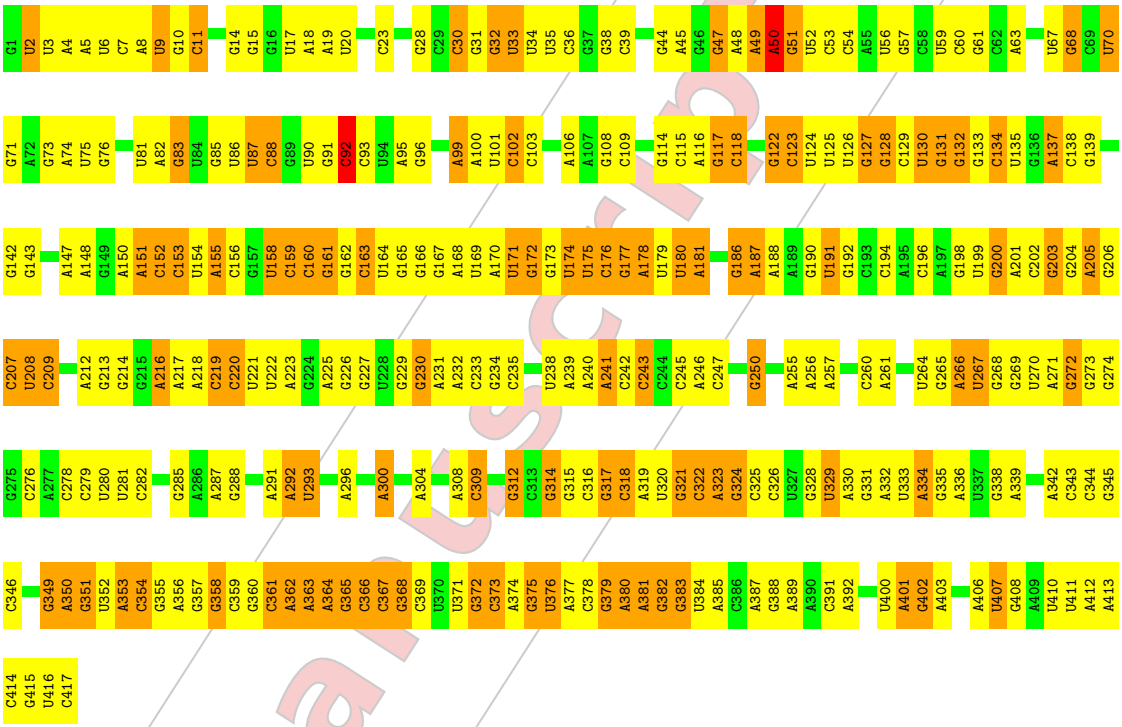
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	27	27	27	0
4	C	2	Total	Ca	0
			2	2	

3 Residue-property plots (i)

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.

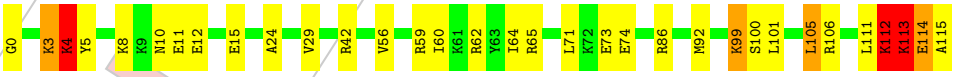
• Molecule 1: RNase P RNA (417-MER)

Chain A:



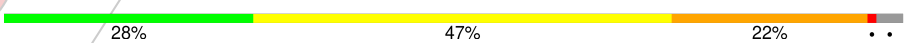
• Molecule 2: Ribonuclease P protein component

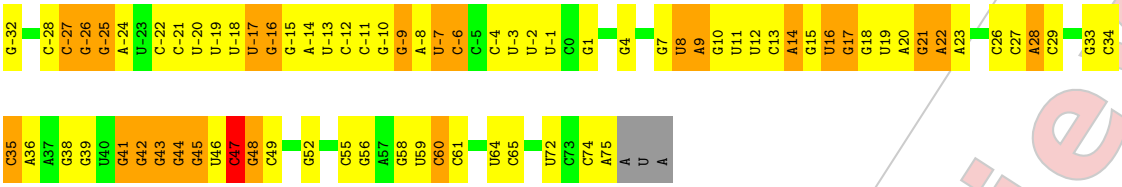
Chain B:



• Molecule 3: precursor tRNA (108-MER)

Chain C:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	483540	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.532	Depositor
Minimum map value	-0.167	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.54	0/10038	0.89	4/15661 (0.0%)
2	B	0.57	1/962 (0.1%)	0.75	1/1281 (0.1%)
3	C	0.59	0/2558	0.90	1/3984 (0.0%)
All	All	0.55	1/13558 (0.0%)	0.88	6/20926 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	SER	CA-CB	-6.88	1.42	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	C	O3'-P-O5'	-6.47	94.29	104.00
1	A	200	G	O3'-P-O5'	-5.49	95.76	104.00
1	A	50	A	O3'-P-O5'	-5.43	95.85	104.00
1	A	191	U	O3'-P-O5'	-5.43	95.86	104.00
3	C	47	C	C1'-C2'-O2'	-5.43	103.66	111.80
2	B	4	LYS	N-CA-C	-5.04	105.98	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8962	0	4510	249	0
2	B	947	0	1008	28	0
3	C	2293	0	1162	56	0
4	A	27	0	0	1	0
4	C	2	0	0	0	0
All	All	12231	0	6680	323	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 19.

All (323) 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:159:C:H6	1:A:159:C:OP2	1.10	1.26
3:C:43:G:H3'	3:C:44:G:H3'	1.26	1.16
1:A:159:C:OP2	1:A:159:C:C6	2.02	1.12
1:A:364:A:C4	1:A:365:G:H1'	1.96	0.99
2:B:105:LEU:HB3	2:B:111:LEU:HG	1.51	0.93
1:A:371:U:H5"	1:A:372:G:H5'	1.54	0.90
1:A:363:A:H2'	1:A:364:A:C4	2.13	0.83
1:A:158:U:H2'	1:A:159:C:C6	2.14	0.83
2:B:106:ARG:HH11	2:B:113:LYS:HA	1.44	0.83
1:A:367:C:H2'	1:A:368:G:C8	2.15	0.81
1:A:350:A:H3'	1:A:351:G:H8	1.45	0.81
1:A:315:G:H2'	1:A:316:C:C6	2.16	0.80
1:A:314:G:H1	1:A:323:A:H61	1.30	0.80
1:A:50:A:C8	1:A:50:A:H5"	2.18	0.78
1:A:127:G:H2'	1:A:128:G:H4'	1.66	0.78
1:A:378:C:H3'	1:A:379:G:C8	2.19	0.76
1:A:45:A:H62	2:B:62:ARG:NH2	1.84	0.75
1:A:160:C:H1'	1:A:167:G:H22	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:G:H3'	3:C:42:G:H8	1.52	0.73
3:C:43:G:H3'	3:C:44:G:C3'	2.14	0.73
1:A:45:A:C2	1:A:388:G:H2'	2.24	0.73
1:A:47:G:H1	1:A:385:A:H62	1.39	0.70
1:A:349:G:H22	1:A:379:G:H1'	1.55	0.70
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.68
1:A:364:A:C5	1:A:365:G:H1'	2.27	0.68
3:C:21:G:H2'	3:C:22:A:H5"	1.75	0.68
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.68
1:A:9:U:H2'	1:A:10:G:H8	1.57	0.67
1:A:158:U:H6	1:A:158:U:O5'	1.76	0.67
1:A:352:U:H2'	1:A:353:A:C8	2.29	0.67
1:A:364:A:H3'	1:A:365:G:O4'	1.95	0.67
1:A:174:U:H2'	1:A:175:U:C6	2.31	0.66
1:A:378:C:H3'	1:A:379:G:H8	1.59	0.66
3:C:-26:G:H2'	3:C:-25:G:H5'	1.78	0.65
3:C:27:C:H2'	3:C:28:A:C8	2.30	0.65
1:A:308:A:N1	1:A:329:U:H5	1.95	0.65
1:A:363:A:O3'	1:A:364:A:O4'	2.15	0.65
1:A:102:C:H2'	1:A:103:C:O4'	1.97	0.65
2:B:112:LYS:O	2:B:114:GLU:N	2.31	0.64
1:A:374:A:H2'	1:A:375:G:C8	2.32	0.64
1:A:18:A:H2'	1:A:19:A:H8	1.62	0.64
1:A:272:G:H5"	1:A:272:G:H8	1.62	0.64
1:A:203:G:C5	1:A:205:A:H1'	2.32	0.63
3:C:41:G:H3'	3:C:42:G:C8	2.33	0.63
1:A:350:A:H3'	1:A:351:G:C8	2.30	0.62
2:B:56:VAL:O	2:B:60:ILE:HG13	2.00	0.62
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.61
1:A:176:C:H2'	1:A:177:G:C8	2.35	0.61
1:A:308:A:N1	1:A:329:U:C5	2.69	0.61
1:A:196:C:OP2	4:A:525:CA:CA	1.77	0.61
1:A:3:U:H2'	1:A:4:A:C8	2.36	0.61
1:A:167:G:H2'	1:A:168:A:C8	2.36	0.61
1:A:314:G:H1	1:A:323:A:N6	1.99	0.61
1:A:45:A:H62	2:B:62:ARG:HH22	1.47	0.61
1:A:159:C:H5'	1:A:161:G:N1	2.16	0.60
3:C:42:G:H2'	3:C:43:G:C8	2.37	0.60
1:A:360:G:H22	1:A:363:A:H5"	1.67	0.60
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.84	0.60
1:A:154:U:O2'	1:A:217:A:N3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:G:H2'	1:A:166:G:C8	2.37	0.59
1:A:379:G:H4'	1:A:380:A:H8	1.66	0.59
1:A:379:G:H4'	1:A:380:A:C8	2.37	0.59
2:B:113:LYS:C	2:B:115:ALA:H	2.08	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
3:C:11:U:H2'	3:C:12:U:C6	2.38	0.59
3:C:9:A:N6	3:C:22:A:C8	2.69	0.59
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.58
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.58
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.58
2:B:4:LYS:HD3	2:B:5:TYR:HE1	1.68	0.58
3:C:-17:U:H3'	3:C:-16:G:H8	1.68	0.58
1:A:315:G:C5	1:A:316:C:C4	2.91	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:353:A:H2'	1:A:354:C:O4'	2.04	0.58
1:A:354:C:H2'	1:A:355:G:O4'	2.04	0.57
2:B:112:LYS:O	2:B:113:LYS:C	2.47	0.57
1:A:32:G:H22	1:A:34:U:H1'	1.67	0.57
1:A:218:A:C5	1:A:219:C:H1'	2.39	0.57
1:A:272:G:H5"	1:A:272:G:C8	2.40	0.57
1:A:6:U:H2'	1:A:7:C:C6	2.40	0.57
1:A:154:U:H4'	1:A:218:A:H4'	1.87	0.57
1:A:155:A:H2'	1:A:156:C:C6	2.39	0.57
3:C:43:G:C3'	3:C:44:G:H3'	2.17	0.57
1:A:3:U:H2'	1:A:4:A:H8	1.68	0.57
1:A:172:G:H3'	1:A:173:G:H8	1.70	0.57
1:A:10:G:H2'	1:A:11:C:H6	1.70	0.56
1:A:2:U:H2'	1:A:3:U:C6	2.40	0.56
1:A:308:A:C2	1:A:329:U:H5	2.23	0.56
1:A:315:G:H2'	1:A:316:C:H6	1.67	0.56
2:B:74:GLU:OE1	2:B:111:LEU:HD22	2.04	0.56
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.56
1:A:207:C:H2'	1:A:208:U:C6	2.41	0.56
1:A:241:A:H2'	1:A:242:C:C6	2.41	0.56
2:B:4:LYS:HD3	2:B:5:TYR:CE1	2.40	0.56
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.56
1:A:364:A:H3'	1:A:364:A:OP2	2.06	0.56
1:A:364:A:OP2	1:A:365:G:O4'	2.21	0.56
2:B:86:ARG:HH12	3:C:-32:G:H1'	1.71	0.56
1:A:5:A:H2'	1:A:6:U:C6	2.41	0.55
1:A:412:A:H2'	1:A:413:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:A:H62	1:A:177:G:H21	1.54	0.55
3:C:-15:G:H2'	3:C:-14:A:H8	1.70	0.55
1:A:4:A:H2'	1:A:5:A:H8	1.70	0.55
1:A:14:G:H2'	1:A:385:A:N1	2.21	0.55
3:C:60:C:H2'	3:C:61:C:H6	1.71	0.55
1:A:364:A:OP1	1:A:365:G:N7	2.36	0.55
3:C:17:G:O2'	3:C:56:G:N2	2.35	0.55
1:A:5:A:H2'	1:A:6:U:H6	1.71	0.55
1:A:59:U:H2'	1:A:60:C:C6	2.42	0.54
1:A:172:G:H1'	1:A:217:A:H61	1.72	0.54
1:A:414:C:H2'	1:A:415:G:H8	1.72	0.54
1:A:7:C:H2'	1:A:8:A:H8	1.72	0.54
2:B:106:ARG:HH11	2:B:113:LYS:CA	2.16	0.54
1:A:198:G:N2	1:A:200:G:H3'	2.23	0.53
1:A:4:A:H2'	1:A:5:A:C8	2.44	0.53
1:A:122:G:H3'	1:A:123:C:H5"	1.90	0.53
1:A:264:U:H2'	1:A:265:G:O4'	2.09	0.53
1:A:364:A:C3'	1:A:365:G:O4'	2.56	0.53
1:A:199:U:C5	1:A:206:G:H1'	2.44	0.52
1:A:155:A:H2	1:A:170:A:N6	2.07	0.52
1:A:168:A:H2'	1:A:169:U:C6	2.44	0.52
1:A:50:A:H3'	1:A:51:G:H8	1.74	0.52
1:A:186:G:N2	1:A:188:A:H3'	2.24	0.52
1:A:222:U:H2'	1:A:223:A:C8	2.45	0.52
3:C:44:G:H4'	3:C:45:G:H5'	1.92	0.51
1:A:124:U:H2'	1:A:125:U:O4'	2.11	0.51
3:C:-25:G:N2	3:C:-11:C:H1'	2.26	0.51
3:C:34:C:H2'	3:C:35:C:C6	2.44	0.51
1:A:6:U:H2'	1:A:7:C:H6	1.74	0.51
1:A:49:A:N1	1:A:387:A:O2'	2.37	0.51
1:A:208:U:H2'	1:A:209:C:O4'	2.10	0.51
1:A:128:G:H2'	1:A:129:C:C6	2.46	0.51
1:A:148:A:H62	1:A:177:G:N2	2.09	0.51
3:C:47:C:H5"	3:C:49:C:OP2	2.11	0.51
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.50
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.50
1:A:99:A:H2'	1:A:100:A:C8	2.45	0.50
3:C:-13:U:H2'	3:C:-12:C:C6	2.47	0.50
1:A:317:G:N1	1:A:321:G:C2	2.79	0.50
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.50
1:A:373:C:H2'	1:A:374:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:C:H2'	3:C:61:C:C6	2.46	0.50
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.50
1:A:351:G:H3'	1:A:352:U:C6	2.47	0.50
3:C:-22:C:H2'	3:C:-21:C:C6	2.47	0.50
3:C:42:G:H2'	3:C:43:G:C1'	2.41	0.50
1:A:356:A:H3'	1:A:357:G:H8	1.77	0.49
1:A:186:G:H5'	1:A:187:A:OP2	2.12	0.49
1:A:130:U:H2'	1:A:131:G:H8	1.78	0.49
1:A:161:G:H4'	1:A:163:C:C5	2.48	0.49
1:A:349:G:N2	1:A:379:G:O2'	2.44	0.49
1:A:363:A:O2'	1:A:364:A:C1'	2.60	0.49
1:A:174:U:H2'	1:A:175:U:H6	1.76	0.49
1:A:267:U:C2	3:C:75:A:C2	3.00	0.49
1:A:137:A:H8	1:A:137:A:H5"	1.78	0.49
1:A:19:A:H2'	1:A:20:U:C6	2.48	0.49
1:A:401:A:H2'	1:A:402:G:O4'	2.13	0.49
3:C:22:A:H2'	3:C:23:A:O4'	2.12	0.49
1:A:350:A:H1'	1:A:380:A:N1	2.28	0.48
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.48
3:C:15:G:H2'	3:C:58:G:O6	2.13	0.48
1:A:115:C:H2'	1:A:116:A:C8	2.48	0.48
1:A:338:G:H2'	1:A:339:A:C8	2.49	0.48
1:A:280:U:H2'	1:A:281:U:C6	2.48	0.48
1:A:23:C:O2	1:A:336:A:O2'	2.28	0.48
1:A:344:C:H2'	1:A:345:G:C8	2.47	0.48
1:A:132:G:H3'	1:A:133:G:H8	1.79	0.48
1:A:280:U:H2'	1:A:281:U:H6	1.79	0.48
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.48
1:A:159:C:OP2	1:A:159:C:O4'	2.31	0.48
1:A:349:G:N2	1:A:379:G:H1'	2.28	0.48
1:A:385:A:H1'	1:A:401:A:C8	2.49	0.48
1:A:217:A:H2'	1:A:218:A:O4'	2.14	0.48
1:A:376:U:H2'	1:A:377:A:C8	2.49	0.48
3:C:-27:C:C4	3:C:-26:G:C8	3.03	0.47
1:A:411:U:H2'	1:A:412:A:C8	2.49	0.47
3:C:44:G:H4'	3:C:45:G:C5'	2.44	0.47
1:A:268:G:O6	3:C:75:A:N6	2.47	0.47
1:A:360:G:H1'	1:A:365:G:N2	2.29	0.47
1:A:7:C:H2'	1:A:8:A:C8	2.49	0.47
1:A:239:A:H4'	1:A:241:A:H5'	1.97	0.47
3:C:14:A:H2'	3:C:15:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:A:H5”	1:A:137:A:C8	2.49	0.47
1:A:199:U:H5	1:A:206:G:N3	2.12	0.47
1:A:335:G:C8	1:A:335:G:H3’	2.49	0.47
2:B:105:LEU:CB	2:B:111:LEU:HG	2.34	0.47
1:A:245:C:H2’	1:A:246:A:C8	2.50	0.47
1:A:371:U:H4’	1:A:373:C:H5	1.79	0.47
1:A:338:G:H2’	1:A:339:A:H8	1.80	0.47
1:A:350:A:H1’	1:A:380:A:C2	2.50	0.47
1:A:151:A:H2’	1:A:152:C:O4’	2.15	0.46
2:B:111:LEU:O	2:B:113:LYS:N	2.46	0.46
3:C:-10:G:H3’	3:C:-9:G:H8	1.81	0.46
1:A:363:A:O2’	1:A:364:A:O4’	2.33	0.46
1:A:285:G:O2’	1:A:300:A:N6	2.49	0.46
3:C:-26:G:H2’	3:C:-25:G:C5’	2.43	0.46
1:A:171:U:H2’	1:A:172:G:O4’	2.16	0.46
1:A:230:G:C6	3:C:55:C:H1’	2.51	0.46
1:A:354:C:O2	1:A:375:G:N1	2.44	0.46
3:C:-7:U:O2’	3:C:-6:C:H5’	2.16	0.46
1:A:159:C:O4’	1:A:159:C:P	2.74	0.46
1:A:199:U:H5	1:A:206:G:H1’	1.80	0.46
3:C:38:G:H2’	3:C:39:G:C8	2.51	0.46
1:A:319:A:H1’	1:A:320:U:C5	2.51	0.46
3:C:-9:G:H2’	3:C:-8:A:O4’	2.15	0.46
1:A:315:G:C6	1:A:316:C:C4	3.03	0.46
1:A:292:A:H2’	1:A:293:U:C6	2.51	0.45
3:C:17:G:N2	3:C:56:G:H2’	2.31	0.45
1:A:50:A:N3	1:A:50:A:H2’	2.31	0.45
1:A:68:G:N3	1:A:68:G:H2’	2.31	0.45
3:C:-20:U:H2’	3:C:-19:U:O4’	2.16	0.45
3:C:-13:U:H2’	3:C:-12:C:H6	1.79	0.45
3:C:-28:C:H2’	3:C:-27:C:C6	2.51	0.45
3:C:9:A:N7	3:C:22:A:N7	2.63	0.45
1:A:268:G:C6	3:C:75:A:N1	2.85	0.45
1:A:246:A:H2’	1:A:247:C:O4’	2.16	0.45
1:A:32:G:H2’	1:A:32:G:N3	2.32	0.45
1:A:170:A:H3’	1:A:171:U:H6	1.81	0.45
1:A:216:A:HO2’	1:A:217:A:H8	1.63	0.45
1:A:229:G:N2	1:A:231:A:H3’	2.32	0.45
1:A:349:G:H22	1:A:379:G:C1’	2.25	0.45
1:A:220:C:H2’	1:A:221:U:C6	2.52	0.45
1:A:292:A:H2’	1:A:293:U:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:A:H2'	1:A:380:A:N3	2.32	0.45
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.45
3:C:35:C:H2'	3:C:36:A:O4'	2.17	0.45
1:A:60:C:H2'	1:A:61:G:H8	1.82	0.45
1:A:114:G:H2'	1:A:115:C:C6	2.52	0.45
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.45
1:A:216:A:O2'	1:A:217:A:H8	1.99	0.45
1:A:222:U:H2'	1:A:223:A:H8	1.81	0.45
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.45
1:A:147:A:H62	1:A:178:A:H62	1.63	0.44
1:A:17:U:H2'	1:A:18:A:H8	1.82	0.44
1:A:331:G:H4'	1:A:332:A:H5'	1.98	0.44
1:A:364:A:H2'	1:A:365:G:O4'	2.18	0.44
2:B:3:LYS:HB3	2:B:8:LYS:HE3	1.98	0.44
1:A:14:G:C2'	1:A:401:A:H61	2.31	0.44
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.44
1:A:358:G:H1	1:A:366:C:H42	1.66	0.44
1:A:365:G:H2'	1:A:365:G:N3	2.33	0.43
1:A:242:C:H2'	1:A:243:C:O4'	2.18	0.43
1:A:312:G:C2	1:A:326:C:C2	3.07	0.43
1:A:355:G:H2'	1:A:356:A:C8	2.53	0.43
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.43
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.80	0.43
1:A:308:A:H2'	1:A:309:C:O4'	2.18	0.43
1:A:123:C:H2'	1:A:124:U:O4'	2.19	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:382:G:H2'	1:A:383:G:O4'	2.18	0.43
1:A:154:U:H2'	1:A:155:A:C4	2.53	0.43
2:B:73:GLU:N	2:B:73:GLU:OE1	2.52	0.43
1:A:166:G:H2'	1:A:167:G:C8	2.54	0.43
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.43
3:C:12:U:H3	3:C:22:A:H61	1.67	0.43
3:C:64:U:H2'	3:C:65:C:C6	2.54	0.43
1:A:324:G:H2'	1:A:325:C:H6	1.84	0.42
1:A:343:C:H2'	1:A:344:C:C6	2.54	0.42
1:A:160:C:H1'	1:A:167:G:N2	2.27	0.42
3:C:-22:C:H2'	3:C:-21:C:H6	1.83	0.42
3:C:8:U:H5'	3:C:48:G:H5'	2.01	0.42
3:C:9:A:N6	3:C:21:G:C8	2.87	0.42
1:A:128:G:H2'	1:A:129:C:H6	1.82	0.42
1:A:95:A:H2'	1:A:96:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:A:H2'	1:A:96:G:H8	1.85	0.42
1:A:260:C:H2'	1:A:261:A:O4'	2.20	0.42
1:A:364:A:H3'	1:A:364:A:P	2.60	0.42
1:A:414:C:H2'	1:A:415:G:C8	2.53	0.42
3:C:26:C:H2'	3:C:27:C:C6	2.55	0.42
1:A:17:U:H2'	1:A:18:A:C8	2.55	0.42
2:B:11:GLU:O	2:B:15:GLU:HG3	2.19	0.42
1:A:82:A:H2'	1:A:83:G:O4'	2.19	0.42
1:A:406:A:H2'	1:A:407:U:O4'	2.20	0.42
3:C:43:G:H2'	3:C:43:G:N3	2.34	0.42
1:A:38:G:H2'	1:A:39:C:C6	2.55	0.42
3:C:-11:C:C2	3:C:-10:G:C8	3.08	0.42
1:A:87:U:H2'	1:A:88:C:C6	2.55	0.42
1:A:153:C:H1'	1:A:173:G:N2	2.34	0.42
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.42
1:A:334:A:H62	2:B:10:ASN:ND2	2.17	0.42
1:A:335:G:C8	1:A:335:G:C3'	3.03	0.42
1:A:170:A:H3'	1:A:171:U:C6	2.55	0.41
1:A:221:U:H2'	1:A:222:U:C6	2.55	0.41
1:A:335:G:H3'	1:A:335:G:H8	1.85	0.41
1:A:10:G:C6	1:A:406:A:N1	2.88	0.41
1:A:115:C:H2'	1:A:116:A:H8	1.85	0.41
1:A:279:C:H2'	1:A:280:U:C6	2.55	0.41
1:A:377:A:H3'	1:A:378:C:H6	1.86	0.41
1:A:219:C:H2'	1:A:220:C:C6	2.55	0.41
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.41
1:A:50:A:C8	1:A:50:A:C5'	2.98	0.41
1:A:334:A:H62	2:B:10:ASN:HD22	1.68	0.41
1:A:344:C:H2'	1:A:345:G:H8	1.85	0.41
1:A:9:U:C2	1:A:10:G:C8	3.09	0.41
2:B:99:LYS:HB2	2:B:99:LYS:HE3	1.71	0.41
2:B:113:LYS:C	2:B:115:ALA:N	2.74	0.41
1:A:45:A:H2	1:A:388:G:H2'	1.82	0.41
1:A:83:G:O6	1:A:250:G:H1'	2.20	0.41
1:A:56:U:H2'	1:A:57:G:H8	1.85	0.41
1:A:134:C:H2'	1:A:135:U:C6	2.56	0.41
1:A:266:A:N3	1:A:266:A:H2'	2.36	0.41
1:A:315:G:C2	1:A:323:A:C2	3.08	0.41
1:A:59:U:H2'	1:A:60:C:H6	1.84	0.41
1:A:156:C:H1'	1:A:216:A:C2	2.55	0.41
1:A:281:U:H2'	1:A:282:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:A:H3'	1:A:357:G:C8	2.56	0.41
3:C:17:G:H21	3:C:56:G:H2'	1.86	0.41
1:A:287:A:H3'	1:A:288:G:H8	1.85	0.41
1:A:352:U:H2'	1:A:353:A:H8	1.83	0.41
1:A:380:A:C2	1:A:381:A:N9	2.89	0.41
1:A:180:U:O2'	1:A:181:A:H5'	2.21	0.40
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.40
1:A:117:G:H3'	1:A:118:C:H6	1.86	0.40
1:A:158:U:O5'	1:A:158:U:C6	2.65	0.40
1:A:352:U:O2	1:A:377:A:H2	2.05	0.40
3:C:16:U:H5	3:C:58:G:O6	2.04	0.40
3:C:34:C:H2'	3:C:35:C:H6	1.86	0.40
1:A:19:A:H2'	1:A:20:U:H6	1.85	0.40
1:A:357:G:H22	1:A:367:C:H42	1.70	0.40
1:A:32:G:H3'	1:A:33:U:C6	2.57	0.40
1:A:92:C:H2'	1:A:93:C:C6	2.57	0.40
1:A:155:A:C6	1:A:156:C:N4	2.90	0.40
1:A:268:G:C6	3:C:75:A:C6	3.10	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
2	B	114/116 (98%)	109 (96%)	3 (3%)	2 (2%)	7 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	113	LYS
2	B	112	LYS

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
2	B	99/99 (100%)	90 (91%)	9 (9%)	7 19

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

Mol	Chain	Res	Type
2	B	3	LYS
2	B	4	LYS
2	B	71	LEU
2	B	92	MET
2	B	99	LYS
2	B	105	LEU
2	B	112	LYS
2	B	113	LYS
2	B	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN
2	B	87	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	180 (43%)	17 (4%)
3	C	107/111 (96%)	44 (41%)	10 (9%)
All	All	523/528 (99%)	224 (42%)	27 (5%)

All (224) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	9	U
1	A	11	C
1	A	15	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	44	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	53	C
1	A	54	C
1	A	63	A
1	A	67	U
1	A	68	G
1	A	70	U
1	A	74	A
1	A	75	U
1	A	76	G
1	A	81	U
1	A	83	G
1	A	85	G
1	A	86	U
1	A	87	U
1	A	88	C
1	A	90	U
1	A	91	G
1	A	92	C
1	A	99	A
1	A	101	U
1	A	102	C
1	A	106	A
1	A	108	G
1	A	109	C
1	A	117	G
1	A	118	C

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Mol	Chain	Res	Type
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	130	U
1	A	131	G
1	A	132	G
1	A	134	C
1	A	137	A
1	A	138	C
1	A	139	G
1	A	142	G
1	A	143	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	153	C
1	A	155	A
1	A	158	U
1	A	159	C
1	A	160	C
1	A	161	G
1	A	162	G
1	A	163	C
1	A	164	U
1	A	171	U
1	A	172	G
1	A	174	U
1	A	175	U
1	A	177	G
1	A	178	A
1	A	179	U
1	A	180	U
1	A	181	A
1	A	186	G
1	A	187	A
1	A	190	G
1	A	191	U
1	A	192	G
1	A	194	C
1	A	202	C

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Mol	Chain	Res	Type
1	A	203	G
1	A	204	G
1	A	205	A
1	A	207	C
1	A	208	U
1	A	209	C
1	A	212	A
1	A	213	G
1	A	214	G
1	A	216	A
1	A	219	C
1	A	220	C
1	A	225	A
1	A	226	G
1	A	227	G
1	A	230	G
1	A	233	C
1	A	234	G
1	A	235	C
1	A	238	U
1	A	240	A
1	A	241	A
1	A	243	C
1	A	250	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	266	A
1	A	267	U
1	A	269	G
1	A	270	U
1	A	271	A
1	A	272	G
1	A	273	G
1	A	274	G
1	A	276	C
1	A	278	C
1	A	291	A
1	A	292	A
1	A	293	U
1	A	296	A
1	A	300	A

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Mol	Chain	Res	Type
1	A	304	A
1	A	309	C
1	A	312	G
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	342	A
1	A	346	C
1	A	349	G
1	A	350	A
1	A	351	G
1	A	353	A
1	A	354	C
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G

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Mol	Chain	Res	Type
1	A	384	U
1	A	389	A
1	A	391	C
1	A	392	A
1	A	400	U
1	A	401	A
1	A	402	G
1	A	403	A
1	A	407	U
1	A	408	G
1	A	410	U
3	C	-27	C
3	C	-26	G
3	C	-25	G
3	C	-24	A
3	C	-18	U
3	C	-17	U
3	C	-16	G
3	C	-9	G
3	C	-7	U
3	C	-6	C
3	C	-4	C
3	C	-3	U
3	C	-2	U
3	C	-1	U
3	C	1	G
3	C	4	G
3	C	8	U
3	C	9	A
3	C	10	G
3	C	13	C
3	C	14	A
3	C	16	U
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	21	G
3	C	22	A
3	C	28	A
3	C	29	C
3	C	33	G

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Mol	Chain	Res	Type
3	C	35	C
3	C	41	G
3	C	42	G
3	C	43	G
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	52	G
3	C	60	C
3	C	72	U
3	C	74	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	50	A
1	A	52	U
1	A	67	U
1	A	75	U
1	A	122	G
1	A	126	U
1	A	137	A
1	A	176	C
1	A	201	A
1	A	232	A
1	A	240	A
1	A	271	A
1	A	272	G
1	A	292	A
1	A	349	G
1	A	363	A
1	A	365	G
3	C	-18	U
3	C	-4	C
3	C	-2	U
3	C	7	G
3	C	17	G
3	C	19	U
3	C	44	G
3	C	46	U

Continued on next page...

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Mol	Chain	Res	Type
3	C	47	C
3	C	59	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

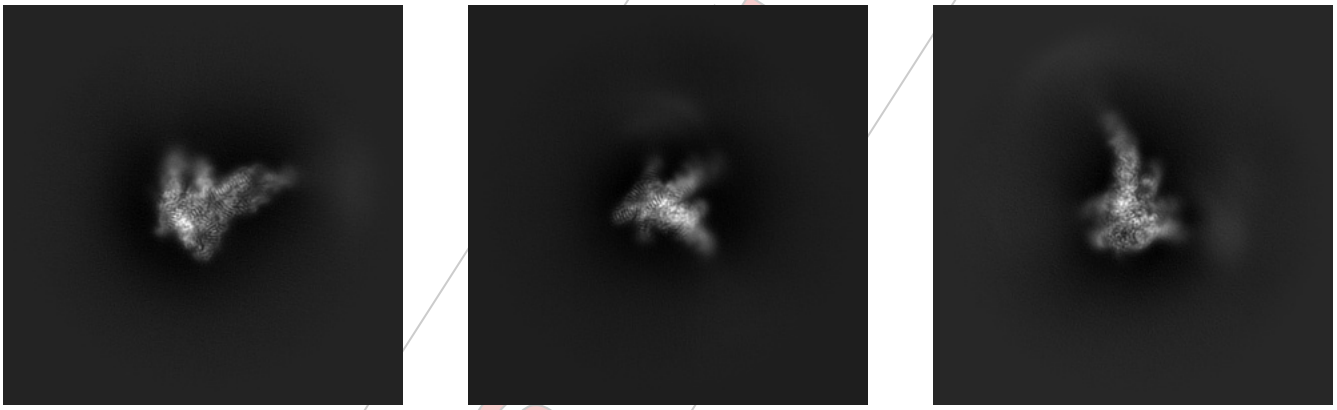
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70948. 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.

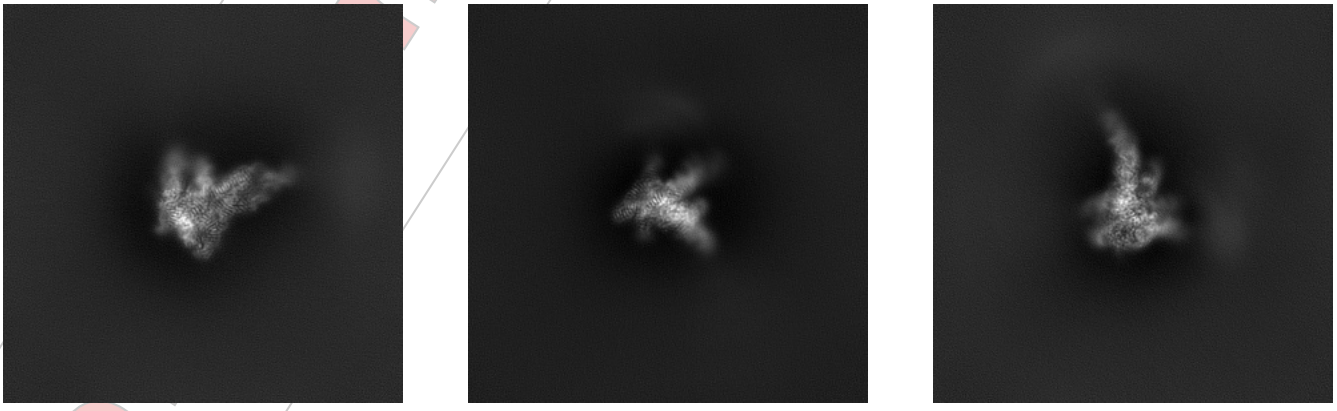
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

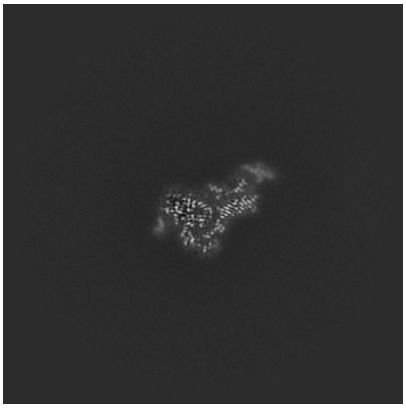


X Y Z

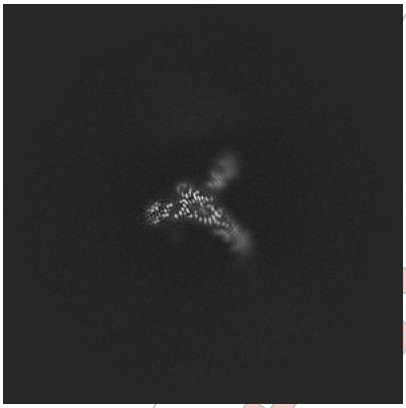
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

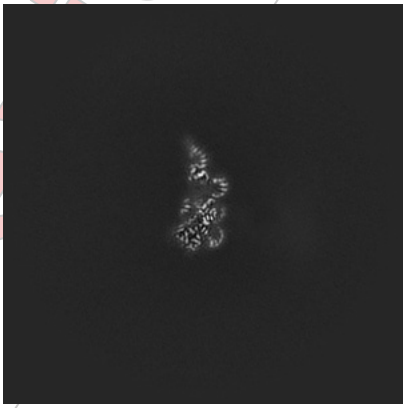
6.2.1 Primary map



X Index: 200

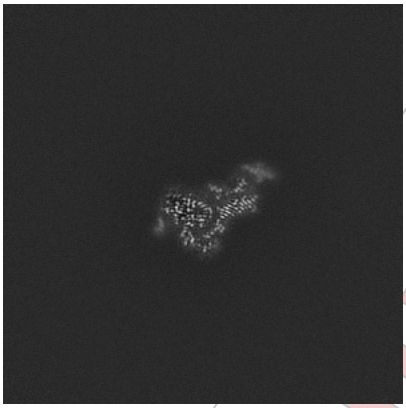


Y Index: 200

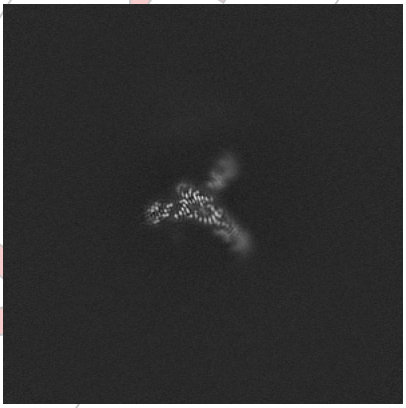


Z Index: 200

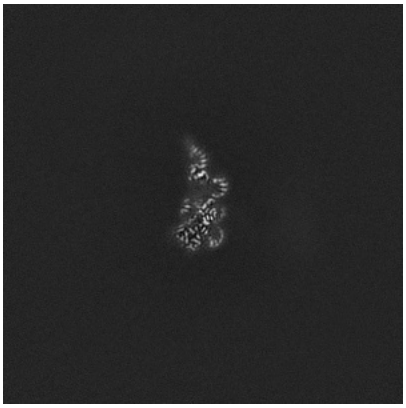
6.2.2 Raw map



X Index: 200



Y Index: 200

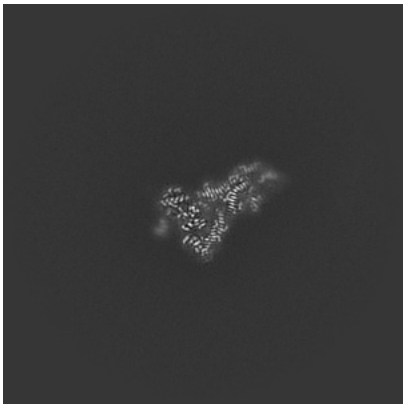


Z Index: 200

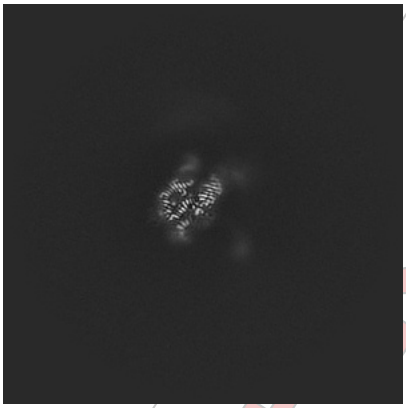
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

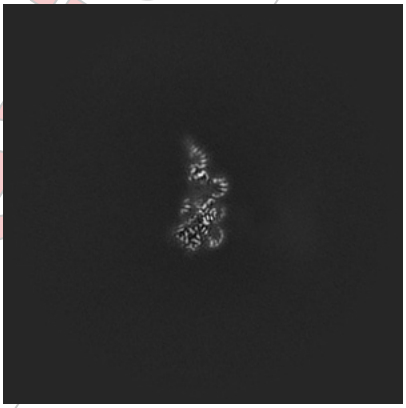
6.3.1 Primary map



X Index: 195

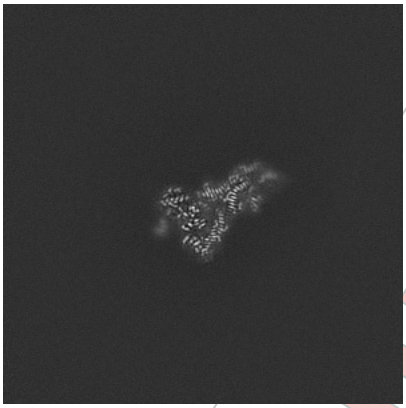


Y Index: 186

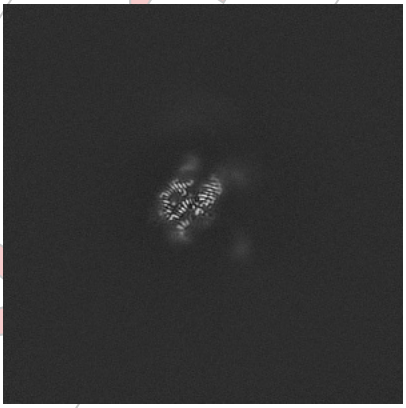


Z Index: 200

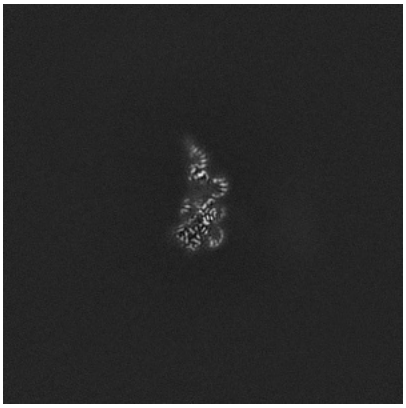
6.3.2 Raw map



X Index: 195



Y Index: 186

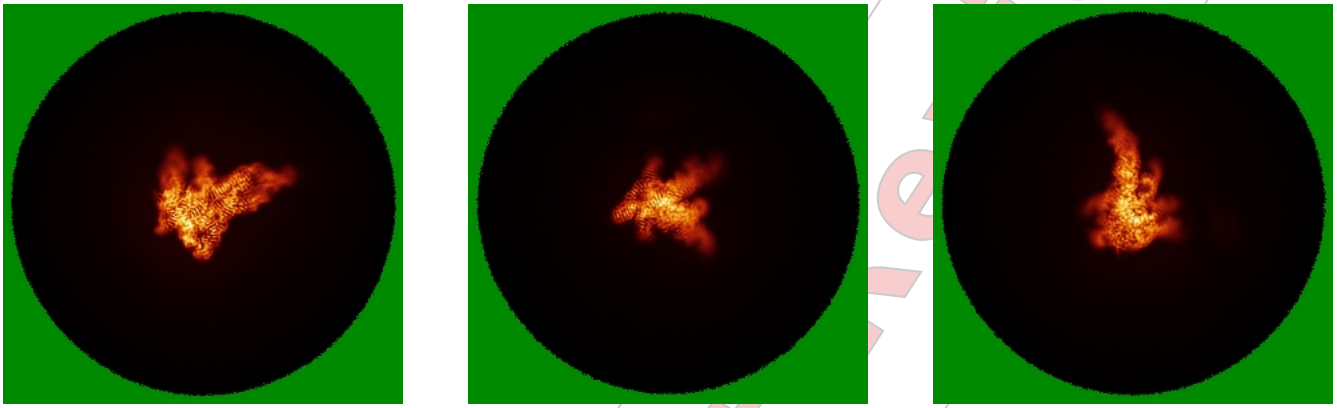


Z Index: 200

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

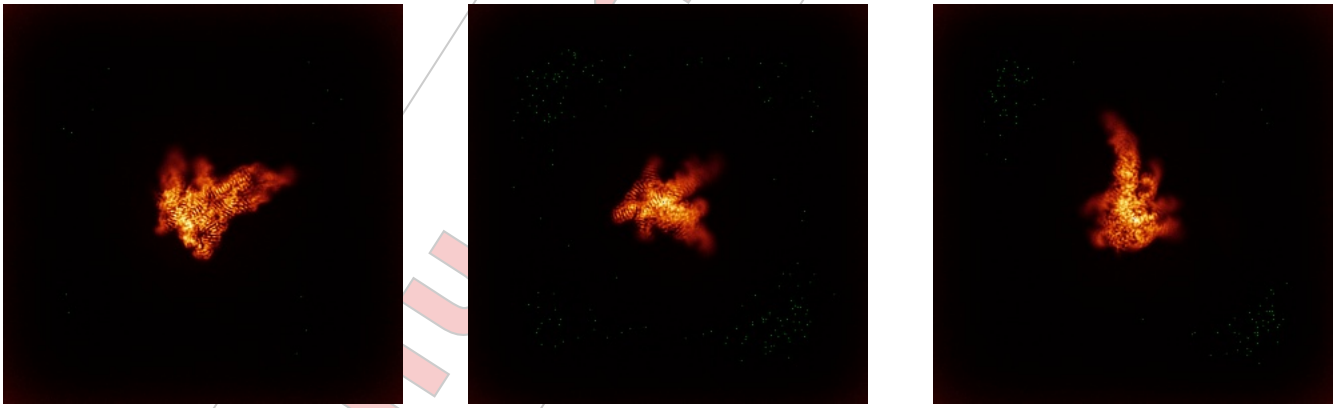
6.4 Orthogonal standard-deviation projections (False-color)

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.

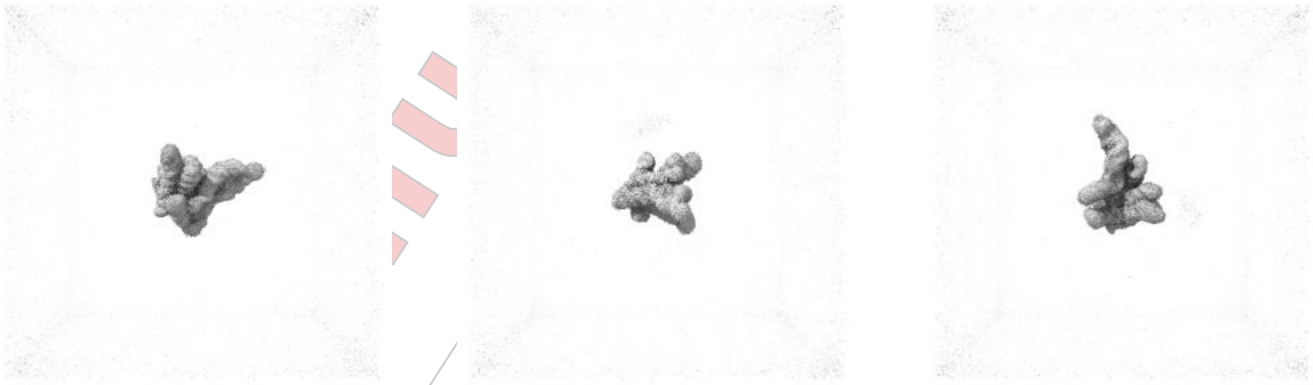
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

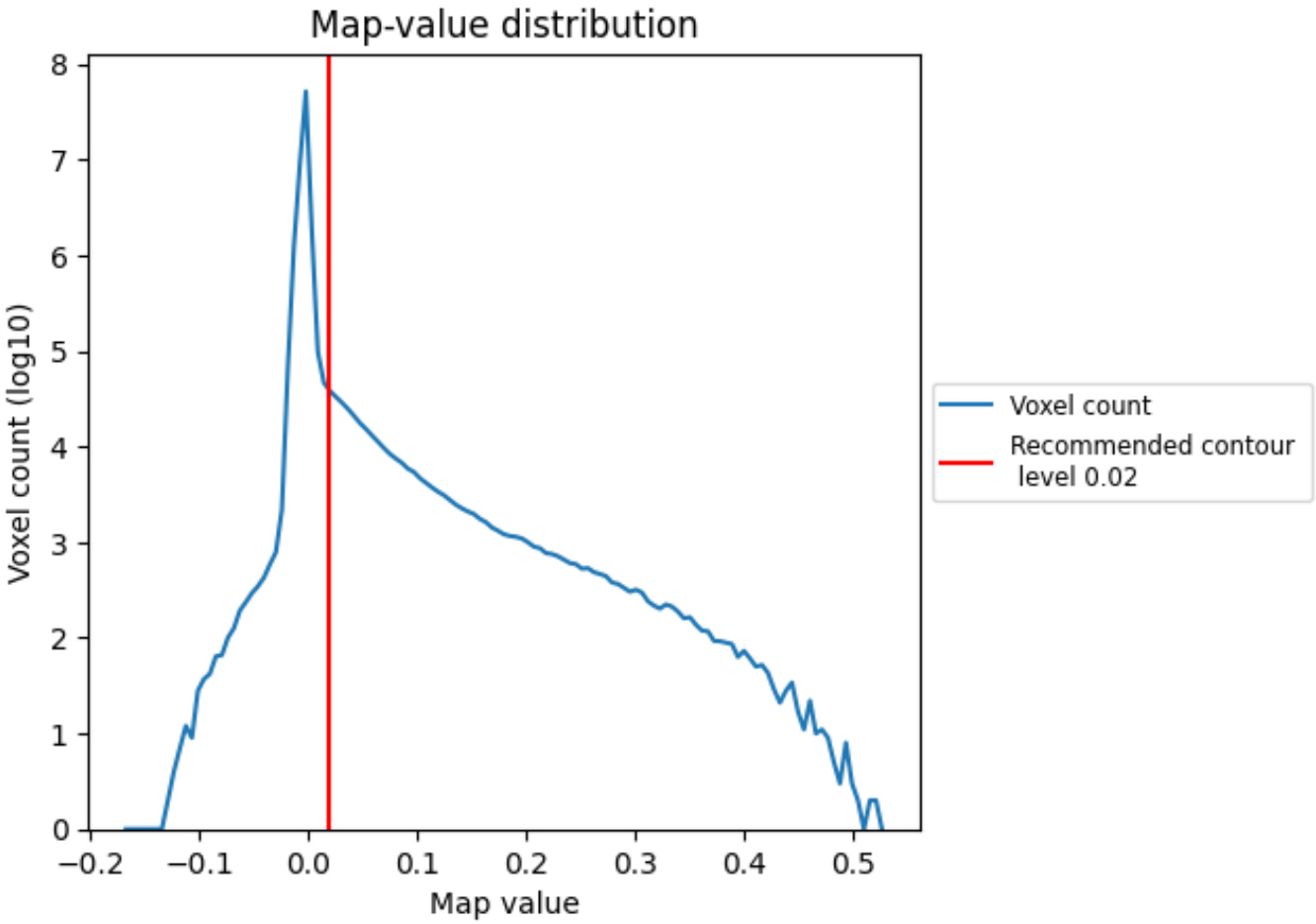
6.6 Mask visualisation (i)

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

7 Map analysis

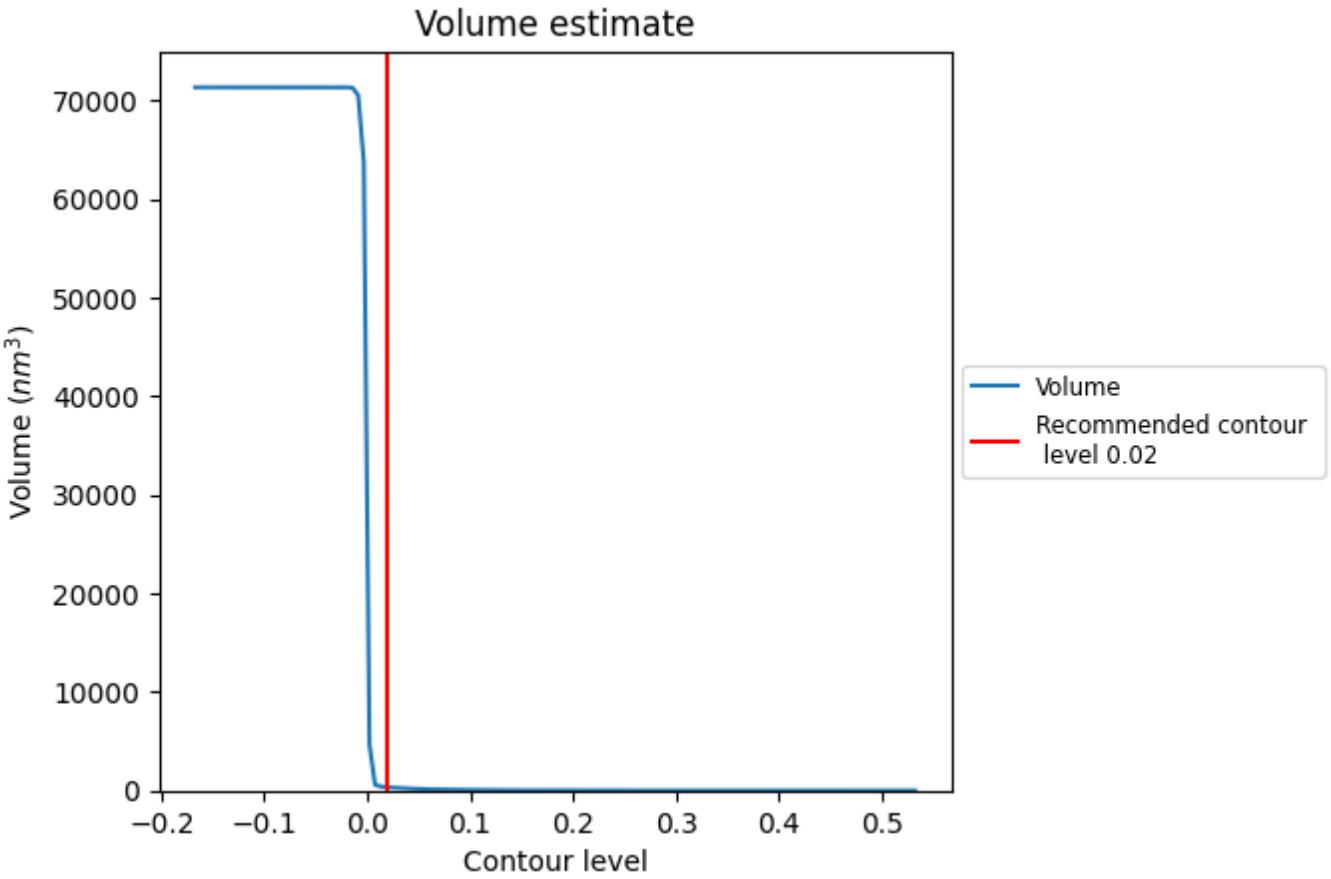
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

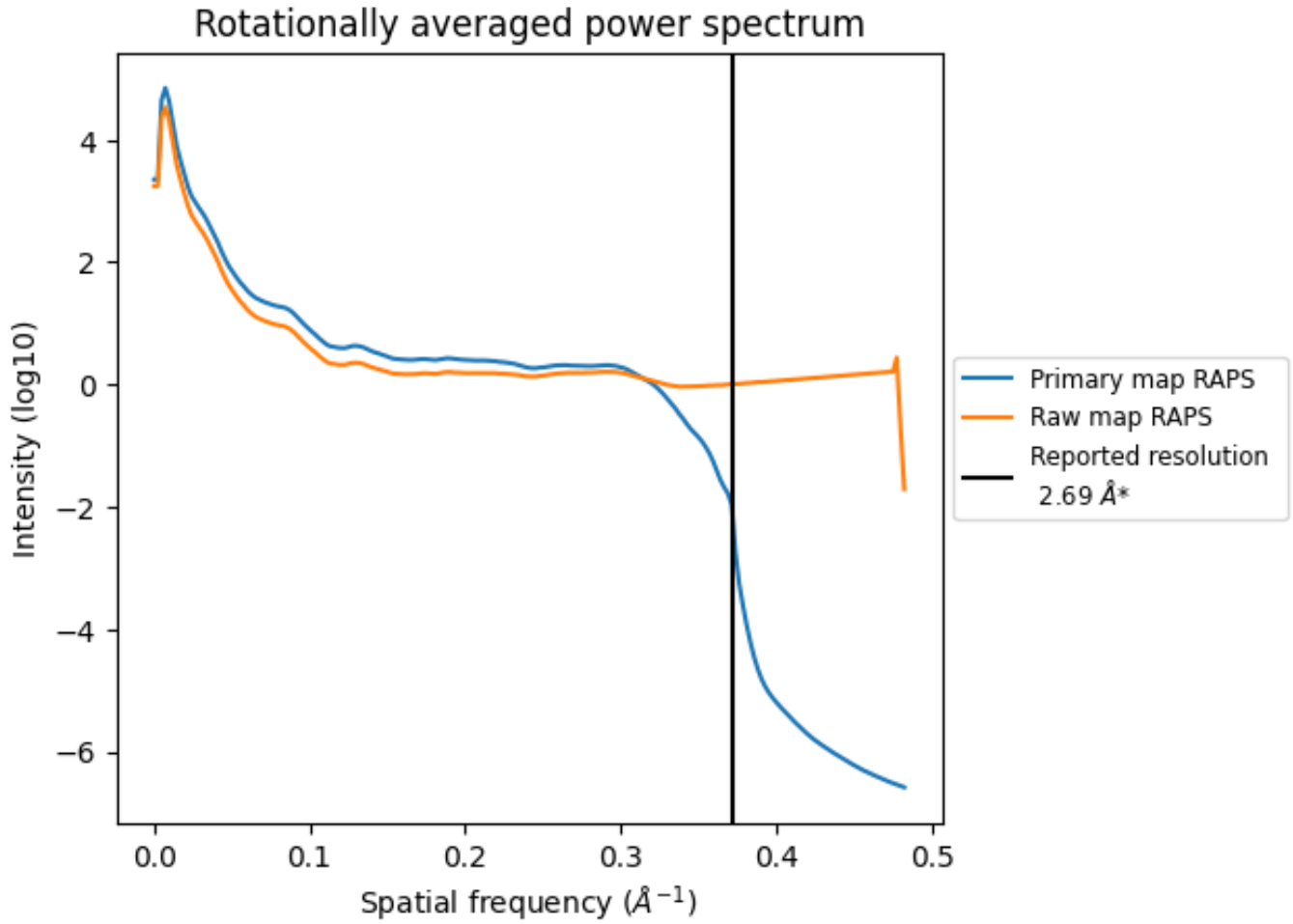
7.2 Volume estimate (i)



The volume at the recommended contour level is 338 nm^3; this corresponds to an approximate mass of 305 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 (i)

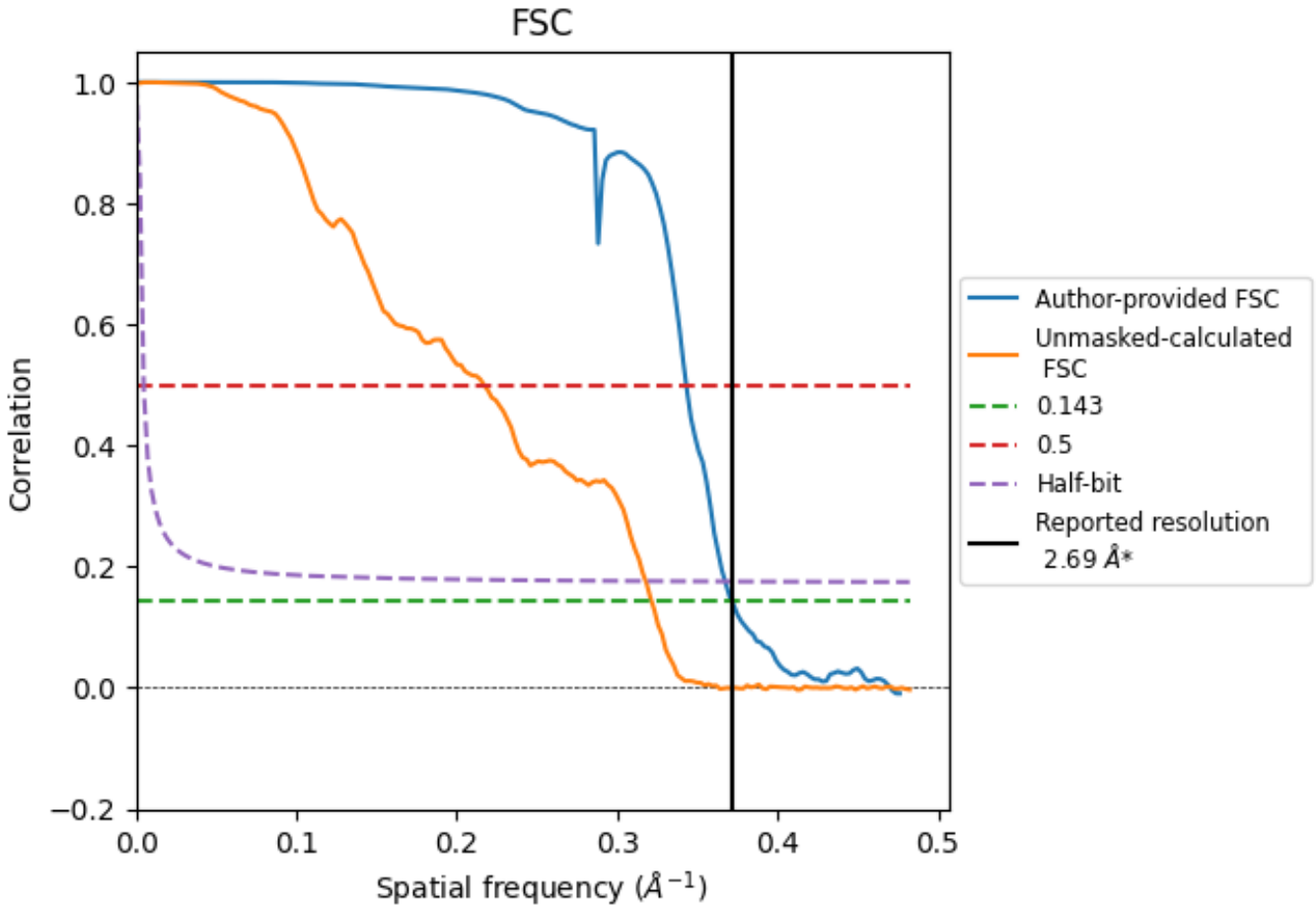


*Reported resolution corresponds to spatial frequency of 0.372 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.372 Å^{-1}

8.2 Resolution estimates (i)

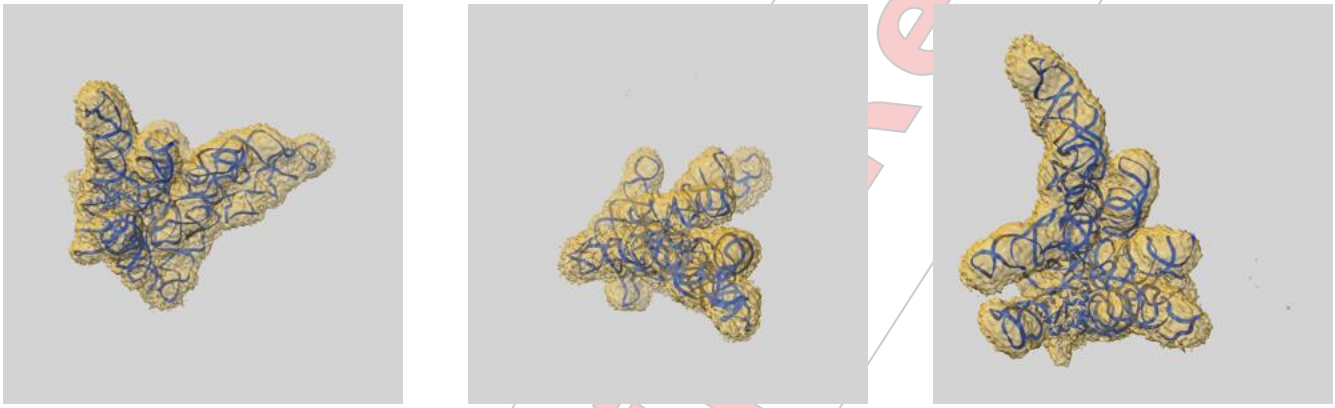
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	2.91	2.72
Unmasked-calculated*	3.11	4.61	3.15

*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 3.11 differs from the reported value 2.69 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70948 and PDB model 9OWY. Per-residue inclusion information can be found in section 3 on page 4.

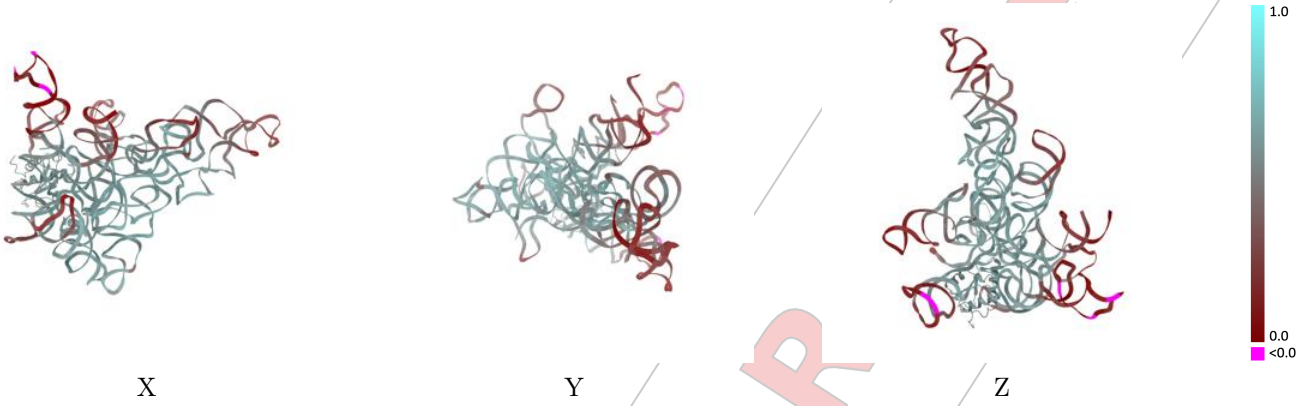
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

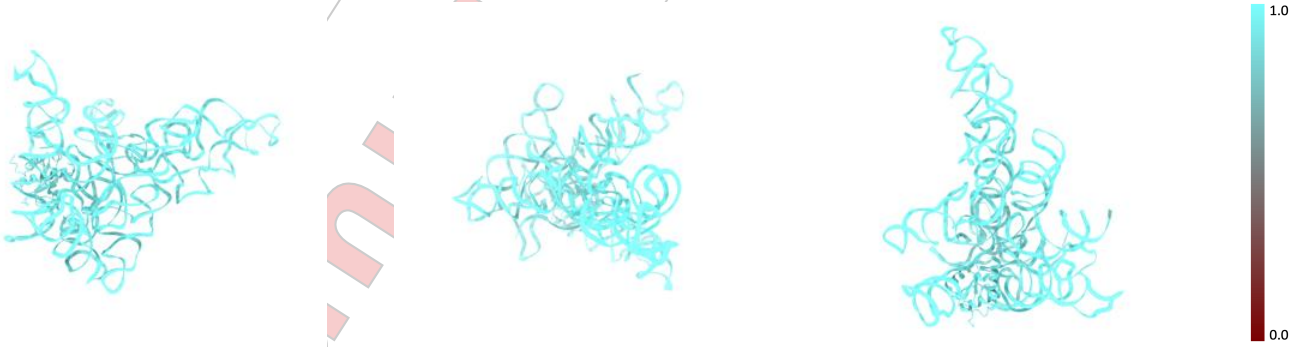
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

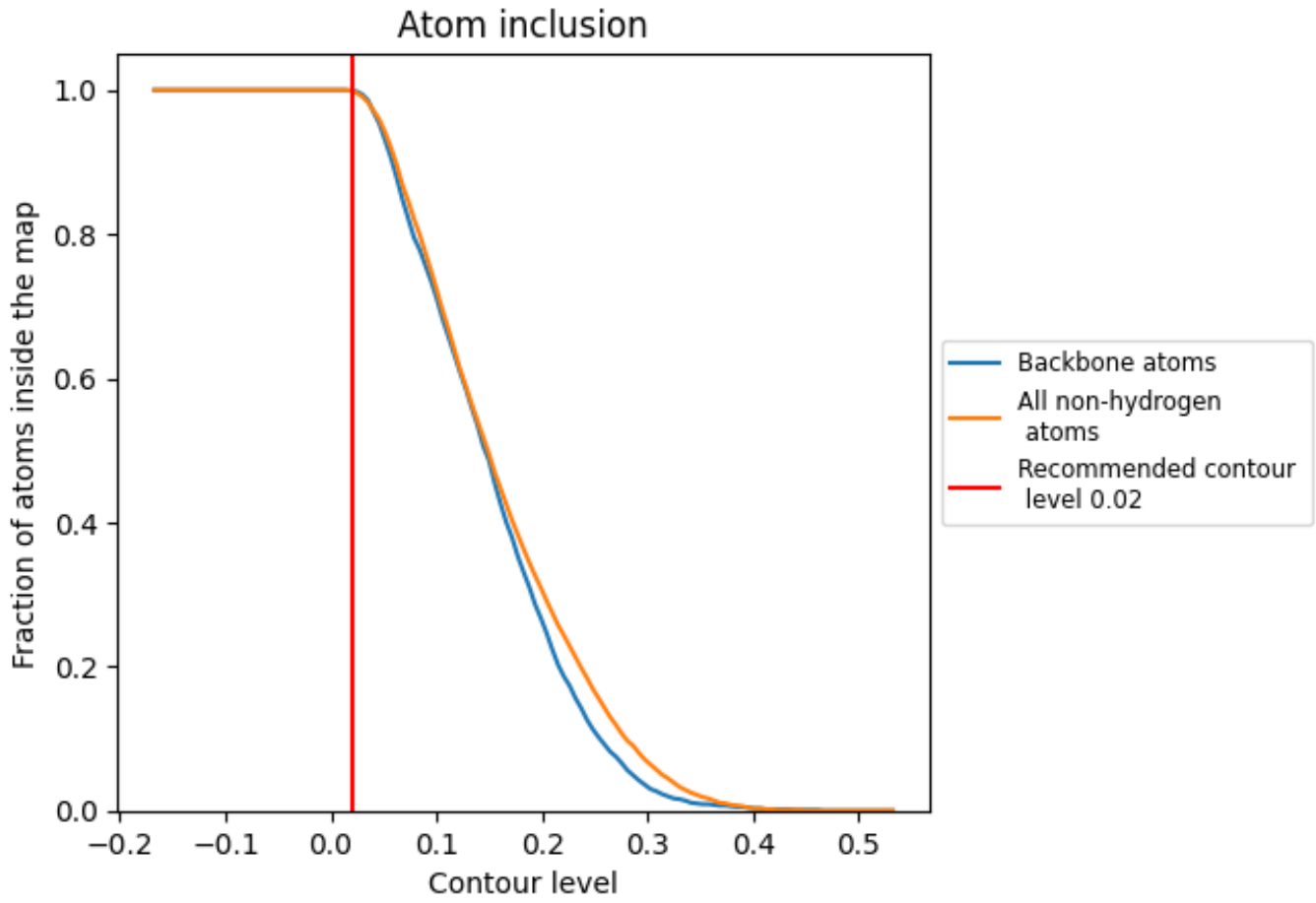
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9990	0.4740
A	0.9990	0.4760
B	0.9980	0.5530
C	0.9990	0.4310

Full wwPDB EM Validation Report ⓘ

Jun 6, 2025 – 03:58 PM EDT

PDB ID	:	9OY5 / pdb_00009oy5
EMDB ID	:	EMD-70997
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme tetraloop mutant (sub-conformation 1)
Deposited on	:	2025-06-04
Resolution	:	3.02 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

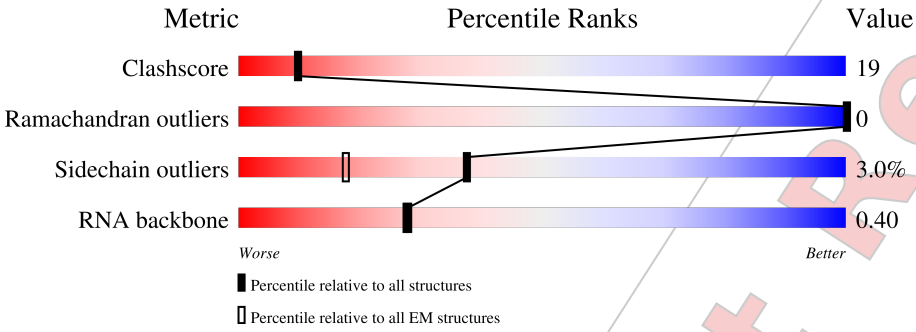
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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 <=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	417	6% 27% 54% 19%
2	B	116	12% 69% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9924 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 RNA chain called RNase P RNA component tetraloop mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8953	3992	1648	2896	417	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	U	C	conflict	GB 143442
A	215	U	G	engineered mutation	GB 143442
A	216	U	A	engineered mutation	GB 143442
A	217	U	A	engineered mutation	GB 143442
A	218	U	A	engineered mutation	GB 143442
A	417	C	G	conflict	GB 143442

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

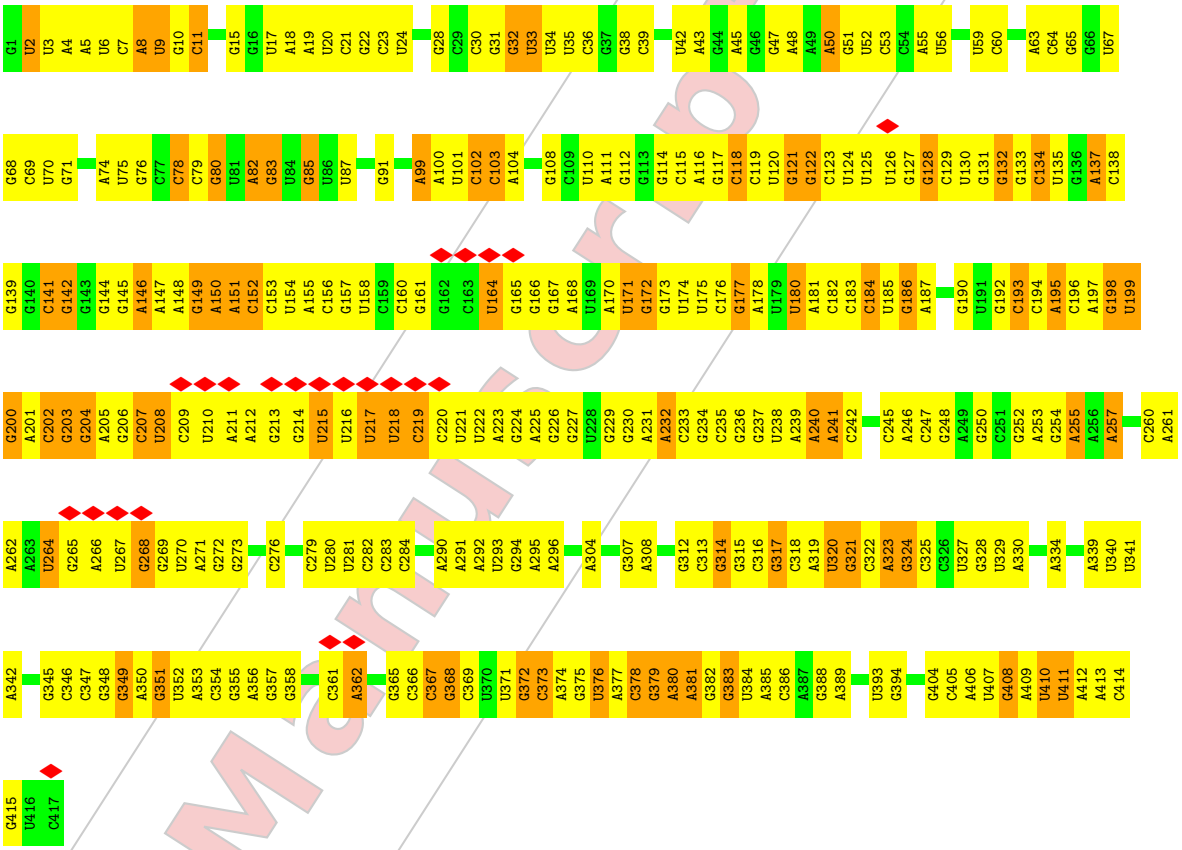
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	24	24	24	0

3 Residue-property plots (i)

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.

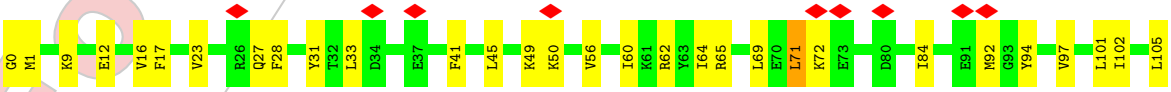
• Molecule 1: RNase P RNA component tetraloop mutant

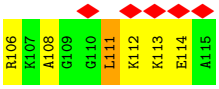
Chain A:



• Molecule 2: Ribonuclease P protein component

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	-0.148	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.28	4/10025 (0.0%)	0.43	0/15639
2	B	0.19	0/962	0.44	0/1281
All	All	0.27	4/10987 (0.0%)	0.43	0/16920

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	U	C1'-N1	6.37	1.58	1.48
1	A	218	U	C1'-N1	6.37	1.58	1.48
1	A	217	U	C1'-N1	6.31	1.57	1.48
1	A	215	U	C1'-N1	5.57	1.56	1.48

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	8953	0	4505	265	0
2	B	947	0	1008	25	0
3	A	24	0	0	0	0
All	All	9924	0	5513	289	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 19.

All (289) 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:314:G:H1	1:A:323:A:H61	1.04	0.90
1:A:350:A:H1'	1:A:380:A:C6	2.09	0.87
1:A:371:U:H5"	1:A:372:G:H5'	1.58	0.83
2:B:50:LYS:H	2:B:50:LYS:HD2	1.43	0.83
1:A:158:U:H3	1:A:168:A:H61	1.25	0.82
1:A:314:G:H1	1:A:323:A:N6	1.75	0.82
1:A:316:C:H2'	1:A:317:G:C8	2.19	0.76
1:A:120:U:H3	1:A:131:G:H1	1.33	0.76
1:A:348:G:N2	1:A:380:A:N7	2.35	0.75
1:A:200:G:O6	1:A:231:A:N1	2.19	0.74
1:A:290:A:H61	1:A:295:A:H3'	1.50	0.73
2:B:105:LEU:HD23	2:B:111:LEU:HD23	1.72	0.72
1:A:349:G:H21	1:A:350:A:H62	1.39	0.70
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.72	0.70
1:A:141:C:H42	1:A:241:A:H62	1.39	0.70
2:B:27:GLN:HG2	2:B:92:MET:HE1	1.75	0.67
1:A:180:U:H2'	1:A:181:A:H8	1.57	0.67
1:A:215:U:H2'	1:A:217:U:H5	1.62	0.65
1:A:18:A:H2'	1:A:19:A:H8	1.61	0.65
1:A:9:U:H2'	1:A:10:G:H8	1.62	0.65
1:A:211:A:H2'	1:A:212:A:C8	2.31	0.64
1:A:352:U:H2'	1:A:353:A:H8	1.63	0.64
1:A:374:A:H2'	1:A:375:G:C8	2.33	0.64
1:A:148:A:H61	1:A:177:G:H1'	1.64	0.62
1:A:130:U:H2'	1:A:131:G:H8	1.64	0.62
1:A:115:C:H2'	1:A:116:A:H8	1.63	0.62
1:A:148:A:N6	1:A:177:G:H1'	2.13	0.62
1:A:204:G:H2'	1:A:205:A:H8	1.63	0.62
1:A:172:G:H2'	1:A:173:G:H8	1.65	0.62
1:A:211:A:H2'	1:A:212:A:H8	1.65	0.61
1:A:9:U:H2'	1:A:10:G:C8	2.34	0.61
1:A:199:U:H2'	1:A:200:G:C8	2.36	0.61
1:A:316:C:H2'	1:A:317:G:N7	2.14	0.61
1:A:379:G:C5'	1:A:380:A:H5"	2.30	0.61
1:A:411:U:H2'	1:A:412:A:C8	2.36	0.61
1:A:352:U:H2'	1:A:353:A:C8	2.35	0.60
1:A:349:G:H1	1:A:379:G:H1'	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:A:H2'	1:A:19:A:C8	2.37	0.60
1:A:315:G:H2'	1:A:316:C:C6	2.37	0.59
1:A:70:U:H2'	1:A:71:G:O4'	2.02	0.59
1:A:130:U:H2'	1:A:131:G:C8	2.38	0.59
1:A:99:A:H2'	1:A:100:A:C8	2.38	0.59
1:A:219:C:H2'	1:A:220:C:C6	2.38	0.59
1:A:349:G:H22	1:A:379:G:C1'	2.16	0.59
1:A:195:A:H2'	1:A:196:C:C6	2.38	0.59
1:A:376:U:C2	1:A:377:A:C8	2.90	0.58
2:B:56:VAL:O	2:B:60:ILE:HG13	2.03	0.58
1:A:85:G:O2'	1:A:87:U:O4	2.21	0.58
1:A:201:A:H61	1:A:230:G:H1	1.50	0.58
1:A:204:G:H2'	1:A:205:A:C8	2.37	0.58
1:A:373:C:H2'	1:A:374:A:H8	1.67	0.58
1:A:71:G:H1'	1:A:291:A:H61	1.69	0.58
1:A:146:A:H3'	1:A:178:A:H61	1.68	0.58
1:A:378:C:H3'	1:A:379:G:H8	1.69	0.58
1:A:293:U:H3'	1:A:294:G:C8	2.39	0.58
1:A:172:G:H2'	1:A:173:G:C8	2.39	0.57
1:A:124:U:H2'	1:A:125:U:O4'	2.03	0.57
1:A:45:A:H62	2:B:62:ARG:NH2	2.03	0.57
1:A:137:A:H3'	1:A:240:A:H62	1.69	0.57
1:A:272:G:H2'	1:A:273:G:H8	1.69	0.57
1:A:215:U:O2'	1:A:217:U:O4	2.16	0.57
1:A:220:C:H2'	1:A:221:U:C6	2.40	0.56
1:A:102:C:H2'	1:A:103:C:O4'	2.05	0.56
1:A:121:G:H1	1:A:130:U:H3	1.53	0.56
1:A:210:U:H2'	1:A:211:A:C8	2.40	0.56
1:A:367:C:H2'	1:A:368:G:C8	2.40	0.56
1:A:411:U:H2'	1:A:412:A:H8	1.70	0.56
1:A:323:A:H2'	1:A:324:G:H5'	1.88	0.56
1:A:197:A:H2'	1:A:199:U:C6	2.41	0.56
1:A:151:A:H2'	1:A:152:C:O4'	2.05	0.55
1:A:341:U:H2'	1:A:342:A:H8	1.70	0.55
1:A:373:C:H2'	1:A:374:A:C8	2.42	0.55
1:A:141:C:H5'	1:A:239:A:H61	1.71	0.55
2:B:112:LYS:HB2	2:B:114:GLU:HG2	1.88	0.55
1:A:379:G:C4'	1:A:380:A:H5"	2.37	0.55
1:A:174:U:H2'	1:A:175:U:C6	2.42	0.55
1:A:3:U:H2'	1:A:4:A:C8	2.42	0.54
1:A:194:C:C2	1:A:195:A:H1'	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:C:H2'	1:A:116:A:C8	2.42	0.54
1:A:3:U:H2'	1:A:4:A:H8	1.72	0.54
1:A:175:U:H2'	1:A:176:C:C6	2.44	0.53
1:A:245:C:H2'	1:A:246:A:H8	1.74	0.53
1:A:59:U:H2'	1:A:60:C:C6	2.44	0.53
1:A:141:C:H4'	1:A:142:G:H5"	1.90	0.53
1:A:206:G:H3'	1:A:207:C:H5"	1.89	0.53
1:A:281:U:H2'	1:A:282:C:H6	1.74	0.53
1:A:380:A:H3'	1:A:381:A:H8	1.74	0.52
1:A:6:U:H2'	1:A:7:C:C6	2.44	0.52
1:A:214:G:H2'	1:A:215:U:H6	1.73	0.52
1:A:380:A:C6	1:A:381:A:C4	2.97	0.52
1:A:176:C:H2'	1:A:177:G:H5'	1.91	0.52
1:A:208:U:H2'	1:A:209:C:C6	2.44	0.52
1:A:215:U:O2	1:A:218:U:O4	2.28	0.52
1:A:110:U:H2'	1:A:111:A:H8	1.75	0.52
1:A:381:A:H2'	1:A:382:G:O4'	2.09	0.52
1:A:193:C:H2'	1:A:194:C:C6	2.44	0.52
1:A:377:A:H3'	1:A:378:C:H6	1.75	0.51
1:A:5:A:H2'	1:A:6:U:C6	2.45	0.51
1:A:218:U:O5'	1:A:218:U:H6	1.94	0.51
1:A:82:A:H2'	1:A:83:G:O4'	2.10	0.51
1:A:200:G:H1	1:A:231:A:H2	1.58	0.51
1:A:262:A:H2	1:A:270:U:H3	1.56	0.51
1:A:120:U:H2'	1:A:121:G:C8	2.45	0.51
1:A:293:U:H3'	1:A:294:G:H8	1.76	0.51
1:A:324:G:H2'	1:A:325:C:H6	1.75	0.51
1:A:350:A:C5	1:A:380:A:C8	2.98	0.50
1:A:412:A:H2'	1:A:413:A:C8	2.46	0.50
1:A:42:U:H2'	1:A:43:A:C8	2.47	0.50
1:A:10:G:H2'	1:A:11:C:H6	1.76	0.50
1:A:166:G:H2'	1:A:167:G:C8	2.46	0.50
1:A:341:U:H2'	1:A:342:A:C8	2.47	0.50
1:A:197:A:H4'	1:A:198:G:C8	2.47	0.50
1:A:407:U:H2'	1:A:408:G:C8	2.46	0.50
1:A:408:G:H2'	1:A:409:A:H8	1.77	0.50
1:A:69:C:H2'	1:A:70:U:C6	2.46	0.50
1:A:379:G:H4'	1:A:380:A:H5"	1.92	0.50
2:B:49:LYS:HD3	2:B:49:LYS:N	2.27	0.50
1:A:19:A:H2'	1:A:20:U:C6	2.46	0.49
1:A:321:G:H2'	1:A:322:C:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:G:H2'	1:A:11:C:C6	2.48	0.49
1:A:167:G:H2'	1:A:168:A:C8	2.47	0.49
1:A:210:U:H2'	1:A:211:A:H8	1.78	0.49
1:A:215:U:H2'	1:A:217:U:C5	2.45	0.49
1:A:128:G:H2'	1:A:129:C:C6	2.48	0.49
1:A:6:U:H2'	1:A:7:C:H6	1.76	0.49
1:A:111:A:H2'	1:A:112:G:H8	1.78	0.49
1:A:382:G:H2'	1:A:383:G:O4'	2.13	0.49
1:A:144:G:H2'	1:A:145:G:O4'	2.13	0.48
1:A:374:A:H2'	1:A:375:G:H8	1.76	0.48
1:A:110:U:H2'	1:A:111:A:C8	2.47	0.48
2:B:50:LYS:H	2:B:50:LYS:CD	2.20	0.48
1:A:55:A:H2'	1:A:56:U:C6	2.49	0.48
1:A:196:C:H2'	1:A:197:A:C8	2.48	0.48
1:A:314:G:C2	1:A:315:G:N7	2.81	0.48
1:A:17:U:H2'	1:A:18:A:H8	1.79	0.48
1:A:121:G:C6	1:A:131:G:C6	3.02	0.48
1:A:346:C:H2'	1:A:347:C:H6	1.79	0.48
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.96	0.48
1:A:349:G:N1	1:A:379:G:H1'	2.28	0.47
1:A:349:G:N2	1:A:379:G:O4'	2.42	0.47
2:B:94:TYR:HA	2:B:97:VAL:HG12	1.95	0.47
1:A:121:G:H3'	1:A:122:G:H8	1.79	0.47
1:A:147:A:H2'	1:A:148:A:C8	2.49	0.47
1:A:166:G:H2'	1:A:167:G:H8	1.79	0.47
1:A:183:C:H2'	1:A:184:C:C6	2.49	0.47
1:A:71:G:H1'	1:A:291:A:N6	2.30	0.47
1:A:355:G:H21	1:A:373:C:H42	1.62	0.47
1:A:412:A:H2'	1:A:413:A:H8	1.79	0.47
1:A:173:G:H2'	1:A:174:U:C6	2.49	0.47
1:A:201:A:N6	1:A:230:G:H1	2.10	0.47
1:A:384:U:H5"	1:A:385:A:OP1	2.15	0.47
1:A:209:C:H2'	1:A:210:U:C6	2.50	0.47
1:A:64:C:O2	1:A:82:A:N6	2.49	0.46
1:A:111:A:H2'	1:A:112:G:C8	2.50	0.46
1:A:307:G:H2'	1:A:308:A:H8	1.80	0.46
1:A:149:G:H3'	1:A:150:A:H8	1.81	0.46
1:A:229:G:H2'	1:A:230:G:C8	2.50	0.46
1:A:280:U:H2'	1:A:281:U:H6	1.78	0.46
1:A:119:C:H2'	1:A:120:U:H6	1.81	0.46
1:A:156:C:O2'	1:A:157:G:H8	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:C:H2'	1:A:24:U:C6	2.50	0.46
1:A:247:C:H2'	1:A:248:G:H8	1.81	0.46
1:A:378:C:H3'	1:A:379:G:C8	2.50	0.46
1:A:324:G:H2'	1:A:325:C:C6	2.50	0.46
1:A:383:G:H5"	1:A:384:U:OP2	2.16	0.46
1:A:223:A:H2'	1:A:224:G:C8	2.51	0.46
1:A:118:C:H2'	1:A:119:C:C6	2.50	0.46
1:A:280:U:H2'	1:A:281:U:C6	2.51	0.46
1:A:339:A:H2'	1:A:340:U:C6	2.51	0.46
1:A:198:G:H1	1:A:235:C:H1'	1.80	0.46
2:B:16:VAL:HG12	2:B:31:TYR:HB3	1.97	0.46
1:A:208:U:H2'	1:A:209:C:H6	1.79	0.46
1:A:155:A:H2'	1:A:156:C:O4'	2.16	0.45
2:B:71:LEU:HD22	2:B:102:ILE:HD11	1.98	0.45
2:B:106:ARG:HG2	2:B:111:LEU:HB3	1.97	0.45
1:A:79:C:H2'	1:A:80:G:O4'	2.16	0.45
2:B:23:VAL:HG21	2:B:108:ALA:HA	1.97	0.45
1:A:19:A:H2'	1:A:20:U:H6	1.81	0.45
1:A:313:C:H2'	1:A:314:G:C8	2.51	0.45
1:A:315:G:C2	1:A:316:C:C4	3.05	0.45
1:A:114:G:H2'	1:A:115:C:H6	1.81	0.45
1:A:131:G:H2'	1:A:132:G:O4'	2.17	0.45
2:B:50:LYS:HD2	2:B:50:LYS:N	2.22	0.45
1:A:319:A:H1'	1:A:320:U:C5	2.52	0.45
2:B:113:LYS:HE2	2:B:113:LYS:HB2	1.60	0.45
1:A:281:U:H2'	1:A:282:C:C6	2.52	0.45
1:A:357:G:H2'	1:A:358:G:H8	1.82	0.45
1:A:393:U:H2'	1:A:394:G:C8	2.52	0.45
1:A:356:A:H3'	1:A:357:G:H8	1.82	0.45
1:A:377:A:C2	1:A:378:C:H1'	2.52	0.45
1:A:410:U:C2	1:A:411:U:C5	3.04	0.45
2:B:16:VAL:HA	2:B:33:LEU:HD22	1.99	0.45
1:A:186:G:H5'	1:A:187:A:OP2	2.16	0.45
1:A:153:C:H2'	1:A:154:U:C6	2.52	0.45
1:A:282:C:H2'	1:A:283:C:H6	1.82	0.45
1:A:32:G:H3'	1:A:33:U:C6	2.52	0.44
1:A:317:G:O6	1:A:321:G:C2	2.70	0.44
1:A:31:G:C2	1:A:32:G:C8	3.05	0.44
1:A:64:C:H2'	1:A:65:G:H8	1.83	0.44
1:A:232:A:H2'	1:A:233:C:C6	2.52	0.44
1:A:351:G:H2'	1:A:352:U:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:A:C6	1:A:382:G:C4	3.05	0.44
1:A:50:A:H5'	1:A:388:G:H5"	1.99	0.44
1:A:200:G:C6	1:A:231:A:N1	2.86	0.44
1:A:381:A:C2	1:A:382:G:H1'	2.52	0.44
1:A:157:G:H1	1:A:170:A:H1'	1.81	0.44
1:A:260:C:H2'	1:A:261:A:O4'	2.18	0.44
1:A:5:A:H2'	1:A:6:U:H6	1.82	0.44
1:A:118:C:H2'	1:A:119:C:H6	1.82	0.44
1:A:2:U:H2'	1:A:3:U:C6	2.53	0.44
1:A:315:G:C6	1:A:316:C:N4	2.86	0.43
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.43
1:A:128:G:H2'	1:A:129:C:H6	1.84	0.43
1:A:252:G:H2'	1:A:253:A:H8	1.83	0.43
1:A:380:A:C5	1:A:381:A:C8	3.06	0.43
2:B:1:MET:HE3	2:B:1:MET:HA	1.99	0.43
1:A:45:A:C2	1:A:388:G:H2'	2.53	0.43
1:A:201:A:H2'	1:A:202:C:C6	2.54	0.43
1:A:361:C:O2'	1:A:362:A:H3'	2.18	0.43
1:A:59:U:H2'	1:A:60:C:H6	1.82	0.43
1:A:247:C:H2'	1:A:248:G:C8	2.54	0.43
1:A:408:G:H2'	1:A:409:A:C8	2.53	0.43
1:A:55:A:H2'	1:A:56:U:H6	1.83	0.43
1:A:171:U:C5	1:A:172:G:C8	3.07	0.43
1:A:350:A:H3'	1:A:351:G:H8	1.84	0.43
2:B:45:LEU:HD11	2:B:65:ARG:HG3	2.00	0.43
1:A:32:G:H1	1:A:34:U:H1'	1.82	0.43
1:A:380:A:C6	1:A:381:A:C5	3.07	0.43
1:A:172:G:C2	1:A:173:G:C5	3.07	0.43
1:A:224:G:H2'	1:A:225:A:C8	2.53	0.43
1:A:380:A:C2	1:A:381:A:H1'	2.54	0.43
1:A:414:C:C2	1:A:415:G:C8	3.07	0.43
1:A:164:U:H2'	1:A:165:G:O4'	2.19	0.42
1:A:350:A:C5	1:A:351:G:C5	3.08	0.42
1:A:264:U:C2	1:A:266:A:H5"	2.55	0.42
1:A:7:C:H2'	1:A:8:A:C8	2.54	0.42
1:A:17:U:H2'	1:A:18:A:C8	2.55	0.42
1:A:32:G:H22	1:A:34:U:H1'	1.83	0.42
1:A:114:G:H2'	1:A:115:C:C6	2.54	0.42
1:A:214:G:H2'	1:A:215:U:C6	2.54	0.42
1:A:230:G:H2'	1:A:231:A:C8	2.54	0.42
1:A:345:G:H2'	1:A:346:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:U:H2'	1:A:21:C:C6	2.54	0.42
1:A:103:C:H3'	1:A:104:A:H8	1.85	0.42
2:B:9:LYS:HB2	2:B:12:GLU:HG2	2.02	0.42
1:A:131:G:C6	1:A:132:G:C5	3.08	0.42
1:A:160:C:C2	1:A:161:G:C8	3.08	0.42
1:A:282:C:C2	1:A:283:C:C5	3.07	0.42
1:A:350:A:H2'	1:A:350:A:N3	2.35	0.42
1:A:307:G:H2'	1:A:308:A:C8	2.54	0.42
1:A:347:C:C2	1:A:348:G:C8	3.08	0.42
1:A:59:U:H1'	1:A:257:A:N3	2.35	0.42
1:A:63:A:H2'	1:A:64:C:C6	2.55	0.42
1:A:268:G:H8	1:A:268:G:OP2	2.03	0.42
1:A:47:G:H1	1:A:385:A:H62	1.68	0.42
1:A:119:C:H2'	1:A:120:U:C6	2.54	0.41
1:A:385:A:H2'	1:A:386:C:O4'	2.19	0.41
1:A:78:C:H2'	1:A:79:C:C6	2.55	0.41
2:B:17:PHE:CE1	2:B:84:ILE:HD11	2.55	0.41
1:A:196:C:H2'	1:A:197:A:H8	1.85	0.41
1:A:283:C:H2'	1:A:284:C:H6	1.85	0.41
1:A:200:G:N1	1:A:232:A:C2	2.88	0.41
1:A:38:G:H2'	1:A:39:C:C6	2.55	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.84	0.41
1:A:279:C:H2'	1:A:280:U:H6	1.85	0.41
1:A:354:C:C2	1:A:355:G:C8	3.08	0.41
1:A:170:A:O2'	1:A:171:U:H5'	2.20	0.41
1:A:314:G:C2	1:A:315:G:C8	3.09	0.41
1:A:323:A:C2'	1:A:324:G:H5'	2.50	0.41
1:A:133:G:H2'	1:A:134:C:C6	2.56	0.41
1:A:180:U:H2'	1:A:181:A:C8	2.46	0.41
1:A:197:A:H61	1:A:233:C:H42	1.69	0.41
1:A:222:U:H2'	1:A:223:A:C8	2.56	0.41
1:A:255:A:O4'	1:A:257:A:C8	2.74	0.41
1:A:349:G:C2	1:A:378:C:N3	2.89	0.41
1:A:350:A:H1'	1:A:380:A:N1	2.36	0.41
2:B:28:PHE:CE2	2:B:97:VAL:HG23	2.56	0.41
1:A:23:C:H2'	1:A:24:U:H6	1.86	0.41
1:A:230:G:H2'	1:A:231:A:H8	1.86	0.41
2:B:41:PHE:CZ	2:B:72:LYS:HG3	2.56	0.41
1:A:262:A:H1'	1:A:271:A:N6	2.37	0.40
1:A:246:A:H2'	1:A:247:C:H6	1.87	0.40
1:A:202:C:H2'	1:A:203:G:C8	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:G:H2'	1:A:316:C:C5	2.56	0.40
1:A:404:G:H2'	1:A:405:C:O4'	2.22	0.40
1:A:221:U:H2'	1:A:222:U:C6	2.57	0.40
1:A:327:U:C2	1:A:328:G:C8	3.09	0.40
2:B:17:PHE:HA	2:B:31:TYR:CD2	2.57	0.40
1:A:219:C:H2'	1:A:220:C:H6	1.85	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	
2	B	114/116 (98%)	111 (97%)	3 (3%)	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	
2	B	99/99 (100%)	96 (97%)	3 (3%)	36	68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	LEU
2	B	71	LEU
2	B	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	132 (31%)	3 (0%)

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	8	A
1	A	9	U
1	A	11	C
1	A	15	G
1	A	22	G
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	48	A
1	A	50	A
1	A	51	G
1	A	52	U
1	A	53	C
1	A	67	U
1	A	68	G
1	A	74	A
1	A	75	U
1	A	76	G
1	A	78	C
1	A	80	G
1	A	82	A
1	A	83	G
1	A	85	G

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Mol	Chain	Res	Type
1	A	91	G
1	A	99	A
1	A	101	U
1	A	102	C
1	A	103	C
1	A	108	G
1	A	117	G
1	A	118	C
1	A	121	G
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	132	G
1	A	134	C
1	A	135	U
1	A	137	A
1	A	138	C
1	A	139	G
1	A	141	C
1	A	142	G
1	A	146	A
1	A	149	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	164	U
1	A	171	U
1	A	172	G
1	A	177	G
1	A	180	U
1	A	182	C
1	A	184	C
1	A	185	U
1	A	186	G
1	A	190	G
1	A	192	G
1	A	193	C
1	A	195	A
1	A	198	G
1	A	199	U

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Mol	Chain	Res	Type
1	A	200	G
1	A	202	C
1	A	203	G
1	A	204	G
1	A	207	C
1	A	208	U
1	A	213	G
1	A	219	C
1	A	226	G
1	A	227	G
1	A	232	A
1	A	234	G
1	A	236	G
1	A	237	G
1	A	238	U
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	254	G
1	A	255	A
1	A	257	A
1	A	264	U
1	A	265	G
1	A	267	U
1	A	268	G
1	A	269	G
1	A	276	C
1	A	292	A
1	A	296	A
1	A	304	A
1	A	312	G
1	A	314	G
1	A	317	G
1	A	318	C
1	A	320	U
1	A	321	G
1	A	323	A
1	A	324	G
1	A	329	U
1	A	330	A
1	A	334	A

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Mol	Chain	Res	Type
1	A	349	G
1	A	351	G
1	A	362	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	376	U
1	A	378	C
1	A	379	G
1	A	380	A
1	A	381	A
1	A	383	G
1	A	389	A
1	A	406	A
1	A	408	G
1	A	410	U
1	A	411	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	122	G
1	A	126	U
1	A	141	C

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 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

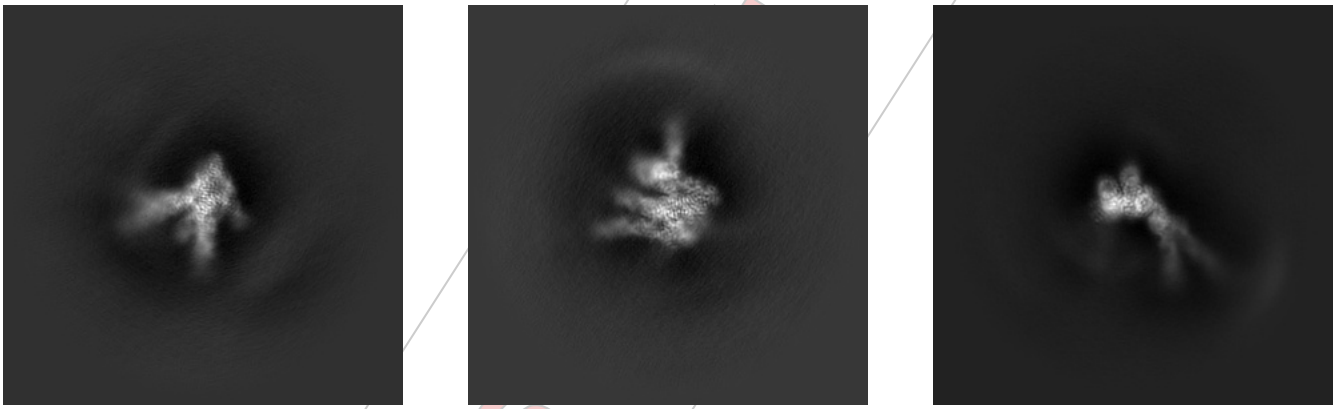
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70997. 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.

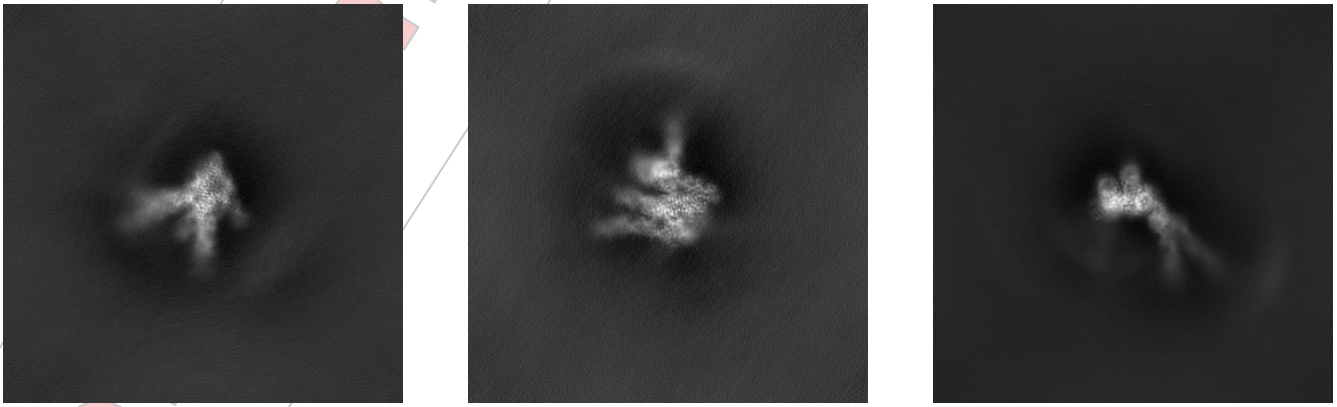
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

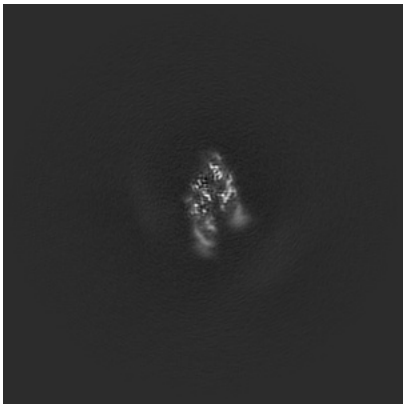


X Y Z

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

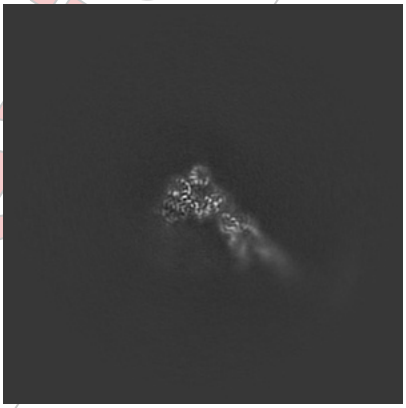
6.2 Central slices (i)

6.2.1 Primary map



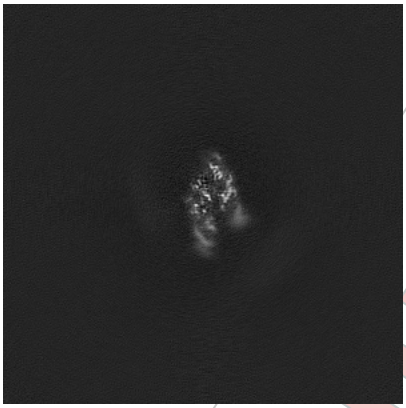
X Index: 200

Y Index: 200



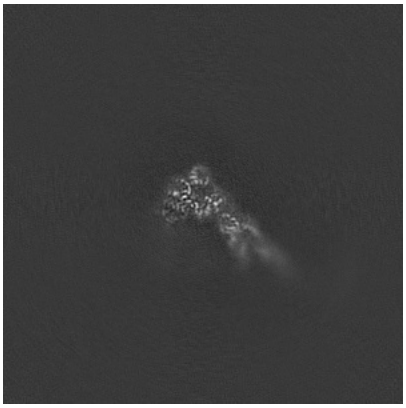
Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

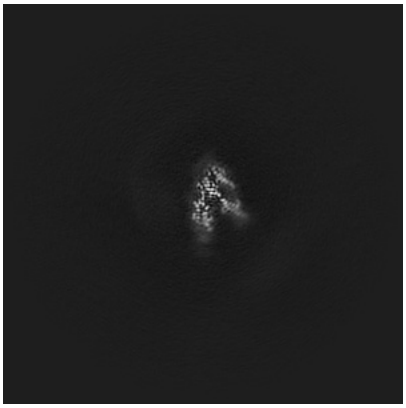


Z Index: 200

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

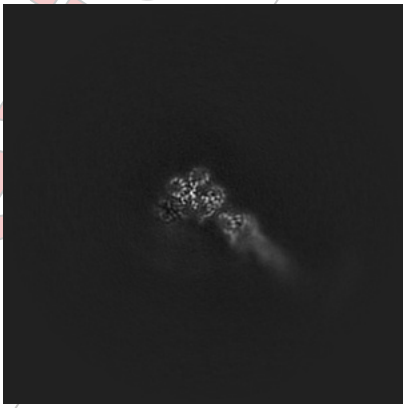
6.3 Largest variance slices (i)

6.3.1 Primary map



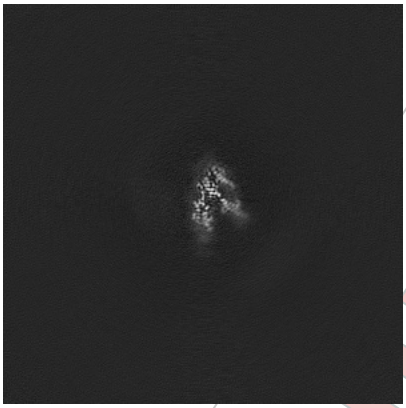
X Index: 193

Y Index: 200



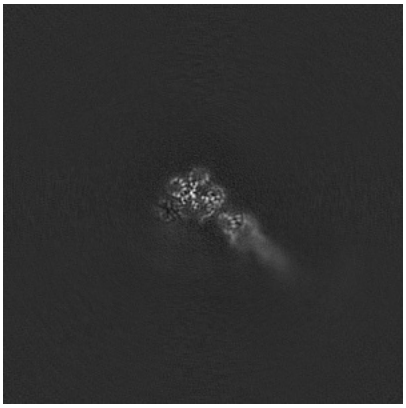
Z Index: 204

6.3.2 Raw map



X Index: 193

Y Index: 200

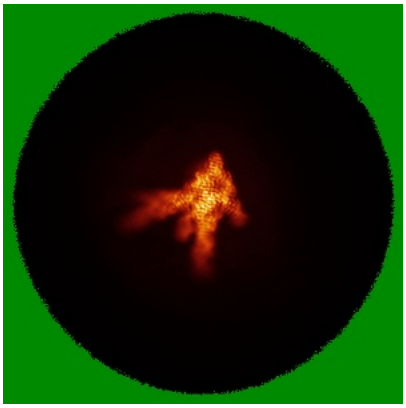


Z Index: 204

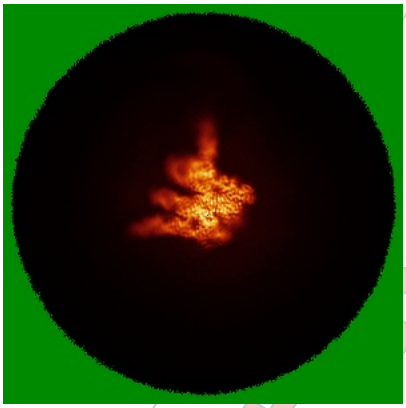
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

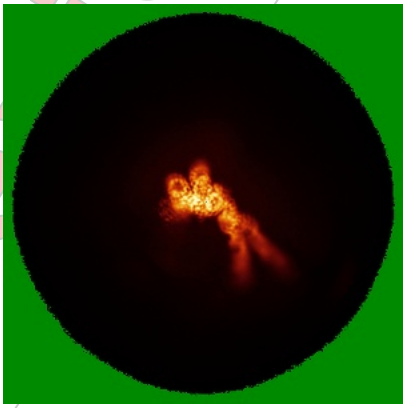
6.4.1 Primary map



X

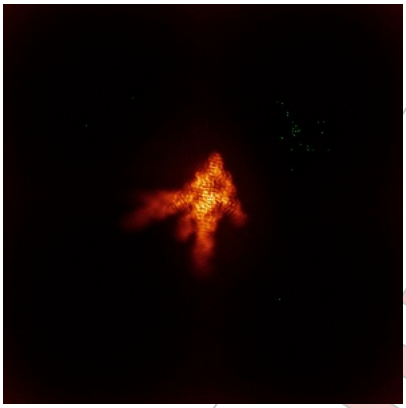


Y

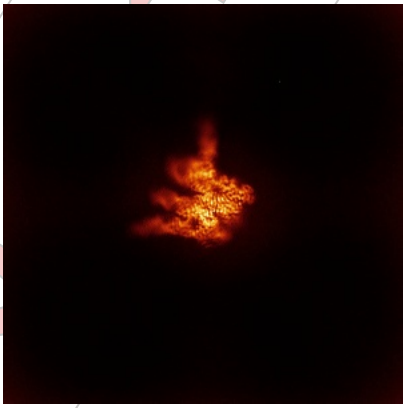


Z

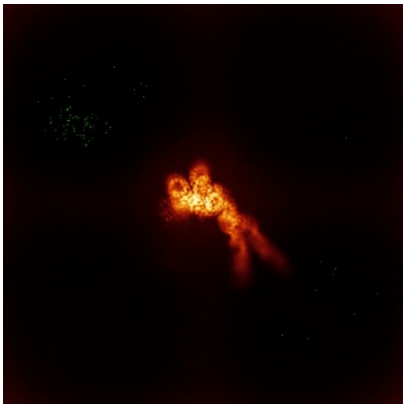
6.4.2 Raw map



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.

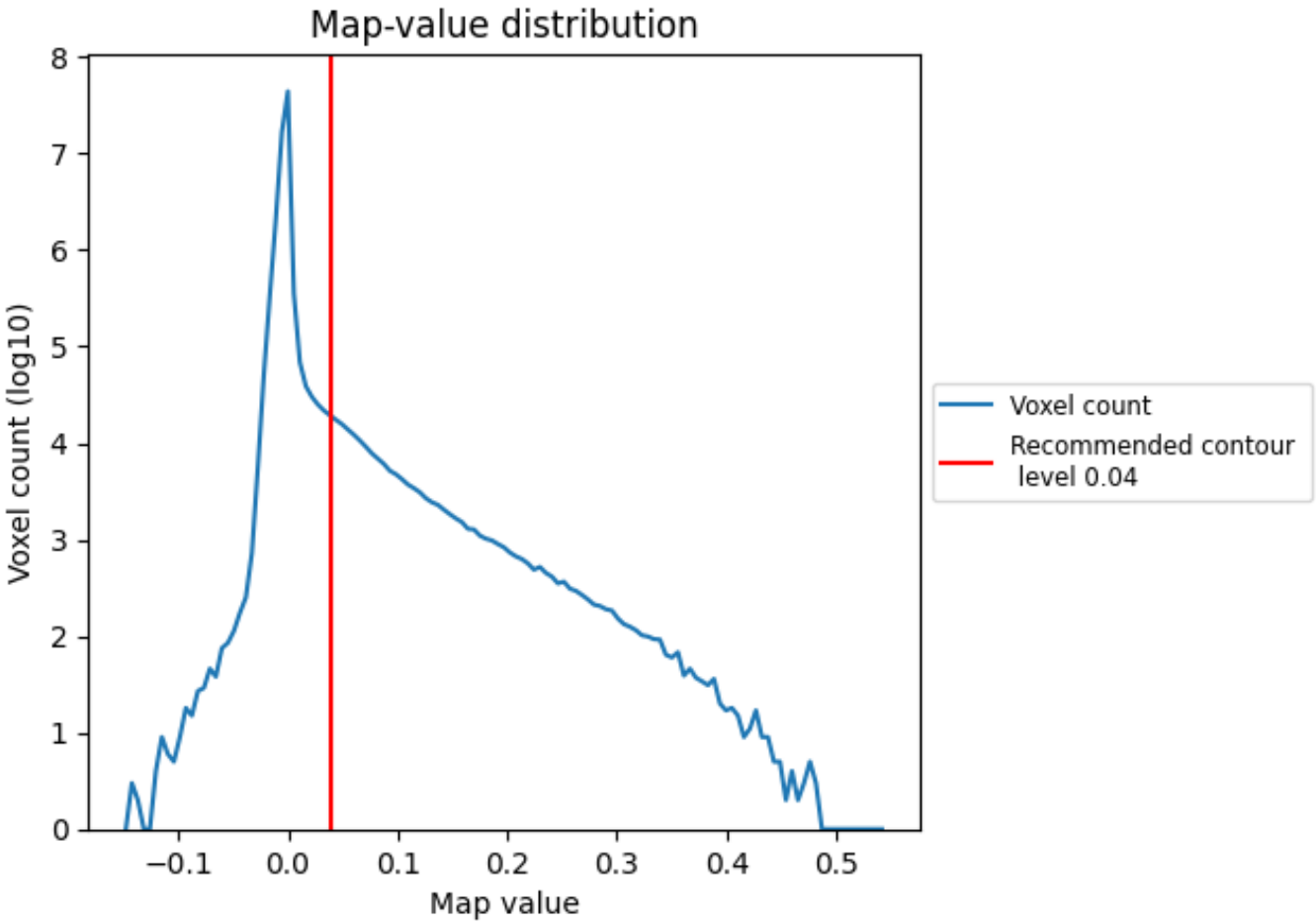
6.6 Mask visualisation (i)

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

7 Map analysis

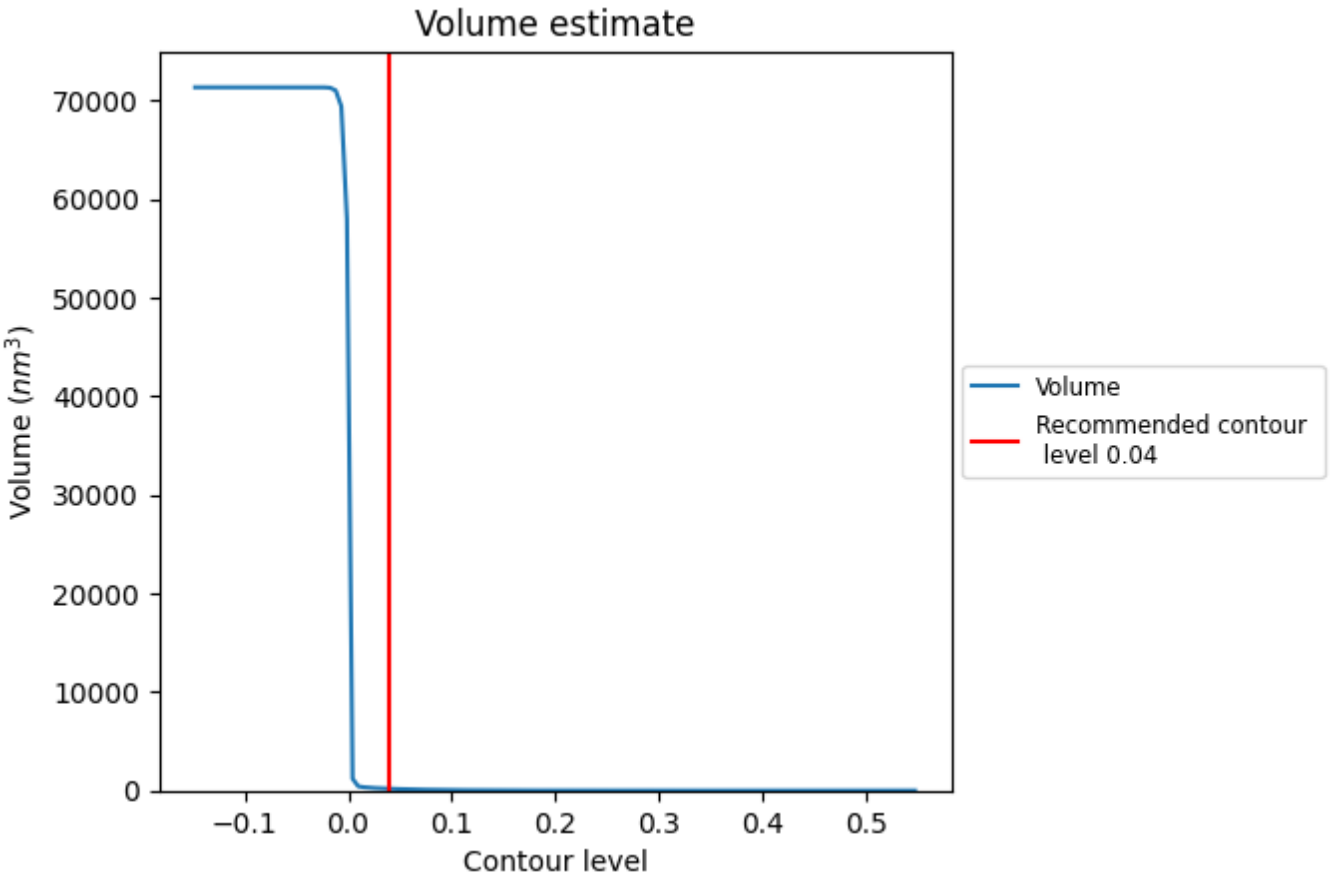
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

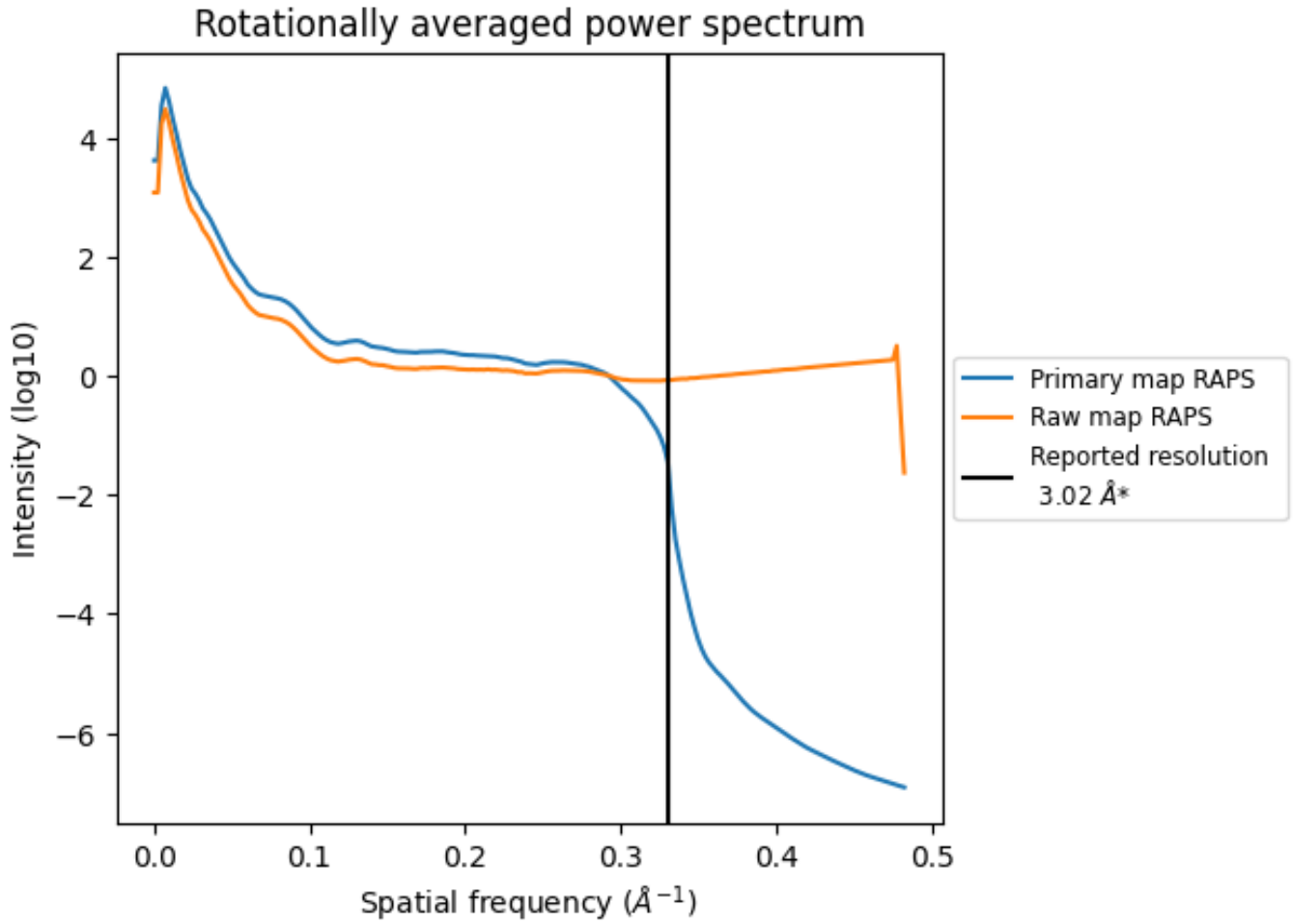
7.2 Volume estimate (i)



The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 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 (i)

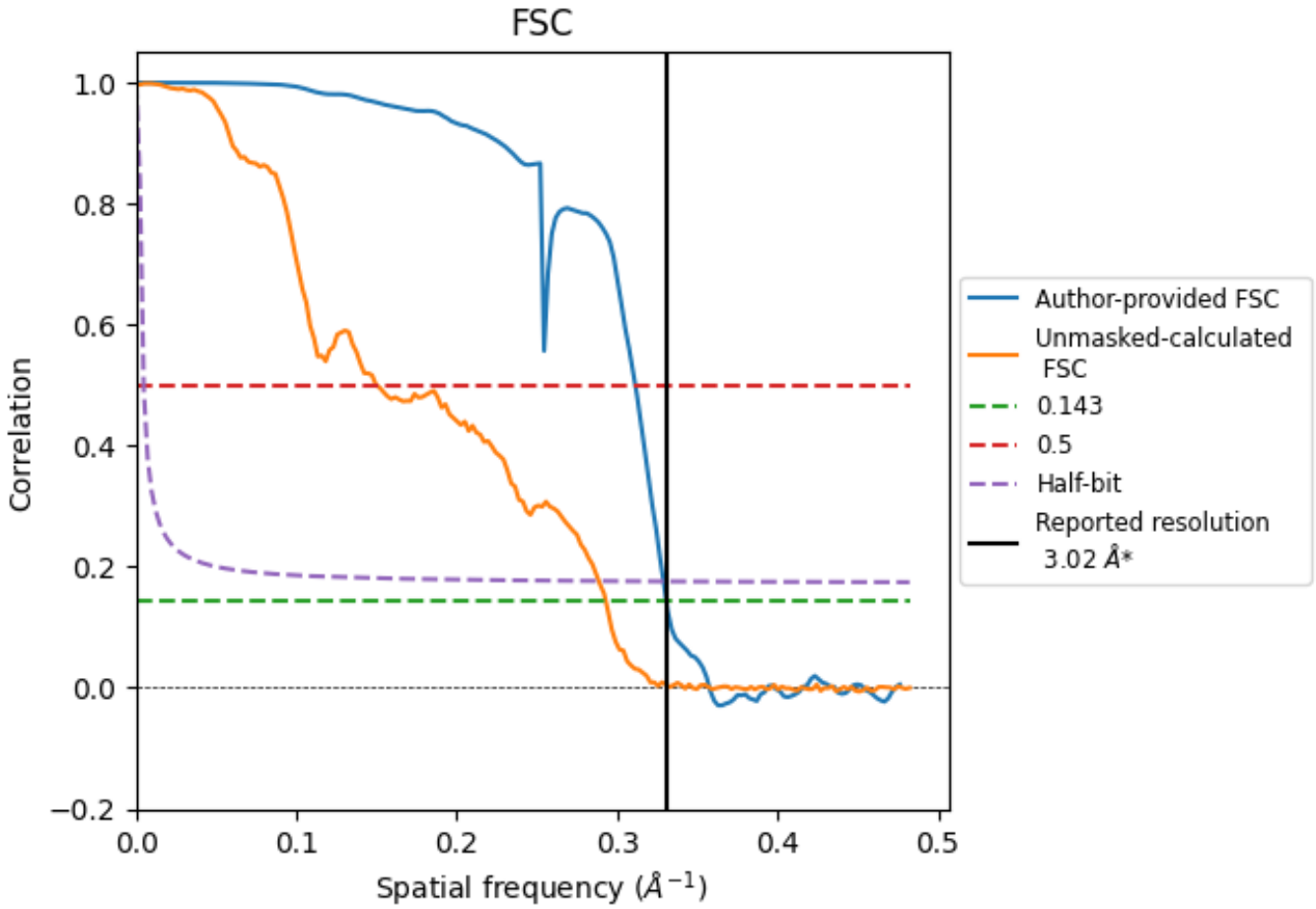


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates (i)

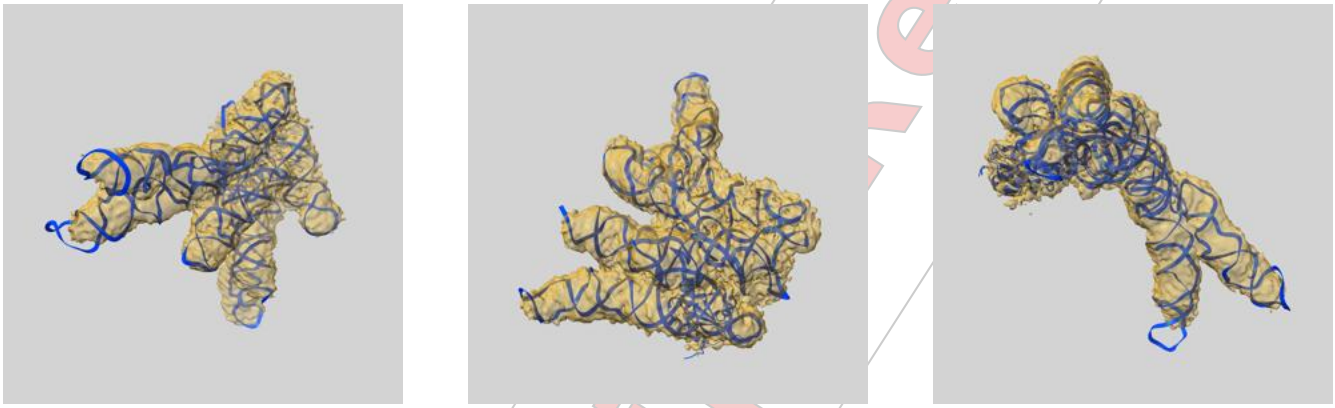
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.21	3.04
Unmasked-calculated*	3.42	6.67	3.47

*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 3.42 differs from the reported value 3.02 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70997 and PDB model 9OY5. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay



X Y Z

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

X Y Z

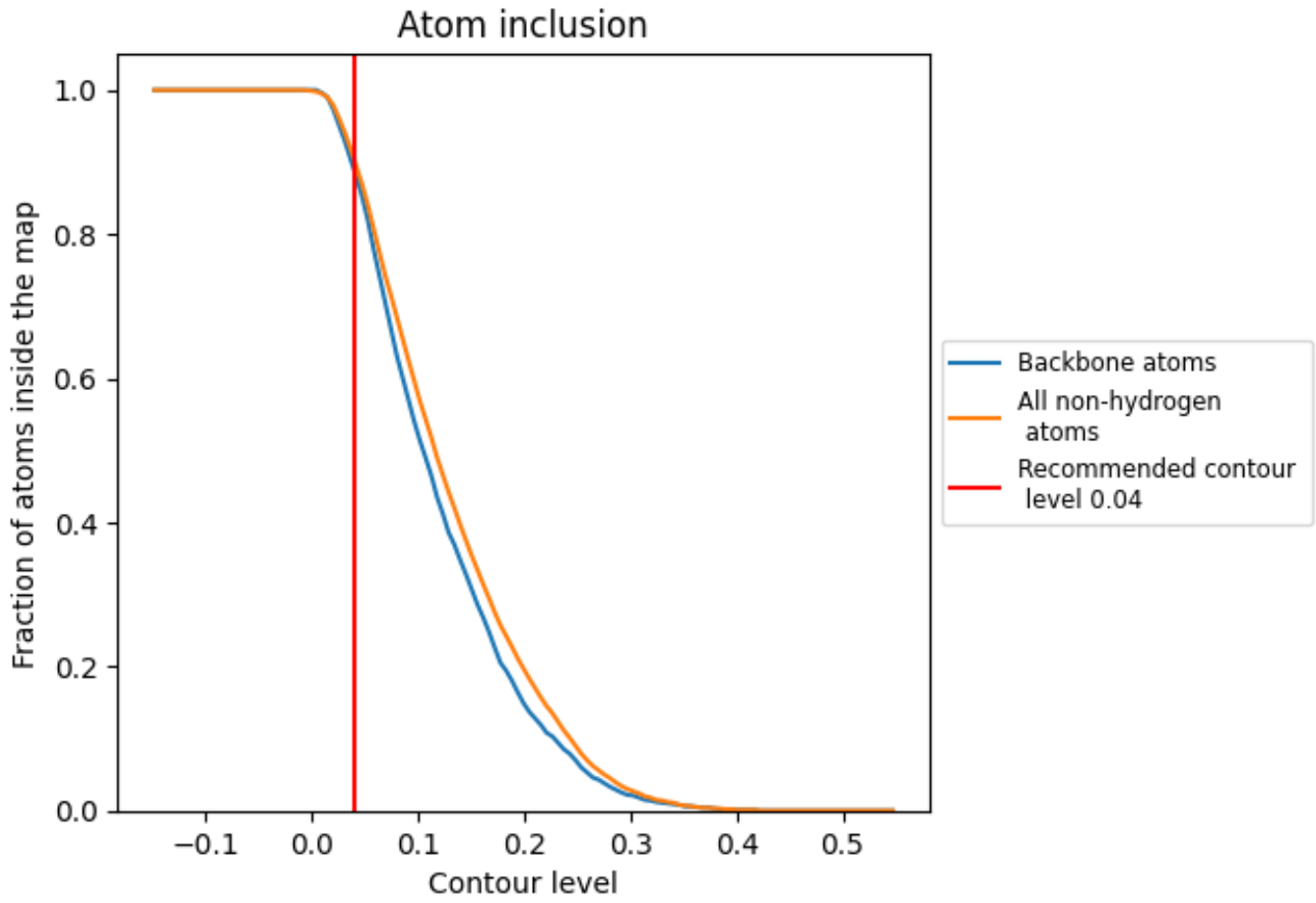
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9050	0.3520
A	0.9210	0.3440
B	0.7530	0.4260

Full wwPDB EM Validation Report ⓘ

Jun 6, 2025 – 12:13 PM EDT

PDB ID	:	9OY6 / pdb_00009oy6
EMDB ID	:	EMD-70998
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme tetraloop mutant (sub-conformation 2)
Deposited on	:	2025-06-04
Resolution	:	2.96 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

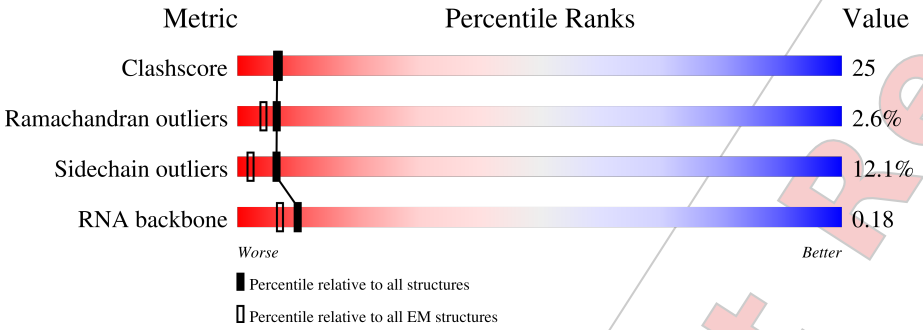
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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 <=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	417	18% 49% 31%
2	B	116	63% 26% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	517	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9925 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 RNA chain called RNase P RNA tetraloop mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8953	3992	1648	2896	417	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	U	C	conflict	GB 143442
A	215	U	G	engineered mutation	GB 143442
A	216	U	A	engineered mutation	GB 143442
A	217	U	A	engineered mutation	GB 143442
A	218	U	A	engineered mutation	GB 143442
A	417	C	G	conflict	GB 143442

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

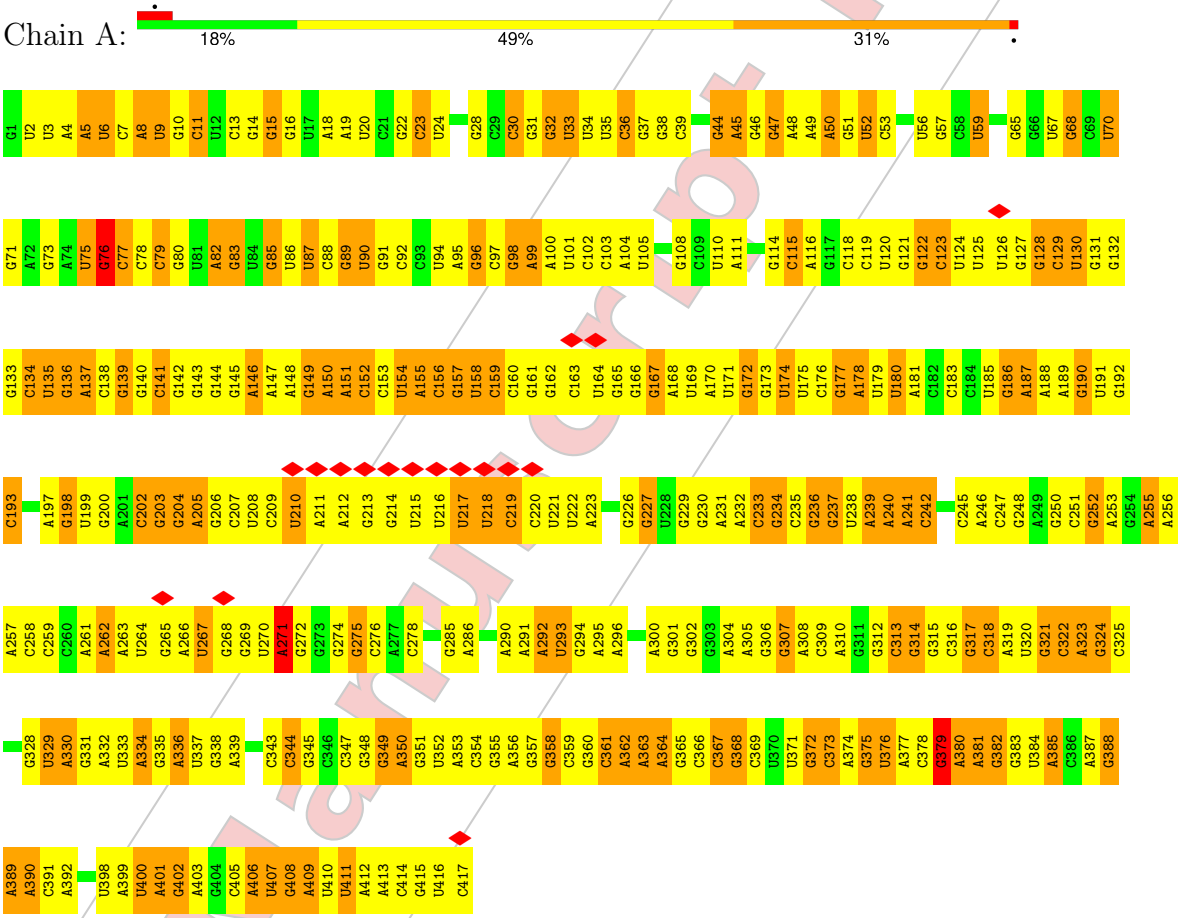
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	25	25	25	0

3 Residue-property plots (i)

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.

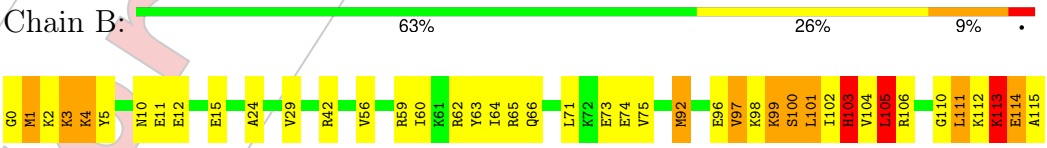
- Molecule 1: RNase P RNA tetraloop mutant

Chain A:



- Molecule 2: Ribonuclease P protein component

Chain B:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.567	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	0.65	2/10025 (0.0%)	1.01	9/15639 (0.1%)
2	B	0.52	1/962 (0.1%)	0.83	4/1281 (0.3%)
All	All	0.64	3/10987 (0.0%)	1.00	13/16920 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	SER	CA-CB	-5.19	1.44	1.53
1	A	218	U	C1'-N1	5.04	1.56	1.48
1	A	217	U	C1'-N1	5.00	1.55	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	C	O3'-P-O5'	-8.27	91.60	104.00
1	A	388	G	C2'-C3'-O3'	-6.92	103.31	113.70
1	A	379	G	O3'-P-O5'	-6.16	94.76	104.00
2	B	4	LYS	CA-C-N	-6.12	112.94	122.37
2	B	4	LYS	C-N-CA	-6.12	112.94	122.37
1	A	390	A	O3'-P-O5'	6.00	113.00	104.00
1	A	258	C	C1'-C2'-O2'	-5.67	99.90	108.40
1	A	44	G	O3'-P-O5'	5.35	112.03	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	103	HIS	CB-CA-C	-5.34	99.80	110.42
1	A	271	A	C4'-C3'-C2'	-5.18	97.42	102.60
1	A	262	A	C3'-C2'-C1'	-5.16	96.14	101.30
2	B	105	LEU	N-CA-C	-5.12	105.39	111.69
1	A	76	G	O3'-P-O5'	-5.07	96.40	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	59	ARG	Sidechain

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	8953	0	4505	314	0
2	B	947	0	1008	44	0
3	A	25	0	0	3	0
All	All	9925	0	5513	352	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 25.

All (352) 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:158:U:H2'	1:A:159:C:C6	1.59	1.37
1:A:158:U:O2'	1:A:159:C:O5'	1.63	1.15
1:A:155:A:H8	1:A:155:A:O5'	1.30	1.11
1:A:141:C:H5'	1:A:239:A:H61	1.17	1.05
1:A:157:G:OP2	1:A:158:U:O4	1.76	1.03
1:A:158:U:H2'	1:A:159:C:C5	1.93	1.02
1:A:156:C:O2	1:A:156:C:H2'	1.57	1.02
1:A:293:U:P	3:A:517:CA:CA	1.77	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:U:H2'	1:A:159:C:H6	1.21	0.96
1:A:155:A:O5'	1:A:155:A:C8	2.21	0.93
1:A:262:A:H2	1:A:270:U:H3	1.15	0.92
1:A:157:G:OP2	1:A:158:U:C4	2.22	0.92
1:A:215:U:H2'	1:A:217:U:H5	1.35	0.91
1:A:155:A:H2'	1:A:156:C:H1'	1.50	0.91
1:A:155:A:H2'	1:A:156:C:C1'	2.01	0.91
1:A:236:G:H2'	1:A:237:G:C8	2.08	0.88
1:A:141:C:H5'	1:A:239:A:N6	1.89	0.88
1:A:371:U:H5"	1:A:372:G:H5'	1.57	0.87
1:A:158:U:C2'	1:A:159:C:O5'	2.24	0.86
1:A:349:G:N2	1:A:379:G:H1'	1.89	0.85
1:A:215:U:O2'	1:A:217:U:O4	1.97	0.82
1:A:293:U:OP2	3:A:517:CA:CA	0.41	0.82
1:A:262:A:H2'	1:A:263:A:H5'	1.60	0.81
1:A:157:G:OP2	1:A:158:U:C5	2.33	0.81
1:A:215:U:H2'	1:A:217:U:C5	2.17	0.80
1:A:349:G:H22	1:A:379:G:H1'	1.44	0.80
1:A:156:C:O2	1:A:156:C:C2'	2.28	0.78
1:A:367:C:H2'	1:A:368:G:C8	2.19	0.78
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.68	0.76
1:A:158:U:HO2'	1:A:159:C:C5'	1.99	0.75
1:A:158:U:C2'	1:A:159:C:C6	2.55	0.74
1:A:350:A:H1'	1:A:380:A:N1	2.02	0.74
1:A:157:G:H3'	1:A:158:U:C5	2.24	0.73
1:A:3:U:H2'	1:A:4:A:C8	2.24	0.72
1:A:414:C:H2'	1:A:415:G:H8	1.53	0.71
1:A:313:C:H2'	1:A:314:G:C8	2.25	0.71
1:A:36:C:C4	1:A:37:G:N7	2.59	0.71
1:A:7:C:H2'	1:A:8:A:C8	2.25	0.71
1:A:158:U:H6	1:A:158:U:O5'	1.74	0.70
1:A:215:U:O2	1:A:218:U:O4	2.09	0.70
1:A:36:C:C2	1:A:37:G:C8	2.80	0.69
2:B:63:TYR:HB3	2:B:97:VAL:HG11	1.73	0.69
1:A:363:A:C8	1:A:363:A:H5"	2.28	0.69
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.75	0.68
1:A:45:A:C2	1:A:388:G:H2'	2.28	0.68
1:A:155:A:H2'	1:A:156:C:C4'	2.24	0.68
1:A:414:C:H2'	1:A:415:G:C8	2.28	0.68
1:A:52:U:C6	1:A:52:U:H5"	2.30	0.67
1:A:350:A:H1'	1:A:380:A:C6	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:U:H2'	1:A:131:G:C8	2.29	0.67
1:A:155:A:C2'	1:A:156:C:H4'	2.24	0.66
1:A:334:A:H62	2:B:10:ASN:HD22	1.42	0.66
1:A:180:U:H2'	1:A:181:A:H8	1.60	0.66
1:A:206:G:H1	1:A:227:G:H22	1.42	0.66
1:A:155:A:C4	1:A:156:C:H1'	2.32	0.65
2:B:101:LEU:O	2:B:105:LEU:HB2	1.97	0.65
1:A:274:G:H2'	1:A:275:G:H5'	1.78	0.65
1:A:381:A:C2	1:A:382:G:H1'	2.33	0.64
1:A:180:U:H2'	1:A:181:A:C8	2.33	0.64
1:A:262:A:C2'	1:A:263:A:H5'	2.27	0.64
1:A:274:G:C2'	1:A:275:G:H5'	2.28	0.64
1:A:380:A:C2	1:A:381:A:H1'	2.33	0.64
2:B:110:GLY:O	2:B:111:LEU:HD23	1.99	0.63
1:A:236:G:H2'	1:A:237:G:H8	1.59	0.62
1:A:316:C:H2'	1:A:317:G:C8	2.35	0.62
1:A:159:C:O5'	1:A:159:C:H6	1.83	0.62
1:A:148:A:H61	1:A:177:G:H1'	1.64	0.62
1:A:270:U:C2'	1:A:271:A:H5'	2.30	0.61
1:A:158:U:C2'	1:A:159:C:H6	2.05	0.61
1:A:157:G:H3'	1:A:158:U:C6	2.36	0.61
2:B:56:VAL:O	2:B:60:ILE:HG13	2.00	0.61
1:A:71:G:O2'	1:A:73:G:N7	2.31	0.61
1:A:141:C:C5'	1:A:239:A:H61	2.03	0.61
1:A:349:G:H21	1:A:350:A:H62	1.48	0.61
1:A:390:A:OP2	3:A:520:CA:CA	1.78	0.61
1:A:71:G:H1'	1:A:291:A:H61	1.66	0.60
1:A:82:A:H2'	1:A:83:G:O4'	2.01	0.60
1:A:85:G:O2'	1:A:87:U:O4	2.19	0.60
1:A:140:G:O6	1:A:239:A:H2'	1.99	0.60
1:A:198:G:H1	1:A:235:C:H1'	1.65	0.60
1:A:161:G:H3'	1:A:162:G:H8	1.67	0.60
1:A:155:A:H2'	1:A:156:C:H4'	1.84	0.60
2:B:112:LYS:HB2	2:B:114:GLU:HG2	1.83	0.60
1:A:38:G:H2'	1:A:39:C:C6	2.37	0.59
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.67	0.59
1:A:32:G:H22	1:A:34:U:H1'	1.67	0.59
1:A:360:G:H22	1:A:363:A:H5"	1.67	0.59
1:A:219:C:H2'	1:A:220:C:C6	2.37	0.59
1:A:158:U:C2'	1:A:159:C:C5	2.77	0.59
1:A:158:U:O5'	1:A:158:U:C6	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:U:C2	1:A:159:C:C5	2.90	0.59
1:A:334:A:H62	2:B:10:ASN:ND2	2.01	0.58
1:A:9:U:H2'	1:A:10:G:C8	2.39	0.58
1:A:360:G:N2	1:A:363:A:H5"	2.18	0.58
1:A:130:U:H2'	1:A:131:G:H8	1.67	0.58
1:A:36:C:N3	1:A:37:G:N7	2.52	0.58
1:A:114:G:H3'	1:A:115:C:H6	1.69	0.58
1:A:251:C:C2'	1:A:252:G:H5'	2.34	0.58
1:A:158:U:O2'	1:A:159:C:C5'	2.48	0.58
1:A:10:G:N1	1:A:405:C:O2	2.30	0.57
1:A:114:G:H3'	1:A:115:C:C6	2.40	0.57
1:A:315:G:H2'	1:A:316:C:C6	2.40	0.57
2:B:3:LYS:C	2:B:5:TYR:H	2.12	0.57
1:A:47:G:H1	1:A:385:A:H62	1.52	0.57
1:A:110:U:H2'	1:A:111:A:C8	2.40	0.56
2:B:105:LEU:HB3	2:B:111:LEU:HG	1.87	0.56
1:A:18:A:H2'	1:A:19:A:C8	2.42	0.56
1:A:141:C:N4	1:A:238:U:H3'	2.21	0.56
1:A:349:G:H1'	1:A:350:A:C8	2.41	0.56
1:A:14:G:C2'	1:A:401:A:H61	2.18	0.55
1:A:267:U:H2'	1:A:268:G:C8	2.41	0.55
1:A:217:U:H3'	1:A:218:U:C5	2.41	0.55
1:A:378:C:H3'	1:A:379:G:H8	1.70	0.55
1:A:360:G:H22	1:A:363:A:C5'	2.19	0.55
1:A:374:A:H2'	1:A:375:G:C8	2.41	0.55
1:A:186:G:H5'	1:A:187:A:OP2	2.06	0.55
1:A:236:G:C2'	1:A:237:G:C8	2.86	0.55
1:A:115:C:H2'	1:A:116:A:C8	2.41	0.55
1:A:241:A:H2'	1:A:242:C:C5	2.41	0.55
1:A:308:A:H2'	1:A:309:C:C6	2.41	0.55
1:A:136:G:H2'	1:A:138:C:C5	2.42	0.55
1:A:176:C:H2'	1:A:177:G:H5'	1.88	0.55
1:A:159:C:H2'	1:A:160:C:C6	2.42	0.54
1:A:308:A:N1	1:A:329:U:H5	2.06	0.54
2:B:92:MET:HB3	2:B:97:VAL:HG23	1.88	0.54
2:B:100:SER:O	2:B:101:LEU:C	2.47	0.54
1:A:10:G:H2'	1:A:11:C:C6	2.43	0.54
1:A:154:U:H3'	1:A:155:A:C8	2.43	0.54
1:A:146:A:H3'	1:A:178:A:H61	1.73	0.54
1:A:360:G:O2'	1:A:364:A:N6	2.42	0.53
1:A:155:A:C2'	1:A:156:C:C4'	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:G:H2'	1:A:198:G:N3	2.24	0.53
1:A:270:U:H2'	1:A:271:A:H5'	1.88	0.53
1:A:378:C:H3'	1:A:379:G:C8	2.44	0.53
1:A:136:G:O2'	1:A:137:A:H5'	2.09	0.53
1:A:203:G:H1	1:A:229:G:H22	1.55	0.53
1:A:236:G:C2'	1:A:237:G:H8	2.20	0.53
2:B:102:ILE:O	2:B:103:HIS:C	2.52	0.53
1:A:85:G:H4'	1:A:85:G:OP1	2.09	0.53
1:A:222:U:H2'	1:A:223:A:C8	2.43	0.53
1:A:262:A:H2	1:A:270:U:N3	1.97	0.52
2:B:3:LYS:C	2:B:5:TYR:N	2.67	0.52
1:A:350:A:C2	1:A:380:A:H1'	2.45	0.51
1:A:38:G:H2'	1:A:39:C:H6	1.75	0.51
1:A:158:U:C2	1:A:159:C:C4	2.99	0.51
1:A:292:A:C8	1:A:292:A:H5"	2.44	0.51
1:A:134:C:H2'	1:A:135:U:O4'	2.10	0.51
1:A:363:A:H5"	1:A:363:A:H8	1.74	0.51
1:A:157:G:O5'	1:A:157:G:H8	1.93	0.51
1:A:9:U:H2'	1:A:10:G:H8	1.75	0.51
1:A:16:G:C2	1:A:344:C:C2	2.99	0.51
1:A:233:C:H2'	1:A:234:G:C8	2.46	0.51
1:A:307:G:C2	1:A:308:A:C5	2.99	0.51
1:A:70:U:H2'	1:A:71:G:O4'	2.10	0.50
1:A:71:G:N2	1:A:73:G:H3'	2.26	0.50
1:A:155:A:C2'	1:A:156:C:H1'	2.31	0.50
2:B:113:LYS:NZ	2:B:115:ALA:OXT	2.44	0.50
1:A:148:A:N6	1:A:177:G:H1'	2.26	0.50
1:A:305:A:H2'	1:A:306:G:O4'	2.11	0.50
1:A:14:G:H1'	1:A:402:G:N2	2.26	0.50
1:A:6:U:H2'	1:A:7:C:C6	2.47	0.50
1:A:358:G:N2	1:A:367:C:O2	2.45	0.50
1:A:155:A:N3	1:A:156:C:H1'	2.27	0.49
1:A:348:G:H3'	1:A:349:G:C8	2.46	0.49
1:A:23:C:H5"	2:B:1:MET:HA	1.94	0.49
1:A:317:G:N1	1:A:321:G:C2	2.79	0.49
1:A:155:A:H2'	1:A:156:C:O4'	2.13	0.49
1:A:122:G:H3'	1:A:123:C:H5"	1.94	0.49
1:A:371:U:H4'	1:A:373:C:H5	1.78	0.49
1:A:193:C:N4	1:A:237:G:C6	2.72	0.49
1:A:15:G:N2	1:A:345:G:H1'	2.28	0.49
1:A:161:G:H3'	1:A:162:G:C8	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:VAL:HG22	2:B:111:LEU:CD2	2.42	0.49
1:A:263:A:O5'	1:A:263:A:H8	1.96	0.49
1:A:56:U:H2'	1:A:57:G:O4'	2.13	0.49
1:A:75:U:HO2'	1:A:76:G:P	2.36	0.49
1:A:241:A:HO2'	1:A:242:C:H6	1.61	0.49
1:A:361:C:O2'	1:A:362:A:H3'	2.12	0.49
2:B:112:LYS:O	2:B:114:GLU:N	2.46	0.49
1:A:240:A:N3	1:A:240:A:H2'	2.26	0.48
1:A:412:A:H2'	1:A:413:A:C8	2.47	0.48
1:A:4:A:H2'	1:A:5:A:C8	2.48	0.48
1:A:216:U:H3'	1:A:217:U:C6	2.47	0.48
1:A:411:U:H2'	1:A:412:A:C8	2.47	0.48
2:B:96:GLU:HA	2:B:99:LYS:HE2	1.94	0.48
1:A:398:U:O5'	1:A:398:U:H6	1.96	0.48
1:A:5:A:C2	1:A:411:U:C2	3.02	0.48
1:A:376:U:H2'	1:A:377:A:C8	2.47	0.48
1:A:380:A:C6	1:A:381:A:C4	3.00	0.48
1:A:331:G:H4'	1:A:332:A:H5'	1.95	0.48
1:A:124:U:H2'	1:A:125:U:O4'	2.13	0.48
1:A:190:G:H2'	1:A:191:U:O4'	2.13	0.48
1:A:30:C:H2'	1:A:31:G:C8	2.49	0.47
1:A:89:G:H2'	1:A:90:U:C6	2.49	0.47
1:A:313:C:H2'	1:A:314:G:H8	1.74	0.47
2:B:75:VAL:HG22	2:B:111:LEU:HD21	1.95	0.47
1:A:187:A:H8	1:A:187:A:OP1	1.98	0.47
1:A:167:G:H2'	1:A:168:A:C8	2.50	0.47
1:A:352:U:H2'	1:A:353:A:C8	2.49	0.47
1:A:356:A:H1'	1:A:373:C:H42	1.80	0.47
1:A:13:C:C2	1:A:403:A:C2	3.03	0.47
1:A:210:U:H2'	1:A:211:A:C8	2.50	0.47
1:A:216:U:H3'	1:A:217:U:H6	1.79	0.47
2:B:113:LYS:HE3	2:B:113:LYS:HB3	1.54	0.47
1:A:406:A:C6	1:A:407:U:C4	3.04	0.46
2:B:105:LEU:HD12	2:B:105:LEU:HA	1.76	0.46
1:A:119:C:H2'	1:A:120:U:C6	2.51	0.46
1:A:8:A:H3'	1:A:9:U:H6	1.80	0.46
1:A:203:G:H1	1:A:229:G:N2	2.13	0.46
1:A:71:G:H1'	1:A:291:A:N6	2.29	0.46
1:A:239:A:O2'	1:A:242:C:H5	1.99	0.46
1:A:319:A:H1'	1:A:320:U:C5	2.51	0.46
2:B:103:HIS:O	2:B:105:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LYS:O	2:B:115:ALA:N	2.49	0.46
1:A:45:A:H62	2:B:62:ARG:NH2	2.12	0.46
1:A:206:G:H1	1:A:227:G:N2	2.11	0.46
1:A:261:A:C2	1:A:272:G:C6	3.04	0.46
1:A:240:A:H4'	1:A:241:A:OP2	2.16	0.46
1:A:149:G:H3'	1:A:150:A:H8	1.81	0.45
1:A:241:A:H2'	1:A:242:C:C6	2.50	0.45
1:A:217:U:H3'	1:A:218:U:C6	2.52	0.45
1:A:308:A:N1	1:A:329:U:C5	2.83	0.45
1:A:408:G:C2	1:A:409:A:C4	3.04	0.45
1:A:143:G:C2	1:A:144:G:C8	3.04	0.45
1:A:164:U:H2'	1:A:165:G:O4'	2.16	0.45
1:A:36:C:N3	1:A:37:G:C5	2.85	0.45
1:A:239:A:H1'	1:A:242:C:H41	1.81	0.45
1:A:77:C:H2'	1:A:78:C:O4'	2.16	0.45
1:A:157:G:OP2	1:A:158:U:H5	1.96	0.45
1:A:97:C:C2'	1:A:98:G:H5'	2.47	0.45
2:B:12:GLU:HG2	2:B:42:ARG:NH2	2.32	0.45
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.98	0.45
1:A:79:C:H2'	1:A:80:G:O4'	2.17	0.45
1:A:68:G:N3	1:A:68:G:H2'	2.31	0.45
1:A:157:G:O5'	1:A:157:G:C8	2.69	0.45
1:A:238:U:H2'	1:A:241:A:N7	2.32	0.45
2:B:98:LYS:O	2:B:99:LYS:C	2.59	0.45
1:A:37:G:N1	1:A:38:G:C5	2.85	0.44
1:A:150:A:H3'	1:A:151:A:H8	1.82	0.44
1:A:204:G:H2'	1:A:205:A:C8	2.52	0.44
1:A:416:U:H2'	1:A:417:C:O4'	2.17	0.44
2:B:74:GLU:CD	2:B:111:LEU:HD22	2.42	0.44
2:B:112:LYS:C	2:B:114:GLU:N	2.74	0.44
1:A:99:A:H2'	1:A:100:A:C8	2.52	0.44
1:A:193:C:N4	1:A:237:G:H1	2.15	0.44
2:B:74:GLU:OE1	2:B:111:LEU:HD22	2.18	0.44
1:A:197:A:O3'	1:A:198:G:H3'	2.18	0.44
1:A:377:A:H3'	1:A:378:C:C6	2.52	0.44
1:A:32:G:H2'	1:A:32:G:N3	2.32	0.44
1:A:115:C:H2'	1:A:116:A:H8	1.83	0.44
1:A:251:C:H2'	1:A:252:G:H5'	1.99	0.44
1:A:309:C:O2'	1:A:310:A:H5'	2.18	0.44
2:B:103:HIS:O	2:B:104:VAL:C	2.60	0.44
1:A:301:G:H2'	1:A:302:G:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:C:N3	1:A:37:G:C8	2.86	0.44
1:A:52:U:H6	1:A:52:U:H2'	1.62	0.44
1:A:193:C:N4	1:A:237:G:N1	2.64	0.44
1:A:202:C:H2'	1:A:203:G:C8	2.52	0.44
1:A:275:G:OP2	1:A:276:C:O2'	2.36	0.44
1:A:360:G:H3'	1:A:361:C:H6	1.82	0.44
1:A:385:A:H8	1:A:400:U:O2'	1.99	0.44
1:A:187:A:N3	1:A:245:C:O2'	2.41	0.44
1:A:19:A:H2'	1:A:20:U:C6	2.52	0.43
1:A:301:G:C2'	1:A:302:G:H5'	2.48	0.43
1:A:14:G:C2	1:A:402:G:C6	3.06	0.43
1:A:161:G:N2	1:A:164:U:H3'	2.33	0.43
1:A:408:G:H2'	1:A:409:A:O4'	2.18	0.43
1:A:409:A:C8	1:A:409:A:H5"	2.52	0.43
1:A:23:C:H5"	2:B:1:MET:CA	2.48	0.43
1:A:169:U:H2'	1:A:170:A:C8	2.53	0.43
1:A:239:A:O2'	1:A:242:C:OP2	2.35	0.43
1:A:399:A:H2'	1:A:400:U:H5'	2.01	0.43
2:B:99:LYS:HE2	2:B:99:LYS:HB2	1.52	0.43
2:B:103:HIS:C	2:B:105:LEU:N	2.71	0.43
1:A:317:G:C5	1:A:318:C:N3	2.86	0.43
1:A:401:A:H2'	1:A:402:G:O4'	2.18	0.43
1:A:7:C:H2'	1:A:8:A:H8	1.79	0.43
1:A:50:A:H5'	1:A:388:G:H5"	2.00	0.43
1:A:314:G:C5	1:A:315:G:N7	2.87	0.43
1:A:339:A:H1'	2:B:66:GLN:NE2	2.32	0.43
1:A:377:A:H3'	1:A:378:C:H6	1.84	0.43
1:A:123:C:H2'	1:A:124:U:O4'	2.18	0.43
1:A:356:A:H3'	1:A:357:G:H8	1.83	0.43
1:A:4:A:C2	1:A:412:A:C2	3.06	0.43
1:A:32:G:N2	1:A:34:U:H1'	2.32	0.43
1:A:157:G:N2	1:A:170:A:H1'	2.34	0.43
1:A:45:A:H5"	1:A:389:A:N6	2.33	0.43
1:A:177:G:C6	1:A:178:A:C6	3.07	0.43
1:A:89:G:C2	1:A:248:G:C2	3.06	0.42
1:A:94:U:H2'	1:A:95:A:C8	2.55	0.42
1:A:110:U:H2'	1:A:111:A:H8	1.84	0.42
1:A:139:G:H21	1:A:188:A:H2	1.67	0.42
1:A:221:U:H2'	1:A:222:U:C6	2.53	0.42
1:A:363:A:H2'	1:A:364:A:C8	2.54	0.42
2:B:1:MET:HE3	2:B:1:MET:HB3	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:U:H1'	1:A:257:A:N3	2.34	0.42
1:A:174:U:H2'	1:A:175:U:C6	2.54	0.42
1:A:373:C:H2'	1:A:374:A:C8	2.54	0.42
2:B:11:GLU:O	2:B:15:GLU:HG3	2.19	0.42
2:B:74:GLU:OE2	2:B:111:LEU:HD22	2.19	0.42
1:A:255:A:OP1	1:A:256:A:O2'	2.34	0.42
1:A:385:A:C8	1:A:400:U:O2'	2.73	0.42
1:A:217:U:H3'	1:A:218:U:H5	1.84	0.42
1:A:8:A:N6	1:A:406:A:H61	2.18	0.42
1:A:330:A:O2'	1:A:336:A:N1	2.50	0.42
1:A:14:G:H2'	1:A:385:A:N1	2.34	0.42
1:A:136:G:H2'	1:A:138:C:H5	1.82	0.42
1:A:235:C:H2'	1:A:236:G:O4'	2.20	0.42
1:A:321:G:H2'	1:A:322:C:C6	2.55	0.42
1:A:322:C:H2'	1:A:323:A:C8	2.55	0.42
1:A:236:G:C3'	1:A:237:G:H8	2.33	0.42
1:A:354:C:H2'	1:A:355:G:O4'	2.20	0.42
1:A:353:A:H62	1:A:371:U:H3	1.68	0.41
2:B:73:GLU:N	2:B:73:GLU:OE1	2.52	0.41
1:A:153:C:H2'	1:A:154:U:C6	2.55	0.41
1:A:186:G:N2	1:A:189:A:C4	2.88	0.41
2:B:75:VAL:CG2	2:B:111:LEU:HD21	2.50	0.41
1:A:172:G:H2'	1:A:173:G:C8	2.55	0.41
1:A:353:A:H3'	1:A:354:C:C6	2.55	0.41
1:A:149:G:C6	1:A:177:G:C2	3.08	0.41
1:A:262:A:H8	1:A:262:A:O5'	2.02	0.41
1:A:158:U:H2'	1:A:159:C:O5'	2.15	0.41
1:A:263:A:H1'	1:A:269:G:O6	2.20	0.41
1:A:324:G:H2'	1:A:325:C:H6	1.84	0.41
1:A:408:G:C4	1:A:409:A:C8	3.08	0.41
1:A:16:G:N2	1:A:344:C:H1'	2.35	0.41
1:A:37:G:C2	1:A:38:G:C5	3.09	0.41
1:A:154:U:O5'	1:A:155:A:OP2	2.38	0.41
1:A:234:G:H2'	1:A:235:C:C6	2.56	0.41
1:A:350:A:C4	1:A:380:A:C5	3.08	0.41
2:B:103:HIS:O	2:B:106:ARG:N	2.54	0.41
1:A:165:G:C4	1:A:166:G:H1'	2.55	0.41
1:A:246:A:H2'	1:A:247:C:O4'	2.21	0.41
1:A:300:A:H2'	1:A:301:G:O4'	2.20	0.41
1:A:262:A:H3'	1:A:262:A:C8	2.55	0.41
1:A:128:G:H2'	1:A:129:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:U:C2'	1:A:217:U:C5	2.98	0.41
1:A:314:G:C6	1:A:315:G:N7	2.89	0.41
1:A:380:A:C6	1:A:381:A:C5	3.09	0.41
1:A:385:A:H1'	1:A:401:A:C8	2.56	0.41
1:A:408:G:H2'	1:A:409:A:C8	2.56	0.41
1:A:229:G:H2'	1:A:230:G:C8	2.56	0.40
1:A:355:G:H2'	1:A:356:A:C8	2.56	0.40
1:A:95:A:H2'	1:A:96:G:O4'	2.21	0.40
1:A:338:G:H2'	1:A:339:A:C8	2.56	0.40
1:A:349:G:H1'	1:A:350:A:H8	1.85	0.40
1:A:32:G:H3'	1:A:33:U:C6	2.57	0.40
1:A:151:A:H2'	1:A:152:C:O4'	2.21	0.40
1:A:157:G:H3'	1:A:158:U:H5	1.81	0.40
1:A:381:A:C6	1:A:382:G:C4	3.09	0.40
1:A:218:U:C5	1:A:219:C:H1'	2.56	0.40
1:A:338:G:H2'	1:A:339:A:H8	1.87	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
2	B	114/116 (98%)	102 (90%)	9 (8%)	3 (3%)	4 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	103	HIS
2	B	114	GLU
2	B	113	LYS

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
2	B	99/99 (100%)	87 (88%)	12 (12%)	4 12

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET
2	B	2	LYS
2	B	3	LYS
2	B	4	LYS
2	B	71	LEU
2	B	92	MET
2	B	97	VAL
2	B	99	LYS
2	B	101	LEU
2	B	105	LEU
2	B	111	LEU
2	B	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	ASN
2	B	14	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	205 (49%)	15 (3%)

All (205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	5	A
1	A	6	U
1	A	8	A
1	A	9	U
1	A	11	C
1	A	15	G
1	A	22	G
1	A	23	C
1	A	24	U
1	A	28	G
1	A	30	C
1	A	32	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	44	G
1	A	45	A
1	A	46	G
1	A	47	G
1	A	48	A
1	A	49	A
1	A	50	A
1	A	51	G
1	A	53	C
1	A	59	U
1	A	65	G
1	A	67	U
1	A	68	G
1	A	70	U
1	A	76	G
1	A	79	C
1	A	82	A
1	A	83	G
1	A	85	G
1	A	86	U
1	A	87	U
1	A	88	C
1	A	89	G
1	A	90	U
1	A	91	G
1	A	92	C
1	A	96	G

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Mol	Chain	Res	Type
1	A	98	G
1	A	99	A
1	A	101	U
1	A	102	C
1	A	103	C
1	A	104	A
1	A	105	U
1	A	108	G
1	A	115	C
1	A	118	C
1	A	121	G
1	A	122	G
1	A	123	C
1	A	126	U
1	A	127	G
1	A	128	G
1	A	129	C
1	A	130	U
1	A	132	G
1	A	133	G
1	A	134	C
1	A	135	U
1	A	136	G
1	A	137	A
1	A	139	G
1	A	141	C
1	A	142	G
1	A	145	G
1	A	146	A
1	A	147	A
1	A	149	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	154	U
1	A	155	A
1	A	156	C
1	A	157	G
1	A	159	C
1	A	163	C
1	A	167	G
1	A	171	U

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Mol	Chain	Res	Type
1	A	172	G
1	A	174	U
1	A	177	G
1	A	178	A
1	A	179	U
1	A	180	U
1	A	183	C
1	A	185	U
1	A	186	G
1	A	187	A
1	A	190	G
1	A	192	G
1	A	193	C
1	A	198	G
1	A	199	U
1	A	200	G
1	A	202	C
1	A	203	G
1	A	204	G
1	A	205	A
1	A	207	C
1	A	208	U
1	A	209	C
1	A	210	U
1	A	212	A
1	A	213	G
1	A	214	G
1	A	219	C
1	A	226	G
1	A	227	G
1	A	231	A
1	A	232	A
1	A	233	C
1	A	234	G
1	A	236	G
1	A	237	G
1	A	239	A
1	A	240	A
1	A	241	A
1	A	242	C
1	A	250	G
1	A	252	G

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Mol	Chain	Res	Type
1	A	253	A
1	A	255	A
1	A	259	C
1	A	264	U
1	A	265	G
1	A	266	A
1	A	267	U
1	A	271	A
1	A	275	G
1	A	278	C
1	A	285	G
1	A	286	A
1	A	290	A
1	A	292	A
1	A	293	U
1	A	294	G
1	A	295	A
1	A	296	A
1	A	304	A
1	A	307	G
1	A	312	G
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	322	C
1	A	323	A
1	A	324	G
1	A	328	G
1	A	329	U
1	A	330	A
1	A	333	U
1	A	334	A
1	A	335	G
1	A	336	A
1	A	337	U
1	A	343	C
1	A	344	C
1	A	347	C
1	A	349	G
1	A	350	A

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Mol	Chain	Res	Type
1	A	351	G
1	A	358	G
1	A	359	C
1	A	361	C
1	A	362	A
1	A	363	A
1	A	364	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	375	G
1	A	376	U
1	A	379	G
1	A	380	A
1	A	381	A
1	A	382	G
1	A	383	G
1	A	384	U
1	A	385	A
1	A	387	A
1	A	389	A
1	A	391	C
1	A	392	A
1	A	400	U
1	A	401	A
1	A	402	G
1	A	406	A
1	A	407	U
1	A	408	G
1	A	409	A
1	A	410	U
1	A	411	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	45	A
1	A	52	U

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Mol	Chain	Res	Type
1	A	67	U
1	A	75	U
1	A	126	U
1	A	136	G
1	A	158	U
1	A	232	A
1	A	240	A
1	A	255	A
1	A	292	A
1	A	334	A
1	A	349	G
1	A	363	A
1	A	383	G

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 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

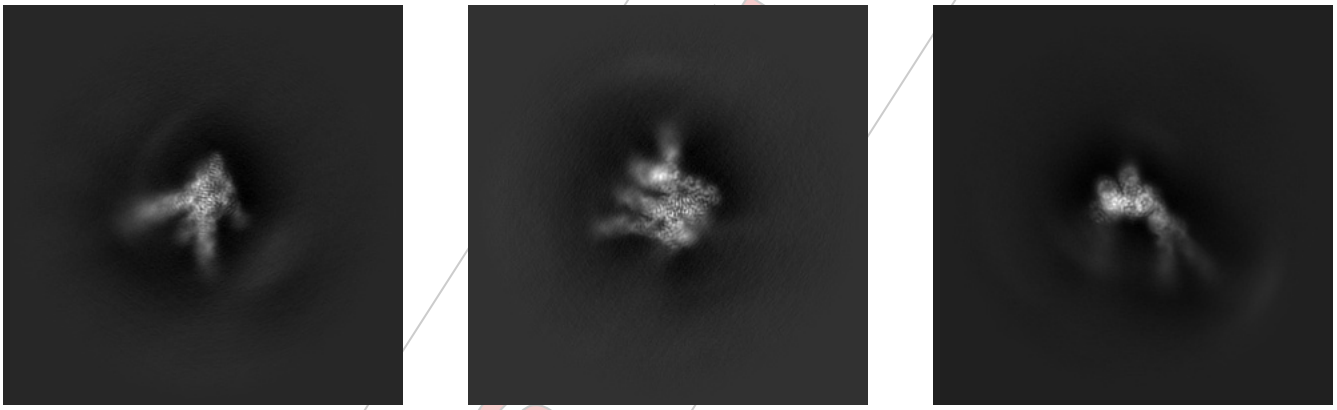
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70998. 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.

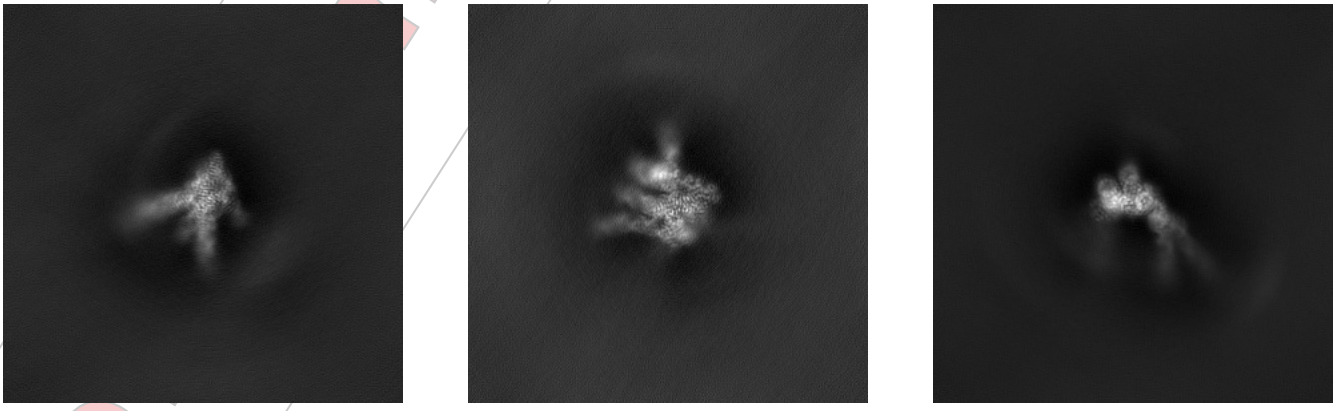
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

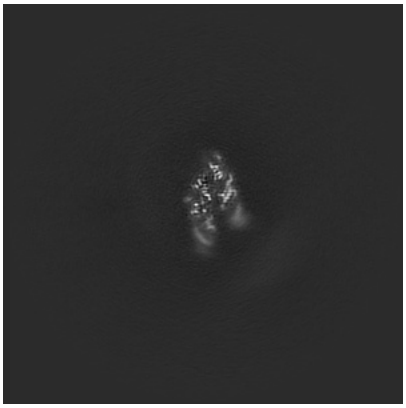


X Y Z

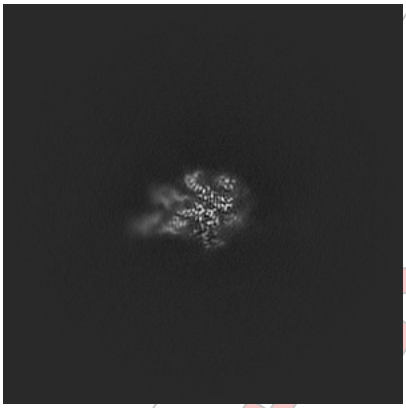
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

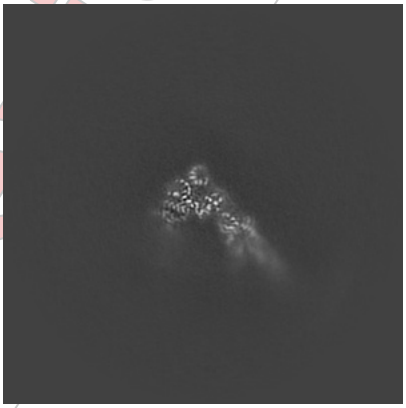
6.2.1 Primary map



X Index: 200

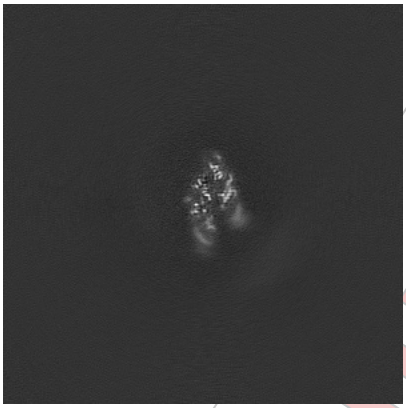


Y Index: 200



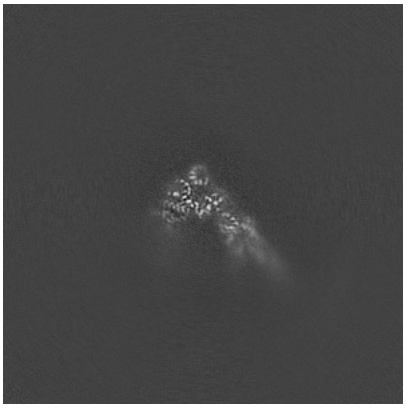
Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

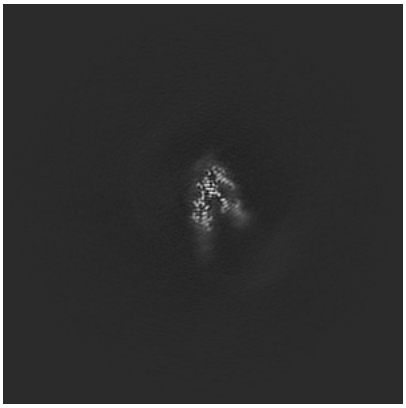


Z Index: 200

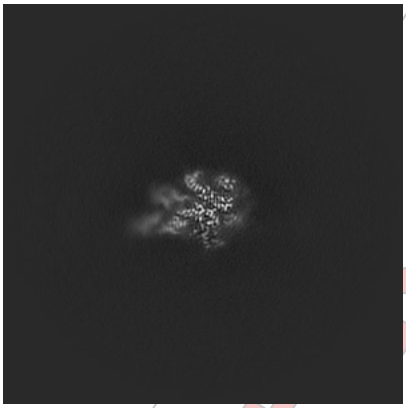
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

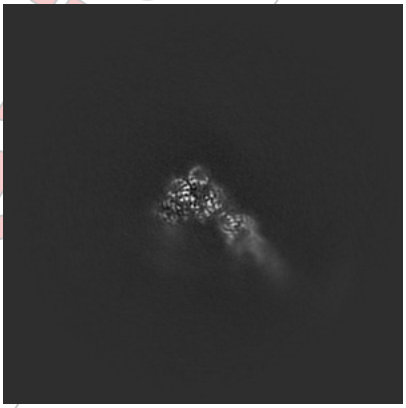
6.3.1 Primary map



X Index: 193

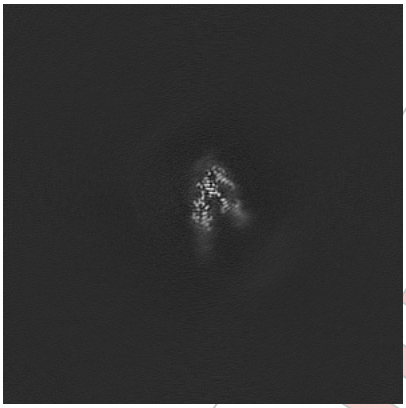


Y Index: 200



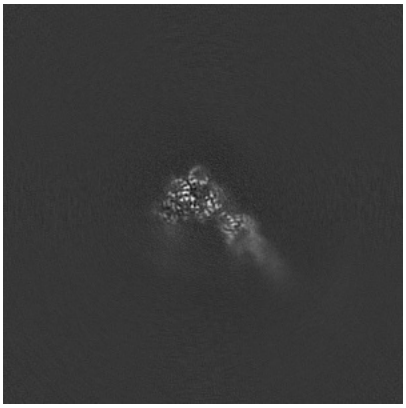
Z Index: 202

6.3.2 Raw map



X Index: 193

Y Index: 200

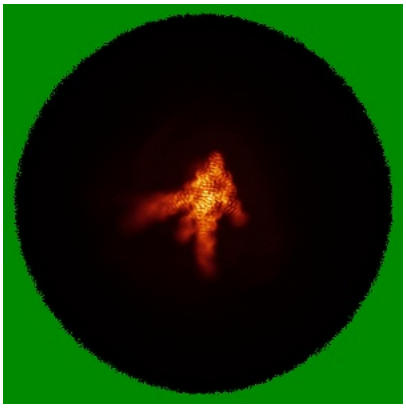


Z Index: 202

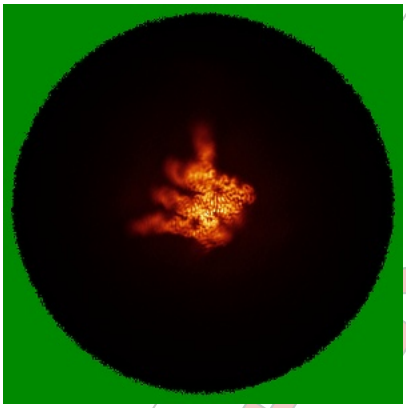
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

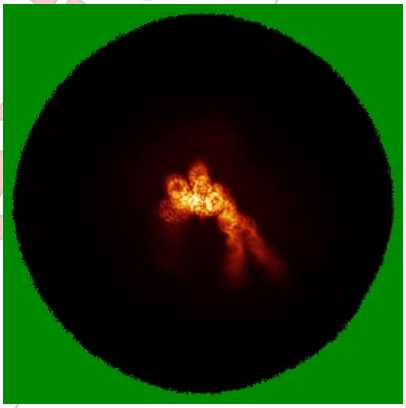
6.4.1 Primary map



X

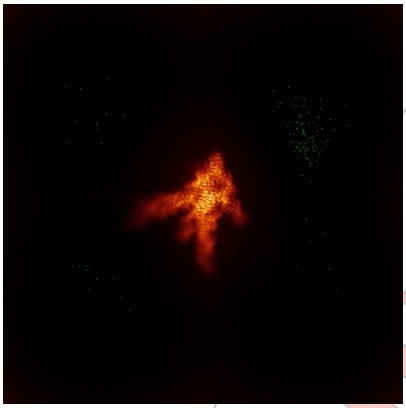


Y

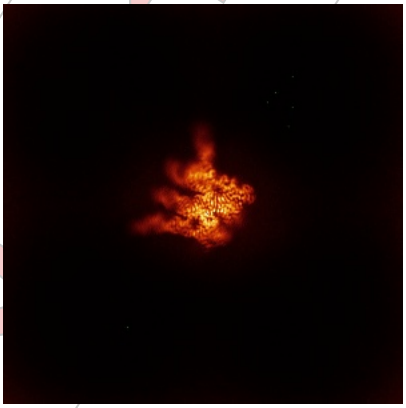


Z

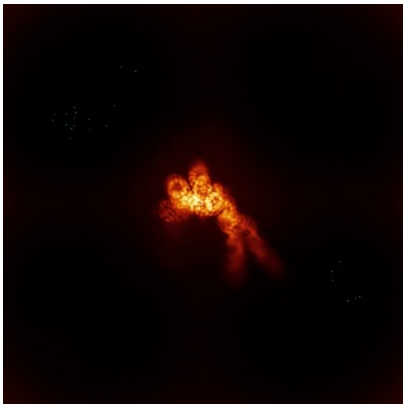
6.4.2 Raw map



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 0.033. 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.

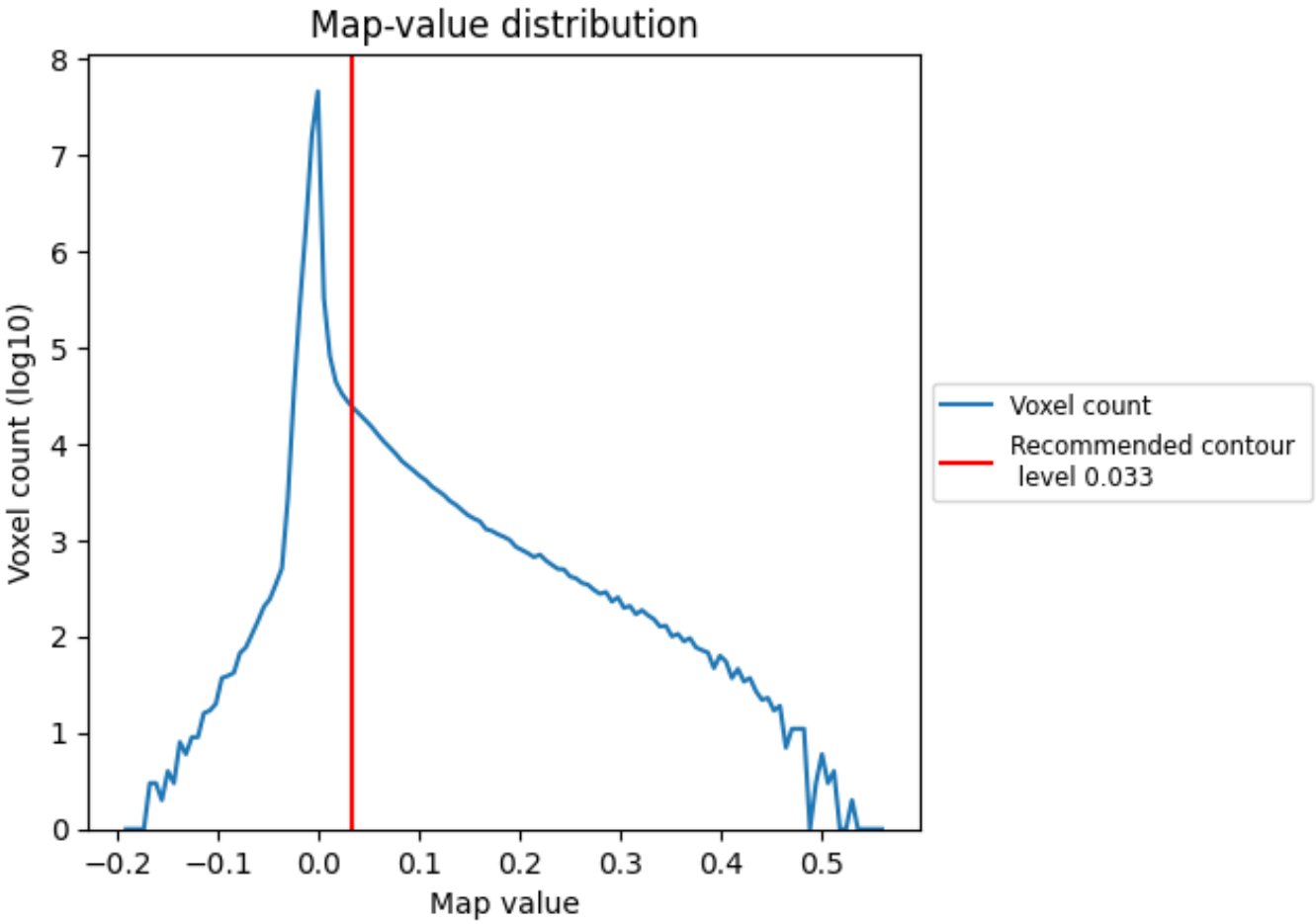
6.6 Mask visualisation (i)

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

7 Map analysis

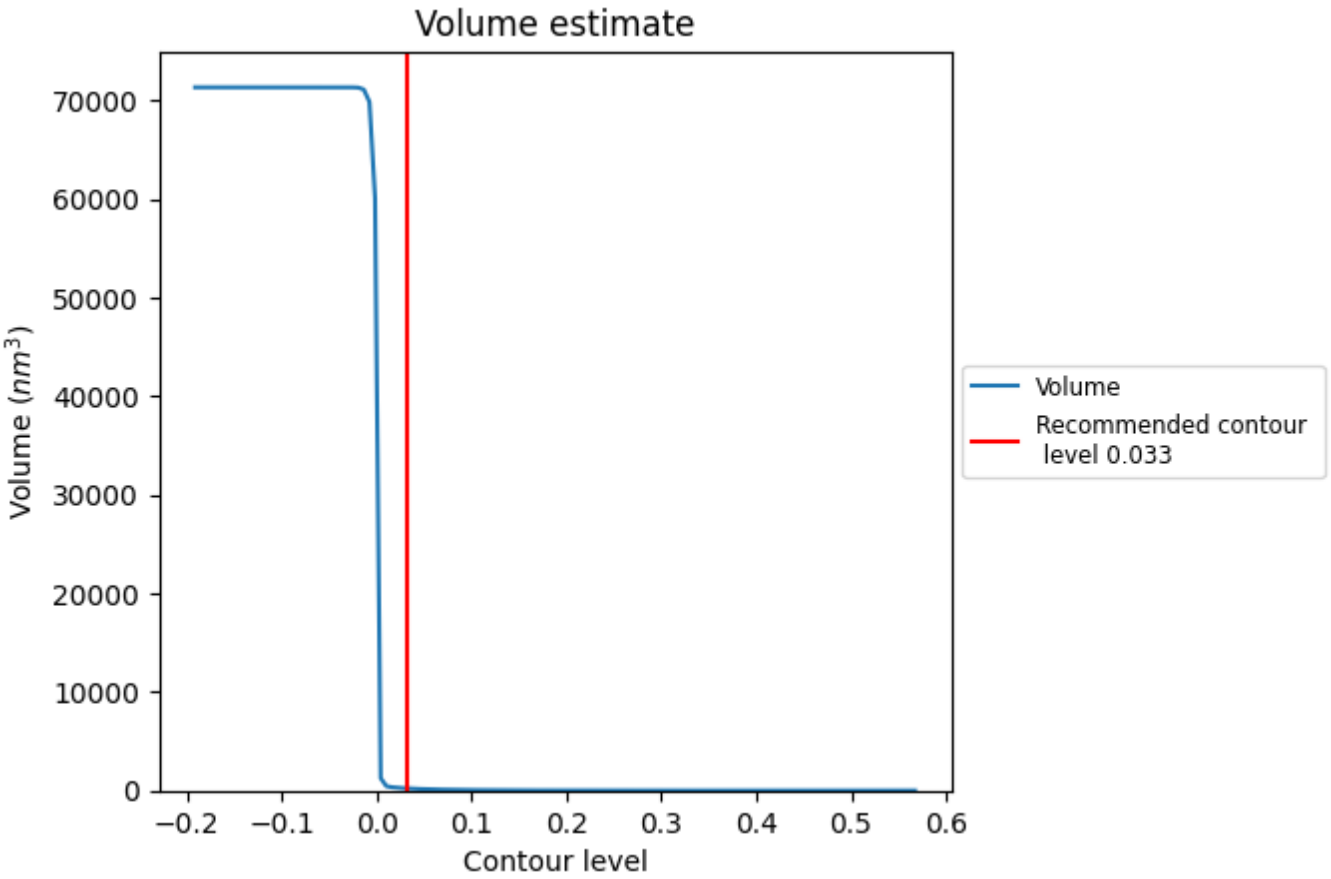
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

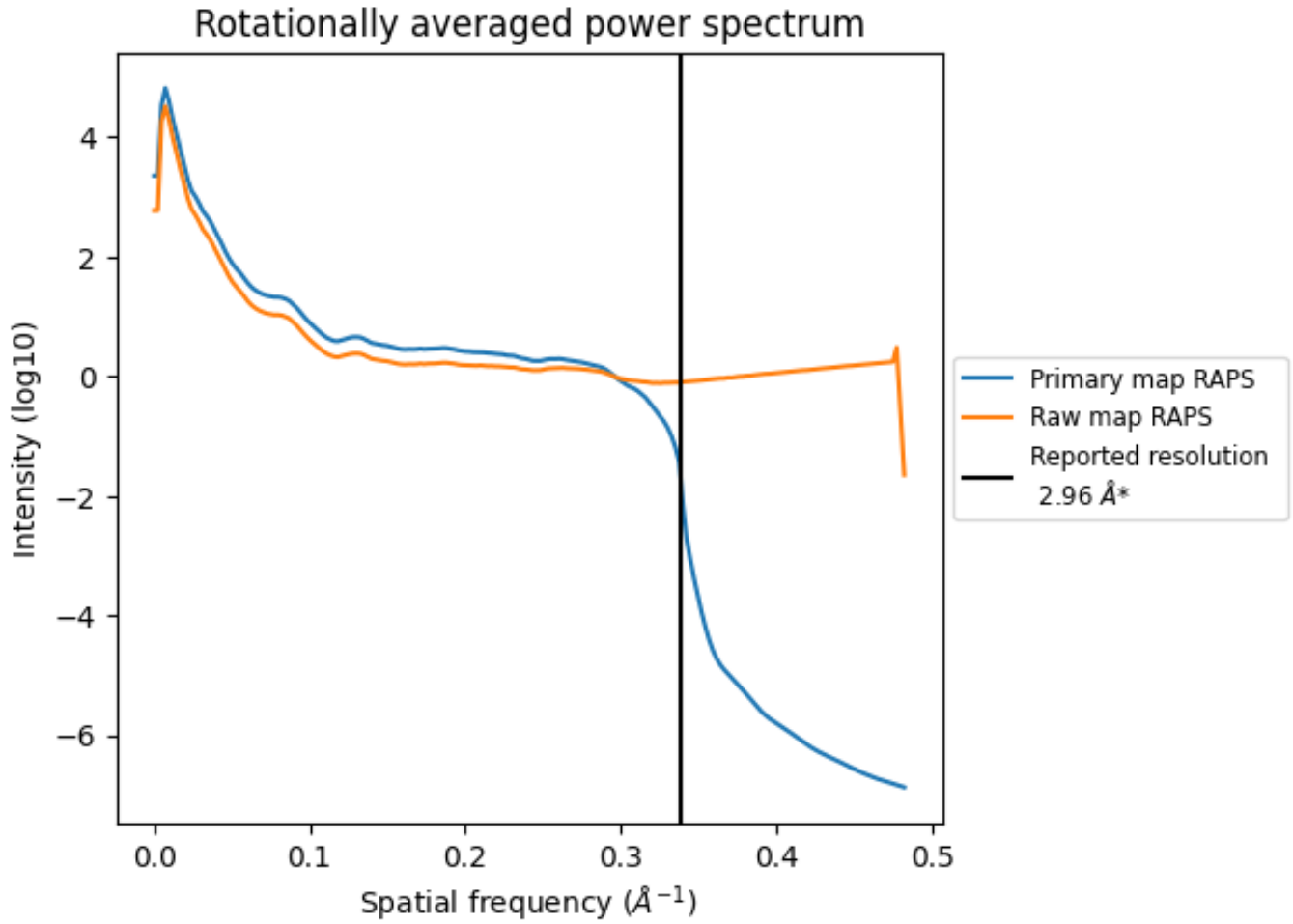
7.2 Volume estimate (i)



The volume at the recommended contour level is 215 nm^3; this corresponds to an approximate mass of 194 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 (i)

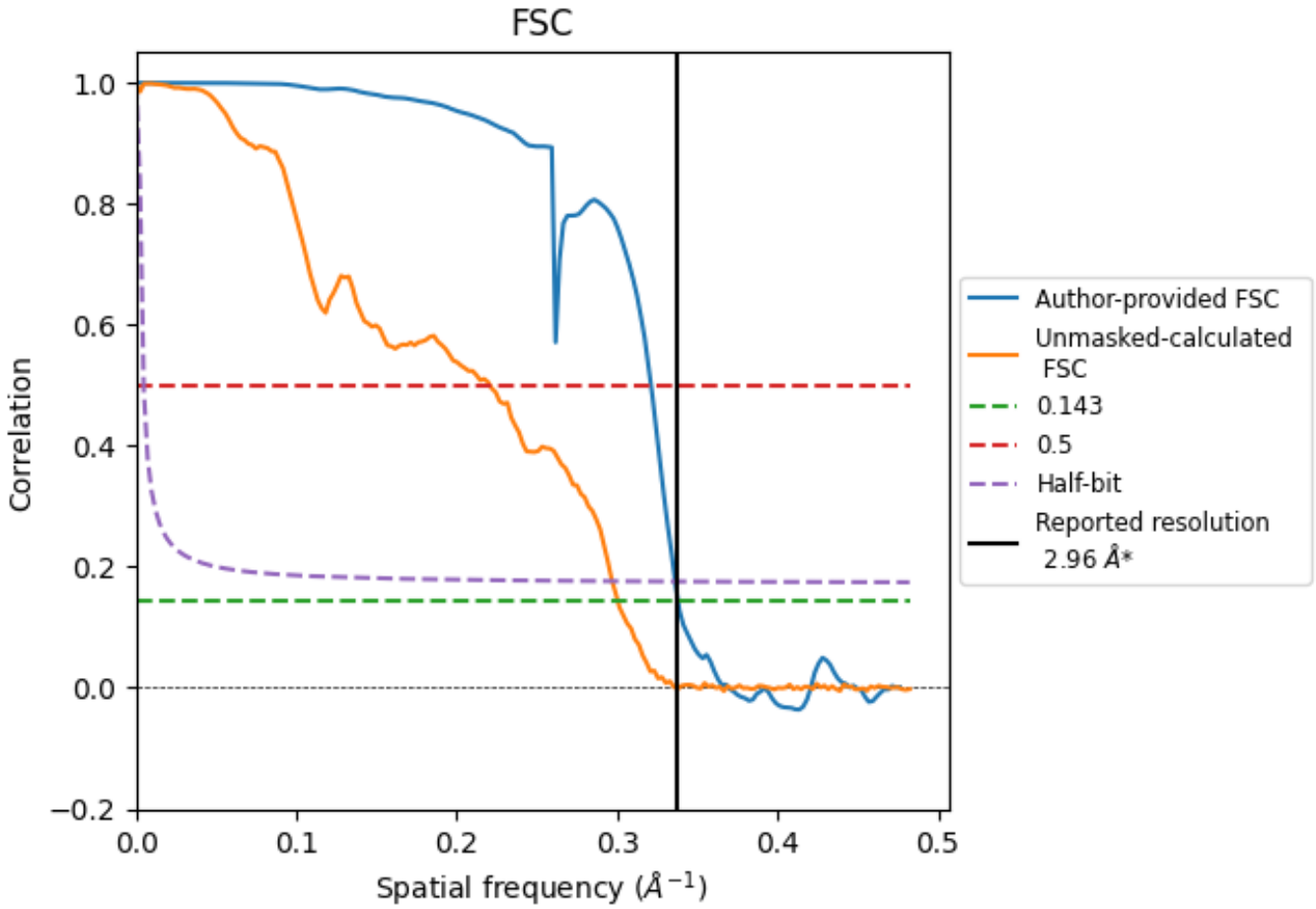


*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

8.2 Resolution estimates (i)

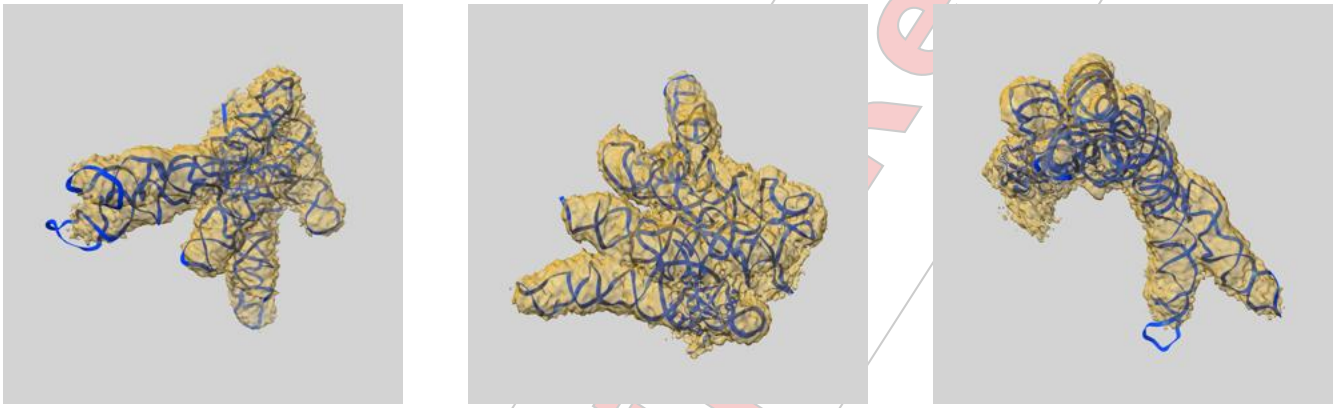
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.11	2.98
Unmasked-calculated*	3.33	4.53	3.37

*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 3.33 differs from the reported value 2.96 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70998 and PDB model 9OY6. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay



X Y Z

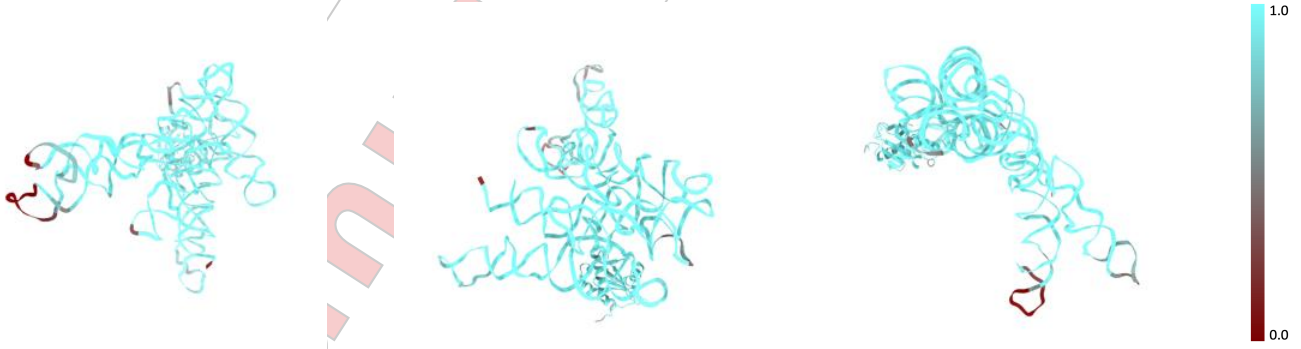
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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.

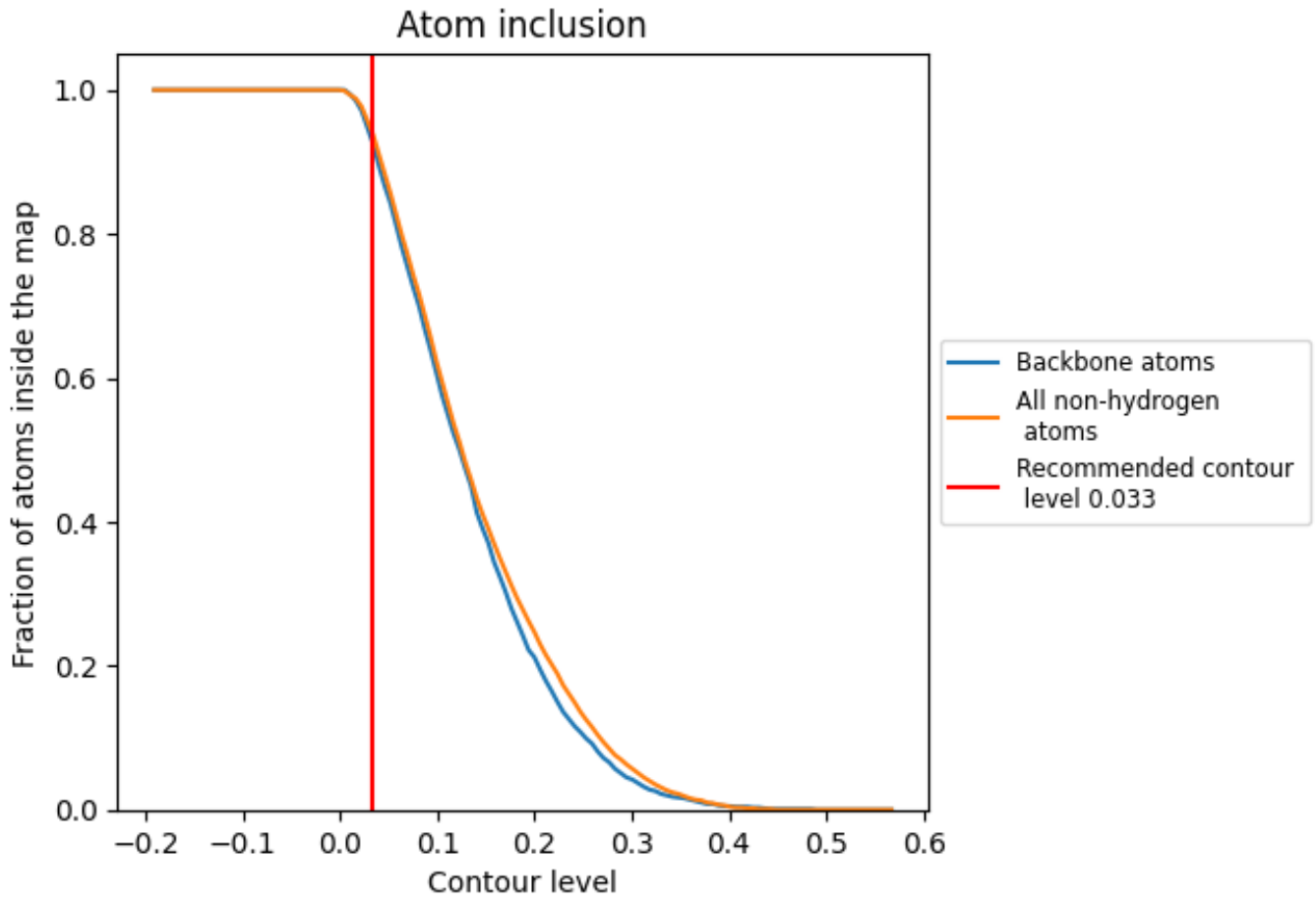
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.033).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.3670
A	0.9400	0.3580
B	0.9460	0.4500

Full wwPDB EM Validation Report ⓘ

Jun 8, 2025 – 04:05 PM EDT

PDB ID	:	9OY7 / pdb_00009oy7
EMDB ID	:	EMD-71000
Title	:	Structure of Geobacillus stearothermophilus RNase P holoenzyme tetraloop mutant in complex with precursor tRNA
Deposited on	:	2025-06-04
Resolution	:	2.94 Å(reported)
Based on initial model	:	2A64

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

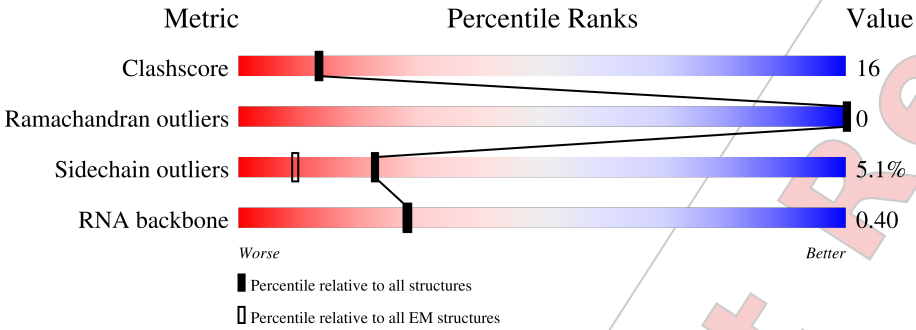
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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 <=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	417	29% 52% 18%
2	B	116	75% 24%
3	C	92	38% 46% 12%
3	E	92	90%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12001 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 RNA chain called RNase P RNA component tetraloop mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	417	8953	3992	1649	2895	417	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	U	G	engineered mutation	GB 143442
A	216	U	A	engineered mutation	GB 143442
A	217	U	A	engineered mutation	GB 143442
A	218	U	A	engineered mutation	GB 143442
A	417	C	G	conflict	GB 143442

- Molecule 2 is a protein called Ribonuclease P protein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	116	947	608	174	162	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A150N245
B	64	ILE	VAL	conflict	UNP A0A150N245

- Molecule 3 is a RNA chain called precursor RNA (89-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	89	1889	842	326	632	89	0	0
			Total	C	N	O	P		
3	E	9	188	84	29	66	9	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	G	C	conflict	GB 1919315002
C	-9	U	A	conflict	GB 1919315002
C	-8	U	A	conflict	GB 1919315002
C	-6	C	G	conflict	GB 1919315002
C	-5	C	A	conflict	GB 1919315002
C	-4	C	U	conflict	GB 1919315002
C	-1	U	G	conflict	GB 1919315002
C	0	C	G	conflict	GB 1919315002
C	76	A	U	conflict	GB 1919315002
C	78	A	U	conflict	GB 1919315002
E	-12	G	C	conflict	GB 1919315002
E	-9	U	A	conflict	GB 1919315002
E	-8	U	A	conflict	GB 1919315002
E	-6	C	G	conflict	GB 1919315002
E	-5	C	A	conflict	GB 1919315002
E	-4	C	U	conflict	GB 1919315002
E	-1	U	G	conflict	GB 1919315002
E	0	C	G	conflict	GB 1919315002
E	76	A	U	conflict	GB 1919315002
E	78	A	U	conflict	GB 1919315002

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

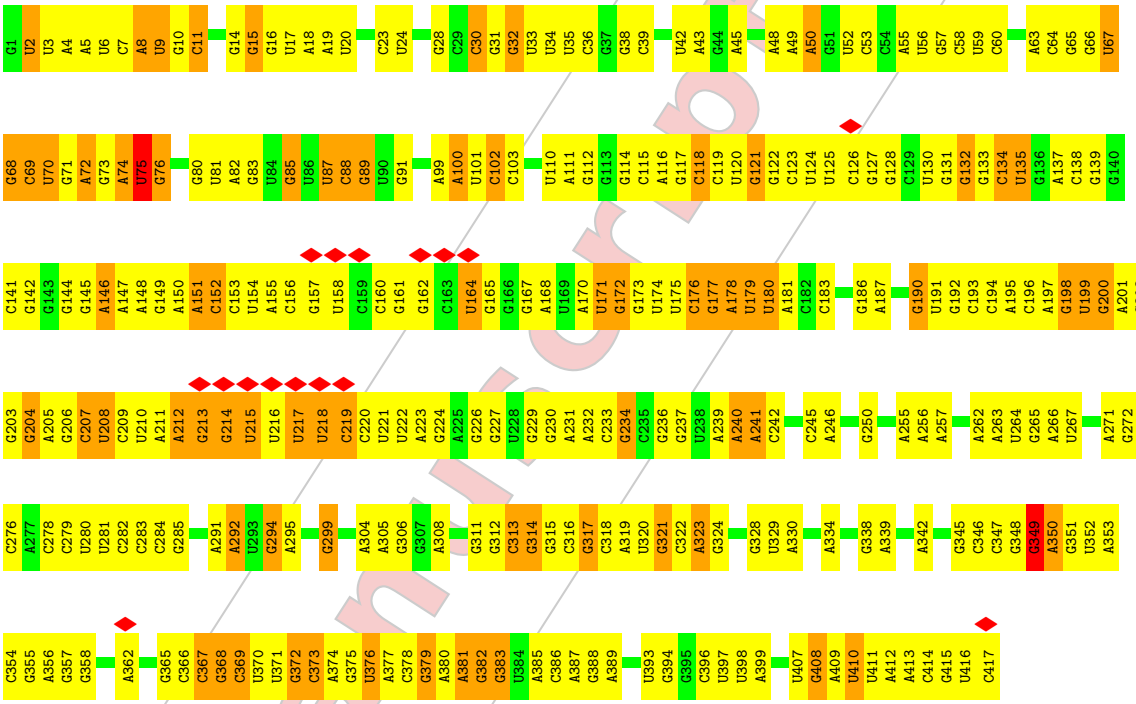
Mol	Chain	Residues	Atoms	AltConf
4	A	23	Total Ca 23 23	0
4	C	1	Total Ca 1 1	0

3 Residue-property plots (i)

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.

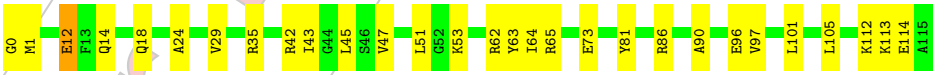
• Molecule 1: RNase P RNA component tetraloop mutant

Chain A:



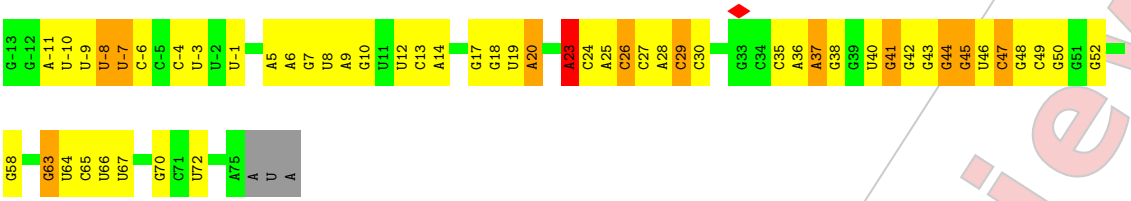
• Molecule 2: Ribonuclease P protein component

Chain B:

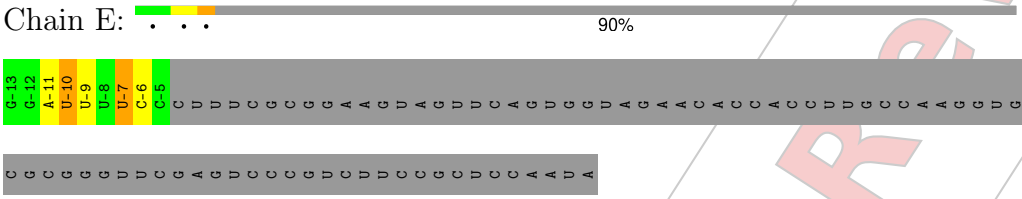


• Molecule 3: precursor RNA (89-MER)

Chain C:



• Molecule 3: precursor RNA (89-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	309996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.143	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0368, 1.0368, 1.0368	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: CA

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	4/10025 (0.0%)	0.53	2/15639 (0.0%)
2	B	0.18	0/962	0.42	0/1281
3	C	0.36	0/2107	0.63	1/3281 (0.0%)
3	E	0.08	0/208	0.19	0/321
All	All	0.30	4/13302 (0.0%)	0.53	3/20522 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	U	C1'-N1	6.38	1.58	1.48
1	A	218	U	C1'-N1	6.36	1.57	1.48
1	A	217	U	C1'-N1	6.34	1.57	1.48
1	A	215	U	C1'-N1	5.53	1.56	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	U	C2'-C3'-O3'	6.64	119.46	109.50
1	A	349	G	O3'-P-O5'	-6.48	94.28	104.00
3	C	23	A	C4'-C3'-C2'	-5.13	97.47	102.60

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	8953	0	4507	231	0
2	B	947	0	1008	17	0
3	C	1889	0	957	44	0
3	E	188	0	96	2	0
4	A	23	0	0	0	0
4	C	1	0	0	0	0
All	All	12001	0	6568	291	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 16.

All (291) 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)
3:C:43:G:H3'	3:C:44:G:H3'	1.56	0.84
1:A:349:G:H22	1:A:379:G:H1'	1.45	0.82
1:A:371:U:H5"	1:A:372:G:H5'	1.60	0.81
1:A:349:G:H21	1:A:350:A:H62	1.30	0.79
1:A:313:C:H2'	1:A:314:G:C8	2.19	0.77
3:C:-11:A:H2'	3:C:-10:U:C6	2.21	0.74
1:A:316:C:H2'	1:A:317:G:C8	2.22	0.73
2:B:0:GLY:HA3	2:B:65:ARG:HB3	1.72	0.72
1:A:158:U:H3	1:A:168:A:H61	1.38	0.72
1:A:199:U:H2'	1:A:200:G:C8	2.28	0.69
1:A:180:U:H2'	1:A:181:A:H8	1.59	0.68
3:C:41:G:H2'	3:C:42:G:C8	2.27	0.68
1:A:115:C:H2'	1:A:116:A:H8	1.59	0.67
2:B:12:GLU:HG2	2:B:42:ARG:HH22	1.60	0.67
1:A:215:U:H2'	1:A:217:U:H5	1.59	0.66
1:A:313:C:H2'	1:A:314:G:H8	1.60	0.65
1:A:195:A:H2'	1:A:196:C:C6	2.32	0.64
1:A:197:A:H61	1:A:233:C:H42	1.45	0.64
1:A:308:A:N1	1:A:329:U:H5	1.95	0.64
1:A:130:U:H2'	1:A:131:G:H8	1.62	0.64
3:C:43:G:H3'	3:C:44:G:C3'	2.27	0.63
1:A:212:A:H2'	1:A:213:G:C8	2.33	0.62
3:C:9:A:N3	3:C:44:G:H1'	2.14	0.62
1:A:146:A:H3'	1:A:178:A:H61	1.65	0.62
1:A:72:A:H2'	1:A:73:G:C8	2.35	0.61
1:A:374:A:H2'	1:A:375:G:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:C:H2'	1:A:317:G:N7	2.16	0.60
1:A:115:C:H2'	1:A:116:A:C8	2.35	0.60
1:A:314:G:H1	1:A:323:A:H61	1.48	0.60
2:B:47:VAL:HG13	2:B:51:LEU:HD12	1.83	0.60
1:A:9:U:H2'	1:A:10:G:H8	1.66	0.60
1:A:338:G:H2'	1:A:339:A:H8	1.67	0.59
1:A:315:G:H2'	1:A:316:C:C6	2.38	0.59
1:A:411:U:H2'	1:A:412:A:C8	2.38	0.59
1:A:71:G:N2	1:A:73:G:H3'	2.17	0.59
1:A:211:A:H2'	1:A:212:A:C8	2.38	0.59
3:C:9:A:C2	3:C:44:G:H1'	2.38	0.58
1:A:411:U:H2'	1:A:412:A:H8	1.67	0.58
1:A:233:C:H2'	1:A:234:G:C8	2.38	0.58
3:C:-11:A:H2'	3:C:-10:U:H6	1.68	0.58
3:C:27:C:H2'	3:C:28:A:H8	1.68	0.58
1:A:172:G:H2'	1:A:173:G:H8	1.69	0.58
1:A:110:U:H2'	1:A:111:A:H8	1.68	0.58
3:C:43:G:C3'	3:C:44:G:H3'	2.31	0.58
1:A:352:U:H2'	1:A:353:A:H8	1.69	0.57
3:C:27:C:H2'	3:C:28:A:C8	2.39	0.57
1:A:204:G:H2'	1:A:205:A:H8	1.69	0.57
1:A:210:U:H2'	1:A:211:A:C8	2.39	0.57
1:A:204:G:H2'	1:A:205:A:C8	2.40	0.57
1:A:69:C:H2'	1:A:70:U:C6	2.39	0.56
1:A:130:U:H2'	1:A:131:G:C8	2.39	0.56
1:A:50:A:H5'	1:A:388:G:H5"	1.87	0.56
1:A:240:A:H4'	1:A:241:A:OP2	2.06	0.56
1:A:3:U:H2'	1:A:4:A:H8	1.71	0.55
1:A:352:U:H2'	1:A:353:A:C8	2.40	0.55
1:A:378:C:H3'	1:A:379:G:H8	1.72	0.55
1:A:215:U:O2'	1:A:217:U:O4	2.17	0.55
1:A:120:U:H3	1:A:131:G:H1	1.53	0.55
1:A:256:A:H1'	3:C:72:U:H5'	1.88	0.55
3:C:-8:U:HO2'	3:C:-7:U:H6	1.55	0.55
1:A:42:U:H2'	1:A:43:A:C8	2.41	0.55
1:A:215:U:H2'	1:A:217:U:C5	2.41	0.55
1:A:245:C:H2'	1:A:246:A:H8	1.71	0.55
1:A:17:U:H2'	1:A:18:A:H8	1.72	0.54
2:B:51:LEU:HD22	2:B:90:ALA:HB2	1.89	0.54
1:A:18:A:H2'	1:A:19:A:H8	1.72	0.54
1:A:211:A:H2'	1:A:212:A:H8	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:C:H2'	1:A:374:A:H8	1.70	0.54
1:A:5:A:H2'	1:A:6:U:C6	2.42	0.54
1:A:367:C:H2'	1:A:368:G:C8	2.42	0.54
1:A:124:U:H2'	1:A:125:U:O4'	2.08	0.54
1:A:102:C:H2'	1:A:103:C:O4'	2.07	0.54
1:A:232:A:H2'	1:A:233:C:C6	2.43	0.54
1:A:280:U:H2'	1:A:281:U:H6	1.73	0.54
1:A:194:C:H2'	1:A:195:A:C8	2.43	0.53
1:A:208:U:H2'	1:A:209:C:C6	2.43	0.53
3:C:26:C:H2'	3:C:27:C:C6	2.43	0.53
1:A:196:C:H2'	1:A:197:A:C8	2.43	0.53
1:A:347:C:C2	1:A:383:G:N2	2.77	0.53
1:A:200:G:O6	1:A:231:A:N1	2.42	0.53
1:A:32:G:H1	1:A:34:U:H1'	1.73	0.52
1:A:241:A:H2'	1:A:242:C:C6	2.44	0.52
1:A:73:G:N2	1:A:291:A:H2'	2.25	0.52
1:A:215:U:O2	1:A:218:U:O4	2.27	0.52
1:A:378:C:H3'	1:A:379:G:C8	2.45	0.52
1:A:172:G:H2'	1:A:173:G:C8	2.44	0.52
1:A:15:G:N2	1:A:345:G:H1'	2.25	0.52
1:A:218:U:O5'	1:A:218:U:H6	1.93	0.52
1:A:3:U:H2'	1:A:4:A:C8	2.44	0.52
1:A:14:G:H2'	1:A:385:A:C6	2.44	0.52
1:A:18:A:H2'	1:A:19:A:C8	2.45	0.52
1:A:285:G:H22	1:A:299:G:H1'	1.75	0.52
3:C:24:C:H2'	3:C:25:A:H8	1.74	0.52
1:A:233:C:H2'	1:A:234:G:H8	1.74	0.52
3:C:42:G:H2'	3:C:43:G:C8	2.44	0.52
1:A:9:U:H2'	1:A:10:G:C8	2.44	0.51
1:A:219:C:H2'	1:A:220:C:C6	2.45	0.51
1:A:280:U:H2'	1:A:281:U:C6	2.45	0.51
1:A:175:U:H2'	1:A:176:C:C6	2.46	0.51
1:A:180:U:H2'	1:A:181:A:C8	2.43	0.51
1:A:374:A:H2'	1:A:375:G:H8	1.75	0.51
3:C:24:C:H2'	3:C:25:A:C8	2.46	0.51
1:A:208:U:H2'	1:A:209:C:H6	1.76	0.51
1:A:373:C:H2'	1:A:374:A:C8	2.46	0.51
1:A:338:G:H2'	1:A:339:A:C8	2.45	0.51
1:A:17:U:H2'	1:A:18:A:C8	2.46	0.51
1:A:230:G:H2'	1:A:231:A:C8	2.46	0.51
2:B:24:ALA:HB2	2:B:29:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:A:O3'	1:A:198:G:H3'	2.12	0.50
1:A:408:G:H2'	1:A:409:A:H8	1.76	0.50
1:A:45:A:H62	2:B:62:ARG:NH2	2.10	0.49
1:A:206:G:H3'	1:A:207:C:H5"	1.93	0.49
1:A:30:C:H2'	1:A:31:G:C8	2.47	0.49
1:A:279:C:H2'	1:A:280:U:H6	1.77	0.49
1:A:153:C:H2'	1:A:154:U:C6	2.47	0.49
3:C:5:A:H2'	3:C:6:A:C8	2.47	0.49
1:A:147:A:H2'	1:A:148:A:H8	1.78	0.49
1:A:200:G:H2'	1:A:201:A:C8	2.47	0.49
1:A:67:U:H4'	1:A:68:G:OP1	2.10	0.49
1:A:223:A:H2'	1:A:224:G:C8	2.47	0.49
1:A:85:G:O2'	1:A:87:U:O4	2.23	0.49
1:A:190:G:H2'	1:A:191:U:O4'	2.13	0.49
3:C:-9:U:H2'	3:C:-8:U:C6	2.48	0.49
3:C:23:A:H2'	3:C:24:C:O4'	2.13	0.49
1:A:118:C:H2'	1:A:119:C:C6	2.48	0.49
2:B:14:GLN:O	2:B:18:GLN:HG2	2.13	0.49
1:A:147:A:H2'	1:A:148:A:C8	2.47	0.49
1:A:167:G:H2'	1:A:168:A:C8	2.47	0.49
1:A:30:C:H2'	1:A:31:G:H8	1.78	0.48
3:C:5:A:H2'	3:C:6:A:H8	1.79	0.48
3:C:37:A:H2'	3:C:38:G:C8	2.48	0.48
1:A:319:A:H1'	1:A:320:U:C5	2.49	0.48
1:A:5:A:H2'	1:A:6:U:H6	1.78	0.48
1:A:74:A:O2'	1:A:76:G:N7	2.44	0.48
1:A:179:U:C4	1:A:233:C:H5'	2.49	0.48
3:C:20:A:N7	3:C:45:G:C5	2.82	0.48
1:A:85:G:H4'	1:A:85:G:OP1	2.14	0.47
2:B:63:TYR:HB3	2:B:97:VAL:HG11	1.97	0.47
3:C:40:U:H2'	3:C:41:G:C8	2.49	0.47
1:A:201:A:H2'	1:A:202:C:C6	2.49	0.47
3:C:-10:U:H2'	3:C:-9:U:C6	2.48	0.47
1:A:209:C:H2'	1:A:210:U:C6	2.48	0.47
1:A:212:A:H2'	1:A:213:G:H8	1.79	0.47
1:A:110:U:H2'	1:A:111:A:C8	2.47	0.47
1:A:197:A:H2'	1:A:199:U:C6	2.49	0.47
1:A:220:C:H2'	1:A:221:U:C6	2.49	0.47
1:A:349:G:H8	1:A:349:G:OP2	1.98	0.47
1:A:386:C:H2'	1:A:387:A:O4'	2.15	0.47
1:A:10:G:H2'	1:A:11:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:C:H2'	1:A:24:U:C6	2.50	0.47
1:A:245:C:H2'	1:A:246:A:C8	2.49	0.47
1:A:281:U:H2'	1:A:282:C:H6	1.80	0.47
1:A:196:C:H2'	1:A:197:A:H8	1.80	0.47
1:A:279:C:H2'	1:A:280:U:C6	2.50	0.47
1:A:2:U:H2'	1:A:3:U:C6	2.50	0.47
1:A:10:G:H2'	1:A:11:C:H6	1.80	0.47
1:A:157:G:H1	1:A:170:A:H1'	1.80	0.47
1:A:114:G:H2'	1:A:115:C:C6	2.51	0.46
1:A:59:U:H1'	1:A:257:A:N3	2.30	0.46
1:A:294:G:H2'	1:A:295:A:C8	2.50	0.46
1:A:2:U:H2'	1:A:3:U:H6	1.81	0.46
1:A:19:A:H2'	1:A:20:U:C6	2.50	0.46
1:A:398:U:H2'	1:A:399:A:H8	1.80	0.46
2:B:43:ILE:HD12	2:B:45:LEU:HD21	1.98	0.46
1:A:32:G:N1	1:A:34:U:H1'	2.30	0.46
1:A:42:U:H2'	1:A:43:A:H8	1.79	0.46
1:A:355:G:H21	1:A:373:C:H42	1.64	0.46
1:A:407:U:H2'	1:A:408:G:C8	2.51	0.46
1:A:111:A:H2'	1:A:112:G:H8	1.81	0.46
1:A:133:G:H2'	1:A:134:C:C6	2.51	0.46
1:A:263:A:H2'	1:A:264:U:C6	2.51	0.46
1:A:134:C:H2'	1:A:135:U:O4'	2.15	0.46
1:A:376:U:C2	1:A:377:A:C8	3.04	0.46
3:C:20:A:C2	3:C:47:C:C2	3.04	0.46
1:A:71:G:N1	1:A:74:A:OP2	2.49	0.46
1:A:195:A:H2'	1:A:196:C:H6	1.80	0.45
2:B:64:ILE:HG23	2:B:101:LEU:HD21	1.98	0.45
1:A:121:G:C6	1:A:131:G:C6	3.05	0.45
1:A:214:G:H2'	1:A:215:U:H6	1.82	0.45
1:A:144:G:H2'	1:A:145:G:O4'	2.17	0.45
1:A:264:U:H2'	1:A:265:G:O4'	2.16	0.45
1:A:356:A:H3'	1:A:357:G:H8	1.81	0.45
3:C:64:U:H2'	3:C:65:C:C6	2.51	0.45
1:A:6:U:H2'	1:A:7:C:C6	2.52	0.45
1:A:57:G:H2'	1:A:58:C:O4'	2.17	0.44
1:A:70:U:H2'	1:A:71:G:O4'	2.16	0.44
1:A:164:U:H2'	1:A:165:G:O4'	2.17	0.44
1:A:315:G:C2	1:A:316:C:C4	3.06	0.44
3:C:65:C:H2'	3:C:66:U:C6	2.53	0.44
1:A:118:C:H2'	1:A:119:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:C:H2'	1:A:284:C:H6	1.82	0.44
3:C:24:C:C2'	3:C:25:A:H8	2.30	0.44
3:C:49:C:H2'	3:C:50:G:C8	2.52	0.44
1:A:210:U:H2'	1:A:211:A:H8	1.82	0.44
1:A:214:G:C4	1:A:215:U:C5	3.05	0.44
2:B:51:LEU:HD21	2:B:86:ARG:O	2.18	0.44
1:A:155:A:H2'	1:A:156:C:O4'	2.18	0.44
1:A:179:U:H1'	1:A:234:G:OP1	2.17	0.44
1:A:132:G:H2'	1:A:133:G:C8	2.53	0.43
1:A:175:U:H2'	1:A:176:C:H6	1.82	0.43
1:A:214:G:H2'	1:A:215:U:C6	2.53	0.43
1:A:412:A:H2'	1:A:413:A:C8	2.53	0.43
3:C:63:G:H2'	3:C:64:U:O4'	2.17	0.43
1:A:314:G:C2	1:A:315:G:N7	2.86	0.43
1:A:82:A:H2'	1:A:83:G:O4'	2.18	0.43
1:A:102:C:O5'	1:A:102:C:H6	2.02	0.43
1:A:393:U:H2'	1:A:394:G:C8	2.53	0.43
1:A:63:A:H2'	1:A:64:C:O4'	2.18	0.43
1:A:148:A:H61	1:A:177:G:H1'	1.83	0.43
3:E:-7:U:H2'	3:E:-6:C:C6	2.53	0.43
1:A:55:A:H2'	1:A:56:U:C6	2.53	0.43
1:A:221:U:H2'	1:A:222:U:C6	2.53	0.43
1:A:416:U:H2'	1:A:417:C:O4'	2.19	0.43
1:A:321:G:H2'	1:A:322:C:O4'	2.19	0.43
1:A:119:C:H2'	1:A:120:U:H6	1.84	0.43
1:A:314:G:H1	1:A:323:A:N6	2.15	0.43
1:A:173:G:H2'	1:A:174:U:H6	1.84	0.42
3:E:-10:U:H2'	3:E:-9:U:C6	2.54	0.42
1:A:7:C:H2'	1:A:8:A:C8	2.54	0.42
2:B:105:LEU:HD23	2:B:105:LEU:HA	1.80	0.42
1:A:32:G:H2'	1:A:32:G:N3	2.35	0.42
3:C:29:C:H2'	3:C:30:C:C6	2.54	0.42
3:C:40:U:H2'	3:C:41:G:O4'	2.20	0.42
1:A:6:U:H2'	1:A:7:C:H6	1.83	0.42
1:A:167:G:H2'	1:A:168:A:H8	1.84	0.42
3:C:43:G:H3'	3:C:44:G:C2'	2.49	0.42
1:A:151:A:H2'	1:A:152:C:O4'	2.20	0.42
1:A:156:C:O2'	1:A:157:G:H8	2.02	0.42
1:A:197:A:N6	1:A:233:C:H42	2.14	0.42
1:A:354:C:C2	1:A:355:G:C8	3.07	0.42
2:B:73:GLU:C	2:B:73:GLU:OE1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:G:H2'	3:C:43:G:C1'	2.49	0.42
1:A:68:G:N3	1:A:68:G:H2'	2.35	0.42
1:A:174:U:H2'	1:A:175:U:C6	2.53	0.42
1:A:393:U:H2'	1:A:394:G:H8	1.84	0.42
1:A:356:A:H3'	1:A:357:G:C8	2.55	0.42
1:A:410:U:C2	1:A:411:U:C5	3.08	0.42
1:A:201:A:H61	1:A:230:G:H1	1.67	0.42
1:A:315:G:C6	1:A:316:C:N4	2.87	0.42
3:C:37:A:H2'	3:C:38:G:H8	1.85	0.42
3:C:44:G:H3'	3:C:44:G:P	2.60	0.42
1:A:45:A:C2	1:A:388:G:H2'	2.54	0.42
3:C:41:G:H2'	3:C:42:G:O4'	2.19	0.42
1:A:292:A:H2'	1:A:292:A:N3	2.34	0.41
1:A:369:C:H2'	1:A:370:U:C6	2.55	0.41
1:A:16:G:H2'	1:A:17:U:H6	1.85	0.41
1:A:75:U:O2'	1:A:76:G:P	2.78	0.41
1:A:170:A:O2'	1:A:171:U:H5'	2.19	0.41
1:A:313:C:C2	1:A:314:G:N7	2.88	0.41
1:A:408:G:H2'	1:A:409:A:C8	2.54	0.41
2:B:112:LYS:HB2	2:B:114:GLU:HG2	2.02	0.41
3:C:24:C:C3'	3:C:25:A:H8	2.33	0.41
3:C:49:C:H2'	3:C:50:G:H8	1.85	0.41
1:A:59:U:O4'	1:A:257:A:H2	2.03	0.41
1:A:161:G:H2'	1:A:162:G:O4'	2.20	0.41
1:A:387:A:H5"	2:B:53:LYS:HD3	2.01	0.41
1:A:120:U:H2'	1:A:121:G:C8	2.55	0.41
1:A:380:A:C2	1:A:381:A:H1'	2.55	0.41
1:A:193:C:H2'	1:A:194:C:C6	2.55	0.41
1:A:262:A:H2'	1:A:263:A:C8	2.56	0.41
1:A:56:U:O2'	1:A:100:A:N1	2.51	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.85	0.41
1:A:198:G:N3	1:A:198:G:H2'	2.35	0.41
1:A:305:A:H2'	1:A:306:G:O4'	2.21	0.41
3:C:35:C:H2'	3:C:36:A:O4'	2.20	0.41
1:A:88:C:H2'	1:A:89:G:C8	2.56	0.41
3:C:66:U:H2'	3:C:67:U:C6	2.55	0.41
1:A:4:A:H2'	1:A:5:A:C8	2.56	0.41
1:A:131:G:H2'	1:A:132:G:O4'	2.20	0.41
1:A:197:A:C6	1:A:199:U:C4	3.09	0.41
3:C:20:A:N7	3:C:45:G:N7	2.68	0.41
1:A:119:C:H2'	1:A:120:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:C:H2'	1:A:220:C:H6	1.84	0.41
1:A:229:G:H2'	1:A:230:G:C8	2.56	0.41
1:A:315:G:H2'	1:A:316:C:C5	2.56	0.41
1:A:412:A:H2'	1:A:413:A:H8	1.86	0.41
1:A:38:G:H2'	1:A:39:C:C6	2.56	0.41
2:B:51:LEU:HD23	2:B:51:LEU:HA	1.92	0.41
3:C:9:A:C2	3:C:45:G:C6	3.08	0.41
3:C:40:U:H2'	3:C:41:G:H8	1.86	0.41
1:A:282:C:H2'	1:A:283:C:H6	1.86	0.40
1:A:357:G:H21	1:A:368:G:H1	1.69	0.40
1:A:160:C:C2	1:A:161:G:C8	3.09	0.40
1:A:222:U:H2'	1:A:223:A:C8	2.56	0.40
1:A:381:A:C2	1:A:382:G:H1'	2.57	0.40
2:B:43:ILE:HA	2:B:81:TYR:O	2.21	0.40
1:A:357:G:H2'	1:A:358:G:H8	1.86	0.40
1:A:414:C:C2	1:A:415:G:C8	3.09	0.40
1:A:31:G:C2	1:A:32:G:C8	3.09	0.40
1:A:173:G:H2'	1:A:174:U:C6	2.56	0.40
1:A:396:C:H2'	1:A:397:U:C6	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	
2	B	114/116 (98%)	113 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	99/99 (100%)	94 (95%)	5 (5%)	20 42

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET
2	B	12	GLU
2	B	35	ARG
2	B	96	GLU
2	B	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	416/417 (99%)	135 (32%)	10 (2%)
3	C	88/92 (95%)	30 (34%)	3 (3%)
3	E	8/92 (8%)	3 (37%)	0
All	All	512/601 (85%)	168 (32%)	13 (2%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	8	A
1	A	9	U
1	A	11	C
1	A	15	G
1	A	28	G
1	A	30	C
1	A	32	G

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Mol	Chain	Res	Type
1	A	33	U
1	A	35	U
1	A	36	C
1	A	48	A
1	A	49	A
1	A	50	A
1	A	52	U
1	A	53	C
1	A	60	C
1	A	65	G
1	A	66	G
1	A	67	U
1	A	68	G
1	A	69	C
1	A	70	U
1	A	72	A
1	A	74	A
1	A	75	U
1	A	76	G
1	A	80	G
1	A	81	U
1	A	85	G
1	A	87	U
1	A	88	C
1	A	89	G
1	A	91	G
1	A	99	A
1	A	100	A
1	A	101	U
1	A	102	C
1	A	117	G
1	A	118	C
1	A	121	G
1	A	122	G
1	A	123	C
1	A	126	C
1	A	127	G
1	A	128	G
1	A	132	G
1	A	134	C
1	A	135	U
1	A	137	A

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Mol	Chain	Res	Type
1	A	138	C
1	A	139	G
1	A	141	C
1	A	142	G
1	A	146	A
1	A	149	G
1	A	150	A
1	A	151	A
1	A	152	C
1	A	164	U
1	A	171	U
1	A	172	G
1	A	177	G
1	A	178	A
1	A	179	U
1	A	180	U
1	A	183	C
1	A	186	G
1	A	187	A
1	A	190	G
1	A	192	G
1	A	198	G
1	A	199	U
1	A	200	G
1	A	203	G
1	A	204	G
1	A	207	C
1	A	208	U
1	A	213	G
1	A	214	G
1	A	219	C
1	A	226	G
1	A	227	G
1	A	234	G
1	A	236	G
1	A	237	G
1	A	239	A
1	A	240	A
1	A	241	A
1	A	250	G
1	A	255	A
1	A	266	A

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Mol	Chain	Res	Type
1	A	267	U
1	A	271	A
1	A	272	G
1	A	276	C
1	A	278	C
1	A	292	A
1	A	294	G
1	A	299	G
1	A	304	A
1	A	311	G
1	A	312	G
1	A	313	C
1	A	314	G
1	A	317	G
1	A	318	C
1	A	321	G
1	A	323	A
1	A	324	G
1	A	328	G
1	A	330	A
1	A	334	A
1	A	342	A
1	A	346	C
1	A	348	G
1	A	349	G
1	A	350	A
1	A	351	G
1	A	362	A
1	A	365	G
1	A	366	C
1	A	367	C
1	A	368	G
1	A	369	C
1	A	372	G
1	A	373	C
1	A	376	U
1	A	379	G
1	A	381	A
1	A	382	G
1	A	383	G
1	A	389	A
1	A	408	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	U
3	C	-8	U
3	C	-7	U
3	C	-6	C
3	C	-4	C
3	C	-3	U
3	C	-1	U
3	C	7	G
3	C	8	U
3	C	10	G
3	C	12	U
3	C	13	C
3	C	14	A
3	C	17	G
3	C	18	G
3	C	19	U
3	C	20	A
3	C	23	A
3	C	26	C
3	C	29	C
3	C	37	A
3	C	41	G
3	C	44	G
3	C	45	G
3	C	46	U
3	C	47	C
3	C	48	G
3	C	52	G
3	C	58	G
3	C	63	G
3	C	70	G
3	E	-11	A
3	E	-10	U
3	E	-7	U

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	67	U
1	A	75	U
1	A	122	G
1	A	126	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	A
1	A	176	C
1	A	212	A
1	A	239	A
1	A	240	A
1	A	349	G
3	C	-4	C
3	C	19	U
3	C	46	U

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 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

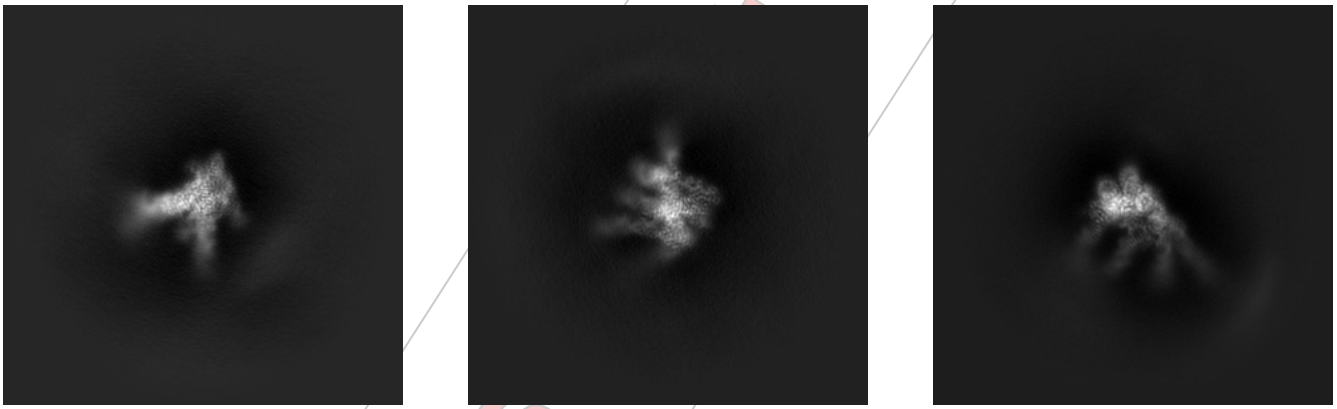
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71000. 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.

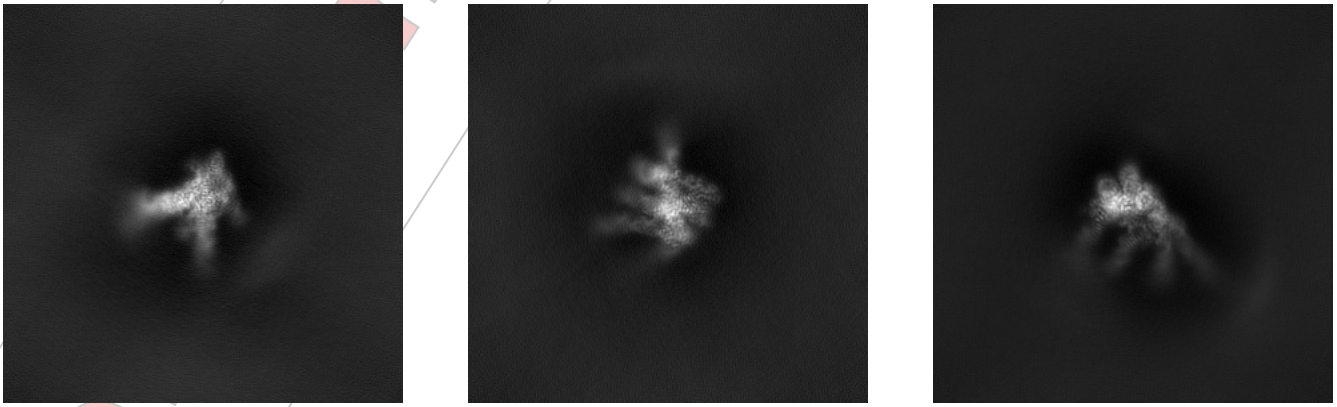
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

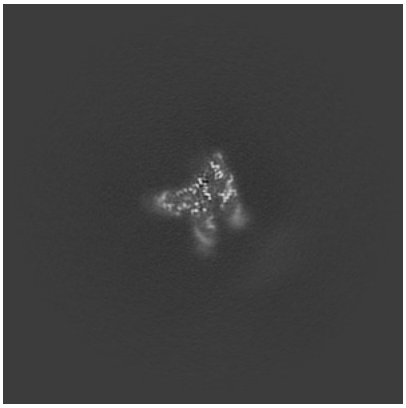


X Y Z

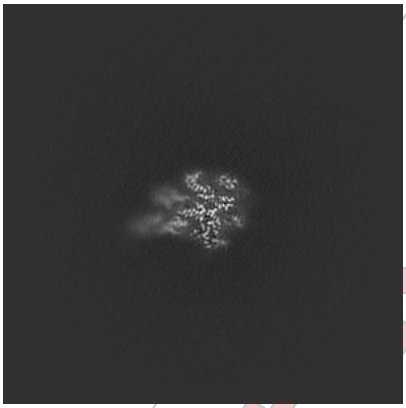
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

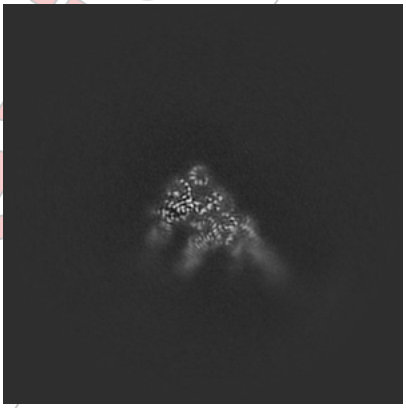
6.2.1 Primary map



X Index: 200

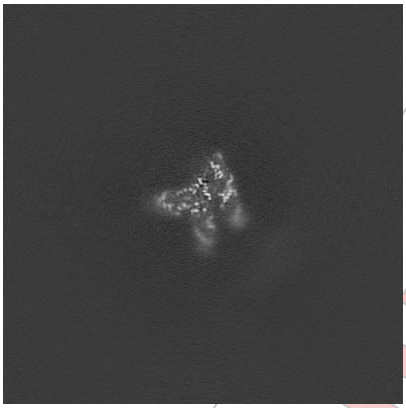


Y Index: 200

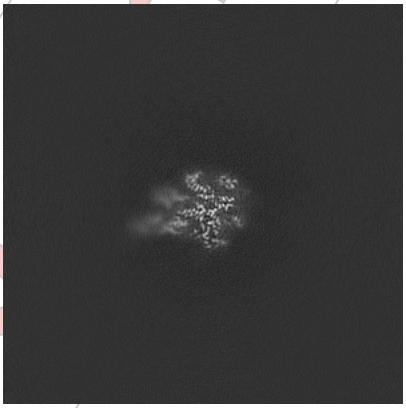


Z Index: 200

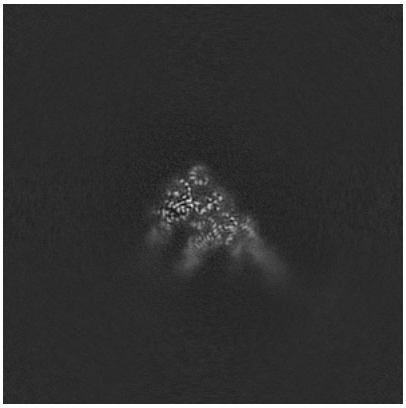
6.2.2 Raw map



X Index: 200



Y Index: 200

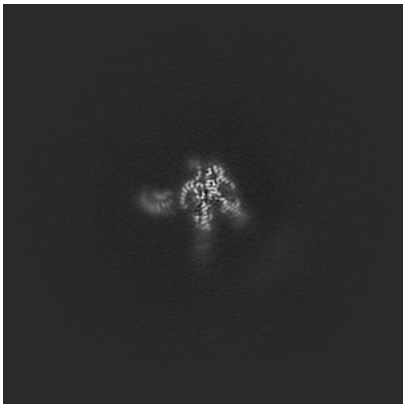


Z Index: 200

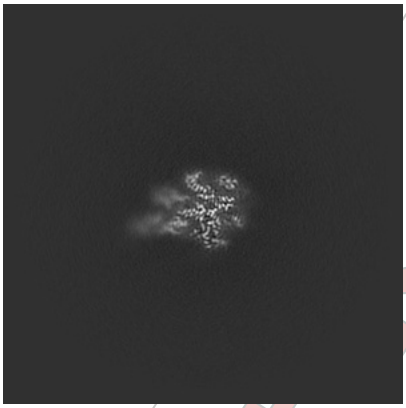
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

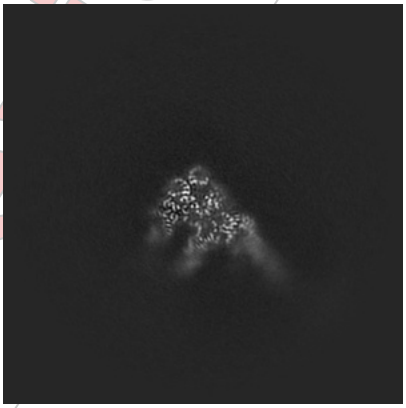
6.3.1 Primary map



X Index: 192

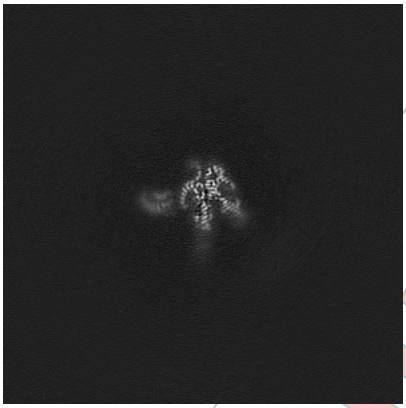


Y Index: 200

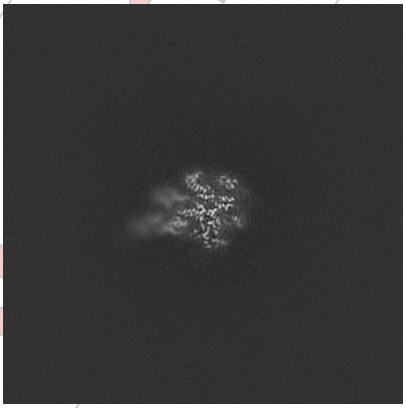


Z Index: 202

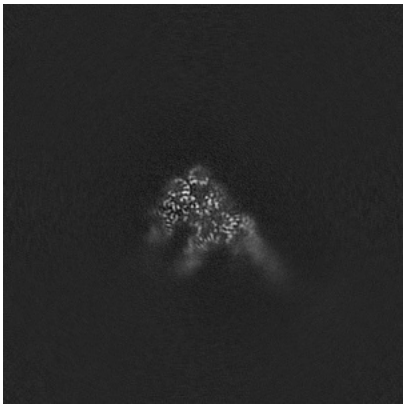
6.3.2 Raw map



X Index: 192



Y Index: 200

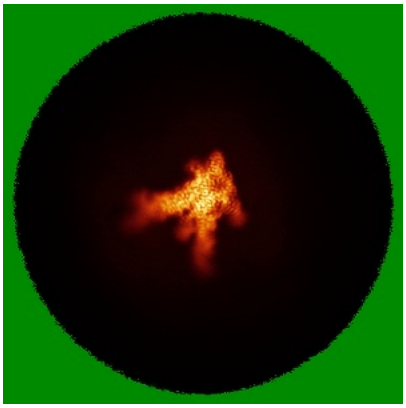


Z Index: 202

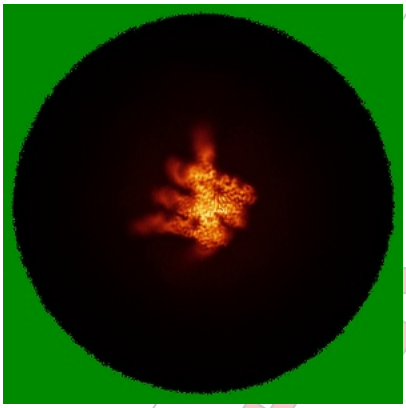
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

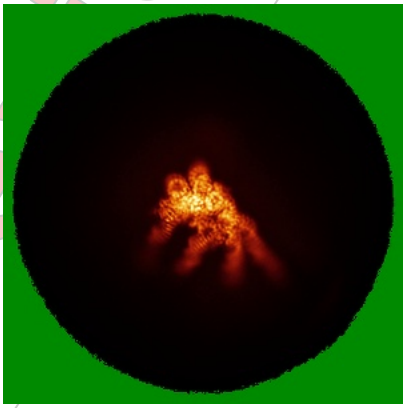
6.4.1 Primary map



X

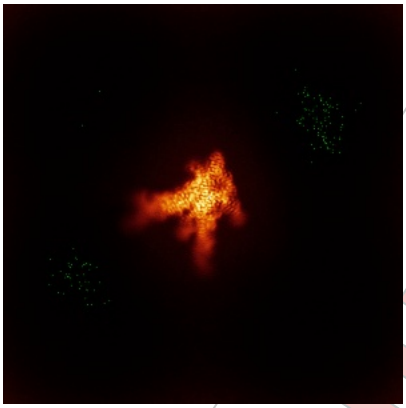


Y

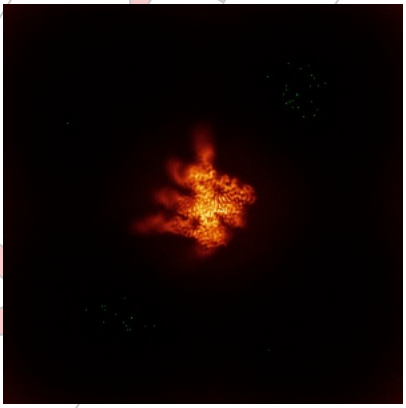


Z

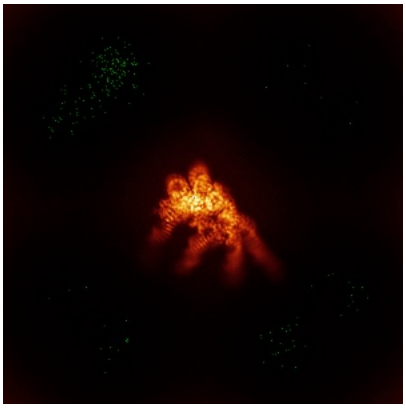
6.4.2 Raw map



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 0.035. 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.

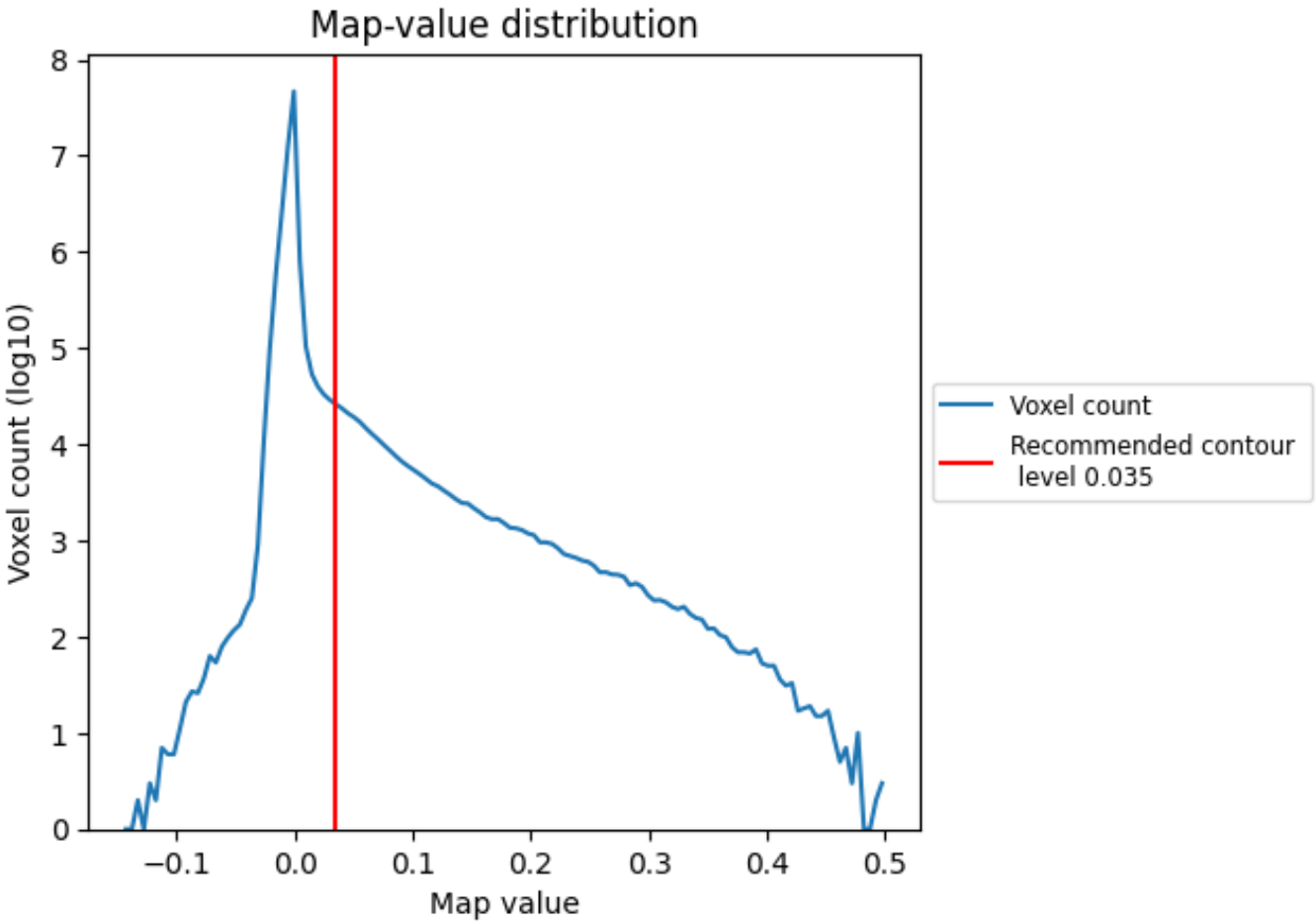
6.6 Mask visualisation (i)

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

7 Map analysis

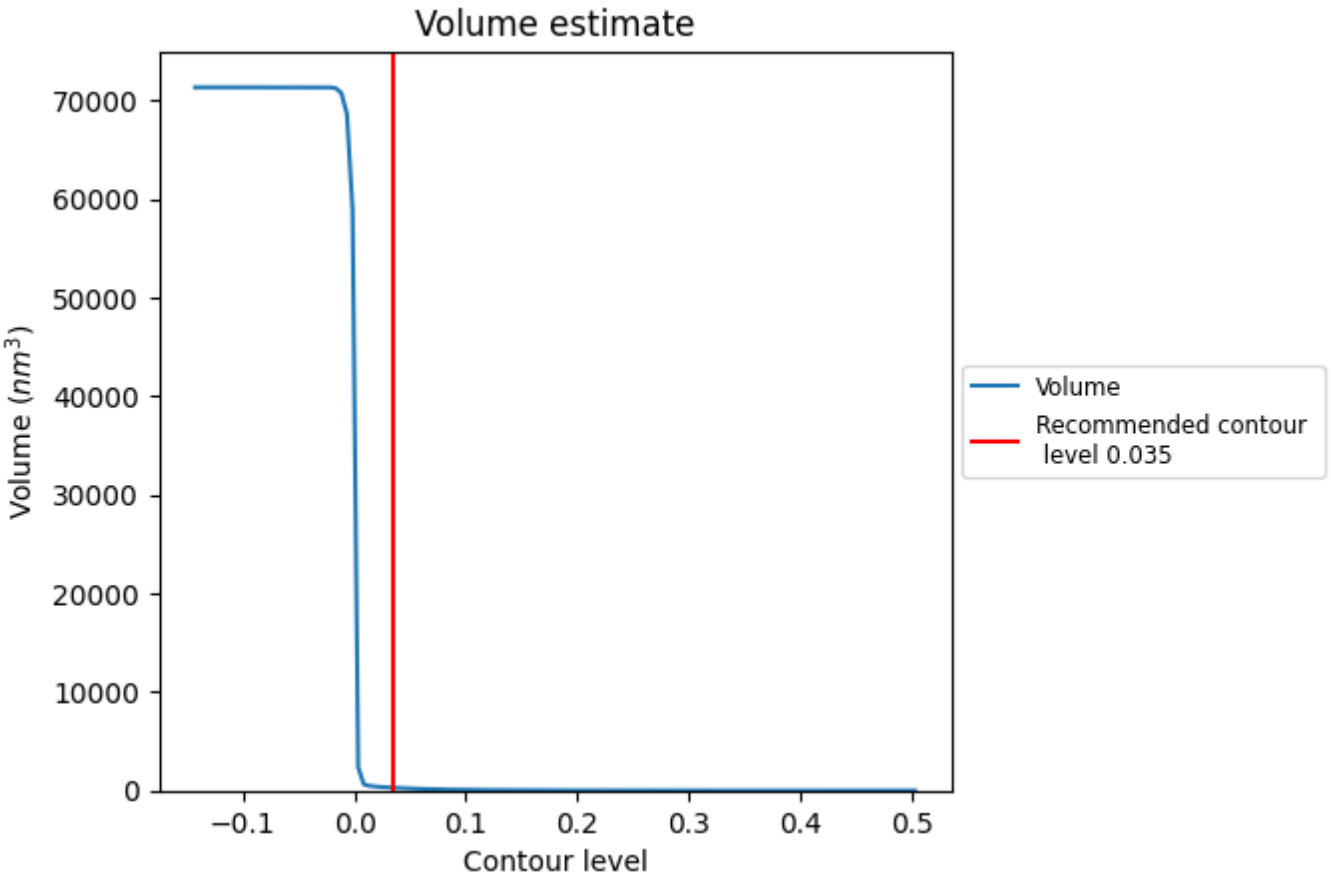
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

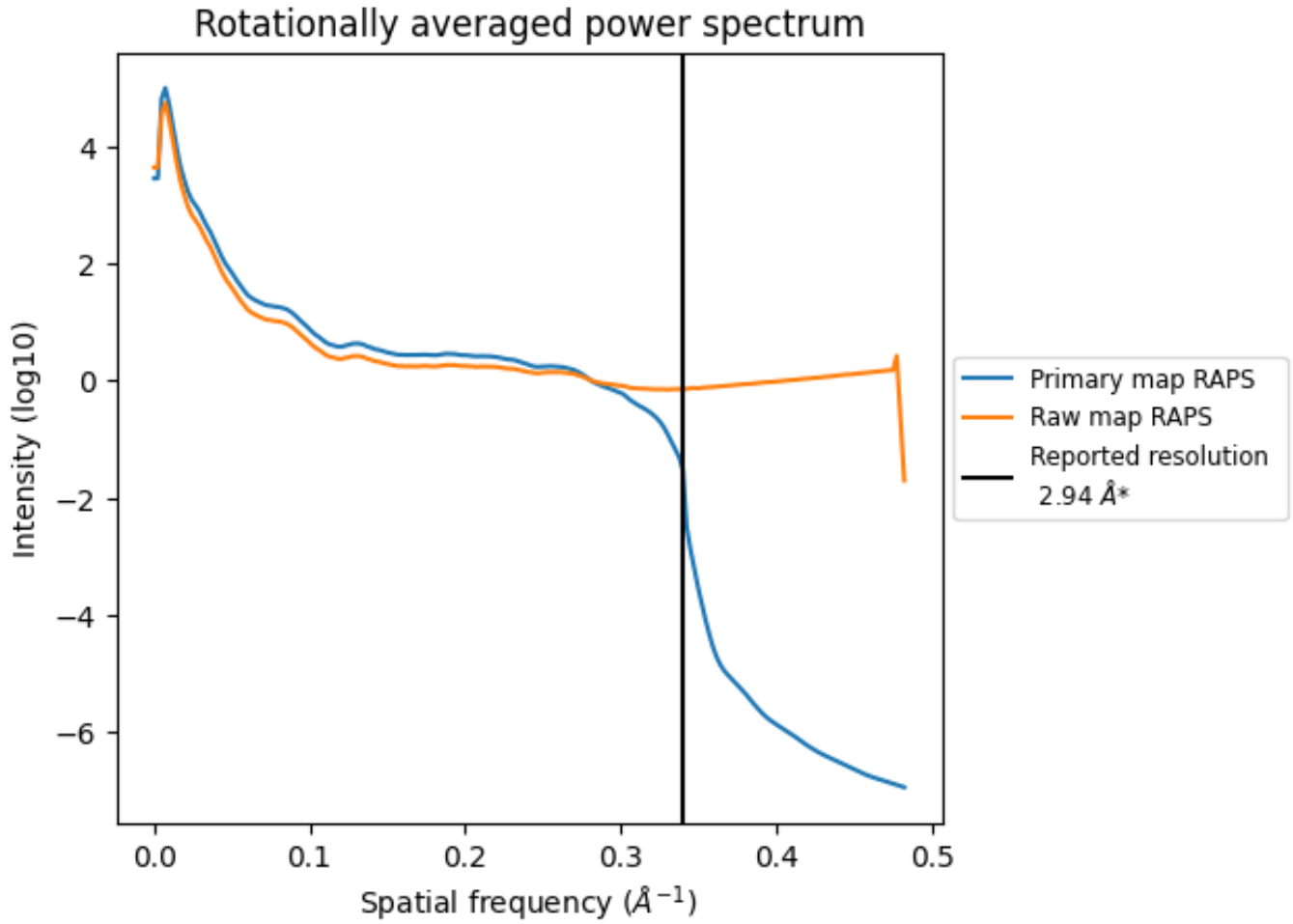
7.2 Volume estimate (i)



The volume at the recommended contour level is 282 nm^3; this corresponds to an approximate mass of 255 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 (i)

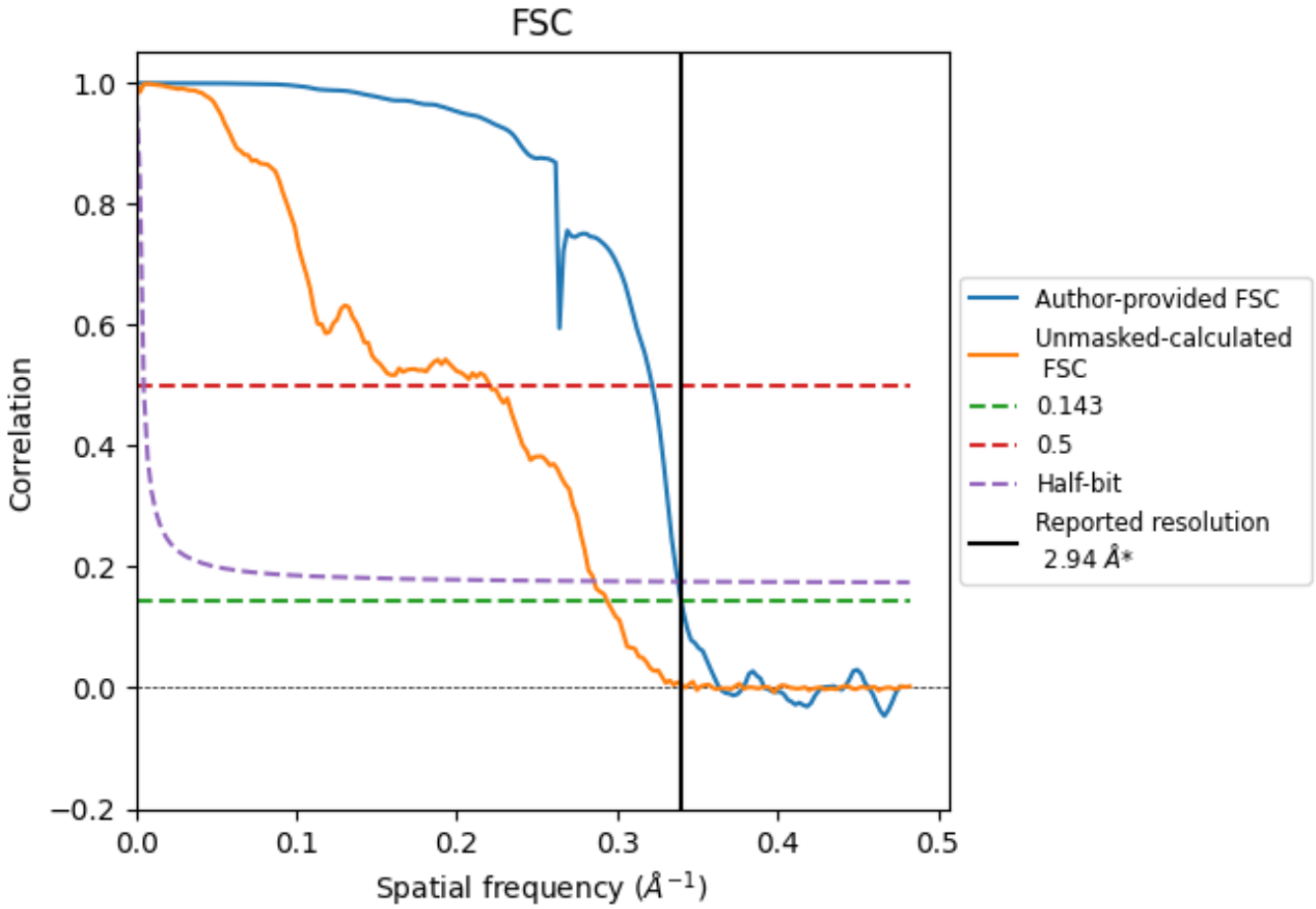


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8.2 Resolution estimates (i)

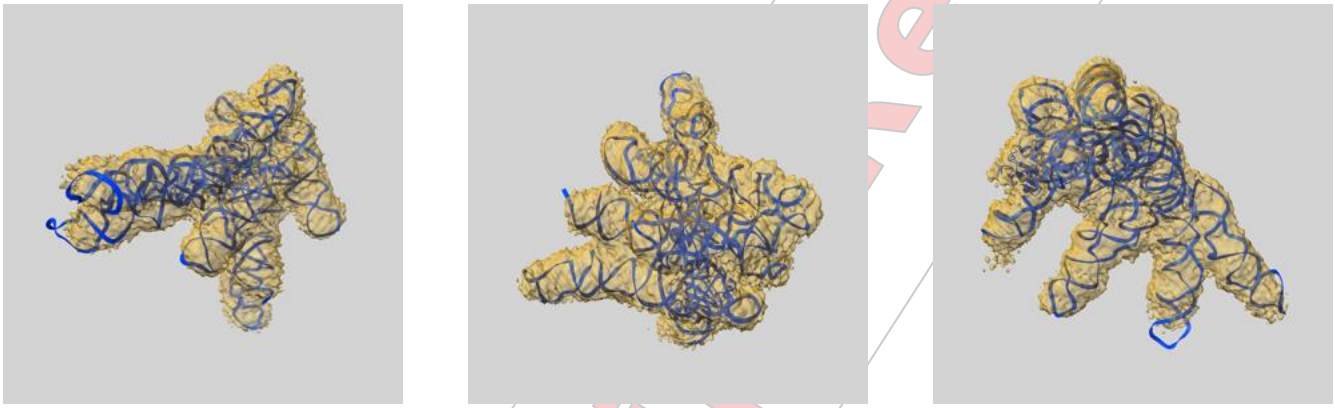
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.11	2.96
Unmasked-calculated*	3.40	4.53	3.50

*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 3.40 differs from the reported value 2.94 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71000 and PDB model 9OY7. Per-residue inclusion information can be found in section 3 on page 5.

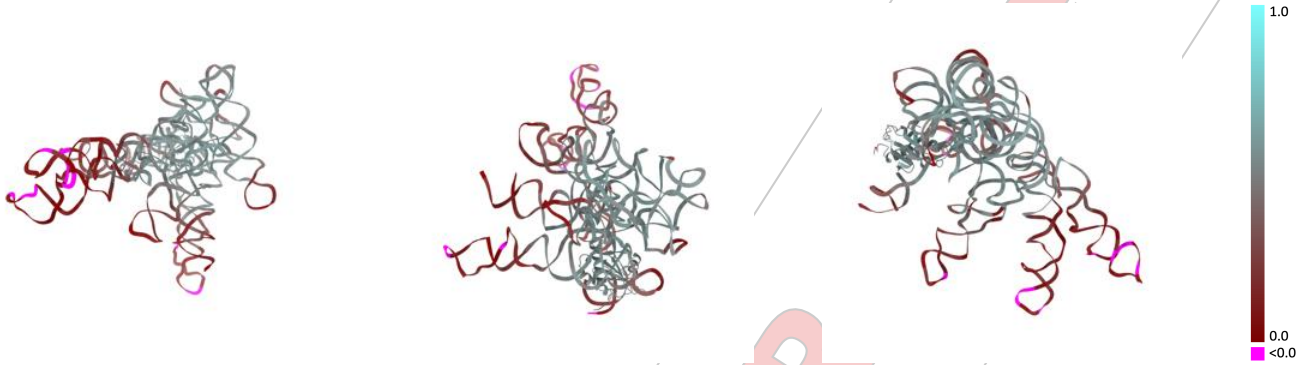
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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



X Y Z

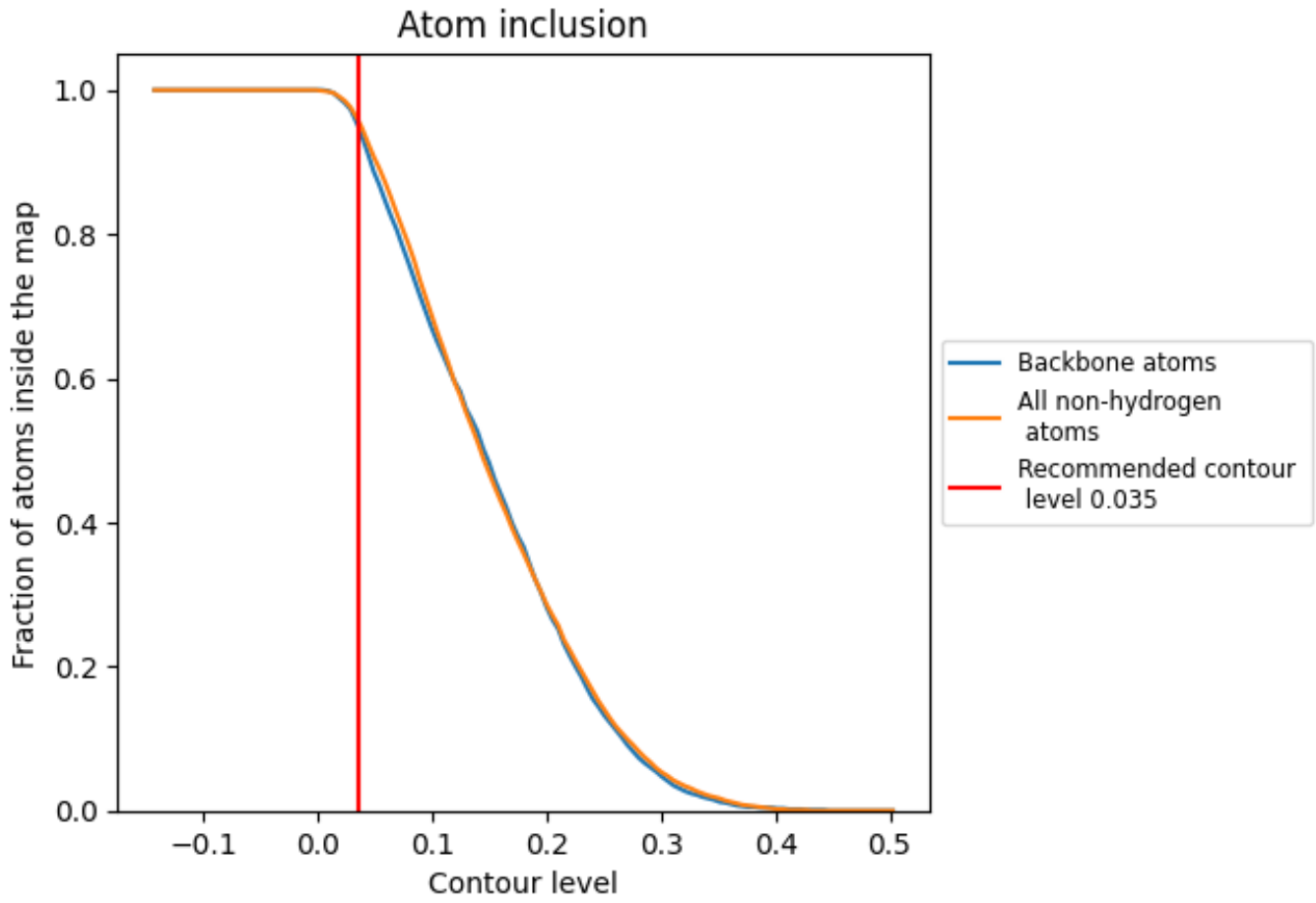
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.3880
A	0.9510	0.3730
B	0.9960	0.5390
C	0.9830	0.3920
E	0.9250	0.2820