Full wwPDB EM Validation Report ⓘ

Jul 18, 2024 – 05:00 PM EDT

PDB ID	:	9CL9
EMDB ID	:	EMD-45666
Title	:	WT 12C IM fraction, B-b3 with RluB bound
Authors	:	Lee, J.; Sheng, K.; Williamson, J.R.
Deposited on	:	2024-07-10
Resolution	:	5.04 Å(reported)
Based on initial models	:	., 8RPY, 4YBB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

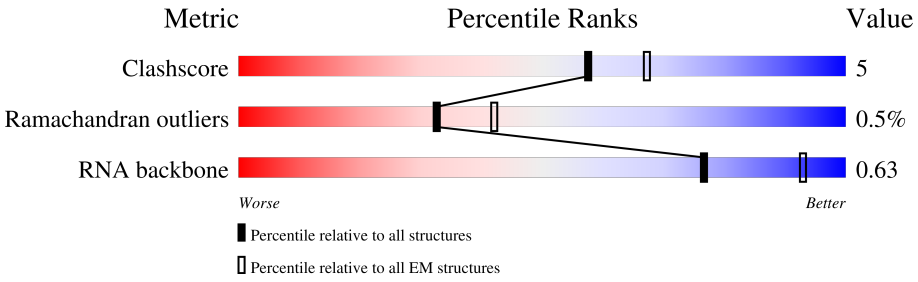
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 5.04 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	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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	Q	117	99%
2	R	103	99%
3	T	90	16% 97%
4	2	37	5% 100%
5	A	283	29% 96%
6	CA	2904	7% 39% 12% 47%
7	D	209	6% 72% 25%
8	E	201	75% 23%

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Mol	Chain	Length	Quality of chain
9	J	142	99%
10	S	110	5% 87% 11%
11	U	102	96%
12	Y	60	98%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 56342 atoms, of which 17846 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	Q	117	698	234	230	117	117	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	R	103	607	206	195	103	103	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	T	90	534	180	174	90	90	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
4	2	37	218	74	70	37	37	0	0

- Molecule 5 is a protein called Ribosomal large subunit pseudouridine synthase B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	A	278	1630	556	518	278	278	0	0

- Molecule 6 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	CA	1543	49803	14785	16659	6119	10697	1543	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	747	C	U	conflict	GB 802133627

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	D	157	Total	C	N	O	0	0
			628	314	157	157		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	154	Total	C	N	O	0	0
			616	308	154	154		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	142	Total	C	N	O	0	0
			568	284	142	142		

- Molecule 10 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	98	Total	C	N	O	0	0
			392	196	98	98		

- Molecule 11 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	102	Total	C	N	O	0	0
			408	204	102	102		

- Molecule 12 is a protein called Large ribosomal subunit protein uL29.

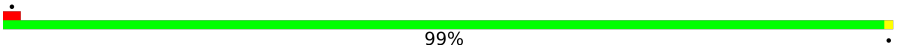
Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	60	Total	C	N	O	0	0
			240	120	60	60		

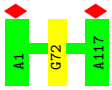
3 Residue-property plots (i)

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: Large ribosomal subunit protein bL20

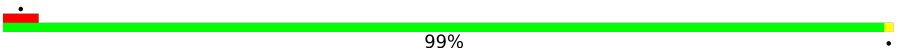
Chain Q:

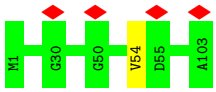




• Molecule 2: Large ribosomal subunit protein bL21

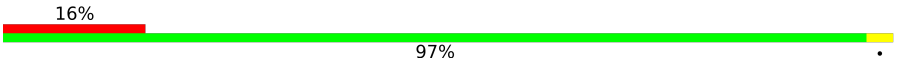
Chain R:

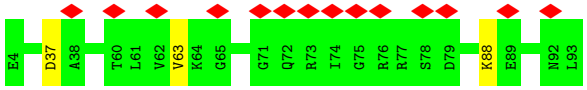




• Molecule 3: Large ribosomal subunit protein uL23

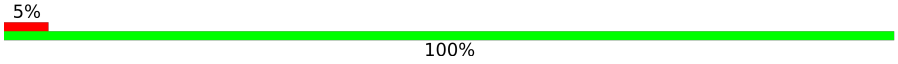
Chain T:

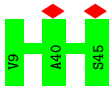




• Molecule 4: Large ribosomal subunit protein bL34

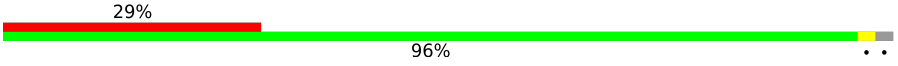
Chain 2:

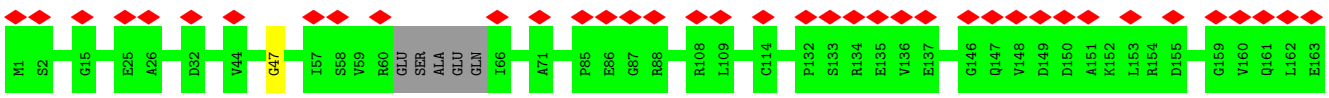


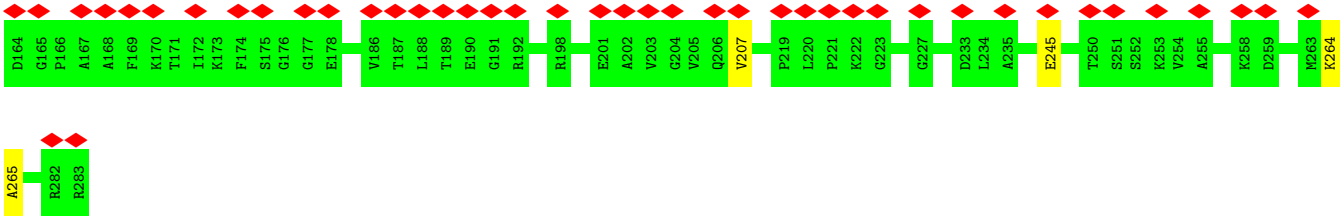


• Molecule 5: Ribosomal large subunit pseudouridine synthase B

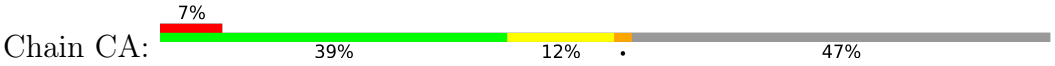
Chain A:

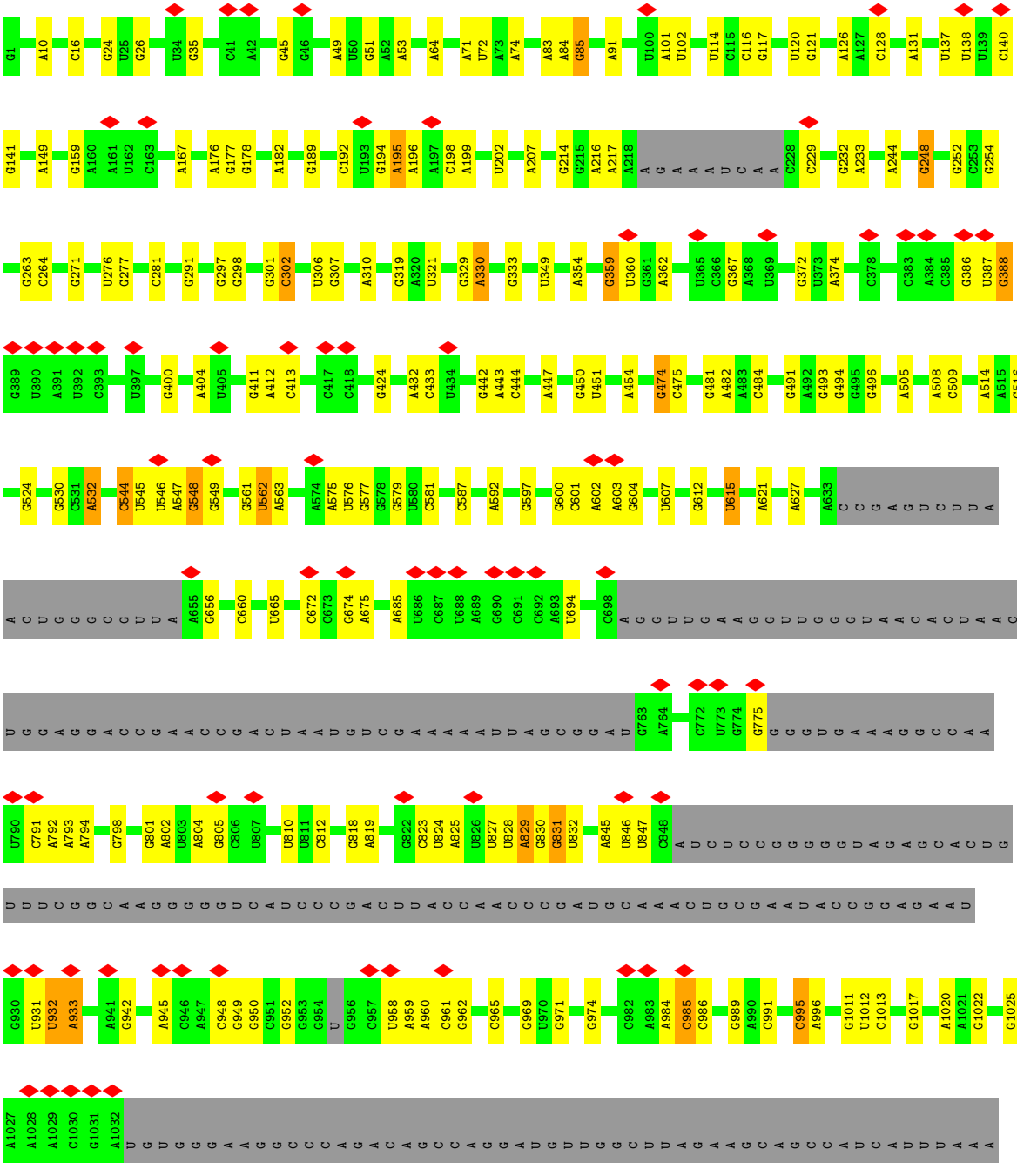


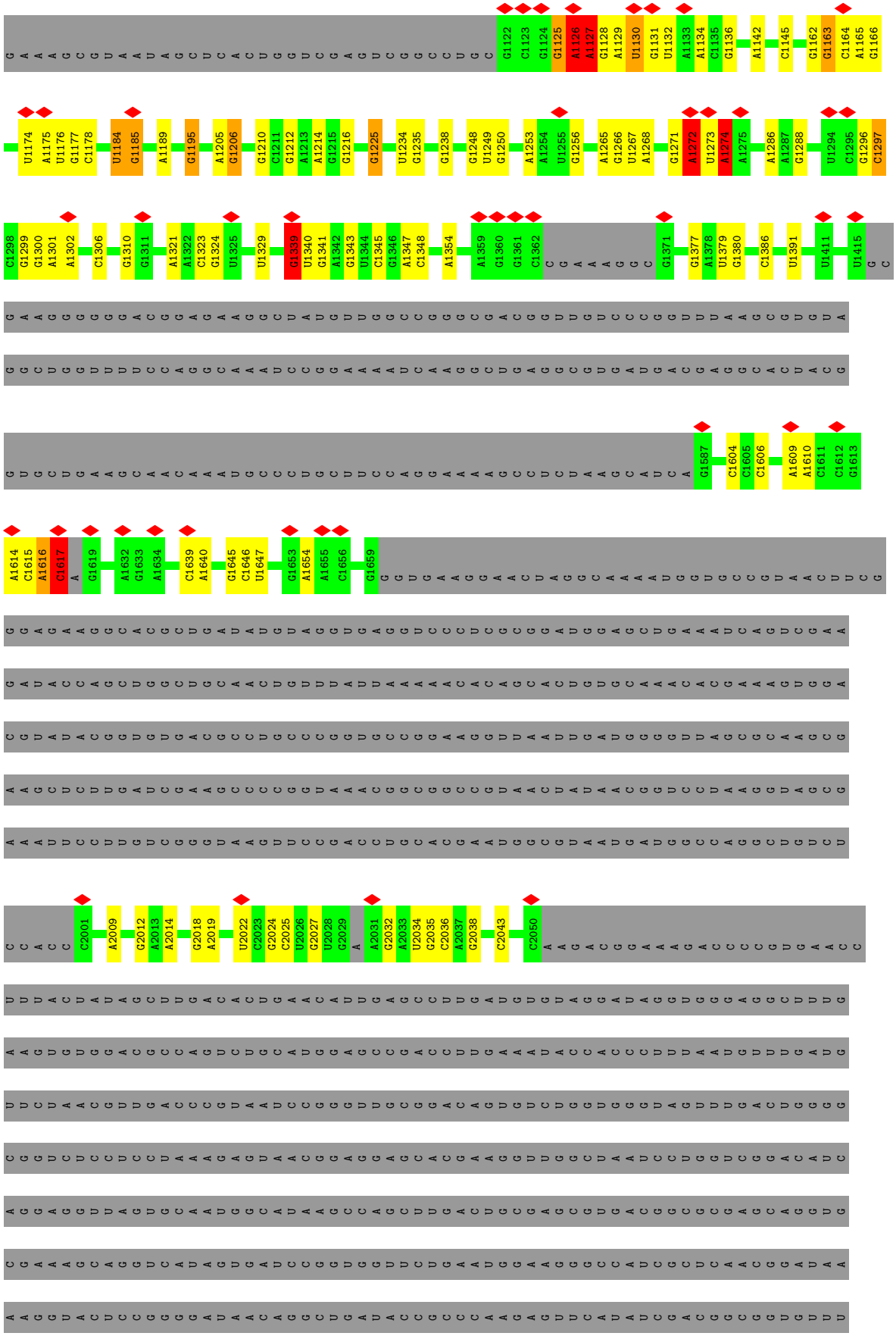


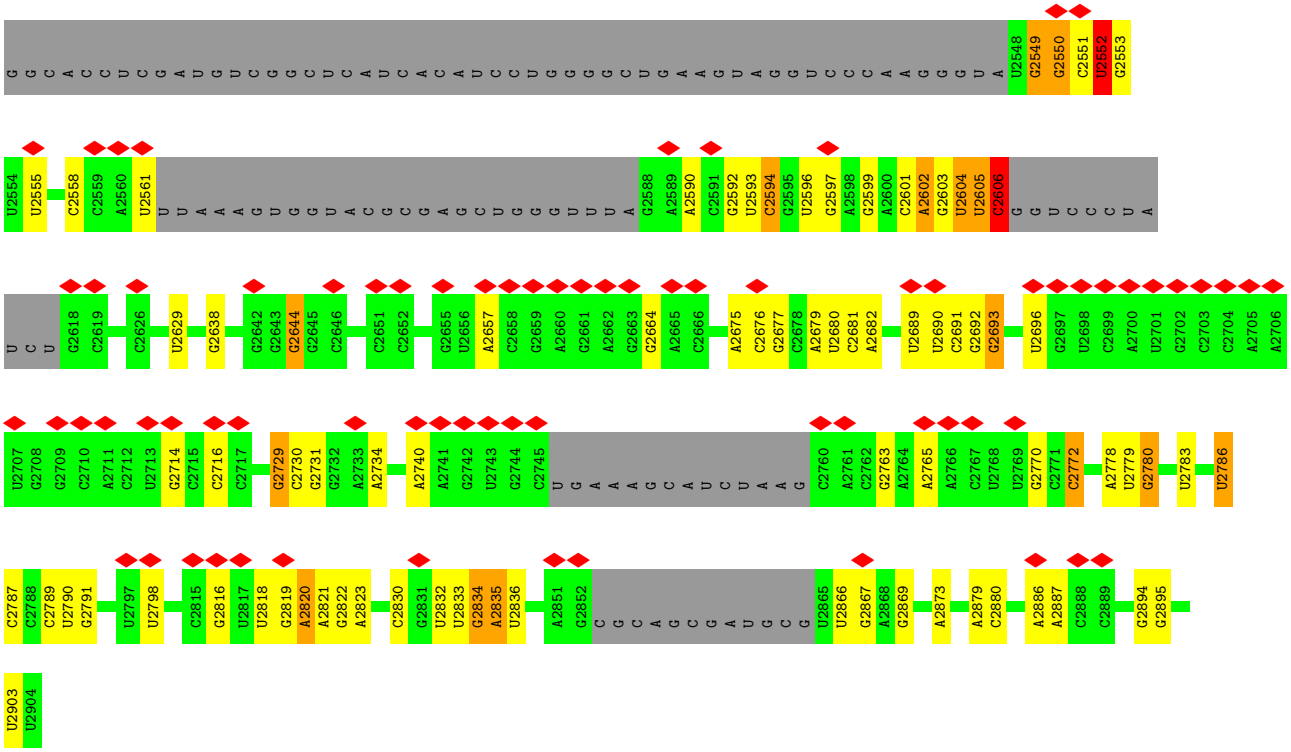


• Molecule 6: 23S rRNA

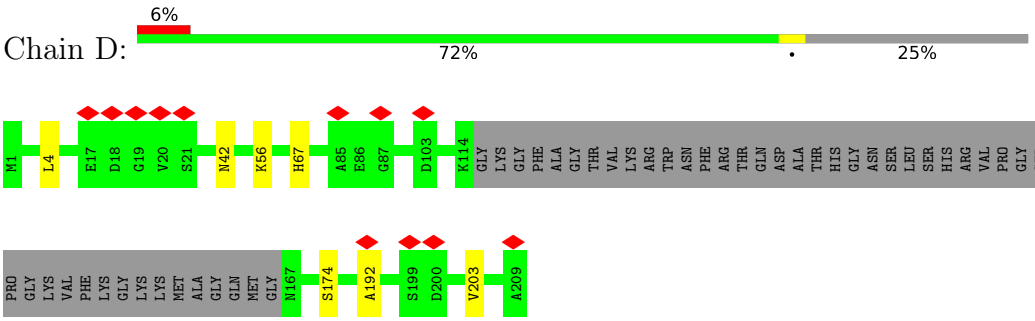




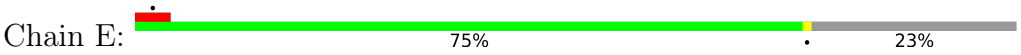


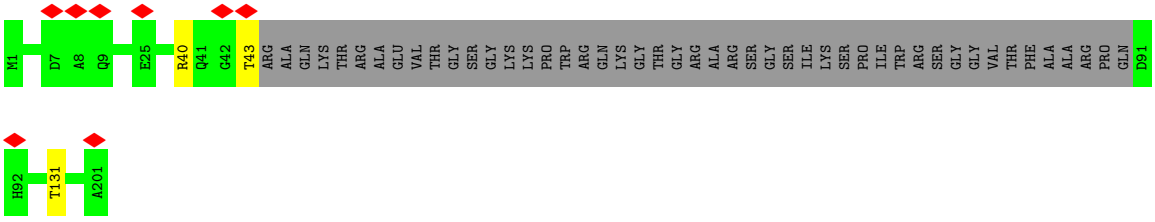


• Molecule 7: Large ribosomal subunit protein uL3

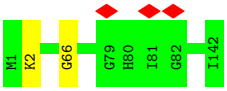


• Molecule 8: Large ribosomal subunit protein uL4



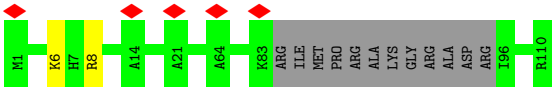


• Molecule 9: Large ribosomal subunit protein uL13



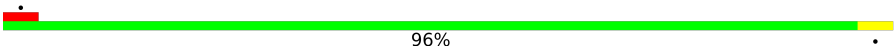
• Molecule 10: Large ribosomal subunit protein uL22

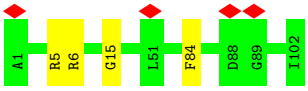
Chain S:



• Molecule 11: Large ribosomal subunit protein uL24

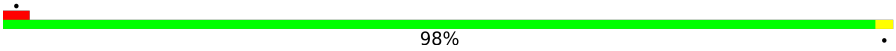
Chain U:

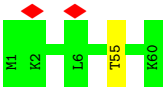




• Molecule 12: Large ribosomal subunit protein uL29

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22502	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction were performed by Patch CTF Estimation of cryoSPARC	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.216	Depositor
Minimum map value	-0.377	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	386.4, 386.4, 386.4	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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	Q	0.21	0/467	0.39	0/582
2	R	0.24	0/411	0.52	0/512
3	T	0.21	0/359	0.47	0/447
4	2	0.21	0/147	0.42	0/182
5	A	0.40	0/1110	0.56	0/1384
6	CA	1.32	32/37084 (0.1%)	1.12	62/57811 (0.1%)
7	D	0.27	0/626	0.52	0/779
8	E	0.23	0/614	0.46	0/764
9	J	0.25	0/567	0.46	0/707
10	S	0.25	0/390	0.48	0/484
11	U	0.25	0/407	0.53	0/507
12	Y	0.23	0/239	0.42	0/297
All	All	1.24	32/42421 (0.1%)	1.08	62/64456 (0.1%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CA	1274	A	N3-C4	77.52	1.81	1.34
6	CA	1274	A	C6-N1	68.61	1.83	1.35
6	CA	1127	A	N3-C4	67.54	1.75	1.34
6	CA	1272	A	N3-C4	64.88	1.73	1.34
6	CA	1272	A	C6-N1	63.04	1.79	1.35
6	CA	1127	A	C6-N1	57.06	1.75	1.35
6	CA	1274	A	C5-C4	53.53	1.76	1.38
6	CA	1127	A	C5-C4	52.62	1.75	1.38
6	CA	1272	A	C5-C4	49.67	1.73	1.38
6	CA	1274	A	N1-C2	49.06	1.78	1.34
6	CA	1274	A	C2-N3	48.33	1.77	1.33
6	CA	1272	A	N1-C2	47.30	1.76	1.34
6	CA	1274	A	C5-C6	45.23	1.81	1.41
6	CA	1127	A	C2-N3	44.42	1.73	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CA	1272	A	C5-C6	43.50	1.80	1.41
6	CA	1272	A	C2-N3	42.93	1.72	1.33
6	CA	1127	A	N1-C2	42.80	1.72	1.34
6	CA	1127	A	C5-C6	42.28	1.79	1.41
6	CA	1617	C	P-O5'	39.70	1.99	1.59
6	CA	1125	G	O3'-P	38.14	2.06	1.61
6	CA	1297	C	C1'-N1	36.94	2.04	1.48
6	CA	1339	G	C6-N1	34.12	1.63	1.39
6	CA	1297	C	N1-C6	31.62	1.56	1.37
6	CA	1339	G	N1-C2	30.76	1.62	1.37
6	CA	1297	C	N1-C2	30.70	1.70	1.40
6	CA	1339	G	N3-C4	26.29	1.53	1.35
6	CA	1339	G	C2-N3	24.43	1.52	1.32
6	CA	1339	G	C5-C4	21.25	1.53	1.38
6	CA	1339	G	C5-C6	18.17	1.60	1.42
6	CA	1125	G	C3'-O3'	16.26	1.65	1.42
6	CA	1617	C	O5'-C5'	13.28	1.65	1.44
6	CA	1297	C	C2-N3	9.61	1.43	1.35

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CA	1297	C	C6-N1-C2	-164.95	54.32	120.30
6	CA	1297	C	C4-C5-C6	-62.29	86.26	117.40
6	CA	1297	C	C5-C6-N1	58.90	150.45	121.00
6	CA	1297	C	N3-C2-O2	-30.38	100.64	121.90
6	CA	1297	C	C2-N1-C1'	29.22	150.94	118.80
6	CA	1297	C	C6-N1-C1'	27.96	154.35	120.80
6	CA	1274	A	N1-C2-N3	-27.85	115.38	129.30
6	CA	1125	G	P-O3'-C3'	27.81	153.07	119.70
6	CA	1272	A	N1-C2-N3	-27.60	115.50	129.30
6	CA	1127	A	N1-C2-N3	-26.61	116.00	129.30
6	CA	1297	C	N3-C4-C5	-25.53	111.69	121.90
6	CA	1272	A	C2-N3-C4	25.45	123.33	110.60
6	CA	1274	A	C2-N3-C4	24.53	122.86	110.60
6	CA	1127	A	C2-N3-C4	24.20	122.70	110.60
6	CA	1297	C	N1-C2-N3	21.56	134.29	119.20
6	CA	2604	U	O3'-P-O5'	-20.45	65.14	104.00
6	CA	1617	C	P-O5'-C5'	19.31	151.80	120.90
6	CA	1127	A	N7-C8-N9	16.31	121.95	113.80
6	CA	1274	A	N7-C8-N9	15.66	121.63	113.80
6	CA	1339	G	C2-N3-C4	15.33	119.56	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CA	1272	A	N7-C8-N9	14.61	121.11	113.80
6	CA	1274	A	C4-C5-N7	-13.98	103.71	110.70
6	CA	1127	A	N3-C4-N9	12.63	137.50	127.40
6	CA	1272	A	C4-C5-N7	-12.38	104.51	110.70
6	CA	1127	A	C4-C5-N7	-11.81	104.80	110.70
6	CA	1297	C	O4'-C1'-N1	11.61	117.49	108.20
6	CA	1126	A	O5'-P-OP1	-11.42	95.42	105.70
6	CA	2604	U	OP1-P-O3'	-11.35	80.24	105.20
6	CA	1339	G	N1-C2-N3	-11.22	117.17	123.90
6	CA	1274	A	N3-C4-N9	11.16	136.33	127.40
6	CA	1297	C	N1-C1'-C2'	11.00	128.29	114.00
6	CA	1617	C	O5'-P-OP2	10.49	123.29	110.70
6	CA	1297	C	N1-C2-O2	10.23	125.04	118.90
6	CA	1126	A	O5'-P-OP2	-10.19	96.53	105.70
6	CA	1127	A	N9-C4-C5	-10.10	101.76	105.80
6	CA	1125	G	OP2-P-O3'	9.90	126.99	105.20
6	CA	1127	A	C6-N1-C2	9.79	124.47	118.60
6	CA	1272	A	N3-C4-N9	9.78	135.23	127.40
6	CA	2604	U	OP2-P-O3'	-9.69	83.89	105.20
6	CA	1274	A	C6-N1-C2	8.94	123.97	118.60
6	CA	1126	A	OP1-P-OP2	-8.87	106.29	119.60
6	CA	1127	A	N3-C4-C5	-8.67	120.73	126.80
6	CA	1272	A	C6-N1-C2	8.38	123.63	118.60
6	CA	1272	A	N9-C4-C5	-8.19	102.52	105.80
6	CA	1297	C	C2-N3-C4	8.19	123.99	119.90
6	CA	1274	A	N3-C4-C5	-8.15	121.09	126.80
6	CA	1274	A	N9-C4-C5	-8.08	102.57	105.80
6	CA	1272	A	C6-C5-N7	7.57	137.60	132.30
6	CA	1127	A	C6-C5-N7	7.46	137.53	132.30
6	CA	1274	A	C6-C5-N7	7.37	137.46	132.30
6	CA	1297	C	N3-C4-N4	7.25	123.07	118.00
6	CA	1617	C	OP1-P-OP2	-7.22	108.77	119.60
6	CA	1297	C	C5-C4-N4	7.20	125.24	120.20
6	CA	1339	G	C4-C5-N7	-7.13	107.95	110.80
6	CA	1272	A	N3-C4-C5	-6.57	122.20	126.80
6	CA	1339	G	N7-C8-N9	6.45	116.32	113.10
6	CA	1339	G	N3-C4-N9	6.42	129.85	126.00
6	CA	2602	A	OP1-P-O3'	5.62	117.58	105.20
6	CA	1339	G	N3-C4-C5	-5.33	125.94	128.60
6	CA	2606	C	C1'-O4'-C4'	-5.29	105.67	109.90
6	CA	2550	G	OP2-P-O3'	5.08	116.37	105.20
6	CA	2596	U	OP2-P-O3'	5.06	116.34	105.20

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	Q	468	230	131	0	0
2	R	412	195	128	0	0
3	T	360	174	96	1	0
4	2	148	70	42	0	0
5	A	1112	518	321	1	0
6	CA	33144	16659	16690	243	0
7	D	628	0	186	7	0
8	E	616	0	165	3	0
9	J	568	0	162	7	0
10	S	392	0	104	4	0
11	U	408	0	121	11	0
12	Y	240	0	64	3	0
All	All	38496	17846	18210	245	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 5.

All (245) 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)
6:CA:1272:A:C6	6:CA:1272:A:C5	1.80	1.65
6:CA:1274:A:C6	6:CA:1274:A:C5	1.81	1.63
6:CA:1127:A:C6	6:CA:1127:A:C5	1.79	1.61
6:CA:1272:A:C2	6:CA:1272:A:N3	1.72	1.58
6:CA:1127:A:C2	6:CA:1127:A:N1	1.72	1.56
6:CA:1127:A:C4	6:CA:1127:A:N3	1.75	1.54
6:CA:1272:A:C2	6:CA:1272:A:N1	1.76	1.53
6:CA:1274:A:C5	6:CA:1274:A:C4	1.76	1.53
6:CA:1127:A:C2	6:CA:1127:A:N3	1.73	1.52
6:CA:1127:A:C6	6:CA:1127:A:N1	1.75	1.52
6:CA:1272:A:N3	6:CA:1272:A:C4	1.73	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:1274:A:C2	6:CA:1274:A:N3	1.77	1.51
6:CA:1274:A:C2	6:CA:1274:A:N1	1.78	1.49
6:CA:1272:A:C6	6:CA:1272:A:N1	1.79	1.46
6:CA:1274:A:C4	6:CA:1274:A:N3	1.81	1.45
6:CA:1274:A:C6	6:CA:1274:A:N1	1.83	1.44
6:CA:1125:G:C3'	6:CA:1125:G:O3'	1.64	1.42
6:CA:1617:C:O5'	6:CA:1617:C:C5'	1.65	1.42
6:CA:1272:A:C4	6:CA:1617:C:O5'	1.69	1.41
6:CA:1274:A:C4	6:CA:1297:C:N1	1.86	1.41
6:CA:1127:A:C5	6:CA:1127:A:C4	1.75	1.40
6:CA:1274:A:C2	6:CA:1297:C:N1	1.91	1.38
6:CA:1125:G:O3'	6:CA:1127:A:C2	1.75	1.38
6:CA:1272:A:C5	6:CA:1617:C:O5'	1.75	1.37
6:CA:1274:A:C6	6:CA:1297:C:N1	1.92	1.36
6:CA:1274:A:C5	6:CA:1297:C:N1	1.92	1.35
6:CA:1272:A:C6	6:CA:1617:C:O5'	1.80	1.31
6:CA:1126:A:P	6:CA:1127:A:C4	2.25	1.30
6:CA:1125:G:O3'	6:CA:1127:A:C6	1.84	1.27
6:CA:1274:A:N1	6:CA:1297:C:N1	1.82	1.27
6:CA:1274:A:N3	6:CA:1297:C:N1	1.84	1.25
6:CA:1126:A:P	6:CA:1127:A:C5	2.29	1.25
6:CA:1274:A:N3	6:CA:1297:C:H1'	1.51	1.23
6:CA:1125:G:O3'	6:CA:1127:A:C4	1.90	1.22
6:CA:1125:G:O3'	6:CA:1127:A:N1	1.66	1.22
6:CA:1272:A:C2	6:CA:1617:C:O5'	1.91	1.22
6:CA:1272:A:C2	6:CA:1617:C:P	2.33	1.21
6:CA:1126:A:P	6:CA:1127:A:C6	2.34	1.21
6:CA:1297:C:N1	6:CA:1297:C:C1'	2.04	1.21
6:CA:1617:C:O5'	6:CA:1617:C:P	1.99	1.20
6:CA:1272:A:N3	6:CA:1617:C:O5'	1.76	1.19
6:CA:1125:G:O3'	6:CA:1127:A:C5	1.96	1.18
6:CA:1272:A:C6	6:CA:1617:C:P	2.37	1.17
6:CA:1125:G:O3'	6:CA:1127:A:N3	1.77	1.15
6:CA:1272:A:N1	6:CA:1617:C:P	2.20	1.14
6:CA:1272:A:N1	6:CA:1617:C:O5'	1.81	1.14
6:CA:1274:A:C2	6:CA:1297:C:C1'	2.30	1.14
6:CA:1125:G:O3'	6:CA:1126:A:P	2.06	1.13
6:CA:1274:A:C6	6:CA:1297:C:C6	2.37	1.11
6:CA:1274:A:C6	6:CA:1297:C:C1'	2.34	1.11
6:CA:1274:A:C4	6:CA:1297:C:C2	2.40	1.08
6:CA:1274:A:C2	6:CA:1297:C:H1'	1.88	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:1274:A:C4	6:CA:1297:C:C1'	2.36	1.07
6:CA:1126:A:P	6:CA:1127:A:C2	2.47	1.07
6:CA:1125:G:H3'	6:CA:1127:A:C4	1.94	1.02
6:CA:1272:A:C4	6:CA:1617:C:P	2.54	1.01
6:CA:1126:A:P	6:CA:1127:A:N3	2.34	1.00
6:CA:1125:G:C3'	6:CA:1127:A:C4	2.44	1.00
6:CA:1274:A:N1	6:CA:1297:C:C1'	2.24	1.00
6:CA:1274:A:C5	6:CA:1297:C:C1'	2.45	0.99
6:CA:1274:A:N3	6:CA:1297:C:C1'	2.24	0.99
6:CA:1272:A:C2	6:CA:1617:C:C5'	2.46	0.99
6:CA:1272:A:C5	6:CA:1617:C:P	2.56	0.98
6:CA:1272:A:N1	6:CA:1617:C:C5'	2.26	0.97
6:CA:1274:A:N1	6:CA:1297:C:C6	2.32	0.97
6:CA:1274:A:N3	6:CA:1297:C:C2	2.32	0.97
6:CA:1126:A:P	6:CA:1127:A:N1	2.40	0.94
6:CA:1125:G:C3'	6:CA:1127:A:C5	2.50	0.93
6:CA:329:G:O6	11:U:15:GLY:HA3	1.69	0.92
6:CA:1272:A:C6	6:CA:1617:C:C5'	2.53	0.91
6:CA:1272:A:N3	6:CA:1617:C:P	2.44	0.90
6:CA:297:G:O3'	11:U:84:PHE:O	1.89	0.89
6:CA:1272:A:C2	6:CA:1617:C:H5'	2.12	0.83
6:CA:329:G:O6	11:U:15:GLY:CA	2.26	0.82
6:CA:1125:G:H3'	6:CA:1127:A:C5	2.15	0.81
6:CA:1274:A:C4	6:CA:1297:C:C2'	2.66	0.78
6:CA:1274:A:N1	6:CA:1297:C:O4'	2.16	0.78
6:CA:1274:A:C5	6:CA:1297:C:C6	2.73	0.77
6:CA:443:A:OP1	8:E:40:ARG:CA	2.34	0.76
6:CA:2549:G:H22	6:CA:2552:OMU:C4	2.00	0.74
6:CA:1126:A:OP2	6:CA:1127:A:C5	2.41	0.74
6:CA:189:G:H21	6:CA:207:A:H62	1.36	0.74
6:CA:1274:A:C4	6:CA:1297:C:H1'	2.23	0.73
6:CA:2786:U:O2'	7:D:67:HIS:N	2.21	0.73
6:CA:1272:A:C5	6:CA:1616:A:O3'	2.43	0.71
6:CA:1274:A:C2	6:CA:1297:C:C2	2.77	0.71
6:CA:1274:A:C2	6:CA:1297:C:C6	2.80	0.70
6:CA:53:A:H62	6:CA:117:G:H21	1.40	0.69
6:CA:1274:A:C4	6:CA:1297:C:H2'	2.28	0.69
6:CA:298:G:OP1	11:U:84:PHE:N	2.24	0.69
6:CA:1272:A:C6	6:CA:1617:C:H5"	2.28	0.68
6:CA:1125:G:C3'	6:CA:1127:A:C6	2.77	0.68
6:CA:1126:A:O5'	6:CA:1127:A:N3	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:329:G:C6	11:U:15:GLY:HA2	2.29	0.68
6:CA:1274:A:C5	6:CA:1297:C:C2'	2.76	0.68
6:CA:1310:G:H1	6:CA:1604:C:H42	1.42	0.67
6:CA:1020:A:N1	9:J:66:GLY:HA2	2.09	0.67
6:CA:72:U:N3	12:Y:55:THR:CA	2.58	0.67
6:CA:1272:A:N1	6:CA:1617:C:OP2	2.28	0.67
6:CA:374:A:H62	6:CA:400:G:H21	1.43	0.66
6:CA:1354:A:H62	6:CA:1377:G:H21	1.42	0.65
6:CA:1020:A:N1	9:J:66:GLY:CA	2.60	0.64
6:CA:1125:G:H5"	6:CA:1127:A:H2'	1.80	0.64
6:CA:442:G:N2	8:E:43:THR:O	2.27	0.62
6:CA:1272:A:C5	6:CA:1617:C:C5'	2.84	0.61
6:CA:1274:A:C6	6:CA:1297:C:C5	2.87	0.61
6:CA:1020:A:H61	9:J:66:GLY:HA2	1.65	0.61
6:CA:2605:U:H4'	6:CA:2606:C:O5'	2.00	0.60
6:CA:72:U:C2	12:Y:55:THR:CA	2.84	0.60
6:CA:1297:C:N1	6:CA:1297:C:H1'	2.12	0.60
6:CA:1125:G:C3'	6:CA:1125:G:HO3'	2.08	0.60
6:CA:1126:A:OP2	6:CA:1127:A:C4	2.55	0.59
6:CA:612:G:H1	6:CA:615:U:H5"	1.67	0.59
6:CA:597:G:H1	6:CA:660:C:H42	1.51	0.59
6:CA:952:G:H1	6:CA:965:C:H42	1.51	0.59
6:CA:1020:A:N6	9:J:66:GLY:HA2	2.17	0.59
6:CA:1274:A:C4	6:CA:1297:C:O2	2.55	0.59
6:CA:1125:G:C3'	6:CA:1127:A:N3	2.66	0.58
6:CA:2729:G:N2	7:D:192:ALA:H	1.99	0.58
6:CA:1274:A:N3	6:CA:1297:C:O2	2.36	0.58
6:CA:116:C:HO2'	6:CA:126:A:HO2'	1.52	0.57
6:CA:2019:A:H61	6:CA:2035:G:H1	1.51	0.57
6:CA:159:G:H21	6:CA:167:A:H62	1.52	0.56
3:T:63:VAL:CA	6:CA:1339:G:N1	2.68	0.56
6:CA:1214:A:H62	6:CA:1235:G:H21	1.52	0.56
6:CA:1274:A:C5	6:CA:1297:C:H2'	2.40	0.56
6:CA:1126:A:OP1	6:CA:1127:A:N1	2.38	0.56
6:CA:281:C:H42	6:CA:359:G:H1	1.53	0.56
6:CA:544:C:H42	6:CA:548:G:H3'	1.71	0.56
6:CA:1274:A:C5	6:CA:1297:C:C2	2.93	0.56
6:CA:447:A:OP2	6:CA:474:G:N2	2.39	0.56
6:CA:329:G:O6	11:U:15:GLY:HA2	2.04	0.55
6:CA:1274:A:C6	6:CA:1297:C:O4'	2.59	0.55
6:CA:1020:A:C6	9:J:66:GLY:HA2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:1272:A:N3	6:CA:1617:C:C5'	2.70	0.55
6:CA:1272:A:C4	6:CA:1617:C:C5'	2.90	0.54
6:CA:321:U:OP2	8:E:131:THR:N	2.38	0.54
6:CA:995:C:N4	9:J:2:LYS:C	2.60	0.54
6:CA:530:G:N2	6:CA:2024:G:OP2	2.41	0.54
6:CA:24:G:H1	6:CA:516:C:H42	1.56	0.53
6:CA:818:G:H21	6:CA:1189:A:H62	1.55	0.53
6:CA:2590:A:N6	6:CA:2606:C:H42	2.06	0.53
6:CA:484:C:H42	6:CA:496:G:H1	1.54	0.53
6:CA:1272:A:N3	6:CA:1617:C:OP1	2.42	0.53
6:CA:298:G:P	11:U:84:PHE:H	2.32	0.52
6:CA:1125:G:H5'	6:CA:1127:A:N3	2.24	0.52
6:CA:16:C:H42	6:CA:524:G:H1	1.56	0.52
6:CA:1272:A:N1	6:CA:1617:C:H5"	2.20	0.52
6:CA:306:U:H3	6:CA:310:A:H62	1.58	0.51
6:CA:1296:G:O6	6:CA:1645:G:N2	2.43	0.51
6:CA:1125:G:C2'	6:CA:1127:A:C6	2.93	0.51
6:CA:530:G:N2	6:CA:2034:U:O2'	2.44	0.51
6:CA:298:G:P	11:U:84:PHE:O	2.69	0.51
6:CA:1323:C:N4	6:CA:1324:G:O6	2.44	0.50
6:CA:1299:G:N1	6:CA:1640:A:OP2	2.45	0.50
6:CA:1126:A:O5'	6:CA:1127:A:C2	2.64	0.50
6:CA:2789:C:O2	6:CA:2894:G:N1	2.39	0.50
6:CA:291:G:H1	6:CA:349:U:H3	1.60	0.50
6:CA:2638:G:H21	6:CA:2778:A:H62	1.59	0.50
6:CA:386:G:OP2	6:CA:388:G:N2	2.46	0.49
6:CA:1017:G:H1	6:CA:1145:C:H42	1.61	0.49
6:CA:85:G:OP1	11:U:5:ARG:CA	2.61	0.49
6:CA:2605:U:H4'	6:CA:2606:C:C5'	2.42	0.49
6:CA:2692:G:H3'	6:CA:2693:G:H8	1.77	0.49
6:CA:116:C:O2'	6:CA:126:A:O2'	2.27	0.49
6:CA:72:U:H3	12:Y:55:THR:CA	2.26	0.49
6:CA:2552:OMU:C4	6:CA:2558:C:H42	2.24	0.49
6:CA:141:G:N2	6:CA:141:G:OP2	2.46	0.48
6:CA:1306:C:OP2	6:CA:1606:C:N4	2.46	0.48
6:CA:301:G:H21	6:CA:302:C:H41	1.60	0.48
6:CA:2834:G:O2'	6:CA:2835:A:O5'	2.25	0.48
6:CA:532:A:N6	6:CA:561:G:O6	2.46	0.48
6:CA:2657:A:H62	6:CA:2664:G:H21	1.62	0.48
6:CA:1125:G:C3'	6:CA:1127:A:C2	2.96	0.47
6:CA:2644:G:H21	6:CA:2772:C:H5'	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:829:A:H62	6:CA:831:G:H21	1.62	0.47
6:CA:1216:G:N2	6:CA:1234:U:O2	2.47	0.47
6:CA:2552:OMU:H6	6:CA:2552:OMU:HM23	1.97	0.47
6:CA:505:A:HO2'	6:CA:509:C:HO2'	1.60	0.47
6:CA:494:G:C1'	10:S:6:LYS:O	2.63	0.47
6:CA:1286:A:H1'	6:CA:1288:G:H1	1.79	0.47
6:CA:202:U:H5'	6:CA:252:G:H21	1.80	0.47
6:CA:1126:A:OP1	6:CA:1127:A:C6	2.66	0.46
6:CA:2835:A:OP2	7:D:56:LYS:CA	2.63	0.46
6:CA:579:G:H4'	6:CA:2018:G:H4'	1.97	0.46
6:CA:969:G:H2'	6:CA:985:C:H5'	1.98	0.46
6:CA:1020:A:N1	9:J:66:GLY:HA3	2.29	0.46
6:CA:991:C:H4'	6:CA:1185:G:H8	1.81	0.46
6:CA:562:U:H1'	6:CA:2036:C:H1'	1.98	0.45
6:CA:493:G:HO2'	10:S:8:ARG:H	1.62	0.45
6:CA:1274:A:OP2	6:CA:1302:A:N6	2.45	0.45
6:CA:2740:A:OP2	6:CA:2763:G:N2	2.45	0.45
6:CA:1130:U:H1'	6:CA:2027:G:H4'	1.97	0.45
6:CA:1195:G:O2'	6:CA:1225:G:N1	2.50	0.45
6:CA:450:G:N1	6:CA:454:A:OP2	2.43	0.45
6:CA:2593:U:C5	6:CA:2594:C:C5	3.05	0.45
6:CA:2593:U:H3	6:CA:2601:C:H42	1.66	0.44
6:CA:2675:A:H61	6:CA:2731:G:H22	1.66	0.44
6:CA:1614:A:N1	6:CA:1615:C:N4	2.66	0.44
6:CA:2730:C:O2'	7:D:174:SER:O	2.23	0.44
6:CA:319:G:H1'	6:CA:333:G:H22	1.81	0.44
6:CA:2783:U:O2'	7:D:42:ASN:O	2.35	0.44
6:CA:26:G:H21	6:CA:514:A:H62	1.65	0.44
6:CA:85:G:OP1	11:U:6:ARG:N	2.51	0.44
6:CA:307:G:H21	6:CA:330:A:H61	1.66	0.43
6:CA:827:U:H2'	6:CA:828:U:H2'	1.99	0.43
6:CA:2549:G:H22	6:CA:2552:OMU:C5	2.29	0.43
6:CA:2820:A:H1'	6:CA:2873:A:H4'	2.00	0.43
6:CA:64:A:N1	6:CA:91:A:N6	2.67	0.43
6:CA:198:C:H42	6:CA:248:G:H1	1.66	0.43
6:CA:2552:OMU:H6	6:CA:2552:OMU:CM2	2.48	0.43
6:CA:948:C:H2'	6:CA:949:G:C8	2.53	0.43
6:CA:1265:A:N6	6:CA:2014:A:OP2	2.49	0.43
6:CA:45:G:H1	6:CA:432:A:H61	1.67	0.42
6:CA:182:A:N3	6:CA:433:C:O2'	2.46	0.42
6:CA:932:U:H4'	6:CA:933:A:H2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CA:194:G:H2'	6:CA:195:A:H4'	2.02	0.42
6:CA:494:G:O4'	10:S:6:LYS:O	2.37	0.42
6:CA:991:C:O4'	6:CA:1184:U:O2'	2.38	0.42
5:A:264:LYS:O	5:A:265:ALA:C	2.56	0.42
6:CA:1268:A:H62	6:CA:2012:G:H21	1.67	0.42
6:CA:592:A:H61	6:CA:665:U:H3	1.67	0.42
6:CA:969:G:N2	6:CA:985:C:O2'	2.50	0.42
6:CA:202:U:O2'	6:CA:252:G:O2'	2.37	0.41
6:CA:207:A:H2	6:CA:798:G:H21	1.68	0.41
6:CA:607:U:H3	6:CA:621:A:H62	1.68	0.41
6:CA:244:A:H62	6:CA:254:G:H21	1.67	0.41
6:CA:1272:A:C6	6:CA:1616:A:O3'	2.74	0.41
6:CA:2779:U:H5"	6:CA:2780:G:H8	1.84	0.41
6:CA:214:G:O2'	6:CA:217:A:OP1	2.39	0.41
6:CA:192:C:H1'	6:CA:802:A:H2	1.85	0.41
6:CA:824:U:H2'	6:CA:825:A:C8	2.56	0.41
6:CA:2025:C:H42	6:CA:2038:G:H1	1.69	0.41
6:CA:85:G:OP1	11:U:5:ARG:C	2.59	0.41
6:CA:271:G:N1	6:CA:367:G:O6	2.54	0.41
6:CA:450:G:OP1	6:CA:1248:G:N2	2.54	0.41
6:CA:576:U:H2'	6:CA:577:G:C8	2.56	0.41
6:CA:949:G:H2'	6:CA:950:G:C8	2.56	0.41
6:CA:1205:A:H5"	6:CA:1206:G:C8	2.56	0.41
6:CA:2729:G:H21	7:D:192:ALA:H	1.66	0.41
6:CA:494:G:H1'	10:S:6:LYS:O	2.22	0.41
6:CA:1267:U:H2'	6:CA:1268:A:H8	1.87	0.40
6:CA:514:A:N3	6:CA:581:C:O2'	2.47	0.40
6:CA:1162:G:N2	6:CA:1163:G:O6	2.55	0.40
7:D:4:LEU:N	7:D:203:VAL:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Q	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17 56
2	R	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15 54
3	T	88/90 (98%)	76 (86%)	10 (11%)	2 (2%)	6 36
4	2	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
5	A	274/283 (97%)	228 (83%)	43 (16%)	3 (1%)	14 52
7	D	153/209 (73%)	147 (96%)	6 (4%)	0	100 100
8	E	150/201 (75%)	147 (98%)	3 (2%)	0	100 100
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100 100
10	S	94/110 (86%)	90 (96%)	4 (4%)	0	100 100
11	U	100/102 (98%)	89 (89%)	11 (11%)	0	100 100
12	Y	58/60 (97%)	56 (97%)	2 (3%)	0	100 100
All	All	1308/1454 (90%)	1192 (91%)	109 (8%)	7 (0%)	32 68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	54	VAL
3	T	37	ASP
5	A	47	GLY
3	T	88	LYS
5	A	245	GLU
1	Q	72	GLY
5	A	207	VAL

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	CA	1523/2904 (52%)	242 (15%)	12 (0%)

All (242) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	CA	10	A

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Mol	Chain	Res	Type
6	CA	35	G
6	CA	49	A
6	CA	51	G
6	CA	71	A
6	CA	74	A
6	CA	83	A
6	CA	84	A
6	CA	85	G
6	CA	101	A
6	CA	102	U
6	CA	114	U
6	CA	120	U
6	CA	121	G
6	CA	128	C
6	CA	131	A
6	CA	138	U
6	CA	140	C
6	CA	149	A
6	CA	177	G
6	CA	178	G
6	CA	195	A
6	CA	196	A
6	CA	199	A
6	CA	216	A
6	CA	229	C
6	CA	232	G
6	CA	233	A
6	CA	248	G
6	CA	263	G
6	CA	264	C
6	CA	276	U
6	CA	277	G
6	CA	302	C
6	CA	330	A
6	CA	354	A
6	CA	360	U
6	CA	362	A
6	CA	372	G
6	CA	387	U
6	CA	388	G
6	CA	404	A
6	CA	411	G

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Mol	Chain	Res	Type
6	CA	412	A
6	CA	413	C
6	CA	424	G
6	CA	444	C
6	CA	451	U
6	CA	474	G
6	CA	475	C
6	CA	481	G
6	CA	482	A
6	CA	491	G
6	CA	508	A
6	CA	532	A
6	CA	544	C
6	CA	545	U
6	CA	546	U
6	CA	547	A
6	CA	548	G
6	CA	549	G
6	CA	562	U
6	CA	563	A
6	CA	575	A
6	CA	587	C
6	CA	600	G
6	CA	601	C
6	CA	602	A
6	CA	603	A
6	CA	604	G
6	CA	615	U
6	CA	627	A
6	CA	656	G
6	CA	672	C
6	CA	674	G
6	CA	675	A
6	CA	685	A
6	CA	694	U
6	CA	775	G
6	CA	791	C
6	CA	792	A
6	CA	793	A
6	CA	794	A
6	CA	801	G
6	CA	804	A

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Mol	Chain	Res	Type
6	CA	805	G
6	CA	810	U
6	CA	812	C
6	CA	819	A
6	CA	823	C
6	CA	830	G
6	CA	831	G
6	CA	832	U
6	CA	845	A
6	CA	846	U
6	CA	847	U
6	CA	931	U
6	CA	932	U
6	CA	933	A
6	CA	942	G
6	CA	945	A
6	CA	958	U
6	CA	959	A
6	CA	960	A
6	CA	961	C
6	CA	962	G
6	CA	971	G
6	CA	974	G
6	CA	984	A
6	CA	985	C
6	CA	986	C
6	CA	989	G
6	CA	995	C
6	CA	996	A
6	CA	1011	G
6	CA	1012	U
6	CA	1013	C
6	CA	1022	G
6	CA	1025	G
6	CA	1026	G
6	CA	1126	A
6	CA	1127	A
6	CA	1128	G
6	CA	1129	A
6	CA	1130	U
6	CA	1131	G
6	CA	1132	U

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Mol	Chain	Res	Type
6	CA	1134	A
6	CA	1136	G
6	CA	1142	A
6	CA	1163	G
6	CA	1164	C
6	CA	1165	A
6	CA	1166	G
6	CA	1174	U
6	CA	1175	A
6	CA	1176	U
6	CA	1177	G
6	CA	1178	C
6	CA	1185	G
6	CA	1195	G
6	CA	1206	G
6	CA	1210	G
6	CA	1212	G
6	CA	1225	G
6	CA	1238	G
6	CA	1249	U
6	CA	1250	G
6	CA	1253	A
6	CA	1256	G
6	CA	1266	G
6	CA	1271	G
6	CA	1272	A
6	CA	1273	U
6	CA	1274	A
6	CA	1300	G
6	CA	1301	A
6	CA	1321	A
6	CA	1329	U
6	CA	1339	G
6	CA	1340	U
6	CA	1341	G
6	CA	1343	G
6	CA	1345	C
6	CA	1348	C
6	CA	1380	G
6	CA	1386	C
6	CA	1391	U
6	CA	1609	A

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Mol	Chain	Res	Type
6	CA	1610	A
6	CA	1616	A
6	CA	1617	C
6	CA	1639	C
6	CA	1646	C
6	CA	1647	U
6	CA	1654	A
6	CA	2009	A
6	CA	2022	U
6	CA	2032	G
6	CA	2043	C
6	CA	2549	G
6	CA	2550	G
6	CA	2551	C
6	CA	2552	OMU
6	CA	2553	G
6	CA	2555	U
6	CA	2561	U
6	CA	2592	G
6	CA	2594	C
6	CA	2597	G
6	CA	2599	G
6	CA	2602	A
6	CA	2603	G
6	CA	2604	U
6	CA	2605	U
6	CA	2606	C
6	CA	2629	U
6	CA	2644	G
6	CA	2676	C
6	CA	2677	G
6	CA	2679	A
6	CA	2681	C
6	CA	2682	A
6	CA	2689	U
6	CA	2690	U
6	CA	2691	C
6	CA	2693	G
6	CA	2696	U
6	CA	2714	G
6	CA	2716	C
6	CA	2729	G

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Mol	Chain	Res	Type
6	CA	2734	A
6	CA	2765	A
6	CA	2770	G
6	CA	2772	C
6	CA	2780	G
6	CA	2786	U
6	CA	2787	C
6	CA	2790	U
6	CA	2791	G
6	CA	2798	U
6	CA	2816	G
6	CA	2818	U
6	CA	2819	G
6	CA	2820	A
6	CA	2821	A
6	CA	2822	G
6	CA	2823	A
6	CA	2830	C
6	CA	2832	U
6	CA	2833	U
6	CA	2835	A
6	CA	2836	U
6	CA	2866	U
6	CA	2867	G
6	CA	2869	G
6	CA	2879	A
6	CA	2880	C
6	CA	2886	A
6	CA	2887	A
6	CA	2895	G
6	CA	2903	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	CA	137	U
6	CA	176	A
6	CA	359	G
6	CA	829	A
6	CA	1129	A
6	CA	1184	U
6	CA	1347	A

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Mol	Chain	Res	Type
6	CA	1379	U
6	CA	2602	A
6	CA	2605	U
6	CA	2680	U
6	CA	2834	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	OMU	CA	2552	6	19,22,23	0.25	0	26,31,34	0.92	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMU	CA	2552	6	-	6/9/27/28	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	CA	2552	OMU	C3'-C2'-C1'	-2.79	97.65	102.89
6	CA	2552	OMU	O2'-C2'-C1'	2.16	113.29	109.08
6	CA	2552	OMU	O4'-C1'-C2'	-2.04	103.00	106.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CA	2552	OMU	O4'-C1'-N1-C2
6	CA	2552	OMU	O4'-C1'-N1-C6
6	CA	2552	OMU	O4'-C4'-C5'-O5'
6	CA	2552	OMU	C2'-C1'-N1-C6
6	CA	2552	OMU	C2'-C1'-N1-C2
6	CA	2552	OMU	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CA	2552	OMU	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	CA	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CA	972:A	O3'	973:A	P	14.67
1	CA	2830:C	O3'	2831:G	P	11.87
1	CA	1125:G	O3'	1126:A	P	2.06

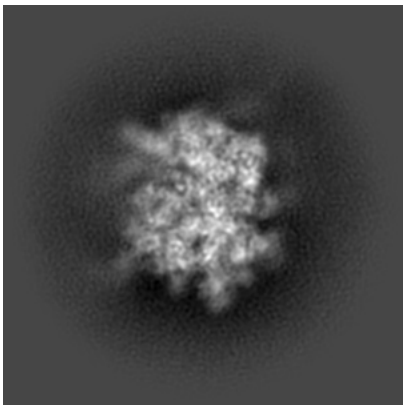
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45666. These allow visual inspection of the internal detail of the map and identification of artifacts.

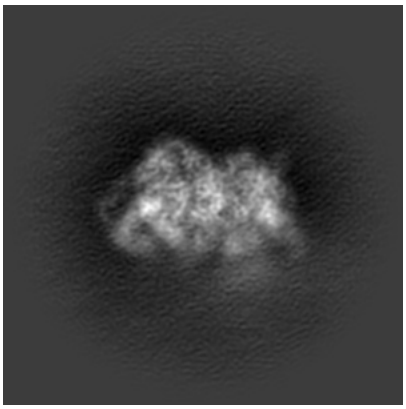
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

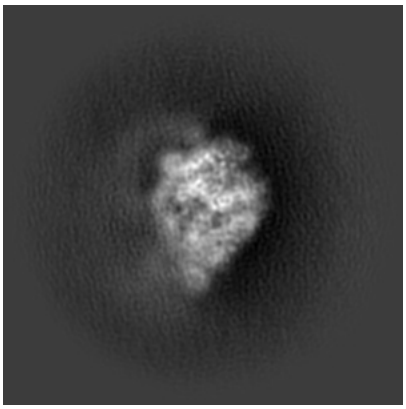
6.1.1 Primary map



X

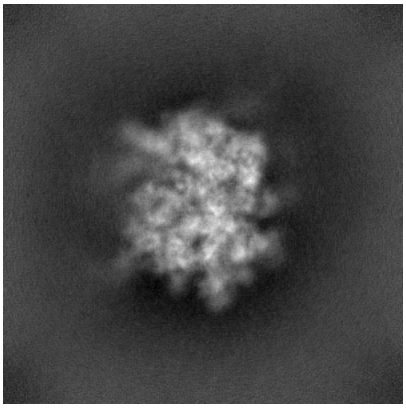


Y

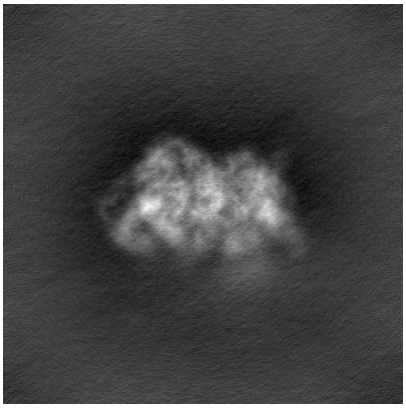


Z

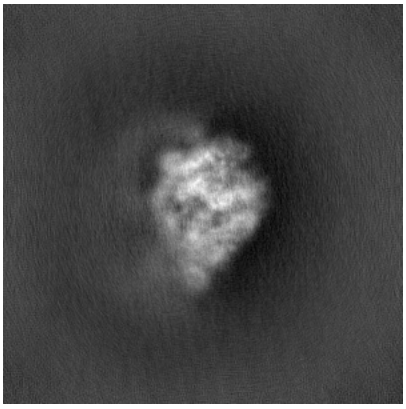
6.1.2 Raw map



X



Y

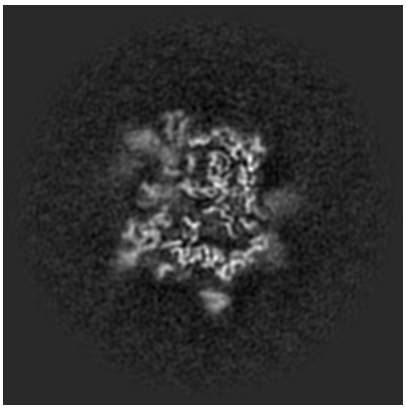


Z

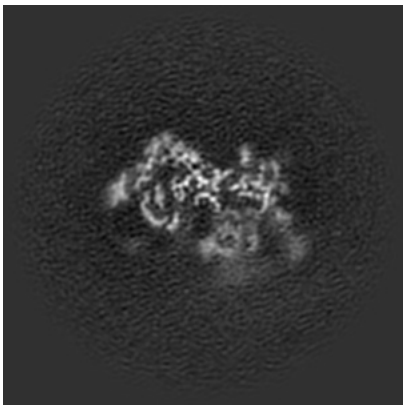
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

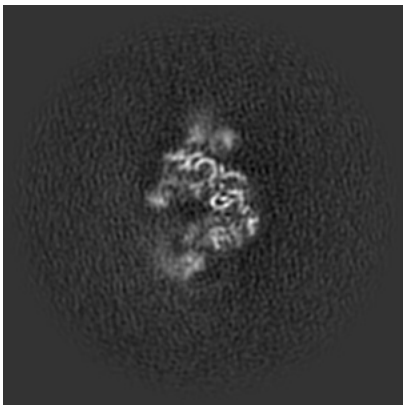
6.2.1 Primary map



X Index: 168

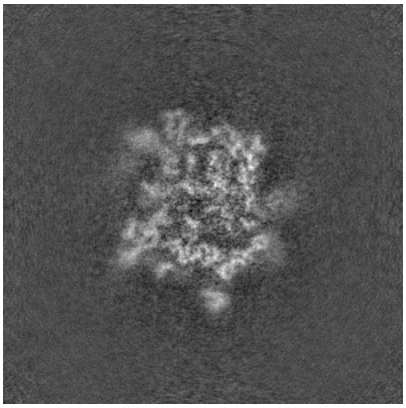


Y Index: 168

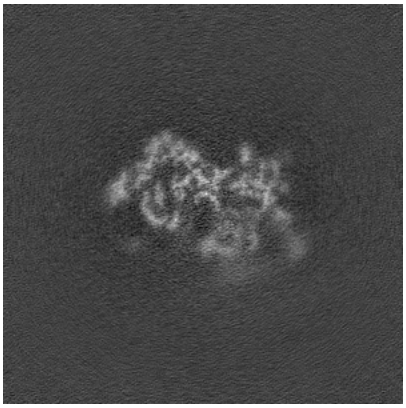


Z Index: 168

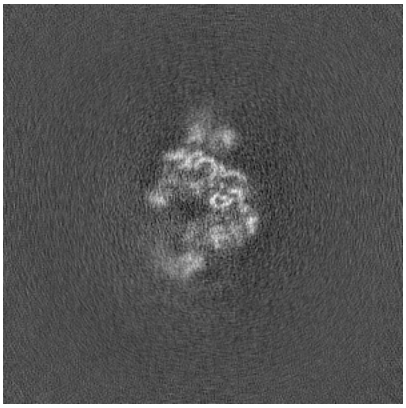
6.2.2 Raw map



X Index: 168



Y Index: 168

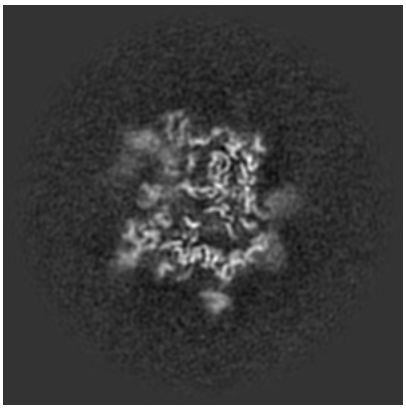


Z Index: 168

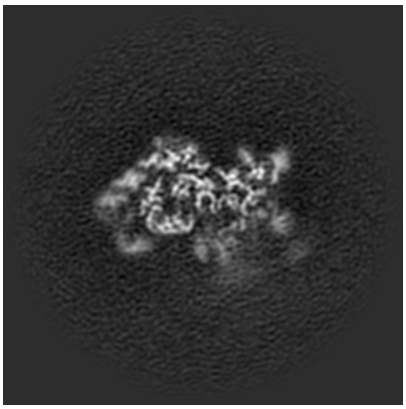
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

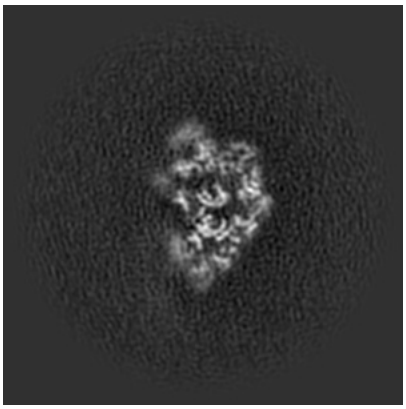
6.3.1 Primary map



X Index: 167

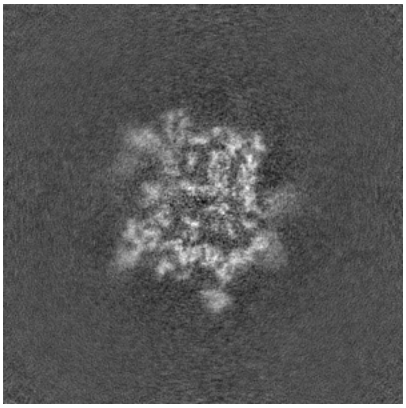


Y Index: 174

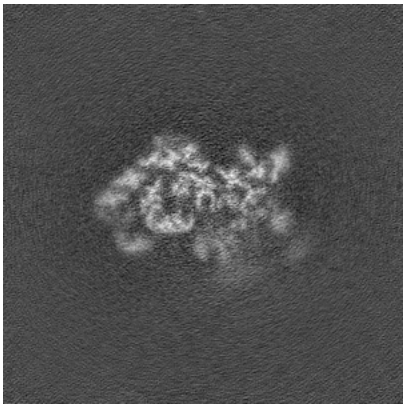


Z Index: 130

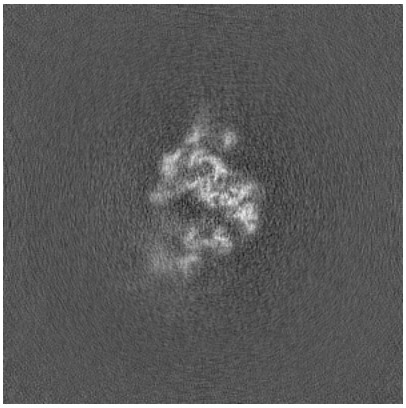
6.3.2 Raw map



X Index: 167



Y Index: 174

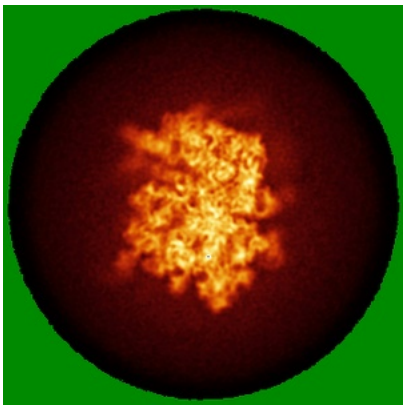


Z Index: 164

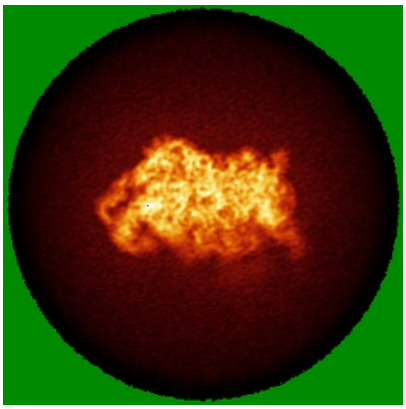
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

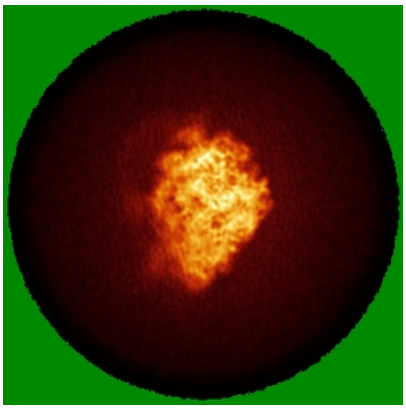
6.4.1 Primary map



X

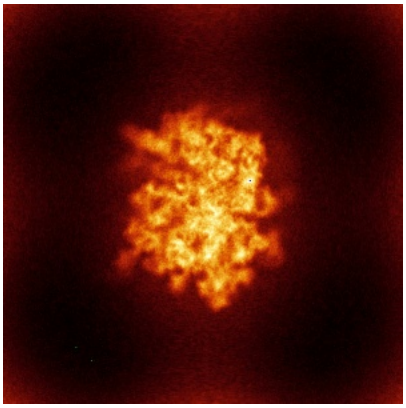


Y

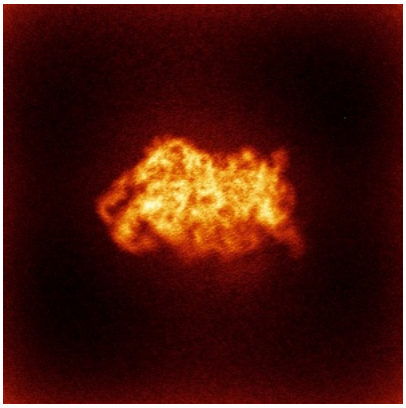


Z

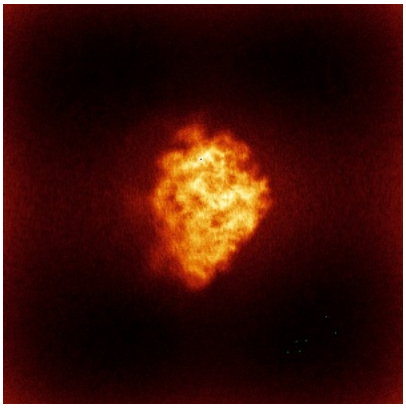
6.4.2 Raw map



X



Y



Z

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

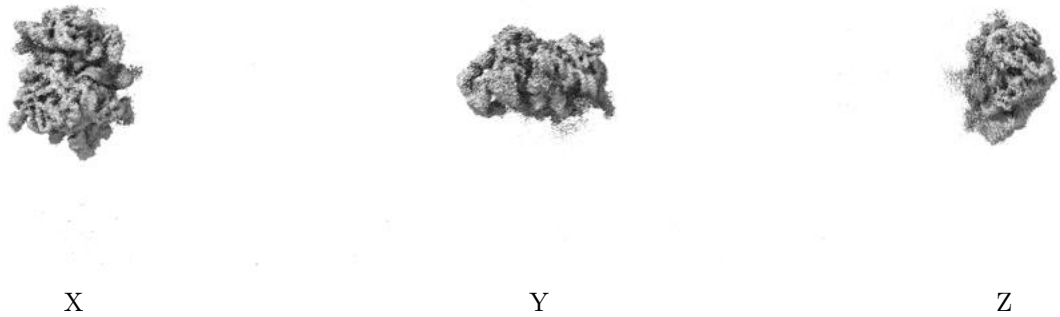
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

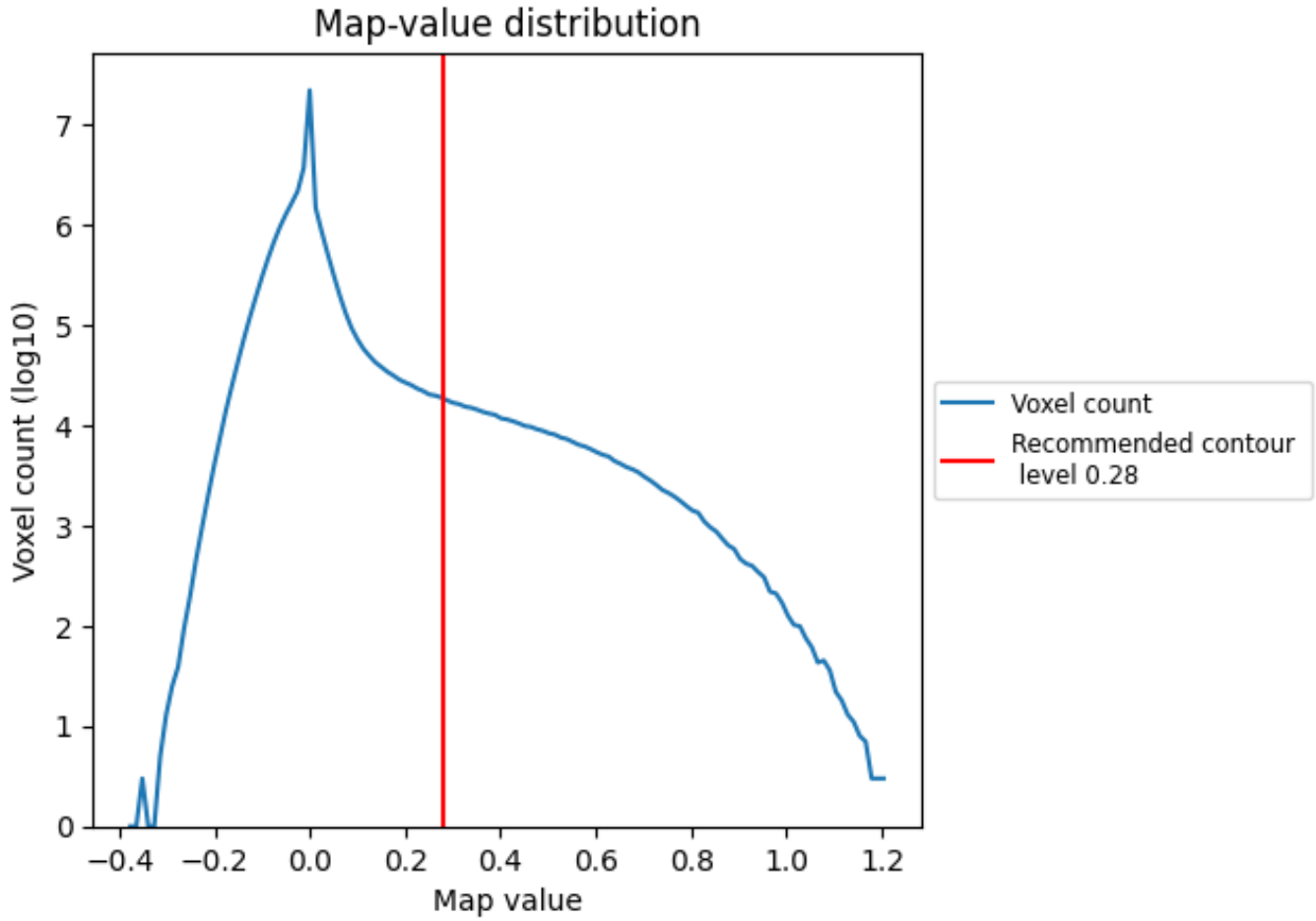
6.6 Mask visualisation (i)

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

7 Map analysis

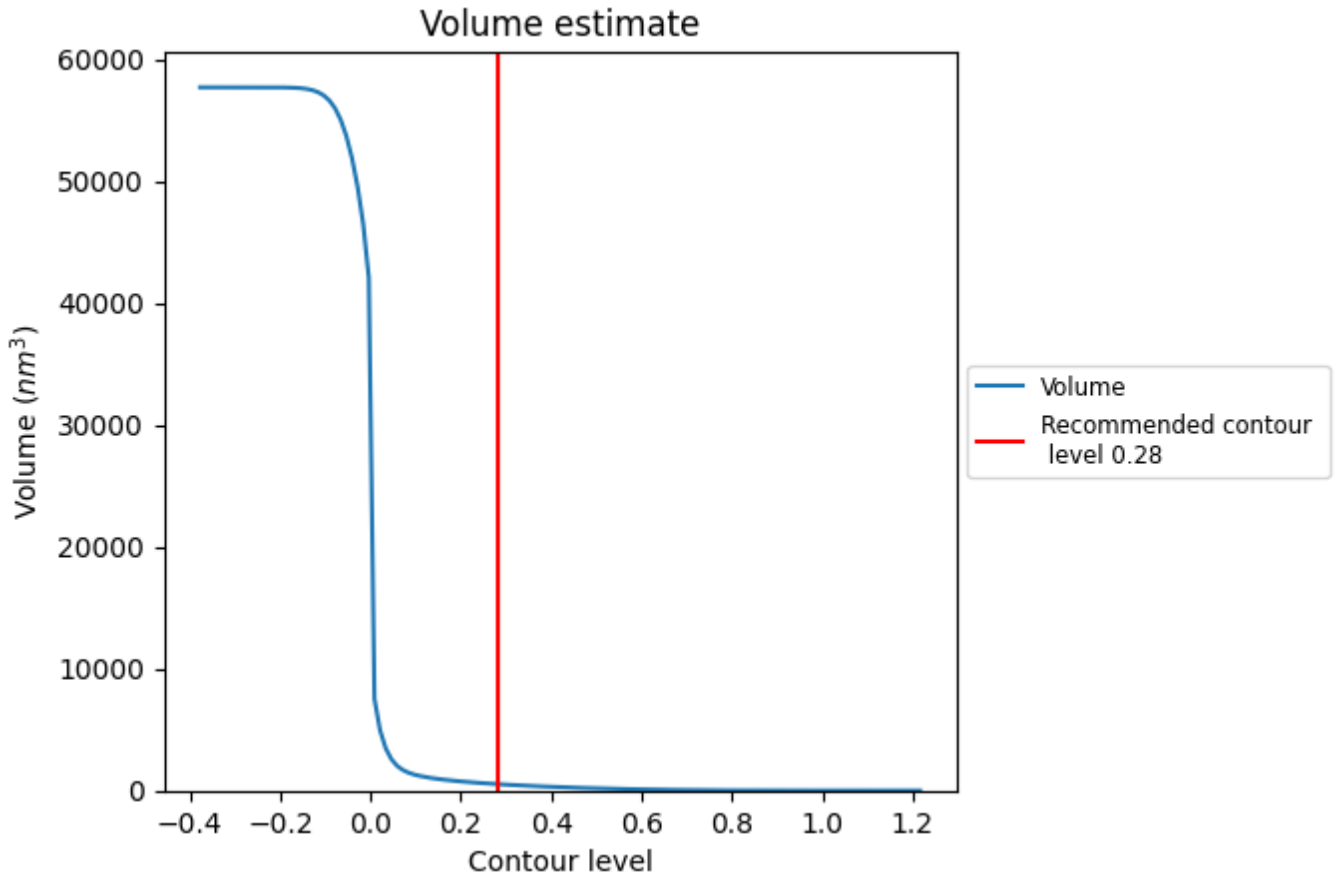
This section contains the results of statistical analysis of the map.

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.

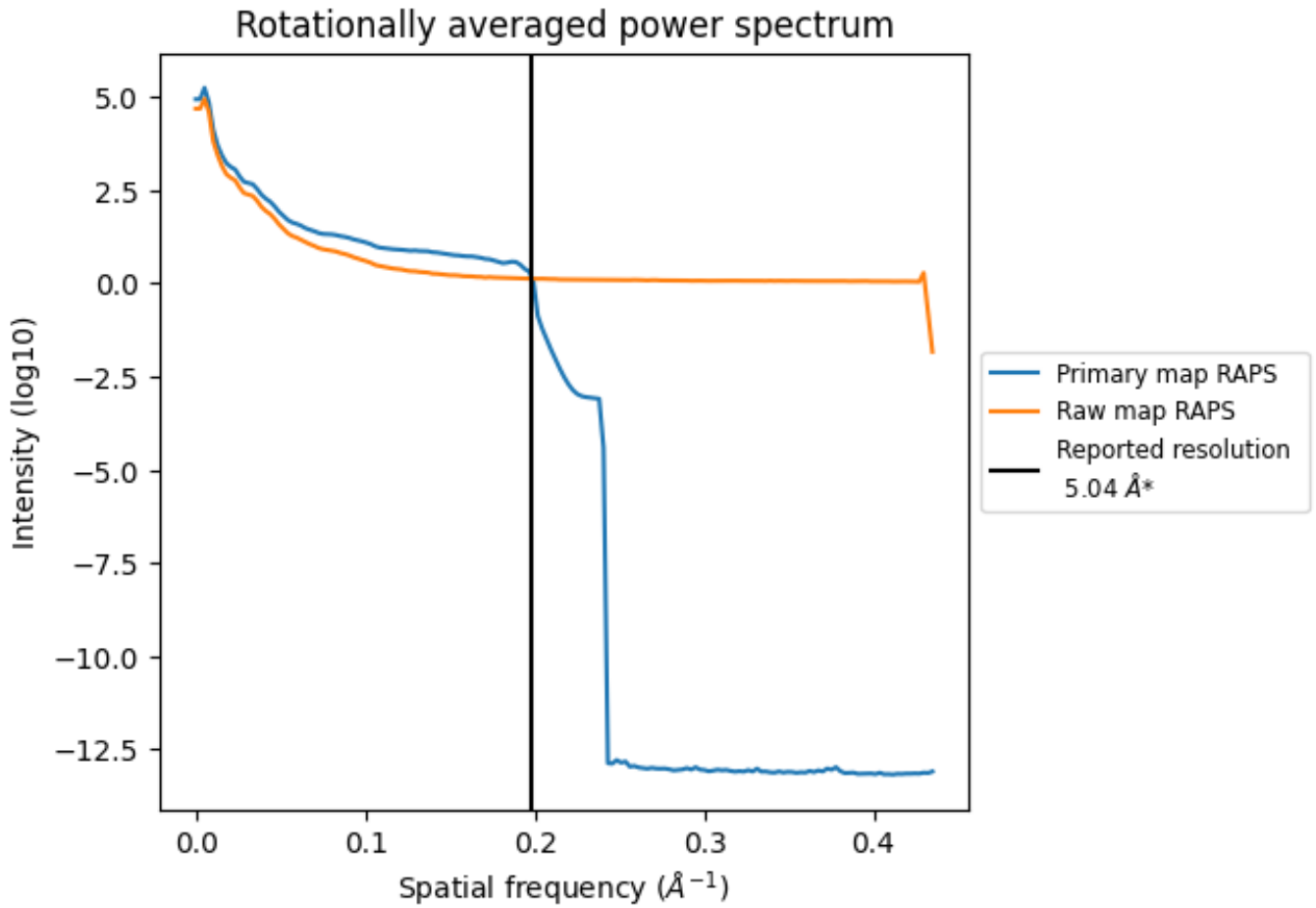
7.2 Volume estimate



The volume at the recommended contour level is 530 nm^3; this corresponds to an approximate mass of 478 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)

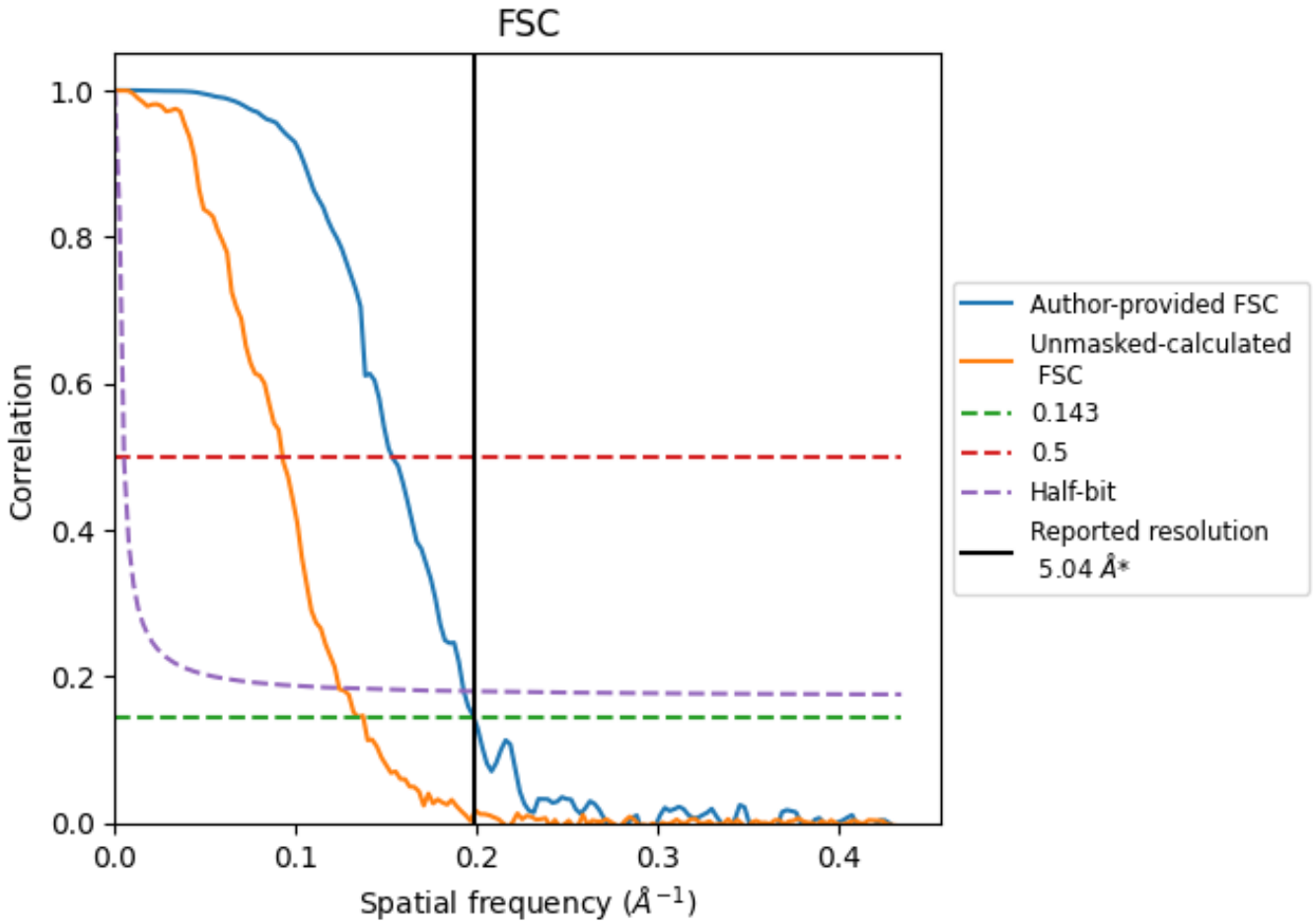


*Reported resolution corresponds to spatial frequency of 0.198 $Å^{-1}$

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 0.198 Å^{-1}

8.2 Resolution estimates (i)

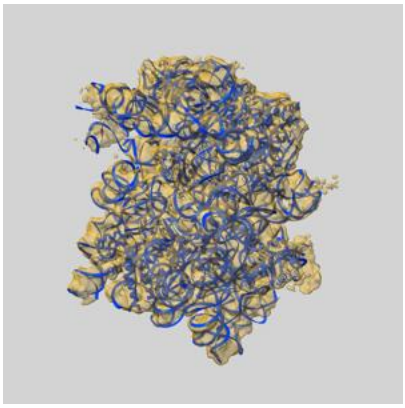
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.04	-	-
Author-provided FSC curve	5.04	6.52	5.18
Unmasked-calculated*	7.28	10.79	8.06

*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 7.28 differs from the reported value 5.04 by more than 10 %

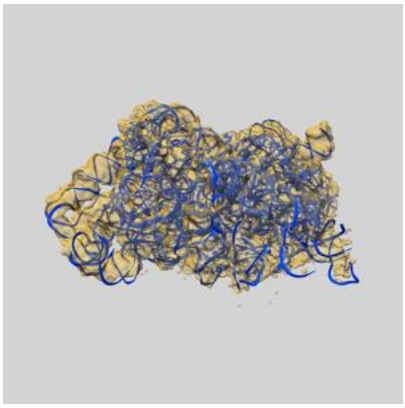
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45666 and PDB model 9CL9. Per-residue inclusion information can be found in section 3 on page 6.

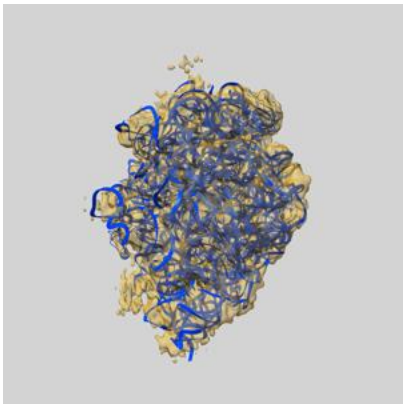
9.1 Map-model overlay



X



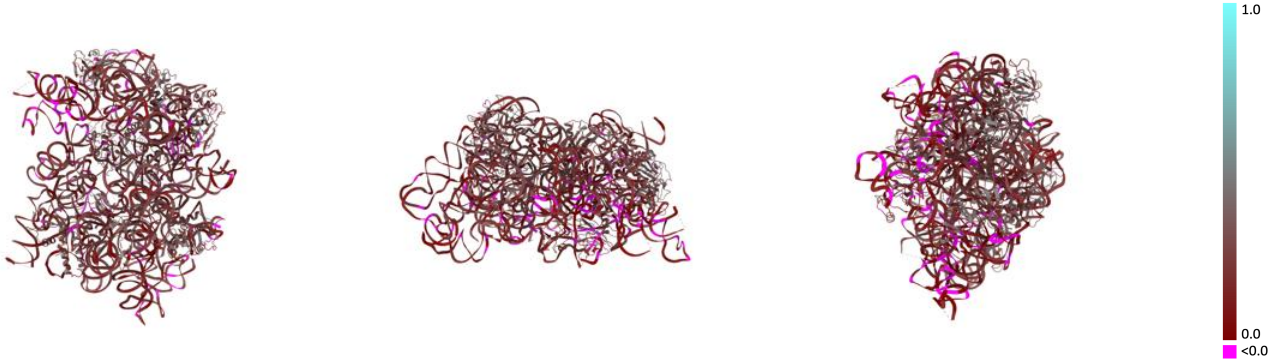
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 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.

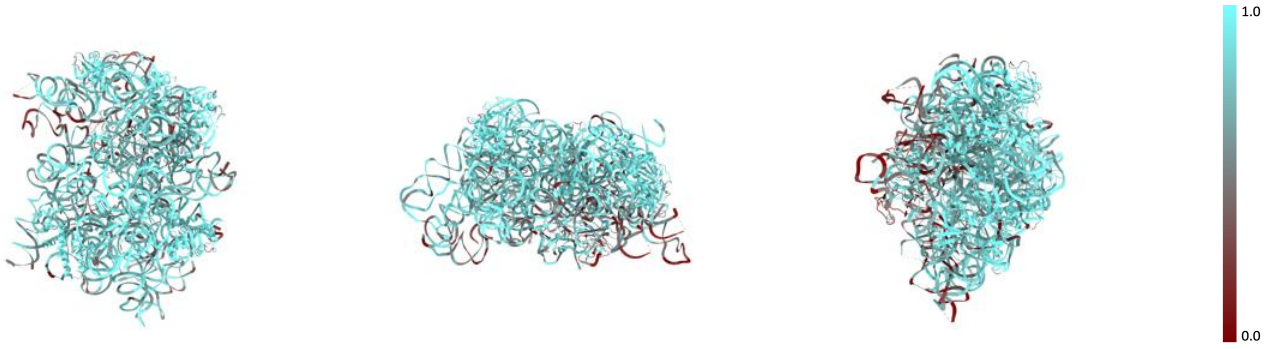
9.2 Q-score mapped to coordinate model (i)



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.

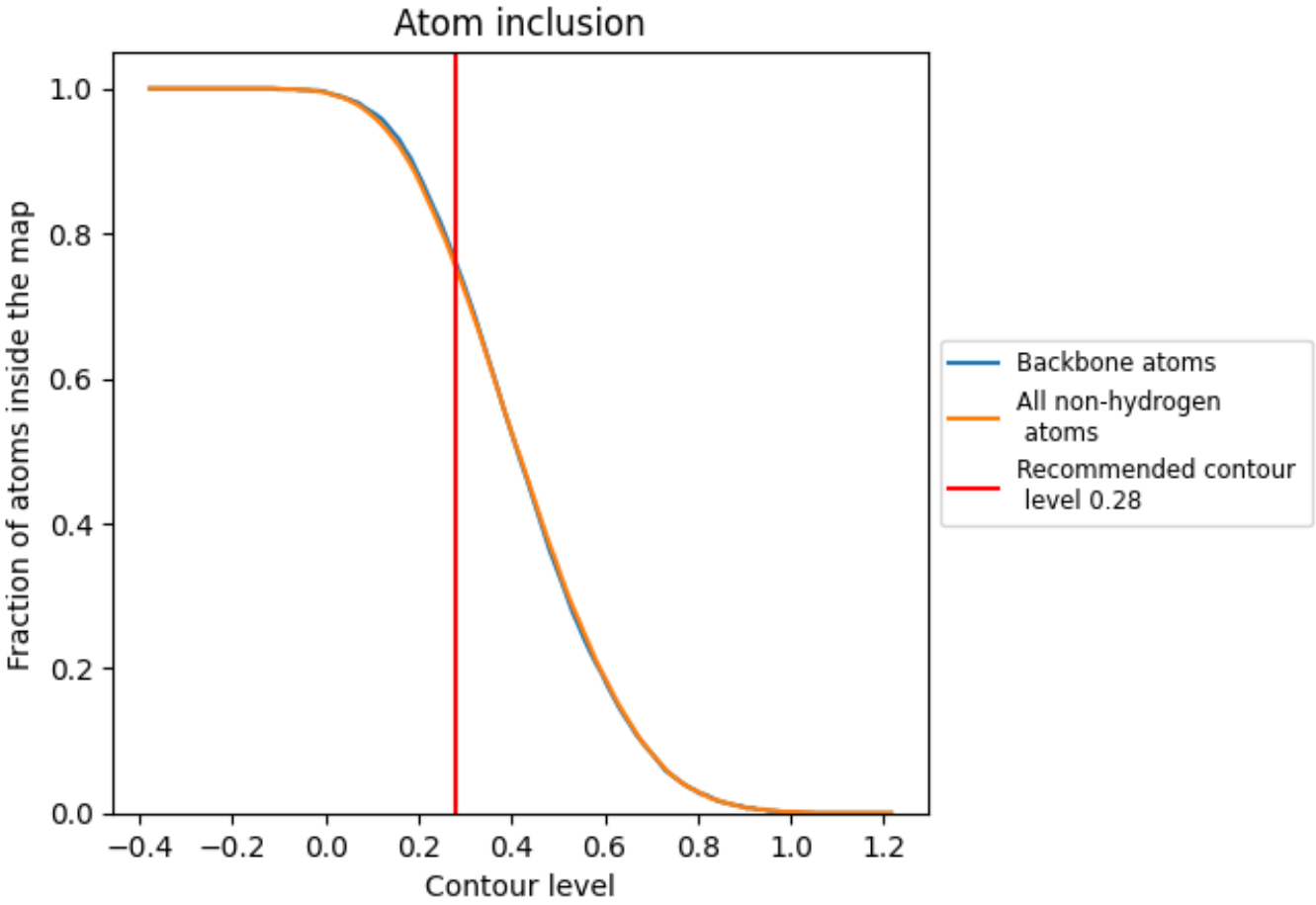
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7540	0.1810
2	0.9120	0.2680
A	0.6050	0.2480
CA	0.7370	0.1640
D	0.8690	0.2890
E	0.8980	0.3000
J	0.9490	0.3370
Q	0.9440	0.2770
R	0.9030	0.3050
S	0.9060	0.2850
T	0.8220	0.2780
U	0.9310	0.3090
Y	0.9250	0.2670