Full wwPDB EM Validation Report (i)

Aug 17, 2026 – 10:24 pm BST

PDB ID	:	9T1A / pdb_00009t1a
EMDB ID	:	EMD-55428
Title	:	E. coli 70S ribosome from delta-RlmE strain, PTC class 1
Authors	:	Larsson, D.S.D.; Selmer, M.
Deposited on	:	2025-10-21
Resolution	:	2.39 Å(reported)
Based on initial model	:	9SYH

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 (i) 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 (1)) were used in the production of this report:

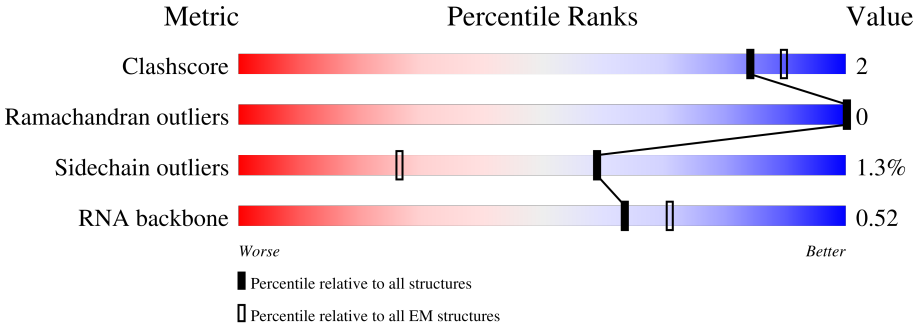
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

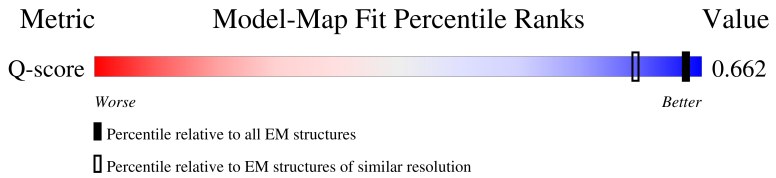
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	Y	76	• 8% 7% 84%
2	Z	77	17% 6% 77%
3	a	2904	15% 5% • 79%

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Mol	Chain	Length	Quality of chain
4	b	120	97%
5	c	273	8% 90%
6	d	209	16% 79%
7	e	201	9% 89%
8	i	142	5% 94%
9	k	144	17% 82%
10	l	136	31% 65%
11	q	103	7% 93%
12	r	110	6% 94%
13	v	85	18% 81%
14	z	57	7% 7% 86%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 15298 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 tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Y	12	257	114	48	83	12	0	0

- Molecule 2 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	Z	18	384	171	72	123	18	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	a	596	12772	5710	2332	4134	596	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	b	4	80	36	10	30	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	26	191	116	41	33	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	d	43	333	206	68	58	1	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	e	23	182	115	39	28	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	i	8	55	34	12	9	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	k	26	182	106	42	33	1	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	48	386	242	81	60	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A7ZSK2

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	q	7	75	48	19	8	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	r	7	53	30	14	9	0	0

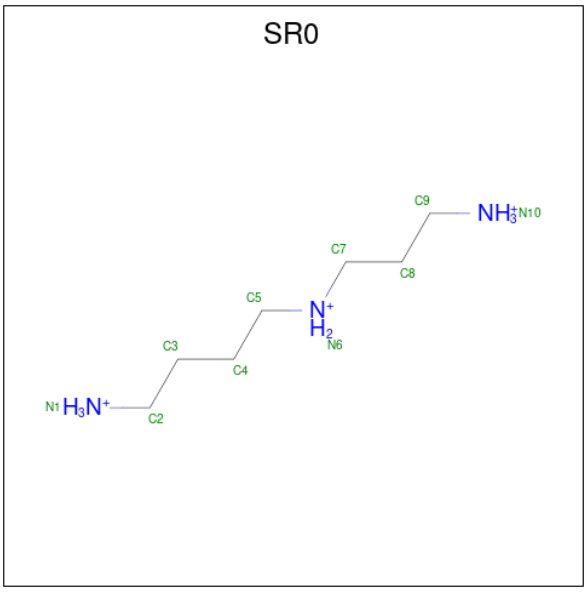
- Molecule 13 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	v	16	116	65	27	24	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein bL32.

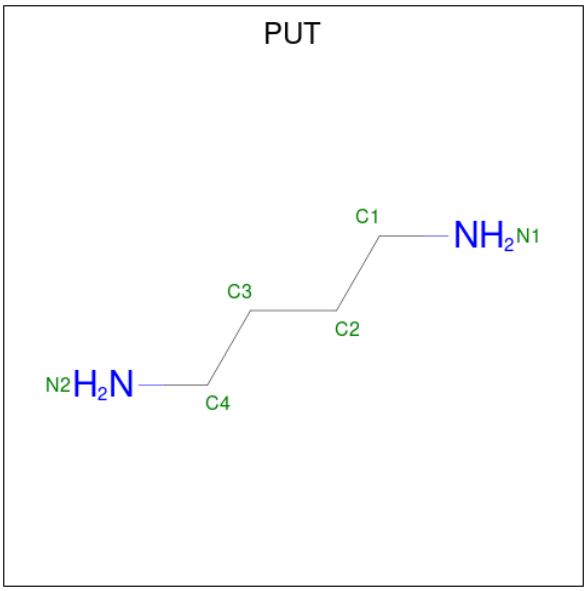
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	z	8	61	37	12	12	0	0

- Molecule 15 is N 1 -(3-azaniumylpropyl)butane-1,4-diaminium (CCD ID: SR0) (formula: $C_7H_{22}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
15	a	1	10	7	3	0
15	a	1	Total	C	N	0
			10	7	3	

- Molecule 16 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
16	a	1	6	4	2	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
17	a	100	100	100	0
17	d	1	1	1	0
17	z	1	1	1	0

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K).

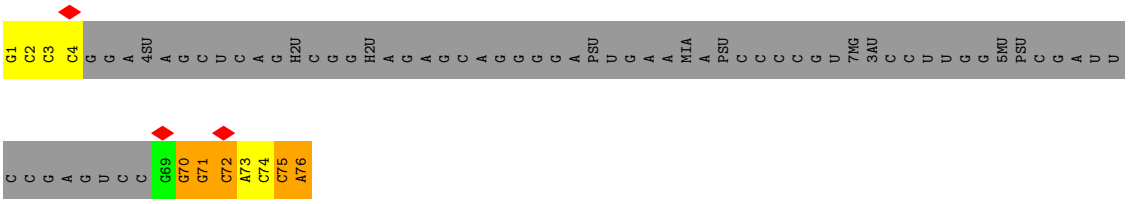
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
18	a	42	42	42	0
18	e	1	1	1	0

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.

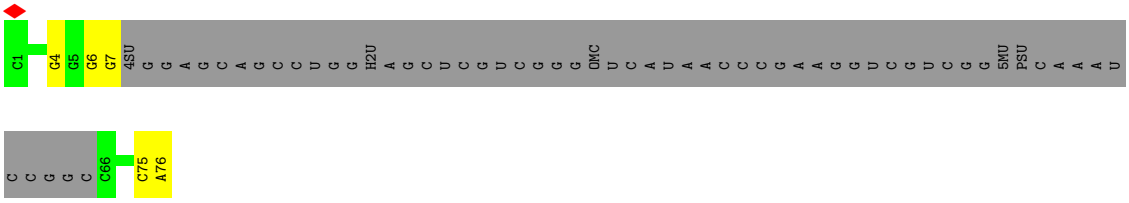
- Molecule 1: tRNA(Phe)

Chain Y: 8% 7% 84%



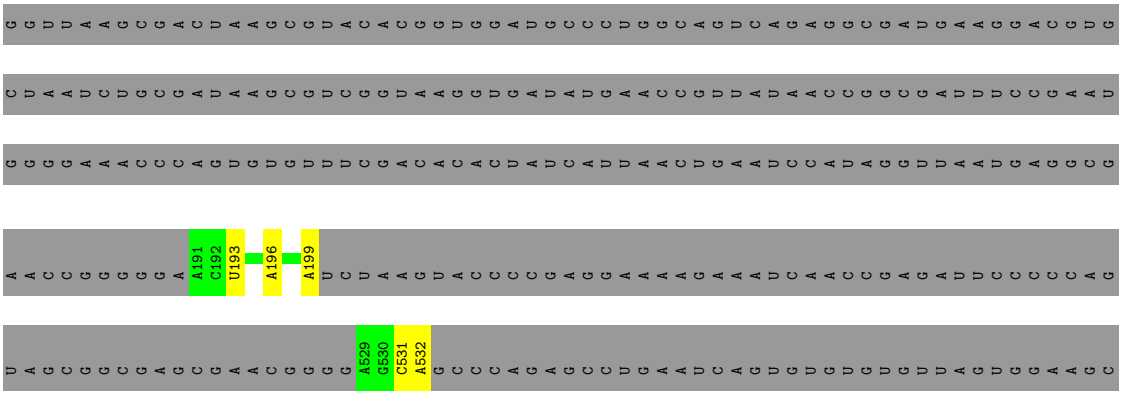
- Molecule 2: tRNA(fMet)

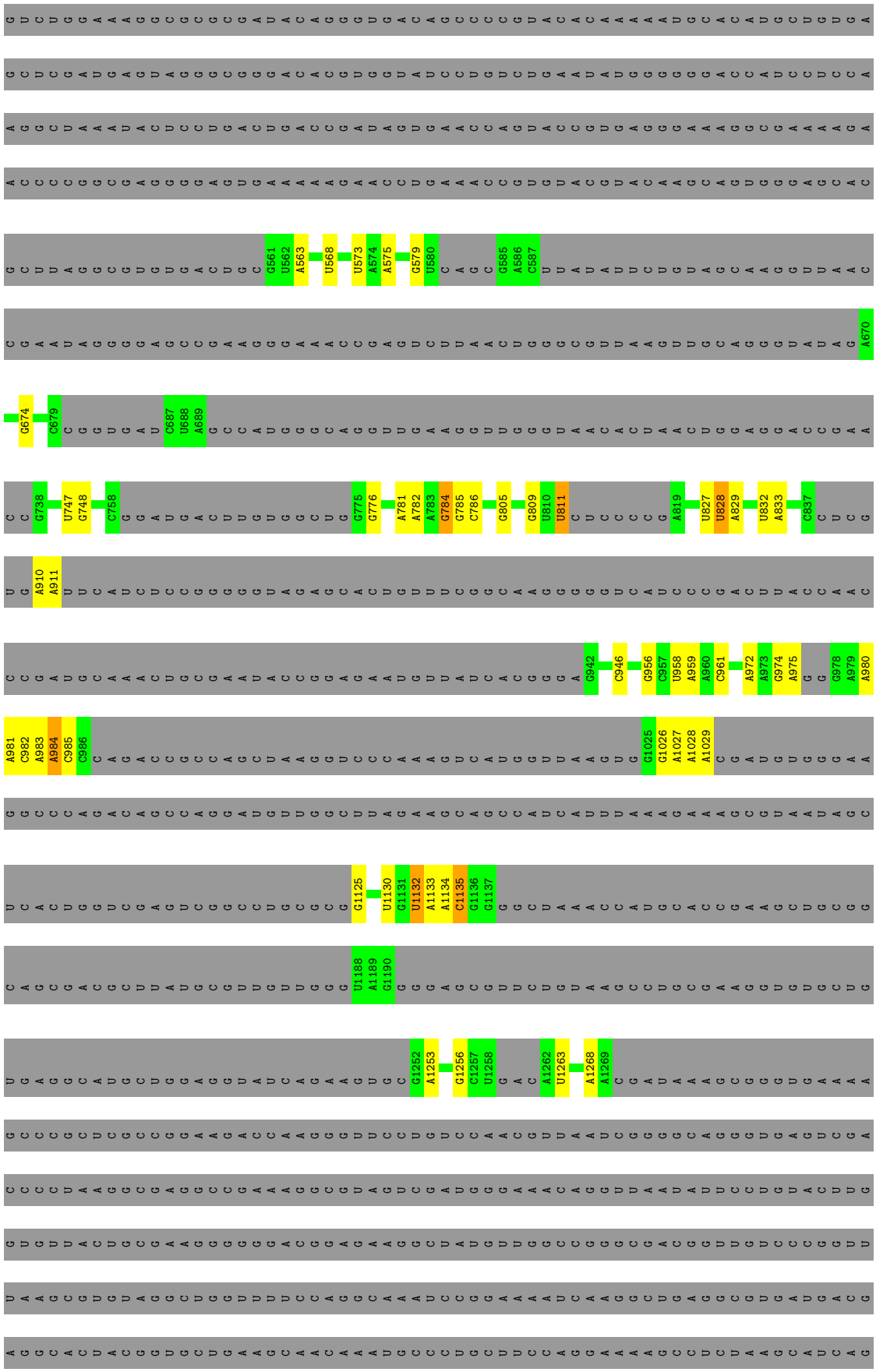
Chain Z: 17% 6% 77%



- Molecule 3: 23S rRNA

Chain a: 15% 5% 79%




G674
C679
G738
U747
G748
G758
C687
U688
A689
A670
G561
U562
A563
U568
U573
A574
A575
G579
U580
G585
A586
C587
A910
A911
G775
G776
A781
A782
A783
G784
G785
C786
G805
G809
U810
U811
A819
U827
U828
A829
U832
A833
C837
G942
C946
G956
C957
U958
A959
A960
C961
A972
A973
G974
A975
G978
A979
A980
A981
C982
A983
A984
C985
C986
G1025
G1026
A1027
A1028
A1029
G1125
U1130
G1131
U1132
A1133
A1134
C1135
G1136
G1137
U1188
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G1190
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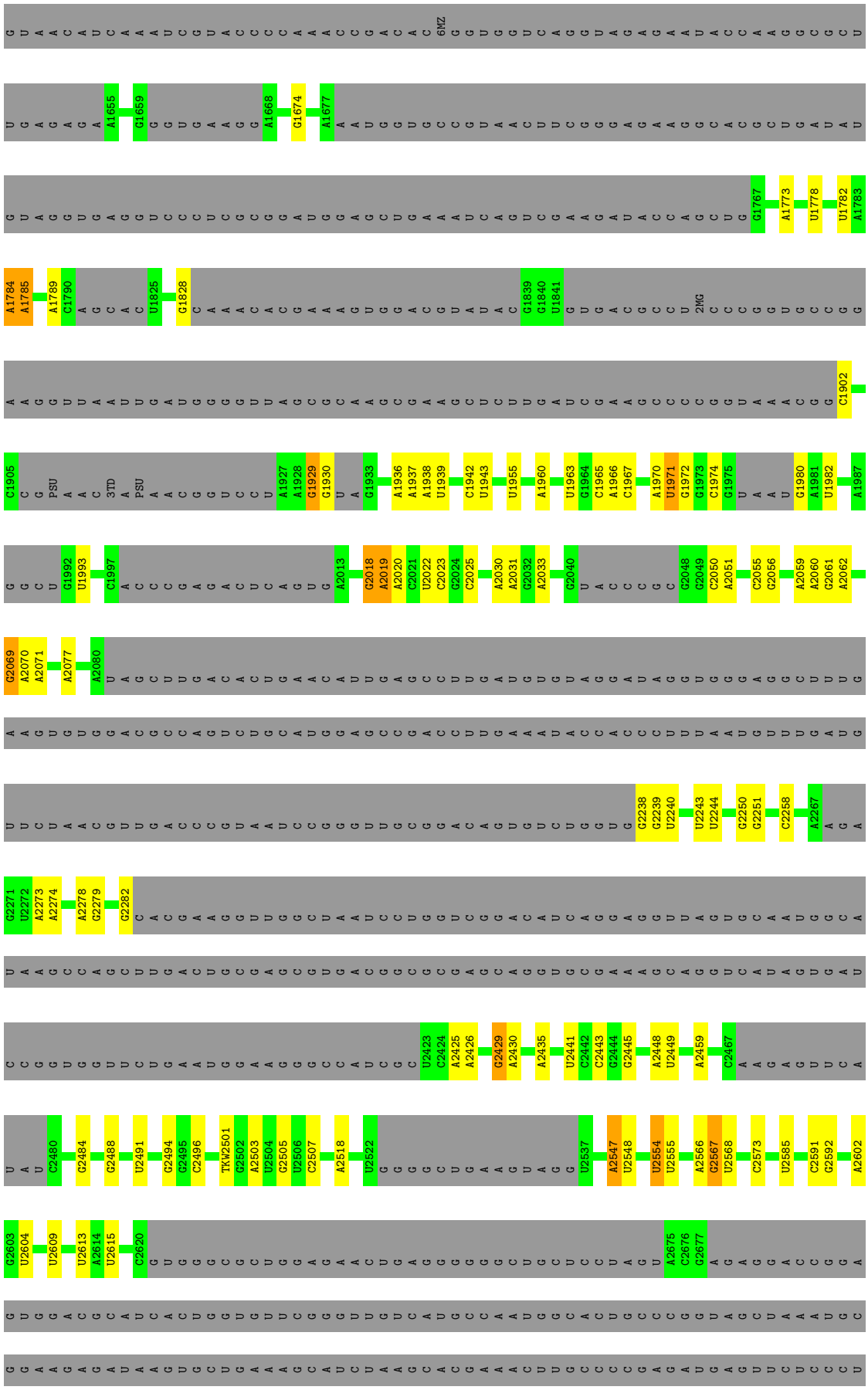
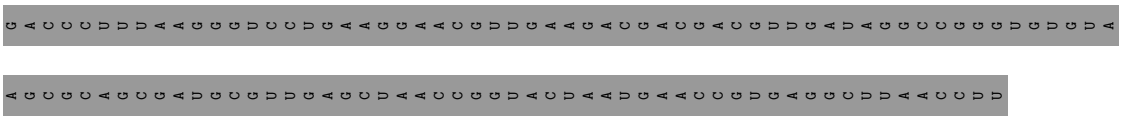
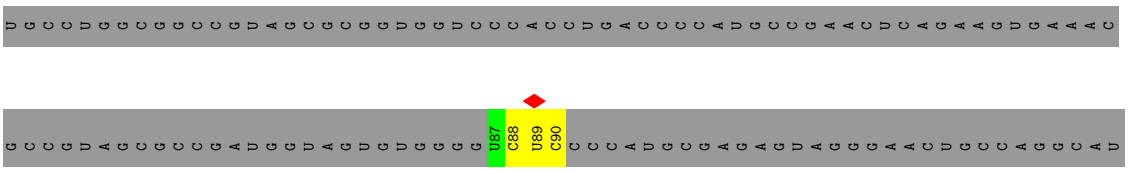
A1253
G1256
C1257
U1258
A1262
U1263
A1268
A1269

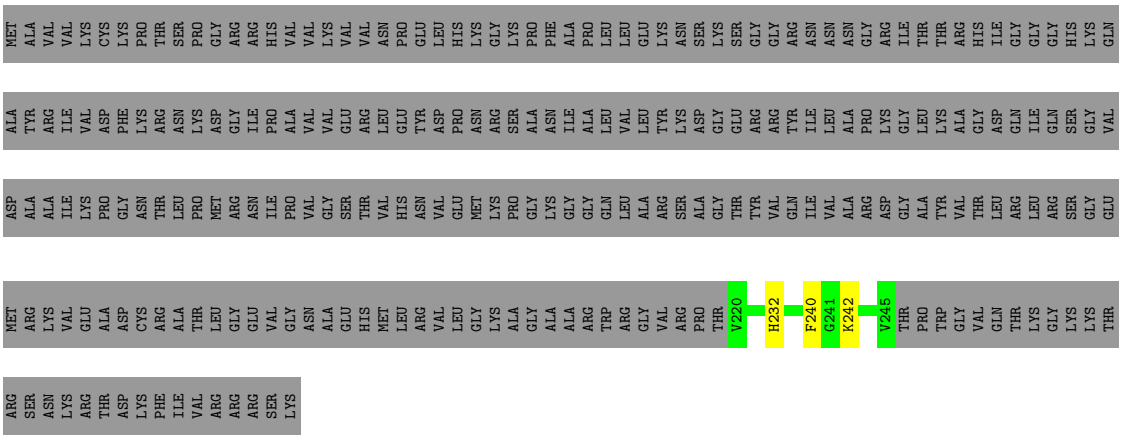

G2603 U2604 U2609 U2613 A2614 U2615 C2620
U A U C2480 G2484 G2488 U2491 G2494 G2495 C2496 TKW2501 G2502 A2503 U2504 G2505 U2506 C2507 A2518 U2522 U2537 A2547 U2548 U2554 U2555 A2566 G2567 U2568 C2573 U2585 C2591 G2592 A2602
C U2423 C2424 A2425 A2426 G2429 A2430 A2435 U2441 C2442 C2443 G2444 G2445 A2448 U2449 A2459 C2467
U2271 U2272 A2273 A2274 A2278 G2279 G2282
G2069 A2070 A2071 A2077 A2080
G G C U G1992 U1993 C1997 A2013 G2018 A2019 A2020 C2021 U2022 C2023 G2024 C2025 A2030 A2031 G2032 A2033 G2040 G2048 G2049 C2050 A2051 C2055 G2056 A2059 A2060 G2061 A2062
C1905 C G PSU A A C 3TD A PSU A A C G G U C C U A1927 A1928 G1929 G1930 U A G1933 A1936 A1937 A1938 U1939 C1942 U1943 U1955 A1960 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1973 C1974 G1975 U A A U G1980 A1981 U1982 A1987
A1784 A1785 A1789 C1790 A G C A C U1825 G1828 C A A A C A C G A A A G U G G A C U A A C G1839 G1840 U1841 G U U G A C C G C U C C U 2MG C C U C G G U G C C G G
G1767 A1773 U1778 U1782 A1783
U G A G A G A A1655 G1659 G G U G A A G G A1668 G1674 A1677 A A U G G U G C C A C G G C U G A G A G G U A A C U U C G G G A U A U
G U A A G G A C C A A U C 6MZ C A A A U C A C C C C A A A C C G G A C G A A A U A C C A A A G G C G C U
A A G U G G A C C C C A G U U G G G C C U U G G A A U U G G C C A A G G G U A G A G A A A C C C C A A A U C C U U U G A U G G G A A A U A A A G G U U G G G U C C A G G A A A C C C C A A A U U U G
U U U C U A A C G U U G A C C G G U A A U C C G G U A A C C G G U G G G U G G G A A A U U U G G C C C C





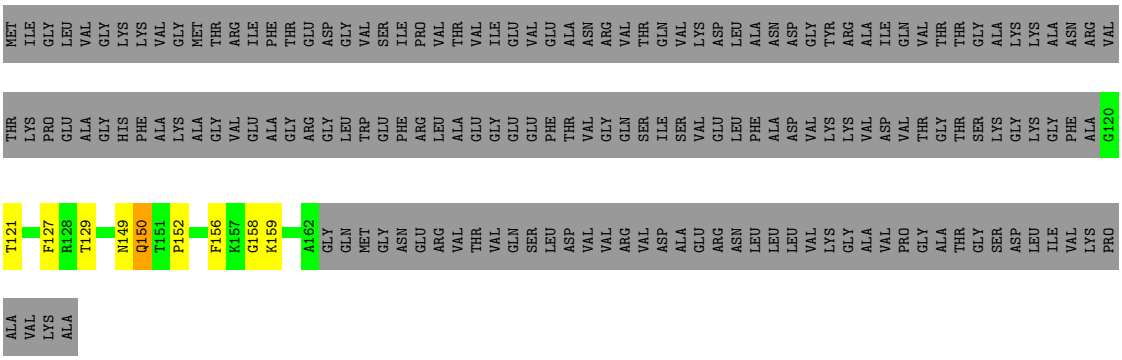
• Molecule 5: Large ribosomal subunit protein uL2

Chain c: 8% 90%



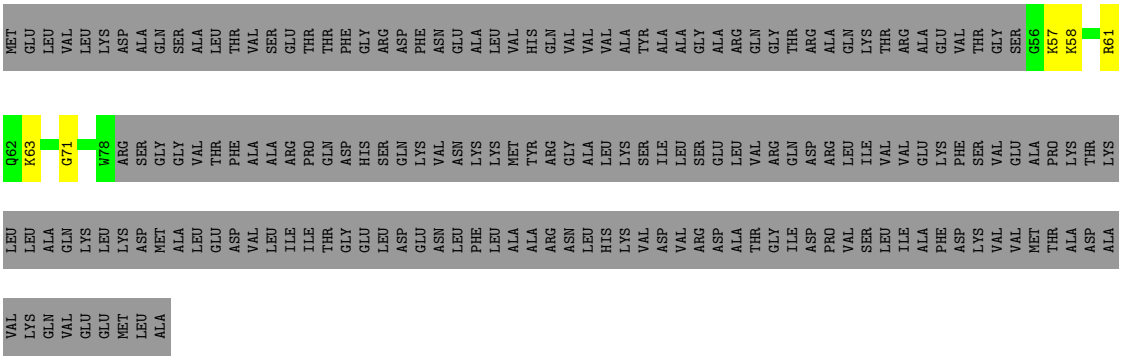
• Molecule 6: Large ribosomal subunit protein uL3

Chain d: 16% 79%



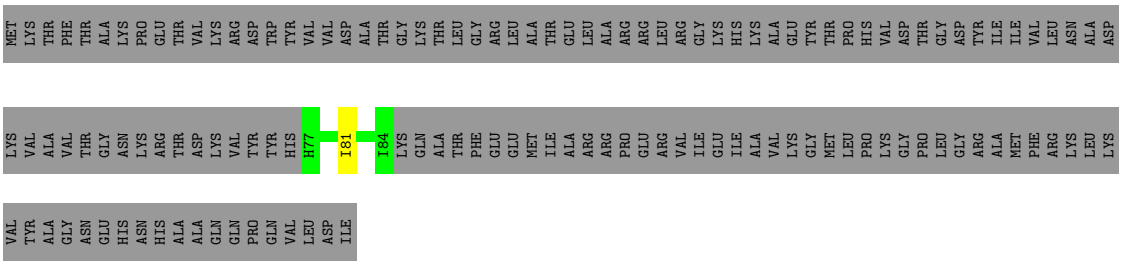
• Molecule 7: Large ribosomal subunit protein uL4

Chain e: 9% 89%



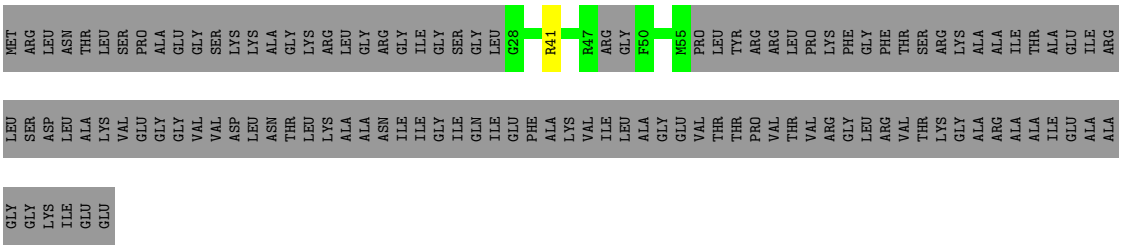
• Molecule 8: Large ribosomal subunit protein uL13

Chain i: 5% • 94%



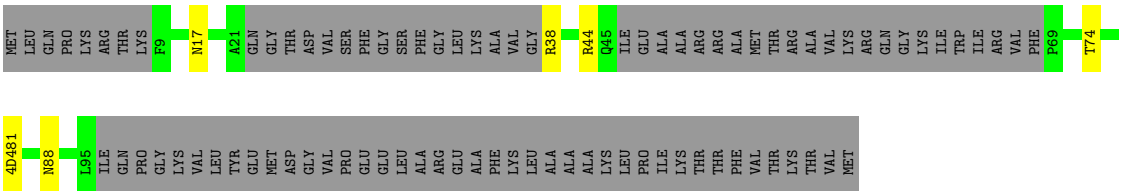
• Molecule 9: Large ribosomal subunit protein uL15

Chain k: 17% • 82%



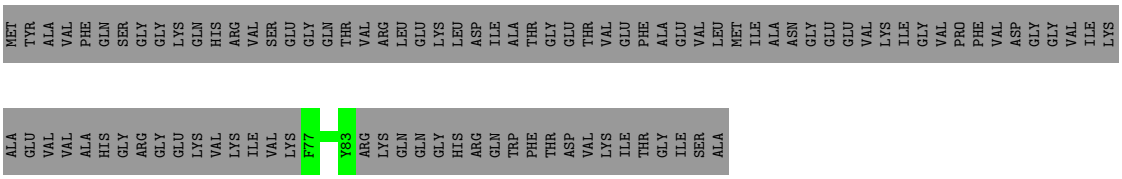
• Molecule 10: Large ribosomal subunit protein uL16

Chain l: 31% • 65%



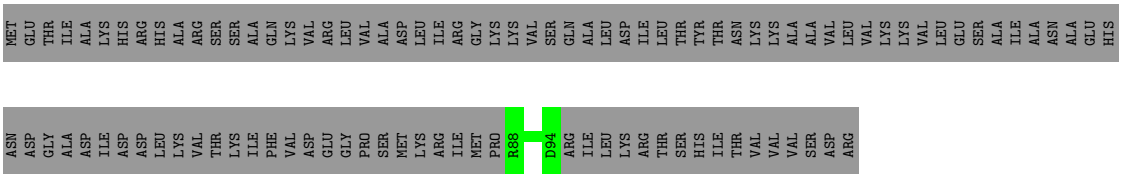
• Molecule 11: Large ribosomal subunit protein bL21

Chain q: 7% 93%



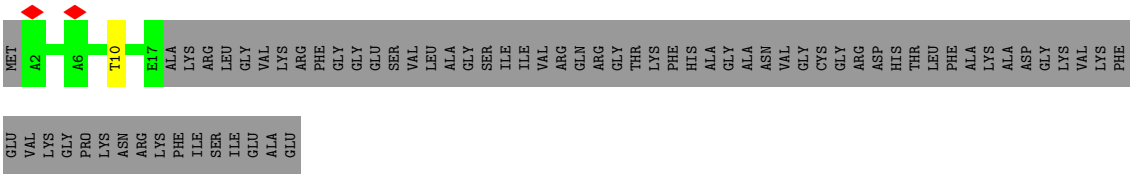
• Molecule 12: Large ribosomal subunit protein uL22

Chain r: 6% 94%



• Molecule 13: Large ribosomal subunit protein bL27

Chain v: 18% 81%



• Molecule 14: Large ribosomal subunit protein bL32

Chain z: 7% 7% 86%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.500	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	421.2736, 421.2736, 421.2736	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8228, 0.8228, 0.8228	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: 4D4, 1MG, 6MZ, OMG, H2U, 2MA, G7M, PUT, 5MC, 2MG, K, OMC, PSU, MS6, 5MU, MG, TKW, MEQ, SR0

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	Y	0.62	0/285	0.90	0/438
2	Z	0.56	0/427	0.85	0/661
3	a	0.56	1/13812 (0.0%)	1.05	41/21450 (0.2%)
4	b	0.57	0/87	1.09	0/132
5	c	0.73	0/197	0.95	0/265
6	d	0.70	0/329	1.15	1/438 (0.2%)
7	e	0.69	0/187	0.96	0/248
8	i	0.70	0/56	1.14	0/74
9	k	0.77	0/182	1.19	0/232
10	l	0.67	0/370	1.03	0/487
11	q	0.75	0/77	1.17	0/99
12	r	0.69	0/52	0.95	0/66
13	v	0.69	0/116	0.94	0/151
14	z	0.74	0/61	1.10	1/82 (1.2%)
All	All	0.57	1/16238 (0.0%)	1.04	43/24823 (0.2%)

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
7	e	0	1
9	k	0	1
10	l	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	2069	G7M	O3'-P	5.53	1.61	1.56

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1132	U	O3'-P-O5'	-19.13	75.30	104.00
3	a	980	A	O3'-P-O5'	-12.45	85.33	104.00
3	a	1971	U	O3'-P-O5'	-10.36	88.46	104.00
3	a	980	A	C4'-C3'-O3'	8.85	126.28	113.00
3	a	2018	G	O3'-P-O5'	-8.11	91.84	104.00
3	a	781	A	O3'-P-O5'	-8.07	91.89	104.00
3	a	2278	A	O3'-P-O5'	-7.90	92.16	104.00
3	a	1974	C	O3'-P-O5'	-7.75	92.38	104.00
3	a	2051	A	O3'-P-O5'	-7.18	93.22	104.00
3	a	1902	C	O3'-P-O5'	-6.93	93.60	104.00
3	a	972	A	O3'-P-O5'	-6.76	93.86	104.00
3	a	1785	A	O3'-P-O5'	-6.62	94.07	104.00
3	a	982	C	C2'-C3'-O3'	-6.46	104.02	113.70
6	d	129	THR	CA-CB-OG1	-6.09	100.47	109.60
3	a	2018	G	C4'-C3'-O3'	-6.01	103.99	113.00
3	a	784	G	O3'-P-O5'	-5.92	95.11	104.00
3	a	748	G	C1'-O4'-C4'	-5.90	104.00	109.90
3	a	2025	C	C2'-C3'-O3'	-5.88	104.89	113.70
3	a	2279	G	O3'-P-O5'	-5.79	95.31	104.00
3	a	2019	A	O3'-P-O5'	-5.76	95.36	104.00
3	a	1966	A	O3'-P-O5'	-5.72	95.42	104.00
3	a	1971	U	C2'-C3'-O3'	-5.70	105.15	113.70
3	a	811	U	C2'-C3'-O3'	5.59	117.89	109.50
3	a	2022	U	O3'-P-O5'	-5.59	95.62	104.00
3	a	784	G	C2'-C3'-O3'	-5.47	105.49	113.70
3	a	193	U	O3'-P-O5'	-5.46	95.81	104.00
3	a	975	A	C4'-C3'-O3'	5.46	121.18	113.00
3	a	2240	U	O3'-P-O5'	5.41	112.11	104.00
3	a	674	G	O3'-P-O5'	-5.39	95.91	104.00
3	a	1929	G	O3'-P-O5'	-5.38	95.93	104.00
3	a	2429	G	C2'-C3'-O3'	-5.34	105.68	113.70
3	a	786	C	C3'-C2'-O2'	5.34	118.71	110.70
3	a	1960	A	C4'-C3'-O3'	-5.34	104.99	113.00
3	a	1135	C	C4'-C3'-O3'	-5.33	105.00	113.00
3	a	1789	A	O3'-P-O5'	-5.28	96.08	104.00
3	a	2238	G	C2'-C3'-O3'	5.22	117.34	109.50
3	a	2050	C	C4'-C3'-O3'	-5.21	105.18	113.00
3	a	1268	A	C2'-C3'-O3'	-5.19	105.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1936	A	C1'-O4'-C4'	-5.19	104.51	109.70
3	a	1936	A	O4'-C1'-C2'	-5.16	100.64	105.80
14	z	5	GLN	CB-CA-C	-5.15	99.91	109.29
3	a	1828	G	C2'-C3'-O3'	5.14	117.22	109.50
3	a	809	G	C4'-C3'-O3'	-5.13	105.31	113.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	e	61	ARG	Sidechain
9	k	41	ARG	Sidechain
10	l	44	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	Y	257	0	134	8	0
2	Z	384	0	200	2	0
3	a	12772	0	6465	34	0
4	b	80	0	43	0	0
5	c	191	0	177	2	0
6	d	333	0	336	5	0
7	e	182	0	193	2	0
8	i	55	0	51	1	0
9	k	182	0	179	0	0
10	l	386	0	399	2	0
11	q	75	0	76	0	0
12	r	53	0	55	0	0
13	v	116	0	110	0	0
14	z	61	0	62	4	0
15	a	20	0	0	2	0
16	a	6	0	12	0	0
17	a	100	0	0	0	0
17	d	1	0	0	0	0
17	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	42	0	0	0	0
18	e	1	0	0	0	0
All	All	15298	0	8492	54	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 2.

All (54) 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:a:568:U:H1'	3:a:2030:6MZ:H9C1	1.64	0.79
10:l:17:ASN:O	10:l:38:ARG:HD3	1.93	0.68
5:c:232:HIS:HA	5:c:242:LYS:HD2	1.76	0.68
3:a:2547:A:H2'	3:a:2548:U:C6	2.33	0.63
3:a:1778:U:H2'	3:a:1784:A:N6	2.16	0.60
1:Y:2:C:H2'	1:Y:3:C:C6	2.37	0.58
3:a:1028:A:H2'	3:a:1029:A:C8	2.42	0.54
6:d:156:PHE:CE1	8:i:81:ILE:HD13	2.42	0.54
3:a:2020:A:H5'	14:z:9:THR:CG2	2.38	0.53
3:a:2273:A:H2'	3:a:2274:A:C8	2.44	0.53
3:a:2243:U:H2'	3:a:2244:U:C6	2.45	0.52
10:l:74:THR:HA	10:l:88:ASN:O	2.10	0.52
3:a:1028:A:N6	3:a:1125:G:H2'	2.26	0.51
1:Y:3:C:H2'	1:Y:4:C:C6	2.48	0.49
1:Y:1:G:H22	1:Y:72:C:H1'	1.77	0.48
3:a:2020:A:H5'	14:z:9:THR:HG21	1.95	0.47
3:a:2591:C:H2'	3:a:2592:G:C8	2.49	0.47
3:a:2554:U:H2'	3:a:2555:U:C6	2.49	0.47
3:a:832:U:H2'	3:a:833:A:C8	2.50	0.47
3:a:1939:5MU:OP1	3:a:2604:PSU:O2'	2.33	0.47
3:a:829:A:OP2	15:a:3001:SR0:N10	2.50	0.45
7:e:58:LYS:HG3	7:e:71:GLY:HA2	1.99	0.45
3:a:579:G:O2'	3:a:2019:A:OP1	2.35	0.44
3:a:1963:U:O2	3:a:1963:U:H2'	2.18	0.43
3:a:2567:G:H2'	3:a:2568:U:C6	2.53	0.43
3:a:1980:G:O2'	3:a:1982:U:OP2	2.33	0.43
3:a:2250:G:O2'	3:a:2496:C:OP1	2.37	0.43
5:c:240:PHE:O	5:c:242:LYS:HE3	2.19	0.42
3:a:956:G:N2	3:a:959:A:H3'	2.34	0.42
3:a:910:A:C6	3:a:911:A:C6	3.06	0.42
1:Y:2:C:H2'	1:Y:3:C:H6	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:828:U:OP2	15:a:3001:SR0:N10	2.52	0.42
6:d:121:THR:HB	6:d:127:PHE:CD2	2.54	0.42
2:Z:75:C:H2'	2:Z:76:A:C8	2.55	0.42
3:a:2070:A:H2'	3:a:2071:A:O4'	2.20	0.42
1:Y:71:G:H3'	1:Y:72:C:C6	2.55	0.42
2:Z:75:C:H3'	2:Z:76:A:H3'	2.01	0.42
6:d:152:PRO:HG3	6:d:156:PHE:CZ	2.55	0.42
3:a:2251:OMG:H1'	3:a:2251:OMG:HM23	1.60	0.42
3:a:2615:U:C2	14:z:4:GLN:HA	2.55	0.42
6:d:149:ASN:OD1	6:d:150:MEQ:N	2.53	0.41
1:Y:70:G:H2'	1:Y:71:G:C8	2.56	0.41
3:a:1942:C:H3'	3:a:1943:U:H2'	2.02	0.41
6:d:158:GLY:O	6:d:159:LYS:C	2.63	0.41
3:a:1263:U:O2'	14:z:8:PRO:HD2	2.19	0.41
3:a:984:A:H2'	3:a:984:A:N3	2.35	0.41
3:a:2018:G:H2'	3:a:2019:A:O4'	2.21	0.41
3:a:2018:G:O2'	3:a:2019:A:H5'	2.21	0.41
3:a:2258:C:O2'	3:a:2426:A:H4'	2.21	0.41
3:a:2445:2MG:HM21	3:a:2449:H2U:O4	2.21	0.41
1:Y:70:G:H2'	1:Y:71:G:H8	1.85	0.40
1:Y:75:C:H2'	1:Y:76:A:C8	2.56	0.40
3:a:2443:C:OP1	7:e:63:LYS:HD3	2.21	0.40
3:a:1027:A:C2	3:a:2488:G:H5'	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	
5	c	24/273 (9%)	23 (96%)	1 (4%)	0	100	100
6	d	40/209 (19%)	36 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	e	21/201 (10%)	20 (95%)	1 (5%)	0	100	100
8	i	6/142 (4%)	6 (100%)	0	0	100	100
9	k	22/144 (15%)	20 (91%)	2 (9%)	0	100	100
10	l	40/136 (29%)	39 (98%)	1 (2%)	0	100	100
11	q	5/103 (5%)	5 (100%)	0	0	100	100
12	r	5/110 (4%)	5 (100%)	0	0	100	100
13	v	14/85 (16%)	13 (93%)	1 (7%)	0	100	100
14	z	6/57 (10%)	6 (100%)	0	0	100	100
All	All	183/1460 (12%)	173 (94%)	10 (6%)	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	
5	c	19/218 (9%)	19 (100%)	0	100	100
6	d	34/163 (21%)	34 (100%)	0	100	100
7	e	18/165 (11%)	17 (94%)	1 (6%)	19	33
8	i	5/116 (4%)	5 (100%)	0	100	100
9	k	16/103 (16%)	16 (100%)	0	100	100
10	l	36/107 (34%)	36 (100%)	0	100	100
11	q	7/84 (8%)	7 (100%)	0	100	100
12	r	4/93 (4%)	4 (100%)	0	100	100
13	v	11/63 (18%)	10 (91%)	1 (9%)	9	14
14	z	7/48 (15%)	7 (100%)	0	100	100
All	All	157/1160 (14%)	155 (99%)	2 (1%)	59	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	e	57	LYS
13	v	10	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
8	i	80	HIS
9	k	54	GLN
13	v	3	HIS
14	z	6	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Y	10/76 (13%)	7 (70%)	1 (10%)
2	Z	16/77 (20%)	3 (18%)	0
3	a	559/2904 (19%)	83 (14%)	0
4	b	3/120 (2%)	3 (100%)	0
All	All	588/3177 (18%)	96 (16%)	1 (0%)

All (96) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Y	70	G
1	Y	71	G
1	Y	72	C
1	Y	73	A
1	Y	74	C
1	Y	75	C
1	Y	76	A
2	Z	4	G
2	Z	6	G
2	Z	7	G
3	a	196	A
3	a	199	A
3	a	531	C
3	a	532	A
3	a	563	A
3	a	573	U
3	a	575	A
3	a	747	5MU

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Mol	Chain	Res	Type
3	a	776	G
3	a	782	A
3	a	784	G
3	a	785	G
3	a	805	G
3	a	811	U
3	a	827	U
3	a	828	U
3	a	946	C
3	a	958	U
3	a	961	C
3	a	974	G
3	a	981	A
3	a	983	A
3	a	984	A
3	a	985	C
3	a	1026	G
3	a	1130	U
3	a	1132	U
3	a	1133	A
3	a	1134	A
3	a	1135	C
3	a	1253	A
3	a	1256	G
3	a	1674	G
3	a	1773	A
3	a	1782	U
3	a	1784	A
3	a	1785	A
3	a	1929	G
3	a	1930	G
3	a	1937	A
3	a	1938	A
3	a	1955	U
3	a	1965	C
3	a	1967	C
3	a	1970	A
3	a	1971	U
3	a	1972	G
3	a	1993	U
3	a	2023	C
3	a	2031	A

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Mol	Chain	Res	Type
3	a	2033	A
3	a	2055	C
3	a	2056	G
3	a	2059	A
3	a	2060	A
3	a	2061	G
3	a	2062	A
3	a	2069	G7M
3	a	2077	A
3	a	2239	G
3	a	2282	G
3	a	2425	A
3	a	2429	G
3	a	2430	A
3	a	2435	A
3	a	2441	U
3	a	2448	A
3	a	2459	A
3	a	2484	G
3	a	2491	U
3	a	2494	G
3	a	2505	G
3	a	2507	C
3	a	2518	A
3	a	2547	A
3	a	2554	U
3	a	2566	A
3	a	2567	G
3	a	2573	C
3	a	2585	U
3	a	2602	A
3	a	2609	U
3	a	2613	U
4	b	88	C
4	b	89	U
4	b	90	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Y	73	A

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

22 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
3	TKW	a	2501	3,18	18,22,23	0.42	0	28,32,35	0.87	1 (3%)
6	MEQ	d	150	6	8,9,10	0.69	0	5,10,12	1.17	1 (20%)
3	PSU	a	2504	3,18	18,21,22	0.36	0	22,30,33	0.41	0
3	PSU	a	2580	3	18,21,22	0.33	0	22,30,33	0.56	0
3	PSU	a	746	17,3	18,21,22	0.37	0	22,30,33	0.41	0
10	MS6	l	82	10	5,7,8	0.25	0	2,7,9	0.40	0
3	2MG	a	2445	3	23,26,27	0.43	0	32,38,41	0.35	0
3	5MU	a	1939	3,18	19,22,23	0.51	0	28,32,35	0.54	0
3	1MG	a	745	3	22,26,27	0.59	0	33,39,42	0.47	0
3	PSU	a	955	3	18,21,22	0.36	0	22,30,33	0.32	0
10	4D4	l	81	10	9,11,12	0.79	0	8,13,15	0.92	1 (12%)
3	PSU	a	2605	3	18,21,22	0.33	0	22,30,33	0.42	0
3	PSU	a	2604	3	18,21,22	0.33	0	22,30,33	0.41	0
3	OMG	a	2251	3,18,2	23,26,27	0.39	0	33,38,41	0.27	0
3	H2U	a	2449	3	18,21,22	0.45	0	21,30,33	0.43	0
3	PSU	a	2457	3	18,21,22	0.33	0	22,30,33	0.37	0
3	OMC	a	2498	17,3	19,22,23	0.27	0	26,31,34	0.41	0
3	6MZ	a	2030	3	22,25,26	0.33	0	30,36,39	0.43	0
3	5MC	a	1962	3,18	18,22,23	0.34	0	26,32,35	0.33	0
3	G7M	a	2069	3,18	23,26,27	0.37	0	35,39,42	0.49	0
3	5MU	a	747	3	19,22,23	0.33	0	28,32,35	0.44	0
3	2MA	a	2503	17,3,18	22,25,26	0.98	1 (4%)	33,37,40	1.15	3 (9%)

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
3	TKW	a	2501	3,18	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MEQ	d	150	6	-	3/8/9/11	-
3	PSU	a	2504	3,18	-	0/7/25/26	0/2/2/2
3	PSU	a	2580	3	-	0/7/25/26	0/2/2/2
3	PSU	a	746	17,3	-	1/7/25/26	0/2/2/2
10	MS6	l	82	10	-	1/4/6/8	-
3	2MG	a	2445	3	-	0/9/27/28	0/3/3/3
3	5MU	a	1939	3,18	-	0/7/25/26	0/2/2/2
3	1MG	a	745	3	-	0/7/25/26	0/3/3/3
3	PSU	a	955	3	-	0/7/25/26	0/2/2/2
10	4D4	l	81	10	-	0/11/12/14	-
3	PSU	a	2605	3	-	0/7/25/26	0/2/2/2
3	PSU	a	2604	3	-	0/7/25/26	0/2/2/2
3	OMG	a	2251	3,18,2	-	1/9/27/28	0/3/3/3
3	H2U	a	2449	3	-	0/7/38/39	0/2/2/2
3	PSU	a	2457	3	-	0/7/25/26	0/2/2/2
3	OMC	a	2498	17,3	-	0/9/27/28	0/2/2/2
3	6MZ	a	2030	3	-	2/9/27/28	0/3/3/3
3	5MC	a	1962	3,18	-	0/7/25/26	0/2/2/2
3	G7M	a	2069	3,18	-	2/7/25/26	0/3/3/3
3	5MU	a	747	3	-	0/7/25/26	0/2/2/2
3	2MA	a	2503	17,3,18	-	3/7/25/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	2503	2MA	C6-N6	-3.48	1.25	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	2503	2MA	N6-C6-N1	4.17	122.93	117.03
3	a	2501	TKW	OAC-C5-C4	3.76	120.11	114.43
3	a	2503	2MA	C2-N1-C6	3.02	122.80	118.08
3	a	2503	2MA	C5-C6-N1	-2.90	114.02	119.01
10	l	81	4D4	O-C-CA	-2.19	119.04	124.78
6	d	150	MEQ	CG-CD-NE2	2.11	119.22	116.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	d	150	MEQ	C-CA-CB-CG
3	a	2030	6MZ	O4'-C4'-C5'-O5'
3	a	2251	OMG	C1'-C2'-O2'-CM2
3	a	2030	6MZ	C3'-C4'-C5'-O5'
6	d	150	MEQ	NE2-CD-CG-CB
6	d	150	MEQ	OE1-CD-CG-CB
3	a	2501	TKW	C2'-C1'-N1-C6
3	a	2069	G7M	C4'-C5'-O5'-P
3	a	2501	TKW	O4'-C1'-N1-C6
3	a	2503	2MA	C4'-C5'-O5'-P
3	a	2501	TKW	O4'-C1'-N1-C2
3	a	2503	2MA	O4'-C4'-C5'-O5'
3	a	2501	TKW	C2'-C1'-N1-C2
3	a	2503	2MA	O4'-C1'-N9-C8
10	l	82	MS6	CB-CG-SD-CE
3	a	746	PSU	O4'-C1'-C5-C6
3	a	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	d	150	MEQ	1	0
3	a	2445	2MG	1	0
3	a	1939	5MU	1	0
3	a	2604	PSU	1	0
3	a	2251	OMG	1	0
3	a	2449	H2U	1	0
3	a	2030	6MZ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 148 ligands modelled in this entry, 145 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	SR0	a	3001	-	9,9,9	0.50	0	8,8,8	0.47	0
16	PUT	a	3003	-	5,5,5	0.27	0	4,4,4	0.23	0
15	SR0	a	3002	-	9,9,9	0.54	0	8,8,8	0.47	0

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
15	SR0	a	3001	-	-	2/7/7/7	-
16	PUT	a	3003	-	-	0/3/3/3	-
15	SR0	a	3002	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	a	3002	SR0	N6-C7-C8-C9
15	a	3002	SR0	C8-C7-N6-C5
15	a	3002	SR0	C2-C3-C4-C5
15	a	3001	SR0	N1-C2-C3-C4
15	a	3001	SR0	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a	3001	SR0	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

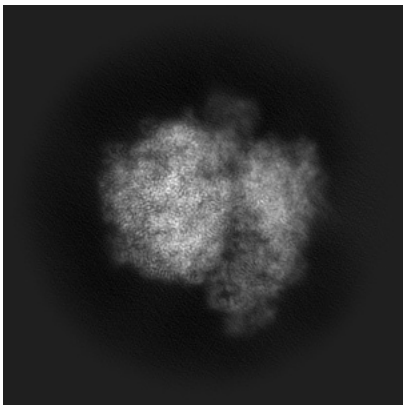
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55428. These allow visual inspection of the internal detail of the map and identification of artifacts.

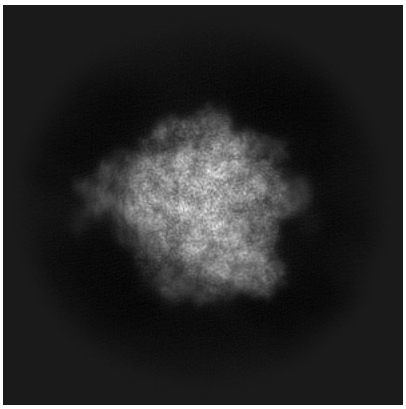
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

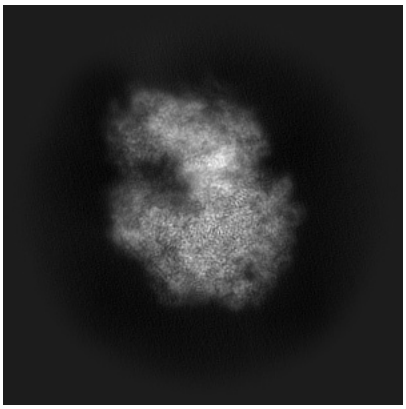
6.1.1 Primary map



X

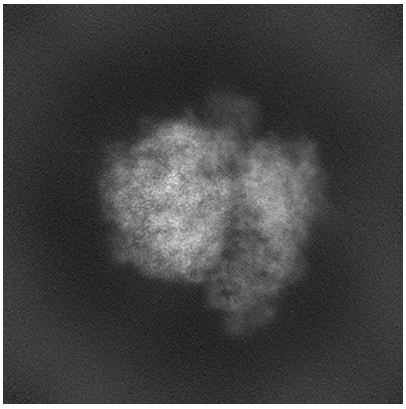


Y

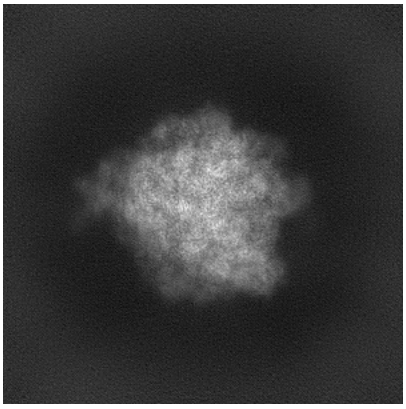


Z

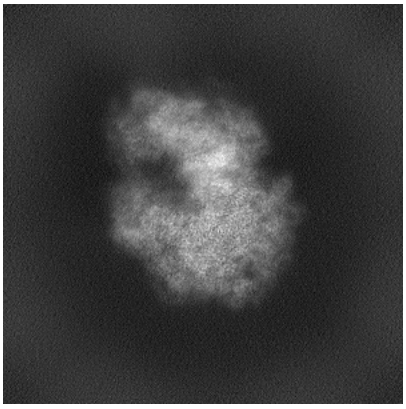
6.1.2 Raw map



X



Y

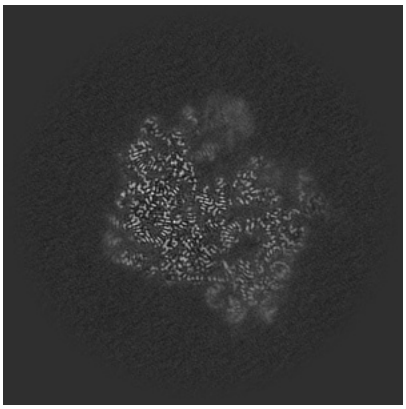


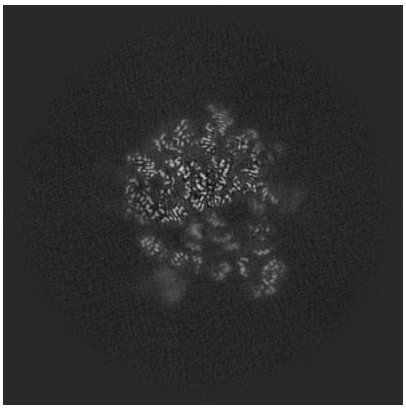
Z

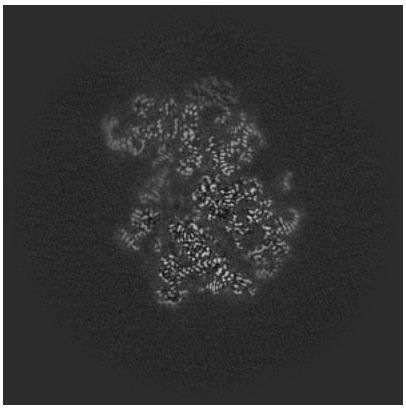
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

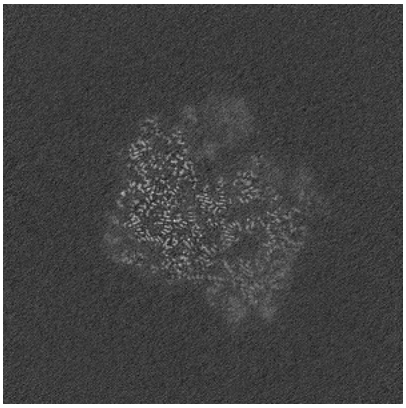
6.2.1 Primary map

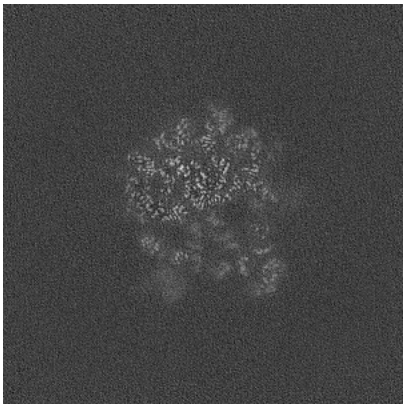

X Index: 256

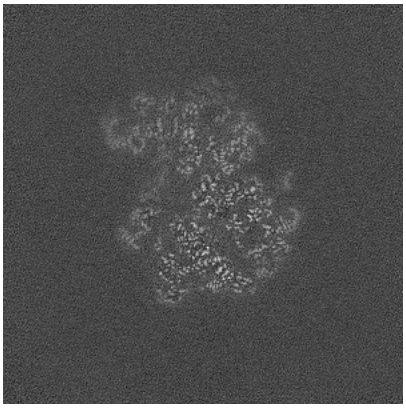

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

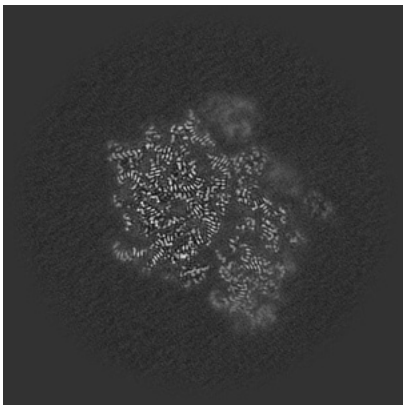

Y Index: 256


Z Index: 256

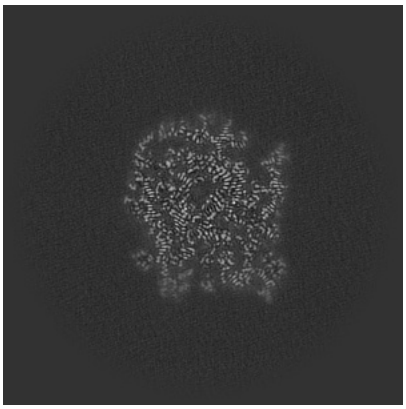
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

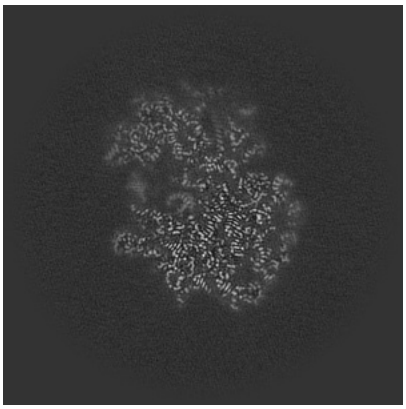
6.3.1 Primary map



X Index: 268

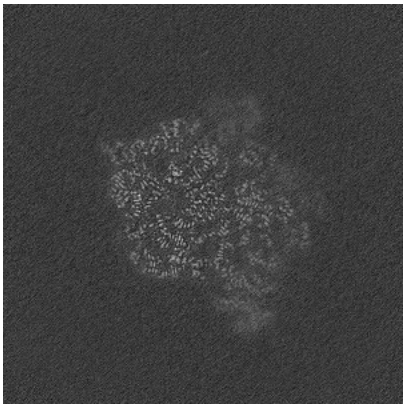


Y Index: 222

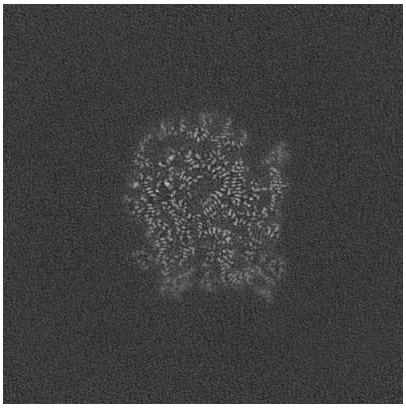


Z Index: 270

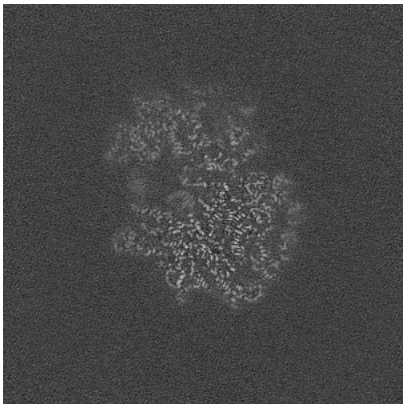
6.3.2 Raw map



X Index: 279



Y Index: 221

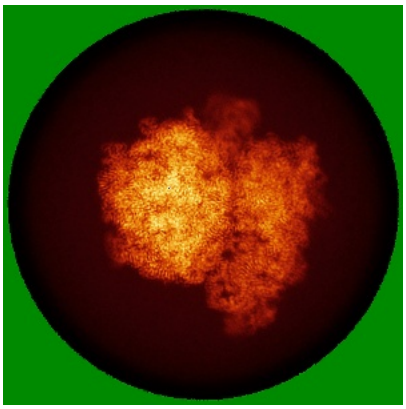


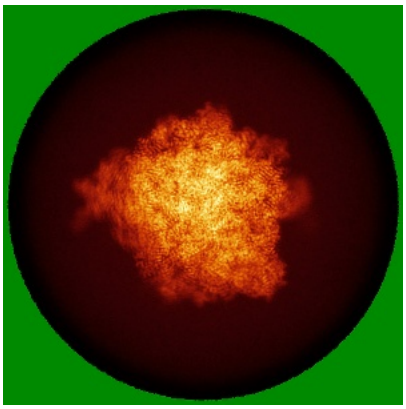
Z Index: 269

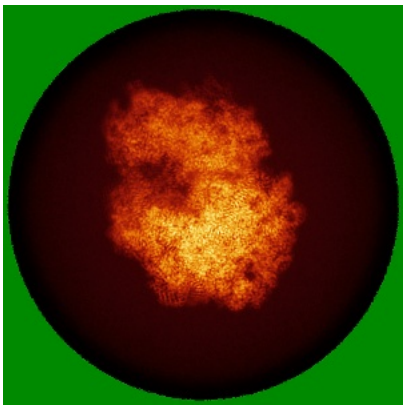
The images above show the largest variance slices of the map in three orthogonal directions.

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

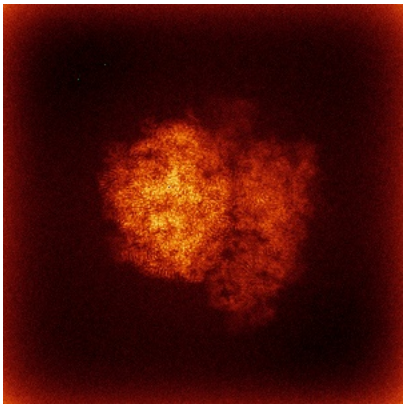
6.4.1 Primary map

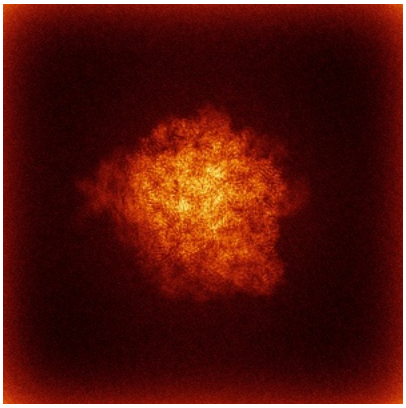

X

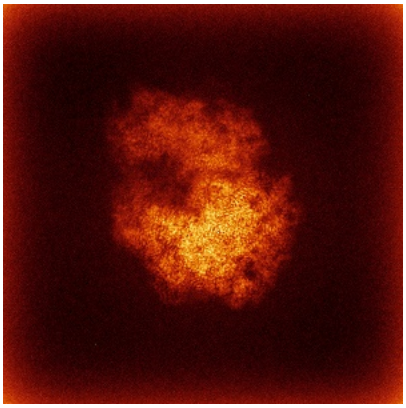

Y


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.

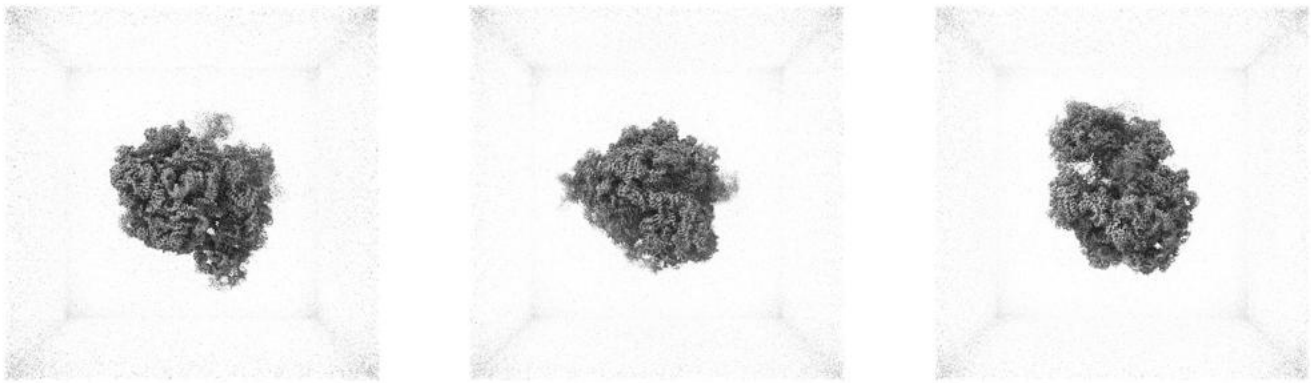
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

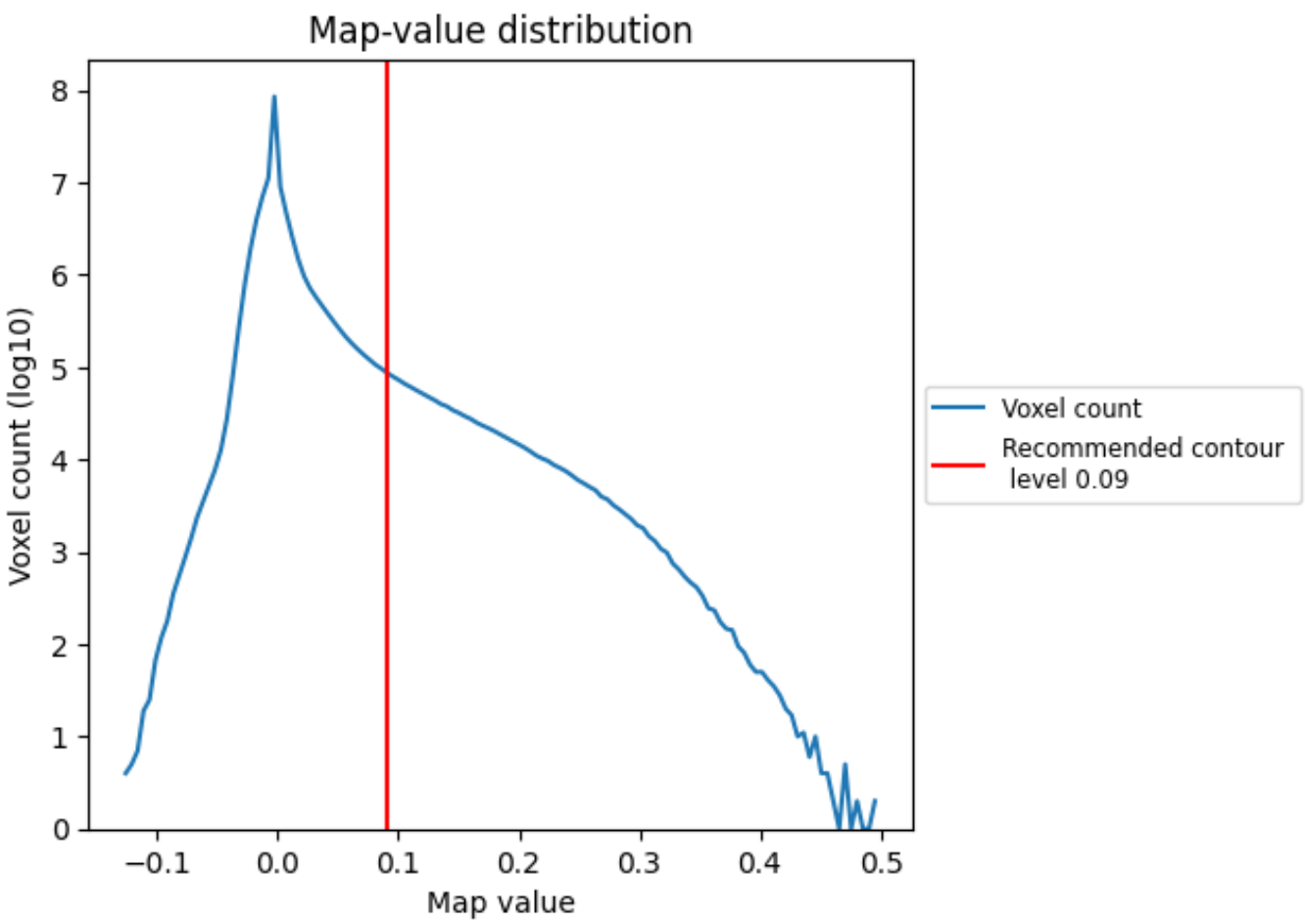
6.6 Mask visualisation (i)

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

7 Map analysis (i)

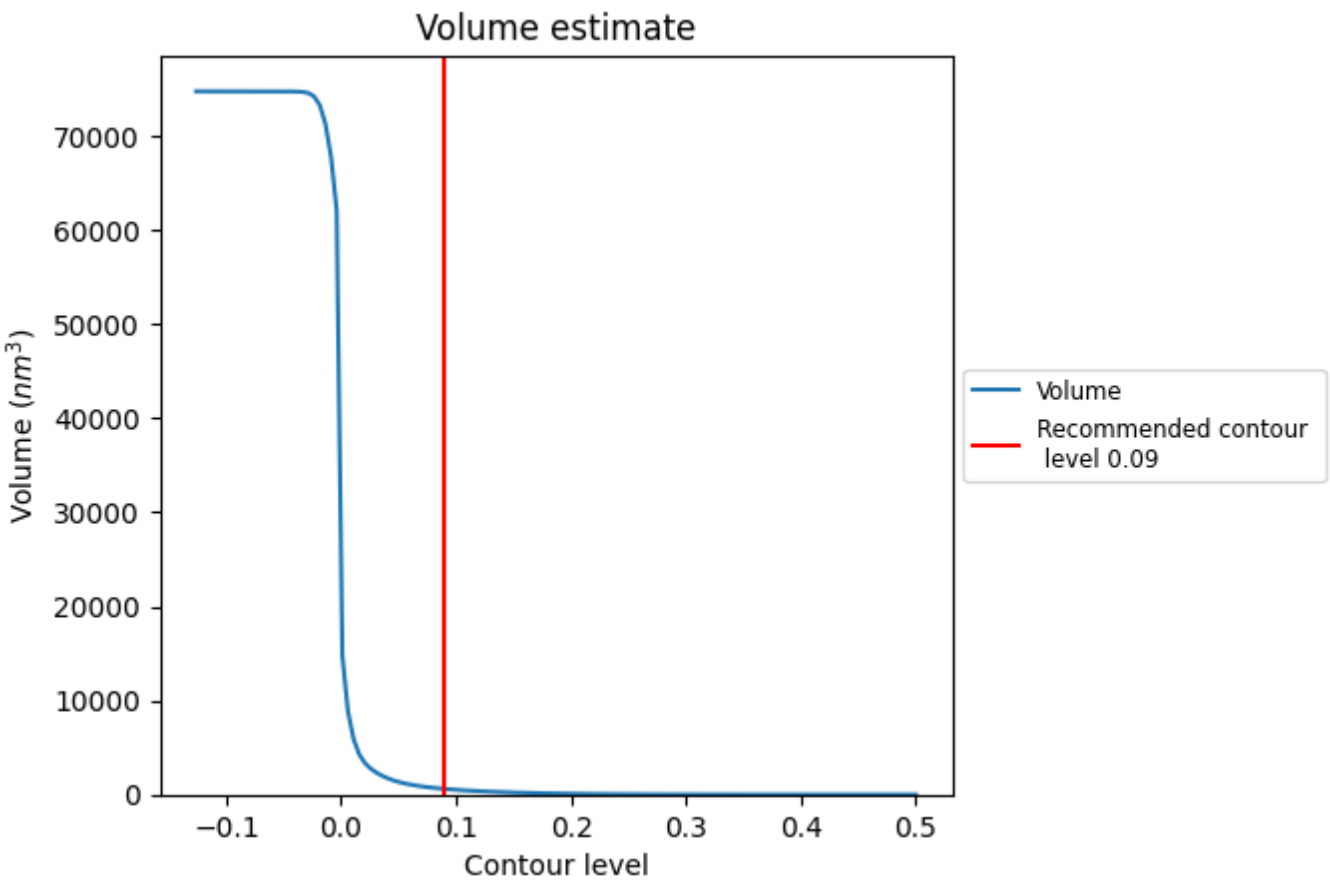
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

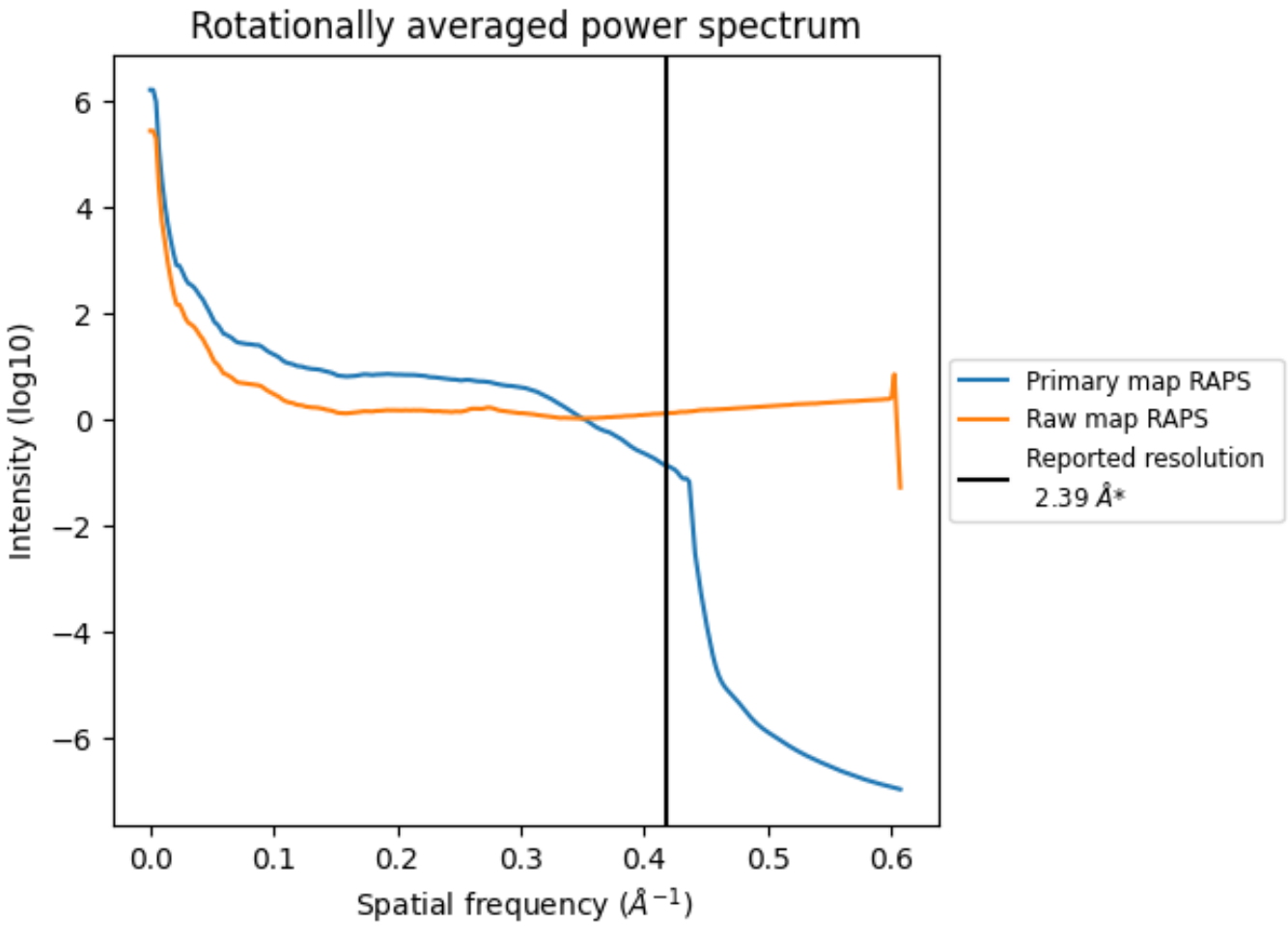
7.2 Volume estimate (i)



The volume at the recommended contour level is 600 nm^3; this corresponds to an approximate mass of 542 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)

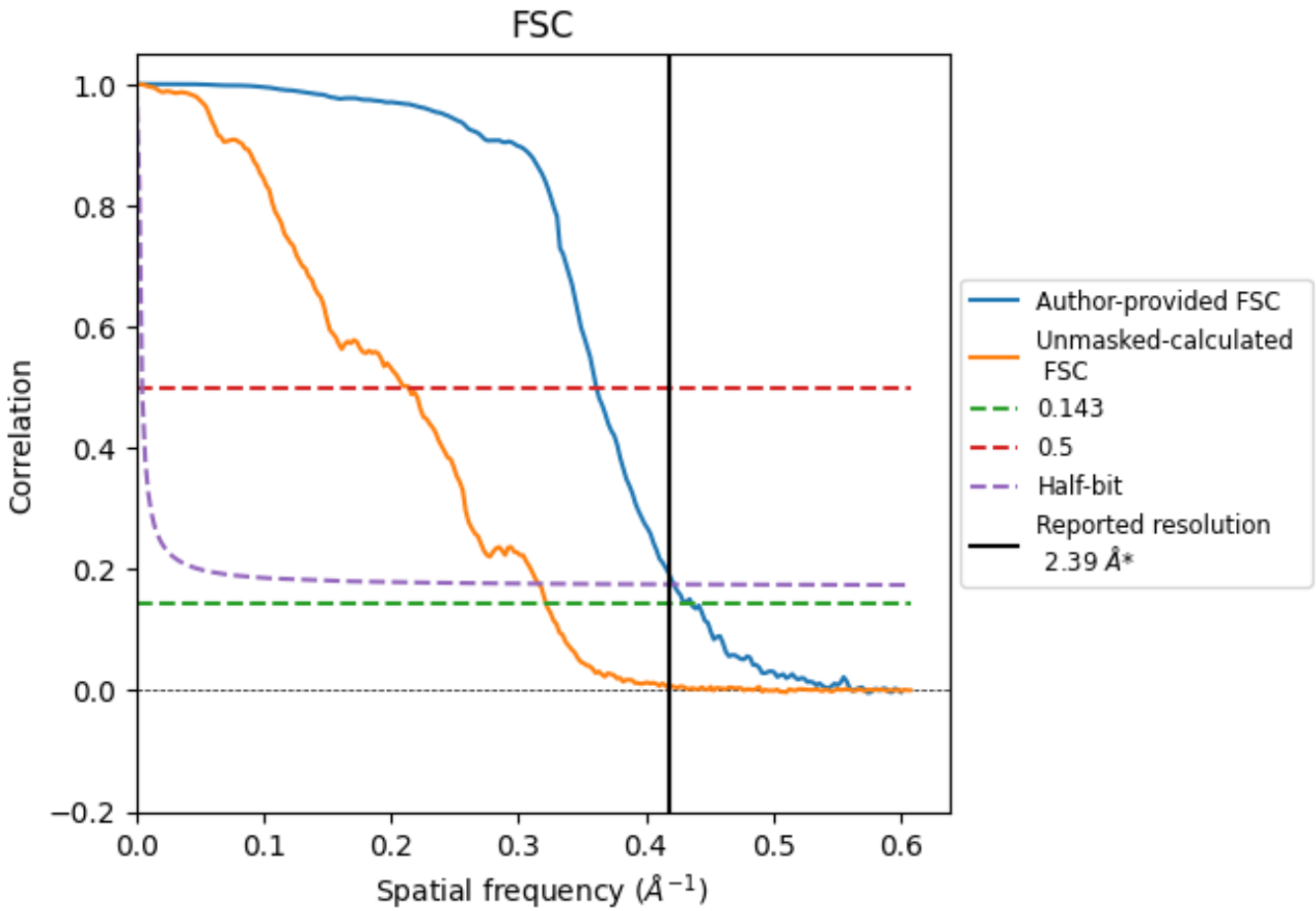


*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8.2 Resolution estimates (i)

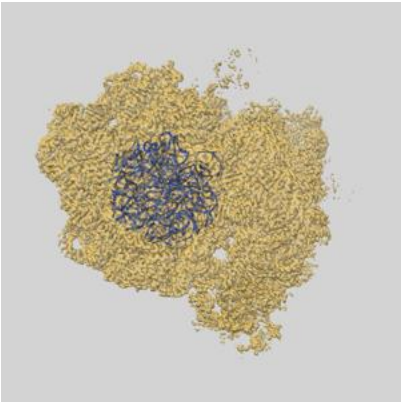
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.29	2.77	2.37
Unmasked-calculated*	3.11	4.68	3.17

*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 2.39 by more than 10 %

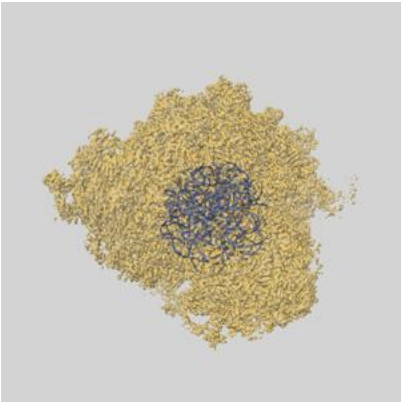
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55428 and PDB model 9T1A. Per-residue inclusion information can be found in section 3 on page 8.

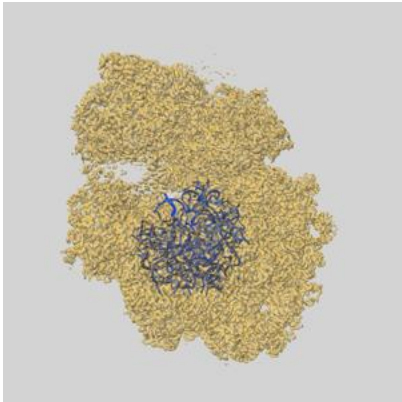
9.1 Map-model overlay (i)



X



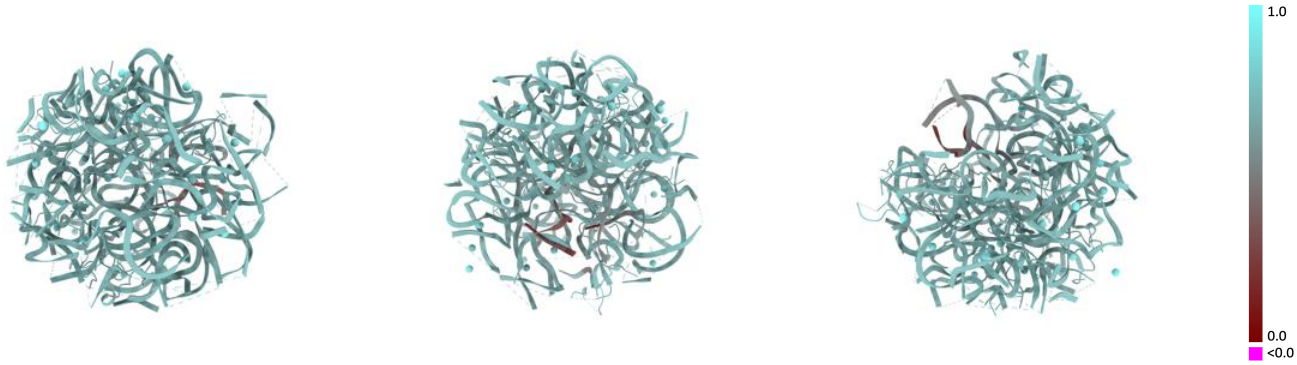
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

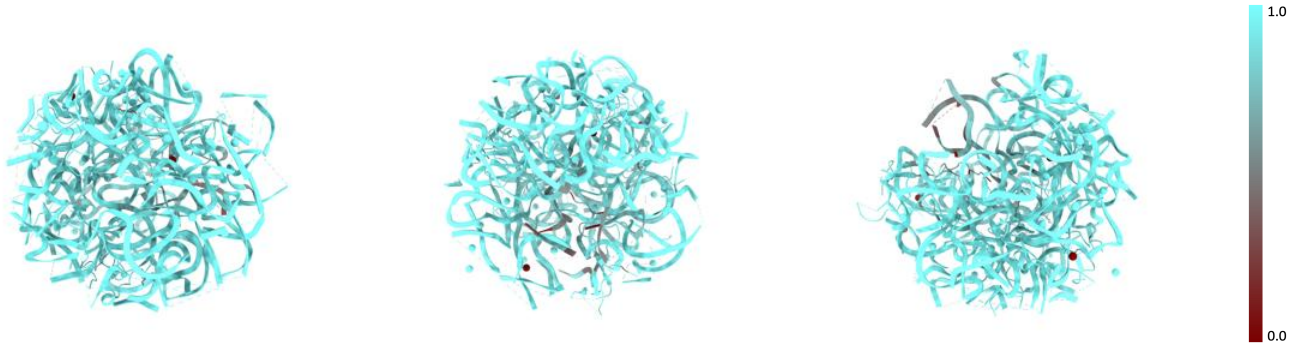
9.2 Q-score mapped to coordinate model (i)



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.

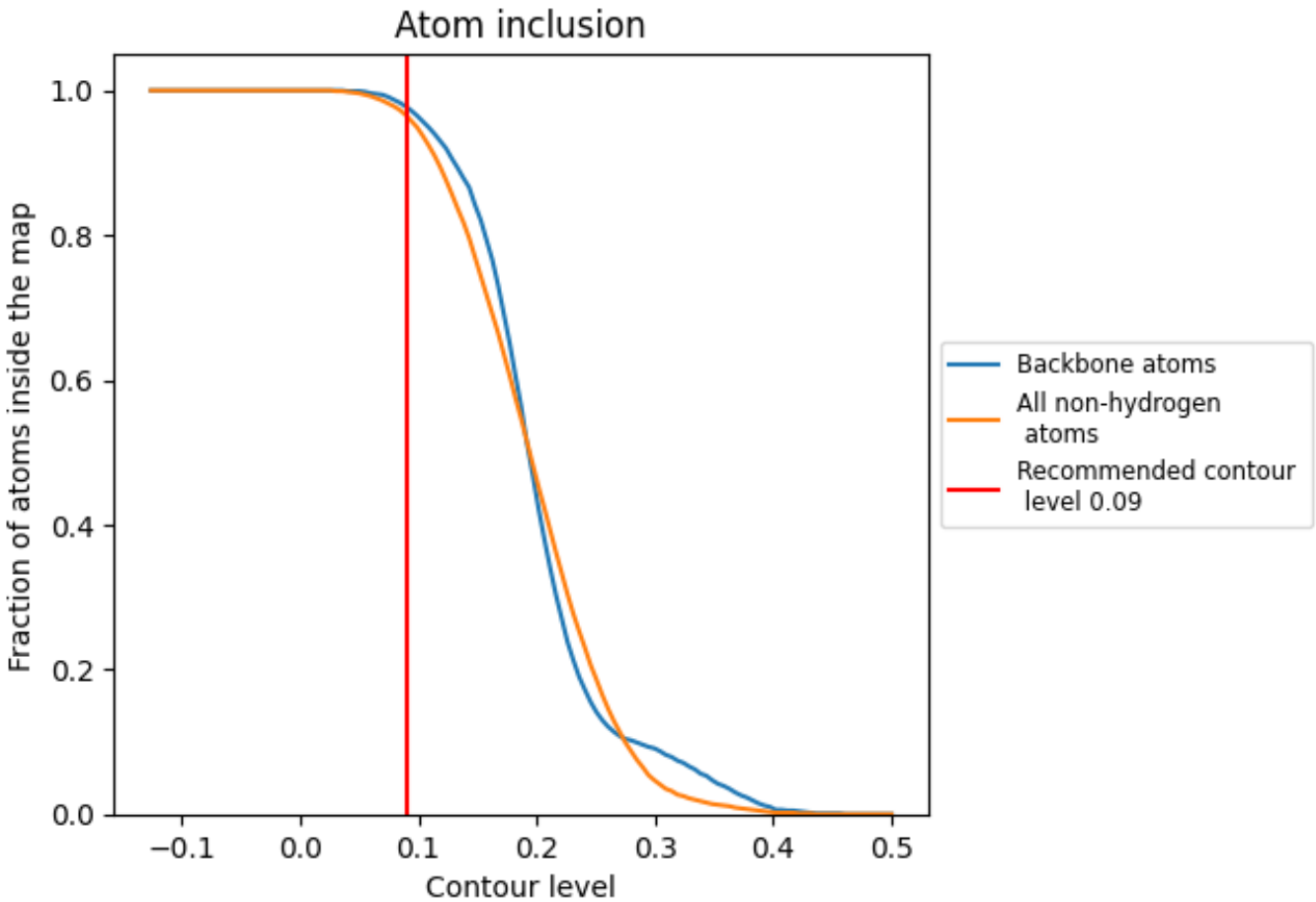
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 98% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.6620
Y	0.5370	0.3710
Z	0.7030	0.5150
a	0.9860	0.6710
b	0.7130	0.5580
c	0.9730	0.6870
d	0.9690	0.6830
e	0.9490	0.6780
i	0.9820	0.6890
k	0.9720	0.6860
l	0.9080	0.6690
q	1.0000	0.6940
r	0.8160	0.6510
v	0.7230	0.6090
z	1.0000	0.6900