Full wwPDB EM Validation Report (i)

Aug 17, 2026 – 09:08 pm BST

PDB ID	:	9T1B / pdb_00009t1b
EMDB ID	:	EMD-55429
Title	:	E. coli 70S ribosome from delta-RlmE strain, PTC class 2
Authors	:	Larsson, D.S.D.; Selmer, M.
Deposited on	:	2025-10-21
Resolution	:	2.32 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:

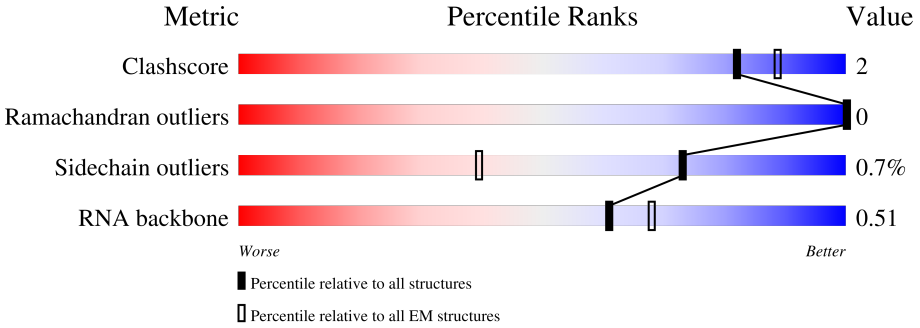
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal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

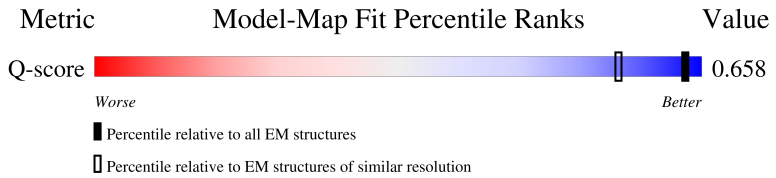
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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	4359 (1.82 - 2.82)

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	14% · 9% · 84%
2	Z	77	· 17% 5% · 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	8% 92%
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	19% 81%
14	z	57	9% 5% 86%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 15254 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	17	138	90	28	20	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

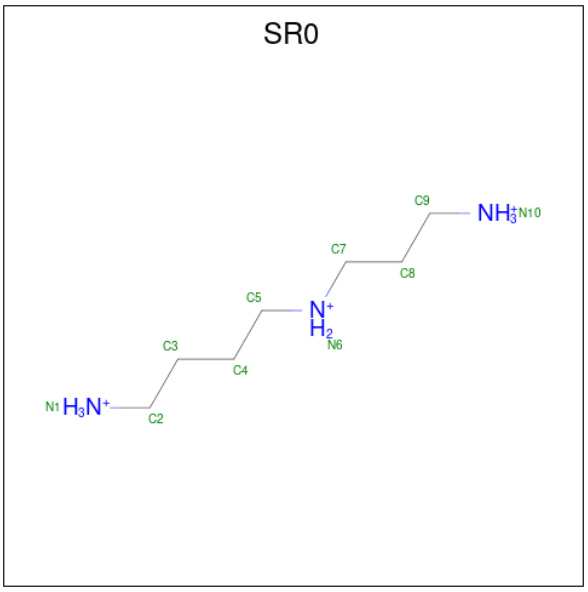
- Molecule 13 is a protein called Large ribosomal subunit protein bL27.

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

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

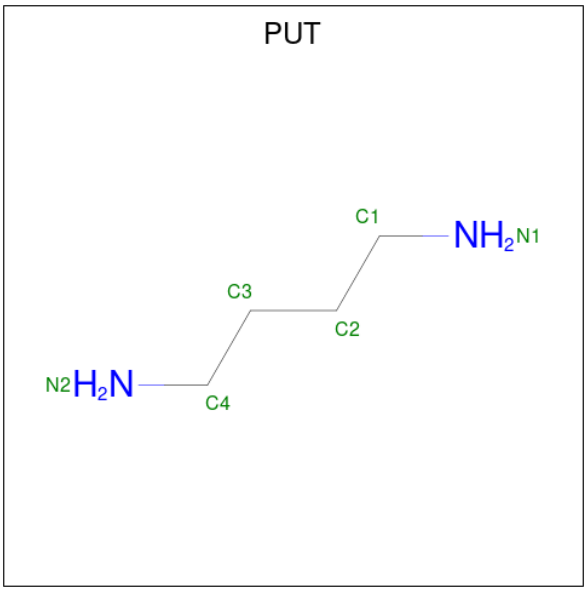
Mol	Chain	Residues	Atoms				AltConf	Trace
14	z	8	Total 61	C 37	N 12	O 12	0	0

- 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
15	a	1	Total 10	C 7	N 3	0
15	a	1	Total 10	C 7	N 3	0

- 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	101	101	101	0
17	d	1	1	1	0

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

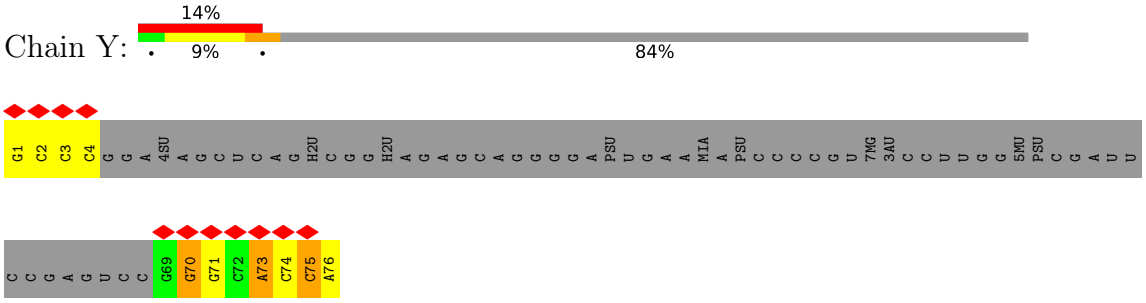
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
18	a	42	42	42	0
18	e	1	1	1	0

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.

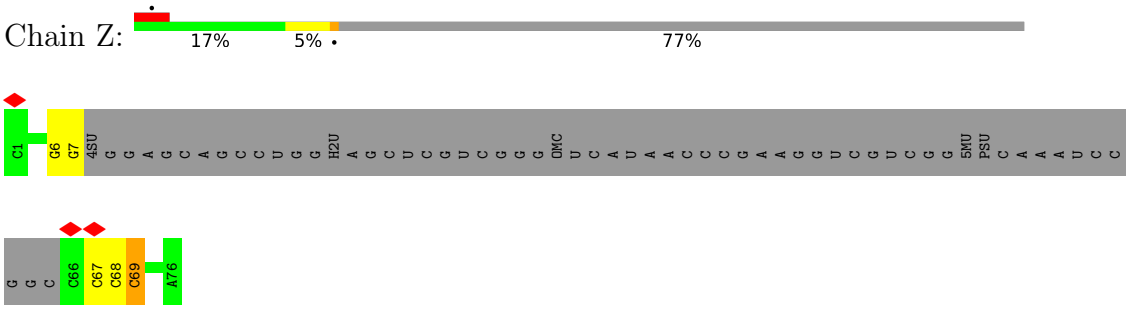
- Molecule 1: tRNA(Phe)

Chain Y:



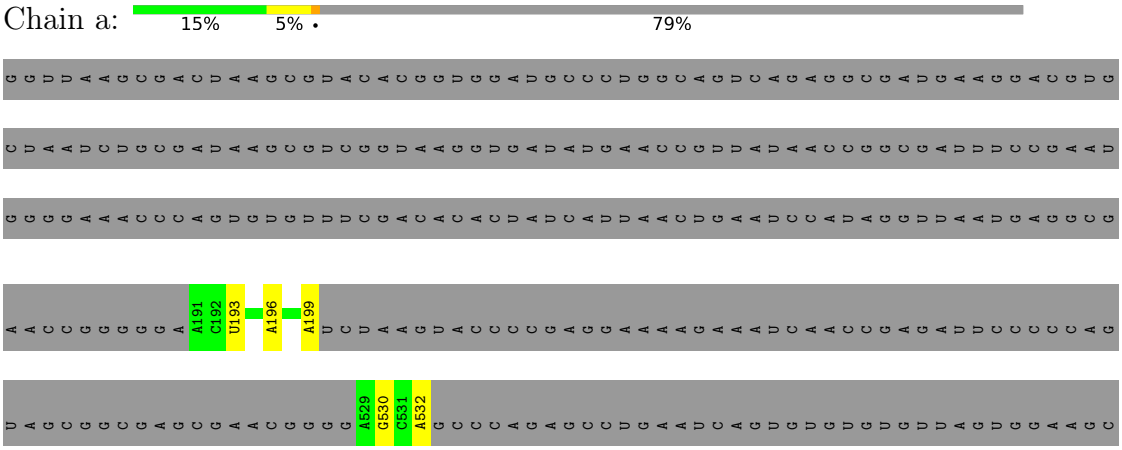
- Molecule 2: tRNA(fMet)

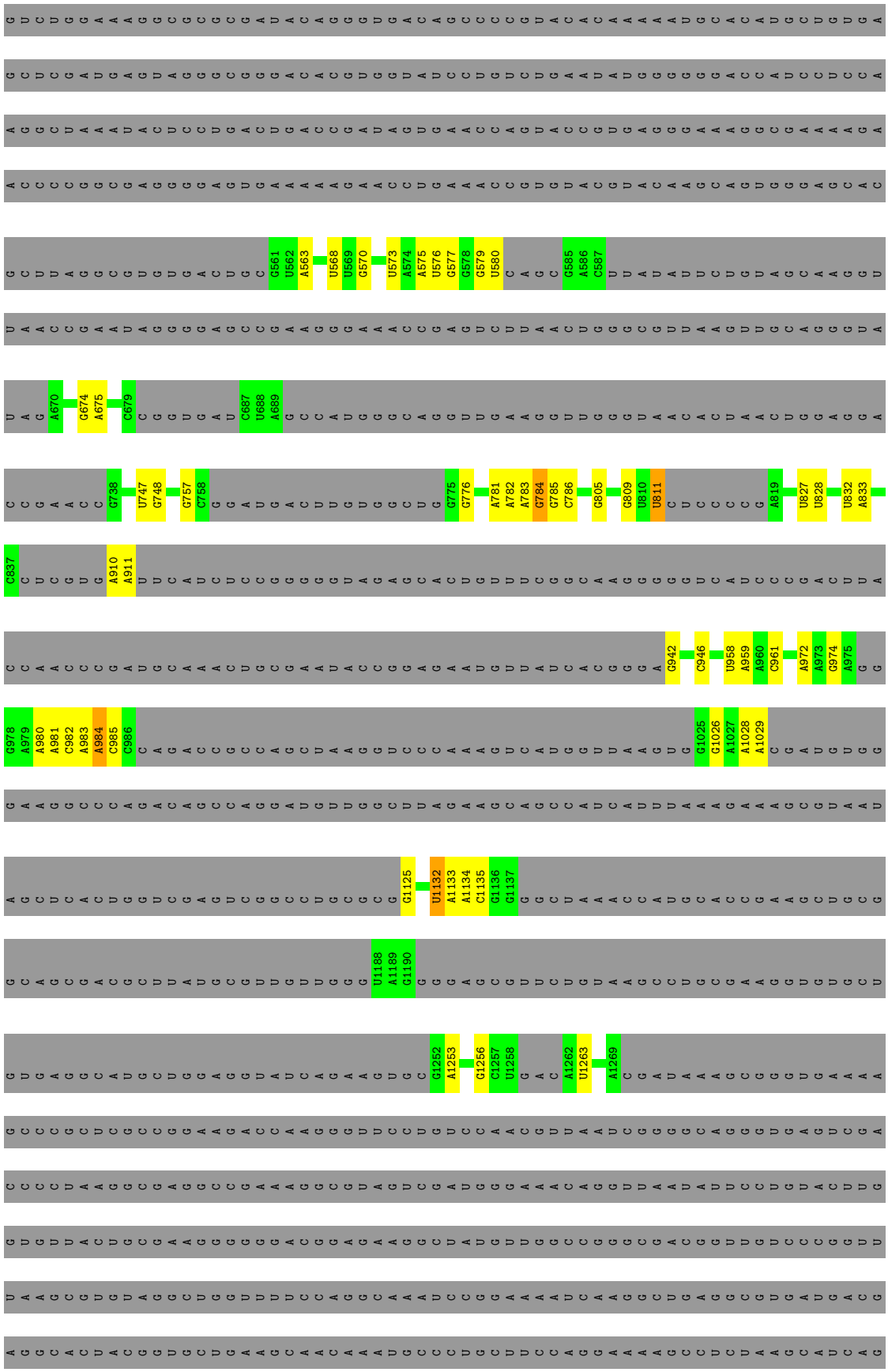
Chain Z:

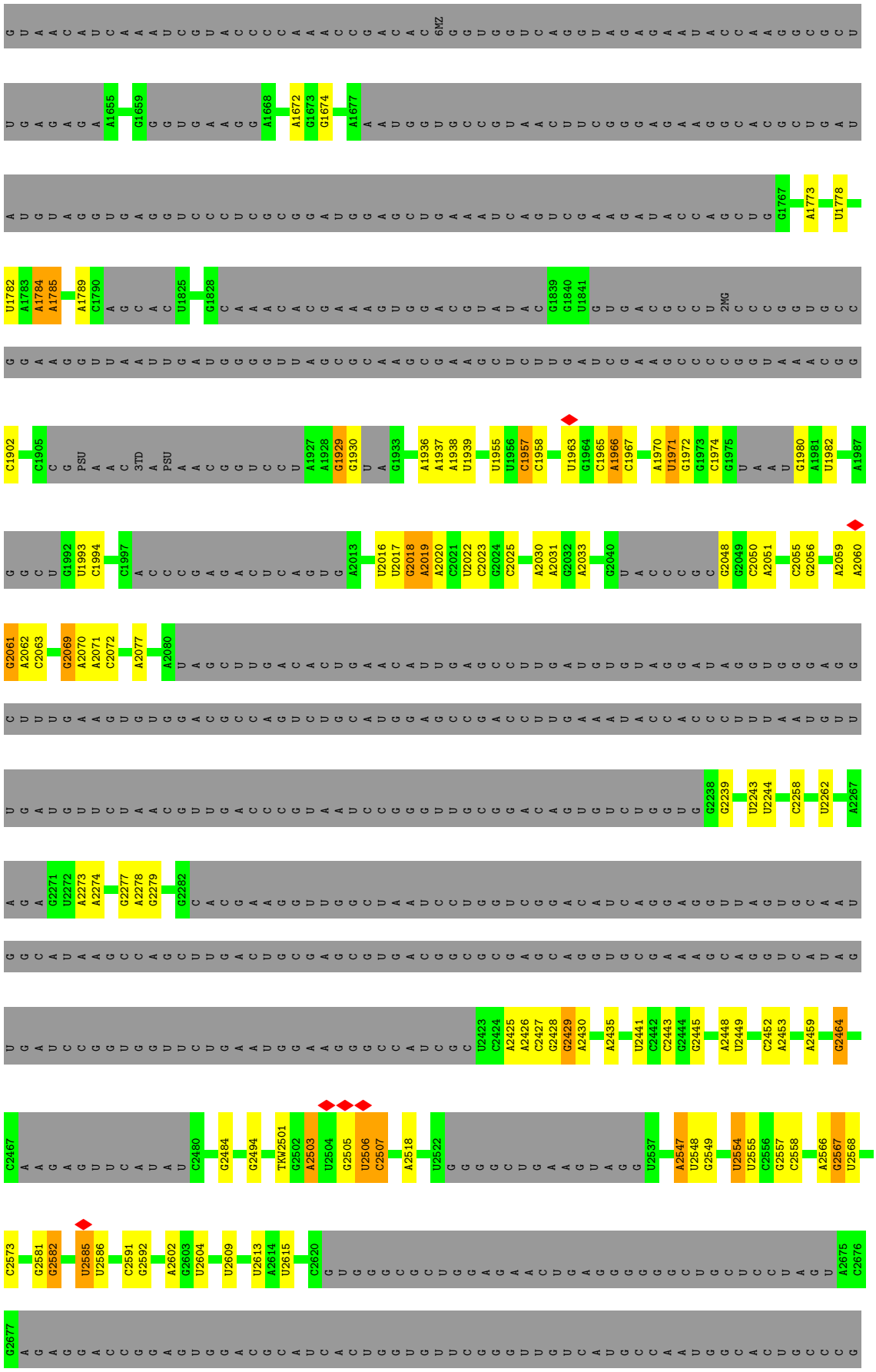


- Molecule 3: 23S rRNA

Chain a:




G561 U562 A563 U568 U569 G570 U573 A574 A575 U576 G577 G578 G579 U580 G585 A586 C587
A670 G674 A675 C679 C687 U688 A689
G738 U747 G748 G757 C758 G775 G776 A781 A782 A783 G784 G785 C786 G805 G809 U810 U811 A819 U827 U828 U832 A833
C837 A910 A911
G942 C946 U958 A959 A960 C961 A972 A973 G974 A975
G978 A979 A980 A981 C982 A983 A984 C985 C986 G1025 G1026 A1027 A1028 A1029
G1125 U1132 A1133 A1134 C1135 G1136 G1137
U1188 A1189 G1190
G1252 A1253 G1256 C1257 U1258 A1262 U1263 A1269


6MZ
A1655
G1659
A1668
A1672
G1673
G1674
A1677
G1767
A1773
U1778
U1782
A1783
A1784
A1785
A1789
C1790
U1825
G1828
G1839
G1840
U1841
2MG
C1902
C1905
PSU
3TD
PSU
A1927
A1928
G1929
G1930
G1933
A1936
A1937
A1938
U1939
U1955
U1956
C1957
C1958
U1963
G1964
C1965
A1966
C1967
A1970
U1971
G1972
G1973
C1974
G1975
G1980
A1981
U1982
A1987
G1992
U1993
C1994
C1997
A2013
U2016
U2017
G2018
A2019
A2020
C2021
U2022
C2023
G2024
C2025
A2030
A2031
G2032
A2033
G2040
C2048
G2049
C2050
A2051
C2055
G2056
A2059
A2060
G2061
A2062
C2063
G2069
A2070
A2071
C2072
A2077
A2080
G2238
G2239
U2243
U2244
C2258
U2262
A2267
G2271
U2272
A2273
A2274
G2277
A2278
G2279
G2282
U2423
C2424
A2425
A2426
C2427
G2428
G2429
A2430
A2435
U2441
C2442
C2443
G2444
G2445
A2448
U2449
C2452
A2453
A2459
G2464
C2467
C2480
G2484
G2494
TKW2501
G2502
A2503
U2504
G2505
U2506
C2507
A2518
U2522
U2537
A2547
U2548
G2549
U2554
U2555
C2556
C2557
C2558
A2566
G2567
U2568
C2573
G2581
G2582
U2585
U2586
C2591
G2592
A2602
G2603
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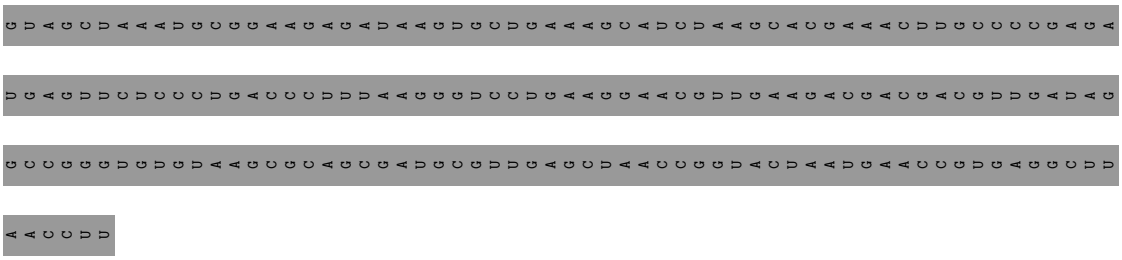
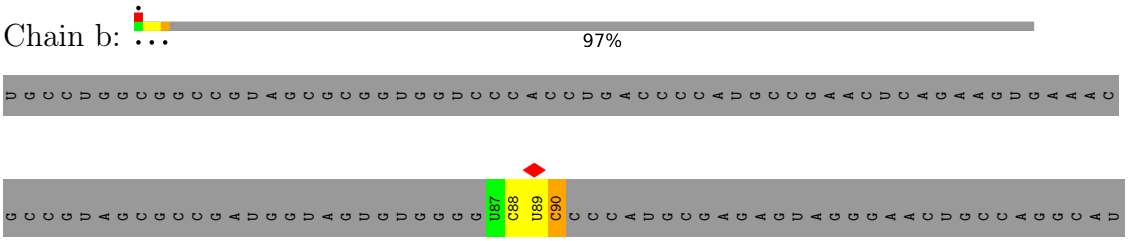
U2609
U2613
A2614
U2615
C2620
A2675
C2676
G2677



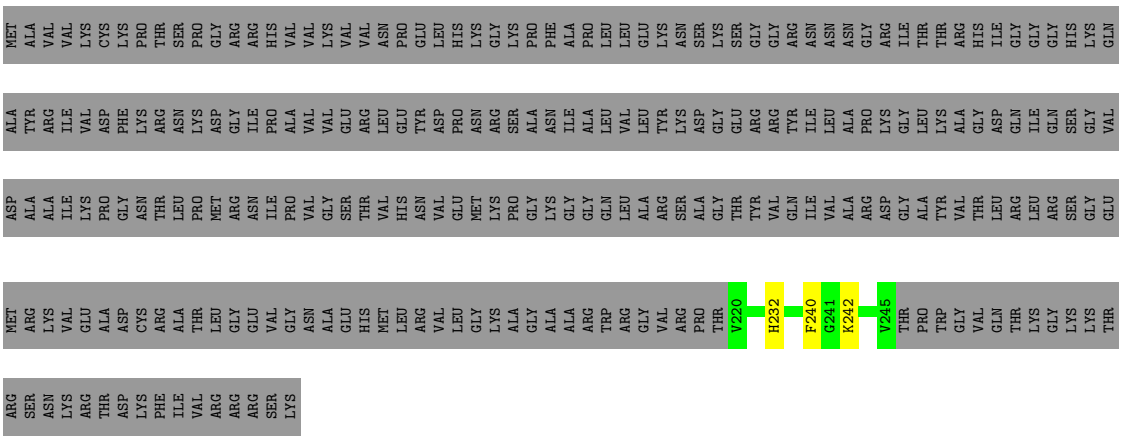
• Molecule 4: 5S rRNA

Chain b: 97%



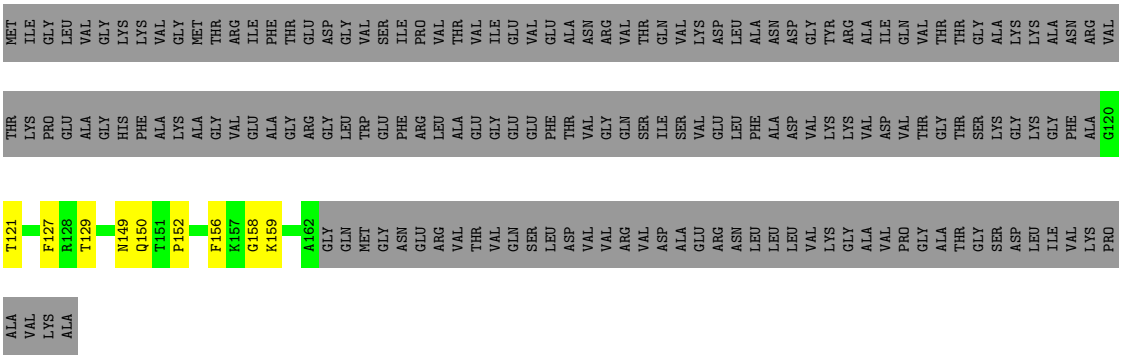
• Molecule 5: Large ribosomal subunit protein uL2

Chain c: 8% 90%



• Molecule 6: Large ribosomal subunit protein uL3

Chain d: 16% 79%



• Molecule 7: Large ribosomal subunit protein uL4

Chain e: 8% 92%

MET GLU LEU VAL LEU LYS ASP ALA GLN SER ALA LEU THR VAL SER GLU THR THR PHE GLY ARG ASP PHE ASN GLU ALA LEU VAL HIS GLN VAL VAL VAL ALA TYR ALA ALA GLY ALA ARG GLN GLY THR ARG ALA GLN LYS THR ARG ALA GLU VAL THR GLY SER G56 K57 K58 P59 W60

R61 GLN LYS GLY THR GLY ARG A68 R69 S70 W78 ARG SER GLY GLY VAL THR PHE ALA ALA ARG PRO GLN ASP HIS SER GLN LYS VAL ASN LYS LYS MET TYR ARG GLY ALA LEU LYS SER ILE LEU SER GLU LEU VAL ARG GLN ASP ARG LEU ILE VAL VAL GLU LYS PHE SER VAL

GLU ALA PRO LYS THR LYS LEU LEU ALA GLN LYS LEU LYS ASP MET ALA LEU GLU ASP VAL LEU ILE ILE THR GLY GLU LEU ASP GLU ASN LEU PHE LEU ALA ALA ARG ASN LEU HIS LYS VAL ASP VAL ARG ASP ALA THR GLY ILE ASP PRO VAL SER LEU ILE ALA PHE ASP LYS VAL

VAL MET THR ALA ASP ALA VAL LYS GLN VAL GLU GLU MET LEU ALA

- Molecule 8: Large ribosomal subunit protein uL13

Chain i: 5% 94%

MET LYS THR PHE THR ALA LYS PRO GLU THR VAL LYS ARG ASP TRP TYR VAL VAL ASP ALA THR GLY LYS THR LEU GLY ARG LEU ALA THR GLU LEU ALA ARG ARG LEU ARG GLY LYS HIS LYS ALA GLU TYR THR PRO HIS VAL ASP THR GLY ASP TYR ILE ILE VAL LEU ASN ALA ASP

LYS VAL ALA VAL THR GLY ASN LYS ARG THR ASP LYS VAL TYR TYR HIS H77 I81 I84 LYS GLN ALA THR PHE GLU GLU MET ILE ALA ARG ARG PRO GLU ARG VAL ILE GLU ILE ALA VAL LYS GLY MET LEU PRO LYS GLY PRO LEU GLY ARG ALA MET PHE ARG LYS LEU LYS

VAL TYR ALA GLY ASN GLU HIS ASN HIS ALA ALA GLN GLN PRO GLN VAL LEU ASP ILE

- Molecule 9: Large ribosomal subunit protein uL15

Chain k: 17% 82%

MET ARG LEU ASN THR LEU SER PRO ALA GLU GLY SER LYS LYS ALA GLY LYS ARG LEU GLY ARG GLY ILE GLY SER GLY LEU G28 R41 R47 ARG GLY F50 M55 PRO LEU TYR ARG ARG LEU PRO LYS PHE GLY PHE THR SER ARG LYS ALA ALA ILE THR ALA GLU ILE ARG

LEU SER ASP LEU ALA LYS VAL GLU GLY GLY VAL VAL ASP LEU ASN THR LEU LYS ALA ALA ASN ILE ILE GLY ILE GLN ILE GLU PHE ALA LYS VAL ILE LEU ALA GLY GLU VAL THR THR PRO VAL THR VAL ARG GLY LEU ARG VAL THR LYS GLY ALA ARG ALA ALA ILE GLU ALA ALA

GLY GLY LYS ILE GLU GLU

- Molecule 10: Large ribosomal subunit protein uL16

Chain l: 31% 65%

MET LEU GLN PRO LYS ARG THR LYS F9 A21 GLN GLY THR ASP VAL SER PHE GLY SER PHE GLY LEU LYS ALA VAL GLY R38 R44 Q45 ILE GLU ALA ALA ARG ARG ALA MET THR ARG ALA VAL LYS ARG GLN GLY LYS ILE TRP ILE ARG VAL PHE P69 T74 E75 4D481

N88 V89 E90 L95 ILE GLN PRO GLY LYS VAL LEU TYR GLU MET ASP GLY VAL PRO GLU GLU LEU ALA ARG GLU ALA PHE LYS LEU ALA ALA ALA LYS LEU PRO ILE LYS THR THR PHE VAL THR LYS THR VAL MET

- Molecule 11: Large ribosomal subunit protein bL21

Chain q: 7% 93%

MET TYR ALA VAL PHE GLN SER GLY GLY LYS GLN HIS ARG VAL SER GLU GLY GLN THR VAL ARG LEU GLU LYS LEU ASP ILE ALA THR GLY GLU THR VAL GLU PHE ALA GLU VAL LEU MET ILE ALA ASN GLY GLU GLU VAL LYS ILE GLY VAL PRO PHE VAL ASP GLY GLY VAL ILE LYS

ALA GLU VAL VAL ALA HIS GLY ARG GLY GLU LYS VAL LYS ILE VAL LYS F77 Y83 ARG LYS GLN GLN GLN GLY HIS ARG GLN TRP PHE THR ASP VAL LYS ILE THR GLY ILE SER ALA

- Molecule 12: Large ribosomal subunit protein uL22

Chain r: 6% 94%

MET GLU THR ILE ALA LYS HIS ARG HIS ALA ARG SER SER ALA GLN LYS VAL ARG LEU VAL ALA ASP LEU ILE ARG GLY LYS LYS VAL SER GLN ALA LEU ASP ILE LEU THR TYR THR ASN LYS LYS ALA ALA VAL LEU VAL LYS LYS VAL LEU GLU SER ALA ILE ALA ASN ALA GLU HIS

ASN ASP GLY ALA ASP ILE ASP ASP LEU LYS VAL THR LYS ILE PHE VAL ASP GLU GLY PRO SER MET LYS ARG ILE MET PRO R88 D94 ARG ILE LEU LYS ARG THR SER HIS ILE THR VAL VAL VAL SER ASP ARG

- Molecule 13: Large ribosomal subunit protein bL27

Chain v: 19% 81%

MET A2 E17 ALA LYS ARG LEU GLY VAL LYS ARG PHE GLY GLY GLU SER VAL LEU ALA GLY SER ILE ILE VAL ARG GLN ARG GLY THR LYS PHE HIS ALA GLY ALA ASN VAL GLY CYS GLY ARG ASP HIS THR LEU PHE ALA LYS ALA ASP GLY LYS VAL LYS PHE GLU VAL LYS GLY

PRO LYS ASN ARG LYS PHE ILE SER ILE GLU ALA GLU

- Molecule 14: Large ribosomal subunit protein bL32

Chain z: 9% 5% 86%

MET A2 V3 Q4 P8 T9 ARG SER LYS ARG GLY MET ARG ARG SER HIS ASP ALA LEU THR ALA VAL THR SER LEU SER VAL ASP LYS THR SER GLY GLU LYS HIS LEU ARG HIS HIS ILE THR ALA ASP GLY TYR TYR ARG GLY ARG LYS VAL ILE ALA LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53040	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	0.497	Depositor
Minimum map value	-0.133	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: MEQ, 4D4, 2MG, G7M, 6MZ, OMC, 1MG, 5MC, MG, PUT, H2U, K, TKW, SR0, OMG, MS6, 2MA, 5MU, PSU

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	0.61	0/285	0.83	0/438
2	Z	0.56	0/427	0.82	0/661
3	a	0.55	1/13812 (0.0%)	1.06	48/21450 (0.2%)
4	b	0.54	0/87	1.12	1/132 (0.8%)
5	c	0.74	0/197	1.01	0/265
6	d	0.69	0/329	1.11	1/438 (0.2%)
7	e	0.65	0/142	0.93	0/188
8	i	0.65	0/56	1.08	0/74
9	k	0.71	0/182	1.19	0/232
10	l	0.68	0/370	1.02	0/487
11	q	0.69	0/77	1.05	0/99
12	r	0.71	0/52	0.93	0/66
13	v	0.65	0/116	0.99	0/151
14	z	0.75	0/61	0.99	0/82
All	All	0.57	1/16193 (0.0%)	1.05	50/24763 (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
9	k	0	1
10	l	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	2069	G7M	O3'-P	5.24	1.61	1.56

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1132	U	O3'-P-O5'	-20.60	73.09	104.00
3	a	980	A	O3'-P-O5'	-12.69	84.96	104.00
3	a	1957	C	O3'-P-O5'	-11.25	87.13	104.00
3	a	1971	U	O3'-P-O5'	-10.77	87.84	104.00
3	a	980	A	C4'-C3'-O3'	8.73	126.09	113.00
3	a	1974	C	O3'-P-O5'	-8.59	91.12	104.00
3	a	781	A	O3'-P-O5'	-8.39	91.41	104.00
3	a	2278	A	O3'-P-O5'	-7.66	92.51	104.00
3	a	2051	A	O3'-P-O5'	-7.34	92.98	104.00
3	a	972	A	O3'-P-O5'	-7.27	93.10	104.00
3	a	1785	A	O3'-P-O5'	-7.17	93.24	104.00
3	a	1966	A	O3'-P-O5'	-6.68	93.98	104.00
3	a	982	C	C2'-C3'-O3'	-6.62	103.77	113.70
3	a	2018	G	C4'-C3'-O3'	-6.57	103.15	113.00
6	d	129	THR	CA-CB-OG1	-6.27	100.20	109.60
3	a	2279	G	O3'-P-O5'	-6.21	94.69	104.00
3	a	674	G	O3'-P-O5'	-6.14	94.79	104.00
3	a	2050	C	O3'-P-O5'	-6.10	94.84	104.00
3	a	2429	G	C2'-C3'-O3'	-6.05	104.63	113.70
3	a	2428	G	O3'-P-O5'	-5.87	95.20	104.00
3	a	2048	G	O3'-P-O5'	-5.84	95.23	104.00
3	a	1902	C	O3'-P-O5'	-5.83	95.26	104.00
3	a	1971	U	C2'-C3'-O3'	-5.81	104.98	113.70
3	a	2018	G	O3'-P-O5'	-5.81	95.29	104.00
3	a	1957	C	C4'-C3'-O3'	-5.77	104.35	113.00
3	a	2025	C	C2'-C3'-O3'	-5.73	105.11	113.70
3	a	1929	G	O3'-P-O5'	-5.70	95.46	104.00
3	a	2262	U	P-O3'-C3'	-5.68	111.68	120.20
3	a	2277	G	O3'-P-O5'	-5.67	95.50	104.00
3	a	748	G	C1'-O4'-C4'	-5.61	104.29	109.90
3	a	2022	U	O3'-P-O5'	-5.58	95.64	104.00
3	a	193	U	O3'-P-O5'	-5.57	95.64	104.00
3	a	786	C	C3'-C2'-O2'	5.48	118.92	110.70
3	a	2585	U	O3'-P-O5'	-5.40	95.89	104.00
3	a	2464	G	C3'-C2'-O2'	-5.34	102.69	110.70
3	a	811	U	C2'-C3'-O3'	5.29	117.44	109.50
3	a	784	G	O3'-P-O5'	-5.29	96.07	104.00
3	a	2050	C	C4'-C3'-O3'	-5.28	105.08	113.00
3	a	784	G	C2'-C3'-O3'	-5.25	105.83	113.70
3	a	580	U	C4'-C3'-O3'	5.24	120.86	113.00
3	a	2059	A	C2'-C3'-O3'	-5.24	105.85	113.70
3	a	2019	A	O3'-P-O5'	-5.19	96.22	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	1789	A	O3'-P-O5'	-5.18	96.23	104.00
3	a	1936	A	C1'-O4'-C4'	-5.17	104.53	109.70
4	b	90	C	C4'-C3'-C2'	-5.12	97.48	102.60
3	a	1936	A	O4'-C1'-C2'	-5.10	100.70	105.80
3	a	757	G	C4'-C3'-C2'	-5.06	97.54	102.60
3	a	809	G	C4'-C3'-O3'	-5.06	105.41	113.00
3	a	783	A	O3'-P-O5'	-5.05	96.43	104.00
3	a	942	G	C2'-C3'-O3'	-5.04	106.13	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	7	0
2	Z	384	0	200	2	0
3	a	12772	0	6469	41	0
4	b	80	0	43	0	0
5	c	191	0	177	2	0
6	d	333	0	336	5	0
7	e	138	0	145	0	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	0	0
16	a	6	0	12	1	0
17	a	101	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	d	1	0	0	0	0
18	a	42	0	0	0	0
18	e	1	0	0	0	0
All	All	15254	0	8448	59	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 (59) 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	1.63	0.79
1:Y:73:A:H2'	1:Y:74:C:C6	2.31	0.66
3:a:2061:G:H1'	3:a:2503:2MA:CM2	2.25	0.66
3:a:1778:U:H2'	3:a:1784:A:N6	2.14	0.63
5:c:232:HIS:HA	5:c:242:LYS:HD2	1.82	0.60
3:a:2547:A:H2'	3:a:2548:U:C6	2.40	0.57
3:a:2061:G:H1'	3:a:2503:2MA:HM23	1.85	0.57
3:a:1028:A:H2'	3:a:1029:A:C8	2.40	0.56
6:d:156:PHE:CE1	8:i:81:ILE:HD13	2.40	0.56
3:a:2273:A:H2'	3:a:2274:A:C8	2.42	0.55
1:Y:2:C:H2'	1:Y:3:C:C6	2.42	0.54
3:a:2020:A:H5'	14:z:9:THR:CG2	2.38	0.54
1:Y:74:C:H2'	1:Y:75:C:C2	2.43	0.53
3:a:1028:A:N6	3:a:1125:G:H2'	2.25	0.52
10:l:74:THR:HA	10:l:88:ASN:O	2.10	0.52
3:a:2061:G:H1'	3:a:2503:2MA:HN1	1.76	0.51
3:a:2243:U:H2'	3:a:2244:U:C6	2.46	0.51
3:a:2591:C:H2'	3:a:2592:G:C8	2.46	0.51
3:a:2445:2MG:HM21	3:a:2449:H2U:O4	2.11	0.49
3:a:2506:U:H2'	3:a:2507:C:H5'	1.94	0.49
10:l:75:GLU:HB2	10:l:90:GLU:HG3	1.93	0.49
2:Z:68:C:H2'	2:Z:69:C:O4'	2.13	0.48
3:a:832:U:H2'	3:a:833:A:C8	2.50	0.47
3:a:1994:C:OP1	16:a:3003:PUT:H41	2.14	0.47
1:Y:3:C:H2'	1:Y:4:C:C6	2.50	0.46
3:a:2452:C:H2'	3:a:2453:A:C8	2.50	0.46
3:a:1672:A:C2	3:a:2582:G:H5'	2.50	0.46
3:a:579:G:O2'	3:a:2019:A:OP1	2.35	0.45
3:a:1963:U:O2	3:a:1963:U:H2'	2.18	0.44
3:a:2016:U:H2'	3:a:2017:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:2554:U:H2'	3:a:2555:U:C6	2.53	0.43
5:c:240:PHE:O	5:c:242:LYS:HE3	2.18	0.43
3:a:1939:5MU:OP1	3:a:2604:PSU:O2'	2.36	0.43
3:a:1966:A:N3	3:a:2592:G:O2'	2.45	0.43
3:a:2567:G:H2'	3:a:2568:U:C6	2.54	0.43
6:d:152:PRO:HG3	6:d:156:PHE:CZ	2.54	0.43
3:a:2020:A:H5'	14:z:9:THR:HG21	2.00	0.42
3:a:2258:C:O2'	3:a:2426:A:H4'	2.20	0.42
3:a:2557:G:H2'	3:a:2558:C:C6	2.54	0.42
1:Y:70:G:H2'	1:Y:71:G:H8	1.83	0.42
1:Y:73:A:H2'	1:Y:74:C:H6	1.81	0.42
6:d:121:THR:HB	6:d:127:PHE:CD2	2.54	0.42
6:d:149:ASN:OD1	6:d:150:MEQ:N	2.52	0.42
3:a:570:G:H2'	3:a:2030:6MZ:N7	2.35	0.42
3:a:1957:C:H2'	3:a:1958:C:C6	2.55	0.42
3:a:2258:C:O2'	3:a:2427:C:OP2	2.31	0.41
1:Y:1:G:H2'	1:Y:2:C:C6	2.55	0.41
3:a:2615:U:C2	14:z:4:GLN:HA	2.56	0.41
3:a:2071:A:H2'	3:a:2072:C:C6	2.55	0.41
3:a:576:U:H2'	3:a:577:G:C8	2.56	0.41
3:a:2018:G:O2'	3:a:2019:A:H5'	2.21	0.41
3:a:675:A:N3	3:a:2443:C:O2'	2.47	0.40
3:a:984:A:H2'	3:a:984:A:N3	2.36	0.40
3:a:2070:A:H2'	3:a:2071:A:O4'	2.21	0.40
3:a:1980:G:O2'	3:a:1982:U:OP2	2.35	0.40
6:d:158:GLY:O	6:d:159:LYS:C	2.64	0.40
3:a:910:A:C6	3:a:911:A:C6	3.09	0.40
2:Z:67:C:H2'	2:Z:68:C:C6	2.56	0.40
3:a:1263:U:O2'	14:z:8:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	c	24/273 (9%)	23 (96%)	1 (4%)	0	100	100
6	d	40/209 (19%)	36 (90%)	4 (10%)	0	100	100
7	e	13/201 (6%)	13 (100%)	0	0	100	100
8	i	6/142 (4%)	6 (100%)	0	0	100	100
9	k	22/144 (15%)	19 (86%)	3 (14%)	0	100	100
10	l	40/136 (29%)	40 (100%)	0	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%)	12 (86%)	2 (14%)	0	100	100
14	z	6/57 (10%)	6 (100%)	0	0	100	100
All	All	175/1460 (12%)	165 (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	14/165 (8%)	13 (93%)	1 (7%)	13	18
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%)	11 (100%)	0	100	100
14	z	7/48 (15%)	7 (100%)	0	100	100
All	All	153/1160 (13%)	152 (99%)	1 (1%)	73	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	e	70	SER

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

Mol	Chain	Res	Type
9	k	54	GLN
14	z	6	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Y	10/76 (13%)	4 (40%)	0
2	Z	16/77 (20%)	3 (18%)	0
3	a	559/2904 (19%)	87 (15%)	0
4	b	3/120 (2%)	3 (100%)	0
All	All	588/3177 (18%)	97 (16%)	0

All (97) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Y	70	G
1	Y	73	A
1	Y	75	C
1	Y	76	A
2	Z	6	G
2	Z	7	G
2	Z	69	C
3	a	196	A
3	a	199	A
3	a	530	G
3	a	532	A
3	a	563	A
3	a	573	U
3	a	575	A
3	a	747	5MU
3	a	776	G
3	a	782	A
3	a	784	G
3	a	785	G

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Mol	Chain	Res	Type
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	959	A
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	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
3	a	2033	A
3	a	2055	C
3	a	2056	G
3	a	2060	A

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Mol	Chain	Res	Type
3	a	2061	G
3	a	2062	A
3	a	2063	C
3	a	2069	G7M
3	a	2077	A
3	a	2239	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	2464	G
3	a	2484	G
3	a	2494	G
3	a	2505	G
3	a	2506	U
3	a	2507	C
3	a	2518	A
3	a	2547	A
3	a	2549	G
3	a	2554	U
3	a	2566	A
3	a	2567	G
3	a	2573	C
3	a	2581	G
3	a	2582	G
3	a	2585	U
3	a	2586	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

There are no RNA pucker outliers to report.

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	2MG	a	2445	3	23,26,27	0.42	0	32,38,41	0.37	0
3	PSU	a	955	3	18,21,22	0.37	0	22,30,33	0.34	0
3	5MU	a	747	3	19,22,23	0.33	0	28,32,35	0.41	0
3	6MZ	a	2030	3	22,25,26	0.28	0	30,36,39	0.39	0
3	PSU	a	2604	3	18,21,22	0.33	0	22,30,33	0.40	0
3	OMC	a	2498	17,3	19,22,23	0.25	0	26,31,34	0.35	0
10	MS6	l	82	10	5,7,8	0.21	0	2,7,9	0.18	0
3	PSU	a	2457	3	18,21,22	0.34	0	22,30,33	0.35	0
3	TKW	a	2501	18,3	18,22,23	0.35	0	28,32,35	0.92	1 (3%)
3	G7M	a	2069	18,3	23,26,27	0.39	0	35,39,42	0.50	0
3	PSU	a	2580	18,3	18,21,22	0.30	0	22,30,33	0.58	0
10	4D4	l	81	10	9,11,12	0.62	0	8,13,15	1.65	3 (37%)
3	2MA	a	2503	17,18,3	22,25,26	1.10	4 (18%)	33,37,40	1.27	3 (9%)
3	H2U	a	2449	3	18,21,22	0.33	0	21,30,33	0.40	0
3	5MC	a	1962	18,3	18,22,23	0.30	0	26,32,35	0.33	0
3	5MU	a	1939	18,3	19,22,23	0.44	0	28,32,35	0.50	0
3	PSU	a	2504	18,3	18,21,22	0.24	0	22,30,33	0.41	0
3	PSU	a	2605	3	18,21,22	0.32	0	22,30,33	0.45	0
3	OMG	a	2251	18,3,2	23,26,27	0.39	0	33,38,41	0.27	0
6	MEQ	d	150	6	8,9,10	0.70	0	5,10,12	1.11	0
3	1MG	a	745	3	22,26,27	0.63	0	33,39,42	0.45	0
3	PSU	a	746	17,3	18,21,22	0.35	0	22,30,33	0.40	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
3	2MG	a	2445	3	-	0/9/27/28	0/3/3/3
3	PSU	a	955	3	-	0/7/25/26	0/2/2/2
3	5MU	a	747	3	-	0/7/25/26	0/2/2/2
3	6MZ	a	2030	3	-	2/9/27/28	0/3/3/3
3	PSU	a	2604	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	a	2498	17,3	-	0/9/27/28	0/2/2/2
10	MS6	l	82	10	-	1/4/6/8	-
3	PSU	a	2457	3	-	0/7/25/26	0/2/2/2
3	TKW	a	2501	18,3	-	4/7/25/26	0/2/2/2
3	G7M	a	2069	18,3	-	2/7/25/26	0/3/3/3
3	PSU	a	2580	18,3	-	0/7/25/26	0/2/2/2
10	4D4	l	81	10	-	1/11/12/14	-
3	2MA	a	2503	17,18,3	-	3/7/25/26	0/3/3/3
3	H2U	a	2449	3	-	0/7/38/39	0/2/2/2
3	5MC	a	1962	18,3	-	0/7/25/26	0/2/2/2
3	5MU	a	1939	18,3	-	0/7/25/26	0/2/2/2
3	PSU	a	2504	18,3	-	2/7/25/26	0/2/2/2
3	PSU	a	2605	3	-	0/7/25/26	0/2/2/2
3	OMG	a	2251	18,3,2	-	1/9/27/28	0/3/3/3
6	MEQ	d	150	6	-	3/8/9/11	-
3	1MG	a	745	3	-	0/7/25/26	0/3/3/3
3	PSU	a	746	17,3	-	1/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	2503	2MA	C6-N6	-3.07	1.26	1.34
3	a	2503	2MA	C2-N3	-2.36	1.29	1.34
3	a	2503	2MA	C6-N1	2.20	1.38	1.35
3	a	2503	2MA	C2-N1	2.12	1.37	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	2503	2MA	N6-C6-N1	4.74	123.73	117.03
3	a	2501	TKW	OAC-C5-C4	3.99	120.45	114.43
3	a	2503	2MA	C5-C6-N1	-3.13	113.61	119.01
10	l	81	4D4	O-C-CA	-3.01	116.90	124.78
3	a	2503	2MA	C2-N1-C6	2.80	122.44	118.08
10	l	81	4D4	NE-CZ-NH2	2.79	125.59	120.70
10	l	81	4D4	NH1-CZ-NE	-2.00	114.57	119.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	d	150	MEQ	C-CA-CB-CG
3	a	2251	OMG	C1'-C2'-O2'-CM2
3	a	2030	6MZ	O4'-C4'-C5'-O5'
3	a	2504	PSU	O4'-C4'-C5'-O5'
3	a	2504	PSU	C3'-C4'-C5'-O5'
6	d	150	MEQ	NE2-CD-CG-CB
6	d	150	MEQ	OE1-CD-CG-CB
3	a	2030	6MZ	C3'-C4'-C5'-O5'
3	a	2501	TKW	C2'-C1'-N1-C6
3	a	2503	2MA	C4'-C5'-O5'-P
3	a	2501	TKW	O4'-C1'-N1-C6
3	a	2069	G7M	C4'-C5'-O5'-P
3	a	2501	TKW	O4'-C1'-N1-C2
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'
3	a	2503	2MA	O4'-C4'-C5'-O5'
10	l	81	4D4	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	a	2445	2MG	1	0
3	a	2030	6MZ	2	0
3	a	2604	PSU	1	0
3	a	2503	2MA	3	0
3	a	2449	H2U	1	0
3	a	1939	5MU	1	0
6	d	150	MEQ	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	0.47	0	8,8,8	0.40	0
16	PUT	a	3003	-	5,5,5	0.35	0	4,4,4	0.17	0
15	SR0	a	3002	-	9,9,9	0.58	0	8,8,8	0.52	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	-	-	1/7/7/7	-
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 (4) 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	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	3003	PUT	1	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.

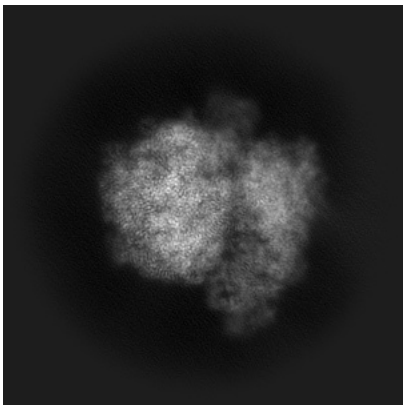
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55429. These allow visual inspection of the internal detail of the map and identification of artifacts.

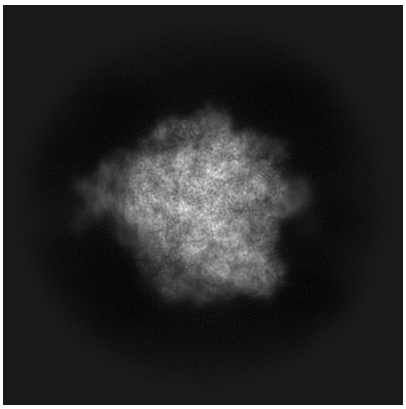
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

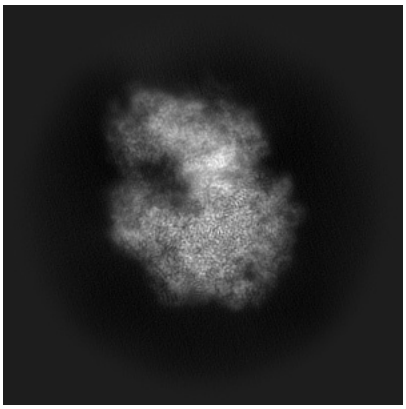
6.1.1 Primary map



X

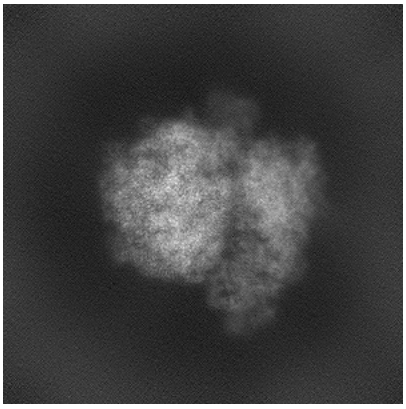


Y

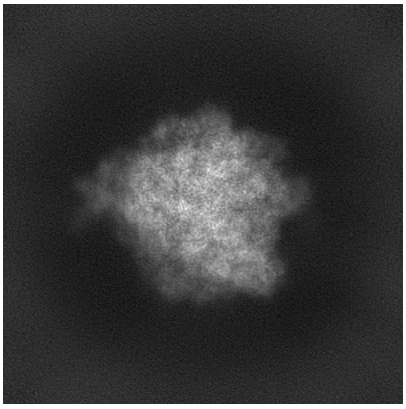


Z

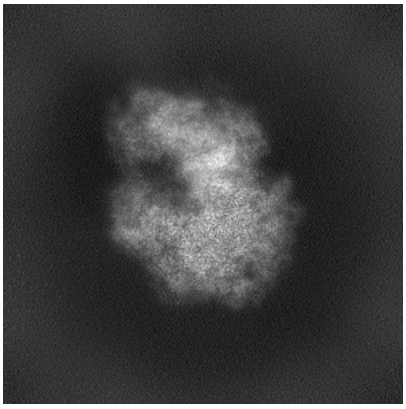
6.1.2 Raw map



X



Y

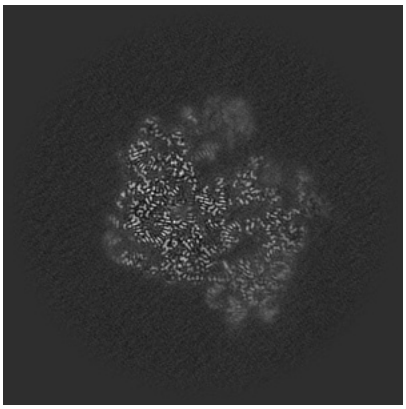


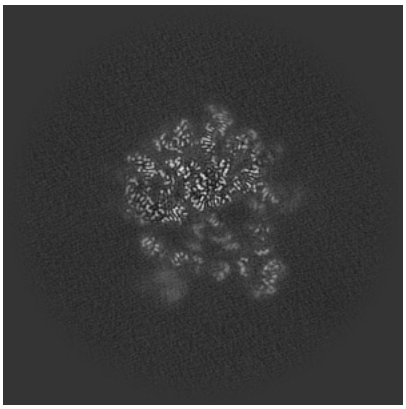
Z

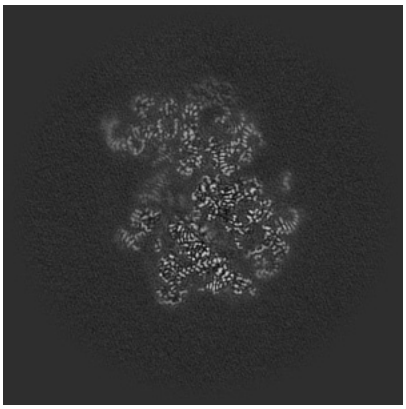
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

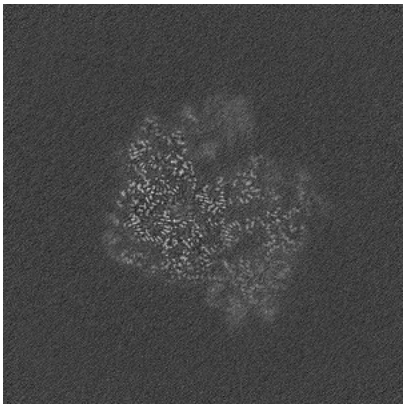
6.2.1 Primary map

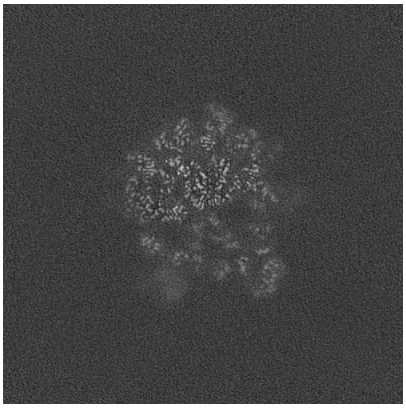

X Index: 256

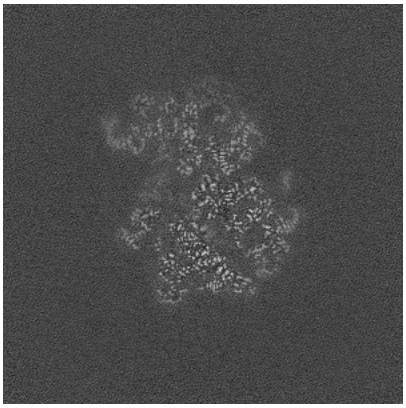

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

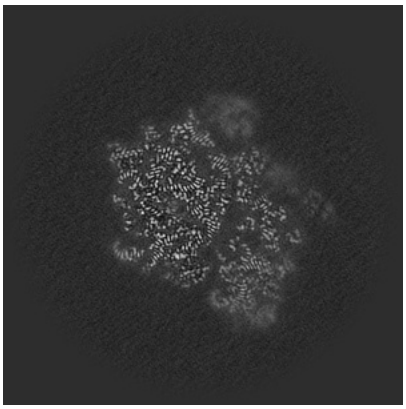

Y Index: 256

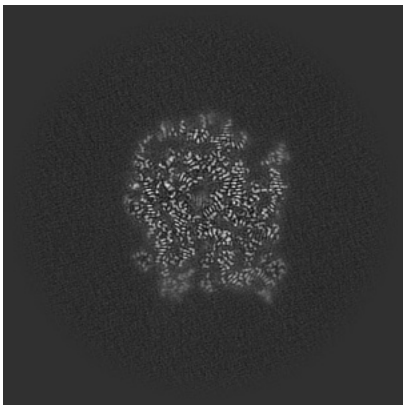

Z Index: 256

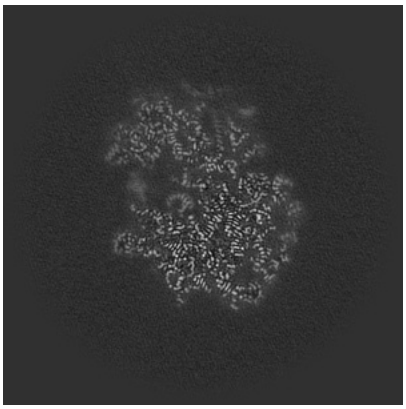
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

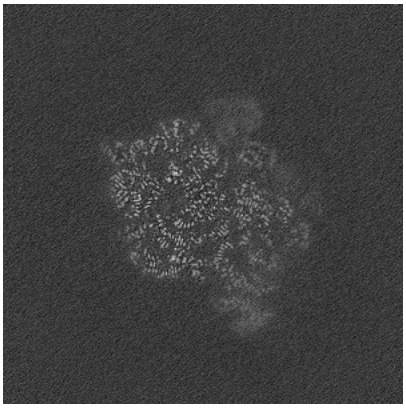
6.3.1 Primary map

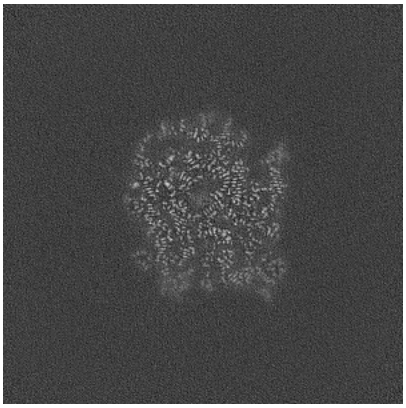

X Index: 267

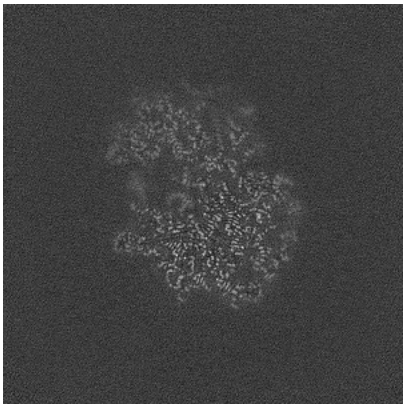

Y Index: 221


Z Index: 270

6.3.2 Raw map


X Index: 279

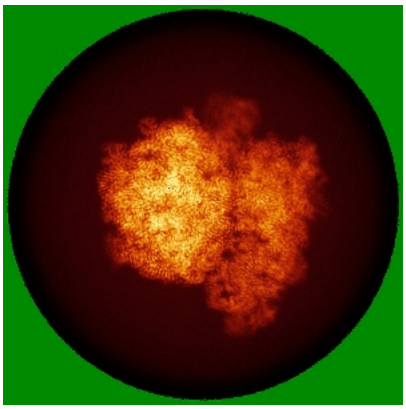

Y Index: 221

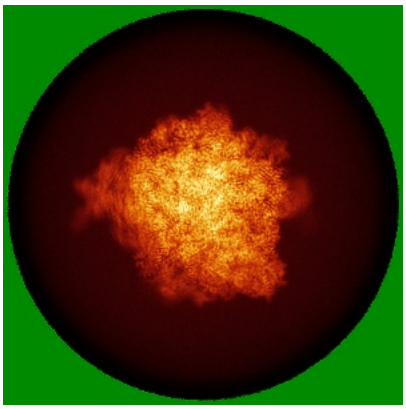

Z Index: 270

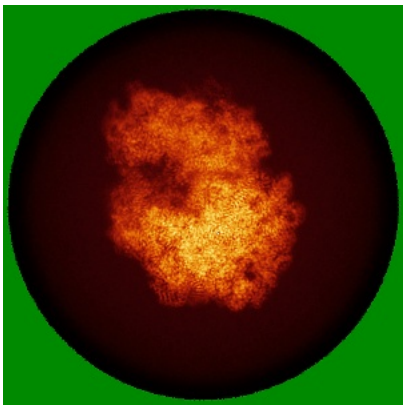
The images above show the largest variance slices of the map in three orthogonal directions.

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

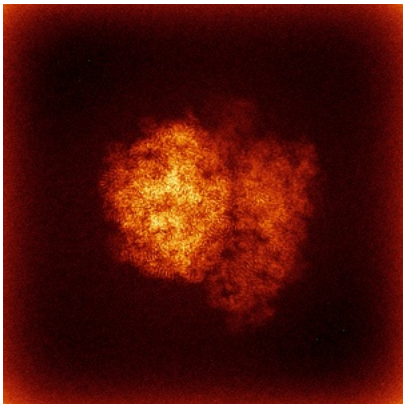
6.4.1 Primary map

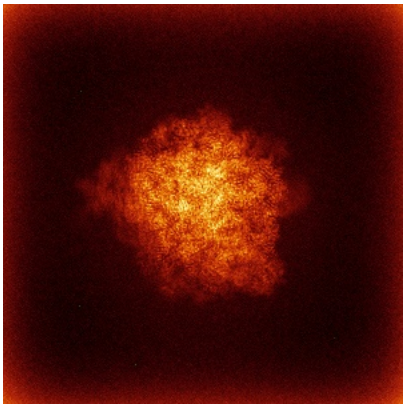

X

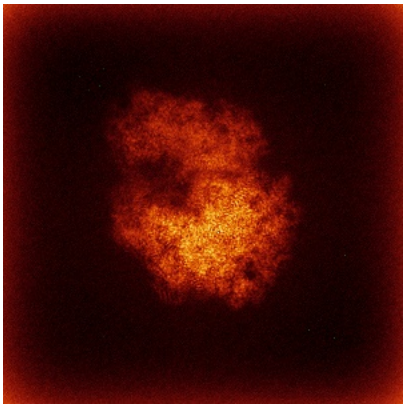

Y


Z

6.4.2 Raw map


X


Y

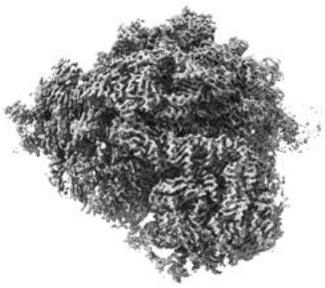

Z

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.

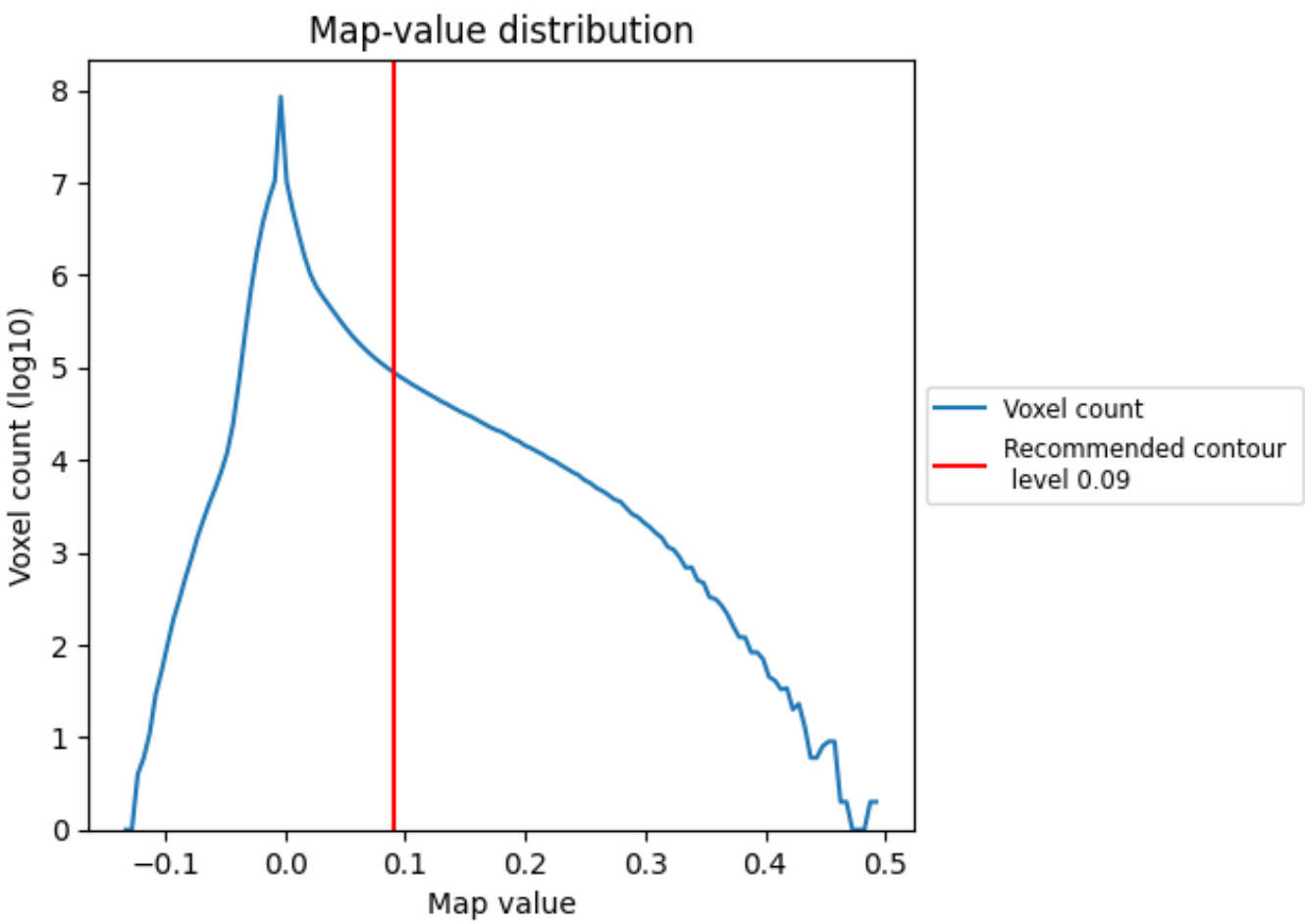
6.6 Mask visualisation (i)

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

7 Map analysis (i)

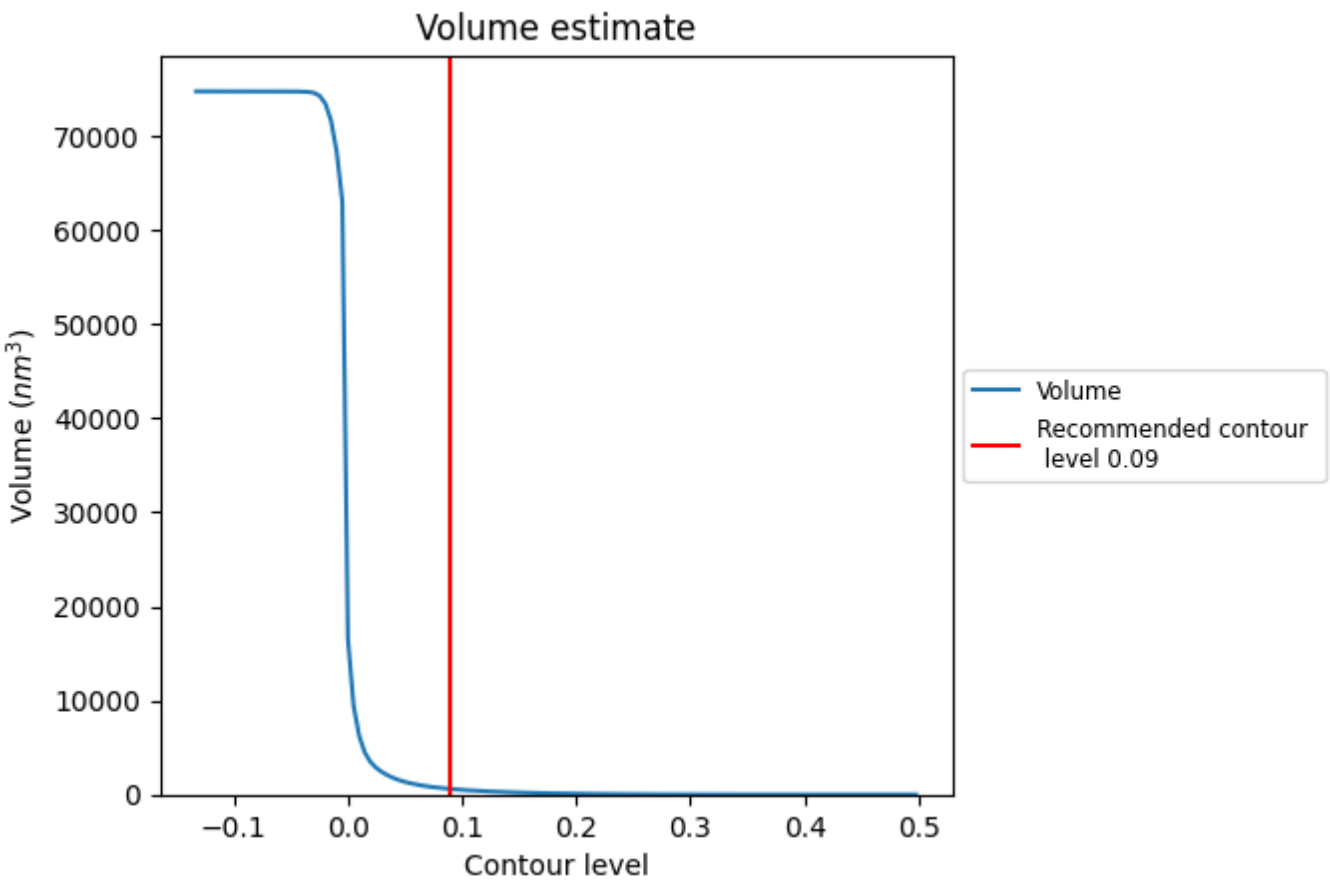
This section contains the results of statistical analysis of the map.

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.

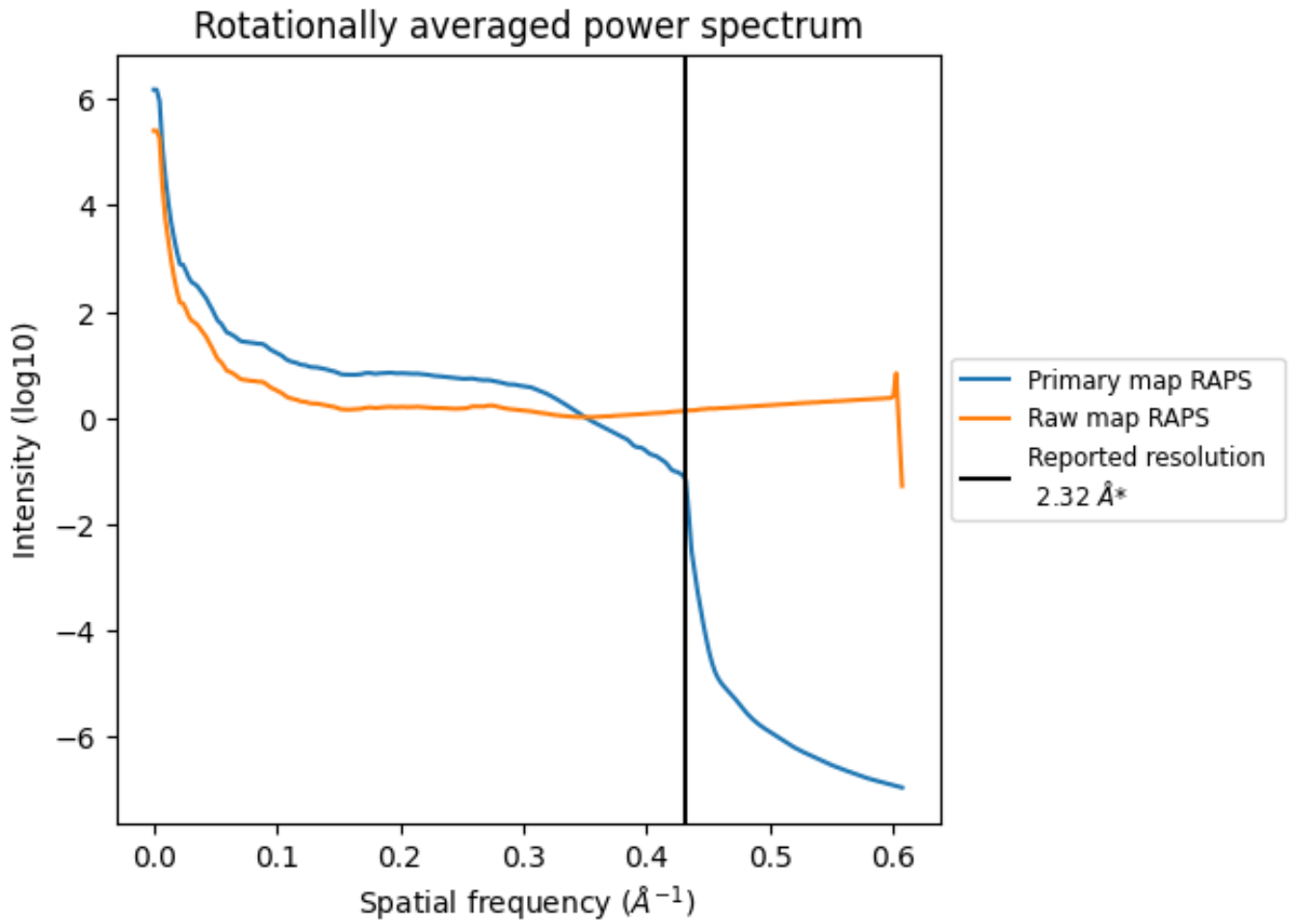
7.2 Volume estimate (i)



The volume at the recommended contour level is 598 nm^3; this corresponds to an approximate mass of 540 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)

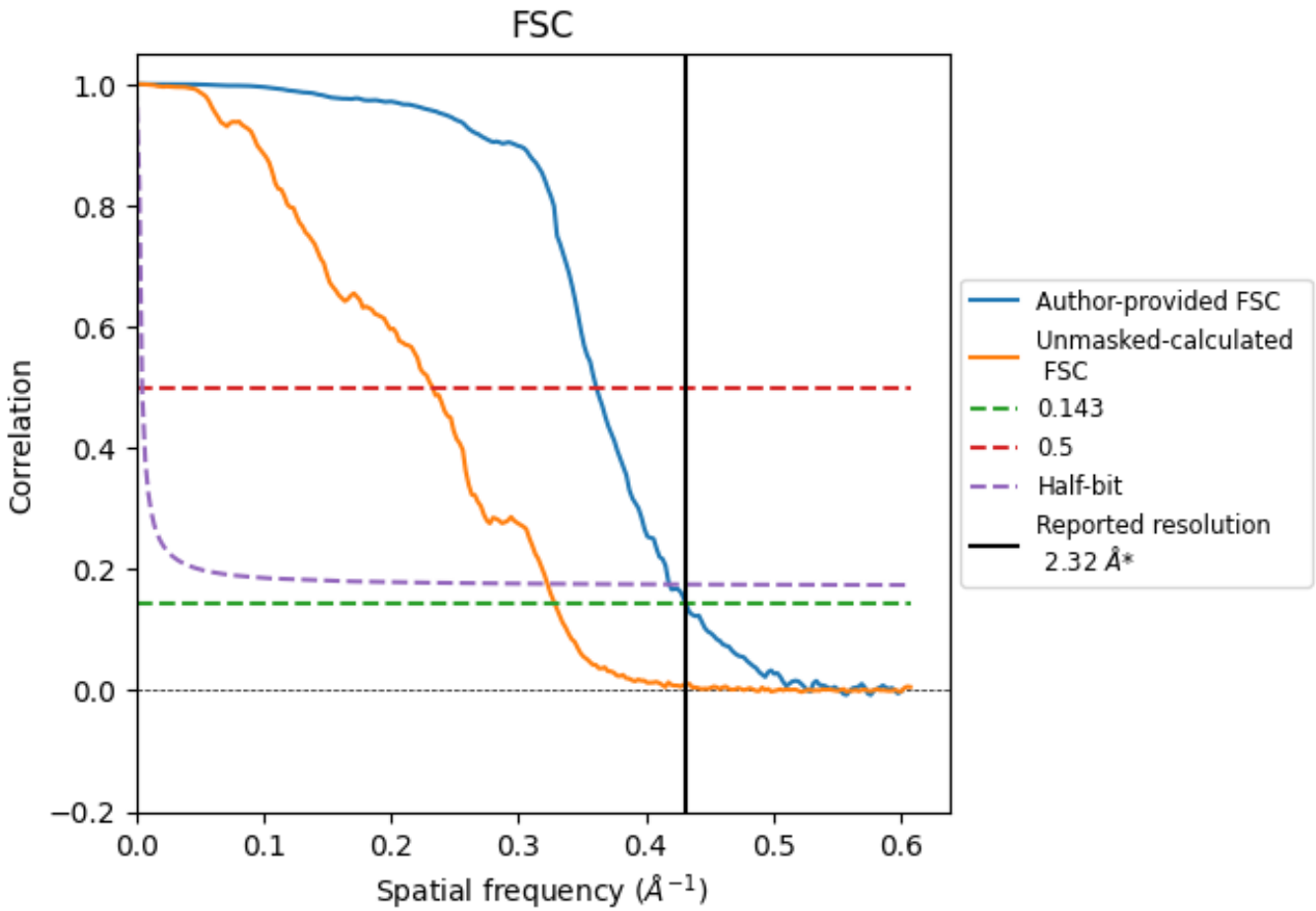


*Reported resolution corresponds to spatial frequency of 0.431 Å^{-1}

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 0.431 Å^{-1}

8.2 Resolution estimates (i)

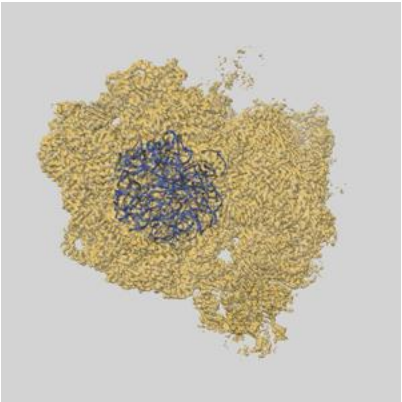
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.32	-	-
Author-provided FSC curve	2.32	2.77	2.39
Unmasked-calculated*	3.04	4.30	3.10

*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 3.04 differs from the reported value 2.32 by more than 10 %

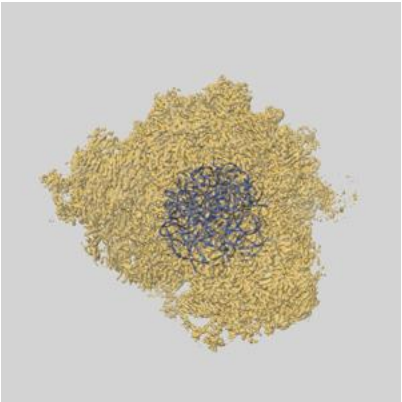
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55429 and PDB model 9T1B. Per-residue inclusion information can be found in section 3 on page 8.

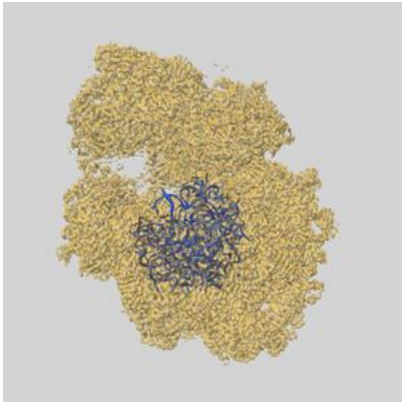
9.1 Map-model overlay (i)



X



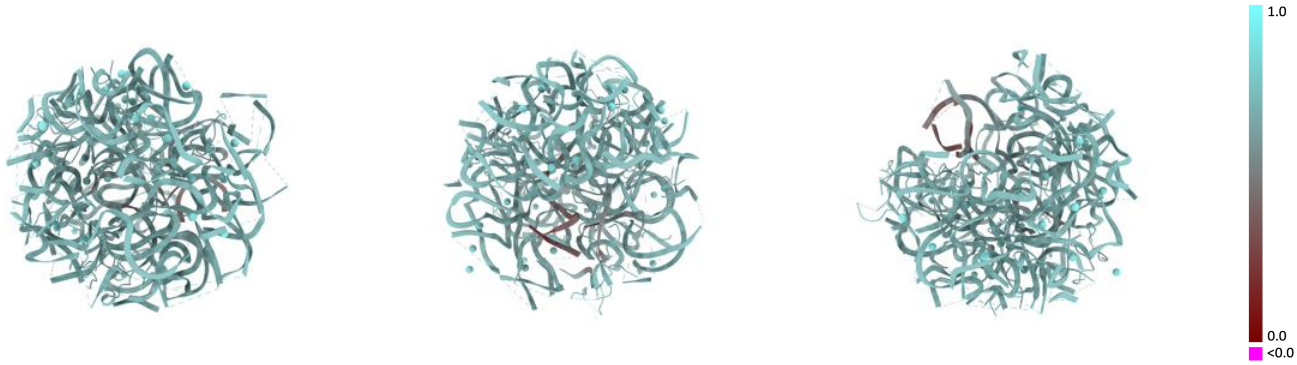
Y



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.

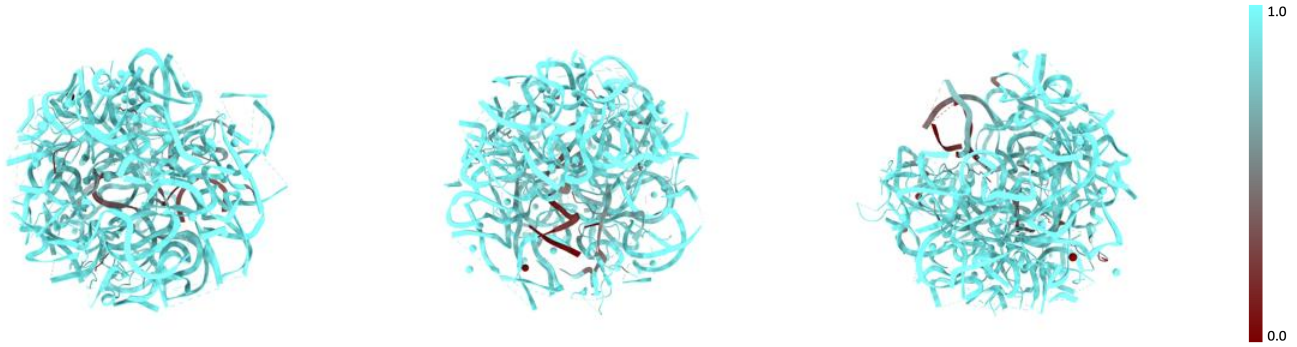
9.2 Q-score mapped to coordinate model (i)



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.

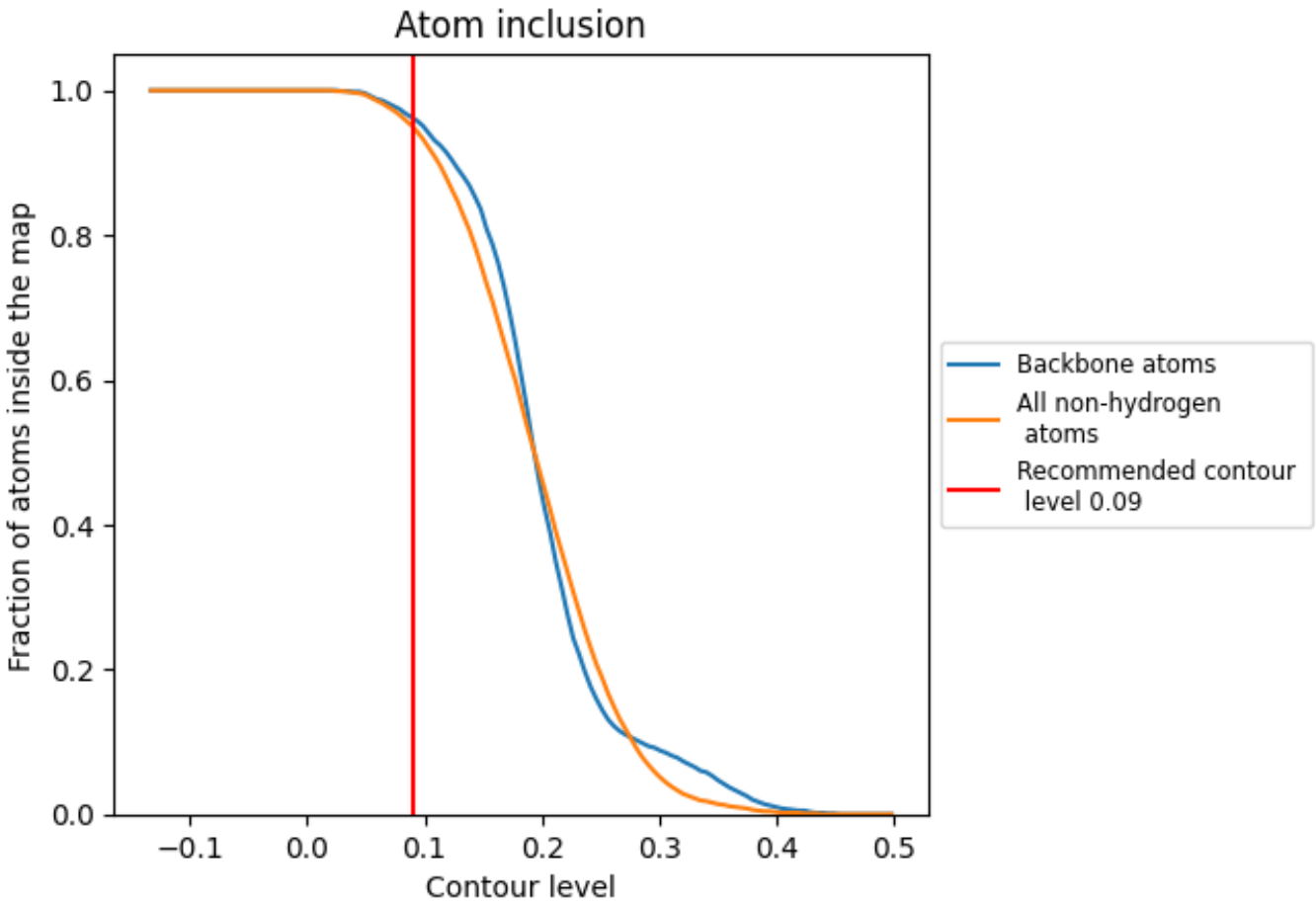
9.3 Atom inclusion mapped to coordinate model (i)



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, 96% of all backbone atoms, 95% 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	0.9500	0.6580
Y	0.1560	0.3550
Z	0.6800	0.5280
a	0.9800	0.6670
b	0.6880	0.5600
c	0.9570	0.6840
d	0.9540	0.6810
e	0.6390	0.5870
i	0.9820	0.6820
k	0.9660	0.6820
l	0.9220	0.6720
q	1.0000	0.6880
r	0.8570	0.6600
v	0.7680	0.6380
z	0.9840	0.6870