Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:13 am GMT

PDB ID	:	6HMA
EMDB ID	:	EMD-0243
Title	:	Improved model derived from cryo-EM map of Staphylococcus aureus large ribosomal subunit
Authors	:	Eyal, Z.; Cimicata, G.; Matzov, D.; Fox, T.; de Val, N.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on	:	2018-09-12
Resolution	:	2.65 Å(reported)

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

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

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

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

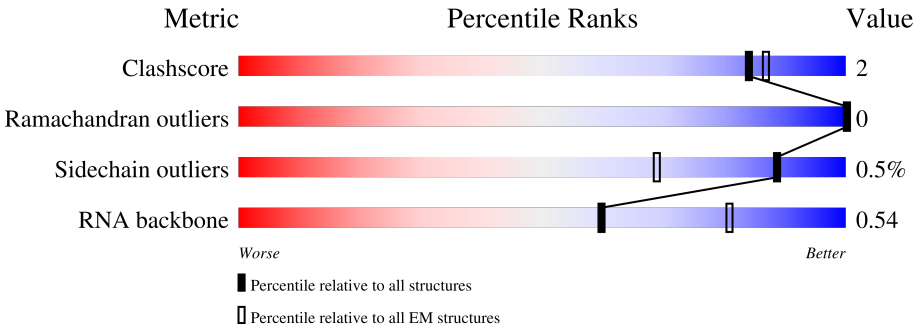
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2923	19% 75% 19%
2	B	115	61% 83% 17%
3	C	274	9% 92% 8%
4	D	215	9% 90% 10%
5	E	206	21% 92% 8%
6	F	158	100% 97%
7	G	175	98% 93% 6%

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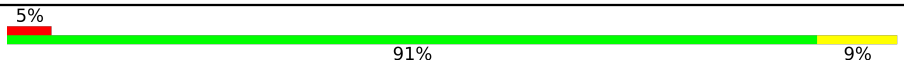
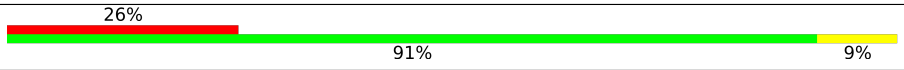
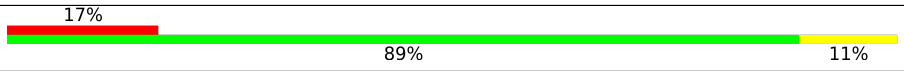
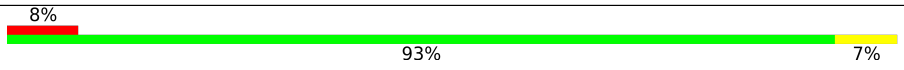
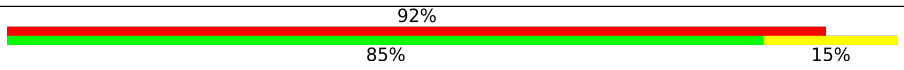
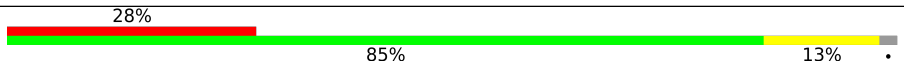
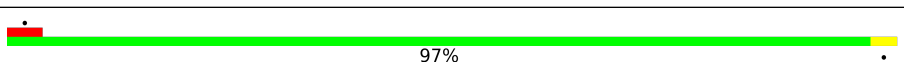
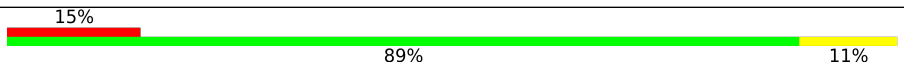
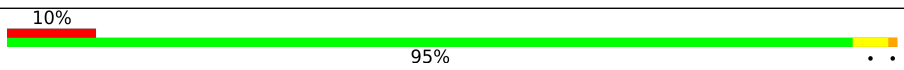
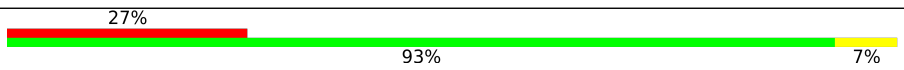
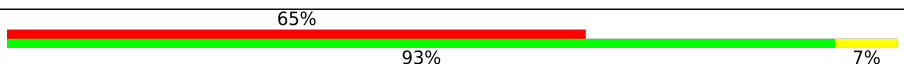
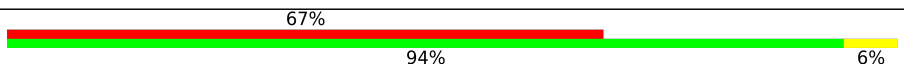
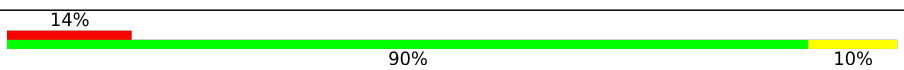
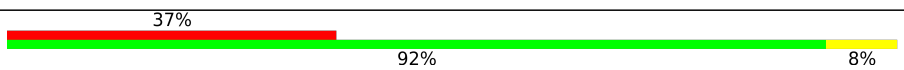
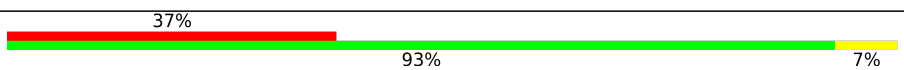
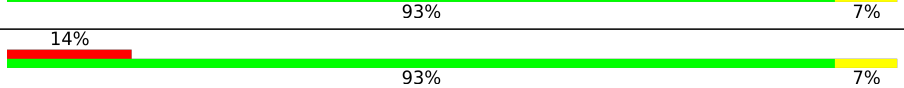
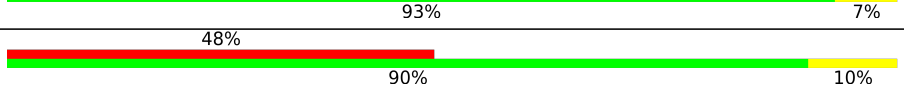
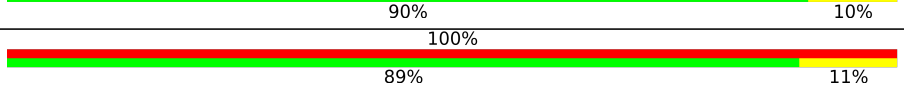
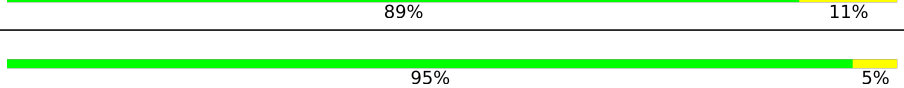
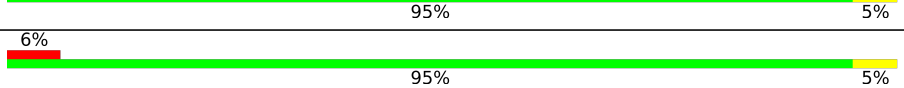
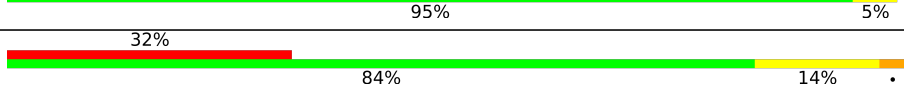
Mol	Chain	Length	Quality of chain
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	119	
14	N	116	
15	O	116	
16	P	102	
17	Q	112	
18	R	89	
19	S	103	
20	T	94	
21	U	79	
22	V	49	
23	W	67	
24	X	58	
25	Z	48	
26	1	47	
27	2	43	
28	3	64	
29	4	37	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 86401 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2834	60769	27128	11118	19689	2834	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	115	2448	1094	436	803	115	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	274	2094	1303	415	371	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	215	1627	1018	299	305	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	206	1572	986	288	296	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	158	778	462	158	158	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1263	790	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	119	Total	C	N	O	0	0
			882	549	174	159		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	114	Total 889	C 563	N 175	O 151	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	116	Total 942	C 593	N 189	O 156	S 4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total 790	C 503	N 142	O 144	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total 854	C 534	N 164	O 153	S 3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total 715	C 453	N 127	O 131	S 4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total 770	C 486	N 142	O 141	S 1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	94	Total 722	C 463	N 130	O 129	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	79	Total 597	C 369	N 117	O 111	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	49	Total 379	C 234	N 82	O 63	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	67	Total 541	C 333	N 102	O 106	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	58	Total 449	C 280	N 85	O 84	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	48	Total 360	C 222	N 77	O 59	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	47	Total 390	C 238	N 78	O 70	S 4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total 367	C 225	N 89	O 52	S 1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

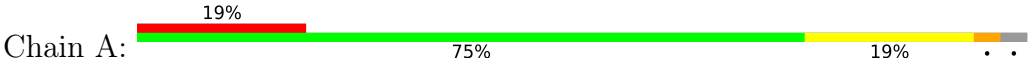
Mol	Chain	Residues	Atoms		AltConf
30	A	229	Total	Mg	0
			229	229	
30	B	2	Total	Mg	0
			2	2	
30	C	2	Total	Mg	0
			2	2	
30	J	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	U	1	Total	Mg	0
			1	1	
30	Z	1	Total	Mg	0
			1	1	

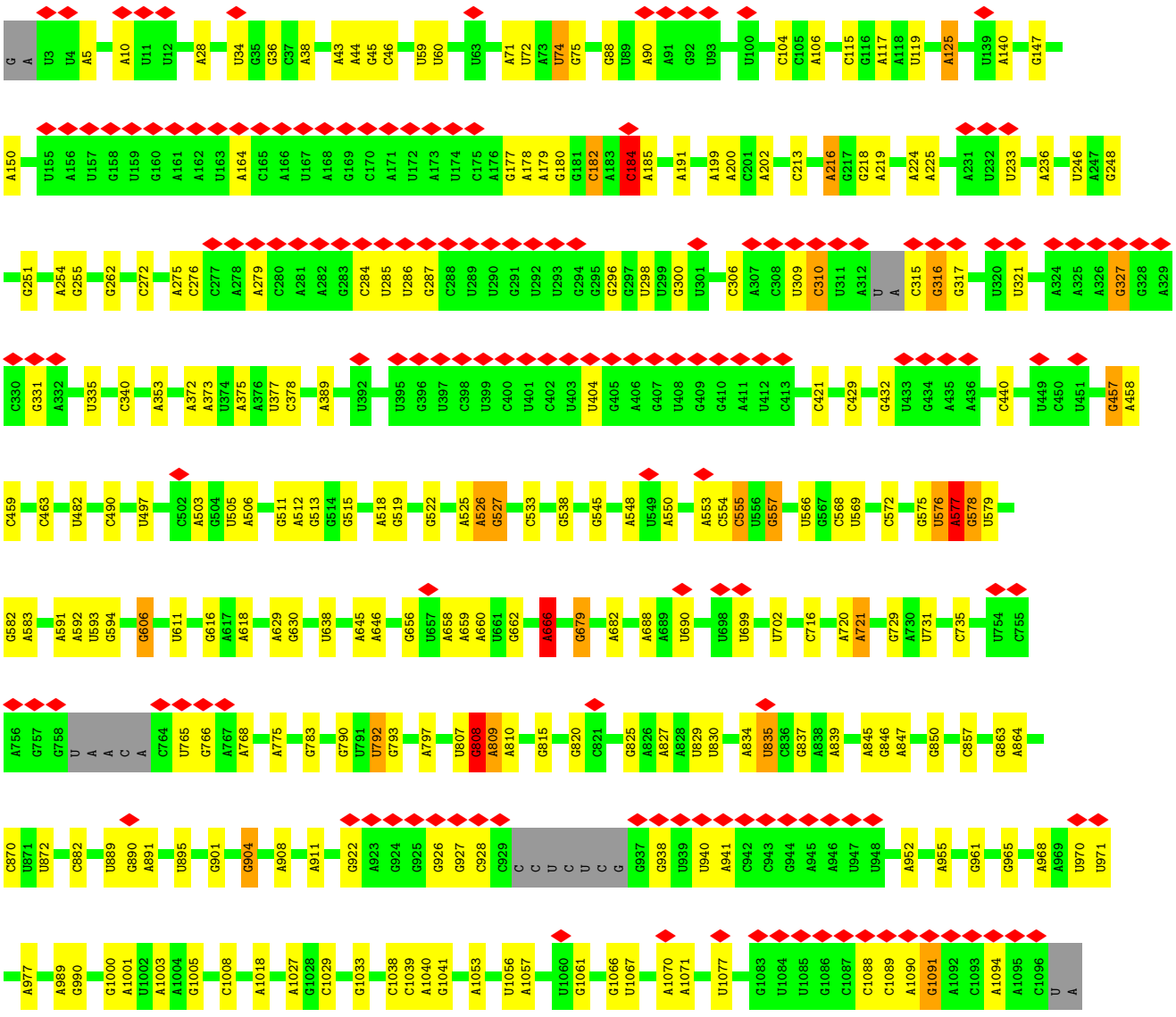
3 Residue-property plots (i)

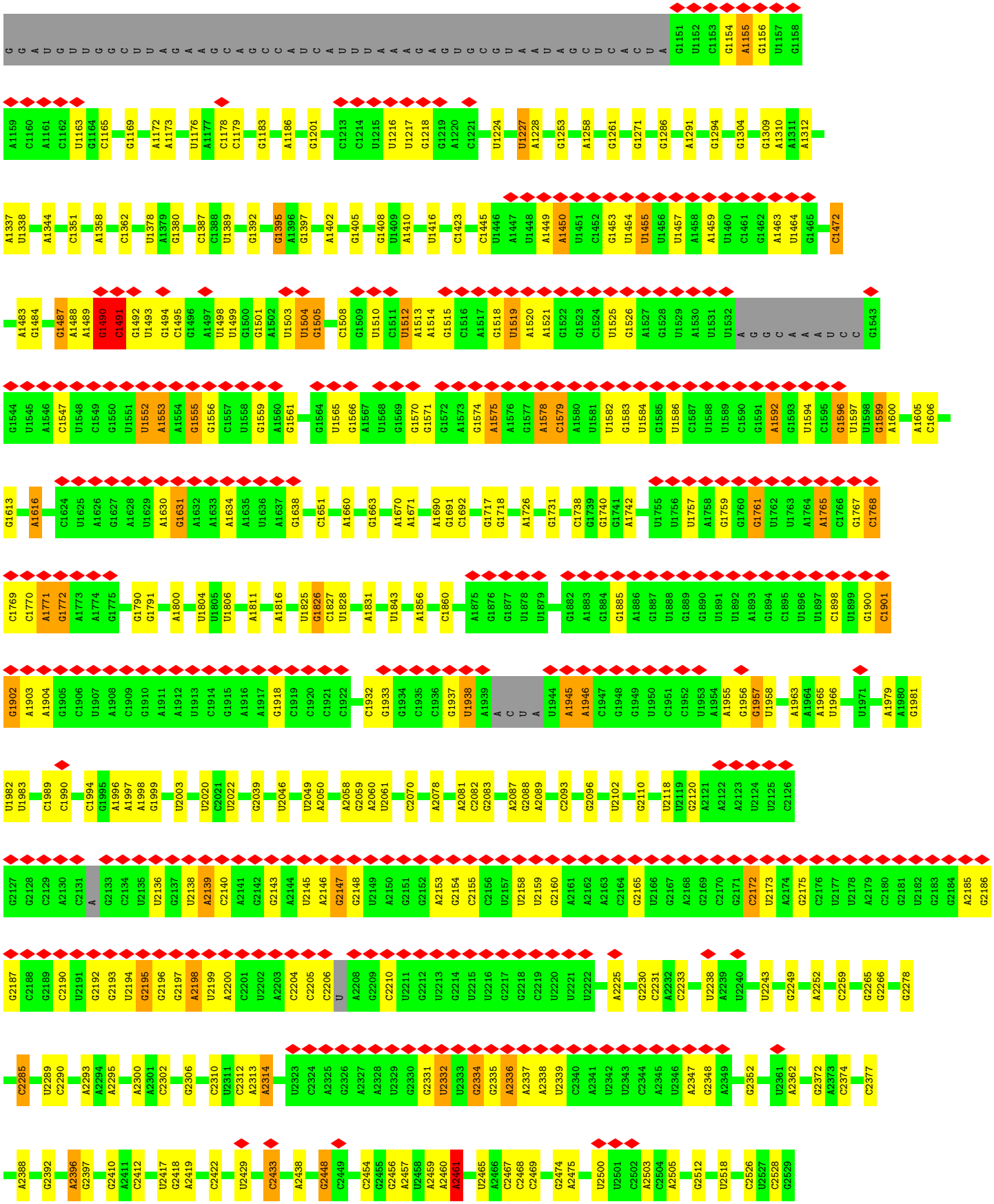
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

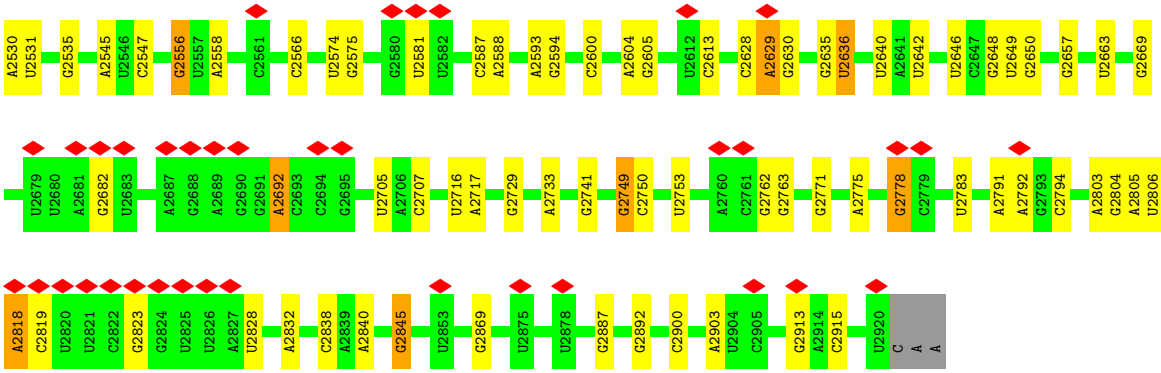
- Molecule 1: 23S ribosomal RNA

Chain A:

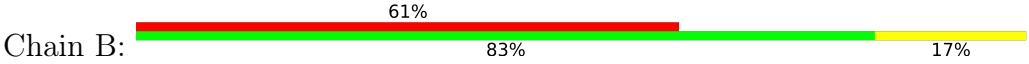


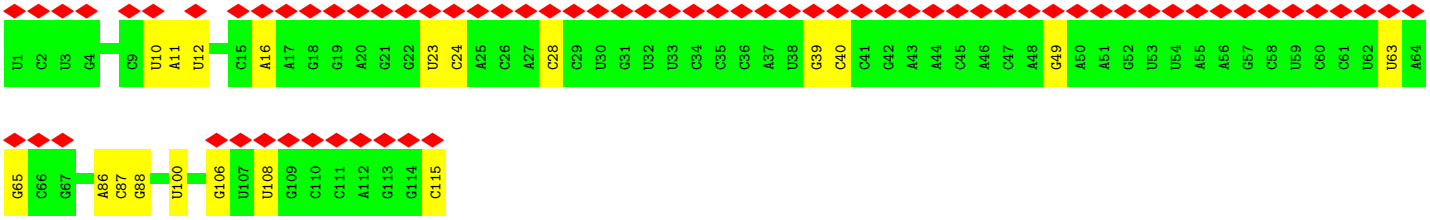




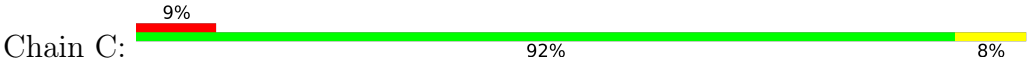


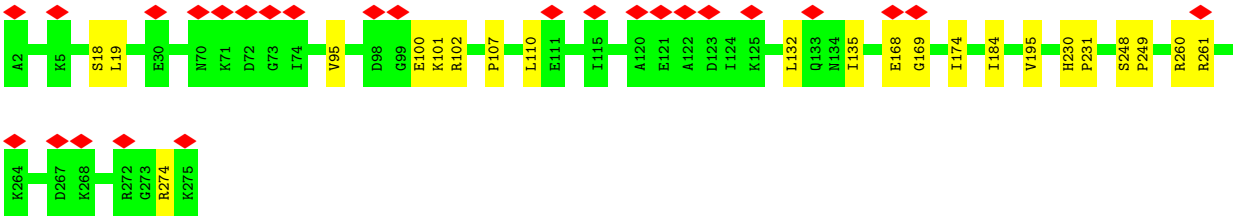
• Molecule 2: 5S ribosomal RNA



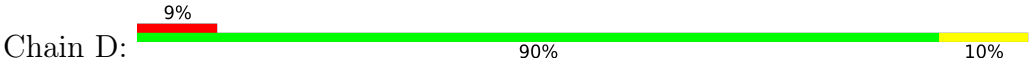


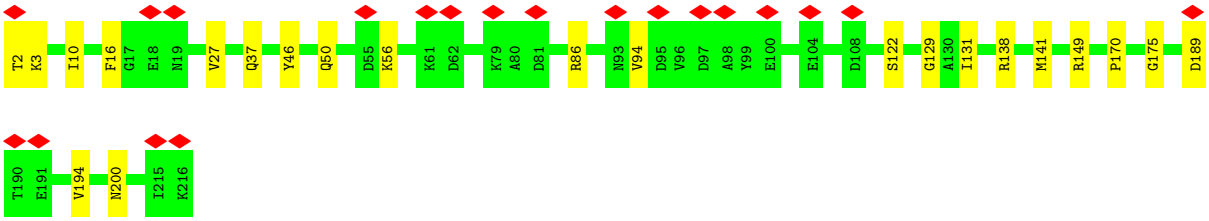
• Molecule 3: 50S ribosomal protein L2



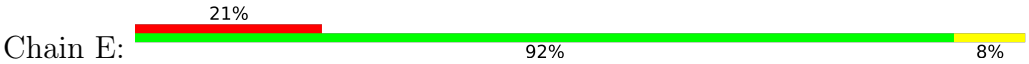


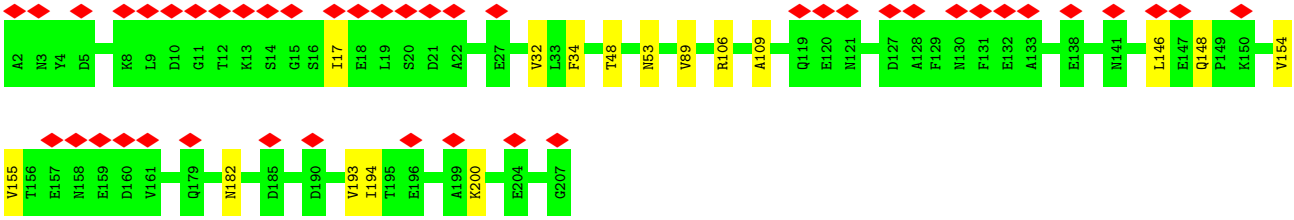
• Molecule 4: 50S ribosomal protein L3



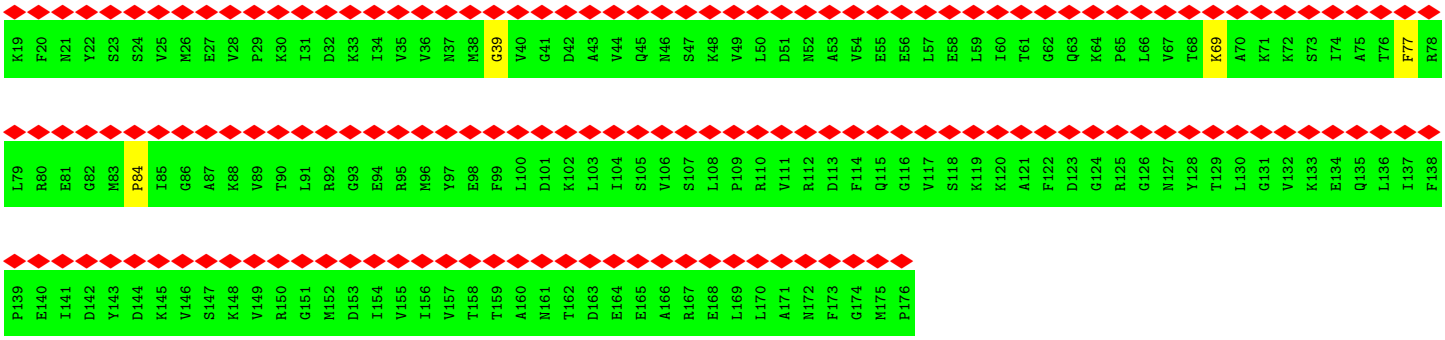


• Molecule 5: 50S ribosomal protein L4

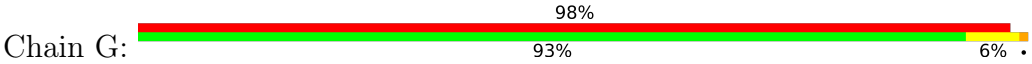


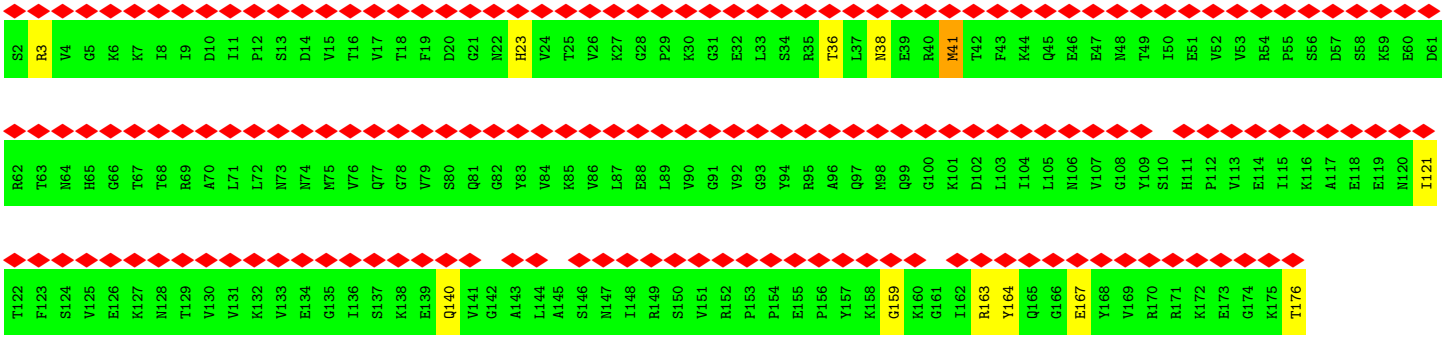


• Molecule 6: 50S ribosomal protein L5

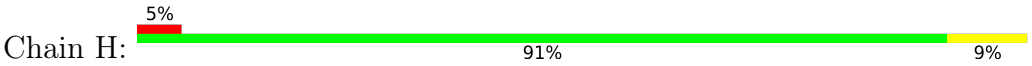


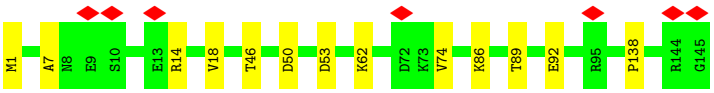
• Molecule 7: 50S ribosomal protein L6



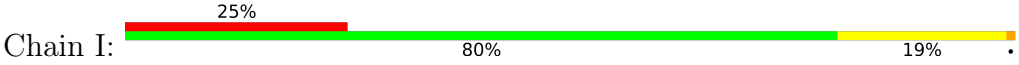


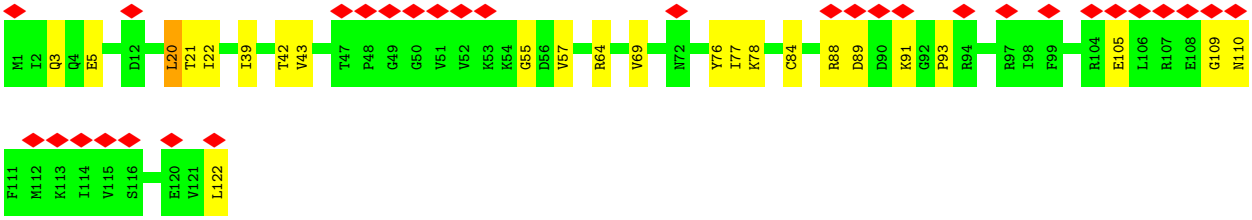
• Molecule 8: 50S ribosomal protein L13



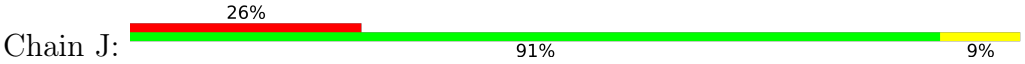


• Molecule 9: 50S ribosomal protein L14

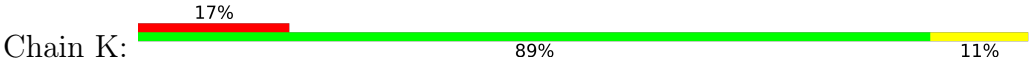


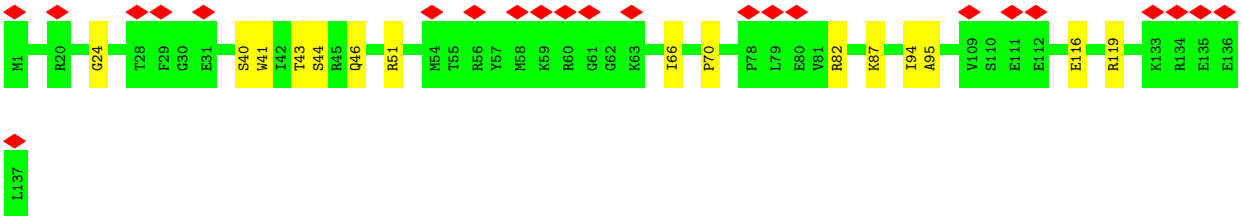


• Molecule 10: 50S ribosomal protein L15

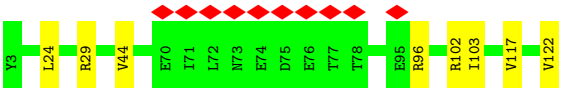


• Molecule 11: 50S ribosomal protein L16

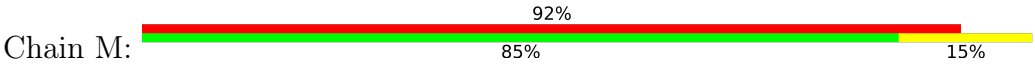


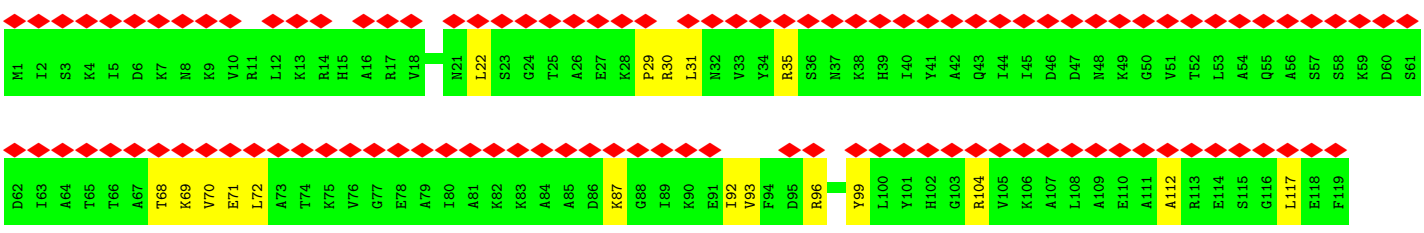


• Molecule 12: 50S ribosomal protein L17



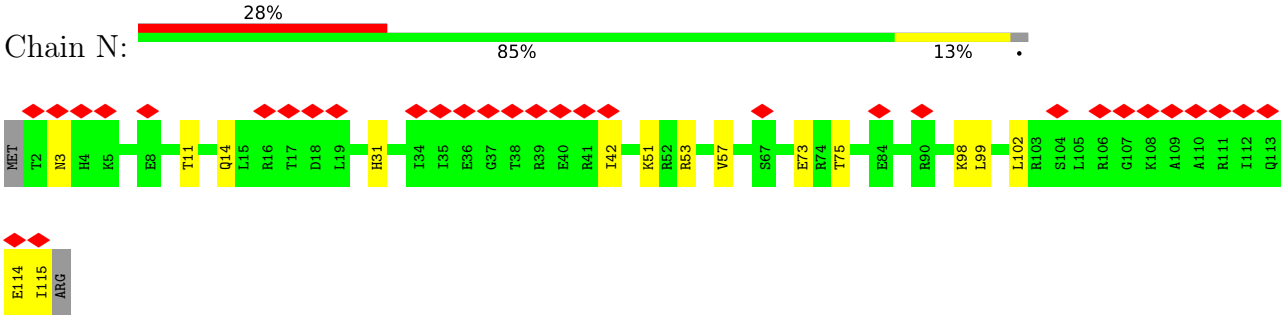
• Molecule 13: 50S ribosomal protein L18





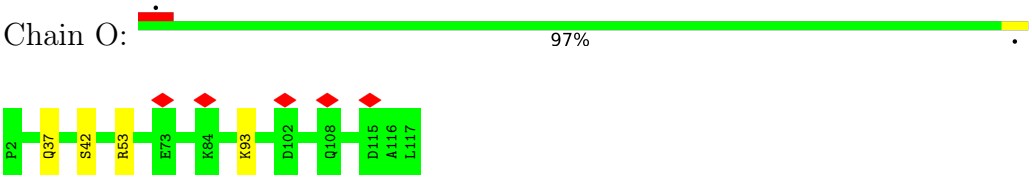
• Molecule 14: 50S ribosomal protein L19

Chain N:



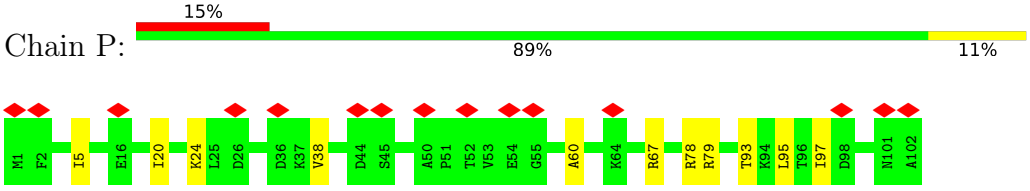
• Molecule 15: 50S ribosomal protein L20

Chain O:



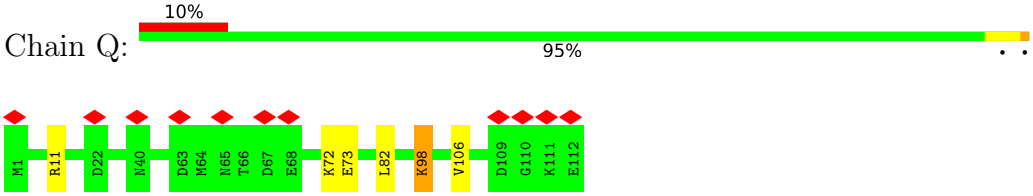
• Molecule 16: 50S ribosomal protein L21

Chain P:



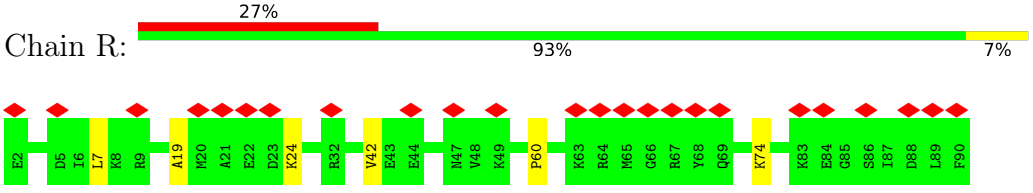
• Molecule 17: 50S ribosomal protein L22

Chain Q:



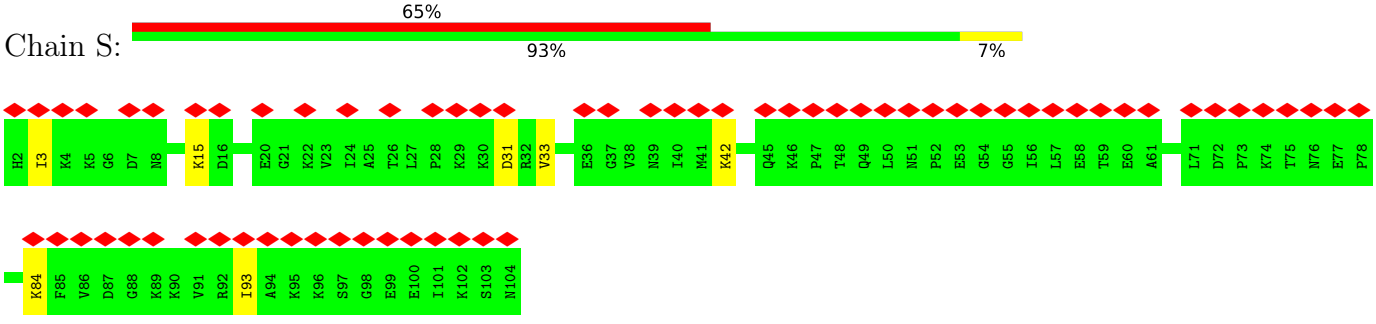
• Molecule 18: 50S ribosomal protein L23

Chain R:



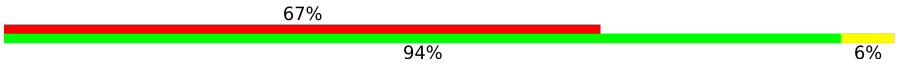
• Molecule 19: 50S ribosomal protein L24

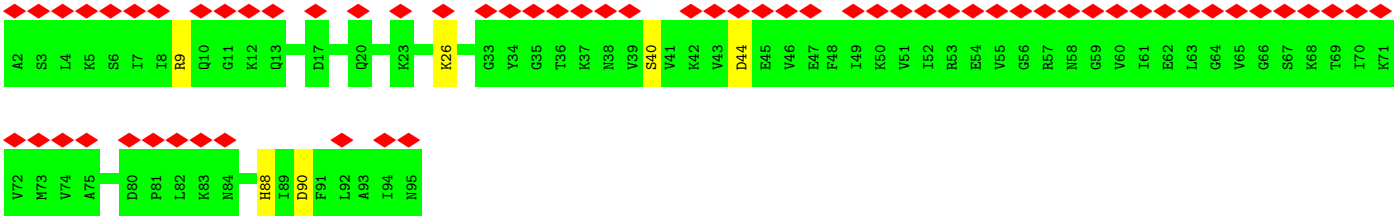
Chain S:



• Molecule 20: 50S ribosomal protein L25

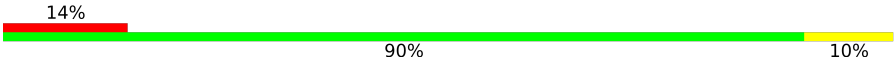
Chain T:

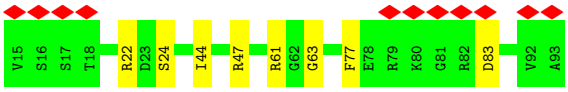




• Molecule 21: 50S ribosomal protein L27

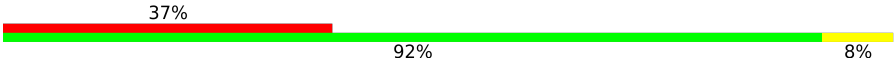
Chain U:

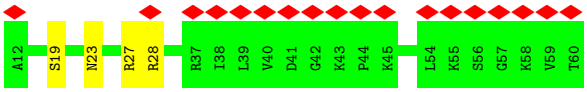




• Molecule 22: 50S ribosomal protein L28

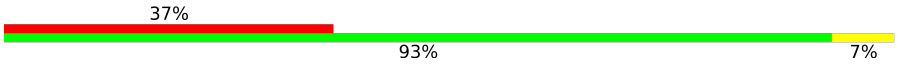
Chain V:

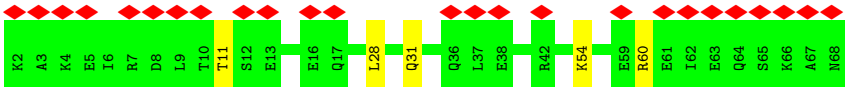




• Molecule 23: 50S ribosomal protein L29

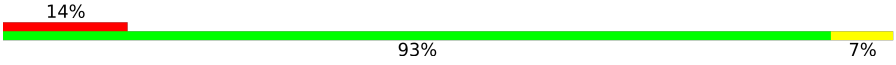
Chain W:

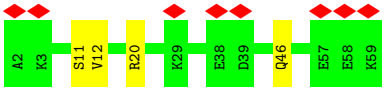




• Molecule 24: 50S ribosomal protein L30

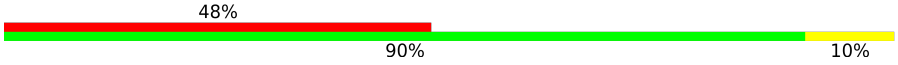
Chain X:

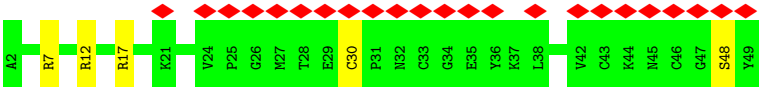




• Molecule 25: 50S ribosomal protein L32

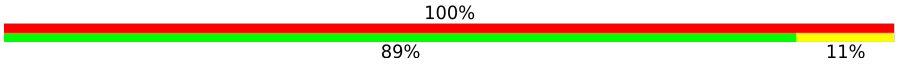
Chain Z:

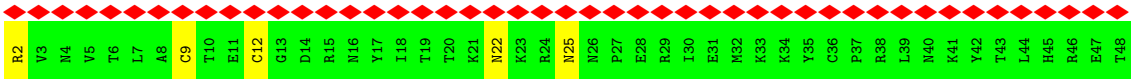




• Molecule 26: 50S ribosomal protein L33

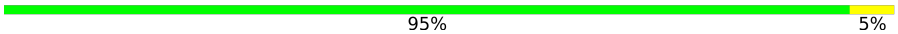
Chain 1:





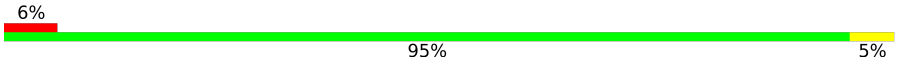
• Molecule 27: 50S ribosomal protein L34

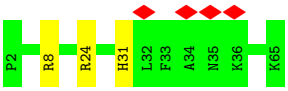
Chain 2:



• Molecule 28: 50S ribosomal protein L35

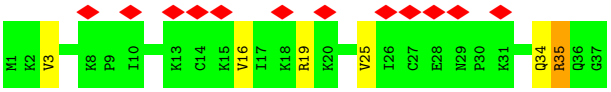
Chain 3:





• Molecule 29: 50S ribosomal protein L36

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211046	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.691	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	281.42398, 281.42398, 281.42398	wwPDB
Map dimensions	328, 328, 328	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8579999, 0.8579999, 0.8579999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, 2MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.19	15/67975 (0.0%)	1.12	142/105995 (0.1%)
2	B	0.97	0/2736	1.04	11/4261 (0.3%)
3	C	0.67	0/2129	0.64	0/2858
4	D	0.70	0/1651	0.66	0/2215
5	E	0.64	0/1595	0.65	0/2154
6	F	0.25	0/777	0.48	0/1079
7	G	0.39	0/1281	0.55	0/1736
8	H	0.69	0/1165	0.67	1/1570 (0.1%)
9	I	0.67	1/925 (0.1%)	0.73	2/1242 (0.2%)
10	J	0.67	0/1100	0.71	0/1467
11	K	0.64	0/1095	0.60	0/1472
12	L	0.63	0/936	0.70	0/1253
13	M	0.43	0/891	0.62	1/1194 (0.1%)
14	N	0.65	0/901	0.63	0/1209
15	O	0.73	0/954	0.65	0/1264
16	P	0.69	0/800	0.69	0/1070
17	Q	0.66	0/862	0.68	0/1161
18	R	0.65	0/723	0.63	0/966
19	S	0.53	0/779	0.66	1/1043 (0.1%)
20	T	0.51	0/730	0.65	0/981
21	U	0.74	0/603	0.66	0/802
22	V	0.56	0/384	0.62	0/515
23	W	0.55	0/542	0.68	0/722
24	X	0.63	0/451	0.62	0/606
25	Z	0.61	0/366	0.63	0/489
26	1	0.33	0/395	0.56	0/530
27	2	0.77	0/371	0.70	0/484
28	3	0.62	0/526	0.63	0/690
29	4	0.56	0/298	0.60	0/392
All	All	1.07	16/93941 (0.0%)	1.03	158/141420 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	5MU	O3'-P	-35.00	1.19	1.61
1	A	790	G	O3'-P	-22.26	1.34	1.61
1	A	1224	U	O3'-P	-11.14	1.47	1.61
1	A	1966	5MU	O3'-P	-10.64	1.48	1.61
1	A	1599	G	N3-C4	-7.42	1.30	1.35
1	A	1599	G	C2-N3	-7.01	1.27	1.32
1	A	1228	A	N3-C4	-6.90	1.30	1.34
1	A	1227	U	N3-C4	-6.71	1.32	1.38
1	A	1227	U	C2-N3	-6.65	1.33	1.37
1	A	1228	A	N9-C4	-6.46	1.33	1.37
1	A	1228	A	N7-C5	-6.27	1.35	1.39
1	A	721	A	N9-C4	-5.47	1.34	1.37
9	I	84	CYS	CB-SG	-5.41	1.73	1.81
1	A	1599	G	N9-C4	-5.13	1.33	1.38
1	A	254	A	N9-C4	-5.11	1.34	1.37
1	A	1228	A	C5-C6	-5.05	1.36	1.41

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2397	G	O5'-P-OP1	-30.54	74.06	110.70
1	A	2397	G	OP1-P-OP2	-26.01	80.58	119.60
1	A	2397	G	O5'-P-OP2	20.15	134.88	110.70
1	A	1599	G	N3-C2-N2	-14.67	109.63	119.90
1	A	2396	A	OP2-P-O3'	-13.24	76.06	105.20
1	A	1227	U	N3-C2-O2	-13.15	112.99	122.20
1	A	2396	A	OP1-P-O3'	12.62	132.96	105.20
1	A	790	G	P-O3'-C3'	11.06	132.97	119.70
1	A	1228	A	N7-C8-N9	11.00	119.30	113.80
1	A	1228	A	C5-N7-C8	-10.49	98.65	103.90
1	A	790	G	OP2-P-O3'	-9.61	84.07	105.20
1	A	2762	G	O3'-P-O5'	-9.39	86.17	104.00
2	B	100	U	C2-N1-C1'	9.03	128.53	117.70
1	A	1228	A	C8-N9-C4	-9.03	102.19	105.80
1	A	1599	G	N1-C2-N2	9.02	124.32	116.20
1	A	790	G	O3'-P-O5'	8.72	120.57	104.00
1	A	576	U	C2-N1-C1'	8.51	127.91	117.70
1	A	1599	G	N9-C4-C5	8.40	108.76	105.40
1	A	1227	U	N1-C2-O2	8.39	128.67	122.80
1	A	792	5MU	OP2-P-O3'	-8.25	87.05	105.20
1	A	1599	G	N3-C4-N9	-8.22	121.07	126.00
1	A	2210	C	N3-C2-O2	-8.19	116.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	A	N1-C6-N6	8.09	123.45	118.60
1	A	792	5MU	O3'-P-O5'	8.01	119.22	104.00
1	A	1508	C	N1-C2-O2	7.88	123.62	118.90
1	A	1499	U	N3-C2-O2	-7.69	116.81	122.20
1	A	1227	U	C2-N1-C1'	7.67	126.91	117.70
1	A	1490	G	N9-C4-C5	-7.55	102.38	105.40
1	A	1227	U	C5-C4-O4	7.43	130.36	125.90
2	B	100	U	N3-C2-O2	-7.42	117.01	122.20
1	A	2762	G	OP2-P-O3'	7.41	121.50	105.20
1	A	2210	C	N1-C2-O2	7.40	123.34	118.90
1	A	2419	A	C4-C5-N7	7.21	114.31	110.70
1	A	2636	U	C2-N1-C1'	7.20	126.34	117.70
1	A	125	A	C5-N7-C8	-7.18	100.31	103.90
1	A	1597	U	N3-C2-O2	-7.14	117.20	122.20
13	M	31	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	721	A	N1-C6-N6	7.05	122.83	118.60
2	B	100	U	N1-C2-O2	6.97	127.68	122.80
1	A	576	U	P-O3'-C3'	6.93	128.02	119.70
1	A	2419	A	C5-N7-C8	-6.92	100.44	103.90
1	A	576	U	N3-C2-O2	-6.88	117.39	122.20
1	A	1351	C	C6-N1-C2	-6.76	117.59	120.30
1	A	577	A	C2-N3-C4	6.72	113.96	110.60
2	B	100	U	C6-N1-C1'	-6.66	111.88	121.20
1	A	2302	C	N1-C2-O2	6.60	122.86	118.90
1	A	1351	C	C2-N1-C1'	6.60	126.06	118.80
1	A	721	A	C5-N7-C8	-6.56	100.62	103.90
1	A	125	A	C5-C6-N6	-6.56	118.45	123.70
1	A	1228	A	C4-C5-N7	6.56	113.98	110.70
1	A	863	G	C2-N3-C4	-6.55	108.62	111.90
1	A	557	G	O4'-C1'-N9	6.55	113.44	108.20
1	A	327	G	O4'-C1'-N9	6.51	113.41	108.20
9	I	20	LEU	CA-CB-CG	6.49	130.24	115.30
1	A	125	A	C4-C5-N7	6.36	113.88	110.70
1	A	2636	U	N1-C2-O2	6.23	127.16	122.80
1	A	1599	G	OP2-P-O3'	6.21	118.87	105.20
1	A	808	G	N7-C8-N9	6.17	116.18	113.10
1	A	1483	A	O3'-P-O5'	6.16	115.70	104.00
2	B	108	U	C2-N1-C1'	6.14	125.07	117.70
1	A	1596	G	N3-C2-N2	-6.14	115.60	119.90
1	A	882	C	C2-N1-C1'	6.13	125.55	118.80
1	A	125	A	N7-C8-N9	6.12	116.86	113.80
1	A	576	U	N1-C2-O2	6.10	127.07	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2422	C	N1-C2-O2	6.09	122.56	118.90
1	A	216	A	C5-C6-N6	-6.07	118.84	123.70
1	A	1491	C	O4'-C1'-N1	6.04	113.03	108.20
1	A	1816	A	C4-C5-N7	6.03	113.71	110.70
1	A	1227	U	N3-C4-O4	-6.02	115.19	119.40
1	A	1816	A	N1-C6-N6	6.01	122.21	118.60
1	A	2528	C	C5-C4-N4	-6.01	115.99	120.20
1	A	2636	U	N3-C2-O2	-6.00	118.00	122.20
1	A	216	A	N1-C6-N6	5.99	122.19	118.60
1	A	1816	A	C5-C6-N6	-5.93	118.96	123.70
8	H	1	MET	CG-SD-CE	-5.91	90.75	100.20
1	A	533	C	N1-C2-O2	5.90	122.44	118.90
1	A	2419	A	N1-C6-N6	5.89	122.14	118.60
1	A	2845	G	N3-C4-C5	5.88	131.54	128.60
1	A	1597	U	N1-C2-O2	5.84	126.89	122.80
1	A	1387	C	C2-N1-C1'	5.81	125.19	118.80
1	A	1508	C	C5-C6-N1	5.81	123.91	121.00
2	B	108	U	N3-C2-O2	-5.78	118.15	122.20
1	A	2845	G	C2-N3-C4	-5.78	109.01	111.90
1	A	2419	A	N9-C4-C5	-5.75	103.50	105.80
1	A	1957	G	C4'-C3'-O3'	5.74	124.48	113.00
1	A	1816	A	C5-N7-C8	-5.73	101.03	103.90
1	A	593	U	N3-C2-O2	-5.73	118.19	122.20
1	A	1227	U	N1-C2-N3	5.71	118.33	114.90
1	A	1512	U	N3-C2-O2	-5.70	118.21	122.20
1	A	882	C	N3-C2-O2	-5.68	117.92	121.90
1	A	808	G	C4-C5-N7	5.68	113.07	110.80
1	A	1491	C	N1-C2-O2	5.66	122.30	118.90
1	A	593	U	N1-C2-O2	5.65	126.75	122.80
1	A	808	G	C6-C5-N7	-5.64	127.02	130.40
2	B	86	A	N7-C8-N9	5.64	116.62	113.80
1	A	1380	G	C4-N9-C1'	5.59	133.76	126.50
1	A	835	U	C2-N1-C1'	5.57	124.39	117.70
2	B	86	A	C8-N9-C4	-5.57	103.57	105.80
1	A	1490	G	C8-N9-C4	5.56	108.63	106.40
1	A	2249	G	O4'-C1'-N9	5.53	112.62	108.20
1	A	1487	G	N3-C2-N2	-5.52	116.03	119.90
1	A	335	U	C5-C4-O4	-5.50	122.60	125.90
1	A	1508	C	N3-C2-O2	-5.50	118.05	121.90
1	A	1395	G	N1-C2-N2	-5.50	111.25	116.20
1	A	2102	U	N3-C4-O4	5.49	123.24	119.40
1	A	555	C	N1-C2-O2	5.48	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	86	A	C5-N7-C8	-5.47	101.17	103.90
1	A	1490	G	C4-C5-N7	5.46	112.98	110.80
1	A	2285	C	N1-C2-O2	5.45	122.17	118.90
1	A	1395	G	N3-C2-N2	5.44	123.71	119.90
1	A	1726	A	N9-C4-C5	-5.44	103.62	105.80
2	B	12	U	N3-C2-O2	-5.40	118.42	122.20
1	A	1378	U	C2-N1-C1'	5.39	124.17	117.70
1	A	1029	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1387	C	N1-C2-O2	5.38	122.13	118.90
1	A	576	U	C6-N1-C2	-5.36	117.78	121.00
1	A	808	G	C5-N7-C8	-5.34	101.63	104.30
1	A	2302	C	N3-C2-O2	-5.34	118.16	121.90
1	A	1169	G	C2-N3-C4	-5.33	109.23	111.90
1	A	2302	C	C2-N1-C1'	5.32	124.66	118.80
1	A	2419	A	C6-C5-N7	-5.32	128.58	132.30
1	A	1932	C	C2-N1-C1'	5.30	124.63	118.80
1	A	666	A	C5-N7-C8	-5.28	101.26	103.90
1	A	1490	G	C6-C5-N7	-5.26	127.24	130.40
1	A	527	G	O4'-C1'-N9	5.23	112.39	108.20
1	A	2419	A	C5-C6-N6	-5.23	119.52	123.70
1	A	2419	A	N7-C8-N9	5.23	116.41	113.80
1	A	2448	G	N3-C4-N9	5.21	129.13	126.00
1	A	1804	U	N3-C2-O2	-5.21	118.56	122.20
1	A	1491	C	C2-N1-C1'	5.20	124.52	118.80
1	A	2461	A	N1-C6-N6	5.19	121.71	118.60
1	A	1201	G	C4-N9-C1'	5.18	133.23	126.50
1	A	2792	A	O4'-C1'-N9	-5.18	104.06	108.20
1	A	1491	C	C5-C6-N1	5.17	123.59	121.00
1	A	1029	C	C2-N1-C1'	5.17	124.49	118.80
1	A	1599	G	C8-N9-C4	-5.16	104.34	106.40
1	A	1490	G	N3-C4-N9	5.15	129.09	126.00
1	A	721	A	C4-C5-N7	5.14	113.27	110.70
9	I	64	ARG	CA-CB-CG	5.14	124.71	113.40
1	A	568	C	C5-C4-N4	-5.14	116.60	120.20
1	A	1380	G	C8-N9-C1'	-5.14	120.32	127.00
1	A	666	A	N1-C6-N6	5.09	121.66	118.60
1	A	847	A	C5-C6-N6	-5.08	119.64	123.70
1	A	1228	A	C2-N3-C4	-5.08	108.06	110.60
1	A	125	A	C6-C5-N7	-5.07	128.75	132.30
1	A	2003	U	C2'-C3'-O3'	5.07	121.81	113.70
2	B	28	C	N1-C2-O2	5.07	121.94	118.90
1	A	2461	A	C5-C6-N6	-5.05	119.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	793	G	O4'-C1'-N9	5.05	112.24	108.20
1	A	2749	G	P-O3'-C3'	5.05	125.75	119.70
1	A	184	C	N3-C2-O2	-5.04	118.37	121.90
1	A	825	G	C2-N3-C4	-5.04	109.38	111.90
1	A	1351	C	N1-C2-O2	5.04	121.92	118.90
1	A	2845	G	N3-C4-N9	-5.04	122.98	126.00
1	A	1201	G	C6-C5-N7	-5.03	127.38	130.40
1	A	1804	U	C2-N1-C1'	5.03	123.73	117.70
19	S	31	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	1487	G	N1-C2-N2	5.01	120.71	116.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60769	0	30549	154	0
2	B	2448	0	1239	1	0
3	C	2094	0	2205	15	0
4	D	1627	0	1667	14	0
5	E	1572	0	1619	22	0
6	F	778	0	348	4	0
7	G	1263	0	1225	9	0
8	H	1143	0	1134	7	0
9	I	918	0	981	19	0
10	J	1086	0	1125	14	0
11	K	1071	0	1123	10	0
12	L	932	0	983	4	0
13	M	882	0	900	9	0
14	N	889	0	937	8	0
15	O	942	0	1014	4	0
16	P	790	0	830	6	0
17	Q	854	0	914	6	0
18	R	715	0	748	3	0
19	S	770	0	809	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	722	0	766	3	0
21	U	597	0	604	5	0
22	V	379	0	400	3	0
23	W	541	0	563	3	0
24	X	449	0	491	3	0
25	Z	360	0	358	4	0
26	1	390	0	394	3	0
27	2	367	0	415	2	0
28	3	521	0	586	3	0
29	4	295	0	340	5	0
30	A	229	0	0	0	0
30	B	2	0	0	0	0
30	C	2	0	0	0	0
30	J	1	0	0	0	0
30	K	1	0	0	0	0
30	U	1	0	0	0	0
30	Z	1	0	0	0	0
All	All	86401	0	55267	287	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 (287) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2338:A:C2	6:F:77:PHE:CB	2.50	0.95
5:E:34:PHE:CE1	10:J:6:LEU:HD13	2.08	0.88
1:A:2669:G:OP2	8:H:86:LYS:NZ	2.09	0.86
4:D:131:ILE:HD11	4:D:149:ARG:CZ	2.07	0.84
1:A:1825:U:OP2	3:C:274:ARG:NH2	2.14	0.80
1:A:1938:U:O2'	1:A:1945:A:N6	2.16	0.79
3:C:230:HIS:ND1	3:C:231:PRO:HD2	1.98	0.79
1:A:2259:C:OP2	22:V:27:ARG:NH2	2.14	0.79
1:A:2334:G:O2'	1:A:2337:A:OP2	2.03	0.76
5:E:34:PHE:HE1	10:J:6:LEU:HD13	1.51	0.76
1:A:2136:U:O4	1:A:2206:C:N4	2.18	0.75
1:A:1501:G:H22	1:A:2729:G:H22	1.35	0.74
1:A:1091:G:O2'	1:A:1155:A:N6	2.21	0.73
8:H:7:ALA:H	8:H:46:THR:HG21	1.53	0.73
1:A:2022:U:O2	9:I:3:GLN:NE2	2.22	0.72
1:A:2338:A:H2	6:F:77:PHE:CB	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:A:N6	1:A:1634:A:N1	2.38	0.72
5:E:34:PHE:HE1	10:J:6:LEU:CD1	2.03	0.71
5:E:154:VAL:HG12	5:E:193:VAL:HG23	1.73	0.71
1:A:1826:G:OP1	3:C:260:ARG:HD2	1.91	0.70
1:A:1455:U:O2'	1:A:1457:U:O4	2.04	0.69
5:E:34:PHE:CD1	10:J:6:LEU:HD13	2.27	0.69
1:A:926:G:O2'	1:A:941:A:N1	2.22	0.69
9:I:91:LYS:NZ	9:I:110:ASN:HB2	2.08	0.69
1:A:1979:A:N3	1:A:2587:C:O2'	2.25	0.69
1:A:2778:G:N2	7:G:3:ARG:HH21	1.92	0.68
1:A:1552:U:O2'	1:A:1553:A:O4'	2.12	0.67
1:A:1491:C:H6	1:A:1574:G:N2	1.93	0.67
1:A:1512:U:H2'	1:A:1513:A:C8	2.31	0.66
13:M:68:THR:HG1	13:M:71:GLU:H	1.42	0.66
1:A:2778:G:N2	7:G:3:ARG:NH2	2.43	0.66
7:G:38:ASN:ND2	7:G:41:MET:SD	2.69	0.66
1:A:2649:U:O2'	1:A:2845:G:N2	2.29	0.65
4:D:10:ILE:HB	4:D:27:VAL:HG13	1.78	0.65
16:P:60:ALA:HB2	16:P:97:ILE:HD13	1.78	0.65
5:E:154:VAL:HG12	5:E:193:VAL:CG2	2.27	0.65
1:A:1039:C:O2'	15:O:93:LYS:NZ	2.27	0.65
1:A:1757:U:O4	1:A:1771:A:N6	2.31	0.64
9:I:89:ASP:OD1	9:I:89:ASP:O	2.15	0.63
1:A:2285:C:O2'	1:A:2454:C:OP2	2.17	0.62
17:Q:11:ARG:O	17:Q:11:ARG:NH2	2.32	0.62
1:A:1493:U:H3	1:A:1505:G:H1	1.48	0.62
1:A:1008:C:O2'	1:A:2300:A:N3	2.28	0.61
7:G:164:TYR:HB2	7:G:167:GLU:HB2	1.81	0.61
1:A:2448:G:N7	28:3:31:HIS:NE2	2.38	0.61
19:S:3:ILE:HD11	19:S:33:VAL:HG11	1.81	0.61
1:A:2783:U:OP2	29:4:19:ARG:NE	2.34	0.61
9:I:77:ILE:HD11	9:I:122:LEU:HD13	1.82	0.60
1:A:315:C:O2'	1:A:316:G:N7	2.24	0.60
1:A:60:U:O2	1:A:74:U:O2'	2.18	0.60
4:D:16:PHE:O	14:N:14:GLN:NE2	2.34	0.59
13:M:96:ARG:NH2	13:M:99:TYR:O	2.34	0.59
1:A:545:G:N1	1:A:548:A:OP2	2.35	0.59
1:A:2278:G:OP1	11:K:82:ARG:NH2	2.36	0.59
1:A:1770:C:N4	1:A:1771:A:N3	2.50	0.59
1:A:1765:A:O2'	1:A:1767:G:N7	2.35	0.58
1:A:2628:C:OP2	1:A:2629:A:N6	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:VAL:HG22	3:C:101:LYS:HG2	1.87	0.57
9:I:91:LYS:NZ	9:I:109:GLY:O	2.30	0.57
9:I:21:THR:HG22	9:I:39:ILE:HD13	1.86	0.57
1:A:577:A:O2'	1:A:578:G:OP1	2.20	0.57
1:A:1487:G:H1	1:A:1596:G:H1	1.53	0.57
9:I:76:TYR:HB2	14:N:75:THR:HB	1.86	0.57
3:C:107:PRO:HD2	3:C:110:LEU:HD22	1.87	0.57
1:A:1901:C:O2'	1:A:1902:G:O4'	2.21	0.57
1:A:1512:U:H2'	1:A:1513:A:H8	1.68	0.57
1:A:457:G:OP2	1:A:2433:C:O2'	2.24	0.56
1:A:1759:G:N7	1:A:1761:G:N2	2.53	0.56
1:A:2558:A:N7	7:G:176:THR:HA	2.20	0.56
20:T:26:LYS:NZ	20:T:44:ASP:OD1	2.39	0.56
1:A:895:U:O2	24:X:46:GLN:NE2	2.39	0.56
5:E:155:VAL:HB	5:E:194:ILE:HG22	1.87	0.56
8:H:14:ARG:NH1	8:H:50:ASP:O	2.38	0.56
1:A:1575:A:N1	1:A:1592:A:N6	2.52	0.56
1:A:1555:G:O2'	1:A:1556:G:N7	2.28	0.55
1:A:2049:U:OP2	25:Z:12:ARG:NH2	2.39	0.55
1:A:46:C:N4	1:A:184:C:O2	2.40	0.55
1:A:2500:U:OP1	1:A:2556:G:N2	2.38	0.55
5:E:146:LEU:O	5:E:146:LEU:HD12	2.06	0.55
1:A:660:A:H8	5:E:182:ASN:HB3	1.72	0.55
1:A:1663:G:HO2'	27:2:2:VAL:N	2.04	0.55
1:A:1806:U:OP2	1:A:1811:A:N6	2.38	0.55
1:A:1514:A:H61	1:A:1566:G:H1	1.53	0.55
1:A:2293:A:N6	1:A:2300:A:OP2	2.40	0.55
1:A:2140:C:N3	1:A:2195:G:O2'	2.39	0.54
14:N:31:HIS:HB3	14:N:42:ILE:HD11	1.88	0.54
22:V:27:ARG:NH1	22:V:28:ARG:O	2.40	0.54
1:A:1484:G:H1	1:A:1599:G:H22	1.56	0.54
1:A:1515:G:H22	1:A:1565:U:H3	1.55	0.54
1:A:1518:G:HO2'	1:A:1519:U:P	2.31	0.54
1:A:656:G:H21	1:A:660:A:H2	1.56	0.54
1:A:1510:U:H3	1:A:1571:G:H1	1.56	0.54
23:W:11:THR:OG1	23:W:60:ARG:NH2	2.41	0.54
1:A:2192:G:O6	1:A:2198:A:N6	2.41	0.54
4:D:129:GLY:HA2	4:D:170:PRO:HB3	1.90	0.53
1:A:522:G:N1	1:A:525:A:OP2	2.41	0.53
4:D:2:THR:OG1	4:D:3:LYS:N	2.39	0.53
5:E:146:LEU:CD1	5:E:148:GLN:HE21	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:SER:HB2	4:D:175:GLY:HA2	1.89	0.53
9:I:42:THR:HG22	9:I:57:VAL:HG22	1.89	0.53
1:A:2650:G:O5'	1:A:2845:G:N2	2.42	0.52
7:G:121:ILE:HD11	7:G:140:GLN:HG3	1.91	0.52
1:A:1900:G:O2'	1:A:1902:G:N7	2.27	0.52
9:I:91:LYS:HZ1	9:I:110:ASN:HB2	1.72	0.52
1:A:606:G:H21	15:O:37:GLN:HE22	1.58	0.52
9:I:122:LEU:HD12	9:I:122:LEU:C	2.30	0.52
1:A:1472:C:O2'	1:A:1616:A:OP2	2.17	0.52
1:A:1518:G:O2'	1:A:1519:U:O5'	2.28	0.52
5:E:146:LEU:HD13	5:E:148:GLN:HE21	1.74	0.52
7:G:159:GLY:O	7:G:163:ARG:NH1	2.43	0.52
1:A:2147:G:O6	1:A:2199:U:O2'	2.25	0.52
18:R:7:LEU:HD21	18:R:42:VAL:HG12	1.91	0.52
12:L:96:ARG:HH12	12:L:122:VAL:HG22	1.75	0.52
8:H:89:THR:OG1	8:H:92:GLU:HG2	2.10	0.51
10:J:125:ALA:HB3	10:J:128:PHE:HE1	1.75	0.51
1:A:46:C:N4	1:A:182:C:N3	2.59	0.51
3:C:100:GLU:OE2	3:C:102:ARG:NH2	2.44	0.51
1:A:1489:A:O2'	1:A:1490:G:N7	2.31	0.50
12:L:102:ARG:HH21	12:L:122:VAL:HG21	1.76	0.50
1:A:38:A:N3	5:E:48:THR:OG1	2.44	0.50
1:A:2154:G:O2'	1:A:2155:C:O4'	2.13	0.50
4:D:2:THR:HA	4:D:94:VAL:HA	1.92	0.50
13:M:29:PRO:HD2	13:M:92:ILE:HG22	1.92	0.50
8:H:53:ASP:OD1	8:H:53:ASP:N	2.43	0.50
24:X:12:VAL:HG22	24:X:20:ARG:HG2	1.93	0.50
1:A:662:G:OP2	5:E:106:ARG:NH2	2.38	0.50
13:M:69:LYS:HA	13:M:72:LEU:HD12	1.94	0.50
14:N:114:GLU:HG2	14:N:115:ILE:HG13	1.94	0.50
1:A:716:C:OP1	10:J:43:GLY:N	2.36	0.50
1:A:904:G:O2'	1:A:961:G:O6	2.19	0.50
13:M:70:VAL:HG22	13:M:104:ARG:HG2	1.94	0.50
1:A:679:G:O6	10:J:71:ARG:NH2	2.45	0.49
1:A:808:G:O2'	1:A:809:A:OP1	2.25	0.49
1:A:2195:G:N2	1:A:2197:G:O6	2.44	0.49
1:A:284:C:O2'	1:A:287:G:N2	2.39	0.49
13:M:22:LEU:HG	13:M:93:VAL:HG11	1.93	0.49
3:C:107:PRO:HA	3:C:195:VAL:HA	1.94	0.49
1:A:1491:C:C6	1:A:1574:G:N2	2.77	0.49
2:B:16:A:H61	2:B:63:U:H3	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:LEU:HD23	13:M:30:ARG:HD3	1.94	0.49
29:4:3:VAL:HG12	29:4:35:ARG:HG3	1.95	0.48
25:Z:30:CYS:SG	25:Z:48:SER:N	2.78	0.48
1:A:1395:G:N1	1:A:1408:G:N7	2.61	0.48
9:I:77:ILE:HD11	9:I:122:LEU:CD1	2.42	0.48
1:A:2512:G:OP1	11:K:46:GLN:NE2	2.44	0.48
4:D:56:LYS:HD3	4:D:86:ARG:HG2	1.95	0.48
12:L:103:ILE:HG23	12:L:117:VAL:CG1	2.44	0.48
21:U:44:ILE:HD13	21:U:47:ARG:HH21	1.79	0.48
1:A:309:U:O2'	1:A:310:C:O5'	2.30	0.48
1:A:927:G:OP2	1:A:927:G:N2	2.45	0.48
1:A:2465:U:O2'	1:A:2467:C:OP1	2.30	0.48
12:L:24:LEU:HD12	12:L:44:VAL:HG21	1.95	0.48
7:G:23:HIS:HB3	7:G:36:THR:HG22	1.95	0.47
1:A:1945:A:N7	1:A:1946:A:N6	2.62	0.47
10:J:74:TYR:HE2	10:J:127:LYS:HE2	1.78	0.47
1:A:115:C:HO2'	1:A:125:A:H8	1.60	0.47
3:C:132:LEU:HD23	3:C:135:ILE:HD12	1.96	0.47
9:I:78:LYS:HB2	14:N:73:GLU:HB2	1.96	0.47
11:K:51:ARG:HG3	11:K:66:ILE:HD11	1.96	0.47
29:4:16:VAL:HG22	29:4:25:VAL:HG12	1.96	0.47
11:K:44:SER:HB2	11:K:70:PRO:HG3	1.97	0.47
14:N:11:THR:HB	14:N:57:VAL:HG21	1.97	0.47
1:A:276:C:O2'	1:A:306:C:OP1	2.25	0.47
1:A:846:G:O6	5:E:53:ASN:ND2	2.48	0.47
3:C:174:ILE:HG21	3:C:184:ILE:HD12	1.97	0.47
5:E:146:LEU:HD12	5:E:148:GLN:HG2	1.97	0.47
11:K:116:GLU:OE2	11:K:119:ARG:NH2	2.39	0.47
1:A:1304:G:OP2	25:Z:17:ARG:NH2	2.45	0.47
16:P:78:ARG:HG2	16:P:79:ARG:HD2	1.97	0.47
14:N:51:LYS:HB2	14:N:98:LYS:HE2	1.97	0.47
1:A:579:U:H5'	15:O:42:SER:HB2	1.98	0.46
1:A:1038:C:OP1	15:O:53:ARG:NH2	2.48	0.46
23:W:28:LEU:HA	23:W:31:GLN:HG2	1.97	0.46
4:D:138:ARG:HE	4:D:141:MET:HE3	1.81	0.46
6:F:69:LYS:HA	6:F:84:PRO:HA	1.97	0.46
1:A:1455:U:O4	1:A:1631:G:N1	2.48	0.46
9:I:91:LYS:HZ2	9:I:110:ASN:HB2	1.80	0.46
22:V:19:SER:OG	22:V:23:ASN:OD1	2.28	0.46
1:A:2046:U:OP1	25:Z:7:ARG:NH2	2.39	0.46
1:A:72:U:OP2	23:W:54:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:G:OP1	16:P:67:ARG:NH2	2.47	0.46
1:A:1491:C:H1'	1:A:1574:G:H22	1.80	0.46
1:A:1981:G:O2'	1:A:1983:U:O4	2.20	0.46
1:A:2332:U:O4	6:F:39:GLY:HA3	2.16	0.46
1:A:721:A:HO2'	1:A:2469:C:HO2'	1.61	0.45
1:A:2682:G:N2	1:A:2692:A:OP2	2.42	0.45
21:U:83:ASP:N	21:U:83:ASP:OD1	2.48	0.45
1:A:59:U:O2'	1:A:74:U:OP2	2.29	0.45
3:C:230:HIS:CE1	3:C:231:PRO:HD2	2.52	0.45
11:K:40:SER:OG	11:K:41:TRP:N	2.50	0.45
1:A:2817:A:O2'	1:A:2818:A:OP2	2.33	0.45
9:I:5:GLU:HA	9:I:20:LEU:HD13	1.99	0.45
17:Q:11:ARG:NH1	17:Q:98:LYS:HG3	2.32	0.45
1:A:2138:U:O2'	1:A:2172:C:N4	2.50	0.45
1:A:275:A:H62	1:A:296:G:H21	1.64	0.45
1:A:1767:G:OP1	1:A:1769:C:N4	2.50	0.45
17:Q:82:LEU:HB2	17:Q:98:LYS:HB2	1.98	0.45
29:4:25:VAL:HG22	29:4:34:GLN:HB2	1.97	0.45
5:E:182:ASN:OD1	5:E:182:ASN:N	2.44	0.45
1:A:2312:C:OP2	26:1:2:ARG:NH2	2.40	0.45
8:H:18:VAL:HG23	8:H:138:PRO:HB2	1.99	0.45
1:A:1491:C:H6	1:A:1574:G:H21	1.63	0.44
1:A:1938:U:H1'	1:A:1946:A:H61	1.83	0.44
1:A:178:A:O2'	1:A:179:A:H5'	2.18	0.44
1:A:1484:G:H1	1:A:1599:G:N2	2.15	0.44
4:D:131:ILE:HD11	4:D:149:ARG:NH1	2.31	0.44
1:A:1488:A:H3'	1:A:1489:A:C8	2.53	0.44
13:M:22:LEU:CD2	13:M:30:ARG:HD3	2.47	0.44
1:A:1757:U:O2	1:A:1772:G:N2	2.47	0.44
1:A:2392:G:OP1	21:U:63:GLY:N	2.48	0.44
1:A:262:G:H21	1:A:666:A:H8	1.64	0.44
1:A:2289:U:OP2	21:U:24:SER:OG	2.26	0.44
1:A:2663:U:HO2'	4:D:46:TYR:HH	1.64	0.44
1:A:901:G:O2'	21:U:77:PHE:HD2	2.00	0.44
26:1:22:ASN:ND2	26:1:25:ASN:OD1	2.42	0.44
1:A:2187:G:N2	1:A:2200:A:O2'	2.50	0.43
9:I:43:VAL:HG23	9:I:55:GLY:H	1.82	0.43
1:A:1494:G:H1	1:A:1504:U:H3	1.64	0.43
9:I:88:ARG:NH2	9:I:93:PRO:O	2.51	0.43
1:A:200:A:N1	1:A:2461:A:N6	2.66	0.43
20:T:88:HIS:NE2	20:T:90:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:C:H1'	10:J:54:GLN:HE21	1.84	0.43
1:A:1488:A:H3'	1:A:1489:A:H8	1.83	0.43
11:K:70:PRO:HA	11:K:95:ALA:HB2	2.00	0.43
13:M:112:ALA:HB1	13:M:117:LEU:HD12	1.99	0.43
3:C:168:GLU:HG3	3:C:169:GLY:H	1.84	0.43
9:I:22:ILE:HD11	9:I:42:THR:HG23	2.00	0.43
1:A:375:A:O2'	1:A:377:U:OP2	2.29	0.43
4:D:189:ASP:HB3	4:D:194:VAL:HG22	2.01	0.43
1:A:629:A:H5'	5:E:89:VAL:HG21	2.00	0.43
3:C:231:PRO:HG2	3:C:248:SER:O	2.19	0.43
5:E:146:LEU:HD13	5:E:148:GLN:NE2	2.34	0.42
19:S:84:LYS:HE3	19:S:93:ILE:HD11	2.01	0.42
9:I:69:VAL:HG21	9:I:105:GLU:HG3	2.00	0.42
16:P:5:ILE:HG22	16:P:38:VAL:HG22	2.01	0.42
10:J:79:LEU:HB2	10:J:113:GLY:HA2	2.02	0.42
1:A:592:A:N3	1:A:592:A:O2'	2.47	0.42
1:A:1599:G:H2'	1:A:1600:A:H5'	2.02	0.42
1:A:1767:G:OP2	1:A:1768:C:N4	2.38	0.42
10:J:6:LEU:HD12	10:J:6:LEU:O	2.20	0.42
1:A:2574:U:O2'	1:A:2575:G:O5'	2.31	0.42
18:R:60:PRO:HG3	18:R:74:LYS:HB3	2.02	0.42
20:T:9:ARG:NH1	20:T:40:SER:HB2	2.34	0.42
1:A:1767:G:P	1:A:1768:C:H41	2.41	0.42
1:A:2778:G:H22	7:G:3:ARG:NH2	2.14	0.42
16:P:20:ILE:HD11	16:P:95:LEU:HB2	2.02	0.42
17:Q:72:LYS:HE3	17:Q:72:LYS:HB3	1.89	0.42
4:D:37:GLN:HB3	4:D:50:GLN:HG2	2.01	0.41
5:E:17:ILE:HD11	5:E:200:LYS:HE3	2.01	0.41
10:J:61:LEU:HD21	28:3:24:ARG:HD2	2.01	0.41
1:A:1395:G:O2'	1:A:1410:A:N6	2.53	0.41
18:R:19:ALA:HB1	18:R:24:LYS:HB2	2.02	0.41
1:A:660:A:C8	5:E:182:ASN:HB3	2.54	0.41
17:Q:73:GLU:HB2	17:Q:106:VAL:HG22	2.02	0.41
1:A:1963:A:OP2	1:A:1989:C:N4	2.49	0.41
1:A:2334:G:O2'	1:A:2336:A:OP2	2.37	0.41
8:H:74:VAL:HG12	8:H:89:THR:HG22	2.03	0.41
1:A:372:A:H61	19:S:15:LYS:HG2	1.84	0.41
1:A:952:A:OP1	11:K:24:GLY:N	2.53	0.41
3:C:230:HIS:HE2	3:C:249:PRO:HG3	1.86	0.41
14:N:99:LEU:HB3	14:N:102:LEU:HD13	2.03	0.41
1:A:2566:C:H5'	29:4:3:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:VAL:HG12	5:E:109:ALA:HB2	2.03	0.41
5:E:34:PHE:CE1	10:J:6:LEU:CD1	2.82	0.41
1:A:526:A:O2'	19:S:42:LYS:O	2.39	0.41
1:A:1552:U:O2'	1:A:1553:A:O5'	2.39	0.41
1:A:1831:A:OP2	3:C:261:ARG:NH2	2.54	0.41
1:A:2139:A:H61	1:A:2148:G:P	2.44	0.41
11:K:43:THR:HG22	11:K:94:ILE:HG22	2.03	0.41
1:A:2313:A:H4'	1:A:2314:A:O4'	2.21	0.41
9:I:88:ARG:O	9:I:88:ARG:HG2	2.21	0.41
10:J:55:LEU:O	10:J:60:ARG:NH1	2.54	0.41
1:A:275:A:H62	1:A:296:G:N2	2.19	0.40
1:A:1000:G:OP2	11:K:87:LYS:NZ	2.54	0.40
1:A:1578:A:O2'	1:A:1579:C:O4'	2.39	0.40
1:A:2331:G:H22	1:A:2339:U:H3	1.68	0.40
1:A:2707:C:H1'	4:D:200:ASN:ND2	2.35	0.40
1:A:246:U:OP2	28:3:8:ARG:NH1	2.55	0.40
1:A:864:A:C8	1:A:1227:U:O4	2.74	0.40
1:A:928:C:N4	1:A:938:G:OP2	2.54	0.40
1:A:2039:G:OP1	17:Q:11:ARG:NH1	2.41	0.40
1:A:1033:G:OP2	24:X:11:SER:HB2	2.20	0.40
3:C:18:SER:OG	3:C:19:LEU:N	2.54	0.40
16:P:24:LYS:HA	16:P:93:THR:HG23	2.04	0.40
1:A:688:A:N1	1:A:2396:A:O2'	2.50	0.40
27:2:4:ARG:HD3	27:2:4:ARG:HA	1.87	0.40
26:1:9:CYS:HB3	26:1:12:CYS:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	272/274 (99%)	259 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	156/158 (99%)	140 (90%)	16 (10%)	0	100	100
7	G	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
8	H	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
9	I	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
11	K	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
12	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
13	M	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
14	N	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
17	Q	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	S	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
20	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
21	U	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
22	V	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
23	W	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
26	1	45/47 (96%)	45 (100%)	0	0	100	100
27	2	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
28	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
29	4	35/37 (95%)	35 (100%)	0	0	100	100
All	All	2985/3041 (98%)	2766 (93%)	219 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	221/221 (100%)	221 (100%)	0	100 100
4	D	173/173 (100%)	173 (100%)	0	100 100
5	E	168/168 (100%)	168 (100%)	0	100 100
7	G	124/153 (81%)	123 (99%)	1 (1%)	81 89
8	H	122/123 (99%)	121 (99%)	1 (1%)	81 89
9	I	100/100 (100%)	100 (100%)	0	100 100
10	J	109/112 (97%)	109 (100%)	0	100 100
11	K	108/114 (95%)	108 (100%)	0	100 100
12	L	96/101 (95%)	95 (99%)	1 (1%)	76 86
13	M	83/95 (87%)	81 (98%)	2 (2%)	49 67
14	N	93/102 (91%)	91 (98%)	2 (2%)	52 70
15	O	96/96 (100%)	96 (100%)	0	100 100
16	P	84/86 (98%)	84 (100%)	0	100 100
17	Q	89/91 (98%)	88 (99%)	1 (1%)	73 85
18	R	78/80 (98%)	78 (100%)	0	100 100
19	S	81/88 (92%)	81 (100%)	0	100 100
20	T	78/82 (95%)	78 (100%)	0	100 100
21	U	59/62 (95%)	57 (97%)	2 (3%)	37 53
22	V	39/41 (95%)	39 (100%)	0	100 100
23	W	58/60 (97%)	58 (100%)	0	100 100
24	X	52/52 (100%)	52 (100%)	0	100 100
25	Z	35/44 (80%)	35 (100%)	0	100 100
26	1	44/45 (98%)	44 (100%)	0	100 100
27	2	39/39 (100%)	39 (100%)	0	100 100
28	3	55/55 (100%)	55 (100%)	0	100 100
29	4	35/35 (100%)	34 (97%)	1 (3%)	42 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2319/2418 (96%)	2308 (100%)	11 (0%)	89 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	41	MET
8	H	62	LYS
12	L	29	ARG
13	M	35	ARG
13	M	87	LYS
14	N	3	ASN
14	N	53	ARG
17	Q	98	LYS
21	U	22	ARG
21	U	61	ARG
29	4	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	53	HIS
3	C	232	HIS
5	E	40	GLN
10	J	4	HIS
10	J	54	GLN
14	N	3	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2820/2923 (96%)	450 (15%)	6 (0%)
2	B	114/115 (99%)	12 (10%)	0
All	All	2934/3038 (96%)	462 (15%)	6 (0%)

All (462) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	10	A

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Mol	Chain	Res	Type
1	A	28	A
1	A	34	U
1	A	36	G
1	A	43	A
1	A	44	A
1	A	45	G
1	A	71	A
1	A	74	U
1	A	75	G
1	A	88	G
1	A	90	A
1	A	104	C
1	A	106	A
1	A	117	A
1	A	119	U
1	A	140	A
1	A	147	G
1	A	150	A
1	A	164	A
1	A	177	G
1	A	180	G
1	A	182	C
1	A	184	C
1	A	185	A
1	A	191	A
1	A	199	A
1	A	202	A
1	A	213	C
1	A	216	A
1	A	218	G
1	A	219	A
1	A	224	A
1	A	225	A
1	A	233	U
1	A	236	A
1	A	248	G
1	A	251	G
1	A	255	G
1	A	272	C
1	A	279	A
1	A	285	U
1	A	286	U

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Mol	Chain	Res	Type
1	A	298	U
1	A	300	G
1	A	310	C
1	A	316	G
1	A	317	G
1	A	321	U
1	A	327	G
1	A	331	G
1	A	340	C
1	A	353	A
1	A	373	A
1	A	378	C
1	A	389	A
1	A	404	U
1	A	421	C
1	A	429	C
1	A	432	G
1	A	440	C
1	A	457	G
1	A	458	A
1	A	459	C
1	A	463	C
1	A	482	U
1	A	490	C
1	A	497	U
1	A	503	A
1	A	505	U
1	A	506	A
1	A	511	G
1	A	512	A
1	A	513	G
1	A	515	G
1	A	518	A
1	A	519	G
1	A	526	A
1	A	527	G
1	A	538	G
1	A	550	A
1	A	553	A
1	A	554	C
1	A	555	C
1	A	557	G

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Mol	Chain	Res	Type
1	A	566	U
1	A	569	U
1	A	572	C
1	A	575	G
1	A	576	U
1	A	577	A
1	A	578	G
1	A	582	G
1	A	583	A
1	A	591	A
1	A	594	G
1	A	606	G
1	A	611	U
1	A	616	G
1	A	618	A
1	A	630	G
1	A	638	U
1	A	645	A
1	A	646	A
1	A	658	A
1	A	659	A
1	A	666	A
1	A	679	G
1	A	682	A
1	A	690	U
1	A	699	U
1	A	702	U
1	A	720	A
1	A	729	G
1	A	731	U
1	A	735	C
1	A	765	U
1	A	766	G
1	A	768	A
1	A	775	A
1	A	783	G
1	A	792	5MU
1	A	797	A
1	A	807	U
1	A	809	A
1	A	810	A
1	A	815	G

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Mol	Chain	Res	Type
1	A	820	G
1	A	827	A
1	A	829	U
1	A	830	U
1	A	834	A
1	A	835	U
1	A	837	G
1	A	839	A
1	A	845	A
1	A	850	G
1	A	857	C
1	A	872	U
1	A	889	U
1	A	890	G
1	A	891	A
1	A	904	G
1	A	908	A
1	A	911	A
1	A	922	G
1	A	940	U
1	A	955	A
1	A	965	G
1	A	968	A
1	A	970	U
1	A	971	U
1	A	977	A
1	A	989	A
1	A	990	G
1	A	1001	A
1	A	1003	A
1	A	1005	G
1	A	1018	A
1	A	1027	A
1	A	1040	A
1	A	1041	G
1	A	1053	A
1	A	1056	U
1	A	1057	A
1	A	1061	G
1	A	1066	G
1	A	1067	U
1	A	1070	A

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Mol	Chain	Res	Type
1	A	1071	A
1	A	1077	U
1	A	1088	C
1	A	1089	C
1	A	1090	A
1	A	1091	G
1	A	1094	A
1	A	1154	G
1	A	1155	A
1	A	1156	G
1	A	1163	U
1	A	1165	C
1	A	1172	A
1	A	1173	A
1	A	1176	U
1	A	1178	C
1	A	1179	C
1	A	1183	G
1	A	1186	A
1	A	1216	U
1	A	1217	U
1	A	1218	G
1	A	1253	G
1	A	1258	A
1	A	1271	G
1	A	1286	G
1	A	1291	A
1	A	1294	G
1	A	1309	G
1	A	1310	A
1	A	1312	A
1	A	1337	A
1	A	1338	U
1	A	1344	A
1	A	1358	A
1	A	1362	C
1	A	1389	U
1	A	1392	G
1	A	1397	G
1	A	1402	A
1	A	1405	G
1	A	1416	U

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Mol	Chain	Res	Type
1	A	1423	C
1	A	1445	C
1	A	1449	A
1	A	1450	A
1	A	1453	G
1	A	1454	U
1	A	1455	U
1	A	1459	A
1	A	1463	A
1	A	1464	U
1	A	1472	C
1	A	1490	G
1	A	1491	C
1	A	1492	G
1	A	1495	C
1	A	1498	U
1	A	1503	U
1	A	1504	U
1	A	1505	G
1	A	1519	U
1	A	1520	A
1	A	1521	A
1	A	1525	U
1	A	1526	G
1	A	1547	C
1	A	1552	U
1	A	1553	A
1	A	1555	G
1	A	1559	G
1	A	1561	G
1	A	1570	G
1	A	1575	A
1	A	1578	A
1	A	1579	C
1	A	1582	U
1	A	1583	G
1	A	1584	U
1	A	1586	U
1	A	1592	A
1	A	1594	U
1	A	1605	A
1	A	1606	C

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Mol	Chain	Res	Type
1	A	1613	G
1	A	1616	A
1	A	1630	A
1	A	1631	G
1	A	1638	G
1	A	1651	C
1	A	1660	A
1	A	1671	A
1	A	1690	A
1	A	1691	G
1	A	1692	C
1	A	1717	G
1	A	1718	G
1	A	1731	G
1	A	1738	C
1	A	1740	G
1	A	1742	A
1	A	1761	G
1	A	1765	A
1	A	1768	C
1	A	1771	A
1	A	1772	G
1	A	1790	G
1	A	1791	G
1	A	1800	A
1	A	1826	G
1	A	1827	C
1	A	1828	U
1	A	1843	U
1	A	1856	A
1	A	1860	C
1	A	1885	G
1	A	1898	C
1	A	1901	C
1	A	1902	G
1	A	1903	A
1	A	1904	A
1	A	1918	G
1	A	1933	G
1	A	1937	G
1	A	1938	U
1	A	1945	A

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Mol	Chain	Res	Type
1	A	1946	A
1	A	1955	A
1	A	1956	G
1	A	1958	U
1	A	1965	A
1	A	1982	U
1	A	1990	C
1	A	1994	C
1	A	1996	A
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2020	U
1	A	2050	A
1	A	2058	A
1	A	2059	G
1	A	2060	A
1	A	2061	U
1	A	2070	C
1	A	2078	A
1	A	2081	A
1	A	2082	C
1	A	2083	G
1	A	2087	A
1	A	2088	G
1	A	2089	A
1	A	2093	C
1	A	2096	G
1	A	2110	G
1	A	2118	U
1	A	2120	G
1	A	2139	A
1	A	2143	G
1	A	2145	U
1	A	2146	A
1	A	2147	G
1	A	2153	A
1	A	2158	U
1	A	2159	U
1	A	2160	G
1	A	2165	G
1	A	2172	C

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Mol	Chain	Res	Type
1	A	2173	U
1	A	2175	G
1	A	2185	A
1	A	2186	G
1	A	2190	C
1	A	2193	G
1	A	2194	U
1	A	2195	G
1	A	2196	G
1	A	2198	A
1	A	2204	C
1	A	2205	C
1	A	2225	A
1	A	2230	G
1	A	2231	C
1	A	2233	C
1	A	2238	U
1	A	2243	U
1	A	2252	A
1	A	2265	G
1	A	2266	G
1	A	2290	C
1	A	2295	A
1	A	2306	G
1	A	2310	C
1	A	2314	A
1	A	2332	U
1	A	2334	G
1	A	2335	G
1	A	2336	A
1	A	2347	A
1	A	2348	G
1	A	2352	G
1	A	2362	A
1	A	2372	G
1	A	2374	C
1	A	2377	C
1	A	2388	A
1	A	2410	G
1	A	2412	C
1	A	2417	U
1	A	2418	G

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Mol	Chain	Res	Type
1	A	2429	U
1	A	2433	C
1	A	2438	A
1	A	2456	G
1	A	2457	A
1	A	2459	A
1	A	2460	A
1	A	2461	A
1	A	2468	C
1	A	2474	G
1	A	2475	A
1	A	2503	A
1	A	2505	A
1	A	2518	U
1	A	2526	C
1	A	2531	U
1	A	2535	G
1	A	2545	A
1	A	2547	C
1	A	2556	G
1	A	2581	U
1	A	2588	A
1	A	2593	A
1	A	2594	G
1	A	2600	C
1	A	2604	A
1	A	2605	G
1	A	2613	C
1	A	2629	A
1	A	2630	G
1	A	2635	G
1	A	2636	U
1	A	2640	U
1	A	2642	U
1	A	2646	U
1	A	2648	G
1	A	2657	G
1	A	2692	A
1	A	2705	U
1	A	2716	U
1	A	2717	A
1	A	2733	A

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Mol	Chain	Res	Type
1	A	2741	G
1	A	2750	C
1	A	2753	U
1	A	2763	G
1	A	2771	G
1	A	2775	A
1	A	2778	G
1	A	2791	A
1	A	2794	C
1	A	2803	A
1	A	2804	G
1	A	2805	A
1	A	2806	U
1	A	2817	A
1	A	2818	A
1	A	2819	C
1	A	2823	G
1	A	2828	U
1	A	2832	A
1	A	2838	C
1	A	2840	A
1	A	2869	G
1	A	2887	G
1	A	2892	G
1	A	2900	C
1	A	2903	A
1	A	2913	G
1	A	2915	C
2	B	10	U
2	B	11	A
2	B	23	U
2	B	24	C
2	B	39	G
2	B	40	C
2	B	49	G
2	B	65	G
2	B	87	C
2	B	88	G
2	B	106	G
2	B	115	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	576	U
1	A	577	A
1	A	808	G
1	A	1670	A
1	A	1957	G
1	A	2749	G

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

3 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	$\#\|Z\| > 2$
1	5MU	A	792	1	19,22,23	4.51	7 (36%)	28,32,35	3.85	10 (35%)
1	2MA	A	2530	30,1	17,25,26	1.05	0	17,37,40	1.35	3 (17%)
1	5MU	A	1966	1	19,22,23	4.61	7 (36%)	28,32,35	3.83	10 (35%)

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
1	5MU	A	792	1	-	2/7/25/26	0/2/2/2
1	2MA	A	2530	30,1	-	2/3/25/26	0/3/3/3
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1966	5MU	C2-N1	9.99	1.54	1.38
1	A	792	5MU	C2-N1	9.89	1.54	1.38
1	A	1966	5MU	C6-N1	9.73	1.54	1.38
1	A	792	5MU	C6-N1	9.39	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1966	5MU	C4-C5	9.18	1.60	1.44
1	A	792	5MU	C4-N3	-8.90	1.22	1.38
1	A	792	5MU	C4-C5	8.56	1.59	1.44
1	A	1966	5MU	C4-N3	-8.52	1.23	1.38
1	A	1966	5MU	C6-C5	5.44	1.43	1.34
1	A	792	5MU	C6-C5	4.85	1.42	1.34
1	A	792	5MU	O4-C4	-3.43	1.17	1.23
1	A	792	5MU	O2-C2	-3.17	1.17	1.23
1	A	1966	5MU	O4-C4	-3.13	1.17	1.23
1	A	1966	5MU	O2-C2	-3.04	1.17	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	792	5MU	C5-C4-N3	12.99	126.40	115.31
1	A	1966	5MU	C5-C4-N3	12.45	125.94	115.31
1	A	1966	5MU	C5-C6-N1	-11.06	111.96	123.34
1	A	792	5MU	C5-C6-N1	-10.44	112.59	123.34
1	A	792	5MU	O4-C4-C5	-5.97	117.98	124.90
1	A	1966	5MU	C4-N3-C2	-5.43	120.32	127.35
1	A	1966	5MU	O4-C4-C5	-5.36	118.69	124.90
1	A	792	5MU	C4-N3-C2	-5.35	120.42	127.35
1	A	1966	5MU	N3-C2-N1	4.81	121.28	114.89
1	A	792	5MU	N3-C2-N1	4.63	121.04	114.89
1	A	1966	5MU	C5M-C5-C6	-3.70	117.91	122.85
1	A	792	5MU	C5M-C5-C6	-3.49	118.19	122.85
1	A	1966	5MU	O2-C2-N1	-3.28	118.42	122.79
1	A	792	5MU	C5M-C5-C4	3.28	122.38	118.77
1	A	1966	5MU	C5M-C5-C4	3.01	122.08	118.77
1	A	2530	2MA	C5-C6-N1	2.76	118.79	114.02
1	A	1966	5MU	O4-C4-N3	-2.47	115.37	120.12
1	A	2530	2MA	C8-N7-C5	2.45	107.66	102.99
1	A	1966	5MU	C6-C5-C4	2.36	120.01	118.03
1	A	792	5MU	O4-C4-N3	-2.35	115.61	120.12
1	A	2530	2MA	O3'-C3'-C4'	-2.35	104.26	111.05
1	A	792	5MU	C1'-N1-C2	2.33	121.79	117.57
1	A	792	5MU	O2-C2-N1	-2.03	120.08	122.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	792	5MU	O4'-C4'-C5'-O5'
1	A	792	5MU	C3'-C4'-C5'-O5'
1	A	2530	2MA	O4'-C4'-C5'-O5'
1	A	2530	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 237 ligands modelled in this entry, 237 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1299:U	O3'	1300:G	P	3.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1232:G	O3'	1233:A	P	3.01
1	A	1294:G	O3'	1295:C	P	2.95
1	A	790:G	O3'	791:U	P	1.34
1	A	792:5MU	O3'	793:G	P	1.19

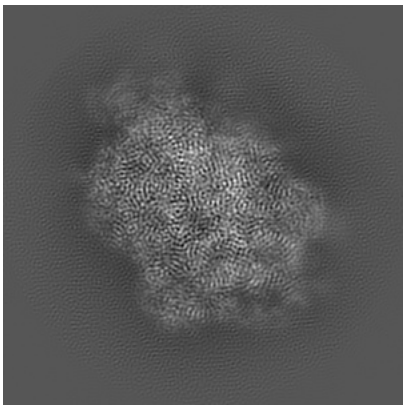
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0243. These allow visual inspection of the internal detail of the map and identification of artifacts.

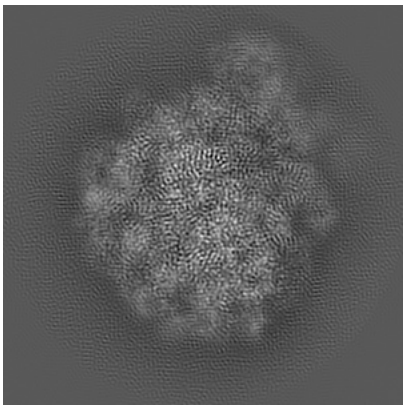
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

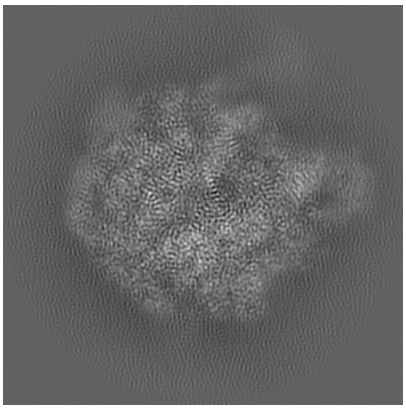
6.1.1 Primary map



X

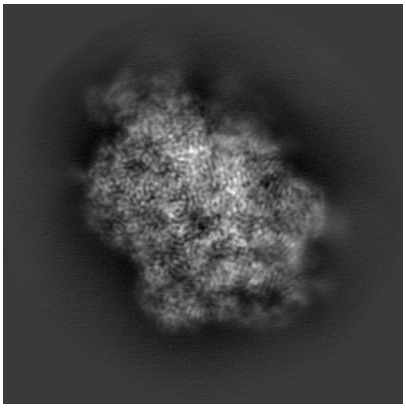


Y

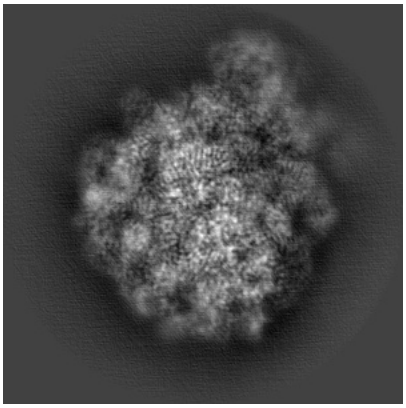


Z

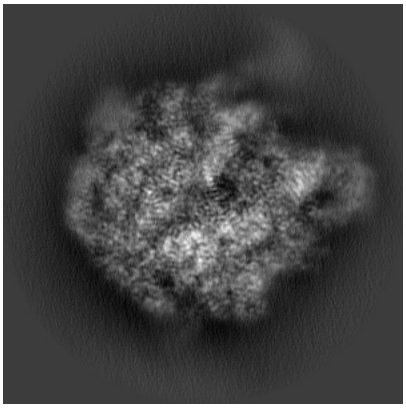
6.1.2 Raw map



X



Y

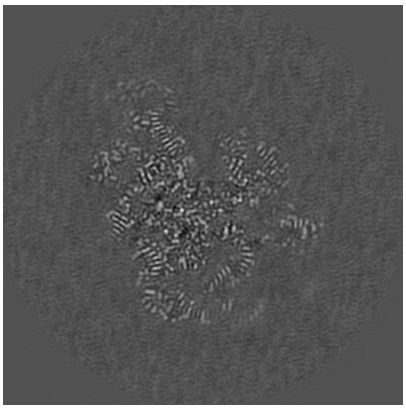


Z

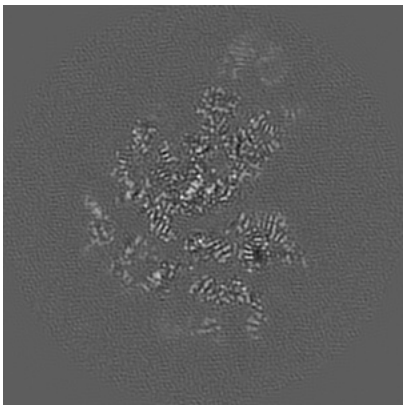
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

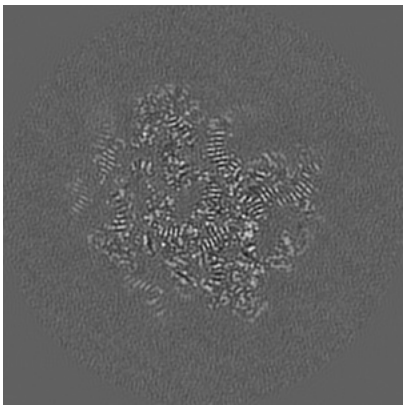
6.2.1 Primary map



X Index: 164

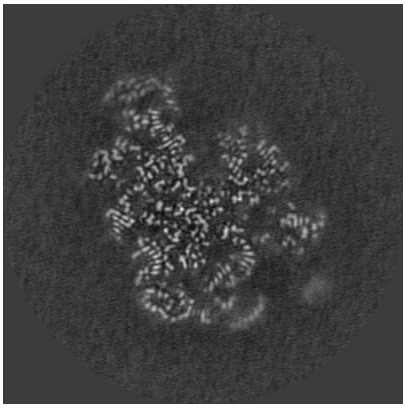


Y Index: 164

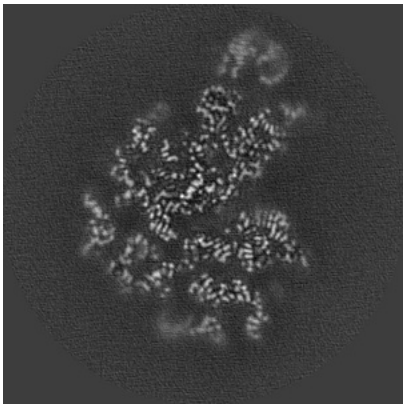


Z Index: 164

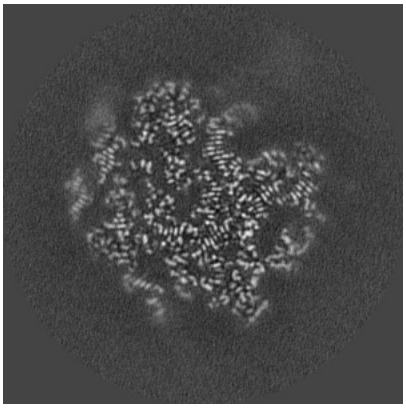
6.2.2 Raw map



X Index: 164



Y Index: 164

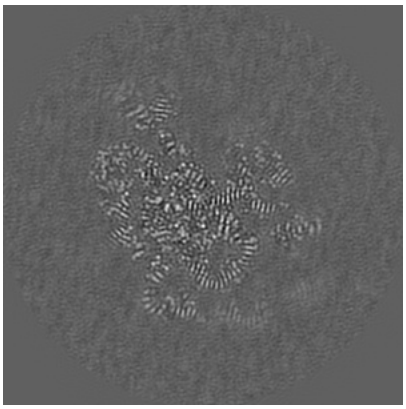


Z Index: 164

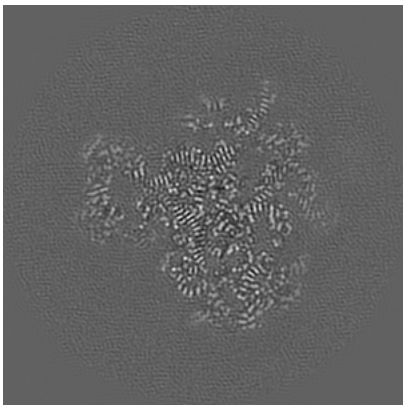
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

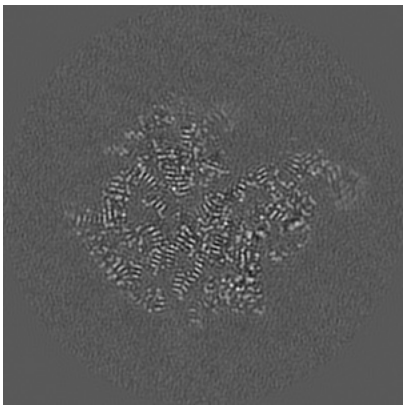
6.3.1 Primary map



X Index: 170

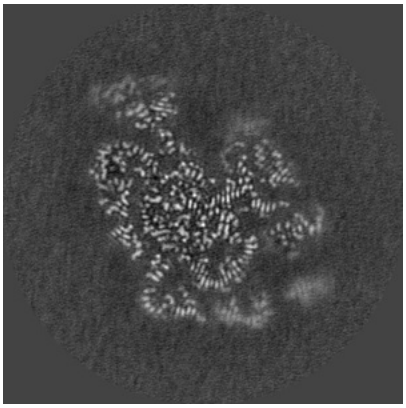


Y Index: 138

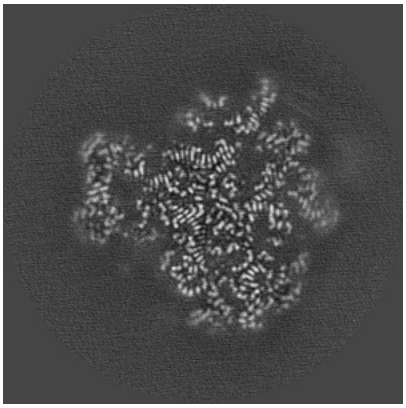


Z Index: 181

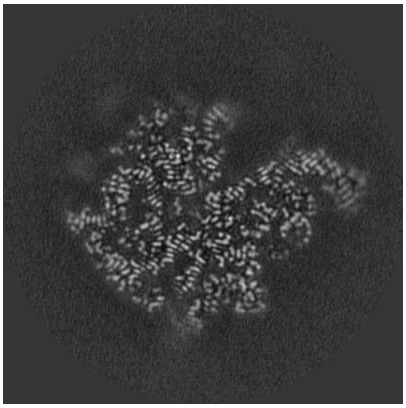
6.3.2 Raw map



X Index: 170



Y Index: 138



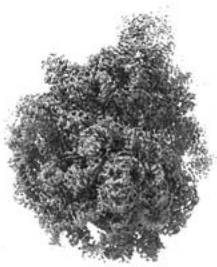
Z Index: 183

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

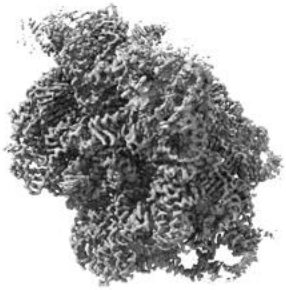


Y

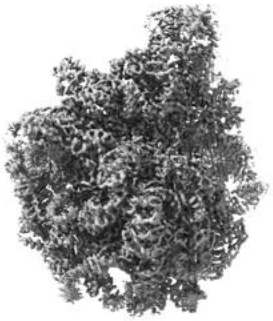
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

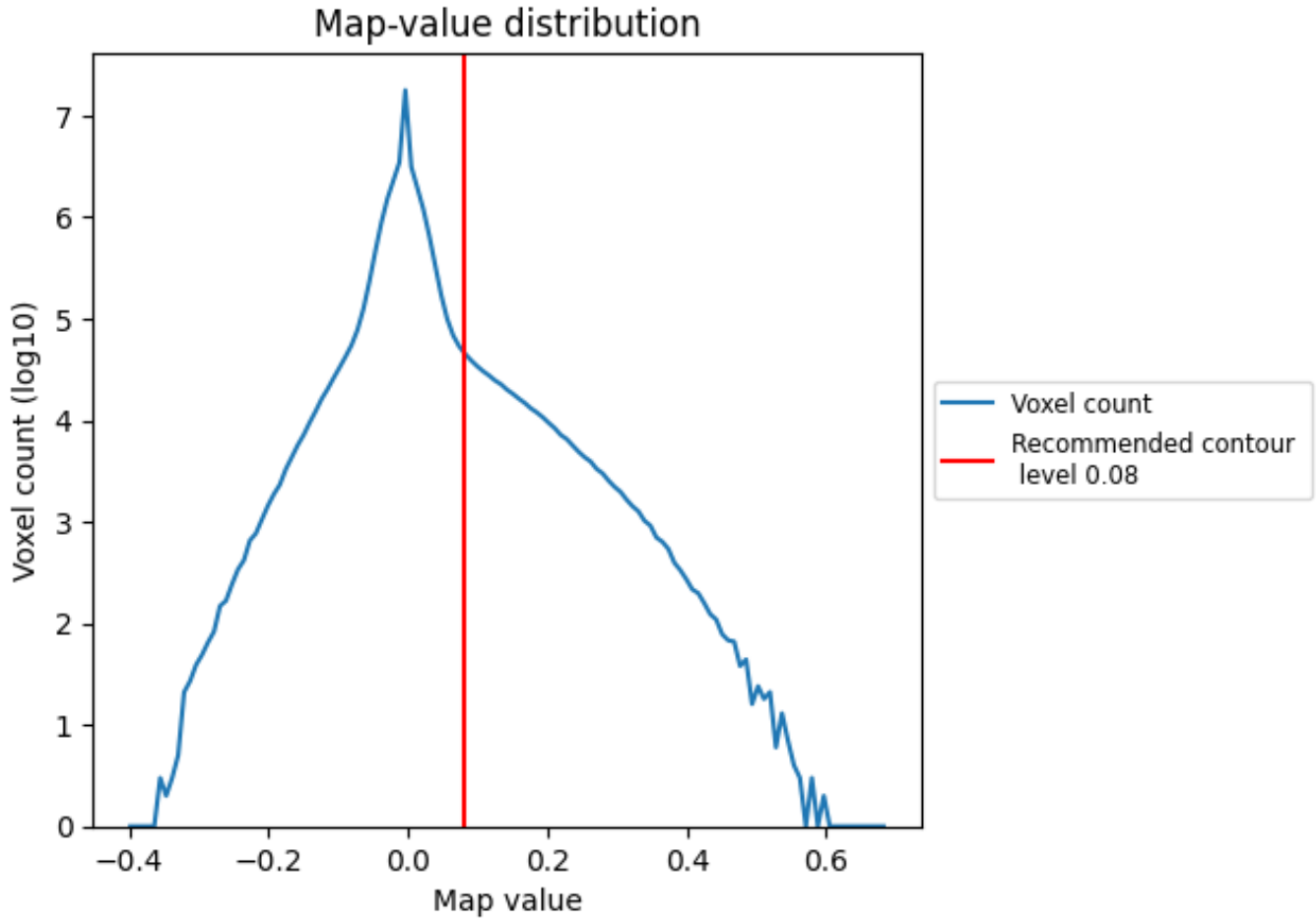
6.5 Mask visualisation (i)

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

7 Map analysis

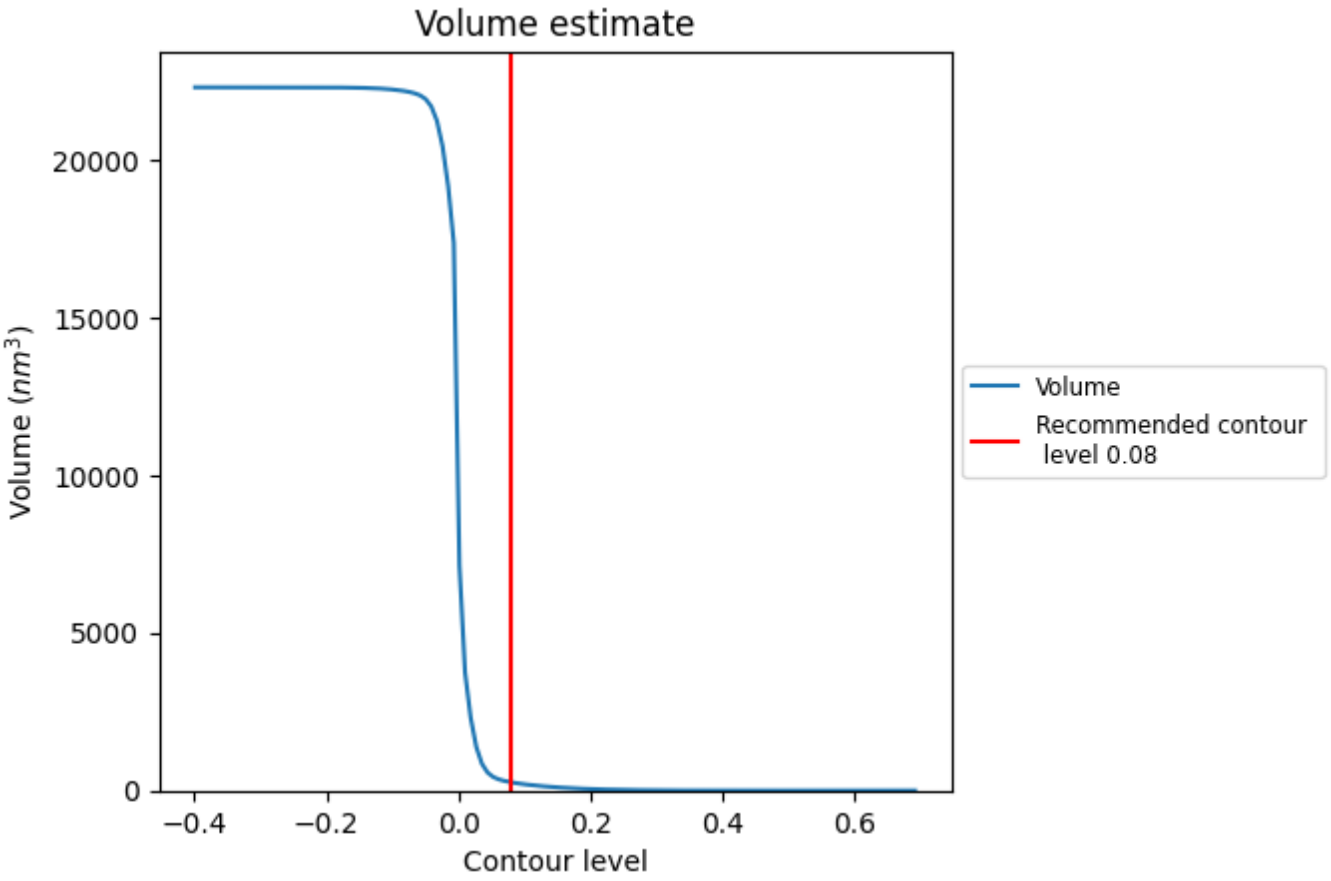
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

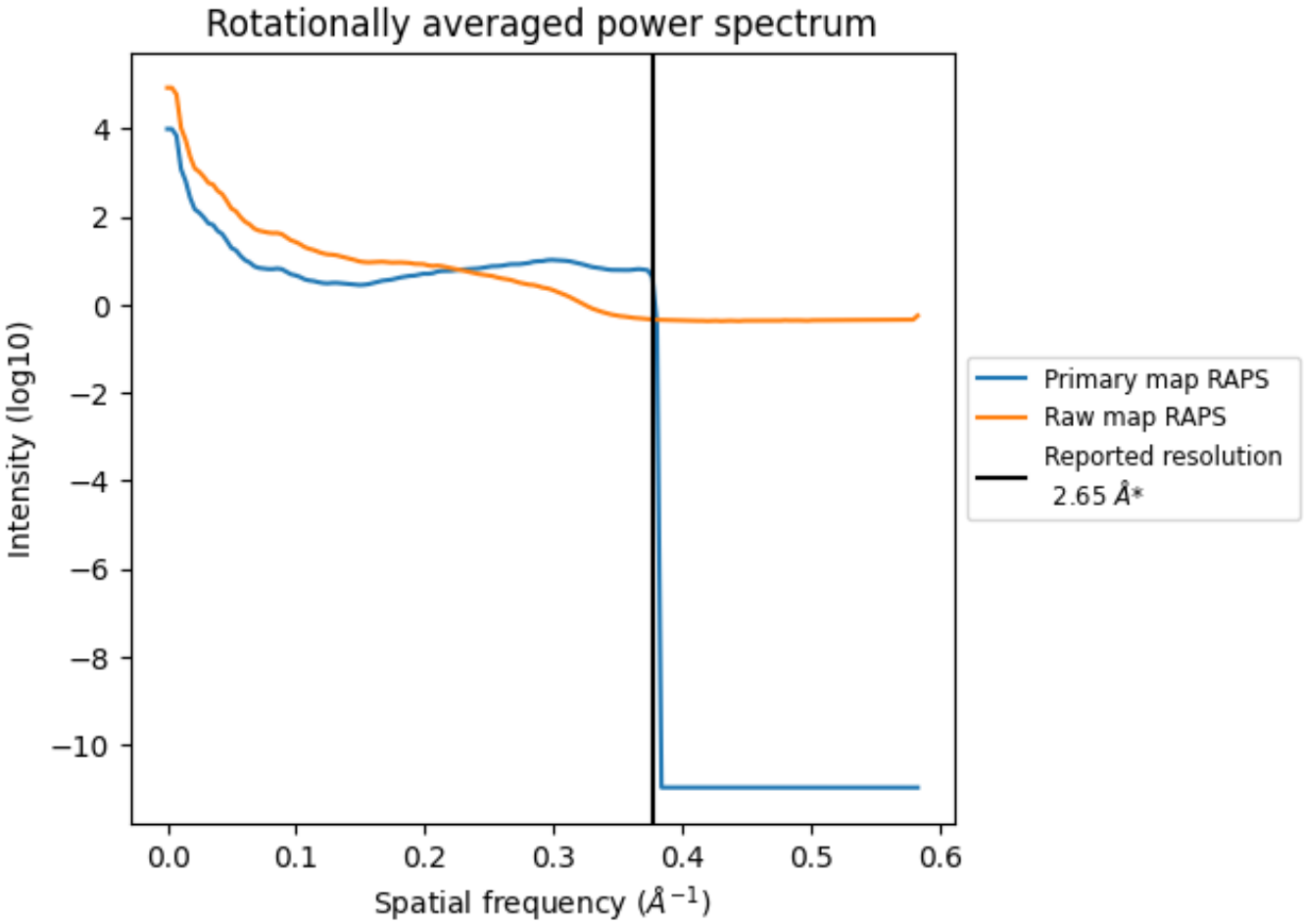
7.2 Volume estimate



The volume at the recommended contour level is 261 nm^3; this corresponds to an approximate mass of 236 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)

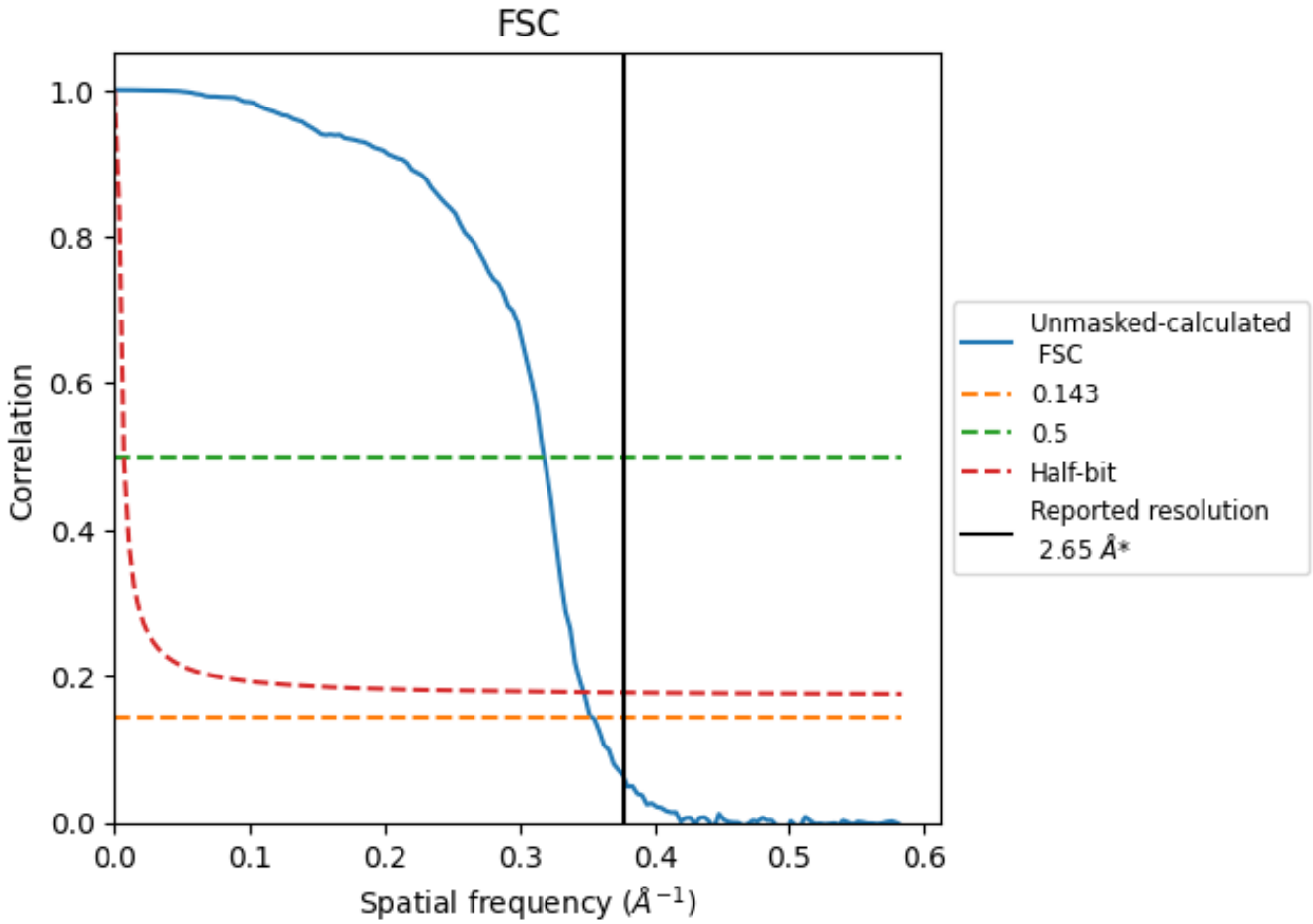


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

8.2 Resolution estimates (i)

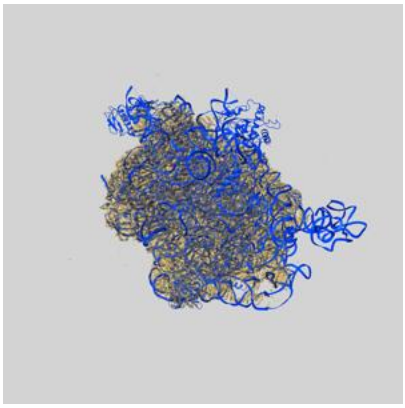
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.14	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

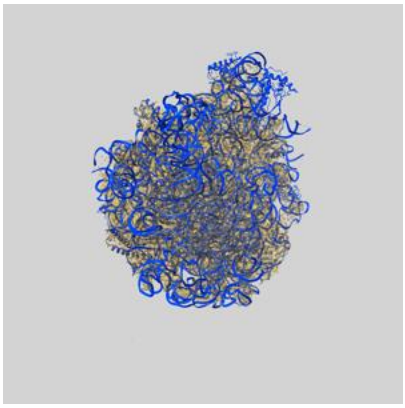
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0243 and PDB model 6HMA. Per-residue inclusion information can be found in section 3 on page 9.

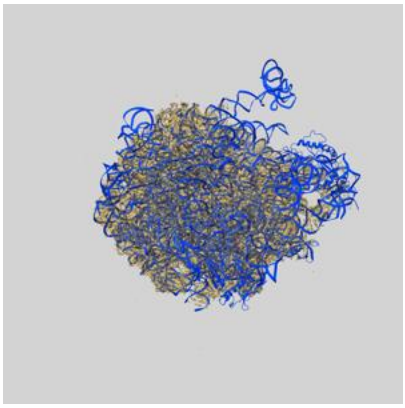
9.1 Map-model overlay



X



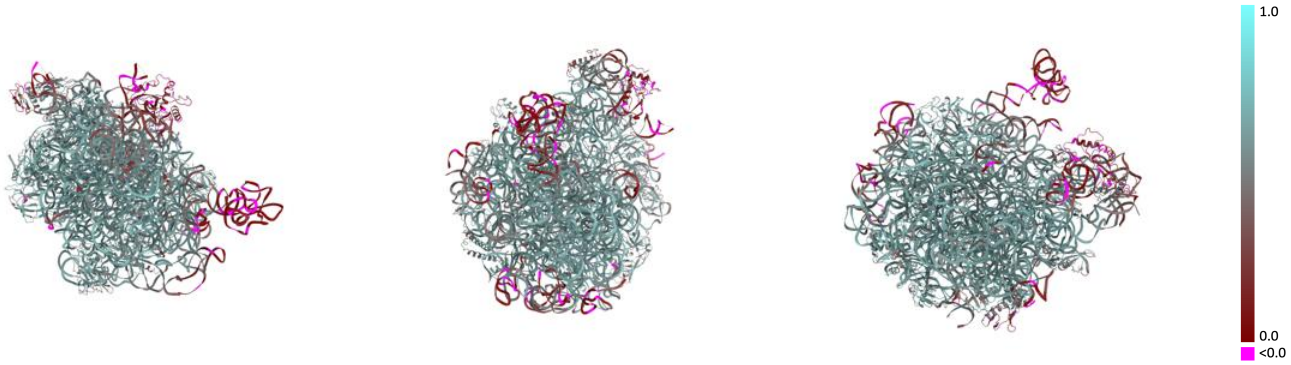
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

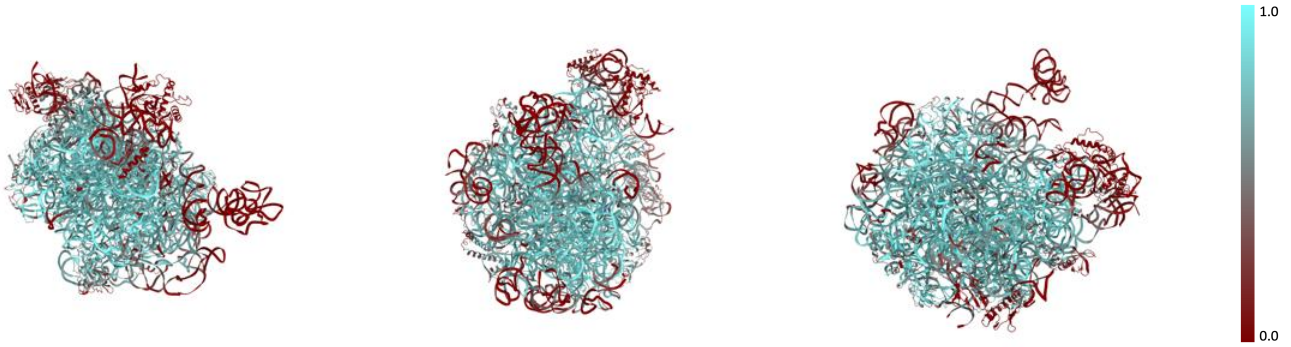
9.2 Q-score mapped to coordinate model (i)



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.

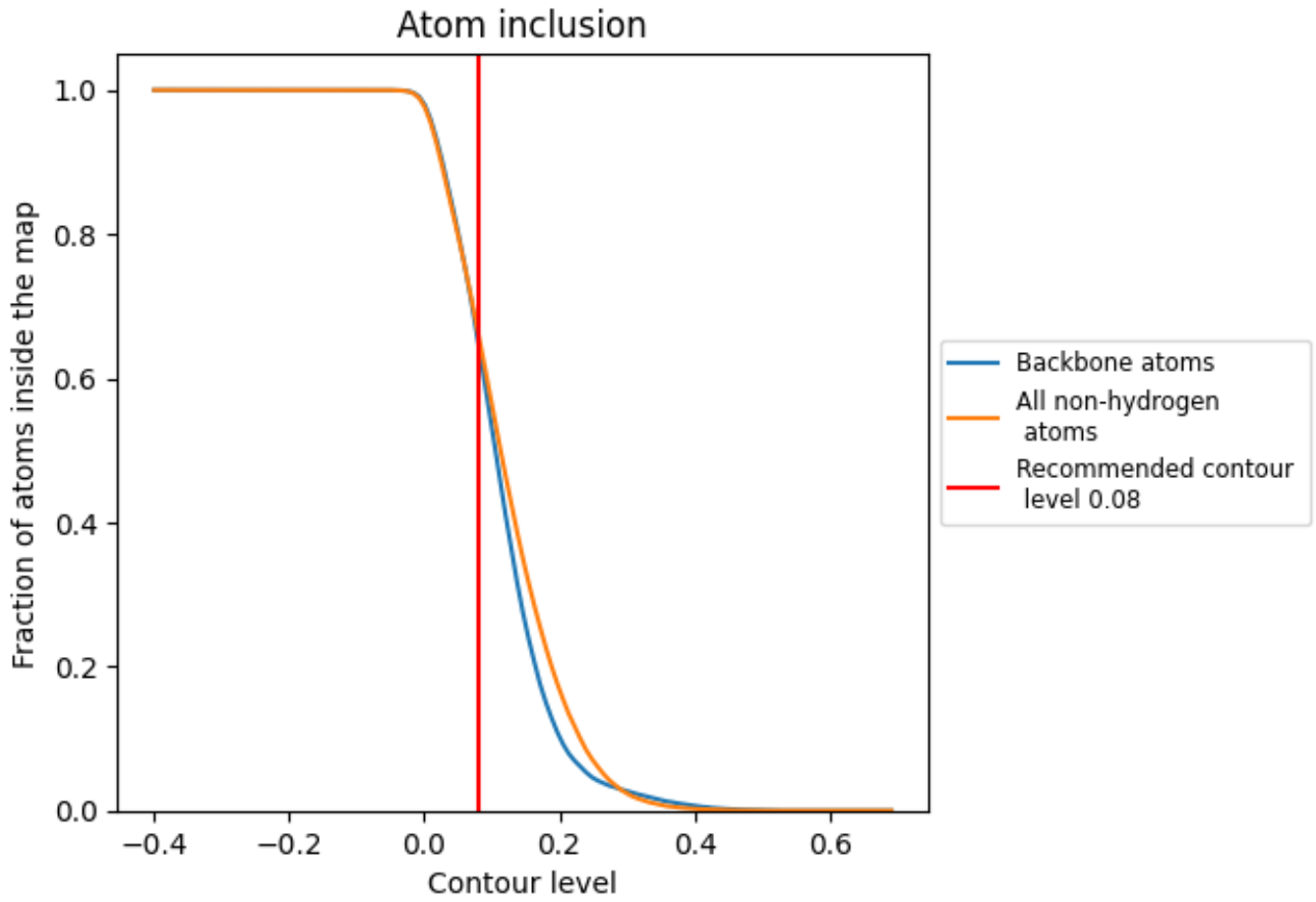
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6635	0.5630
1	0.0347	0.4330
2	0.9017	0.6430
3	0.7689	0.6250
4	0.4810	0.5720
A	0.7047	0.5680
B	0.3527	0.4900
C	0.7490	0.6210
D	0.7636	0.6120
E	0.6639	0.5980
F	0.0000	0.1450
G	0.0696	0.3980
H	0.7825	0.6160
I	0.6279	0.5790
J	0.6325	0.5870
K	0.7055	0.6070
L	0.7620	0.6140
M	0.1570	0.4320
N	0.5984	0.5720
O	0.8405	0.6470
P	0.7057	0.5890
Q	0.7680	0.6190
R	0.6052	0.5630
S	0.3001	0.4710
T	0.3032	0.5070
U	0.7478	0.5990
V	0.5288	0.5280
W	0.4819	0.5290
X	0.7392	0.5970
Z	0.5489	0.5390