



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 08:32 AM JST

PDB ID : 5Z3G
EMDB ID : EMD-6878
Title : Cryo-EM structure of a nucleolar pre-60S ribosome (Rpf1-TAP)
Authors : Zhu, X.; Zhou, D.; Ye, K.
Deposited on : 2018-01-06
Resolution : 3.65 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:

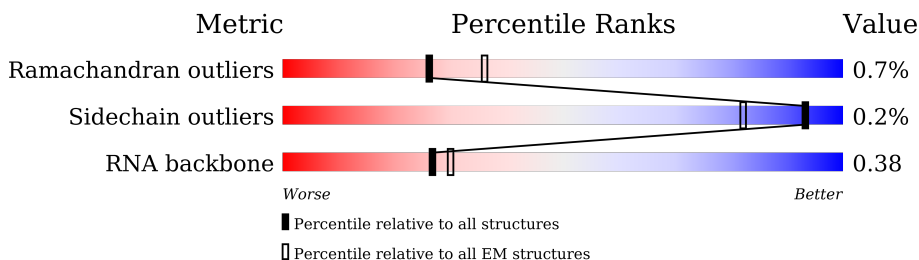
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.65 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.




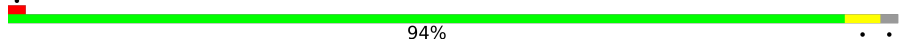
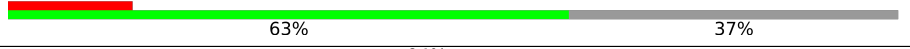
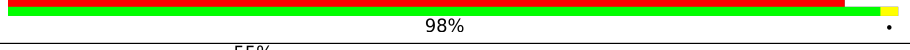

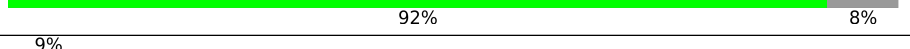
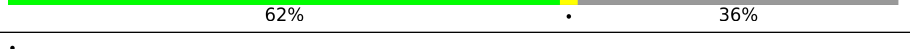

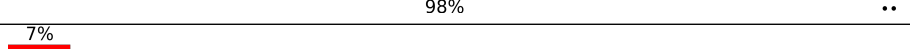
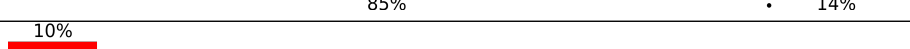
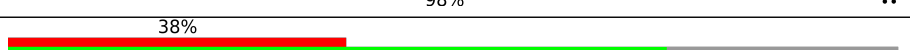

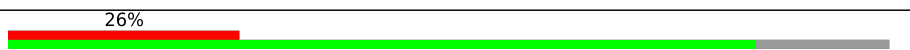
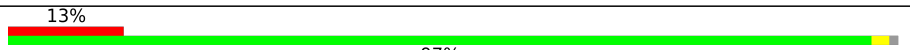
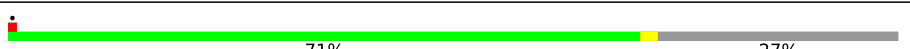




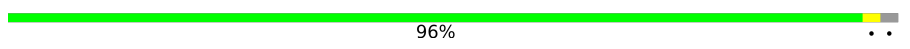
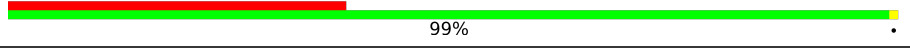
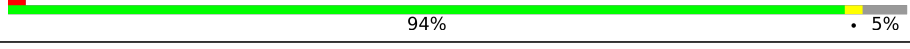
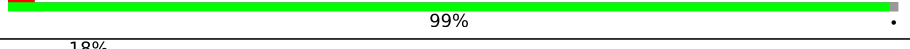
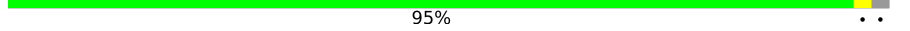

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	3396	
2	B	158	
3	C	232	
4	D	322	
5	E	220	
6	F	387	
7	G	362	
8	H	376	



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Mol	Chain	Length	Quality of chain
9	I	176	
10	J	244	
11	K	256	
12	L	191	
13	M	605	
14	N	245	
15	O	295	
16	P	199	
17	Q	138	
18	R	204	
19	S	199	
20	T	184	
21	U	186	
22	V	463	
23	W	172	
24	X	278	
25	Y	505	
26	Z	306	
27	a	291	
28	b	427	
29	c	127	
30	d	154	
31	i	130	
32	j	107	
33	l	120	

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Mol	Chain	Length	Quality of chain
34	m	100	 <p>33% 67% 33%</p>
35	n	88	 <p>81% 18%</p>

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 85899 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1501	32146	14349	5813	10483	1501	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	156	3313	1482	582	1093	156	0	0

- Molecule 3 is a RNA chain called ITS2 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	65	1370	614	228	463	65	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	247	1956	1248	348	357	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	133	1107	716	198	189	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	336	2670	1696	493	475	6	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 8 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	256	Total	C	N	O	S	0	0
			2063	1332	341	387	3		

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	150	Total	C	N	O	S	0	0
			1198	775	214	208	1		

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	Total	C	N	O	S	0	0
			1918	1235	348	334	1		

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	162	Total	C	N	O	S	0	0
			1247	804	212	229	2		

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 13 is a protein called Nucleolar protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 14 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	226	Total	C	N	O	S	0	0
			1709	1060	296	346	7		

- Molecule 15 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	190	Total	C	N	O	S	0	0
			1591	1031	277	281	2		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	108	Total	C	N	O	0	0
			867	543	182	142		

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	175	Total	C	N	O	S	0	0
			1498	940	315	242	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	136	Total	C	N	O	0	0
			1057	663	197	197		

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	134	1035	659	196	179	1	0	0

- Molecule 22 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	392	3096	1982	522	581	11	0	0

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	170	1425	916	265	241	3	0	0

- Molecule 24 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	202	1718	1121	298	295	4	0	0

- Molecule 25 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	438	3486	2245	600	629	12	0	0

- Molecule 26 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	169	1410	887	269	245	9	0	0

- Molecule 27 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	212	1747	1125	309	307	6	0	0

- Molecule 28 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	82	689	437	122	129	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	125	984	620	191	173		0	0

- Molecule 30 is a protein called Unassigned.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	154	770	462	154	154		0	0

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	i	124	1001	635	202	163	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	j	106	850	540	165	144	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	l	117	959	609	184	165	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	m	67	533	329	111	92	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L37-A.

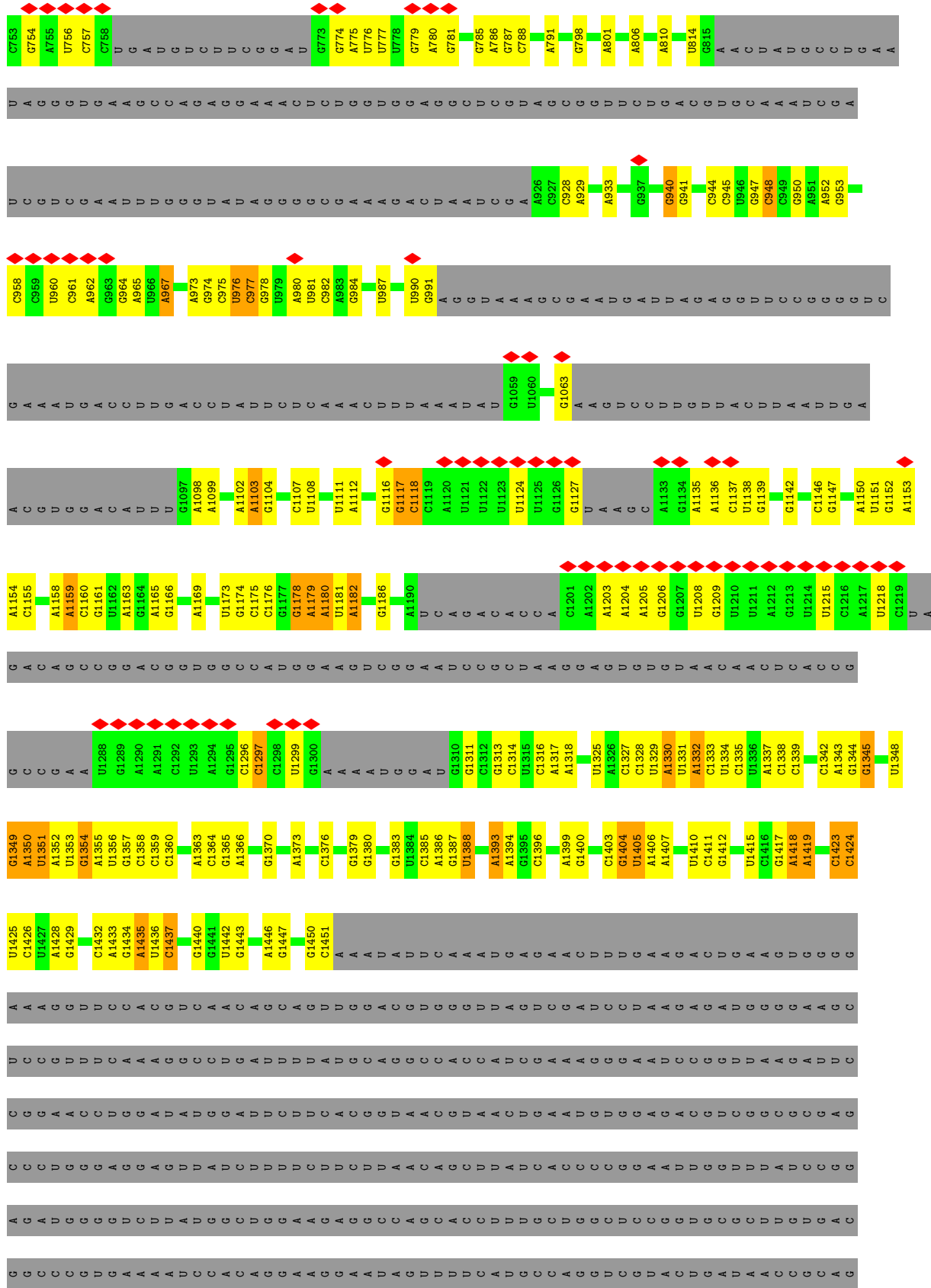
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	n	72	575	350	125	95	5	0	0

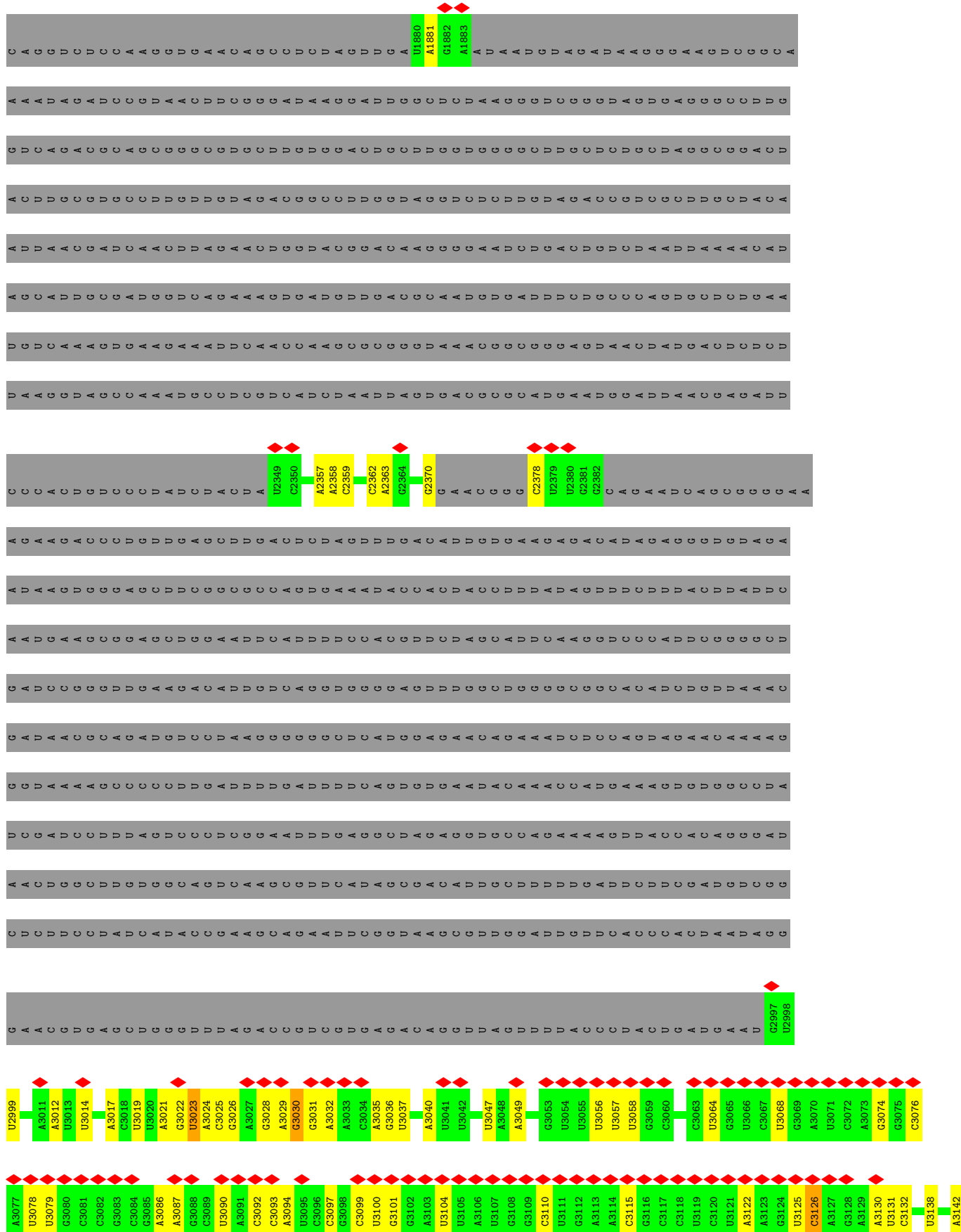
3 Residue-property plots

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.

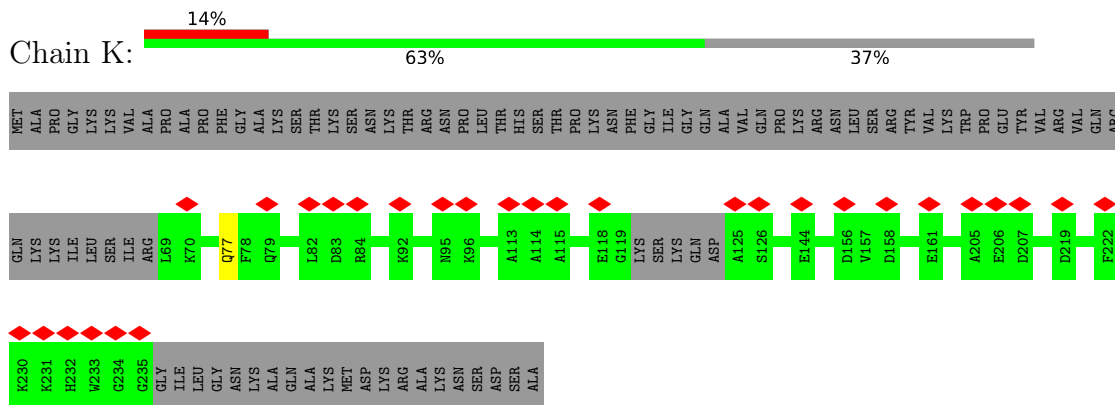
• Molecule 1: 25S rRNA



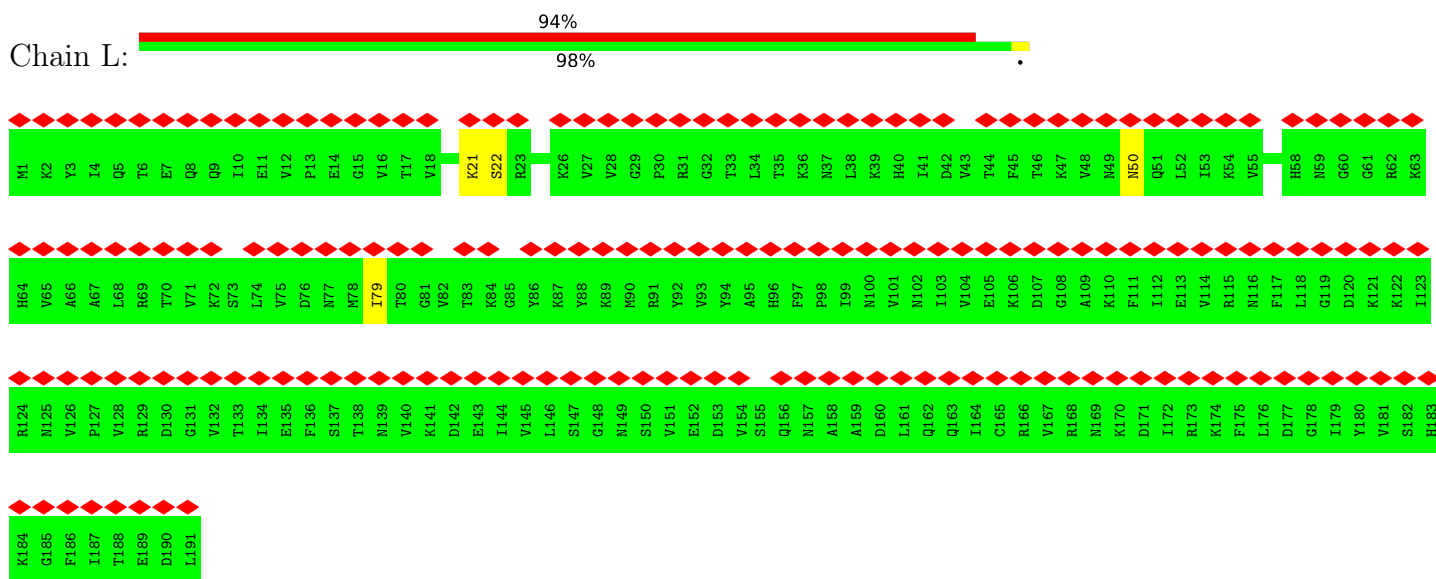




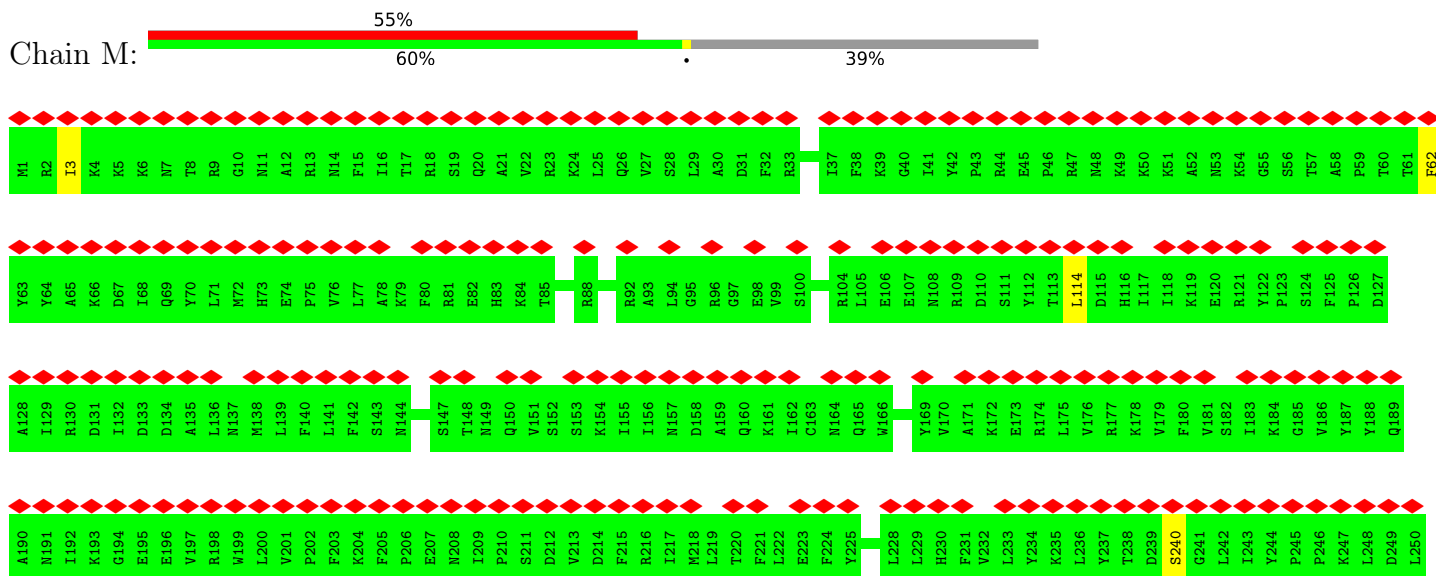
• Molecule 11: 60S ribosomal protein L8-A

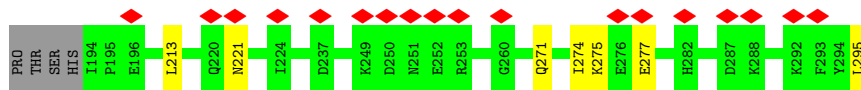


• Molecule 12: 60S ribosomal protein L9-A

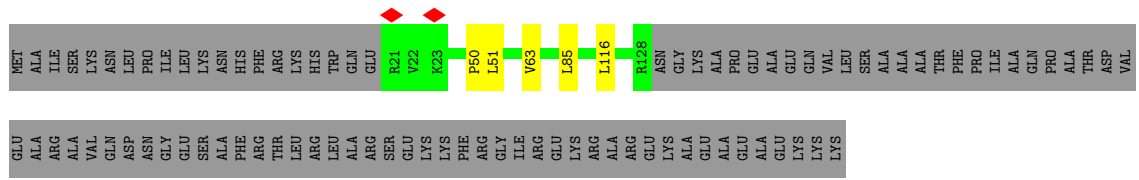


• Molecule 13: Nucleolar protein 7

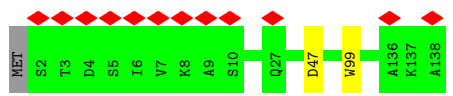




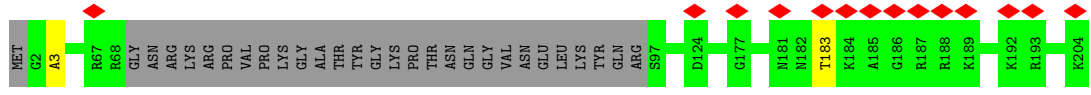
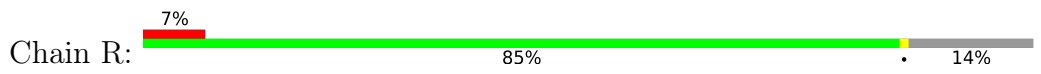
• Molecule 16: 60S ribosomal protein L13-A



• Molecule 17: 60S ribosomal protein L14-A



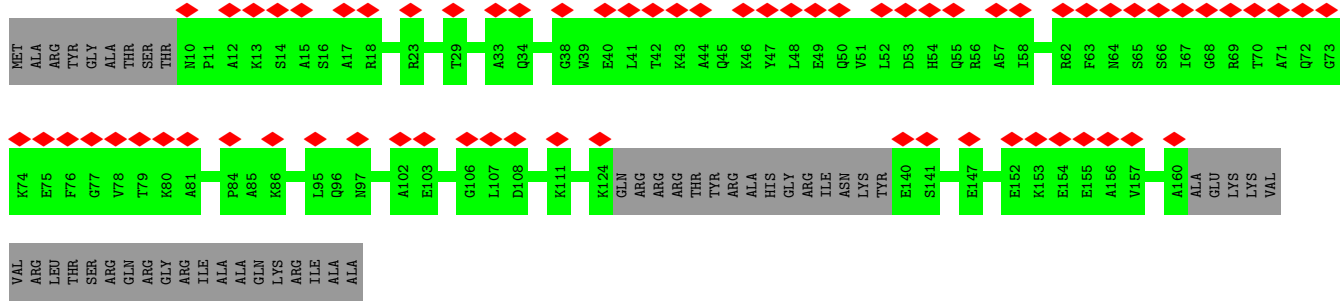
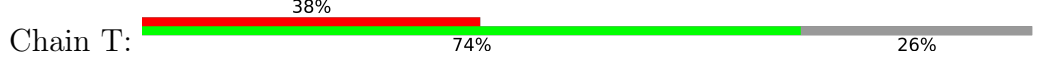
• Molecule 18: 60S ribosomal protein L15-A



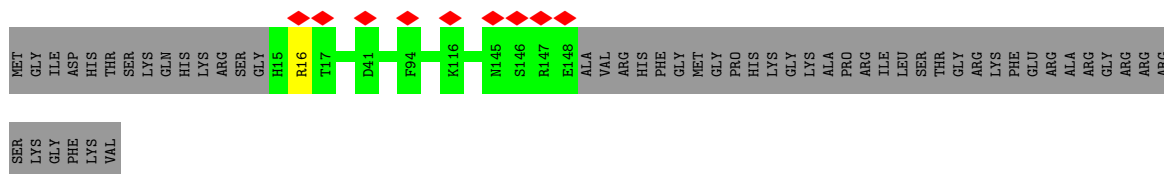
• Molecule 19: 60S ribosomal protein L16-A



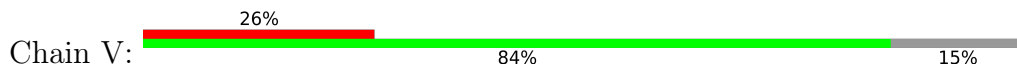
• Molecule 20: 60S ribosomal protein L17-A



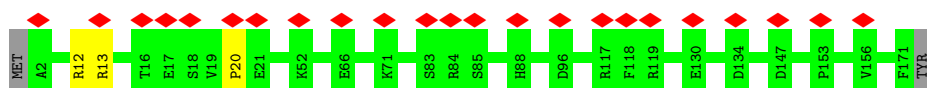
- Molecule 21: 60S ribosomal protein L18-A



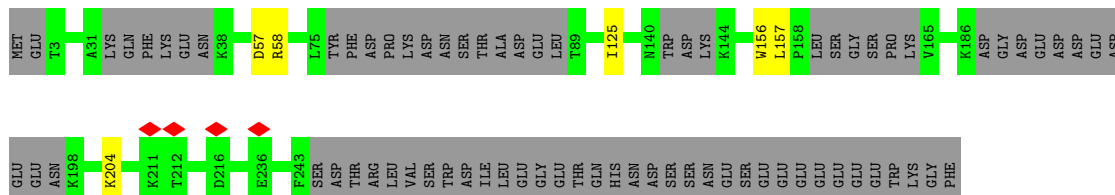
- Molecule 22: Ribosome biogenesis protein NSA1



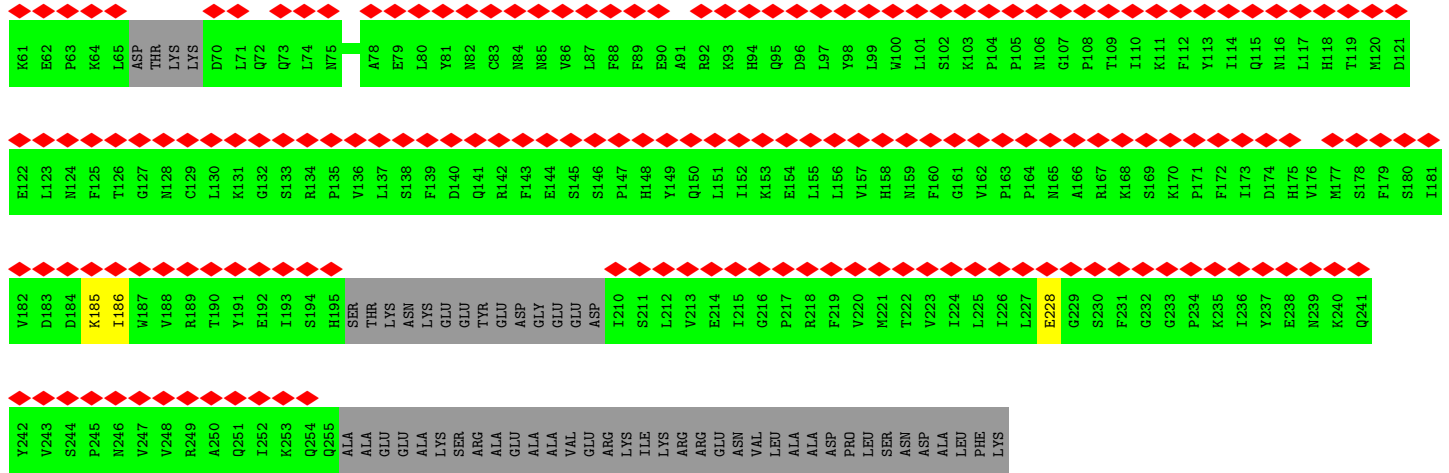
- Molecule 23: 60S ribosomal protein L20-A



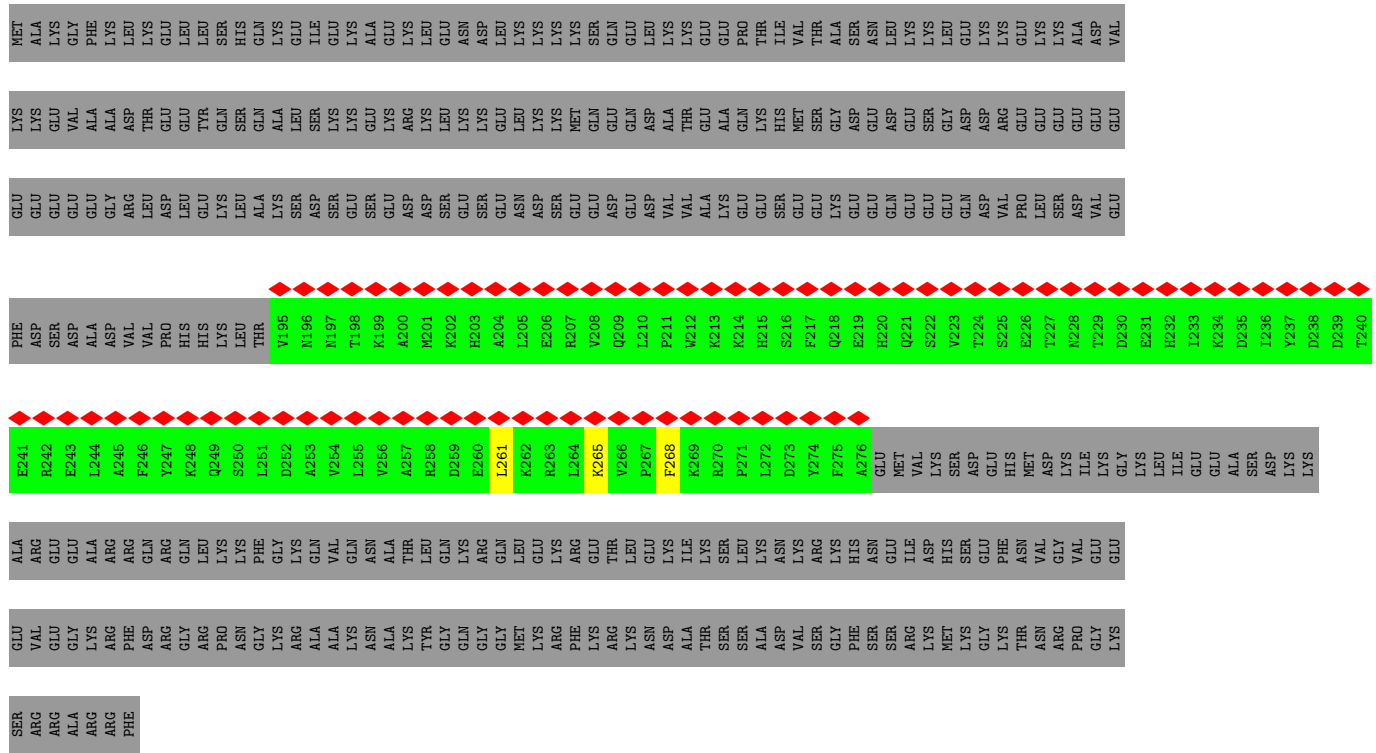
- Molecule 24: Ribosomal RNA-processing protein 1



- Molecule 25: ATP-dependent RNA helicase HAS1



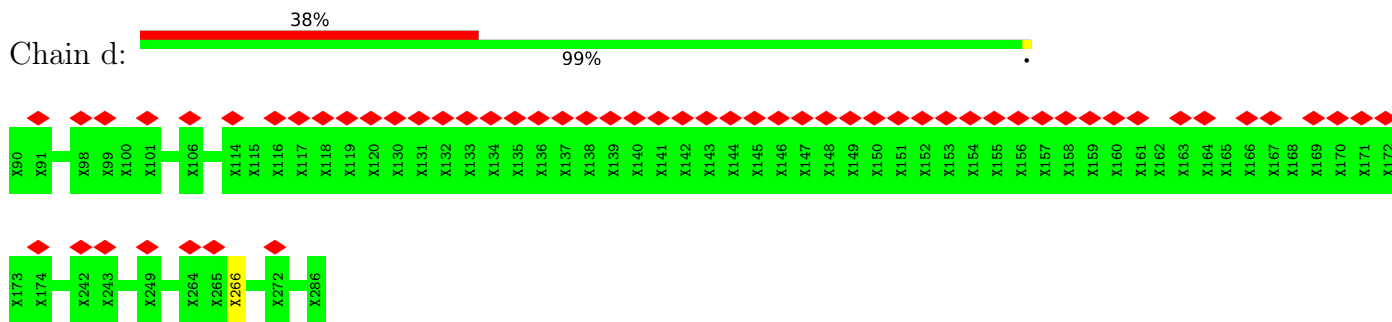
• Molecule 28: rRNA-processing protein EBP2



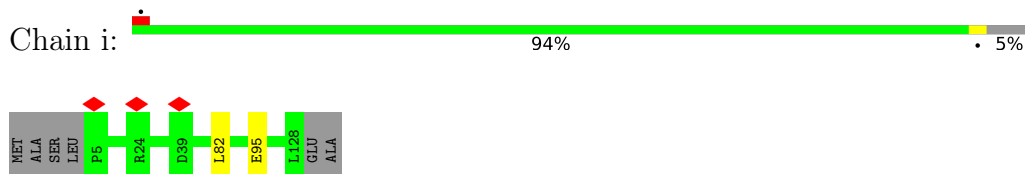
• Molecule 29: 60S ribosomal protein L26-A



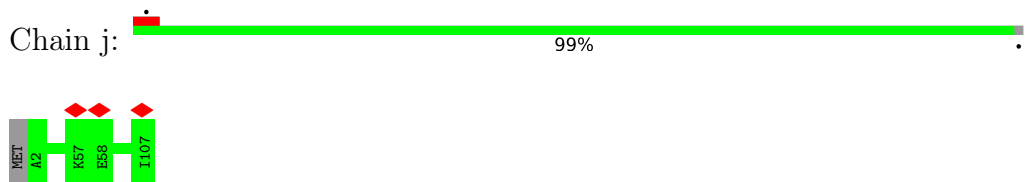
• Molecule 30: Unassigned



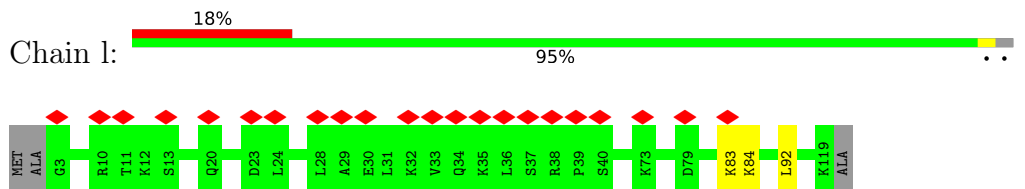
• Molecule 31: 60S ribosomal protein L32



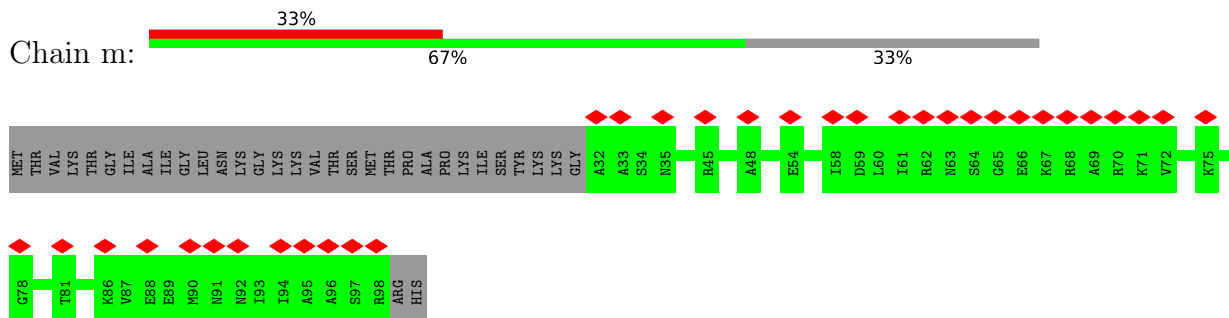
• Molecule 32: 60S ribosomal protein L33-A



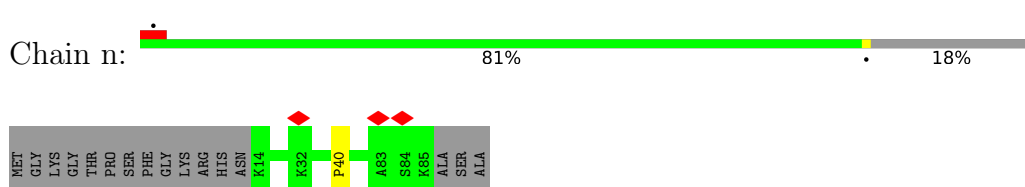
• Molecule 33: 60S ribosomal protein L35-A



• Molecule 34: 60S ribosomal protein L36-A



• Molecule 35: 60S ribosomal protein L37-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.564	Depositor
Minimum map value	-0.265	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality i

5.1 Standard geometry i

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	1.49	246/35968 (0.7%)	1.31	241/56046 (0.4%)
2	B	1.50	18/3702 (0.5%)	1.32	22/5764 (0.4%)
3	C	0.79	0/1527	1.11	6/2371 (0.3%)
4	D	0.42	0/1982	0.65	2/2668 (0.1%)
5	E	0.47	0/1129	0.62	0/1502
6	F	0.47	0/2724	0.66	0/3659
7	G	0.94	2/2801 (0.1%)	0.83	4/3792 (0.1%)
8	H	0.44	0/2097	0.65	1/2828 (0.0%)
9	I	0.77	0/1218	0.69	0/1637
10	J	0.81	0/1956	0.75	1/2631 (0.0%)
11	K	0.65	0/1268	0.71	0/1716
12	L	0.42	0/1539	0.62	0/2073
13	M	0.40	0/3101	0.64	1/4187 (0.0%)
14	N	0.36	0/1730	0.65	0/2354
15	O	0.67	0/1623	0.73	1/2178 (0.0%)
16	P	0.87	0/880	0.77	1/1182 (0.1%)
17	Q	0.73	1/1074 (0.1%)	0.69	0/1446
18	R	0.83	0/1529	0.71	0/2046
19	S	0.80	0/1585	0.69	0/2128
20	T	0.53	0/1075	0.65	0/1448
21	U	0.86	0/1050	0.82	2/1419 (0.1%)
22	V	0.58	0/3151	0.68	0/4244
23	W	0.67	0/1460	0.66	0/1962
24	X	0.79	1/1751 (0.1%)	0.79	2/2348 (0.1%)
25	Y	0.46	0/3552	0.69	1/4789 (0.0%)
26	Z	1.02	3/1437 (0.2%)	0.84	0/1927
27	a	0.43	0/1790	0.64	1/2418 (0.0%)
28	b	0.45	0/704	0.62	0/949
29	c	0.74	0/995	0.73	1/1329 (0.1%)
31	i	0.88	0/1022	0.76	1/1367 (0.1%)
32	j	1.12	0/868	0.79	0/1168
33	l	0.64	0/968	0.68	1/1287 (0.1%)
34	m	0.51	0/536	0.64	0/711
35	n	0.90	0/587	0.77	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.11	271/90379 (0.3%)	1.04	289/130352 (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
4	D	0	2
6	F	0	1
8	H	0	1
10	J	0	3
11	K	0	1
13	M	0	4
15	O	0	3
17	Q	0	1
18	R	0	2
22	V	0	1
23	W	0	3
24	X	0	2
25	Y	0	7
26	Z	0	1
27	a	0	1
28	b	0	3
30	d	0	1
31	i	0	1
33	l	0	1
All	All	0	39

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1366	A	N9-C4	-8.81	1.32	1.37
1	A	1354	G	N9-C4	-8.31	1.31	1.38
1	A	219	A	N9-C4	-7.89	1.33	1.37
1	A	340	C	N1-C6	-7.84	1.32	1.37
1	A	63	A	N9-C4	-7.55	1.33	1.37
1	A	346	C	N1-C6	-7.53	1.32	1.37
1	A	1354	G	N3-C4	-7.48	1.30	1.35
1	A	1330	A	N9-C4	-7.43	1.33	1.37
1	A	324	A	N9-C4	-7.34	1.33	1.37
1	A	27	C	N1-C6	-7.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	A	N9-C4	-7.12	1.33	1.37
1	A	657	A	N3-C4	-7.06	1.30	1.34
1	A	228	U	N1-C2	-7.03	1.32	1.38
1	A	1403	C	N1-C6	-7.02	1.32	1.37
1	A	945	C	N1-C6	-7.00	1.32	1.37
1	A	1147	G	N9-C8	-6.93	1.32	1.37
1	A	324	A	N3-C4	-6.87	1.30	1.34
1	A	941	G	N9-C8	-6.85	1.33	1.37
1	A	1376	C	N1-C6	-6.79	1.33	1.37
1	A	74	G	N9-C4	-6.79	1.32	1.38
1	A	334	A	N9-C4	-6.76	1.33	1.37
1	A	77	A	N9-C4	-6.68	1.33	1.37
1	A	1180	A	N9-C4	-6.67	1.33	1.37
1	A	1146	C	N1-C6	-6.67	1.33	1.37
7	G	194	TYR	CD2-CE2	-6.65	1.29	1.39
1	A	1387	G	C5-C4	-6.62	1.33	1.38
1	A	516	A	N9-C4	-6.61	1.33	1.37
1	A	296	A	N9-C4	-6.60	1.33	1.37
1	A	690	A	N9-C4	-6.60	1.33	1.37
1	A	1158	A	N9-C4	-6.59	1.33	1.37
1	A	199	A	N9-C4	-6.58	1.33	1.37
1	A	341	G	C6-N1	-6.58	1.34	1.39
1	A	504	A	N9-C4	-6.55	1.33	1.37
2	B	35	C	N1-C6	-6.54	1.33	1.37
1	A	327	A	N9-C4	-6.54	1.33	1.37
1	A	630	A	N9-C4	-6.53	1.33	1.37
1	A	123	A	N9-C4	-6.50	1.33	1.37
1	A	219	A	N7-C5	-6.47	1.35	1.39
24	X	156	TRP	CB-CG	-6.47	1.38	1.50
1	A	219	A	N3-C4	-6.43	1.30	1.34
1	A	409	A	N9-C8	-6.38	1.32	1.37
1	A	1388	U	N1-C2	-6.32	1.32	1.38
1	A	340	C	N3-C4	-6.32	1.29	1.33
1	A	367	A	N9-C4	-6.31	1.34	1.37
26	Z	28	CYS	CB-SG	-6.27	1.71	1.82
1	A	1433	A	N9-C4	-6.26	1.34	1.37
1	A	396	A	N9-C4	-6.25	1.34	1.37
1	A	1169	A	N7-C5	-6.25	1.35	1.39
1	A	1159	A	N9-C4	-6.22	1.34	1.37
1	A	399	A	N3-C4	-6.21	1.31	1.34
1	A	407	A	N9-C4	-6.19	1.34	1.37
1	A	3172	A	N9-C4	-6.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	G	N3-C4	-6.17	1.31	1.35
1	A	685	G	N7-C5	-6.17	1.35	1.39
1	A	323	A	N9-C4	-6.16	1.34	1.37
1	A	1418	A	C5-C4	-6.16	1.34	1.38
1	A	1335	C	N1-C6	-6.14	1.33	1.37
1	A	1404	G	C5-C4	-6.14	1.34	1.38
1	A	373	A	N9-C4	-6.12	1.34	1.37
1	A	1161	G	C5-C4	-6.12	1.34	1.38
1	A	584	G	C5-C4	-6.11	1.34	1.38
1	A	1405	U	N1-C2	-6.11	1.33	1.38
2	B	28	C	N1-C6	-6.10	1.33	1.37
1	A	62	A	N9-C4	-6.09	1.34	1.37
1	A	1419	A	C6-N1	-6.07	1.31	1.35
1	A	77	A	N3-C4	-6.06	1.31	1.34
1	A	215	G	C5-C4	-6.04	1.34	1.38
1	A	657	A	N7-C5	-6.02	1.35	1.39
2	B	36	G	C5-C4	-6.01	1.34	1.38
2	B	36	G	N7-C5	-6.00	1.35	1.39
1	A	325	A	N9-C4	-6.00	1.34	1.37
1	A	199	A	N3-C4	-6.00	1.31	1.34
1	A	24	G	N9-C4	-5.99	1.33	1.38
1	A	409	A	N7-C5	-5.99	1.35	1.39
1	A	107	A	C5-C4	-5.98	1.34	1.38
1	A	656	A	N3-C4	-5.97	1.31	1.34
1	A	317	A	N9-C4	-5.96	1.34	1.37
2	B	105	A	N7-C5	-5.95	1.35	1.39
1	A	1327	C	N1-C6	-5.95	1.33	1.37
1	A	1330	A	N3-C4	-5.94	1.31	1.34
1	A	1380	G	C5-C4	-5.91	1.34	1.38
1	A	589	A	N7-C5	-5.91	1.35	1.39
1	A	235	A	N9-C4	-5.89	1.34	1.37
1	A	1426	C	N1-C6	-5.89	1.33	1.37
1	A	941	G	N7-C5	-5.89	1.35	1.39
1	A	341	G	N7-C5	-5.89	1.35	1.39
1	A	318	A	N9-C4	-5.88	1.34	1.37
26	Z	15	CYS	CB-SG	-5.88	1.72	1.81
1	A	1166	G	C5-C4	-5.87	1.34	1.38
2	B	24	G	C6-N1	-5.87	1.35	1.39
1	A	197	G	N9-C4	-5.86	1.33	1.38
1	A	339	C	N1-C6	-5.84	1.33	1.37
1	A	22	G	N7-C5	-5.83	1.35	1.39
1	A	327	A	N3-C4	-5.82	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	C	N1-C6	-5.82	1.33	1.37
1	A	267	G	N3-C4	-5.82	1.31	1.35
1	A	929	A	N3-C4	-5.81	1.31	1.34
1	A	321	C	N1-C6	-5.80	1.33	1.37
1	A	65	A	C5-C4	-5.80	1.34	1.38
1	A	350	C	N1-C6	-5.79	1.33	1.37
1	A	1437	C	N1-C6	-5.78	1.33	1.37
1	A	211	A	N9-C4	-5.77	1.34	1.37
1	A	1393	A	C5-C6	-5.76	1.35	1.41
1	A	344	A	N7-C5	-5.75	1.35	1.39
1	A	1317	A	N9-C4	-5.75	1.34	1.37
1	A	1342	C	N1-C6	-5.74	1.33	1.37
1	A	341	G	C5-C6	-5.74	1.36	1.42
1	A	656	A	N7-C5	-5.74	1.35	1.39
1	A	1433	A	C5-C4	-5.73	1.34	1.38
1	A	1332	A	N7-C5	-5.73	1.35	1.39
1	A	342	A	N3-C4	-5.73	1.31	1.34
1	A	1366	A	N3-C4	-5.72	1.31	1.34
1	A	1388	U	C2-N3	-5.71	1.33	1.37
1	A	665	A	N9-C4	-5.70	1.34	1.37
2	B	45	C	N1-C6	-5.70	1.33	1.37
1	A	657	A	C5-C4	-5.70	1.34	1.38
1	A	589	A	C5-C4	-5.68	1.34	1.38
17	Q	99	TRP	CB-CG	-5.68	1.40	1.50
1	A	1158	A	N3-C4	-5.68	1.31	1.34
1	A	342	A	C5-C4	-5.67	1.34	1.38
1	A	504	A	N3-C4	-5.66	1.31	1.34
1	A	64	G	N9-C8	-5.66	1.33	1.37
1	A	1424	C	N1-C6	-5.65	1.33	1.37
1	A	26	A	N7-C5	-5.65	1.35	1.39
1	A	610	G	N9-C8	-5.61	1.33	1.37
1	A	344	A	C5-C4	-5.60	1.34	1.38
1	A	952	A	N9-C4	-5.60	1.34	1.37
1	A	327	A	C5-C4	-5.59	1.34	1.38
1	A	1418	A	N3-C4	-5.59	1.31	1.34
1	A	349	A	N9-C4	-5.57	1.34	1.37
1	A	1176	C	N1-C2	-5.56	1.34	1.40
1	A	657	A	N9-C4	-5.56	1.34	1.37
1	A	103	G	N7-C5	-5.54	1.35	1.39
1	A	214	G	C6-N1	-5.54	1.35	1.39
1	A	576	C	N1-C6	-5.53	1.33	1.37
1	A	1175	C	N1-C6	-5.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1161	G	N3-C4	-5.50	1.31	1.35
1	A	1423	C	N1-C6	-5.50	1.33	1.37
1	A	610	G	C6-N1	-5.49	1.35	1.39
1	A	213	A	N7-C5	-5.49	1.35	1.39
1	A	57	A	N9-C4	-5.49	1.34	1.37
1	A	678	G	N7-C5	-5.48	1.35	1.39
1	A	611	A	N9-C4	-5.47	1.34	1.37
1	A	678	G	C6-N1	-5.47	1.35	1.39
1	A	344	A	N9-C4	-5.46	1.34	1.37
1	A	1365	G	N3-C4	-5.46	1.31	1.35
1	A	339	C	N3-C4	-5.45	1.30	1.33
1	A	674	G	N9-C8	-5.44	1.34	1.37
2	B	78	G	N9-C4	-5.43	1.33	1.38
1	A	1383	G	C5-C4	-5.43	1.34	1.38
1	A	1379	G	C6-N1	-5.43	1.35	1.39
1	A	1425	U	N1-C2	-5.42	1.33	1.38
1	A	1158	A	N7-C5	-5.42	1.35	1.39
2	B	17	A	N3-C4	-5.42	1.31	1.34
1	A	1173	U	N1-C2	-5.41	1.33	1.38
1	A	338	A	N7-C5	-5.41	1.36	1.39
1	A	1418	A	C6-N1	-5.41	1.31	1.35
1	A	1163	A	N9-C4	-5.40	1.34	1.37
1	A	1176	C	N1-C6	-5.40	1.33	1.37
1	A	1328	C	N1-C6	-5.39	1.33	1.37
1	A	219	A	C5-C6	-5.39	1.36	1.41
1	A	692	A	N7-C5	-5.39	1.36	1.39
1	A	1165	A	C5-C4	-5.39	1.34	1.38
1	A	296	A	N3-C4	-5.39	1.31	1.34
1	A	1343	A	N9-C4	-5.38	1.34	1.37
1	A	1412	G	C5-C4	-5.38	1.34	1.38
1	A	655	C	N1-C6	-5.37	1.33	1.37
1	A	1419	A	C5-C4	-5.37	1.34	1.38
1	A	1432	C	N1-C6	-5.37	1.33	1.37
1	A	1342	C	N3-C4	-5.37	1.30	1.33
1	A	1180	A	C5-C4	-5.36	1.35	1.38
1	A	65	A	N3-C4	-5.36	1.31	1.34
1	A	1345	G	N3-C4	-5.35	1.31	1.35
1	A	653	A	N3-C4	-5.35	1.31	1.34
1	A	657	A	C6-N1	-5.35	1.31	1.35
1	A	23	A	N9-C4	-5.35	1.34	1.37
1	A	63	A	N3-C4	-5.35	1.31	1.34
1	A	787	G	C6-N1	-5.34	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1344	G	N3-C4	-5.34	1.31	1.35
1	A	1364	C	N1-C6	-5.34	1.33	1.37
1	A	611	A	N7-C5	-5.33	1.36	1.39
1	A	1415	U	N1-C2	-5.33	1.33	1.38
1	A	193	C	N1-C6	-5.32	1.33	1.37
1	A	377	A	N9-C4	-5.32	1.34	1.37
1	A	407	A	N3-C4	-5.31	1.31	1.34
1	A	947	G	N7-C5	-5.29	1.36	1.39
1	A	1179	A	N9-C4	-5.28	1.34	1.37
1	A	653	A	N9-C4	-5.28	1.34	1.37
1	A	1180	A	N9-C8	-5.26	1.33	1.37
1	A	1339	C	N1-C6	-5.26	1.33	1.37
1	A	324	A	C6-N1	-5.26	1.31	1.35
1	A	503	C	N1-C6	-5.26	1.33	1.37
1	A	31	C	N1-C6	-5.26	1.33	1.37
1	A	67	A	N9-C4	-5.25	1.34	1.37
1	A	427	C	C4-C5	-5.25	1.38	1.43
2	B	39	G	N3-C4	-5.25	1.31	1.35
1	A	336	A	N7-C5	-5.24	1.36	1.39
1	A	1396	C	N1-C6	-5.24	1.34	1.37
1	A	222	A	C5-C6	-5.23	1.36	1.41
1	A	660	A	C5-C4	-5.23	1.35	1.38
1	A	1147	G	C5-C4	-5.23	1.34	1.38
1	A	1411	C	N1-C6	-5.21	1.34	1.37
1	A	332	C	N1-C6	-5.21	1.34	1.37
2	B	39	G	C5-C4	-5.21	1.34	1.38
1	A	342	A	C6-N1	-5.20	1.31	1.35
1	A	1158	A	C5-C6	-5.20	1.36	1.41
1	A	187	A	N9-C4	-5.20	1.34	1.37
2	B	17	A	N7-C5	-5.20	1.36	1.39
1	A	598	A	N9-C4	-5.19	1.34	1.37
1	A	801	A	C6-N1	-5.19	1.31	1.35
2	B	44	A	C5-C6	-5.19	1.36	1.41
1	A	338	A	N3-C4	-5.19	1.31	1.34
2	B	30	C	N1-C6	-5.18	1.34	1.37
1	A	559	A	N9-C4	-5.18	1.34	1.37
1	A	660	A	N9-C4	-5.18	1.34	1.37
1	A	791	A	N3-C4	-5.18	1.31	1.34
1	A	1419	A	N3-C4	-5.18	1.31	1.34
1	A	1379	G	N9-C8	-5.18	1.34	1.37
1	A	399	A	N9-C4	-5.17	1.34	1.37
1	A	466	G	C5-C4	-5.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	G	N9-C8	-5.15	1.34	1.37
1	A	1333	C	N1-C6	-5.15	1.34	1.37
26	Z	100	TRP	CB-CG	-5.15	1.41	1.50
1	A	22	G	N3-C4	-5.15	1.31	1.35
1	A	395	A	N9-C4	-5.14	1.34	1.37
1	A	639	G	C5-C4	-5.14	1.34	1.38
1	A	1182	A	N9-C4	-5.14	1.34	1.37
1	A	408	A	N3-C4	-5.13	1.31	1.34
1	A	1417	G	N7-C5	-5.13	1.36	1.39
1	A	105	C	N1-C6	-5.13	1.34	1.37
1	A	357	A	C5-C4	-5.13	1.35	1.38
1	A	197	G	N3-C4	-5.12	1.31	1.35
1	A	1419	A	N9-C4	-5.12	1.34	1.37
1	A	690	A	N3-C4	-5.12	1.31	1.34
1	A	1334	U	N1-C6	-5.12	1.33	1.38
1	A	228	U	C2-N3	-5.12	1.34	1.37
1	A	295	A	N9-C4	-5.12	1.34	1.37
1	A	52	A	N9-C4	-5.12	1.34	1.37
1	A	1350	A	N3-C4	-5.11	1.31	1.34
1	A	1380	G	N3-C4	-5.11	1.31	1.35
1	A	363	G	N9-C8	-5.10	1.34	1.37
7	G	250	TRP	CB-CG	-5.10	1.41	1.50
2	B	27	U	N1-C6	-5.09	1.33	1.38
1	A	222	A	N7-C5	-5.09	1.36	1.39
2	B	44	A	C5-C4	-5.09	1.35	1.38
1	A	940	G	N7-C5	-5.08	1.36	1.39
1	A	3215	A	N9-C4	-5.08	1.34	1.37
1	A	1365	G	C5-C4	-5.08	1.34	1.38
1	A	1406	A	N9-C4	-5.08	1.34	1.37
1	A	787	G	N7-C5	-5.07	1.36	1.39
1	A	1363	A	N7-C5	-5.07	1.36	1.39
1	A	810	A	N9-C4	-5.07	1.34	1.37
1	A	1365	G	N9-C4	-5.07	1.33	1.38
1	A	333	G	N9-C8	-5.07	1.34	1.37
1	A	322	U	N1-C2	-5.07	1.33	1.38
1	A	1415	U	C2-N3	-5.06	1.34	1.37
1	A	656	A	C6-N1	-5.05	1.32	1.35
1	A	1423	C	C4-C5	-5.05	1.39	1.43
1	A	952	A	N3-C4	-5.05	1.31	1.34
1	A	334	A	N3-C4	-5.04	1.31	1.34
1	A	610	G	N7-C5	-5.04	1.36	1.39
1	A	1358	C	N1-C6	-5.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	C	N1-C6	-5.03	1.34	1.37
1	A	1344	G	C5-C4	-5.03	1.34	1.38
1	A	791	A	N7-C5	-5.03	1.36	1.39
2	B	104	A	N3-C4	-5.02	1.31	1.34
1	A	683	U	N1-C2	-5.01	1.34	1.38
1	A	1165	A	N3-C4	-5.01	1.31	1.34
1	A	346	C	C4-C5	-5.01	1.39	1.43
1	A	3147	G	N9-C4	-5.00	1.33	1.38
1	A	289	A	N9-C4	-5.00	1.34	1.37

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	C	N1-C2-O2	-11.10	112.24	118.90
1	A	1354	G	O4'-C1'-N9	-10.44	99.84	108.20
1	A	544	C	C2-N3-C4	-9.76	115.02	119.90
1	A	1423	C	C6-N1-C2	-8.66	116.84	120.30
1	A	544	C	C2-N1-C1'	-8.63	109.31	118.80
1	A	1354	G	C2-N3-C4	-8.59	107.61	111.90
1	A	547	G	N3-C2-N2	-8.58	113.89	119.90
1	A	638	C	C6-N1-C2	-8.21	117.02	120.30
1	A	544	C	C6-N1-C1'	8.11	130.53	120.80
1	A	1108	U	C2-N1-C1'	7.99	127.28	117.70
1	A	141	C	N3-C2-O2	-7.95	116.34	121.90
1	A	340	C	N3-C2-O2	-7.95	116.34	121.90
1	A	74	G	N3-C4-N9	-7.93	121.24	126.00
1	A	544	C	N1-C2-N3	7.85	124.70	119.20
1	A	660	A	O5'-P-OP1	-7.76	98.72	105.70
1	A	1354	G	N3-C4-N9	-7.68	121.39	126.00
1	A	1349	G	C2-N3-C4	-7.67	108.07	111.90
1	A	228	U	C2-N1-C1'	-7.65	108.52	117.70
1	A	341	G	C6-C5-N7	-7.63	125.82	130.40
7	G	21	PRO	C-N-CA	-7.57	102.77	121.70
1	A	1103	A	C8-N9-C4	7.49	108.80	105.80
1	A	57	A	C2-N3-C4	-7.42	106.89	110.60
1	A	1435	A	O5'-P-OP1	-7.39	99.04	105.70
3	C	33	U	N1-C2-O2	7.33	127.93	122.80
1	A	74	G	N3-C4-C5	7.29	132.25	128.60
1	A	1354	G	N3-C4-C5	7.28	132.24	128.60
1	A	400	G	C8-N9-C4	7.26	109.31	106.40
1	A	220	G	C8-N9-C1'	-7.24	117.58	127.00
1	A	75	G	C4-N9-C1'	7.20	135.86	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	G	O4'-C1'-N9	7.07	113.86	108.20
24	X	157	LEU	CA-CB-CG	6.99	131.38	115.30
2	B	78	G	N3-C4-C5	6.97	132.09	128.60
1	A	333	G	C8-N9-C1'	-6.94	117.97	127.00
15	O	119	PRO	N-CA-CB	6.94	111.63	103.30
3	C	33	U	C2-N1-C1'	6.88	125.96	117.70
7	G	134	LEU	CA-CB-CG	-6.88	99.48	115.30
1	A	140	C	N3-C2-O2	-6.87	117.09	121.90
1	A	641	C	C2-N1-C1'	-6.86	111.25	118.80
1	A	547	G	N9-C4-C5	6.86	108.14	105.40
1	A	678	G	C4-N9-C1'	6.86	135.42	126.50
2	B	152	G	N3-C4-N9	-6.83	121.90	126.00
3	C	48	A	O4'-C1'-N9	6.81	113.65	108.20
1	A	1351	U	C2-N1-C1'	6.78	125.84	117.70
1	A	404	G	N9-C4-C5	-6.78	102.69	105.40
1	A	1415	U	C5-C6-N1	-6.78	119.31	122.70
1	A	56	G	C8-N9-C4	-6.75	103.70	106.40
21	U	16	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	B	94	C	C6-N1-C2	6.74	123.00	120.30
1	A	588	G	N3-C4-C5	-6.73	125.24	128.60
1	A	439	C	C2-N1-C1'	6.70	126.17	118.80
1	A	333	G	C4-N9-C1'	6.70	135.20	126.50
1	A	678	G	C6-C5-N7	-6.66	126.40	130.40
1	A	352	A	O5'-P-OP2	-6.64	99.72	105.70
1	A	439	C	C6-N1-C1'	-6.64	112.83	120.80
1	A	694	C	C6-N1-C2	-6.62	117.65	120.30
3	C	33	U	N3-C2-O2	-6.60	117.58	122.20
2	B	78	G	N3-C4-N9	-6.59	122.05	126.00
1	A	75	G	C8-N9-C1'	-6.59	118.44	127.00
2	B	56	G	N1-C6-O6	-6.57	115.96	119.90
2	B	152	G	N3-C4-C5	6.56	131.88	128.60
1	A	1118	C	N1-C2-O2	-6.50	115.00	118.90
1	A	656	A	N1-C2-N3	6.49	132.54	129.30
1	A	1358	C	C5-C6-N1	-6.48	117.76	121.00
1	A	721	G	N9-C4-C5	-6.47	102.81	105.40
1	A	220	G	C4-N9-C1'	6.46	134.90	126.50
1	A	678	G	N3-C4-N9	6.45	129.87	126.00
1	A	700	C	N1-C2-O2	6.42	122.75	118.90
1	A	682	U	C2-N1-C1'	-6.42	110.00	117.70
29	c	126	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	976	U	C5-C6-N1	6.39	125.90	122.70
1	A	228	U	C6-N1-C1'	6.37	130.12	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	C	N3-C2-O2	-6.36	117.45	121.90
2	B	24	G	C5-C6-O6	6.36	132.41	128.60
1	A	515	C	C2-N1-C1'	6.35	125.78	118.80
1	A	1415	U	C2-N1-C1'	-6.29	110.15	117.70
1	A	953	G	N3-C4-C5	6.29	131.75	128.60
1	A	2378	C	C2-N1-C1'	6.28	125.70	118.80
1	A	266	A	C8-N9-C4	-6.27	103.29	105.80
1	A	385	A	N1-C6-N6	6.22	122.33	118.60
1	A	678	G	N3-C4-C5	-6.21	125.50	128.60
1	A	547	G	N3-C4-N9	-6.19	122.28	126.00
1	A	334	A	C6-N1-C2	-6.17	114.90	118.60
1	A	1338	C	C6-N1-C2	-6.16	117.84	120.30
1	A	3126	C	N1-C2-O2	6.12	122.57	118.90
1	A	439	C	N1-C2-O2	6.12	122.57	118.90
1	A	1118	C	C2-N1-C1'	-6.11	112.08	118.80
1	A	1366	A	C8-N9-C4	6.09	108.24	105.80
1	A	630	A	C2-N3-C4	-6.09	107.56	110.60
1	A	637	C	O4'-C1'-N1	6.08	113.07	108.20
1	A	220	G	N3-C4-N9	6.07	129.64	126.00
1	A	700	C	N3-C2-O2	-6.06	117.66	121.90
1	A	197	G	N3-C4-N9	-6.05	122.37	126.00
1	A	656	A	C8-N9-C4	-6.04	103.38	105.80
1	A	462	C	C6-N1-C1'	6.01	128.01	120.80
21	U	16	ARG	CG-CD-NE	-6.01	99.19	111.80
1	A	457	C	N1-C2-O2	5.99	122.50	118.90
1	A	341	G	C4-N9-C1'	5.98	134.27	126.50
1	A	263	C	N3-C2-O2	-5.97	117.72	121.90
7	G	182	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	1108	U	C5-C6-N1	5.96	125.68	122.70
1	A	948	C	C6-N1-C2	-5.94	117.92	120.30
1	A	267	G	C2-N3-C4	-5.94	108.93	111.90
1	A	141	C	N1-C2-O2	5.94	122.46	118.90
7	G	156	LEU	CA-CB-CG	5.94	128.95	115.30
1	A	685	G	C6-C5-N7	-5.93	126.84	130.40
1	A	641	C	C6-N1-C1'	5.92	127.91	120.80
1	A	1425	U	C2-N3-C4	-5.92	123.45	127.00
1	A	74	G	C2-N3-C4	-5.91	108.94	111.90
1	A	207	U	C2-N1-C1'	5.90	124.78	117.70
1	A	260	C	C6-N1-C2	5.90	122.66	120.30
1	A	1117	G	N3-C4-N9	-5.89	122.47	126.00
4	D	224	PRO	N-CA-C	-5.87	96.84	112.10
1	A	641	C	N1-C2-O2	-5.85	115.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1118	C	C6-N1-C1'	5.85	127.82	120.80
1	A	1435	A	N7-C8-N9	5.84	116.72	113.80
1	A	940	G	O5'-P-OP1	-5.83	100.45	105.70
1	A	360	G	C8-N9-C4	5.82	108.73	106.40
1	A	267	G	N3-C4-C5	5.82	131.51	128.60
1	A	682	U	C5-C6-N1	-5.81	119.80	122.70
1	A	3239	G	N1-C6-O6	-5.81	116.42	119.90
1	A	590	G	C4-C5-N7	5.81	113.12	110.80
2	B	127	U	N1-C2-O2	5.79	126.85	122.80
1	A	1435	A	C5-N7-C8	-5.76	101.02	103.90
1	A	41	G	C4-N9-C1'	5.76	133.99	126.50
1	A	63	A	C2-N3-C4	-5.76	107.72	110.60
1	A	404	G	C8-N9-C4	5.76	108.70	106.40
1	A	547	G	C4-C5-N7	-5.76	108.50	110.80
1	A	294	U	O5'-P-OP1	-5.76	100.52	105.70
1	A	215	G	N3-C4-N9	-5.75	122.55	126.00
1	A	399	A	O5'-P-OP2	-5.74	100.53	105.70
2	B	39	G	N9-C4-C5	5.74	107.70	105.40
1	A	24	G	N3-C4-C5	5.74	131.47	128.60
2	B	29	U	N1-C2-O2	-5.73	118.79	122.80
10	J	103	LEU	CA-CB-CG	-5.68	102.23	115.30
1	A	678	G	C8-N9-C1'	-5.68	119.61	127.00
1	A	960	U	N1-C2-O2	5.67	126.77	122.80
1	A	3147	G	N3-C4-C5	5.67	131.43	128.60
1	A	227	G	C4-N9-C1'	5.66	133.86	126.50
1	A	227	G	C6-C5-N7	-5.66	127.00	130.40
1	A	315	C	N3-C2-O2	-5.66	117.94	121.90
1	A	745	C	N1-C2-O2	-5.66	115.51	118.90
1	A	3023	U	C2-N1-C1'	5.64	124.47	117.70
1	A	1338	C	C6-N1-C1'	5.63	127.56	120.80
1	A	544	C	C5-C6-N1	-5.62	118.19	121.00
3	C	21	G	N1-C6-O6	-5.61	116.53	119.90
1	A	407	A	O4'-C1'-N9	-5.61	103.71	108.20
24	X	125	ILE	CG1-CB-CG2	-5.61	99.06	111.40
1	A	428	A	C6-N1-C2	-5.59	115.25	118.60
1	A	3247	G	N3-C4-N9	-5.59	122.65	126.00
1	A	515	C	N1-C2-O2	5.59	122.25	118.90
1	A	1124	U	C2-N1-C1'	5.58	124.40	117.70
2	B	4	C	C2-N1-C1'	5.58	124.94	118.80
2	B	39	G	N3-C2-N2	-5.58	116.00	119.90
1	A	430	U	C5-C6-N1	5.58	125.49	122.70
1	A	24	G	N3-C4-N9	-5.56	122.66	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	A	C6-N1-C2	-5.56	115.27	118.60
1	A	1297	C	C6-N1-C2	-5.56	118.08	120.30
1	A	1328	C	C2-N3-C4	-5.55	117.12	119.90
1	A	457	C	C4-C5-C6	-5.55	114.62	117.40
4	D	163	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	3019	U	N3-C2-O2	-5.54	118.32	122.20
1	A	588	G	C6-N1-C2	-5.54	121.78	125.10
1	A	1159	A	O5'-P-OP2	-5.53	100.72	105.70
1	A	950	G	C6-C5-N7	-5.52	127.09	130.40
13	M	376	LEU	CA-CB-CG	5.52	127.99	115.30
2	B	83	C	C6-N1-C2	5.50	122.50	120.30
1	A	3126	C	N3-C2-O2	-5.50	118.05	121.90
1	A	58	G	C5-C6-O6	5.50	131.90	128.60
1	A	75	G	C6-C5-N7	-5.49	127.10	130.40
1	A	1107	C	N1-C2-O2	-5.49	115.60	118.90
1	A	341	G	C8-N9-C1'	-5.49	119.87	127.00
1	A	547	G	C8-N9-C1'	5.48	134.13	127.00
1	A	612	U	C2-N3-C4	-5.47	123.72	127.00
1	A	266	A	C4-C5-C6	5.46	119.73	117.00
1	A	341	G	N1-C2-N2	-5.46	111.28	116.20
1	A	274	G	C8-N9-C4	5.46	108.58	106.40
1	A	445	G	C4-C5-N7	5.45	112.98	110.80
1	A	1103	A	N7-C8-N9	-5.44	111.08	113.80
1	A	361	A	C6-C5-N7	-5.44	128.49	132.30
1	A	515	C	C6-N1-C1'	-5.44	114.27	120.80
1	A	110	G	N3-C4-C5	-5.43	125.88	128.60
1	A	638	C	C5-C6-N1	5.43	123.72	121.00
1	A	140	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1349	G	N3-C4-C5	5.43	131.31	128.60
1	A	1415	U	C6-N1-C2	5.42	124.25	121.00
1	A	27	C	N3-C2-O2	-5.41	118.11	121.90
1	A	311	C	N1-C2-O2	5.41	122.14	118.90
1	A	526	C	C6-N1-C2	5.40	122.46	120.30
25	Y	280	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	967	A	C5-N7-C8	-5.40	101.20	103.90
1	A	721	G	C4-C5-N7	5.39	112.95	110.80
1	A	364	G	C6-C5-N7	-5.38	127.17	130.40
1	A	457	C	C5-C6-N1	5.38	123.69	121.00
1	A	3023	U	N3-C2-O2	-5.38	118.44	122.20
1	A	217	U	C2-N1-C1'	-5.38	111.25	117.70
1	A	110	G	N3-C4-N9	5.37	129.22	126.00
1	A	1349	G	N1-C6-O6	5.36	123.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3176	G	C4-N9-C1'	5.36	133.47	126.50
1	A	1165	A	C6-N1-C2	-5.34	115.39	118.60
1	A	977	C	N1-C2-O2	5.34	122.10	118.90
1	A	684	G	C4-C5-N7	5.34	112.94	110.80
1	A	81	C	C6-N1-C2	-5.33	118.17	120.30
1	A	41	G	N3-C4-N9	5.33	129.20	126.00
1	A	341	G	N3-C4-N9	5.33	129.20	126.00
1	A	337	G	N3-C4-N9	-5.32	122.81	126.00
1	A	166	C	C5-C6-N1	5.32	123.66	121.00
1	A	517	G	C4-C5-N7	5.32	112.93	110.80
2	B	91	C	C6-N1-C2	-5.31	118.17	120.30
1	A	418	A	C8-N9-C4	-5.30	103.68	105.80
1	A	341	G	C4-C5-N7	5.30	112.92	110.80
2	B	56	G	C5-C6-O6	5.30	131.78	128.60
1	A	650	C	C5-C6-N1	5.30	123.65	121.00
16	P	116	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	547	G	C6-N1-C2	-5.29	121.92	125.10
1	A	1103	A	OP1-P-O3'	5.29	116.84	105.20
1	A	950	G	C8-N9-C1'	-5.29	120.13	127.00
1	A	950	G	N9-C4-C5	-5.29	103.29	105.40
1	A	928	C	N3-C2-O2	-5.28	118.21	121.90
1	A	3030	G	P-O3'-C3'	5.27	126.03	119.70
1	A	427	C	N3-C4-C5	5.27	124.01	121.90
8	H	291	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	3378	C	N1-C2-O2	5.26	122.06	118.90
1	A	360	G	N9-C4-C5	-5.26	103.30	105.40
31	i	82	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	298	U	C2-N1-C1'	5.25	124.00	117.70
1	A	404	G	N3-C4-N9	5.25	129.15	126.00
1	A	977	C	C2-N1-C1'	5.24	124.56	118.80
1	A	222	A	C6-C5-N7	-5.24	128.63	132.30
1	A	262	U	C2-N1-C1'	5.23	123.98	117.70
1	A	468	G	O5'-P-OP1	-5.23	100.99	105.70
1	A	3147	G	N3-C4-N9	-5.23	122.86	126.00
1	A	1169	A	C6-C5-N7	-5.23	128.64	132.30
1	A	1108	U	N1-C2-O2	5.22	126.45	122.80
1	A	1176	C	C6-N1-C2	5.22	122.39	120.30
27	a	186	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	A	1137	C	C2-N1-C1'	5.21	124.54	118.80
1	A	1388	U	C2-N3-C4	-5.21	123.87	127.00
1	A	340	C	N1-C2-O2	5.21	122.03	118.90
1	A	1108	U	N3-C2-O2	-5.21	118.55	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	G	C6-C5-N7	-5.19	127.28	130.40
1	A	409	A	N7-C8-N9	5.19	116.39	113.80
1	A	948	C	C5-C6-N1	5.19	123.59	121.00
1	A	1425	U	C6-N1-C2	5.18	124.11	121.00
2	B	135	G	N3-C4-C5	5.18	131.19	128.60
1	A	188	U	C2-N1-C1'	-5.17	111.49	117.70
1	A	222	A	C4-C5-N7	5.17	113.29	110.70
1	A	430	U	C2-N1-C1'	5.17	123.91	117.70
1	A	217	U	N1-C2-N3	5.17	118.00	114.90
1	A	1365	G	O4'-C1'-N9	-5.17	104.07	108.20
1	A	1379	G	N3-C4-C5	-5.16	126.02	128.60
33	l	92	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	1358	C	C2-N3-C4	-5.15	117.32	119.90
1	A	454	C	N1-C2-O2	5.15	121.99	118.90
1	A	659	G	OP2-P-O3'	5.14	116.52	105.20
1	A	544	C	O4'-C1'-N1	5.14	112.31	108.20
1	A	798	G	N9-C4-C5	5.12	107.45	105.40
1	A	505	G	C4-N9-C1'	5.12	133.16	126.50
1	A	56	G	N9-C4-C5	5.12	107.45	105.40
1	A	1351	U	C6-N1-C1'	-5.11	114.04	121.20
1	A	1379	G	N1-C6-O6	-5.11	116.84	119.90
2	B	107	G	C4-C5-N7	5.11	112.84	110.80
1	A	612	U	C5-C6-N1	-5.09	120.16	122.70
1	A	650	C	C6-N1-C2	-5.09	118.27	120.30
1	A	1174	G	C4-C5-N7	5.09	112.83	110.80
1	A	517	G	C6-C5-N7	-5.08	127.35	130.40
1	A	3076	C	C5-C6-N1	5.08	123.54	121.00
1	A	404	G	C4-C5-N7	5.08	112.83	110.80
1	A	720	A	P-O3'-C3'	5.08	125.80	119.70
1	A	1180	A	C8-N9-C4	5.07	107.83	105.80
3	C	232	A	N1-C2-N3	5.07	131.84	129.30
1	A	227	G	C8-N9-C1'	-5.06	120.42	127.00
1	A	1328	C	C5-C6-N1	-5.06	118.47	121.00
1	A	1354	G	C5-N7-C8	-5.05	101.77	104.30
1	A	1108	U	C6-N1-C1'	-5.05	114.14	121.20
1	A	1159	A	N1-C6-N6	5.05	121.63	118.60
1	A	454	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	547	G	C4-N9-C1'	-5.04	119.95	126.50
2	B	135	G	N3-C4-N9	-5.04	122.98	126.00
1	A	3228	C	P-O3'-C3'	5.03	125.74	119.70
1	A	267	G	C4-C5-N7	5.03	112.81	110.80
1	A	587	U	N3-C2-O2	5.03	125.72	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	94	C	C5-C6-N1	-5.03	118.49	121.00
1	A	1311	G	C6-C5-N7	-5.02	127.39	130.40
1	A	1178	G	N3-C4-N9	5.02	129.01	126.00
1	A	517	G	N1-C6-O6	5.02	122.91	119.90
1	A	294	U	C2-N1-C1'	-5.01	111.68	117.70
1	A	186	U	C5-C6-N1	-5.01	120.20	122.70
1	A	3288	G	N3-C4-C5	5.00	131.10	128.60
2	B	70	G	N3-C4-N9	-5.00	123.00	126.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	245	ILE	Peptide
4	D	270	PRO	Peptide
6	F	187	SER	Peptide
8	H	285	ARG	Peptide
10	J	177	GLY	Peptide
10	J	219	LYS	Peptide
10	J	232	ARG	Peptide
11	K	77	GLN	Peptide
13	M	114	LEU	Peptide
13	M	240	SER	Peptide
13	M	3	ILE	Peptide
13	M	62	PHE	Peptide
15	O	221	ASN	Peptide
15	O	271	GLN	Peptide
15	O	275	LYS	Peptide
17	Q	47	ASP	Peptide
18	R	183	THR	Peptide
18	R	3	ALA	Peptide
22	V	59	SER	Peptide
23	W	12	ARG	Peptide
23	W	13	ARG	Peptide
23	W	20	PRO	Peptide
24	X	57	ASP	Peptide
24	X	58	ARG	Peptide
25	Y	110	LYS	Peptide
25	Y	186	VAL	Peptide
25	Y	187	PHE	Peptide
25	Y	365	ASP	Peptide
25	Y	368	ASP	Peptide

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Mol	Chain	Res	Type	Group
25	Y	414	GLU	Peptide
25	Y	478	GLY	Peptide
26	Z	56	ASP	Peptide
27	a	185	LYS	Peptide
28	b	261	LEU	Peptide
28	b	265	LYS	Peptide
28	b	268	PHE	Peptide
30	d	266	UNK	Peptide
31	i	95	GLU	Peptide
33	l	83	LYS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
4	D	243/322 (76%)	198 (82%)	41 (17%)	4 (2%)	9	43
5	E	131/220 (60%)	109 (83%)	20 (15%)	2 (2%)	10	44
6	F	332/387 (86%)	290 (87%)	40 (12%)	2 (1%)	25	62
7	G	359/362 (99%)	317 (88%)	40 (11%)	2 (1%)	25	62
8	H	252/376 (67%)	218 (86%)	33 (13%)	1 (0%)	34	69
9	I	146/176 (83%)	133 (91%)	13 (9%)	0	100	100
10	J	237/244 (97%)	212 (90%)	20 (8%)	5 (2%)	7	38
11	K	158/256 (62%)	132 (84%)	26 (16%)	0	100	100
12	L	189/191 (99%)	167 (88%)	18 (10%)	4 (2%)	7	38
13	M	365/605 (60%)	305 (84%)	58 (16%)	2 (0%)	29	66
14	N	224/245 (91%)	199 (89%)	25 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	184/295 (62%)	152 (83%)	29 (16%)	3 (2%)	9	43
16	P	106/199 (53%)	84 (79%)	19 (18%)	3 (3%)	5	33
17	Q	135/138 (98%)	113 (84%)	22 (16%)	0	100	100
18	R	171/204 (84%)	148 (86%)	23 (14%)	0	100	100
19	S	195/199 (98%)	179 (92%)	15 (8%)	1 (0%)	29	66
20	T	132/184 (72%)	116 (88%)	16 (12%)	0	100	100
21	U	132/186 (71%)	121 (92%)	11 (8%)	0	100	100
22	V	386/463 (83%)	362 (94%)	24 (6%)	0	100	100
23	W	168/172 (98%)	145 (86%)	23 (14%)	0	100	100
24	X	190/278 (68%)	160 (84%)	29 (15%)	1 (0%)	29	66
25	Y	434/505 (86%)	372 (86%)	59 (14%)	3 (1%)	22	59
26	Z	167/306 (55%)	144 (86%)	22 (13%)	1 (1%)	25	62
27	a	206/291 (71%)	191 (93%)	14 (7%)	1 (0%)	29	66
28	b	80/427 (19%)	70 (88%)	10 (12%)	0	100	100
29	c	123/127 (97%)	115 (94%)	6 (5%)	2 (2%)	9	43
31	i	122/130 (94%)	111 (91%)	11 (9%)	0	100	100
32	j	104/107 (97%)	94 (90%)	10 (10%)	0	100	100
33	l	115/120 (96%)	104 (90%)	10 (9%)	1 (1%)	17	54
34	m	65/100 (65%)	58 (89%)	7 (11%)	0	100	100
35	n	70/88 (80%)	65 (93%)	4 (6%)	1 (1%)	11	45
All	All	5921/7903 (75%)	5184 (88%)	698 (12%)	39 (1%)	26	59

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	339	LEU
15	O	119	PRO
8	H	284	ASN
26	Z	158	ILE
6	F	34	LYS
12	L	22	SER
12	L	50	ASN
16	P	51	LEU
25	Y	477	TYR
29	c	45	ILE

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Mol	Chain	Res	Type
4	D	224	PRO
5	E	194	LYS
13	M	378	PHE
16	P	63	VAL
19	S	187	GLU
24	X	204	LYS
33	l	84	LYS
4	D	260	SER
6	F	35	ASP
10	J	147	LEU
10	J	157	ASN
10	J	158	LYS
13	M	433	PHE
25	Y	78	ALA
25	Y	199	ASP
27	a	228	GLU
4	D	270	PRO
12	L	21	LYS
15	O	213	LEU
29	c	14	LYS
35	n	40	PRO
10	J	168	ILE
16	P	50	PRO
5	E	147	ILE
7	G	317	PRO
10	J	178	ILE
15	O	274	ILE
4	D	235	VAL
12	L	79	ILE

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
4	D	218/287 (76%)	218 (100%)	0	100 100
5	E	118/199 (59%)	118 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	282/323 (87%)	281 (100%)	1 (0%)	91	95
7	G	288/289 (100%)	288 (100%)	0	100	100
8	H	236/346 (68%)	236 (100%)	0	100	100
9	I	130/153 (85%)	129 (99%)	1 (1%)	81	89
10	J	202/205 (98%)	201 (100%)	1 (0%)	88	94
11	K	129/208 (62%)	129 (100%)	0	100	100
12	L	171/171 (100%)	171 (100%)	0	100	100
13	M	334/548 (61%)	333 (100%)	1 (0%)	92	96
14	N	194/211 (92%)	194 (100%)	0	100	100
15	O	176/276 (64%)	174 (99%)	2 (1%)	73	85
16	P	87/159 (55%)	86 (99%)	1 (1%)	73	85
17	Q	108/109 (99%)	108 (100%)	0	100	100
18	R	152/176 (86%)	152 (100%)	0	100	100
19	S	160/162 (99%)	160 (100%)	0	100	100
20	T	109/146 (75%)	109 (100%)	0	100	100
21	U	110/151 (73%)	110 (100%)	0	100	100
22	V	345/410 (84%)	344 (100%)	1 (0%)	92	96
23	W	154/156 (99%)	154 (100%)	0	100	100
24	X	186/257 (72%)	186 (100%)	0	100	100
25	Y	380/440 (86%)	378 (100%)	2 (0%)	88	94
26	Z	153/274 (56%)	152 (99%)	1 (1%)	84	91
27	a	198/263 (75%)	198 (100%)	0	100	100
28	b	76/383 (20%)	76 (100%)	0	100	100
29	c	108/110 (98%)	108 (100%)	0	100	100
31	i	107/111 (96%)	107 (100%)	0	100	100
32	j	90/91 (99%)	90 (100%)	0	100	100
33	l	104/105 (99%)	104 (100%)	0	100	100
34	m	55/82 (67%)	55 (100%)	0	100	100
35	n	60/71 (84%)	60 (100%)	0	100	100
All	All	5220/6872 (76%)	5209 (100%)	11 (0%)	93	97

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

Mol	Chain	Res	Type
6	F	85	VAL
9	I	101	PHE
10	J	44	ILE
13	M	442	VAL
15	O	277	GLU
15	O	295	LEU
16	P	85	LEU
22	V	293	ARG
25	Y	145	PHE
25	Y	149	ILE
26	Z	38	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	242	HIS
4	D	291	GLN
5	E	100	HIS
5	E	113	GLN
5	E	130	ASN
6	F	211	GLN
6	F	212	ASN
6	F	273	HIS
6	F	293	ASN
6	F	319	ASN
7	G	5	GLN
7	G	48	GLN
7	G	59	GLN
7	G	114	ASN
7	G	320	ASN
8	H	84	ASN
8	H	101	ASN
8	H	212	HIS
8	H	245	ASN
8	H	295	GLN
9	I	57	HIS
10	J	52	GLN
10	J	64	GLN
11	K	137	ASN
11	K	138	HIS
11	K	155	ASN
11	K	232	HIS
12	L	9	GLN

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Mol	Chain	Res	Type
12	L	50	ASN
12	L	163	GLN
13	M	11	ASN
13	M	14	ASN
13	M	20	GLN
13	M	53	ASN
13	M	189	GLN
14	N	178	GLN
15	O	200	ASN
15	O	201	ASN
15	O	220	GLN
15	O	221	ASN
15	O	233	HIS
15	O	235	GLN
15	O	262	GLN
16	P	25	HIS
16	P	106	GLN
18	R	15	GLN
18	R	23	GLN
18	R	37	HIS
18	R	117	ASN
18	R	138	GLN
18	R	139	HIS
19	S	42	ASN
19	S	50	ASN
20	T	97	ASN
20	T	118	GLN
21	U	45	ASN
22	V	24	ASN
22	V	233	GLN
22	V	283	HIS
22	V	290	GLN
22	V	298	GLN
22	V	310	GLN
22	V	337	ASN
22	V	375	HIS
23	W	3	HIS
23	W	46	GLN
23	W	62	ASN
23	W	74	ASN
24	X	73	HIS
24	X	172	HIS

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Mol	Chain	Res	Type
24	X	229	ASN
24	X	230	ASN
25	Y	51	GLN
25	Y	178	HIS
25	Y	266	GLN
25	Y	288	GLN
25	Y	300	ASN
25	Y	330	ASN
25	Y	363	GLN
25	Y	397	ASN
26	Z	47	ASN
26	Z	110	GLN
27	a	85	ASN
27	a	115	GLN
27	a	141	GLN
27	a	195	HIS
28	b	197	ASN
28	b	209	GLN
28	b	215	HIS
28	b	221	GLN
29	c	120	GLN
32	j	42	GLN
32	j	75	HIS
32	j	88	ASN
34	m	35	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1482/3396 (43%)	506 (34%)	38 (2%)
2	B	155/158 (98%)	50 (32%)	3 (1%)
3	C	63/232 (27%)	34 (53%)	0
All	All	1700/3786 (44%)	590 (34%)	41 (2%)

All (590) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	U
1	A	6	A
1	A	7	C

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Mol	Chain	Res	Type
1	A	12	A
1	A	13	A
1	A	14	U
1	A	15	C
1	A	22	G
1	A	25	U
1	A	26	A
1	A	28	C
1	A	38	U
1	A	40	A
1	A	41	G
1	A	42	C
1	A	43	A
1	A	48	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	69	C
1	A	71	A
1	A	73	C
1	A	74	G
1	A	76	G
1	A	78	U
1	A	85	A
1	A	91	G
1	A	92	G
1	A	93	C
1	A	96	G
1	A	104	G
1	A	106	A
1	A	108	A
1	A	109	A
1	A	110	G
1	A	111	C
1	A	112	U
1	A	113	C
1	A	116	A
1	A	117	U
1	A	120	G
1	A	122	A

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Mol	Chain	Res	Type
1	A	123	A
1	A	124	U
1	A	131	C
1	A	133	U
1	A	134	U
1	A	135	C
1	A	136	G
1	A	147	U
1	A	148	G
1	A	149	U
1	A	155	G
1	A	156	G
1	A	157	A
1	A	161	G
1	A	165	A
1	A	166	C
1	A	170	G
1	A	173	G
1	A	187	A
1	A	190	U
1	A	191	U
1	A	192	C
1	A	193	C
1	A	200	C
1	A	206	G
1	A	210	U
1	A	211	A
1	A	212	G
1	A	218	G
1	A	219	A
1	A	221	A
1	A	225	C
1	A	226	C
1	A	228	U
1	A	233	C
1	A	237	G
1	A	240	U
1	A	241	G
1	A	243	G
1	A	244	G
1	A	245	U
1	A	248	U

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Mol	Chain	Res	Type
1	A	249	U
1	A	250	U
1	A	251	G
1	A	252	U
1	A	253	A
1	A	259	C
1	A	265	A
1	A	267	G
1	A	268	A
1	A	269	G
1	A	270	U
1	A	277	G
1	A	281	G
1	A	282	G
1	A	284	A
1	A	285	A
1	A	286	U
1	A	287	G
1	A	295	A
1	A	298	U
1	A	299	G
1	A	304	G
1	A	316	U
1	A	323	A
1	A	326	U
1	A	329	U
1	A	330	G
1	A	332	C
1	A	337	G
1	A	338	A
1	A	339	C
1	A	346	C
1	A	349	A
1	A	352	A
1	A	354	U
1	A	356	C
1	A	375	A
1	A	376	G
1	A	386	A
1	A	390	G
1	A	392	G
1	A	396	A

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Mol	Chain	Res	Type
1	A	397	A
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	407	A
1	A	410	U
1	A	412	G
1	A	417	A
1	A	421	G
1	A	422	A
1	A	424	G
1	A	438	A
1	A	439	C
1	A	440	A
1	A	441	U
1	A	446	U
1	A	453	C
1	A	464	U
1	A	465	U
1	A	466	G
1	A	467	U
1	A	468	G
1	A	473	G
1	A	475	G
1	A	487	U
1	A	490	A
1	A	494	G
1	A	495	G
1	A	498	A
1	A	501	A
1	A	510	G
1	A	512	U
1	A	515	C
1	A	517	G
1	A	520	U
1	A	521	A
1	A	523	A
1	A	525	C
1	A	530	G

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Mol	Chain	Res	Type
1	A	534	U
1	A	535	G
1	A	540	U
1	A	541	U
1	A	543	C
1	A	544	C
1	A	545	U
1	A	546	C
1	A	547	G
1	A	548	G
1	A	550	A
1	A	551	A
1	A	552	G
1	A	555	U
1	A	557	A
1	A	558	U
1	A	559	A
1	A	568	G
1	A	572	A
1	A	578	A
1	A	579	G
1	A	592	A
1	A	593	C
1	A	597	G
1	A	604	G
1	A	608	A
1	A	609	G
1	A	610	G
1	A	611	A
1	A	616	G
1	A	619	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	627	U
1	A	635	G
1	A	636	C
1	A	637	C
1	A	642	U
1	A	643	U
1	A	644	G
1	A	645	A

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Mol	Chain	Res	Type
1	A	646	A
1	A	647	A
1	A	649	A
1	A	650	C
1	A	659	G
1	A	660	A
1	A	661	G
1	A	668	G
1	A	669	U
1	A	675	C
1	A	676	G
1	A	677	A
1	A	679	U
1	A	681	U
1	A	682	U
1	A	683	U
1	A	684	G
1	A	686	G
1	A	688	G
1	A	689	U
1	A	691	A
1	A	705	A
1	A	721	G
1	A	722	G
1	A	726	G
1	A	734	C
1	A	735	A
1	A	742	G
1	A	747	A
1	A	752	C
1	A	754	G
1	A	756	U
1	A	757	C
1	A	774	G
1	A	775	A
1	A	776	U
1	A	777	U
1	A	779	G
1	A	780	A
1	A	781	G
1	A	785	G
1	A	786	A

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Mol	Chain	Res	Type
1	A	806	A
1	A	814	U
1	A	933	A
1	A	940	G
1	A	944	C
1	A	948	C
1	A	958	C
1	A	961	C
1	A	962	A
1	A	964	G
1	A	965	A
1	A	967	A
1	A	973	A
1	A	974	G
1	A	975	C
1	A	976	U
1	A	977	C
1	A	978	G
1	A	980	A
1	A	981	U
1	A	982	C
1	A	984	G
1	A	987	U
1	A	990	U
1	A	991	G
1	A	1063	G
1	A	1098	A
1	A	1099	A
1	A	1103	A
1	A	1104	G
1	A	1111	U
1	A	1112	A
1	A	1116	G
1	A	1117	G
1	A	1118	C
1	A	1127	G
1	A	1135	A
1	A	1136	A
1	A	1138	U
1	A	1139	G
1	A	1142	G
1	A	1150	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	1151	U
1	A	1153	A
1	A	1155	C
1	A	1159	A
1	A	1160	C
1	A	1178	G
1	A	1179	A
1	A	1180	A
1	A	1181	U
1	A	1182	A
1	A	1186	G
1	A	1204	A
1	A	1206	G
1	A	1208	U
1	A	1209	G
1	A	1215	U
1	A	1218	U
1	A	1296	C
1	A	1297	C
1	A	1299	U
1	A	1313	G
1	A	1314	C
1	A	1316	C
1	A	1318	A
1	A	1325	U
1	A	1330	A
1	A	1331	U
1	A	1332	A
1	A	1337	A
1	A	1345	G
1	A	1348	U
1	A	1349	G
1	A	1350	A
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1359	C
1	A	1360	C

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Mol	Chain	Res	Type
1	A	1370	G
1	A	1373	A
1	A	1385	C
1	A	1386	A
1	A	1388	U
1	A	1393	A
1	A	1394	A
1	A	1399	A
1	A	1400	G
1	A	1404	G
1	A	1405	U
1	A	1410	U
1	A	1418	A
1	A	1419	A
1	A	1423	C
1	A	1424	C
1	A	1428	A
1	A	1429	G
1	A	1434	G
1	A	1435	A
1	A	1436	U
1	A	1437	C
1	A	1440	G
1	A	1442	U
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1450	G
1	A	1451	C
1	A	1881	A
1	A	2357	A
1	A	2358	A
1	A	2359	C
1	A	2362	C
1	A	2363	A
1	A	2370	G
1	A	2999	U
1	A	3012	A
1	A	3014	U
1	A	3017	A
1	A	3021	A
1	A	3022	G

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Mol	Chain	Res	Type
1	A	3023	U
1	A	3024	A
1	A	3025	C
1	A	3026	G
1	A	3028	G
1	A	3029	A
1	A	3031	G
1	A	3032	A
1	A	3035	A
1	A	3036	G
1	A	3037	U
1	A	3040	A
1	A	3047	U
1	A	3049	A
1	A	3056	U
1	A	3057	U
1	A	3058	U
1	A	3064	U
1	A	3068	U
1	A	3074	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3087	A
1	A	3090	U
1	A	3092	C
1	A	3093	C
1	A	3094	A
1	A	3097	C
1	A	3099	C
1	A	3100	U
1	A	3101	G
1	A	3104	U
1	A	3110	C
1	A	3115	C
1	A	3122	A
1	A	3125	U
1	A	3126	C
1	A	3130	A
1	A	3131	U
1	A	3132	C
1	A	3138	U

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Mol	Chain	Res	Type
1	A	3142	A
1	A	3143	C
1	A	3144	G
1	A	3150	A
1	A	3165	A
1	A	3166	C
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3180	A
1	A	3181	C
1	A	3184	A
1	A	3187	A
1	A	3188	G
1	A	3196	U
1	A	3199	G
1	A	3207	U
1	A	3208	G
1	A	3210	A
1	A	3212	C
1	A	3213	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3223	A
1	A	3224	G
1	A	3226	A
1	A	3227	A
1	A	3229	G
1	A	3232	G
1	A	3242	G
1	A	3244	A
1	A	3245	A
1	A	3246	G
1	A	3251	U
1	A	3253	G
1	A	3254	G
1	A	3259	U
1	A	3260	G
1	A	3263	G
1	A	3265	C

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Mol	Chain	Res	Type
1	A	3267	A
1	A	3268	A
1	A	3269	U
1	A	3270	U
1	A	3271	G
1	A	3273	A
1	A	3275	U
1	A	3276	G
1	A	3277	U
1	A	3278	C
1	A	3279	A
1	A	3286	G
1	A	3289	G
1	A	3292	A
1	A	3293	U
1	A	3295	A
1	A	3304	U
1	A	3309	G
1	A	3310	A
1	A	3314	A
1	A	3316	A
1	A	3317	U
1	A	3320	A
1	A	3324	C
1	A	3327	G
1	A	3328	G
1	A	3330	A
1	A	3333	G
1	A	3334	U
1	A	3335	A
1	A	3336	A
1	A	3338	C
1	A	3368	U
1	A	3369	G
1	A	3370	A
1	A	3374	U
1	A	3375	A
1	A	3378	C
1	A	3381	U
1	A	3382	U
2	B	2	A
2	B	4	C

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Mol	Chain	Res	Type
2	B	7	U
2	B	20	U
2	B	22	U
2	B	23	U
2	B	34	U
2	B	39	G
2	B	42	G
2	B	51	G
2	B	52	A
2	B	59	A
2	B	62	C
2	B	63	G
2	B	71	A
2	B	77	A
2	B	78	G
2	B	81	U
2	B	82	U
2	B	83	C
2	B	84	C
2	B	86	U
2	B	87	G
2	B	89	A
2	B	90	U
2	B	95	G
2	B	99	C
2	B	100	U
2	B	104	A
2	B	106	C
2	B	109	A
2	B	111	A
2	B	112	U
2	B	113	U
2	B	114	G
2	B	116	G
2	B	123	G
2	B	124	G
2	B	125	U
2	B	126	A
2	B	128	U
2	B	129	C
2	B	130	C
2	B	131	A

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Mol	Chain	Res	Type
2	B	144	G
2	B	148	G
2	B	149	A
2	B	151	C
2	B	152	G
2	B	154	C
3	C	2	C
3	C	4	U
3	C	5	C
3	C	6	U
3	C	7	C
3	C	10	A
3	C	15	C
3	C	16	U
3	C	17	G
3	C	24	A
3	C	26	U
3	C	29	G
3	C	33	U
3	C	34	A
3	C	38	U
3	C	40	U
3	C	41	G
3	C	42	G
3	C	43	A
3	C	45	U
3	C	47	A
3	C	48	A
3	C	49	C
3	C	52	G
3	C	53	A
3	C	54	A
3	C	55	A
3	C	56	U
3	C	58	G
3	C	59	C
3	C	229	U
3	C	230	A
3	C	231	A
3	C	232	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	13	A
1	A	75	G
1	A	160	G
1	A	239	G
1	A	250	U
1	A	315	C
1	A	385	A
1	A	420	G
1	A	452	G
1	A	486	U
1	A	618	C
1	A	621	A
1	A	645	A
1	A	646	A
1	A	649	A
1	A	661	G
1	A	720	A
1	A	976	U
1	A	1102	A
1	A	1103	A
1	A	1152	G
1	A	1154	A
1	A	1159	A
1	A	1203	A
1	A	1205	A
1	A	1329	U
1	A	1351	U
1	A	2362	C
1	A	3030	G
1	A	3035	A
1	A	3078	U
1	A	3218	A
1	A	3228	C
1	A	3269	U
1	A	3276	G
1	A	3292	A
1	A	3316	A
2	B	21	C
2	B	123	G
2	B	151	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	d	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	174:UNK	C	180:UNK	N	119.43
1	d	120:UNK	C	130:UNK	N	51.93
1	d	233:UNK	C	240:UNK	N	39.23
1	d	213:UNK	C	220:UNK	N	26.40
1	d	250:UNK	C	259:UNK	N	16.25
1	d	190:UNK	C	200:UNK	N	13.74

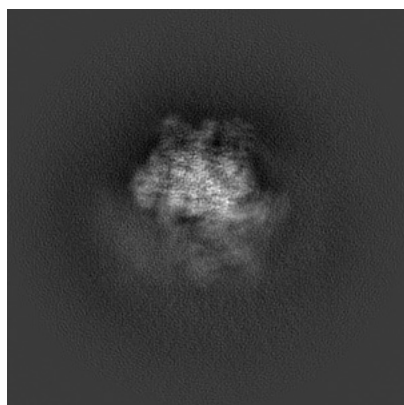
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6878. These allow visual inspection of the internal detail of the map and identification of artifacts.

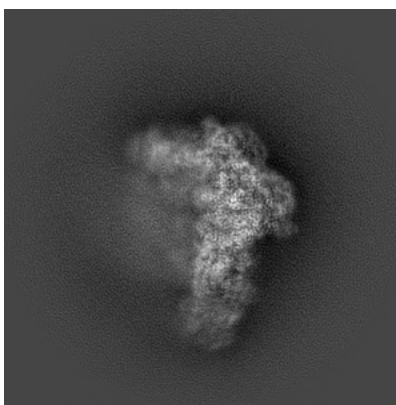
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

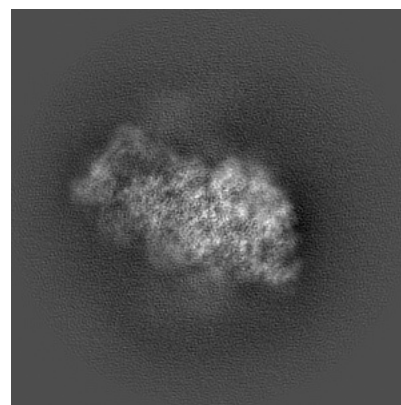
6.1.1 Primary map



X



Y

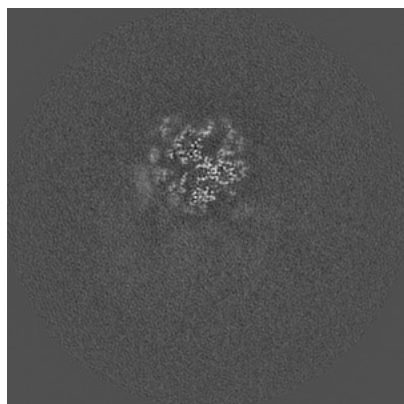


Z

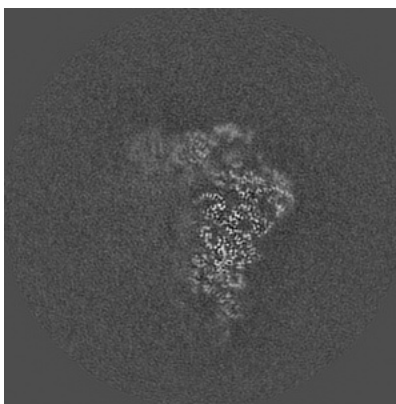
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

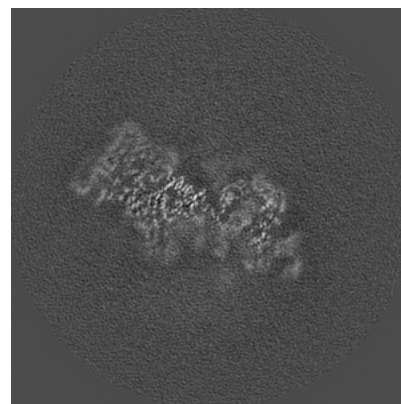
6.2.1 Primary map



X Index: 180



Y Index: 180

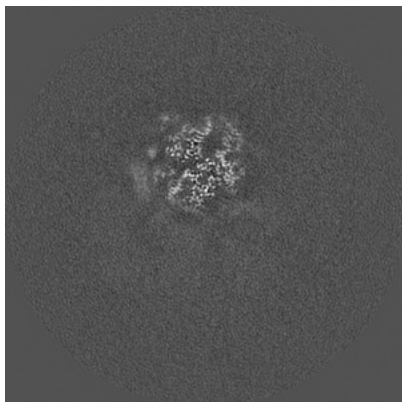


Z Index: 180

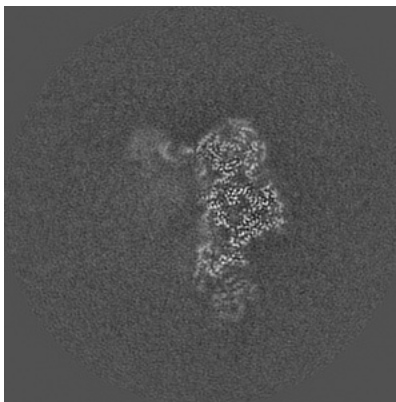
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

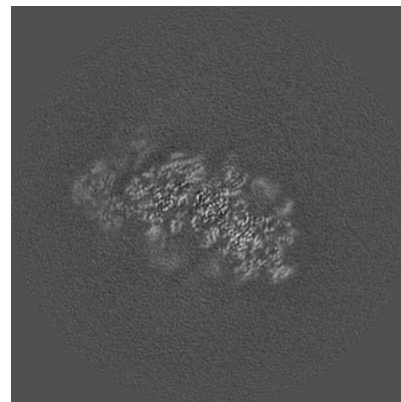
6.3.1 Primary map



X Index: 182



Y Index: 168



Z Index: 195

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 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

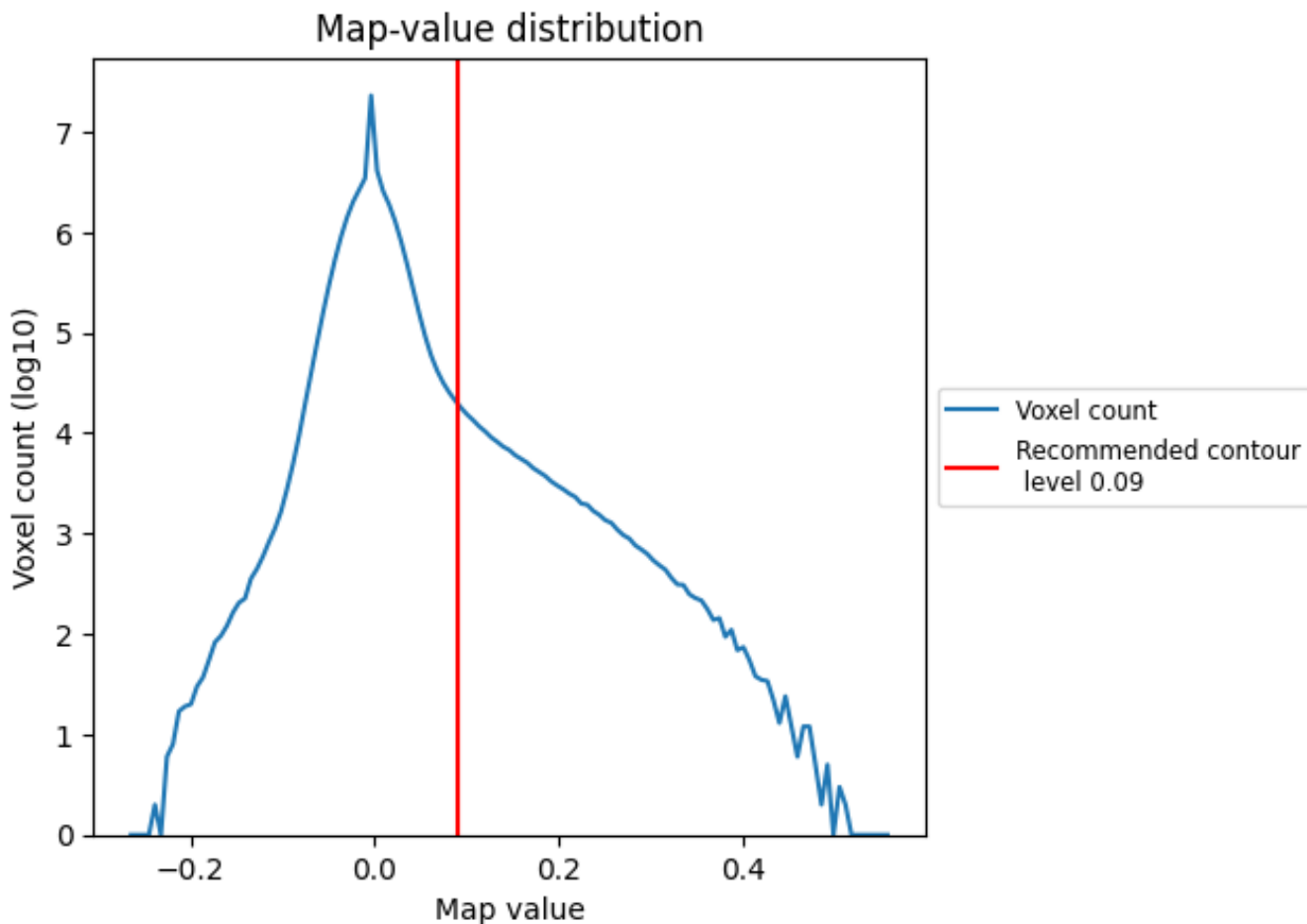
6.5 Mask visualisation

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

7 Map analysis [i](#)

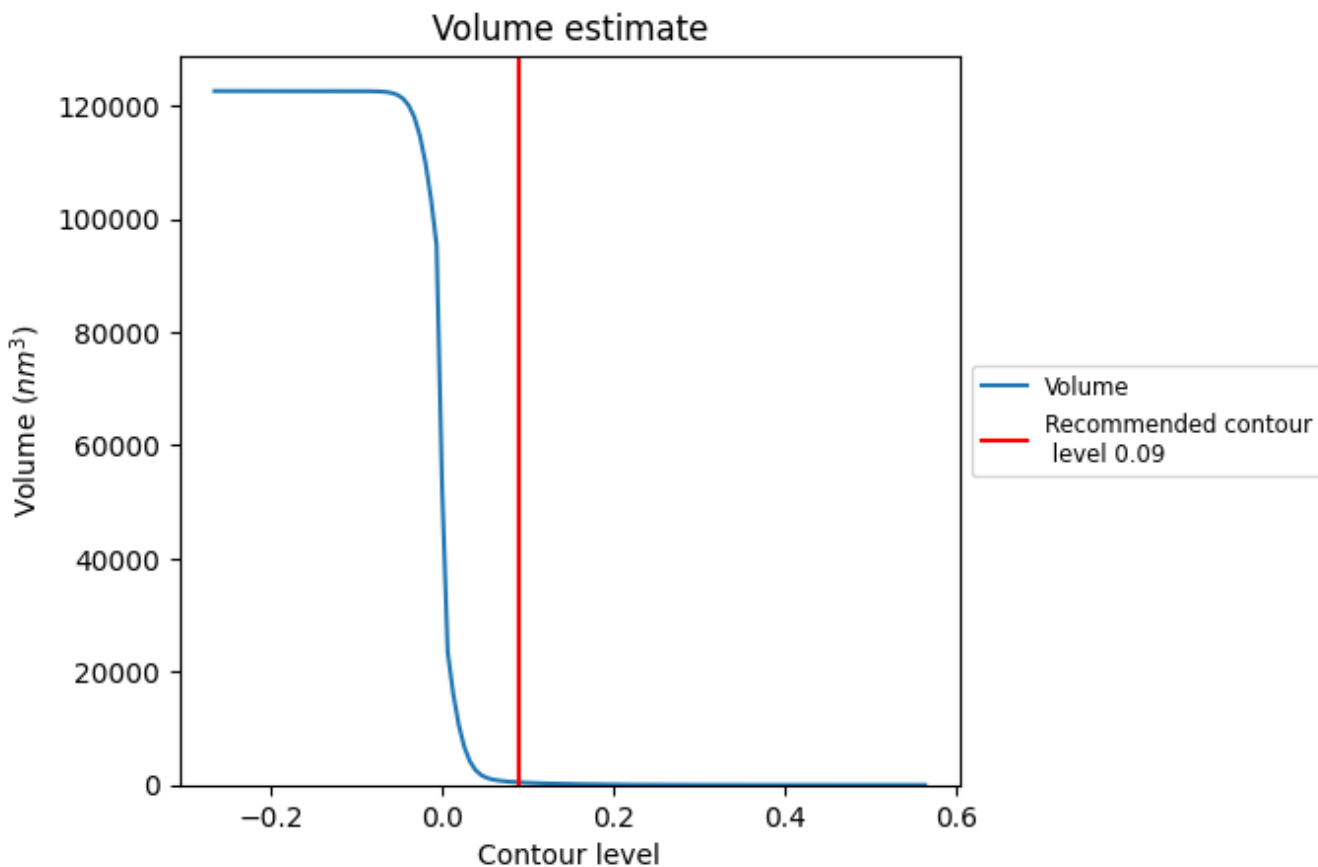
This section contains the results of statistical analysis of the map.

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.

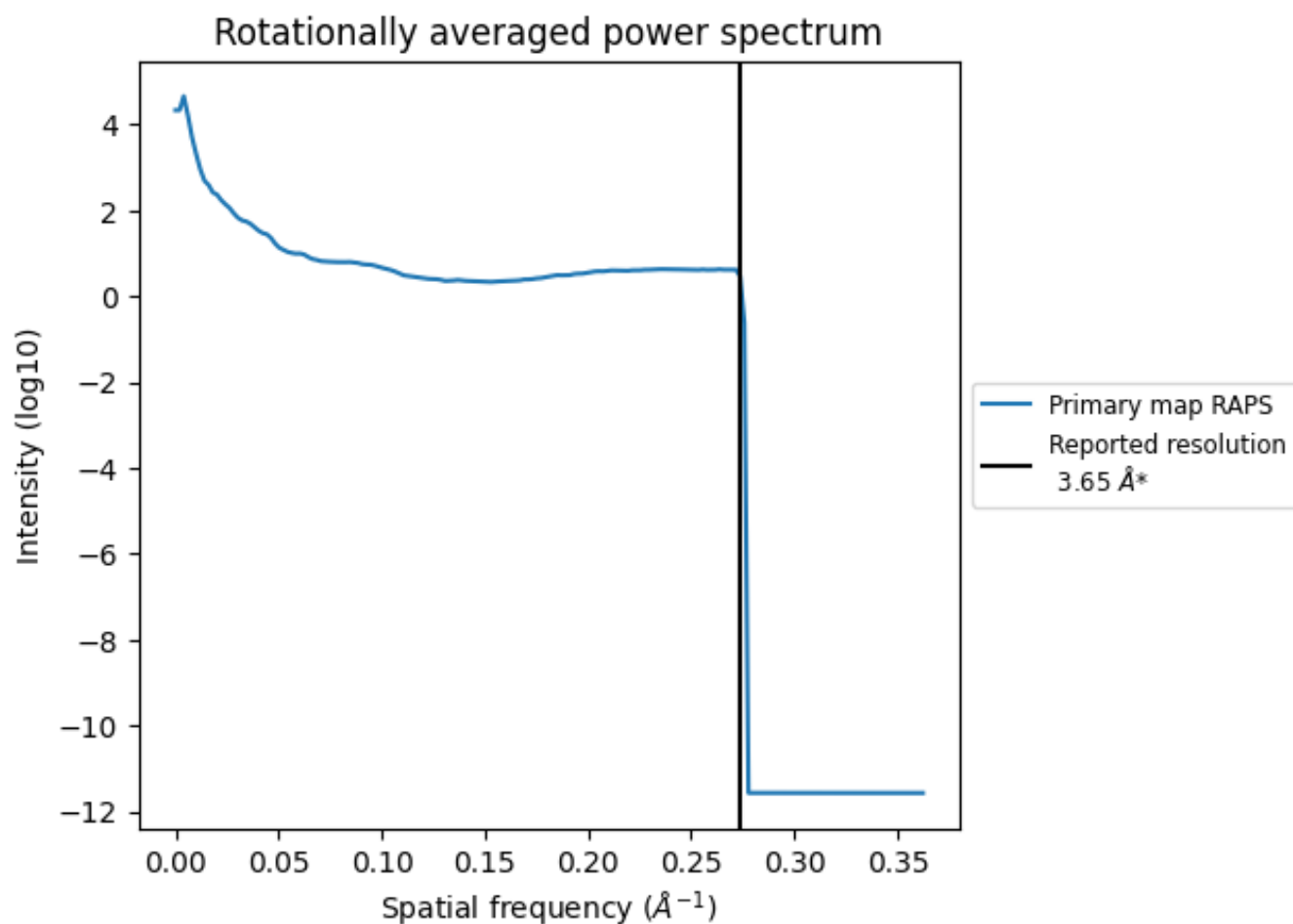
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 459 nm³; this corresponds to an approximate mass of 415 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 [\(i\)](#)

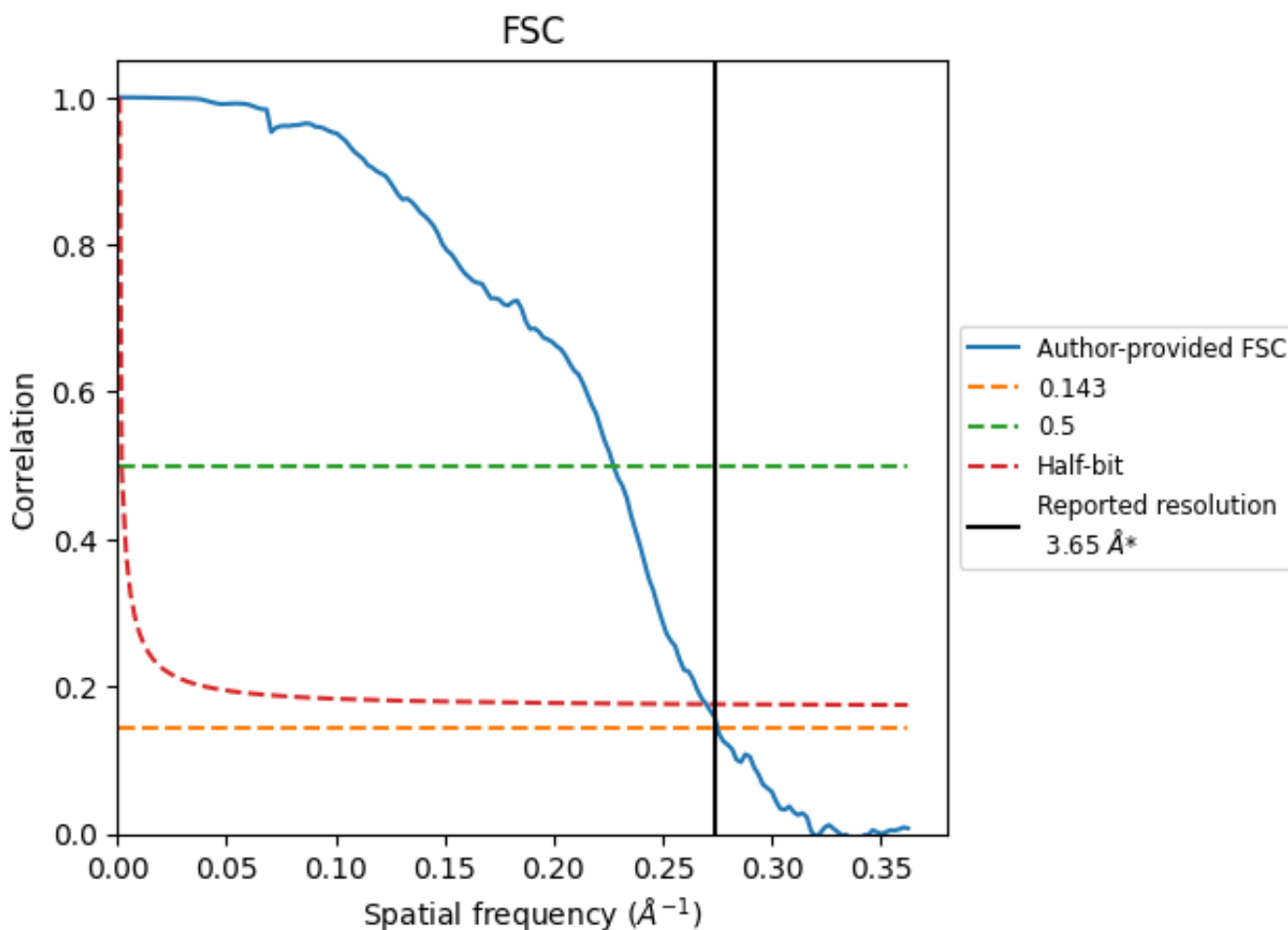


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

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 0.274 Å⁻¹

8.2 Resolution estimates [i](#)

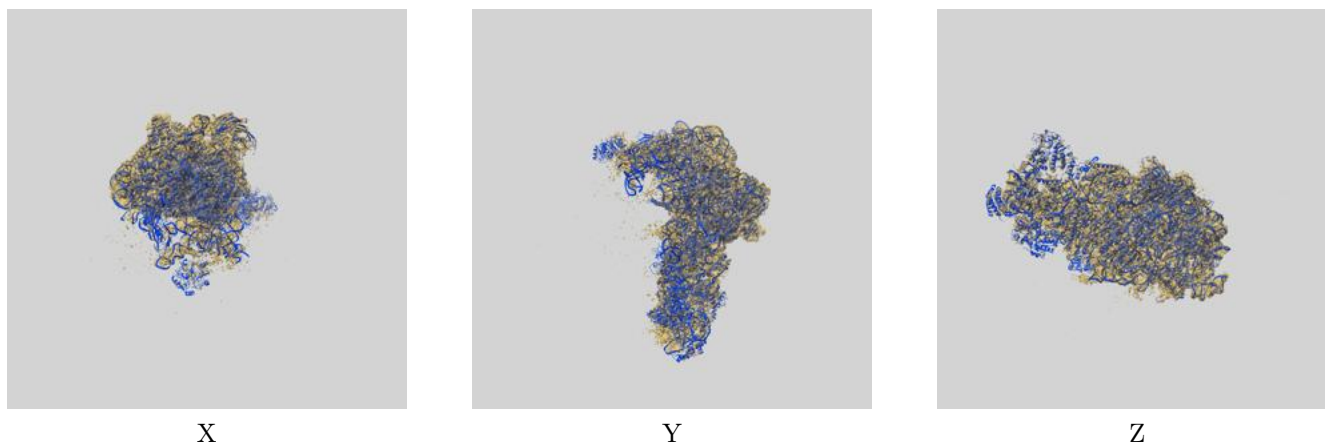
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.64	4.40	3.71
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

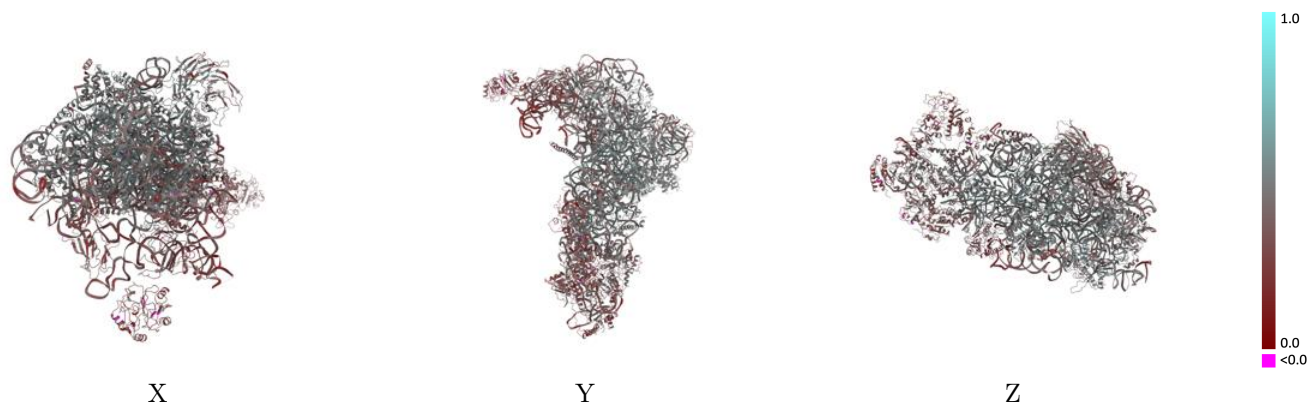
This section contains information regarding the fit between EMDB map EMD-6878 and PDB model 5Z3G. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



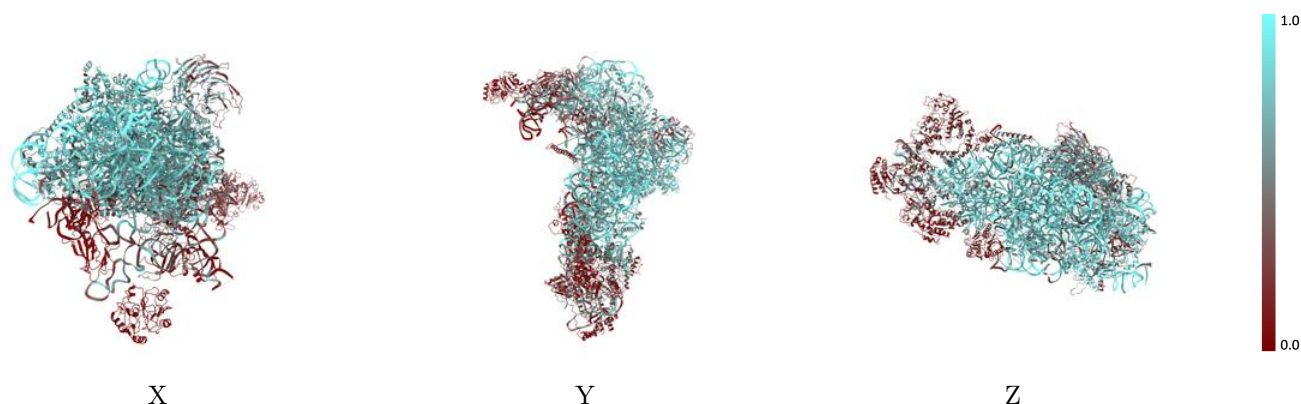
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



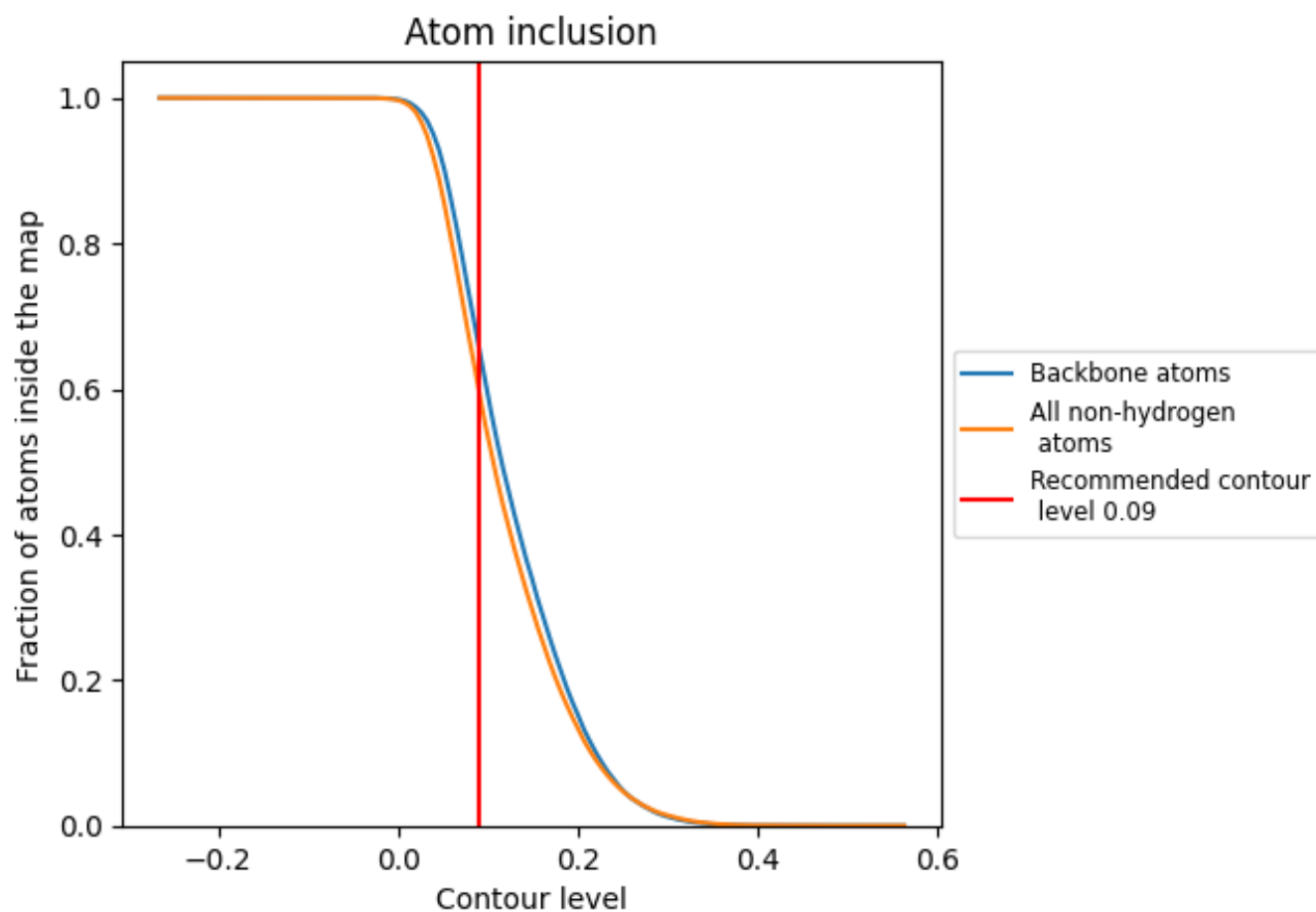
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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, 66% of all backbone atoms, 60% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6007	 0.4220
A	 0.7607	 0.4290
B	 0.7797	 0.4320
C	 0.5095	 0.3770
D	 0.2748	 0.3480
E	 0.2922	 0.3550
F	 0.3700	 0.3670
G	 0.7678	 0.5190
H	 0.2450	 0.3530
I	 0.7654	 0.4890
J	 0.7788	 0.4920
K	 0.5772	 0.4550
L	 0.0987	 0.3730
M	 0.1376	 0.2980
N	 0.0458	 0.2850
O	 0.6263	 0.4490
P	 0.7687	 0.4960
Q	 0.7374	 0.4630
R	 0.6894	 0.4930
S	 0.7160	 0.4770
T	 0.4006	 0.4380
U	 0.7378	 0.4870
V	 0.5215	 0.4380
W	 0.6500	 0.4530
X	 0.7729	 0.4610
Y	 0.1908	 0.3440
Z	 0.7962	 0.4920
a	 0.1033	 0.3090
b	 0.0119	 0.2690
c	 0.7534	 0.4970
d	 0.5727	 0.4430
i	 0.7538	 0.5340
j	 0.8173	 0.5310
l	 0.5981	 0.4430
m	 0.4627	 0.4030
n	 0.8040	 0.5170

