



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 06:33 PM JST

PDB ID : 7BT6  
EMDB ID : EMD-30170  
Title : Cryo-EM structure of pre-60S ribosome from *Saccharomyces cerevisiae* rpl4delta63-87 strain at 3.12 Angstroms resolution(state R1)  
Authors : Li, Y.; Wilson, D.M.  
Deposited on : 2020-03-31  
Resolution : 3.12 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](mailto: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>.

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

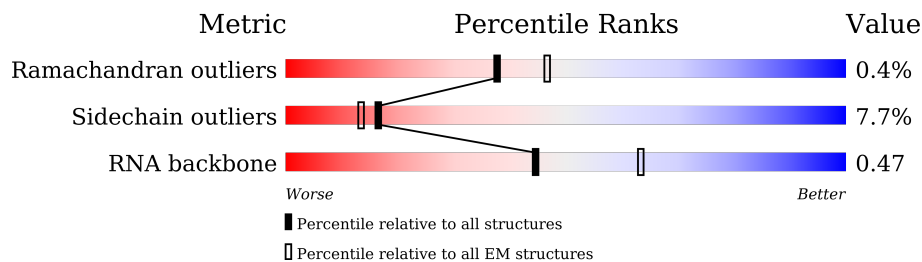
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal 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 3.12 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.



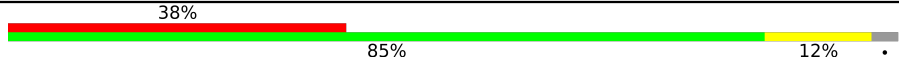

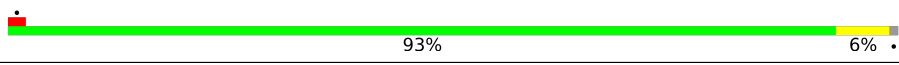

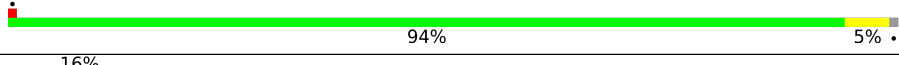
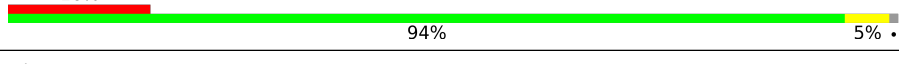
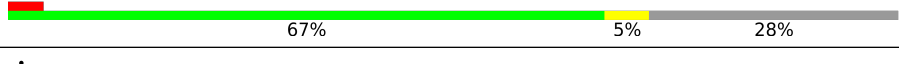

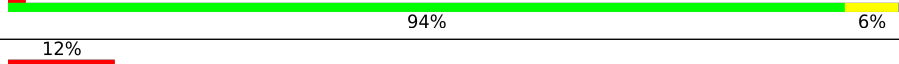


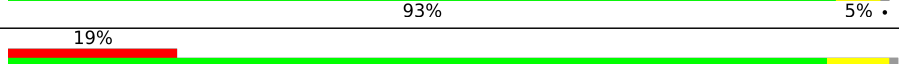
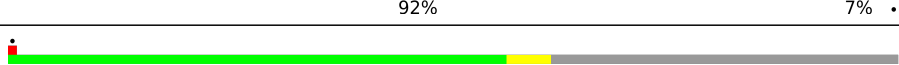
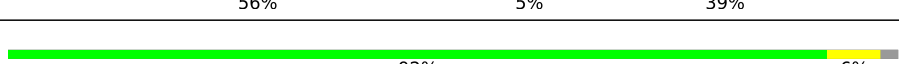
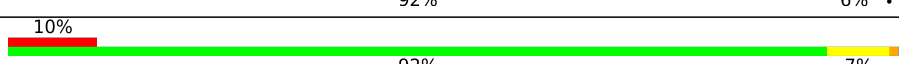
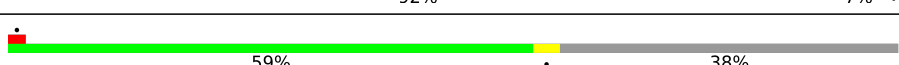
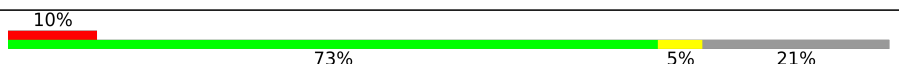
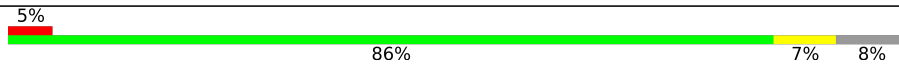
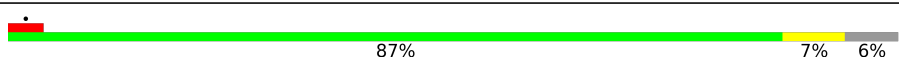
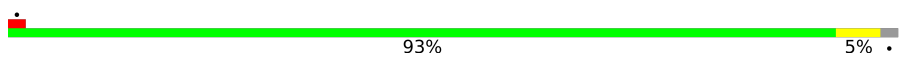
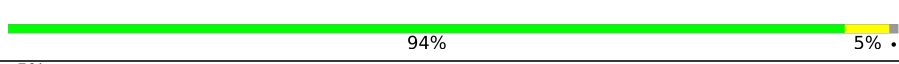
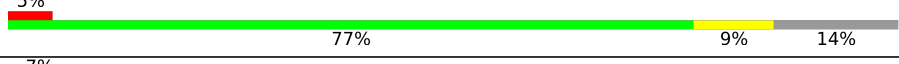
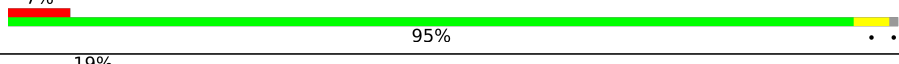
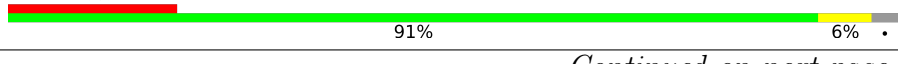

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	254	
2	B	387	
3	C	362	
4	D	297	
5	E	176	
6	F	244	
7	G	256	
8	H	191	

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Mol	Chain	Length	Quality of chain
9	J	174	
10	L	199	
11	M	138	
12	N	204	
13	O	199	
14	P	184	
15	Q	186	
16	R	189	
17	S	172	
18	T	160	
19	U	121	
20	V	137	
21	W	236	
22	X	142	
23	Y	127	
24	Z	136	
25	a	149	
26	b	647	
27	c	105	
28	d	113	
29	e	130	
30	f	107	
31	g	121	
32	h	120	
33	i	100	

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Mol	Chain	Length	Quality of chain
34	j	88	
35	k	78	
36	m	486	
37	p	92	
38	r	261	
39	u	199	
40	v	344	
41	w	203	
42	x	515	
43	y	245	
44	z	106	
45	1	3396	
46	2	158	
47	3	121	

## 2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 133299 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 protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	178	1377	869	269	239	0	0

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	386	3081	1956	584	533	8	0	0

- Molecule 3 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	334	2559	1619	478	459	3	0	0

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	271	2176	1376	384	414	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	156	1239	800	222	216	1	0	0

- Molecule 6 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	222	1784	1151	324	308	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	162	1249	801	213	233	2	0	0

- Molecule 8 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	190	1510	957	273	276	4	0	0

- Molecule 9 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	169	1353	847	253	249	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	L	182	1459	907	300	252	0	0

- Molecule 11 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	183	1570	984	332	253	1	0	0

- Molecule 13 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	P	183	1442	896	287	259	0	0

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	R	154	1241	772	262	207	0	0

- Molecule 17 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	171	1437	925	266	243	3	0	0

- Molecule 18 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	119	943	595	180	165	3	0	0

- Molecule 19 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	U	102	812	526	134	152	0	0

- Molecule 20 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	135	997	625	188	177	7	0	0

- Molecule 21 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 22 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	86	Total	C	N	O	S	0	0
			687	441	114	130	2		

- Molecule 23 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Y	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 24 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 25 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 26 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	510	Total	C	N	O	S	0	0
			4146	2629	726	773	18		

- Molecule 27 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 28 is a protein called 60S ribosomal protein L31-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	d	106	865	549	164	151	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	e	127	1020	647	205	167	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 31 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	104	819	509	168	138	4	0	0

- Molecule 32 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	h	119	969	615	186	167	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	i	97	750	469	149	130	2	0	0

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	j	77	603	365	131	102	5	0	0

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 36 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	452	Total	C	N	O	S	0	0
			3639	2302	655	673	9		

- Molecule 37 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 39 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	144	Total	C	N	O	S	0	0
			1216	763	245	199	9		

- Molecule 40 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 41 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 42 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	x	488	Total	C	N	O	S	0	0
			3807	2398	677	711	21		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 44 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 45 is a RNA chain called RDN25-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	2962	Total	C	N	O	P	0	0
			63385	28311	11449	20663	2962		

- Molecule 46 is a RNA chain called RDN5.8-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 47 is a RNA chain called RDN5-2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

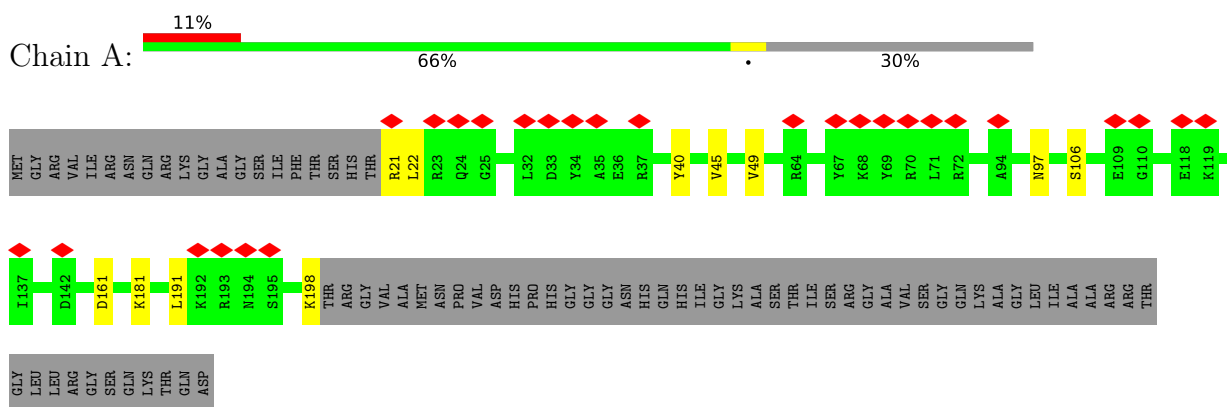
- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



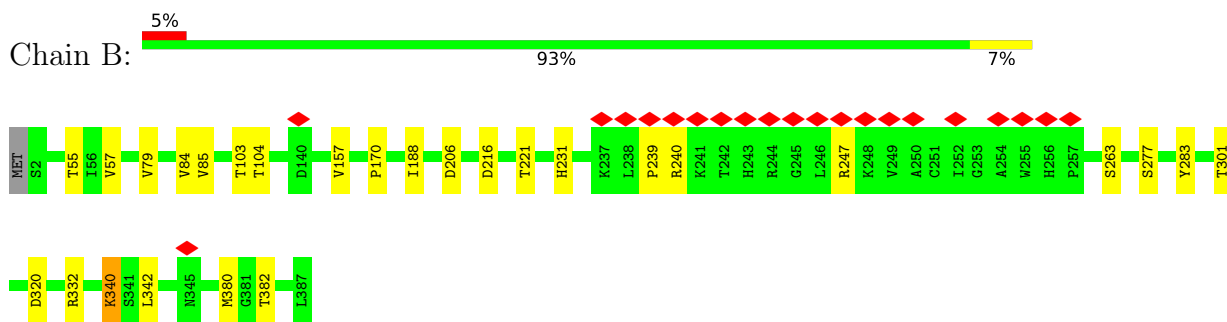
### 3 Residue-property plots [i](#)

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.

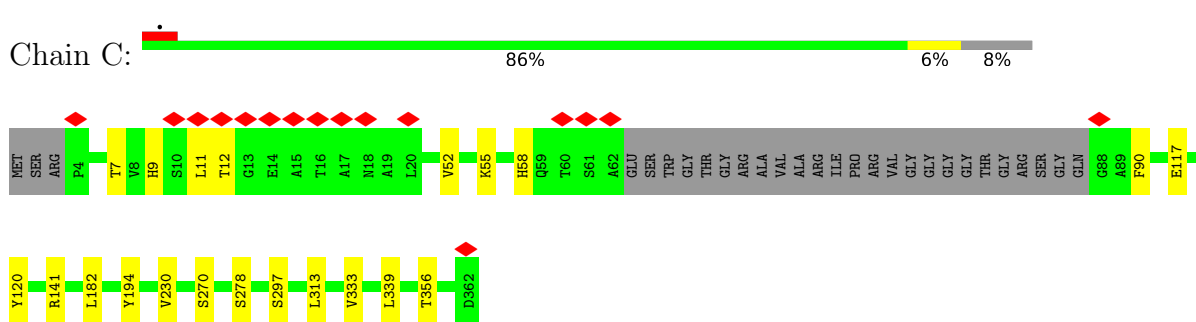
- Molecule 1: 60S ribosomal protein L2-A



- Molecule 2: 60S ribosomal protein L3

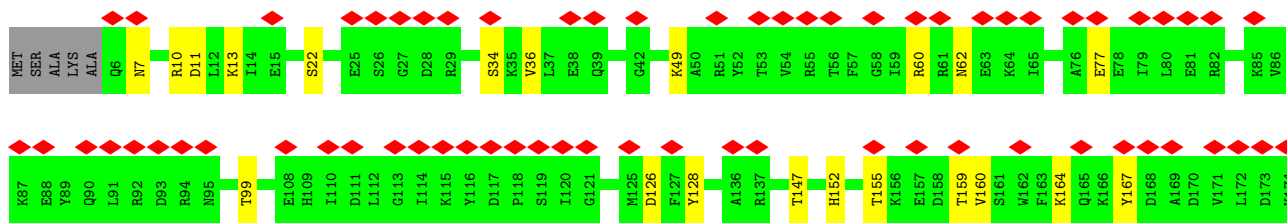


- Molecule 3: 60S ribosomal protein L4-A

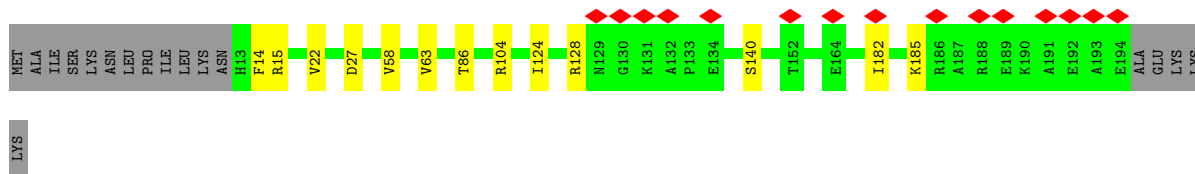
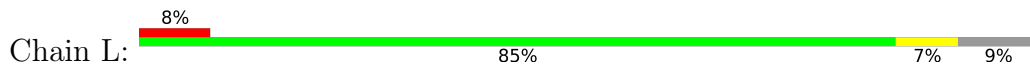


- Molecule 4: 60S ribosomal protein L5

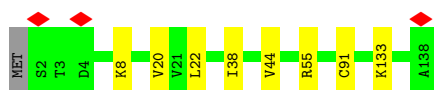




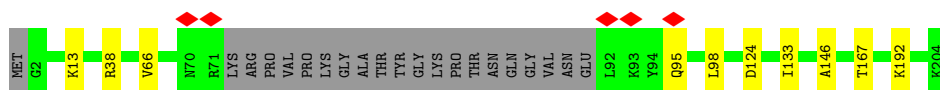
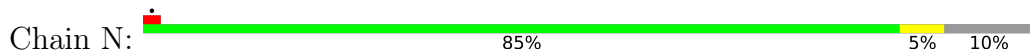
• Molecule 10: 60S ribosomal protein L13-A



• Molecule 11: 60S ribosomal protein L14-A



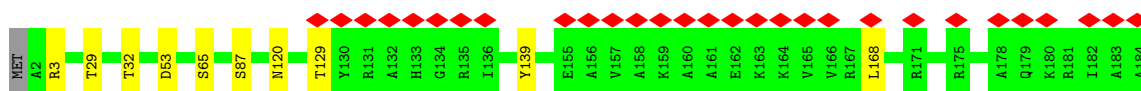
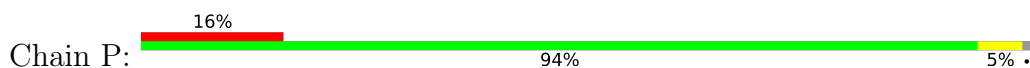
• Molecule 12: 60S ribosomal protein L15-A



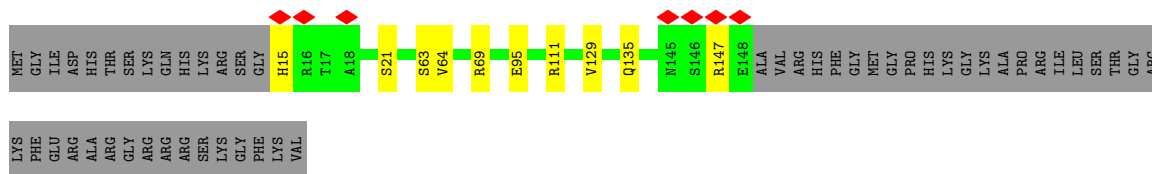
• Molecule 13: 60S ribosomal protein L16-A



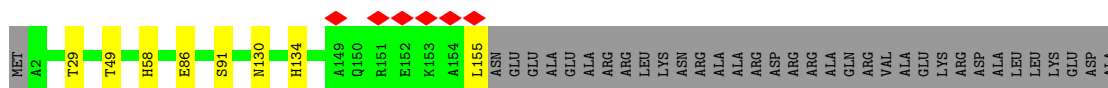
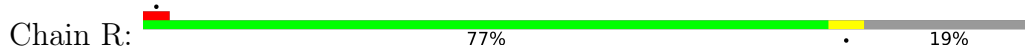
• Molecule 14: 60S ribosomal protein L17-A



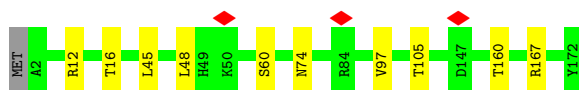
• Molecule 15: 60S ribosomal protein L18-A



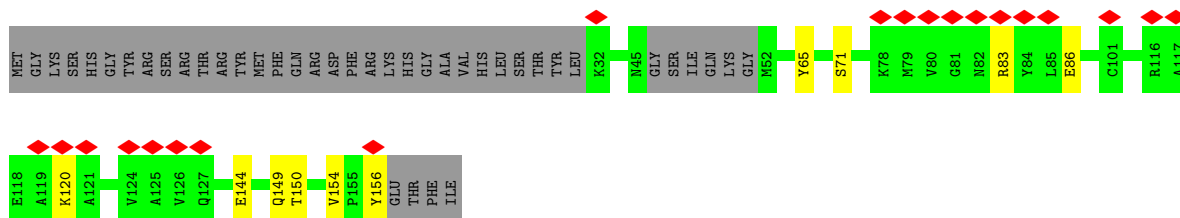
• Molecule 16: 60S ribosomal protein L19-A



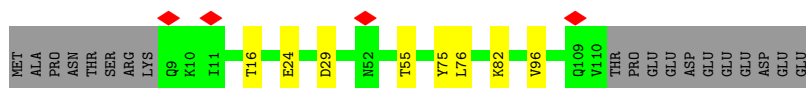
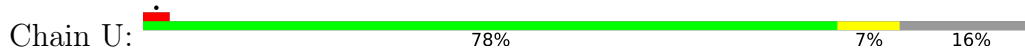
• Molecule 17: 60S ribosomal protein L20-A



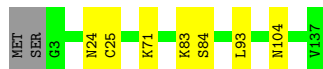
• Molecule 18: 60S ribosomal protein L21-A



• Molecule 19: 60S ribosomal protein L22-A

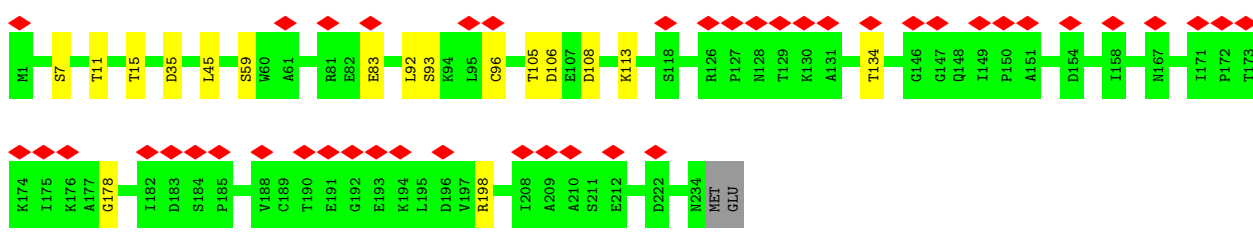
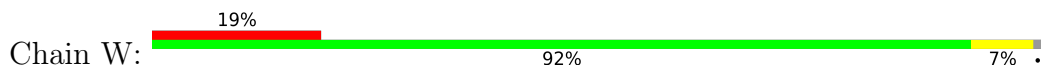


• Molecule 20: 60S ribosomal protein L23-A

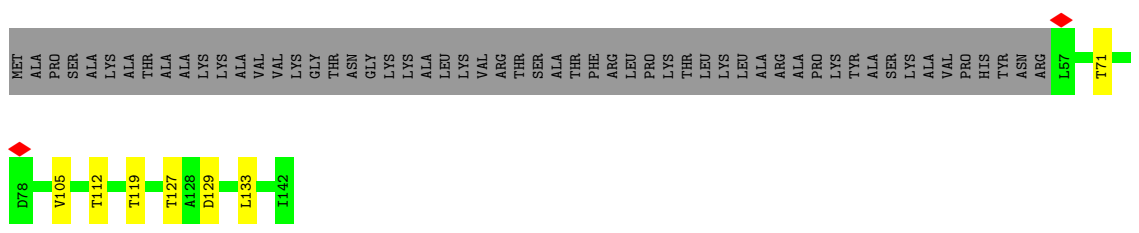


• Molecule 21: Ribosome assembly factor MRT4

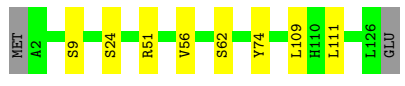
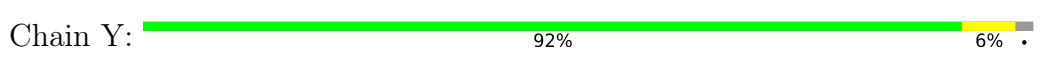




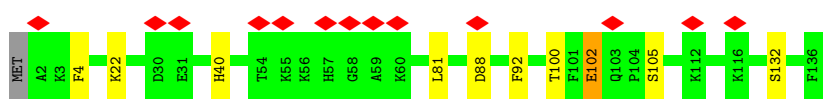
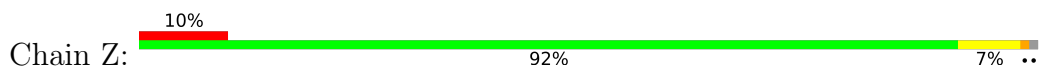
• Molecule 22: 60S ribosomal protein L25



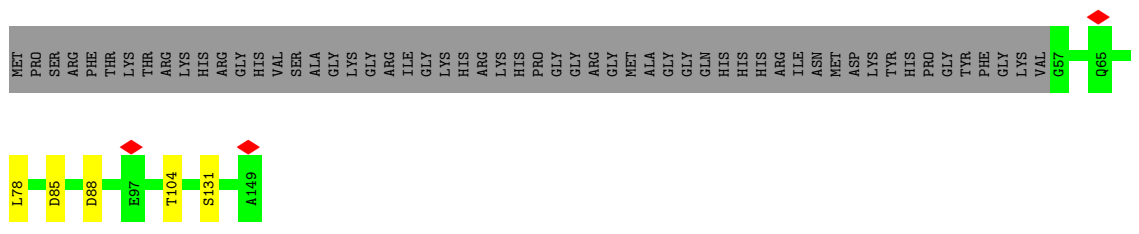
• Molecule 23: 60S ribosomal protein L26-A



• Molecule 24: 60S ribosomal protein L27-A



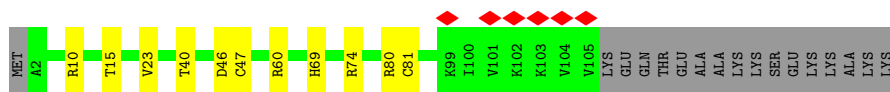
• Molecule 25: 60S ribosomal protein L28



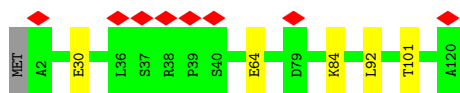
• Molecule 26: Nucleolar GTP-binding protein 1



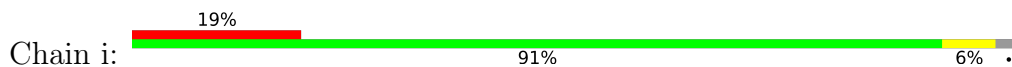




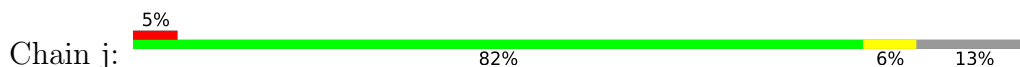
- Molecule 32: 60S ribosomal protein L35-A



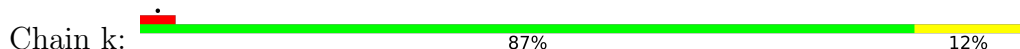
- Molecule 33: 60S ribosomal protein L36-A



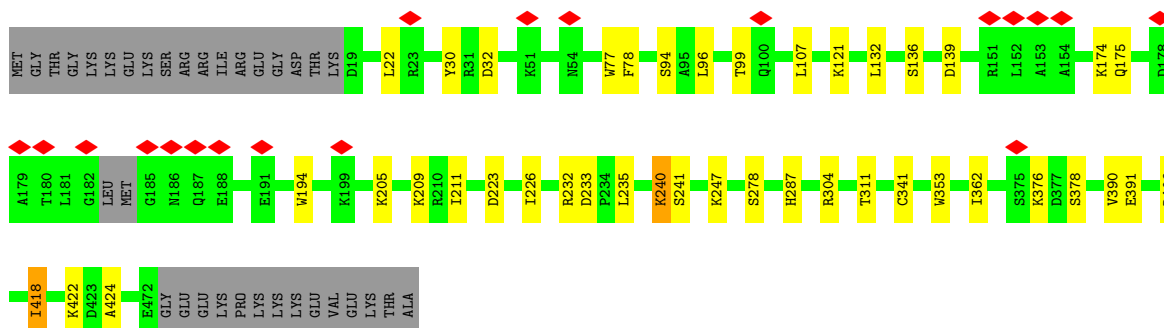
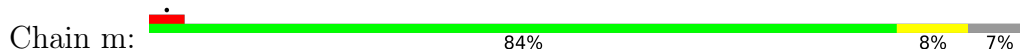
- Molecule 34: 60S ribosomal protein L37-A



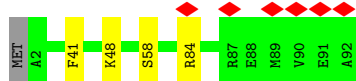
- Molecule 35: 60S ribosomal protein L38



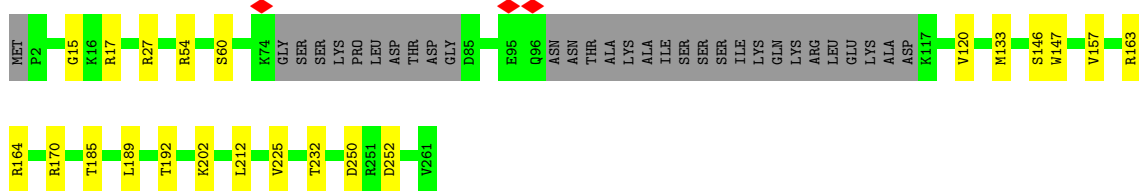
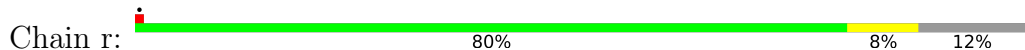
- Molecule 36: Nucleolar GTP-binding protein 2



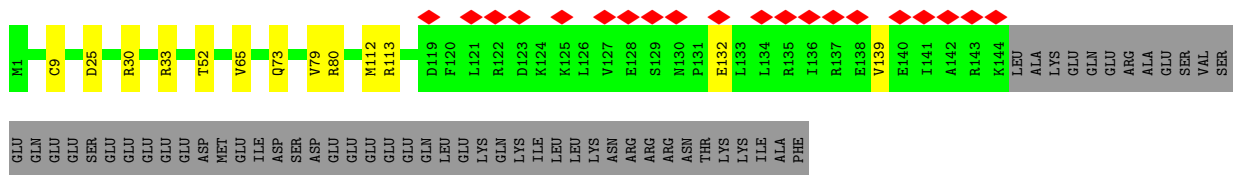
- Molecule 37: 60S ribosomal protein L43-A



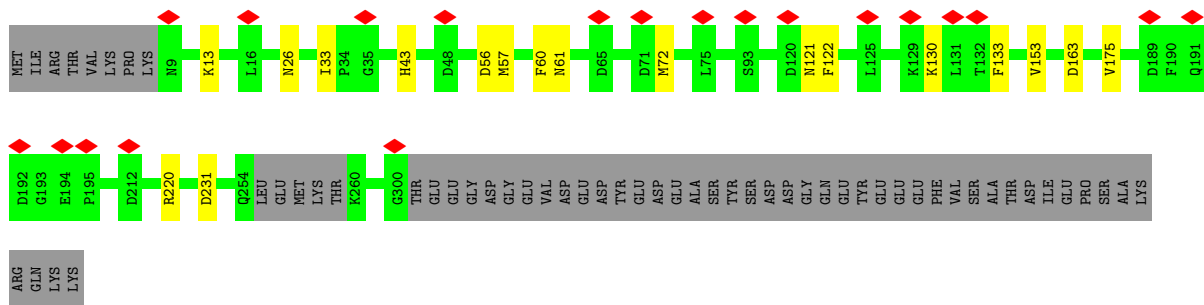
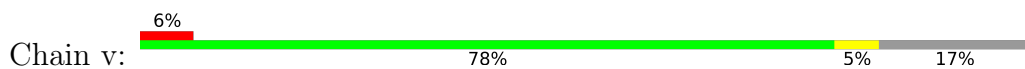
• Molecule 38: Ribosome biogenesis protein NSA2



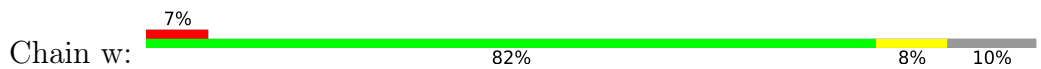
• Molecule 39: Ribosome biogenesis protein RLP24

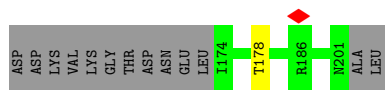


• Molecule 40: Ribosome biogenesis protein RPF2

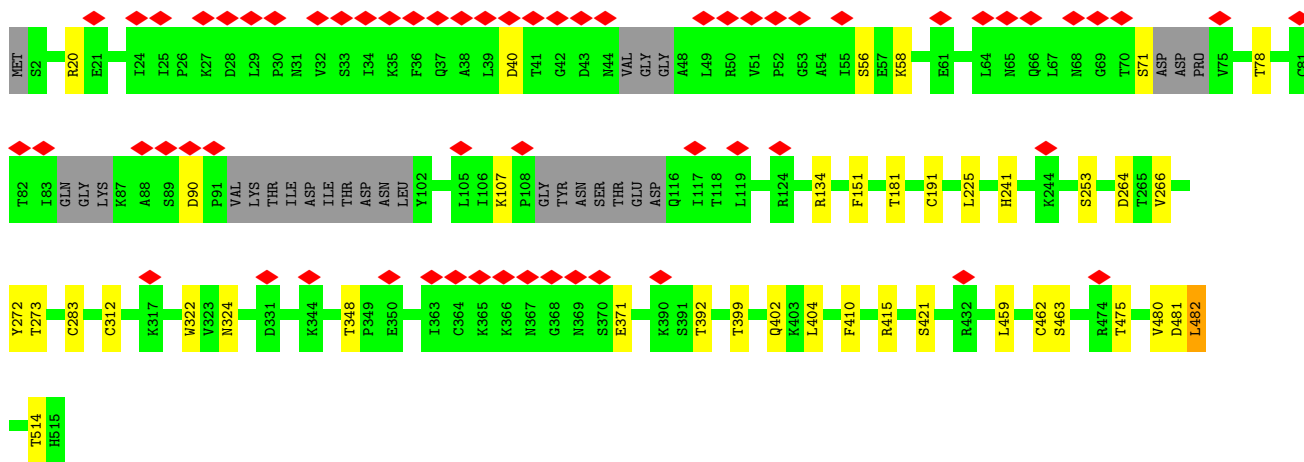
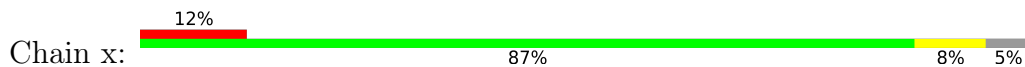


• Molecule 41: Regulator of ribosome biosynthesis





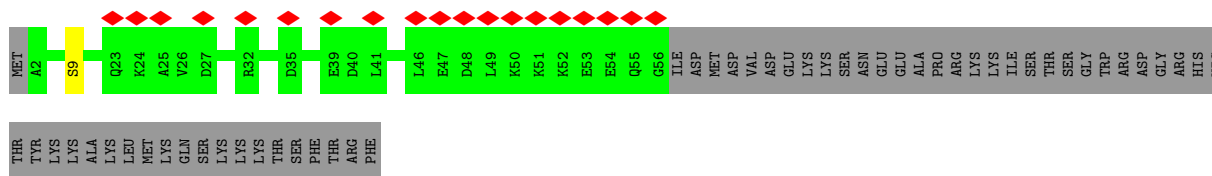
• Molecule 42: Ribosome assembly protein 4



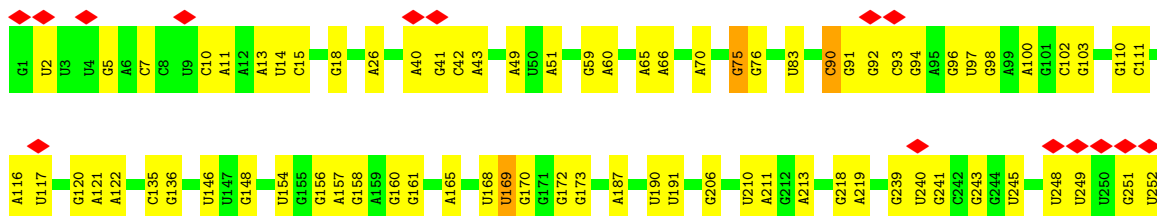
• Molecule 43: Eukaryotic translation initiation factor 6



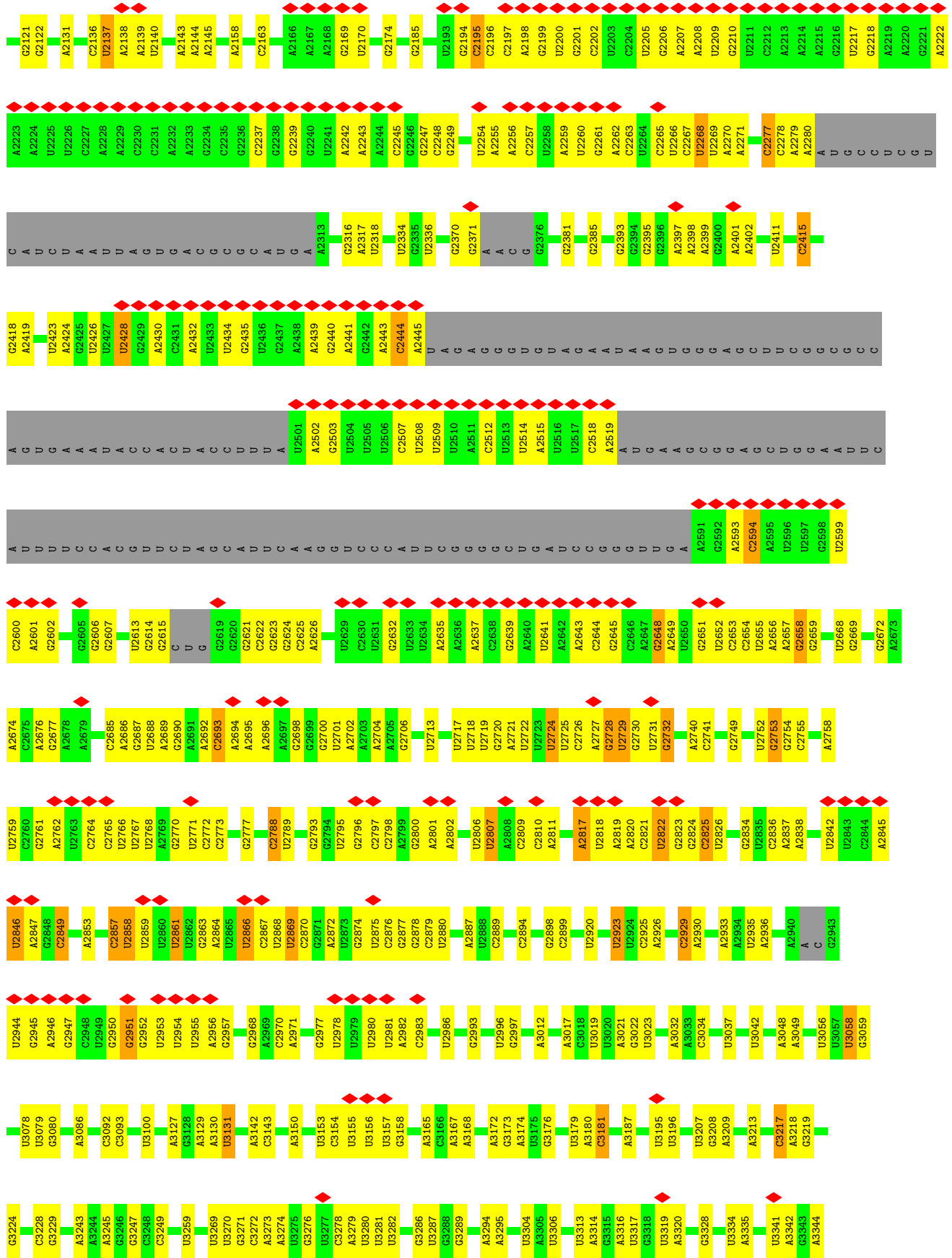
• Molecule 44: UPF0642 protein YBL028C



• Molecule 45: RDN25-1 rRNA

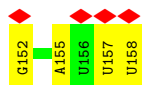
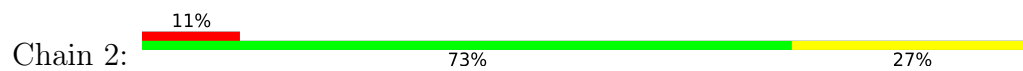




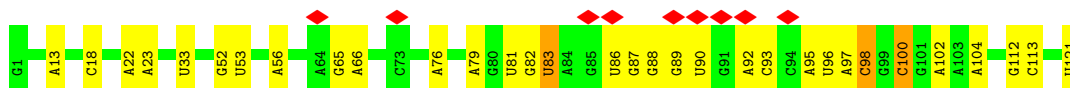
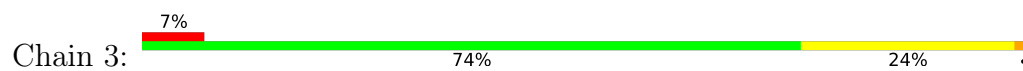




- Molecule 46: RDN5.8-1 rRNA



- Molecule 47: RDN5-2 rRNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103319	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 ( $e^-/\text{\AA}^2$ )	1.9	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	0.228	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	412.02, 412.02, 412.02	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3734, 1.3734, 1.3734	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, ZN

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	0.32	0/1403	0.50	0/1887
2	B	0.41	0/3152	0.51	0/4239
3	C	0.36	0/2607	0.53	1/3530 (0.0%)
4	D	0.30	0/2222	0.48	0/2996
5	E	0.34	0/1260	0.48	0/1694
6	F	0.39	0/1821	0.49	0/2451
7	G	0.28	0/1268	0.51	0/1716
8	H	0.38	0/1531	0.49	0/2062
9	J	0.28	0/1374	0.51	0/1842
10	L	0.33	0/1483	0.49	0/1991
11	M	0.35	0/1074	0.48	0/1446
12	N	0.35	0/1602	0.45	0/2142
13	O	0.44	0/1585	0.49	0/2128
14	P	0.38	0/1465	0.50	0/1968
15	Q	0.33	0/1050	0.47	0/1419
16	R	0.38	0/1258	0.48	0/1679
17	S	0.38	0/1473	0.50	0/1980
18	T	0.30	0/957	0.47	0/1285
19	U	0.34	0/828	0.48	0/1121
20	V	0.40	0/1012	0.53	0/1361
21	W	0.29	0/1918	0.49	0/2586
22	X	0.35	0/695	0.45	0/937
23	Y	0.36	0/995	0.48	0/1329
24	Z	0.33	0/1118	0.47	0/1497
25	a	0.31	0/751	0.46	0/1013
26	b	0.35	0/4220	0.49	0/5687
27	c	0.33	0/751	0.46	0/1008
28	d	0.42	0/879	0.53	0/1180
29	e	0.40	0/1041	0.50	0/1394
30	f	0.43	0/868	0.50	0/1168
31	g	0.41	0/829	0.50	0/1109
32	h	0.30	0/978	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	i	0.27	0/756	0.45	0/1005
34	j	0.37	0/614	0.49	0/813
35	k	0.30	0/618	0.50	0/826
36	m	0.37	0/3713	0.52	0/5006
37	p	0.40	0/701	0.55	0/934
38	r	0.40	0/1892	0.54	0/2528
39	u	0.37	0/1238	0.45	0/1646
40	v	0.30	0/2361	0.48	0/3153
41	w	0.28	0/1471	0.48	0/1980
42	x	0.31	0/3897	0.52	1/5282 (0.0%)
43	y	0.35	0/1872	0.53	0/2548
44	z	0.27	0/445	0.42	0/585
45	1	0.65	0/70950	0.91	114/110603 (0.1%)
46	2	0.58	0/3746	0.84	0/5832
47	3	0.32	0/2883	0.87	7/4491 (0.2%)
All	All	0.53	0/142625	0.76	123/208378 (0.1%)

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
2	B	0	2
6	F	0	1
24	Z	0	1
26	b	0	1
31	g	0	1
36	m	0	2
38	r	0	1
39	u	0	1
41	w	0	1
42	x	0	1
All	All	0	12

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3	83	U	N3-C2-O2	-9.89	115.28	122.20
45	1	3217	C	N1-C2-O2	8.84	124.20	118.90
45	1	3217	C	C2-N1-C1'	8.12	127.74	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	1	2923	U	C2-N1-C1'	7.87	127.14	117.70
45	1	2137	U	C2-N1-C1'	7.71	126.96	117.70
45	1	960	U	N3-C2-O2	-7.71	116.80	122.20
45	1	960	U	C2-N1-C1'	7.63	126.86	117.70
45	1	2239	G	N3-C4-N9	-7.46	121.52	126.00
45	1	2428	U	N3-C2-O2	-7.33	117.07	122.20
45	1	2137	U	N3-C2-O2	-7.31	117.08	122.20
45	1	2428	U	C2-N1-C1'	7.14	126.27	117.70
45	1	960	U	N1-C2-O2	7.08	127.76	122.80
45	1	1255	C	C2-N1-C1'	7.08	126.59	118.80
45	1	2869	U	C2-N1-C1'	7.02	126.12	117.70
45	1	720	A	P-O3'-C3'	6.99	128.09	119.70
45	1	922	U	C2-N1-C1'	6.97	126.07	117.70
45	1	2428	U	N1-C2-O2	6.90	127.63	122.80
45	1	2869	U	N1-C2-O2	6.83	127.58	122.80
45	1	995	U	C2-N1-C1'	6.78	125.84	117.70
45	1	2137	U	N1-C2-O2	6.72	127.50	122.80
45	1	2239	G	C8-N9-C1'	6.67	135.67	127.00
45	1	3217	C	N3-C2-O2	-6.66	117.24	121.90
45	1	3058	U	N1-C2-O2	6.65	127.46	122.80
45	1	1199	C	N1-C2-O2	6.65	122.89	118.90
45	1	2693	C	N1-C2-O2	6.61	122.86	118.90
45	1	1608	C	C2-N1-C1'	6.58	126.04	118.80
45	1	3058	U	C2-N1-C1'	6.47	125.46	117.70
45	1	2923	U	N1-C2-O2	6.46	127.32	122.80
45	1	1283	C	N3-C2-O2	-6.45	117.38	121.90
45	1	2594	C	N1-C2-O2	6.45	122.77	118.90
45	1	995	U	N1-C2-O2	6.29	127.21	122.80
42	x	482	LEU	CA-CB-CG	6.25	129.68	115.30
45	1	2239	G	N9-C4-C5	6.24	107.90	105.40
45	1	2923	U	N3-C2-O2	-6.23	117.84	122.20
45	1	2648	G	N3-C4-N9	-6.17	122.30	126.00
45	1	1227	C	C2-N1-C1'	6.13	125.54	118.80
45	1	3058	U	N3-C2-O2	-6.13	117.91	122.20
45	1	260	C	N3-C2-O2	-6.10	117.63	121.90
45	1	2807	U	N3-C2-O2	-6.07	117.95	122.20
45	1	2866	U	OP2-P-O3'	6.03	118.47	105.20
45	1	2822	U	C2-N1-C1'	6.02	124.92	117.70
45	1	3217	C	C6-N1-C1'	-6.00	113.60	120.80
45	1	90	C	C5-C6-N1	5.99	123.99	121.00
45	1	995	U	N3-C2-O2	-5.98	118.02	122.20
45	1	2239	G	C4-N9-C1'	-5.96	118.75	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	1	1199	C	C2-N1-C1'	5.93	125.33	118.80
45	1	646	A	N9-C1'-C2'	5.89	121.66	114.00
45	1	2869	U	N3-C2-O2	-5.87	118.09	122.20
45	1	3048	A	O4'-C1'-N9	5.84	112.88	108.20
45	1	406	G	O4'-C1'-N9	5.84	112.87	108.20
45	1	720	A	OP2-P-O3'	5.80	117.96	105.20
45	1	2817	A	OP1-P-O3'	5.80	117.96	105.20
45	1	2195	C	N1-C2-O2	5.79	122.37	118.90
45	1	1283	C	N1-C2-O2	5.78	122.37	118.90
45	1	835	G	O4'-C1'-N9	5.77	112.82	108.20
45	1	910	G	C5-C6-O6	-5.74	125.15	128.60
45	1	1349	G	N3-C4-C5	-5.72	125.74	128.60
45	1	2248	C	N1-C2-O2	5.71	122.33	118.90
45	1	75	G	C4-N9-C1'	5.70	133.91	126.50
45	1	2788	C	N1-C2-O2	5.69	122.31	118.90
45	1	2807	U	N1-C2-O2	5.67	126.77	122.80
45	1	2857	C	C6-N1-C2	5.67	122.57	120.30
45	1	2951	G	O4'-C1'-N9	5.65	112.72	108.20
45	1	2849	C	C2-N1-C1'	5.64	125.00	118.80
45	1	3131	U	C2-N1-C1'	5.63	124.45	117.70
45	1	2755	C	N3-C2-O2	-5.62	117.96	121.90
45	1	2732	G	O5'-P-OP1	-5.61	100.66	105.70
45	1	3278	C	C2-N1-C1'	5.58	124.94	118.80
45	1	2137	U	C6-N1-C2	-5.58	117.65	121.00
45	1	2444	C	N1-C2-O2	5.57	122.24	118.90
45	1	2658	G	O4'-C1'-N9	5.55	112.64	108.20
47	3	83	U	N1-C2-N3	5.55	118.23	114.90
45	1	2788	C	N3-C2-O2	-5.53	118.03	121.90
45	1	2693	C	N3-C2-O2	-5.52	118.04	121.90
45	1	2846	U	C2-N1-C1'	5.45	124.23	117.70
45	1	1107	C	C2-N1-C1'	5.44	124.78	118.80
45	1	2268	U	C2-N1-C1'	5.43	124.22	117.70
45	1	648	C	N1-C2-O2	5.39	122.13	118.90
3	C	182	LEU	CA-CB-CG	5.37	127.64	115.30
45	1	90	C	C6-N1-C2	-5.35	118.16	120.30
45	1	1235	U	C5-C4-O4	-5.32	122.71	125.90
47	3	98	C	N1-C2-O2	5.31	122.09	118.90
45	1	2861	U	C2-N1-C1'	5.30	124.06	117.70
45	1	648	C	C2-N1-C1'	5.29	124.62	118.80
45	1	2415	C	C2-N1-C1'	5.26	124.59	118.80
45	1	3306	U	C2-N1-C1'	5.26	124.01	117.70
45	1	2248	C	C2-N1-C1'	5.26	124.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3	83	U	N1-C2-O2	5.25	126.48	122.80
45	1	2825	C	C2-N1-C1'	5.24	124.57	118.80
45	1	75	G	C8-N9-C1'	-5.23	120.20	127.00
45	1	2866	U	P-O3'-C3'	5.23	125.98	119.70
45	1	2428	U	C6-N1-C2	-5.23	117.86	121.00
45	1	922	U	N1-C2-O2	5.23	126.46	122.80
45	1	2693	C	C2-N1-C1'	5.22	124.55	118.80
45	1	2857	C	OP1-P-O3'	5.22	116.69	105.20
45	1	2858	U	O5'-P-OP1	-5.22	101.00	105.70
45	1	2753	G	P-O3'-C3'	5.21	125.96	119.70
45	1	169	U	P-O3'-C3'	5.21	125.95	119.70
45	1	2822	U	N1-C2-O2	5.20	126.44	122.80
45	1	2428	U	C5-C6-N1	5.19	125.30	122.70
45	1	2277	C	OP1-P-O3'	5.16	116.56	105.20
45	1	2857	C	N3-C4-C5	5.14	123.95	121.90
45	1	2728	G	P-O3'-C3'	5.13	125.86	119.70
45	1	2923	U	C6-N1-C1'	-5.13	114.02	121.20
45	1	3350	C	N1-C2-O2	5.12	121.97	118.90
45	1	2594	C	N3-C2-O2	-5.12	118.32	121.90
45	1	2724	U	N3-C2-O2	-5.11	118.62	122.20
45	1	1187	C	C6-N1-C2	-5.10	118.26	120.30
45	1	2248	C	N3-C2-O2	-5.09	118.33	121.90
47	3	100	C	C2-N1-C1'	5.09	124.40	118.80
45	1	2929	C	O4'-C1'-N1	5.09	112.27	108.20
45	1	3181	C	C2-N1-C1'	5.08	124.39	118.80
47	3	97	A	N1-C6-N6	-5.08	115.55	118.60
45	1	1222	G	O4'-C1'-N9	5.07	112.26	108.20
45	1	1187	C	C2-N1-C1'	5.05	124.36	118.80
45	1	292	U	C2-N1-C1'	5.05	123.76	117.70
45	1	2729	U	O4'-C1'-N1	5.04	112.23	108.20
45	1	3019	U	N3-C2-O2	-5.03	118.68	122.20
45	1	2836	C	C2-N1-C1'	5.03	124.33	118.80
45	1	3344	A	O4'-C1'-N9	5.03	112.22	108.20
47	3	113	C	N1-C2-O2	5.03	121.92	118.90
45	1	3278	C	N1-C2-O2	5.02	121.91	118.90
45	1	1349	G	N3-C4-N9	5.01	129.01	126.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	THR	Peptide

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Mol	Chain	Res	Type	Group
2	B	340	LYS	Peptide
6	F	158	LYS	Peptide
24	Z	102	GLU	Peptide
26	b	438	GLY	Peptide
31	g	80	ARG	Peptide
36	m	240	LYS	Peptide
36	m	418	ILE	Peptide
38	r	15	GLY	Peptide
39	u	79	VAL	Peptide
41	w	141	TRP	Peptide
42	x	20	ARG	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	
1	A	176/254 (69%)	164 (93%)	12 (7%)	0	100	100
2	B	384/387 (99%)	332 (86%)	49 (13%)	3 (1%)	19	53
3	C	330/362 (91%)	292 (88%)	37 (11%)	1 (0%)	41	73
4	D	267/297 (90%)	240 (90%)	27 (10%)	0	100	100
5	E	152/176 (86%)	141 (93%)	11 (7%)	0	100	100
6	F	220/244 (90%)	201 (91%)	18 (8%)	1 (0%)	29	63
7	G	160/256 (62%)	140 (88%)	20 (12%)	0	100	100
8	H	188/191 (98%)	167 (89%)	20 (11%)	1 (0%)	29	63
9	J	167/174 (96%)	136 (81%)	31 (19%)	0	100	100
10	L	180/199 (90%)	157 (87%)	22 (12%)	1 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
12	N	179/204 (88%)	165 (92%)	12 (7%)	2 (1%)	14	45
13	O	195/199 (98%)	187 (96%)	8 (4%)	0	100	100
14	P	181/184 (98%)	166 (92%)	15 (8%)	0	100	100
15	Q	132/186 (71%)	126 (96%)	6 (4%)	0	100	100
16	R	152/189 (80%)	145 (95%)	7 (5%)	0	100	100
17	S	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
18	T	115/160 (72%)	101 (88%)	14 (12%)	0	100	100
19	U	100/121 (83%)	87 (87%)	13 (13%)	0	100	100
20	V	133/137 (97%)	125 (94%)	8 (6%)	0	100	100
21	W	232/236 (98%)	209 (90%)	22 (10%)	1 (0%)	34	68
22	X	84/142 (59%)	78 (93%)	6 (7%)	0	100	100
23	Y	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
24	Z	133/136 (98%)	115 (86%)	17 (13%)	1 (1%)	19	53
25	a	91/149 (61%)	80 (88%)	10 (11%)	1 (1%)	14	45
26	b	506/647 (78%)	437 (86%)	64 (13%)	5 (1%)	15	48
27	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
28	d	104/113 (92%)	98 (94%)	6 (6%)	0	100	100
29	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
30	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
31	g	102/121 (84%)	95 (93%)	7 (7%)	0	100	100
32	h	117/120 (98%)	101 (86%)	15 (13%)	1 (1%)	17	51
33	i	95/100 (95%)	86 (90%)	9 (10%)	0	100	100
34	j	74/88 (84%)	69 (93%)	5 (7%)	0	100	100
35	k	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
36	m	448/486 (92%)	384 (86%)	56 (12%)	8 (2%)	8	33
37	p	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
38	r	224/261 (86%)	186 (83%)	34 (15%)	4 (2%)	8	33
39	u	142/199 (71%)	135 (95%)	7 (5%)	0	100	100
40	v	283/344 (82%)	264 (93%)	19 (7%)	0	100	100
41	w	178/203 (88%)	155 (87%)	23 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	x	476/515 (92%)	429 (90%)	47 (10%)	0	100	100
43	y	242/245 (99%)	223 (92%)	19 (8%)	0	100	100
44	z	53/106 (50%)	51 (96%)	2 (4%)	0	100	100
All	All	7910/9080 (87%)	7130 (90%)	750 (10%)	30 (0%)	38	68

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	339	LEU
36	m	209	LYS
36	m	241	SER
10	L	63	VAL
12	N	146	ALA
24	Z	102	GLU
25	a	78	LEU
26	b	369	ARG
26	b	484	SER
36	m	78	PHE
36	m	424	ALA
6	F	158	LYS
8	H	50	ASN
21	W	178	GLY
26	b	399	ALA
36	m	240	LYS
38	r	17	ARG
38	r	147	TRP
2	B	342	LEU
26	b	483	ALA
36	m	136	SER
36	m	378	SER
38	r	163	ARG
12	N	95	GLN
32	h	92	LEU
38	r	146	SER
36	m	77	TRP
2	B	188	ILE
2	B	239	PRO
26	b	9	PRO

### 5.3.2 Protein sidechains

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	
1	A	140/196 (71%)	129 (92%)	11 (8%)	12	39
2	B	322/323 (100%)	299 (93%)	23 (7%)	14	44
3	C	271/289 (94%)	252 (93%)	19 (7%)	15	44
4	D	224/245 (91%)	203 (91%)	21 (9%)	8	32
5	E	134/153 (88%)	125 (93%)	9 (7%)	16	45
6	F	186/205 (91%)	176 (95%)	10 (5%)	22	53
7	G	131/208 (63%)	119 (91%)	12 (9%)	9	32
8	H	170/171 (99%)	162 (95%)	8 (5%)	26	58
9	J	147/150 (98%)	126 (86%)	21 (14%)	3	14
10	L	144/159 (91%)	132 (92%)	12 (8%)	11	37
11	M	108/109 (99%)	100 (93%)	8 (7%)	13	41
12	N	159/176 (90%)	151 (95%)	8 (5%)	24	56
13	O	160/162 (99%)	150 (94%)	10 (6%)	18	47
14	P	145/146 (99%)	135 (93%)	10 (7%)	15	44
15	Q	110/151 (73%)	100 (91%)	10 (9%)	9	33
16	R	127/154 (82%)	119 (94%)	8 (6%)	18	47
17	S	155/156 (99%)	145 (94%)	10 (6%)	17	47
18	T	102/137 (74%)	92 (90%)	10 (10%)	8	29
19	U	89/107 (83%)	81 (91%)	8 (9%)	9	33
20	V	103/105 (98%)	96 (93%)	7 (7%)	16	45
21	W	211/213 (99%)	195 (92%)	16 (8%)	13	41
22	X	76/118 (64%)	69 (91%)	7 (9%)	9	32
23	Y	108/110 (98%)	100 (93%)	8 (7%)	13	41
24	Z	115/116 (99%)	106 (92%)	9 (8%)	12	40
25	a	76/119 (64%)	72 (95%)	4 (5%)	22	53
26	b	458/573 (80%)	427 (93%)	31 (7%)	16	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	c	81/88 (92%)	74 (91%)	7 (9%)	10	36
28	d	93/97 (96%)	85 (91%)	8 (9%)	10	36
29	e	109/111 (98%)	103 (94%)	6 (6%)	21	52
30	f	90/91 (99%)	85 (94%)	5 (6%)	21	51
31	g	89/103 (86%)	79 (89%)	10 (11%)	6	24
32	h	104/105 (99%)	100 (96%)	4 (4%)	33	65
33	i	79/82 (96%)	73 (92%)	6 (8%)	13	41
34	j	62/71 (87%)	57 (92%)	5 (8%)	11	38
35	k	68/69 (99%)	59 (87%)	9 (13%)	4	17
36	m	399/428 (93%)	365 (92%)	34 (8%)	10	36
37	p	71/72 (99%)	67 (94%)	4 (6%)	21	51
38	r	203/229 (89%)	186 (92%)	17 (8%)	11	37
39	u	128/180 (71%)	116 (91%)	12 (9%)	8	32
40	v	258/309 (84%)	240 (93%)	18 (7%)	15	44
41	w	161/179 (90%)	146 (91%)	15 (9%)	9	32
42	x	428/451 (95%)	389 (91%)	39 (9%)	9	33
43	y	210/211 (100%)	195 (93%)	15 (7%)	14	44
44	z	48/95 (50%)	47 (98%)	1 (2%)	53	78
All	All	6852/7722 (89%)	6327 (92%)	525 (8%)	16	40

All (525) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	22	LEU
1	A	40	TYR
1	A	45	VAL
1	A	49	VAL
1	A	97	ASN
1	A	106	SER
1	A	161	ASP
1	A	181	LYS
1	A	191	LEU
1	A	198	LYS
2	B	55	THR
2	B	57	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	79	VAL
2	B	84	VAL
2	B	85	VAL
2	B	103	THR
2	B	104	THR
2	B	157	VAL
2	B	170	PRO
2	B	206	ASP
2	B	216	ASP
2	B	231	HIS
2	B	240	ARG
2	B	247	ARG
2	B	263	SER
2	B	277	SER
2	B	283	TYR
2	B	301	THR
2	B	320	ASP
2	B	332	ARG
2	B	340	LYS
2	B	380	MET
2	B	382	THR
3	C	7	THR
3	C	9	HIS
3	C	11	LEU
3	C	12	THR
3	C	52	VAL
3	C	55	LYS
3	C	58	HIS
3	C	90	PHE
3	C	117	GLU
3	C	120	TYR
3	C	141	ARG
3	C	194	TYR
3	C	230	VAL
3	C	270	SER
3	C	278	SER
3	C	297	SER
3	C	313	LEU
3	C	333	VAL
3	C	356	THR
4	D	8	LYS
4	D	12	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	14	SER
4	D	16	PHE
4	D	18	THR
4	D	40	HIS
4	D	43	LYS
4	D	46	THR
4	D	51	LEU
4	D	59	ASP
4	D	85	ARG
4	D	95	TRP
4	D	137	ASP
4	D	144	VAL
4	D	158	ARG
4	D	173	VAL
4	D	178	ASN
4	D	205	SER
4	D	229	ASP
4	D	232	ASP
4	D	276	LYS
5	E	2	SER
5	E	38	THR
5	E	40	LEU
5	E	62	THR
5	E	64	LEU
5	E	79	VAL
5	E	98	VAL
5	E	104	GLU
5	E	143	LYS
6	F	89	ILE
6	F	110	ARG
6	F	111	ILE
6	F	140	SER
6	F	143	THR
6	F	158	LYS
6	F	179	LEU
6	F	183	ASP
6	F	190	THR
6	F	239	LEU
7	G	90	THR
7	G	92	LYS
7	G	94	PHE
7	G	155	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	180	VAL
7	G	186	LEU
7	G	189	LEU
7	G	194	THR
7	G	197	VAL
7	G	206	GLU
7	G	222	PHE
7	G	227	ASP
8	H	6	THR
8	H	41	ILE
8	H	69	ARG
8	H	92	TYR
8	H	107	ASP
8	H	133	THR
8	H	139	ASN
8	H	151	VAL
9	J	7	ASN
9	J	10	ARG
9	J	11	ASP
9	J	13	LYS
9	J	22	SER
9	J	34	SER
9	J	36	VAL
9	J	49	LYS
9	J	60	ARG
9	J	62	ASN
9	J	77	GLU
9	J	99	THR
9	J	126	ASP
9	J	128	TYR
9	J	147	THR
9	J	152	HIS
9	J	155	THR
9	J	159	THR
9	J	160	VAL
9	J	164	LYS
9	J	167	TYR
10	L	14	PHE
10	L	15	ARG
10	L	22	VAL
10	L	27	ASP
10	L	58	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	L	86	THR
10	L	104	ARG
10	L	124	ILE
10	L	128	ARG
10	L	140	SER
10	L	182	ILE
10	L	185	LYS
11	M	8	LYS
11	M	20	VAL
11	M	22	LEU
11	M	38	ILE
11	M	44	VAL
11	M	55	ARG
11	M	91	CYS
11	M	133	LYS
12	N	13	LYS
12	N	38	ARG
12	N	66	VAL
12	N	98	LEU
12	N	124	ASP
12	N	133	ILE
12	N	167	THR
12	N	192	LYS
13	O	21	SER
13	O	34	VAL
13	O	37	ARG
13	O	48	PHE
13	O	56	ASP
13	O	59	ARG
13	O	92	THR
13	O	117	ARG
13	O	119	VAL
13	O	184	THR
14	P	3	ARG
14	P	29	THR
14	P	32	THR
14	P	53	ASP
14	P	65	SER
14	P	87	SER
14	P	120	ASN
14	P	129	THR
14	P	139	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	P	168	LEU
15	Q	15	HIS
15	Q	21	SER
15	Q	63	SER
15	Q	64	VAL
15	Q	69	ARG
15	Q	95	GLU
15	Q	111	ARG
15	Q	129	VAL
15	Q	135	GLN
15	Q	147	ARG
16	R	29	THR
16	R	49	THR
16	R	58	HIS
16	R	86	GLU
16	R	91	SER
16	R	130	ASN
16	R	134	HIS
16	R	155	LEU
17	S	12	ARG
17	S	16	THR
17	S	45	LEU
17	S	48	LEU
17	S	60	SER
17	S	74	ASN
17	S	97	VAL
17	S	105	THR
17	S	160	THR
17	S	167	ARG
18	T	65	TYR
18	T	71	SER
18	T	83	ARG
18	T	86	GLU
18	T	120	LYS
18	T	144	GLU
18	T	149	GLN
18	T	150	THR
18	T	154	VAL
18	T	156	TYR
19	U	16	THR
19	U	24	GLU
19	U	29	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	U	55	THR
19	U	75	TYR
19	U	76	LEU
19	U	82	LYS
19	U	96	VAL
20	V	24	ASN
20	V	25	CYS
20	V	71	LYS
20	V	83	LYS
20	V	84	SER
20	V	93	LEU
20	V	104	ASN
21	W	7	SER
21	W	11	THR
21	W	15	THR
21	W	35	ASP
21	W	45	LEU
21	W	59	SER
21	W	83	GLU
21	W	92	LEU
21	W	93	SER
21	W	96	CYS
21	W	105	THR
21	W	106	ASP
21	W	108	ASP
21	W	113	LYS
21	W	134	THR
21	W	198	ARG
22	X	71	THR
22	X	105	VAL
22	X	112	THR
22	X	119	THR
22	X	127	THR
22	X	129	ASP
22	X	133	LEU
23	Y	9	SER
23	Y	24	SER
23	Y	51	ARG
23	Y	56	VAL
23	Y	62	SER
23	Y	74	TYR
23	Y	109	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	Y	111	LEU
24	Z	4	PHE
24	Z	22	LYS
24	Z	40	HIS
24	Z	81	LEU
24	Z	88	ASP
24	Z	92	PHE
24	Z	100	THR
24	Z	105	SER
24	Z	132	SER
25	a	85	ASP
25	a	88	ASP
25	a	104	THR
25	a	131	SER
26	b	5	TRP
26	b	24	ARG
26	b	111	ASP
26	b	129	LYS
26	b	170	LEU
26	b	175	TYR
26	b	197	TYR
26	b	212	LYS
26	b	263	THR
26	b	265	GLU
26	b	321	SER
26	b	323	GLN
26	b	324	LEU
26	b	326	GLU
26	b	332	ARG
26	b	338	LYS
26	b	339	LEU
26	b	342	SER
26	b	362	HIS
26	b	398	LEU
26	b	420	TYR
26	b	421	LEU
26	b	427	TRP
26	b	428	LYS
26	b	430	ASP
26	b	439	LYS
26	b	445	LEU
26	b	484	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	b	499	ARG
26	b	510	ARG
26	b	512	SER
27	c	11	ASN
27	c	16	LEU
27	c	48	THR
27	c	76	GLU
27	c	91	SER
27	c	97	ASP
27	c	99	ASP
28	d	27	LYS
28	d	47	ASP
28	d	64	VAL
28	d	76	SER
28	d	87	ASN
28	d	96	VAL
28	d	98	VAL
28	d	106	THR
29	e	23	ASP
29	e	51	SER
29	e	67	SER
29	e	81	ASP
29	e	91	THR
29	e	126	LEU
30	f	15	SER
30	f	53	TYR
30	f	56	SER
30	f	59	VAL
30	f	78	SER
31	g	10	ARG
31	g	15	THR
31	g	23	VAL
31	g	40	THR
31	g	46	ASP
31	g	47	CYS
31	g	60	ARG
31	g	69	HIS
31	g	74	ARG
31	g	81	CYS
32	h	30	GLU
32	h	64	GLU
32	h	84	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	h	101	THR
33	i	2	THR
33	i	3	VAL
33	i	27	SER
33	i	45	ARG
33	i	70	ARG
33	i	90	MET
34	j	46	SER
34	j	59	THR
34	j	67	LEU
34	j	69	HIS
34	j	71	SER
35	k	3	ARG
35	k	5	ILE
35	k	7	ASP
35	k	10	GLN
35	k	31	LEU
35	k	33	LYS
35	k	39	ARG
35	k	57	ASN
35	k	65	LEU
36	m	22	LEU
36	m	30	TYR
36	m	32	ASP
36	m	94	SER
36	m	96	LEU
36	m	99	THR
36	m	107	LEU
36	m	121	LYS
36	m	132	LEU
36	m	139	ASP
36	m	174	LYS
36	m	175	GLN
36	m	194	TRP
36	m	205	LYS
36	m	211	ILE
36	m	223	ASP
36	m	226	ILE
36	m	232	ARG
36	m	233	ASP
36	m	235	LEU
36	m	247	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	m	278	SER
36	m	287	HIS
36	m	304	ARG
36	m	311	THR
36	m	341	CYS
36	m	353	TRP
36	m	362	ILE
36	m	376	LYS
36	m	390	VAL
36	m	391	GLU
36	m	406	ARG
36	m	418	ILE
36	m	422	LYS
37	p	41	PHE
37	p	48	LYS
37	p	58	SER
37	p	84	ARG
38	r	27	ARG
38	r	54	ARG
38	r	60	SER
38	r	120	VAL
38	r	133	MET
38	r	157	VAL
38	r	164	ARG
38	r	170	ARG
38	r	185	THR
38	r	189	LEU
38	r	192	THR
38	r	202	LYS
38	r	212	LEU
38	r	225	VAL
38	r	232	THR
38	r	250	ASP
38	r	252	ASP
39	u	9	CYS
39	u	25	ASP
39	u	30	ARG
39	u	33	ARG
39	u	52	THR
39	u	65	VAL
39	u	73	GLN
39	u	80	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	u	112	MET
39	u	113	ARG
39	u	132	GLU
39	u	139	VAL
40	v	13	LYS
40	v	26	ASN
40	v	33	ILE
40	v	43	HIS
40	v	56	ASP
40	v	57	MET
40	v	60	PHE
40	v	61	ASN
40	v	72	MET
40	v	121	ASN
40	v	122	PHE
40	v	130	LYS
40	v	133	PHE
40	v	153	VAL
40	v	163	ASP
40	v	175	VAL
40	v	220	ARG
40	v	231	ASP
41	w	12	THR
41	w	33	VAL
41	w	40	ASP
41	w	45	ARG
41	w	72	THR
41	w	73	THR
41	w	80	THR
41	w	86	VAL
41	w	94	ASP
41	w	127	GLU
41	w	151	ASN
41	w	152	LYS
41	w	159	LEU
41	w	160	VAL
41	w	178	THR
42	x	40	ASP
42	x	56	SER
42	x	58	LYS
42	x	71	SER
42	x	78	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	x	90	ASP
42	x	107	LYS
42	x	134	ARG
42	x	151	PHE
42	x	181	THR
42	x	191	CYS
42	x	225	LEU
42	x	241	HIS
42	x	253	SER
42	x	264	ASP
42	x	266	VAL
42	x	272	TYR
42	x	273	THR
42	x	283	CYS
42	x	312	CYS
42	x	322	TRP
42	x	324	ASN
42	x	348	THR
42	x	371	GLU
42	x	392	THR
42	x	399	THR
42	x	402	GLN
42	x	404	LEU
42	x	410	PHE
42	x	415	ARG
42	x	421	SER
42	x	459	LEU
42	x	462	CYS
42	x	463	SER
42	x	475	THR
42	x	480	VAL
42	x	481	ASP
42	x	482	LEU
42	x	514	THR
43	y	74	THR
43	y	77	THR
43	y	78	ASP
43	y	128	LEU
43	y	143	SER
43	y	146	ILE
43	y	165	THR
43	y	166	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	y	175	SER
43	y	182	VAL
43	y	198	VAL
43	y	206	THR
43	y	224	LEU
43	y	235	ASN
43	y	239	THR
44	z	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	38	HIS
1	A	139	HIS
2	B	13	HIS
2	B	231	HIS
2	B	256	HIS
3	C	221	ASN
3	C	296	GLN
3	C	307	GLN
4	D	39	GLN
4	D	45	ASN
4	D	90	HIS
4	D	264	GLN
5	E	80	ASN
5	E	138	GLN
5	E	167	ASN
6	F	172	ASN
6	F	194	HIS
7	G	77	GLN
7	G	95	ASN
8	H	125	ASN
8	H	157	ASN
8	H	183	HIS
9	J	62	ASN
9	J	95	ASN
9	J	132	ASN
10	L	17	HIS
11	M	62	GLN
11	M	126	GLN
12	N	181	ASN
13	O	50	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	Q	73	GLN
16	R	34	GLN
16	R	75	HIS
17	S	89	ASN
17	S	122	HIS
17	S	157	GLN
18	T	54	HIS
19	U	25	ASN
19	U	109	GLN
20	V	4	ASN
20	V	81	GLN
21	W	14	GLN
21	W	74	GLN
21	W	88	ASN
21	W	110	ASN
21	W	148	GLN
22	X	137	ASN
23	Y	4	GLN
24	Z	36	HIS
24	Z	57	HIS
25	a	74	ASN
26	b	89	ASN
26	b	120	GLN
26	b	124	GLN
26	b	280	ASN
26	b	333	ASN
26	b	440	ASN
29	e	88	HIS
29	e	104	ASN
31	g	52	GLN
31	g	61	GLN
32	h	68	GLN
33	i	63	ASN
33	i	91	ASN
34	j	13	ASN
34	j	76	ASN
35	k	10	GLN
36	m	111	ASN
36	m	146	GLN
36	m	175	GLN
38	r	4	ASN
38	r	10	HIS

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Mol	Chain	Res	Type
38	r	14	HIS
38	r	211	GLN
39	u	37	HIS
40	v	29	GLN
40	v	36	GLN
40	v	173	GLN
40	v	213	GLN
40	v	249	HIS
41	w	57	ASN
41	w	59	GLN
41	w	83	GLN
41	w	194	GLN
41	w	195	GLN
41	w	198	ASN
42	x	31	ASN
42	x	154	HIS
42	x	241	HIS
42	x	321	HIS
42	x	401	HIS
43	y	9	ASN
43	y	11	ASN
43	y	33	ASN
43	y	106	ASN
43	y	140	GLN
43	y	168	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	1	2950/3396 (86%)	795 (26%)	58 (1%)
46	2	157/158 (99%)	41 (26%)	2 (1%)
47	3	120/121 (99%)	29 (24%)	1 (0%)
All	All	3227/3675 (87%)	865 (26%)	61 (1%)

All (865) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	1	2	U
45	1	5	G
45	1	7	C
45	1	10	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	11	A
45	1	13	A
45	1	14	U
45	1	15	C
45	1	18	G
45	1	26	A
45	1	40	A
45	1	41	G
45	1	42	C
45	1	43	A
45	1	49	A
45	1	51	A
45	1	59	G
45	1	60	A
45	1	65	A
45	1	66	A
45	1	70	A
45	1	75	G
45	1	76	G
45	1	83	U
45	1	90	C
45	1	91	G
45	1	92	G
45	1	93	C
45	1	94	G
45	1	96	G
45	1	97	U
45	1	98	G
45	1	100	A
45	1	102	C
45	1	103	G
45	1	110	G
45	1	111	C
45	1	116	A
45	1	117	U
45	1	120	G
45	1	121	A
45	1	122	A
45	1	135	C
45	1	136	G
45	1	146	U
45	1	148	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	154	U
45	1	156	G
45	1	157	A
45	1	158	G
45	1	160	G
45	1	161	G
45	1	165	A
45	1	168	U
45	1	170	G
45	1	172	G
45	1	173	G
45	1	187	A
45	1	190	U
45	1	191	U
45	1	206	G
45	1	210	U
45	1	211	A
45	1	213	A
45	1	218	G
45	1	219	A
45	1	239	G
45	1	240	U
45	1	241	G
45	1	243	G
45	1	245	U
45	1	248	U
45	1	249	U
45	1	251	G
45	1	252	U
45	1	254	A
45	1	258	G
45	1	260	C
45	1	261	U
45	1	262	U
45	1	263	C
45	1	269	G
45	1	282	G
45	1	284	A
45	1	295	A
45	1	305	U
45	1	306	A
45	1	307	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	323	A
45	1	329	U
45	1	349	A
45	1	352	A
45	1	368	G
45	1	376	G
45	1	395	A
45	1	398	A
45	1	399	A
45	1	401	U
45	1	402	A
45	1	403	C
45	1	421	G
45	1	422	A
45	1	439	C
45	1	440	A
45	1	495	G
45	1	496	C
45	1	498	A
45	1	516	A
45	1	518	G
45	1	521	A
45	1	535	G
45	1	544	C
45	1	545	U
45	1	547	G
45	1	548	G
45	1	549	U
45	1	550	A
45	1	551	A
45	1	553	U
45	1	555	U
45	1	557	A
45	1	558	U
45	1	559	A
45	1	568	G
45	1	578	A
45	1	579	G
45	1	582	G
45	1	592	A
45	1	603	A
45	1	604	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	611	A
45	1	620	U
45	1	621	A
45	1	643	U
45	1	644	G
45	1	645	A
45	1	646	A
45	1	647	A
45	1	650	C
45	1	660	A
45	1	665	A
45	1	677	A
45	1	681	U
45	1	684	G
45	1	689	U
45	1	690	A
45	1	691	A
45	1	695	C
45	1	705	A
45	1	708	G
45	1	712	G
45	1	715	A
45	1	720	A
45	1	721	G
45	1	722	G
45	1	733	G
45	1	735	A
45	1	736	A
45	1	738	A
45	1	762	U
45	1	765	C
45	1	766	U
45	1	767	U
45	1	777	U
45	1	779	G
45	1	780	A
45	1	781	G
45	1	784	A
45	1	785	G
45	1	806	A
45	1	809	G
45	1	817	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	830	A
45	1	837	A
45	1	849	C
45	1	850	U
45	1	861	C
45	1	870	G
45	1	871	U
45	1	872	U
45	1	874	U
45	1	875	G
45	1	879	U
45	1	884	A
45	1	885	U
45	1	886	C
45	1	896	A
45	1	897	U
45	1	907	G
45	1	908	G
45	1	909	G
45	1	914	A
45	1	916	G
45	1	917	A
45	1	918	C
45	1	921	A
45	1	922	U
45	1	924	G
45	1	925	A
45	1	926	A
45	1	936	A
45	1	937	G
45	1	944	C
45	1	956	U
45	1	958	C
45	1	960	U
45	1	971	G
45	1	974	G
45	1	975	C
45	1	977	C
45	1	978	G
45	1	980	A
45	1	991	G
45	1	993	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	994	G
45	1	995	U
45	1	997	A
45	1	999	G
45	1	1000	C
45	1	1002	A
45	1	1003	A
45	1	1048	A
45	1	1049	C
45	1	1052	U
45	1	1053	A
45	1	1054	A
45	1	1057	A
45	1	1058	U
45	1	1059	G
45	1	1064	A
45	1	1065	A
45	1	1066	G
45	1	1074	U
45	1	1085	A
45	1	1086	C
45	1	1088	U
45	1	1089	G
45	1	1090	G
45	1	1093	A
45	1	1094	U
45	1	1095	U
45	1	1096	U
45	1	1097	G
45	1	1098	A
45	1	1103	A
45	1	1104	G
45	1	1105	A
45	1	1111	U
45	1	1112	A
45	1	1117	G
45	1	1118	C
45	1	1127	G
45	1	1129	A
45	1	1132	C
45	1	1145	G
45	1	1155	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	1159	A
45	1	1160	C
45	1	1173	U
45	1	1174	G
45	1	1180	A
45	1	1181	U
45	1	1186	G
45	1	1189	C
45	1	1192	C
45	1	1196	C
45	1	1197	A
45	1	1198	C
45	1	1199	C
45	1	1200	A
45	1	1201	C
45	1	1203	A
45	1	1204	A
45	1	1206	G
45	1	1209	G
45	1	1212	A
45	1	1220	U
45	1	1222	G
45	1	1227	C
45	1	1237	G
45	1	1241	U
45	1	1242	G
45	1	1244	A
45	1	1245	A
45	1	1262	G
45	1	1263	A
45	1	1264	G
45	1	1271	A
45	1	1272	C
45	1	1278	A
45	1	1280	C
45	1	1286	A
45	1	1287	A
45	1	1301	A
45	1	1302	A
45	1	1303	A
45	1	1304	A
45	1	1305	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	1307	G
45	1	1309	U
45	1	1313	G
45	1	1330	A
45	1	1332	A
45	1	1348	U
45	1	1349	G
45	1	1350	A
45	1	1351	U
45	1	1352	A
45	1	1353	U
45	1	1354	G
45	1	1355	A
45	1	1356	U
45	1	1357	G
45	1	1364	C
45	1	1380	G
45	1	1386	A
45	1	1399	A
45	1	1400	G
45	1	1418	A
45	1	1419	A
45	1	1431	G
45	1	1434	G
45	1	1437	C
45	1	1446	A
45	1	1450	G
45	1	1455	U
45	1	1475	A
45	1	1481	A
45	1	1482	A
45	1	1508	C
45	1	1523	U
45	1	1533	U
45	1	1542	G
45	1	1544	G
45	1	1547	G
45	1	1549	U
45	1	1550	C
45	1	1555	U
45	1	1556	C
45	1	1583	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	1587	A
45	1	1589	A
45	1	1593	A
45	1	1607	U
45	1	1619	A
45	1	1623	G
45	1	1629	U
45	1	1639	C
45	1	1641	U
45	1	1643	A
45	1	1657	C
45	1	1716	U
45	1	1717	U
45	1	1718	G
45	1	1724	U
45	1	1725	C
45	1	1736	G
45	1	1741	A
45	1	1742	U
45	1	1743	G
45	1	1750	A
45	1	1751	G
45	1	1752	A
45	1	1760	A
45	1	1762	C
45	1	1763	U
45	1	1765	U
45	1	1770	G
45	1	1780	G
45	1	1796	G
45	1	1797	A
45	1	1813	A
45	1	1814	A
45	1	1815	U
45	1	1816	A
45	1	1817	G
45	1	1820	U
45	1	1821	U
45	1	1839	A
45	1	1841	A
45	1	1842	A
45	1	1847	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	1849	C
45	1	1851	G
45	1	1866	C
45	1	1867	A
45	1	1872	C
45	1	1874	A
45	1	1878	G
45	1	1880	U
45	1	1881	A
45	1	1886	A
45	1	1906	G
45	1	1907	C
45	1	1909	A
45	1	1926	C
45	1	1953	G
45	1	2094	C
45	1	2101	C
45	1	2102	U
45	1	2112	U
45	1	2113	A
45	1	2116	G
45	1	2121	G
45	1	2122	G
45	1	2131	A
45	1	2136	C
45	1	2137	U
45	1	2138	A
45	1	2139	A
45	1	2140	U
45	1	2143	A
45	1	2144	A
45	1	2145	A
45	1	2158	A
45	1	2163	C
45	1	2169	G
45	1	2170	U
45	1	2174	G
45	1	2185	G
45	1	2194	G
45	1	2195	C
45	1	2196	C
45	1	2197	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2198	A
45	1	2199	G
45	1	2200	U
45	1	2201	G
45	1	2202	C
45	1	2205	U
45	1	2206	G
45	1	2207	A
45	1	2208	A
45	1	2209	U
45	1	2210	G
45	1	2218	G
45	1	2222	A
45	1	2237	C
45	1	2242	A
45	1	2243	A
45	1	2245	C
45	1	2247	G
45	1	2249	G
45	1	2254	U
45	1	2255	A
45	1	2256	A
45	1	2257	C
45	1	2259	A
45	1	2260	U
45	1	2261	G
45	1	2262	A
45	1	2263	C
45	1	2265	C
45	1	2266	U
45	1	2267	C
45	1	2268	U
45	1	2269	U
45	1	2270	A
45	1	2271	A
45	1	2277	C
45	1	2278	C
45	1	2279	A
45	1	2280	A
45	1	2316	G
45	1	2317	A
45	1	2318	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2334	U
45	1	2336	U
45	1	2370	G
45	1	2371	G
45	1	2381	G
45	1	2385	G
45	1	2393	G
45	1	2395	G
45	1	2397	A
45	1	2398	A
45	1	2399	A
45	1	2401	A
45	1	2402	A
45	1	2411	U
45	1	2415	C
45	1	2418	G
45	1	2419	A
45	1	2423	U
45	1	2424	A
45	1	2426	U
45	1	2428	U
45	1	2430	A
45	1	2432	A
45	1	2434	U
45	1	2435	G
45	1	2439	A
45	1	2440	G
45	1	2441	A
45	1	2443	A
45	1	2444	C
45	1	2445	A
45	1	2502	A
45	1	2503	G
45	1	2507	C
45	1	2508	U
45	1	2509	U
45	1	2512	C
45	1	2514	U
45	1	2515	A
45	1	2518	C
45	1	2519	A
45	1	2593	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2594	C
45	1	2599	U
45	1	2600	C
45	1	2601	A
45	1	2602	G
45	1	2606	G
45	1	2607	G
45	1	2613	U
45	1	2614	G
45	1	2615	G
45	1	2621	G
45	1	2622	C
45	1	2623	G
45	1	2625	C
45	1	2626	A
45	1	2632	G
45	1	2635	A
45	1	2637	A
45	1	2639	G
45	1	2641	U
45	1	2643	A
45	1	2644	C
45	1	2645	G
45	1	2648	G
45	1	2649	A
45	1	2651	G
45	1	2652	U
45	1	2653	C
45	1	2654	C
45	1	2655	U
45	1	2656	A
45	1	2657	A
45	1	2659	G
45	1	2668	U
45	1	2669	G
45	1	2672	G
45	1	2674	A
45	1	2676	A
45	1	2677	G
45	1	2685	C
45	1	2686	A
45	1	2687	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2688	U
45	1	2689	A
45	1	2690	G
45	1	2692	A
45	1	2693	C
45	1	2694	A
45	1	2695	A
45	1	2696	A
45	1	2698	G
45	1	2700	G
45	1	2701	U
45	1	2702	A
45	1	2704	A
45	1	2706	G
45	1	2713	U
45	1	2717	U
45	1	2718	U
45	1	2719	U
45	1	2720	G
45	1	2721	A
45	1	2722	U
45	1	2724	U
45	1	2725	U
45	1	2726	C
45	1	2727	A
45	1	2728	G
45	1	2729	U
45	1	2730	G
45	1	2731	U
45	1	2732	G
45	1	2740	A
45	1	2741	C
45	1	2749	G
45	1	2752	U
45	1	2754	G
45	1	2758	A
45	1	2759	U
45	1	2762	A
45	1	2764	C
45	1	2765	C
45	1	2766	U
45	1	2767	U

*Continued on next page...*



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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2768	U
45	1	2770	G
45	1	2771	U
45	1	2772	C
45	1	2773	C
45	1	2777	G
45	1	2788	C
45	1	2789	U
45	1	2793	G
45	1	2795	U
45	1	2796	G
45	1	2797	C
45	1	2798	C
45	1	2800	G
45	1	2801	A
45	1	2802	A
45	1	2806	U
45	1	2807	U
45	1	2809	C
45	1	2810	C
45	1	2811	A
45	1	2817	A
45	1	2818	U
45	1	2819	A
45	1	2820	A
45	1	2821	C
45	1	2822	U
45	1	2823	G
45	1	2824	G
45	1	2825	C
45	1	2826	U
45	1	2834	G
45	1	2837	A
45	1	2838	A
45	1	2842	U
45	1	2845	A
45	1	2846	U
45	1	2847	A
45	1	2849	C
45	1	2853	A
45	1	2857	C
45	1	2858	U

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2859	U
45	1	2861	U
45	1	2863	G
45	1	2864	A
45	1	2866	U
45	1	2867	C
45	1	2868	U
45	1	2869	U
45	1	2870	C
45	1	2872	A
45	1	2874	G
45	1	2875	U
45	1	2876	C
45	1	2877	G
45	1	2878	G
45	1	2879	C
45	1	2880	U
45	1	2887	A
45	1	2889	C
45	1	2894	C
45	1	2898	G
45	1	2899	C
45	1	2920	U
45	1	2923	U
45	1	2925	C
45	1	2926	A
45	1	2929	C
45	1	2930	A
45	1	2933	A
45	1	2935	U
45	1	2936	A
45	1	2944	U
45	1	2945	G
45	1	2947	G
45	1	2950	G
45	1	2951	G
45	1	2952	G
45	1	2953	U
45	1	2954	U
45	1	2955	U
45	1	2956	A
45	1	2957	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	2968	G
45	1	2970	C
45	1	2971	A
45	1	2977	G
45	1	2978	U
45	1	2980	U
45	1	2981	U
45	1	2982	A
45	1	2983	C
45	1	2986	U
45	1	2993	G
45	1	2996	U
45	1	2997	G
45	1	3012	A
45	1	3017	A
45	1	3021	A
45	1	3022	G
45	1	3023	U
45	1	3032	A
45	1	3034	C
45	1	3037	U
45	1	3042	U
45	1	3049	A
45	1	3056	U
45	1	3058	U
45	1	3059	G
45	1	3078	U
45	1	3079	U
45	1	3080	G
45	1	3086	A
45	1	3092	C
45	1	3093	C
45	1	3100	U
45	1	3127	A
45	1	3129	A
45	1	3130	A
45	1	3131	U
45	1	3142	A
45	1	3143	C
45	1	3150	A
45	1	3153	U
45	1	3154	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	3155	U
45	1	3156	U
45	1	3157	U
45	1	3158	G
45	1	3165	A
45	1	3167	A
45	1	3168	A
45	1	3172	A
45	1	3173	G
45	1	3174	A
45	1	3176	G
45	1	3179	U
45	1	3180	A
45	1	3181	C
45	1	3187	A
45	1	3195	U
45	1	3196	U
45	1	3207	U
45	1	3208	G
45	1	3209	A
45	1	3213	A
45	1	3217	C
45	1	3218	A
45	1	3219	G
45	1	3224	G
45	1	3228	C
45	1	3229	G
45	1	3243	A
45	1	3245	A
45	1	3247	G
45	1	3249	C
45	1	3259	U
45	1	3270	U
45	1	3271	G
45	1	3272	C
45	1	3273	A
45	1	3274	A
45	1	3276	G
45	1	3279	A
45	1	3280	U
45	1	3281	U
45	1	3282	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	3286	G
45	1	3287	U
45	1	3289	G
45	1	3294	A
45	1	3295	A
45	1	3304	U
45	1	3313	U
45	1	3314	A
45	1	3316	A
45	1	3317	U
45	1	3319	U
45	1	3320	A
45	1	3328	G
45	1	3334	U
45	1	3335	A
45	1	3341	U
45	1	3342	A
45	1	3345	G
45	1	3350	C
45	1	3351	U
45	1	3352	U
45	1	3353	G
45	1	3355	U
45	1	3356	G
45	1	3359	A
45	1	3363	U
45	1	3369	G
45	1	3375	A
45	1	3378	C
45	1	3381	U
45	1	3382	U
45	1	3383	G
45	1	3386	G
45	1	3389	U
45	1	3396	U
46	2	8	C
46	2	23	U
46	2	25	G
46	2	34	U
46	2	35	C
46	2	51	G
46	2	53	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	2	54	A
46	2	59	A
46	2	62	C
46	2	63	G
46	2	75	G
46	2	76	C
46	2	80	A
46	2	82	U
46	2	83	C
46	2	84	C
46	2	85	G
46	2	86	U
46	2	87	G
46	2	90	U
46	2	95	G
46	2	104	A
46	2	106	C
46	2	111	A
46	2	112	U
46	2	113	U
46	2	124	G
46	2	125	U
46	2	126	A
46	2	127	U
46	2	128	U
46	2	129	C
46	2	138	A
46	2	144	G
46	2	150	G
46	2	151	C
46	2	152	G
46	2	155	A
46	2	157	U
46	2	158	U
47	3	13	A
47	3	18	C
47	3	22	A
47	3	23	A
47	3	33	U
47	3	53	U
47	3	56	A
47	3	65	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	3	66	A
47	3	76	A
47	3	79	A
47	3	81	U
47	3	82	G
47	3	83	U
47	3	86	U
47	3	87	G
47	3	88	G
47	3	89	G
47	3	90	U
47	3	92	A
47	3	93	C
47	3	95	A
47	3	96	U
47	3	98	C
47	3	100	C
47	3	102	A
47	3	104	A
47	3	112	G
47	3	121	U

All (61) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	40	A
45	1	90	C
45	1	96	G
45	1	97	U
45	1	160	G
45	1	169	U
45	1	239	G
45	1	649	A
45	1	720	A
45	1	761	A
45	1	784	A
45	1	849	C
45	1	990	U
45	1	1057	A
45	1	1064	A
45	1	1097	G
45	1	1102	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1	1103	A
45	1	1128	U
45	1	1159	A
45	1	1205	A
45	1	1221	A
45	1	1241	U
45	1	1302	A
45	1	1329	U
45	1	1355	A
45	1	1716	U
45	1	1816	A
45	1	2101	C
45	1	2197	C
45	1	2217	U
45	1	2254	U
45	1	2269	U
45	1	2277	C
45	1	2317	A
45	1	2593	A
45	1	2624	G
45	1	2625	C
45	1	2651	G
45	1	2652	U
45	1	2658	G
45	1	2728	G
45	1	2731	U
45	1	2753	G
45	1	2758	A
45	1	2761	G
45	1	2817	A
45	1	2822	U
45	1	2857	C
45	1	2866	U
45	1	2875	U
45	1	2946	A
45	1	3021	A
45	1	3078	U
45	1	3228	C
45	1	3269	U
45	1	3341	U
45	1	3350	C
46	2	123	G

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Mol	Chain	Res	Type
46	2	127	U
47	3	52	G

## 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](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	GTP	m	501	49	26,34,34	1.30	2 (7%)	32,54,54	1.60	6 (18%)
48	GTP	b	701	-	26,34,34	1.11	1 (3%)	32,54,54	1.69	7 (21%)

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
48	GTP	m	501	49	-	3/18/38/38	0/3/3/3
48	GTP	b	701	-	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	m	501	GTP	C5-C6	-4.44	1.38	1.47
48	b	701	GTP	C5-C6	-3.94	1.39	1.47
48	m	501	GTP	O4'-C4'	-2.01	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	b	701	GTP	PA-O3A-PB	-4.12	118.69	132.83
48	b	701	GTP	PB-O3B-PG	-3.53	120.72	132.83
48	b	701	GTP	C5-C6-N1	3.37	119.89	113.95
48	m	501	GTP	PA-O3A-PB	-3.34	121.35	132.83
48	m	501	GTP	C5-C6-N1	3.24	119.67	113.95
48	m	501	GTP	C8-N7-C5	3.11	108.92	102.99
48	b	701	GTP	C8-N7-C5	3.09	108.88	102.99
48	m	501	GTP	C2-N1-C6	-3.02	119.55	125.10
48	b	701	GTP	C3'-C2'-C1'	3.01	105.51	100.98
48	b	701	GTP	C2-N1-C6	-2.85	119.85	125.10
48	m	501	GTP	PB-O3B-PG	-2.74	123.41	132.83
48	m	501	GTP	C3'-C2'-C1'	2.65	104.97	100.98
48	b	701	GTP	O6-C6-C5	-2.03	120.41	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

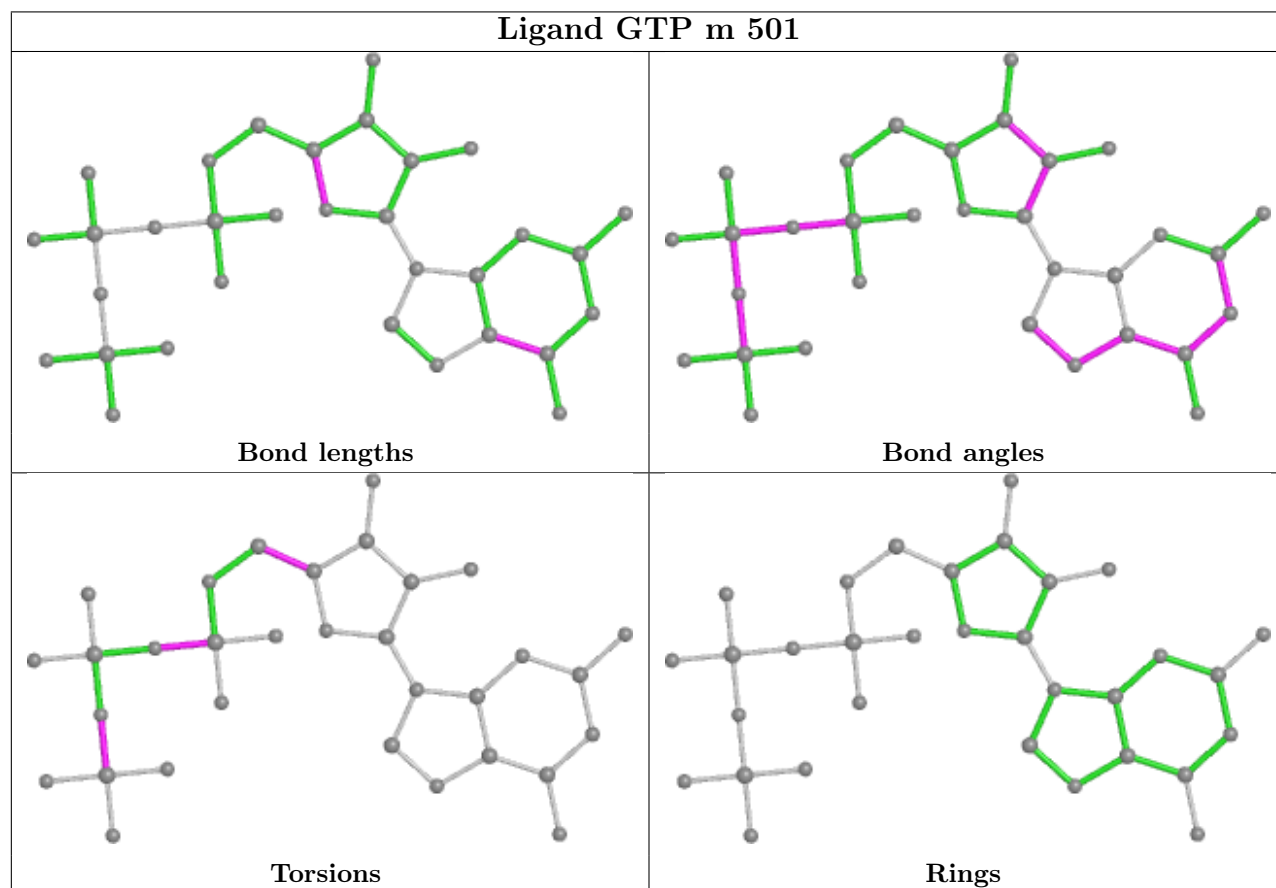
Mol	Chain	Res	Type	Atoms
48	b	701	GTP	C5'-O5'-PA-O3A
48	b	701	GTP	C5'-O5'-PA-O1A
48	m	501	GTP	PB-O3B-PG-O2G
48	b	701	GTP	C4'-C5'-O5'-PA
48	m	501	GTP	O4'-C4'-C5'-O5'
48	m	501	GTP	PB-O3A-PA-O1A

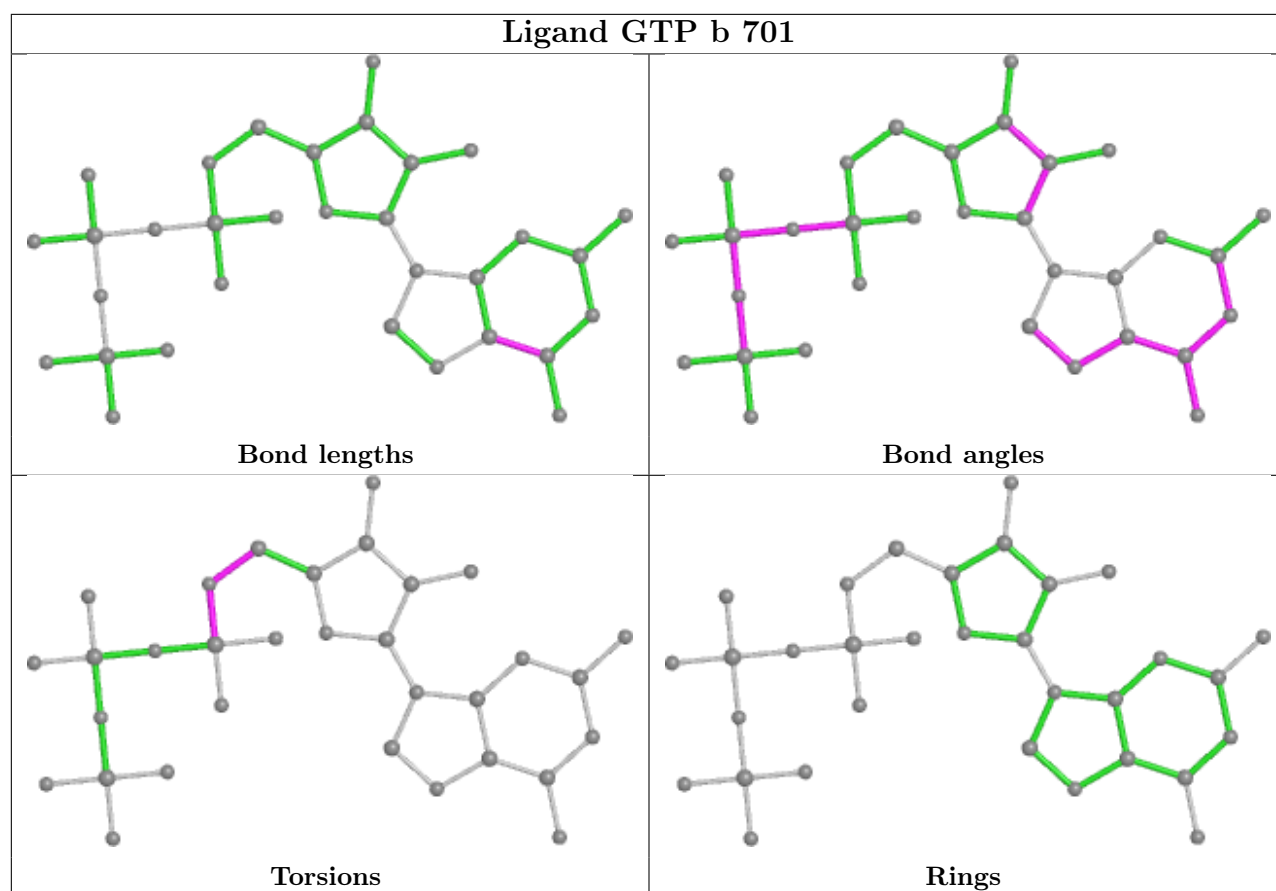
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

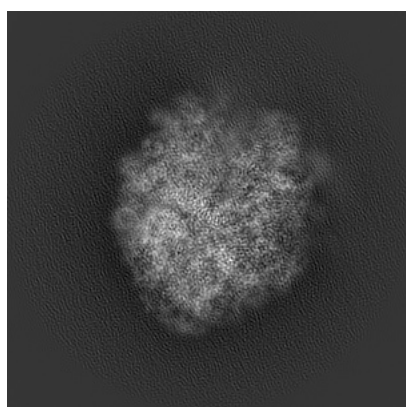
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30170. These allow visual inspection of the internal detail of the map and identification of artifacts.

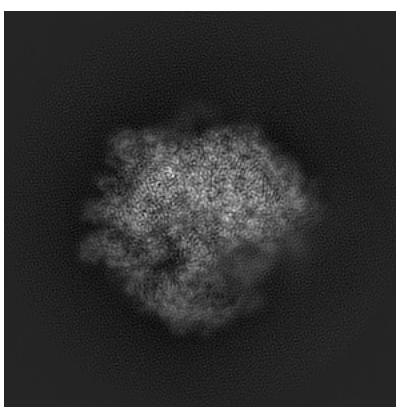
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

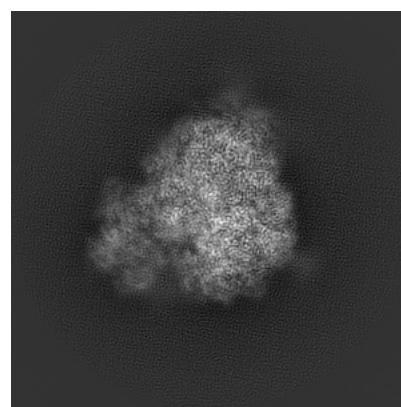
#### 6.1.1 Primary map



X



Y

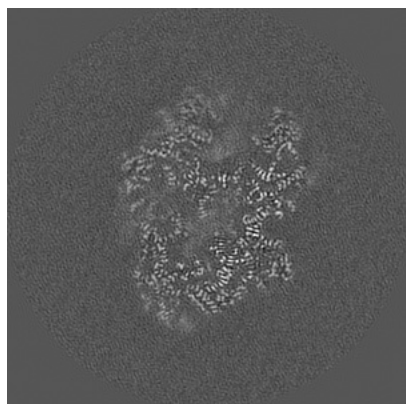


Z

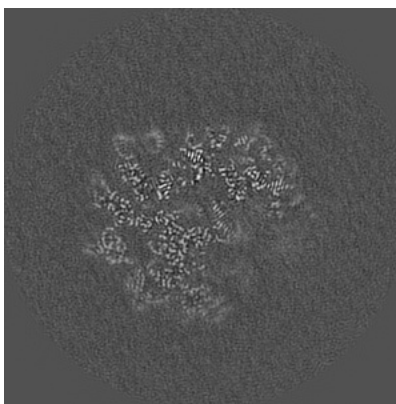
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

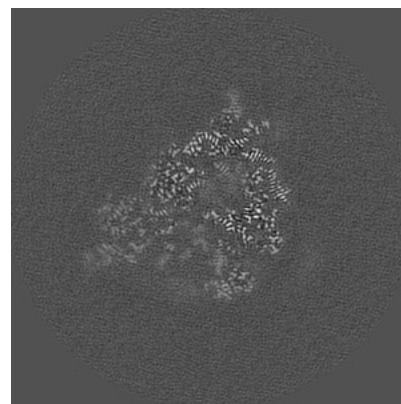
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

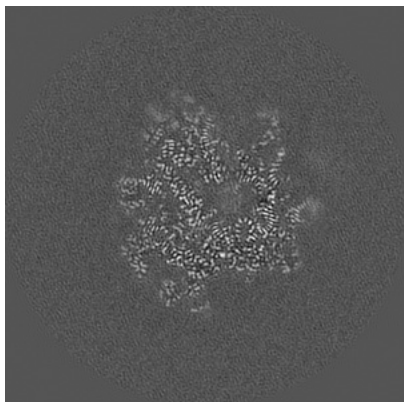


Z Index: 150

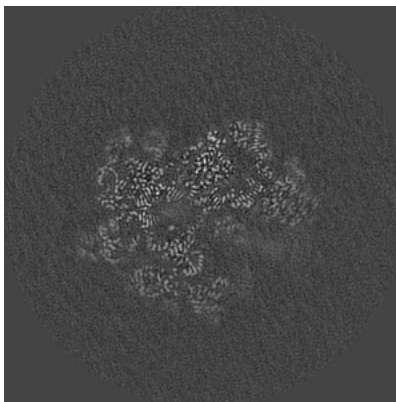
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

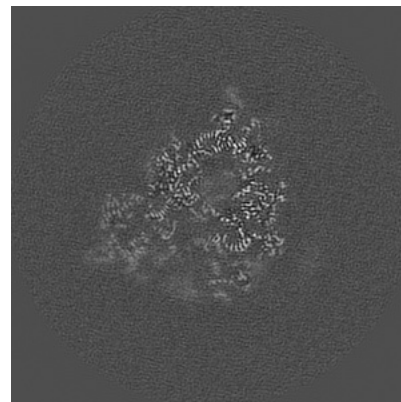
### 6.3.1 Primary map



X Index: 167



Y Index: 143

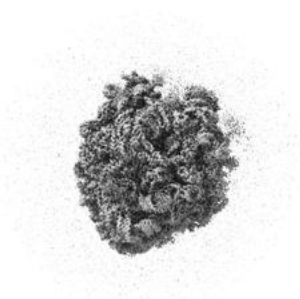


Z Index: 147

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

## 6.4 Orthogonal surface views [i](#)

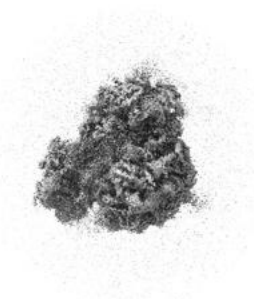
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

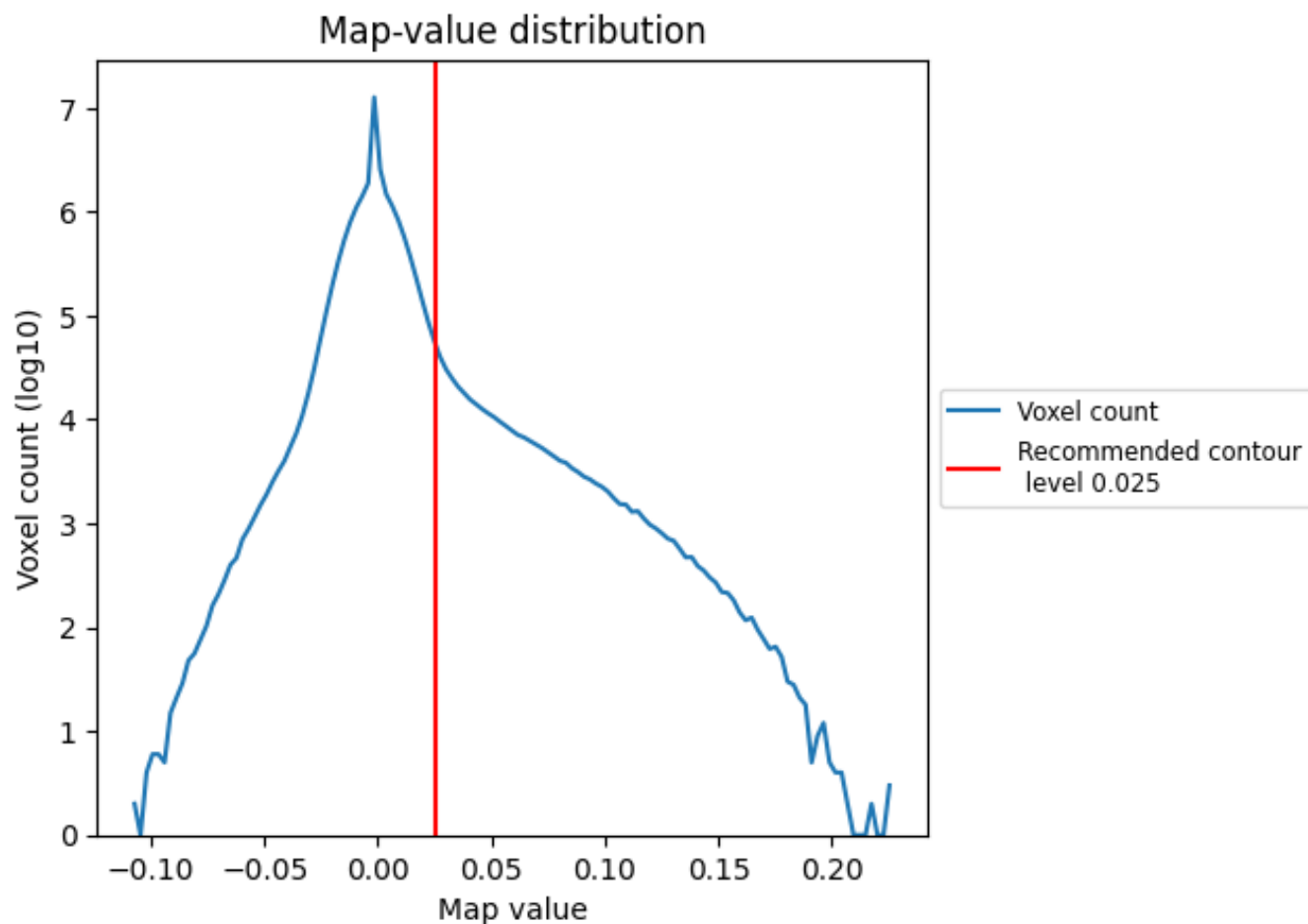
## 6.5 Mask visualisation

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.

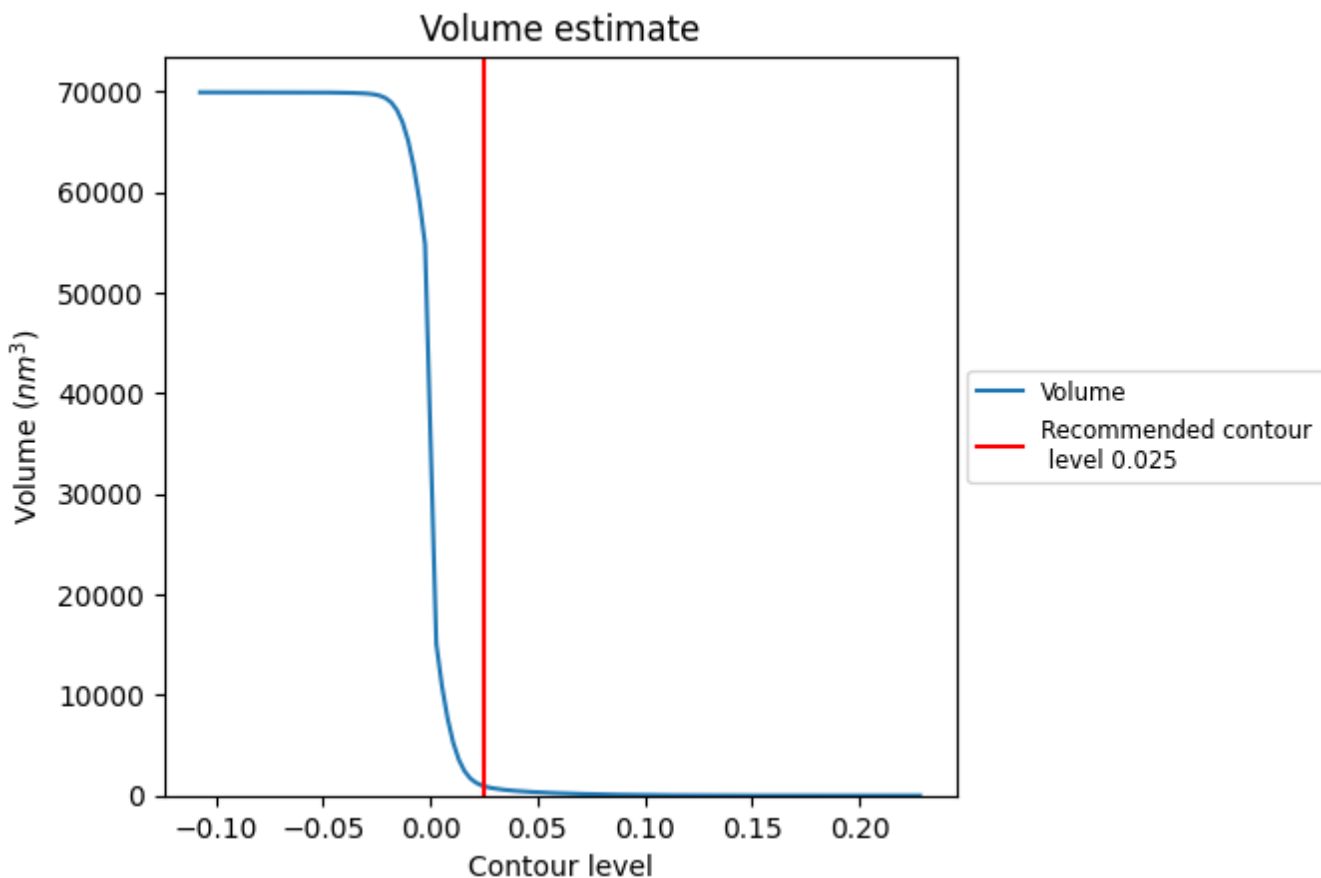
### 7.1 Map-value distribution [i](#)



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.



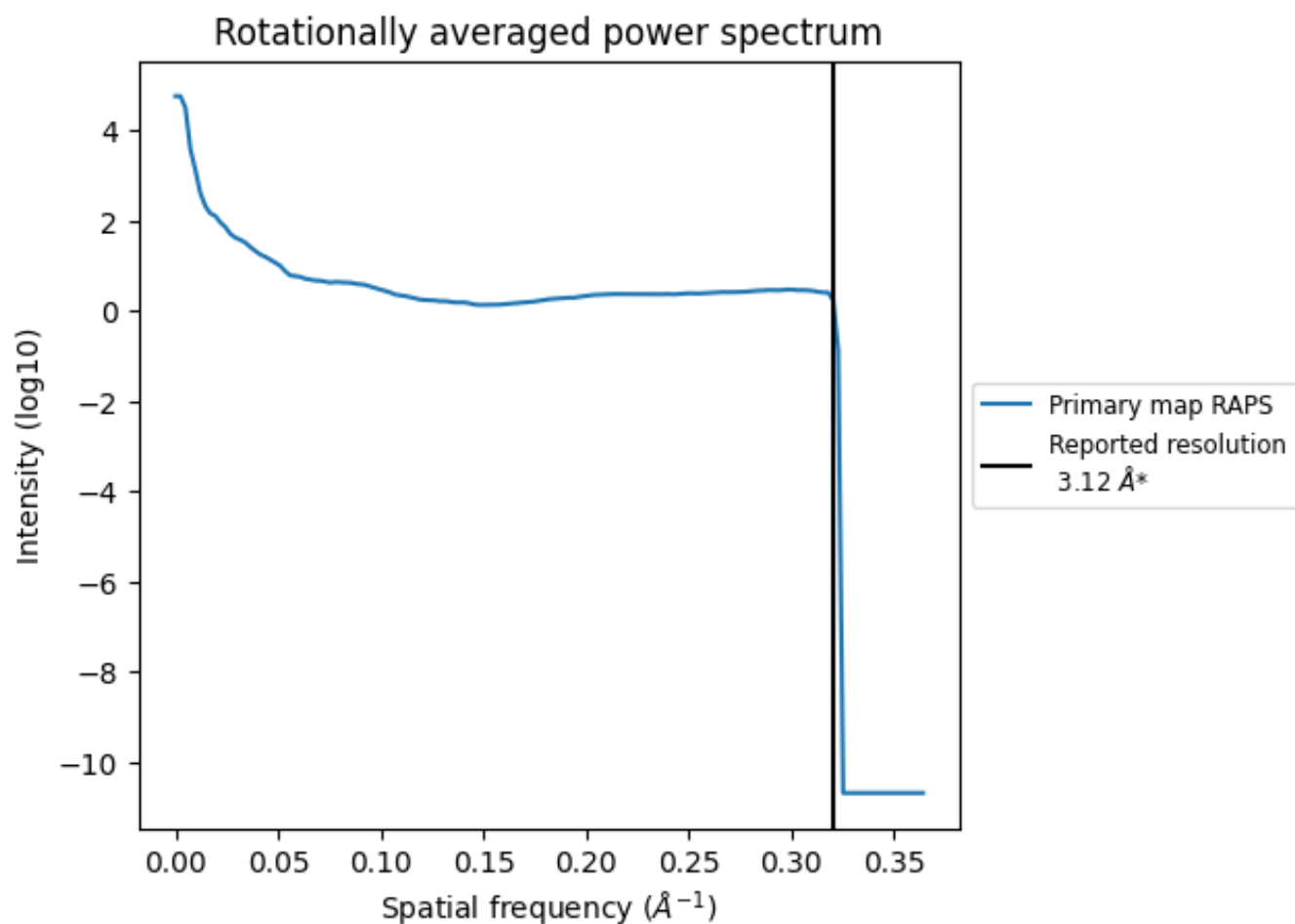
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 945 nm<sup>3</sup>; this corresponds to an approximate mass of 854 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 0.321 Å<sup>-1</sup>

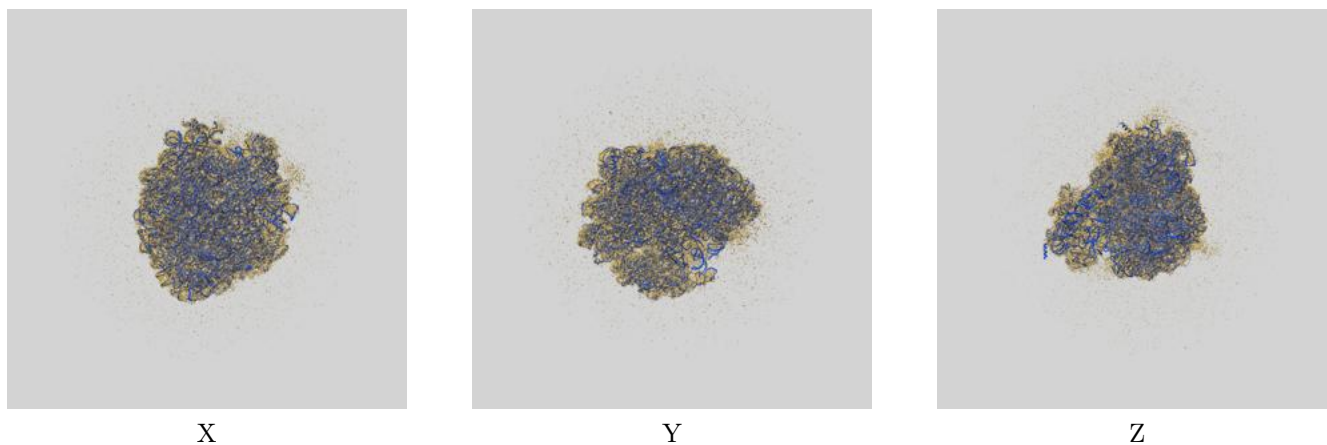
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

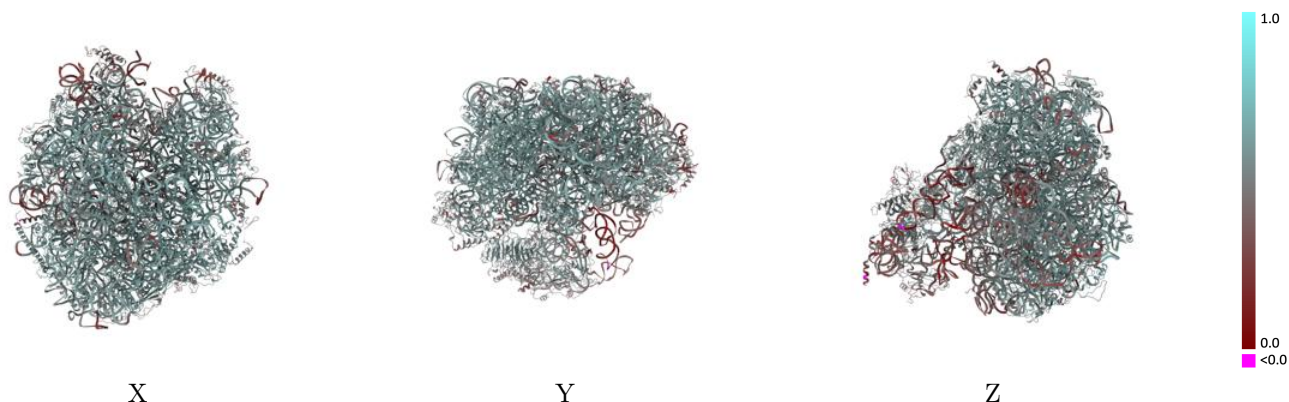
This section contains information regarding the fit between EMDB map EMD-30170 and PDB model 7BT6. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



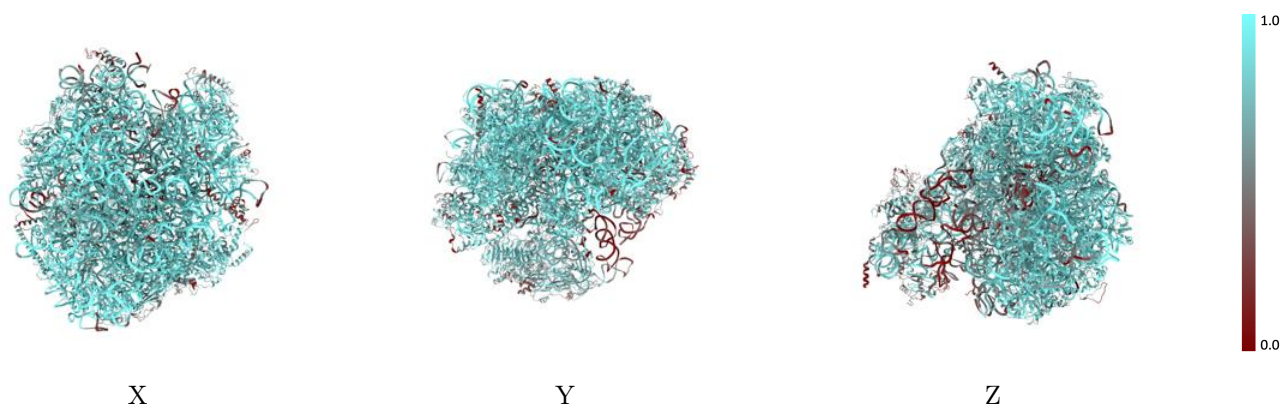
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



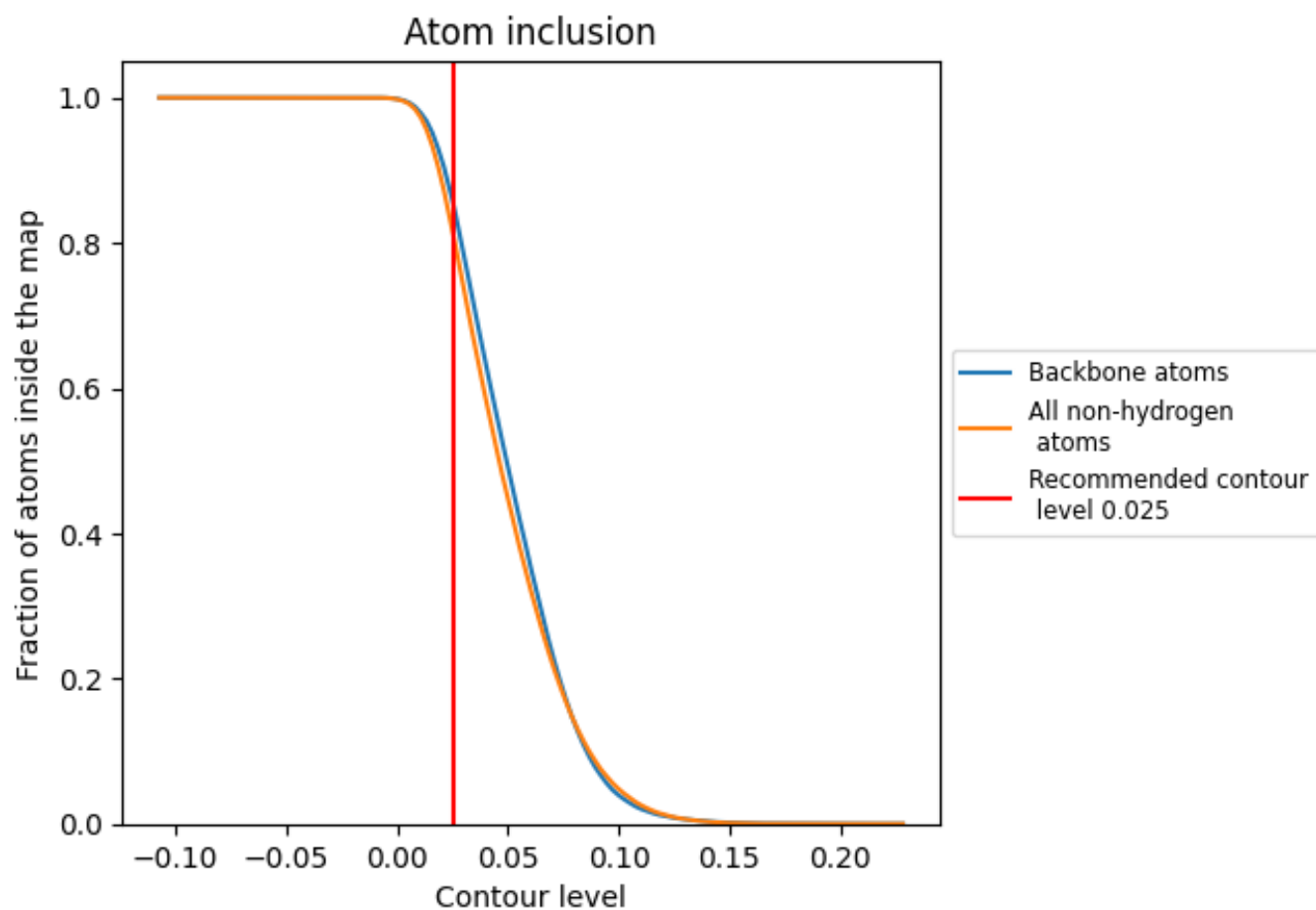
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8162	 0.5330
1	 0.8473	 0.5240
2	 0.8079	 0.5180
3	 0.7553	 0.3910
A	 0.6924	 0.5150
B	 0.8872	 0.5870
C	 0.8569	 0.5820
D	 0.6582	 0.4750
E	 0.8516	 0.5720
F	 0.8961	 0.5880
G	 0.5727	 0.4510
H	 0.8812	 0.5850
J	 0.4791	 0.4120
L	 0.7855	 0.5430
M	 0.8886	 0.5840
N	 0.8362	 0.5600
O	 0.9267	 0.6060
P	 0.7994	 0.5690
Q	 0.8232	 0.5640
R	 0.8686	 0.5890
S	 0.8501	 0.5680
T	 0.6457	 0.5110
U	 0.7882	 0.5340
V	 0.9126	 0.6060
W	 0.6238	 0.4820
X	 0.8178	 0.5580
Y	 0.8798	 0.5870
Z	 0.7180	 0.5060
a	 0.7819	 0.5450
b	 0.7467	 0.5360
c	 0.7565	 0.5280
d	 0.8868	 0.5940
e	 0.8964	 0.6060
f	 0.9342	 0.6170
g	 0.8570	 0.5820



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Chain	Atom inclusion	Q-score
h	 0.7466	 0.5120
i	 0.6309	 0.4790
j	 0.8983	 0.5950
k	 0.7412	 0.5380
m	 0.8287	 0.5650
p	 0.8373	 0.5690
r	 0.8699	 0.5860
u	 0.7945	 0.5660
v	 0.7223	 0.5300
w	 0.6899	 0.5140
x	 0.7227	 0.5150
y	 0.8465	 0.5740
z	 0.5023	 0.5310