



# wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 23, 2017 – 05:00 PM EST

PDB ID : 3JCT  
EMDB ID: : EMD-6615  
Title : Cryo-em structure of eukaryotic pre-60S ribosomal subunits  
Authors : Wu, S.; Kumcuoglu, B.; Yan, K.G.; Brown, H.; Zhang, Y.X.; Tan, D.; Gama-  
linda, M.; Yuan, Y.; Li, Z.F.; Jakovljevic, J.; Ma, C.Y.; Lei, J.L.; Dong, M.Q.;  
Woolford Jr., J.L.; Gao, N.  
Deposited on : 2016-03-09  
Resolution : 3.08 Å (reported)  
Based on PDB ID : 4V88

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

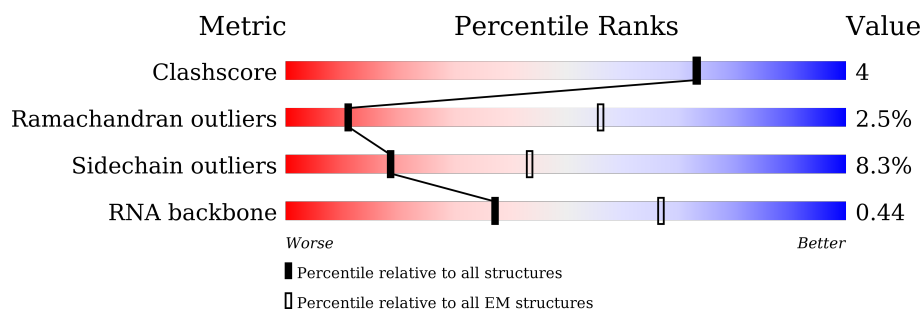
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.08 Å.

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









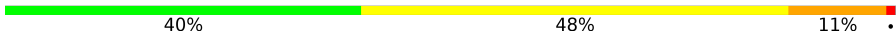




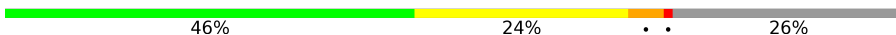




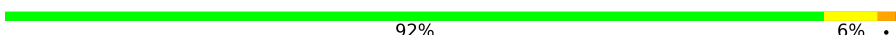








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

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	









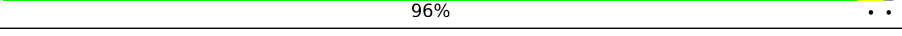

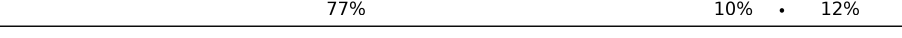
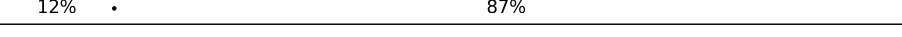

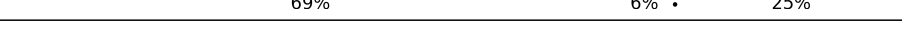


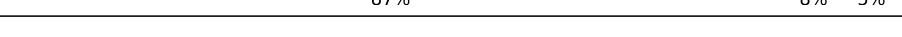

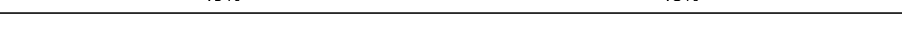






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Mol	Chain	Length	Quality of chain
9	I	166	
10	J	174	
11	K	376	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	W	236	
24	X	142	
25	Y	127	
26	Z	136	
27	a	149	
28	b	647	
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	

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Mol	Chain	Length	Quality of chain
34	h	120	
35	i	100	
36	j	88	
37	k	78	
38	l	51	
39	m	486	
40	n	605	
41	o	220	
42	p	92	
43	q	455	
44	r	261	
45	s	520	
46	t	322	
47	u	199	
48	v	344	
49	w	203	
50	x	515	
51	y	245	
52	z	106	
53	1	3396	
54	2	158	
55	3	121	
56	4	593	
57	5	120	
58	6	232	

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 156562 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
1	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	276	Total	C	N	O	S	0	0
			2211	1397	391	421	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1817	1159	326	329	3		

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

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

- Molecule 9 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 10 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 11 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	256	Total	C	N	O	S	0	0
			2064	1332	342	387	3		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	187	Total	C	N	O	0	0
			1499	934	307	258		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	156	Total	C	N	O	S	0	0
			1258	781	265	212			

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 23 is a protein called Ribosome assembly factor MRT4.

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

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 26 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 27 is a protein called 60S ribosomal protein L28.

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

- Molecule 28 is a protein called Nucleolar GTP-binding protein 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 29 is a protein called 60S ribosomal protein L30.

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

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

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

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

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

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

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 34 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 36 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 37 is a protein called 60S ribosomal protein L38.

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

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 39 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	469	Total	C	N	O	S	0	0
			3774	2381	685	699	9		

- Molecule 40 is a protein called Pescadillo homolog.

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

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

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

- Molecule 42 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 43 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	183	Total	C	N	O	S	0	0
			1514	957	268	288	1		

- Molecule 44 is a protein called Ribosome biogenesis protein NSA2.

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

- Molecule 45 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 46 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 47 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 48 is a protein called Ribosome biogenesis protein RPF2.

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

- Molecule 49 is a protein called Regulator of ribosome biosynthesis.

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

- Molecule 50 is a protein called Ribosome assembly protein 4.

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

- Molecule 51 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 52 is a protein called UPF0642 protein YBL028C.

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

- Molecule 53 is a RNA chain called RDN25-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	3058	Total	C	N	O	P	0	0
			65427	29223	11807	21339	3058		

- Molecule 54 is a RNA chain called RDN58-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 55 is a RNA chain called RDN5-2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 56 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	516	Total	C	N	O	S	0	0
			3999	2530	688	766	15		

- Molecule 57 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

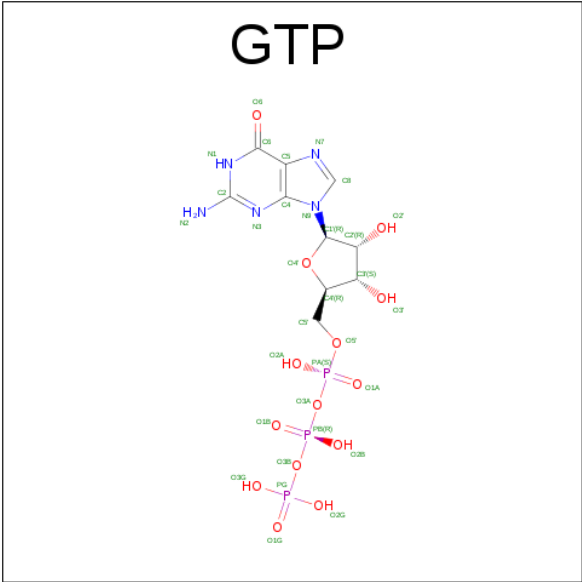
- Molecule 58 is a RNA chain called ITS2-1 miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	p	1	Total	Zn	0
			1	1	
59	j	1	Total	Zn	0
			1	1	
59	I	1	Total	Zn	0
			1	1	
59	u	1	Total	Zn	0
			1	1	

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
60	b	1	Total	C	N	O	P	0
			32	10	5	14	3	
60	m	1	Total	C	N	O	P	0
			32	10	5	14	3	

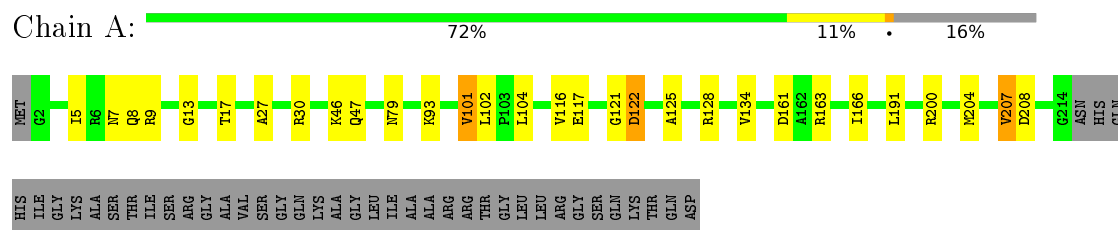
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	b	1	Total	Mg	0
			1	1	
61	m	1	Total	Mg	0
			1	1	

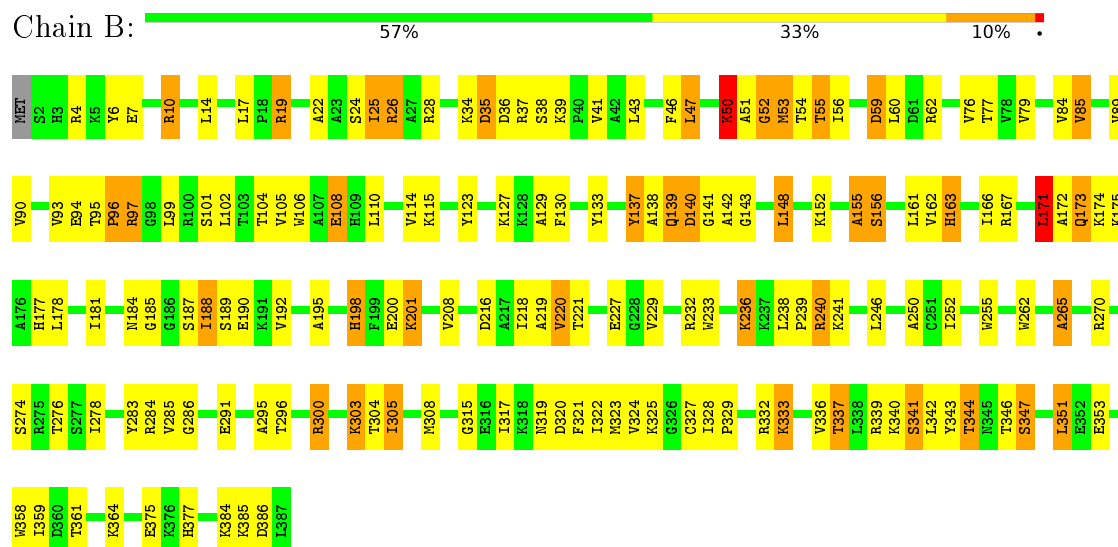
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

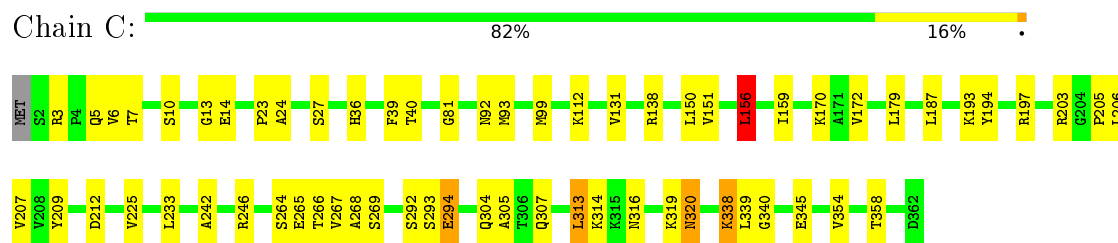
- Molecule 1: 60S ribosomal protein L2-A



- Molecule 2: 60S ribosomal protein L3

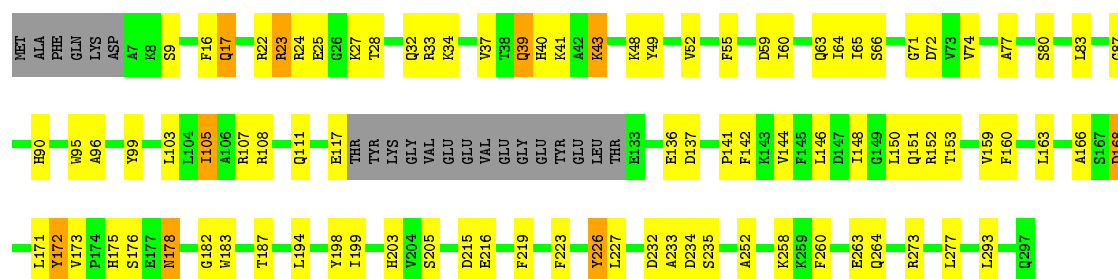


- Molecule 3: 60S ribosomal protein L4-A



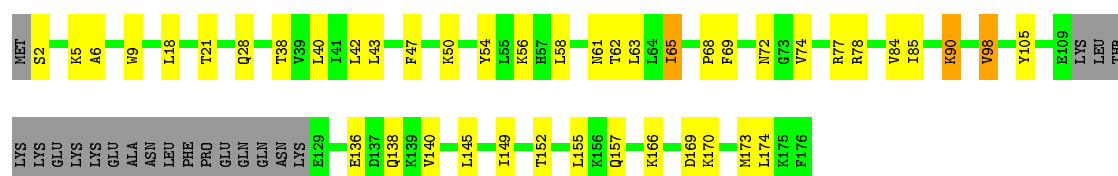
- Molecule 4: 60S ribosomal protein L5

Chain D:  62% 28% 7%



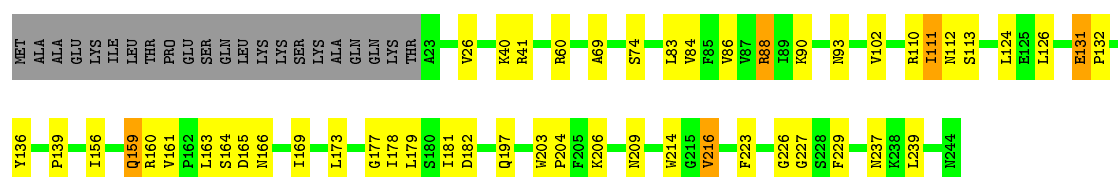
- Molecule 5: 60S ribosomal protein L6-A

Chain E:  64% 23% • 11%



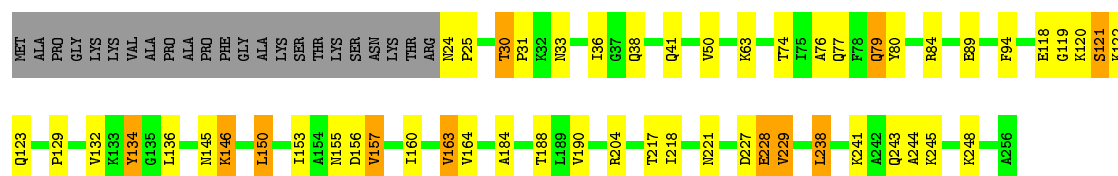
- Molecule 6: 60S ribosomal protein L7-A

Chain F:  70% 19% 9%



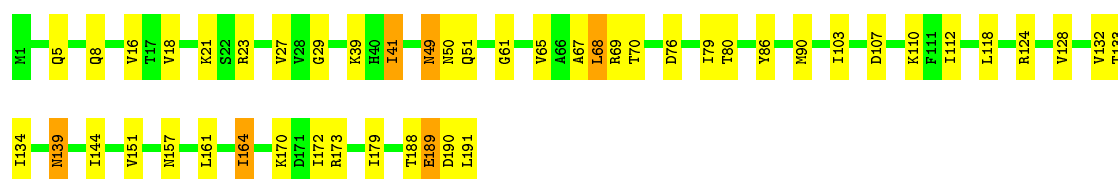
- Molecule 7: 60S ribosomal protein L8-A

Chain G:  70% 17% 9%




- Molecule 8: 60S ribosomal protein L9-A

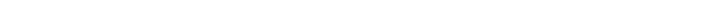
Chain H:  75% 22% .





- Chain M:  80% 19%

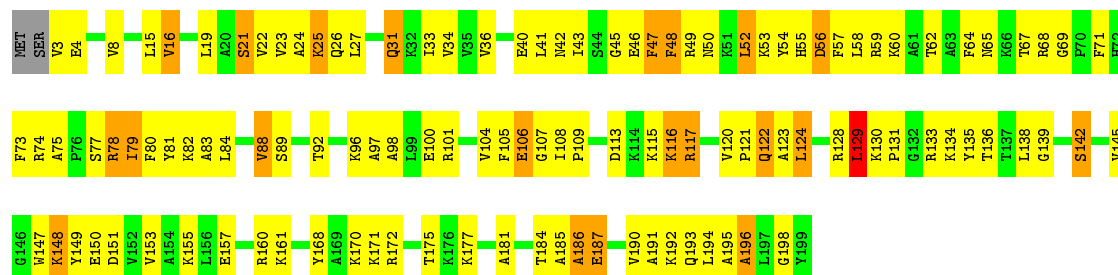
- Molecule 14: 60S ribosomal protein L15-A

Chain N:  88% 11%



- Molecule 15: 60S ribosomal protein L16-A

Chain O:  40% 48% 11%



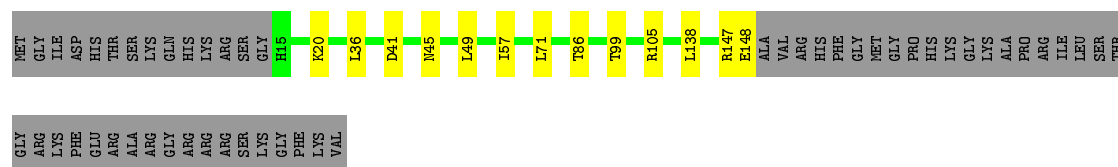
- Molecule 16: 60S ribosomal protein L17-A

Chain P:  88% 11% ..



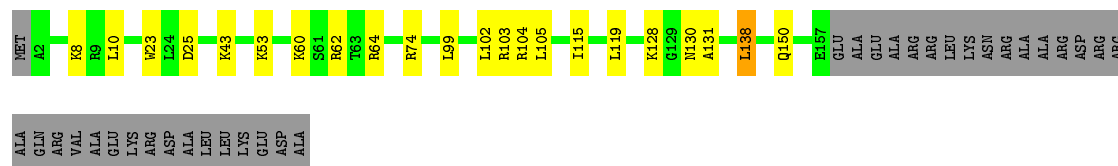
- Molecule 17: 60S ribosomal protein L18-A

Chain Q:  65% 7% 28%



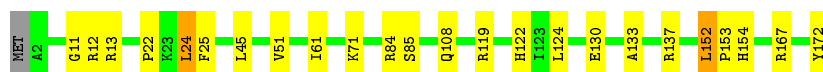
- Molecule 18: 60S ribosomal protein L19-A

Chain R:  71% 11% • 17%

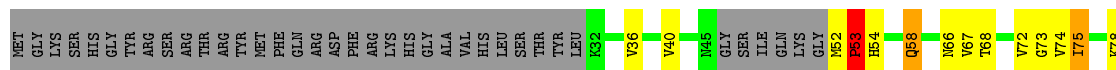


- Molecule 19: 60S ribosomal protein L20-A

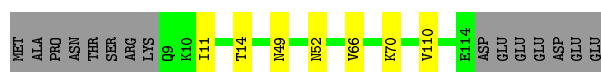
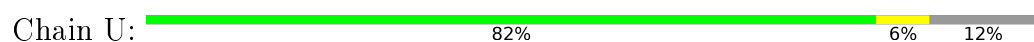
Chain S:  85% 13% .



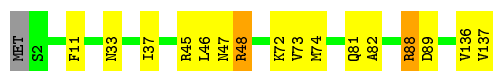
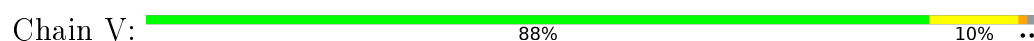
- Molecule 20: 60S ribosomal protein L21-A



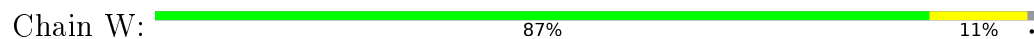
- Molecule 21: 60S ribosomal protein L22-A



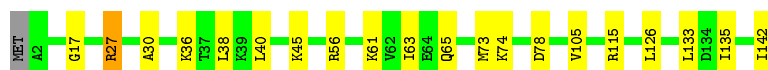
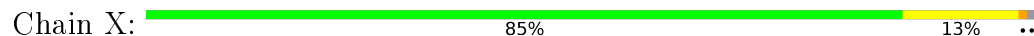
- Molecule 22: 60S ribosomal protein L23-A



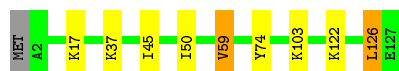
- Molecule 23: Ribosome assembly factor MRT4



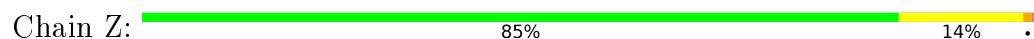
- Molecule 24: 60S ribosomal protein L25



- Molecule 25: 60S ribosomal protein L26-A



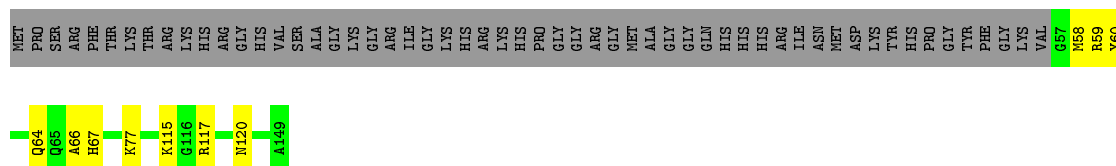
- Molecule 26: 60S ribosomal protein L27-A





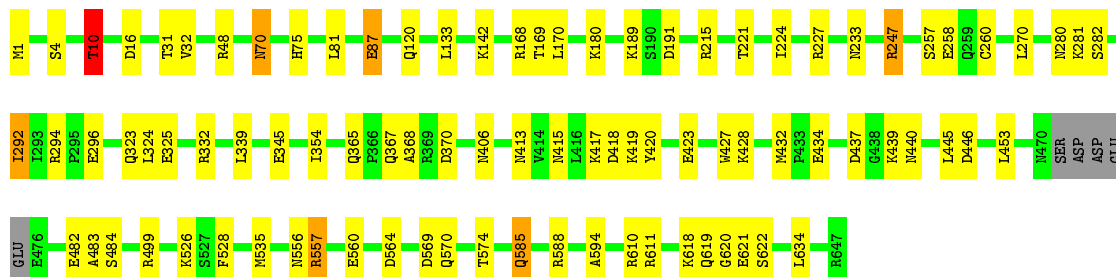
- Molecule 27: 60S ribosomal protein L28

Chain a: 56% 7% 38%



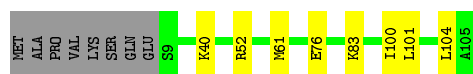
- Molecule 28: Nucleolar GTP-binding protein 1

Chain b: 85% 13% ..



- Molecule 29: 60S ribosomal protein L30

Chain c: 85% 8% 8%



- Molecule 30: 60S ribosomal protein L31-A

Chain d: 83% 11% 5%



- Molecule 31: 60S ribosomal protein L32

Chain e: 92% 6% .

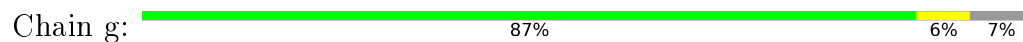


- Molecule 32: 60S ribosomal protein L33-A

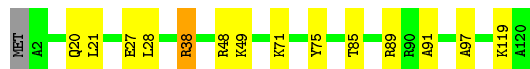
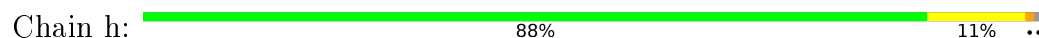
Chain f: 93% 5% ..



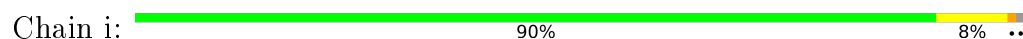
- Molecule 33: 60S ribosomal protein L34-A



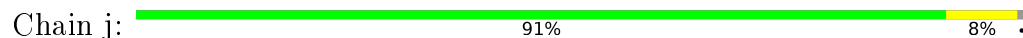
- Molecule 34: 60S ribosomal protein L35-A



- Molecule 35: 60S ribosomal protein L36-A



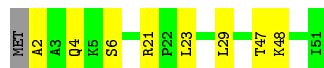
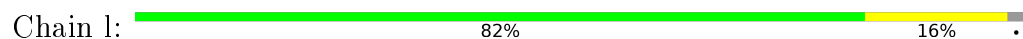
- Molecule 36: 60S ribosomal protein L37-A



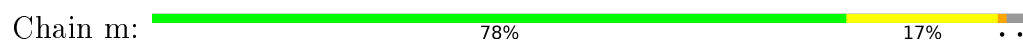
- Molecule 37: 60S ribosomal protein L38

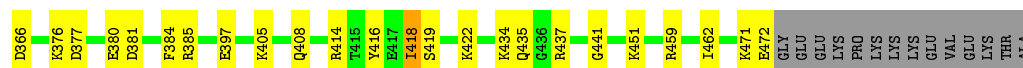


- Molecule 38: 60S ribosomal protein L39



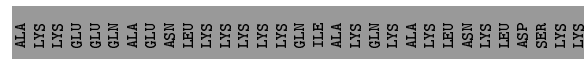
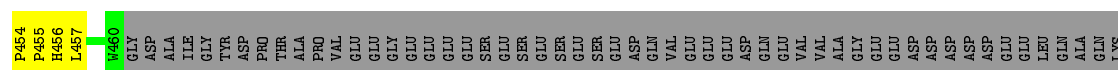
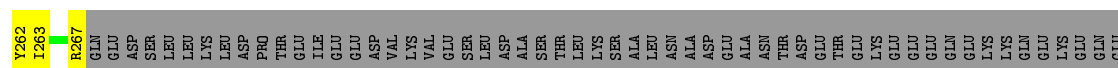
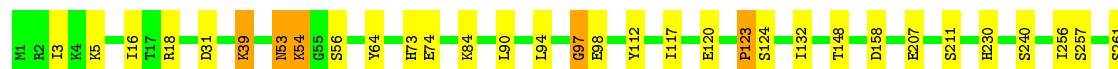
- Molecule 39: Nucleolar GTP-binding protein 2





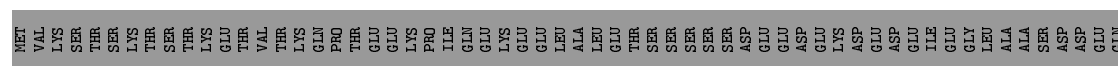
- Molecule 40: Pescadillo homolog

Chain n:  53% 8% 39%



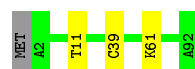
- Molecule 41: Ribosome biogenesis protein 15

Chain o: 



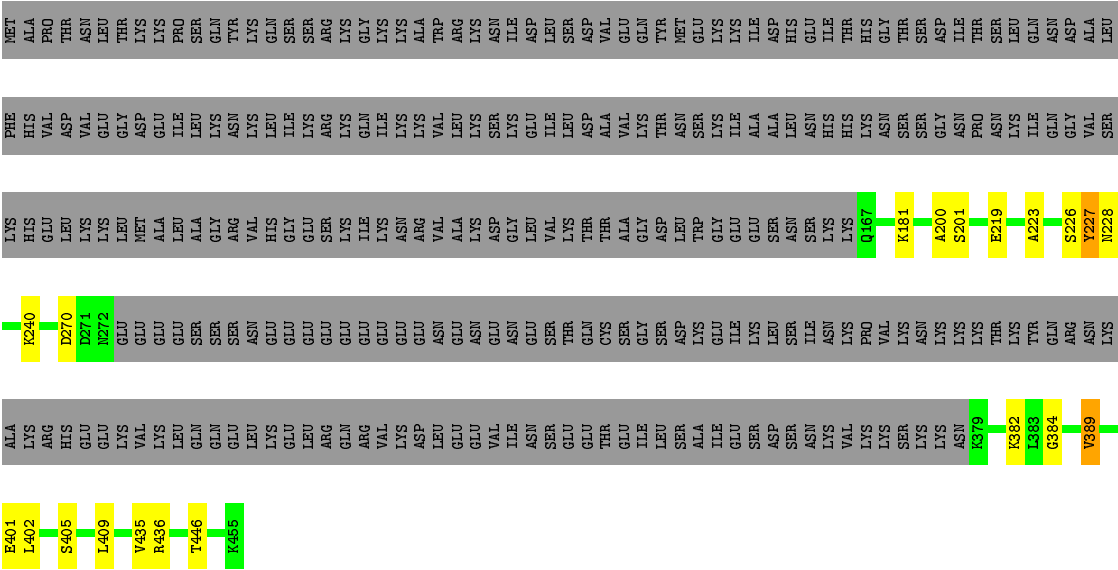
- Molecule 42: 60S ribosomal protein L43-A

Chain p:  96%

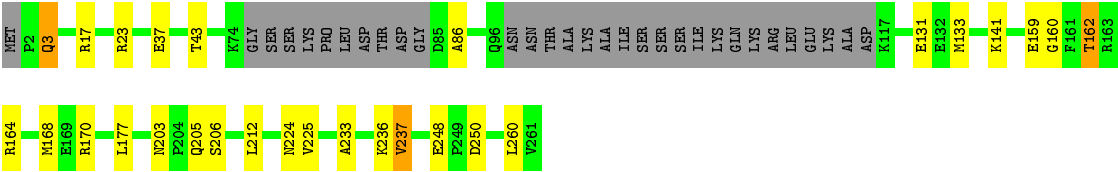


- Molecule 43: Ribosome biogenesis protein NOP53

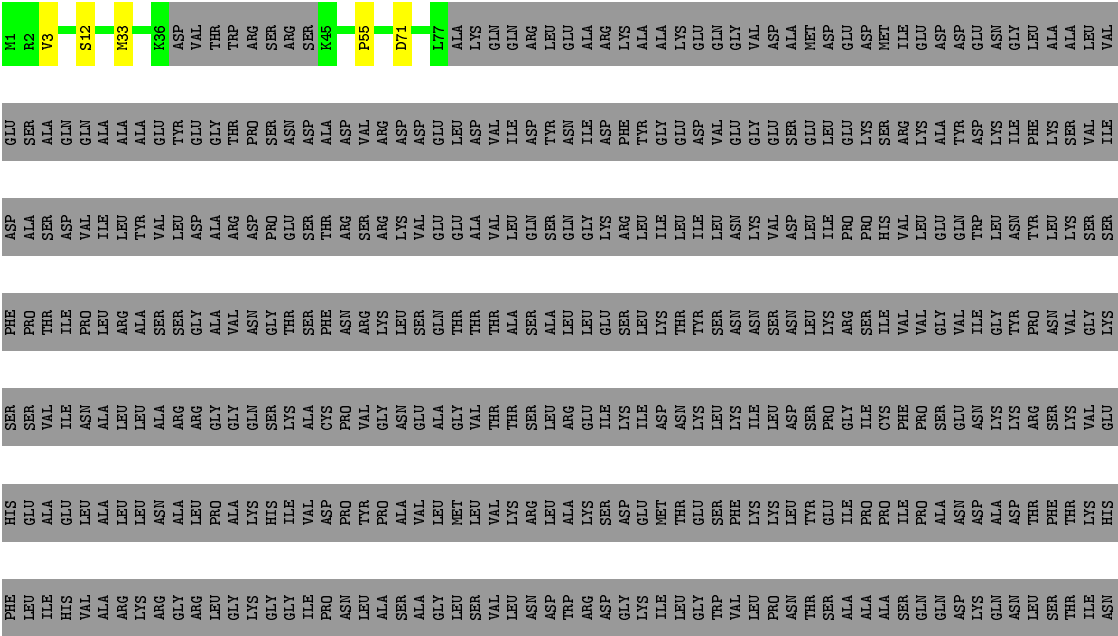
Chain q:  36% . 60%



• Molecule 44: Ribosome biogenesis protein NSA2

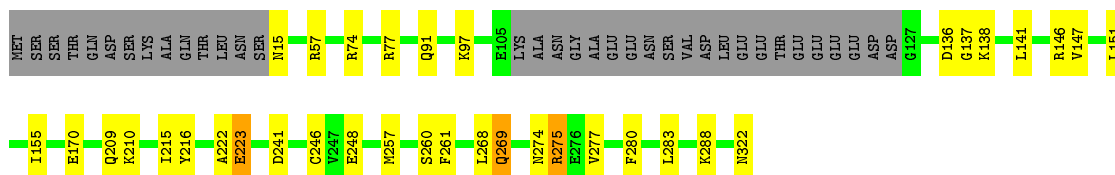


• Molecule 45: Nuclear GTP-binding protein NUG1



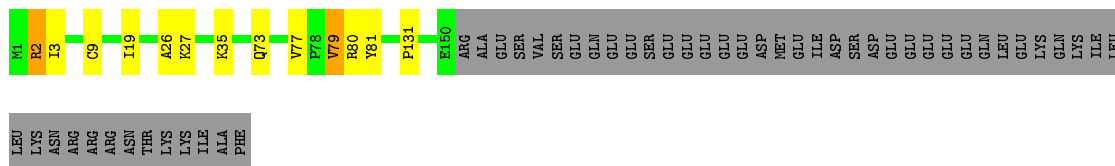
- Molecule 46: Ribosome biogenesis protein RLP7

Chain t:  78% 10% 11%

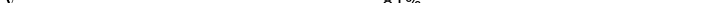


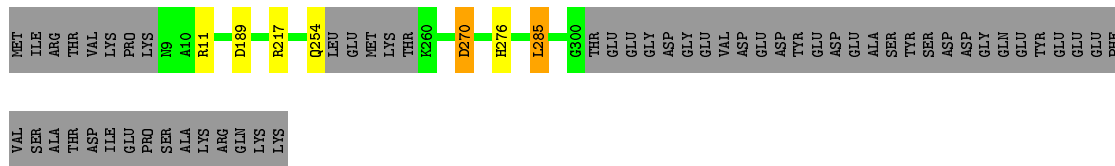
- Molecule 47: Ribosome biogenesis protein RLP24

Chain u:  69% 6% • 25%



- Molecule 48: Ribosome biogenesis protein RPF2

Chain v:  81% .. 17%



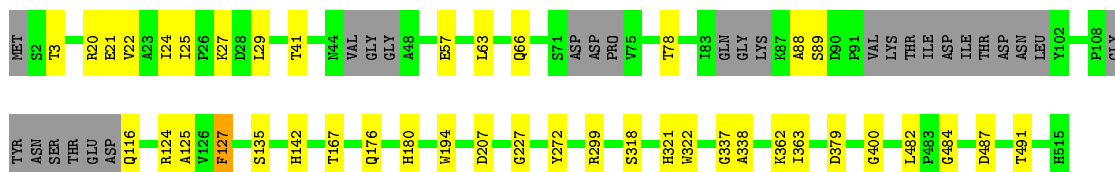
- Molecule 49: Regulator of ribosome biosynthesis

Chain w:  81% 7% • 10%



- Molecule 50: Ribosome assembly protein 4

Chain x:  87% 8% 5%



- Molecule 51: Eukaryotic translation initiation factor 6

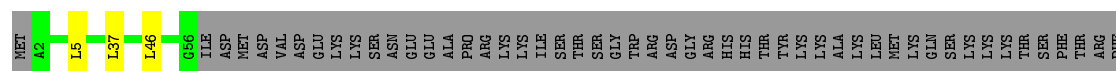


Chain y:  92% 8%



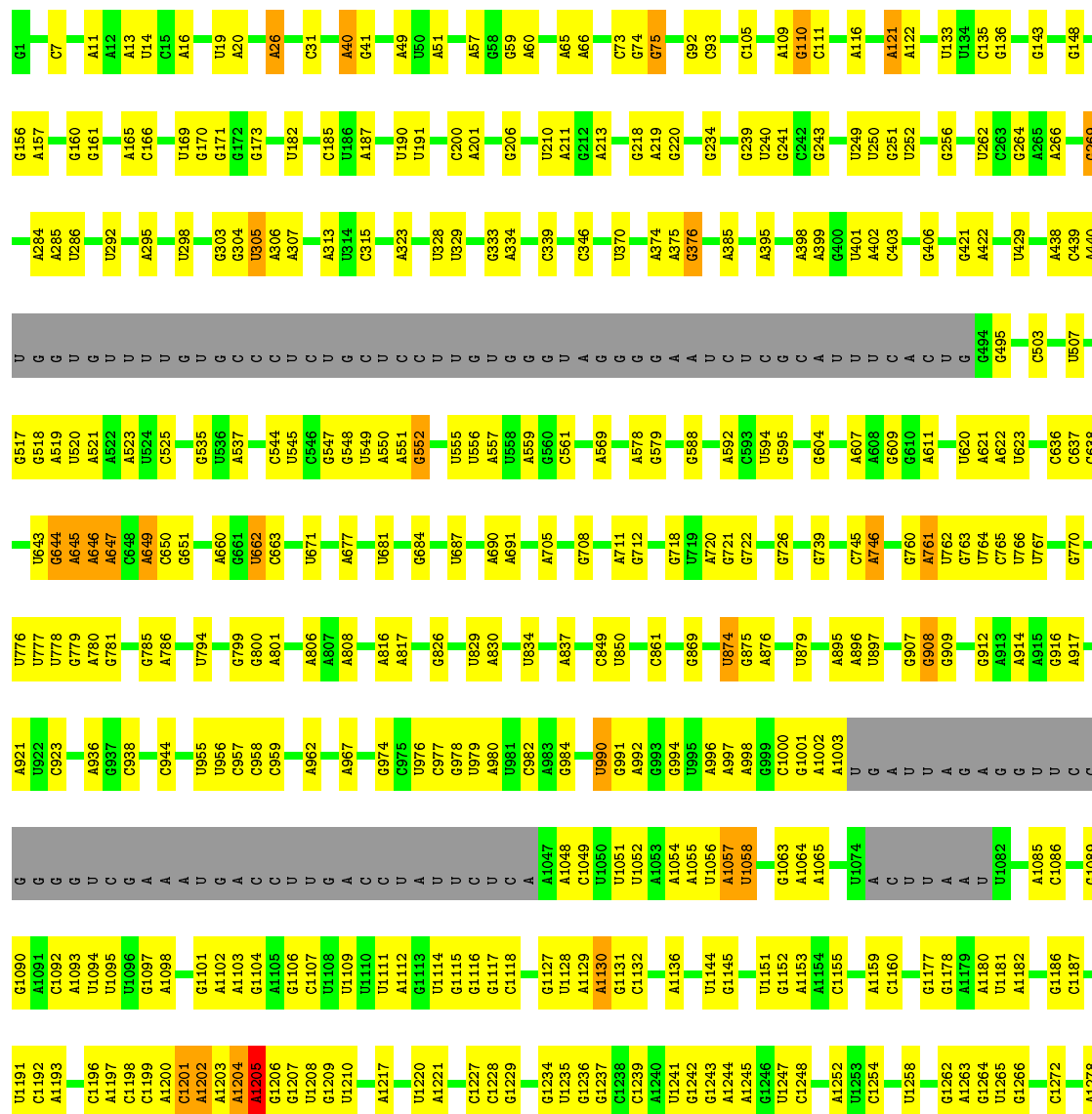
- Molecule 52: UPF0642 protein YBL028C

Chain z:  49% 0% 48%

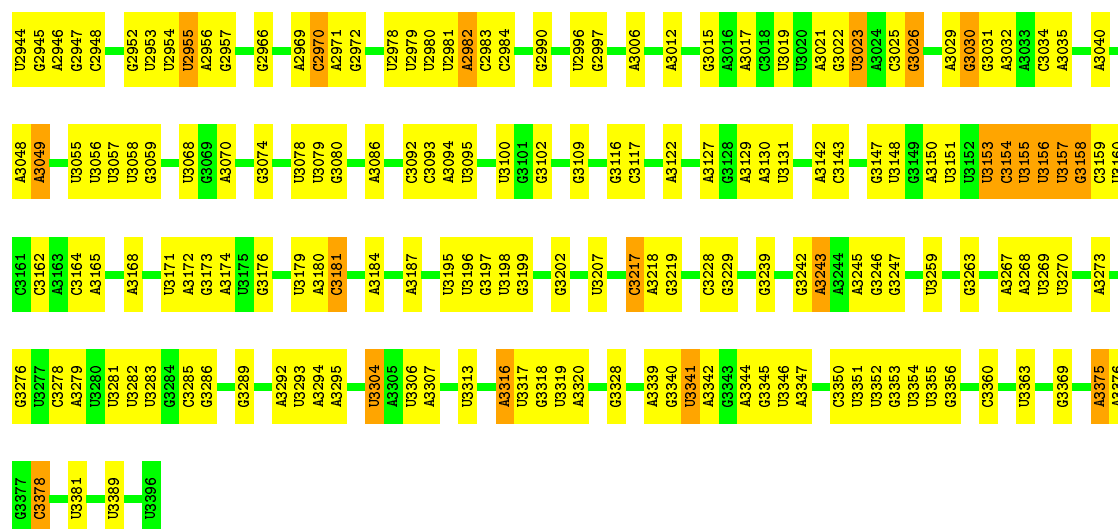


- Molecule 53: RDN25-1 rRNA

Chain 1:  59% 27% 10%

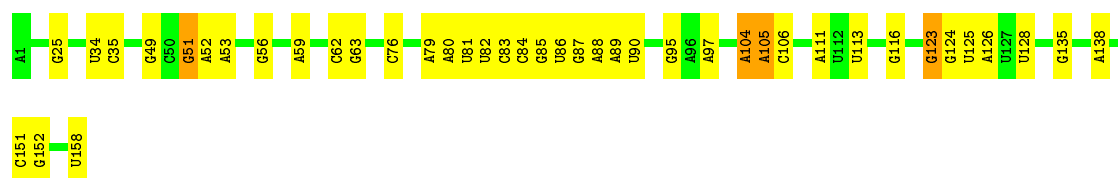


U2846	C2764	U2688	C2583	A2502	G2437	C	C2245	U2137	G	C1866	G1718	A1566	C1420	C1279
A2847	C2765	A2689	C2586	G2503	C2444	A	G2246	U2140	G	A1867	U1721	U1567	G1421	C1280
G2848	U2766	A2690	G2586	U2504	A2445	U	C2247	U2141	A	U1568	U1569	U1568	G1434	G1281
C2857	U2767	A2691	G2586	U2505		U	C2248	A2142	G	U1570	U1724	U1569	U1435	G1282
U2858	A2768	C2693	A2593	C2506	A	A	G2249	A2143	G	A1571	C1725	U1570	C1436	C1283
U2859	G2770	A2694	C2594	U2507	G	G	G2250	A2144	U	U1572	A1741	U1572	C1437	A1286
U2860	U2771	A2695	A2595	U2508	A	A	A2252	A2145	C	U1573	U1746	C1573	G1443	A1287
U2861	C2772	A2696	U2596	U2509	G	G	A2255	C2146	A	C1574	U1746	C1574	G1443	C1296
U2862	C2773	A2697	U2597	C2512	G	G	A2256	G2150	G	A1575	U1746	A1575	G1447	U1299
U2863	C2774	G2698	U2598	U2513	G	U	G2257	G2151	C	G1576	A1750	G1576	G1447	U1299
A2864		G2699	U2599	U2514	U	U	U2258	A2158	U	G1577	G1751	U1577	G1450	A1302
U2865	G2777	U2701	C2600	U2515	G	G	A2259		C	A1580		A1580	A1460	A1303
U2866	G2778	U2702	A2601	A2516	U	A	U2260	C2163	U	C1581	C1759	C1581	A1460	A1304
C2867	A2779	A2703	G2602		U	G	G2261	A2164	G	A1582	A1760	A1582	A1467	
U2868		A2704	G2607	A2522	A	A	A2262	G2169	U	A1583	C1762	A1583	U1471	G1307
G2869	A2785	G2705	G2607	A2523	U	U	A2263	U2170	A	A1587	U1763	A1587	U1471	A1308
G2870	G2786	U2706	G2607	A2524	A	A	U2264		G	U1588	U1764	U1588	A1481	G1313
G2871	G2787	C2707	G2614	A2525	A	A	U2268	G2177	A	A1589	G1766	A1589	A1482	U1322
U2872	U2788	U2712	G2615	C2526	G	G	U2269	U2184	C	A1593	G1770	A1593	G1483	U1329
G2873	U2789	G2713	C	U2528	U	A	A2270	G2185	U	U1606	G1775	U1606	G1485	A1330
G2874	G2790	G2714	U	A2529	U	A	A2271	G2185	U	U1607	G1775	U1607	G1487	A1331
G2875	G2791	A2715	G	U2530	G	G	A2272	U2190	C	C1608		C1608	U1332	
C2876	A2792	U2716	G2619	C2531	G	G	G2273	U2191	U	U1620	G1780	U1620	A1490	U1348
G2877	G2793	U2717	G2620	U2532	G	G	U2274	C2192	C	A1621	G1780	A1621	C1502	A1350
G2878	G2794	U2718	C2621	G2533	A	A	A2275	U2193	U	U1622	G1780	U1622	A1503	U1351
C2879	U2795	U2719	G2622	G2534	G	G	G2276	U2194	U	U1629	G1794	U1629	C1508	U1352
	G2796	G2720	G2623	U2538	C	C	C2277	C2195	G	U1630	U1795	U1630	U1523	U1353
A2887	G2797	A2721	G2624	U2539	U	U	C2278	C2196	C	A1632	G1796	A1632	A1524	G1354
C2888	U2798	U2722	C2625	C2539	C	C	A2279	C2197	U	U1639	U1797	U1639	U1525	A1355
C2889	G2800	U2723	A2626	U2540	U	U	A2280	U2198	A	G1640	U1810	G1640	U1526	U1356
U2890	A2801	U2724	G2645	C2541	G	G		A2198	C	U1641	A1813	U1641	C1527	G1362
	A2802	U2725	U2645	U2542	C	C		G2201	A	A1814	U1815	A1814	C1531	G1367
G2898	A2803	C2726	U2650	U2543	G	G		U2205	A	U1816	U1817	A1816	U1532	G1380
C2899	A2804	G2727	G2651	U2544	C	C		G2206	A	A1642	G1817	A1642	U1533	A1381
A2900		G2728	U2652	C2545	C	C		U2207	U	A1643		A1643	A1539	G1383
G2901		U2729	C2653	C2546	U	U		G2208	A	C1644	U1820	C1644	U1549	A1386
A2902		G2730	U2654	U2547	G	G		U2209	C	U1645	U1821	U1645	C1657	G1387
		U2731	C2655	C2548	U	U		G2210	C		C1822		G1536	A1399
G2918		G2732	U2656	U2549	G	G		U2211	C		U1837	G1658	A1554	U1555
		A2740	A2657	G2549	A	A			A		G1838	G1658	C1557	G1400
C2921	G2814	U2817	G2658	C2552	A	A			C		U1839	G1662	U1701	G1404
G2922	G2815	A2818	U2659	U2553	A	A			C		U1840		U1703	G1404
U2923	U2816	G2752	G2663	G2554	U	U			C				U1716	G1414
U2924	A2748	G2753	G2667	A2561	C	C			C				C1562	
C2925	G2749	G2754	A2674	C2568	A	A			C					
A2926	U2822	C2755	G2677	A2569	U	U			C					
C2927	G2823	G2756	U2677	U2570	A	A			C					
C2928	U2824	G2757	A2680	U2571	C	C			C					
C2929	C2825	U2758	U2681	C2572	U	U			C					
U2935	U2826	U2759	G2685	G2573	U	U			C					
A2936	C2836	U2760	A2685	U2574	U	U			C					
		G2840	A2686	G2575	U	U			C					
U2940	G2841	G2761	C2687	C2576	A	A			C					
C		A2762		U2578	U	U			C					
G2943	G2845	U2763			A	A			C					



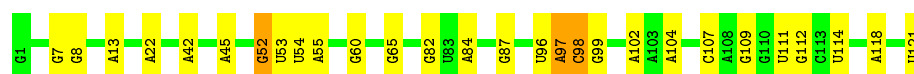
• Molecule 54: RDN58-1 rRNA

Chain 2: 73% 24%



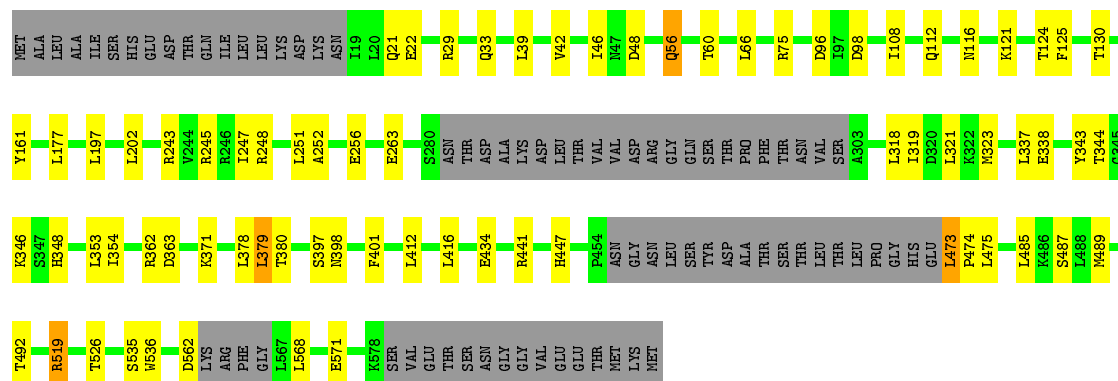
• Molecule 55: RDN5-2 rRNA

Chain 3: 77% 21%

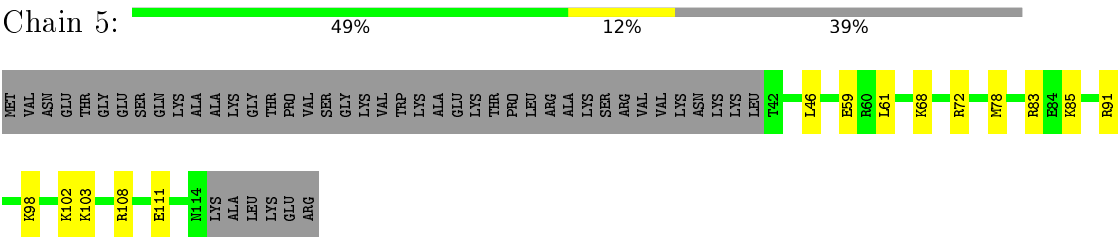


• Molecule 56: Probable metalloprotease ARX1

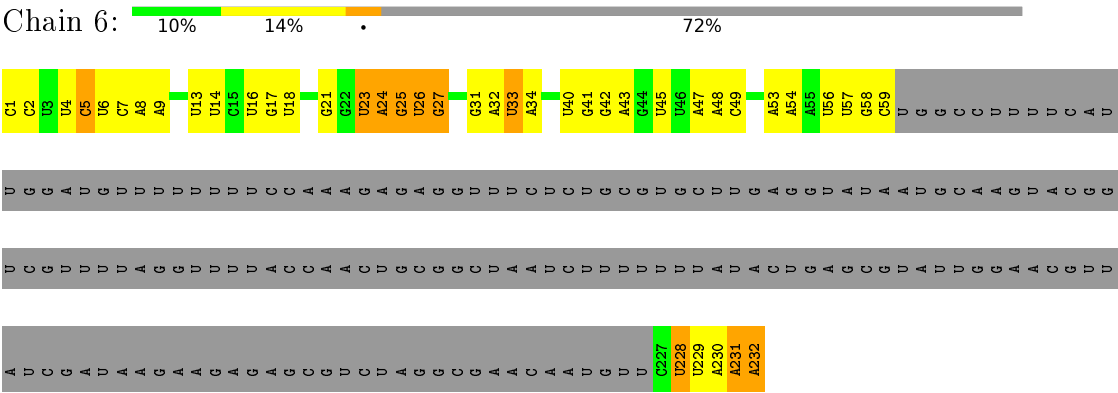
Chain 4: 75% 12% 13%



• Molecule 57: rRNA-processing protein CGR1



● Molecule 58: ITS2-1 miscRNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	191848	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Gatan k2 summit	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.37	0/1666	0.66	0/2241
10	J	0.42	0/1374	0.68	0/1842
11	K	0.38	0/2098	0.49	0/2830
12	L	0.38	0/1524	0.71	1/2046 (0.0%)
13	M	0.33	0/1074	0.58	0/1446
14	N	0.38	0/1757	0.70	0/2354
15	O	0.34	0/1585	0.44	0/2128
16	P	0.35	0/1465	0.63	0/1968
17	Q	0.35	0/1050	0.57	0/1419
18	R	0.34	0/1275	0.60	0/1702
19	S	0.35	0/1473	0.57	0/1980
2	B	0.41	0/3152	0.71	1/4239 (0.0%)
20	T	0.37	0/957	0.63	0/1285
21	U	0.36	0/861	0.49	0/1167
22	V	0.34	0/1018	0.55	0/1369
23	W	0.37	0/1918	0.53	0/2586
24	X	0.34	0/1116	0.54	0/1503
25	Y	0.33	0/1004	0.56	1/1341 (0.1%)
26	Z	0.35	0/1118	0.54	0/1497
27	a	0.36	0/751	0.57	0/1013
28	b	0.38	0/5270	0.59	0/7080
29	c	0.35	0/751	0.52	0/1008
3	C	0.37	0/2801	0.62	0/3792
30	d	0.32	0/887	0.53	0/1191
31	e	0.34	0/1041	0.58	0/1394
32	f	0.35	0/868	0.60	0/1168
33	g	0.34	0/891	0.61	0/1191
34	h	0.34	0/978	0.57	0/1301
35	i	0.37	0/778	0.58	0/1034
36	j	0.39	0/696	0.69	1/923 (0.1%)
37	k	0.36	0/618	0.53	0/826
38	l	0.36	0/443	0.69	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
39	m	0.40	1/3848 (0.0%)	0.59	0/5181
4	D	0.39	0/2257	0.63	0/3043
40	n	0.39	0/3101	0.56	0/4187
41	o	0.38	0/1129	0.54	0/1502
42	p	0.35	0/701	0.60	0/934
43	q	0.38	0/1539	0.54	0/2059
44	r	0.38	0/1892	0.62	0/2528
45	s	0.35	0/577	0.53	0/752
46	t	0.40	1/2333 (0.0%)	0.54	0/3128
47	u	0.38	0/1287	0.62	0/1711
48	v	0.35	0/2361	0.47	0/3153
49	w	0.35	0/1471	0.52	0/1980
5	E	0.36	0/1260	0.61	0/1694
50	x	0.35	0/3897	0.50	0/5282
51	y	0.35	0/1872	0.57	1/2548 (0.0%)
52	z	0.39	0/445	0.63	0/585
53	1	0.23	0/73234	0.70	12/114167 (0.0%)
54	2	0.23	0/3746	0.69	1/5832 (0.0%)
55	3	0.20	0/2883	0.65	1/4491 (0.0%)
56	4	0.37	0/4069	0.52	0/5520
57	5	0.39	0/649	0.59	0/848
58	6	0.26	0/1527	0.77	0/2371
6	F	0.37	0/1821	0.60	0/2451
7	G	0.37	0/1849	0.60	0/2495
8	H	0.35	0/1539	0.61	0/2073
9	I	0.37	0/1075	0.52	0/1443
All	All	0.31	2/166620 (0.0%)	0.65	19/241410 (0.0%)

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
10	J	0	3
11	K	0	3
13	M	0	1
18	R	0	1
19	S	0	6
2	B	0	10
20	T	0	2
21	U	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	V	0	2
23	W	0	3
24	X	0	2
26	Z	0	2
28	b	0	18
3	C	0	1
30	d	0	3
31	e	0	1
32	f	0	1
33	g	0	1
34	h	0	2
36	j	0	1
37	k	0	2
38	l	0	1
39	m	0	16
4	D	0	3
40	n	0	18
41	o	0	4
43	q	0	8
44	r	0	6
46	t	0	7
47	u	0	3
49	w	0	9
50	x	0	8
51	y	0	3
56	4	0	11
6	F	0	1
7	G	0	4
9	I	0	1
All	All	0	169

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	m	182	GLY	C-O	7.46	1.35	1.23
46	t	322	ASN	C-O	6.18	1.35	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	1307	G	C2'-C3'-O3'	7.51	126.02	109.50
53	1	649	A	C2'-C3'-O3'	7.47	125.94	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	2900	A	C2'-C3'-O3'	7.35	125.67	109.50
53	1	3030	G	C2'-C3'-O3'	6.33	123.82	113.70
53	1	3341	U	C2'-C3'-O3'	6.30	123.78	113.70

There are no chirality outliers.

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	156	SER	Peptide
2	B	220	VAL	Peptide
2	B	50	LYS	Peptide
2	B	52	GLY	Peptide
2	B	59	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1685	17	0
2	B	3081	0	3165	86	0
3	C	2749	0	2863	30	0
4	D	2211	0	2175	66	0
5	E	1239	0	1326	22	0
6	F	1784	0	1862	23	0
7	G	1817	0	1908	29	0
8	H	1518	0	1587	25	0
9	I	1059	0	1090	4	0
10	J	1353	0	1383	9	0
11	K	2064	0	2156	16	0
12	L	1499	0	1558	20	0
13	M	1059	0	1154	22	0
14	N	1720	0	1779	9	0
15	O	1555	0	1659	165	0
16	P	1442	0	1485	10	0
17	Q	1035	0	1115	4	0
18	R	1258	0	1341	9	0
19	S	1437	0	1475	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	943	0	994	31	0
21	U	844	0	855	1	0
22	V	1003	0	1048	12	0
23	W	1885	0	1921	3	0
24	X	1100	0	1187	5	0
25	Y	993	0	1081	2	0
26	Z	1092	0	1155	12	0
27	a	735	0	776	0	0
28	b	5185	0	5251	0	0
29	c	743	0	797	0	0
30	d	873	0	914	0	0
31	e	1020	0	1090	0	0
32	f	850	0	880	0	0
33	g	881	0	945	0	0
34	h	969	0	1078	0	0
35	i	771	0	849	0	0
36	j	681	0	683	0	0
37	k	612	0	682	0	0
38	l	436	0	475	0	0
39	m	3774	0	3835	0	0
40	n	3030	0	3107	0	0
41	o	1107	0	1159	0	0
42	p	694	0	734	0	0
43	q	1514	0	1570	0	0
44	r	1860	0	1965	0	0
45	s	573	0	644	0	0
46	t	2306	0	2454	0	0
47	u	1265	0	1314	0	0
48	v	2318	0	2398	0	0
49	w	1448	0	1510	0	0
50	x	3807	0	3790	0	0
51	y	1849	0	1835	0	0
52	z	444	0	478	0	0
53	1	65427	0	32875	328	0
54	2	3353	0	1695	4	0
55	3	2579	0	1303	12	0
56	4	3999	0	4088	7	0
57	5	645	0	688	0	0
58	6	1370	0	692	20	0
59	I	1	0	0	0	0
59	j	1	0	0	0	0
59	p	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	u	1	0	0	0	0
60	b	32	0	12	0	0
60	m	32	0	12	0	0
61	b	1	0	0	0	0
61	m	1	0	0	0	0
All	All	156562	0	123585	939	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 939 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2428:U:C5	53:1:2602:G:N1	1.70	1.54
53:1:2428:U:H5	53:1:2602:G:N1	0.92	1.40
53:1:2255:A:N7	53:1:2261:G:N2	1.70	1.35
53:1:3153:U:O4	53:1:3293:U:N3	1.59	1.35
18:R:62:ARG:NH1	53:1:3068:U:OP2	1.61	1.32

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	211/254 (83%)	205 (97%)	5 (2%)	1 (0%)	34	72
2	B	384/387 (99%)	281 (73%)	67 (17%)	36 (9%)	1	4
3	C	359/362 (99%)	330 (92%)	21 (6%)	8 (2%)	8	36
4	D	272/297 (92%)	246 (90%)	21 (8%)	5 (2%)	11	42
5	E	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	26	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	220/244 (90%)	207 (94%)	8 (4%)	5 (2%)	8	35
7	G	231/256 (90%)	213 (92%)	12 (5%)	6 (3%)	7	32
8	H	189/191 (99%)	181 (96%)	6 (3%)	2 (1%)	17	55
9	I	129/166 (78%)	110 (85%)	18 (14%)	1 (1%)	24	63
10	J	167/174 (96%)	137 (82%)	15 (9%)	15 (9%)	1	5
11	K	252/376 (67%)	226 (90%)	20 (8%)	6 (2%)	7	33
12	L	185/199 (93%)	170 (92%)	8 (4%)	7 (4%)	4	23
13	M	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	26	65
14	N	201/204 (98%)	190 (94%)	9 (4%)	2 (1%)	19	58
15	O	195/199 (98%)	150 (77%)	35 (18%)	10 (5%)	2	15
16	P	181/184 (98%)	169 (93%)	9 (5%)	3 (2%)	11	43
17	Q	132/186 (71%)	126 (96%)	6 (4%)	0	100	100
18	R	154/189 (82%)	149 (97%)	4 (3%)	1 (1%)	30	68
19	S	169/172 (98%)	156 (92%)	9 (5%)	4 (2%)	7	33
20	T	115/160 (72%)	102 (89%)	6 (5%)	7 (6%)	2	11
21	U	104/121 (86%)	94 (90%)	8 (8%)	2 (2%)	10	40
22	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
23	W	232/236 (98%)	214 (92%)	17 (7%)	1 (0%)	39	75
24	X	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
25	Y	124/127 (98%)	114 (92%)	10 (8%)	0	100	100
26	Z	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	24	63
27	a	91/149 (61%)	80 (88%)	9 (10%)	2 (2%)	8	36
28	b	638/647 (99%)	561 (88%)	59 (9%)	18 (3%)	6	30
29	c	95/105 (90%)	93 (98%)	1 (1%)	1 (1%)	17	55
30	d	105/113 (93%)	99 (94%)	4 (4%)	2 (2%)	10	40
31	e	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
32	f	104/107 (97%)	99 (95%)	4 (4%)	1 (1%)	19	58
33	g	110/121 (91%)	107 (97%)	2 (2%)	1 (1%)	21	61
34	h	117/120 (98%)	109 (93%)	6 (5%)	2 (2%)	11	43
35	i	97/100 (97%)	87 (90%)	7 (7%)	3 (3%)	5	28
36	j	85/88 (97%)	75 (88%)	9 (11%)	1 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
38	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
39	m	465/486 (96%)	399 (86%)	53 (11%)	13 (3%)	6	30
40	n	365/605 (60%)	321 (88%)	27 (7%)	17 (5%)	3	17
41	o	131/220 (60%)	116 (88%)	12 (9%)	3 (2%)	8	35
42	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	55
43	q	179/455 (39%)	155 (87%)	18 (10%)	6 (3%)	5	25
44	r	224/261 (86%)	194 (87%)	23 (10%)	7 (3%)	5	28
45	s	65/520 (12%)	59 (91%)	3 (5%)	3 (5%)	3	18
46	t	283/322 (88%)	249 (88%)	24 (8%)	10 (4%)	4	25
47	u	148/199 (74%)	134 (90%)	9 (6%)	5 (3%)	5	25
48	v	283/344 (82%)	269 (95%)	11 (4%)	3 (1%)	17	55
49	w	178/203 (88%)	152 (85%)	21 (12%)	5 (3%)	6	30
50	x	476/515 (92%)	433 (91%)	29 (6%)	14 (3%)	6	29
51	y	242/245 (99%)	222 (92%)	16 (7%)	4 (2%)	11	43
52	z	53/106 (50%)	51 (96%)	2 (4%)	0	100	100
56	4	508/593 (86%)	469 (92%)	31 (6%)	8 (2%)	12	44
57	5	71/120 (59%)	70 (99%)	1 (1%)	0	100	100
All	All	10349/12508 (83%)	9344 (90%)	750 (7%)	255 (2%)	11	33

5 of 255 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	ILE
2	B	34	LYS
2	B	38	SER
2	B	140	ASP
2	B	142	ALA

### 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	166/196 (85%)	157 (95%)	9 (5%)	27	64
2	B	322/323 (100%)	261 (81%)	61 (19%)	2	8
3	C	288/289 (100%)	272 (94%)	16 (6%)	26	63
4	D	227/245 (93%)	206 (91%)	21 (9%)	11	39
5	E	134/153 (88%)	125 (93%)	9 (7%)	20	56
6	F	186/205 (91%)	174 (94%)	12 (6%)	21	57
7	G	191/208 (92%)	175 (92%)	16 (8%)	14	46
8	H	171/171 (100%)	155 (91%)	16 (9%)	11	39
9	I	117/141 (83%)	111 (95%)	6 (5%)	29	66
10	J	147/150 (98%)	125 (85%)	22 (15%)	3	15
11	K	236/346 (68%)	224 (95%)	12 (5%)	29	66
12	L	149/159 (94%)	135 (91%)	14 (9%)	11	39
13	M	108/109 (99%)	105 (97%)	3 (3%)	51	82
14	N	175/176 (99%)	164 (94%)	11 (6%)	22	58
15	O	160/162 (99%)	145 (91%)	15 (9%)	11	39
16	P	145/146 (99%)	135 (93%)	10 (7%)	19	55
17	Q	110/151 (73%)	104 (94%)	6 (6%)	27	63
18	R	129/154 (84%)	119 (92%)	10 (8%)	16	50
19	S	155/156 (99%)	146 (94%)	9 (6%)	25	61
20	T	102/137 (74%)	89 (87%)	13 (13%)	5	22
21	U	93/107 (87%)	91 (98%)	2 (2%)	60	86
22	V	104/105 (99%)	98 (94%)	6 (6%)	25	61
23	W	211/213 (99%)	192 (91%)	19 (9%)	12	41
24	X	117/118 (99%)	103 (88%)	14 (12%)	6	24
25	Y	109/110 (99%)	103 (94%)	6 (6%)	27	63
26	Z	115/116 (99%)	109 (95%)	6 (5%)	29	65
27	a	76/119 (64%)	68 (90%)	8 (10%)	8	32
28	b	568/573 (99%)	506 (89%)	62 (11%)	8	31
29	c	81/88 (92%)	74 (91%)	7 (9%)	13	45
30	d	94/97 (97%)	85 (90%)	9 (10%)	10	37
31	e	109/111 (98%)	102 (94%)	7 (6%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	f	90/91 (99%)	85 (94%)	5 (6%)	26	63
33	g	95/103 (92%)	90 (95%)	5 (5%)	28	64
34	h	104/105 (99%)	93 (89%)	11 (11%)	8	32
35	i	81/82 (99%)	74 (91%)	7 (9%)	13	45
36	j	70/71 (99%)	66 (94%)	4 (6%)	25	62
37	k	68/69 (99%)	65 (96%)	3 (4%)	35	71
38	l	45/46 (98%)	38 (84%)	7 (16%)	3	14
39	m	413/428 (96%)	349 (84%)	64 (16%)	3	14
40	n	334/548 (61%)	310 (93%)	24 (7%)	18	53
41	o	118/199 (59%)	103 (87%)	15 (13%)	5	22
42	p	71/72 (99%)	69 (97%)	2 (3%)	51	82
43	q	171/420 (41%)	163 (95%)	8 (5%)	32	69
44	r	203/229 (89%)	185 (91%)	18 (9%)	12	42
45	s	62/445 (14%)	60 (97%)	2 (3%)	46	80
46	t	256/287 (89%)	235 (92%)	21 (8%)	14	47
47	u	133/180 (74%)	126 (95%)	7 (5%)	28	64
48	v	258/309 (84%)	252 (98%)	6 (2%)	58	84
49	w	161/179 (90%)	154 (96%)	7 (4%)	35	73
50	x	428/451 (95%)	407 (95%)	21 (5%)	31	68
51	y	210/211 (100%)	199 (95%)	11 (5%)	29	65
52	z	48/95 (50%)	45 (94%)	3 (6%)	22	58
56	4	453/520 (87%)	409 (90%)	44 (10%)	10	36
57	5	67/106 (63%)	53 (79%)	14 (21%)	1	6
All	All	9034/10780 (84%)	8288 (92%)	746 (8%)	19	47

5 of 746 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Y	126	LEU
29	c	76	GLU
56	4	22	GLU
27	a	64	GLN
28	b	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	74	GLN
28	b	367	GLN
51	y	106	ASN
23	W	167	ASN
27	a	64	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	1	3048/3396 (89%)	923 (30%)	216 (7%)
54	2	157/158 (99%)	38 (24%)	5 (3%)
55	3	120/121 (99%)	22 (18%)	4 (3%)
58	6	64/232 (27%)	41 (64%)	10 (15%)
All	All	3389/3907 (86%)	1024 (30%)	235 (6%)

5 of 1024 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	1	7	C
53	1	11	A
53	1	13	A
53	1	14	U
53	1	16	A

5 of 235 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	2268	U
53	1	2568	C
54	2	81	U
53	1	2272	G
53	1	2510	U

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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	$\# Z  > 2$
60	GTP	b	701	61	26,34,34	1.15	2 (7%)	29,54,54	1.83	6 (20%)
60	GTP	m	501	61	26,34,34	1.05	2 (7%)	29,54,54	1.64	4 (13%)

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
60	GTP	b	701	61	-	0/18/38/38	0/3/3/3
60	GTP	m	501	61	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	m	501	GTP	C5-C4	2.82	1.46	1.40
60	b	701	GTP	C5-C4	3.04	1.47	1.40
60	m	501	GTP	C6-C5	3.18	1.47	1.41
60	b	701	GTP	C6-C5	3.86	1.49	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	b	701	GTP	C6-C5-C4	-3.71	116.62	120.86
60	b	701	GTP	C5-C6-N1	-3.66	118.73	123.52
60	m	501	GTP	C5-C6-N1	-3.54	118.89	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	b	701	GTP	N3-C2-N1	-3.50	122.79	127.56
60	m	501	GTP	N3-C2-N1	-3.27	123.10	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.