



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 7, 2016 – 05:06 PM EST

PDB ID : 4V3P
EMDB ID: : EMD-2790
Title : The molecular structure of the left-handed supra-molecular helix of eukaryotic polyribosomes
Authors : myasnikov, A.g.; afonina, z.a.; menetret, j.f.; shirokov, v.a.; spirin, A.s.; klaholz, b.p.
Deposited on : 2014-10-20
Resolution : 34.00 Å(reported)
Based on PDB ID : 3IZ6

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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : unknown
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

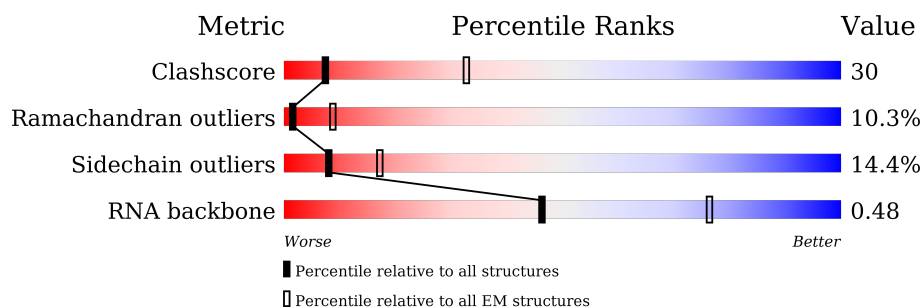
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 34.00 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.



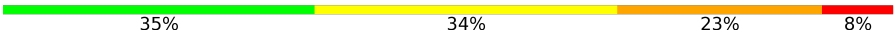

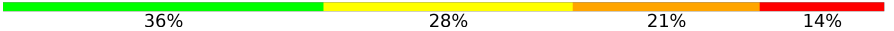

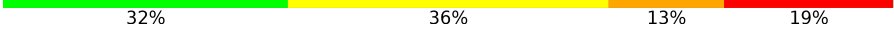



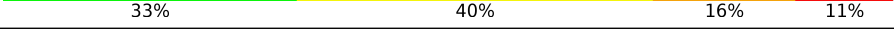


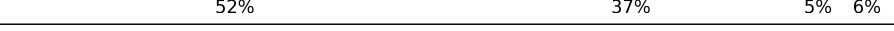
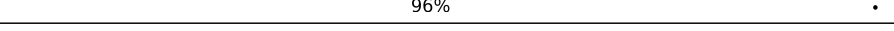
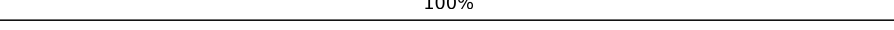





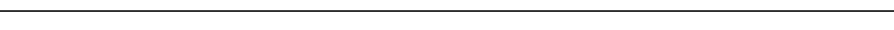

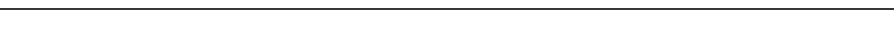
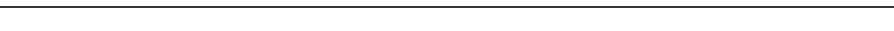


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	Sa	380	65% 26% 7% .
2	SA	260	35% 40% 18% 6%
3	SB	208	32% 34% 25% 9%
4	SD	200	31% 46% 13% 12%
5	SE	263	52% 30% 15% .
6	SF	191	61% 27% 10% .
7	SI	126	53% 30% 11% 6%
8	SJ	128	59% 30% 8% .




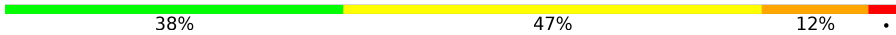
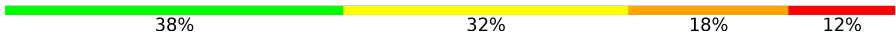






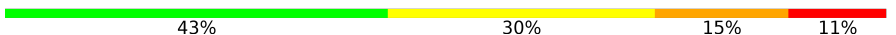
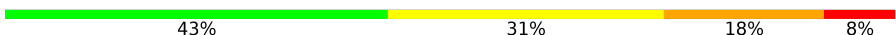

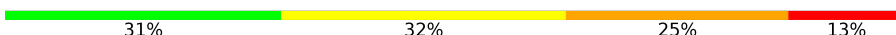










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Mol	Chain	Length	Quality of chain
9	SK	119	
10	SL	142	
11	SM	152	
12	SO	121	
13	SQ	141	
14	SP	85	
15	SS	146	
16	SR	91	
17	SV	100	
18	SW	92	
19	SY	58	
20	SZ	62	
21	Sc	25	
22	Sb	36	
23	SU	98	
24	SX	50	
25	SC	195	
26	SG	143	
27	SH	130	
28	SN	48	
29	ST	82	
30	S3	11	
31	S2	75	
32	S1	1743	
33	L1	3352	

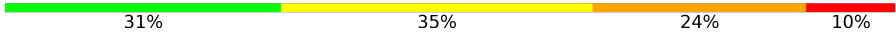



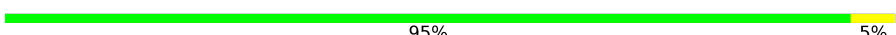

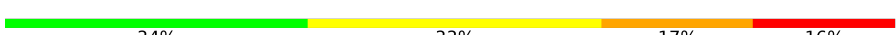




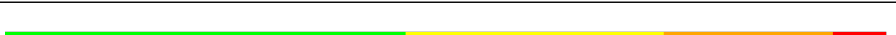

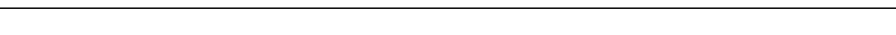
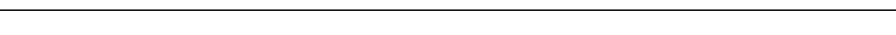
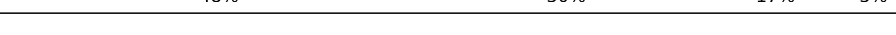

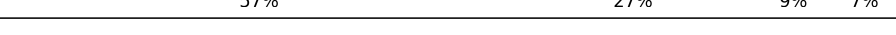

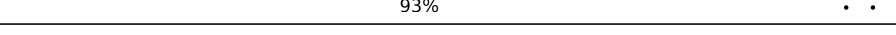





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Mol	Chain	Length	Quality of chain
34	L3	120	
35	L2	159	
36	LA	216	
37	LB	255	
38	LE	170	
39	LF	190	
40	LH	201	
41	LM	140	
42	LP	194	
43	LO	144	
44	LR	163	
45	LQ	304	
46	LT	189	
47	LU	164	
48	LV	171	
49	LX	122	
50	LZ	75	
51	LY	130	
52	Lb	73	
53	Ld	23	
54	Lf	112	
55	Lg	120	
56	Lh	133	
57	Li	94	
58	Ln	69	





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Mol	Chain	Length	Quality of chain
59	Lo	51	
60	Lr	105	
61	Lq	25	
62	Lx	20	
62	Ly	20	
63	Lz	14	
64	LG	219	
65	LL	182	
66	LN	134	
67	LS	167	
68	LW	108	
69	La	99	
70	Li	119	
71	Lj	104	
72	Lk	77	
73	Lp	41	
74	LJ	128	
75	Lt	58	
75	Lu	58	
76	Lv	59	
76	Lw	59	
77	Lc	124	
78	Le	244	
79	Ls	262	
80	LC	389	

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Mol	Chain	Length	Quality of chain
81	LD	372	 52%29%10%9%
82	LK	206	 59%23%13%•
83	Lm	92	 71%18%10%•
84	LI	184	 68%20%9%•

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 195694 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 G protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Sa	380	Total	C	N	O	S	0	0
			2842	1758	512	553	19		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	260	Total	C	N	O	S	0	0
			1946	1220	349	367	10		

- Molecule 3 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SB	208	Total	C	N	O	S	0	0
			1539	964	288	279	8		

- Molecule 4 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	200	Total	C	N	O	S	0	0
			1607	1030	290	283	4		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	263	Total	C	N	O	S	0	0
			2028	1283	385	352	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	191	Total	C	N	O	S	0	0
			1485	925	281	272	7		

- Molecule 7 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SI	126	Total	C	N	O	S	0	0
			1017	648	195	170	4		

- Molecule 8 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	128	Total	C	N	O	S	0	0
			887	541	171	171	4		

- Molecule 9 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	119	Total	C	N	O	S	0	0
			830	508	159	159	4		

- Molecule 10 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SL	142	Total	C	N	O	S	0	0
			952	576	197	175	4		

- Molecule 11 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SM	152	Total	C	N	O	S	0	0
			1167	722	233	206	6		

- Molecule 12 is a protein called 40S ribosomal protein S13-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SO	121	Total	C	N	O	S	0	0
			977	627	180	167	3		

- Molecule 13 is a protein called 40S ribosomal protein S17-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SQ	141	Total	C	N	O	S	0	0
			1129	699	214	210	6		

- Molecule 14 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SP	85	Total	C	N	O	S	0	0
			639	399	130	107	3		

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SS	146	Total	C	N	O	S	0	0
			1155	726	218	207	4		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SR	91	Total	C	N	O	S	0	0
			711	457	130	120	4		

- Molecule 17 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SV	100	Total	C	N	O	S	0	0
			740	458	142	140			

- Molecule 18 is a protein called 40S WHEAT GERM RIBOSOME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SW	92	Total	C	N	O	S	0	0
			460	276	92	92			

- Molecule 19 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SY	58	Total	C	N	O	S	0	0
			442	274	83	82	3		

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SZ	62	Total	C	N	O	S	0	0
			469	289	105	73	2		

- Molecule 21 is a protein called Unknown 40S wheat germ ribosome protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Sc	25	Total	C	N	O	0	0
			126	75	25	26		

- Molecule 22 is a protein called Unknown 40S wheat germ ribosome protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Sb	36	Total	C	N	O	0	0
			181	108	36	37		

- Molecule 23 is a protein called Unknown 40S wheat germ ribosome protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SU	98	Total	C	N	O	S	0	0
			732	466	142	123	1		

- Molecule 24 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SX	50	Total	C	N	O	S	0	0
			375	235	65	68	7		

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SC	195	Total	C	N	O	S	0	0
			1535	958	307	265	5		

- Molecule 26 is a protein called Unknown 40S wheat germ ribosome protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	SG	143	Total	C	N	O	0	0
			716	429	143	144		

- Molecule 27 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SH	130	Total	C	N	O	S	0	0
			1042	667	189	181	5		

- Molecule 28 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SN	48	Total	C	N	O	S	0	0
			313	184	67	56	6		

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	ST	82	Total	C	N	O	S	0	0
			650	400	121	126	3		

- Molecule 30 is a RNA chain called 40S WHEAT GERM RIBOSOME protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S3	11	Total	C	N	O	P	0	0
			236	106	45	74	11		

- Molecule 31 is a RNA chain called 40S rRNA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S2	75	Total	C	N	O	P	0	0
			1599	712	280	532	75		

- Molecule 32 is a RNA chain called Triticum aestivum 18S ribosomal RNA gene.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S1	1743	Total	C	N	O	P	0	11
			33897	14994	5742	11418	1743		

- Molecule 33 is a RNA chain called 26S ribosomal RNA gene.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L1	3352	Total	C	N	O	P	0	39
			69592	30953	12564	22725	3350		

- Molecule 34 is a RNA chain called Wheat 5S DNA short repeating unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L3	120	Total	C	N	O	P	0	0
			2565	1144	461	840	120		

- Molecule 35 is a RNA chain called Triticum aestivum E-2055 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene, complete sequence; and internal transcribed spacer 2, partial sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L2	159	Total	C	N	O	P	0	0
			3192	1415	555	1063	159		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L2	136	G	C	conflict	GB 17016972

- Molecule 36 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LA	216	Total	C	N	O	S	0	0
			1718	1092	309	304	13		

- Molecule 37 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LB	255	Total	C	N	O	S	0	0
			1933	1200	398	326	9		

- Molecule 38 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LE	170	Total	C	N	O	S	0	0
			1376	867	256	244	9		

- Molecule 39 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LF	190	Total	C	N	O	S	0	0
			1500	947	270	277	6		

- Molecule 40 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LH	201	Total	C	N	O	S	0	0
			1564	996	289	273	6		

- Molecule 41 is a protein called Ribosomal Pr 117.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LM	140	Total	C	N	O	S	0	0
			1020	640	192	179	9		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LP	194	Total	C	N	O	S	0	0
			1630	1027	342	257	4		

- Molecule 43 is a protein called 60S ribosomal protein L27a-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LO	144	Total	C	N	O	S	0	0
			1086	691	217	173	5		

- Molecule 44 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LR	163	Total	C	N	O	S	0	0
			1284	810	248	219	7		

- Molecule 45 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LQ	304	Total	C	N	O	S	0	0
			2395	1497	430	461	7		

- Molecule 46 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LT	189	Total	C	N	O	S	0	0
			1569	972	330	257	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	184	GLY	UNK	variant	UNP Q7XY20

- Molecule 47 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LU	164	Total	C	N	O	S	0	0
			1266	789	250	225	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LU	65	TRP	CYS	conflict	UNP W5EIT2

- Molecule 48 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LV	171	Total	C	N	O	S	0	0
			1335	826	266	238	5		

- Molecule 49 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LX	122	Total	C	N	O	S	0	0
			987	634	178	173	2		

- Molecule 50 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LZ	75	Total	C	N	O	S	0	0
			578	366	115	94	3		

- Molecule 51 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LY	130	Total	C	N	O	S	0	0
			1048	647	220	178	3		

- Molecule 52 is a protein called 60S ribosomal protein l28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lb	73	Total	C	N	O	S	0	0
			576	364	107	103	2		

- Molecule 53 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Ld	23	Total	C	N	O	0	0
			199	119	41	39		

- Molecule 54 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lf	112	Total	C	N	O	S	0	0
			825	516	146	157	6		

- Molecule 55 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lg	120	Total	C	N	O	S	0	0
			944	585	185	171	3		

- Molecule 56 is a protein called Ribosomal L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lh	133	Total	C	N	O	S	0	0
			1089	688	216	179	6		

- Molecule 57 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ll	94	Total	C	N	O	S	0	0
			725	438	158	122	7		

- Molecule 58 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ln	69	Total	C	N	O	S	0	0
			547	347	102	96	2		

- Molecule 59 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lo	51	Total	C	N	O	S	0	0
			460	291	100	67	2		

- Molecule 60 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Lr	105	Total	C	N	O	S	0	0
			838	523	166	143	6		

- Molecule 61 is a protein called Unknown 60S wheat germ ribosome protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lq	25	Total	C	N	O	S	0	0
			238	145	62	28	3		

- Molecule 62 is a protein called Unknown 60S wheat germ ribosome protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	Ly	20	Total	C	N	O	0	0
			101	60	20	21		
62	Lx	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 63 is a protein called Unknown 60S wheat germ ribosome protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	Lz	14	Total	C	N	O	0	0
			71	42	14	15		

- Molecule 64 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LG	219	Total	C	N	O	S	0	0
			1730	1106	314	306	4		

- Molecule 65 is a protein called Unknown 60S wheat germ ribosome protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	LL	182	Total	C	N	O	0	0
			910	545	182	183		

- Molecule 66 is a protein called Unknown 60S wheat germ ribosome protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LN	134	Total	C	N	O	S	0	0
			1081	690	201	185	5		

- Molecule 67 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LS	167	Total	C	N	O	S	0	0
			1419	916	263	233	7		

- Molecule 68 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	LW	108	Total	C	N	O	S	0	0
			839	530	152	155	2		

- Molecule 69 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	La	99	Total	C	N	O	S	0	0
			732	463	140	126	3		

- Molecule 70 is a protein called Ribosomal protein l34.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Li	119	Total	C	N	O	S	0	0
			964	606	195	161	2		

- Molecule 71 is a protein called ribosomal protein L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lj	104	Total	C	N	O	S	0	0
			797	498	158	138	3		

- Molecule 72 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lk	77	Total	C	N	O	S	0	0
			613	383	128	100	2		

- Molecule 73 is a protein called Ubiquitin-60S ribosomal protein L40-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lp	41	Total	C	N	O	S	0	0
			344	211	75	53	5		

- Molecule 74 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	LJ	128	Total	C	N	O	S	0	0
			959	601	177	177	4		

- Molecule 75 is a protein called Ribosomal protein P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lt	58	Total	C	N	O	S	0	0
			432	283	69	79	1		
75	Lu	58	Total	C	N	O	S	0	0
			432	283	69	79	1		

- Molecule 76 is a protein called 60S acidic ribosomal protein P2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lv	59	Total	C	N	O	S	0	0
			441	278	69	90	4		
76	Lw	59	Total	C	N	O	S	0	0
			441	278	69	90	4		

- Molecule 77 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lc	124	Total	C	N	O		0	0
			1006	632	202	172			

- Molecule 78 is a protein called Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Le	244	Total	C	N	O	S	0	0
			1984	1271	368	339	6		

- Molecule 79 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ls	262	Total	C	N	O	S	0	0
			1993	1278	330	377	8		

- Molecule 80 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LC	389	Total	C	N	O	S	0	0
			3102	1968	578	538	18		

- Molecule 81 is a protein called 60S ribosomal protein L4/L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	LD	372	Total	C	N	O	S	0	0
			2866	1802	555	502	7		

- Molecule 82 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	LK	206	Total	C	N	O	S	0	0
			1650	1045	320	274	11		

- Molecule 83 is a protein called 60S ribosomal protein L37a, expressed.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lm	92	Total	C	N	O	S	0	0
			715	447	137	124	7		

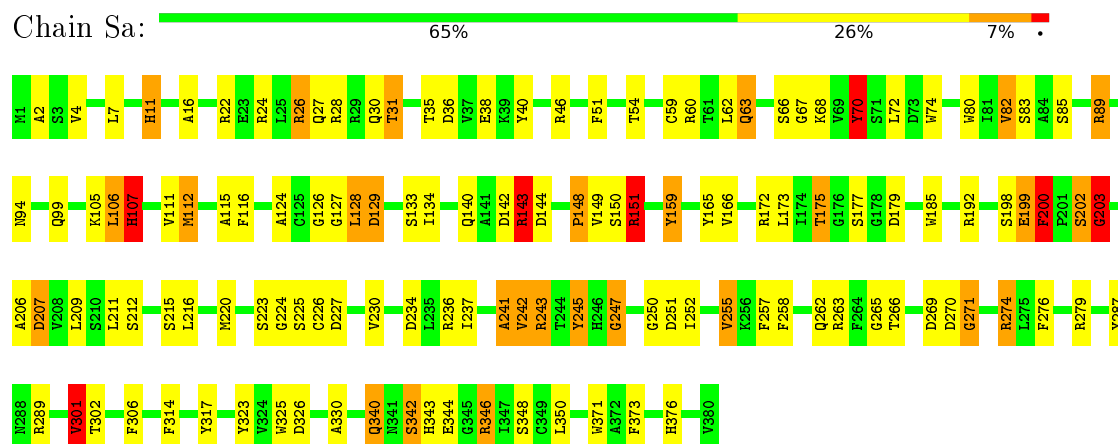
- Molecule 84 is a protein called 60S ribosomal protein L10-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	LI	184	Total	C	N	O	S	0	0
			1468	923	288	245	12		

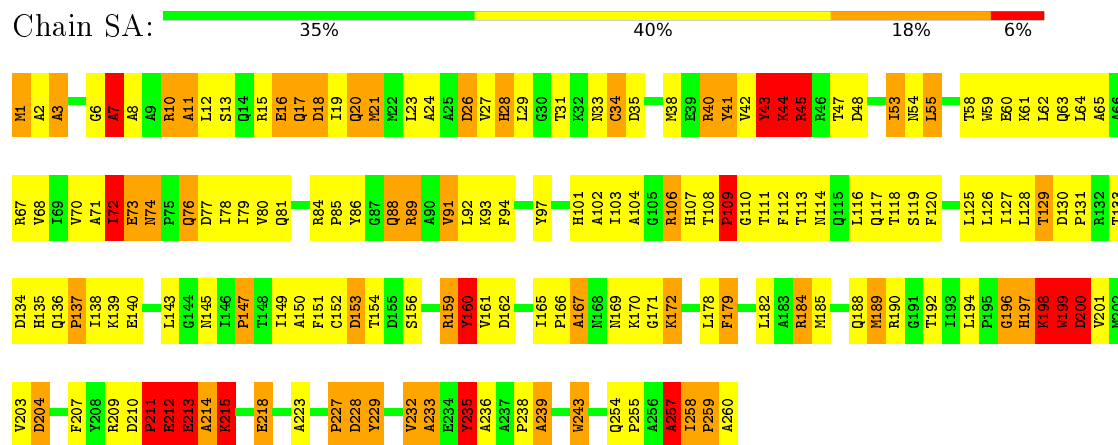
3 Residue-property plots

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.

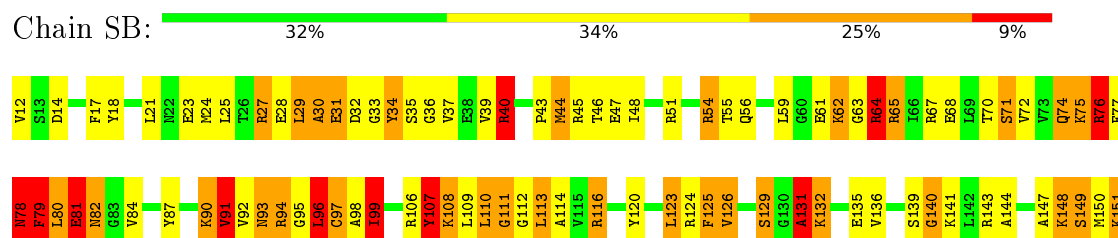
- Molecule 1: G protein beta subunit



- Molecule 2: 40S ribosomal protein SA



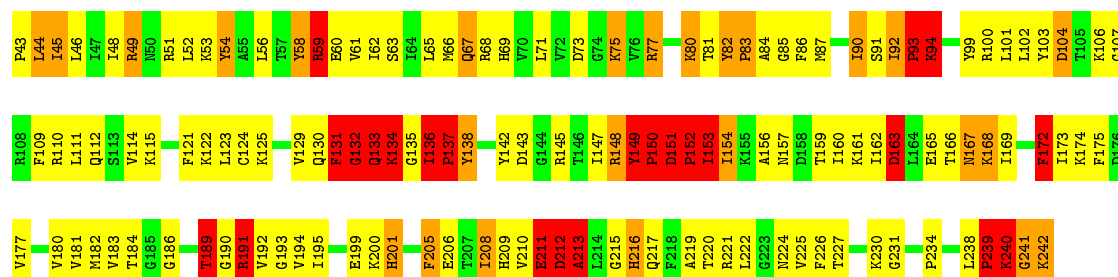
- Molecule 3: Putative 40S ribosomal protein S3





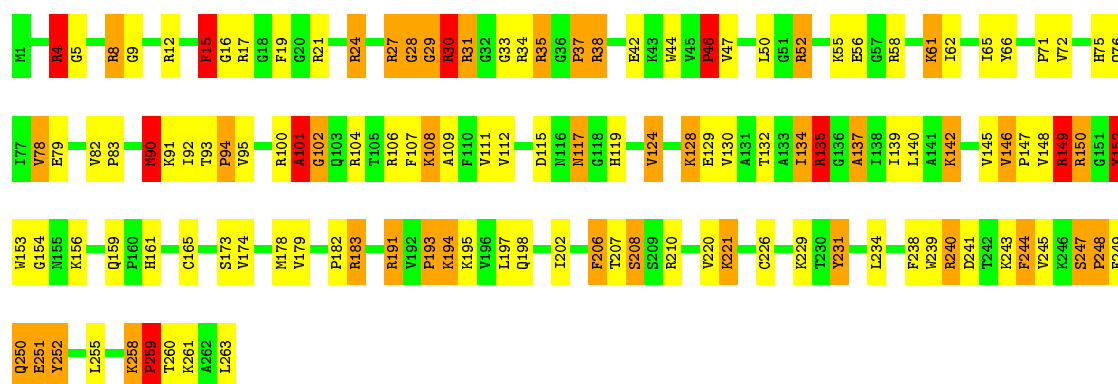
• Molecule 4: 40S ribosomal protein S4

Chain SD: 31% 46% 13% 12%

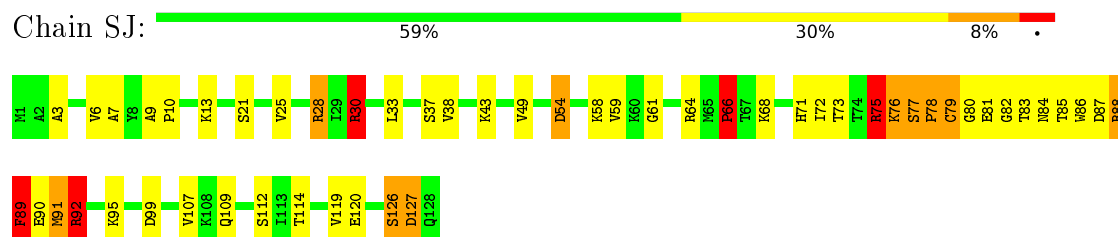


• Molecule 5: 40S ribosomal protein S2

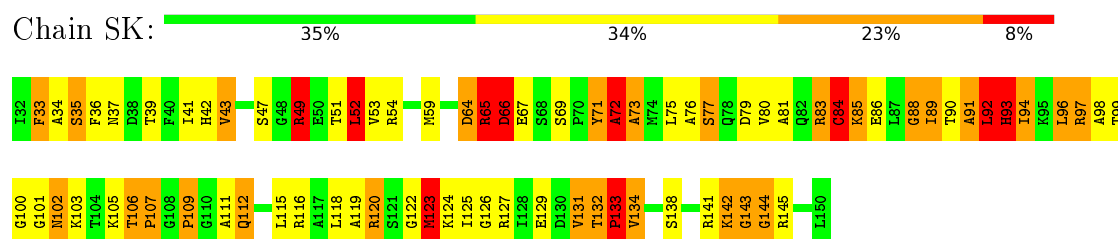
Chain SE: 52% 30% 15% .



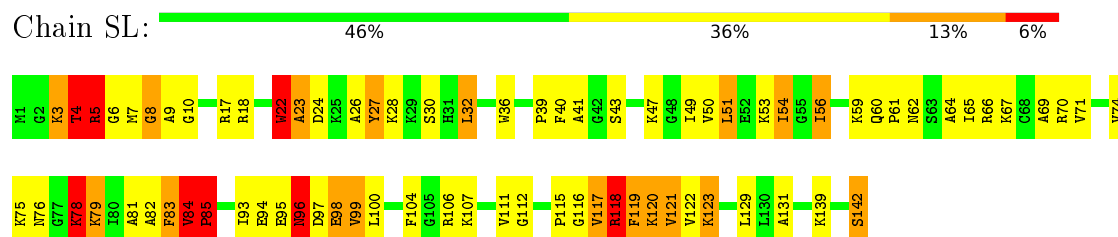
- Molecule 8: 40S ribosomal protein S20



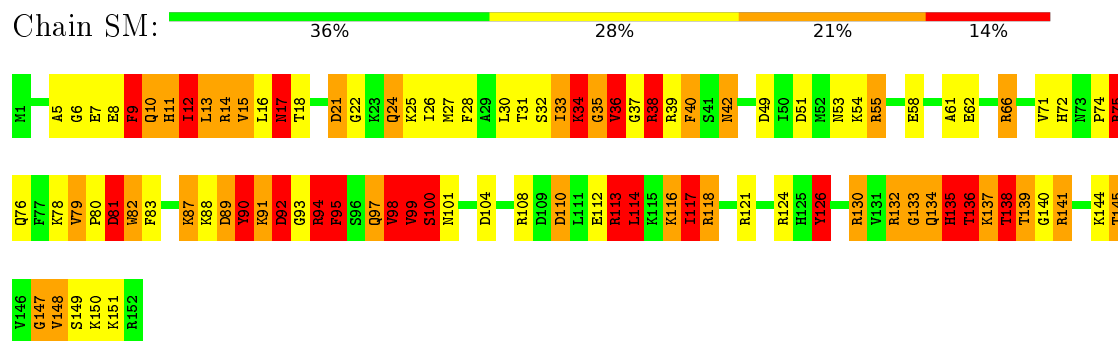
- Molecule 9: 40S ribosomal protein S14



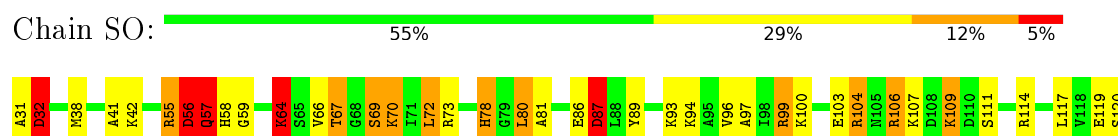
- Molecule 10: 40S ribosomal protein S23

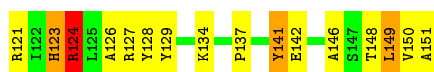


- Molecule 11: 40S ribosomal protein S18



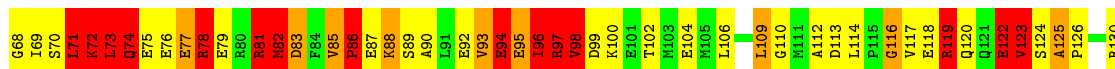
- Molecule 12: 40S ribosomal protein S13-1





- Molecule 13: 40S ribosomal protein S17-4

Chain SQ: 32% 36% 13% 19%



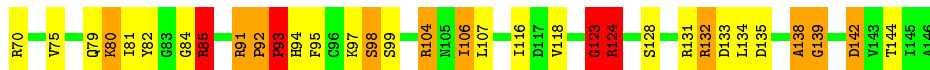
- Molecule 14: 40S ribosomal protein S11

Chain SP: 25% 41% 24% 11%



- Molecule 15: 40S ribosomal protein S19

Chain SS: 47% 27% 16% 10%



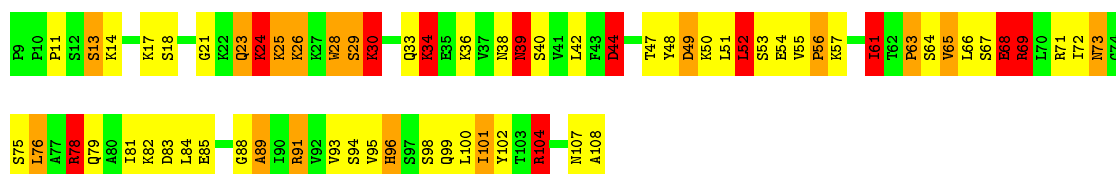
- Molecule 16: 40S ribosomal protein S15

Chain SR: 55% 30% 12%



- Molecule 17: 40S ribosomal protein S25

Chain SV: 33% 40% 16% 11%



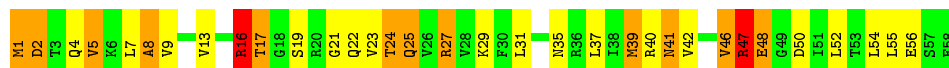
- Molecule 18: 40S WHEAT GERM RIBOSOME1

Chain SW: 67% 29% .



- Molecule 19: 40S ribosomal protein S28

Chain SY: 43% 33% 21% .



- Molecule 20: 40S ribosomal protein S30

Chain SZ: 52% 37% 5% 6%



- Molecule 21: Unknown 40S wheat germ ribosome protein 2

Chain Sc: 96% .



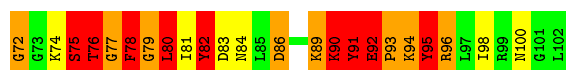
- Molecule 22: Unknown 40S wheat germ ribosome protein 3

Chain Sb: 100%

There are no outlier residues recorded for this chain.

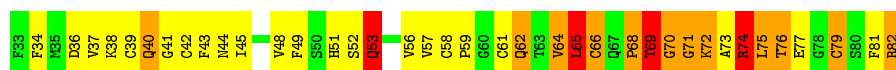
- Molecule 23: Unknown 40S wheat germ ribosome protein 3

Chain SU: 23% 20% 23% 33%



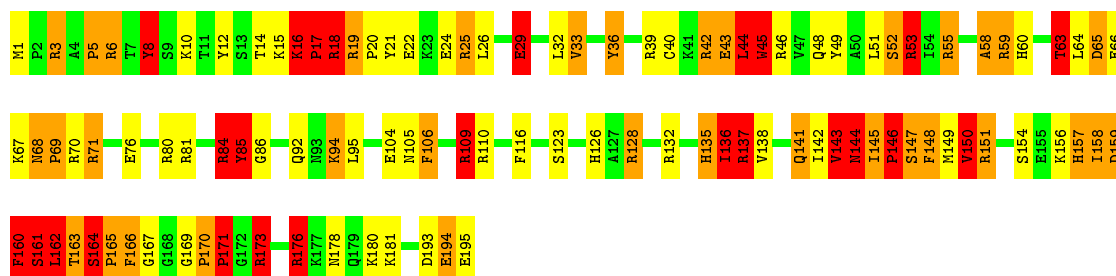
- Molecule 24: 40S ribosomal protein S27

Chain SX: 



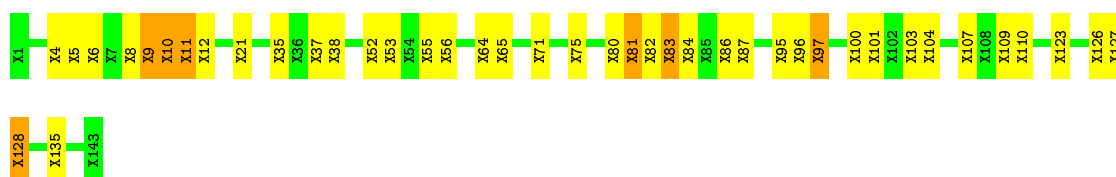
- Molecule 25: 40S ribosomal protein S9

Chain SC: 




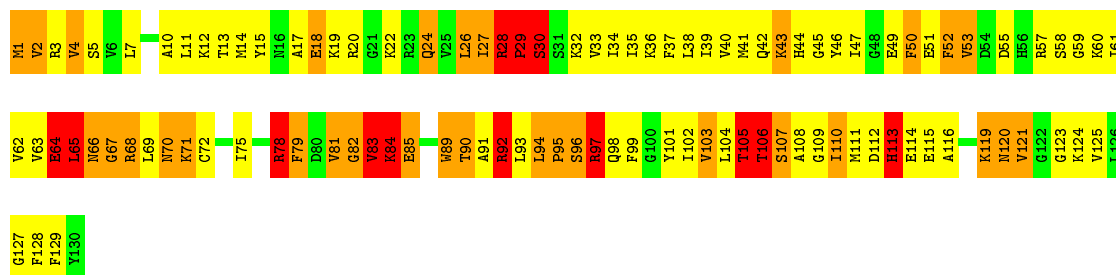
- Molecule 26: Unknown 40S wheat germ ribosome protein 4

Chain SG: 



- Molecule 27: Ribosomal protein S15

Chain SH: 



- Molecule 28: 40S ribosomal protein S29

Chain SN: 



- Molecule 29: 40S ribosomal protein S21

Chain ST: 



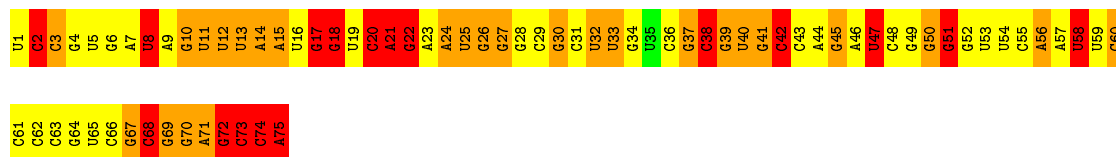
- Molecule 30: 40S WHEAT GERM RIBOSOME protein 4

Chain S3: 9% 36% 36% 18%



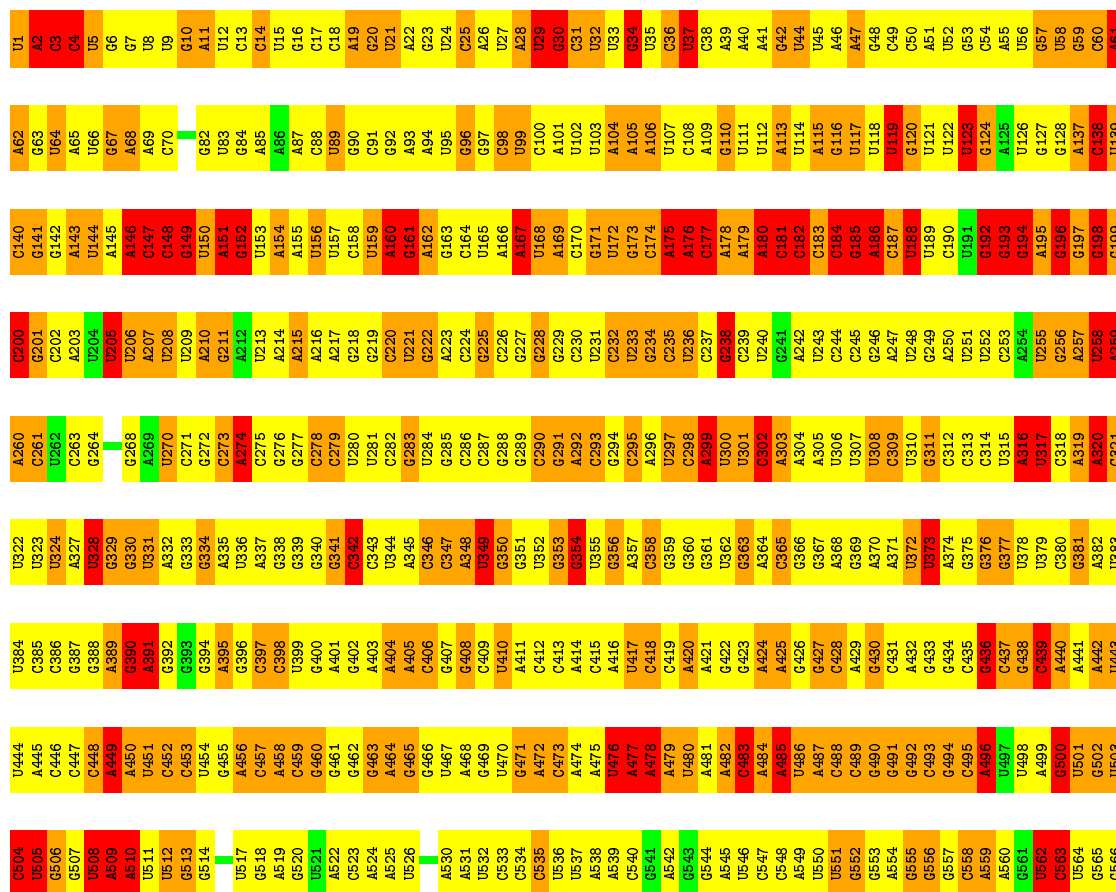
- Molecule 31: 40S rRNA 1

Chain S2: 41% 35% 23%

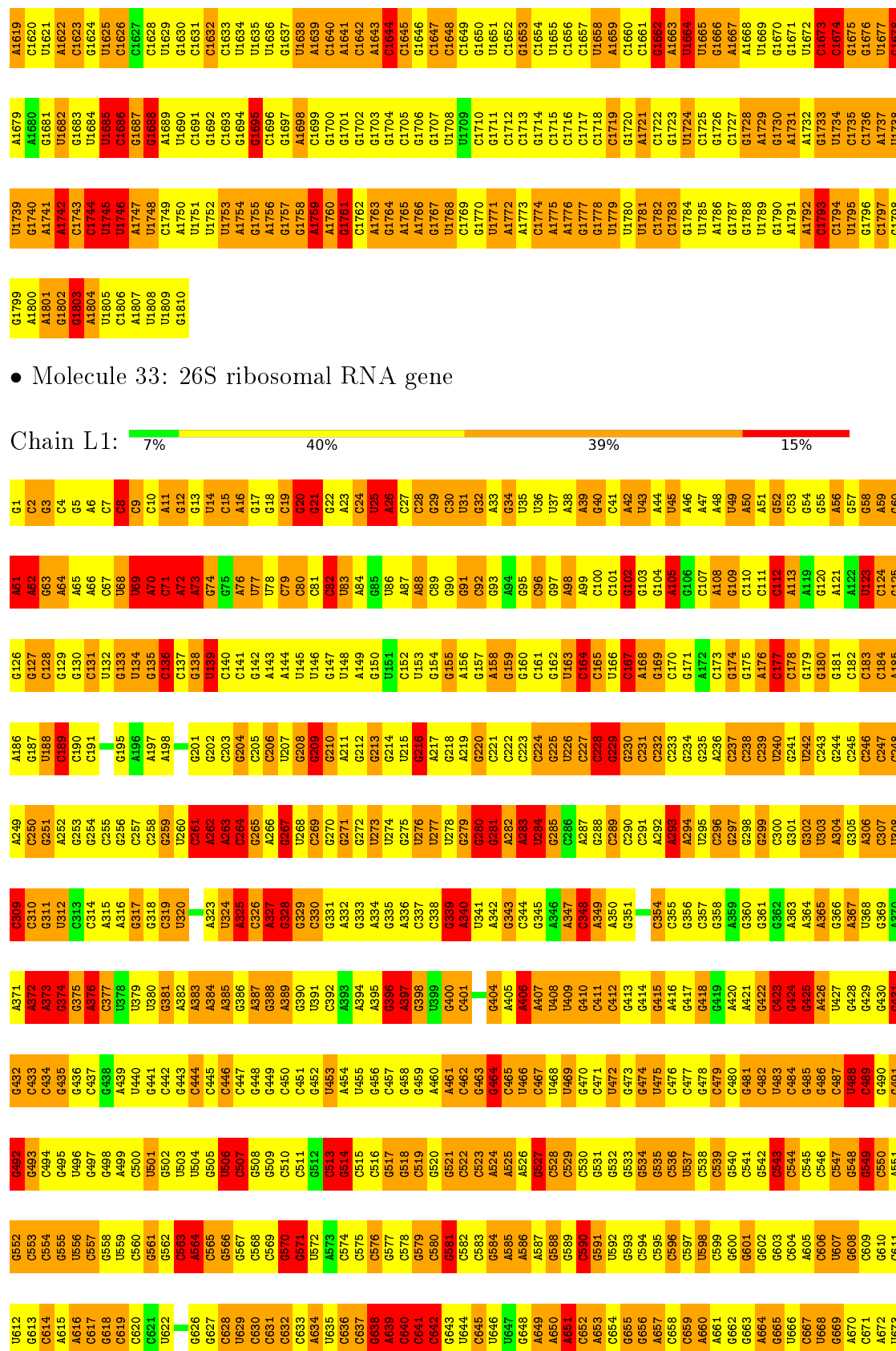


- Molecule 32: Triticum aestivum 18S ribosomal RNA gene

Chain S1: 7% 47% 35% 11%

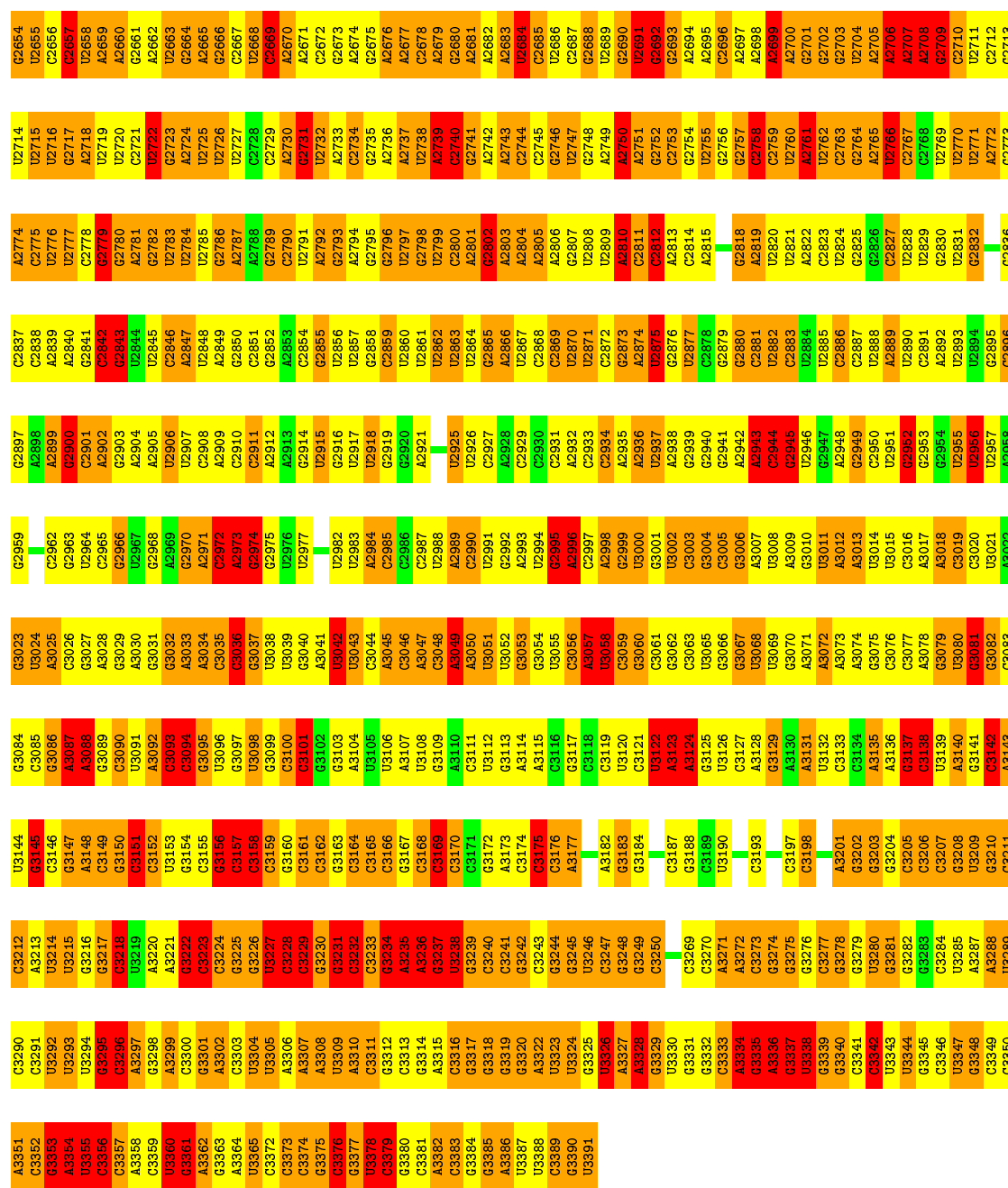


U1559	U1426	C1365	U1305	U1244	C1184	G1124	U1063	U1003	G943	G883	U796	C687	A627	U567
U1560	A1427	A1366	U1306	G1245	U1185	U1125	U1064	U1004	A944	G884	A797	U688	G628	G568
G1561	U1428	U1367	U1307	A1246	A1186	C1126	A1065	C1005	A945	C885	C798	C689	C629	C569
C1562	U1429	C1368	G1308	U1247	A1187	G1127	U1066	A1006	A946	A886	A799	G690	U630	C570
A1563	A1430	C1369	U1309	A1248	U1188	C1128	A1067	G1007	G947	U887	U800	A691	C631	A571
A1564	U1431	C1370	G1310	U1249	U1189	A1129	G1068	A1008	C948	U888	U801	C692	G632	G572
U1565	C1432	U1371	U1311	C1250	U1190	A1130	G1069	U009	A949	C889	A802	C693	U833	C573
U1566	U1433	C1372	G1312	U1251	U1191	A1131	A1070	U009	U950	C890	G803	C694	A634	A574
G1567	G1434	C1373	G1313	U1252	U1192	G1132	C1071	A1010	U951	U891	A823	C701	G635	A575
U1568	U1435	C1374	U1314	U1253	A1193	C1133	U1072	C1012	U952	A892	U824	U715	U637	C577
U1569	U1436	C1375	U1315	U1254	U1194	C1134	C1073	G1013	G953	U893	U825	U716	G638	G578
G1570	G1437	A1376	A1316	C1256	U1195	G1135	G1074	U1014	C954	U894	C826	A716	G639	G579
G1571	U1438	G1377	A1317	U1257	U1196	A1136	G1075	C1015	C955	U895	C827	G717	G640	G580
U1572	G1439	C1378	U1318	U1258	A1197	A1137	C1076	C1016	A956	C896	G828	C718	A640	G581
C1573	U1440	U1379	U1319	U1259	A1198	A1138	C1077	U1017	A957	A897	G829	C719	C641	G582
U1574	A1441	A1380	C1320	A1260	C1199	C1139	G1078	A1018	G958	U898	U830	U720	C642	U583
U1575	A1442	G1381	C1321	U1261	A1200	U1140	G1079	G1019	A959	A899	C831	U724	U644	A583
C1576	U1443	C1382	G1322	U1262	C1201	U1141	C1080	U1020	A960	G900	C832	U725	G645	A584
U1577	G1444	U1383	U1323	C1263	G1202	A1142	A1081	C1021	U961	U901	U833	U726	G646	U585
G1578	C1445	U1384	U1324	U1264	G1203	A1143	C1082	U1022	G962	C902	A834	U731	G647	U586
C1579	U1446	C1385	A1325	U1265	G1204	A1144	C1083	C1023	U963	A903	U835	G732	G648	C587
U1580	C1447	U1386	A1326	U1266	G1205	G1145	U1084	A1024	U964	C904	U836	U733	C649	C588
C1581	U1448	C1387	C1327	G1267	A1206	G1146	U1085	A1025	U965	A905	U837	U734	U644	A589
G1582	U1449	A1388	G1328	G1268	A1207	A1147	A1086	C1026	U966	C906	U838	C734	G650	G590
G1583	A1450	G1389	A1329	G1269	A1208	A1148	U1088	C1027	C967	G907	G839	C735	G651	C591
A1584	A1452	A1390	A1330	U1270	C1209	U1149	A1089	A1028	A968	U908	U840	U736	G652	U592
U1585	U1453	C1391	C1331	G1271	U1210	U1150	G1090	U1029	U969	G909	U841	U740	U653	C593
U1586	G1454	G1392	G1332	G1272	U1211	G1151	A1091	A1030	U970	A910	G842	C741	G654	C594
G1587	U1455	C1393	A1333	U1273	A1212	C1153	A1092	A1031	A971	A911	G843	U741	G655	A595
C1588	A1456	A1394	G1334	G1274	C1213	G1154	A1093	C1032	A972	A912	C844	U742	G656	A596
G1589	U1457	C1395	A1335	G1275	C1214	G1155	U1094	C1033	U973	U913	C845	U743	C657	U597
U1590	U1458	U1396	C1336	U1276	A1215	G1156	C1095	G1034	C974	U914	U846	U744	C658	A598
A1591	G1459	A1397	C1337	G1277	A1216	A1157	A1096	A1035	A975	C915	U847	U745	G659	A599
U1592	U1460	U1398	C1338	C1278	U1217	A1158	A1097	U1036	A976	A916	C848	U746	G660	C600
G1593	G1461	C1399	C1339	A1279	U1218	G1159	G1098	G1037	G977	U917	G849	U747	U661	G601
A1594	C1462	A1400	A1340	U1280	C1219	G1160	G1099	C1038	A978	C918	G850	U748	C662	U602
U1595	G1463	C1401	G1341	G1281	A1220	G1161	U1100	C1039	A979	G919	G851	U749	C663	A603
G1596	C1464	C1402	C1342	G1282	A1221	C1162	C1101	G1040	C980	A920	A852	U750	G664	U604
U1597	A1466	G1403	C1343	C1283	G1222	A1163	U1102	A1041	G981	U921	U853	U751	C665	A605
C1598	C1467	U1404	U1344	C1284	A1223	C1164	U1103	C1042	A982	U922	C854	U752	C666	U606
G1599	G1468	U1405	G1345	G1285	C1224	A1165	U1104	C1043	A983	U923	G855	U753	U667	U607
U1600	C1469	A1406	C1346	U1286	A1225	G1166	G1105	A1044	A984	A924	G856	U754	C668	U608
A1601	U1470	A1407	U1347	U1287	U1226	C1167	G1106	G1045	G985	U925	A857	U755	A669	A609
G1602	A1348	C1408	A1348	U1288	A1227	C1168	G1107	G1046	U986	G926	G858	U756	C670	A610
U1603	U1349	G1409	U1349	U1289	G1228	A1169	U1108	G1047	U987	A927	U859	U757	G671	G611
C1604	C1472	C1410	C1350	U1290	G1229	G1170	U1109	A1048	G988	A928	A860	U758	C672	U612
A1605	U1473	C1411	U1351	A1291	A1230	G1171	U1049	U1049	G989	A929	A861	U759	C673	U613
U1606	A1474	A1412	A1352	G1292	A1231	C1171	C1110	G1050	G990	G930	U862	U760	G674	G614
G1607	C1475	C1413	G1353	U1293	G1232	A1172	G1111	G1051	G991	A931	G871	U761	A675	U615
A1608	U1476	U1294	C1354	U1294	G1233	U1173	G1112	G1052	G992	C932	G872	U762	G676	U616
G1609	A1477	G1414	U1355	U1295	A1234	G1174	G1113	C1053	C993	G933	G873	U763	C677	G617
U1610	G1478	A1415	G1296	G1296	U1235	G1175	G1114	G1054	U994	A934	A874	U764	A678	G618
C1611	U1479	A1416	C1356	U1297	U1236	A1176	G1115	G1055	C995	A935	C875	U765	C679	A619
U1612	G1480	C1417	U1357	U1297	U1237	G1177	G1116	A1056	G996	C936	G876	U766	C680	G620
G1613	A1481	G1358	G1358	U1298	G1237	C1178	A1118	U1057	A997	A937	A877	U767	G681	U621
C1614	U1482	C1359	C1359	U1299	A1238	C1179	A1119	G1058	A998	A938	G877	U768	A682	G622
G1615	G1483	U1421	G1360	A1300	C1239	C1179	G1119	U1059	G999	C939	C879	U769	C683	A623
U1616	U1484	G1422	G1361	G1301	A1240	U1180	U1120	U1060	G999	U940	G880	U770	G684	A624
G1617	U1485	A1423	A1362	C1302	G1241	G1181	U1121	C1061	C1001	G941	G881	U771	U685	A625
U1618	U1486	G1425	G1363	A1242	A1242	G1182	U1122	C1062	G1002	C942	G882	U772	A686	A626

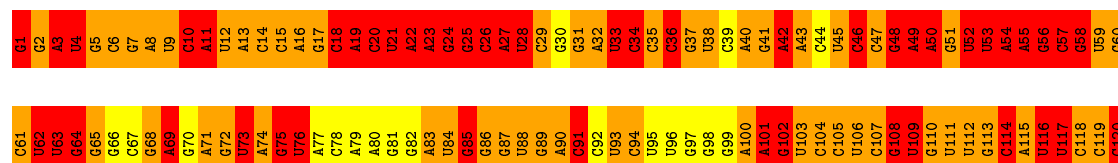
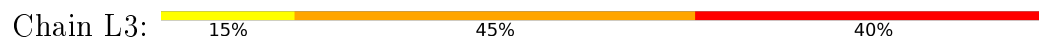


U1587	C1339	U1475	U1536	U1476	U1218	C1158	U1098	C1038	G974	C914	C854	G794	C734	G674
U1588	G1340	G1476	A1537	G1414	C1219	C1159	G1099	C1039	G975	G915	U855	C795	C735	C675
A1589	G1341	A1477	A1538	G1415	U1280	G1160	G1100	C1040	A976	A916	G856	C796	U736	G676
A1600	C1342	A1478	G1539	G1416	A1221	G1161	A1101	C1041	G977	A917	G857	U797	C737	U677
G1601	C1343	G1479	C1344	G1417	U1222	A1162	A1102	C1042	C978	A918	U858	G798	A738	G678
A1602	C1344	G1480	C1345	G1418	U1223	A1163	U1103	C1043	C979	G919	G859	U799	C739	C679
U1603	U1345	G1481	U1346	G1419	A1224	G1164	C1104	C1044	C980	A920	G860	C800	G740	G680
U1604	C1346	C1482	C1347	G1420	U1285	C1165	C1105	U1045	A981	C921	A861	G801	G741	A681
A1605	U1347	G1421	U1348	G1421	A1225	C1166	G1106	U1046	U982	U922	G862	G802	G742	G682
C1607	G1348	G1422	G1349	G1423	C1227	G1167	G1107	C1047	U983	A923	G863	G803	C743	U683
C1608	C1349	G1423	C1350	G1424	C1228	G1168	U1108	U1048	A984	A924	G864	A804	C744	C684
G1609	G1350	G1424	G1351	G1425	U1229	G1169	G1109	C1049	C985	U925	U865	C805	G745	G685
A1610	A1290	A1290	C1351	G1425	G1230	U1170	C1110	A1050	G986	C926	C866	C806	G746	A686
G1611	A1291	A1291	C1351	G1426	C1231	U1171	U1111	A1051	A987	G927	G867	C807	A747	C687
C1612	C1361	C1427	C1362	G1427	U1292	A1172	C1112	A1052	G988	A928	A868	G808	C748	G688
C1613	G1428	G1428	C1363	G1428	C1293	C1173	C1113	C1053	U989	A929	A869	A809	C749	G689
G1614	C1364	A1429	C1365	G1429	A1294	G1174	U1114	U1054	U990	C930	G870	A810	G750	G690
G1615	C1366	C1430	C1367	G1430	A1295	G1175	A1115	U1055	C991	C931	G871	A811	G751	U691
G1616	G1431	A1431	C1368	G1431	A1296	U1176	G1116	U1056	U992	A932	G872	G812	U752	U692
U1618	G1432	G1432	G1367	G1432	G1237	U1177	U1117	A1057	A993	U933	G873	A813	G753	C693
G1619	C1367	U1433	C1368	G1433	G1238	C1178	U1118	A1058	U994	C934	U874	A814	G754	U694
U1620	U1434	U1434	U1369	G1434	C1239	C1179	G1119	A1059	C995	U935	A875	G815	C755	G695
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C1622	A1436	A1436	A1371	G1436	G1241	A1181	C1121	A1061	G997	G937	U877	U817	G757	G697
C1623	G1371	G1371	C1302	U1437	U1242	A1182	C1122	G1062	G998	U938	G878	G818	G758	A698
G1624	U1372	U1372	C1303	G1438	C1243	C1183	A1123	G1063	U999	A939	A879	A819	C759	C699
G1625	C1373	G1439	G1304	U1440	A1244	U1184	U1124	U1064	A1000	G940	C880	A820	C760	C700
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G1637	G1387	U1451	G1316	U1451	A1256	U1196	A1136	G1076	U1012	C952	U892	G832	U772	A712
U1638	C1388	G1317	C1317	U1452	U1257	A1197	G1137	C1077	A1013	G953	C893	G833	G773	G713
C1639	C1389	C1318	C1318	U1453	C1258	A1198	A1138	U1078	G1014	A954	G894	G834	A774	A714
A1640	A1391	U1319	C1320	A1455	C1259	A1199	A1139	G1079	A1015	A955	U895	G835	A775	G715
G1641	U1392	G1320	G1260	A1456	G1260	A1200	C1140	C1080	G1016	G956	C896	G836	A776	A716
G1642	G1393	A1321	C1261	U1457	C1261	C1201	U1141	U1081	G1017	U957	U897	G837	G777	G717
A1643	C1394	A1322	U1262	U1458	U1262	C1202	G1142	U1082	C1018	U958	G898	G838	G778	C718
U1644	A1395	G1323	A1263	G1459	A1263	C1203	G1143	C1083	A1019	U959	A899	A839	U779	U719
G1645	C1398	G1325	G1265	U1461	G1265	C1205	G1145	G1085	C960	C960	U901	G841	C781	G720
U1646	A1399	G1326	A1267	U1462	G1266	A1206	A1146	U1086	U1021	C962	U902	C842	G782	G722
C1647	C1400	C1326	A1267	U1462	A1267	A1207	U1147	G1087	G1023	U963	G903	C843	A783	G723
G1648	C1401	G1329	U1268	U1465	G1268	A1208	G1148	A1088	G1024	C964	G904	A844	G784	A724
U1649	G1403	A1330	U1269	U1466	G1269	C1209	G1149	G1089	A965	G1025	G905	A845	U785	G725
A1651	G1404	C1331	G1270	U1467	G1270	G1210	G1150	C1090	A1026	G966	U906	A846	U786	C726
G1652	G1405	C1332	U1271	U1468	U1271	G1211	G1151	C1091	C1027	G967	A907	G847	G787	G727
A1653	C1333	G1333	G1272	U1469	G1272	U1212	G1152	G1092	G1028	A968	U908	G848	G788	G728
U1654	G1407	A1334	U1273	U1470	U1273	G1213	A1153	U1093	U1034	U969	A909	A849	G789	G729
G1655	C1408	C1335	A1274	U1471	A1274	U1214	U1154	G1094	U1035	A970	G910	A850	G790	A730
C1656	G1409	C1336	U1275	U1472	A1275	U1215	U1155	C1095	G1036	G971	G911	A851	C791	G731
G1657	A1410	C1337	C1276	U1473	C1276	G1216	A1156	C1096	C1037	C972	G912	C852	A792	G732
U1658	G1411	C1338	U1277	U1474	A1277	G1217	A1157	A1097	U1037	U973	G913	U853	C793	G733




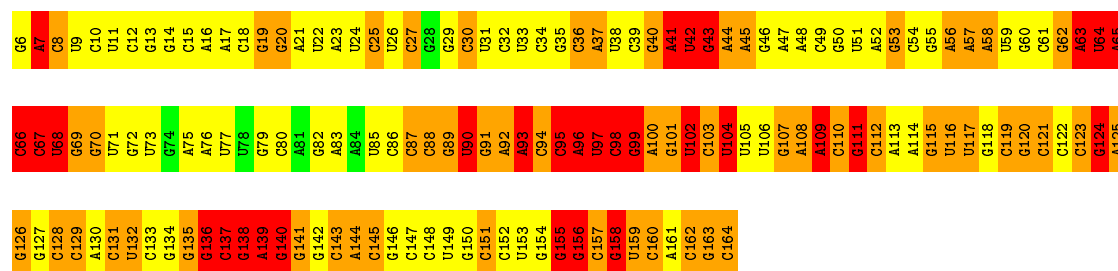



• Molecule 34: Wheat 5S DNA short repeating unit



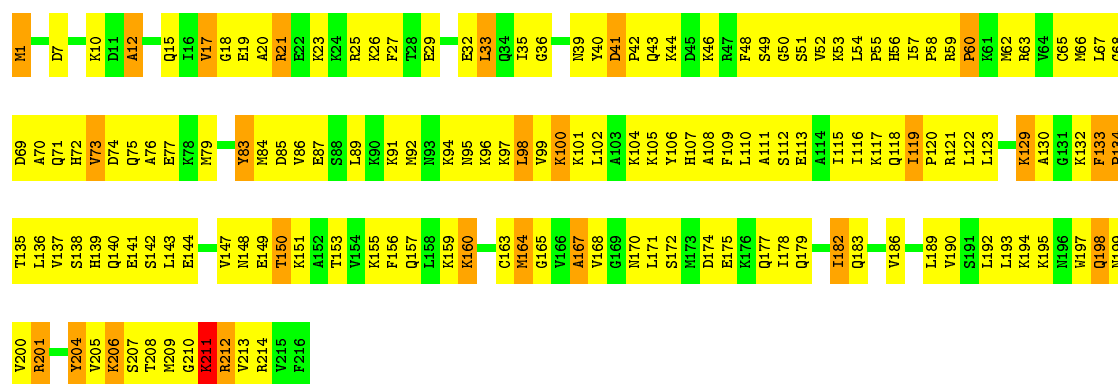
• Molecule 35: Triticum aestivum E-2055 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene, complete sequence; and internal transcribed spacer 2, partial sequence

Chain L2: 




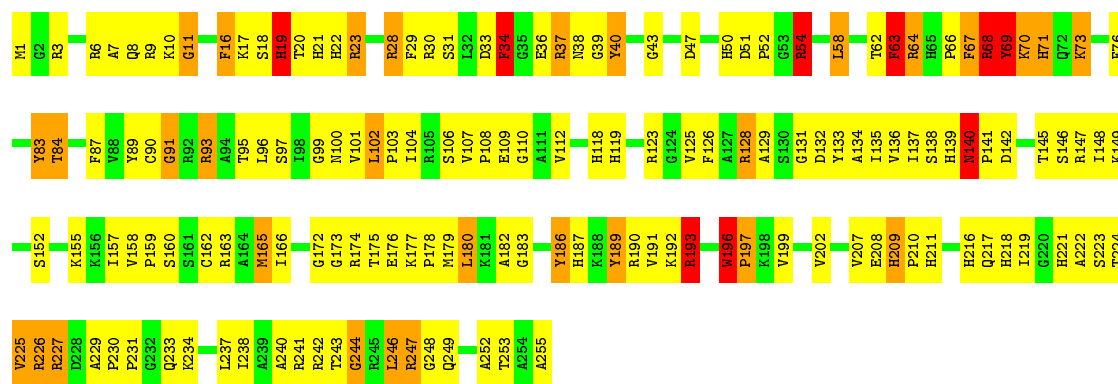
• Molecule 36: Ribosomal protein

Chain LA: 



• Molecule 37: 60S ribosomal protein L2

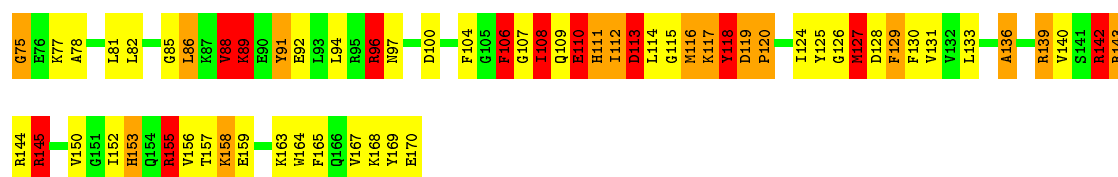
Chain LB: 



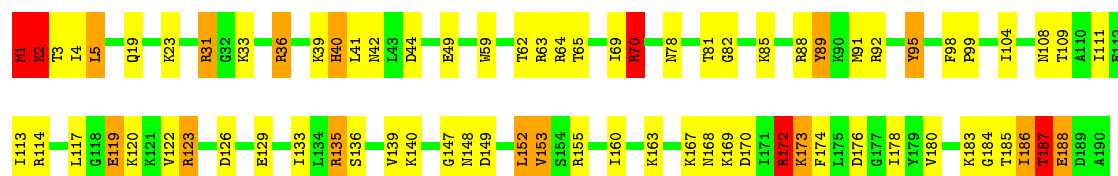
• Molecule 38: Ribosomal protein L11

Chain LE: 

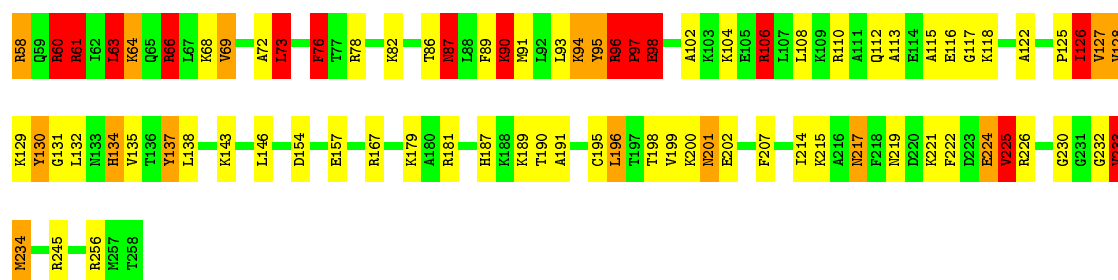




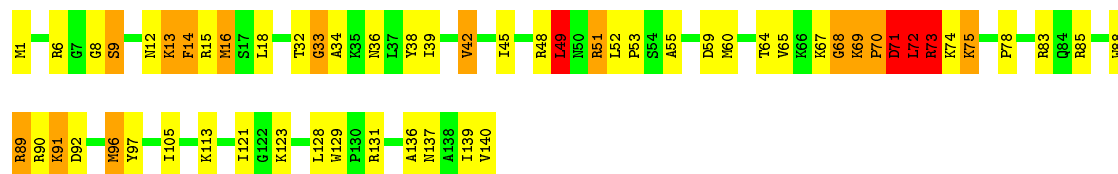
• Molecule 39: 60S ribosomal protein L9



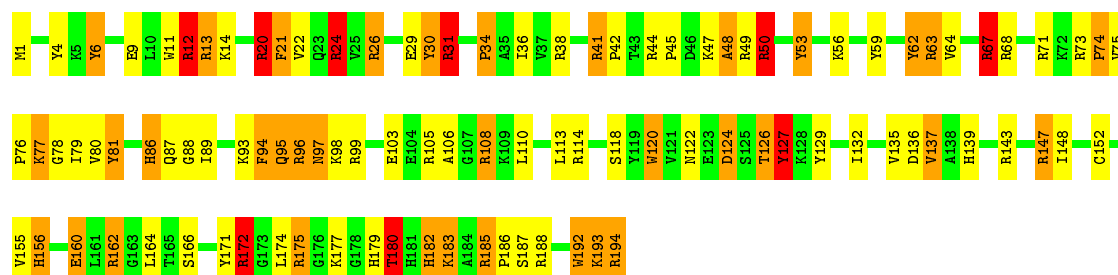
• Molecule 40: 60S ribosomal protein L7a



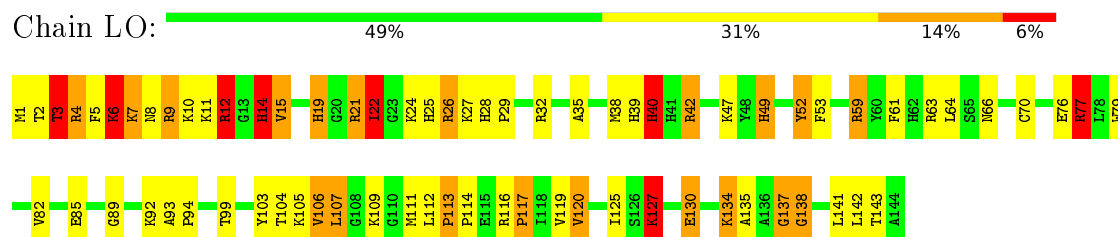
• Molecule 41: Ribosomal Pr 117



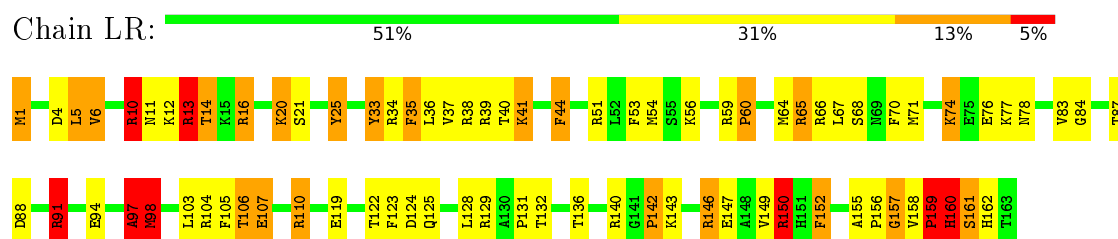
• Molecule 42: Ribosomal protein L15



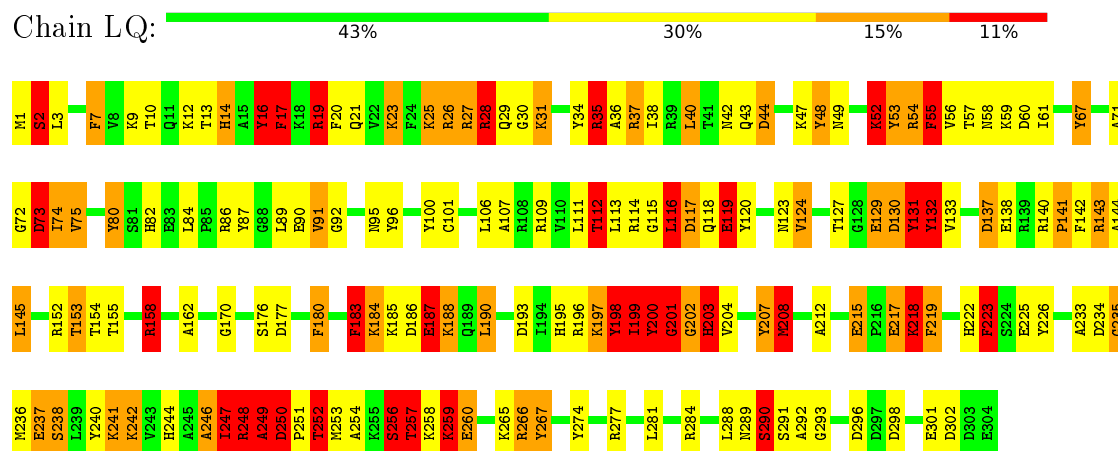
- Molecule 43: 60S ribosomal protein L27a-3



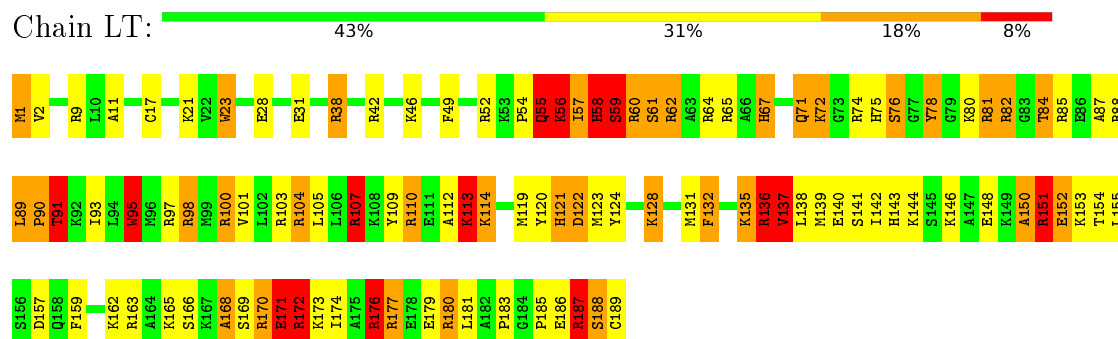
- Molecule 44: 60S ribosomal protein L18



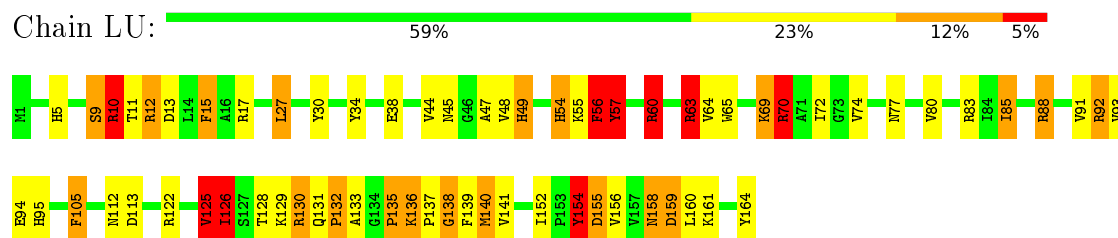
- Molecule 45: 60S ribosomal protein L5



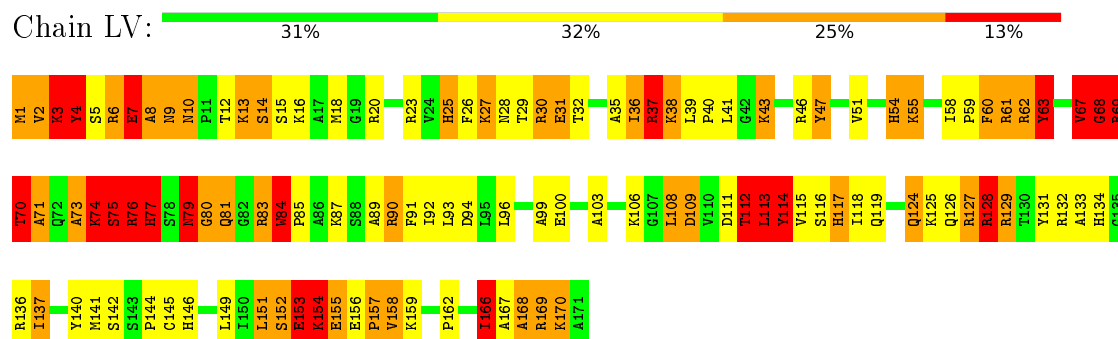
- Molecule 46: Ribosomal protein L19



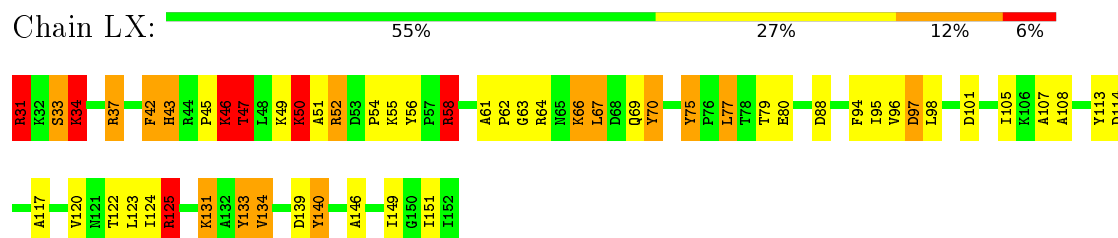
- Molecule 47: 60S ribosomal protein L21



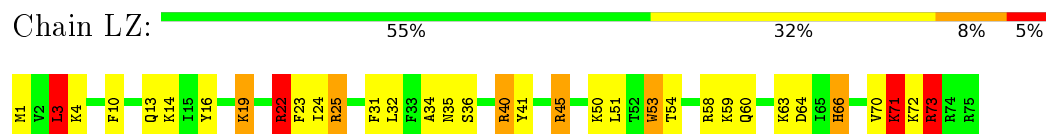
• Molecule 48: 60S ribosomal protein L17



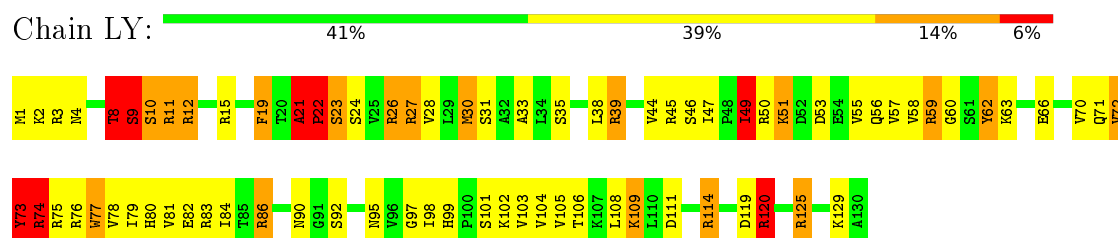
• Molecule 49: 60S ribosomal protein L23a



• Molecule 50: 60S ribosomal protein L24



• Molecule 51: 60S ribosomal protein L26



• Molecule 52: 60S ribosomal protein l28





- Molecule 53: 60S ribosomal protein L29

Chain Ld: 83% 9% 9%



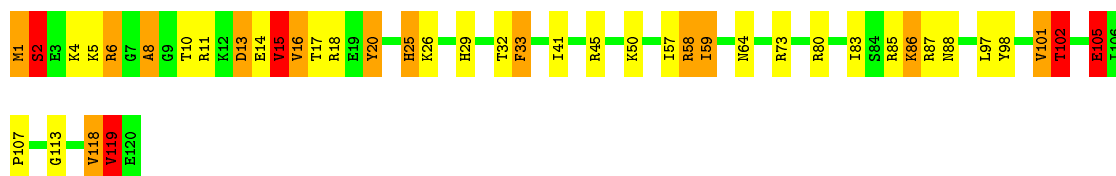
- Molecule 54: 60S ribosomal protein L30

Chain Lf: 71% 19% 7% .



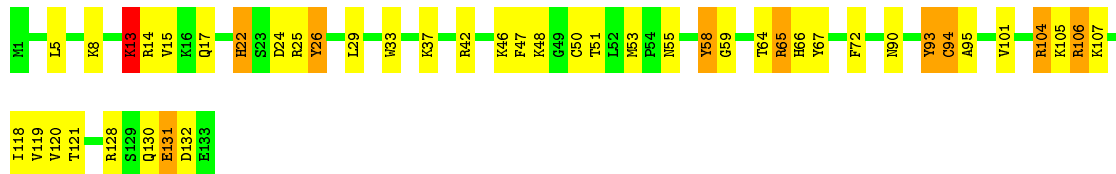
- Molecule 55: 60S ribosomal protein L31

Chain Lg: 64% 21% 11% .



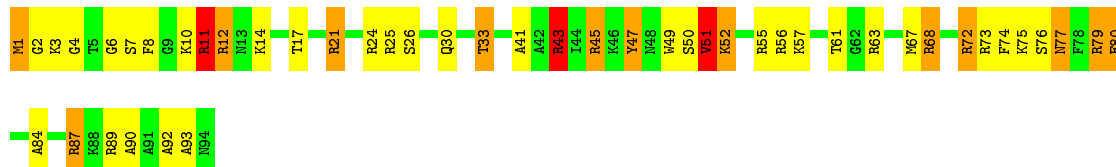
- Molecule 56: Ribosomal L32

Chain Lh: 66% 26% 7% .



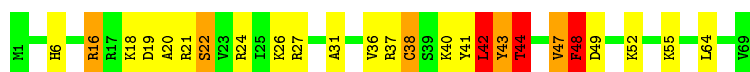
- Molecule 57: Ribosomal protein L37

Chain Ll: 50% 33% 14% .



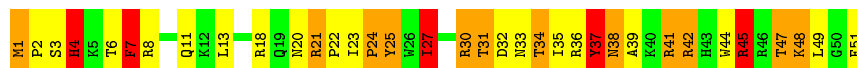
- Molecule 58: 60S ribosomal protein L38

Chain Ln: 64% 25% 7% .



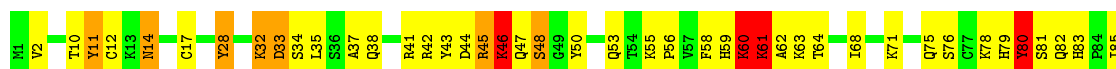
- Molecule 59: Ribosomal protein L39

Chain Lo: 31% 35% 24% 10%



- Molecule 60: 60S ribosomal protein L44

Chain Lr: 50% 35% 11% 4%



- Molecule 61: Unknown 60S wheat germ ribosome protein 1

Chain Lq: 56% 32% 12%



- Molecule 62: Unknown 60S wheat germ ribosome protein 2

Chain Ly: 95% 5%



- Molecule 62: Unknown 60S wheat germ ribosome protein 2

Chain Lx: 80% 20%



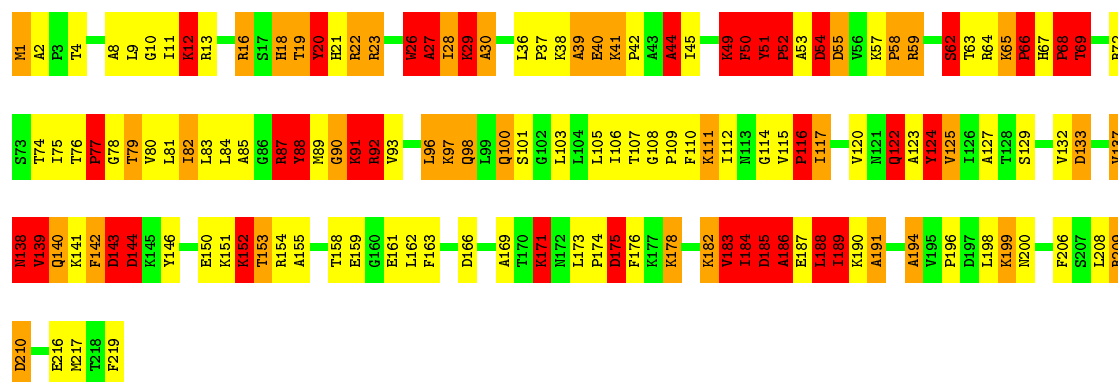
- Molecule 63: Unknown 60S wheat germ ribosome protein 3

Chain Lz: 86% 14%



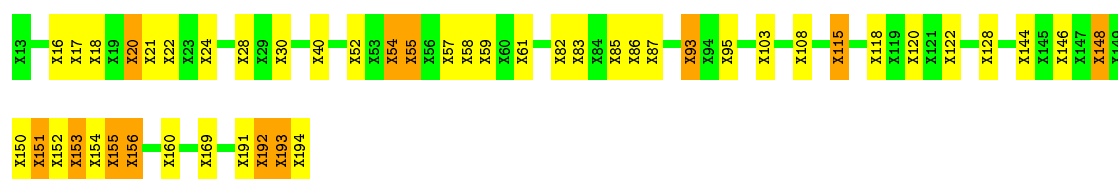
- Molecule 64: 60S ribosomal protein L6

Chain LG: 34% 33% 17% 16%



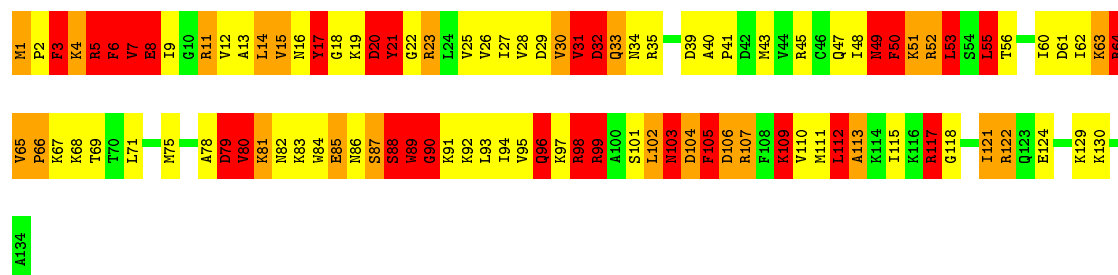
- Molecule 65: Unknown 60S wheat germ ribosome protein 5

Chain LL: 74% 19% 7%



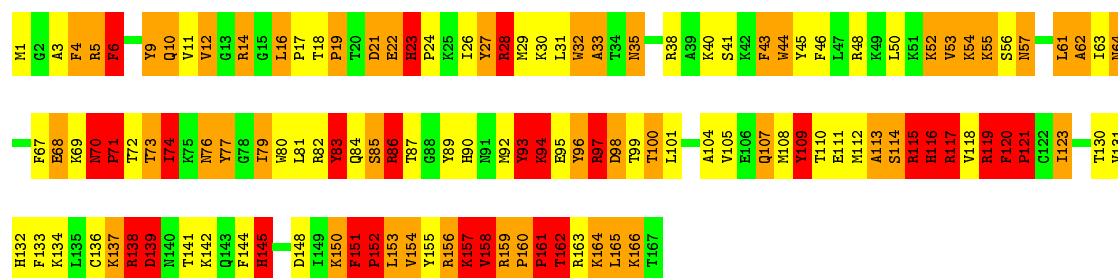
- Molecule 66: Unknown 60S wheat germ ribosome protein 6

Chain LN: 25% 37% 17% 21%



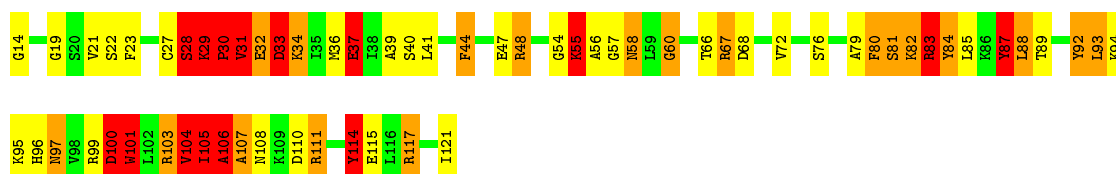
- Molecule 67: 60S ribosomal protein L18a

Chain LS: 25% 31% 28% 16%



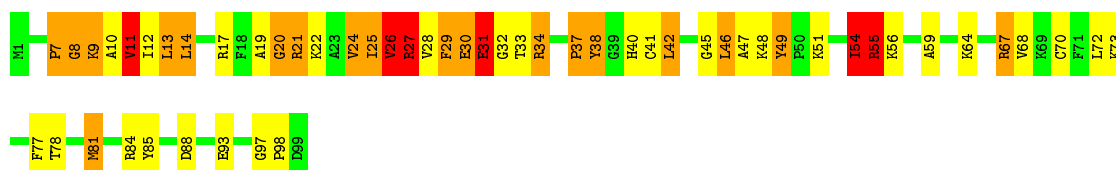
- Molecule 68: 60S ribosomal protein L22

Chain LW: 42% 27% 18% 14%



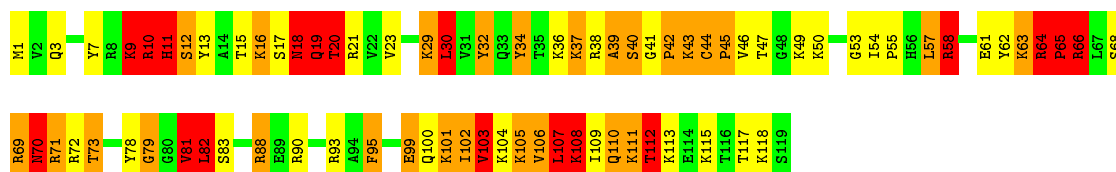
- Molecule 69: 60S ribosomal protein L27

Chain La: 45% 29% 19% 6%



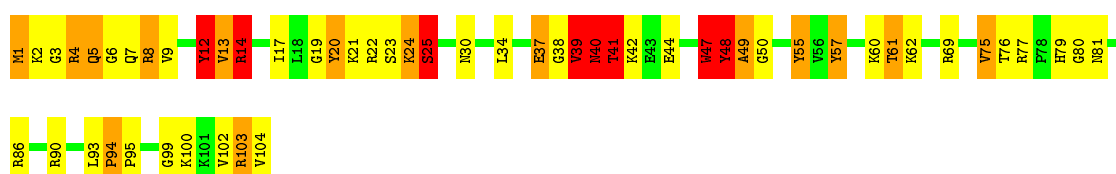
- Molecule 70: Ribosomal protein l34

Chain Li: 34% 28% 23% 15%



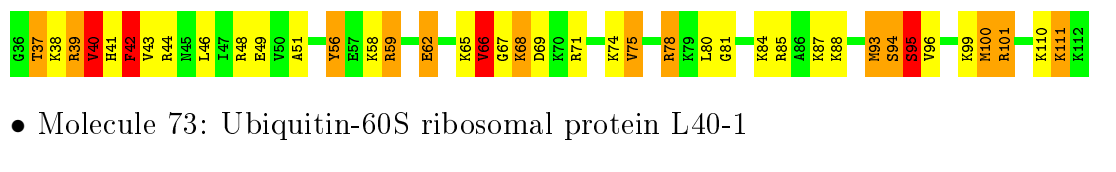
- Molecule 71: ribosomal protein L35A

Chain Lj: 47% 31% 14% 8%



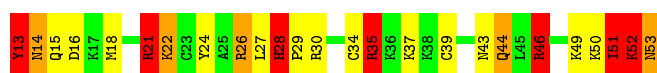
- Molecule 72: 60S ribosomal protein L36

Chain Lk: 48% 30% 17% 5%

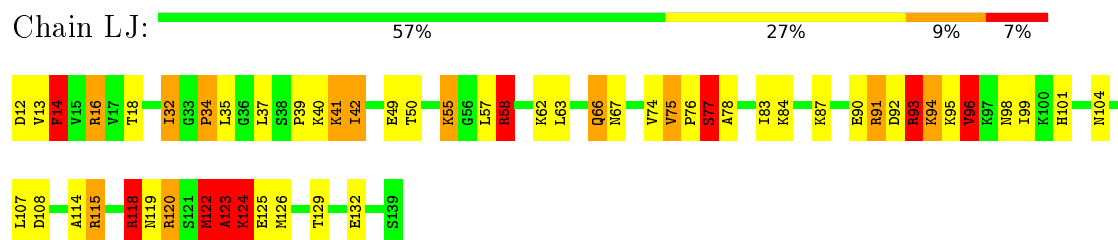


- Molecule 73: Ubiquitin-60S ribosomal protein L40-1

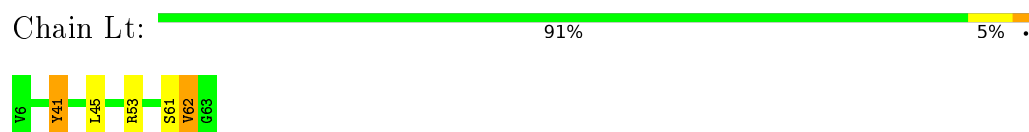
Chain Lp: 39% 32% 12% 17%



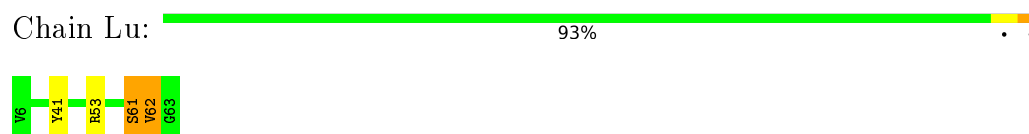
- Molecule 74: 60S ribosomal protein L12



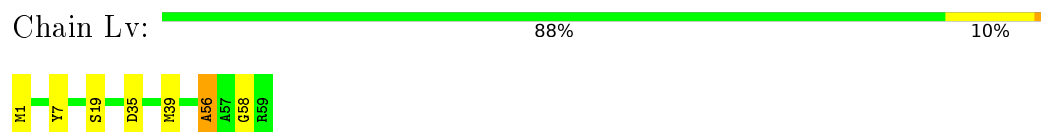
- Molecule 75: Ribosomal protein P1



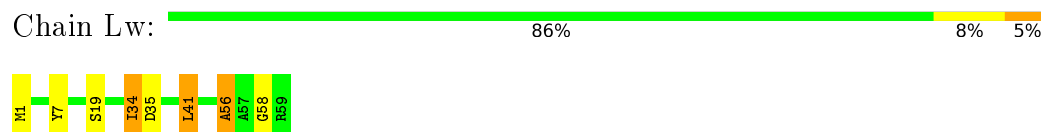
- Molecule 75: Ribosomal protein P1



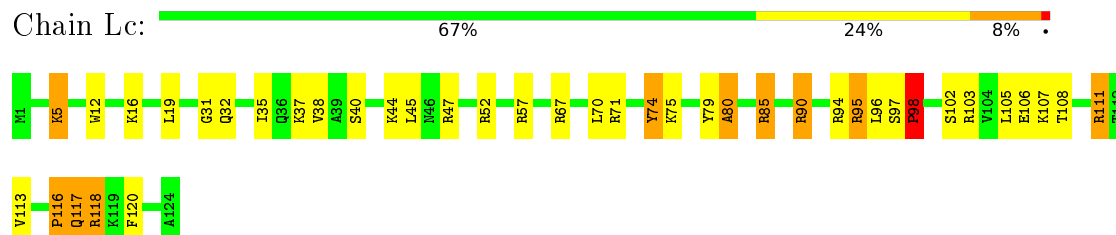
- Molecule 76: 60S acidic ribosomal protein P2A



- Molecule 76: 60S acidic ribosomal protein P2A

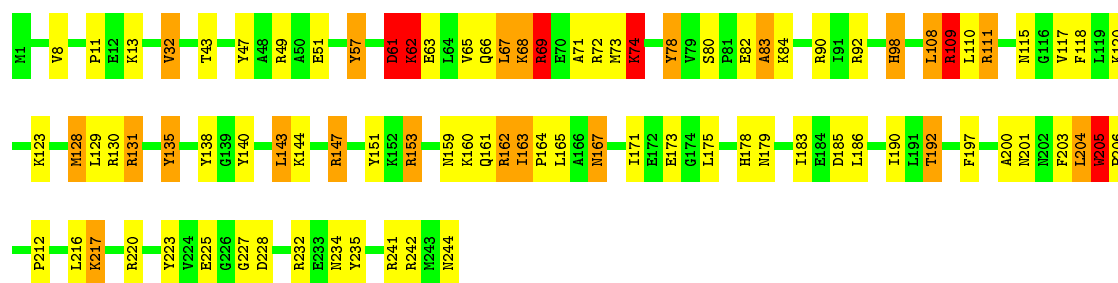


- Molecule 77: 60S ribosomal protein L35



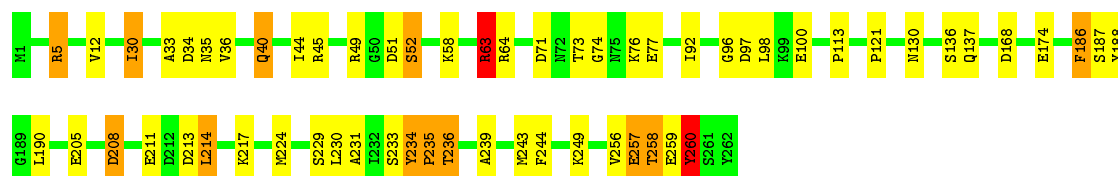
- Molecule 78: Ribosomal protein L7





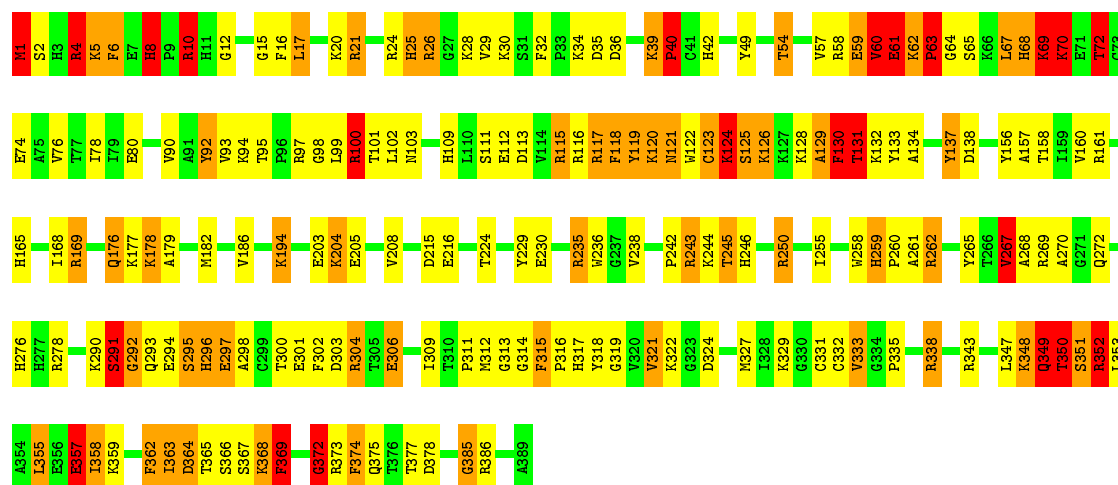
- Molecule 79: 60S acidic ribosomal protein P0

Chain Ls: 77% 18% 5% .



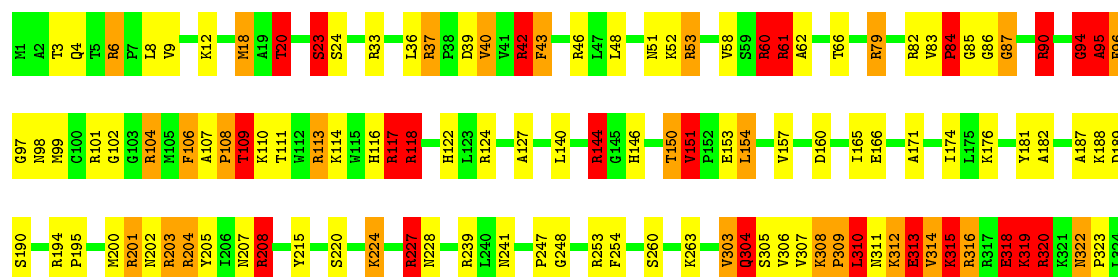
- Molecule 80: Ribosomal protein L3

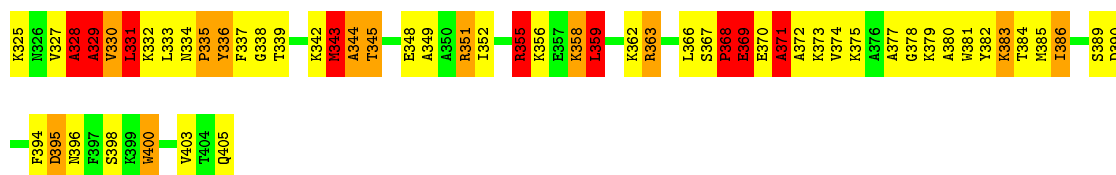
Chain LC: 50% 30% 14% 6%



- Molecule 81: 60S ribosomal protein L4/L1

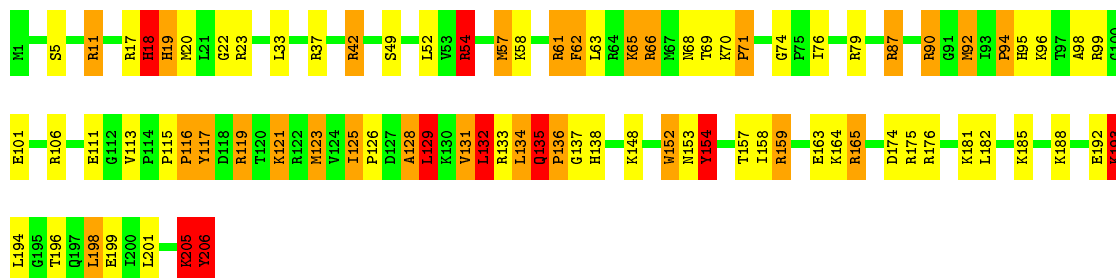
Chain LD: 52% 29% 10% 9%





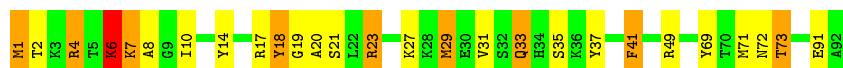
- Molecule 82: Ribosomal protein L13a

Chain LK: 59% 23% 13%



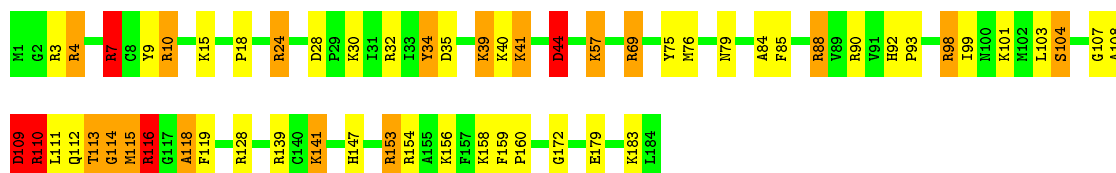
- Molecule 83: 60S ribosomal protein L37a, expressed

Chain Lm: 71% 18% 10%



- Molecule 84: 60S ribosomal protein L10-1

Chain LI: 68% 20% 9%



4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of subtomograms used	106	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	150	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	41176	Depositor
Image detector	FEI FALCON I (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	Sa	1.90	33/2897 (1.1%)	2.28	124/3917 (3.2%)
10	SL	1.68	18/965 (1.9%)	2.24	35/1271 (2.8%)
11	SM	3.93	25/1185 (2.1%)	3.78	113/1574 (7.2%)
12	SO	0.90	2/994 (0.2%)	2.31	29/1332 (2.2%)
13	SQ	1.81	23/1145 (2.0%)	3.16	96/1531 (6.3%)
14	SP	1.91	10/653 (1.5%)	2.85	41/871 (4.7%)
15	SS	1.88	24/1179 (2.0%)	3.02	80/1586 (5.0%)
16	SR	1.50	6/727 (0.8%)	1.91	29/975 (3.0%)
17	SV	1.18	3/748 (0.4%)	1.77	31/994 (3.1%)
19	SY	1.98	8/443 (1.8%)	2.41	20/592 (3.4%)
2	SA	1.63	11/1988 (0.6%)	2.25	83/2697 (3.1%)
20	SZ	1.54	4/476 (0.8%)	2.82	22/623 (3.5%)
23	SU	2.45	34/745 (4.6%)	3.90	126/988 (12.8%)
24	SX	1.65	9/382 (2.4%)	1.96	15/515 (2.9%)
25	SC	3.58	34/1563 (2.2%)	3.62	136/2086 (6.5%)
27	SH	1.53	10/1060 (0.9%)	2.45	52/1419 (3.7%)
28	SN	2.18	7/317 (2.2%)	2.71	27/414 (6.5%)
29	ST	1.52	4/659 (0.6%)	2.09	29/884 (3.3%)
3	SB	2.02	27/1555 (1.7%)	2.91	115/2077 (5.5%)
30	S3	2.62	16/264 (6.1%)	2.41	16/407 (3.9%)
31	S2	3.33	165/1785 (9.2%)	2.83	192/2779 (6.9%)
32	S1	2.97	2435/37672 (6.5%)	2.60	3313/58357 (5.7%)
33	L1	3.27	5613/77720 (7.2%)	2.85	8211/121026 (6.8%)
34	L3	3.13	166/2868 (5.8%)	2.95	328/4468 (7.3%)
35	L2	3.74	298/3553 (8.4%)	3.05	429/5515 (7.8%)
36	LA	1.27	7/1741 (0.4%)	1.66	27/2323 (1.2%)
37	LB	1.57	15/1979 (0.8%)	2.30	63/2659 (2.4%)
38	LE	2.68	30/1397 (2.1%)	2.43	86/1864 (4.6%)
39	LF	1.25	10/1519 (0.7%)	1.98	45/2042 (2.2%)
4	SD	1.94	35/1637 (2.1%)	3.00	96/2202 (4.4%)
40	LH	1.24	9/1586 (0.6%)	2.43	41/2120 (1.9%)
41	LM	1.36	7/1036 (0.7%)	1.97	40/1388 (2.9%)
42	LP	1.72	23/1669 (1.4%)	2.57	80/2235 (3.6%)
43	LO	1.49	11/1113 (1.0%)	2.62	32/1485 (2.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
44	LR	1.36	7/1303 (0.5%)	2.09	41/1748 (2.3%)
45	LQ	1.69	24/2438 (1.0%)	3.26	131/3271 (4.0%)
46	LT	1.73	12/1590 (0.8%)	2.57	88/2100 (4.2%)
47	LU	1.75	9/1290 (0.7%)	2.66	55/1728 (3.2%)
48	LV	2.47	27/1359 (2.0%)	3.07	111/1816 (6.1%)
49	LX	1.71	9/1002 (0.9%)	2.28	42/1340 (3.1%)
5	SE	2.09	32/2068 (1.5%)	2.98	73/2776 (2.6%)
50	LZ	1.42	5/591 (0.8%)	2.45	20/782 (2.6%)
51	LY	1.65	15/1061 (1.4%)	2.37	37/1418 (2.6%)
52	Lb	1.79	9/585 (1.5%)	2.16	31/786 (3.9%)
53	Ld	1.12	0/201	1.55	3/261 (1.1%)
54	Lf	1.22	1/836 (0.1%)	1.85	23/1121 (2.1%)
55	Lg	1.52	7/954 (0.7%)	2.14	42/1272 (3.3%)
56	Lh	1.50	4/1108 (0.4%)	2.35	37/1477 (2.5%)
57	Li	1.67	8/738 (1.1%)	2.57	49/974 (5.0%)
58	Ln	1.11	1/554 (0.2%)	2.46	15/738 (2.0%)
59	Lo	1.87	7/472 (1.5%)	3.05	44/627 (7.0%)
6	SF	0.99	2/1505 (0.1%)	1.58	29/2027 (1.4%)
60	Lr	1.99	14/853 (1.6%)	3.17	41/1124 (3.6%)
61	Lq	1.77	5/239 (2.1%)	3.70	15/302 (5.0%)
64	LG	1.72	25/1765 (1.4%)	3.20	140/2372 (5.9%)
66	LN	1.57	13/1094 (1.2%)	3.36	81/1461 (5.5%)
67	LS	1.93	21/1457 (1.4%)	2.83	120/1957 (6.1%)
68	LW	1.76	14/850 (1.6%)	2.74	55/1135 (4.8%)
69	La	1.69	12/743 (1.6%)	2.67	65/992 (6.6%)
7	SI	1.85	14/1034 (1.4%)	2.36	42/1379 (3.0%)
70	Li	1.87	15/979 (1.5%)	2.91	91/1305 (7.0%)
71	Lj	1.89	20/811 (2.5%)	3.14	58/1083 (5.4%)
72	Lk	1.74	7/618 (1.1%)	3.73	52/809 (6.4%)
73	Lp	2.33	11/349 (3.2%)	3.33	37/458 (8.1%)
74	LJ	1.36	1/967 (0.1%)	2.08	29/1298 (2.2%)
75	Lt	0.83	0/438	1.67	4/596 (0.7%)
75	Lu	0.69	0/438	1.28	2/596 (0.3%)
76	Lv	0.83	0/444	1.42	6/596 (1.0%)
76	Lw	0.97	1/444 (0.2%)	1.61	8/596 (1.3%)
77	Lc	1.69	10/1017 (1.0%)	2.53	27/1351 (2.0%)
78	Le	1.52	13/2018 (0.6%)	2.44	77/2702 (2.8%)
79	Ls	0.90	0/2023	1.71	40/2739 (1.5%)
8	SJ	1.78	13/896 (1.5%)	2.78	34/1193 (2.8%)
80	LC	1.56	35/3168 (1.1%)	3.16	134/4234 (3.2%)
81	LD	1.47	27/2919 (0.9%)	3.04	129/3924 (3.3%)
82	LK	1.33	12/1678 (0.7%)	2.08	44/2246 (2.0%)
83	Lm	1.32	4/724 (0.6%)	2.06	28/958 (2.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
84	LI	0.93	6/1499 (0.4%)	1.88	31/2001 (1.5%)
9	SK	2.29	11/839 (1.3%)	2.92	43/1120 (3.8%)
All	All	2.71	9615/207179 (4.6%)	2.73	16506/304005 (5.4%)

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
1	Sa	1	25
10	SL	0	11
11	SM	1	24
12	SO	0	14
13	SQ	1	37
14	SP	3	6
15	SS	1	25
16	SR	0	4
17	SV	0	5
18	SW	0	12
19	SY	0	6
2	SA	1	24
20	SZ	1	9
21	Sc	0	1
23	SU	3	38
24	SX	0	3
25	SC	6	43
26	SG	8	43
27	SH	0	11
28	SN	1	6
29	ST	2	6
3	SB	0	32
32	S1	9	0
33	L1	49	0
34	L3	2	0
35	L2	4	0
36	LA	0	4
37	LB	0	25
38	LE	1	18
39	LF	0	15
4	SD	1	31
40	LH	0	28

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	LM	0	5
42	LP	0	29
43	LO	0	20
44	LR	0	27
45	LQ	4	59
46	LT	1	26
47	LU	1	21
48	LV	0	29
49	LX	1	11
5	SE	0	23
50	LZ	0	12
51	LY	0	12
52	Lb	0	2
53	Ld	0	2
54	Lf	0	6
55	Lg	0	11
56	Lh	1	13
57	Li	0	11
58	Ln	0	11
59	Lo	0	12
6	SF	0	14
60	Lr	1	28
61	Lq	0	5
62	Lx	0	5
62	Ly	0	1
63	Lz	0	2
64	LG	2	59
65	LL	1	39
66	LN	2	21
67	LS	2	41
68	LW	0	24
69	La	0	28
7	SI	0	5
70	Li	2	43
71	Lj	0	26
72	Lk	1	10
73	Lp	2	10
74	LJ	1	12
75	Lt	0	2
75	Lu	0	3
76	Lv	0	1
76	Lw	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
77	Lc	0	16
78	Le	0	23
79	Ls	1	13
8	SJ	0	16
80	LC	5	58
81	LD	2	58
82	LK	2	26
83	Lm	0	12
84	LI	0	17
9	SK	0	14
All	All	127	1482

The worst 5 of 9615 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	SM	126	TYR	CD2-CE2	112.90	3.08	1.39
25	SC	171	PRO	N-CD	81.71	2.62	1.47
32	S1	1315	U	O3'-P	-72.15	0.74	1.61
32	S1	860	A	O3'-P	-63.70	0.84	1.61
33	L1	2398	A	O3'-P	-57.14	0.92	1.61

The worst 5 of 16506 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	SE	30	ARG	NE-CZ-NH2	-75.84	82.38	120.30
66	LN	64	ARG	NE-CZ-NH2	-64.81	87.90	120.30
11	SM	126	TYR	CZ-CE2-CD2	-63.49	62.66	119.80
33	L1	1395	A	O4'-C1'-N9	60.43	156.54	108.20
33	L1	62	A	O4'-C1'-N9	55.67	152.73	108.20

5 of 127 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Sa	128	LEU	CA
2	SA	199	TRP	CA
4	SD	56	LEU	CA
11	SM	116	LYS	CA
13	SQ	139	ASP	CA

5 of 1482 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Sa	105	LYS	Peptide
1	Sa	26	ARG	Sidechain
1	Sa	63	GLN	Sidechain
1	Sa	70	TYR	Sidechain
1	Sa	82	VAL	Mainchain

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	Sa	2842	0	2691	0	0
2	SA	1946	0	1876	281	0
3	SB	1539	0	1537	60	0
4	SD	1607	0	1675	235	0
5	SE	2028	0	2104	259	0
6	SF	1485	0	1525	103	0
7	SI	1017	0	1080	68	0
8	SJ	887	0	861	48	0
9	SK	830	0	806	104	0
10	SL	952	0	875	82	0
11	SM	1167	0	1141	137	0
12	SO	977	0	1056	106	0
13	SQ	1129	0	1160	66	0
14	SP	639	0	625	269	0
15	SS	1155	0	1173	103	0
16	SR	711	0	758	24	0
17	SV	740	0	746	196	0
18	SW	460	0	111	24	0
19	SY	442	0	467	34	0
20	SZ	469	0	500	24	0
21	Sc	126	0	26	0	0
22	Sb	181	0	39	0	0
23	SU	732	0	740	108	0
24	SX	375	0	367	96	0
25	SC	1535	0	1556	106	0
26	SG	716	0	160	74	0
27	SH	1042	0	1086	309	0
28	SN	313	0	269	33	0
29	ST	650	0	636	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	S3	236	0	120	15	0
31	S2	1599	0	797	277	0
32	S1	33897	0	16592	1570	0
33	L1	69592	0	34889	2810	0
34	L3	2565	0	1293	389	0
35	L2	3192	0	1590	112	0
36	LA	1718	0	1841	311	0
37	LB	1933	0	1932	305	0
38	LE	1376	0	1417	206	0
39	LF	1500	0	1564	88	0
40	LH	1564	0	1658	26	0
41	LM	1020	0	1059	88	0
42	LP	1630	0	1704	74	0
43	LO	1086	0	1127	63	0
44	LR	1284	0	1376	74	0
45	LQ	2395	0	2337	196	0
46	LT	1569	0	1676	382	0
47	LU	1266	0	1268	26	0
48	LV	1335	0	1337	168	0
49	LX	987	0	1083	37	0
50	LZ	578	0	566	27	0
51	LY	1048	0	1130	66	0
52	Lb	576	0	616	0	0
53	Ld	199	0	193	0	0
54	Lf	825	0	830	0	0
55	Lg	944	0	992	0	0
56	Lh	1089	0	1164	0	0
57	Li	725	0	718	0	0
58	Ln	547	0	578	0	0
59	Lo	460	0	490	0	0
60	Lr	838	0	887	0	0
61	Lq	238	0	289	0	0
62	Lx	101	0	24	0	0
62	Ly	101	0	23	0	0
63	Lz	71	0	16	0	0
64	LG	1730	0	1824	123	0
65	LL	910	0	202	82	0
66	LN	1081	0	1170	199	0
67	LS	1419	0	1465	179	0
68	LW	839	0	863	36	0
69	La	732	0	754	0	0
70	Li	964	0	1053	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	Lj	797	0	804	0	0
72	Lk	613	0	684	0	0
73	Lp	344	0	371	0	0
74	LJ	959	0	1039	22	0
75	Lt	432	0	463	0	0
75	Lu	432	0	463	0	0
76	Lv	441	0	453	0	0
76	Lw	441	0	453	0	0
77	Lc	1006	0	1100	0	0
78	Le	1984	0	2090	0	0
79	Ls	1993	0	2086	0	0
80	LC	3102	0	3191	69	0
81	LD	2866	0	2967	261	0
82	LK	1650	0	1771	118	0
83	Lm	715	0	756	0	0
84	LI	1468	0	1506	83	0
All	All	195694	0	140350	8317	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 30.

The worst 5 of 8317 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)
38:LE:91:TYR:CG	38:LE:91:TYR:CD1	1.78	1.70
38:LE:91:TYR:CD2	38:LE:91:TYR:CE2	1.75	1.69
38:LE:91:TYR:CZ	38:LE:91:TYR:CE2	1.80	1.68
38:LE:91:TYR:CD1	38:LE:91:TYR:CE1	1.78	1.68
17:SV:48:TYR:CD1	17:SV:81:ILE:HG23	1.16	1.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Sa	376/380 (99%)	330 (88%)	24 (6%)	22 (6%)	2	27
2	SA	258/260 (99%)	194 (75%)	31 (12%)	33 (13%)	0	8
3	SB	206/208 (99%)	117 (57%)	35 (17%)	54 (26%)	0	1
4	SD	198/200 (99%)	164 (83%)	17 (9%)	17 (9%)	1	17
5	SE	261/263 (99%)	186 (71%)	45 (17%)	30 (12%)	0	9
6	SF	189/191 (99%)	157 (83%)	25 (13%)	7 (4%)	4	38
7	SI	124/126 (98%)	90 (73%)	17 (14%)	17 (14%)	0	6
8	SJ	126/128 (98%)	103 (82%)	14 (11%)	9 (7%)	1	22
9	SK	117/119 (98%)	85 (73%)	13 (11%)	19 (16%)	0	5
10	SL	140/142 (99%)	93 (66%)	18 (13%)	29 (21%)	0	3
11	SM	150/152 (99%)	101 (67%)	22 (15%)	27 (18%)	0	4
12	SO	119/121 (98%)	95 (80%)	11 (9%)	13 (11%)	0	11
13	SQ	139/141 (99%)	87 (63%)	27 (19%)	25 (18%)	0	4
14	SP	83/85 (98%)	64 (77%)	12 (14%)	7 (8%)	1	18
15	SS	144/146 (99%)	119 (83%)	13 (9%)	12 (8%)	1	18
16	SR	89/91 (98%)	65 (73%)	15 (17%)	9 (10%)	1	14
17	SV	98/100 (98%)	70 (71%)	12 (12%)	16 (16%)	0	5
19	SY	56/58 (97%)	38 (68%)	8 (14%)	10 (18%)	0	4
20	SZ	60/62 (97%)	43 (72%)	9 (15%)	8 (13%)	0	7
23	SU	96/98 (98%)	70 (73%)	12 (12%)	14 (15%)	0	6
24	SX	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	18
25	SC	193/195 (99%)	127 (66%)	34 (18%)	32 (17%)	0	5
27	SH	128/130 (98%)	100 (78%)	17 (13%)	11 (9%)	1	17
28	SN	46/48 (96%)	30 (65%)	4 (9%)	12 (26%)	0	1
29	ST	80/82 (98%)	67 (84%)	4 (5%)	9 (11%)	0	10
36	LA	214/216 (99%)	191 (89%)	14 (6%)	9 (4%)	3	34
37	LB	253/255 (99%)	224 (88%)	18 (7%)	11 (4%)	3	34
38	LE	168/170 (99%)	129 (77%)	16 (10%)	23 (14%)	0	6
39	LF	188/190 (99%)	165 (88%)	16 (8%)	7 (4%)	4	38
40	LH	199/201 (99%)	149 (75%)	26 (13%)	24 (12%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LM	138/140 (99%)	123 (89%)	9 (6%)	6 (4%)	3	34
42	LP	192/194 (99%)	169 (88%)	18 (9%)	5 (3%)	7	45
43	LO	142/144 (99%)	106 (75%)	17 (12%)	19 (13%)	0	7
44	LR	161/163 (99%)	127 (79%)	18 (11%)	16 (10%)	1	14
45	LQ	302/304 (99%)	218 (72%)	39 (13%)	45 (15%)	0	5
46	LT	187/189 (99%)	167 (89%)	12 (6%)	8 (4%)	3	34
47	LU	162/164 (99%)	136 (84%)	18 (11%)	8 (5%)	3	31
48	LV	169/171 (99%)	131 (78%)	20 (12%)	18 (11%)	0	11
49	LX	120/122 (98%)	98 (82%)	12 (10%)	10 (8%)	1	18
50	LZ	73/75 (97%)	53 (73%)	13 (18%)	7 (10%)	1	15
51	LY	128/130 (98%)	113 (88%)	9 (7%)	6 (5%)	3	32
52	Lb	71/73 (97%)	48 (68%)	12 (17%)	11 (16%)	0	5
53	Ld	21/23 (91%)	18 (86%)	2 (10%)	1 (5%)	3	32
54	Lf	110/112 (98%)	95 (86%)	8 (7%)	7 (6%)	2	25
55	Lg	118/120 (98%)	96 (81%)	13 (11%)	9 (8%)	1	20
56	Lh	131/133 (98%)	113 (86%)	9 (7%)	9 (7%)	1	23
57	Ll	92/94 (98%)	60 (65%)	18 (20%)	14 (15%)	0	5
58	Ln	67/69 (97%)	51 (76%)	11 (16%)	5 (8%)	1	21
59	Lo	49/51 (96%)	33 (67%)	6 (12%)	10 (20%)	0	3
60	Lr	103/105 (98%)	75 (73%)	16 (16%)	12 (12%)	0	9
61	Lq	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
64	LG	217/219 (99%)	149 (69%)	24 (11%)	44 (20%)	0	3
66	LN	132/134 (98%)	96 (73%)	15 (11%)	21 (16%)	0	5
67	LS	165/167 (99%)	115 (70%)	24 (14%)	26 (16%)	0	5
68	LW	106/108 (98%)	73 (69%)	15 (14%)	18 (17%)	0	5
69	La	97/99 (98%)	68 (70%)	15 (16%)	14 (14%)	0	6
70	Li	117/119 (98%)	72 (62%)	13 (11%)	32 (27%)	0	0
71	Lj	102/104 (98%)	74 (72%)	17 (17%)	11 (11%)	0	11
72	Lk	75/77 (97%)	60 (80%)	5 (7%)	10 (13%)	0	7
73	Lp	39/41 (95%)	28 (72%)	8 (20%)	3 (8%)	1	20
74	LJ	126/128 (98%)	97 (77%)	15 (12%)	14 (11%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	Lt	56/58 (97%)	54 (96%)	1 (2%)	1 (2%)	11	53
75	Lu	56/58 (97%)	54 (96%)	1 (2%)	1 (2%)	11	53
76	Lv	57/59 (97%)	54 (95%)	2 (4%)	1 (2%)	11	53
76	Lw	57/59 (97%)	54 (95%)	2 (4%)	1 (2%)	11	53
77	Lc	122/124 (98%)	106 (87%)	7 (6%)	9 (7%)	1	21
78	Le	239/244 (98%)	212 (89%)	17 (7%)	10 (4%)	3	34
79	Ls	260/262 (99%)	233 (90%)	17 (6%)	10 (4%)	4	37
80	LC	387/389 (100%)	298 (77%)	43 (11%)	46 (12%)	0	9
81	LD	368/372 (99%)	306 (83%)	38 (10%)	24 (6%)	1	25
82	LK	204/206 (99%)	179 (88%)	15 (7%)	10 (5%)	3	31
83	Lm	90/92 (98%)	77 (86%)	9 (10%)	4 (4%)	3	33
84	LI	182/184 (99%)	140 (77%)	26 (14%)	16 (9%)	1	17
All	All	10359/10512 (98%)	8138 (79%)	1149 (11%)	1072 (10%)	1	12

5 of 1072 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Sa	2	ALA
1	Sa	112	MET
1	Sa	129	ASP
1	Sa	149	VAL
1	Sa	150	SER

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	Sa	301/323 (93%)	275 (91%)	26 (9%)	13	47
2	SA	190/204 (93%)	161 (85%)	29 (15%)	3	22
3	SB	150/175 (86%)	126 (84%)	24 (16%)	3	21
4	SD	176/176 (100%)	152 (86%)	24 (14%)	5	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SE	211/211 (100%)	190 (90%)	21 (10%)	9	38
6	SF	158/159 (99%)	144 (91%)	14 (9%)	12	44
7	SI	103/103 (100%)	91 (88%)	12 (12%)	7	32
8	SJ	91/113 (80%)	84 (92%)	7 (8%)	16	52
9	SK	78/94 (83%)	66 (85%)	12 (15%)	3	22
10	SL	79/113 (70%)	71 (90%)	8 (10%)	9	38
11	SM	116/133 (87%)	91 (78%)	25 (22%)	1	9
12	SO	106/106 (100%)	97 (92%)	9 (8%)	13	48
13	SQ	123/127 (97%)	100 (81%)	23 (19%)	2	14
14	SP	63/74 (85%)	53 (84%)	10 (16%)	3	21
15	SS	121/121 (100%)	96 (79%)	25 (21%)	1	10
16	SR	77/77 (100%)	64 (83%)	13 (17%)	2	18
17	SV	76/87 (87%)	70 (92%)	6 (8%)	15	51
19	SY	49/52 (94%)	41 (84%)	8 (16%)	3	20
20	SZ	44/49 (90%)	38 (86%)	6 (14%)	5	27
23	SU	70/84 (83%)	42 (60%)	28 (40%)	0	0
24	SX	44/44 (100%)	40 (91%)	4 (9%)	12	43
25	SC	154/167 (92%)	136 (88%)	18 (12%)	7	32
27	SH	113/113 (100%)	95 (84%)	18 (16%)	3	21
28	SN	27/40 (68%)	24 (89%)	3 (11%)	8	34
29	ST	68/68 (100%)	59 (87%)	9 (13%)	5	28
36	LA	192/192 (100%)	179 (93%)	13 (7%)	20	57
37	LB	193/195 (99%)	175 (91%)	18 (9%)	11	42
38	LE	148/149 (99%)	126 (85%)	22 (15%)	4	23
39	LF	164/164 (100%)	152 (93%)	12 (7%)	17	54
40	LH	164/173 (95%)	135 (82%)	29 (18%)	2	16
41	LM	103/109 (94%)	91 (88%)	12 (12%)	7	32
42	LP	167/167 (100%)	143 (86%)	24 (14%)	4	25
43	LO	104/110 (94%)	88 (85%)	16 (15%)	3	22
44	LR	138/138 (100%)	117 (85%)	21 (15%)	3	22
45	LQ	242/251 (96%)	196 (81%)	46 (19%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	LT	166/166 (100%)	144 (87%)	22 (13%)	5	28
47	LU	129/140 (92%)	110 (85%)	19 (15%)	4	24
48	LV	136/144 (94%)	112 (82%)	24 (18%)	2	16
49	LX	109/109 (100%)	95 (87%)	14 (13%)	5	29
50	LZ	54/66 (82%)	49 (91%)	5 (9%)	11	42
51	LY	115/115 (100%)	98 (85%)	17 (15%)	4	24
52	Lb	64/64 (100%)	57 (89%)	7 (11%)	8	35
53	Ld	21/21 (100%)	20 (95%)	1 (5%)	31	67
54	Lf	90/98 (92%)	72 (80%)	18 (20%)	1	11
55	Lg	99/103 (96%)	85 (86%)	14 (14%)	4	26
56	Lh	119/122 (98%)	111 (93%)	8 (7%)	20	57
57	Ll	72/77 (94%)	61 (85%)	11 (15%)	3	22
58	Ln	59/63 (94%)	48 (81%)	11 (19%)	2	14
59	Lo	48/48 (100%)	37 (77%)	11 (23%)	1	7
60	Lr	91/94 (97%)	75 (82%)	16 (18%)	2	16
61	Lq	24/24 (100%)	22 (92%)	2 (8%)	14	49
64	LG	185/185 (100%)	152 (82%)	33 (18%)	2	16
66	LN	116/116 (100%)	88 (76%)	28 (24%)	1	6
67	LS	153/153 (100%)	123 (80%)	30 (20%)	1	12
68	LW	89/94 (95%)	75 (84%)	14 (16%)	3	21
69	La	73/83 (88%)	56 (77%)	17 (23%)	1	7
70	Li	105/107 (98%)	78 (74%)	27 (26%)	0	6
71	Lj	80/89 (90%)	63 (79%)	17 (21%)	1	9
72	Lk	62/62 (100%)	45 (73%)	17 (27%)	0	4
73	Lp	38/38 (100%)	26 (68%)	12 (32%)	0	2
74	LJ	104/105 (99%)	80 (77%)	24 (23%)	1	7
75	Lt	46/46 (100%)	45 (98%)	1 (2%)	60	83
75	Lu	46/46 (100%)	46 (100%)	0	100	100
76	Lv	48/48 (100%)	47 (98%)	1 (2%)	61	84
76	Lw	48/48 (100%)	46 (96%)	2 (4%)	36	70
77	Lc	107/109 (98%)	99 (92%)	8 (8%)	17	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Le	206/206 (100%)	171 (83%)	35 (17%)	2	18
79	Ls	222/222 (100%)	199 (90%)	23 (10%)	9	36
80	LC	328/335 (98%)	276 (84%)	52 (16%)	3	21
81	LD	294/302 (97%)	257 (87%)	37 (13%)	5	29
82	LK	173/173 (100%)	141 (82%)	32 (18%)	2	14
83	Lm	73/73 (100%)	67 (92%)	6 (8%)	14	49
84	LI	152/156 (97%)	135 (89%)	17 (11%)	7	33
All	All	8547/8911 (96%)	7319 (86%)	1228 (14%)	8	25

5 of 1228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	LQ	31	LYS
51	LY	51	LYS
80	LC	369	PHE
45	LQ	183	PHE
47	LU	60	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
37	LB	71	HIS
43	LO	39	HIS
79	Ls	137	GLN
37	LB	168	GLN
39	LF	162	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	S3	10/11 (90%)	3 (30%)	1 (10%)
31	S2	74/75 (98%)	22 (29%)	5 (6%)
32	S1	1492/1743 (85%)	439 (29%)	156 (10%)
33	L1	3192/3352 (95%)	903 (28%)	413 (12%)
34	L3	120/120 (100%)	49 (40%)	17 (14%)
35	L2	143/159 (89%)	55 (38%)	28 (19%)
All	All	5031/5460 (92%)	1471 (29%)	620 (12%)

5 of 1471 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	S3	13	A
30	S3	14	A
30	S3	18	C
31	S2	2	C
31	S2	8	U

5 of 620 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	L1	1057	A
33	L1	1598	U
33	L1	3389	C
33	L1	1126	U
33	L1	1312	A

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	S1	23

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Mol	Chain	Number of breaks
33	L1	20
26	SG	3
9	SK	2
78	Le	2
2	SA	2
19	SY	2
25	SC	2
14	SP	1
4	SD	1
16	SR	1
5	SE	1
81	LD	1
15	SS	1
28	SN	1
1	Sa	1
3	SB	1
10	SL	1
24	SX	1
18	SW	1

The worst 5 of 68 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	694:C	O3'	701:C	P	33.58
1	S1	803:G	O3'	823:A	P	30.95
1	L1	2547:C	O3'	2561:A	P	30.63
1	S1	744:G	O3'	764:U	P	27.26
1	S1	862:U	O3'	871:G	P	24.78