



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2016 – 01:10 AM EST

PDB ID : 5DGV  
Title : Complex of yeast 80S ribosome with hypusine-containing/non-modified eIF5A and/or a peptidyl-tRNA analog  
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.  
Deposited on : 2015-08-28  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

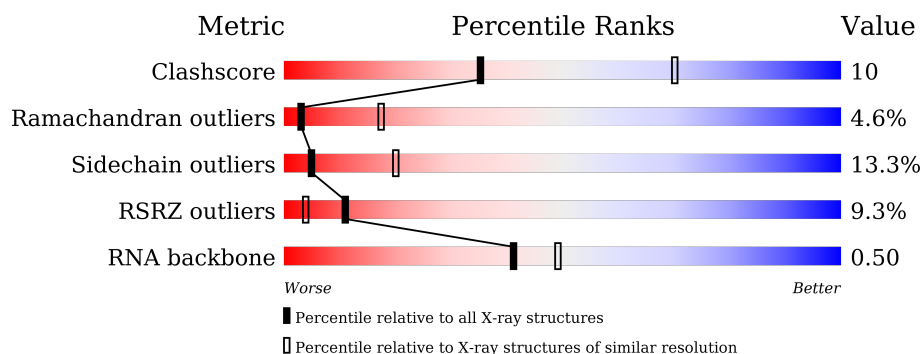
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	<div> <div>8%</div> <div>48%</div> <div>38%</div> <div>12%</div> <div>..</div> </div>
1	6	1800	<div> <div>6%</div> <div>51%</div> <div>37%</div> <div>11%</div> </div>
2	S0	251	<div> <div>27%</div> <div>32%</div> <div>44%</div> <div>6%</div> <div>18%</div> </div>
2	s0	251	<div> <div>12%</div> <div>66%</div> <div>15%</div> <div>18%</div> </div>
3	S1	254	<div> <div>20%</div> <div>27%</div> <div>44%</div> <div>11%</div> <div>16%</div> </div>
3	s1	254	<div> <div>15%</div> <div>70%</div> <div>14%</div> <div>15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	263	
35	sM	263	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	




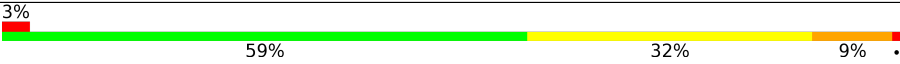
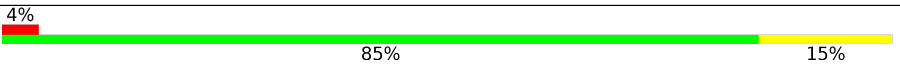

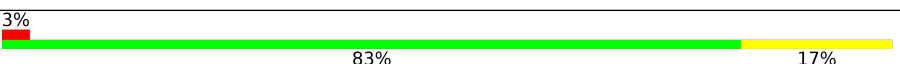
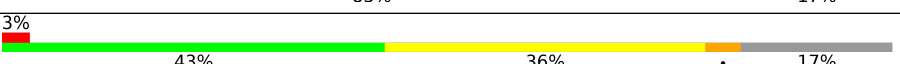
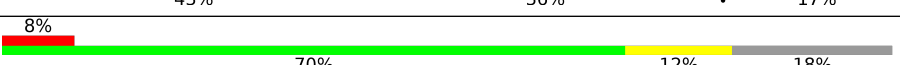
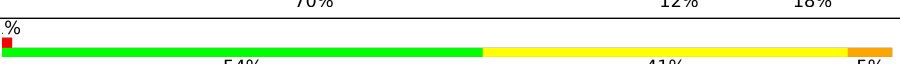
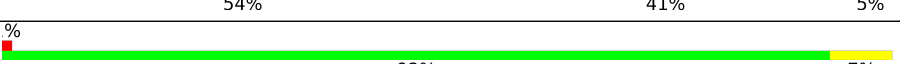
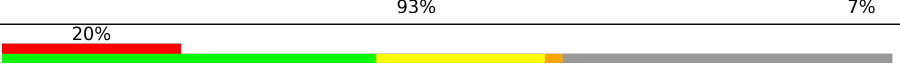
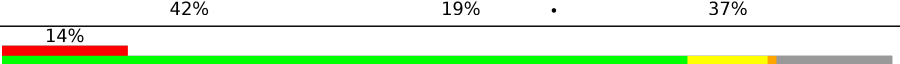




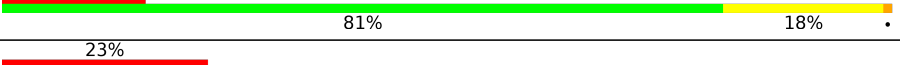

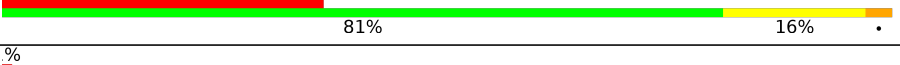
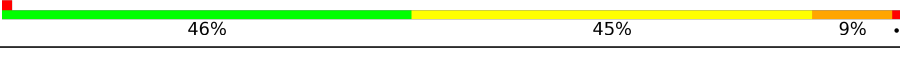


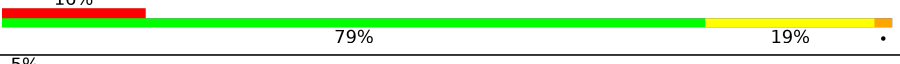
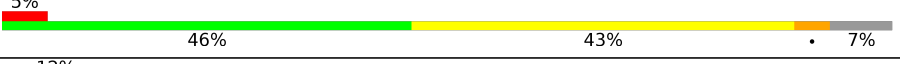
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	
85	C	5	
85	D	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	MG	C	3402	-	-	-	X
88	MG	D	3402	-	-	-	X

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 402683 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* S288c RDN37-1 miscRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	S	0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O	S	0	0	0
			1491	957	267	267				

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	91	ALA	GLY	conflict	UNP Q08745

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			681	404	140	137				

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3148	Total	C	N	O	P	0	0	0
			67333	30076	12137	21972	3148			
36	5	3149	Total	C	N	O	P	0	0	0
			67354	30085	12140	21981	3148			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A (eL8).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O		0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O		0	0	0
			1548	965	316	267				

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O		0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O		0	0	0
			1227	764	238	225				

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	S	0	0	0
			796	516	131	149				
58	n2	98	Total	C	N	O	S	0	0	0
			778	505	127	146				

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	S	0	0	0
			993	625	192	176				

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	?	-	LYS	deletion	UNP P87262
o4	?	-	LYS	deletion	UNP P87262

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O	S	0	0	0
			608	388	114	106				

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called 60S ribosomal protein L12-A (uL11).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 83 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 84 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 85 is a RNA chain called DNA (5'-R(\*CP\*CP\*(8AN)\*(Pro)\*(Pro))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	C	5	Total	C	N	O	P	0	0	0
			73	38	14	19	2			
85	D	5	Total	C	N	O	P	0	0	0
			76	38	14	21	3			

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

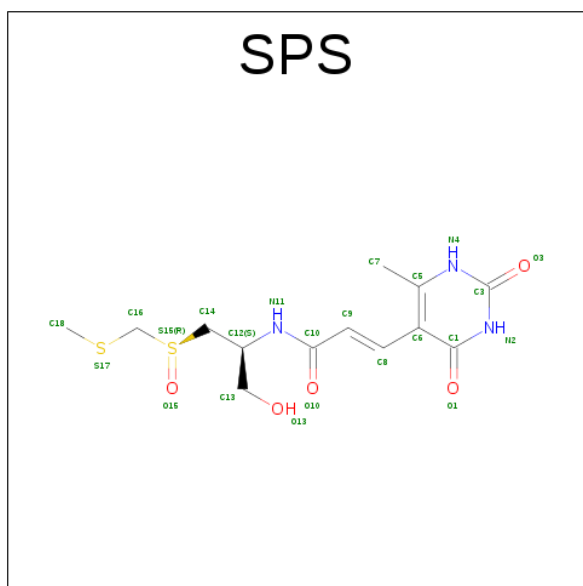
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	q0	1	Total	Zn	0	0
			1	1		
86	D6	1	Total	Zn	0	0
			1	1		
86	Q2	1	Total	Zn	0	0
			1	1		
86	e1	1	Total	Zn	0	0
			1	1		
86	Q3	1	Total	Zn	0	0
			1	1		
86	D9	1	Total	Zn	0	0
			1	1		
86	E1	1	Total	Zn	0	0
			1	1		
86	Q0	1	Total	Zn	0	0
			1	1		
86	d7	1	Total	Zn	0	0
			1	1		
86	q3	1	Total	Zn	0	0
			1	1		
86	d9	1	Total	Zn	0	0
			1	1		
86	D7	1	Total	Zn	0	0
			1	1		
86	d6	1	Total	Zn	0	0
			1	1		
86	o7	1	Total	Zn	0	0
			1	1		
86	O7	1	Total	Zn	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	q2	1	Total	Zn	0	0
			1	1		

- Molecule 87 is SPARSOMYCIN (three-letter code: SPS) (formula:  $C_{13}H_{19}N_3O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
87	C	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
87	D	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

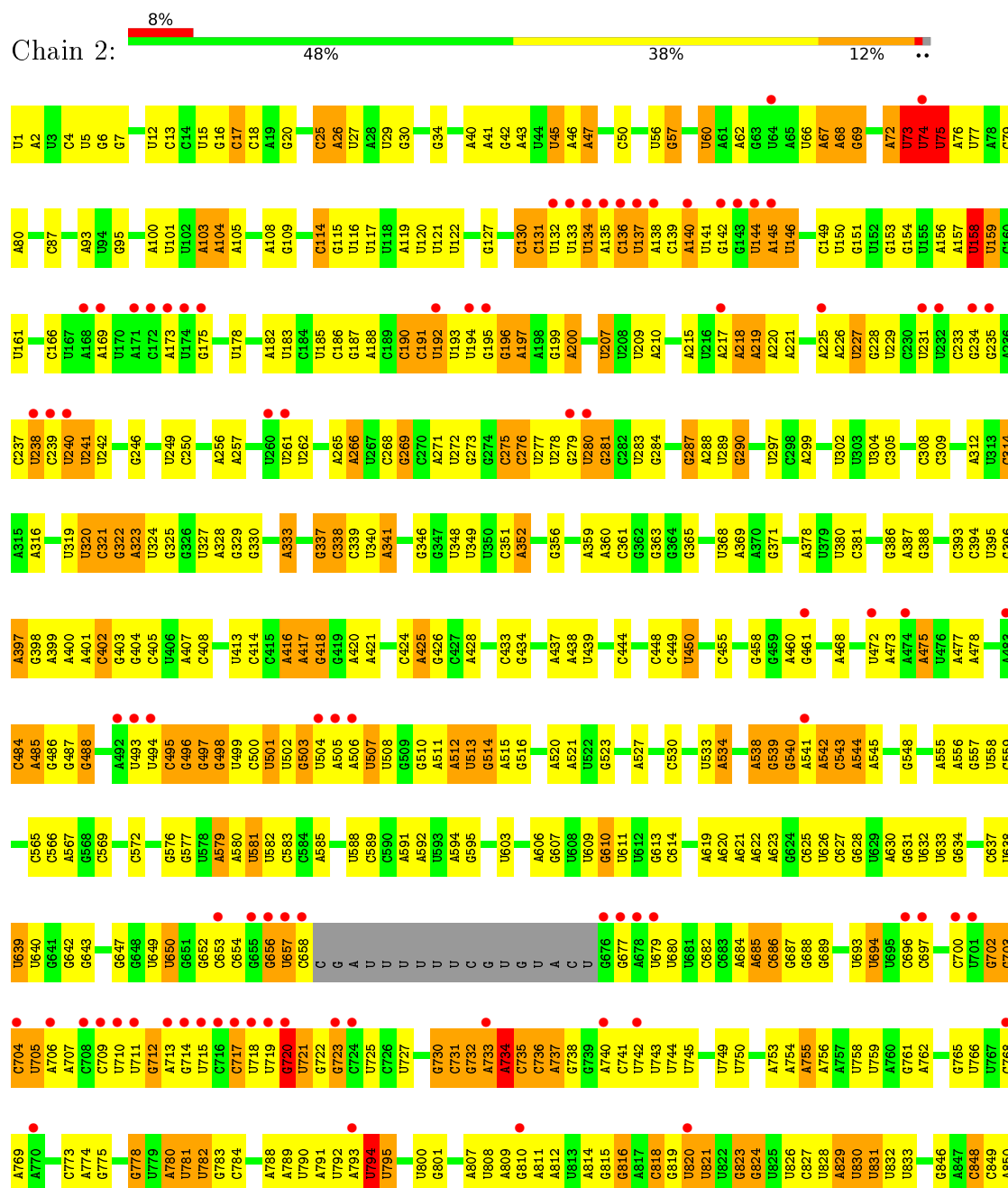
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	D	1	Total	Mg	0	0
			1	1		
88	C	1	Total	Mg	0	0
			1	1		

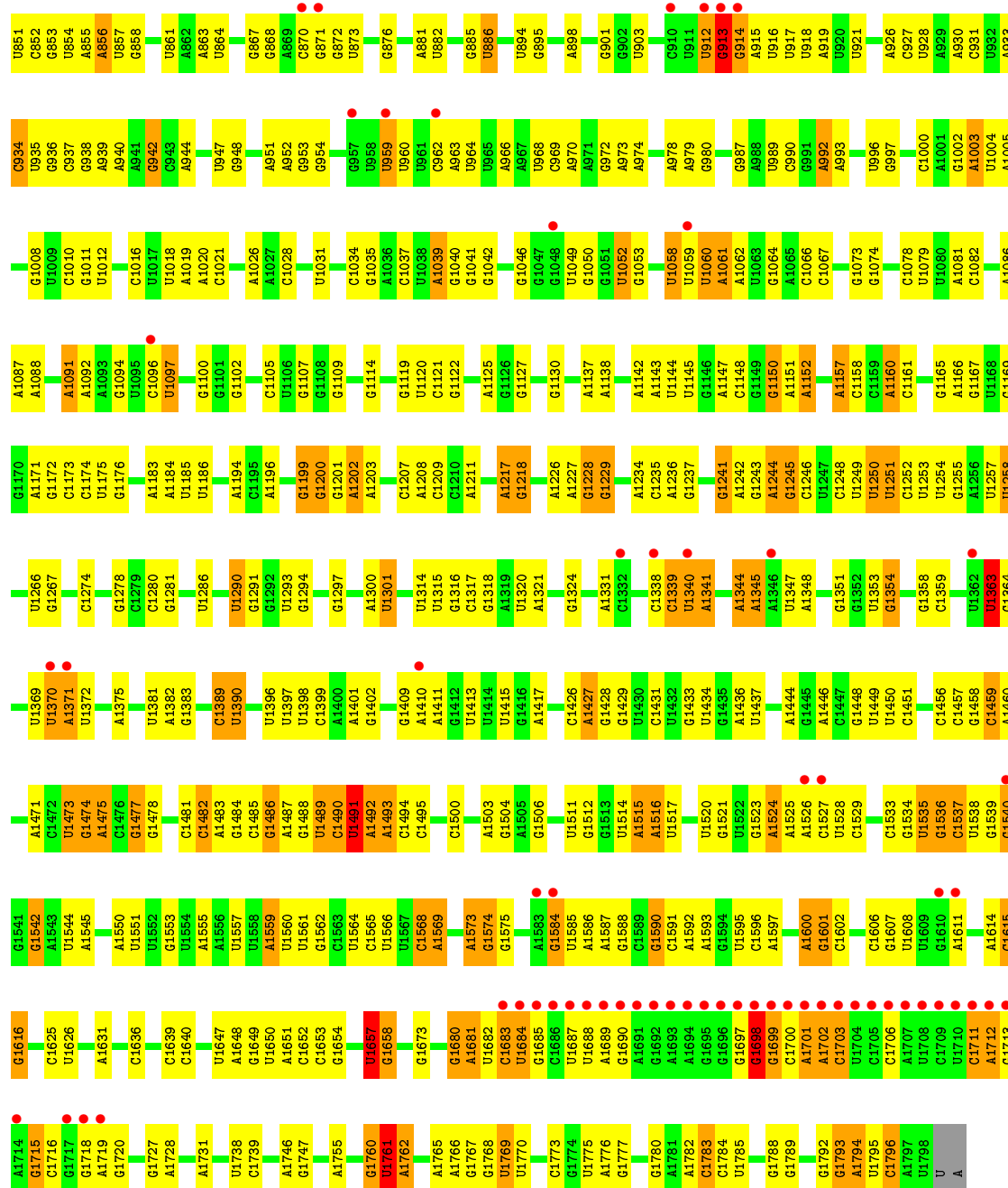
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

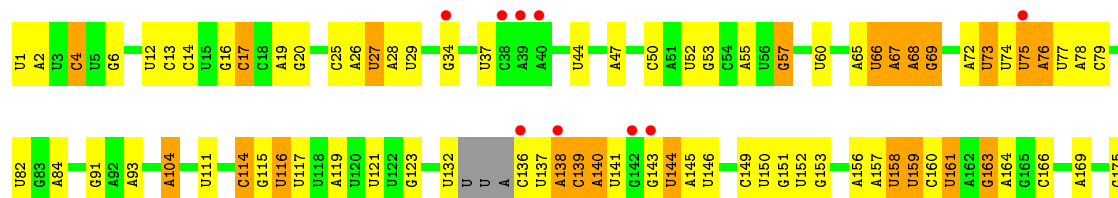
- Molecule 1: *Saccharomyces cerevisiae* S288c RDN37-1 miscRNA





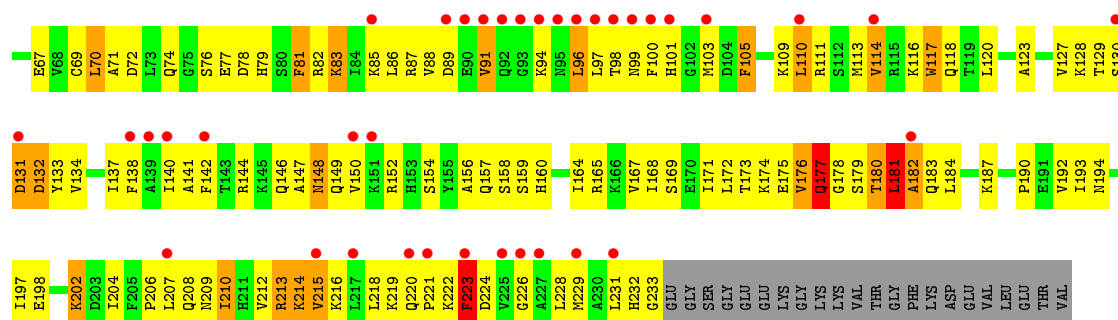


● Molecule 1: *Saccharomyces cerevisiae* S288c RDN37-1 miscRNA

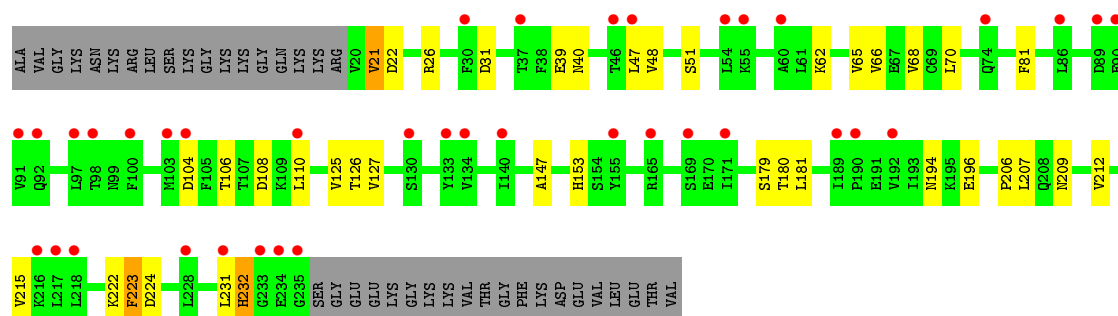




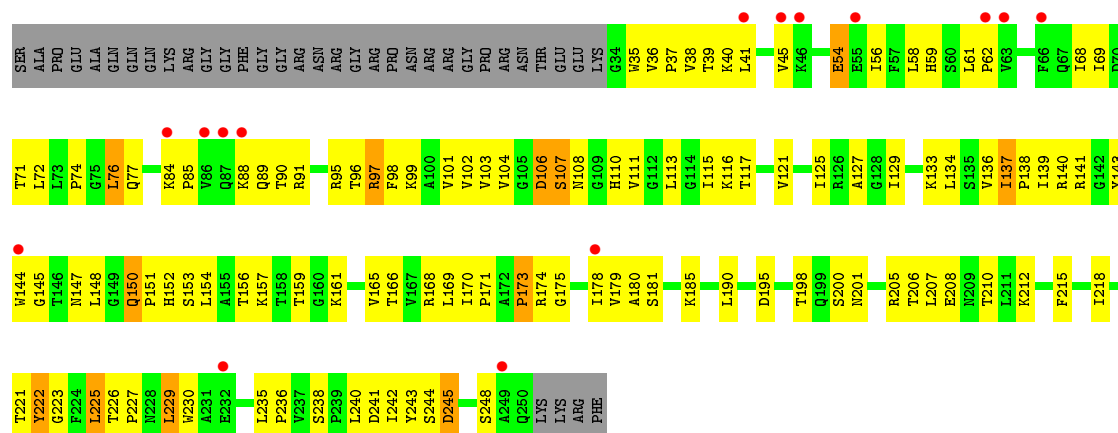
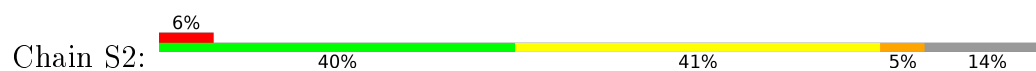




• Molecule 3: 40S ribosomal protein S1-A



• Molecule 4: 40S ribosomal protein S2



• Molecule 4: 40S ribosomal protein S2

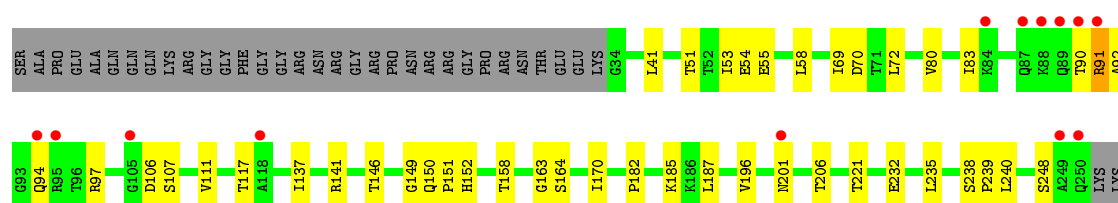
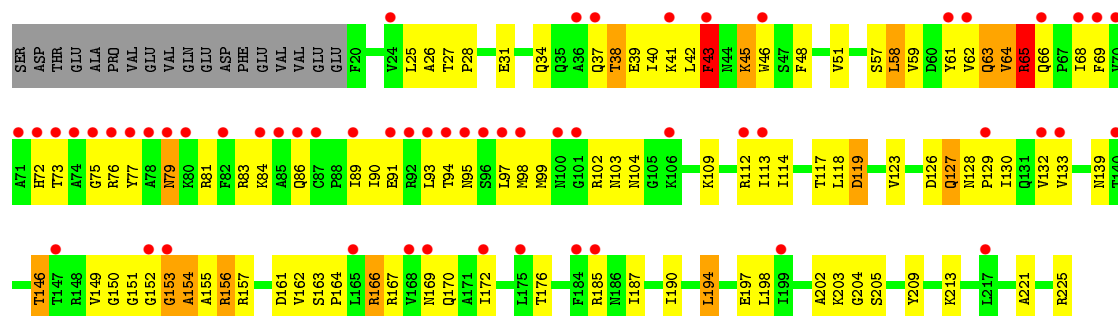


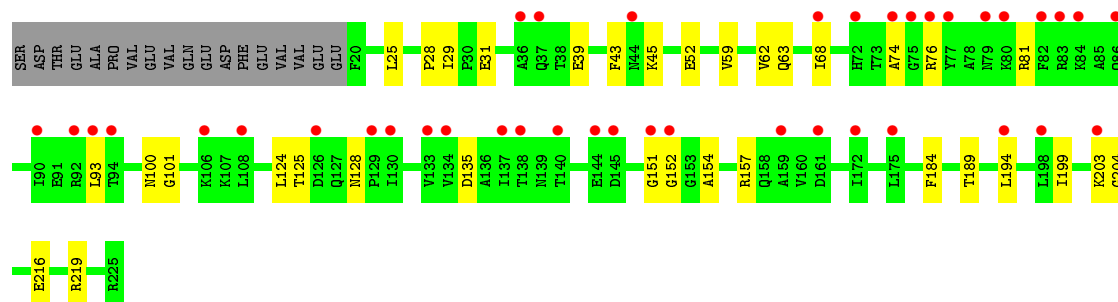
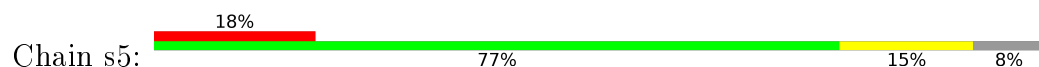
Figure 1: A horizontal bar chart showing the distribution of 1000 samples across 26 categories. The categories are labeled A2, K6, L9, K10, R11, L12, A13, A14, P15, R22, L23, S24, G25, C26, R30, L38, R39, E40, S41, L42, R49, N50, R51, T64, Q67, R68, H69, V70, T81, I90, A94, L101, D104, G107, R113, L123, L131, G132, K133, T159, and D162. The bars are colored in a repeating pattern of green, yellow, and red. The height of each bar represents the number of samples in that category. The total number of samples is 1000.



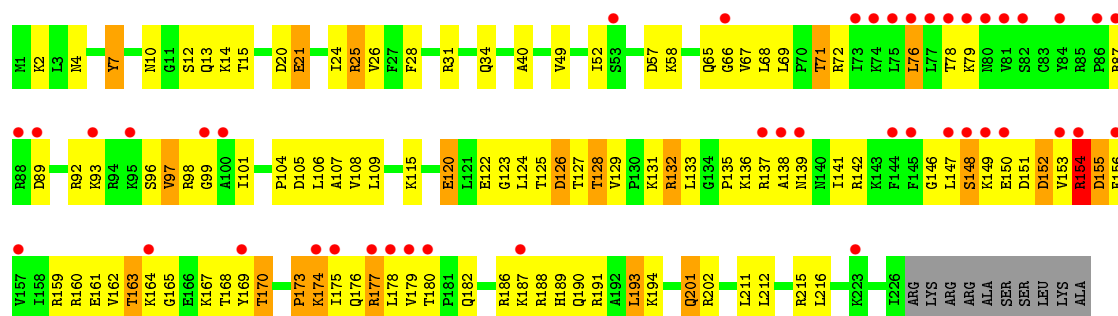
• Molecule 7: 40S ribosomal protein S5



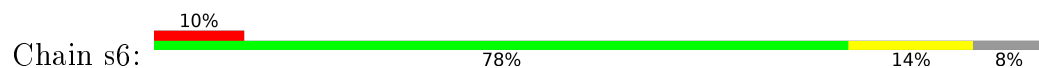
• Molecule 7: 40S ribosomal protein S5

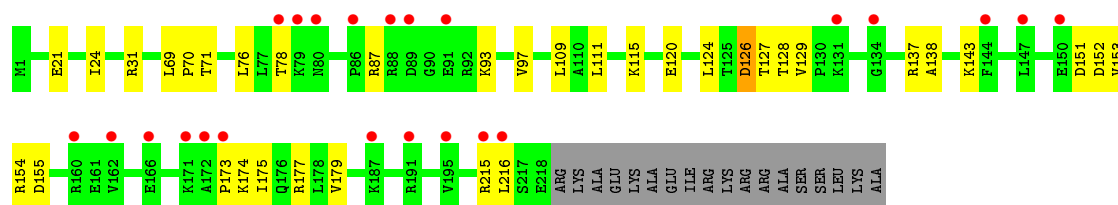


• Molecule 8: 40S ribosomal protein S6-A

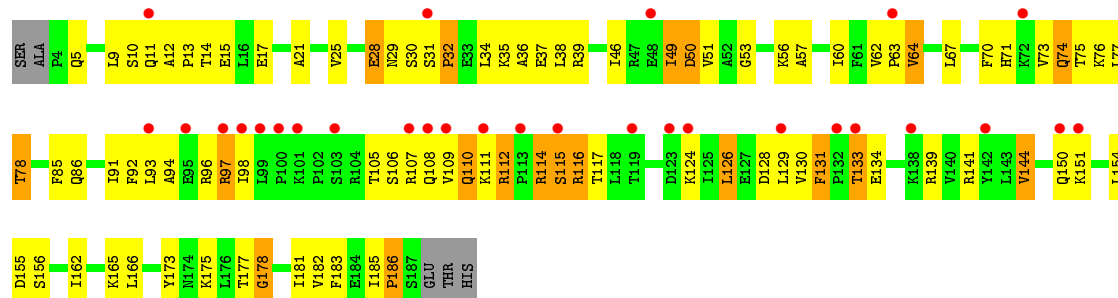


• Molecule 8: 40S ribosomal protein S6-A

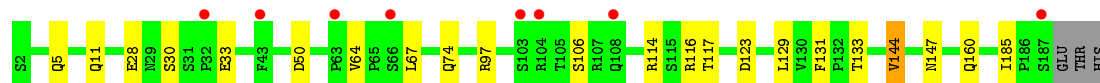
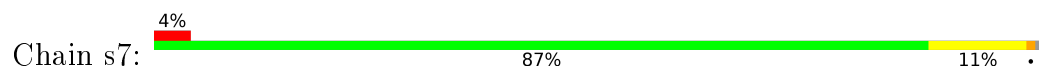




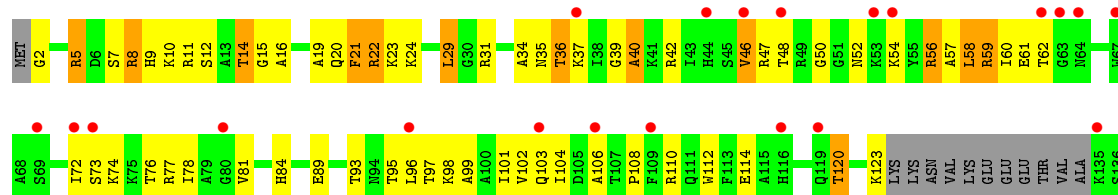
• Molecule 9: 40S ribosomal protein S7-A



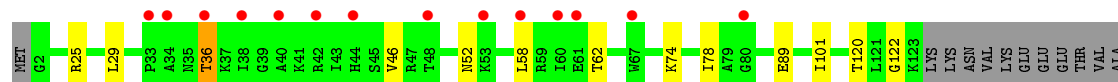
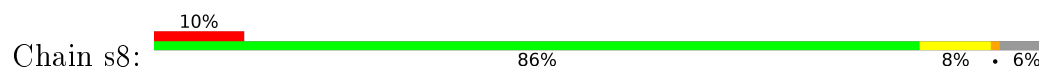
• Molecule 9: 40S ribosomal protein S7-A

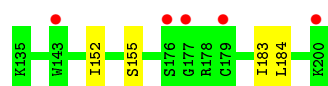


• Molecule 10: 40S ribosomal protein S8-A

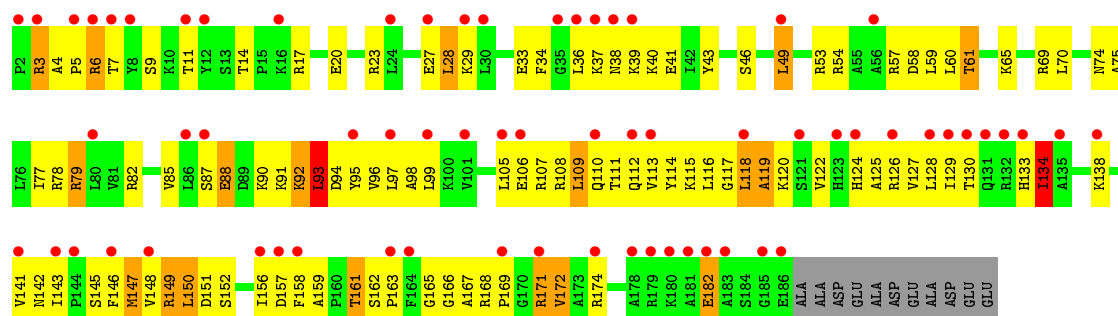
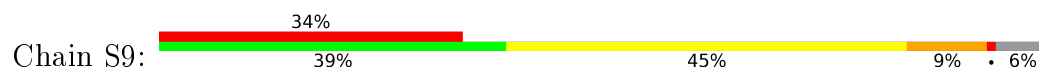


• Molecule 10: 40S ribosomal protein S8-A

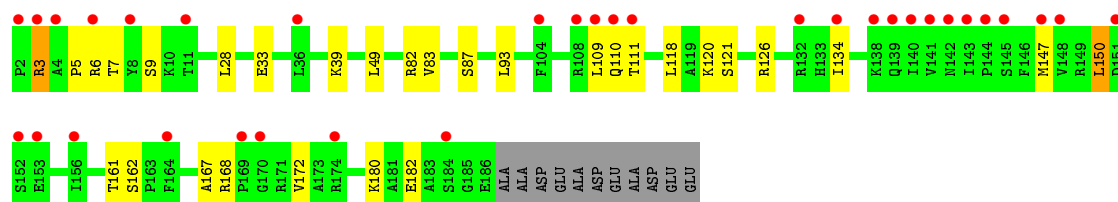
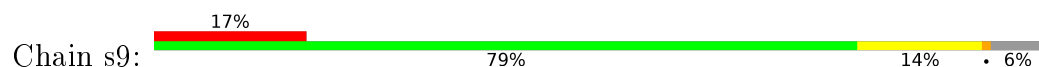




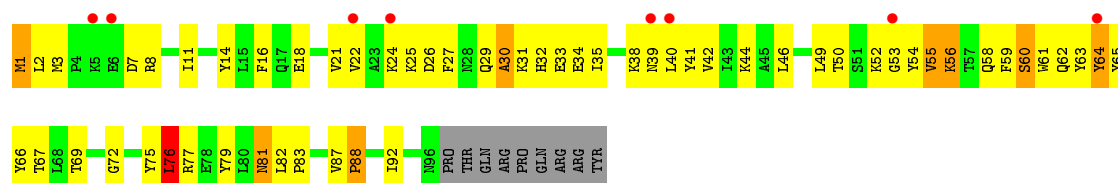
- Molecule 11: 40S ribosomal protein S9-A



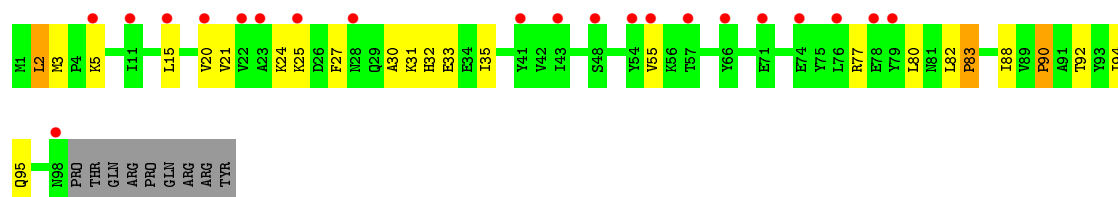
- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S10-A



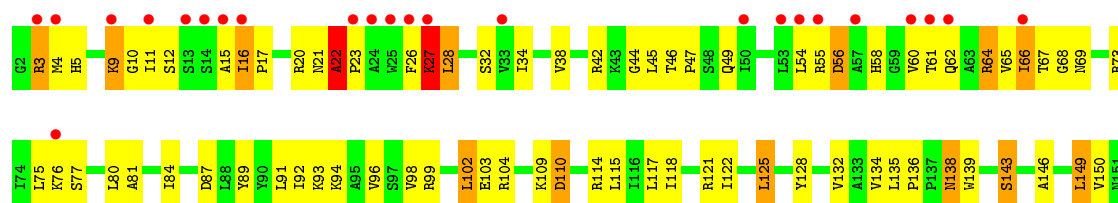
- Molecule 12: 40S ribosomal protein S10-A



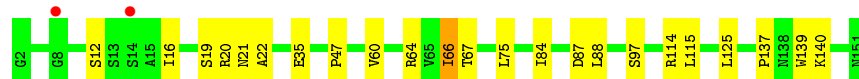
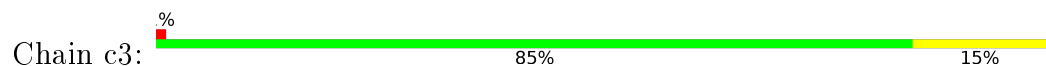
- Molecule 13: 40S ribosomal protein S11-A



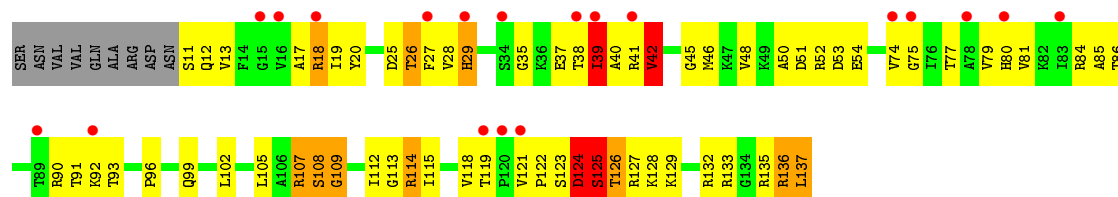
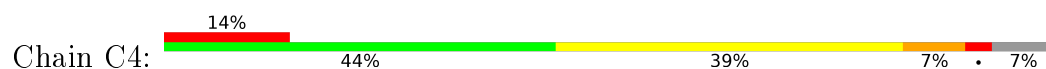




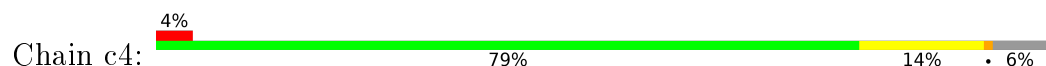
- Molecule 15: 40S ribosomal protein S13



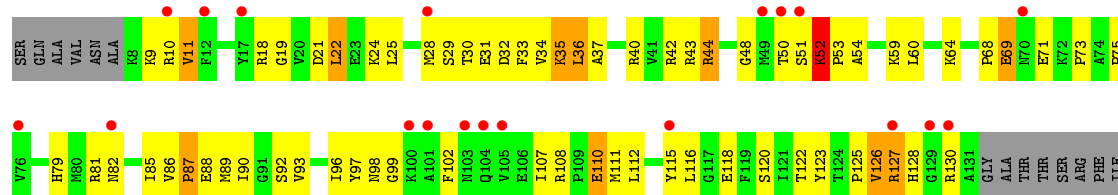
- Molecule 16: 40S ribosomal protein S14-A



- Molecule 16: 40S ribosomal protein S14-A

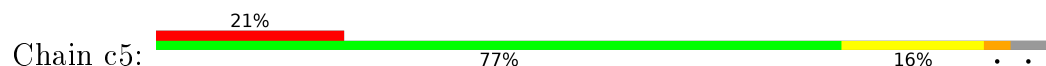


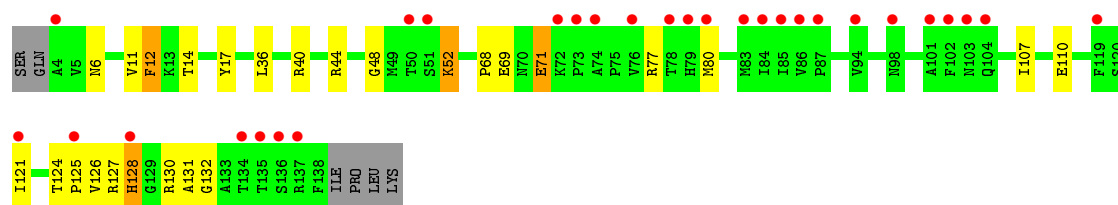
- Molecule 17: 40S ribosomal protein S15



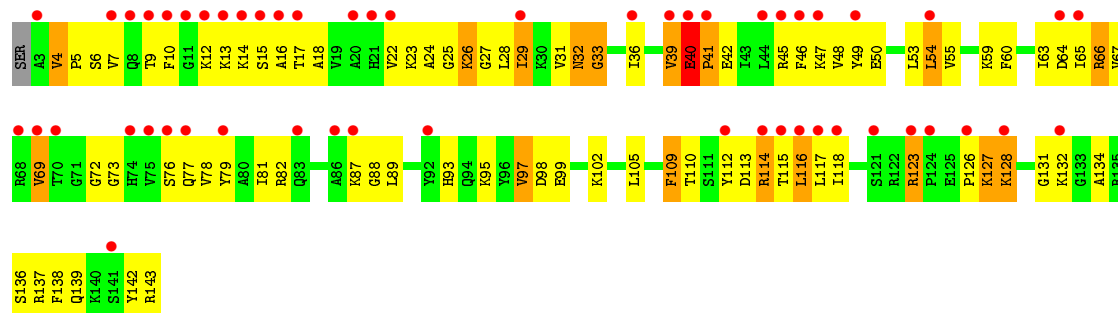
PRO  
LEU  
LYS

- Molecule 17: 40S ribosomal protein S15

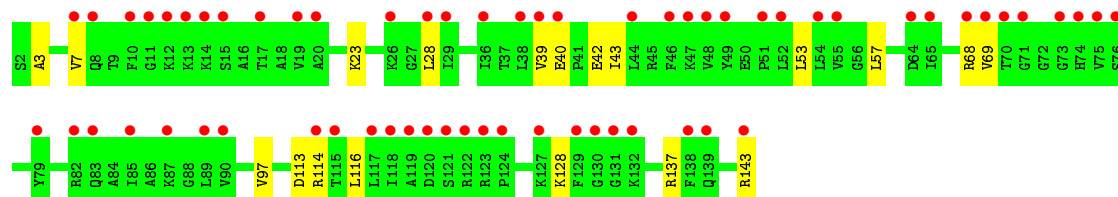
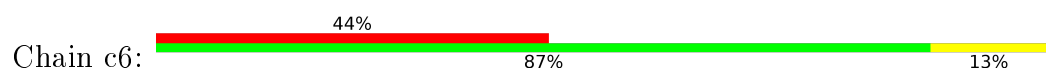




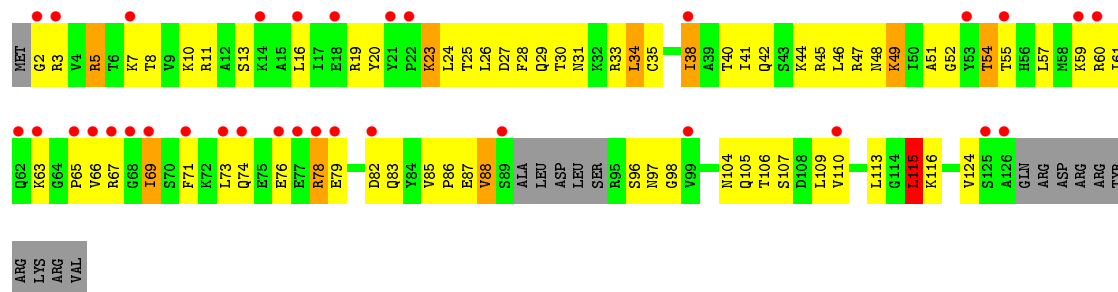
• Molecule 18: 40S ribosomal protein S16-A



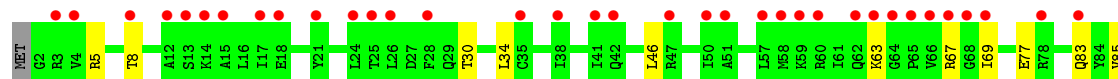
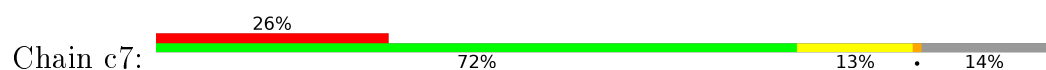
• Molecule 18: 40S ribosomal protein S16-A

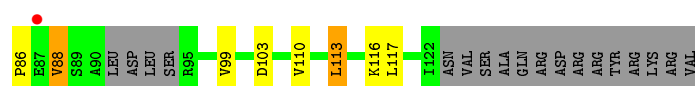


• Molecule 19: 40S ribosomal protein S17-A

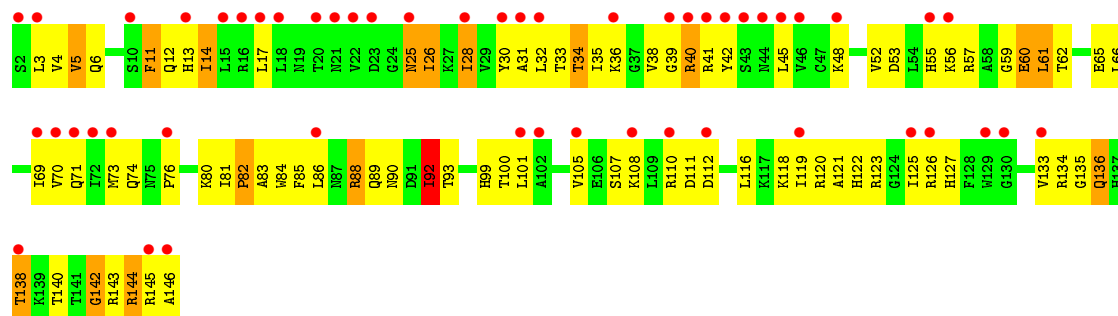
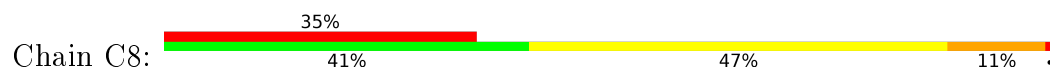


• Molecule 19: 40S ribosomal protein S17-A

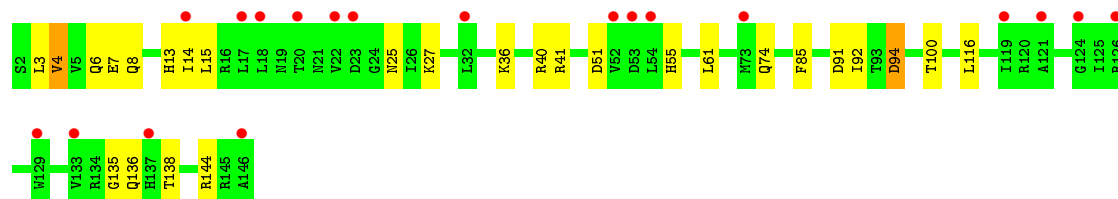
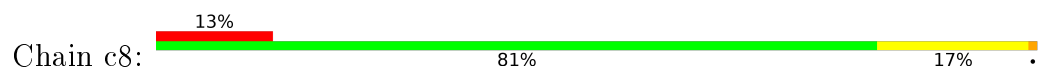




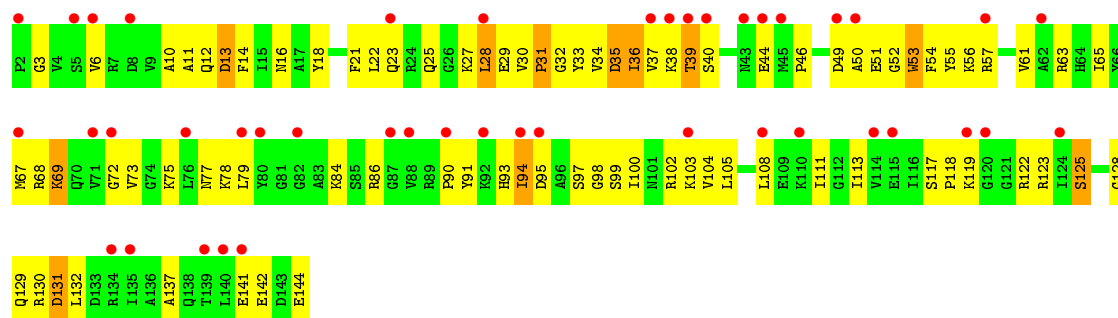
- Molecule 20: 40S ribosomal protein S18-A



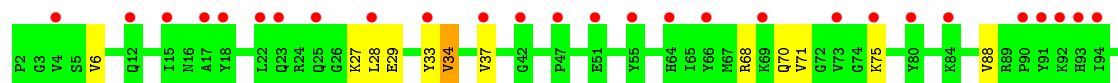
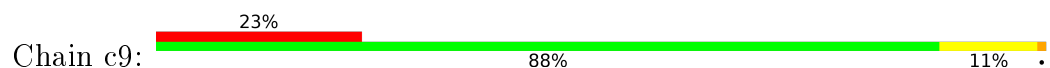
- Molecule 20: 40S ribosomal protein S18-A

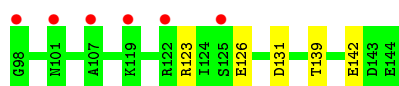


- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A

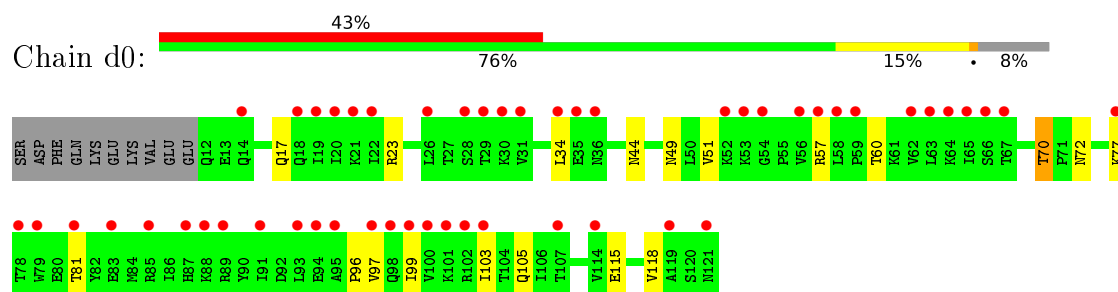




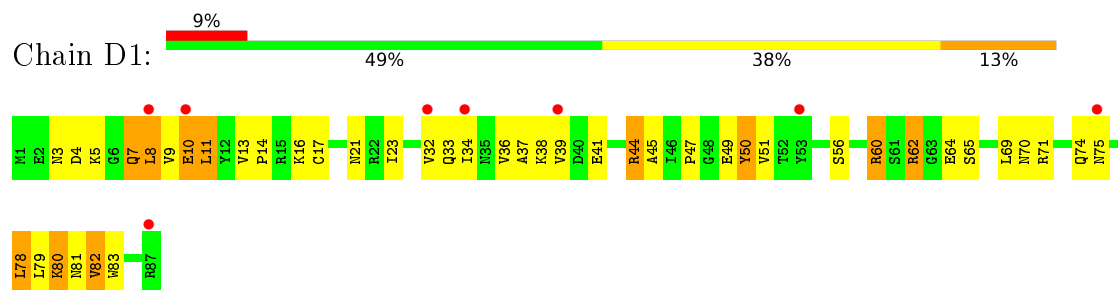
- Molecule 22: 40S ribosomal protein S20



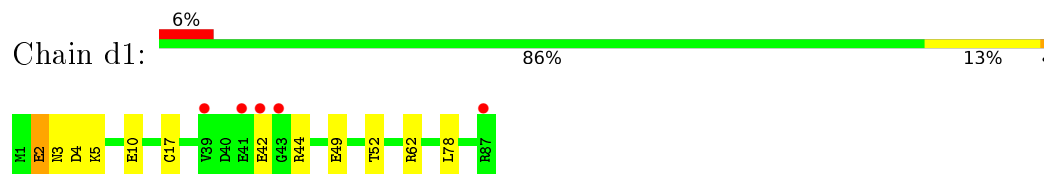
- Molecule 22: 40S ribosomal protein S20



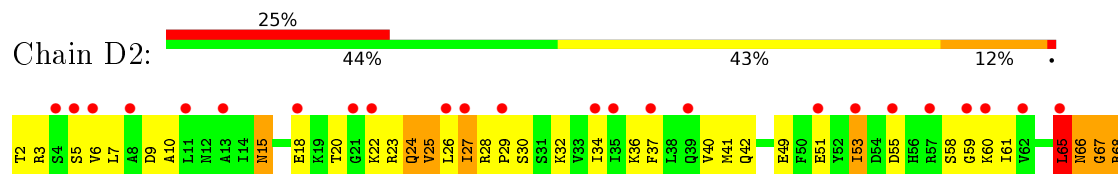
- Molecule 23: 40S ribosomal protein S21-A

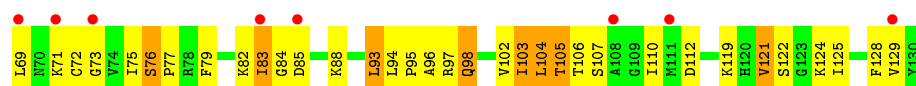


- Molecule 23: 40S ribosomal protein S21-A

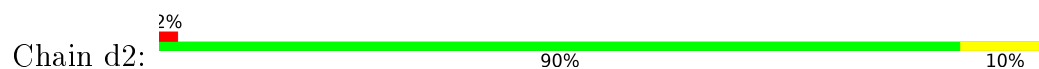


- Molecule 24: 40S ribosomal protein S22-A

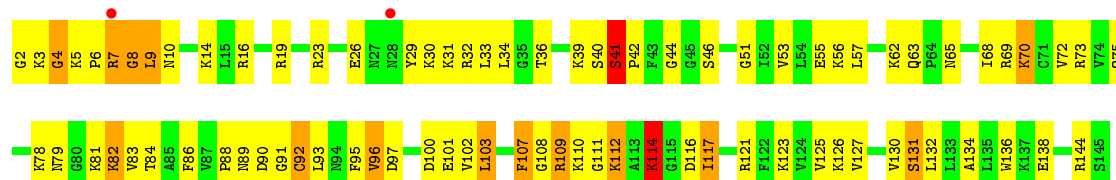
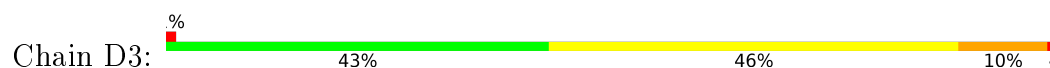




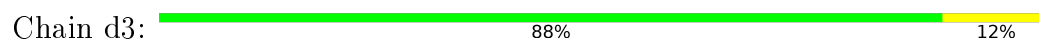
- Molecule 24: 40S ribosomal protein S22-A



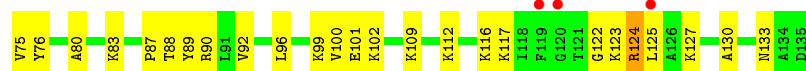
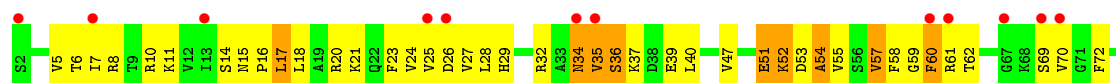
- Molecule 25: 40S ribosomal protein S23-A



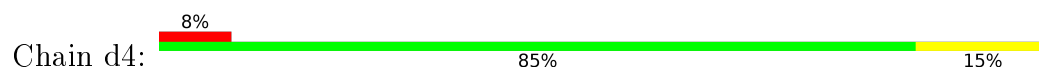
- Molecule 25: 40S ribosomal protein S23-A



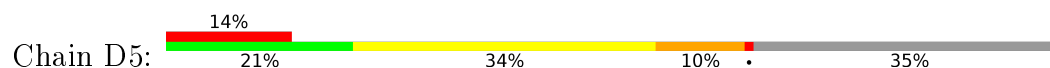
- Molecule 26: 40S ribosomal protein S24-A

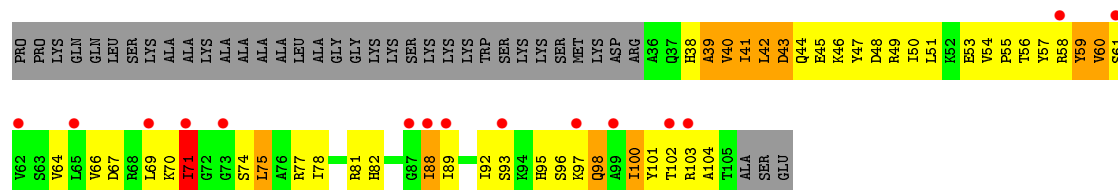


- Molecule 26: 40S ribosomal protein S24-A

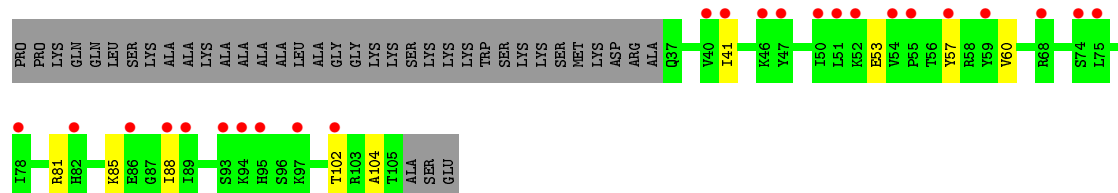


- Molecule 27: 40S ribosomal protein S25-A

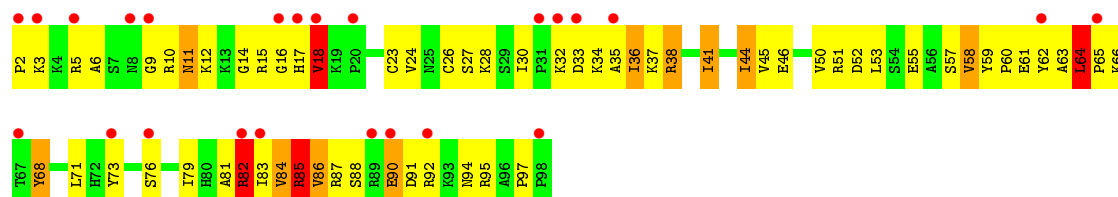




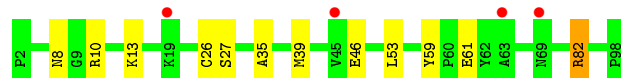
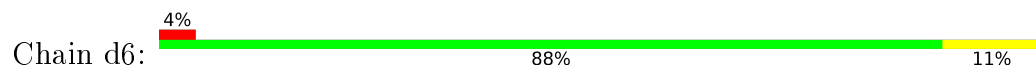
- Molecule 27: 40S ribosomal protein S25-A



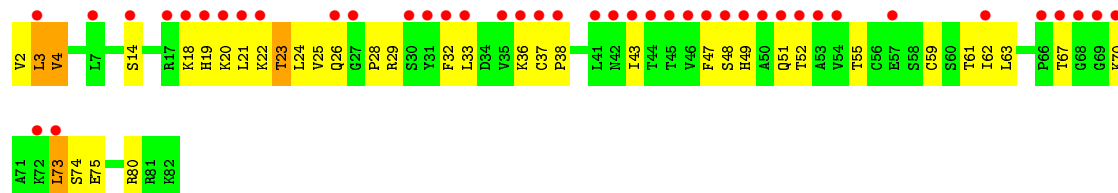
- Molecule 28: 40S ribosomal protein S26-B



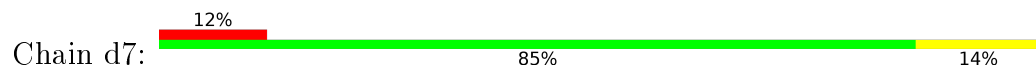
- Molecule 28: 40S ribosomal protein S26-B

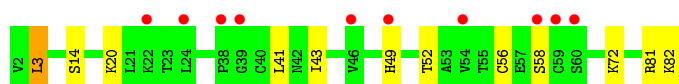


- Molecule 29: 40S ribosomal protein S27-A



- Molecule 29: 40S ribosomal protein S27-A

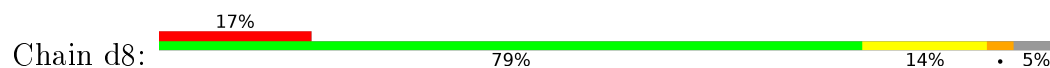




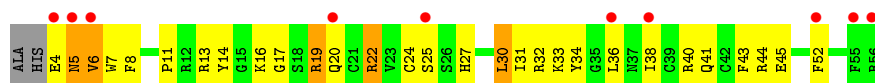
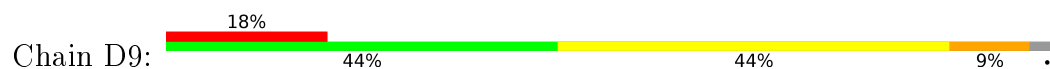
- Molecule 30: 40S ribosomal protein S28-A



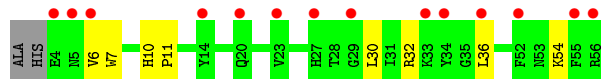
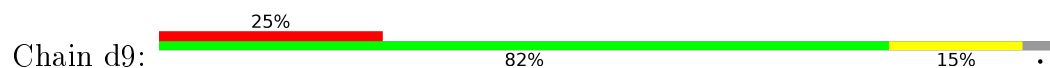
- Molecule 30: 40S ribosomal protein S28-A



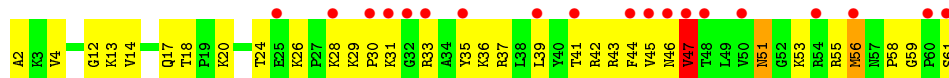
- Molecule 31: 40S ribosomal protein S29-A



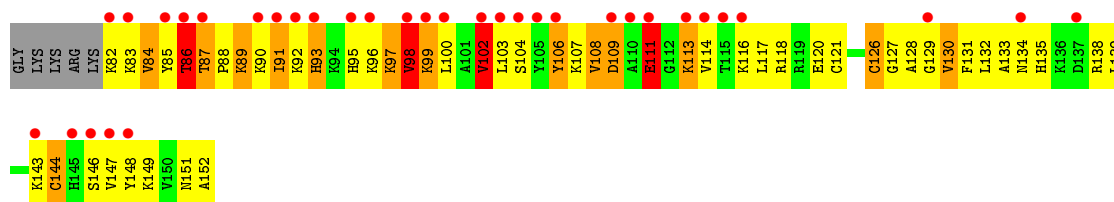
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: Ubiquitin-40S ribosomal protein S31

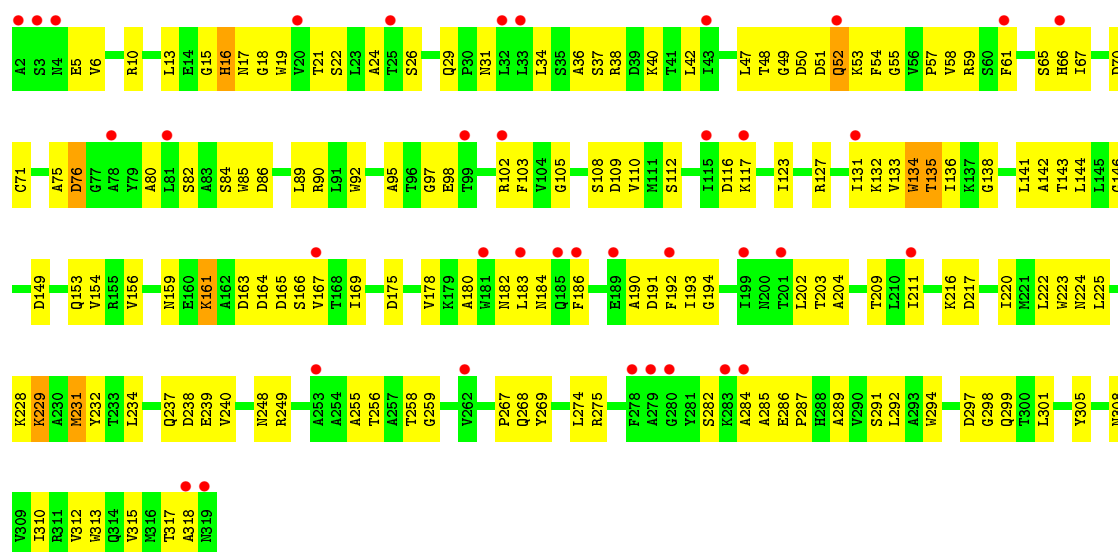


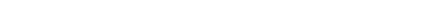
- Molecule 33: Ubiquitin-40S ribosomal protein S31

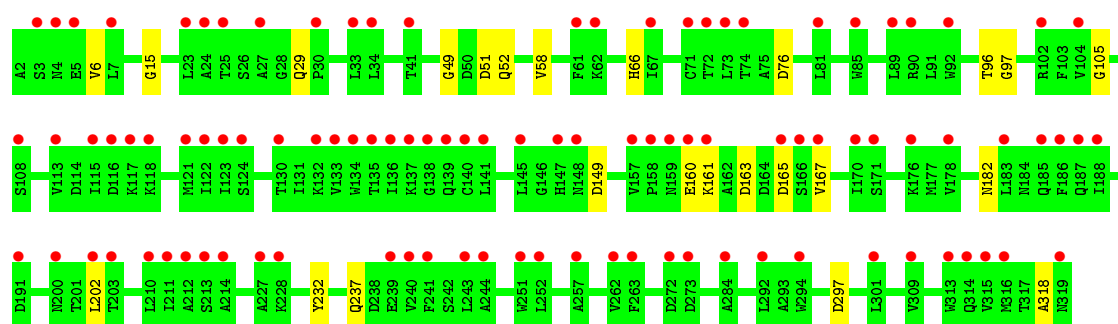


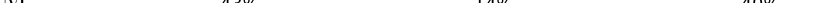
Year	Publications
1977	7
1978	10
1979	12
1980	15
1981	18
1982	20
1983	22
1984	25
1985	28
1986	30
1987	32
1988	35
1989	38
1990	40
1991	42
1992	45
1993	48
1994	50
1995	52
1996	55
1997	58
1998	60
1999	62
2000	65
2001	68
2002	70
2003	72
2004	75
2005	78
2006	80
2007	82
2008	85
2009	88
2010	90
2011	92
2012	95
2013	98
2014	100
2015	102
2016	105
2017	108
2018	110
2019	112
2020	115

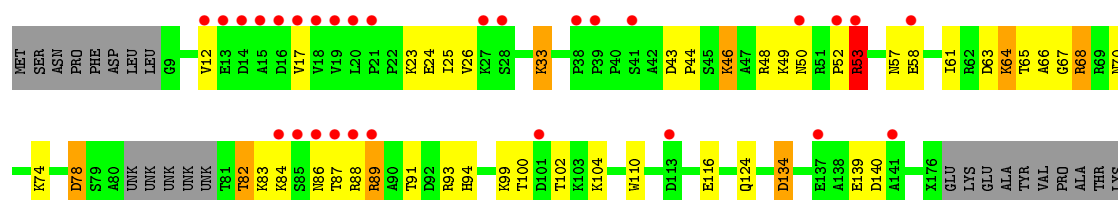
- Chain SR: 

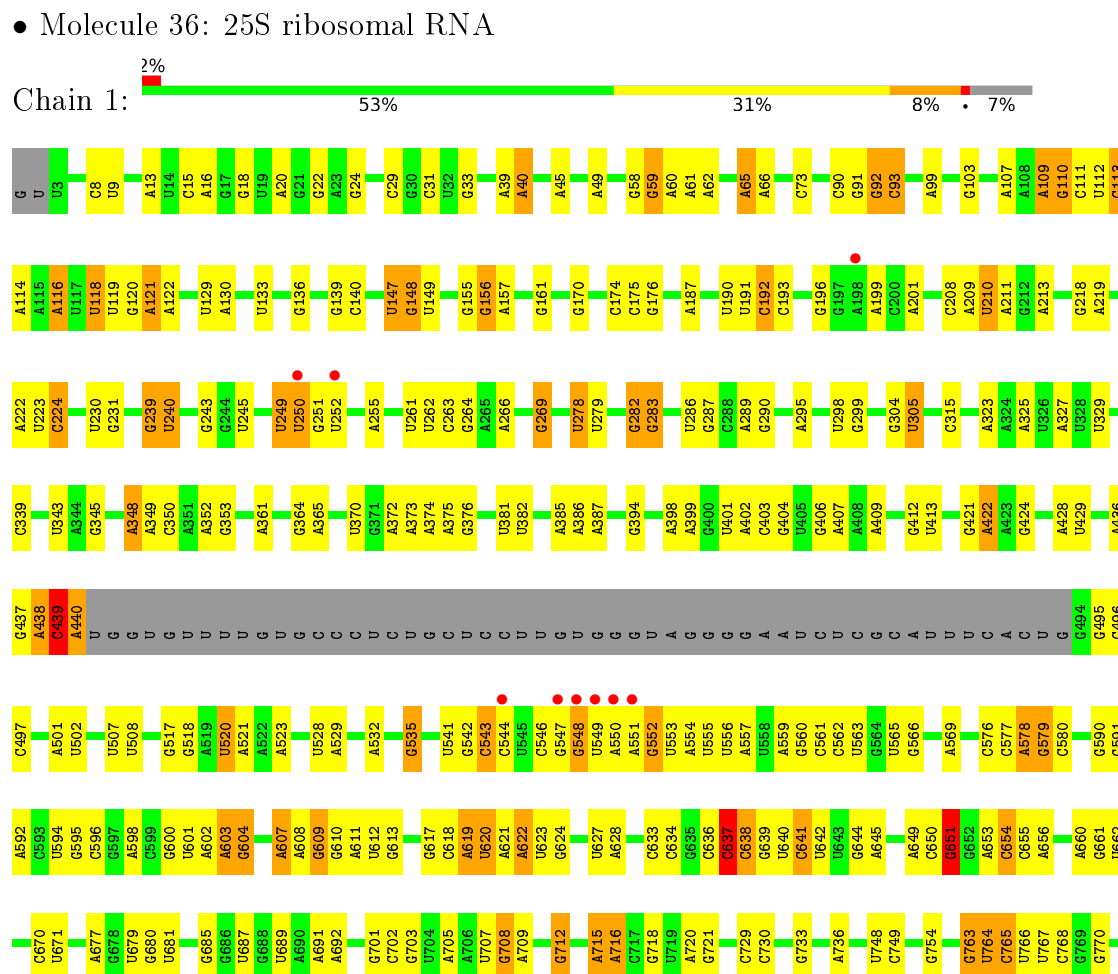


- Chain sR: 



- Chain SM: 



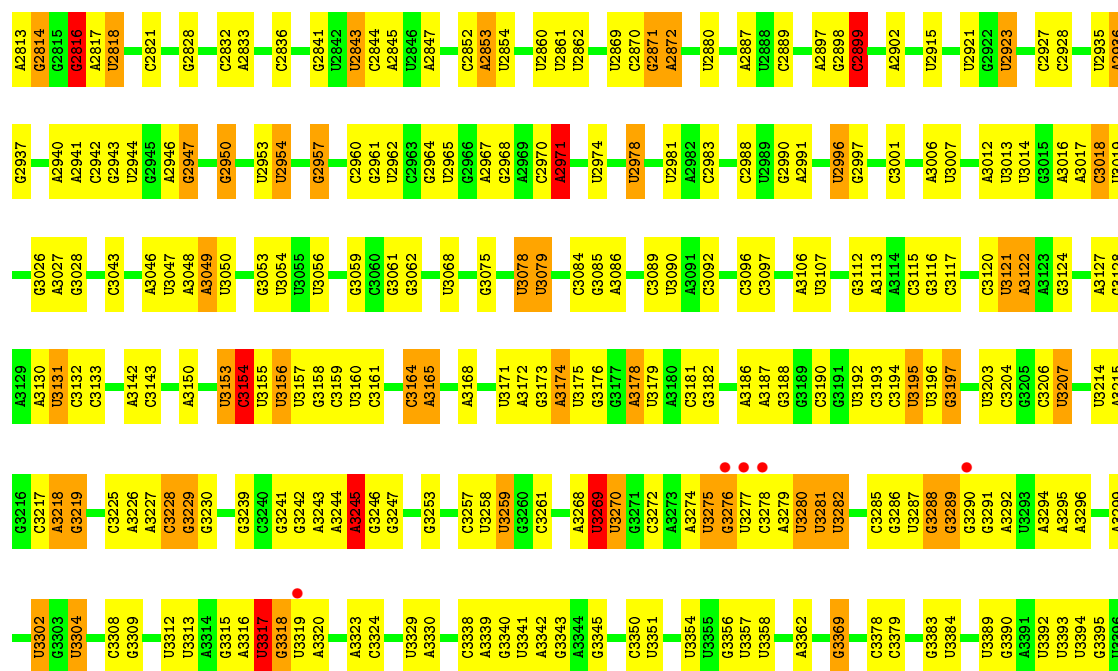


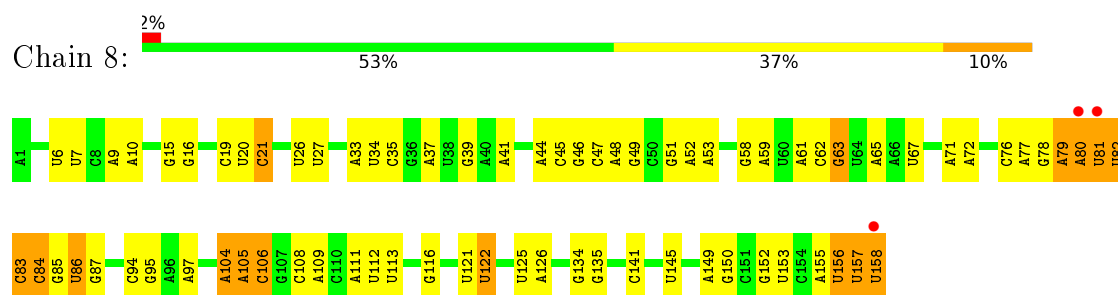
C G U G C C U U G U U G U A G A C G G G C C C U U U G G G U U A A G G G U C U C U U U G U U A G A A C C G G U C G C G C U U G U G C U U A C A A A U U A

C3888	U3306	U3138	U3042	G3950	U2869	U2768	G2661	G2556	C	A2419	U2297	A2198	C2094
U3889	A3307	A3141	C3043	G2951	C2870	C2771	G2662	A2557	C	C2420	U2298	U2203	G2095
G3390	U3313	A3142	U3047	G2952	G2871	C2772	G2663	C2560	A	U2421	A2299	U2204	A2096
U3393	C3233	C3143	A3048	U2954	G2873	C2776	G2672	A2562	U	G2424	G2307	U2205	A2100
U3394	A3234	A3150	A3049	C2980	U2875	G2777	A2674	A2567	U	G2425	C2308	G2206	C2101
G3395	C3235	U3151	G3053	G2961	U2878	C2778	A2675	U2565	C	U2433	A2309	A2207	U2102
U3396	G3239	U3152	A3056	U2969	C2879	G2779	A2676	C2566	C	U2434	U2311	A2208	U2103
	G3242	U3153	U3057	C2970	U2880	A2781	A2677	C2567	U	G2435	G2312	G2210	C2107
	A3243	U3154	U3058	U2971	C2881	G2784	A2678	U2569	A	A2438	A2313	A2213	C2108
	A3244	U3155	G3059	G2972	U2882	U2795	C2682	U2571	U2501	A2439	G2315	A2214	G2111
	A3245	G3158	U3066	U2973	U2883	U2796	U2683	C2572	A2502	G2440	C2331	A2215	U2112
	G3246	C3067	C3067	U2978	C2884	G2797	U2684	C2573	U2503	C2444	U2332	G2216	A2113
	G3247	U3160	U3068	U2979	U2886	C2798	A2685	C2574	U2504	A2445	C2333	A2219	G2115
		C3161		C2983	A2887	U2799	A2686	U2581	C2507	U	U2334	A2220	A2120
	G3252		C3072	U2986	U2888	G2800	A2687	G2607	U2508	A	G2335	A2223	G2121
	G3253	C3164	A3073	C2987	C2889	A2801	U2688	G2585	U2509	G	U2336	A2224	G2122
	G3254	A3165	A3077	U2987	A2890	A2802	A2689	G2586	U2510	A	C2337	A2225	A2121
	U3255	C3166	U3078	C2988	C2894	A2803	A2691	G2592	A2511	G	C2338	U2226	A2131
	G3256	A3167	U3079	U2989	G2895		A2694	C2593	C2512	G	C2339	U2227	
	A3259	A3168	G3080	U2990	A2896		A2695	C2594	U2513	U		A2228	C2136
	G3260	U3169		A2991	A2897	C2810	A2696		A2514	G	A2352	A2229	U2137
	C3261	A3170		U2992	G2898			G2606	A2515	U	G2355		A2138
			C3084	G2993	C2899	G2814		G2607	U2516	A	A2356	A2242	U2140
	A3267	G3173	G3085	G2996	C2900	G2815	A2703		A2520	G	A	A2243	
	G3268	U3174	A3086	U2996	G2901	G2816	A2704	G2610	U2521	G	A2263	A2244	
	U3269	U3175	A3087	C2997	G2902	A2817	A2705	U2611	G2522	A	A		A2144
	G3270	G3176	G3088	G2997	U2904	U2818	G2706	U2612	A2523	U	A2372	G2249	A2145
	G3271	A3177	U3089	U3000	U2905	A2819		U2613	A2524	A	A2373	G2250	C2146
	C3272	U3178	U3090	C3001	G2914	A2820	G2714	G2615	G2525	G	C2374	U2254	
		A3180		A3005	G2915		G2719	G2616	A2529	U	G2375	A2255	G2150
	U3275	C3093	C3093	A3006	U2916	G2827		U2617		G	A2384	A2256	
	G3276	A3094	A3094	U3007	U2917	G2828			U2532	G	G2385	A2257	G2155
	U3277	U3095	U3095	A3012	A2919	G2834	U2723	G2621	U2533	G			
	C3278	C3096	C3097	U3013	U2923	U2835	U2724	C2622	G2534	G	G2391	G2261	A2158
	U3280		G3101	U3014	U2923	C2836	U2725	G2623	A2535	A	C2392	C2267	U2162
	C3281	U3195		C2927	C2928	A2837	A2726	G2624	A2536	C	C2393	U2268	C2163
		U3196	U3104	G3022	C2928	A2838	G2728		U2537	U	G2394		
	G3284	G3197		U3023	C2929	G2839	U2729	G2632	U2538	C		G2272	A2168
	C3285	U3198		A3024	U2933	U2842	A2736	A2637	C2539	U	A2397	G2273	G2169
	U3287	G3199	G3112	C3025	A2934	U2843	C2737		A2540	G	G2400		U2170
	G3288		A3113	G3028	U2935	C2844		G2645	U2542	G	A	C2278	
	G3289	C3204	A3114	G3028	A2936	A2845	A2746	C2646	U2543	C	A2402	A2280	G2174
		G3205		A3029	A2936	U2846	A2747	A2647	U2544	C	G2403	A2281	U2175
	U3293	U3207	C3120	G3030	A2940	A2847	A2748		C2545	C	A2404	U2282	G2180
	A3294	U3208	U3121	A3033	A2941		G2749	G2651	C2546	A	C2405	G2283	G2185
	G3295	A3209	A3122	C3034	C2942	C2852	U2752	U2652	A2547	G	C2406	C2284	U2186
	A3296		A3123	C3034	G2943	U2854	G2753	U2655	G2549	U	C2407	C2285	C2407
	U3297	U3214	A3129	U3037	U2944	C2855		U2656		G	U2408		G2187
	C3298	A3215	U3130	U3038	G2945	U2856	G2761	A2657	C2552	A	U2411	G2288	A2188
		G3216	U3131	U3039	A2946	C2857	A2762	G2658	U2553	A			U2193
	G3303	A3217	A3134	C3040	C2947	U2867		G2659	A2554	U	U2417	U2294	G2194
	U3304			U3041	U2949	U2868	U2767	G2660	G2555	A		A2296	

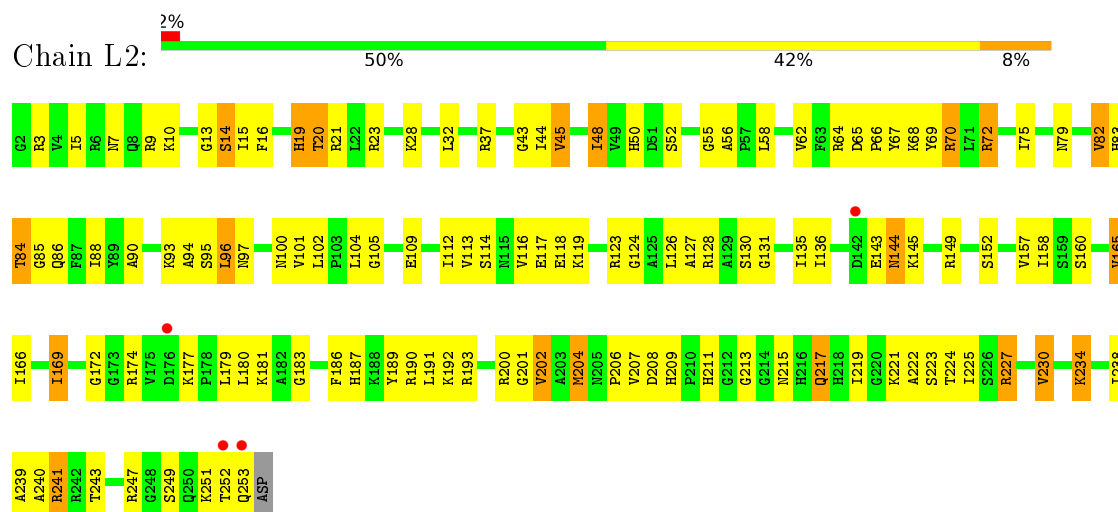
[illegible]



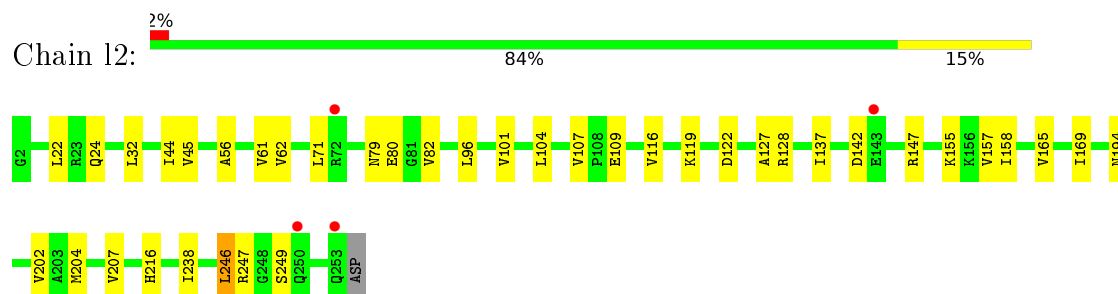




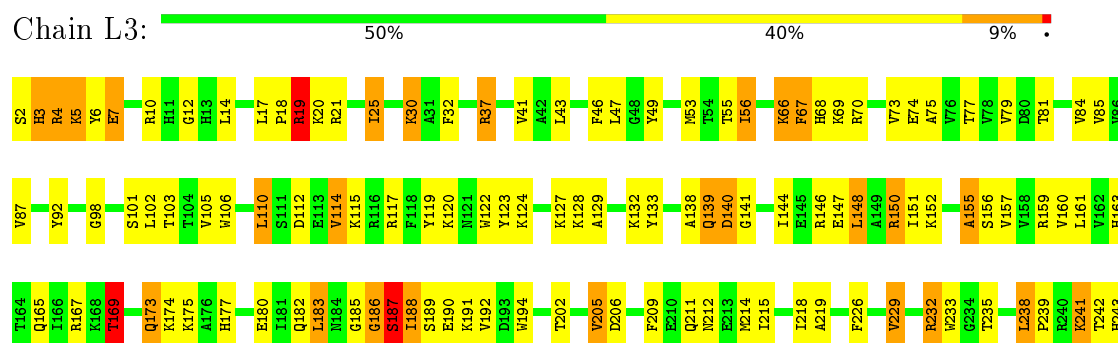
• Molecule 39: 60S ribosomal protein L2-A



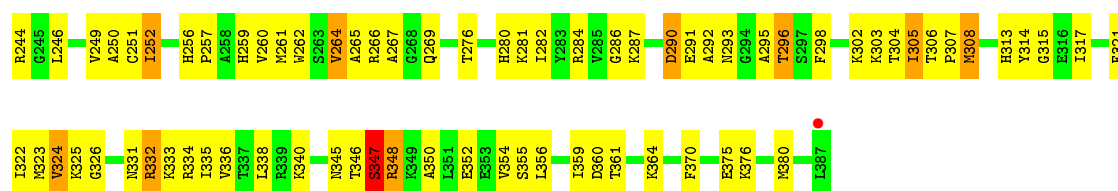
• Molecule 39: 60S ribosomal protein L2-A



• Molecule 40: 60S ribosomal protein L3

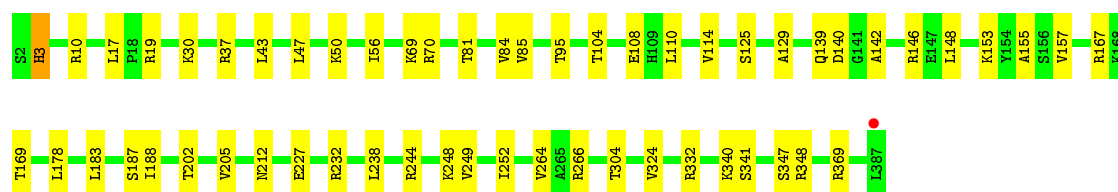






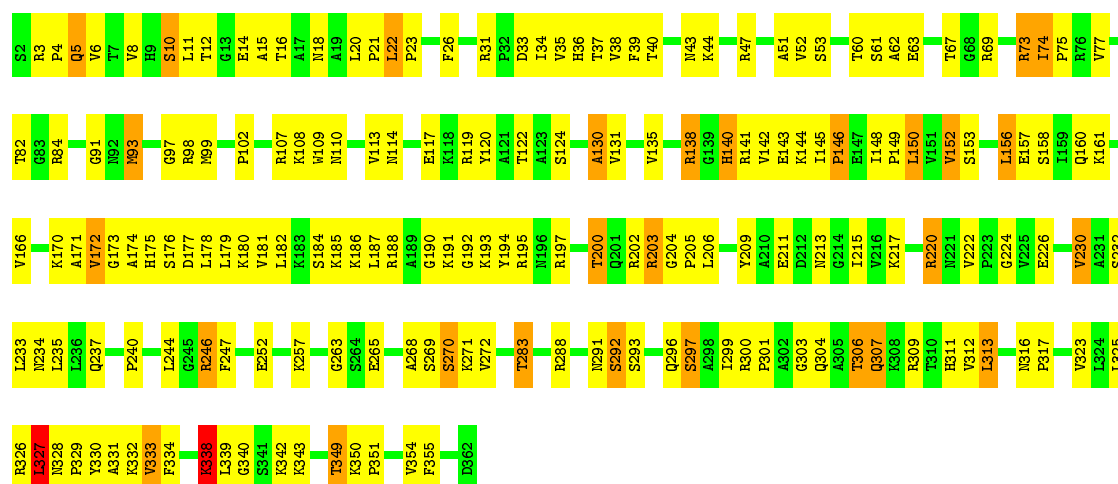
• Molecule 40: 60S ribosomal protein L3

Chain l3: 85% 14%



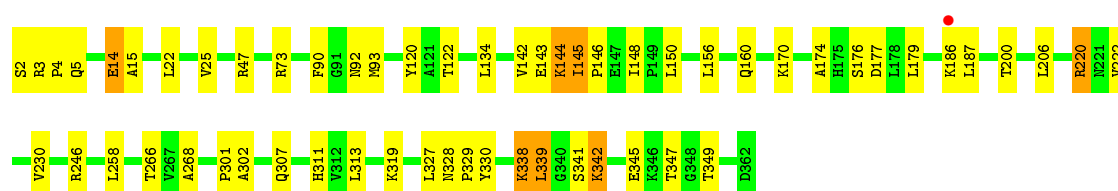
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 49% 42% 8%



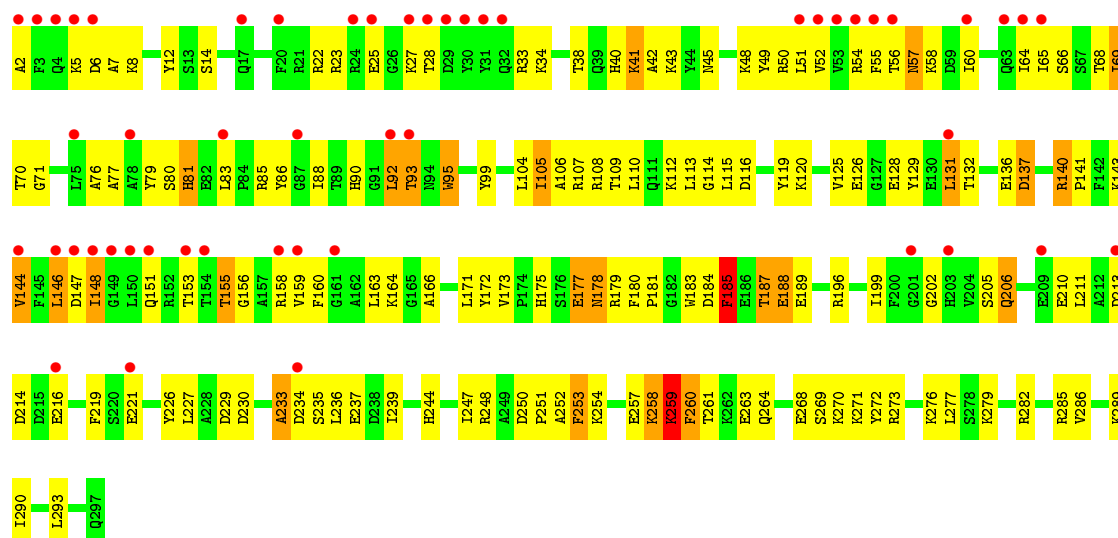
• Molecule 41: 60S ribosomal protein L4-A

Chain l4: 84% 14%

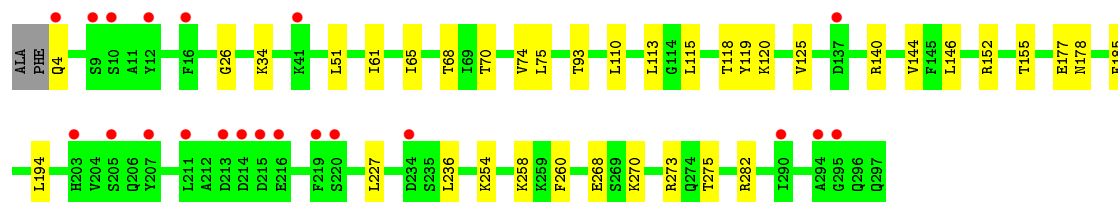
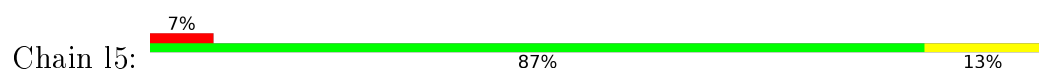


• Molecule 42: 60S ribosomal protein L5

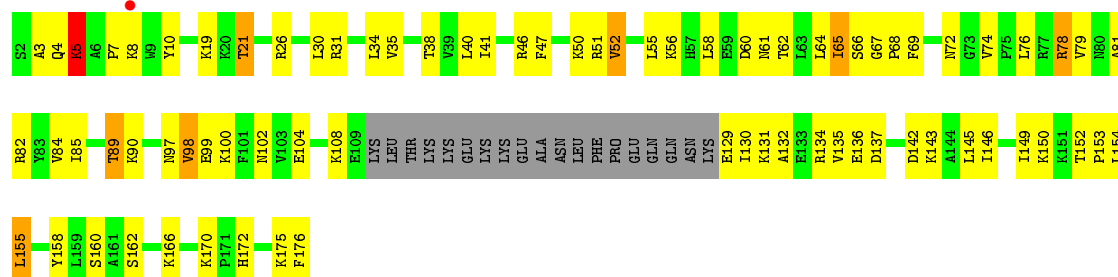
Chain L5: 17% 47% 45% 8%



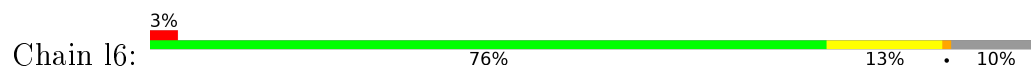
• Molecule 42: 60S ribosomal protein L5



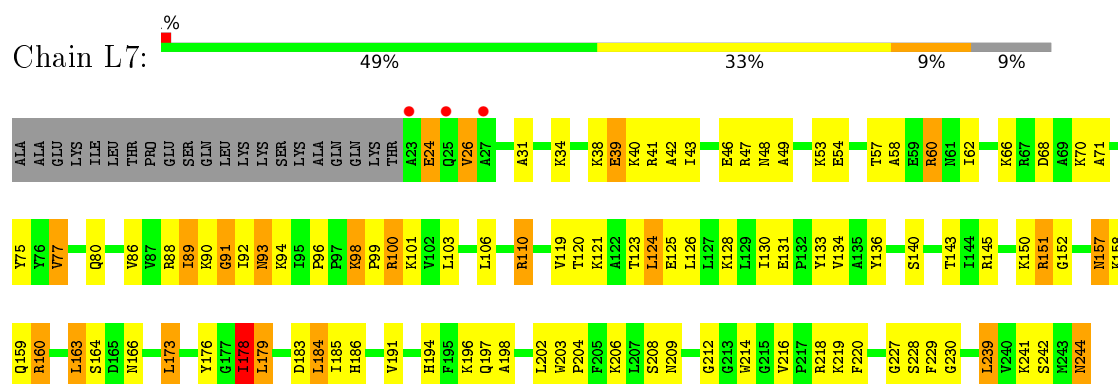
• Molecule 43: 60S ribosomal protein L6-A



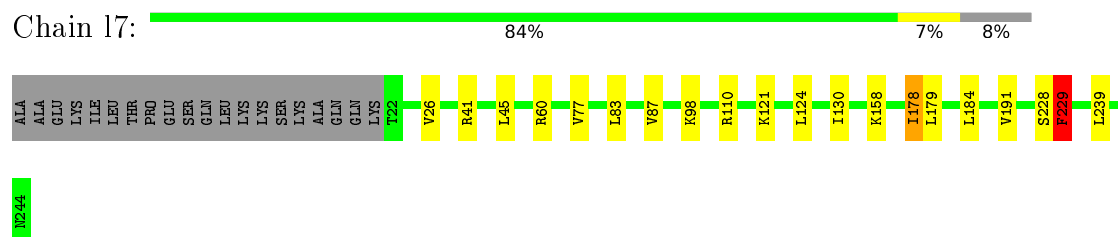
• Molecule 43: 60S ribosomal protein L6-A



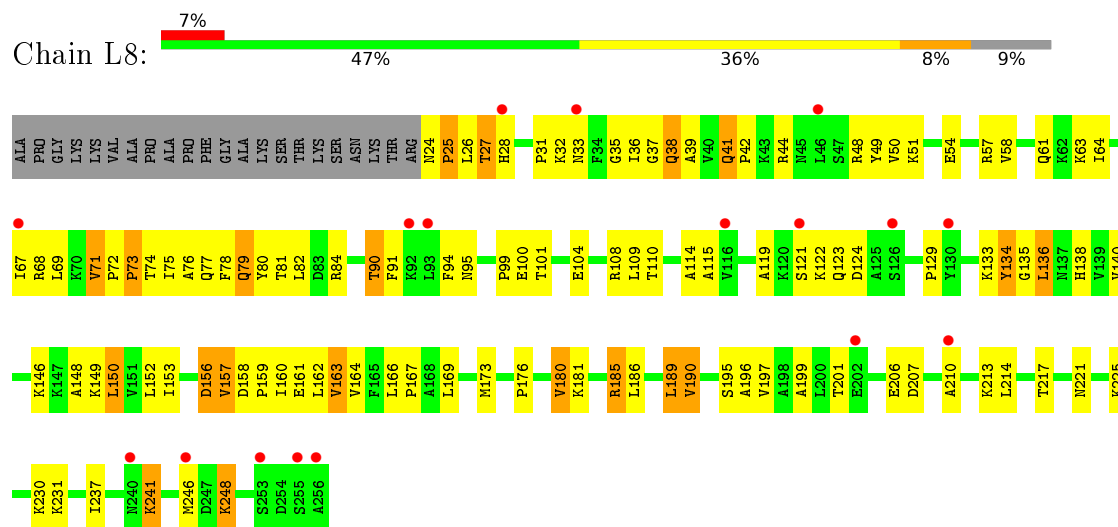
• Molecule 44: 60S ribosomal protein L7-A



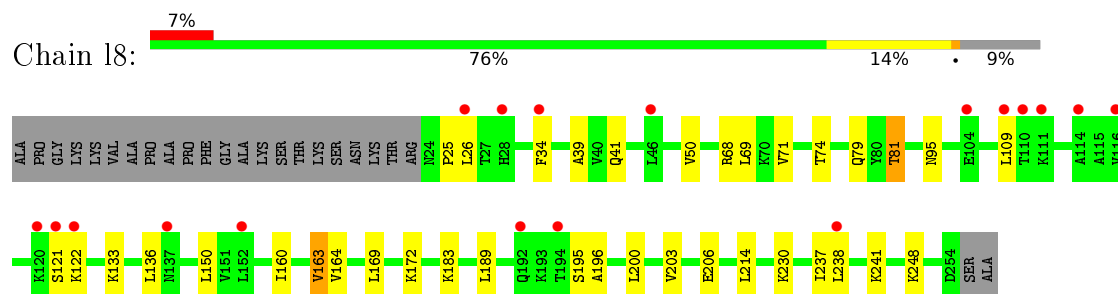
- Molecule 44: 60S ribosomal protein L7-A



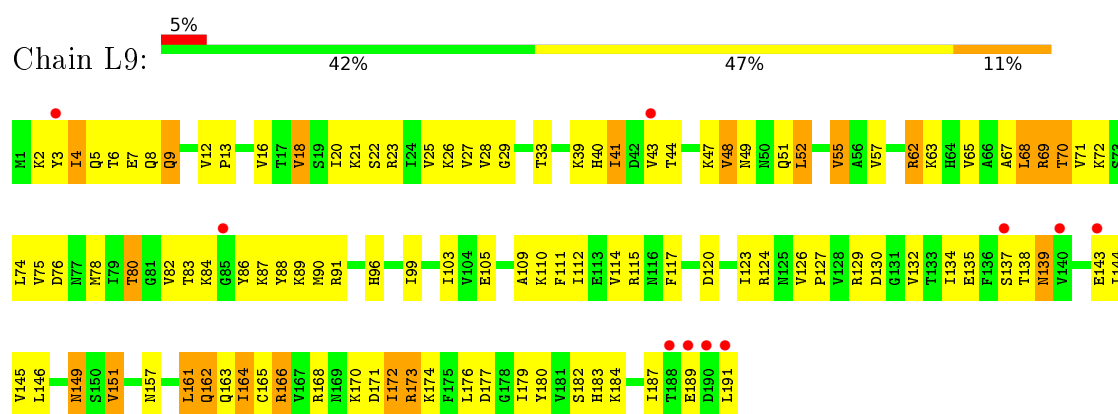
- Molecule 45: 60S ribosomal protein L8-A (eL8)



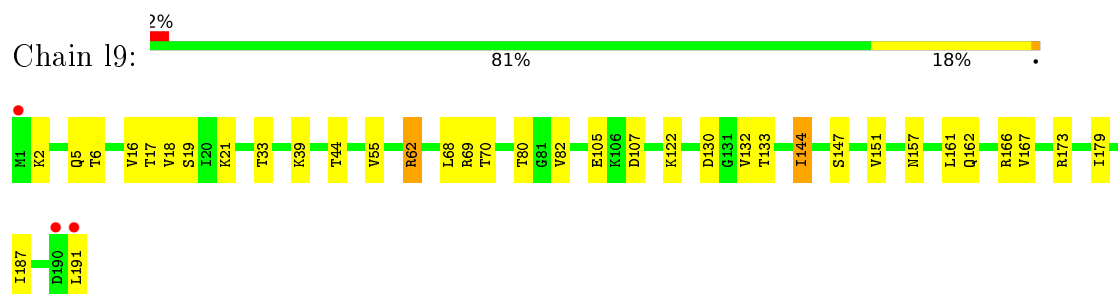
- Molecule 45: 60S ribosomal protein L8-A (eL8)



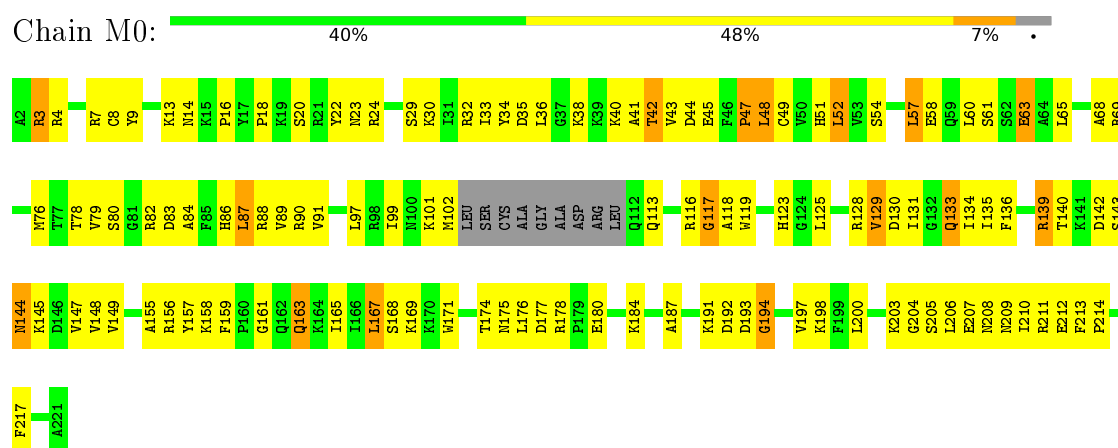
- Molecule 46: 60S ribosomal protein L9-A



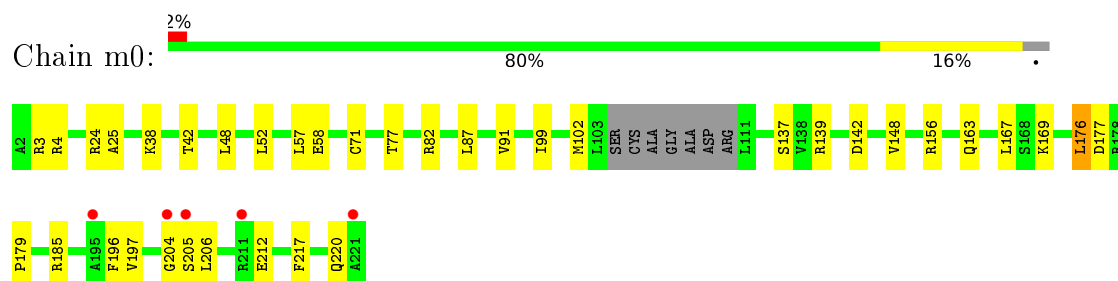
- Molecule 46: 60S ribosomal protein L9-A



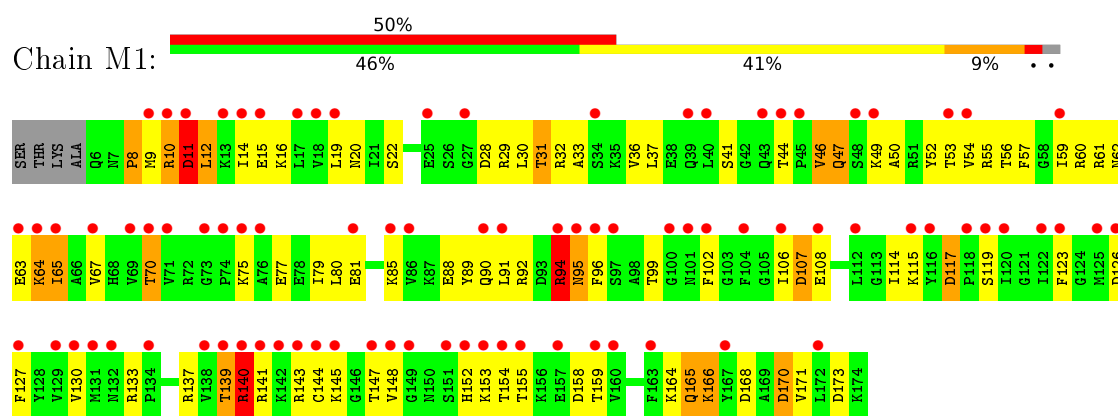
- Molecule 47: 60S ribosomal protein L10



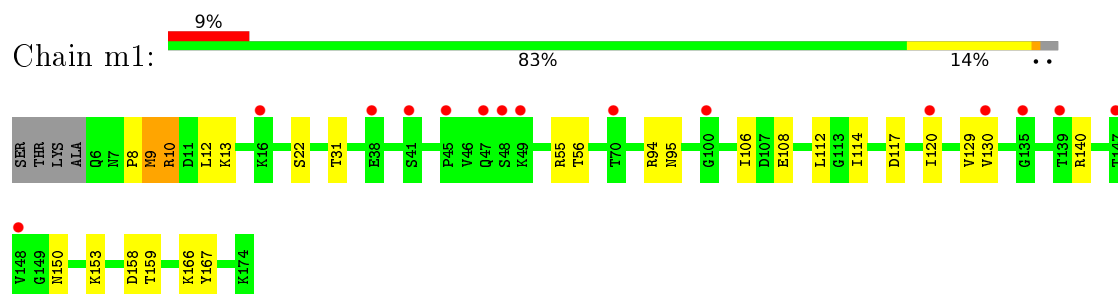
- Molecule 47: 60S ribosomal protein L10



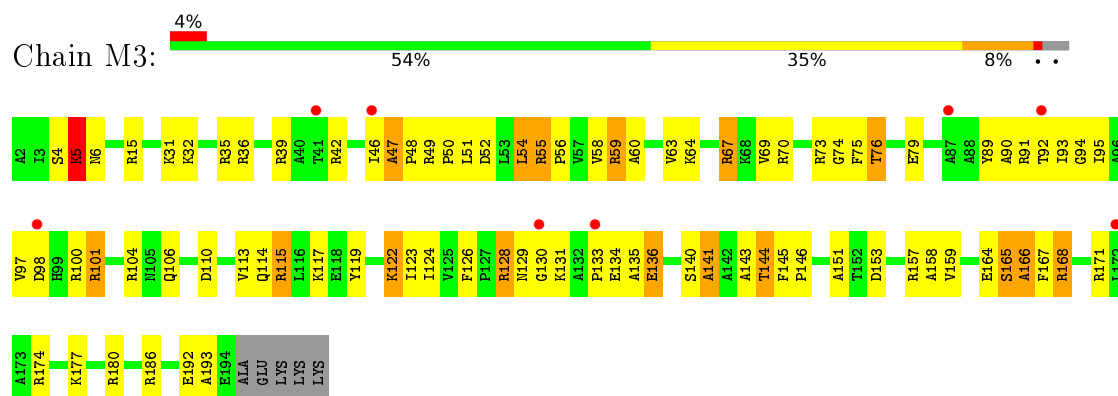
- Molecule 48: 60S ribosomal protein L11-B



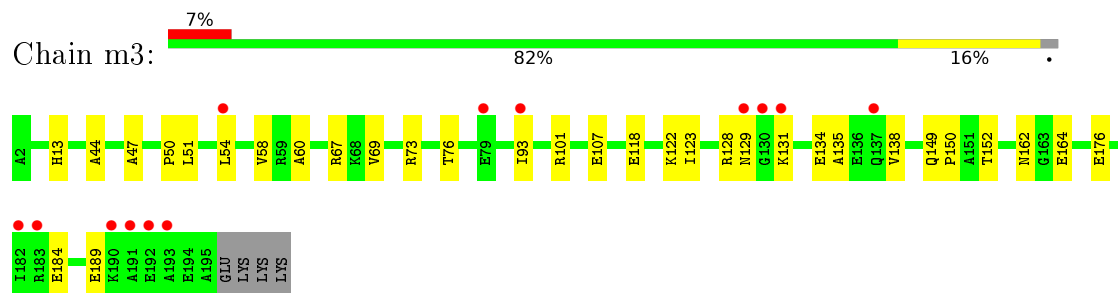
• Molecule 48: 60S ribosomal protein L11-B



• Molecule 49: 60S ribosomal protein L13-A

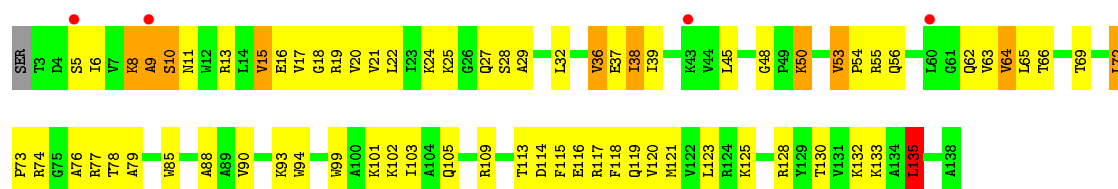


• Molecule 49: 60S ribosomal protein L13-A



• Molecule 50: 60S ribosomal protein L14-A





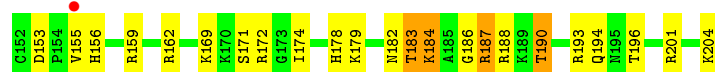
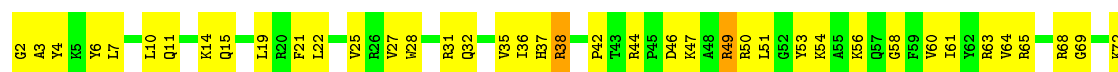
• Molecule 50: 60S ribosomal protein L14-A

Chain m4: 88% 12%



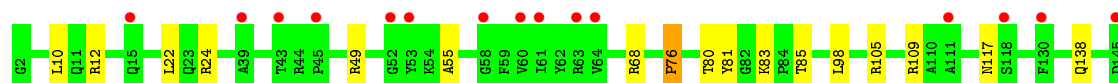
• Molecule 51: 60S ribosomal protein L15-A

Chain M5: 48% 45% 7%



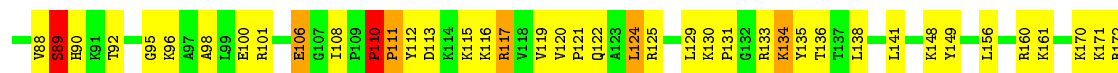
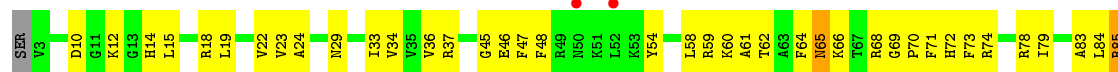
• Molecule 51: 60S ribosomal protein L15-A

Chain m5: 9% 90% 10%

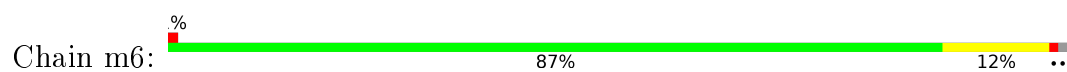


• Molecule 52: 60S ribosomal protein L16-A

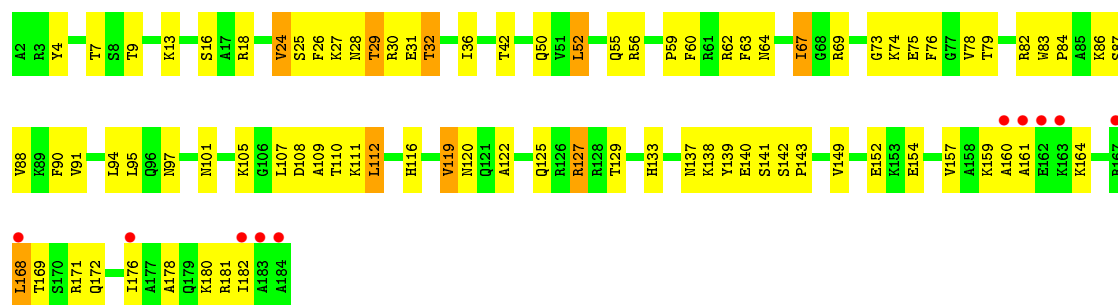
Chain M6: % 53% 42% . . .



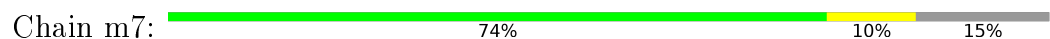
• Molecule 52: 60S ribosomal protein L16-A



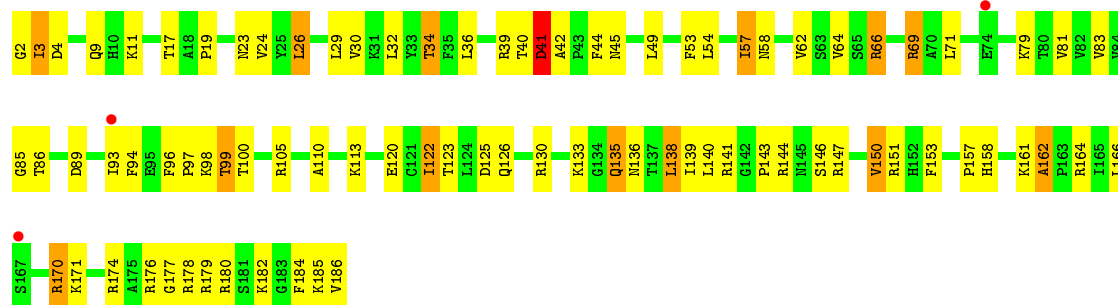
- Molecule 53: 60S ribosomal protein L17-A



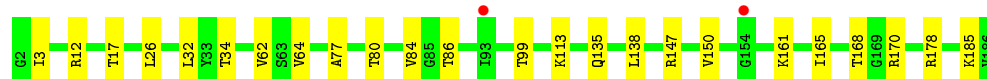
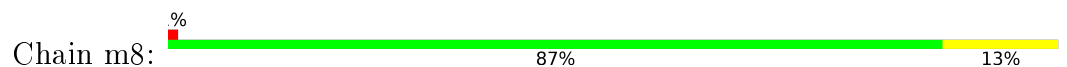
- Molecule 53: 60S ribosomal protein L17-A



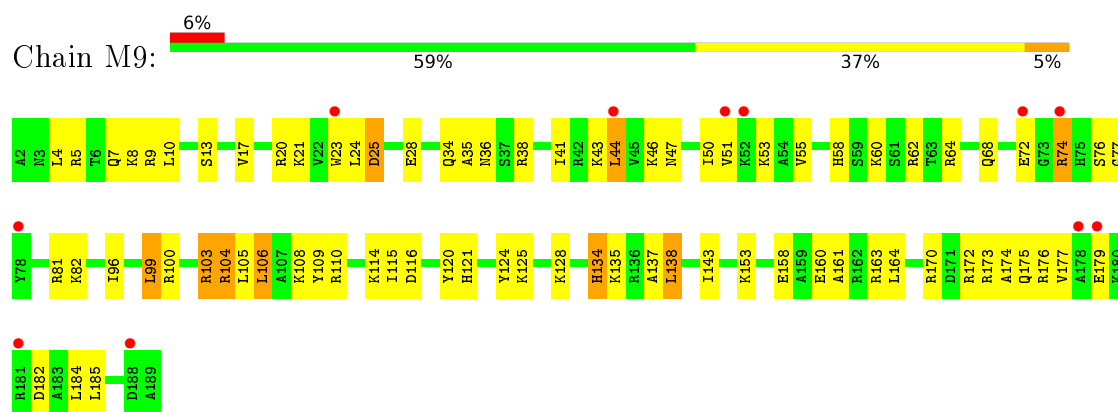
- Molecule 54: 60S ribosomal protein L18-A



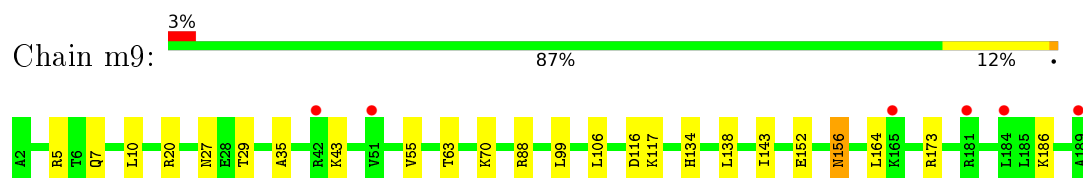
- Molecule 54: 60S ribosomal protein L18-A



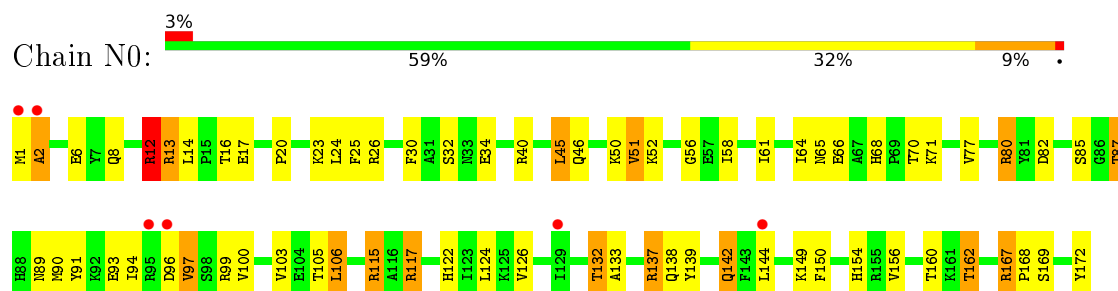
- Molecule 55: 60S ribosomal protein L19-A



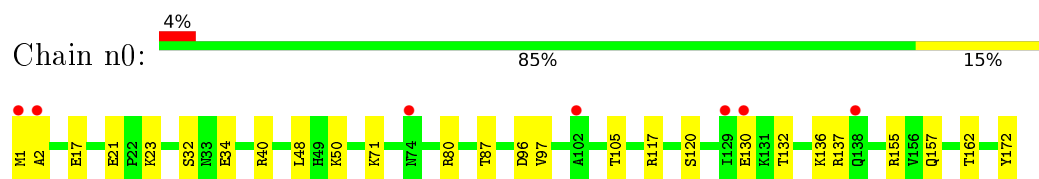
- Molecule 55: 60S ribosomal protein L19-A



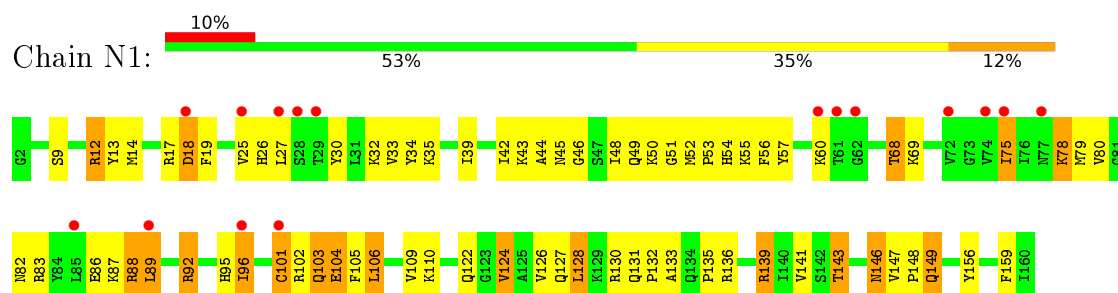
- Molecule 56: 60S ribosomal protein L20-A



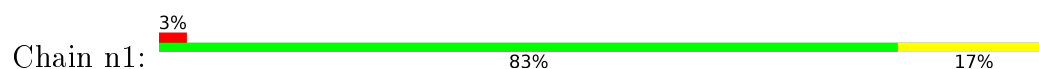
- Molecule 56: 60S ribosomal protein L20-A



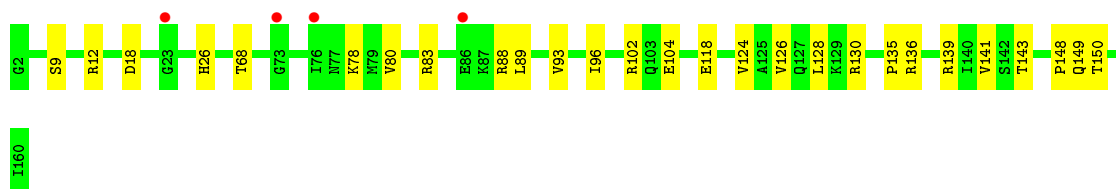
- Molecule 57: 60S ribosomal protein L21-A



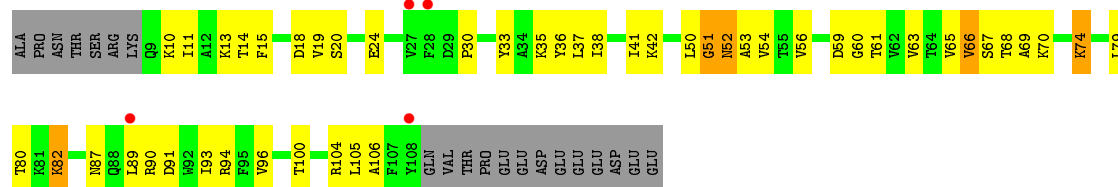
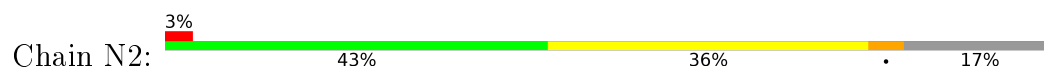
- Molecule 57: 60S ribosomal protein L21-A







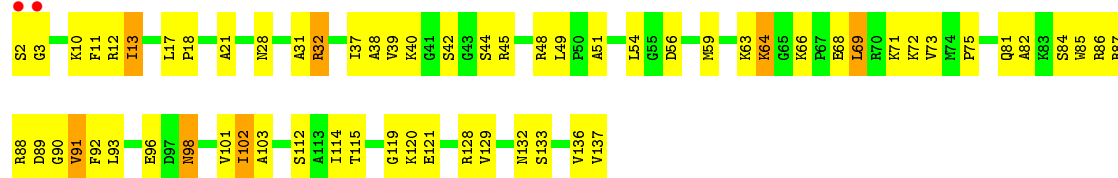
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



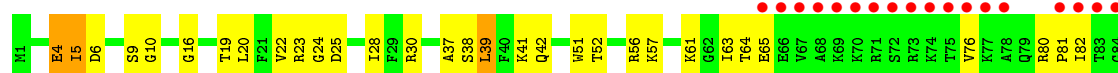
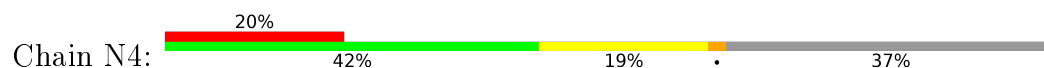
- Molecule 59: 60S ribosomal protein L23-A



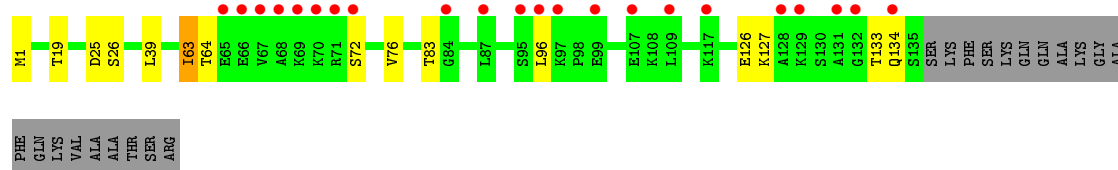
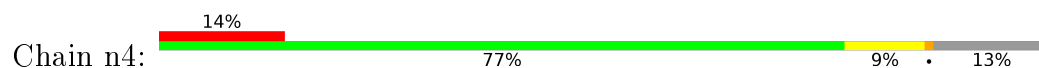
- Molecule 59: 60S ribosomal protein L23-A



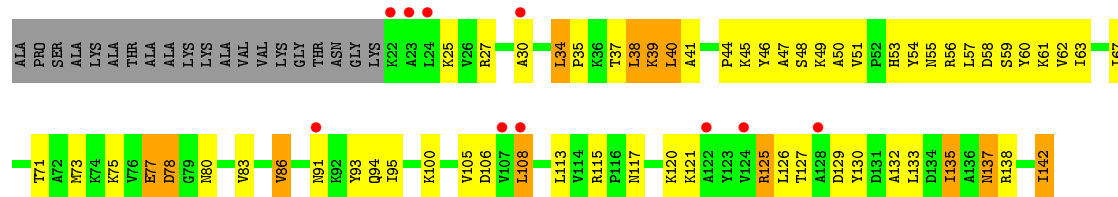
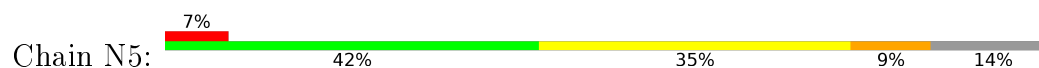
- Molecule 60: 60S ribosomal protein L24-A



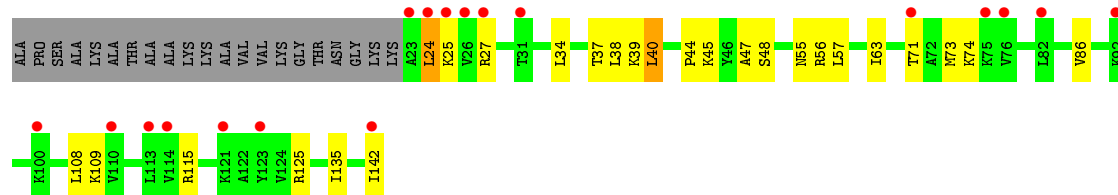
- Molecule 60: 60S ribosomal protein L24-A



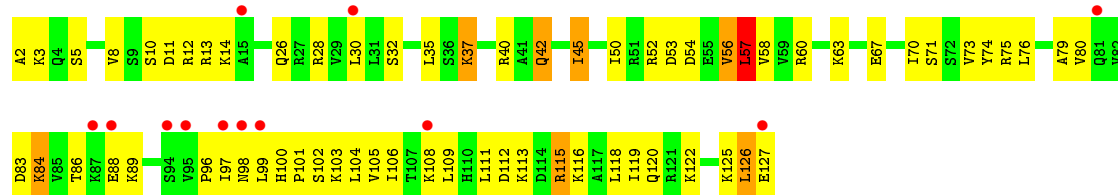
- Molecule 61: 60S ribosomal protein L25



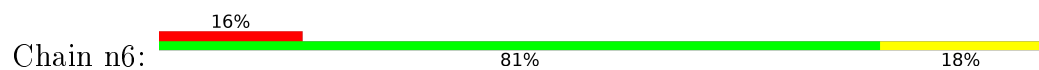
- Molecule 61: 60S ribosomal protein L25

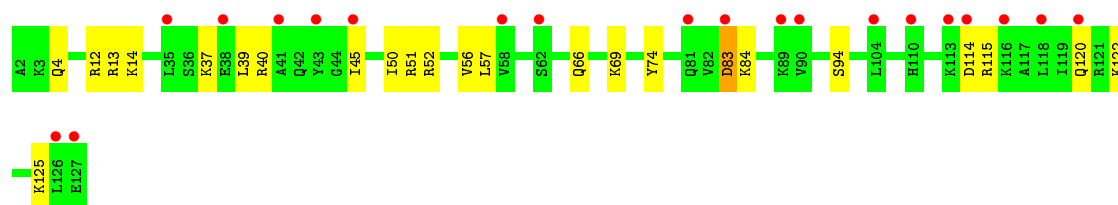


- Molecule 62: 60S ribosomal protein L26-A

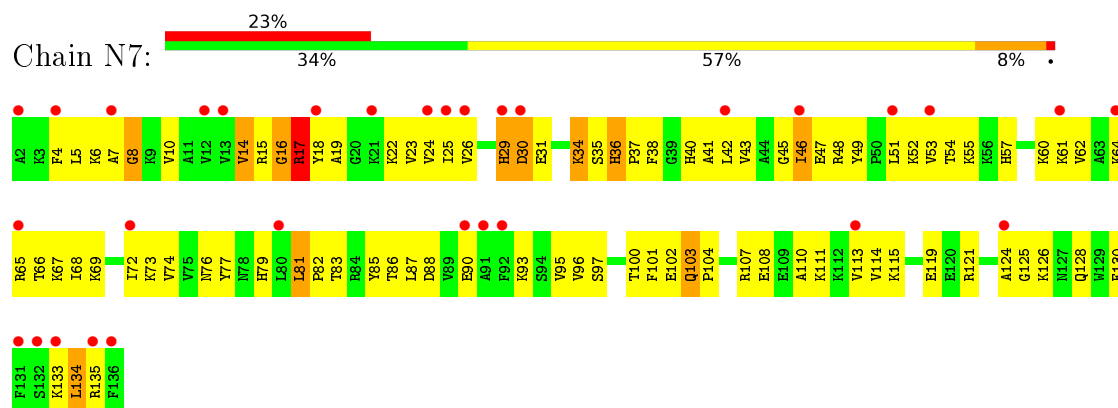


- Molecule 62: 60S ribosomal protein L26-A

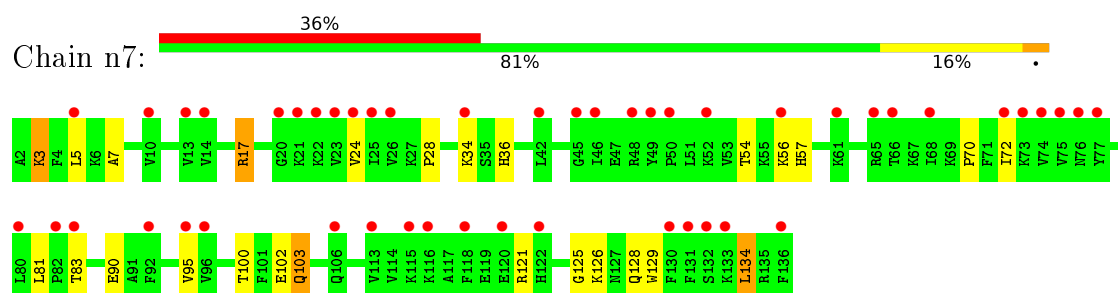




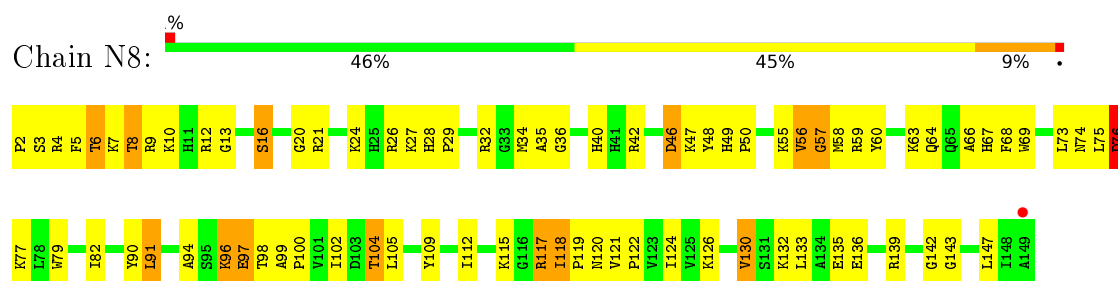
- Molecule 63: 60S ribosomal protein L27-A



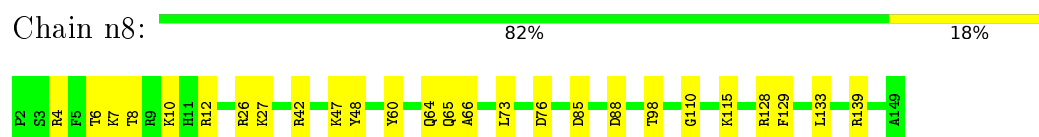
- Molecule 63: 60S ribosomal protein L27-A



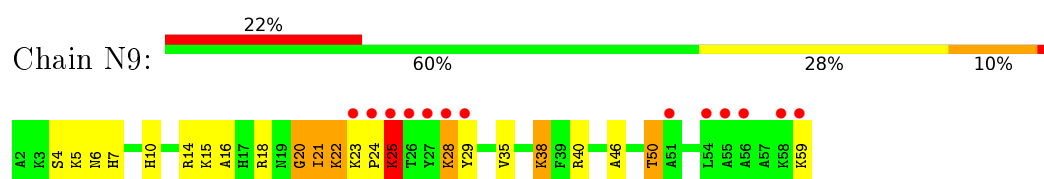
- Molecule 64: 60S ribosomal protein L28



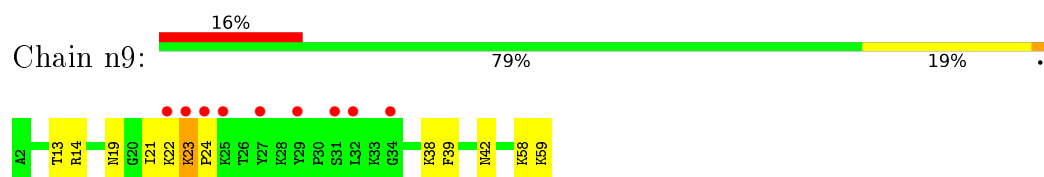
- Molecule 64: 60S ribosomal protein L28



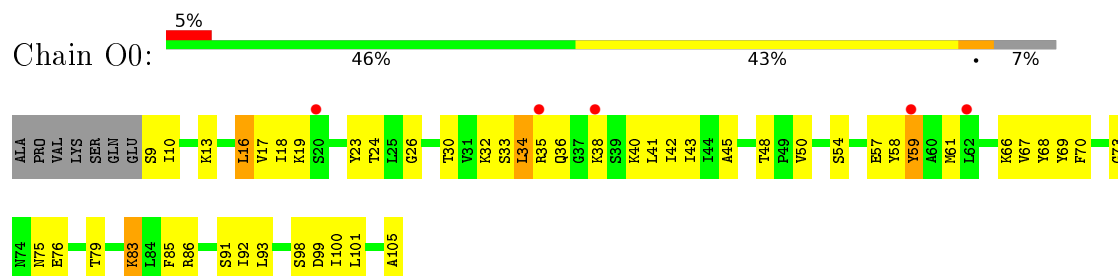
- Molecule 65: 60S ribosomal protein L29



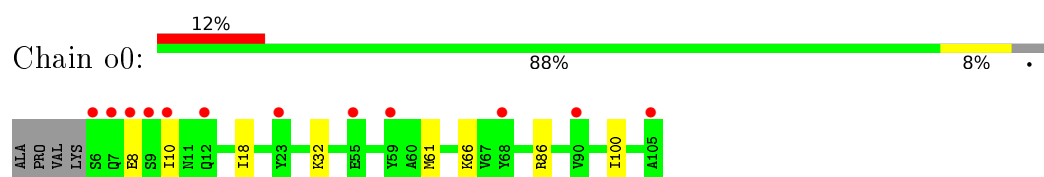
- Molecule 65: 60S ribosomal protein L29



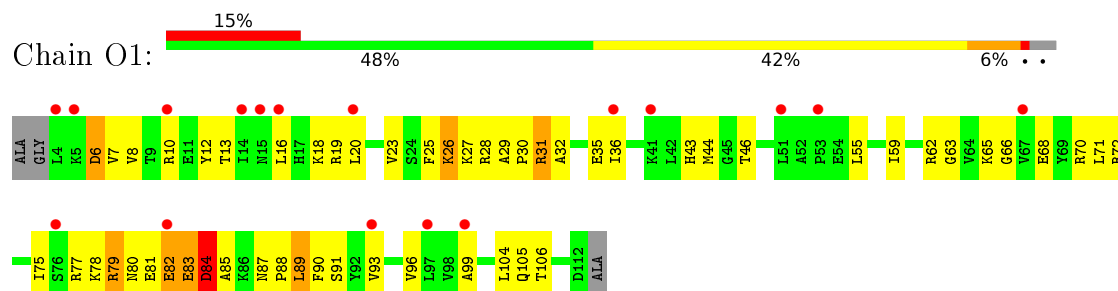
- Molecule 66: 60S ribosomal protein L30



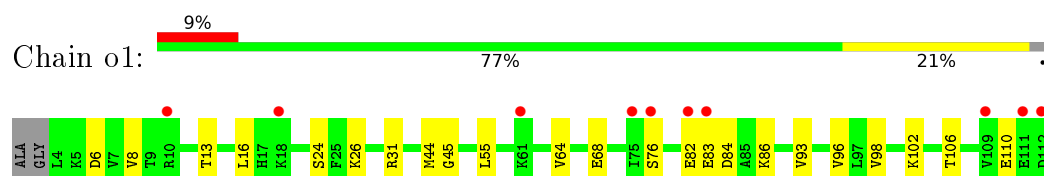
- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A



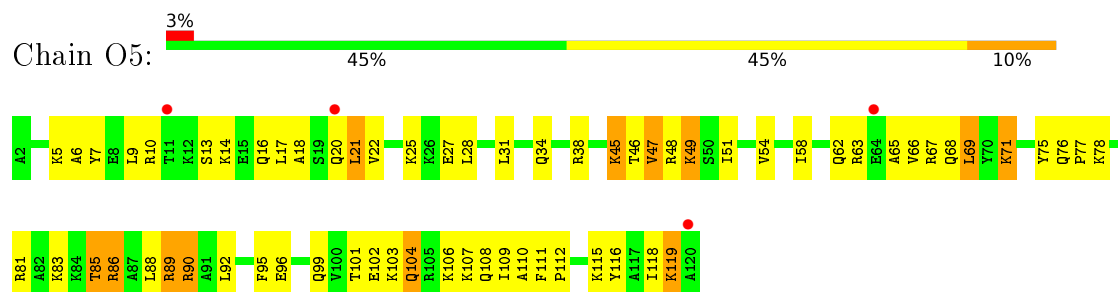
- Molecule 67: 60S ribosomal protein L31-A



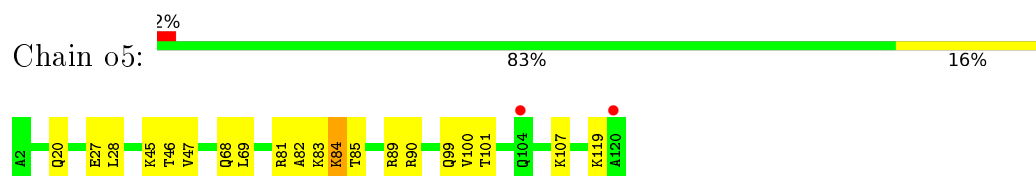
- Molecule 68: 60S ribosomal protein L32



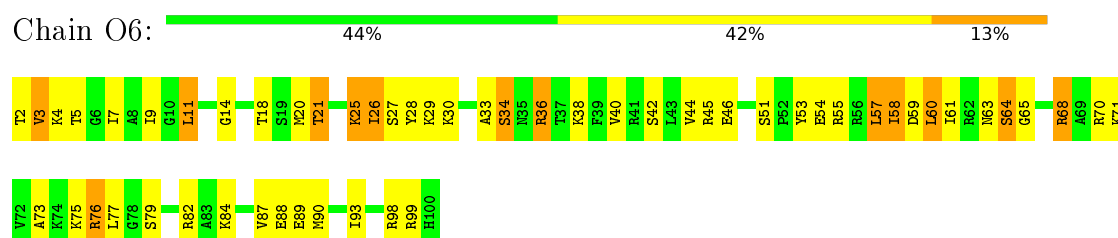
## • Molecule 71: 60S ribosomal protein L35-A



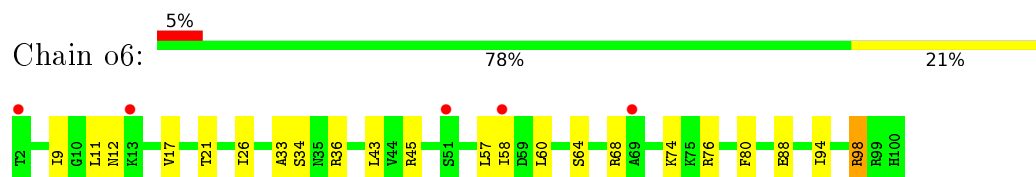
## • Molecule 71: 60S ribosomal protein L35-A



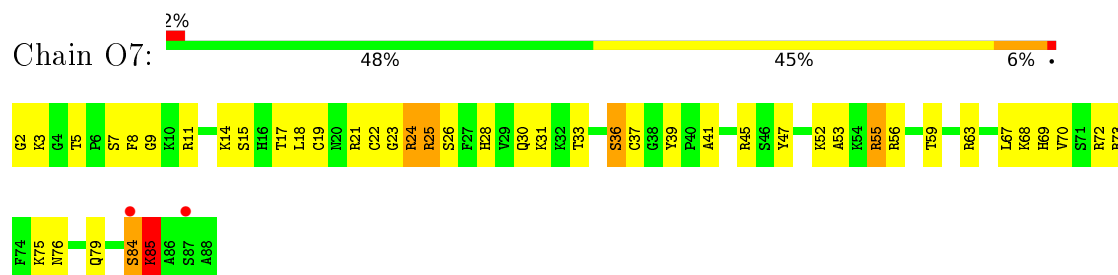
## • Molecule 72: 60S ribosomal protein L36-A



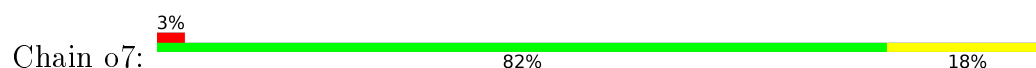
## • Molecule 72: 60S ribosomal protein L36-A



## • Molecule 73: 60S ribosomal protein L37-A

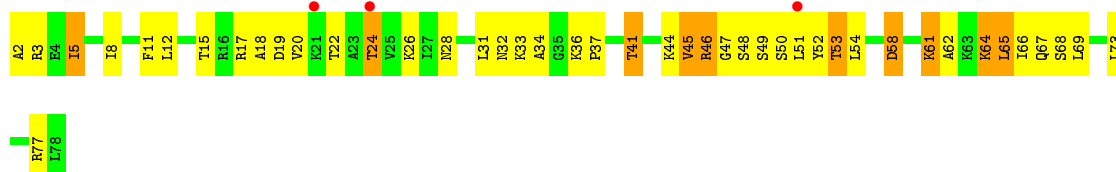


## • Molecule 73: 60S ribosomal protein L37-A

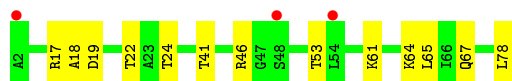
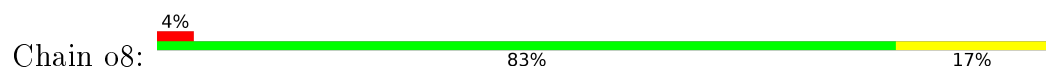




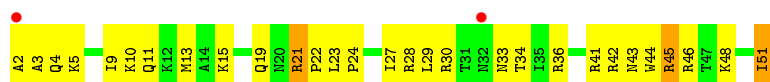
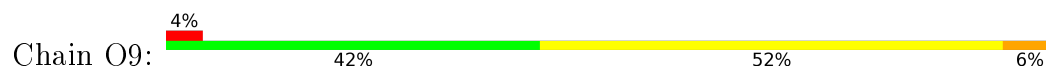
- Molecule 74: 60S ribosomal protein L38



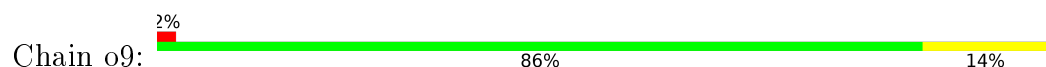
- Molecule 74: 60S ribosomal protein L38



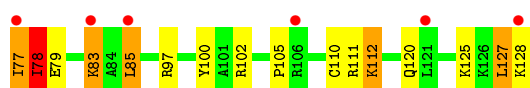
- Molecule 75: 60S ribosomal protein L39



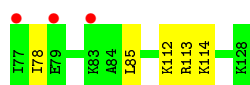
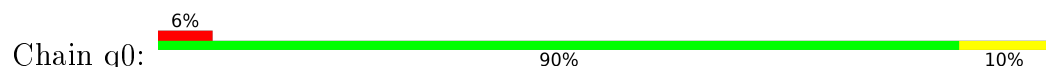
- Molecule 75: 60S ribosomal protein L39



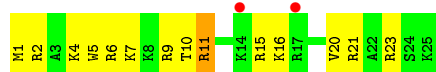
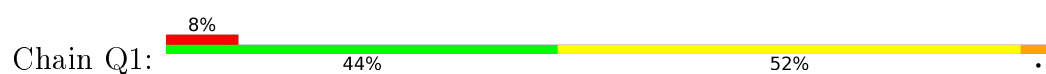
- Molecule 76: Ubiquitin-60S ribosomal protein L40



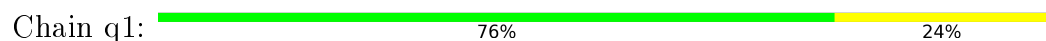
- Molecule 76: Ubiquitin-60S ribosomal protein L40



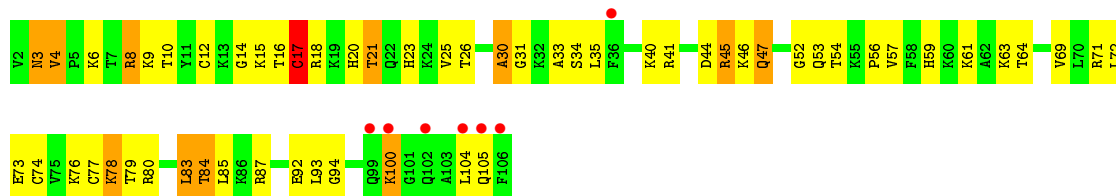
- Molecule 77: 60S ribosomal protein L41-A



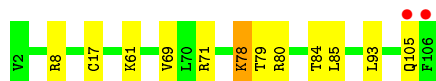
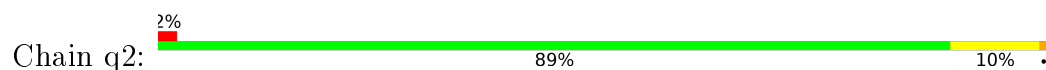
- Molecule 77: 60S ribosomal protein L41-A



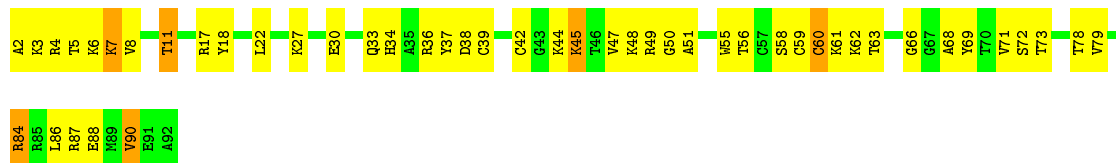
- Molecule 78: 60S ribosomal protein L42-A



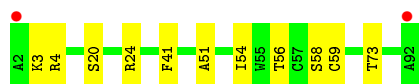
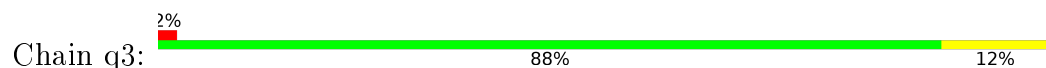
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A

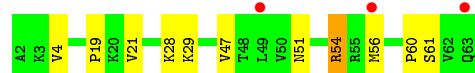
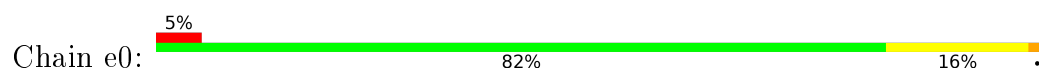


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S30-A

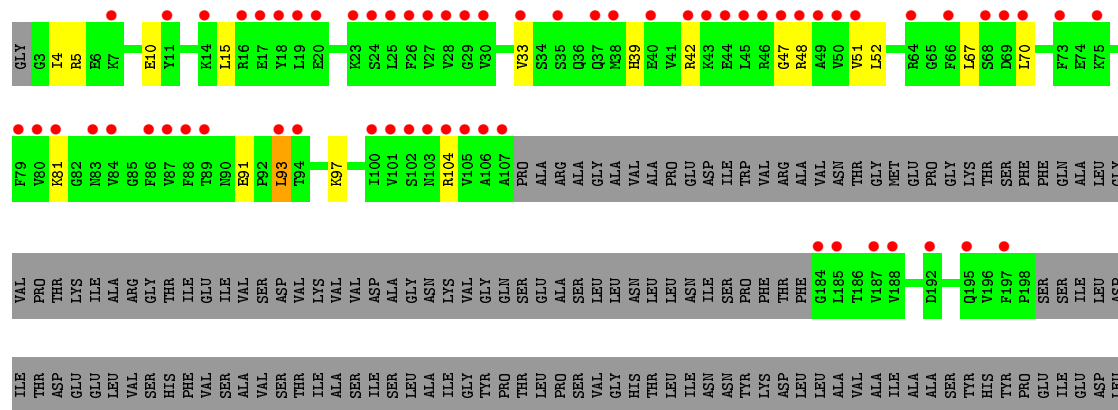
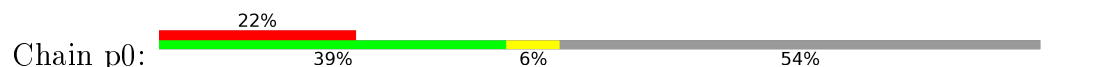




- Molecule 81: 60S ribosomal protein L12-A (uL11)



- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: 60S ribosomal protein P1 alpha/P2 beta



There are no outlier residues recorded for this chain.

- Molecule 84: 60S ribosomal protein P1 alpha/P2 beta



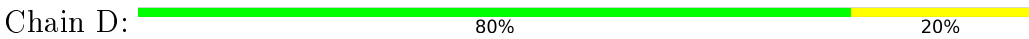
There are no outlier residues recorded for this chain.

- Molecule 85: DNA (5'-R(\*CP\*CP\*(8AN)\*(Pro)\*(Pro))-3')



There are no outlier residues recorded for this chain.

- Molecule 85: DNA (5'-R(\*CP\*CP\*(8AN)\*(Pro)\*(Pro))-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	437.14Å 287.91Å 303.85Å 90.00° 98.76° 90.00°	Depositor
Resolution (Å)	149.05 – 3.10 149.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (149.05-3.10) 99.9 (149.04-3.10)	Depositor EDS
$R_{merge}$	0.56	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.238 , 0.284 0.248 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	73.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	402683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SPS, MG, 8AN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	2	0.36	0/42467	0.88	40/66169 (0.1%)
1	6	0.41	0/42790	0.91	34/66673 (0.1%)
2	S0	0.25	0/1617	0.47	0/2215
2	s0	0.27	0/1623	0.51	0/2222
3	S1	0.25	0/1735	0.50	0/2335
3	s1	0.30	0/1748	0.52	0/2352
4	S2	0.28	0/1665	0.48	0/2263
4	s2	0.32	0/1665	0.54	0/2263
5	S3	0.27	0/1759	0.46	0/2368
5	s3	0.25	0/1759	0.44	0/2368
6	S4	0.29	0/2109	0.53	0/2839
6	s4	0.30	0/2109	0.54	0/2839
7	S5	0.25	0/1629	0.48	0/2202
7	s5	0.25	0/1629	0.47	0/2202
8	S6	0.29	0/1823	0.48	0/2439
8	s6	0.31	0/1779	0.51	0/2379
9	S7	0.26	0/1506	0.50	0/2028
9	s7	0.27	0/1516	0.48	0/2043
10	S8	0.32	0/1514	0.51	0/2021
10	s8	0.33	0/1514	0.53	0/2021
11	S9	0.27	0/1519	0.47	0/2035
11	s9	0.30	0/1519	0.49	0/2035
12	C0	0.28	0/790	0.53	2/1069 (0.2%)
12	c0	0.27	0/777	0.52	2/1049 (0.2%)
13	C1	0.32	0/1239	0.51	0/1673
13	c1	0.36	0/1194	0.56	1/1610 (0.1%)
14	C2	0.24	0/900	0.46	0/1224
14	c2	0.22	0/900	0.45	0/1224
15	C3	0.29	0/1215	0.51	1/1638 (0.1%)
15	c3	0.32	0/1215	0.51	0/1638
16	C4	0.26	0/901	0.51	0/1217
16	c4	0.31	0/960	0.53	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.30	0/998	0.51	0/1341
17	c5	0.28	0/1060	0.50	0/1426
18	C6	0.28	0/1125	0.53	1/1510 (0.1%)
18	c6	0.27	0/1131	0.49	0/1518
19	C7	0.27	0/935	0.50	0/1254
19	c7	0.25	0/914	0.49	0/1224
20	C8	0.27	0/1211	0.49	0/1628
20	c8	0.27	0/1211	0.49	0/1628
21	C9	0.27	0/1130	0.45	0/1517
21	c9	0.27	0/1130	0.45	0/1517
22	D0	0.27	0/865	0.48	0/1169
22	d0	0.27	0/892	0.50	0/1205
23	D1	0.27	0/693	0.45	0/935
23	d1	0.28	0/693	0.47	0/935
24	D2	0.30	0/1038	0.57	2/1395 (0.1%)
24	d2	0.33	0/1038	0.54	1/1395 (0.1%)
25	D3	0.35	0/1139	0.56	0/1518
25	d3	0.36	0/1139	0.54	0/1518
26	D4	0.28	0/1087	0.45	0/1449
26	d4	0.30	0/1087	0.52	0/1449
27	D5	0.26	0/571	0.56	0/768
27	d5	0.23	0/566	0.43	0/761
28	D6	0.29	0/782	0.52	0/1047
28	d6	0.32	0/782	0.54	0/1047
29	D7	0.26	0/620	0.49	0/838
29	d7	0.28	0/620	0.51	0/838
30	D8	0.24	0/499	0.45	0/670
30	d8	0.25	0/499	0.48	0/670
31	D9	0.30	0/452	0.51	0/600
31	d9	0.31	0/452	0.52	0/600
32	E0	0.27	0/483	0.45	0/643
33	E1	0.27	0/577	0.56	0/770
33	e1	0.28	0/619	0.61	0/822
34	SR	0.24	0/2490	0.45	0/3389
34	sR	0.22	0/2495	0.42	0/3395
35	SM	0.31	0/984	0.51	1/1323 (0.1%)
35	sM	0.32	0/585	0.48	0/788
36	1	0.55	0/75368	1.03	147/117502 (0.1%)
36	5	0.57	1/75388 (0.0%)	1.04	135/117532 (0.1%)
37	3	0.44	0/2883	0.86	0/4491
37	7	0.56	0/2883	1.00	3/4491 (0.1%)
38	4	0.54	0/3746	0.97	2/5832 (0.0%)
38	8	0.49	0/3746	0.93	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.39	0/1948	0.59	0/2617
39	l2	0.39	0/1946	0.62	1/2614 (0.0%)
40	L3	0.40	0/3146	0.57	0/4228
40	l3	0.43	0/3146	0.59	0/4228
41	L4	0.41	0/2800	0.62	1/3790 (0.0%)
41	l4	0.40	0/2800	0.61	1/3790 (0.0%)
42	L5	0.33	0/2425	0.51	0/3271
42	l5	0.40	0/2408	0.56	0/3248
43	L6	0.38	0/1260	0.54	0/1694
43	l6	0.41	0/1269	0.57	0/1705
44	L7	0.41	0/1821	0.57	0/2451
44	l7	0.43	0/1828	0.61	1/2461 (0.0%)
45	L8	0.32	0/1836	0.53	0/2481
45	l8	0.31	0/1796	0.51	0/2431
46	L9	0.36	0/1539	0.51	0/2073
46	l9	0.38	0/1539	0.56	0/2073
47	M0	0.38	0/1741	0.53	1/2335 (0.0%)
47	m0	0.43	0/1758	0.58	0/2358
48	M1	0.29	0/1374	0.49	0/1842
48	m1	0.37	0/1374	0.57	0/1842
49	M3	0.38	0/1568	0.58	0/2106
49	m3	0.36	0/1573	0.57	0/2113
50	M4	0.37	0/1068	0.56	0/1438
50	m4	0.40	0/1074	0.57	0/1446
51	M5	0.40	0/1757	0.58	0/2354
51	m5	0.36	0/1757	0.54	0/2354
52	M6	0.28	0/1585	0.46	0/2128
52	m6	0.31	0/1585	0.47	0/2128
53	M7	0.42	0/1443	0.58	0/1944
53	m7	0.44	0/1250	0.58	0/1683
54	M8	0.39	0/1465	0.60	0/1965
54	m8	0.40	0/1465	0.61	0/1965
55	M9	0.31	0/1538	0.47	0/2050
55	m9	0.33	0/1538	0.48	0/2050
56	N0	0.39	0/1481	0.55	0/1990
56	n0	0.42	0/1481	0.57	0/1990
57	N1	0.39	0/1300	0.54	0/1743
57	n1	0.45	0/1300	0.56	0/1743
58	N2	0.28	0/812	0.47	0/1099
58	n2	0.30	0/794	0.51	0/1076
59	N3	0.40	0/1018	0.56	0/1369
59	n3	0.46	0/1018	0.64	0/1369
60	N4	0.33	0/712	0.47	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.34	0/1052	0.53	0/1398
61	N5	0.34	0/979	0.56	0/1321
61	n5	0.37	0/974	0.57	0/1314
62	N6	0.36	0/1004	0.59	1/1341 (0.1%)
62	n6	0.36	0/1004	0.55	0/1341
63	N7	0.31	0/1118	0.52	0/1497
63	n7	0.30	0/1118	0.50	0/1497
64	N8	0.42	0/1204	0.61	0/1612
64	n8	0.41	0/1204	0.59	1/1612 (0.1%)
65	N9	0.39	0/473	0.53	0/629
65	n9	0.43	0/473	0.76	1/629 (0.2%)
66	O0	0.30	0/751	0.47	0/1008
66	o0	0.30	0/775	0.46	0/1040
67	O1	0.35	0/890	0.51	0/1196
67	o1	0.40	0/897	0.57	0/1205
68	O2	0.42	0/1041	0.59	0/1394
68	o2	0.46	0/1041	0.63	0/1394
69	O3	0.46	0/868	0.57	0/1168
69	o3	0.47	0/868	0.61	0/1168
70	O4	0.35	0/890	0.58	1/1189 (0.1%)
70	o4	0.35	0/890	0.57	0/1189
71	O5	0.37	0/978	0.58	1/1301 (0.1%)
71	o5	0.33	0/974	0.50	0/1297
72	O6	0.35	0/778	0.53	0/1034
72	o6	0.31	0/777	0.52	0/1033
73	O7	0.44	0/696	0.60	0/923
73	o7	0.41	0/696	0.59	0/923
74	O8	0.30	0/618	0.49	0/826
74	o8	0.30	0/614	0.47	0/822
75	O9	0.40	0/443	0.58	0/588
75	o9	0.39	0/443	0.55	0/588
76	Q0	0.44	0/423	0.59	0/562
76	q0	0.47	0/423	0.62	0/562
77	Q1	0.35	0/234	0.68	0/300
77	q1	0.41	0/234	0.56	0/300
78	Q2	0.52	1/860 (0.1%)	0.64	0/1136
78	q2	0.51	1/860 (0.1%)	0.61	1/1136 (0.1%)
79	Q3	0.40	0/701	0.55	0/934
79	q3	0.45	0/701	0.56	0/934
80	e0	0.30	0/499	0.53	0/665
82	p0	0.26	0/1091	0.51	2/1472 (0.1%)
85	C	0.74	0/54	1.28	0/76
85	D	0.47	0/57	0.96	0/80

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.45	3/430695 (0.0%)	0.84	385/632350 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
22	d0	0	1
39	L2	0	1
52	M6	0	1
52	m6	0	1
64	n8	0	1
65	N9	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	8.29	1.96	1.82
78	q2	17	CYS	CB-SG	7.90	1.95	1.82
36	5	1152	G	N9-C4	-6.74	1.32	1.38

The worst 5 of 385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-15.26	116.84	126.00
36	5	1152	G	N3-C4-C5	14.46	135.83	128.60
36	1	2403	G	N1-C6-O6	10.51	126.21	119.90
36	5	1152	G	C8-N9-C1'	9.79	139.73	127.00
36	1	2617	U	C5-C4-O4	9.68	131.71	125.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	L2	19	HIS	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide
22	d0	70	THR	Peptide
52	m6	110	PRO	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	2	37970	0	19106	617	1
1	6	38260	0	19252	600	0
2	S0	1577	0	1567	102	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	132	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	89	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	96	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	127	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	74	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	106	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	73	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	89	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	104	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	50	0
12	c0	762	0	700	0	0
13	C1	1213	0	1257	66	0
13	c1	1168	0	1233	0	0
14	C2	892	0	891	44	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	75	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	67	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	62	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	74	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	c7	906	0	909	0	0
20	C8	1192	0	1222	89	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	70	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	50	0
22	d0	882	0	939	0	0
23	D1	684	0	672	44	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	67	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	70	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	62	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	44	0
27	d5	558	0	598	0	0
28	D6	769	0	814	66	0
28	d6	769	0	814	0	0
29	D7	610	0	630	38	0
29	d7	610	0	631	0	0
30	D8	497	0	535	32	0
30	d8	497	0	535	0	0
31	D9	442	0	428	24	0
31	d9	442	0	428	0	0
32	E0	475	0	525	36	0
33	E1	566	0	602	48	0
33	e1	608	0	657	0	0
34	SR	2437	0	2386	92	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	969	52	0
35	sM	681	0	591	0	0
36	1	67333	0	33838	846	0
36	5	67354	0	33851	839	1
37	3	2579	0	1304	33	0
37	7	2579	0	1304	33	0
38	4	3353	0	1695	38	0
38	8	3353	0	1695	57	0
39	L2	1914	0	1981	127	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	163	0
40	l3	3075	0	3142	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	L4	2748	0	2859	160	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	155	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	62	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	87	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	89	0
45	l8	1764	0	1821	0	0
46	L9	1518	0	1587	104	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	105	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	70	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	75	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	69	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	95	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	81	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	75	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	78	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	67	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	57	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	70	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	35	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	52	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	19	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	53	0
61	n5	959	0	1023	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	N6	993	0	1081	51	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	79	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	79	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	26	0
65	n9	462	0	491	0	0
66	O0	743	0	797	33	0
66	o0	767	0	816	0	0
67	O1	876	0	912	34	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	58	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	40	0
69	o3	850	0	880	0	0
70	O4	880	0	945	56	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	66	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	42	0
72	o6	770	0	846	0	0
73	O7	681	0	683	51	0
73	o7	681	0	683	0	0
74	O8	612	0	682	29	0
74	o8	608	0	671	0	0
75	O9	436	0	475	32	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	12	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	16	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	50	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	45	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	180	0	0
82	p0	1076	0	1076	0	0
83	p1	235	0	53	0	0
84	p2	230	0	49	0	0
85	C	73	0	48	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	D	76	0	48	1	0
86	D6	1	0	0	0	0
86	D7	1	0	0	0	0
86	D9	1	0	0	0	0
86	E1	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
86	d6	1	0	0	0	0
86	d7	1	0	0	0	0
86	d9	1	0	0	0	0
86	e1	1	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q2	1	0	0	0	0
86	q3	1	0	0	0	0
87	C	23	0	18	1	0
87	D	23	0	18	6	0
88	C	1	0	0	0	0
88	D	1	0	0	0	0
All	All	402683	0	297750	6748	1

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 10.

The worst 5 of 6748 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)
5:S3:94:ARG:NH2	35:SM:134:ASP:OD1	1.86	1.07
40:L3:296:THR:HG22	40:L3:298:PHE:H	4.58	0.95
1:6:1636:C:H4'	1:6:1637:C:H5'	1.46	0.94
71:O5:85:THR:HG22	71:O5:88:LEU:H	1.33	0.94
64:N8:21:ARG:NH2	36:5:640:U:OP1	182.08	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.13	0.07

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
2	S0	204/251 (81%)	166 (81%)	26 (13%)	12 (6%)	2	12
2	s0	204/251 (81%)	162 (79%)	27 (13%)	15 (7%)	1	7
3	S1	212/254 (84%)	156 (74%)	27 (13%)	29 (14%)	0	1
3	s1	214/254 (84%)	167 (78%)	34 (16%)	13 (6%)	2	11
4	S2	215/253 (85%)	178 (83%)	27 (13%)	10 (5%)	3	17
4	s2	215/253 (85%)	185 (86%)	18 (8%)	12 (6%)	2	13
5	S3	221/239 (92%)	192 (87%)	21 (10%)	8 (4%)	4	24
5	s3	221/239 (92%)	185 (84%)	24 (11%)	12 (5%)	2	14
6	S4	258/260 (99%)	213 (83%)	31 (12%)	14 (5%)	2	14
6	s4	258/260 (99%)	209 (81%)	38 (15%)	11 (4%)	3	19
7	S5	204/224 (91%)	169 (83%)	21 (10%)	14 (7%)	1	8
7	s5	204/224 (91%)	157 (77%)	33 (16%)	14 (7%)	1	8
8	S6	224/236 (95%)	191 (85%)	21 (9%)	12 (5%)	2	14
8	s6	216/236 (92%)	190 (88%)	17 (8%)	9 (4%)	3	19
9	S7	182/189 (96%)	138 (76%)	27 (15%)	17 (9%)	1	4
9	s7	184/189 (97%)	148 (80%)	28 (15%)	8 (4%)	3	19
10	S8	184/200 (92%)	160 (87%)	18 (10%)	6 (3%)	5	26
10	s8	184/200 (92%)	161 (88%)	17 (9%)	6 (3%)	5	26
11	S9	183/196 (93%)	158 (86%)	17 (9%)	8 (4%)	3	18
11	s9	183/196 (93%)	152 (83%)	21 (12%)	10 (6%)	2	13
12	C0	94/105 (90%)	71 (76%)	16 (17%)	7 (7%)	1	7
12	c0	92/105 (88%)	62 (67%)	14 (15%)	16 (17%)	0	0
13	C1	153/155 (99%)	129 (84%)	18 (12%)	6 (4%)	4	22
13	c1	144/155 (93%)	120 (83%)	18 (12%)	6 (4%)	3	19
14	C2	122/142 (86%)	77 (63%)	31 (25%)	14 (12%)	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	78 (64%)	30 (25%)	14 (12%)	0	2
15	C3	148/150 (99%)	126 (85%)	16 (11%)	6 (4%)	3	20
15	c3	148/150 (99%)	118 (80%)	23 (16%)	7 (5%)	3	17
16	C4	125/136 (92%)	92 (74%)	21 (17%)	12 (10%)	1	4
16	c4	126/136 (93%)	102 (81%)	18 (14%)	6 (5%)	3	17
17	C5	122/141 (86%)	90 (74%)	22 (18%)	10 (8%)	1	6
17	c5	133/141 (94%)	98 (74%)	18 (14%)	17 (13%)	0	1
18	C6	139/142 (98%)	116 (84%)	14 (10%)	9 (6%)	1	9
18	c6	140/142 (99%)	123 (88%)	10 (7%)	7 (5%)	3	16
19	C7	116/136 (85%)	91 (78%)	18 (16%)	7 (6%)	2	11
19	c7	113/136 (83%)	90 (80%)	13 (12%)	10 (9%)	1	5
20	C8	143/145 (99%)	121 (85%)	13 (9%)	9 (6%)	2	10
20	c8	143/145 (99%)	116 (81%)	18 (13%)	9 (6%)	2	10
21	C9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	3	19
21	c9	141/143 (99%)	124 (88%)	13 (9%)	4 (3%)	6	30
22	D0	105/120 (88%)	90 (86%)	11 (10%)	4 (4%)	4	22
22	d0	108/120 (90%)	84 (78%)	18 (17%)	6 (6%)	2	13
23	D1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	2	12
23	d1	85/87 (98%)	67 (79%)	13 (15%)	5 (6%)	2	12
24	D2	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	12	44
24	d2	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	24	63
25	D3	142/144 (99%)	111 (78%)	19 (13%)	12 (8%)	1	5
25	d3	142/144 (99%)	127 (89%)	10 (7%)	5 (4%)	4	24
26	D4	132/134 (98%)	110 (83%)	13 (10%)	9 (7%)	1	8
26	d4	132/134 (98%)	112 (85%)	12 (9%)	8 (6%)	2	11
27	D5	68/107 (64%)	53 (78%)	8 (12%)	7 (10%)	1	4
27	d5	67/107 (63%)	56 (84%)	9 (13%)	2 (3%)	5	28
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	71 (75%)	18 (19%)	6 (6%)	2	10
29	D7	79/81 (98%)	66 (84%)	11 (14%)	2 (2%)	7	32
29	d7	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	4	22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	48 (79%)	12 (20%)	1 (2%)	12	44
30	d8	61/66 (92%)	46 (75%)	11 (18%)	4 (7%)	1	9
31	D9	51/55 (93%)	40 (78%)	9 (18%)	2 (4%)	4	22
31	d9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	12
32	E0	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	5	25
33	E1	69/76 (91%)	37 (54%)	18 (26%)	14 (20%)	0	0
33	e1	74/76 (97%)	35 (47%)	20 (27%)	19 (26%)	0	0
34	SR	316/318 (99%)	273 (86%)	30 (10%)	13 (4%)	3	20
34	sR	316/318 (99%)	268 (85%)	38 (12%)	10 (3%)	5	26
35	SM	131/263 (50%)	105 (80%)	16 (12%)	10 (8%)	1	7
35	sM	80/263 (30%)	61 (76%)	8 (10%)	11 (14%)	0	1
39	L2	250/253 (99%)	230 (92%)	15 (6%)	5 (2%)	9	38
39	l2	250/253 (99%)	209 (84%)	32 (13%)	9 (4%)	4	24
40	L3	384/386 (100%)	340 (88%)	28 (7%)	16 (4%)	3	19
40	l3	384/386 (100%)	346 (90%)	30 (8%)	8 (2%)	9	37
41	L4	359/361 (99%)	308 (86%)	32 (9%)	19 (5%)	2	14
41	l4	359/361 (99%)	297 (83%)	39 (11%)	23 (6%)	2	10
42	L5	294/296 (99%)	254 (86%)	22 (8%)	18 (6%)	2	11
42	l5	292/296 (99%)	263 (90%)	22 (8%)	7 (2%)	7	33
43	L6	152/175 (87%)	136 (90%)	14 (9%)	2 (1%)	15	50
43	l6	153/175 (87%)	128 (84%)	21 (14%)	4 (3%)	7	32
44	L7	220/243 (90%)	198 (90%)	14 (6%)	8 (4%)	4	24
44	l7	221/243 (91%)	200 (90%)	17 (8%)	4 (2%)	11	42
45	L8	231/255 (91%)	193 (84%)	29 (13%)	9 (4%)	4	22
45	l8	229/255 (90%)	197 (86%)	20 (9%)	12 (5%)	2	15
46	L9	189/191 (99%)	163 (86%)	24 (13%)	2 (1%)	17	55
46	l9	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	9	37
47	M0	207/220 (94%)	180 (87%)	21 (10%)	6 (3%)	6	29
47	m0	209/220 (95%)	174 (83%)	27 (13%)	8 (4%)	4	22
48	M1	167/173 (96%)	134 (80%)	21 (13%)	12 (7%)	1	7
48	m1	167/173 (96%)	145 (87%)	10 (6%)	12 (7%)	1	7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	162 (85%)	18 (9%)	11 (6%)	2	12
49	m3	192/198 (97%)	157 (82%)	22 (12%)	13 (7%)	1	8
50	M4	134/137 (98%)	117 (87%)	8 (6%)	9 (7%)	1	9
50	m4	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	4	24
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	5	28
52	M6	195/198 (98%)	182 (93%)	9 (5%)	4 (2%)	9	37
52	m6	195/198 (98%)	181 (93%)	10 (5%)	4 (2%)	9	37
53	M7	181/183 (99%)	151 (83%)	21 (12%)	9 (5%)	3	16
53	m7	153/183 (84%)	141 (92%)	11 (7%)	1 (1%)	26	65
54	M8	183/185 (99%)	164 (90%)	15 (8%)	4 (2%)	8	36
54	m8	183/185 (99%)	162 (88%)	17 (9%)	4 (2%)	8	36
55	M9	186/188 (99%)	169 (91%)	16 (9%)	1 (0%)	34	72
55	m9	186/188 (99%)	168 (90%)	16 (9%)	2 (1%)	17	55
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	7	33
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	16	52
57	N1	157/159 (99%)	140 (89%)	15 (10%)	2 (1%)	15	50
57	n1	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	15	50
58	N2	98/120 (82%)	81 (83%)	15 (15%)	2 (2%)	9	38
58	n2	96/120 (80%)	83 (86%)	12 (12%)	1 (1%)	19	58
59	N3	134/136 (98%)	123 (92%)	10 (8%)	1 (1%)	26	65
59	n3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	26	65
60	N4	96/155 (62%)	80 (83%)	10 (10%)	6 (6%)	2	10
60	n4	133/155 (86%)	110 (83%)	14 (10%)	9 (7%)	1	8
61	N5	119/141 (84%)	107 (90%)	8 (7%)	4 (3%)	5	25
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	7
62	N6	124/126 (98%)	113 (91%)	10 (8%)	1 (1%)	24	63
62	n6	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	7	33
63	N7	133/135 (98%)	114 (86%)	10 (8%)	9 (7%)	1	8
63	n7	133/135 (98%)	99 (74%)	21 (16%)	13 (10%)	1	4
64	N8	146/148 (99%)	120 (82%)	19 (13%)	7 (5%)	3	17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	129 (88%)	13 (9%)	4 (3%)	6	31
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	4	24
65	n9	56/58 (97%)	41 (73%)	11 (20%)	4 (7%)	1	8
66	O0	95/104 (91%)	89 (94%)	6 (6%)	0	100	100
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	19	58
67	O1	107/112 (96%)	98 (92%)	3 (3%)	6 (6%)	2	13
67	o1	107/112 (96%)	91 (85%)	11 (10%)	5 (5%)	3	17
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	24	63
68	o2	125/129 (97%)	110 (88%)	11 (9%)	4 (3%)	5	26
69	O3	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
69	o3	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	6	29
70	O4	110/119 (92%)	98 (89%)	11 (10%)	1 (1%)	21	61
70	o4	110/119 (92%)	96 (87%)	11 (10%)	3 (3%)	6	31
71	O5	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	21	61
71	o5	117/119 (98%)	101 (86%)	12 (10%)	4 (3%)	5	25
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	2	15
72	o6	97/99 (98%)	80 (82%)	13 (13%)	4 (4%)	3	20
73	O7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	7	33
73	o7	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	3	17
74	O8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	4	21
74	o8	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	15	50
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	9	37
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	4	21
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	9	38
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	79 (77%)	21 (20%)	3 (3%)	6	29
78	q2	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	19	58
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	5	25
79	q3	89/91 (98%)	82 (92%)	5 (6%)	2 (2%)	8	36

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	38 (63%)	16 (27%)	6 (10%)	1	4
82	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	6	29
All	All	22291/24121 (92%)	18907 (85%)	2362 (11%)	1022 (5%)	3	17

5 of 1022 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	190	ASP
2	S0	191	ARG
3	S1	35	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	S0	164/209 (78%)	146 (89%)	18 (11%)	8	30
2	s0	165/209 (79%)	138 (84%)	27 (16%)	3	12
3	S1	191/223 (86%)	164 (86%)	27 (14%)	4	18
3	s1	192/223 (86%)	163 (85%)	29 (15%)	3	15
4	S2	176/204 (86%)	154 (88%)	22 (12%)	6	22
4	s2	176/204 (86%)	143 (81%)	33 (19%)	2	8
5	S3	182/194 (94%)	159 (87%)	23 (13%)	5	22
5	s3	182/194 (94%)	159 (87%)	23 (13%)	5	22
6	S4	221/221 (100%)	194 (88%)	27 (12%)	6	24
6	s4	221/221 (100%)	196 (89%)	25 (11%)	7	28
7	S5	173/190 (91%)	158 (91%)	15 (9%)	13	44
7	s5	173/190 (91%)	153 (88%)	20 (12%)	7	27
8	S6	188/201 (94%)	161 (86%)	27 (14%)	4	17
8	s6	187/201 (93%)	160 (86%)	27 (14%)	4	17

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	150 (91%)	15 (9%)	12	40
9	s7	165/169 (98%)	150 (91%)	15 (9%)	12	40
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	16
10	s8	150/161 (93%)	138 (92%)	12 (8%)	15	48
11	S9	158/165 (96%)	134 (85%)	24 (15%)	3	14
11	s9	158/165 (96%)	136 (86%)	22 (14%)	4	19
12	C0	77/98 (79%)	69 (90%)	8 (10%)	9	32
12	c0	73/98 (74%)	64 (88%)	9 (12%)	6	23
13	C1	129/136 (95%)	116 (90%)	13 (10%)	9	33
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	11
14	C2	88/118 (75%)	75 (85%)	13 (15%)	4	16
14	c2	88/118 (75%)	73 (83%)	15 (17%)	2	11
15	C3	127/127 (100%)	112 (88%)	15 (12%)	6	25
15	c3	127/127 (100%)	110 (87%)	17 (13%)	5	20
16	C4	81/104 (78%)	68 (84%)	13 (16%)	3	13
16	c4	97/104 (93%)	82 (84%)	15 (16%)	3	14
17	C5	101/117 (86%)	93 (92%)	8 (8%)	15	49
17	c5	103/117 (88%)	90 (87%)	13 (13%)	5	22
18	C6	117/118 (99%)	104 (89%)	13 (11%)	8	29
18	c6	118/118 (100%)	106 (90%)	12 (10%)	9	33
19	C7	94/124 (76%)	77 (82%)	17 (18%)	2	9
19	c7	92/124 (74%)	81 (88%)	11 (12%)	6	24
20	C8	128/128 (100%)	110 (86%)	18 (14%)	4	18
20	c8	128/128 (100%)	108 (84%)	20 (16%)	3	14
21	C9	115/115 (100%)	100 (87%)	15 (13%)	5	21
21	c9	115/115 (100%)	101 (88%)	14 (12%)	6	24
22	D0	100/113 (88%)	90 (90%)	10 (10%)	9	34
22	d0	103/113 (91%)	90 (87%)	13 (13%)	5	22
23	D1	74/74 (100%)	64 (86%)	10 (14%)	5	20
23	d1	74/74 (100%)	66 (89%)	8 (11%)	8	30
24	D2	110/110 (100%)	94 (86%)	16 (14%)	4	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	99 (90%)	11 (10%)	9	34
25	D3	119/119 (100%)	104 (87%)	15 (13%)	5	22
25	d3	119/119 (100%)	107 (90%)	12 (10%)	9	33
26	D4	112/112 (100%)	100 (89%)	12 (11%)	8	31
26	d4	112/112 (100%)	100 (89%)	12 (11%)	8	31
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	4
27	d5	61/88 (69%)	54 (88%)	7 (12%)	7	27
28	D6	83/83 (100%)	70 (84%)	13 (16%)	3	13
28	d6	83/83 (100%)	76 (92%)	7 (8%)	14	46
29	D7	70/70 (100%)	63 (90%)	7 (10%)	9	34
29	d7	70/70 (100%)	60 (86%)	10 (14%)	4	17
30	D8	56/59 (95%)	46 (82%)	10 (18%)	2	10
30	d8	56/59 (95%)	47 (84%)	9 (16%)	3	13
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	11
31	d9	47/48 (98%)	42 (89%)	5 (11%)	8	31
32	E0	51/51 (100%)	45 (88%)	6 (12%)	6	25
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	4
33	e1	66/66 (100%)	53 (80%)	13 (20%)	1	7
34	SR	259/261 (99%)	242 (93%)	17 (7%)	21	56
34	sR	260/261 (100%)	246 (95%)	14 (5%)	27	64
35	SM	97/193 (50%)	87 (90%)	10 (10%)	9	32
35	sM	54/193 (28%)	49 (91%)	5 (9%)	11	39
39	L2	193/195 (99%)	166 (86%)	27 (14%)	4	18
39	l2	192/195 (98%)	162 (84%)	30 (16%)	3	14
40	L3	321/322 (100%)	273 (85%)	48 (15%)	3	15
40	l3	319/322 (99%)	270 (85%)	49 (15%)	3	14
41	L4	288/288 (100%)	250 (87%)	38 (13%)	5	20
41	l4	288/288 (100%)	247 (86%)	41 (14%)	4	18
42	L5	244/244 (100%)	215 (88%)	29 (12%)	6	25
42	l5	243/244 (100%)	213 (88%)	30 (12%)	6	23
43	L6	134/152 (88%)	119 (89%)	15 (11%)	7	29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	114 (84%)	21 (16%)	3	14
44	L7	186/204 (91%)	165 (89%)	21 (11%)	7	28
44	l7	187/204 (92%)	169 (90%)	18 (10%)	10	37
45	L8	187/207 (90%)	164 (88%)	23 (12%)	6	23
45	l8	177/207 (86%)	150 (85%)	27 (15%)	3	14
46	L9	171/171 (100%)	143 (84%)	28 (16%)	3	12
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	7
47	M0	177/186 (95%)	153 (86%)	24 (14%)	5	19
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	11
48	M1	147/150 (98%)	124 (84%)	23 (16%)	3	14
48	m1	147/150 (98%)	131 (89%)	16 (11%)	8	30
49	M3	154/158 (98%)	135 (88%)	19 (12%)	6	23
49	m3	154/158 (98%)	135 (88%)	19 (12%)	6	23
50	M4	107/108 (99%)	94 (88%)	13 (12%)	6	24
50	m4	108/108 (100%)	91 (84%)	17 (16%)	3	13
51	M5	175/175 (100%)	152 (87%)	23 (13%)	5	21
51	m5	175/175 (100%)	159 (91%)	16 (9%)	12	40
52	M6	160/161 (99%)	152 (95%)	8 (5%)	30	67
52	m6	160/161 (99%)	139 (87%)	21 (13%)	5	21
53	M7	140/145 (97%)	124 (89%)	16 (11%)	7	28
53	m7	125/145 (86%)	107 (86%)	18 (14%)	4	17
54	M8	150/150 (100%)	130 (87%)	20 (13%)	5	20
54	m8	150/150 (100%)	130 (87%)	20 (13%)	5	20
55	M9	153/153 (100%)	138 (90%)	15 (10%)	10	36
55	m9	153/153 (100%)	130 (85%)	23 (15%)	3	15
56	N0	156/156 (100%)	130 (83%)	26 (17%)	3	11
56	n0	156/156 (100%)	132 (85%)	24 (15%)	3	14
57	N1	136/136 (100%)	107 (79%)	29 (21%)	1	6
57	n1	136/136 (100%)	111 (82%)	25 (18%)	2	9
58	N2	87/106 (82%)	79 (91%)	8 (9%)	11	40
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	93 (89%)	11 (11%)	8	31
59	n3	104/104 (100%)	95 (91%)	9 (9%)	13	44
60	N4	57/129 (44%)	53 (93%)	4 (7%)	19	54
60	n4	100/129 (78%)	93 (93%)	7 (7%)	19	54
61	N5	104/117 (89%)	84 (81%)	20 (19%)	2	8
61	n5	104/117 (89%)	85 (82%)	19 (18%)	2	9
62	N6	109/109 (100%)	94 (86%)	15 (14%)	4	19
62	n6	109/109 (100%)	87 (80%)	22 (20%)	1	7
63	N7	115/115 (100%)	104 (90%)	11 (10%)	10	37
63	n7	115/115 (100%)	98 (85%)	17 (15%)	4	16
64	N8	118/118 (100%)	100 (85%)	18 (15%)	3	14
64	n8	118/118 (100%)	98 (83%)	20 (17%)	2	11
65	N9	46/46 (100%)	40 (87%)	6 (13%)	5	21
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	11
66	O0	81/87 (93%)	71 (88%)	10 (12%)	6	23
66	o0	84/87 (97%)	77 (92%)	7 (8%)	14	46
67	O1	92/96 (96%)	78 (85%)	14 (15%)	3	14
67	o1	94/96 (98%)	76 (81%)	18 (19%)	2	8
68	O2	109/110 (99%)	98 (90%)	11 (10%)	9	33
68	o2	109/110 (99%)	97 (89%)	12 (11%)	8	30
69	O3	90/90 (100%)	76 (84%)	14 (16%)	3	14
69	o3	90/90 (100%)	76 (84%)	14 (16%)	3	14
70	O4	95/101 (94%)	80 (84%)	15 (16%)	3	13
70	o4	95/101 (94%)	81 (85%)	14 (15%)	4	16
71	O5	104/104 (100%)	87 (84%)	17 (16%)	3	12
71	o5	103/104 (99%)	86 (84%)	17 (16%)	3	12
72	O6	81/81 (100%)	66 (82%)	15 (18%)	2	9
72	o6	80/81 (99%)	61 (76%)	19 (24%)	1	3
73	O7	70/70 (100%)	64 (91%)	6 (9%)	13	45
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	11
74	O8	68/68 (100%)	54 (79%)	14 (21%)	1	6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	10
75	O9	45/45 (100%)	38 (84%)	7 (16%)	3	14
75	o9	45/45 (100%)	39 (87%)	6 (13%)	5	20
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	4	15
76	q0	47/47 (100%)	43 (92%)	4 (8%)	13	45
77	Q1	23/23 (100%)	21 (91%)	2 (9%)	13	44
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1	7
78	q2	90/90 (100%)	79 (88%)	11 (12%)	6	24
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	7	28
79	q3	71/71 (100%)	62 (87%)	9 (13%)	5	22
80	e0	53/53 (100%)	47 (89%)	6 (11%)	7	28
82	p0	105/253 (42%)	89 (85%)	16 (15%)	3	14
All	All	18727/20169 (93%)	16232 (87%)	2495 (13%)	5	20

5 of 2495 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	86	ARG
9	s7	28	GLU
64	n8	98	THR
74	O8	46	ARG
4	s2	41	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
44	L7	244	ASN
57	N1	146	ASN
45	l8	61	GLN
47	M0	59	GLN
50	M4	105	GLN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	437 (24%)	50 (2%)
1	6	1792/1800 (99%)	419 (23%)	43 (2%)
36	1	3143/3396 (92%)	618 (19%)	66 (2%)
36	5	3143/3396 (92%)	604 (19%)	63 (2%)
37	3	120/121 (99%)	14 (11%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	0
38	4	157/158 (99%)	32 (20%)	2 (1%)
38	8	157/158 (99%)	31 (19%)	0
85	C	1/5 (20%)	0	0
85	D	1/5 (20%)	0	0
All	All	10410/10960 (94%)	2170 (20%)	225 (2%)

5 of 2170 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 225 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	2818	U
1	6	145	A
36	5	2772	C
36	1	3121	U
36	1	3375	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
85	8AN	C	76	88,85	18,24,25	1.10	1 (5%)	10,35,38	2.27	1 (10%)
85	8AN	D	76	88,85	18,24,25	1.07	1 (5%)	10,35,38	2.22	3 (30%)

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
85	8AN	C	76	88,85	-	0/3/25/26	0/3/3/3
85	8AN	D	76	88,85	-	0/3/25/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	C	76	8AN	C5-C4	2.94	1.47	1.40
85	D	76	8AN	C5-C4	2.97	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	C	76	8AN	N3-C2-N1	-6.21	123.99	128.87
85	D	76	8AN	N3-C2-N1	-5.56	124.50	128.87
85	D	76	8AN	O4'-C1'-N9	-2.53	103.32	108.11
85	D	76	8AN	N6-C6-N1	2.41	122.55	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 18 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	$\# Z  > 2$
87	SPS	C	3401	88	19,23,23	3.46	10 (52%)	16,30,30	3.19	10 (62%)
87	SPS	D	3401	88	19,23,23	3.48	12 (63%)	16,30,30	3.20	11 (68%)

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
87	SPS	C	3401	88	-	0/15/18/18	0/1/1/1
87	SPS	D	3401	88	-	0/15/18/18	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	D	3401	SPS	C9-C10	-8.50	1.31	1.48
87	C	3401	SPS	C9-C10	-8.42	1.31	1.48
87	D	3401	SPS	O13-C13	-5.57	1.18	1.42
87	C	3401	SPS	O13-C13	-5.19	1.19	1.42
87	C	3401	SPS	O10-C10	-3.05	1.18	1.24

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	D	3401	SPS	C12-N11-C10	-5.92	114.57	122.57
87	C	3401	SPS	N2-C3-N4	-5.00	119.27	127.69
87	D	3401	SPS	N2-C3-N4	-4.66	119.84	127.69
87	D	3401	SPS	C7-C5-C6	-3.58	119.35	123.63
87	C	3401	SPS	C7-C5-C6	-3.53	119.41	123.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	C	3401	SPS	1	0
87	D	3401	SPS	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
81	m2	2
35	sM	1
12	c0	1
35	SM	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	153:ALA	C	154:UNK	N	39.08
1	SM	141:ALA	C	151:UNK	N	25.76
1	c0	84:GLU	C	87:HIS	N	8.48
1	m2	23:UNK	C	28:UNK	N	3.80
1	m2	52:UNK	C	54:UNK	N	3.61

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	2	1781/1800 (98%)	0.80	147 (8%) 14 5	47, 88, 194, 293	0
1	6	1795/1800 (99%)	0.60	108 (6%) 25 10	37, 78, 178, 271	0
2	S0	206/251 (82%)	1.43	67 (32%) 1 0	98, 124, 141, 156	0
2	s0	206/251 (82%)	1.01	30 (14%) 3 1	77, 102, 120, 127	0
3	S1	214/254 (84%)	1.33	52 (24%) 1 0	101, 160, 206, 217	0
3	s1	216/254 (85%)	1.10	38 (17%) 2 1	68, 87, 112, 120	0
4	S2	217/253 (85%)	0.53	15 (6%) 20 7	74, 95, 116, 124	0
4	s2	217/253 (85%)	0.33	13 (5%) 25 10	60, 80, 95, 112	0
5	S3	223/239 (93%)	0.52	14 (6%) 23 9	80, 99, 136, 152	0
5	s3	223/239 (93%)	0.68	30 (13%) 4 2	78, 121, 153, 164	0
6	S4	260/260 (100%)	0.81	33 (12%) 5 2	60, 95, 109, 144	0
6	s4	260/260 (100%)	0.53	17 (6%) 22 8	52, 85, 99, 129	0
7	S5	206/224 (91%)	1.36	57 (27%) 1 0	103, 134, 153, 168	0
7	s5	206/224 (91%)	0.96	40 (19%) 1 1	87, 120, 139, 153	0
8	S6	226/236 (95%)	0.85	44 (19%) 1 0	63, 105, 134, 163	0
8	s6	218/236 (92%)	0.51	23 (10%) 8 3	50, 87, 112, 126	0
9	S7	184/189 (97%)	0.70	29 (15%) 3 1	94, 134, 175, 186	0
9	s7	186/189 (98%)	0.36	8 (4%) 39 18	74, 118, 168, 174	0
10	S8	188/200 (94%)	1.06	40 (21%) 1 0	56, 77, 118, 130	0
10	s8	188/200 (94%)	0.60	19 (10%) 9 3	47, 71, 117, 137	0
11	S9	185/196 (94%)	1.63	66 (35%) 0 0	78, 106, 152, 185	0
11	s9	185/196 (94%)	1.14	33 (17%) 2 1	67, 89, 135, 160	0
12	C0	96/105 (91%)	0.61	8 (8%) 14 5	88, 122, 166, 181	0
12	c0	96/105 (91%)	1.09	21 (21%) 1 0	108, 153, 180, 192	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	C1	155/155 (100%)	0.63	17 (10%)	7 2	61, 74, 133, 148	0
13	c1	146/155 (94%)	0.24	2 (1%)	78 60	52, 69, 101, 130	0
14	C2	124/142 (87%)	1.99	58 (46%)	0 0	162, 188, 207, 214	0
14	c2	124/142 (87%)	3.85	87 (70%)	0 0	211, 238, 259, 264	0
15	C3	150/150 (100%)	0.89	24 (16%)	3 1	70, 89, 114, 119	0
15	c3	150/150 (100%)	0.33	2 (1%)	79 62	56, 74, 96, 99	0
16	C4	127/136 (93%)	0.84	19 (14%)	3 1	68, 155, 181, 187	0
16	c4	128/136 (94%)	0.58	6 (4%)	35 16	48, 90, 104, 109	0
17	C5	124/141 (87%)	0.79	19 (15%)	3 1	82, 102, 124, 162	0
17	c5	135/141 (95%)	1.16	29 (21%)	1 0	73, 105, 118, 128	0
18	C6	141/142 (99%)	1.83	53 (37%)	0 0	83, 118, 125, 128	0
18	c6	142/142 (100%)	1.89	62 (43%)	0 0	74, 113, 131, 136	0
19	C7	120/136 (88%)	1.50	33 (27%)	1 0	91, 114, 151, 157	0
19	c7	117/136 (86%)	1.31	36 (30%)	1 0	80, 106, 135, 150	0
20	C8	145/145 (100%)	1.65	51 (35%)	0 0	77, 114, 154, 160	0
20	c8	145/145 (100%)	0.83	19 (13%)	5 2	87, 102, 141, 147	0
21	C9	143/143 (100%)	1.46	43 (30%)	1 0	87, 114, 133, 142	0
21	c9	143/143 (100%)	1.34	33 (23%)	1 0	81, 103, 127, 136	0
22	D0	107/120 (89%)	1.19	23 (21%)	1 0	74, 120, 154, 157	0
22	d0	110/120 (91%)	2.09	51 (46%)	0 0	75, 133, 171, 177	0
23	D1	87/87 (100%)	0.84	8 (9%)	11 4	98, 107, 135, 144	0
23	d1	87/87 (100%)	0.31	5 (5%)	27 11	75, 89, 116, 124	0
24	D2	129/129 (100%)	1.35	32 (24%)	1 0	70, 88, 96, 104	0
24	d2	129/129 (100%)	0.45	2 (1%)	74 55	58, 71, 78, 87	0
25	D3	144/144 (100%)	0.38	2 (1%)	78 60	61, 67, 77, 101	0
25	d3	144/144 (100%)	0.17	0	100 100	50, 56, 71, 91	0
26	D4	134/134 (100%)	0.85	15 (11%)	7 2	73, 107, 120, 134	0
26	d4	134/134 (100%)	0.64	11 (8%)	14 5	61, 92, 108, 118	0
27	D5	70/107 (65%)	1.36	15 (21%)	1 0	130, 149, 160, 161	0
27	d5	69/107 (64%)	1.56	24 (34%)	0 0	106, 132, 148, 150	0
28	D6	97/97 (100%)	1.11	24 (24%)	1 0	72, 89, 178, 180	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	d6	97/97 (100%)	0.50	4 (4%) 41 19	53, 65, 110, 117	0
29	D7	81/81 (100%)	2.02	42 (51%) 0 0	90, 108, 149, 151	0
29	d7	81/81 (100%)	0.99	10 (12%) 5 2	72, 88, 139, 143	0
30	D8	63/66 (95%)	0.74	6 (9%) 10 4	114, 147, 161, 164	0
30	d8	63/66 (95%)	0.98	11 (17%) 2 1	102, 129, 141, 144	0
31	D9	53/55 (96%)	1.04	10 (18%) 2 1	77, 82, 101, 110	0
31	d9	53/55 (96%)	1.58	14 (26%) 1 0	74, 86, 131, 153	0
32	E0	60/60 (100%)	1.21	19 (31%) 1 0	72, 106, 148, 150	0
33	E1	71/76 (93%)	2.02	34 (47%) 0 0	114, 147, 184, 189	0
33	e1	76/76 (100%)	2.66	37 (48%) 0 0	110, 188, 229, 231	0
34	SR	318/318 (100%)	0.83	37 (11%) 6 2	111, 133, 149, 177	0
34	sR	318/318 (100%)	1.56	100 (31%) 1 0	122, 149, 166, 179	0
35	SM	133/263 (50%)	1.50	29 (21%) 1 0	53, 92, 148, 165	0
35	sM	84/263 (31%)	1.06	22 (26%) 1 0	45, 107, 147, 150	0
36	1	3148/3396 (92%)	0.40	80 (2%) 61 37	29, 49, 128, 262	0
36	5	3149/3396 (92%)	0.39	71 (2%) 64 40	26, 46, 119, 209	0
37	3	121/121 (100%)	0.32	0 100 100	37, 69, 84, 91	0
37	7	121/121 (100%)	0.22	1 (0%) 87 75	30, 49, 60, 72	0
38	4	158/158 (100%)	0.18	1 (0%) 90 80	34, 49, 87, 132	0
38	8	158/158 (100%)	0.22	3 (1%) 70 48	37, 55, 91, 120	0
39	L2	252/253 (99%)	0.37	4 (1%) 74 55	33, 51, 66, 86	0
39	l2	252/253 (99%)	0.23	4 (1%) 74 55	32, 53, 70, 75	0
40	L3	386/386 (100%)	-0.00	1 (0%) 94 88	32, 56, 69, 83	0
40	l3	386/386 (100%)	0.02	1 (0%) 94 88	26, 44, 57, 80	0
41	L4	361/361 (100%)	-0.01	0 100 100	30, 49, 68, 75	0
41	l4	361/361 (100%)	-0.05	1 (0%) 94 88	30, 53, 73, 85	0
42	L5	296/296 (100%)	1.10	51 (17%) 2 1	51, 81, 100, 123	0
42	l5	294/296 (99%)	0.65	21 (7%) 19 7	39, 56, 78, 92	0
43	L6	156/175 (89%)	0.02	1 (0%) 90 80	44, 52, 70, 83	0
43	l6	157/175 (89%)	0.15	6 (3%) 44 21	45, 52, 76, 88	0
44	L7	222/243 (91%)	0.18	3 (1%) 78 60	35, 45, 76, 115	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	-0.02	0 100 100	32, 42, 82, 119	0
45	L8	233/255 (91%)	0.58	17 (7%) 18 6	61, 75, 118, 126	0
45	l8	231/255 (90%)	0.66	18 (7%) 16 5	67, 81, 112, 123	0
46	L9	191/191 (100%)	0.66	10 (5%) 31 13	52, 65, 79, 94	0
46	l9	191/191 (100%)	0.13	3 (1%) 74 55	40, 52, 72, 82	0
47	M0	211/220 (95%)	0.07	0 100 100	39, 61, 96, 108	0
47	m0	213/220 (96%)	0.14	5 (2%) 64 40	33, 54, 75, 96	0
48	M1	169/173 (97%)	2.03	86 (50%) 0 0	63, 84, 99, 104	0
48	m1	169/173 (97%)	0.74	15 (8%) 12 4	42, 60, 72, 78	0
49	M3	193/198 (97%)	0.50	8 (4%) 41 19	33, 58, 97, 118	0
49	m3	194/198 (97%)	0.53	13 (6%) 21 7	36, 64, 106, 125	0
50	M4	136/137 (99%)	0.14	4 (2%) 55 31	49, 55, 69, 80	0
50	m4	137/137 (100%)	0.03	0 100 100	44, 50, 66, 87	0
51	M5	203/203 (100%)	0.31	1 (0%) 91 83	31, 48, 58, 62	0
51	m5	203/203 (100%)	0.83	18 (8%) 12 4	35, 53, 66, 69	0
52	M6	197/198 (99%)	0.22	2 (1%) 84 69	35, 42, 57, 59	0
52	m6	197/198 (99%)	0.20	2 (1%) 84 69	30, 36, 55, 58	0
53	M7	183/183 (100%)	0.39	10 (5%) 29 12	36, 47, 115, 160	0
53	m7	155/183 (84%)	-0.06	0 100 100	33, 41, 58, 78	0
54	M8	185/185 (100%)	0.27	3 (1%) 74 55	37, 49, 66, 79	0
54	m8	185/185 (100%)	0.33	2 (1%) 82 66	36, 52, 62, 67	0
55	M9	188/188 (100%)	0.54	11 (5%) 26 11	51, 67, 166, 188	0
55	m9	188/188 (100%)	0.41	6 (3%) 51 27	46, 60, 154, 171	0
56	N0	172/172 (100%)	0.45	6 (3%) 48 23	43, 53, 68, 72	0
56	n0	172/172 (100%)	0.24	7 (4%) 41 19	37, 45, 58, 67	0
57	N1	159/159 (100%)	0.71	16 (10%) 9 3	37, 52, 95, 105	0
57	n1	159/159 (100%)	0.37	4 (2%) 61 37	32, 42, 77, 85	0
58	N2	100/120 (83%)	0.36	4 (4%) 42 20	86, 104, 112, 116	0
58	n2	98/120 (81%)	0.60	9 (9%) 11 4	74, 91, 101, 106	0
59	N3	136/136 (100%)	0.16	2 (1%) 76 58	40, 52, 66, 76	0
59	n3	136/136 (100%)	0.07	2 (1%) 76 58	30, 42, 55, 62	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	2.22	31 (31%) 1 0	52, 64, 164, 171	0
60	n4	135/155 (87%)	1.06	22 (16%) 2 1	42, 96, 146, 170	0
61	N5	121/141 (85%)	0.70	10 (8%) 14 5	49, 62, 75, 108	0
61	n5	120/141 (85%)	0.98	18 (15%) 3 1	49, 63, 79, 92	0
62	N6	126/126 (100%)	1.01	12 (9%) 10 4	40, 58, 69, 76	0
62	n6	126/126 (100%)	1.25	20 (15%) 3 1	43, 59, 74, 81	0
63	N7	135/135 (100%)	1.39	31 (22%) 1 0	71, 88, 99, 102	0
63	n7	135/135 (100%)	1.58	48 (35%) 0 0	75, 91, 103, 108	0
64	N8	148/148 (100%)	0.34	1 (0%) 89 78	28, 50, 73, 83	0
64	n8	148/148 (100%)	0.24	0 100 100	27, 53, 72, 76	0
65	N9	58/58 (100%)	1.16	13 (22%) 1 0	32, 58, 105, 120	0
65	n9	58/58 (100%)	0.82	9 (15%) 3 1	31, 53, 78, 87	0
66	O0	97/104 (93%)	0.43	5 (5%) 31 13	70, 82, 105, 111	0
66	o0	100/104 (96%)	0.87	12 (12%) 6 2	69, 84, 112, 120	0
67	O1	109/112 (97%)	0.97	17 (15%) 3 1	50, 65, 98, 109	0
67	o1	109/112 (97%)	0.85	10 (9%) 11 4	41, 54, 89, 100	0
68	O2	127/129 (98%)	0.24	1 (0%) 87 75	30, 44, 58, 78	0
68	o2	127/129 (98%)	0.33	4 (3%) 52 28	27, 48, 63, 74	0
69	O3	106/106 (100%)	0.07	0 100 100	36, 42, 67, 80	0
69	o3	106/106 (100%)	0.13	1 (0%) 85 72	33, 42, 65, 79	0
70	O4	112/119 (94%)	1.20	23 (20%) 1 0	45, 62, 102, 109	0
70	o4	112/119 (94%)	0.69	3 (2%) 58 34	45, 61, 107, 115	0
71	O5	119/119 (100%)	0.46	4 (3%) 49 24	44, 65, 73, 75	0
71	o5	119/119 (100%)	0.17	2 (1%) 73 52	49, 67, 82, 95	0
72	O6	99/99 (100%)	0.32	0 100 100	55, 64, 97, 112	0
72	o6	99/99 (100%)	0.58	5 (5%) 32 13	58, 70, 95, 115	0
73	O7	87/87 (100%)	0.21	2 (2%) 64 40	33, 39, 59, 68	0
73	o7	87/87 (100%)	0.28	3 (3%) 49 24	34, 43, 69, 81	0
74	O8	77/77 (100%)	0.29	3 (3%) 43 21	72, 87, 111, 117	0
74	o8	77/77 (100%)	0.53	3 (3%) 43 21	71, 87, 102, 105	0
75	O9	50/50 (100%)	0.51	2 (4%) 42 20	43, 48, 53, 54	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	0.49	1 (2%) 68 46	43, 49, 57, 59	0
76	Q0	52/52 (100%)	0.96	6 (11%) 6 2	43, 50, 71, 79	0
76	q0	52/52 (100%)	0.59	3 (5%) 26 11	34, 39, 54, 57	0
77	Q1	25/25 (100%)	0.80	2 (8%) 15 5	51, 56, 58, 60	0
77	q1	25/25 (100%)	0.54	0 100 100	43, 46, 48, 49	0
78	Q2	105/105 (100%)	0.20	7 (6%) 21 7	34, 51, 76, 103	0
78	q2	105/105 (100%)	0.01	2 (1%) 70 48	35, 46, 64, 97	0
79	Q3	91/91 (100%)	-0.00	0 100 100	41, 56, 73, 81	0
79	q3	91/91 (100%)	0.09	2 (2%) 65 42	37, 53, 67, 78	0
80	e0	62/62 (100%)	0.53	3 (4%) 34 15	57, 88, 121, 129	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	1.93	68 (47%) 0 0	98, 131, 238, 246	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
85	C	4/5 (80%)	0.58	0 100 100	34, 36, 37, 37	0
85	D	4/5 (80%)	0.71	0 100 100	33, 34, 34, 39	0
All	All	33054/35334 (93%)	0.64	3074 (9%) 11 4	26, 68, 150, 293	0

The worst 5 of 3074 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	1699	G	19.7
14	c2	22	VAL	19.0
60	N4	86	SER	18.2
14	c2	128	ALA	16.9
60	N4	83	THR	15.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	8AN	C	76	22/23	0.97	0.24	-	34,34,34,34	0
85	8AN	D	76	22/23	0.97	0.22	-	32,33,34,35	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
88	MG	D	3402	1/1	0.95	0.38	3.33	33,33,33,33	0
88	MG	C	3402	1/1	0.90	0.40	3.09	34,34,34,34	0
86	ZN	q3	501	1/1	0.99	0.20	1.14	60,60,60,60	0
87	SPS	D	3401	23/23	0.94	0.28	0.05	29,32,45,48	0
86	ZN	E1	501	1/1	0.90	0.12	-0.65	155,155,155,155	0
86	ZN	o7	501	1/1	0.99	0.18	-0.81	46,46,46,46	0
86	ZN	Q3	501	1/1	0.99	0.16	-0.83	66,66,66,66	0
86	ZN	e1	501	1/1	0.92	0.15	-0.86	200,200,200,200	0
87	SPS	C	3401	23/23	0.95	0.24	-0.90	29,32,46,48	0
86	ZN	Q0	500	1/1	0.97	0.16	-1.00	46,46,46,46	0
86	ZN	O7	100	1/1	0.99	0.15	-1.08	44,44,44,44	0
86	ZN	D6	500	1/1	0.94	0.13	-1.11	88,88,88,88	0
86	ZN	d6	500	1/1	0.98	0.14	-1.14	57,57,57,57	0
86	ZN	d9	101	1/1	0.97	0.14	-1.19	85,85,85,85	0
86	ZN	Q2	501	1/1	0.97	0.08	-1.53	75,75,75,75	0
86	ZN	q0	500	1/1	0.99	0.15	-1.63	38,38,38,38	0
86	ZN	q2	501	1/1	0.95	0.08	-1.73	72,72,72,72	0
86	ZN	d7	101	1/1	0.80	0.20	-1.95	148,148,148,148	0
86	ZN	D9	101	1/1	0.98	0.11	-2.77	85,85,85,85	0
86	ZN	D7	101	1/1	0.27	0.18	-	165,165,165,165	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.