



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2017 – 04:16 AM EDT

PDB ID : 5DC3  
Title : Complex of yeast 80S ribosome with non-modified eIF5A  
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.;  
Dever, T.E.; Yusupov, M.  
Deposited on : unknown  
Resolution : 3.25 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

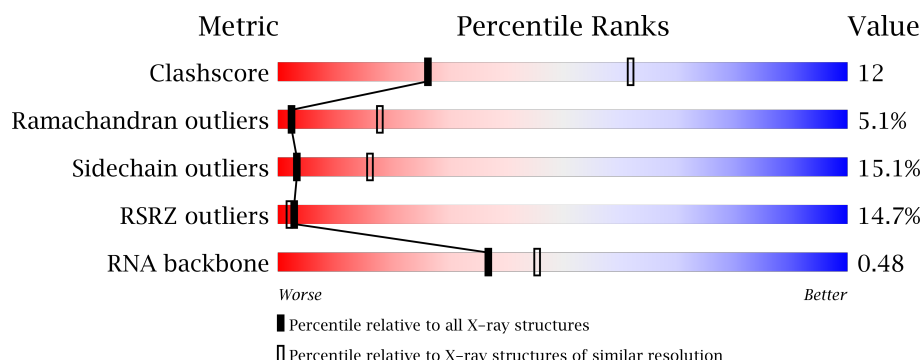
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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.



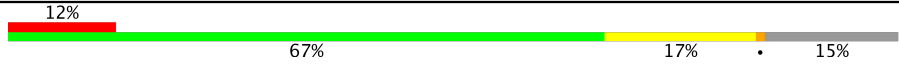

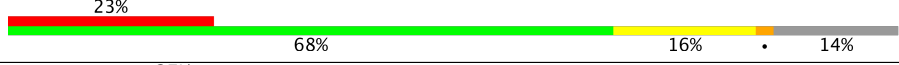
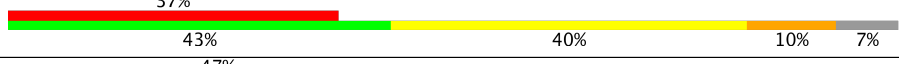

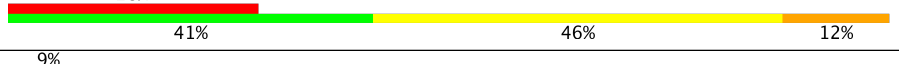
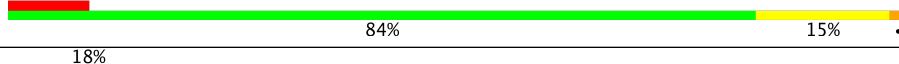
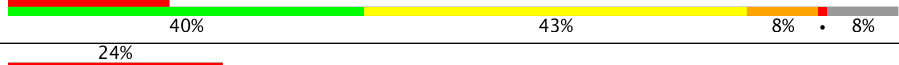
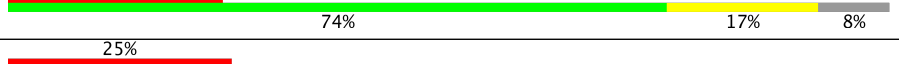
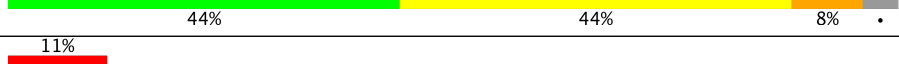

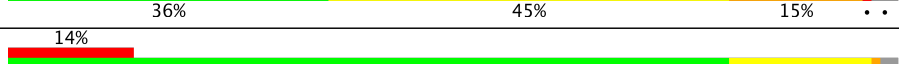
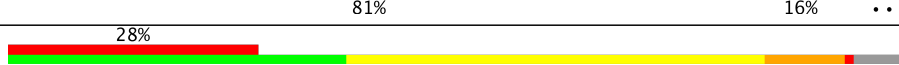
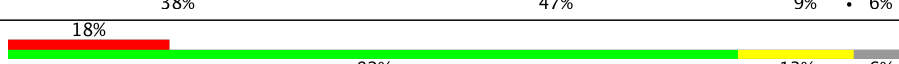
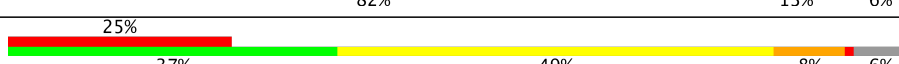
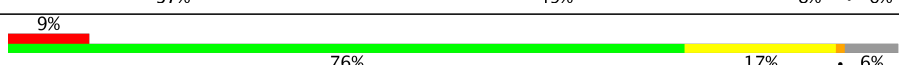
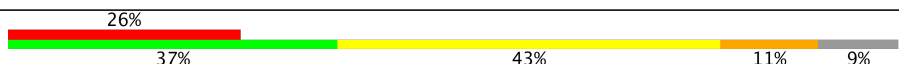

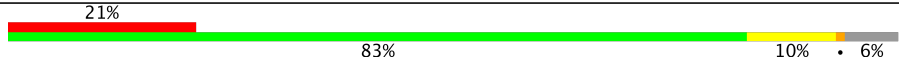


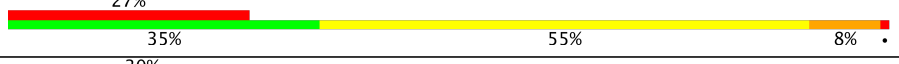
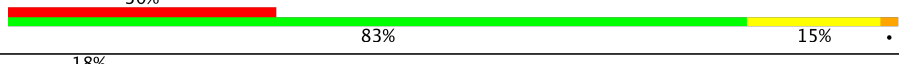
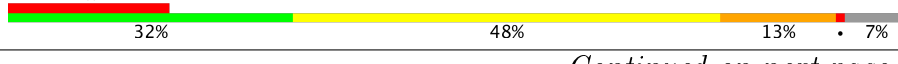

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)
RNA backbone	2435	1085 (3.72-2.80)

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>12%</div> <div> <div>43%</div> <div>42%</div> <div>13%</div> <div>..</div> </div> </div>
1	6	1800	<div> <div>5%</div> <div> <div>45%</div> <div>41%</div> <div>12%</div> <div>.</div> </div> </div>
2	S0	251	<div> <div>48%</div> <div> <div>30%</div> <div>41%</div> <div>11%</div> <div>18%</div> </div> </div>
2	s0	251	<div> <div>31%</div> <div> <div>68%</div> <div>14%</div> <div>18%</div> </div> </div>
3	S1	254	<div> <div>13%</div> <div> <div>24%</div> <div>47%</div> <div>13%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	s1	254	
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	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	

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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	

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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	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
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	

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Mol	Chain	Length	Quality of chain
41	l4	361	
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	

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Mol	Chain	Length	Quality of chain
54	M8	185	
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	

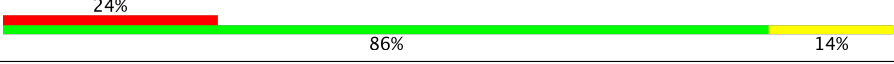
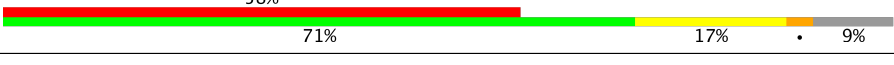
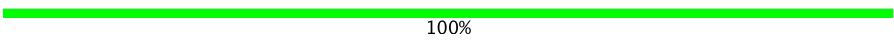

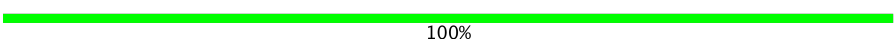
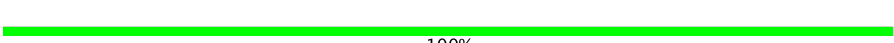

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Mol	Chain	Length	Quality of chain
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	

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Mol	Chain	Length	Quality of chain
79	Q3	91	
79	q3	91	
80	c0	105	
81	m2	150	
82	p0	311	
83	p1	47	
84	p2	46	
85	f	157	

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 404042 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 18S ribosomal RNA.

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	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	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			

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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
			772	499	126	145	2			

- 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
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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			
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			

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

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

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

- 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			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E1	77	ALA	GLY	conflict	UNP P05759
e1	77	ALA	GLY	conflict	UNP P05759

- 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
			679	402	140	137				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3169	Total	C	N	O	P	0	0	0
			67780	30276	12216	22120	3168			

- 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	l5	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	l6	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	l7	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	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			
46	l9	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O	S	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	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	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	0	0	0
			993	625	192	176			
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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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		0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O		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 S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- 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.

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 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 protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	f	148	Total	C	N	O	S	0	0	0
			1116	692	188	227	9			

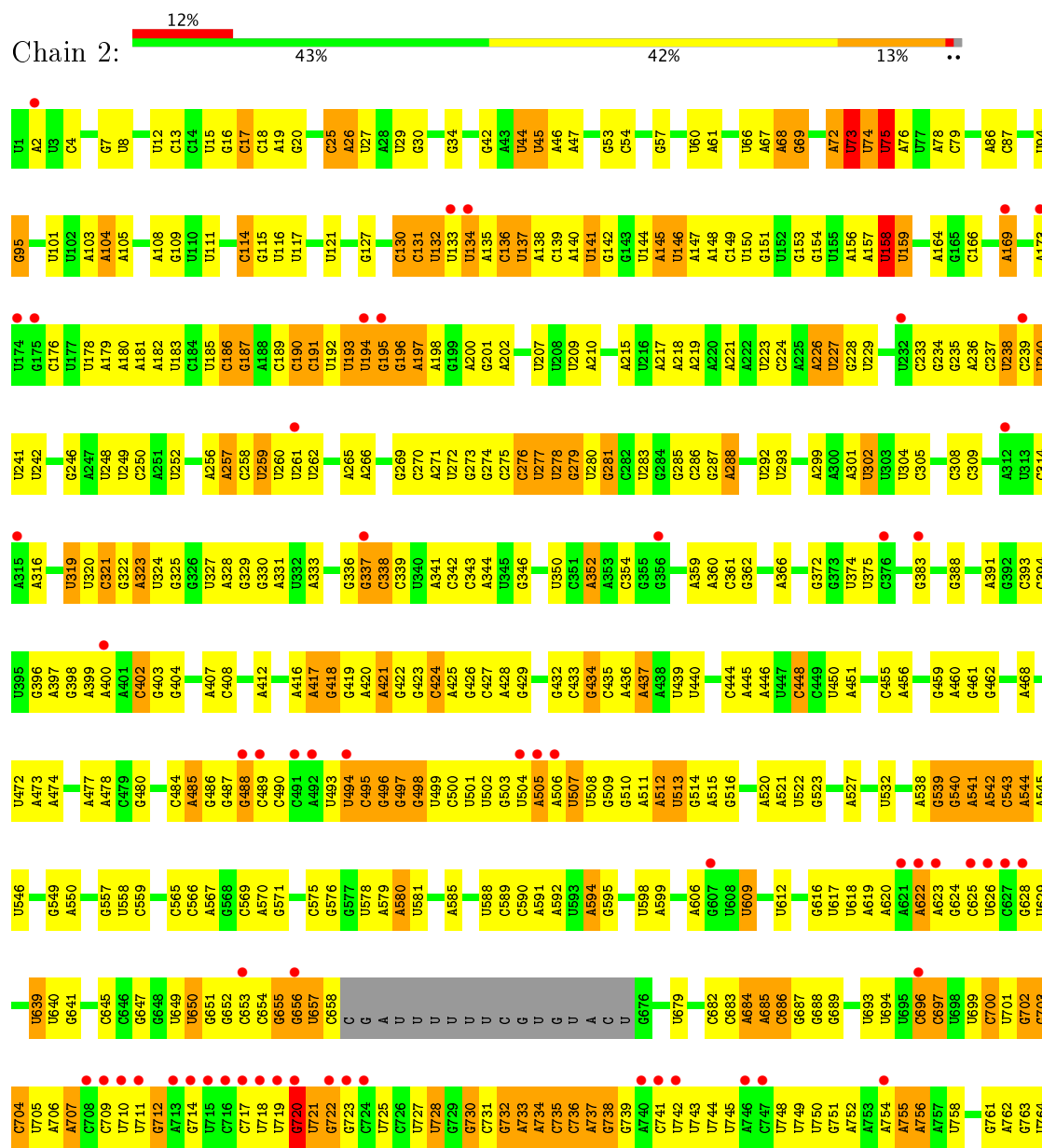
- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	q0	1	Total 1	Zn 1	0	0
86	D6	1	Total 1	Zn 1	0	0
86	Q2	1	Total 1	Zn 1	0	0
86	e1	1	Total 1	Zn 1	0	0
86	Q3	1	Total 1	Zn 1	0	0
86	D9	1	Total 1	Zn 1	0	0
86	E1	1	Total 1	Zn 1	0	0
86	Q0	1	Total 1	Zn 1	0	0
86	d7	1	Total 1	Zn 1	0	0
86	q3	1	Total 1	Zn 1	0	0
86	d9	1	Total 1	Zn 1	0	0
86	D7	1	Total 1	Zn 1	0	0
86	d6	1	Total 1	Zn 1	0	0
86	o7	1	Total 1	Zn 1	0	0
86	O7	1	Total 1	Zn 1	0	0
86	q2	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

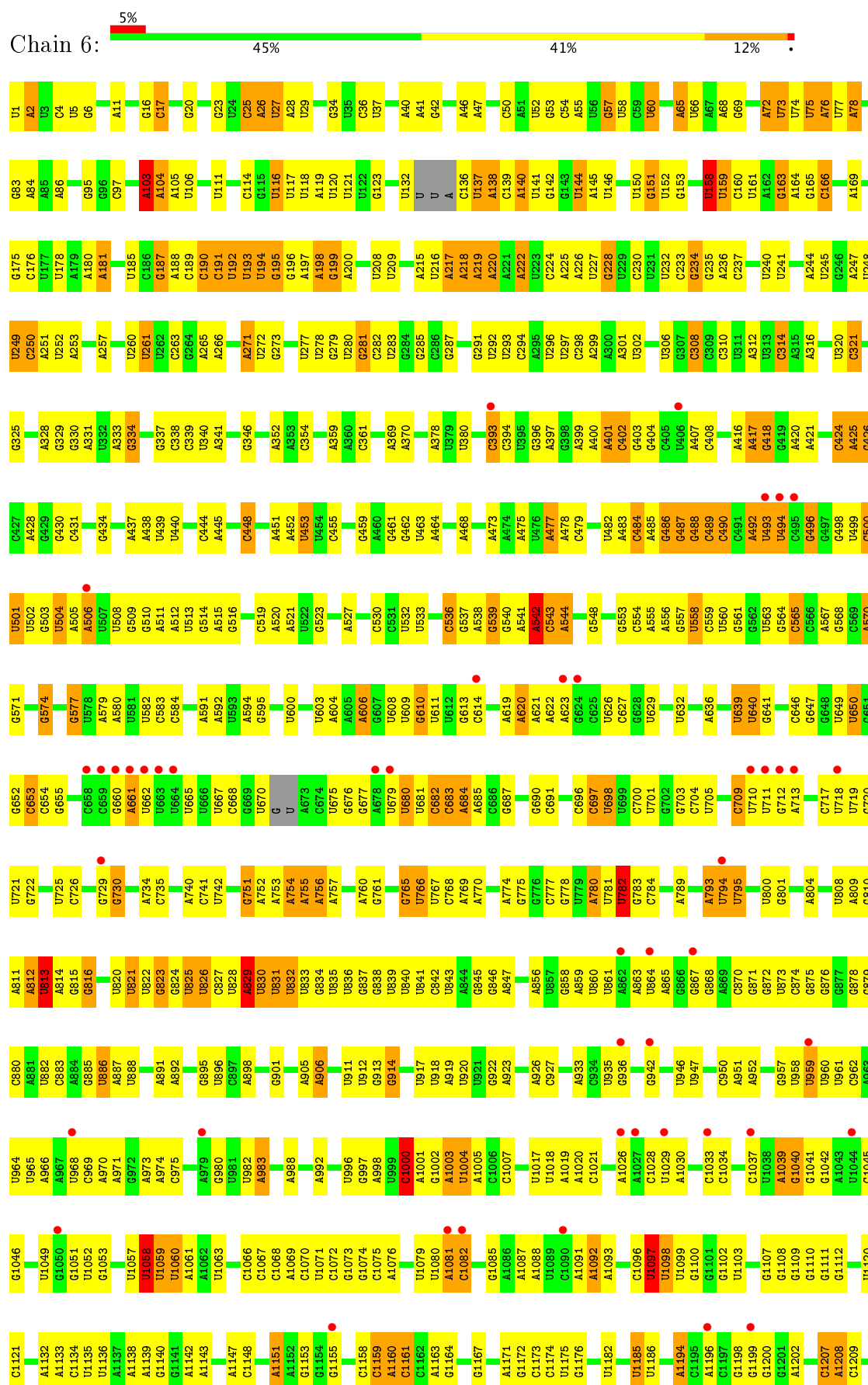
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 18S ribosomal RNA



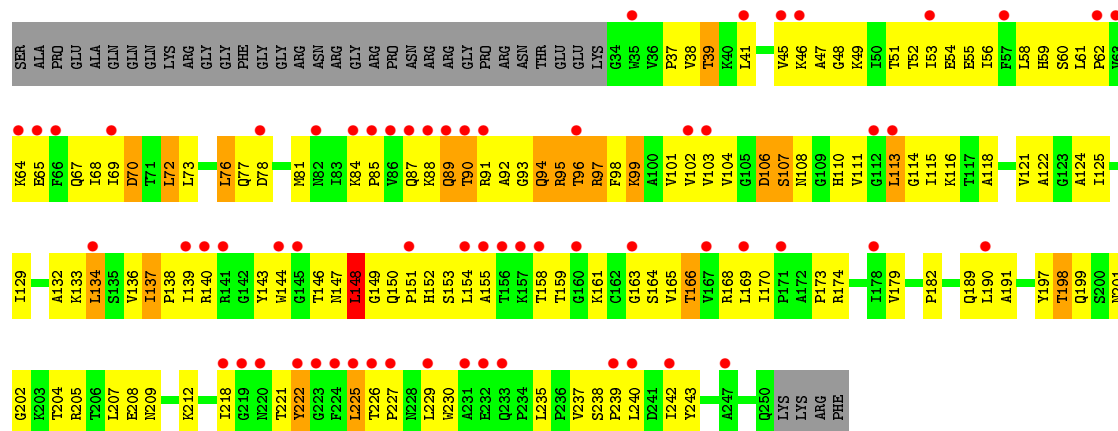




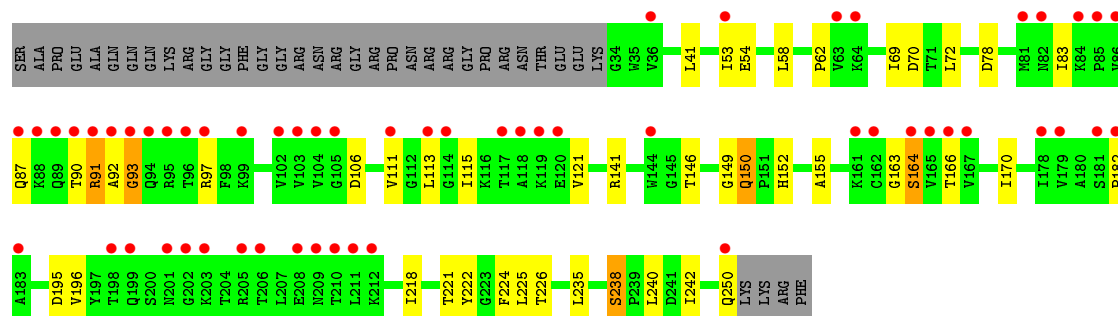




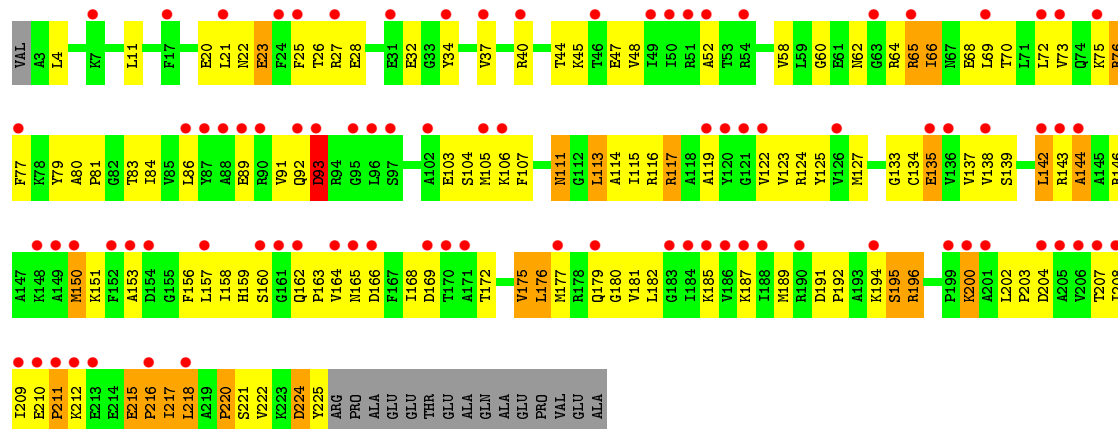
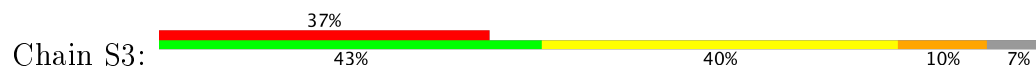




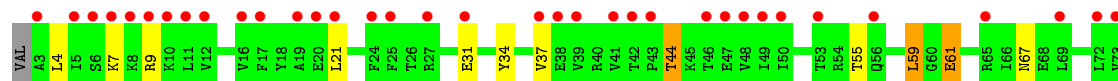
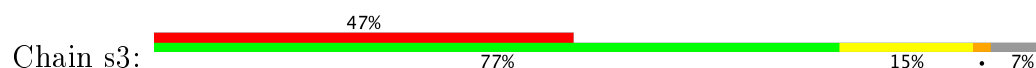
• Molecule 4: 40S ribosomal protein S2

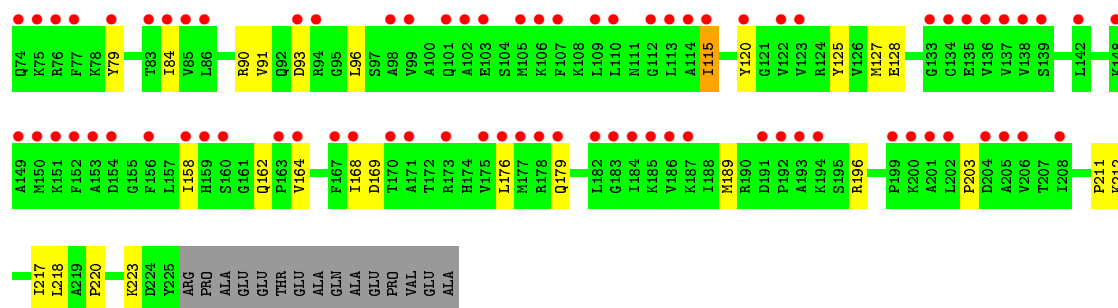


• Molecule 5: 40S ribosomal protein S3

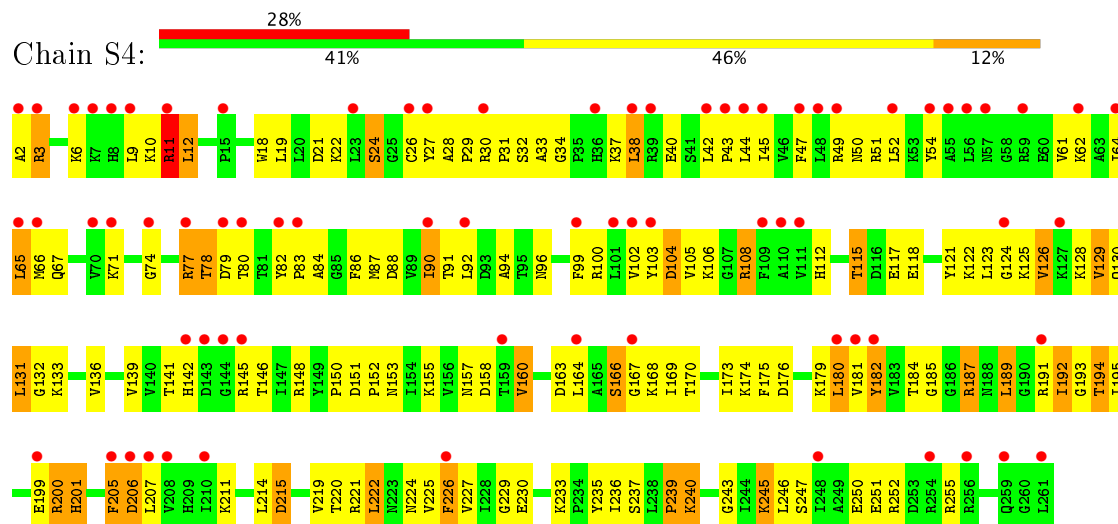


• Molecule 5: 40S ribosomal protein S3

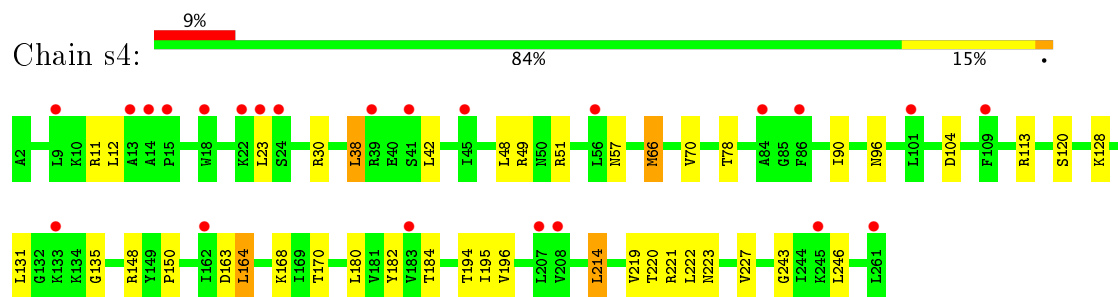




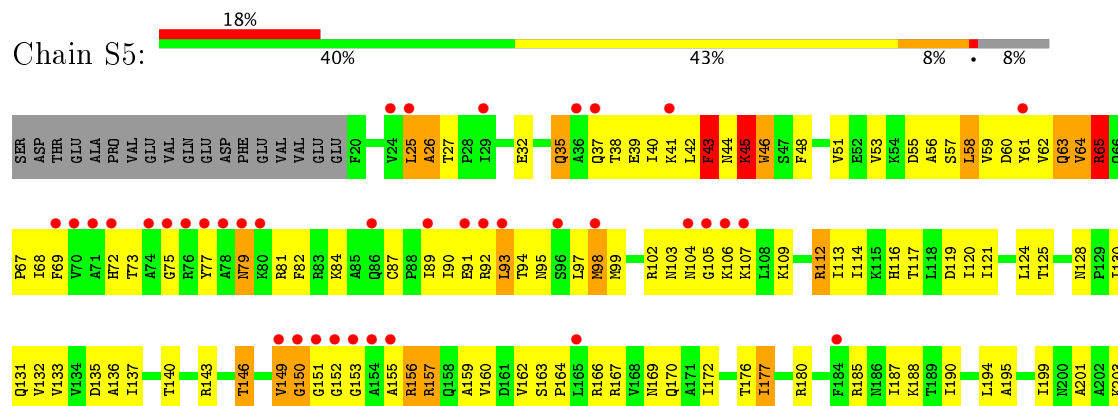
• Molecule 6: 40S ribosomal protein S4-A

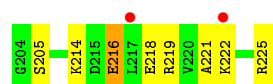


• Molecule 6: 40S ribosomal protein S4-A

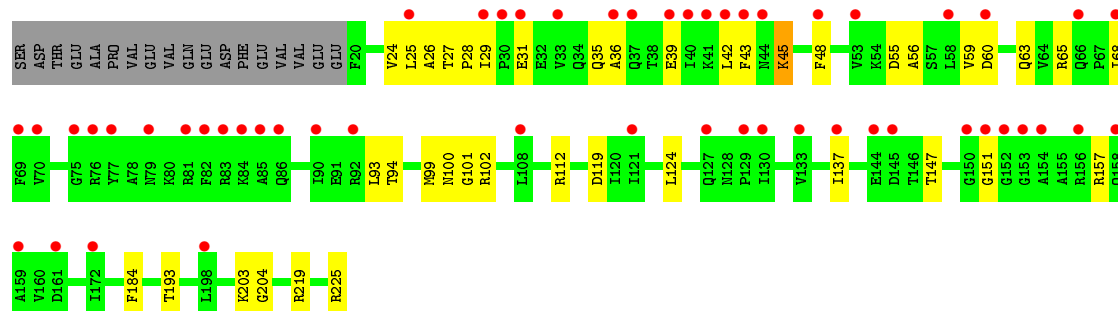
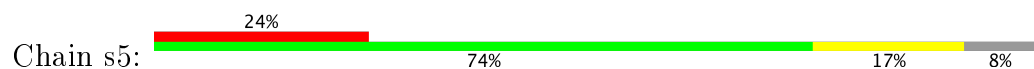


• Molecule 7: 40S ribosomal protein S5

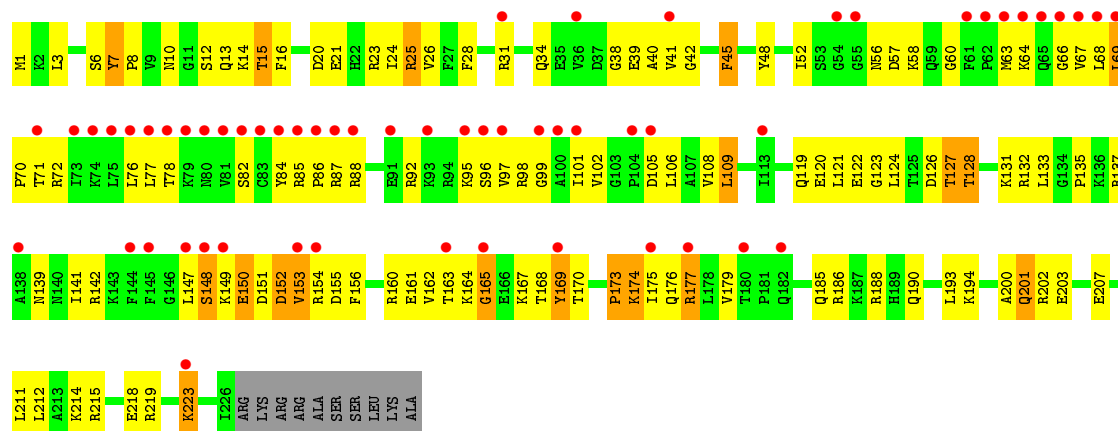
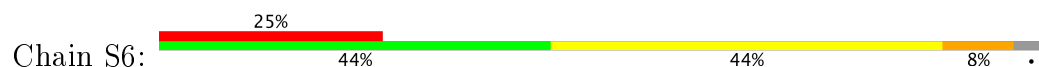




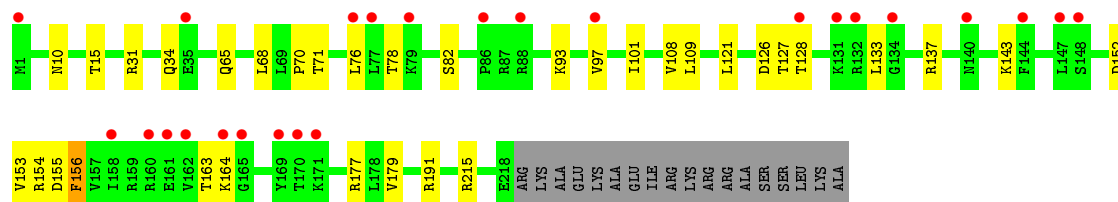
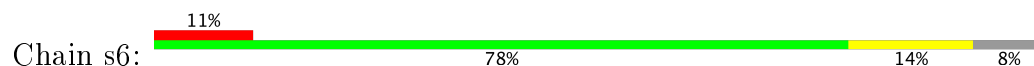
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6-A



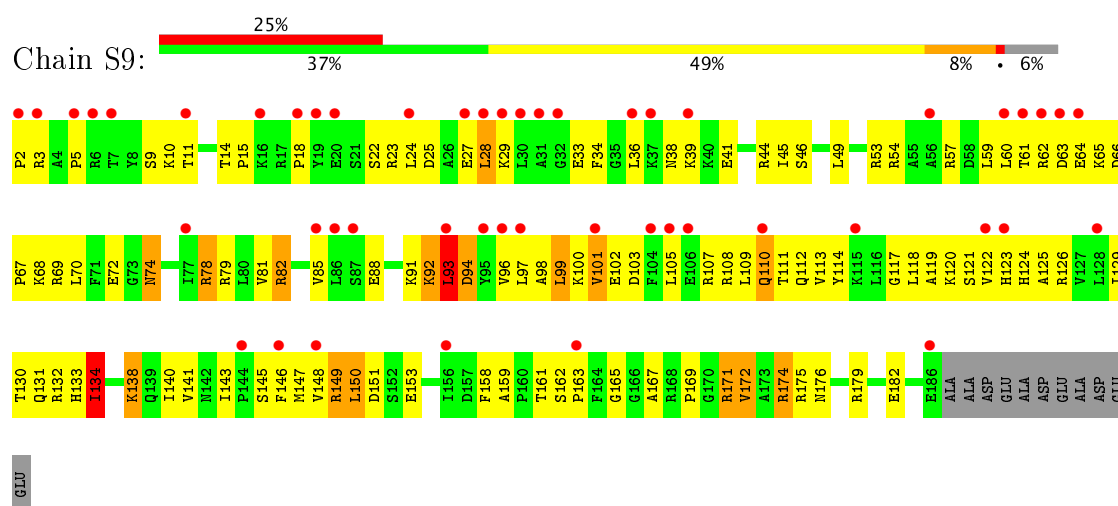
• Molecule 8: 40S ribosomal protein S6-A



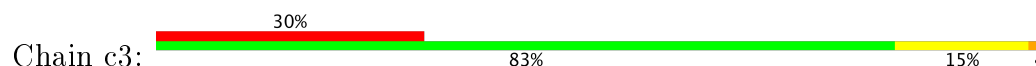
• Molecule 9: 40S ribosomal protein S7-A

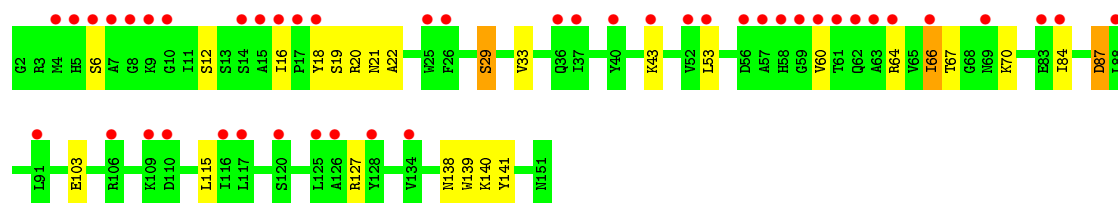




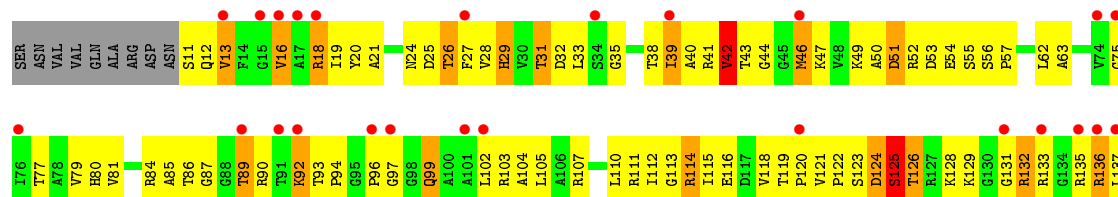




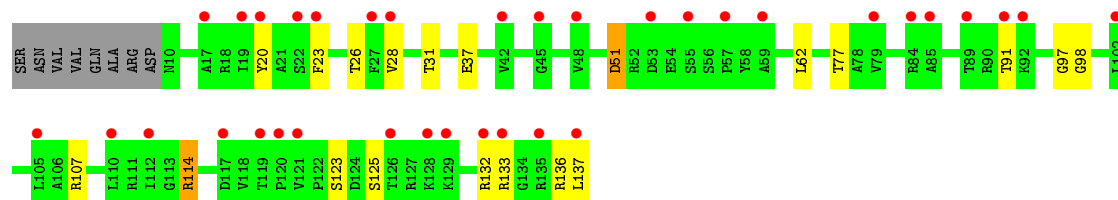
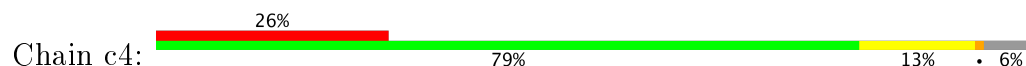




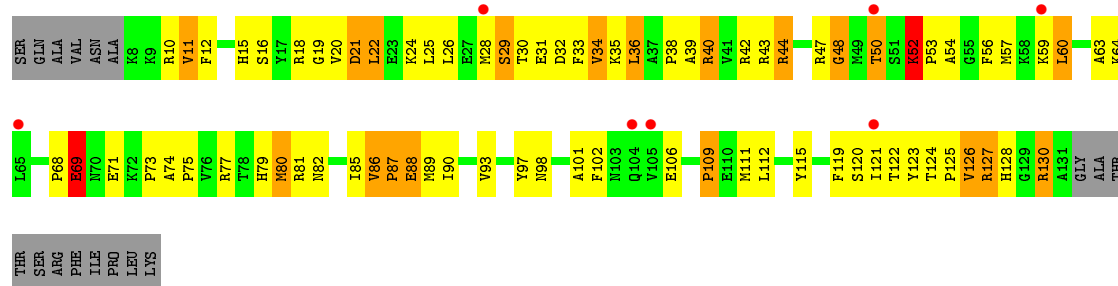
• Molecule 16: 40S ribosomal protein S14-A



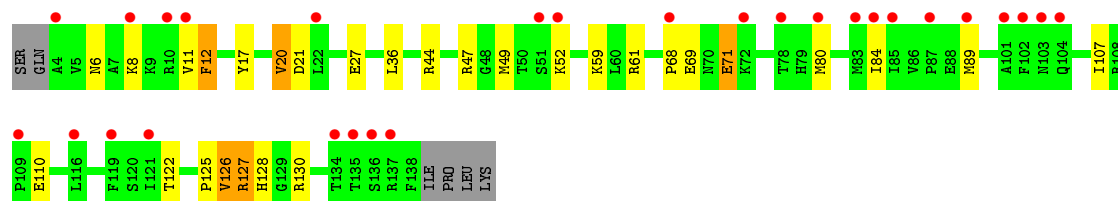
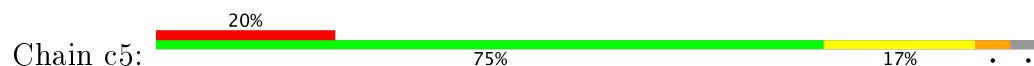
• Molecule 16: 40S ribosomal protein S14-A



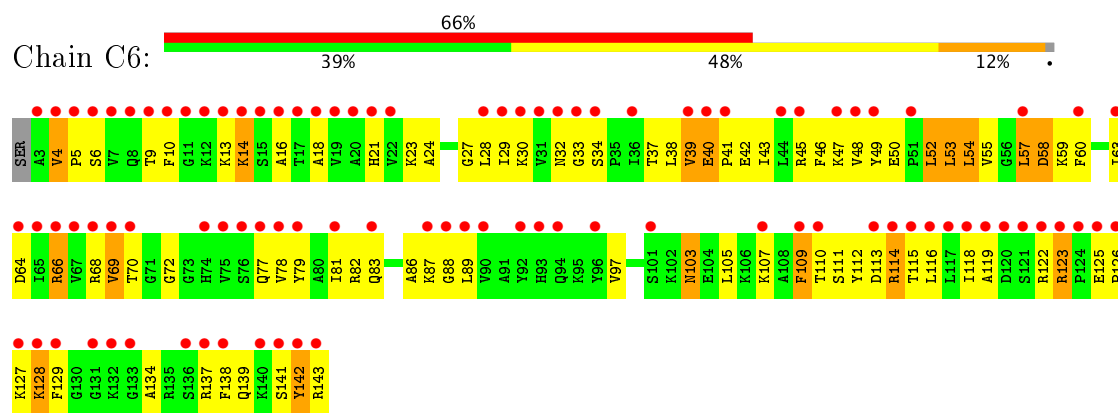
• Molecule 17: 40S ribosomal protein S15



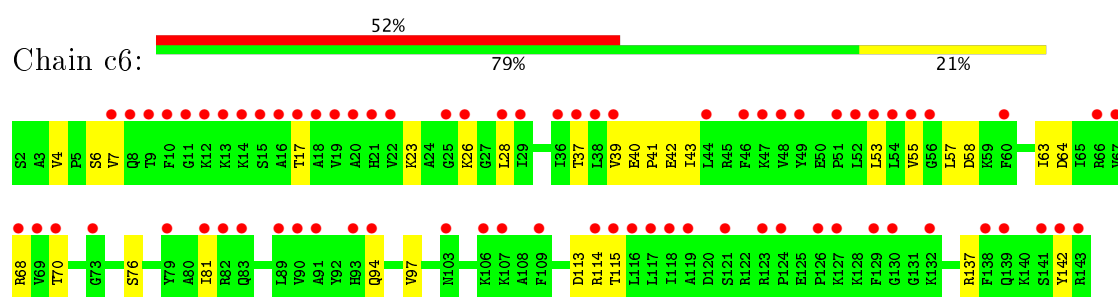
• Molecule 17: 40S ribosomal protein S15



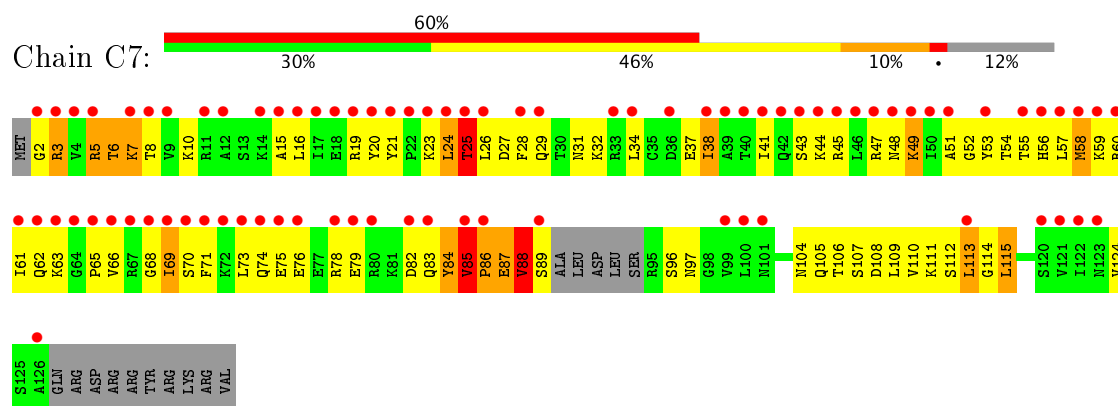
- Molecule 18: 40S ribosomal protein S16-A

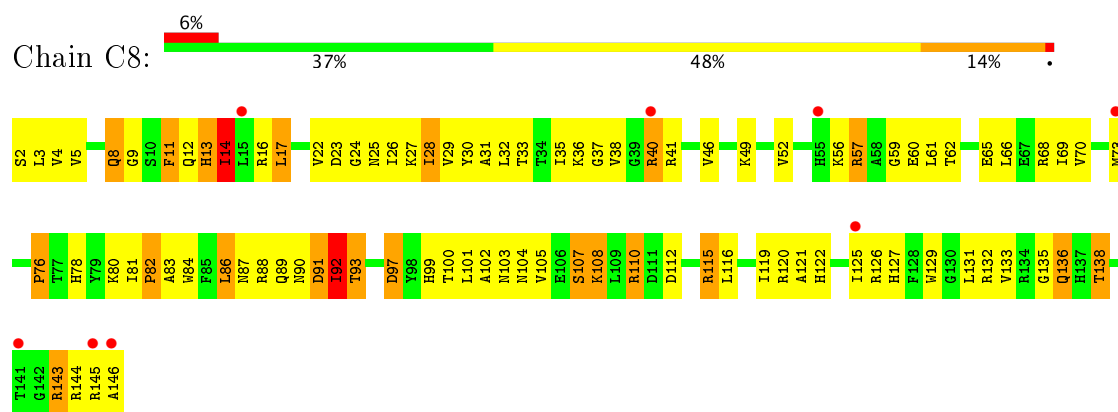


- Molecule 18: 40S ribosomal protein S16-A

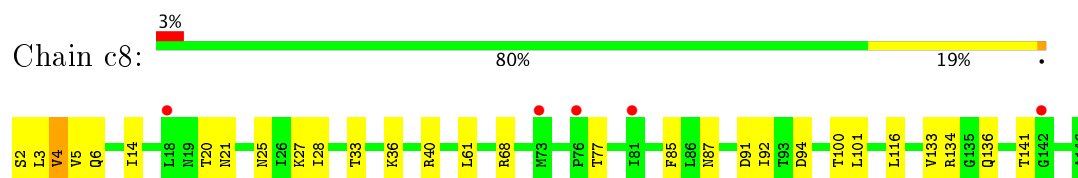


- Molecule 19: 40S ribosomal protein S17-A

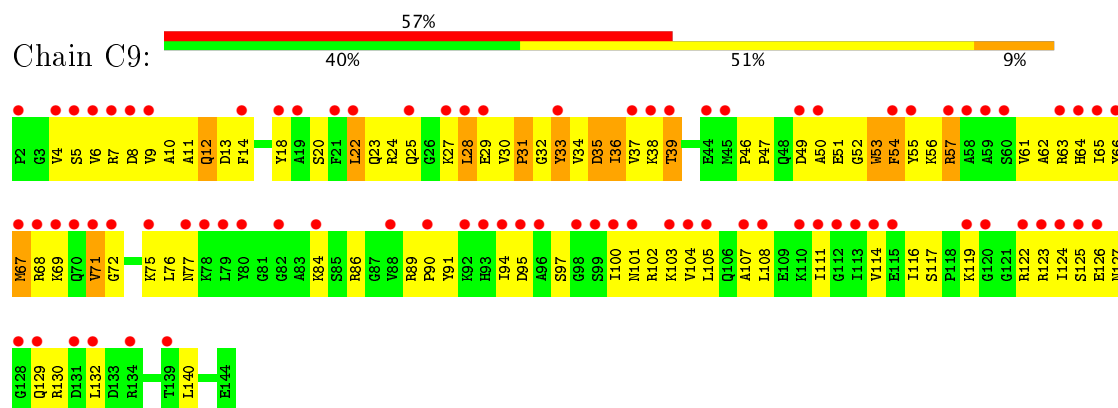




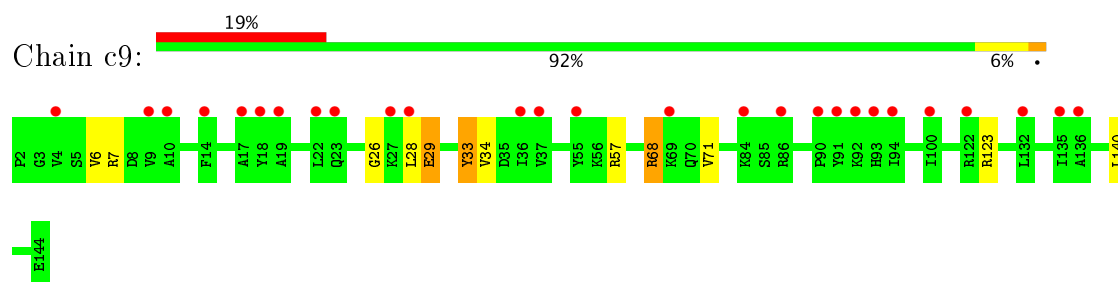
• Molecule 20: 40S ribosomal protein S18-A



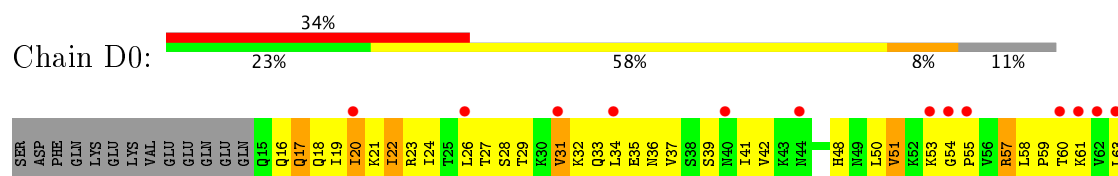
• Molecule 21: 40S ribosomal protein S19-A

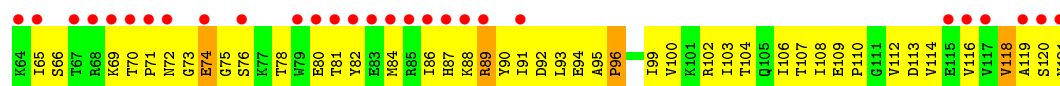


• Molecule 21: 40S ribosomal protein S19-A

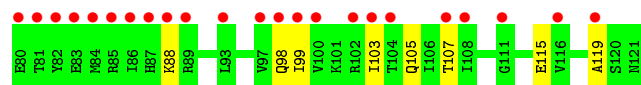
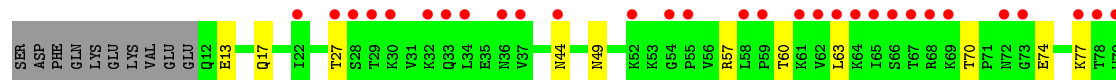
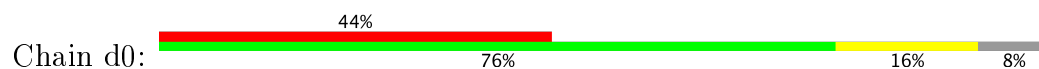


• Molecule 22: 40S ribosomal protein S20

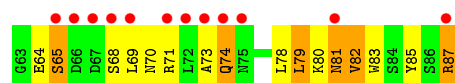
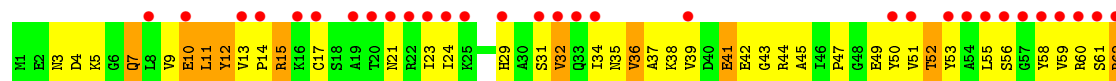




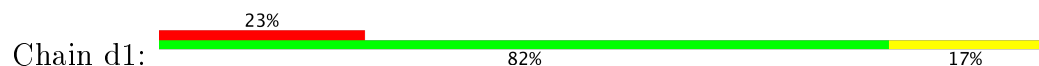
• Molecule 22: 40S ribosomal protein S20



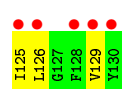
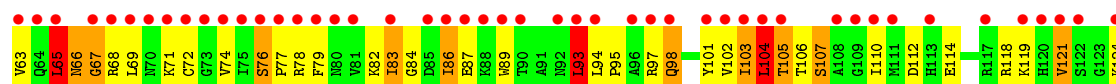
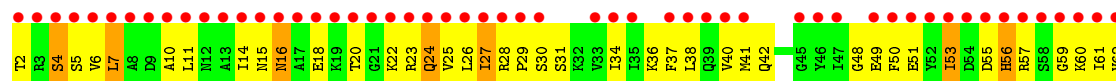
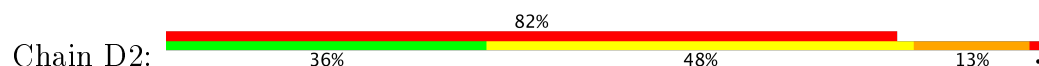
• Molecule 23: 40S ribosomal protein S21-A



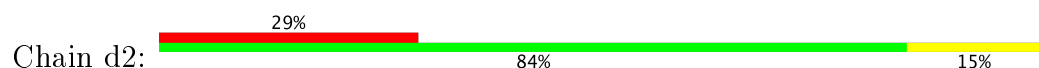
• Molecule 23: 40S ribosomal protein S21-A

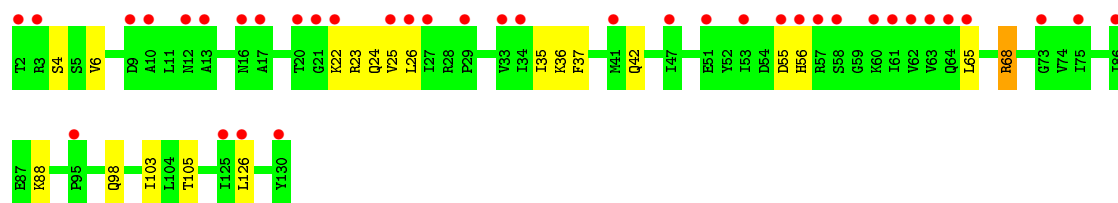


• Molecule 24: 40S ribosomal protein S22-A

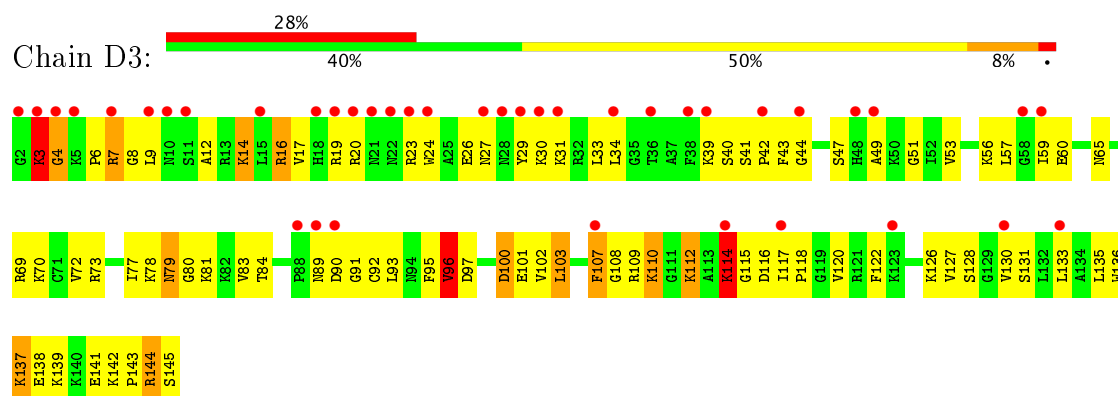


• Molecule 24: 40S ribosomal protein S22-A

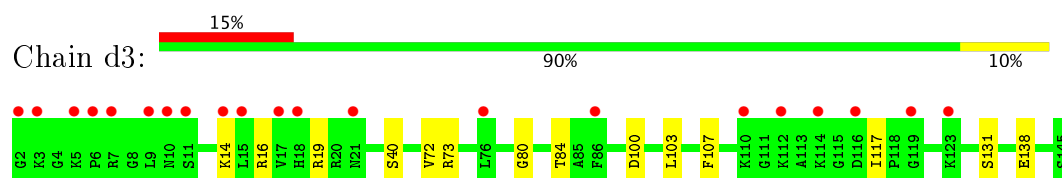




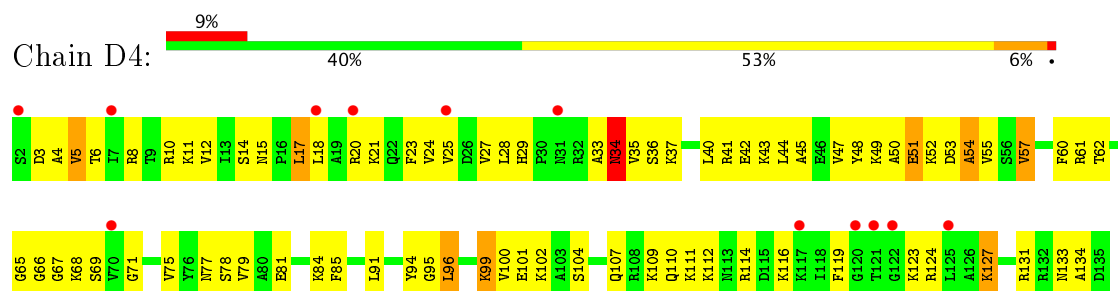
• Molecule 25: 40S ribosomal protein S23-A



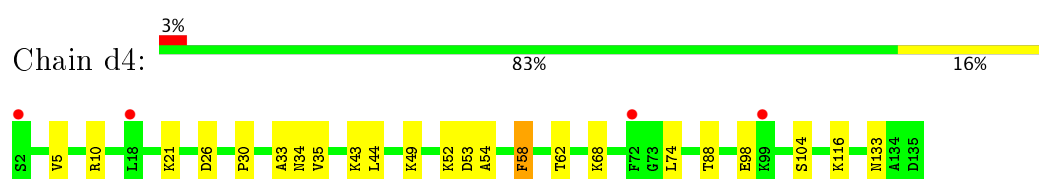
• Molecule 25: 40S ribosomal protein S23-A



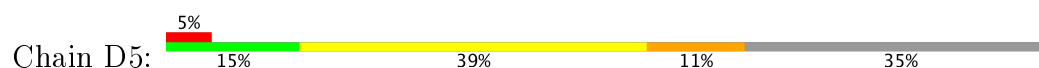
• Molecule 26: 40S ribosomal protein S24-A

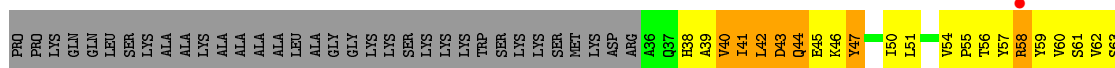


• Molecule 26: 40S ribosomal protein S24-A

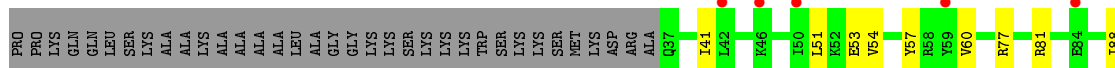


• Molecule 27: 40S ribosomal protein S25-A

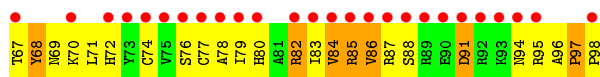
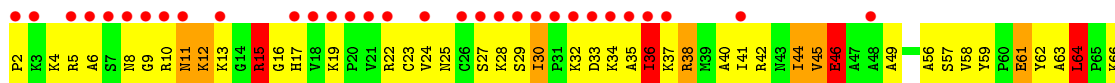




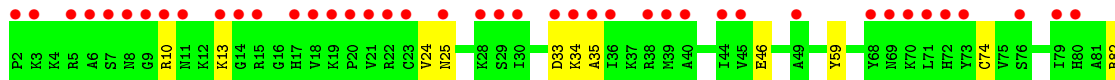
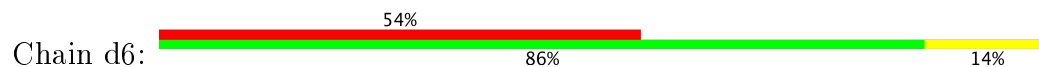
• Molecule 27: 40S ribosomal protein S25-A



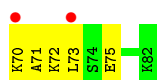
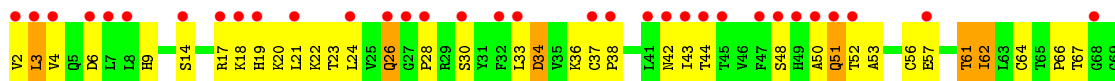
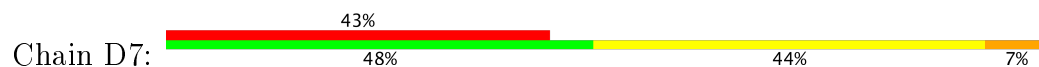
• Molecule 28: 40S ribosomal protein S26-B



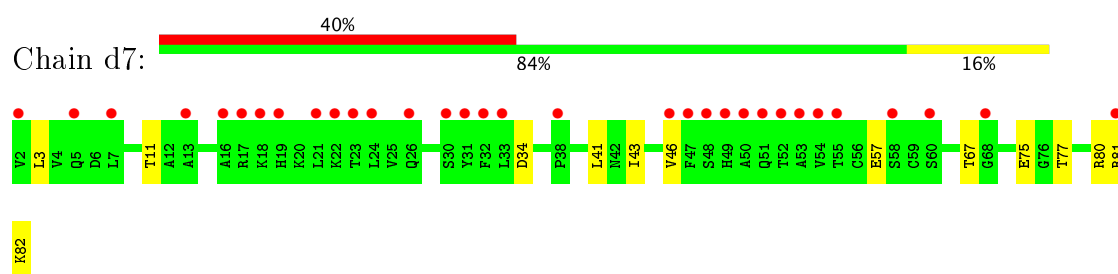
• Molecule 28: 40S ribosomal protein S26-B



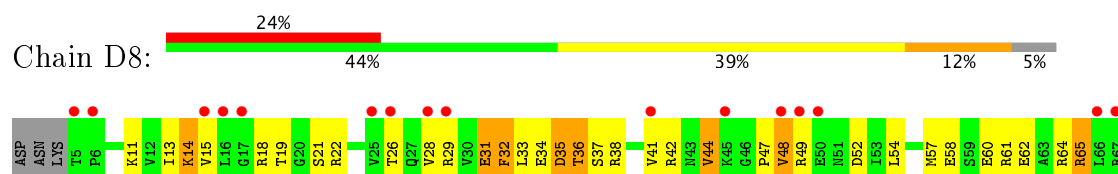
• Molecule 29: 40S ribosomal protein S27-A



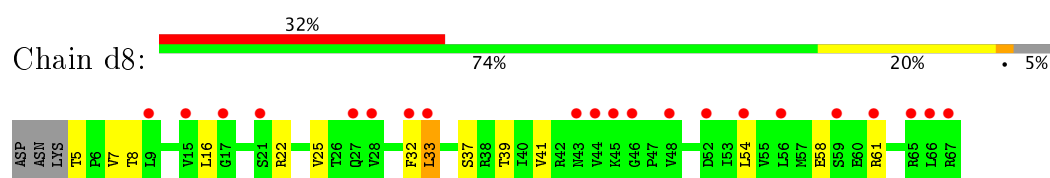
• Molecule 29: 40S ribosomal protein S27-A



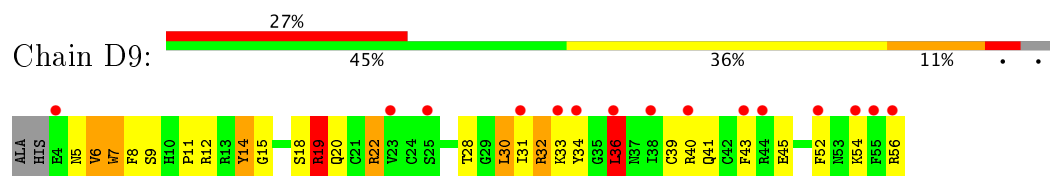
- Molecule 30: 40S ribosomal protein S28-A



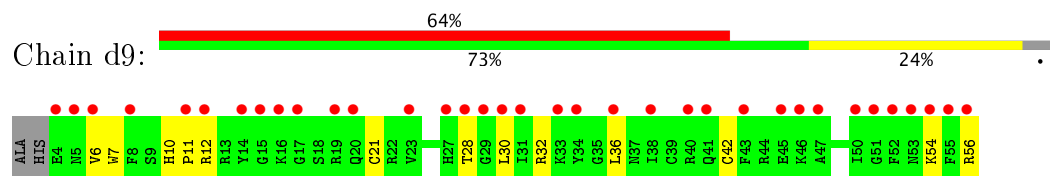
- Molecule 30: 40S ribosomal protein S28-A



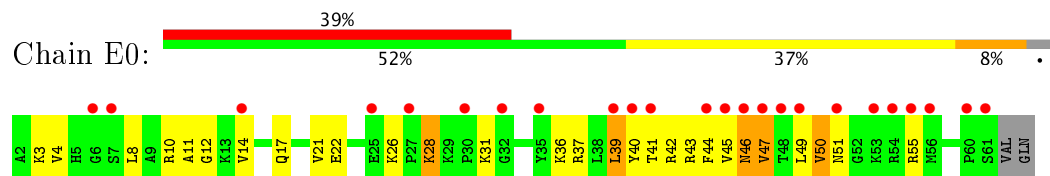
- Molecule 31: 40S ribosomal protein S29-A



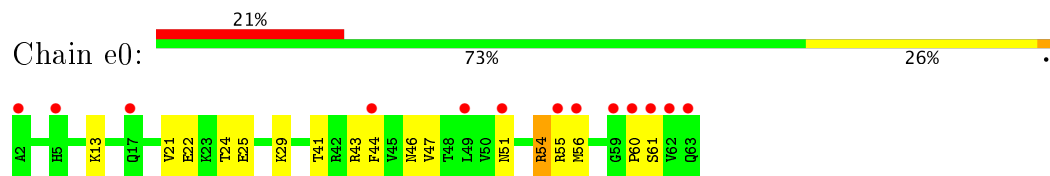
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

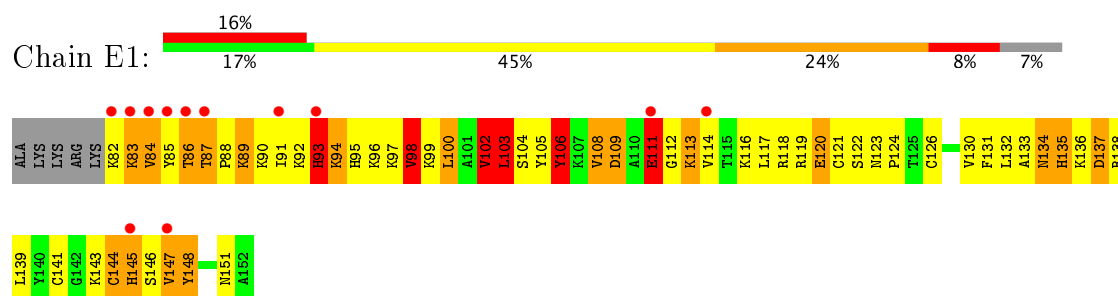


- Molecule 32: 40S ribosomal protein S30-A

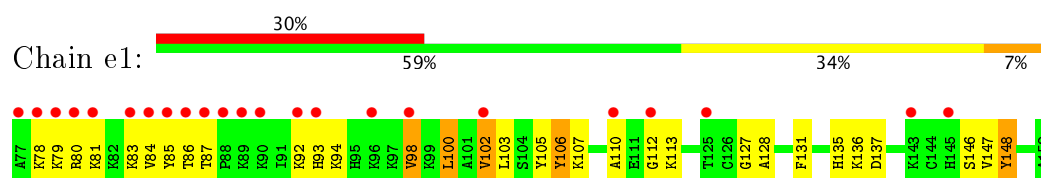




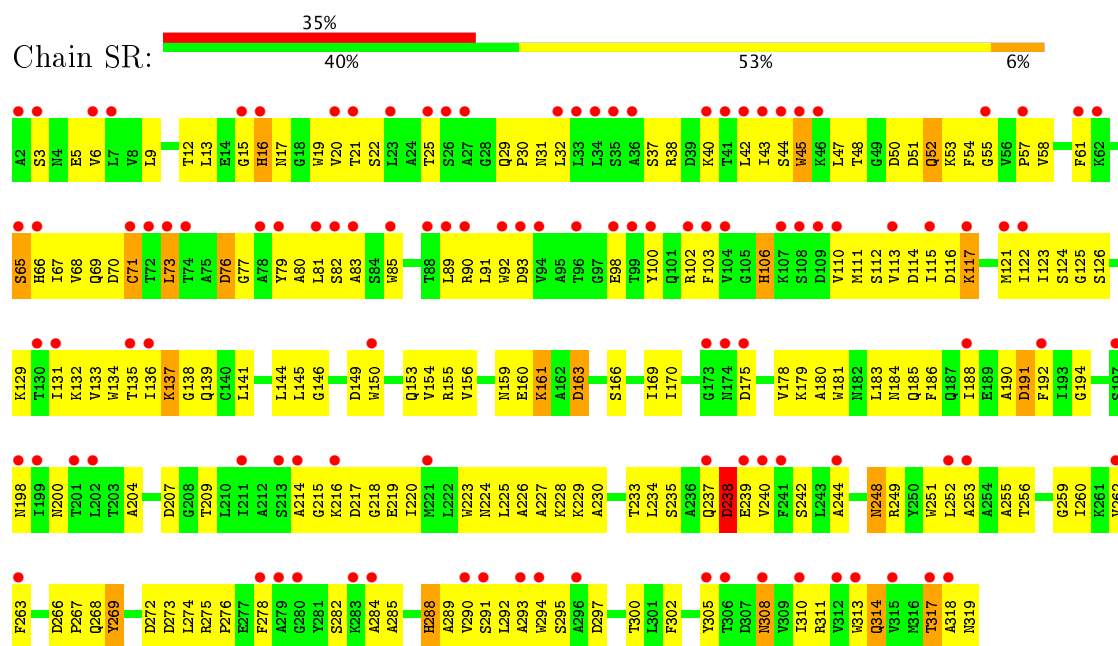
- Molecule 33: Ubiquitin-40S ribosomal protein S31



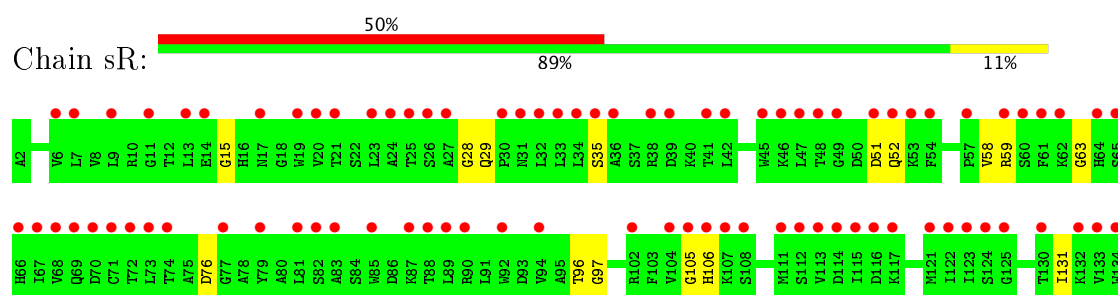
- Molecule 33: Ubiquitin-40S ribosomal protein S31



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



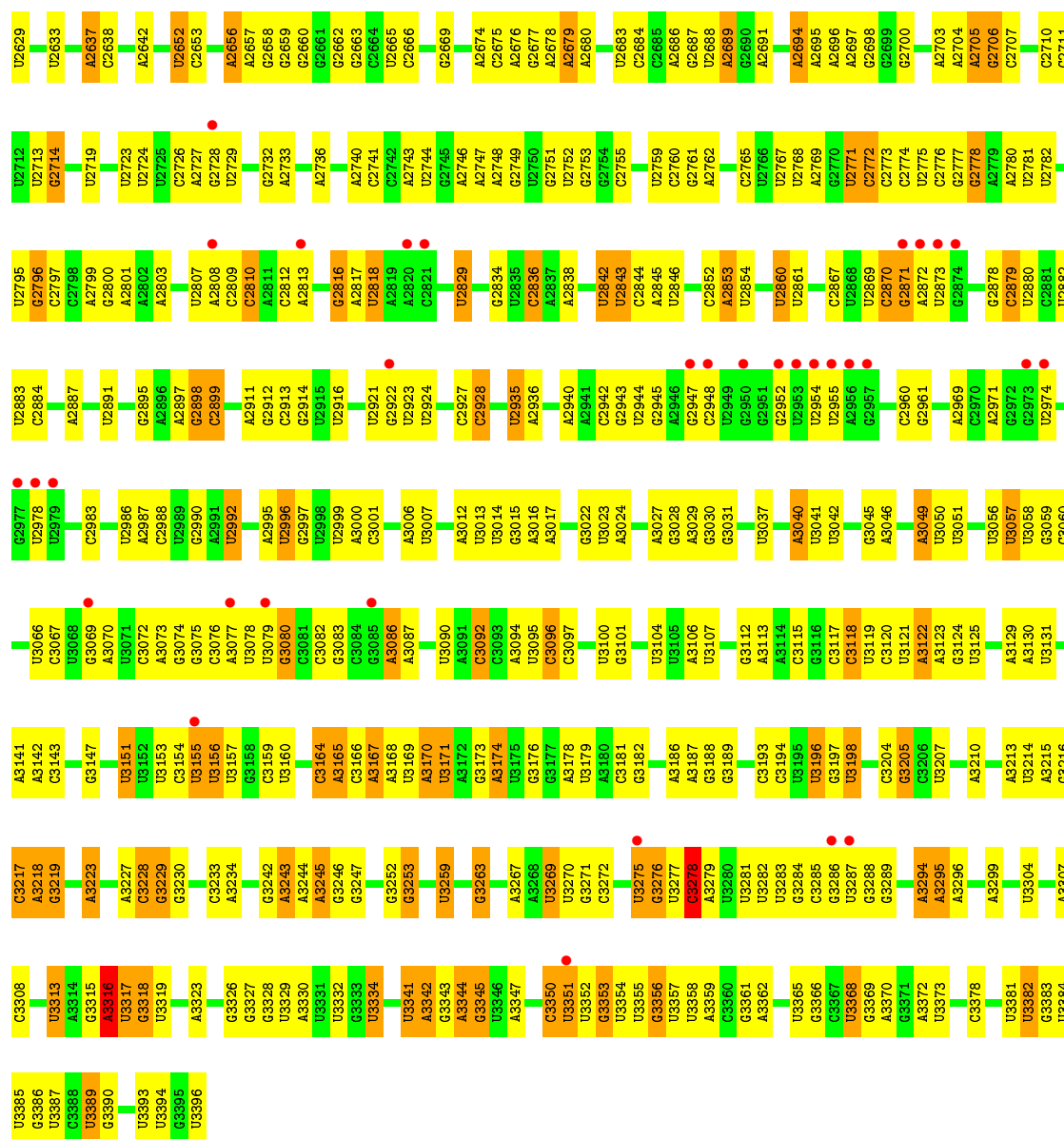
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



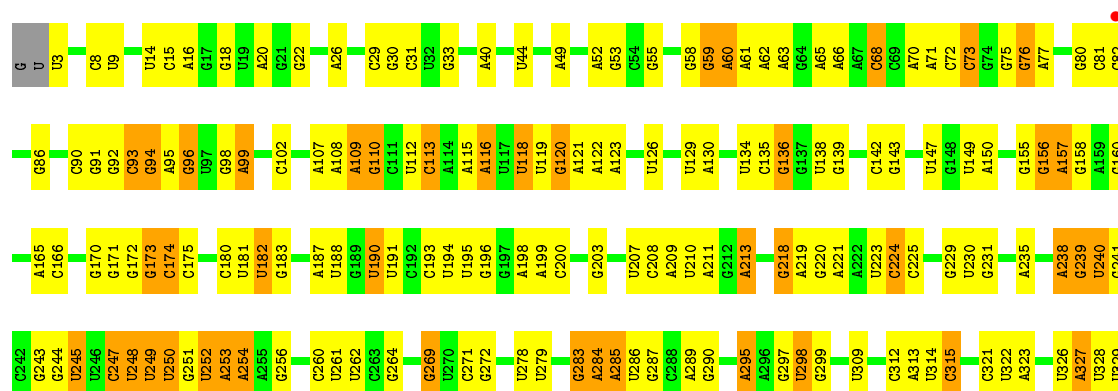


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G1344	C1254	G1175	C1076	A1001	G745	G658	A578	U	G420	C339	U257	U168
U1347	G1255	G1176	A1080	G916	A746	G659	G579	C	G421	U343	G170	G170
U1348	G1256	G1177	A1081	A917	A747	A660	A579	A	G422	U344	C174	C174
C1257	U1258	G1178	U1082	G918	A748	G661	G583	C	A423	G345	U262	C175
U1350	A1259	A1179	U1083	A919	G749	G662	G584	U	G424	C346	G264	G176
U1351	G1260	U1180	A1094	U922	A751	G663	A585	G	G425	G346	C263	C177
A1352	G1261	G1013	G1090	G923	G754	U664	C586	U	G426	A349	U177	U178
U1353	G1262	U1014	G1090	G924	G754	A665	U587	G494	G426	C350	A266	C179
G1354	G1263	U1015	G1090	G925	G754	G670	G588	G495	A436	G353	G267	G180
A1355	G1264	G1016	A1093	A926	G760	U671	G588	A498	G437	U354	A268	C180
U1356	U1265	C1017	U1094	A929	G763	A672	G591	A501	A438	G355	G269	U181
G1357	G1266	G1018	U1095	U930	U764	U673	A592	U502	C439	A355	U270	A187
C1360	U1269	G1019	G1097	C931	C765	G674	C596	C503	A440	U359	G274	U190
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A1394	G1306	G1117	G1117	U959	U790	C695	A621	G542	U	U382	U294	C224
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C1411	A1318	A1054	A1054	U976	A806	A715	G635	A550	G	G392	G304	U230
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A1420	G1322	G1155	G1063	U980	A816	U719	C641	U555	G	U401	A318	C233
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G1422	C1324	U1162	U1065	G982	C818	G721	U643	A557	G	G403	A323	U240
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		G993	G993	A982	C824	G735	G654	C561	U	A407	U329	G244
		G994	G994	G993	A913	A736	C654	U563	U	A408	U329	U245
		G994	G994	G994	A914	A737	C655	U565	C	A409	U329	U245
		G994	G994	G994	A914	A737	C655	U565	C	G412	U249	U249
		G994	G994	G994	A914	A737	C655	U565	C	G412	U249	U249

U2543	G2395	G2221	A2319	A2149	C	U1955	U1853	C1779	G1604	G1527	G1434
U2544	G2396	A2222	U2319	G2150	G	A	C1854	G1780	A1699	C1627	A1435
G2545	A2397	A2223	A2324	G2151	C	G	C1855	U1855	U1700	U1533	U1436
G2549	A2398	A2224	A2325	U2154	U	G	C1856	U1781	C1608	U1533	U1437
U2550	A2399	U2225	G2325	U2155	C	G	C1857	U1782	C1609	A1534	U1438
U2551	G2400	G2226	G2326	U2156	A	A	A1858	U1783	G1710	A1535	U1439
G2552	A2401	C2227	C2327	A2158	U	G	A1859	U1784	C1711	G1543	G1440
G2553	A2402	A2228	U2334	U2159	U	G	A1864	G1785	G1712	G1544	G1441
A2554	A2403	A2229	G2335	U2162	G	C	A1865	G1786	G1713	G1545	
G2555	A2404	A2230	U2336	C2163	C	C	C1866	A1787	G1714	A1546	
G2556	C2405	A2242	C2337	A2164	U	C	C1867	A1788	A1715	G1547	
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	U2408	G2245	C2339	A2166	C	U	A1874	U1717	U1622		
		G2246	U2340	A2167	A	U	G1875	G1718	U1629		
G2560	U2411	G2249	A2341	A2168	U	G	A1876	G1719	U1630		
A2561	A2412	G2250	U2342	U2169	A	C	G1878	U1720	U1631		
A2562	A2413	G2251	U2343	U2170	U	C	A1879	U1721	C1632		
	G2414	U2170	U2344	U2171	A	G	U1880	U1722	U1633		
U2565			A2345		A2093	C	G1889	A1799	G1725		
G2566	G2418	U2254		G2174	C2094	C	A1896	A1800	G1634		
G2567	A2419	A2255		U2175	G2095	C	A1897	C1726	U1635		
A2568		A2256		U2176	A2100	G	G1898	G1727	U1636		
A2569	C2422	C2257		A2176	C2101	C	U1903	G1728	A1638		
U2570	U2423	U2258		A2178	U2102	C	C1904	A1729	C1639		
U2571	A2424	G2261		G2180	U2103	U	C1905	G1730	G1640		
C2572	G2425	A2262		C2181	A2107	G	G1906	G1731	U1641		
G2573	G2426	C2263		A2182	C2108	C	C1907	G1732	A1642		
G2575		U2264		U2183	U2109	U	A1910	G1733	A1643		
G2576	G2437	C2265		G2185	G2111	C	A1915	G1734	U1644		
				U2186	U2112	G	U1916	G1735	U1645		
U2581	G2442	G2272		G2187	U2113	U	A1922	G1736			
	A2443	G2273		U2188	C2114	A	C1923	U1739	U1651		
G2585	A2445			U2189	G2115	C	U1924	U1740	G1652		
G2586		C2278		U2190		A	U1925	A1741	U1657		
U2587		A2279		U2191	A2120	C	U1926	U1742	A1656		
G2588		A2280		C2192	G2121	G	G1927	G1743	G1657		
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A2591		U2282		G2194	C2123	C	U1933	U1745	G1576		
G2592		G2283		C2195	U2126	C	U1934	U1746	G1577		
A2593		C2284		A2198	A2130	G	U1935	G1747	C1578		
G2594		U2287		U2199	G2131	U	A1936	A1667	C1579		
		U2298		G2200	C2132	C	U1937	G1748	A1581		
G2606		A2299		C2202	U2133	G	U1938	A1749	C1582		
G2607		G2300		U2205	G2134	U	G1939	G1751	U1584		
		U2301		U2208	U2137	A	A1940	A1752	C1585		
G2614		G2302		U2209	U2138	G	U1941	G1761	C1586		
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G2618		C2308		A2213	U2142	C	U1945	U1765	G1590		
		U2309		A2214	A2143	U	G1946	G1766	C1591		
G2621		U2310		A2215	A2144	C	U1947	C1767	U1687		
G2622		U2311		U2217	A2145	U	U1950	U1768	U1688		
G2623		A2313		U2218	A2146	A	C1951	U1769	U1689		
G2624		U2314		A2219	C2147	U	G1952	G1770	C1690		
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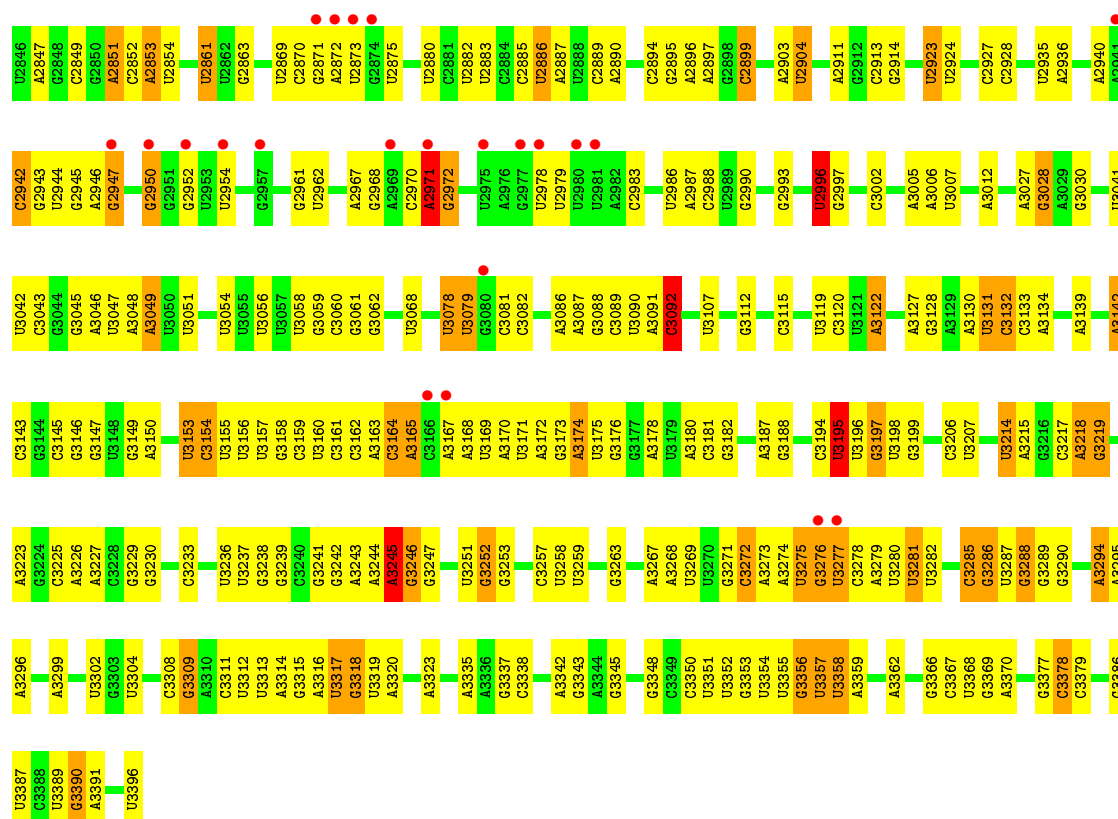


• Molecule 36: 25S ribosomal RNA

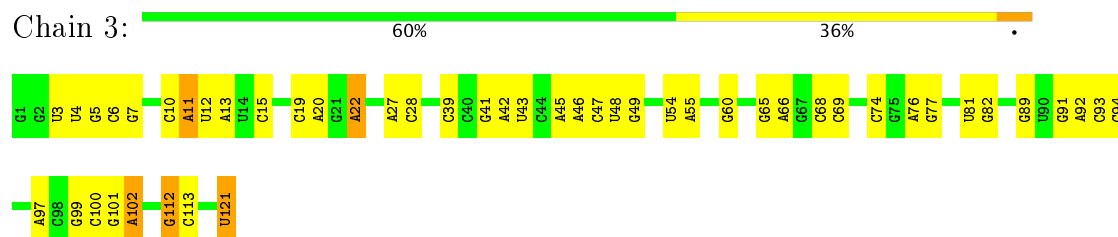




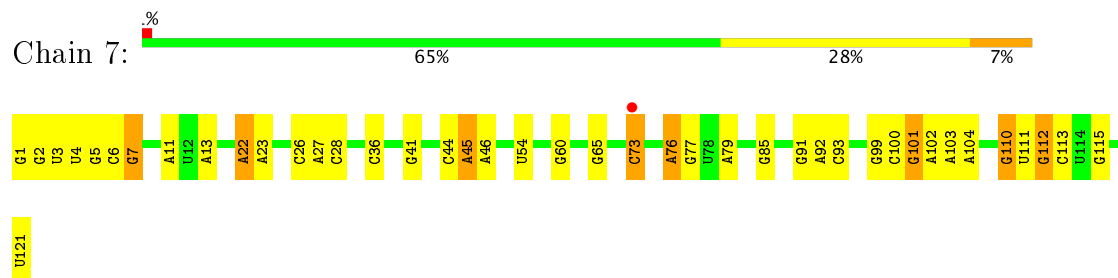
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A2762	A2676	C2572	G2503	C2443	A2357	A2262	A2182	A2103	G	A1884	C1804	A1715	G1623
G2763	G2677	G2574	U2504	A2444	A2358	U2263	U2184	A2104	C	U1903	C1805	U1716	G1624
C2764	U2683	G2584	C2507	U2445	A2359	U2264	G2187	G2106	G	G1906	C1806	U1717	A1625
C2765	C2684	G2585	U2508	A2447	C2360	G2265	U2188	G2111	U	G1907	G1807	G1718	C1628
U2766	G2687	G2586	U2509	G2448	G2364	U2266	U2189	U2112	A	A1908	G1812	U1719	U1629
U2771	U2688	G2592	U2513	G2449	G2370	G2270	C2192	A2113	G	A1913	A1813	U1720	U1630
C2772	A2689	A2593	U2514	G2450	G2371	A2271	U2193	C2114	C	A1914	A1814	U1721	A1631
C2773	G2690	C2594	A2515	G2452	A2372	G2272	U2194	G2115	U	G1915	U1815	U1722	A1632
C2774	A2691	A2595	U2516	U	A2373	G2273	C2197	A2117	G	U1916	G1817	U1723	G1633
G2777	A2694	C2600	U2517	G	C2374	A2276	A2198	C2118	C	U1925	U1818	C1725	G1635
C2778	A2695	A2601	C2518	A	G2375	G2277	G2201	A2119	A	C1926	U1819	G1728	C1639
A2779	A2696	G2602	A2520	G	G2376	C2278	C2202	A2120	C	U1944	A1750	U1729	G1640
A2780	A2697	U2603	U2521	A	C2378	A2279	U2203	G2121	U	G1945	U1751	G1730	U1641
G2786	G2700	U2604	G2522	U	U2379	A2280	C2204	G2122	C	A1932	U1824	G1738	A1642
U2795	U2701	G2605	A2523	A	U2381	A2281	U2205	A2131	U	A1933	U1831	G1747	A1643
G2796	A2702	G2606	A2524	A	G2385	U2282	G2206	G2134	G	G1940	U1832	U1748	C1644
A2799	A2703	U2611	C2525	G	A2386	G2283	A2207	G2135	U	U1943	G1833	U1749	U1645
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A2801	A2705	U2613	G2530	G	C2394	G2288	G2210	A2138	U	U1945	U1837	G1751	U1649
A2802	G2706	G2614	C2531	A	G2395	A2291	A2213	U2140	C	A1946	U1838	C1756	A1654
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C2809	G2708	U2617	A2535	C	A2398	A2299	G2218	A2144	U	G1948	A1841	G1758	C1657
C2810	C2709	G2618	U2536	U	A2399	A2300	A2219	A2145	C	G1949	U1842	G1759	G1658
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G2816	U2633	U2544	C2544	C	C2406	G2311	A2229	C2151	U	G	G1849	U1765	A1667
A2817	A2636	C2545	U2545	A	C2407	A2312	C2230	U2153	C	U	C1850	G1766	G1668
U2818	G2637	A2546	C2546	G	U2411	A2313	C2231	G2155	A	G	C1856	U1767	G1675
G2822	U2645	A2547	C2547	U	C2415	U2314	C2236	C2156	U	G	U1857	G1770	A1676
G2823	G2648	U2549	C2549	G	G2418	G2315	U2236	G2157	C	G	A1858	G1677	G1677
U2827	A2649	U2550	U2550	A	A2419	A2324	U2241	A2158	C	C	G1863	G1773	U1682
G2828	U2652	U2551	C2552	U	U2425	A2332	A2242	U2159	A	C	A1864	G1774	A1683
G2830	U2655	G2555	C2555	C	G2426	C2333	A2243	G2165	C	U	C1865	G1778	U1686
A2833	A2656	A2556	A2557	C	U2427	U2334	A2244	A2166	C	G	C1866	G1779	U1687
C2836	G2657	C2557	C2557	A	G2428	G2335	C2245	A2167	A	U	U1871	G1780	U1688
A2837	U2658	C2560	C2560	U	G2429	U2336	G2249	A2168	U	C	G1875	U1782	U1689
A2838	G2659	G2563	C2563	C	U2433	A2341	G2250	U2170	A	U	U1876	U1783	U1692
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U2842	C2664	C2567	C2567	U	G2437	U2343	A2252	A2172	C	A	G1878	G1786	U1694
C2843	U2665	U2665	U2665	U	A2438	U2344	G2253	U2173	C	C	A1879	A1787	U1695
C2844	C2666	C2666	C2666	U	G2439	A2345	U2254	G2174	U	G	U1880	G1792	A1699
A2845	G2754	U2667	A2569	A2500	G2440	U2351	A2255	G2177	C	A	A1886	A1797	G1700
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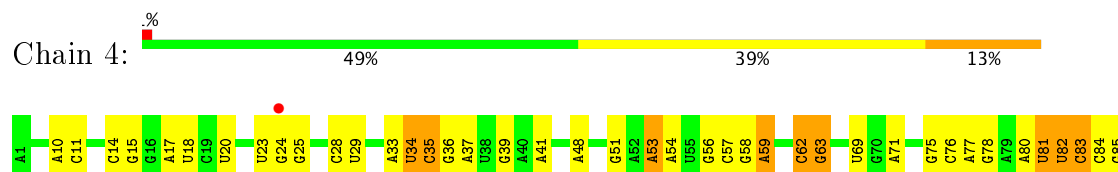
- Molecule 37: 5S ribosomal RNA



- Molecule 37: 5S ribosomal RNA



- Molecule 38: 5.8S ribosomal RNA



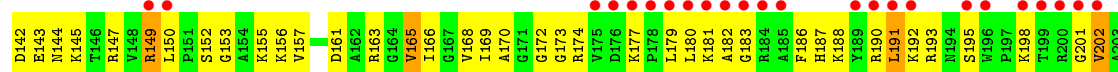
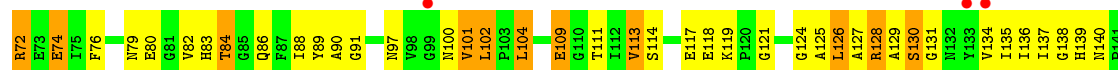




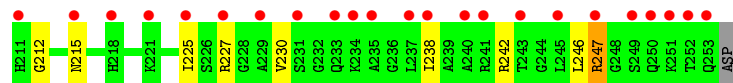
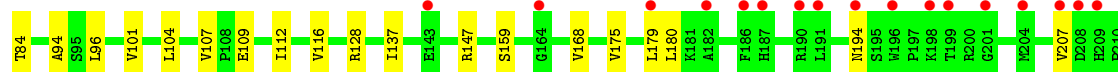
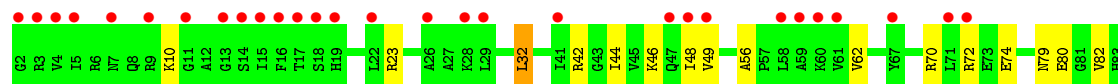
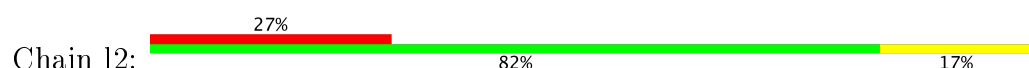
• Molecule 38: 5.8S ribosomal RNA



• Molecule 39: 60S ribosomal protein L2-A

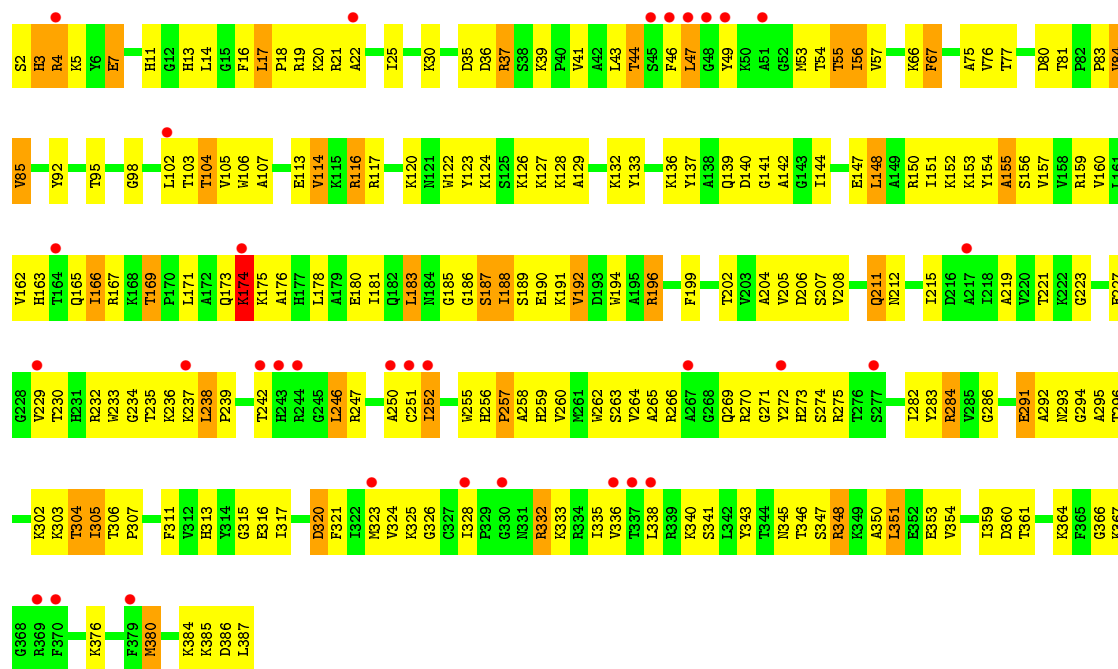


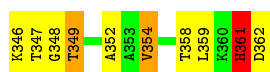
• Molecule 39: 60S ribosomal protein L2-A



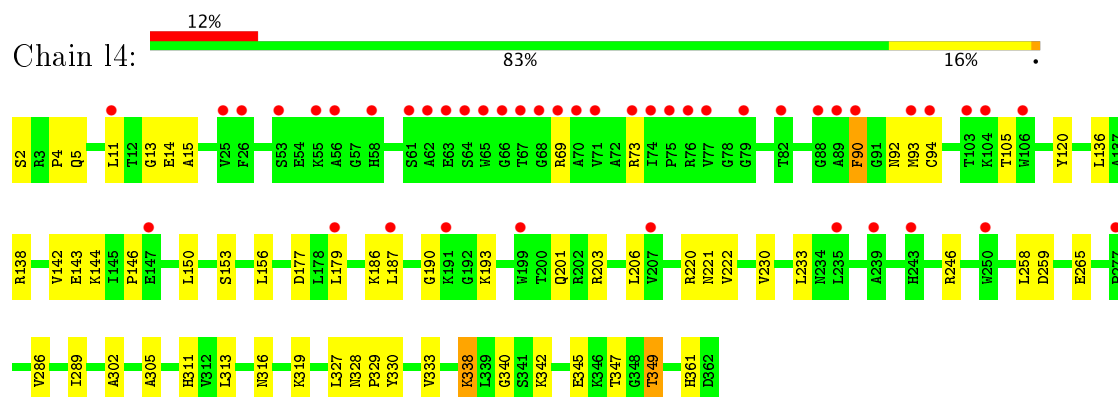
• Molecule 40: 60S ribosomal protein L3



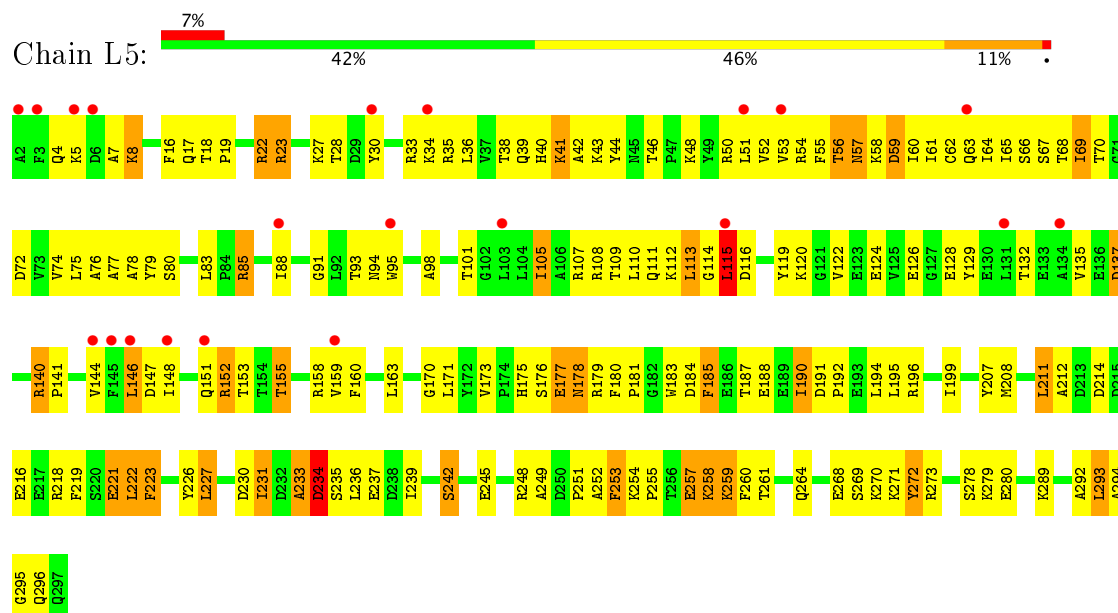




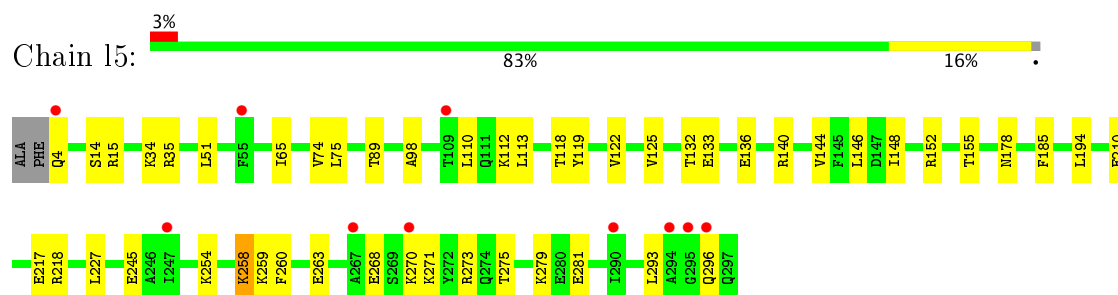
• Molecule 41: 60S ribosomal protein L4-A



• Molecule 42: 60S ribosomal protein L5

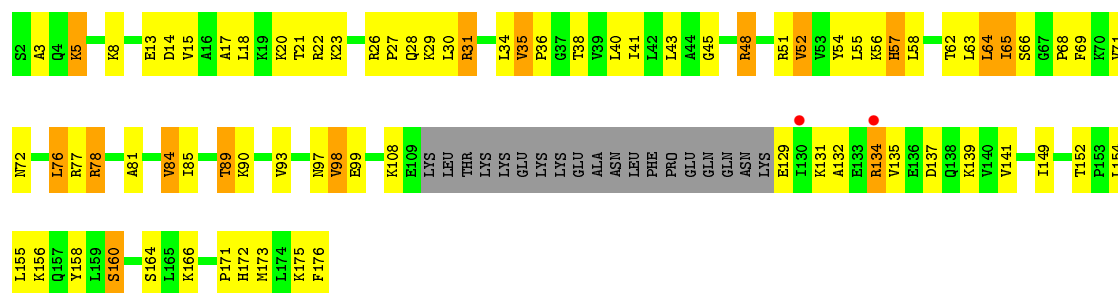


• Molecule 42: 60S ribosomal protein L5

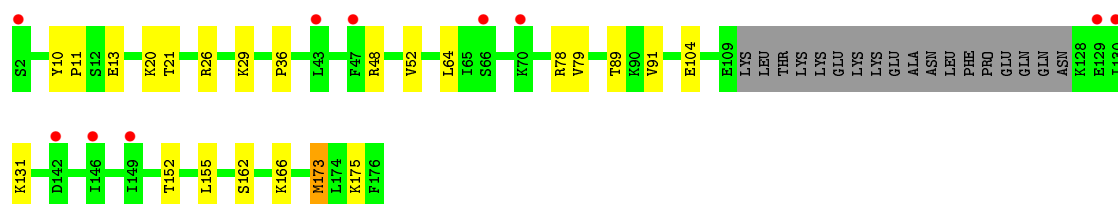
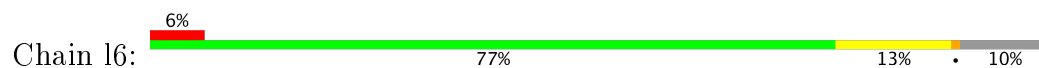


• Molecule 43: 60S ribosomal protein L6-A

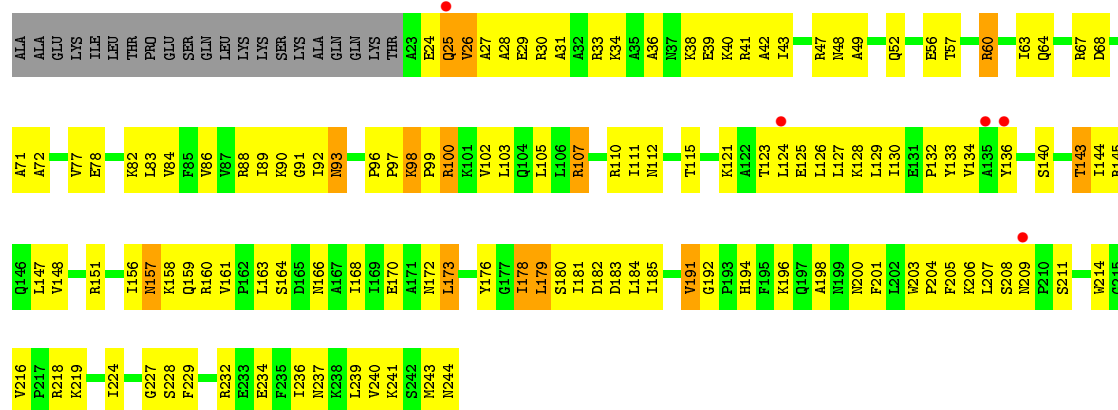




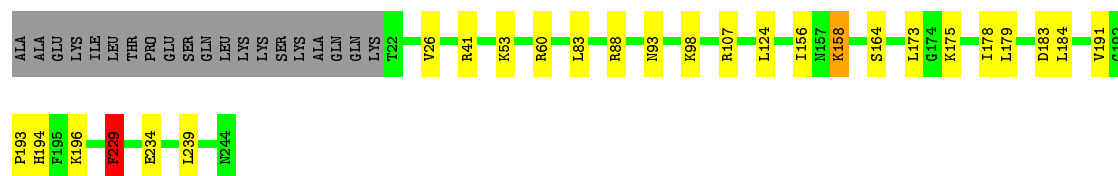
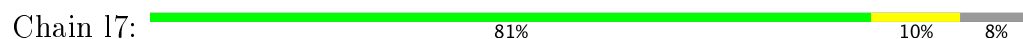
- Molecule 43: 60S ribosomal protein L6-A



- Molecule 44: 60S ribosomal protein L7-A

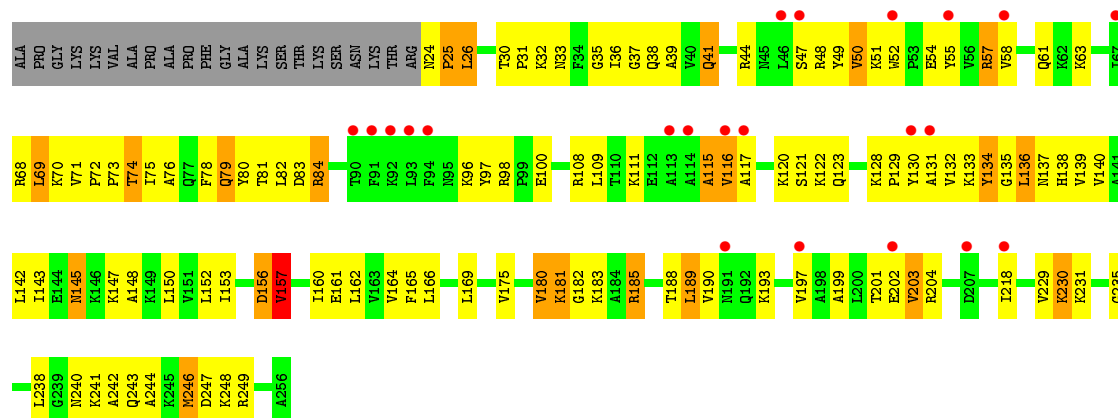


- Molecule 44: 60S ribosomal protein L7-A

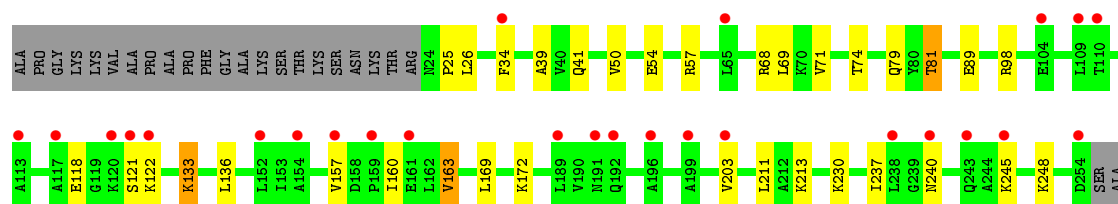
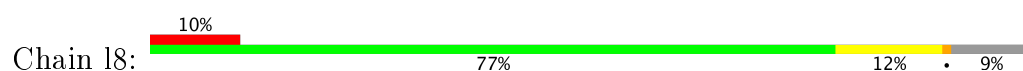


- Molecule 45: 60S ribosomal protein L8-A

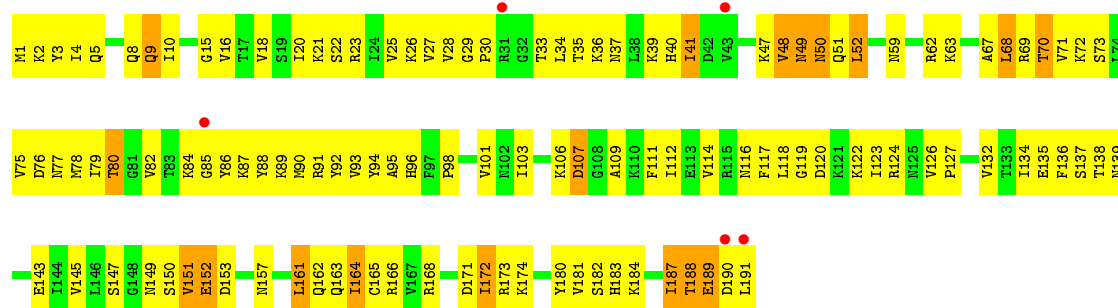




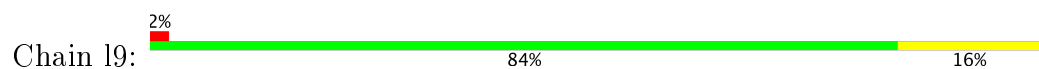
• Molecule 45: 60S ribosomal protein L8-A



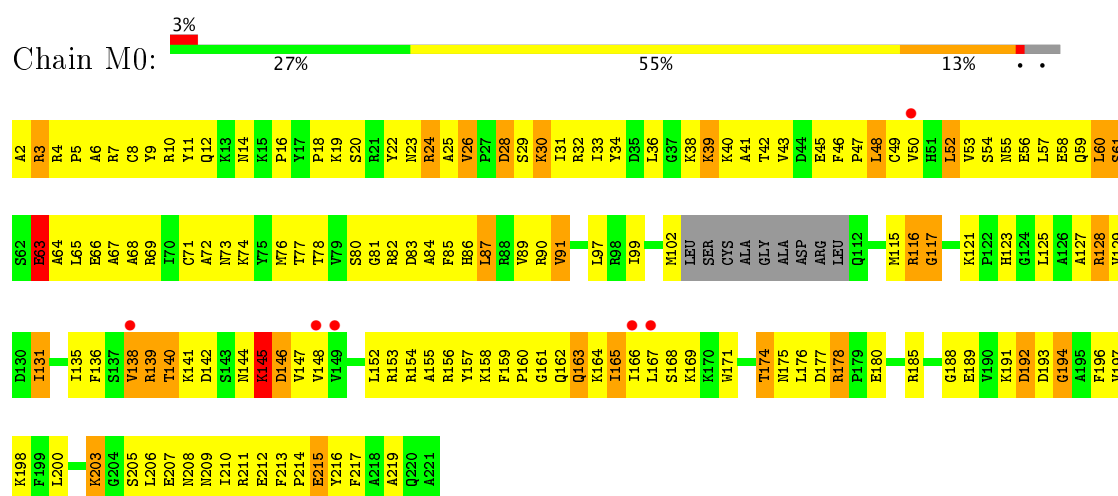
• Molecule 46: 60S ribosomal protein L9-A



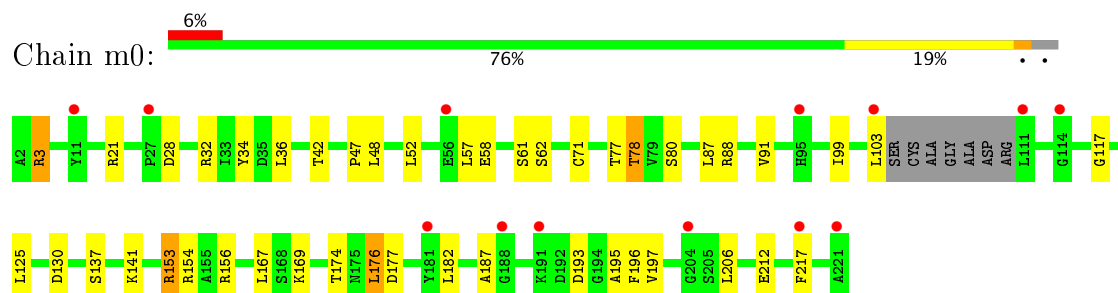
• Molecule 46: 60S ribosomal protein L9-A



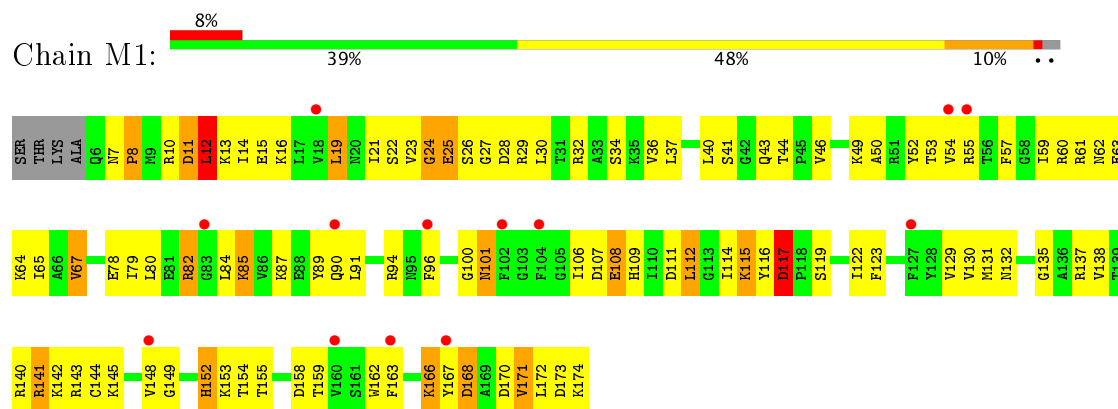
• Molecule 47: 60S ribosomal protein L10



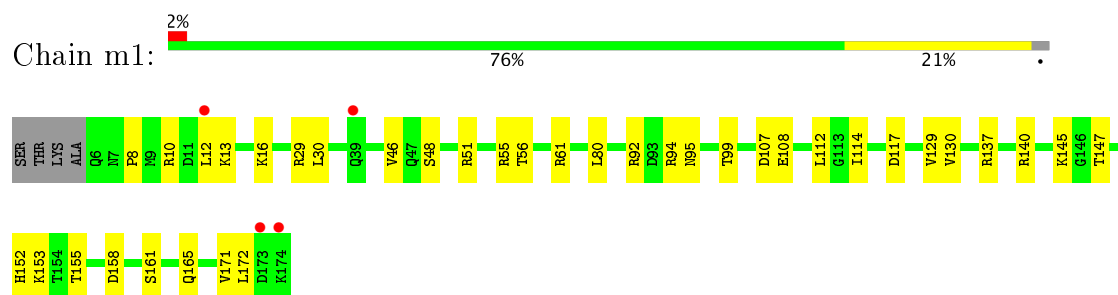
- Molecule 47: 60S ribosomal protein L10



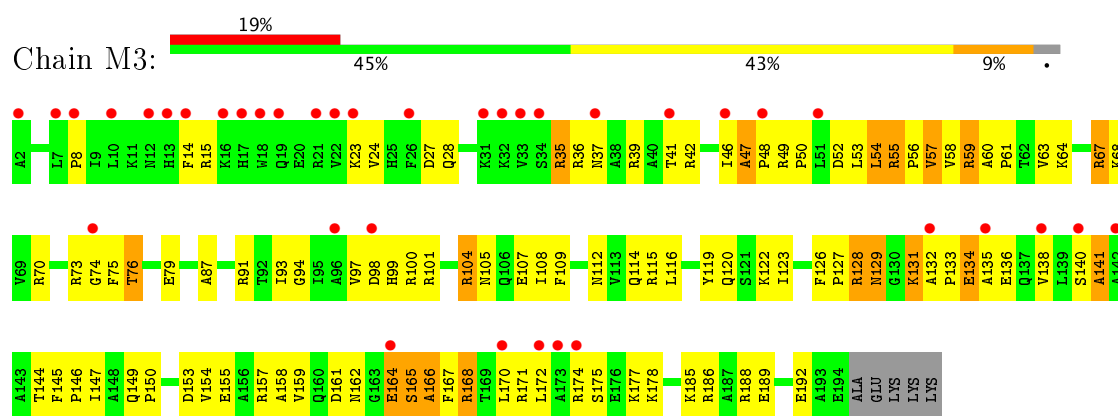
- Molecule 48: 60S ribosomal protein L11-B



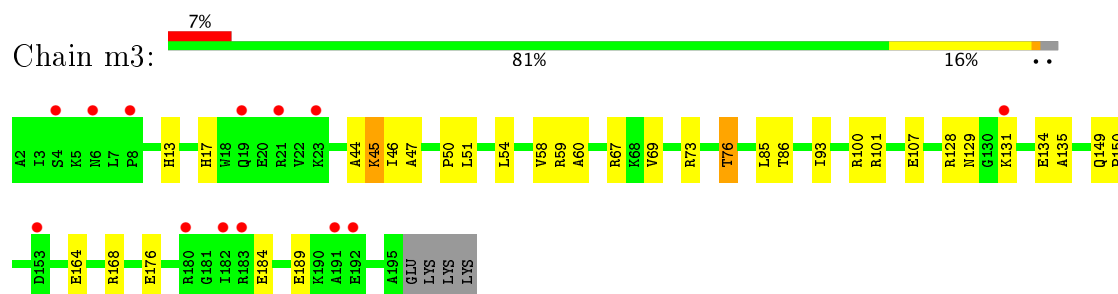
- Molecule 48: 60S ribosomal protein L11-B



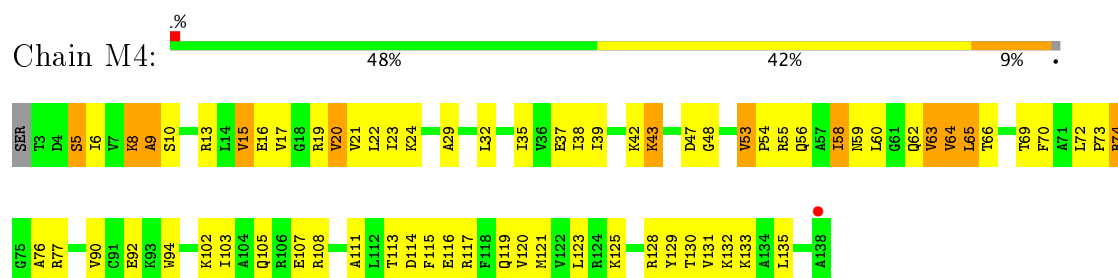
- Molecule 49: 60S ribosomal protein L13-A



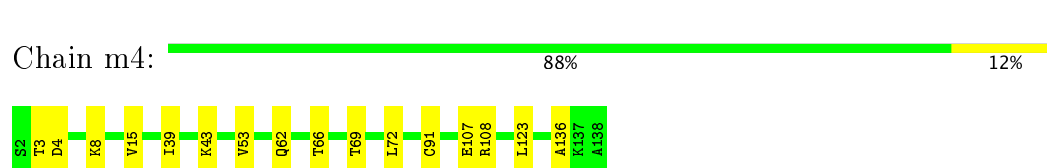
• Molecule 49: 60S ribosomal protein L13-A



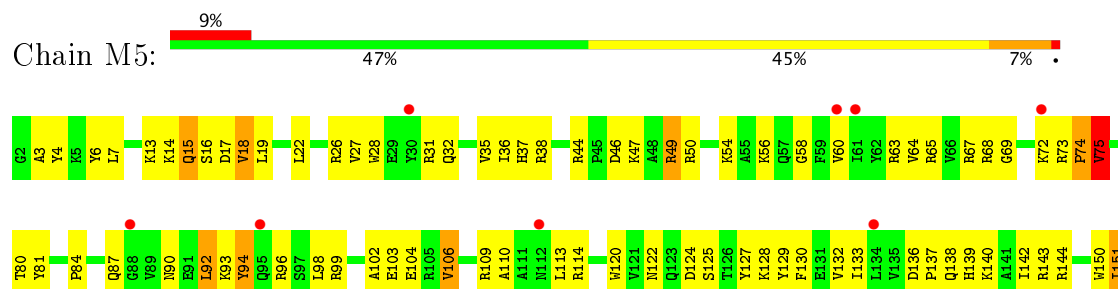
• Molecule 50: 60S ribosomal protein L14-A

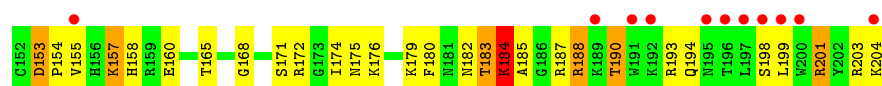


• Molecule 50: 60S ribosomal protein L14-A

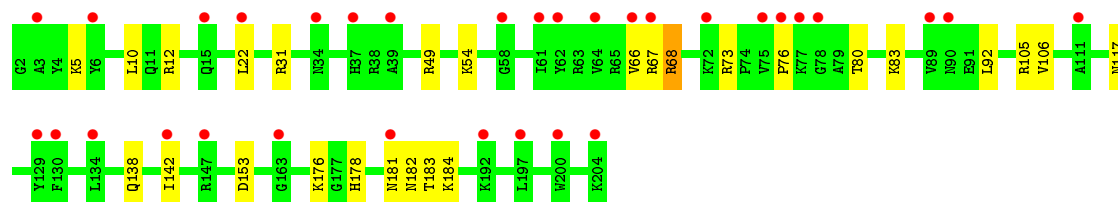
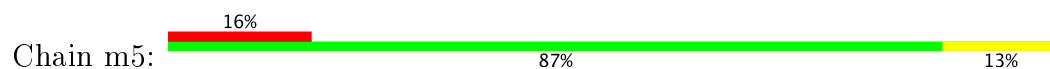


• Molecule 51: 60S ribosomal protein L15-A

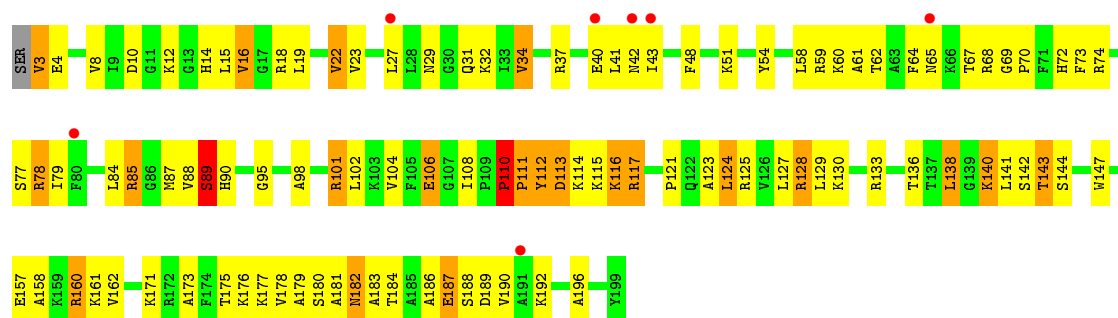




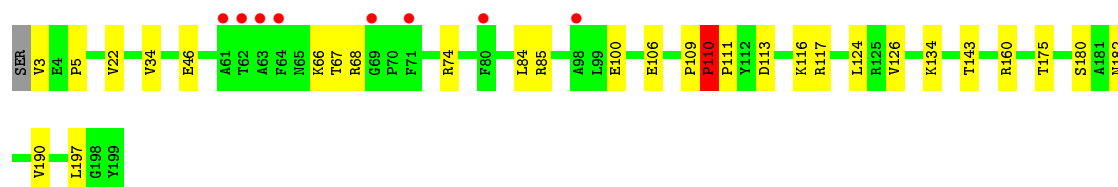
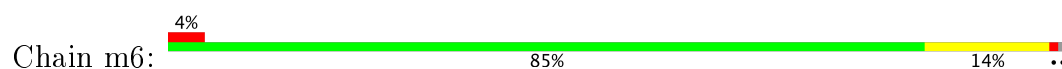
- Molecule 51: 60S ribosomal protein L15-A



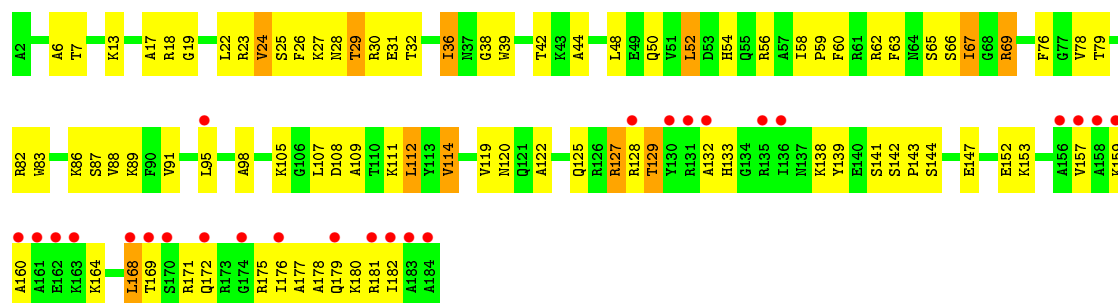
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L16-A

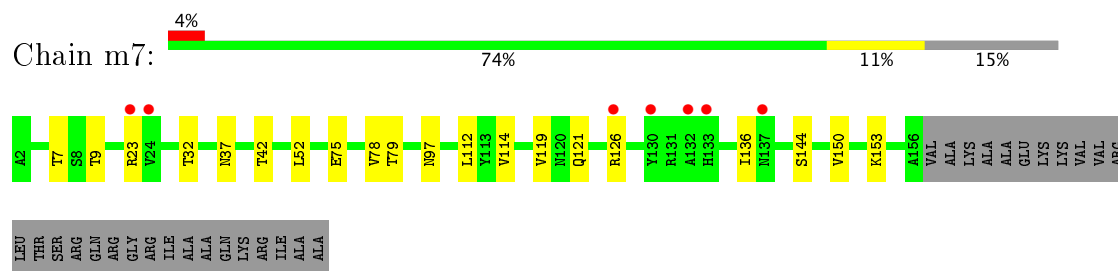


- Molecule 53: 60S ribosomal protein L17-A





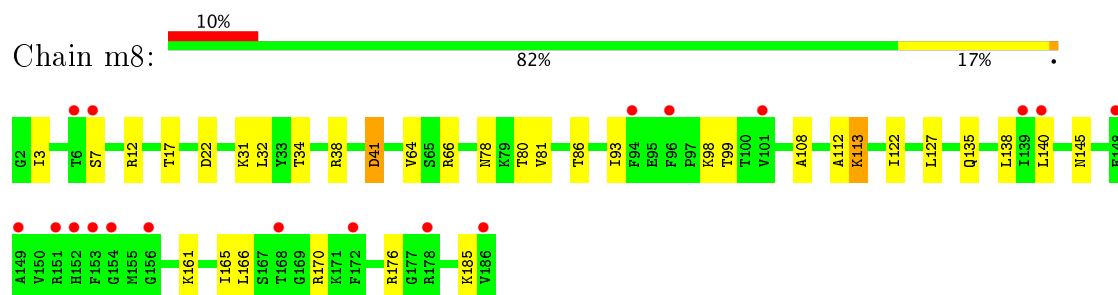
- Molecule 53: 60S ribosomal protein L17-A



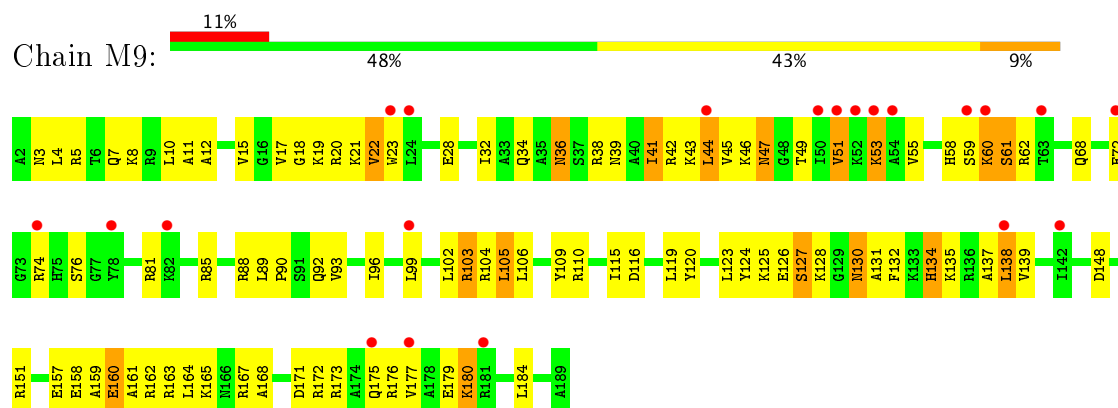
- Molecule 54: 60S ribosomal protein L18-A



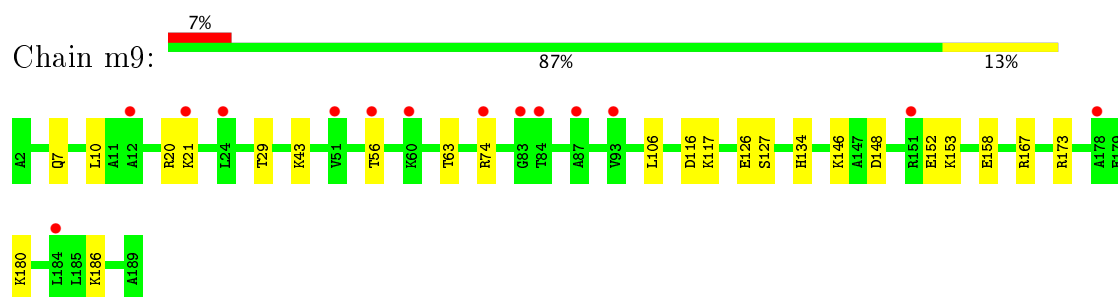
- Molecule 54: 60S ribosomal protein L18-A



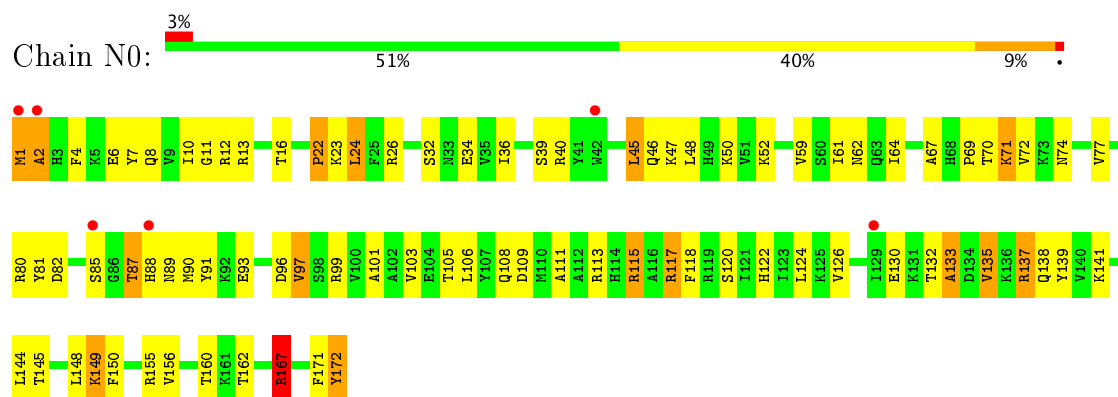
- Molecule 55: 60S ribosomal protein L19-A



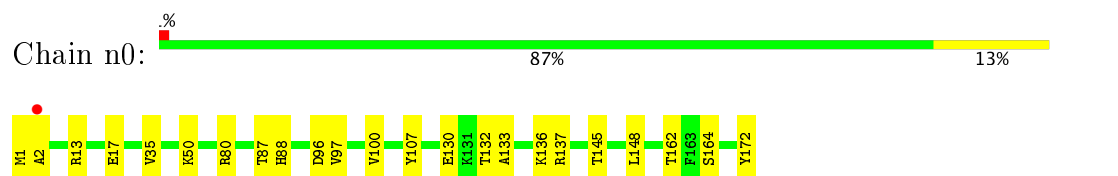
- Molecule 55: 60S ribosomal protein L19-A



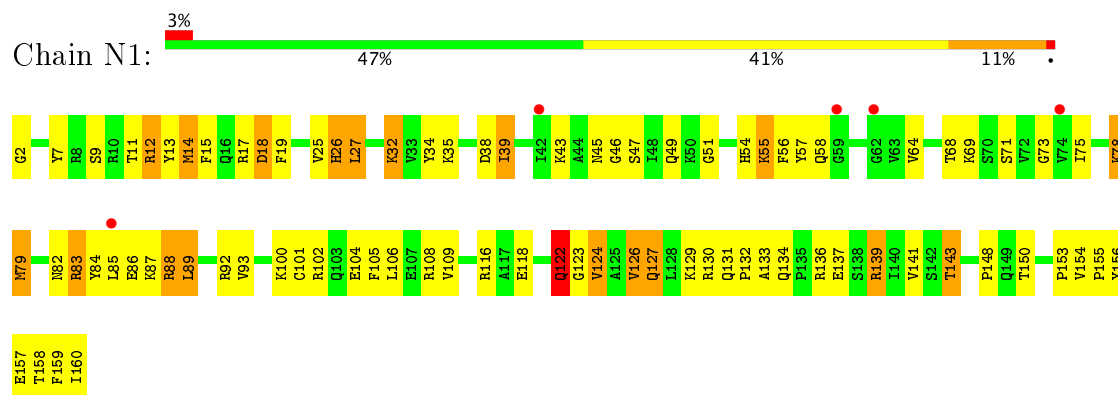
- Molecule 56: 60S ribosomal protein L20-A



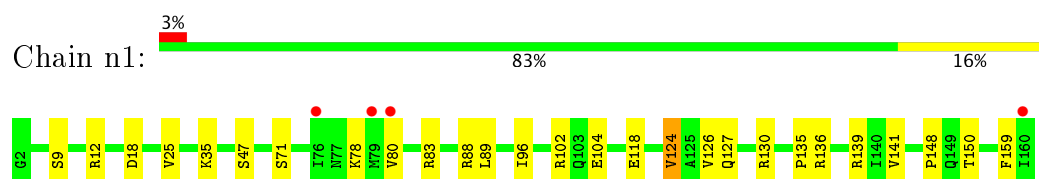
- Molecule 56: 60S ribosomal protein L20-A



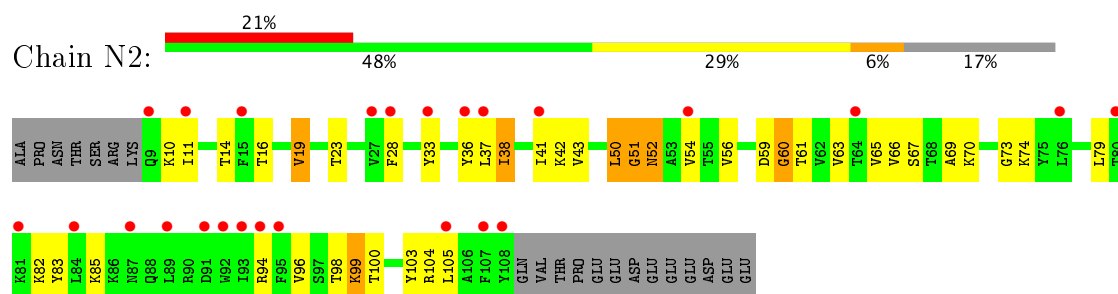
- Molecule 57: 60S ribosomal protein L21-A



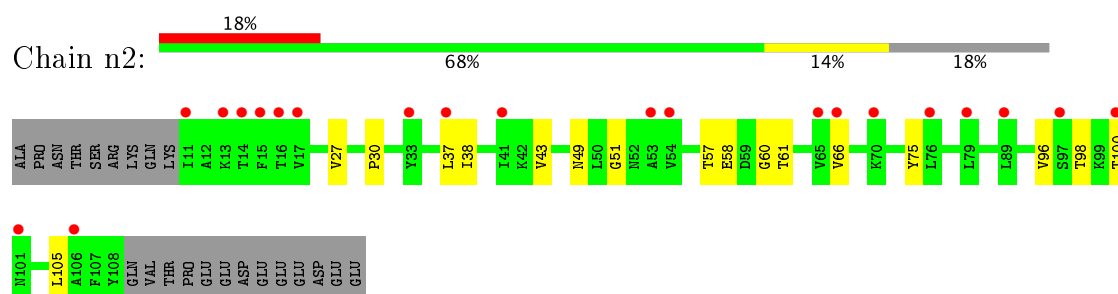
- Molecule 57: 60S ribosomal protein L21-A



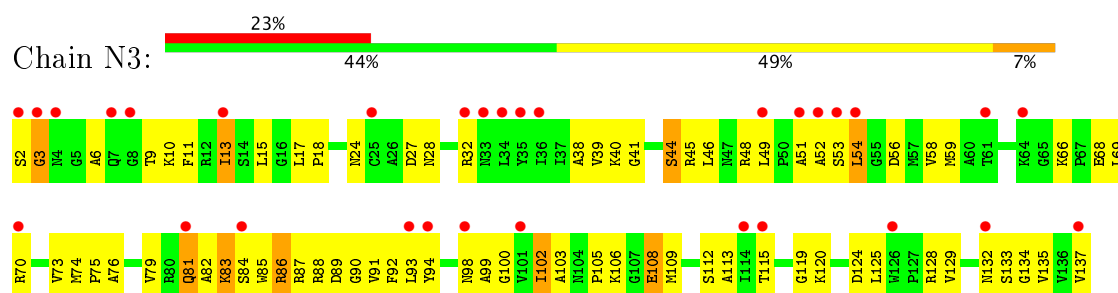
- Molecule 58: 60S ribosomal protein L22-A



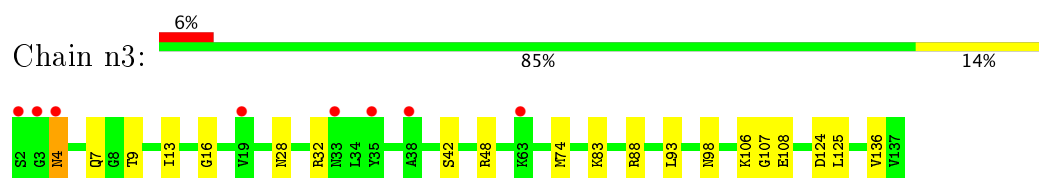
- Molecule 58: 60S ribosomal protein L22-A



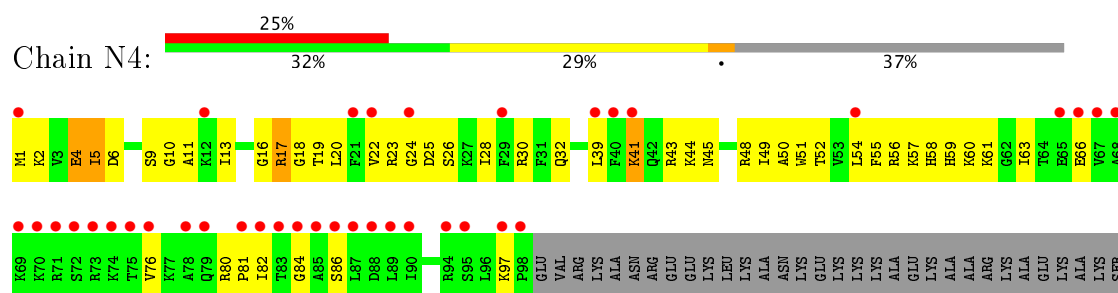
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A



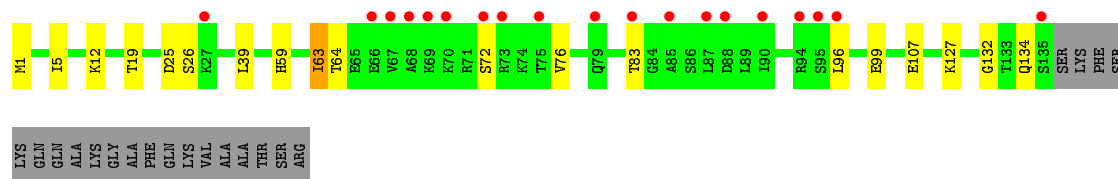
- Molecule 60: 60S ribosomal protein L24-A



ALA  
GLY  
THR  
GLN  
SER  
SER  
LYS  
PHE  
SER  
SER  
GLN  
GLN  
ALA  
LYS  
GLY  
ALA  
PHE  
GLN  
LYS  
VAL  
ALA  
ALA  
THR  
SER  
ARG

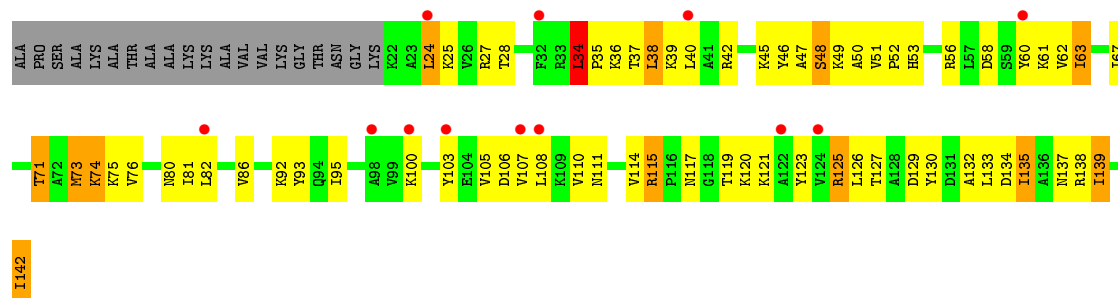
• Molecule 60: 60S ribosomal protein L24-A

Chain n4: 12% 75% 12% 13%



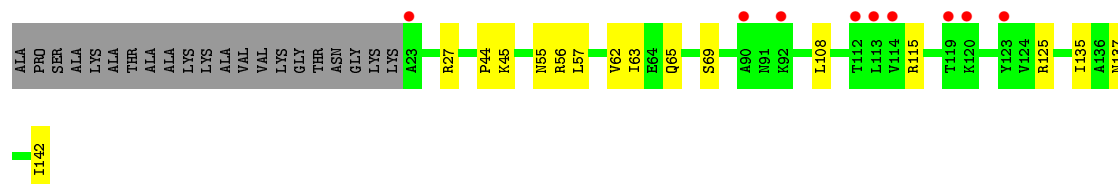
• Molecule 61: 60S ribosomal protein L25

Chain N5: 9% 38% 39% 9% 14%



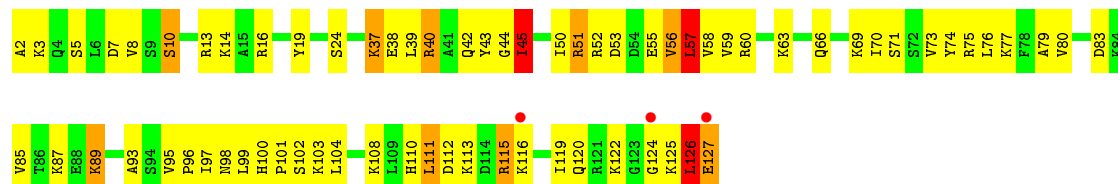
• Molecule 61: 60S ribosomal protein L25

Chain n5: 6% 74% 11% 15%



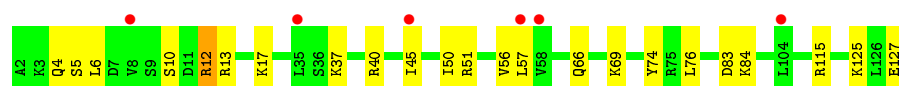
• Molecule 62: 60S ribosomal protein L26-A

Chain N6: 2% 44% 46% 7%



• Molecule 62: 60S ribosomal protein L26-A

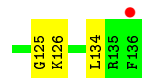
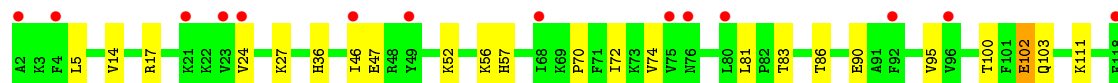
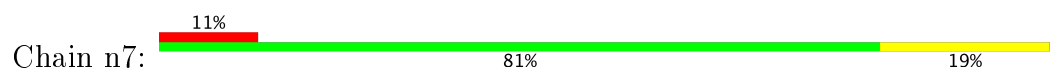
Chain n6: 5% 82% 17%



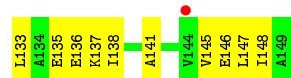
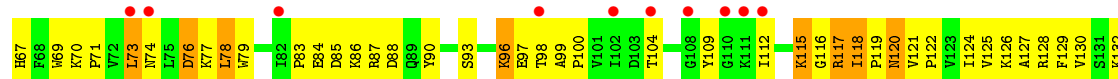
• Molecule 63: 60S ribosomal protein L27-A



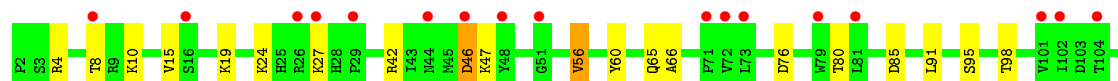
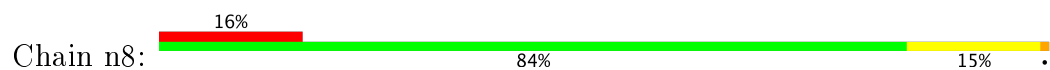
• Molecule 63: 60S ribosomal protein L27-A



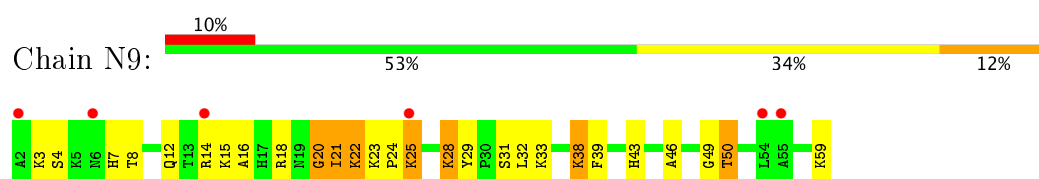
• Molecule 64: 60S ribosomal protein L28



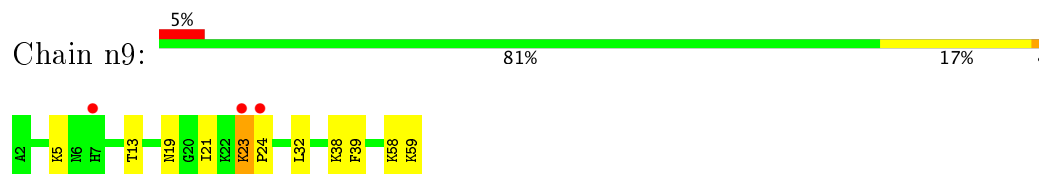
• Molecule 64: 60S ribosomal protein L28



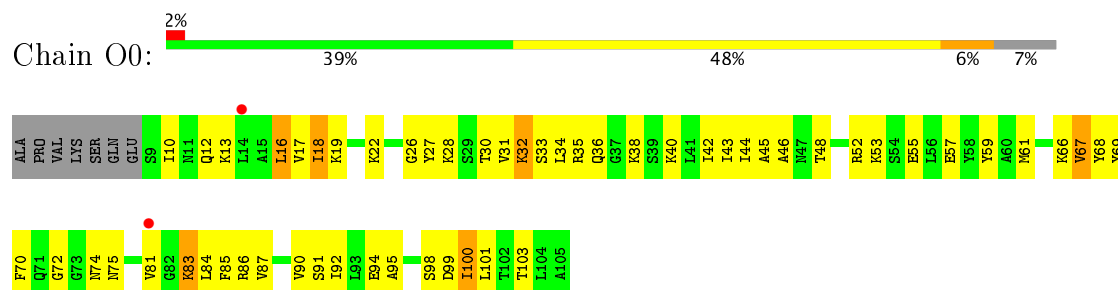
• Molecule 65: 60S ribosomal protein L29



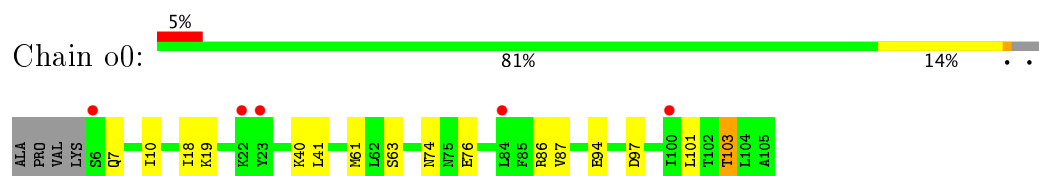
- Molecule 65: 60S ribosomal protein L29



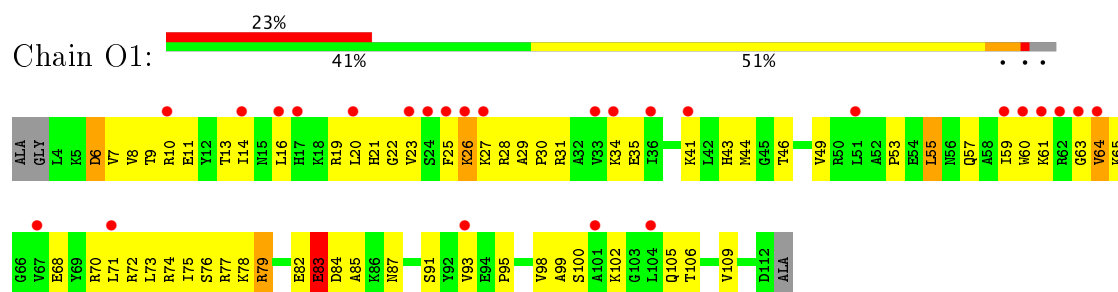
- Molecule 66: 60S ribosomal protein L30



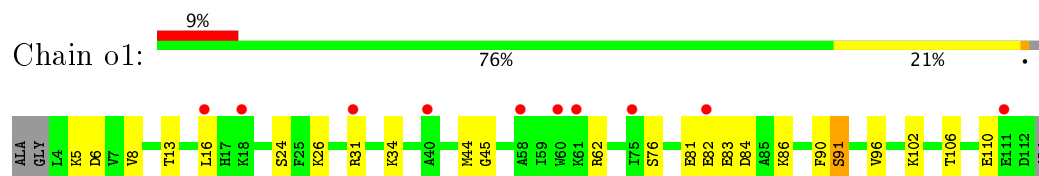
- Molecule 66: 60S ribosomal protein L30



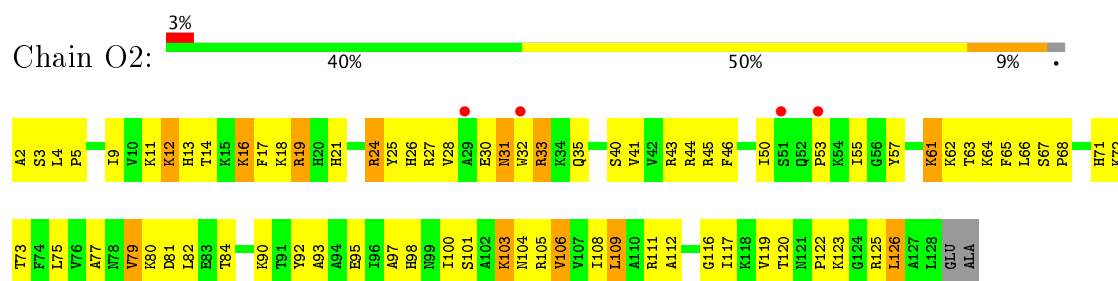
- Molecule 67: 60S ribosomal protein L31-A



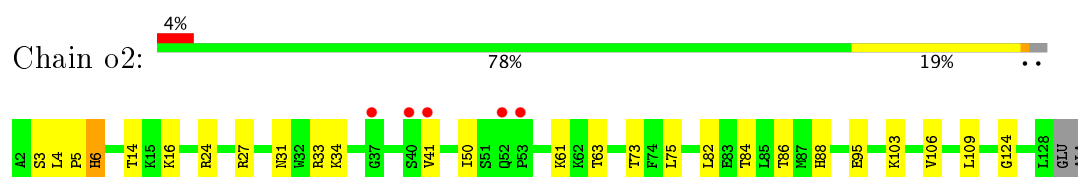
- Molecule 67: 60S ribosomal protein L31-A



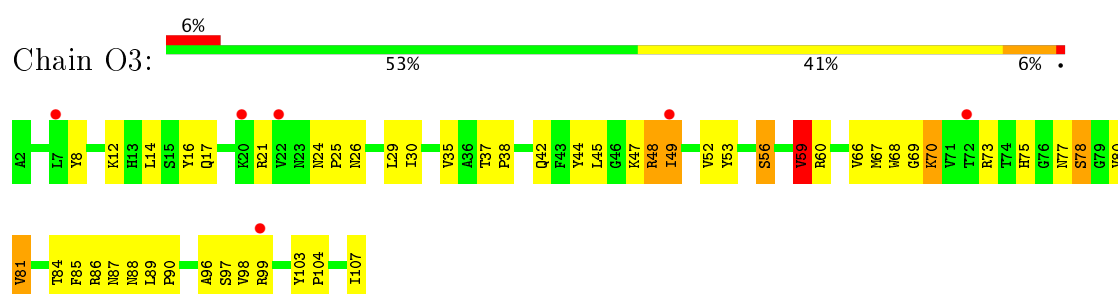
- Molecule 68: 60S ribosomal protein L32



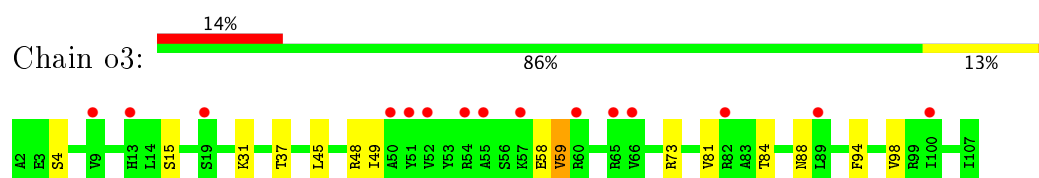
• Molecule 68: 60S ribosomal protein L32



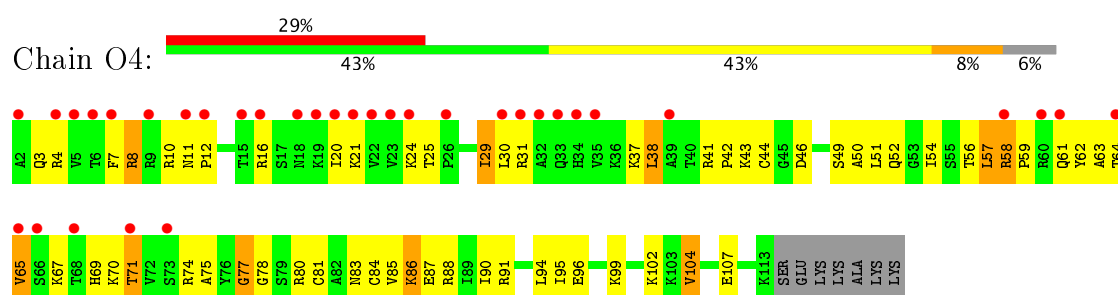
• Molecule 69: 60S ribosomal protein L33-A



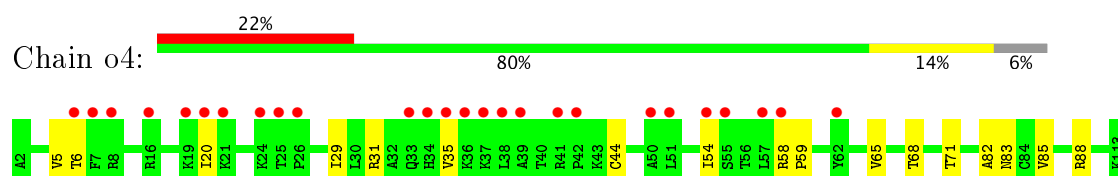
• Molecule 69: 60S ribosomal protein L33-A



• Molecule 70: 60S ribosomal protein L34-A

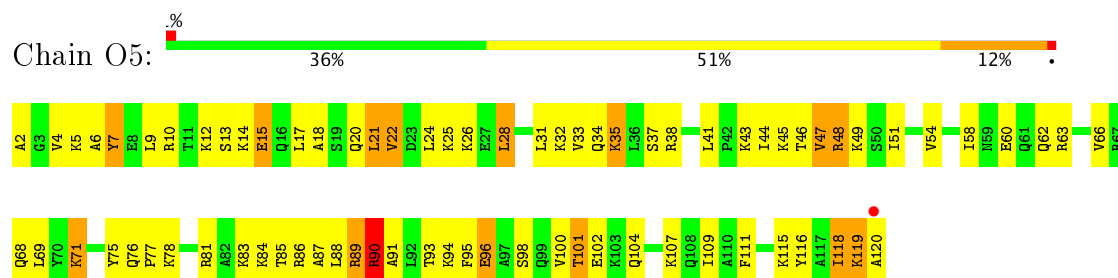


• Molecule 70: 60S ribosomal protein L34-A

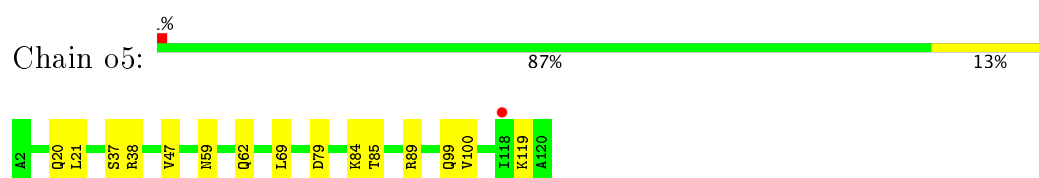


SER  
GLU  
LYS  
LYS  
LYS  
ALA  
LYS  
LYS

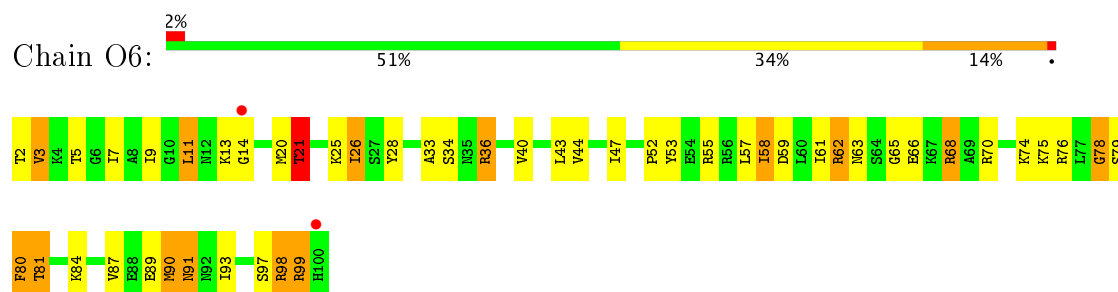
- Molecule 71: 60S ribosomal protein L35-A



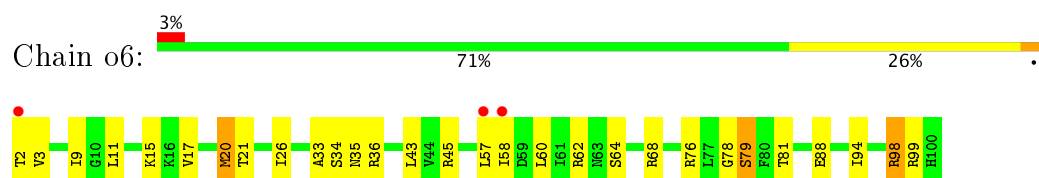
- Molecule 71: 60S ribosomal protein L35-A



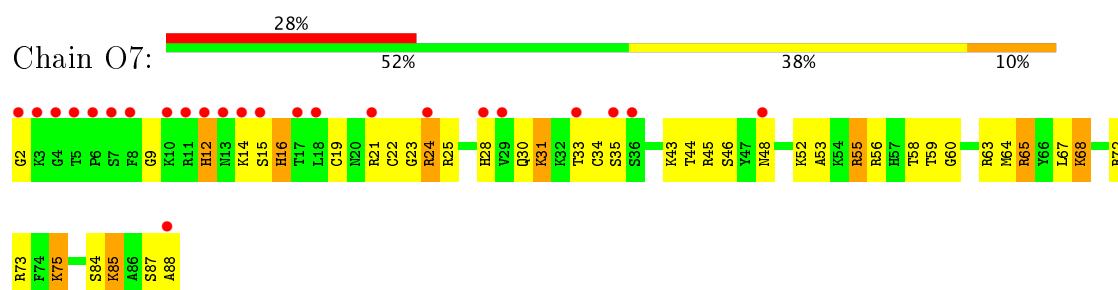
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 72: 60S ribosomal protein L36-A

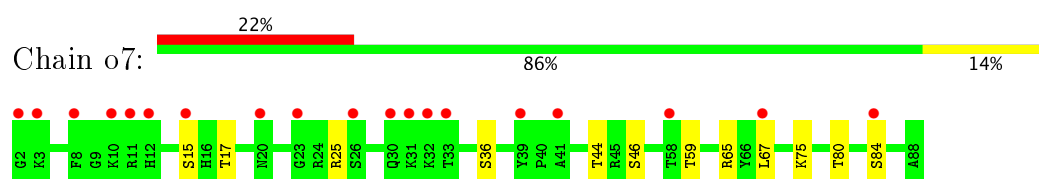


- Molecule 73: 60S ribosomal protein L37-A

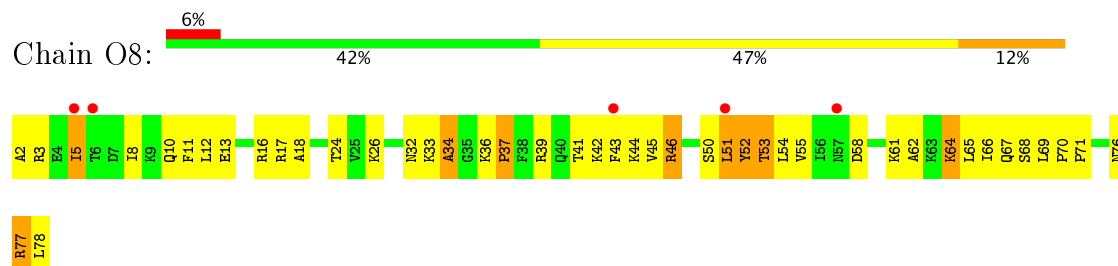


- Molecule 73: 60S ribosomal protein L37-A

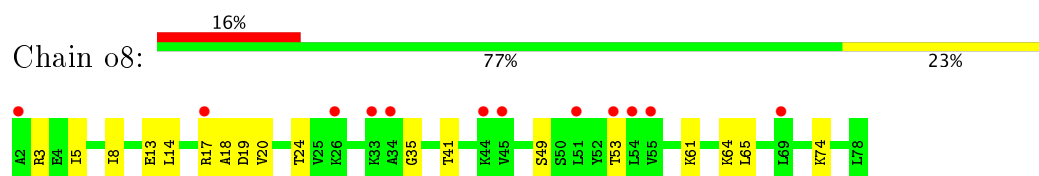




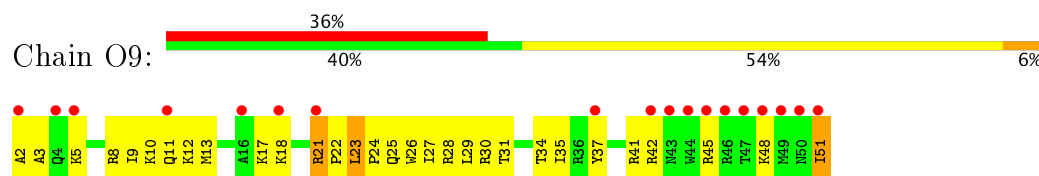
- Molecule 74: 60S ribosomal protein L38



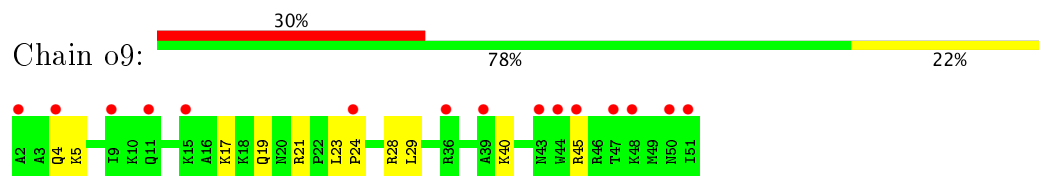
- Molecule 74: 60S ribosomal protein L38



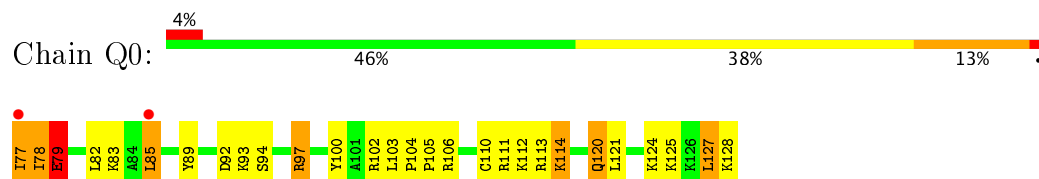
- Molecule 75: 60S ribosomal protein L39



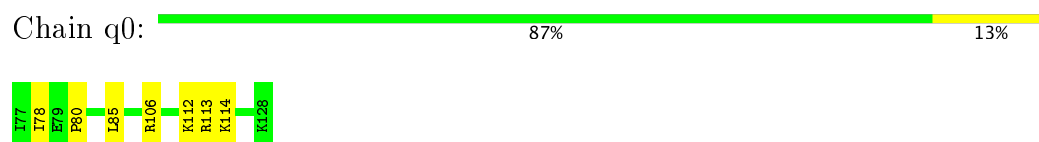
- Molecule 75: 60S ribosomal protein L39



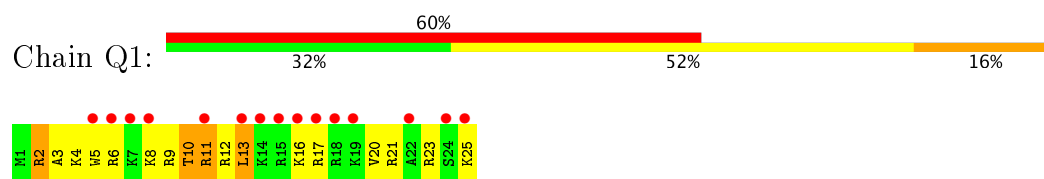
- Molecule 76: Ubiquitin-60S ribosomal protein L40



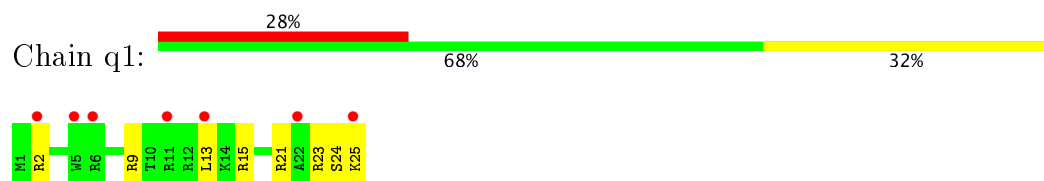
- Molecule 76: Ubiquitin-60S ribosomal protein L40



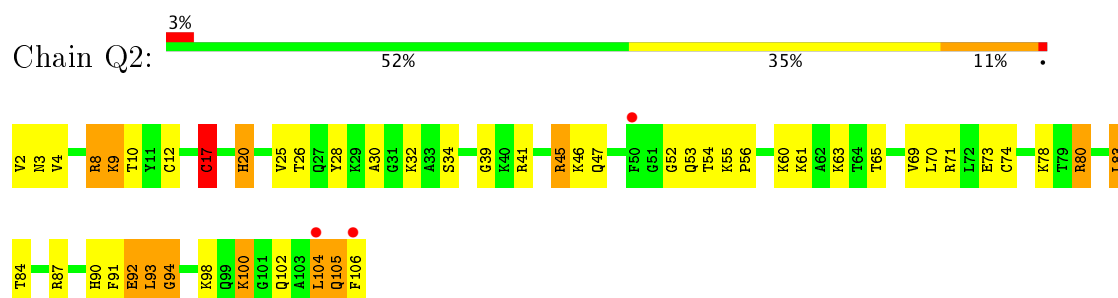
- Molecule 77: 60S ribosomal protein L41-A



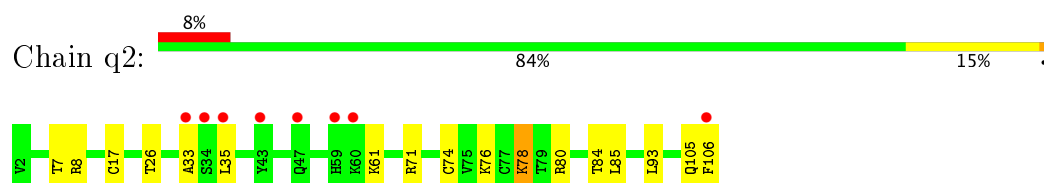
- Molecule 77: 60S ribosomal protein L41-A



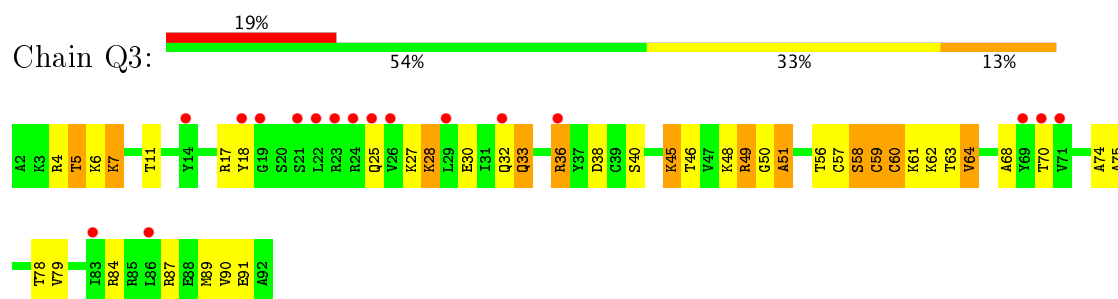
- Molecule 78: 60S ribosomal protein L42-A



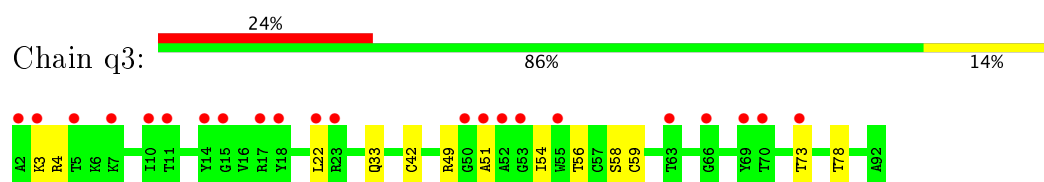
- Molecule 78: 60S ribosomal protein L42-A



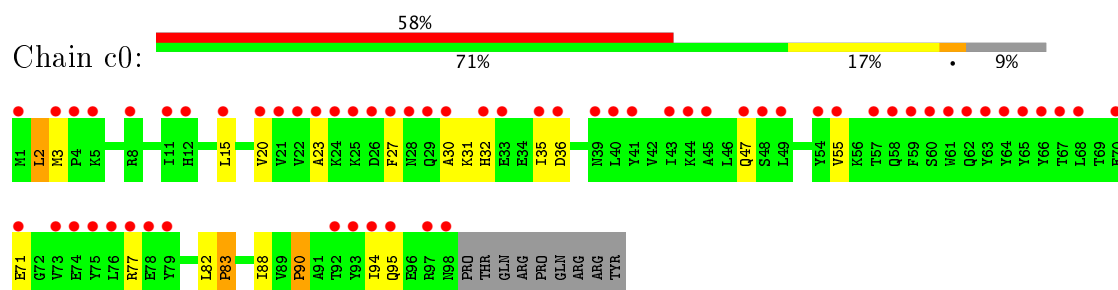
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S10-A

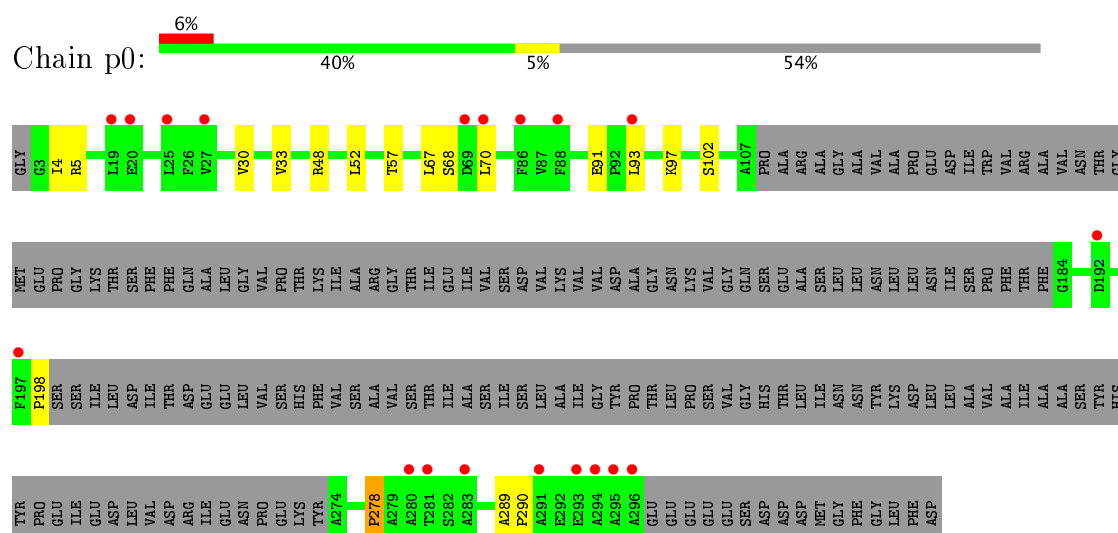


- Molecule 81: 60S ribosomal protein L12-A (uL11)



There are no outlier residues recorded for this chain.

- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: 60S ribosomal protein P1 alpha



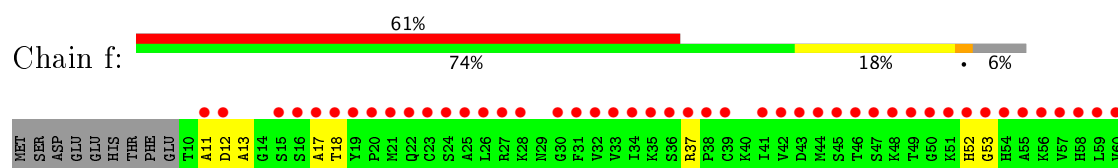
There are no outlier residues recorded for this chain.

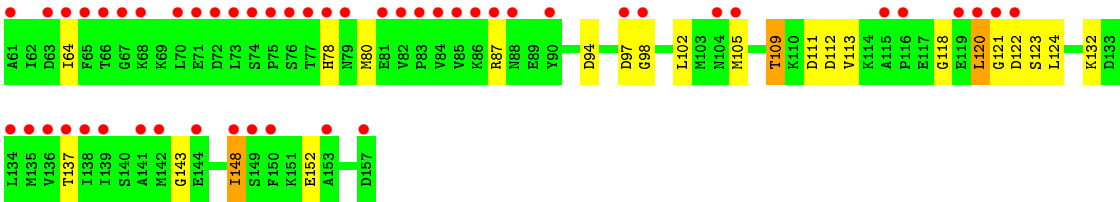
- Molecule 84: 60S ribosomal P2 beta



There are no outlier residues recorded for this chain.

- Molecule 85: Eukaryotic translation initiation factor 5A-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	438.23 Å   289.33 Å   305.47 Å 90.00°   98.95°   90.00°	Depositor
Resolution (Å)	190.48 – 3.25 196.56 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (190.48-3.25) 99.9 (196.56-3.25)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.26 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.252 ,   0.301 0.260 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	86.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 78.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	404042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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

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	0.37	0/42467	0.89	53/66169 (0.1%)
1	6	0.43	0/42790	0.93	47/66673 (0.1%)
2	S0	0.28	0/1617	0.51	0/2215
2	s0	0.30	0/1623	0.52	0/2222
3	S1	0.27	0/1735	0.53	0/2335
3	s1	0.29	0/1748	0.52	0/2352
4	S2	0.30	0/1665	0.52	0/2263
4	s2	0.33	0/1665	0.57	1/2263 (0.0%)
5	S3	0.31	0/1759	0.49	0/2368
5	s3	0.29	0/1759	0.47	0/2368
6	S4	0.29	0/2109	0.53	0/2839
6	s4	0.34	0/2109	0.57	1/2839 (0.0%)
7	S5	0.27	0/1629	0.49	0/2202
7	s5	0.28	0/1629	0.50	0/2202
8	S6	0.29	0/1823	0.48	0/2439
8	s6	0.33	0/1779	0.52	0/2379
9	S7	0.29	0/1506	0.54	0/2028
9	s7	0.29	0/1516	0.53	1/2043 (0.0%)
10	S8	0.32	0/1514	0.51	0/2021
10	s8	0.35	0/1514	0.51	0/2021
11	S9	0.29	0/1519	0.49	0/2035
11	s9	0.31	0/1519	0.51	0/2035
12	C0	0.29	0/789	0.48	1/1067 (0.1%)
13	C1	0.32	0/1239	0.51	0/1673
13	c1	0.36	0/1194	0.52	0/1610
14	C2	0.28	0/898	0.52	1/1220 (0.1%)
14	c2	0.24	0/898	0.49	0/1220
15	C3	0.31	0/1215	0.51	1/1638 (0.1%)
15	c3	0.33	0/1215	0.53	0/1638
16	C4	0.28	0/901	0.54	0/1217
16	c4	0.30	0/960	0.55	0/1290
17	C5	0.31	0/998	0.55	1/1341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	c5	0.31	0/1060	0.50	0/1426
18	C6	0.29	0/1125	0.56	2/1510 (0.1%)
18	c6	0.29	0/1131	0.51	0/1518
19	C7	0.31	0/935	0.54	0/1254
19	c7	0.29	0/914	0.52	0/1224
20	C8	0.30	0/1211	0.52	0/1628
20	c8	0.29	0/1211	0.51	0/1628
21	C9	0.28	0/1130	0.48	0/1517
21	c9	0.29	0/1130	0.47	0/1517
22	D0	0.30	0/865	0.55	0/1169
22	d0	0.28	0/892	0.52	0/1205
23	D1	0.28	0/693	0.51	0/935
23	d1	0.30	0/693	0.49	0/935
24	D2	0.31	0/1038	0.58	3/1395 (0.2%)
24	d2	0.34	0/1038	0.56	0/1395
25	D3	0.34	0/1139	0.54	0/1518
25	d3	0.38	0/1139	0.59	0/1518
26	D4	0.29	0/1087	0.46	0/1449
26	d4	0.31	0/1087	0.52	0/1449
27	D5	0.28	0/571	0.57	0/768
27	d5	0.27	0/566	0.47	0/761
28	D6	0.30	0/782	0.53	0/1047
28	d6	0.35	0/782	0.52	0/1047
29	D7	0.28	0/620	0.51	0/838
29	d7	0.28	0/620	0.50	0/838
30	D8	0.28	0/499	0.48	0/670
30	d8	0.28	0/499	0.54	0/670
31	D9	0.30	0/452	0.53	1/600 (0.2%)
31	d9	0.32	0/452	0.51	0/600
32	E0	0.28	0/483	0.47	0/643
32	e0	0.32	0/499	0.54	0/665
33	E1	0.30	0/577	0.60	0/770
33	e1	0.30	0/619	0.64	0/822
34	SR	0.26	0/2490	0.49	0/3389
34	sR	0.26	0/2495	0.45	0/3395
35	SM	0.32	0/1113	0.55	2/1502 (0.1%)
35	sM	0.32	0/682	0.50	0/921
36	1	0.55	0/75394	1.02	101/117545 (0.1%)
36	5	0.58	2/75865 (0.0%)	1.04	122/118275 (0.1%)
37	3	0.47	0/2883	0.88	0/4491
37	7	0.55	0/2883	1.03	4/4491 (0.1%)
38	4	0.51	0/3746	0.99	5/5832 (0.1%)
38	8	0.50	0/3746	0.95	4/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.37	0/1948	0.58	0/2617
39	l2	0.39	0/1946	0.60	0/2614
40	L3	0.39	0/3146	0.57	0/4228
40	l3	0.43	0/3146	0.58	0/4228
41	L4	0.41	0/2800	0.60	0/3790
41	l4	0.40	1/2800 (0.0%)	0.62	1/3790 (0.0%)
42	L5	0.34	0/2425	0.53	0/3271
42	l5	0.40	0/2408	0.56	0/3248
43	L6	0.38	0/1260	0.56	0/1694
43	l6	0.41	0/1269	0.58	0/1705
44	L7	0.42	0/1821	0.59	0/2451
44	l7	0.44	0/1828	0.63	2/2461 (0.1%)
45	L8	0.31	0/1836	0.52	1/2481 (0.0%)
45	l8	0.33	0/1795	0.52	0/2429
46	L9	0.37	0/1539	0.55	0/2073
46	l9	0.40	0/1539	0.56	0/2073
47	M0	0.41	0/1741	0.55	0/2335
47	m0	0.43	0/1758	0.61	0/2358
48	M1	0.31	0/1374	0.50	0/1842
48	m1	0.34	0/1374	0.56	0/1842
49	M3	0.40	0/1568	0.59	0/2106
49	m3	0.40	0/1573	0.57	0/2113
50	M4	0.40	0/1068	0.54	0/1438
50	m4	0.41	0/1074	0.57	0/1446
51	M5	0.38	0/1757	0.57	0/2354
51	m5	0.37	0/1757	0.56	0/2354
52	M6	0.43	0/1585	0.58	0/2128
52	m6	0.50	0/1585	0.61	0/2128
53	M7	0.42	0/1443	0.55	0/1944
53	m7	0.44	0/1250	0.61	0/1683
54	M8	0.39	0/1465	0.60	0/1965
54	m8	0.40	0/1465	0.62	0/1965
55	M9	0.30	0/1538	0.48	0/2050
55	m9	0.34	0/1538	0.51	0/2050
56	N0	0.39	0/1481	0.59	0/1990
56	n0	0.43	0/1481	0.57	0/1990
57	N1	0.41	0/1300	0.56	0/1743
57	n1	0.44	0/1300	0.55	0/1743
58	N2	0.29	0/812	0.48	0/1099
58	n2	0.32	0/794	0.54	0/1076
59	N3	0.38	0/1018	0.56	0/1369
59	n3	0.45	0/1018	0.64	0/1369
60	N4	0.31	0/712	0.47	0/958



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.36	0/1052	0.53	0/1398
61	N5	0.34	0/979	0.57	1/1321 (0.1%)
61	n5	0.34	0/974	0.56	0/1314
62	N6	0.37	0/1004	0.63	2/1341 (0.1%)
62	n6	0.34	0/1004	0.56	0/1341
63	N7	0.31	0/1118	0.51	0/1497
63	n7	0.31	0/1118	0.51	0/1497
64	N8	0.41	0/1204	0.64	0/1612
64	n8	0.42	0/1204	0.63	0/1612
65	N9	0.38	0/473	0.57	0/629
65	n9	0.45	0/473	0.71	1/629 (0.2%)
66	O0	0.30	0/751	0.46	0/1008
66	o0	0.32	0/775	0.51	0/1040
67	O1	0.36	0/890	0.53	0/1196
67	o1	0.43	0/897	0.59	0/1205
68	O2	0.42	0/1041	0.61	0/1394
68	o2	0.42	0/1041	0.59	0/1394
69	O3	0.44	0/868	0.52	0/1168
69	o3	0.47	0/868	0.58	0/1168
70	O4	0.33	0/890	0.53	1/1189 (0.1%)
70	o4	0.35	0/890	0.56	0/1189
71	O5	0.38	0/978	0.56	0/1301
71	o5	0.33	0/974	0.53	0/1297
72	O6	0.35	0/778	0.57	0/1034
72	o6	0.34	0/777	0.53	0/1033
73	O7	0.41	0/696	0.62	0/923
73	o7	0.39	0/696	0.61	0/923
74	O8	0.31	0/618	0.51	0/826
74	o8	0.32	0/614	0.51	0/822
75	O9	0.38	0/443	0.60	0/588
75	o9	0.37	0/443	0.56	0/588
76	Q0	0.44	0/423	0.60	0/562
76	q0	0.46	0/423	0.62	0/562
77	Q1	0.35	0/234	0.61	0/300
77	q1	0.43	0/234	0.58	0/300
78	Q2	0.51	1/860 (0.1%)	0.64	0/1136
78	q2	0.52	1/860 (0.1%)	0.64	1/1136 (0.1%)
79	Q3	0.38	0/701	0.58	0/934
79	q3	0.42	0/701	0.60	0/934
80	c0	0.28	0/777	0.53	2/1049 (0.2%)
82	p0	0.27	0/1091	0.53	2/1472 (0.1%)
85	f	0.31	0/1131	0.59	1/1522 (0.1%)
All	All	0.45	5/432438 (0.0%)	0.84	366/634802 (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
7	s5	0	1
18	c6	0	2
19	C7	0	1
27	D5	0	1
52	M6	0	1
52	m6	0	1
56	n0	0	1
64	n8	0	2
65	N9	0	1
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	8.72	1.97	1.82
78	Q2	17	CYS	CB-SG	8.11	1.96	1.82
36	5	1152	G	N9-C4	-7.24	1.32	1.38
36	5	2971	A	N9-C4	6.37	1.41	1.37
41	l4	94	CYS	CB-SG	-5.72	1.72	1.81

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	13.24	135.22	128.60
36	5	1152	G	N3-C4-N9	-12.64	118.41	126.00
36	5	1152	G	C2-N3-C4	-10.83	106.48	111.90
36	5	2726	C	C6-N1-C2	-9.83	116.37	120.30
36	1	3217	C	N1-C2-O2	8.77	124.16	118.90

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide
7	s5	99	MET	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	684	1
1	6	38260	0	19252	678	0
2	S0	1577	0	1567	133	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	131	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	111	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1816	104	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	134	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	113	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	107	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	93	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	107	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	115	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	47	0
13	C1	1213	0	1257	73	0
13	c1	1168	0	1233	0	0
14	C2	890	0	887	57	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	82	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	72	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	82	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	78	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	80	0
19	c7	906	0	909	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C8	1192	0	1222	91	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	78	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	75	0
22	d0	882	0	939	0	0
23	D1	684	0	672	61	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	80	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	81	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	75	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	50	0
27	d5	558	0	598	0	0
28	D6	769	0	814	78	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	28	0
30	d8	497	0	535	0	0
31	D9	442	0	428	28	0
31	d9	442	0	428	0	0
32	E0	475	0	525	30	0
32	e0	491	0	542	0	0
33	E1	566	0	602	56	0
33	e1	608	0	655	0	0
34	SR	2437	0	2386	135	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	1002	74	0
35	sM	679	0	615	0	0
36	1	67355	0	33848	1047	0
36	5	67780	0	34065	1002	0
37	3	2579	0	1304	45	0
37	7	2579	0	1304	36	0
38	4	3353	0	1695	61	1
38	8	3353	0	1695	61	0
39	L2	1914	0	1981	138	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	185	0
40	l3	3075	0	3142	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	L4	2748	0	2859	198	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	165	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	74	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	122	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	93	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	112	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	151	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	81	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	111	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	121	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	96	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	79	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	94	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	92	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	76	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	81	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	34	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	64	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	34	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	69	0
61	n5	959	0	1023	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	N6	993	0	1081	61	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	87	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	99	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	38	0
65	n9	462	0	491	0	0
66	O0	743	0	797	46	0
66	o0	767	0	816	0	0
67	O1	876	0	912	46	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	74	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	47	0
69	o3	850	0	880	0	0
70	O4	880	0	945	55	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	92	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	48	0
72	o6	770	0	846	0	0
73	O7	681	0	683	43	0
73	o7	681	0	683	0	0
74	O8	612	0	682	37	0
74	o8	608	0	671	0	0
75	O9	436	0	475	27	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	29	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	17	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	43	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	33	0
79	q3	694	0	734	0	0
80	c0	762	0	700	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	f	1116	0	1108	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	404042	0	298994	8045	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 12.

The worst 5 of 8045 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)
47:M0:174:THR:HG23	47:M0:176:LEU:H	1.29	0.96
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.49	0.95
5:S3:125:TYR:OH	35:SM:134:ASP:OD2	1.87	0.93
79:Q3:57:CYS:SG	79:Q3:60:CYS:HB3	2.10	0.92
50:M4:55:ARG:NH2	50:M4:76:ALA:O	2.18	0.92

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)
1:2:236:A:O2'	38:4:158:U:O2'[2_556]	2.19	0.01

## 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%)	156 (76%)	30 (15%)	18 (9%)	1	5
2	s0	204/251 (81%)	158 (78%)	31 (15%)	15 (7%)	1	9
3	S1	212/254 (84%)	154 (73%)	36 (17%)	22 (10%)	0	3
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	2	16
4	S2	215/253 (85%)	174 (81%)	33 (15%)	8 (4%)	4	26
4	s2	215/253 (85%)	175 (81%)	26 (12%)	14 (6%)	1	12
5	S3	221/239 (92%)	189 (86%)	21 (10%)	11 (5%)	2	18
5	s3	221/239 (92%)	183 (83%)	27 (12%)	11 (5%)	2	18
6	S4	258/260 (99%)	205 (80%)	37 (14%)	16 (6%)	2	13
6	s4	258/260 (99%)	198 (77%)	44 (17%)	16 (6%)	2	13
7	S5	204/224 (91%)	163 (80%)	28 (14%)	13 (6%)	1	12
7	s5	204/224 (91%)	157 (77%)	30 (15%)	17 (8%)	1	6
8	S6	224/236 (95%)	198 (88%)	17 (8%)	9 (4%)	3	24
8	s6	216/236 (92%)	186 (86%)	24 (11%)	6 (3%)	6	34
9	S7	182/189 (96%)	137 (75%)	27 (15%)	18 (10%)	1	4
9	s7	184/189 (97%)	146 (79%)	25 (14%)	13 (7%)	1	9
10	S8	184/200 (92%)	159 (86%)	18 (10%)	7 (4%)	4	25
10	s8	184/200 (92%)	156 (85%)	21 (11%)	7 (4%)	4	25
11	S9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	4	25
11	s9	183/196 (93%)	151 (82%)	24 (13%)	8 (4%)	3	21
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	9
13	C1	153/155 (99%)	123 (80%)	23 (15%)	7 (5%)	3	20
13	c1	144/155 (93%)	122 (85%)	20 (14%)	2 (1%)	13	50
14	C2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	1
14	c2	122/142 (86%)	76 (62%)	30 (25%)	16 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	23
15	c3	148/150 (99%)	117 (79%)	21 (14%)	10 (7%)	1	10
16	C4	125/136 (92%)	92 (74%)	21 (17%)	12 (10%)	1	4
16	c4	126/136 (93%)	98 (78%)	19 (15%)	9 (7%)	1	9
17	C5	122/141 (86%)	90 (74%)	17 (14%)	15 (12%)	0	2
17	c5	133/141 (94%)	98 (74%)	19 (14%)	16 (12%)	0	2
18	C6	139/142 (98%)	111 (80%)	19 (14%)	9 (6%)	1	12
18	c6	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	22
19	C7	116/136 (85%)	89 (77%)	20 (17%)	7 (6%)	2	14
19	c7	113/136 (83%)	89 (79%)	16 (14%)	8 (7%)	1	9
20	C8	143/145 (99%)	109 (76%)	27 (19%)	7 (5%)	2	19
20	c8	143/145 (99%)	116 (81%)	21 (15%)	6 (4%)	3	23
21	C9	141/143 (99%)	115 (82%)	19 (14%)	7 (5%)	2	18
21	c9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	4	28
22	D0	105/120 (88%)	90 (86%)	9 (9%)	6 (6%)	2	15
22	d0	108/120 (90%)	87 (81%)	18 (17%)	3 (3%)	6	34
23	D1	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	1	7
23	d1	85/87 (98%)	71 (84%)	8 (9%)	6 (7%)	1	9
24	D2	127/129 (98%)	111 (87%)	12 (9%)	4 (3%)	5	31
24	d2	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	7	37
25	D3	142/144 (99%)	109 (77%)	20 (14%)	13 (9%)	1	5
25	d3	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	8	41
26	D4	132/134 (98%)	114 (86%)	8 (6%)	10 (8%)	1	8
26	d4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	2	14
27	D5	68/107 (64%)	47 (69%)	15 (22%)	6 (9%)	1	5
27	d5	67/107 (63%)	52 (78%)	14 (21%)	1 (2%)	12	49
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	70 (74%)	20 (21%)	5 (5%)	2	17
29	D7	79/81 (98%)	58 (73%)	18 (23%)	3 (4%)	4	25
29	d7	79/81 (98%)	62 (78%)	15 (19%)	2 (2%)	6	36
30	D8	61/66 (92%)	53 (87%)	6 (10%)	2 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	d8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	11
31	D9	51/55 (93%)	42 (82%)	6 (12%)	3 (6%)	2	14
31	d9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	14
32	E0	58/62 (94%)	48 (83%)	7 (12%)	3 (5%)	2	17
32	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	1	4
33	E1	69/76 (91%)	39 (56%)	12 (17%)	18 (26%)	0	0
33	e1	74/76 (97%)	38 (51%)	12 (16%)	24 (32%)	0	0
34	SR	316/318 (99%)	266 (84%)	34 (11%)	16 (5%)	2	18
34	sR	316/318 (99%)	264 (84%)	39 (12%)	13 (4%)	3	23
35	SM	155/273 (57%)	114 (74%)	22 (14%)	19 (12%)	0	2
35	sM	98/273 (36%)	59 (60%)	28 (29%)	11 (11%)	0	3
39	L2	250/253 (99%)	216 (86%)	25 (10%)	9 (4%)	4	27
39	l2	250/253 (99%)	208 (83%)	32 (13%)	10 (4%)	3	24
40	L3	384/386 (100%)	332 (86%)	39 (10%)	13 (3%)	4	28
40	l3	384/386 (100%)	341 (89%)	38 (10%)	5 (1%)	14	52
41	L4	359/361 (99%)	296 (82%)	38 (11%)	25 (7%)	1	9
41	l4	359/361 (99%)	295 (82%)	42 (12%)	22 (6%)	2	14
42	L5	294/296 (99%)	231 (79%)	38 (13%)	25 (8%)	1	6
42	l5	292/296 (99%)	253 (87%)	31 (11%)	8 (3%)	6	34
43	L6	152/175 (87%)	135 (89%)	13 (9%)	4 (3%)	6	35
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	6	35
44	L7	220/243 (90%)	190 (86%)	24 (11%)	6 (3%)	6	34
44	l7	221/243 (91%)	199 (90%)	17 (8%)	5 (2%)	7	38
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	2	19
45	l8	229/255 (90%)	178 (78%)	37 (16%)	14 (6%)	2	14
46	L9	189/191 (99%)	161 (85%)	20 (11%)	8 (4%)	3	23
46	l9	189/191 (99%)	170 (90%)	16 (8%)	3 (2%)	11	47
47	M0	207/220 (94%)	169 (82%)	32 (16%)	6 (3%)	5	33
47	m0	209/220 (95%)	161 (77%)	35 (17%)	13 (6%)	2	13
48	M1	167/173 (96%)	130 (78%)	25 (15%)	12 (7%)	1	9
48	m1	167/173 (96%)	139 (83%)	18 (11%)	10 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	149 (78%)	34 (18%)	8 (4%)	3	23
49	m3	192/198 (97%)	148 (77%)	30 (16%)	14 (7%)	1	9
50	M4	134/137 (98%)	116 (87%)	14 (10%)	4 (3%)	5	32
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	12	49
51	M5	201/203 (99%)	178 (89%)	16 (8%)	7 (4%)	4	28
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	6	36
52	M6	195/198 (98%)	171 (88%)	17 (9%)	7 (4%)	4	27
52	m6	195/198 (98%)	173 (89%)	18 (9%)	4 (2%)	8	41
53	M7	181/183 (99%)	149 (82%)	26 (14%)	6 (3%)	4	29
53	m7	153/183 (84%)	140 (92%)	11 (7%)	2 (1%)	14	52
54	M8	183/185 (99%)	157 (86%)	22 (12%)	4 (2%)	8	39
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	4	29
55	M9	186/188 (99%)	164 (88%)	19 (10%)	3 (2%)	11	47
55	m9	186/188 (99%)	166 (89%)	20 (11%)	0	100	100
56	N0	170/172 (99%)	150 (88%)	13 (8%)	7 (4%)	3	23
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	28	68
57	N1	157/159 (99%)	135 (86%)	16 (10%)	6 (4%)	4	25
57	n1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	5	30
58	N2	98/120 (82%)	73 (74%)	21 (21%)	4 (4%)	3	23
58	n2	96/120 (80%)	84 (88%)	8 (8%)	4 (4%)	3	23
59	N3	134/136 (98%)	117 (87%)	11 (8%)	6 (4%)	3	21
59	n3	134/136 (98%)	121 (90%)	7 (5%)	6 (4%)	3	21
60	N4	96/155 (62%)	76 (79%)	15 (16%)	5 (5%)	2	17
60	n4	133/155 (86%)	109 (82%)	16 (12%)	8 (6%)	2	14
61	N5	119/141 (84%)	101 (85%)	16 (13%)	2 (2%)	11	46
61	n5	118/141 (84%)	101 (86%)	13 (11%)	4 (3%)	4	28
62	N6	124/126 (98%)	109 (88%)	13 (10%)	2 (2%)	11	47
62	n6	124/126 (98%)	104 (84%)	16 (13%)	4 (3%)	5	30
63	N7	133/135 (98%)	106 (80%)	16 (12%)	11 (8%)	1	6
63	n7	133/135 (98%)	111 (84%)	15 (11%)	7 (5%)	2	17
64	N8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	3	23
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	4	27
65	n9	56/58 (97%)	40 (71%)	10 (18%)	6 (11%)	0	3
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	85 (87%)	9 (9%)	4 (4%)	3	23
67	O1	107/112 (96%)	92 (86%)	9 (8%)	6 (6%)	2	16
67	o1	107/112 (96%)	91 (85%)	9 (8%)	7 (6%)	1	12
68	O2	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	22	62
68	o2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	7	37
69	O3	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	18	58
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	5	33
70	O4	110/119 (92%)	94 (86%)	15 (14%)	1 (1%)	20	60
70	o4	110/119 (92%)	93 (84%)	15 (14%)	2 (2%)	10	45
71	O5	117/119 (98%)	97 (83%)	14 (12%)	6 (5%)	2	18
71	o5	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11	46
72	O6	97/99 (98%)	78 (80%)	12 (12%)	7 (7%)	1	9
72	o6	97/99 (98%)	76 (78%)	13 (13%)	8 (8%)	1	7
73	O7	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	15	54
73	o7	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
74	O8	75/77 (97%)	63 (84%)	9 (12%)	3 (4%)	3	24
74	o8	75/77 (97%)	59 (79%)	10 (13%)	6 (8%)	1	7
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	8	41
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	23
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	14
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	24
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	1	10
78	q2	103/105 (98%)	88 (85%)	11 (11%)	4 (4%)	3	25
79	Q3	89/91 (98%)	77 (86%)	6 (7%)	6 (7%)	1	11
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	1
82	p0	139/311 (45%)	113 (81%)	20 (14%)	6 (4%)	3	22
85	f	146/157 (93%)	98 (67%)	30 (20%)	18 (12%)	0	2
All	All	22479/24300 (92%)	18504 (82%)	2828 (13%)	1147 (5%)	2	18

5 of 1147 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
2	S0	192	THR

### 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%)	138 (84%)	26 (16%)	3	14
2	s0	165/209 (79%)	142 (86%)	23 (14%)	4	19
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	12
3	s1	192/223 (86%)	157 (82%)	35 (18%)	2	10
4	S2	176/204 (86%)	148 (84%)	28 (16%)	3	14
4	s2	176/204 (86%)	141 (80%)	35 (20%)	1	7
5	S3	182/194 (94%)	153 (84%)	29 (16%)	3	14
5	s3	182/194 (94%)	150 (82%)	32 (18%)	2	10
6	S4	221/221 (100%)	188 (85%)	33 (15%)	3	16
6	s4	221/221 (100%)	192 (87%)	29 (13%)	5	22
7	S5	173/190 (91%)	154 (89%)	19 (11%)	7	30
7	s5	173/190 (91%)	150 (87%)	23 (13%)	4	21
8	S6	188/201 (94%)	160 (85%)	28 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	s6	187/201 (93%)	158 (84%)	29 (16%)	3	15
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2	12
9	s7	165/169 (98%)	146 (88%)	19 (12%)	6	28
10	S8	150/161 (93%)	132 (88%)	18 (12%)	6	26
10	s8	150/161 (93%)	132 (88%)	18 (12%)	6	26
11	S9	158/165 (96%)	133 (84%)	25 (16%)	3	14
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	9
12	C0	77/98 (79%)	66 (86%)	11 (14%)	4	18
13	C1	129/136 (95%)	120 (93%)	9 (7%)	18	53
13	c1	129/136 (95%)	113 (88%)	16 (12%)	5	24
14	C2	88/118 (75%)	76 (86%)	12 (14%)	4	20
14	c2	88/118 (75%)	76 (86%)	12 (14%)	4	20
15	C3	127/127 (100%)	107 (84%)	20 (16%)	3	14
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	16
16	C4	81/104 (78%)	62 (76%)	19 (24%)	1	4
16	c4	97/104 (93%)	84 (87%)	13 (13%)	4	21
17	C5	101/117 (86%)	83 (82%)	18 (18%)	2	10
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	11
18	C6	117/118 (99%)	101 (86%)	16 (14%)	4	20
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	9
19	C7	94/124 (76%)	76 (81%)	18 (19%)	2	8
19	c7	92/124 (74%)	80 (87%)	12 (13%)	5	22
20	C8	128/128 (100%)	105 (82%)	23 (18%)	2	10
20	c8	128/128 (100%)	104 (81%)	24 (19%)	2	9
21	C9	115/115 (100%)	99 (86%)	16 (14%)	4	19
21	c9	115/115 (100%)	105 (91%)	10 (9%)	12	42
22	D0	100/113 (88%)	88 (88%)	12 (12%)	6	26
22	d0	103/113 (91%)	87 (84%)	16 (16%)	3	15
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	10
23	d1	74/74 (100%)	63 (85%)	11 (15%)	3	16
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2	13
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	21
25	d3	119/119 (100%)	108 (91%)	11 (9%)	11	38
26	D4	112/112 (100%)	103 (92%)	9 (8%)	14	47
26	d4	112/112 (100%)	96 (86%)	16 (14%)	4	18
27	D5	61/88 (69%)	49 (80%)	12 (20%)	1	7
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	17
28	D6	83/83 (100%)	71 (86%)	12 (14%)	4	18
28	d6	83/83 (100%)	74 (89%)	9 (11%)	7	30
29	D7	70/70 (100%)	64 (91%)	6 (9%)	12	42
29	d7	70/70 (100%)	59 (84%)	11 (16%)	3	14
30	D8	56/59 (95%)	47 (84%)	9 (16%)	3	13
30	d8	56/59 (95%)	45 (80%)	11 (20%)	1	8
31	D9	47/48 (98%)	36 (77%)	11 (23%)	1	4
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	6
32	E0	51/53 (96%)	43 (84%)	8 (16%)	3	14
32	e0	53/53 (100%)	41 (77%)	12 (23%)	1	4
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	2
33	e1	66/66 (100%)	54 (82%)	12 (18%)	2	10
34	SR	259/261 (99%)	230 (89%)	29 (11%)	7	29
34	sR	260/261 (100%)	236 (91%)	24 (9%)	11	38
35	SM	97/228 (42%)	82 (84%)	15 (16%)	3	15
35	sM	54/228 (24%)	46 (85%)	8 (15%)	3	17
39	L2	193/195 (99%)	158 (82%)	35 (18%)	2	10
39	l2	192/195 (98%)	156 (81%)	36 (19%)	2	9
40	L3	320/322 (99%)	274 (86%)	46 (14%)	4	18
40	l3	319/322 (99%)	264 (83%)	55 (17%)	2	11
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	13
41	l4	288/288 (100%)	247 (86%)	41 (14%)	4	18
42	L5	244/244 (100%)	203 (83%)	41 (17%)	2	12
42	l5	243/244 (100%)	201 (83%)	42 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	16
43	l6	135/152 (89%)	115 (85%)	20 (15%)	3	17
44	L7	186/204 (91%)	164 (88%)	22 (12%)	6	27
44	l7	187/204 (92%)	164 (88%)	23 (12%)	5	25
45	L8	187/207 (90%)	160 (86%)	27 (14%)	4	18
45	l8	177/207 (86%)	154 (87%)	23 (13%)	5	22
46	L9	171/171 (100%)	151 (88%)	20 (12%)	6	27
46	l9	171/171 (100%)	142 (83%)	29 (17%)	2	12
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1	7
47	m0	179/186 (96%)	143 (80%)	36 (20%)	1	7
48	M1	147/150 (98%)	124 (84%)	23 (16%)	3	14
48	m1	147/150 (98%)	120 (82%)	27 (18%)	2	9
49	M3	154/158 (98%)	138 (90%)	16 (10%)	8	32
49	m3	154/158 (98%)	132 (86%)	22 (14%)	4	18
50	M4	107/108 (99%)	92 (86%)	15 (14%)	4	19
50	m4	108/108 (100%)	94 (87%)	14 (13%)	5	22
51	M5	175/175 (100%)	153 (87%)	22 (13%)	5	24
51	m5	175/175 (100%)	152 (87%)	23 (13%)	5	22
52	M6	160/161 (99%)	136 (85%)	24 (15%)	3	16
52	m6	160/161 (99%)	134 (84%)	26 (16%)	3	13
53	M7	140/145 (97%)	123 (88%)	17 (12%)	6	25
53	m7	125/145 (86%)	107 (86%)	18 (14%)	4	18
54	M8	150/150 (100%)	136 (91%)	14 (9%)	10	37
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	7
55	M9	153/153 (100%)	132 (86%)	21 (14%)	4	20
55	m9	153/153 (100%)	129 (84%)	24 (16%)	3	14
56	N0	156/156 (100%)	134 (86%)	22 (14%)	4	19
56	n0	156/156 (100%)	135 (86%)	21 (14%)	4	20
57	N1	136/136 (100%)	107 (79%)	29 (21%)	1	6
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	12
58	N2	87/106 (82%)	79 (91%)	8 (9%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	15
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	20
59	n3	104/104 (100%)	89 (86%)	15 (14%)	4	18
60	N4	57/129 (44%)	50 (88%)	7 (12%)	5	25
60	n4	100/129 (78%)	88 (88%)	12 (12%)	6	26
61	N5	104/117 (89%)	86 (83%)	18 (17%)	2	11
61	n5	104/117 (89%)	92 (88%)	12 (12%)	6	28
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	11
62	n6	109/109 (100%)	89 (82%)	20 (18%)	2	9
63	N7	115/115 (100%)	104 (90%)	11 (10%)	10	36
63	n7	115/115 (100%)	95 (83%)	20 (17%)	2	11
64	N8	118/118 (100%)	100 (85%)	18 (15%)	3	15
64	n8	118/118 (100%)	100 (85%)	18 (15%)	3	15
65	N9	46/46 (100%)	40 (87%)	6 (13%)	5	22
65	n9	46/46 (100%)	41 (89%)	5 (11%)	7	30
66	O0	81/87 (93%)	70 (86%)	11 (14%)	4	20
66	o0	84/87 (97%)	71 (84%)	13 (16%)	3	15
67	O1	92/96 (96%)	78 (85%)	14 (15%)	3	16
67	o1	94/96 (98%)	76 (81%)	18 (19%)	2	8
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	13
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	5
69	O3	90/90 (100%)	81 (90%)	9 (10%)	9	34
69	o3	90/90 (100%)	77 (86%)	13 (14%)	4	18
70	O4	95/101 (94%)	84 (88%)	11 (12%)	6	27
70	o4	95/101 (94%)	80 (84%)	15 (16%)	3	14
71	O5	104/104 (100%)	90 (86%)	14 (14%)	4	20
71	o5	103/104 (99%)	90 (87%)	13 (13%)	5	24
72	O6	81/81 (100%)	66 (82%)	15 (18%)	2	9
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	6
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	5
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%)	36 (80%)	9 (20%)	1	7
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	12
76	q0	47/47 (100%)	42 (89%)	5 (11%)	8	31
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	11
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	3	14
78	q2	90/90 (100%)	77 (86%)	13 (14%)	4	18
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	12
79	q3	71/71 (100%)	60 (84%)	11 (16%)	3	15
80	c0	73/98 (74%)	64 (88%)	9 (12%)	5	25
82	p0	105/253 (42%)	94 (90%)	11 (10%)	8	32
85	f	124/133 (93%)	108 (87%)	16 (13%)	5	22
All	All	18850/20374 (92%)	15999 (85%)	2851 (15%)	3	16

5 of 2851 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	102	GLU
9	s7	95	GLU
66	o0	18	ILE
74	O8	52	TYR
4	s2	87	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	144	ASN
3	s1	149	GLN
56	n0	8	GLN
51	M5	15	GLN
54	M8	135	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	454 (25%)	49 (2%)
1	6	1791/1800 (99%)	436 (24%)	35 (1%)
36	1	3145/3396 (92%)	652 (20%)	49 (1%)
36	5	3163/3396 (93%)	650 (20%)	49 (1%)
37	3	120/121 (99%)	11 (9%)	0
37	7	120/121 (99%)	16 (13%)	1 (0%)
38	4	157/158 (99%)	36 (22%)	1 (0%)
38	8	157/158 (99%)	33 (21%)	1 (0%)
All	All	10429/10950 (95%)	2288 (21%)	185 (1%)

5 of 2288 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	2541	U
1	6	158	U
36	5	2446	U
36	1	2593	A
36	1	3275	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
81	m2	2
80	c0	1
36	5	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	7.38
1	2	1716:C	O3'	1717:G	P	5.29
1	5	2437:G	O3'	2438:A	P	3.76
1	m2	52:UNK	C	54:UNK	N	3.58
1	m2	23:UNK	C	28:UNK	N	3.14

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.93	211 (11%) 5 3	60, 99, 172, 210	0
1	6	1795/1800 (99%)	0.61	94 (5%) 28 20	46, 86, 159, 201	0
2	S0	206/251 (82%)	2.50	120 (58%) 0 0	101, 114, 125, 133	0
2	s0	206/251 (82%)	1.65	78 (37%) 0 0	83, 99, 113, 119	0
3	S1	214/254 (84%)	0.78	33 (15%) 2 2	107, 142, 167, 173	0
3	s1	216/254 (85%)	0.83	30 (13%) 3 2	84, 98, 115, 123	0
4	S2	217/253 (85%)	1.54	63 (29%) 1 1	84, 97, 111, 115	0
4	s2	217/253 (85%)	1.42	57 (26%) 1 1	68, 81, 96, 103	0
5	S3	223/239 (93%)	1.73	88 (39%) 0 0	89, 100, 122, 129	0
5	s3	223/239 (93%)	2.19	112 (50%) 0 0	84, 111, 133, 137	0
6	S4	260/260 (100%)	1.35	74 (28%) 1 1	77, 102, 110, 125	0
6	s4	260/260 (100%)	0.69	23 (8%) 11 8	61, 83, 97, 119	0
7	S5	206/224 (91%)	1.02	40 (19%) 1 1	102, 123, 131, 134	0
7	s5	206/224 (91%)	1.25	53 (25%) 1 1	87, 108, 122, 128	0
8	S6	226/236 (95%)	1.15	58 (25%) 1 1	78, 110, 127, 139	0
8	s6	218/236 (92%)	0.77	25 (11%) 5 4	60, 89, 107, 116	0
9	S7	184/189 (97%)	0.93	38 (20%) 1 1	101, 123, 139, 142	0
9	s7	186/189 (98%)	0.79	26 (13%) 3 2	77, 105, 132, 137	0
10	S8	188/200 (94%)	1.50	55 (29%) 1 1	71, 89, 123, 135	0
10	s8	188/200 (94%)	1.08	35 (18%) 1 1	56, 75, 116, 133	0
11	S9	185/196 (94%)	1.33	49 (26%) 1 1	90, 107, 133, 150	0
11	s9	185/196 (94%)	0.82	17 (9%) 10 7	72, 90, 116, 130	0
12	C0	96/105 (91%)	1.39	27 (28%) 1 1	92, 113, 133, 141	0
13	C1	155/155 (100%)	2.03	71 (45%) 0 0	73, 85, 112, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	c1	146/155 (94%)	1.48	32 (21%)	1	1	59, 72, 97, 121	0
14	C2	124/142 (87%)	1.09	30 (24%)	1	1	138, 146, 152, 159	0
14	c2	124/142 (87%)	2.35	51 (41%)	0	0	169, 184, 194, 196	0
15	C3	150/150 (100%)	1.39	41 (27%)	1	1	81, 94, 113, 116	0
15	c3	150/150 (100%)	1.37	45 (30%)	1	1	67, 80, 97, 102	0
16	C4	127/136 (93%)	1.03	25 (19%)	1	1	84, 139, 155, 159	0
16	c4	128/136 (94%)	1.36	35 (27%)	1	1	66, 102, 112, 119	0
17	C5	124/141 (87%)	0.55	7 (5%)	25	18	88, 100, 112, 119	0
17	c5	135/141 (95%)	1.00	28 (20%)	1	1	78, 105, 114, 118	0
18	C6	141/142 (99%)	3.39	94 (66%)	0	0	92, 112, 117, 120	0
18	c6	142/142 (100%)	2.37	74 (52%)	0	0	80, 101, 116, 125	0
19	C7	120/136 (88%)	2.78	81 (67%)	0	0	99, 108, 126, 129	0
19	c7	117/136 (86%)	1.44	40 (34%)	0	0	87, 102, 115, 118	0
20	C8	145/145 (100%)	0.41	8 (5%)	26	19	86, 110, 131, 137	0
20	c8	145/145 (100%)	0.50	5 (3%)	46	36	88, 100, 118, 127	0
21	C9	143/143 (100%)	2.22	82 (57%)	0	0	95, 110, 121, 126	0
21	c9	143/143 (100%)	1.21	27 (18%)	1	1	84, 96, 112, 121	0
22	D0	107/120 (89%)	1.89	41 (38%)	0	0	85, 112, 128, 130	0
22	d0	110/120 (91%)	2.20	53 (48%)	0	0	84, 114, 139, 156	0
23	D1	87/87 (100%)	2.09	43 (49%)	0	0	100, 106, 118, 127	0
23	d1	87/87 (100%)	0.99	20 (22%)	1	1	80, 88, 108, 116	0
24	D2	129/129 (100%)	3.54	106 (82%)	0	0	83, 94, 103, 112	0
24	d2	129/129 (100%)	1.40	38 (29%)	1	1	65, 75, 82, 89	0
25	D3	144/144 (100%)	1.42	40 (27%)	1	1	71, 77, 86, 97	0
25	d3	144/144 (100%)	1.04	21 (14%)	3	2	58, 63, 74, 82	0
26	D4	134/134 (100%)	0.51	12 (8%)	10	8	88, 111, 122, 128	0
26	d4	134/134 (100%)	0.37	4 (2%)	51	41	68, 92, 105, 108	0
27	D5	70/107 (65%)	0.28	5 (7%)	17	13	119, 131, 137, 138	0
27	d5	69/107 (64%)	0.59	6 (8%)	11	8	97, 115, 125, 126	0
28	D6	97/97 (100%)	2.65	57 (58%)	0	0	88, 104, 150, 154	0
28	d6	97/97 (100%)	2.41	52 (53%)	0	0	71, 86, 115, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
29	D7	81/81 (100%)	1.64	35 (43%)	0	0	98, 110, 134, 137	0
29	d7	81/81 (100%)	1.88	32 (39%)	0	0	80, 94, 124, 130	0
30	D8	63/66 (95%)	1.23	16 (25%)	1	1	110, 125, 137, 139	0
30	d8	63/66 (95%)	1.61	21 (33%)	0	1	103, 116, 125, 130	0
31	D9	53/55 (96%)	1.52	15 (28%)	1	1	86, 90, 106, 111	0
31	d9	53/55 (96%)	2.69	35 (66%)	0	0	81, 92, 128, 141	0
32	E0	60/62 (96%)	2.14	24 (40%)	0	0	77, 108, 128, 130	0
32	e0	62/62 (100%)	1.00	13 (20%)	1	1	66, 91, 110, 113	0
33	E1	71/76 (93%)	0.87	12 (16%)	2	1	105, 134, 149, 153	0
33	e1	76/76 (100%)	1.55	23 (30%)	0	1	112, 161, 175, 179	0
34	SR	318/318 (100%)	1.65	110 (34%)	0	0	108, 119, 131, 147	0
34	sR	318/318 (100%)	2.41	159 (50%)	0	0	110, 127, 139, 150	0
35	SM	159/273 (58%)	1.25	45 (28%)	1	1	62, 98, 144, 148	0
35	sM	104/273 (38%)	0.74	16 (15%)	2	2	56, 109, 181, 186	0
36	1	3149/3396 (92%)	0.63	163 (5%)	28	20	38, 61, 124, 213	0
36	5	3169/3396 (93%)	0.65	118 (3%)	42	32	37, 56, 124, 192	0
37	3	121/121 (100%)	0.22	0	100	100	44, 76, 91, 98	0
37	7	121/121 (100%)	0.31	1 (0%)	86	80	41, 62, 74, 80	0
38	4	158/158 (100%)	0.42	2 (1%)	77	69	47, 64, 94, 125	0
38	8	158/158 (100%)	0.45	3 (1%)	67	58	46, 66, 95, 118	0
39	L2	252/253 (99%)	1.22	60 (23%)	1	1	46, 64, 80, 86	0
39	l2	252/253 (99%)	1.40	69 (27%)	1	1	45, 61, 75, 85	0
40	L3	386/386 (100%)	0.63	32 (8%)	12	9	44, 64, 77, 87	0
40	l3	386/386 (100%)	0.43	13 (3%)	46	36	37, 51, 64, 79	0
41	L4	361/361 (100%)	0.57	40 (11%)	6	4	42, 57, 70, 74	0
41	l4	361/361 (100%)	0.77	44 (12%)	5	3	45, 60, 74, 82	0
42	L5	296/296 (100%)	0.46	21 (7%)	17	13	60, 83, 99, 107	0
42	l5	294/296 (99%)	0.36	10 (3%)	46	36	50, 64, 89, 105	0
43	L6	156/175 (89%)	0.48	2 (1%)	77	69	52, 59, 72, 82	0
43	l6	157/175 (89%)	0.50	10 (6%)	20	15	53, 60, 78, 87	0
44	L7	222/243 (91%)	0.55	5 (2%)	61	52	42, 52, 78, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.30	0 100 100	42, 51, 80, 105	0
45	L8	233/255 (91%)	0.64	22 (9%) 9 7	70, 86, 109, 117	0
45	l8	231/255 (90%)	0.79	26 (11%) 6 4	73, 86, 106, 114	0
46	L9	191/191 (100%)	0.30	5 (2%) 56 47	62, 72, 83, 92	0
46	l9	191/191 (100%)	0.37	4 (2%) 64 54	47, 57, 72, 82	0
47	M0	211/220 (95%)	0.55	6 (2%) 53 44	47, 61, 88, 110	0
47	m0	213/220 (96%)	0.72	13 (6%) 22 16	45, 64, 88, 97	0
48	M1	169/173 (97%)	0.66	13 (7%) 14 10	70, 88, 99, 102	0
48	m1	169/173 (97%)	0.31	4 (2%) 59 50	54, 71, 79, 83	0
49	M3	193/198 (97%)	1.06	37 (19%) 1 1	43, 68, 93, 114	0
49	m3	194/198 (97%)	0.56	13 (6%) 19 14	44, 71, 100, 112	0
50	M4	136/137 (99%)	0.23	1 (0%) 87 83	56, 62, 74, 86	0
50	m4	137/137 (100%)	0.12	0 100 100	51, 57, 70, 81	0
51	M5	203/203 (100%)	0.86	19 (9%) 9 7	45, 59, 70, 72	0
51	m5	203/203 (100%)	1.07	32 (15%) 2 2	46, 63, 73, 78	0
52	M6	197/198 (99%)	0.57	7 (3%) 43 33	44, 51, 67, 69	0
52	m6	197/198 (99%)	0.49	8 (4%) 38 30	37, 45, 64, 67	0
53	M7	183/183 (100%)	1.25	26 (14%) 3 2	49, 56, 93, 112	0
53	m7	155/183 (84%)	0.45	7 (4%) 34 26	42, 50, 63, 82	0
54	M8	185/185 (100%)	0.66	11 (5%) 23 17	45, 58, 71, 86	0
54	m8	185/185 (100%)	0.80	18 (9%) 8 6	44, 60, 70, 74	0
55	M9	188/188 (100%)	0.86	21 (11%) 6 4	67, 80, 140, 146	0
55	m9	188/188 (100%)	0.68	14 (7%) 15 12	53, 67, 127, 138	0
56	N0	172/172 (100%)	0.65	6 (3%) 44 34	51, 59, 70, 76	0
56	n0	172/172 (100%)	0.29	1 (0%) 89 85	45, 52, 62, 68	0
57	N1	159/159 (100%)	0.57	5 (3%) 49 40	46, 58, 95, 103	0
57	n1	159/159 (100%)	0.43	4 (2%) 58 48	43, 52, 86, 91	0
58	N2	100/120 (83%)	1.17	25 (25%) 1 1	95, 107, 121, 123	0
58	n2	98/120 (81%)	0.98	21 (21%) 1 1	78, 90, 97, 100	0
59	N3	136/136 (100%)	1.35	31 (22%) 1 1	54, 62, 72, 79	0
59	n3	136/136 (100%)	0.79	8 (5%) 23 17	38, 47, 57, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	2.94	38 (38%) 0 0	63, 75, 134, 138	0
60	n4	135/155 (87%)	1.08	19 (14%) 3 2	47, 94, 119, 124	0
61	N5	121/141 (85%)	0.87	12 (9%) 8 6	62, 73, 86, 99	0
61	n5	120/141 (85%)	0.66	9 (7%) 15 11	58, 72, 86, 98	0
62	N6	126/126 (100%)	0.39	3 (2%) 59 50	53, 66, 76, 81	0
62	n6	126/126 (100%)	0.66	6 (4%) 31 23	55, 68, 79, 85	0
63	N7	135/135 (100%)	0.61	12 (8%) 10 8	87, 98, 107, 111	0
63	n7	135/135 (100%)	0.62	15 (11%) 6 4	80, 92, 102, 106	0
64	N8	148/148 (100%)	1.15	19 (12%) 4 3	38, 60, 79, 86	0
64	n8	148/148 (100%)	1.12	24 (16%) 2 1	38, 61, 75, 78	0
65	N9	58/58 (100%)	0.80	6 (10%) 7 5	41, 63, 89, 95	0
65	n9	58/58 (100%)	0.49	3 (5%) 28 20	41, 60, 82, 89	0
66	O0	97/104 (93%)	0.24	2 (2%) 64 54	85, 93, 107, 109	0
66	o0	100/104 (96%)	0.42	5 (5%) 30 21	74, 83, 101, 111	0
67	O1	109/112 (97%)	1.06	26 (23%) 1 1	62, 73, 92, 98	0
67	o1	109/112 (97%)	0.85	10 (9%) 10 7	49, 60, 84, 98	0
68	O2	127/129 (98%)	0.53	4 (3%) 49 40	39, 53, 65, 71	0
68	o2	127/129 (98%)	0.48	5 (3%) 40 31	38, 56, 69, 72	0
69	O3	106/106 (100%)	0.85	6 (5%) 24 18	44, 49, 70, 78	0
69	o3	106/106 (100%)	1.11	15 (14%) 3 2	42, 49, 70, 78	0
70	O4	112/119 (94%)	1.26	34 (30%) 0 1	61, 78, 107, 113	0
70	o4	112/119 (94%)	1.04	26 (23%) 1 1	54, 72, 102, 107	0
71	O5	119/119 (100%)	0.35	1 (0%) 86 80	58, 74, 82, 87	0
71	o5	119/119 (100%)	0.20	1 (0%) 86 80	62, 75, 89, 98	0
72	O6	99/99 (100%)	0.19	2 (2%) 65 56	64, 72, 94, 105	0
72	o6	99/99 (100%)	0.30	3 (3%) 51 41	66, 75, 87, 101	0
73	O7	87/87 (100%)	1.54	24 (27%) 1 1	46, 53, 71, 76	0
73	o7	87/87 (100%)	1.42	19 (21%) 1 1	43, 52, 76, 93	0
74	O8	77/77 (100%)	0.37	5 (6%) 20 15	86, 97, 109, 114	0
74	o8	77/77 (100%)	0.80	12 (15%) 2 2	80, 91, 101, 103	0
75	O9	50/50 (100%)	1.79	18 (36%) 0 0	55, 60, 64, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	1.44	15 (30%) 1 1	52, 58, 66, 67	0
76	Q0	52/52 (100%)	0.38	2 (3%) 41 32	52, 60, 76, 79	0
76	q0	52/52 (100%)	0.22	0 100 100	43, 47, 56, 59	0
77	Q1	25/25 (100%)	2.53	15 (60%) 0 0	62, 66, 73, 73	0
77	q1	25/25 (100%)	1.56	7 (28%) 1 1	53, 58, 59, 59	0
78	Q2	105/105 (100%)	0.34	3 (2%) 52 43	46, 58, 78, 103	0
78	q2	105/105 (100%)	0.65	8 (7%) 15 11	45, 56, 71, 94	0
79	Q3	91/91 (100%)	1.02	17 (18%) 1 1	56, 68, 82, 90	0
79	q3	91/91 (100%)	1.08	22 (24%) 1 1	47, 60, 76, 85	0
80	c0	96/105 (91%)	2.70	61 (63%) 0 0	104, 135, 149, 151	0
81	m2	0/150	-	-	-	-
82	p0	143/311 (45%)	0.82	19 (13%) 4 3	102, 125, 192, 199	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
85	f	148/157 (94%)	3.43	96 (64%) 0 0	49, 95, 145, 147	148 (100%)
All	All	33261/35493 (93%)	0.93	4886 (14%) 3 2	37, 76, 134, 213	148 (0%)

The worst 5 of 4886 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	M7	161	ALA	23.1
1	2	1699	G	20.2
60	N4	86	SER	15.9
53	M7	160	ALA	14.8
60	N4	88	ASP	13.4

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

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
86	ZN	d7	101	1/1	0.78	0.31	0.32	134,134,134,134	0
86	ZN	q3	501	1/1	0.99	0.18	-0.43	64,64,64,64	0
86	ZN	E1	501	1/1	0.91	0.15	-0.77	133,133,133,133	0
86	ZN	Q3	501	1/1	0.99	0.14	-1.11	74,74,74,74	0
86	ZN	Q0	500	1/1	0.98	0.20	-1.22	57,57,57,57	0
86	ZN	e1	501	1/1	0.72	0.15	-1.27	165,165,165,165	0
86	ZN	d9	101	1/1	0.95	0.13	-1.49	93,93,93,93	0
86	ZN	D9	101	1/1	0.97	0.11	-1.62	89,89,89,89	0
86	ZN	Q2	501	1/1	0.97	0.08	-1.73	78,78,78,78	0
86	ZN	o7	501	1/1	0.99	0.14	-1.89	53,53,53,53	0
86	ZN	O7	100	1/1	1.00	0.13	-1.98	53,53,53,53	0
86	ZN	q2	501	1/1	0.95	0.07	-2.36	74,74,74,74	0
86	ZN	d6	500	1/1	0.94	0.07	-2.57	82,82,82,82	0
86	ZN	D6	500	1/1	0.94	0.06	-3.00	99,99,99,99	0
86	ZN	q0	500	1/1	0.99	0.16	-3.58	48,48,48,48	0
86	ZN	D7	101	1/1	0.76	0.17	-	140,140,140,140	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.