



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2016 – 09:46 PM 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 : 2015-08-23
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

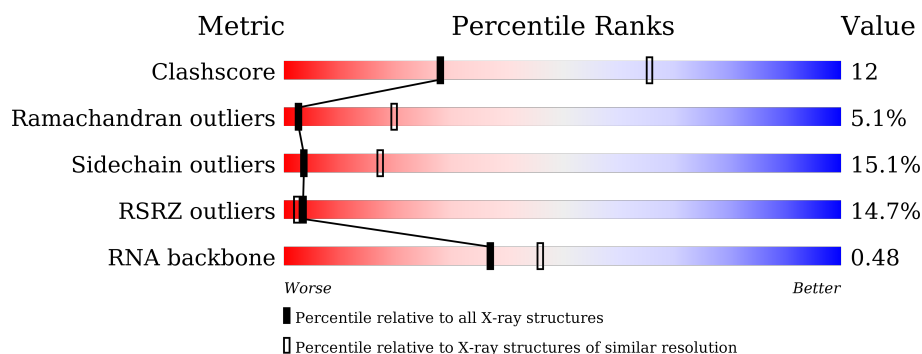
1 Overall quality at a glance ⓘ

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	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)
RNA backbone	2183	1001 (3.76-2.76)

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 ≥ 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>43%</div> <div>42%</div> <div>13%</div> <div>..</div> </div>
1	6	1800	<div> <div>5%</div> <div>45%</div> <div>41%</div> <div>12%</div> <div>.</div> </div>
2	S0	251	<div> <div>48%</div> <div>30%</div> <div>41%</div> <div>11%</div> <div>18%</div> </div>
2	s0	251	<div> <div>31%</div> <div>68%</div> <div>14%</div> <div>.</div> <div>18%</div> </div>
3	S1	254	<div> <div>13%</div> <div>24%</div> <div>47%</div> <div>13%</div> <div>16%</div> </div>
3	s1	254	<div> <div>12%</div> <div>67%</div> <div>17%</div> <div>.</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	

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Mol	Chain	Length	Quality of chain
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	
29	D7	81	

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Mol	Chain	Length	Quality of chain
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	
41	l4	361	

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

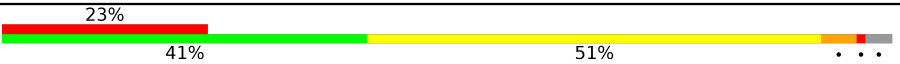


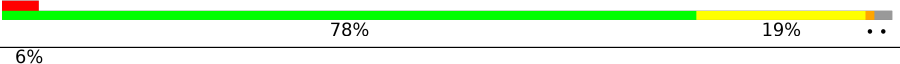
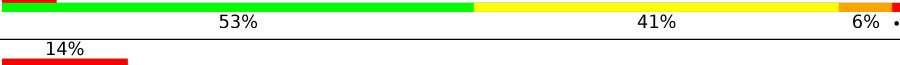
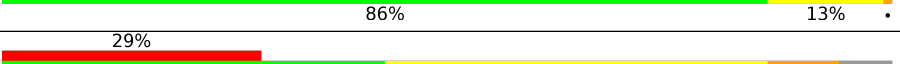
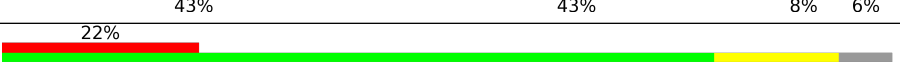
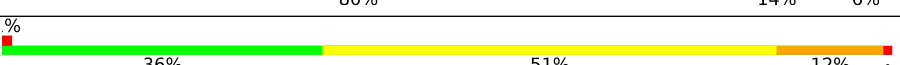
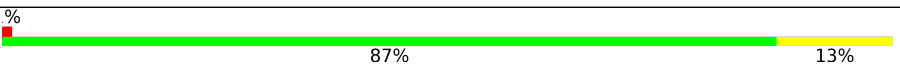

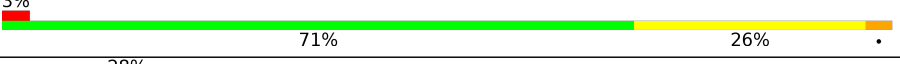
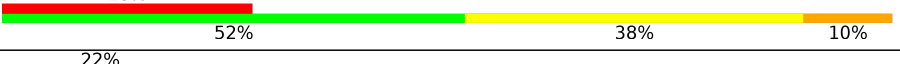



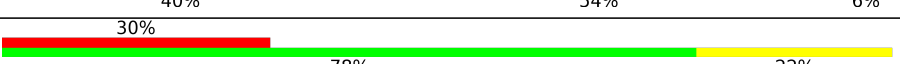
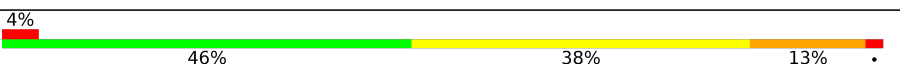
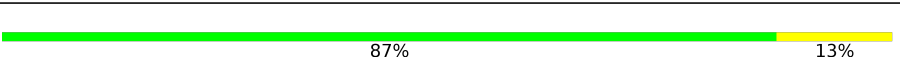




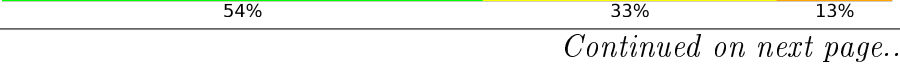


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Mol	Chain	Length	Quality of chain
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8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

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

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Mol	Chain	Length	Quality of chain
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	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

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

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

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

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

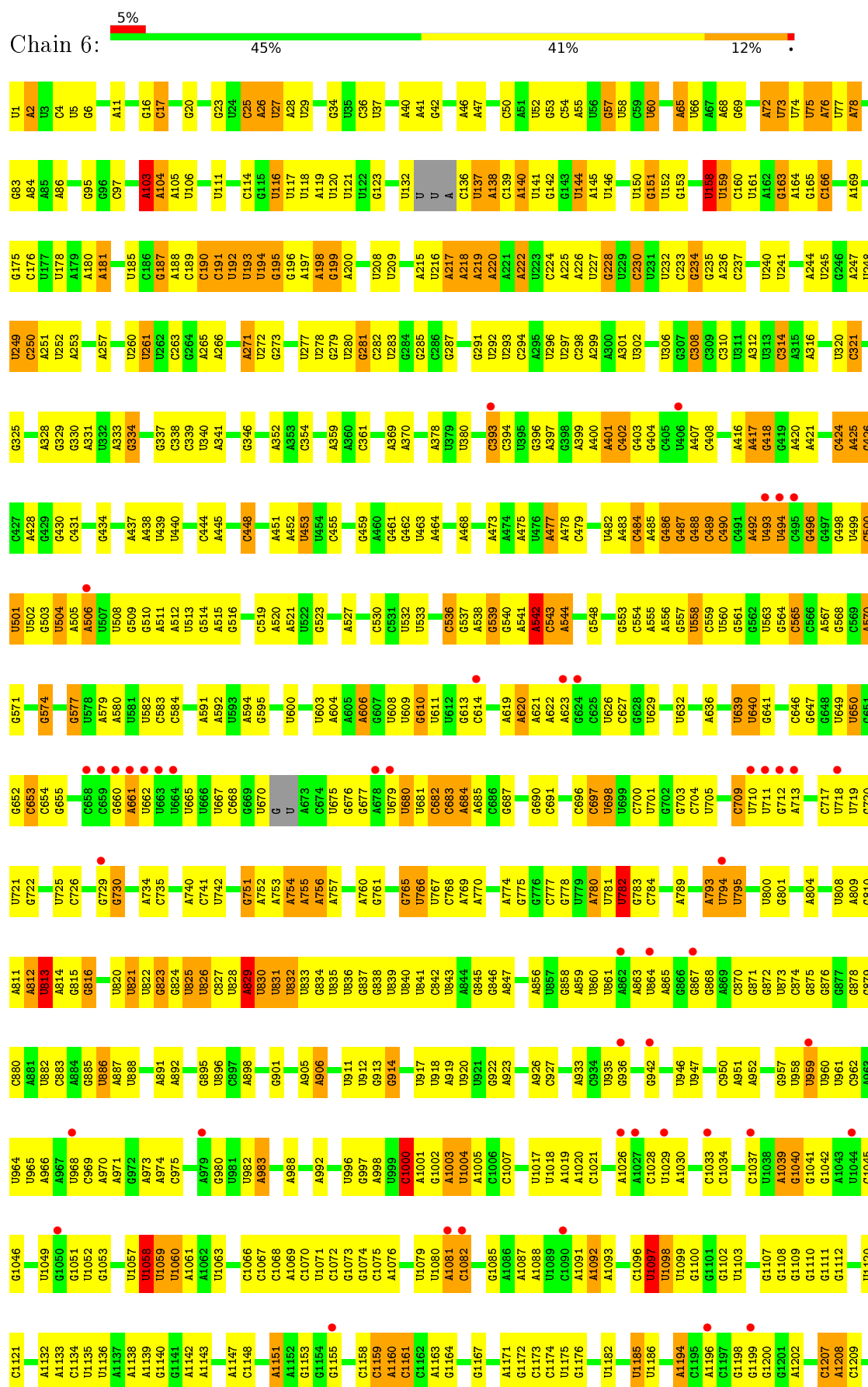
- Molecule 85 is a protein called Eukaryotic translation initiation factor 5A-1.

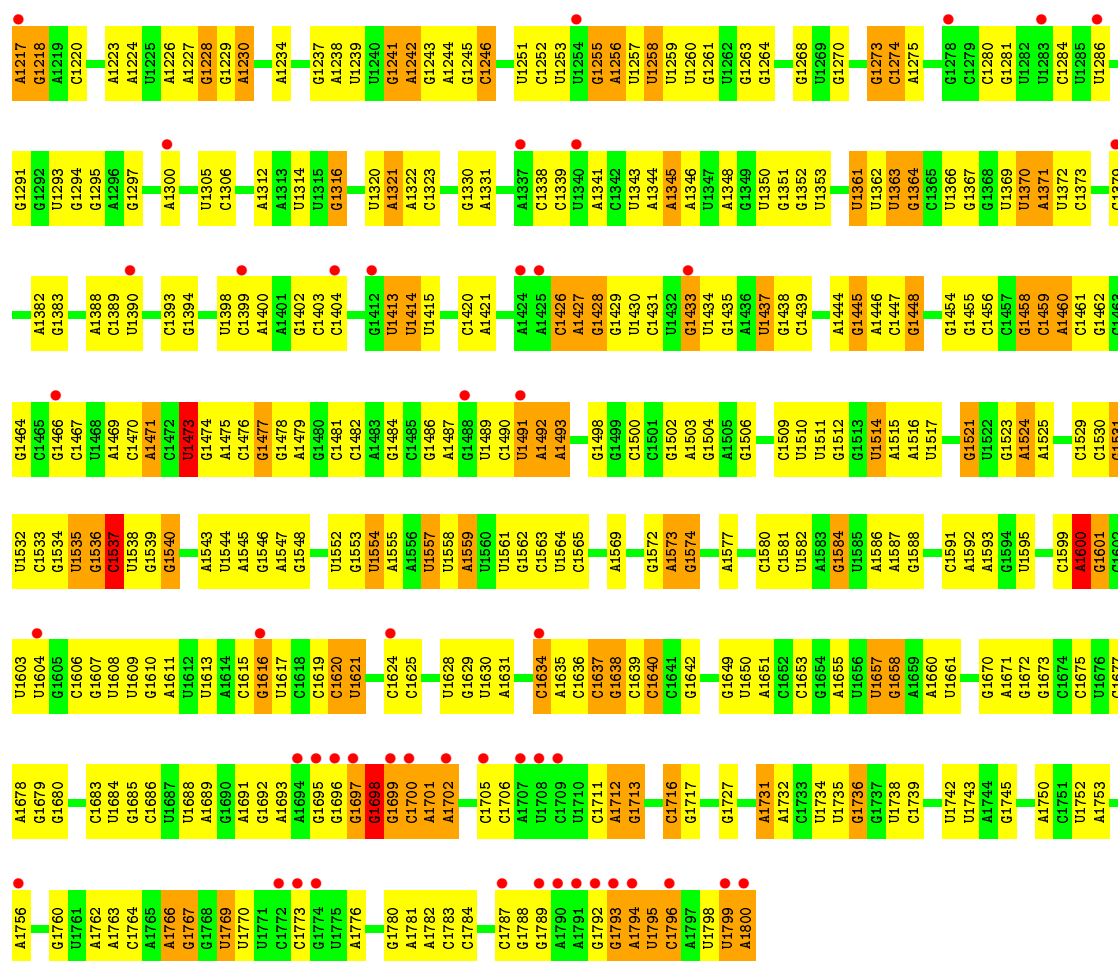
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	f	148	Total	C	N	O	S	0	0	0
			1116	692	188	227	9			

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

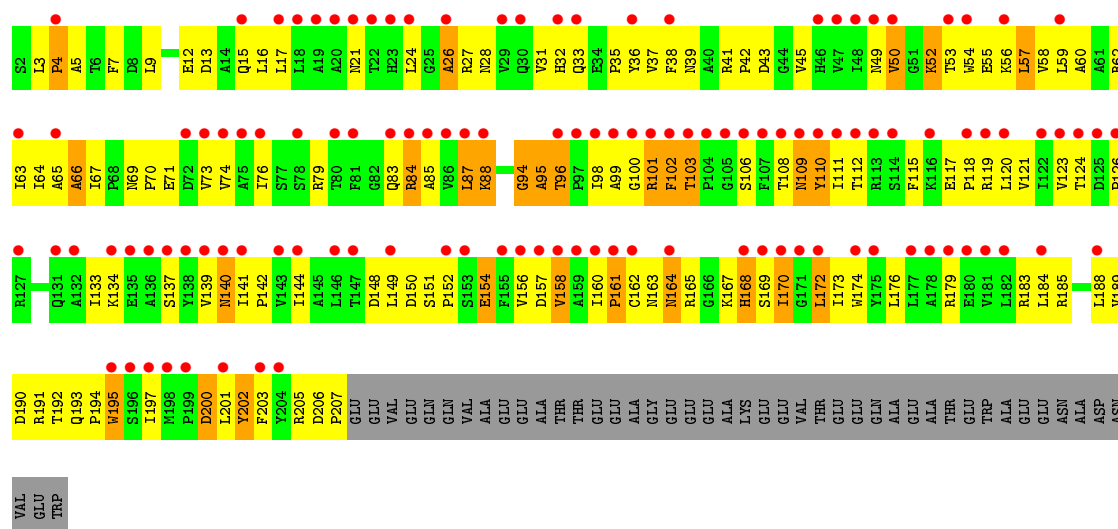
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86	D6	1	Total 1	Zn 1	0	0
86	Q2	1	Total 1	Zn 1	0	0
86	e1	1	Total 1	Zn 1	0	0
86	Q3	1	Total 1	Zn 1	0	0
86	D9	1	Total 1	Zn 1	0	0
86	E1	1	Total 1	Zn 1	0	0
86	Q0	1	Total 1	Zn 1	0	0
86	d7	1	Total 1	Zn 1	0	0
86	q3	1	Total 1	Zn 1	0	0
86	d9	1	Total 1	Zn 1	0	0
86	D7	1	Total 1	Zn 1	0	0
86	d6	1	Total 1	Zn 1	0	0
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86	O7	1	Total 1	Zn 1	0	0
86	q2	1	Total 1	Zn 1	0	0



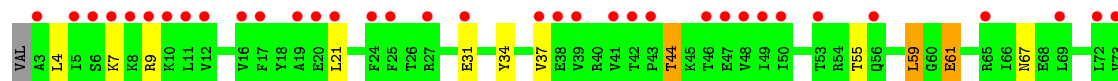


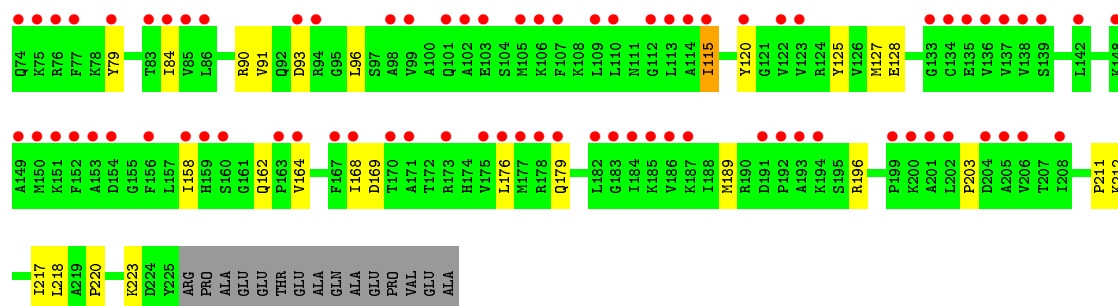


• Molecule 2: 40S ribosomal protein S0-A

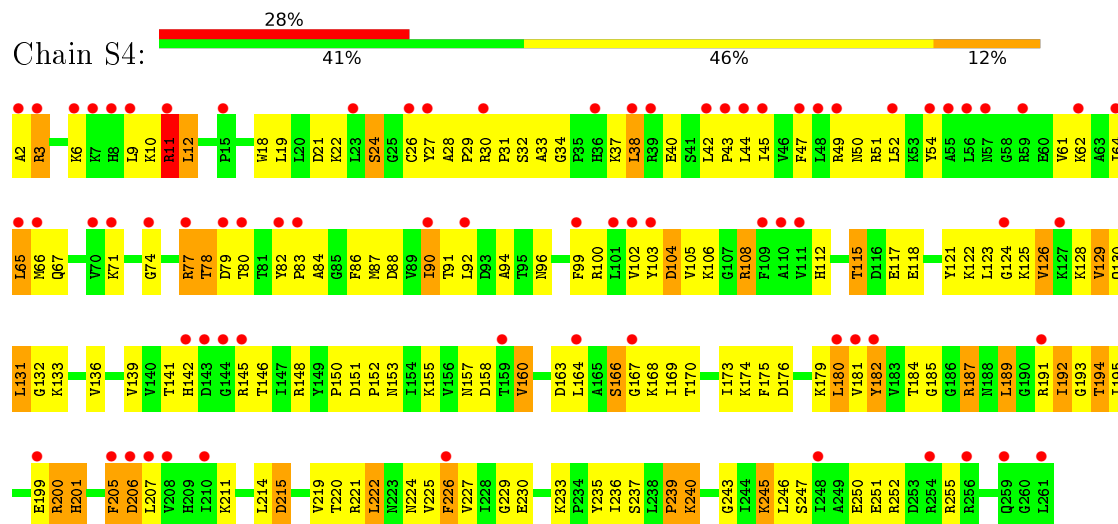


• Molecule 2: 40S ribosomal protein S0-A

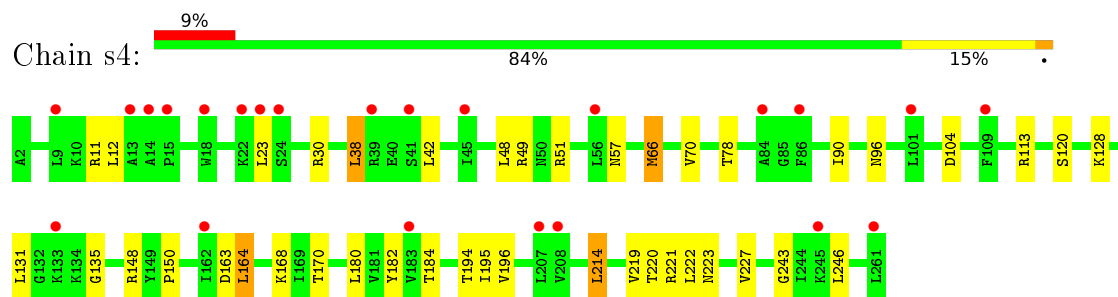




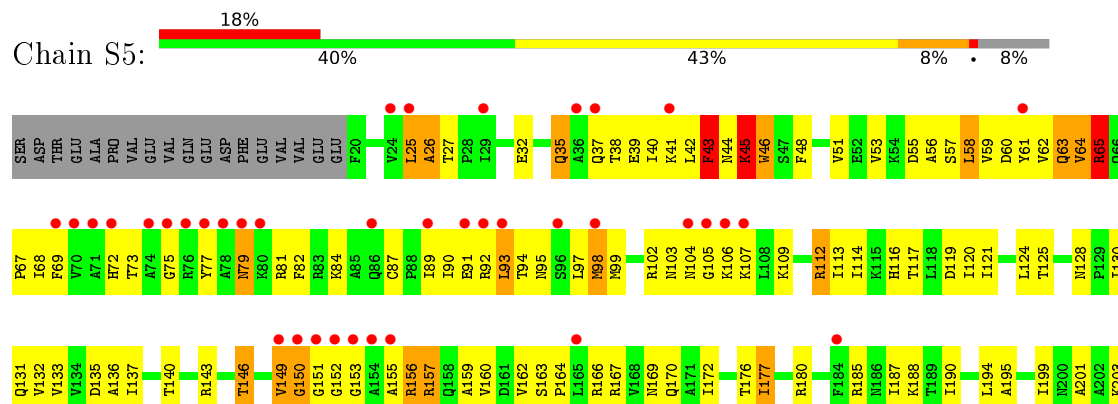
• Molecule 6: 40S ribosomal protein S4-A

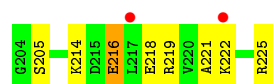


• Molecule 6: 40S ribosomal protein S4-A

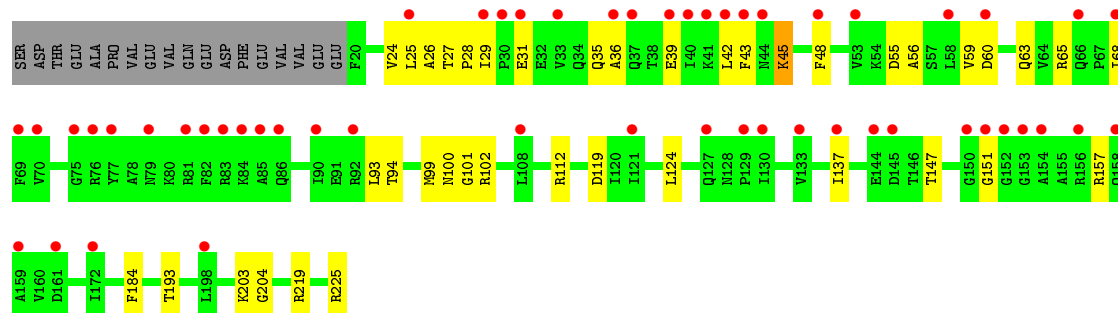
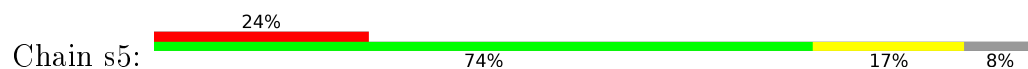


• Molecule 7: 40S ribosomal protein S5

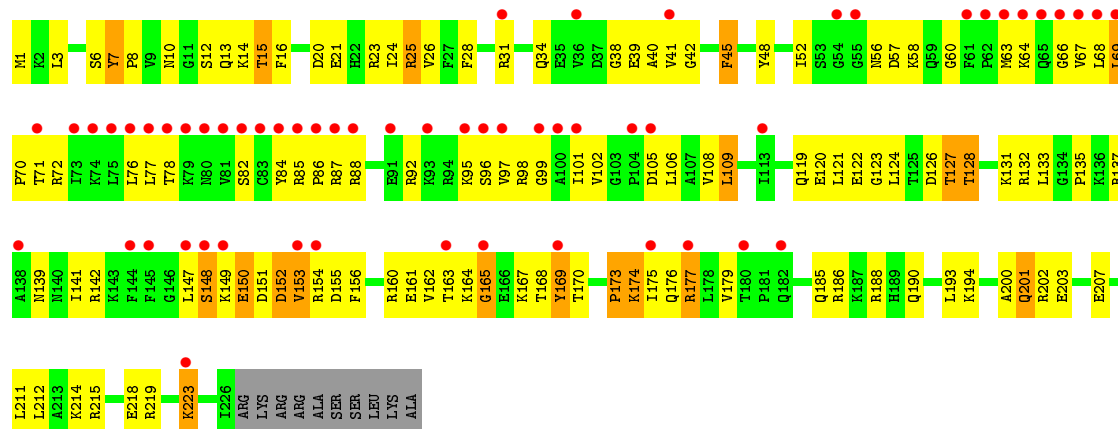
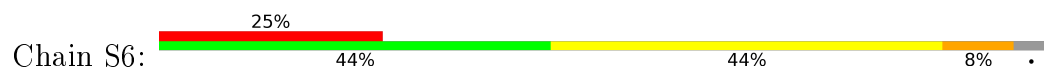




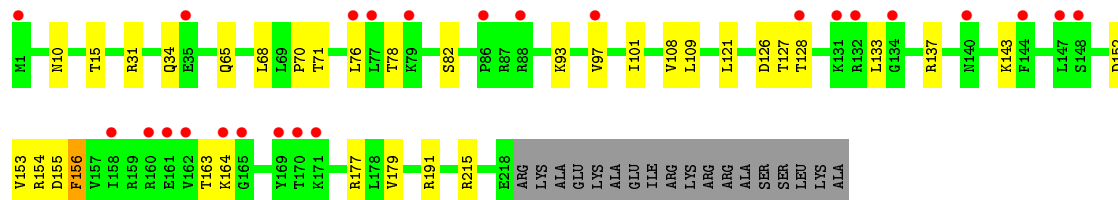
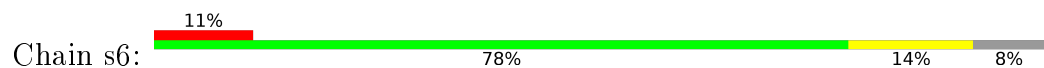
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6-A

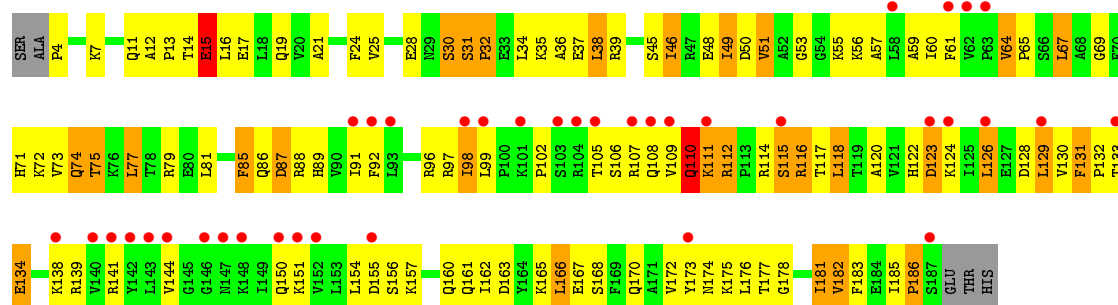


• Molecule 8: 40S ribosomal protein S6-A

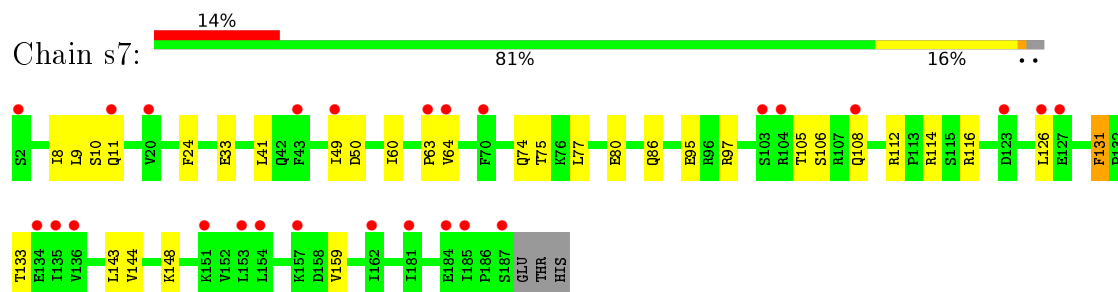


• Molecule 9: 40S ribosomal protein S7-A

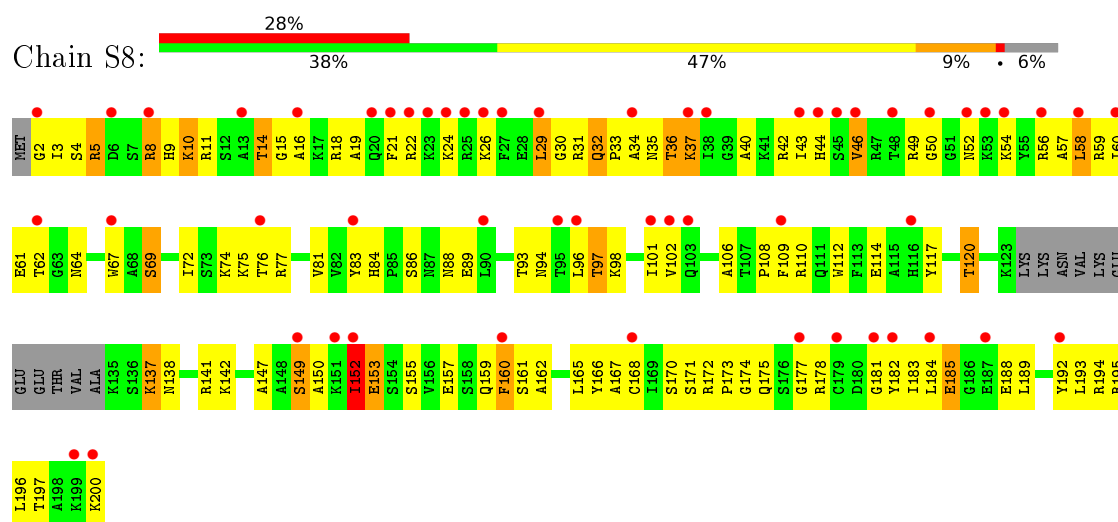




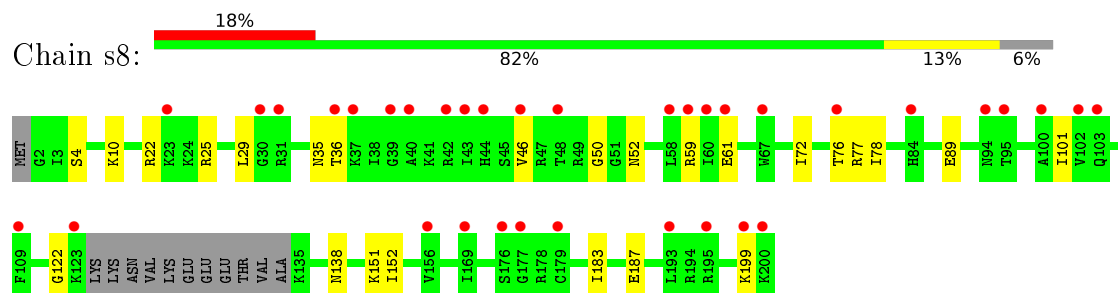
- Molecule 9: 40S ribosomal protein S7-A



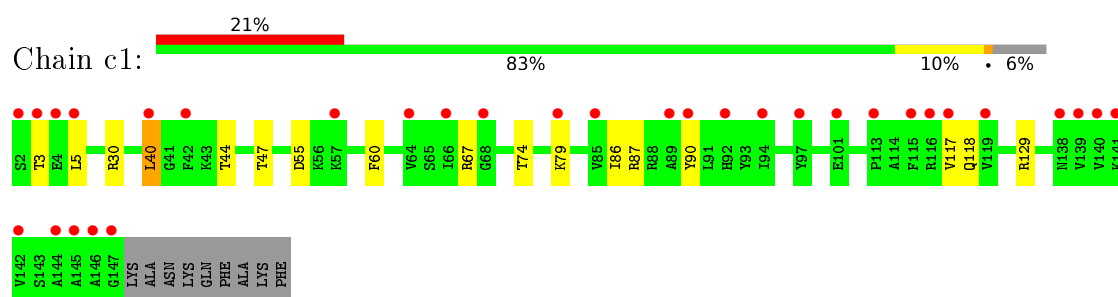
- Molecule 10: 40S ribosomal protein S8-A



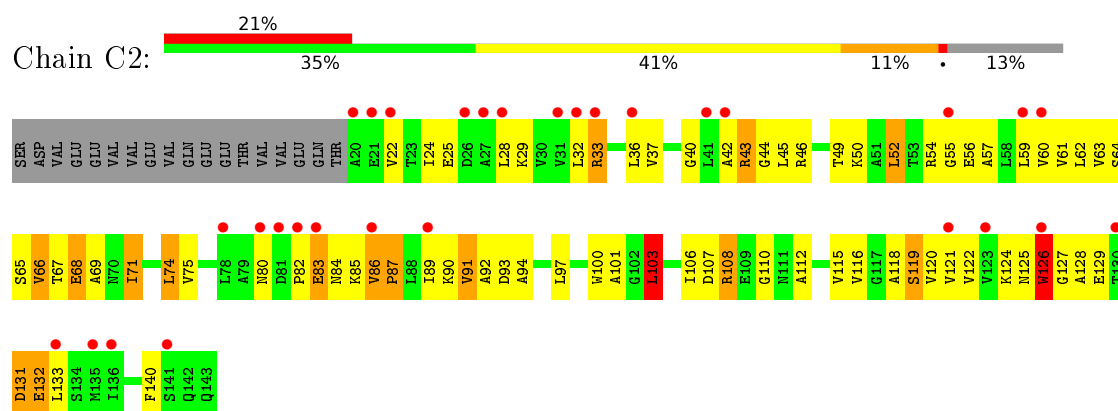
- Molecule 10: 40S ribosomal protein S8-A



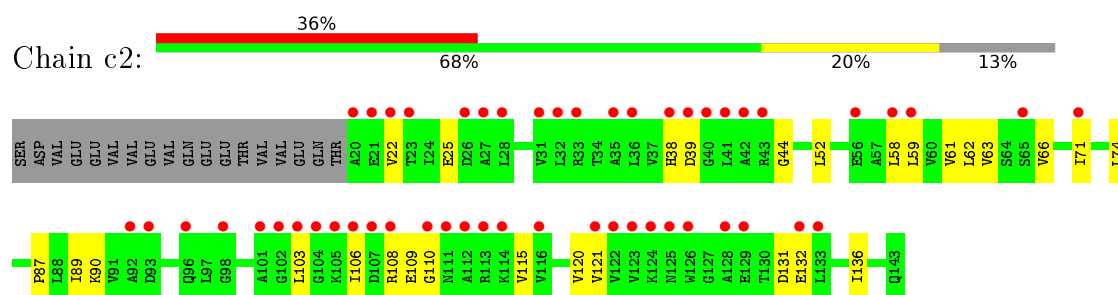
- Molecule 11: 40S ribosomal protein S9-A



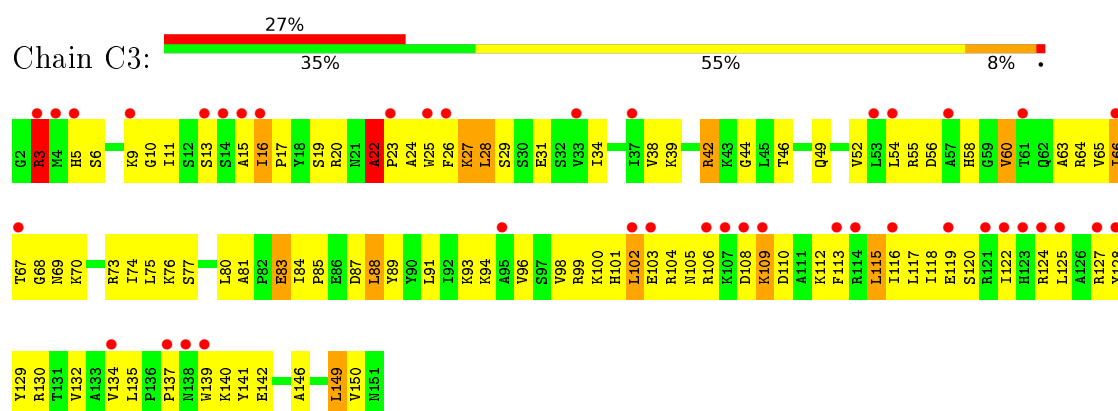
• Molecule 14: 40S ribosomal protein S12



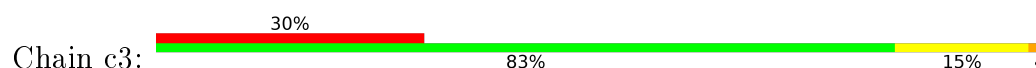
• Molecule 14: 40S ribosomal protein S12

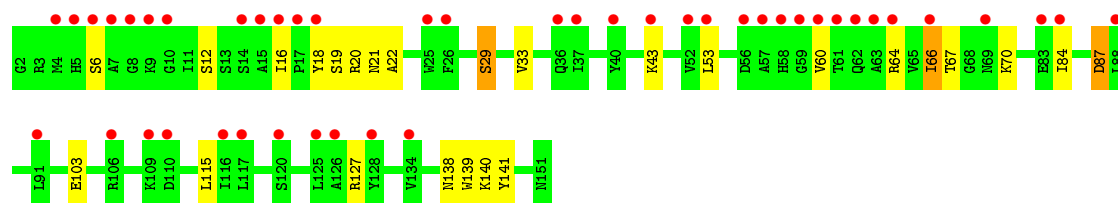


• Molecule 15: 40S ribosomal protein S13

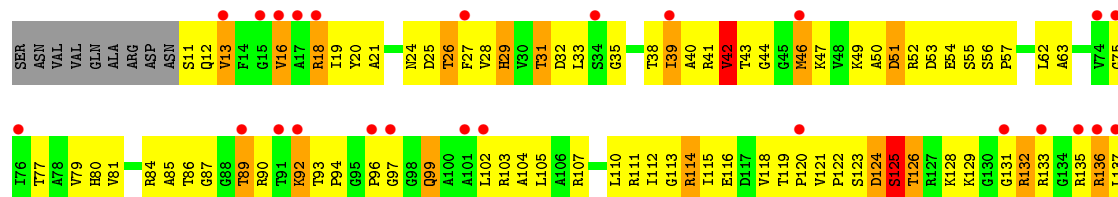


• Molecule 15: 40S ribosomal protein S13

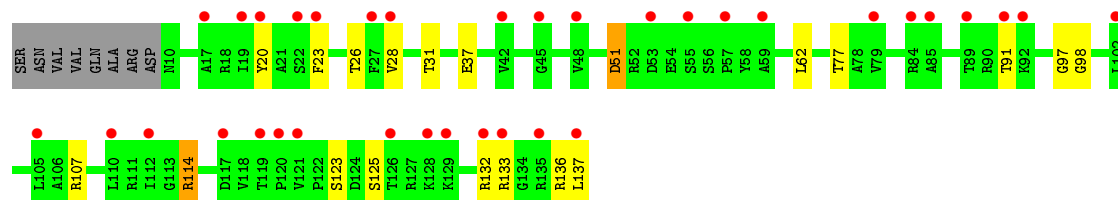
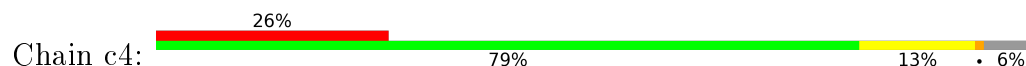




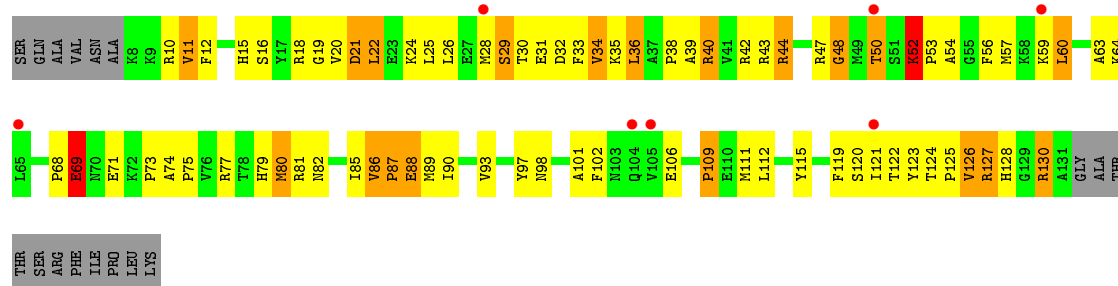
• Molecule 16: 40S ribosomal protein S14-A



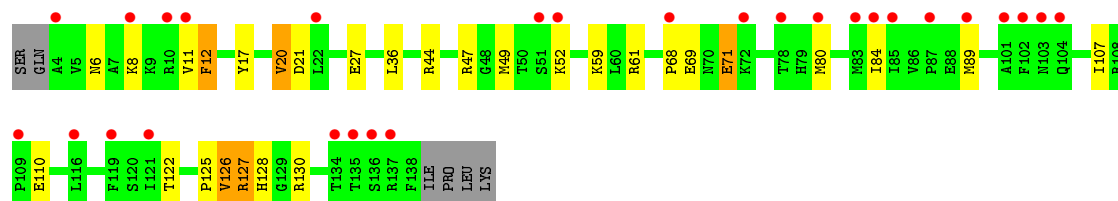
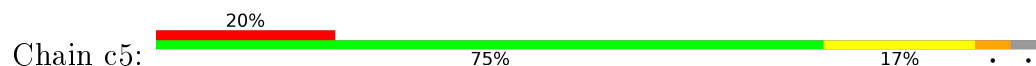
• Molecule 16: 40S ribosomal protein S14-A



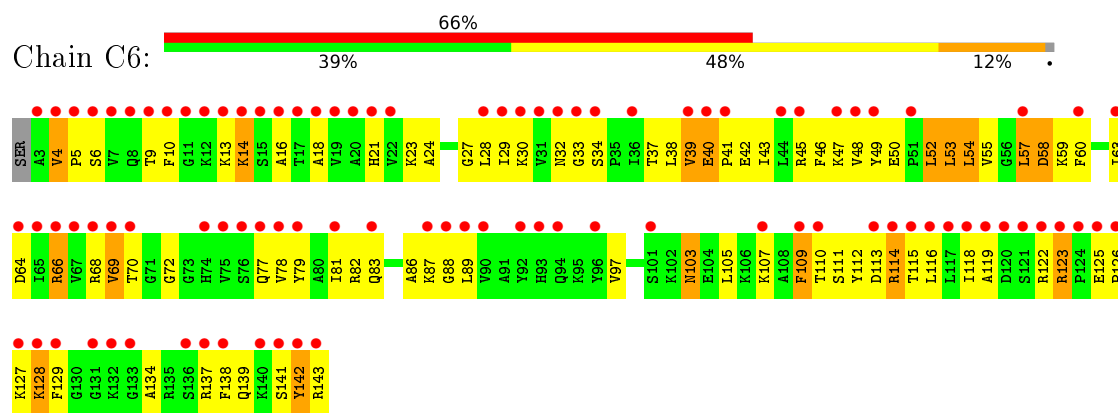
• Molecule 17: 40S ribosomal protein S15



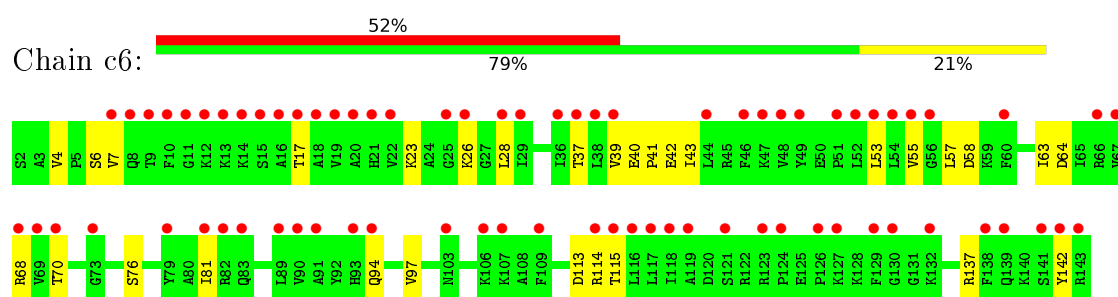
• Molecule 17: 40S ribosomal protein S15



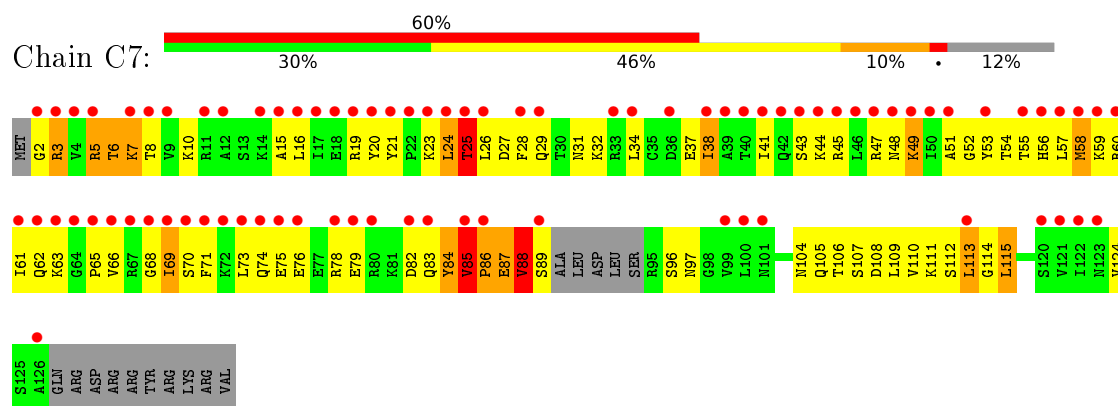
- Molecule 18: 40S ribosomal protein S16-A



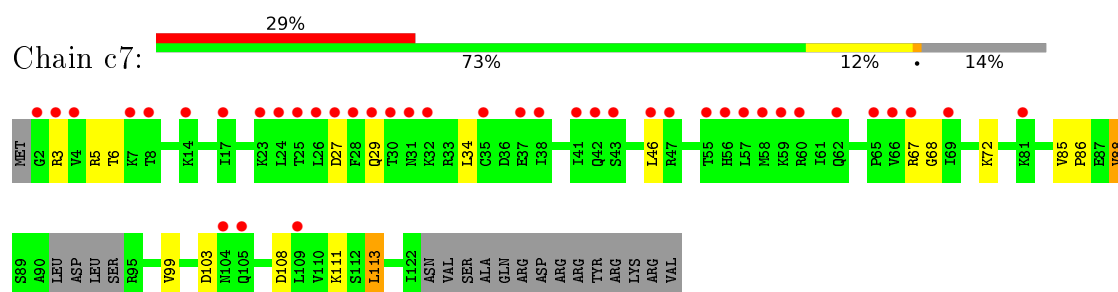
- Molecule 18: 40S ribosomal protein S16-A



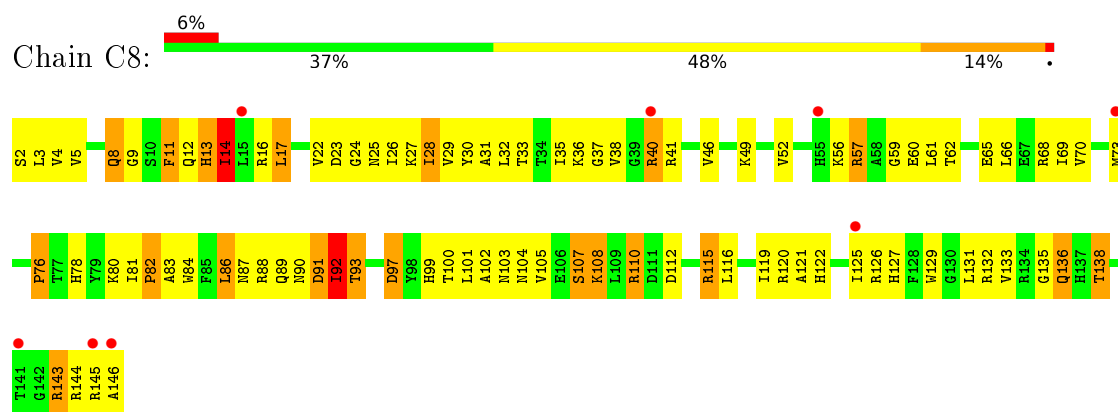
- Molecule 19: 40S ribosomal protein S17-A



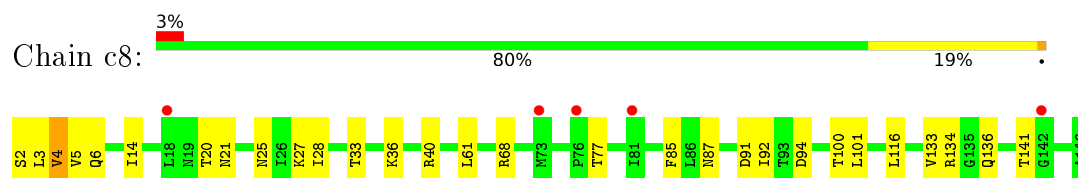
- Molecule 19: 40S ribosomal protein S17-A



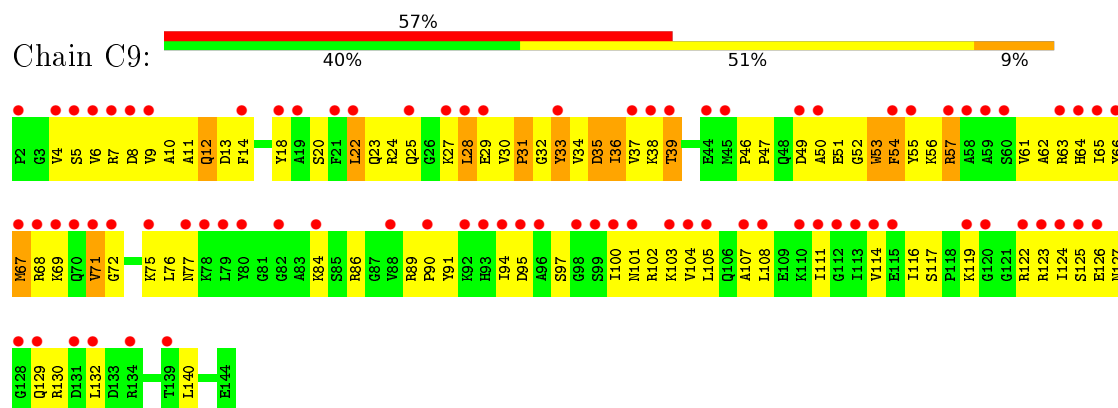
- Molecule 20: 40S ribosomal protein S18-A



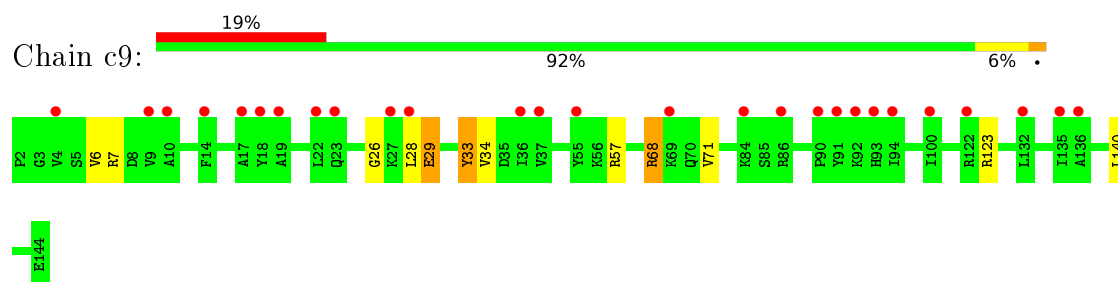
• Molecule 20: 40S ribosomal protein S18-A



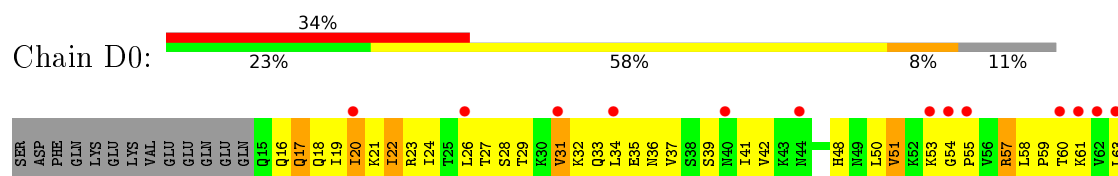
• Molecule 21: 40S ribosomal protein S19-A

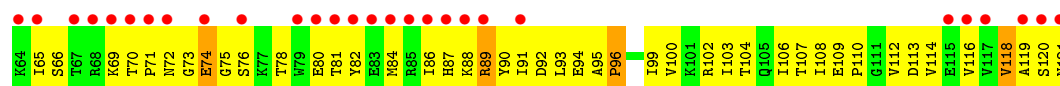


• Molecule 21: 40S ribosomal protein S19-A

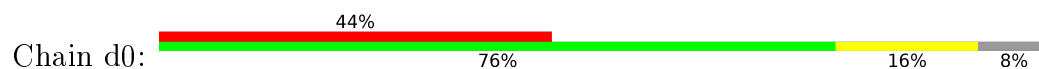


• Molecule 22: 40S ribosomal protein S20

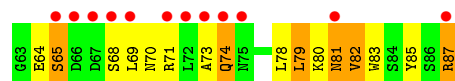
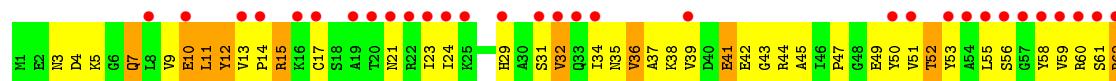




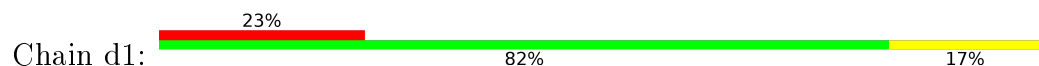
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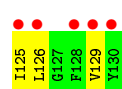
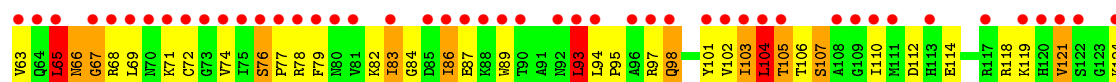
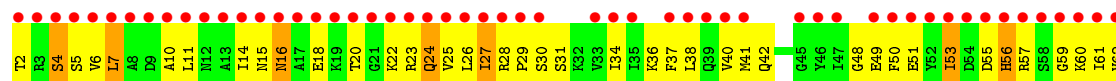
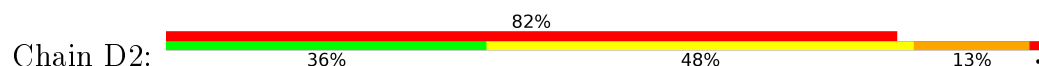
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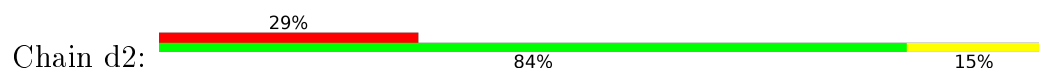
• Molecule 23: 40S ribosomal protein S21-A

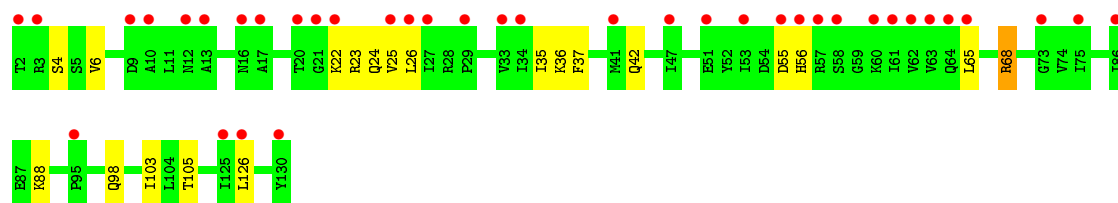


• Molecule 24: 40S ribosomal protein S22-A

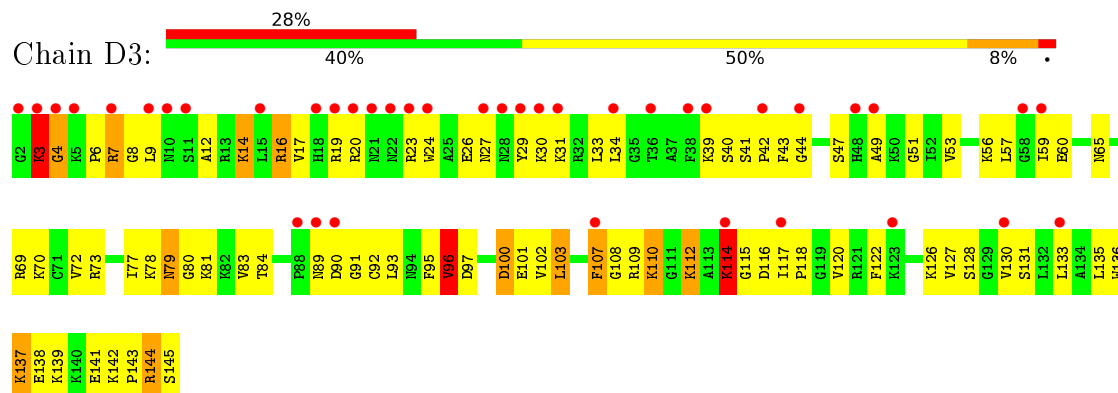


• Molecule 24: 40S ribosomal protein S22-A

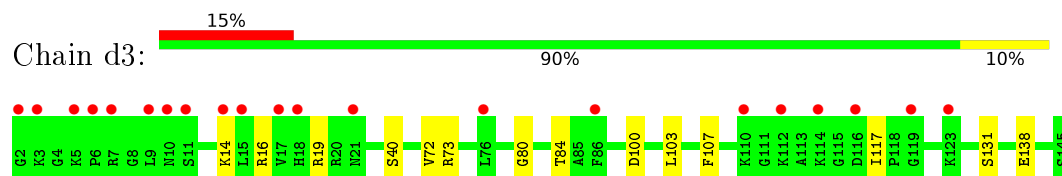




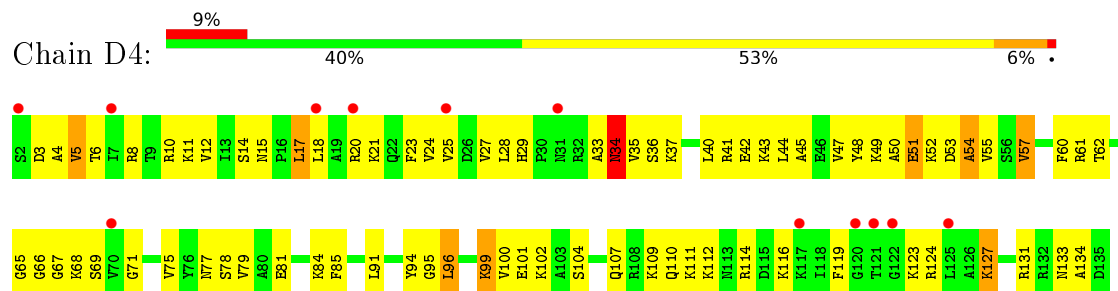
• Molecule 25: 40S ribosomal protein S23-A



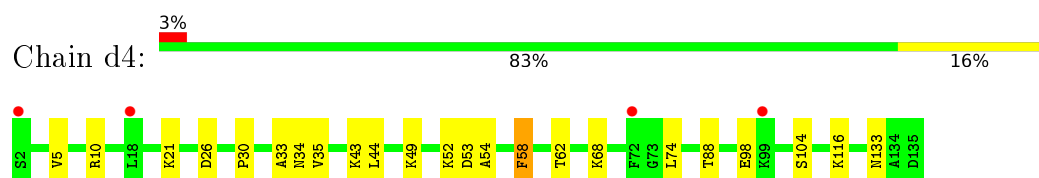
• Molecule 25: 40S ribosomal protein S23-A



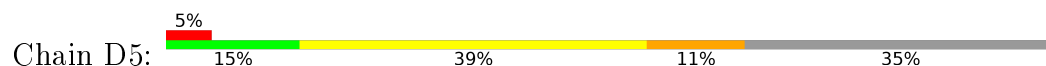
• Molecule 26: 40S ribosomal protein S24-A

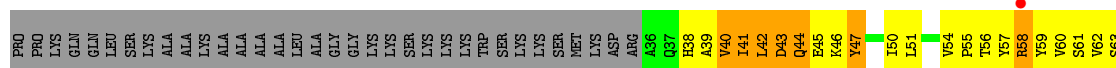


• Molecule 26: 40S ribosomal protein S24-A

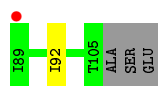
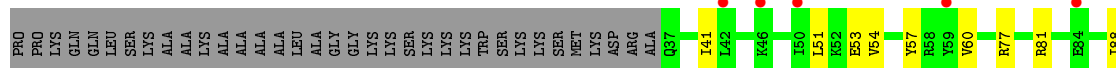


• Molecule 27: 40S ribosomal protein S25-A

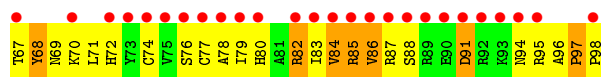
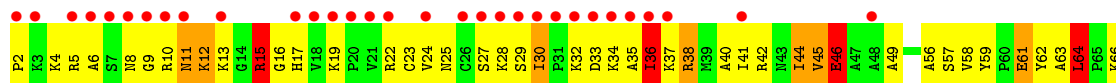




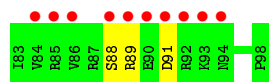
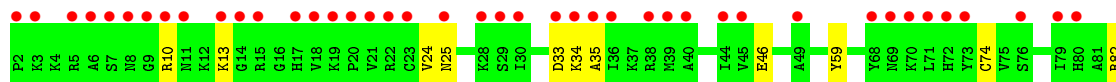
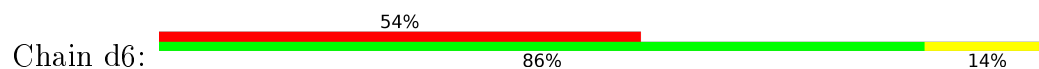
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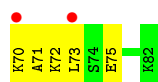
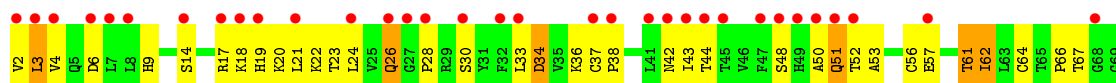
• Molecule 28: 40S ribosomal protein S26-B



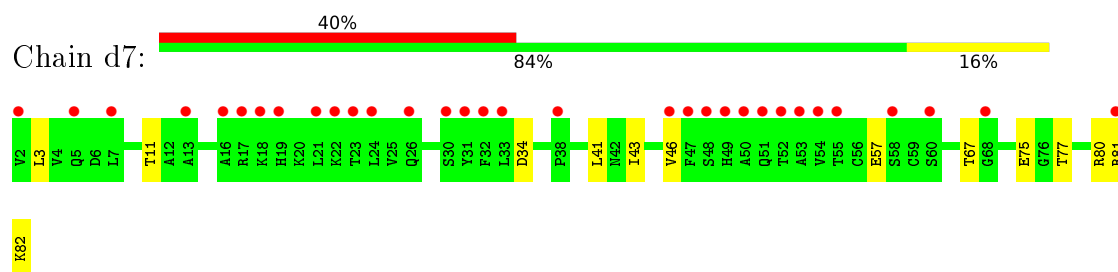
• Molecule 28: 40S ribosomal protein S26-B



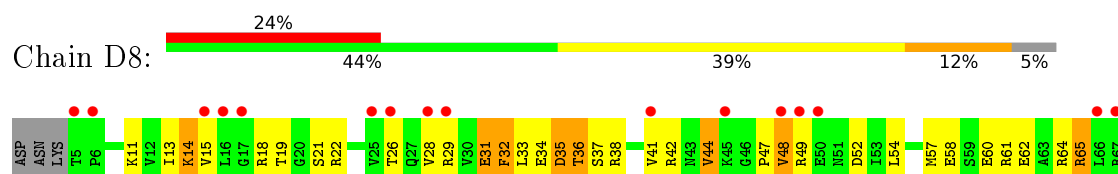
• Molecule 29: 40S ribosomal protein S27-A



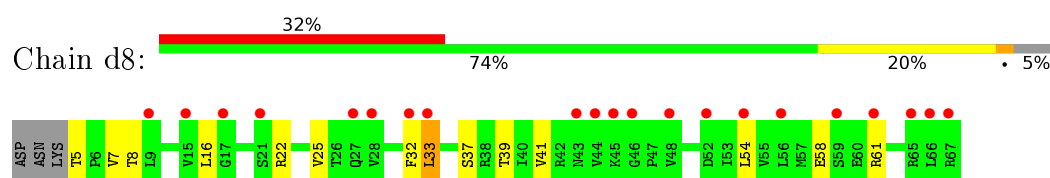
• Molecule 29: 40S ribosomal protein S27-A



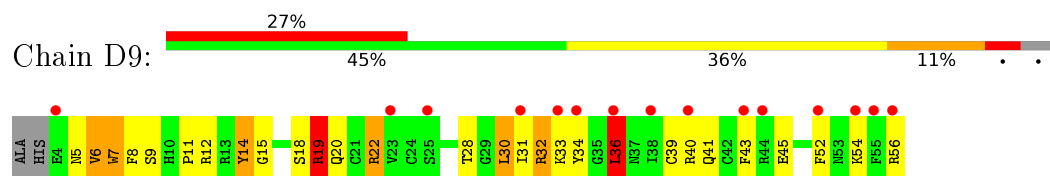
- Molecule 30: 40S ribosomal protein S28-A



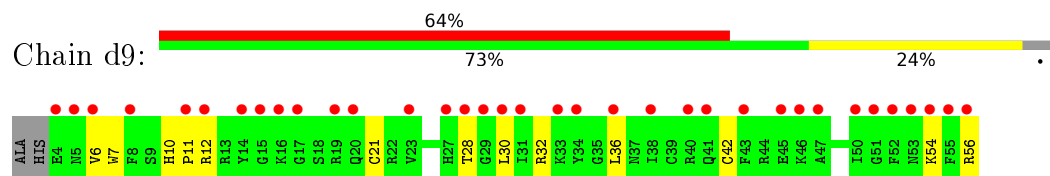
- Molecule 30: 40S ribosomal protein S28-A



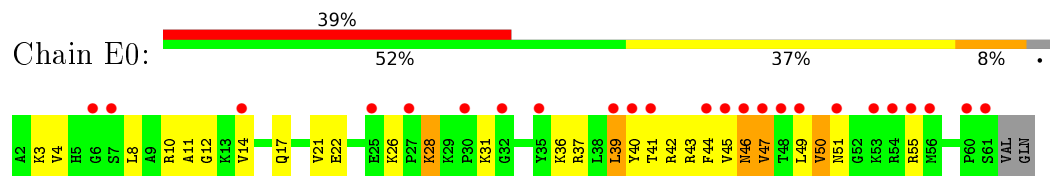
- Molecule 31: 40S ribosomal protein S29-A



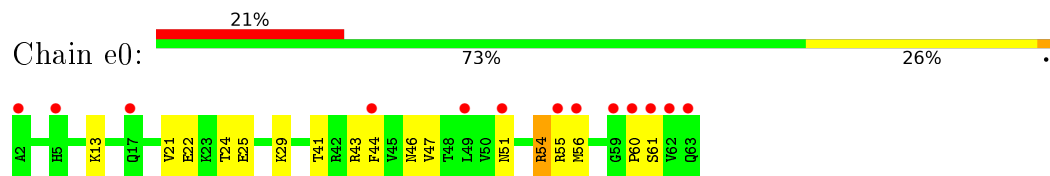
- Molecule 31: 40S ribosomal protein S29-A



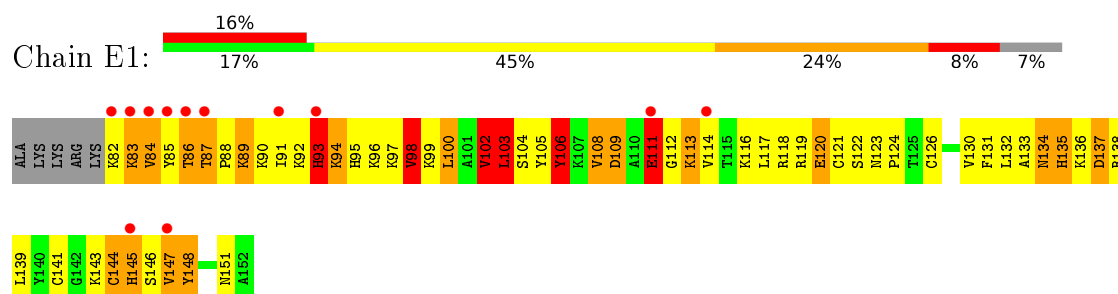
- Molecule 32: 40S ribosomal protein S30-A



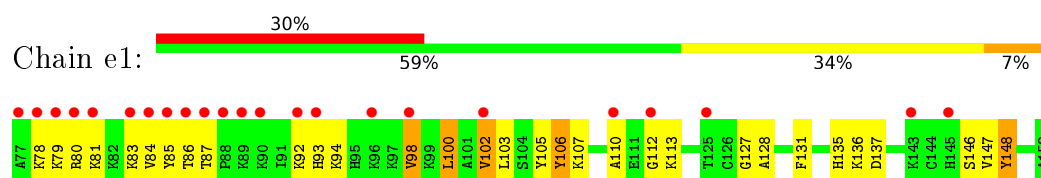
- Molecule 32: 40S ribosomal protein S30-A



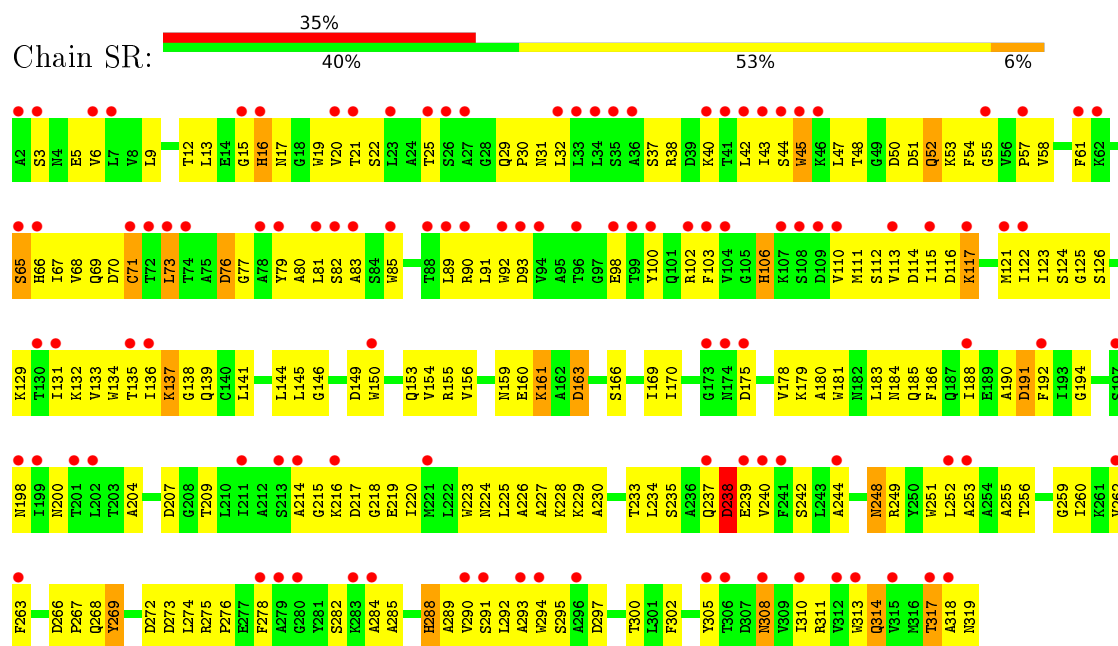
- Molecule 33: Ubiquitin-40S ribosomal protein S31



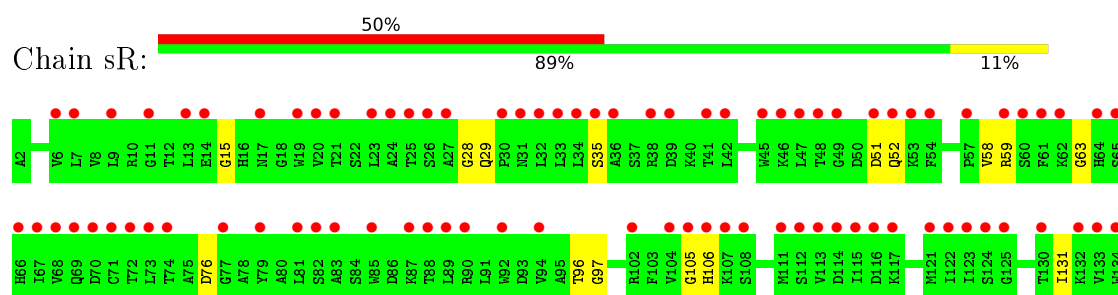
- Molecule 33: Ubiquitin-40S ribosomal protein S31



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

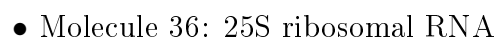


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



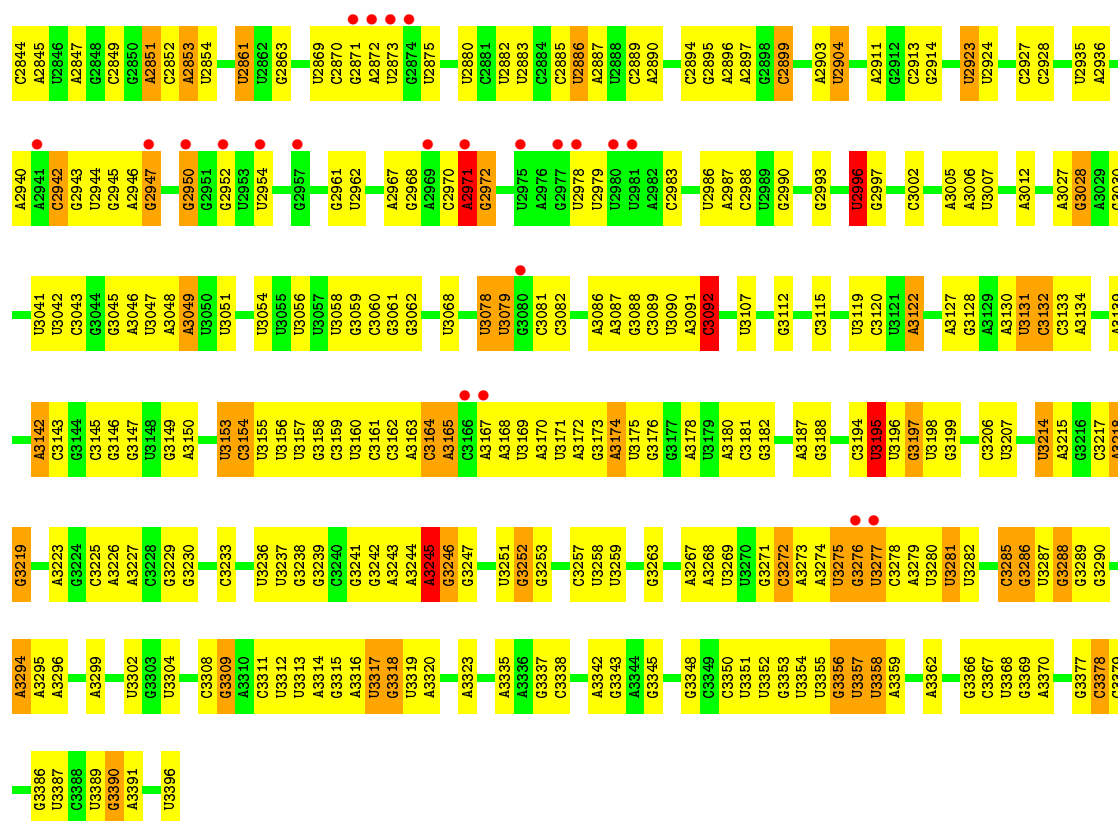
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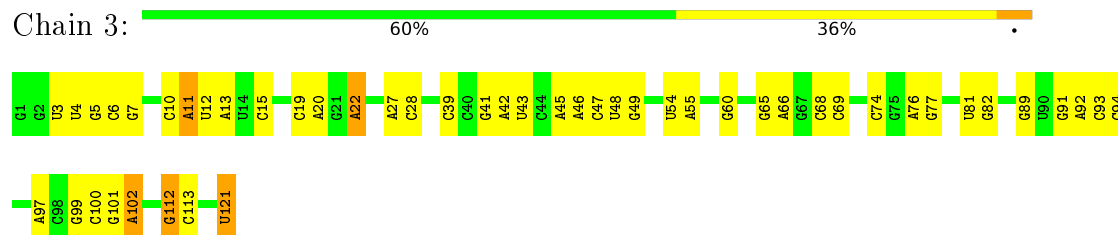




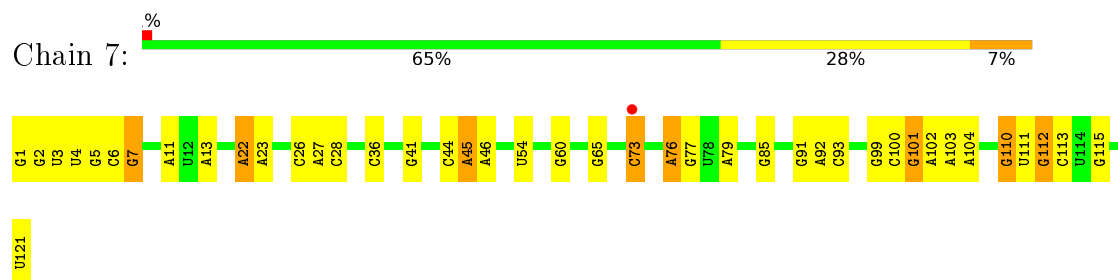
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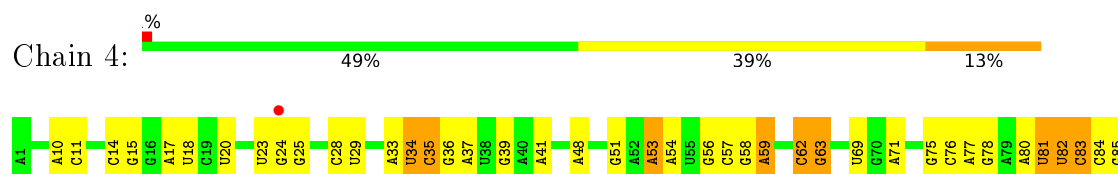
• Molecule 37: 5S ribosomal RNA

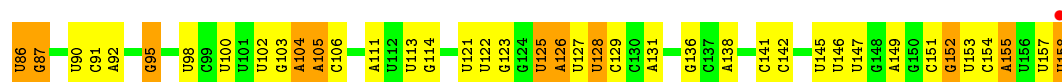


• Molecule 37: 5S ribosomal RNA

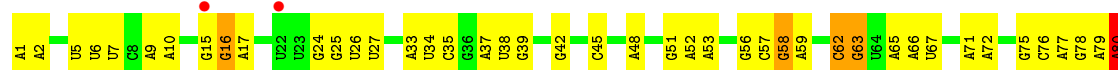


• Molecule 38: 5.8S ribosomal RNA

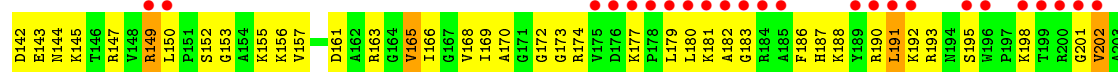
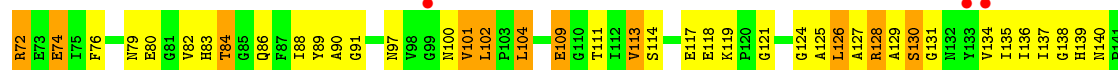




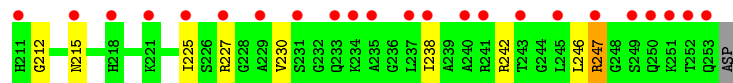
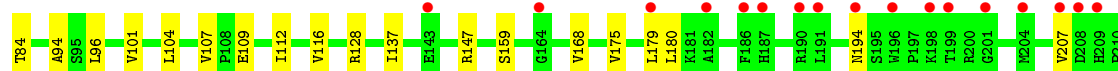
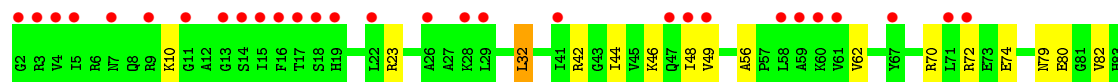
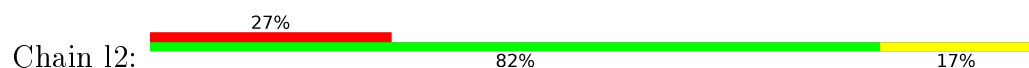
• Molecule 38: 5.8S ribosomal RNA



• Molecule 39: 60S ribosomal protein L2-A

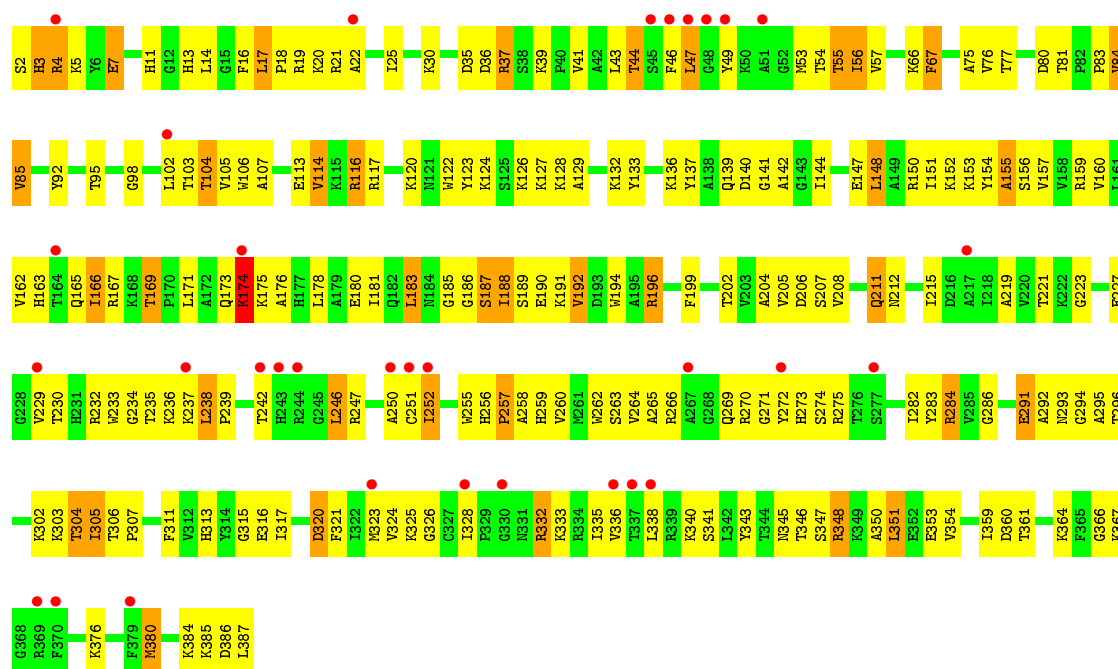


• Molecule 39: 60S ribosomal protein L2-A

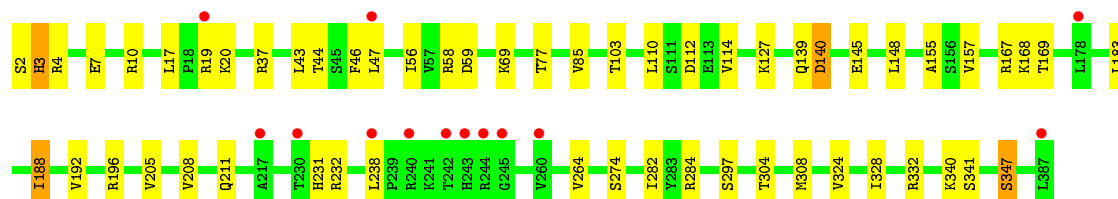
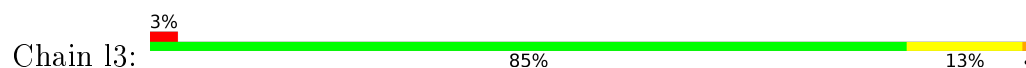


• Molecule 40: 60S ribosomal protein L3

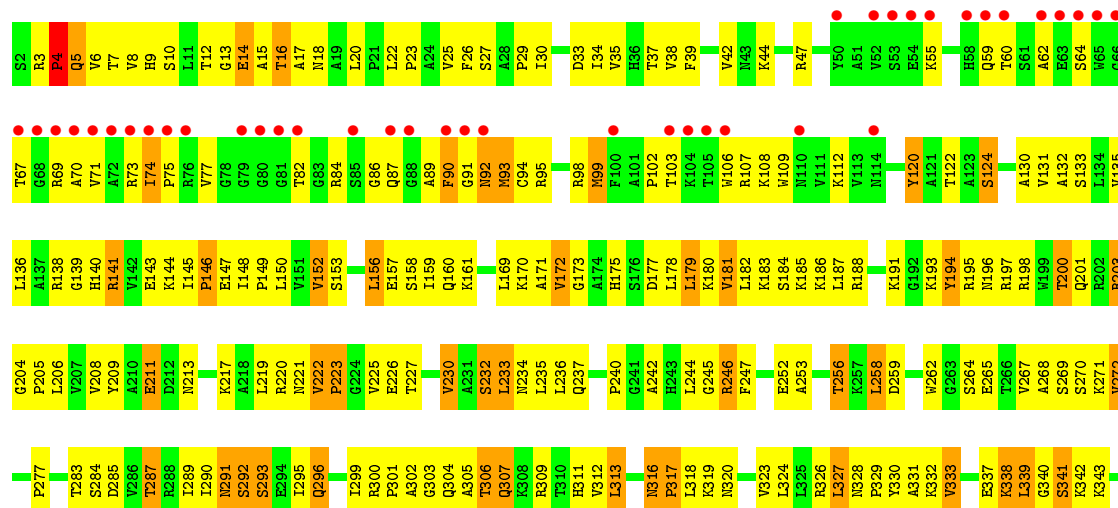
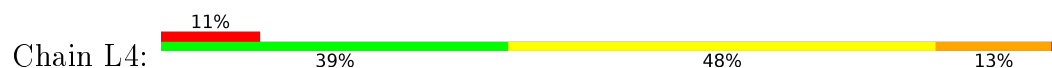


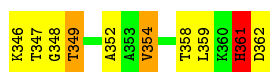


• Molecule 40: 60S ribosomal protein L3



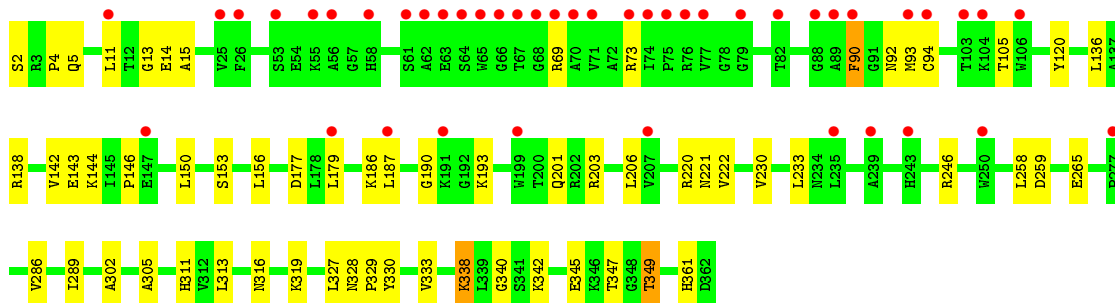
• Molecule 41: 60S ribosomal protein L4-A





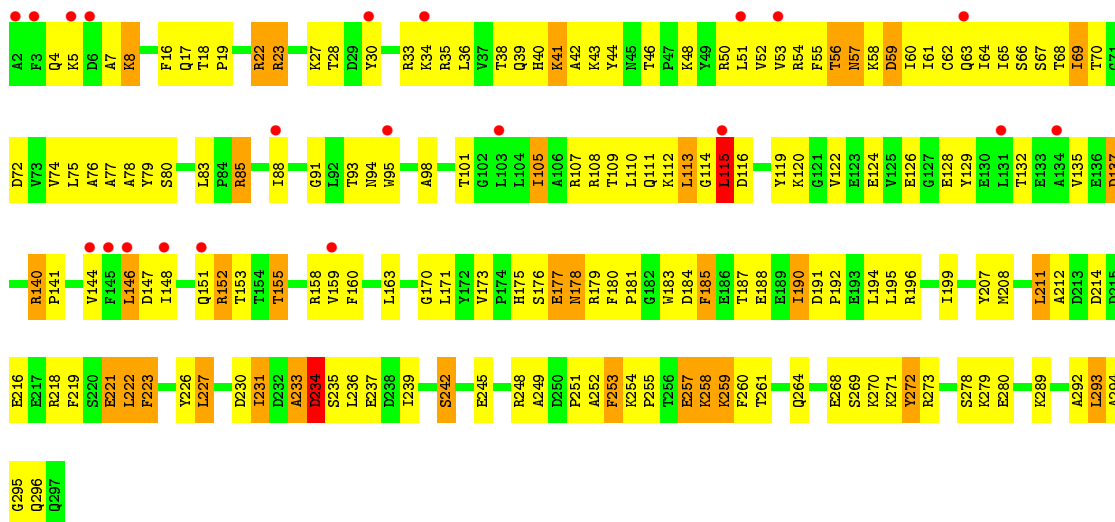
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: .



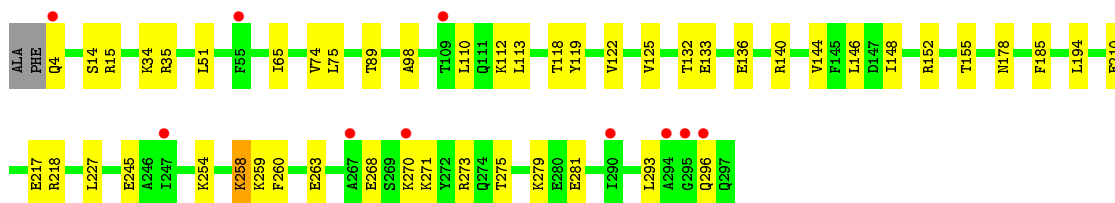
• Molecule 42: 60S ribosomal protein L5

Chain L5: .



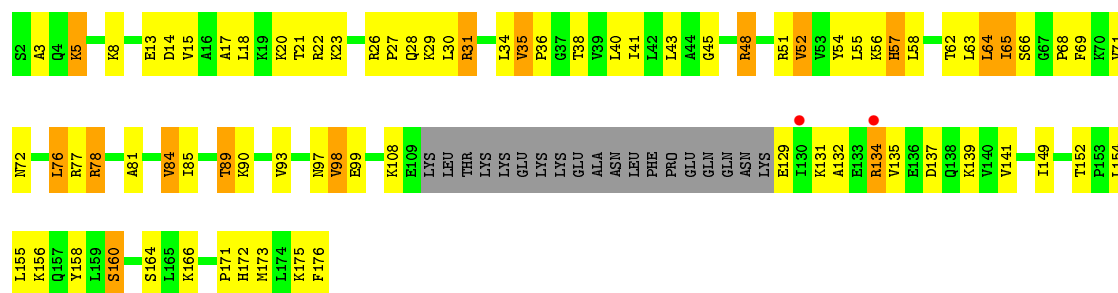
• Molecule 42: 60S ribosomal protein L5

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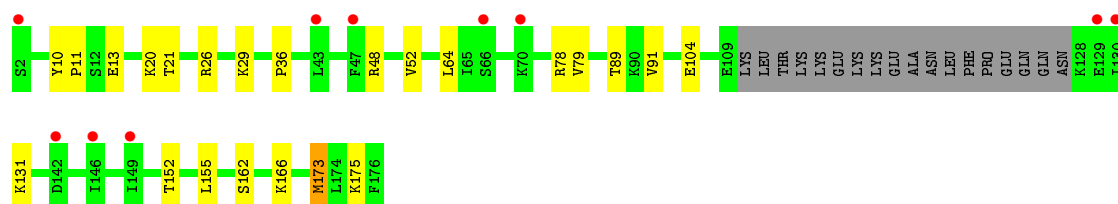
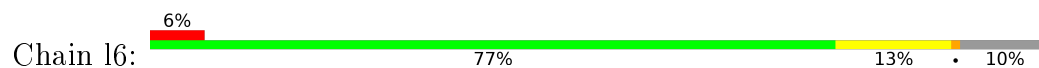


• Molecule 43: 60S ribosomal protein L6-A

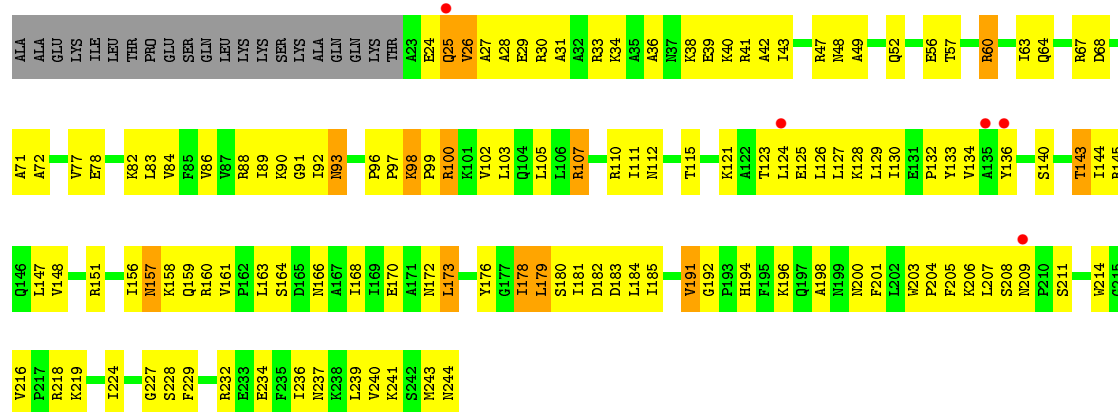
Chain L6: .



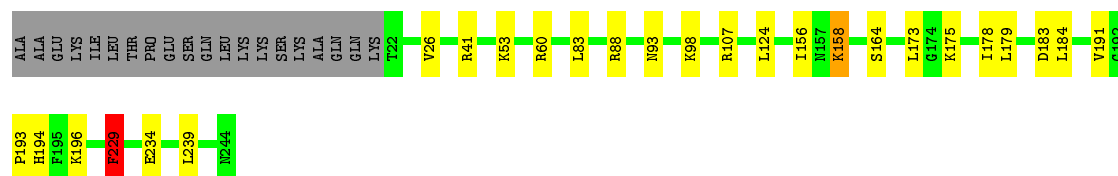
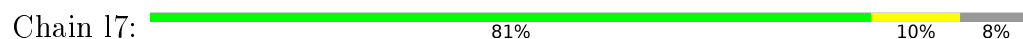
- Molecule 43: 60S ribosomal protein L6-A



- Molecule 44: 60S ribosomal protein L7-A

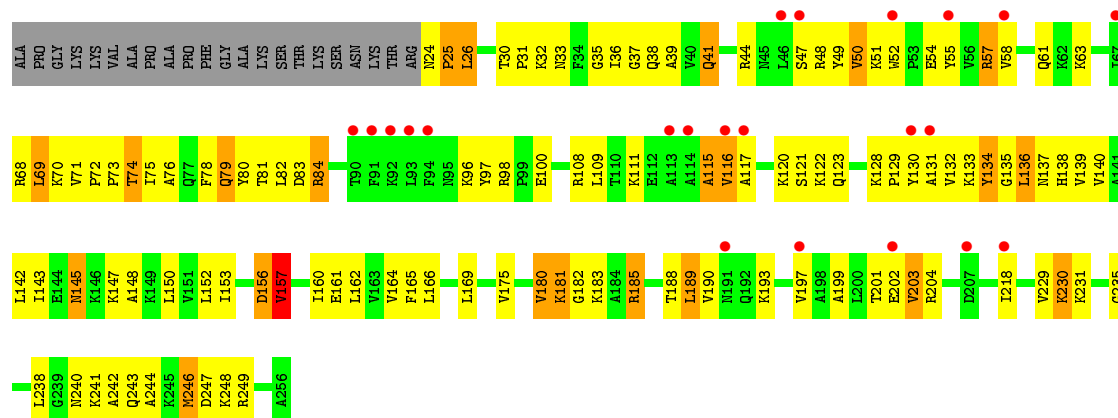


- Molecule 44: 60S ribosomal protein L7-A

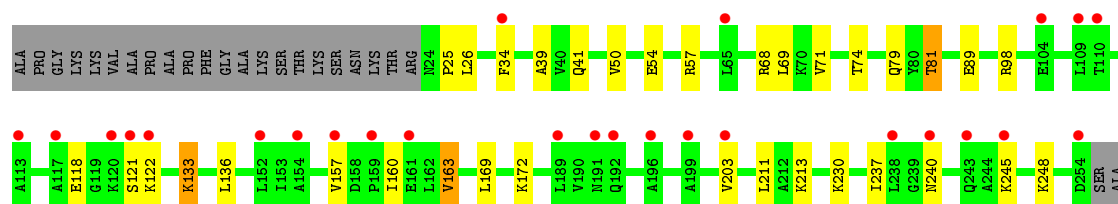
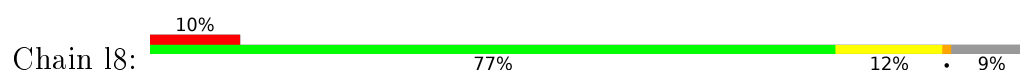


- Molecule 45: 60S ribosomal protein L8-A

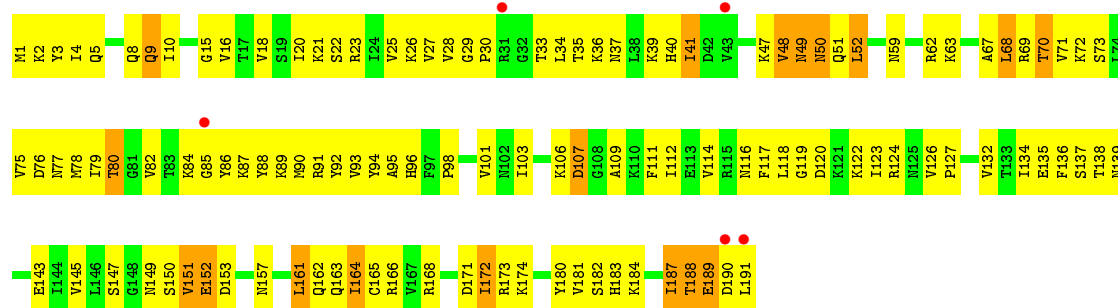




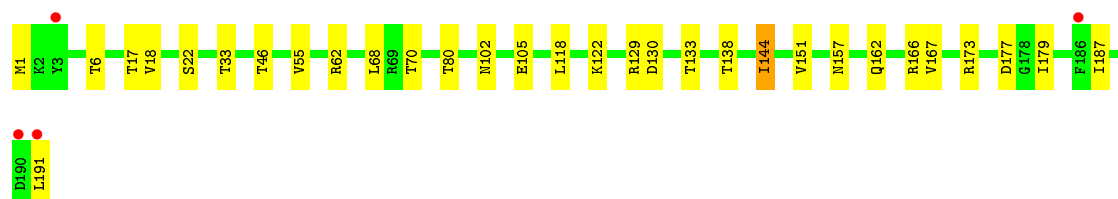
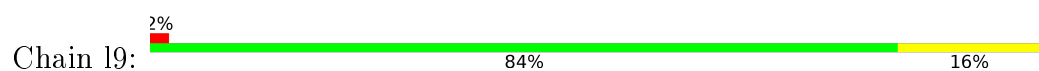
• Molecule 45: 60S ribosomal protein L8-A



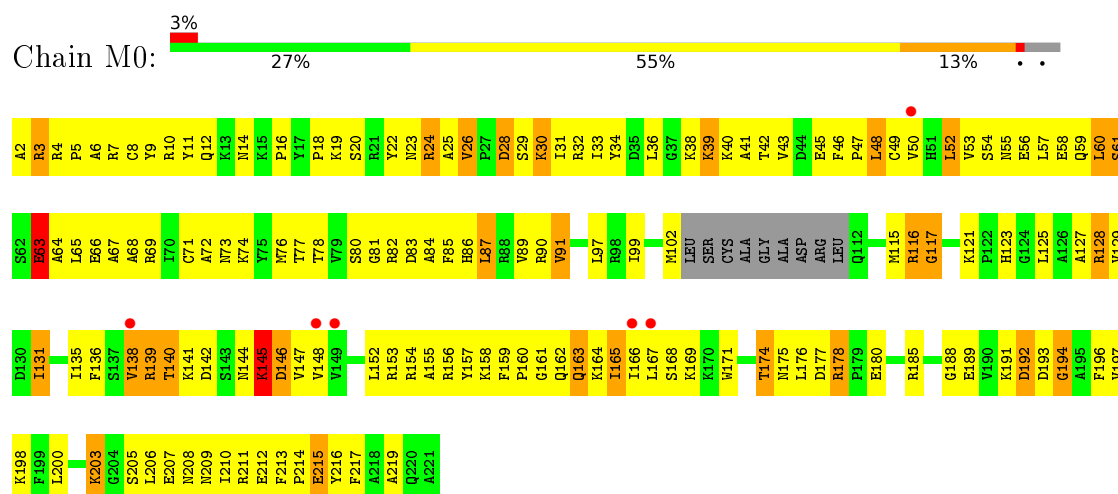
• Molecule 46: 60S ribosomal protein L9-A



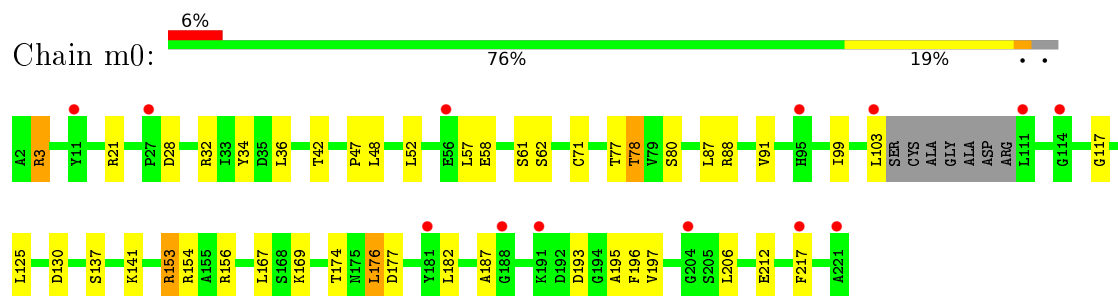
• Molecule 46: 60S ribosomal protein L9-A



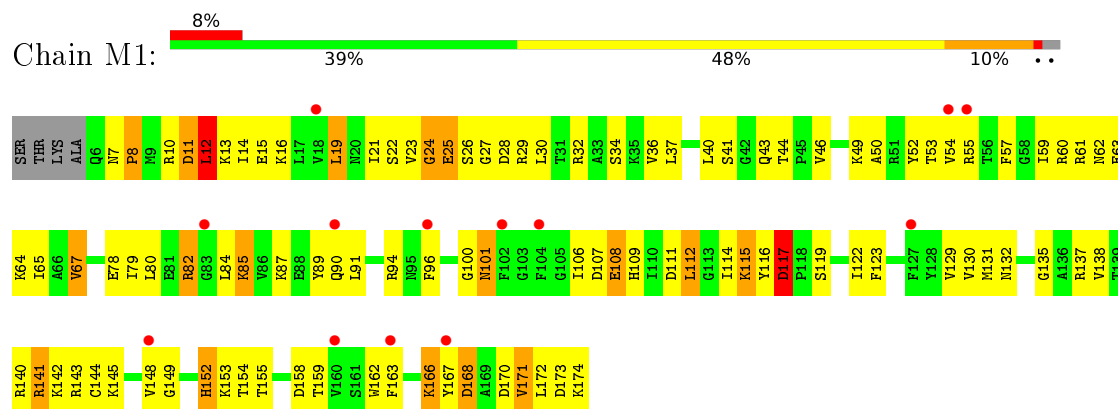
• Molecule 47: 60S ribosomal protein L10



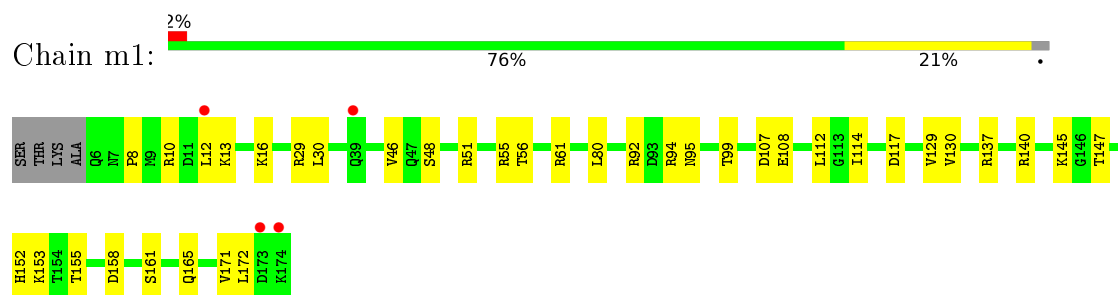
- Molecule 47: 60S ribosomal protein L10



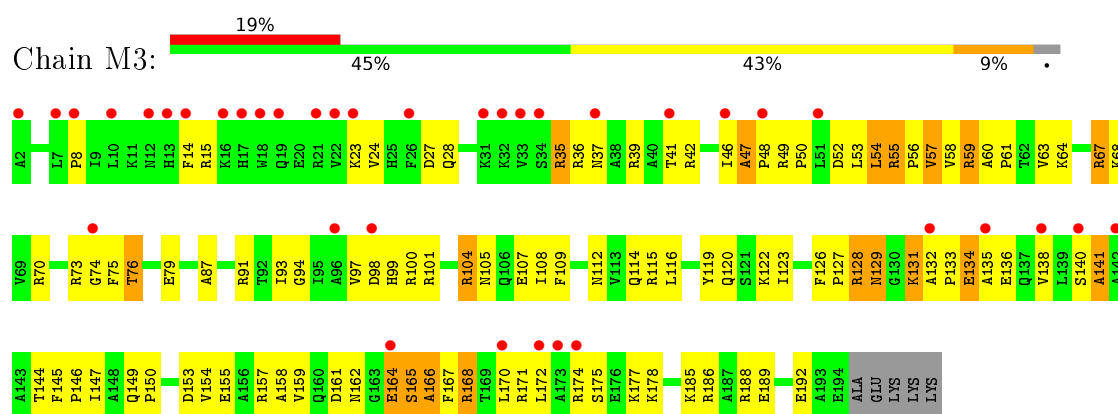
- Molecule 48: 60S ribosomal protein L11-B



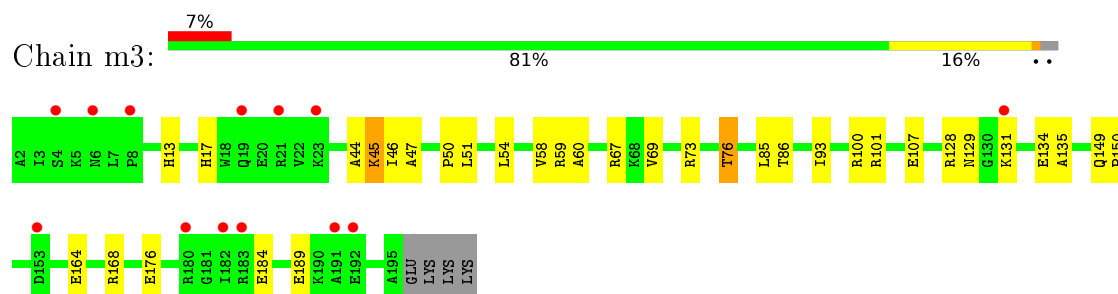
- Molecule 48: 60S ribosomal protein L11-B



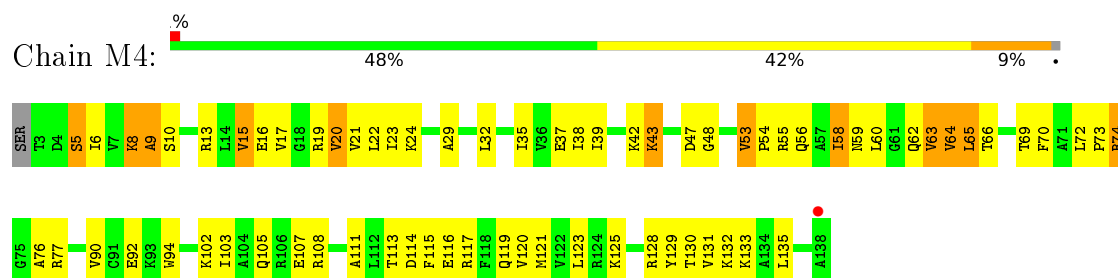
- Molecule 49: 60S ribosomal protein L13-A



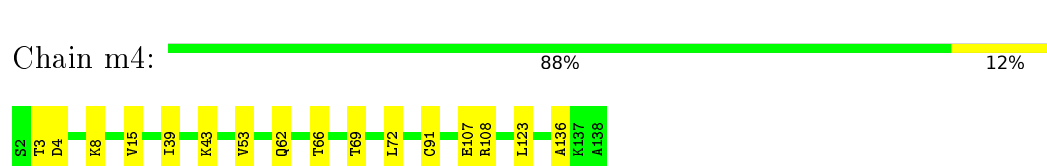
• Molecule 49: 60S ribosomal protein L13-A



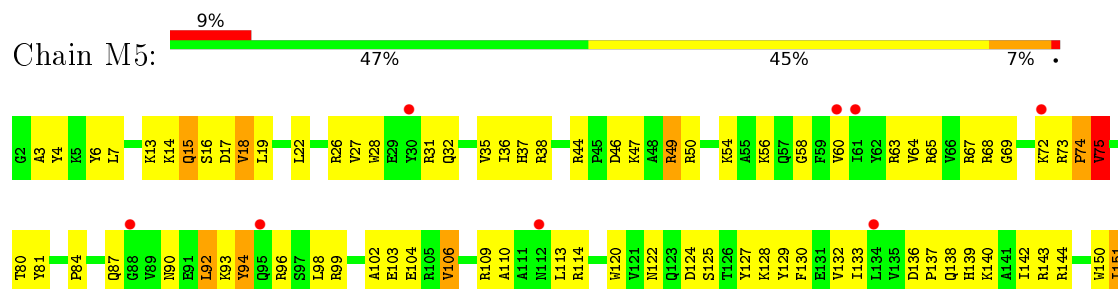
• Molecule 50: 60S ribosomal protein L14-A

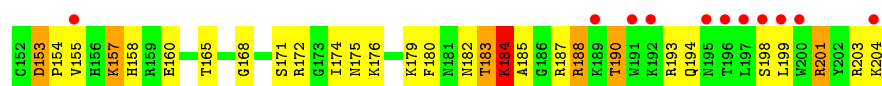


• Molecule 50: 60S ribosomal protein L14-A

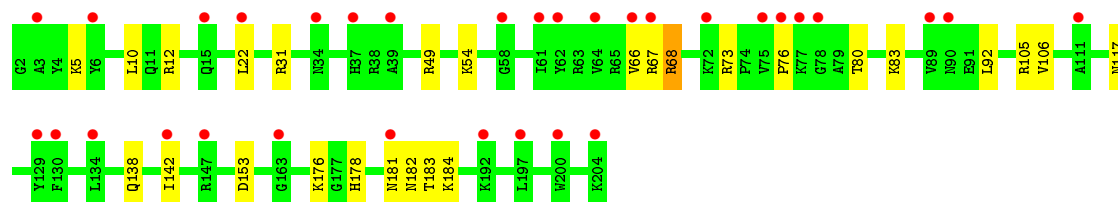
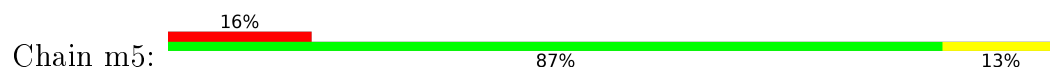


• Molecule 51: 60S ribosomal protein L15-A

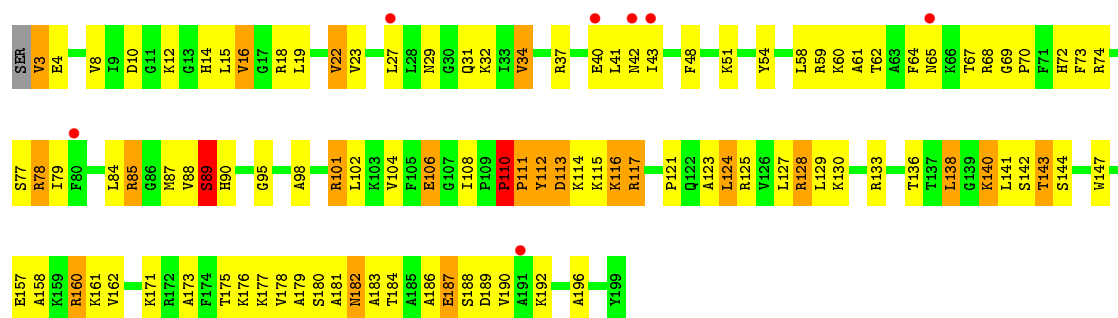




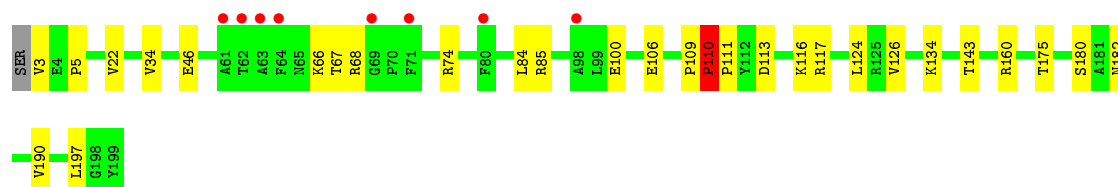
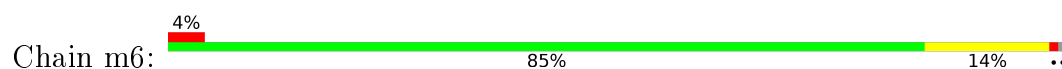
- Molecule 51: 60S ribosomal protein L15-A



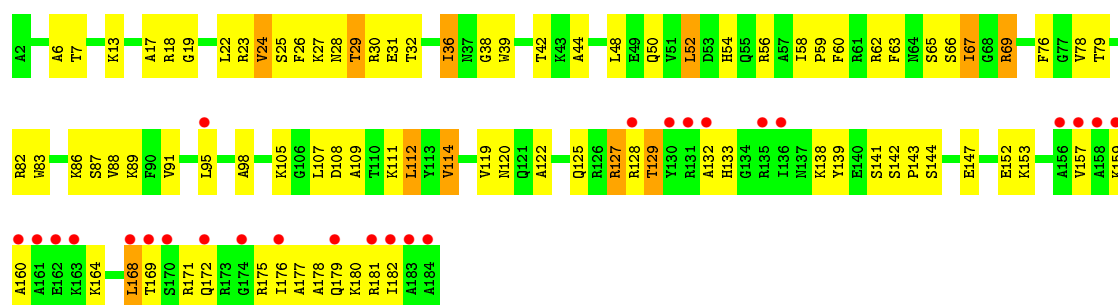
- Molecule 52: 60S ribosomal protein L16-A



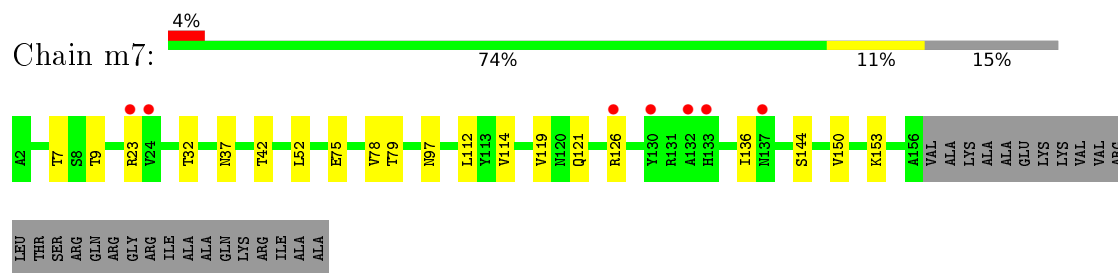
- Molecule 52: 60S ribosomal protein L16-A



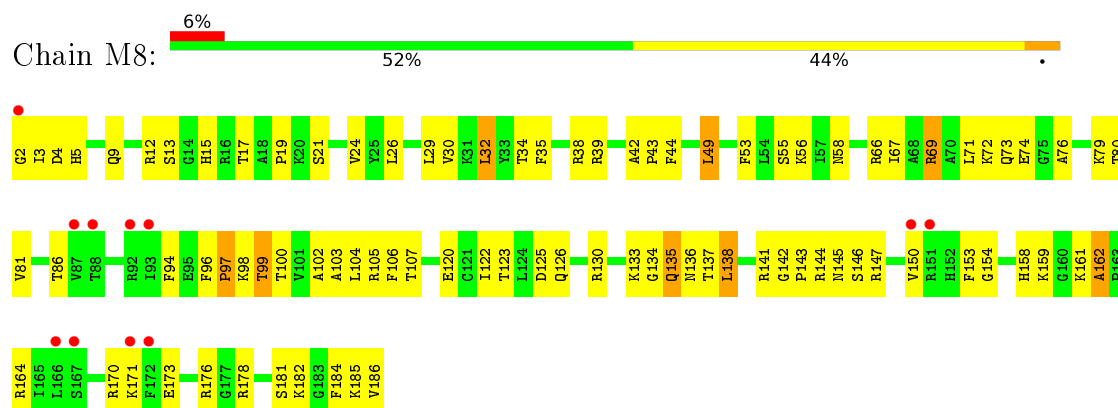
- Molecule 53: 60S ribosomal protein L17-A



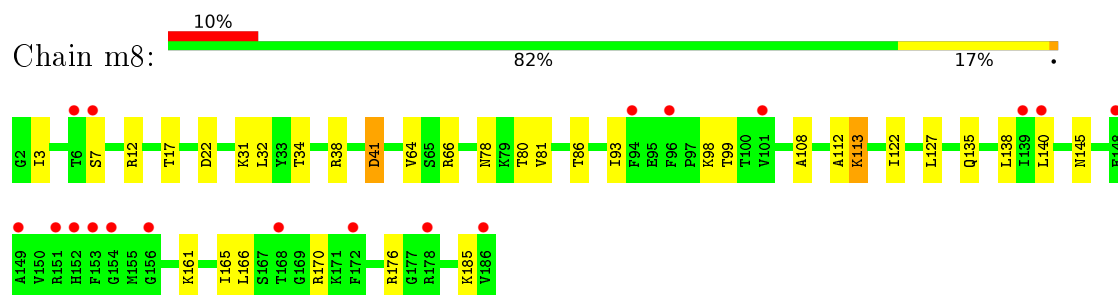
- Molecule 53: 60S ribosomal protein L17-A



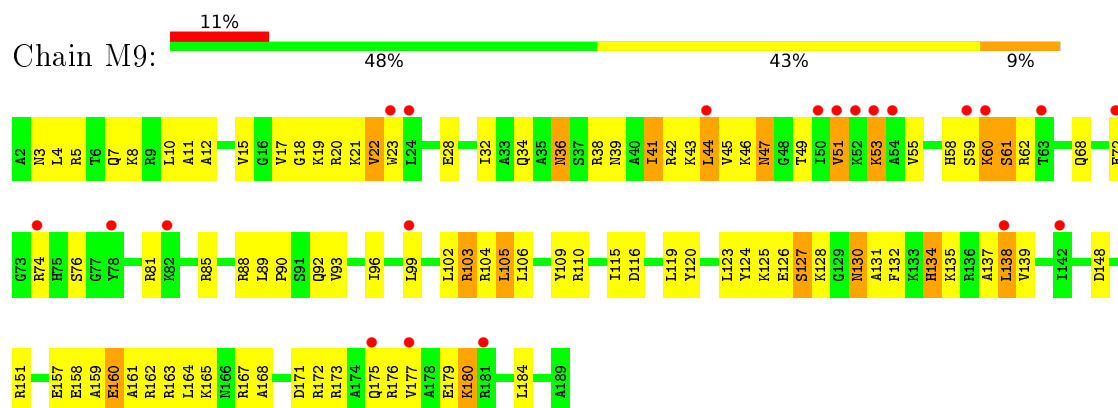
- Molecule 54: 60S ribosomal protein L18-A



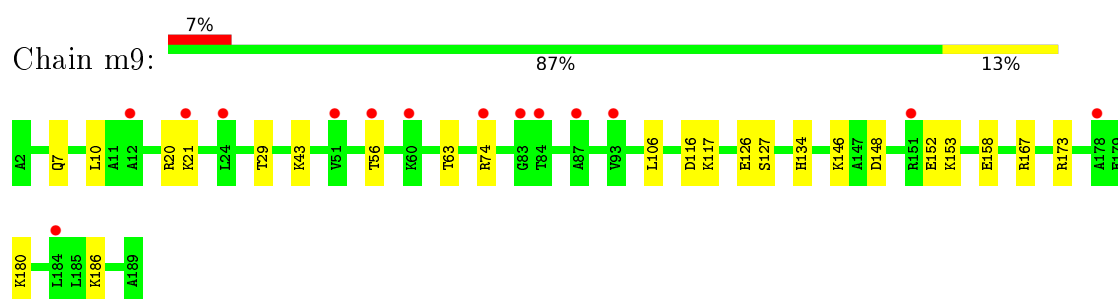
- Molecule 54: 60S ribosomal protein L18-A



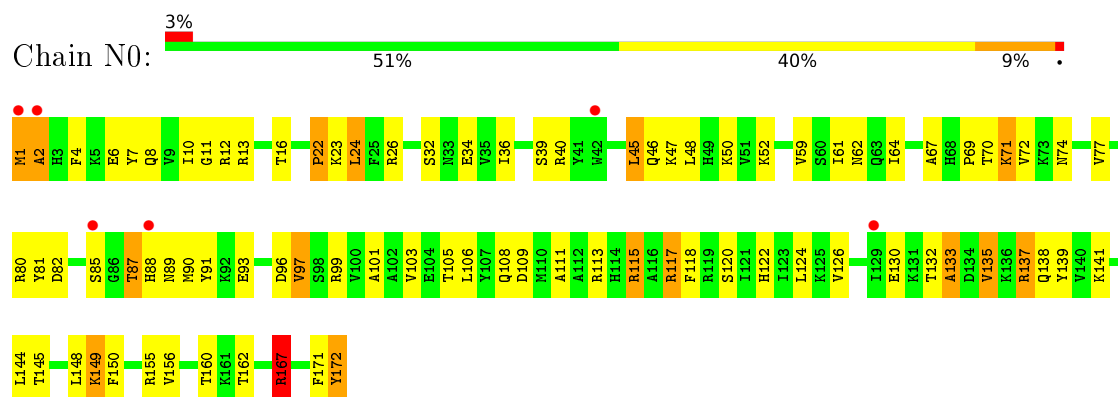
- Molecule 55: 60S ribosomal protein L19-A



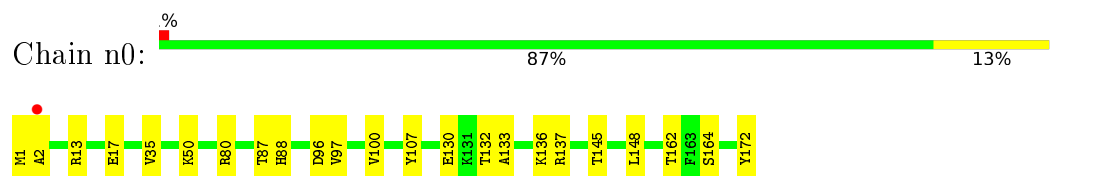
- Molecule 55: 60S ribosomal protein L19-A



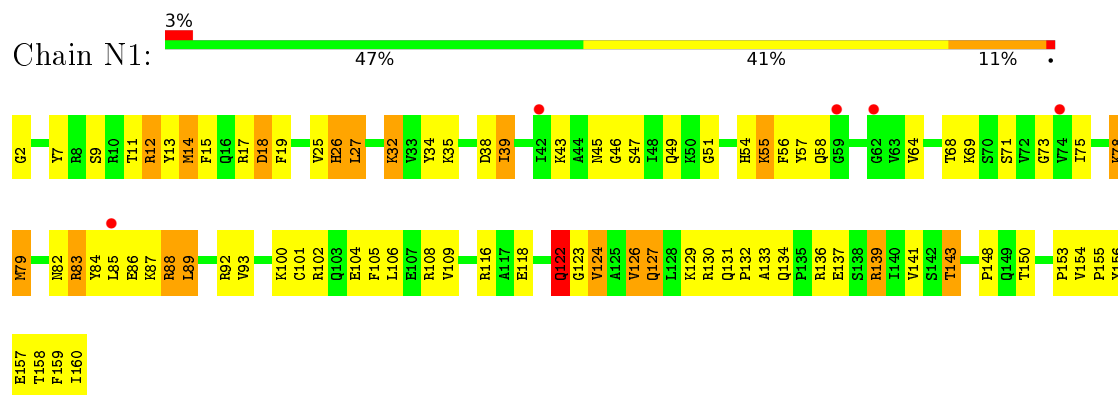
- Molecule 56: 60S ribosomal protein L20-A



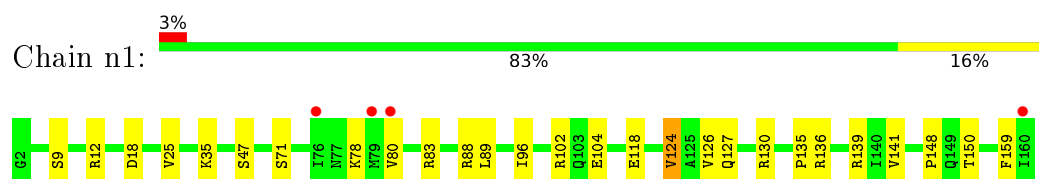
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A



- Molecule 57: 60S ribosomal protein L21-A

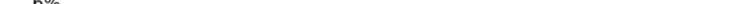


Chain N2:

Position	Amino Acid
1	K31
2	K82
3	Y83
4	L84
5	K85
6	K86
7	N87
8	K88
9	L89
10	R90
11	D91
12	N92
13	I93
14	R94
15	F95
16	V96
17	S97
18	T98
19	K99
20	T100
21	Y103
22	R104
23	L105
24	A106
25	F107
26	Y108
27	GLN
28	VAL
29	THR
30	PRO
31	GLU
32	GLU
33	GLU
34	ASP
35	GLU
36	GLU
37	GLU
38	ASP
39	GLU
40	GLU
41	GLU
42	GLU
43	GLU
44	GLU
45	GLU
46	GLU
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169	GLU
170	GLU
171	GLU
172	GLU
173	GLU
174	GLU
175	GLU
176	GLU
177	GLU
178	GLU
179	GLU
180	GLU

[illegible]

Chain N3:

Chain n3: 

Chain N4:

Sequence logo for Chain N4. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. The logo is divided into three segments: 25% (red), 32% (green), and 29% (yellow). A 37% segment is also indicated at the end.

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%

M1 I5 K12 T19 D25 S26 K27 L39 F59 I63 T64 E65 E66 V67 A68 K69 K70 K71 S72 R73 K74 T75 V76 Q79 T83 G84 A85 S86 L87 D88 L89 I90 R94 S95 L96 E99 E107 K127 G132 T133 Q134 S135 SER LYS PHE SER

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

• Molecule 61: 60S ribosomal protein L25

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

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS VAL VAL LYS GLY THR ASN GLY LYS K22 A23 L24 K25 V26 R27 T28 F32 R33 R34 R35 K36 T37 L38 K39 L40 L41 R42 K45 A47 Y46 S48 S49 A50 V51 P52 H53 R56 L57 D58 S59 Y60 K61 V62 I63 I67

T71 A72 M73 K74 K75 V76 N80 I81 L82 V86 K82 Y83 Q84 I85 A88 V89 K100 E103 E104 V105 D106 V107 L108 K109 V110 N111 V114 R115 P116 M117 G118 T119 K120 K121 A122 Y123 V124 R125 L126 T127 A128 D129 Y130 D131 A132 L133 D134 I135 A136 N137 I138 I139

I142

• Molecule 61: 60S ribosomal protein L25

Chain n5: 6% 74% 11% 15%

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS VAL VAL LYS GLY THR ASN GLY LYS LYS A23 R27 P44 K45 R55 R56 L57 V62 E63 E64 Q65 S69 A90 R91 R92 L108 T112 L113 V114 R115 T119 K120 Y123 V124 R125 I135 A136 N137

I142

• Molecule 62: 60S ribosomal protein L26-A

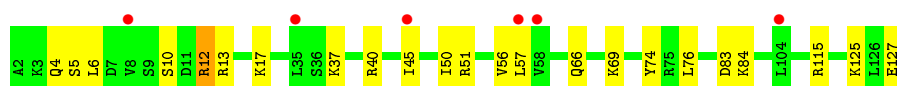
Chain N6: 2% 44% 46% 7%

A2 K3 Q4 S5 L6 D7 V8 S9 S10 R13 K14 A15 R16 Y19 S24 K37 E38 L39 R40 Q41 A42 Y43 G44 I45 I50 R51 R52 D53 E55 V56 L57 V58 V59 R60 K63 Q66 K69 I70 S71 S72 V73 Y74 R75 L76 K77 F78 A79 V80 D83 K84

V85 T86 K87 E88 K89 A93 S94 V95 P96 I97 N98 L99 H100 P101 S102 K103 L104 K108 L109 H110 L111 D112 K113 D114 K115 K116 I119 Q120 R121 K122 G124 K125 L126 E127

• Molecule 62: 60S ribosomal protein L26-A

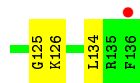
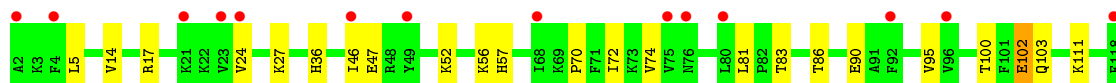
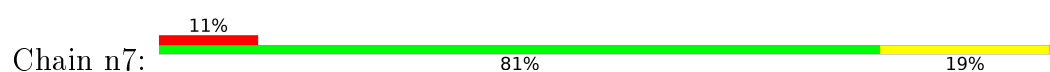
Chain n6: 5% 82% 17%



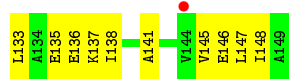
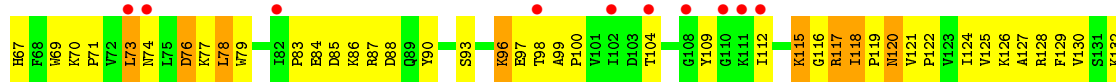
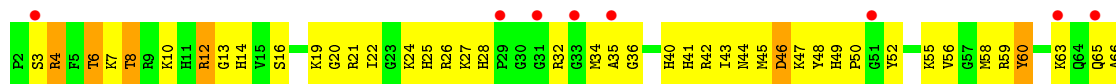
- Molecule 63: 60S ribosomal protein L27-A



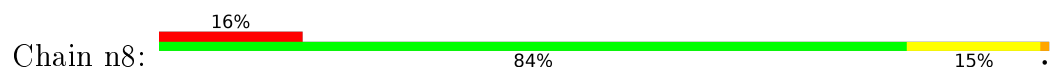
- Molecule 63: 60S ribosomal protein L27-A



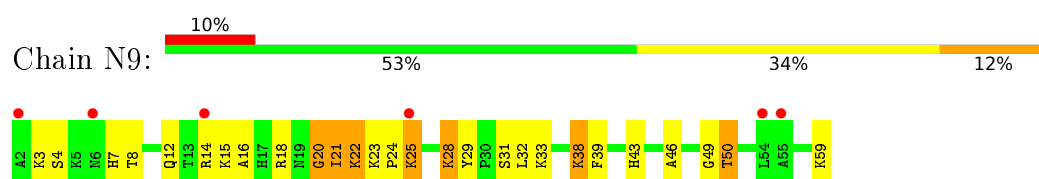
- Molecule 64: 60S ribosomal protein L28



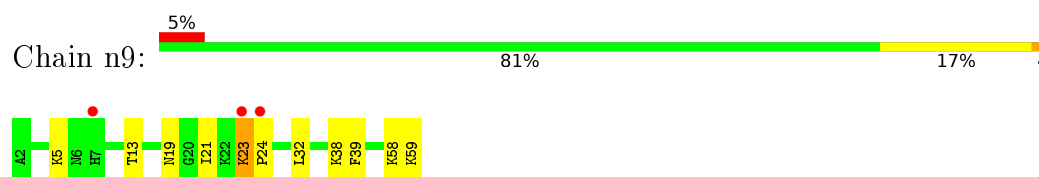
- Molecule 64: 60S ribosomal protein L28



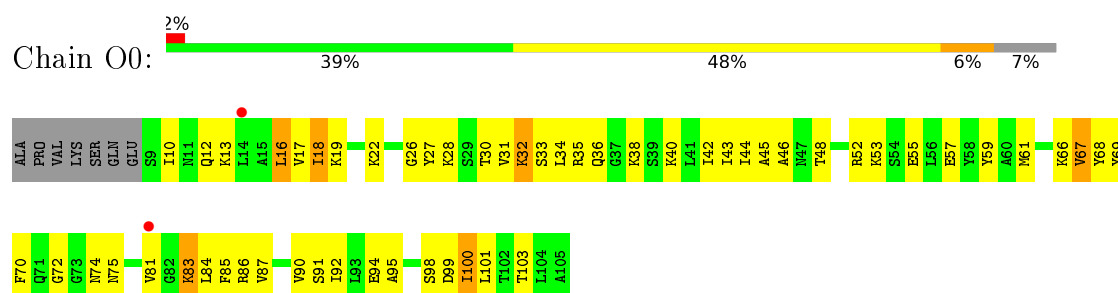
- Molecule 65: 60S ribosomal protein L29



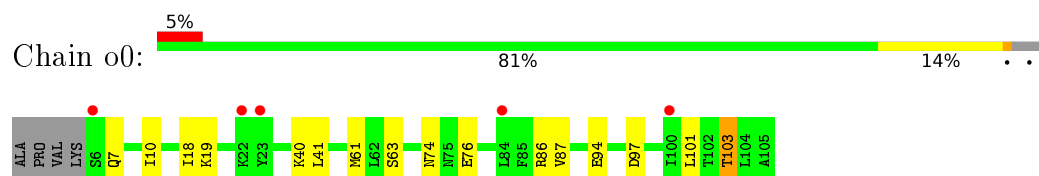
- Molecule 65: 60S ribosomal protein L29



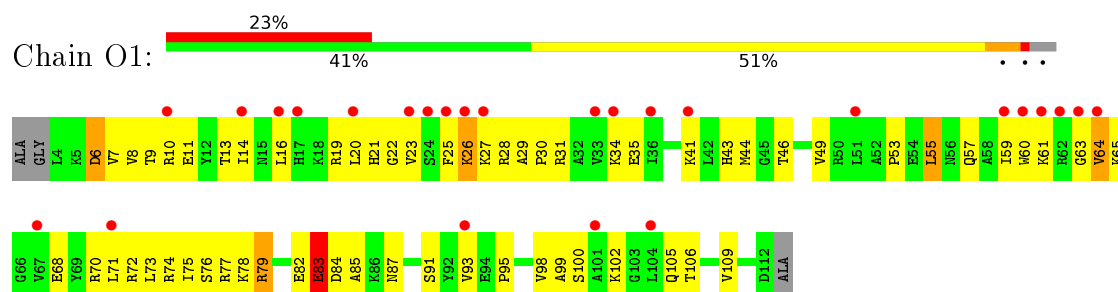
- Molecule 66: 60S ribosomal protein L30



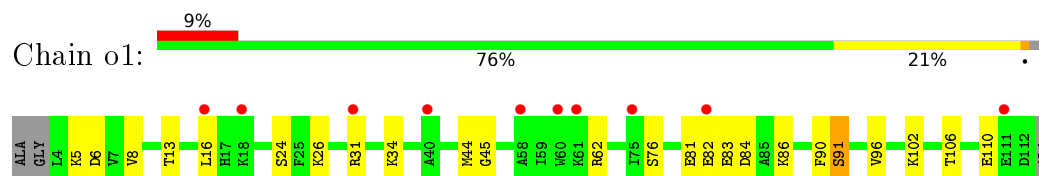
- Molecule 66: 60S ribosomal protein L30



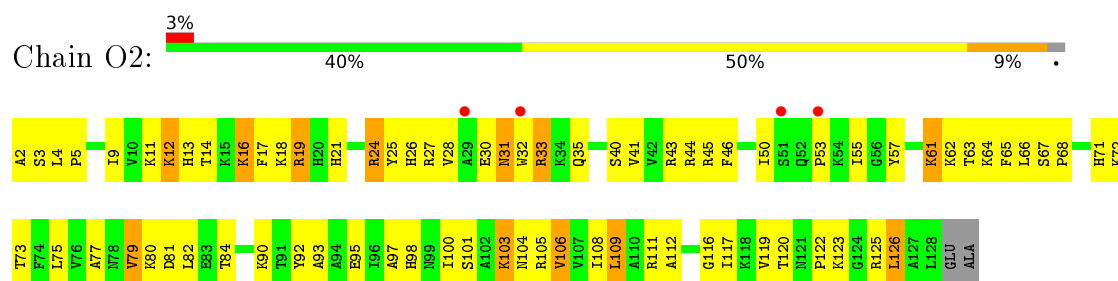
- Molecule 67: 60S ribosomal protein L31-A



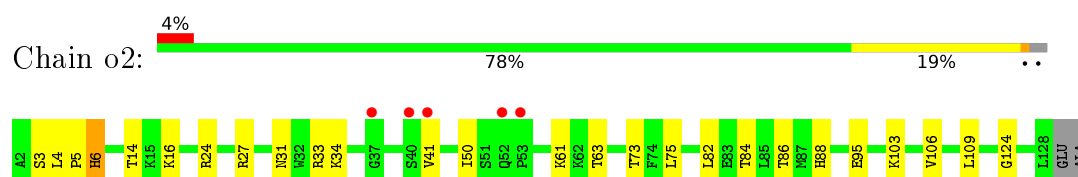
- Molecule 67: 60S ribosomal protein L31-A



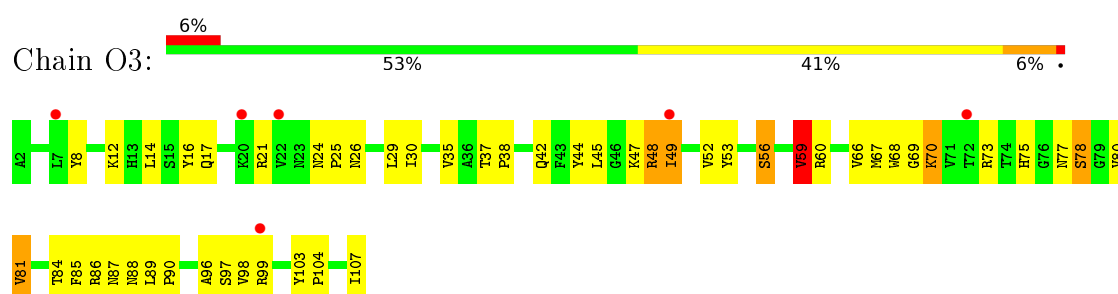
- Molecule 68: 60S ribosomal protein L32



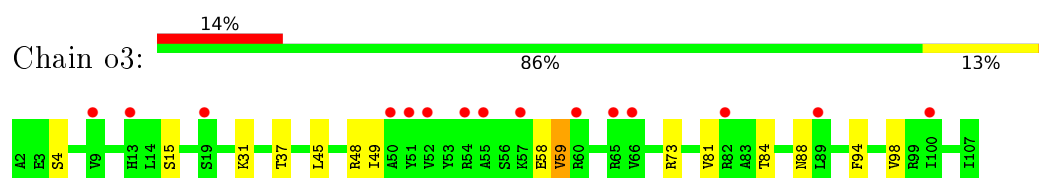
• Molecule 68: 60S ribosomal protein L32



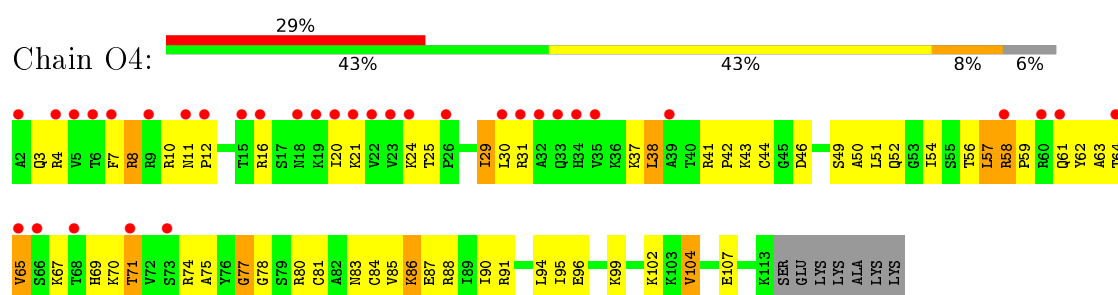
• Molecule 69: 60S ribosomal protein L33-A



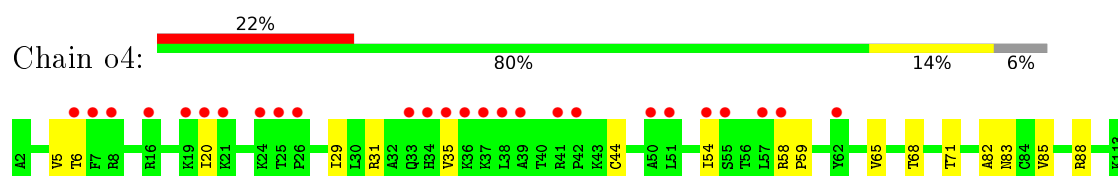
• Molecule 69: 60S ribosomal protein L33-A



• Molecule 70: 60S ribosomal protein L34-A

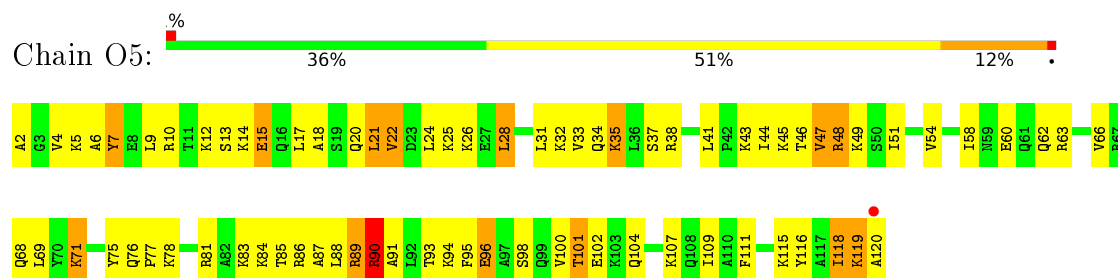


• Molecule 70: 60S ribosomal protein L34-A

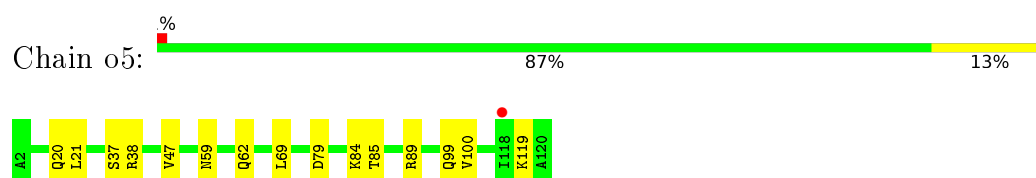


SER
GLU
LYS
LYS
LYS
ALA
LYS
LYS

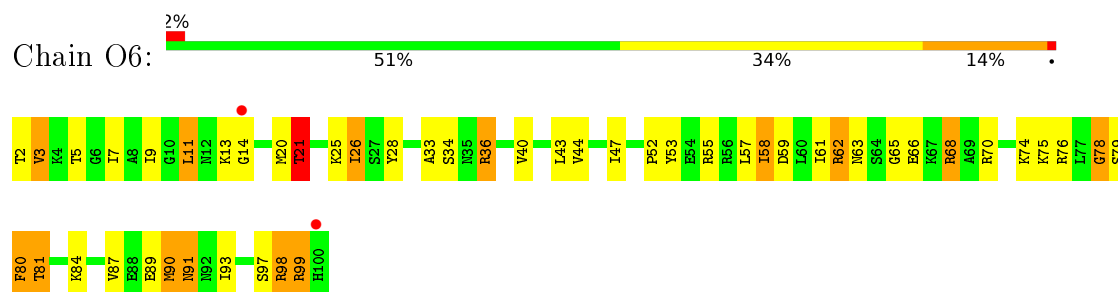
- Molecule 71: 60S ribosomal protein L35-A



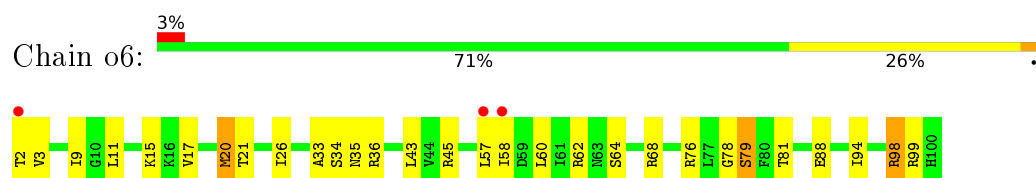
- Molecule 71: 60S ribosomal protein L35-A



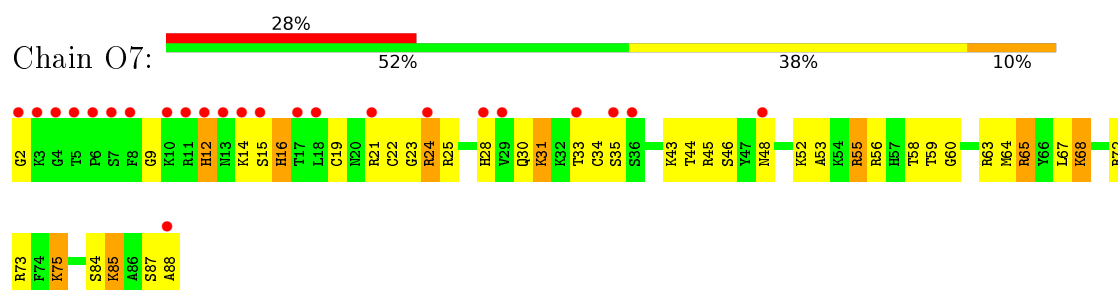
- Molecule 72: 60S ribosomal protein L36-A



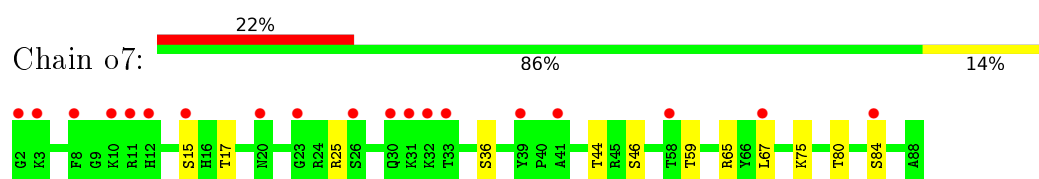
- Molecule 72: 60S ribosomal protein L36-A



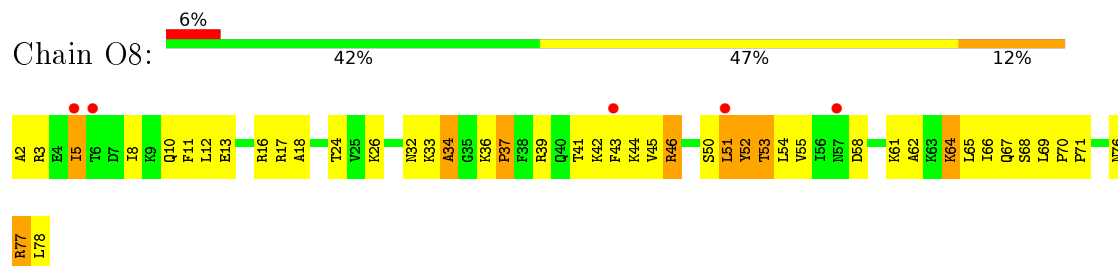
- Molecule 73: 60S ribosomal protein L37-A



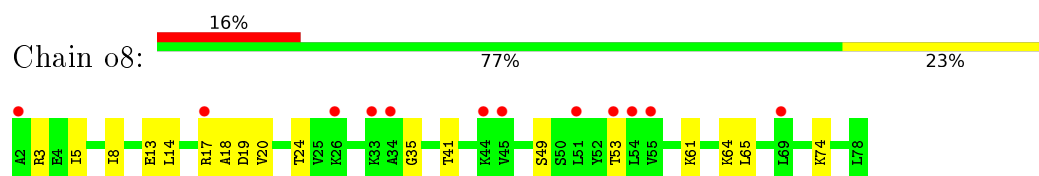
- Molecule 73: 60S ribosomal protein L37-A



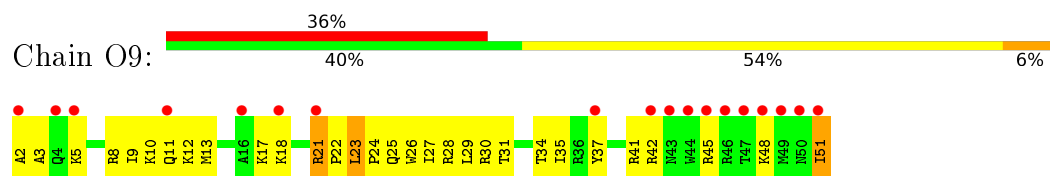
- Molecule 74: 60S ribosomal protein L38



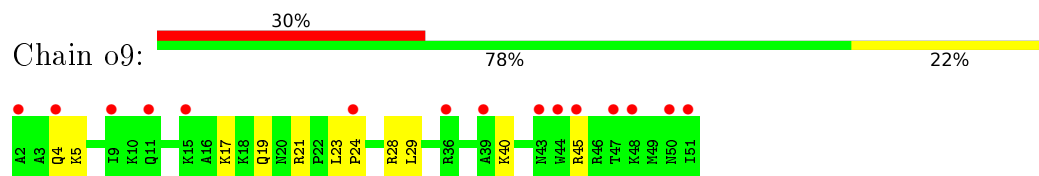
- Molecule 74: 60S ribosomal protein L38



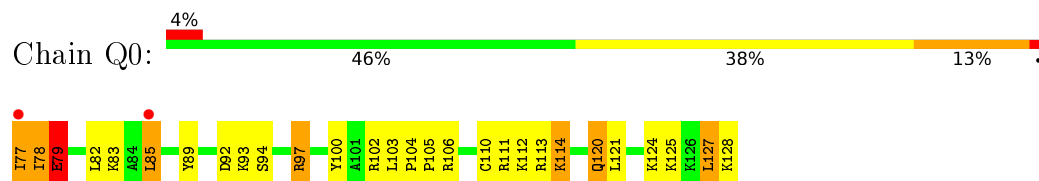
- Molecule 75: 60S ribosomal protein L39



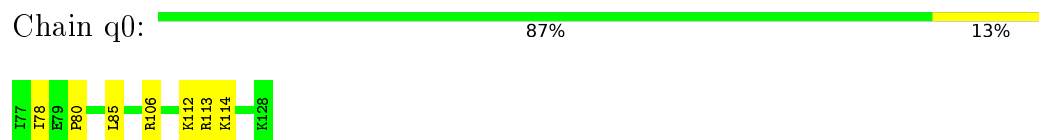
- Molecule 75: 60S ribosomal protein L39



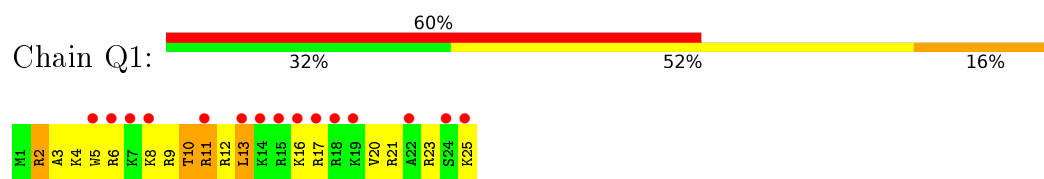
- Molecule 76: Ubiquitin-60S ribosomal protein L40



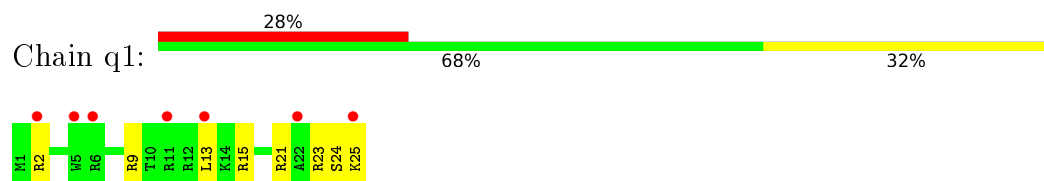
- Molecule 76: Ubiquitin-60S ribosomal protein L40



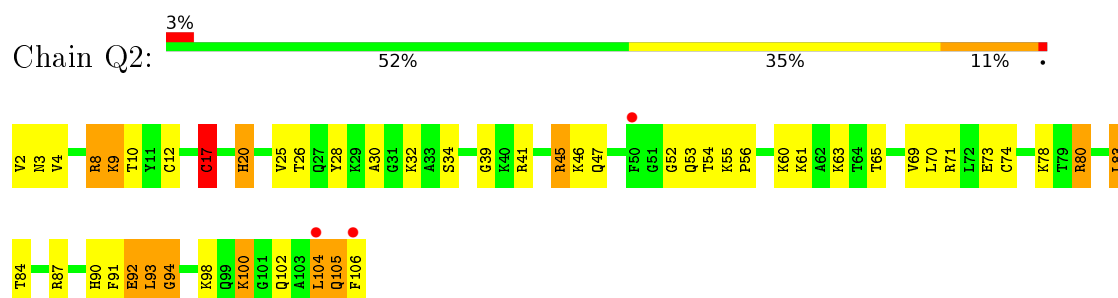
- Molecule 77: 60S ribosomal protein L41-A



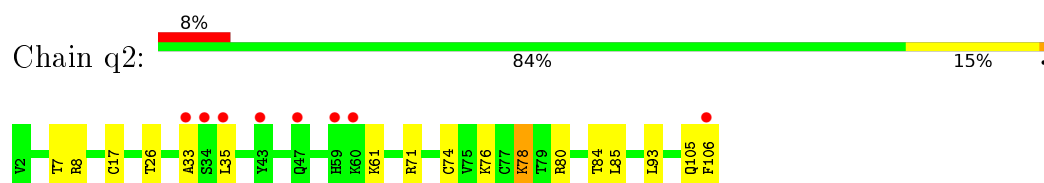
- Molecule 77: 60S ribosomal protein L41-A



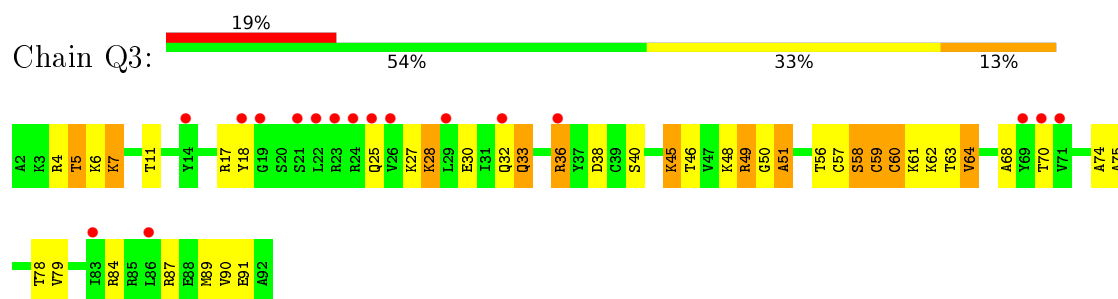
- Molecule 78: 60S ribosomal protein L42-A



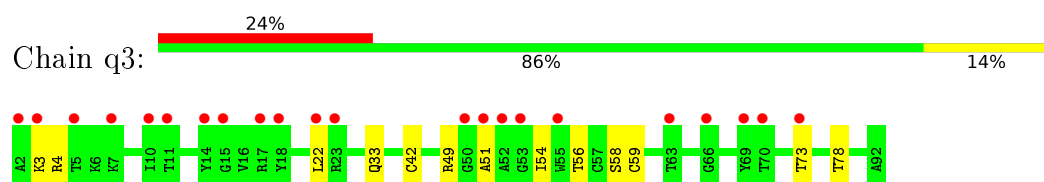
- Molecule 78: 60S ribosomal protein L42-A



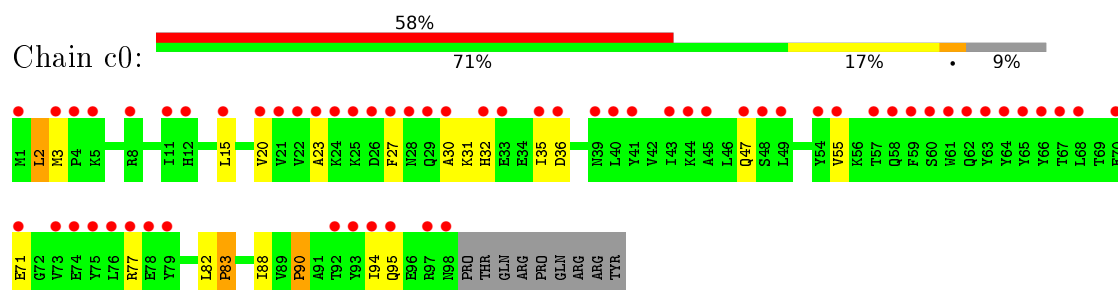
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S10-A

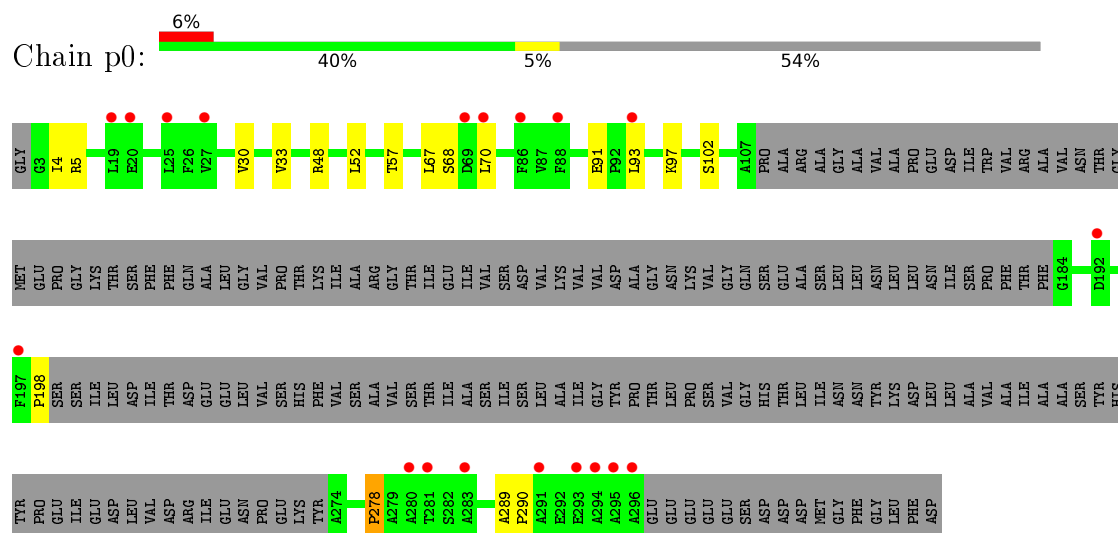


- Molecule 81: 60S ribosomal protein L12-A (uL11)



There are no outlier residues recorded for this chain.

- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: 60S ribosomal protein P1 alpha



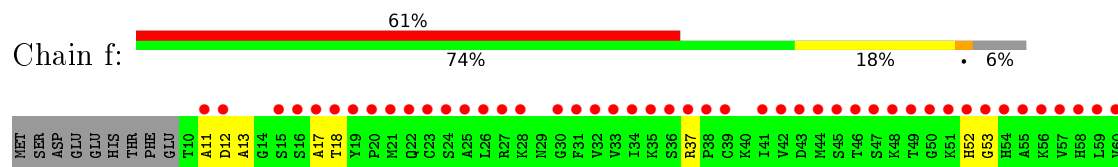
There are no outlier residues recorded for this chain.

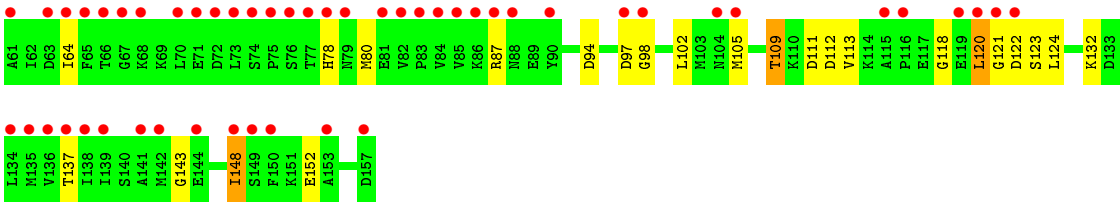
- Molecule 84: 60S ribosomal P2 beta



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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	86.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	14	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	689	1
1	6	38260	0	19252	679	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	1049	0
36	5	67780	0	34065	1005	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	8056	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 8056 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	6
2	s0	204/251 (81%)	158 (78%)	31 (15%)	15 (7%)	1	10
3	S1	212/254 (84%)	154 (73%)	36 (17%)	22 (10%)	1	4
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	2	17
4	S2	215/253 (85%)	174 (81%)	33 (15%)	8 (4%)	4	28
4	s2	215/253 (85%)	175 (81%)	26 (12%)	14 (6%)	1	13
5	S3	221/239 (92%)	189 (86%)	21 (10%)	11 (5%)	3	20
5	s3	221/239 (92%)	183 (83%)	27 (12%)	11 (5%)	3	20
6	S4	258/260 (99%)	205 (80%)	37 (14%)	16 (6%)	2	14
6	s4	258/260 (99%)	198 (77%)	44 (17%)	16 (6%)	2	14
7	S5	204/224 (91%)	163 (80%)	28 (14%)	13 (6%)	2	13
7	s5	204/224 (91%)	157 (77%)	30 (15%)	17 (8%)	1	7
8	S6	224/236 (95%)	198 (88%)	17 (8%)	9 (4%)	4	26
8	s6	216/236 (92%)	186 (86%)	24 (11%)	6 (3%)	6	37
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	10
10	S8	184/200 (92%)	159 (86%)	18 (10%)	7 (4%)	4	28
10	s8	184/200 (92%)	156 (85%)	21 (11%)	7 (4%)	4	28
11	S9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	4	28
11	s9	183/196 (93%)	151 (82%)	24 (13%)	8 (4%)	3	23
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	10
13	C1	153/155 (99%)	123 (80%)	23 (15%)	7 (5%)	3	22
13	c1	144/155 (93%)	122 (85%)	20 (14%)	2 (1%)	14	54
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	26
15	c3	148/150 (99%)	117 (79%)	21 (14%)	10 (7%)	1	11
16	C4	125/136 (92%)	92 (74%)	21 (17%)	12 (10%)	1	5
16	c4	126/136 (93%)	98 (78%)	19 (15%)	9 (7%)	1	10
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	13
18	c6	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	3	25
19	C7	116/136 (85%)	89 (77%)	20 (17%)	7 (6%)	2	15
19	c7	113/136 (83%)	89 (79%)	16 (14%)	8 (7%)	1	10
20	C8	143/145 (99%)	109 (76%)	27 (19%)	7 (5%)	3	21
20	c8	143/145 (99%)	116 (81%)	21 (15%)	6 (4%)	3	25
21	C9	141/143 (99%)	115 (82%)	19 (14%)	7 (5%)	3	20
21	c9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	4	30
22	D0	105/120 (88%)	90 (86%)	9 (9%)	6 (6%)	2	17
22	d0	108/120 (90%)	87 (81%)	18 (17%)	3 (3%)	6	37
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	10
24	D2	127/129 (98%)	111 (87%)	12 (9%)	4 (3%)	5	34
24	d2	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	7	41
25	D3	142/144 (99%)	109 (77%)	20 (14%)	13 (9%)	1	5
25	d3	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	9	45
26	D4	132/134 (98%)	114 (86%)	8 (6%)	10 (8%)	1	9
26	d4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	2	15
27	D5	68/107 (64%)	47 (69%)	15 (22%)	6 (9%)	1	6
27	d5	67/107 (63%)	52 (78%)	14 (21%)	1 (2%)	13	53
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	18
29	D7	79/81 (98%)	58 (73%)	18 (23%)	3 (4%)	4	28
29	d7	79/81 (98%)	62 (78%)	15 (19%)	2 (2%)	7	40
30	D8	61/66 (92%)	53 (87%)	6 (10%)	2 (3%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	d8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	12
31	D9	51/55 (93%)	42 (82%)	6 (12%)	3 (6%)	2	16
31	d9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	16
32	E0	58/62 (94%)	48 (83%)	7 (12%)	3 (5%)	2	19
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	20
34	sR	316/318 (99%)	264 (84%)	39 (12%)	13 (4%)	3	26
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	29
39	l2	250/253 (99%)	208 (83%)	32 (13%)	10 (4%)	4	26
40	L3	384/386 (100%)	332 (86%)	39 (10%)	13 (3%)	5	31
40	l3	384/386 (100%)	341 (89%)	38 (10%)	5 (1%)	15	56
41	L4	359/361 (99%)	296 (82%)	38 (11%)	25 (7%)	1	10
41	l4	359/361 (99%)	295 (82%)	42 (12%)	22 (6%)	2	15
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	37
43	L6	152/175 (87%)	135 (89%)	13 (9%)	4 (3%)	7	39
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	7	39
44	L7	220/243 (90%)	190 (86%)	24 (11%)	6 (3%)	6	37
44	l7	221/243 (91%)	199 (90%)	17 (8%)	5 (2%)	8	42
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	3	21
45	l8	229/255 (90%)	178 (78%)	37 (16%)	14 (6%)	2	15
46	L9	189/191 (99%)	161 (85%)	20 (11%)	8 (4%)	3	25
46	l9	189/191 (99%)	170 (90%)	16 (8%)	3 (2%)	12	52
47	M0	207/220 (94%)	169 (82%)	32 (16%)	6 (3%)	6	36
47	m0	209/220 (95%)	161 (77%)	35 (17%)	13 (6%)	2	14
48	M1	167/173 (96%)	130 (78%)	25 (15%)	12 (7%)	1	10
48	m1	167/173 (96%)	139 (83%)	18 (11%)	10 (6%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	149 (78%)	34 (18%)	8 (4%)	3	25
49	m3	192/198 (97%)	148 (77%)	30 (16%)	14 (7%)	1	10
50	M4	134/137 (98%)	116 (87%)	14 (10%)	4 (3%)	5	35
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	13	53
51	M5	201/203 (99%)	178 (89%)	16 (8%)	7 (4%)	4	30
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	7	40
52	M6	195/198 (98%)	171 (88%)	17 (9%)	7 (4%)	4	29
52	m6	195/198 (98%)	173 (89%)	18 (9%)	4 (2%)	9	45
53	M7	181/183 (99%)	149 (82%)	26 (14%)	6 (3%)	5	32
53	m7	153/183 (84%)	140 (92%)	11 (7%)	2 (1%)	15	56
54	M8	183/185 (99%)	157 (86%)	22 (12%)	4 (2%)	8	43
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	5	32
55	M9	186/188 (99%)	164 (88%)	19 (10%)	3 (2%)	12	52
55	m9	186/188 (99%)	166 (89%)	20 (11%)	0	100	100
56	N0	170/172 (99%)	150 (88%)	13 (8%)	7 (4%)	3	26
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	30	72
57	N1	157/159 (99%)	135 (86%)	16 (10%)	6 (4%)	4	28
57	n1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	5	33
58	N2	98/120 (82%)	73 (74%)	21 (21%)	4 (4%)	3	26
58	n2	96/120 (80%)	84 (88%)	8 (8%)	4 (4%)	3	25
59	N3	134/136 (98%)	117 (87%)	11 (8%)	6 (4%)	3	23
59	n3	134/136 (98%)	121 (90%)	7 (5%)	6 (4%)	3	23
60	N4	96/155 (62%)	76 (79%)	15 (16%)	5 (5%)	2	19
60	n4	133/155 (86%)	109 (82%)	16 (12%)	8 (6%)	2	15
61	N5	119/141 (84%)	101 (85%)	16 (13%)	2 (2%)	11	50
61	n5	118/141 (84%)	101 (86%)	13 (11%)	4 (3%)	5	31
62	N6	124/126 (98%)	109 (88%)	13 (10%)	2 (2%)	12	52
62	n6	124/126 (98%)	104 (84%)	16 (13%)	4 (3%)	5	33
63	N7	133/135 (98%)	106 (80%)	16 (12%)	11 (8%)	1	7
63	n7	133/135 (98%)	111 (84%)	15 (11%)	7 (5%)	2	18
64	N8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	3	26
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	4	29
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	26
67	O1	107/112 (96%)	92 (86%)	9 (8%)	6 (6%)	2	17
67	o1	107/112 (96%)	91 (85%)	9 (8%)	7 (6%)	1	13
68	O2	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	24	66
68	o2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	7	41
69	O3	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	19	62
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	6	36
70	O4	110/119 (92%)	94 (86%)	15 (14%)	1 (1%)	21	64
70	o4	110/119 (92%)	93 (84%)	15 (14%)	2 (2%)	11	49
71	O5	117/119 (98%)	97 (83%)	14 (12%)	6 (5%)	2	20
71	o5	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11	50
72	O6	97/99 (98%)	78 (80%)	12 (12%)	7 (7%)	1	10
72	o6	97/99 (98%)	76 (78%)	13 (13%)	8 (8%)	1	7
73	O7	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	16	58
73	o7	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
74	O8	75/77 (97%)	63 (84%)	9 (12%)	3 (4%)	4	26
74	o8	75/77 (97%)	59 (79%)	10 (13%)	6 (8%)	1	8
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	9	45
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	25
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	15
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	4	26
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	11
78	q2	103/105 (98%)	88 (85%)	11 (11%)	4 (4%)	4	27
79	Q3	89/91 (98%)	77 (86%)	6 (7%)	6 (7%)	1	12
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	8	43

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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	25
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	20

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	15
2	s0	165/209 (79%)	142 (86%)	23 (14%)	4	21
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	13
3	s1	192/223 (86%)	157 (82%)	35 (18%)	2	10
4	S2	176/204 (86%)	148 (84%)	28 (16%)	3	15
4	s2	176/204 (86%)	141 (80%)	35 (20%)	1	8
5	S3	182/194 (94%)	153 (84%)	29 (16%)	3	15
5	s3	182/194 (94%)	150 (82%)	32 (18%)	2	11
6	S4	221/221 (100%)	188 (85%)	33 (15%)	4	17
6	s4	221/221 (100%)	192 (87%)	29 (13%)	5	24
7	S5	173/190 (91%)	154 (89%)	19 (11%)	8	32
7	s5	173/190 (91%)	150 (87%)	23 (13%)	5	23
8	S6	188/201 (94%)	160 (85%)	28 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	s6	187/201 (93%)	158 (84%)	29 (16%)	3	16
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2	13
9	s7	165/169 (98%)	146 (88%)	19 (12%)	7	30
10	S8	150/161 (93%)	132 (88%)	18 (12%)	6	28
10	s8	150/161 (93%)	132 (88%)	18 (12%)	6	28
11	S9	158/165 (96%)	133 (84%)	25 (16%)	3	15
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	9
12	C0	77/98 (79%)	66 (86%)	11 (14%)	4	19
13	C1	129/136 (95%)	120 (93%)	9 (7%)	19	57
13	c1	129/136 (95%)	113 (88%)	16 (12%)	6	26
14	C2	88/118 (75%)	76 (86%)	12 (14%)	5	22
14	c2	88/118 (75%)	76 (86%)	12 (14%)	5	22
15	C3	127/127 (100%)	107 (84%)	20 (16%)	3	15
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	17
16	C4	81/104 (78%)	62 (76%)	19 (24%)	1	4
16	c4	97/104 (93%)	84 (87%)	13 (13%)	5	22
17	C5	101/117 (86%)	83 (82%)	18 (18%)	2	11
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	12
18	C6	117/118 (99%)	101 (86%)	16 (14%)	4	21
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	10
19	C7	94/124 (76%)	76 (81%)	18 (19%)	2	9
19	c7	92/124 (74%)	80 (87%)	12 (13%)	5	24
20	C8	128/128 (100%)	105 (82%)	23 (18%)	2	11
20	c8	128/128 (100%)	104 (81%)	24 (19%)	2	10
21	C9	115/115 (100%)	99 (86%)	16 (14%)	4	21
21	c9	115/115 (100%)	105 (91%)	10 (9%)	13	45
22	D0	100/113 (88%)	88 (88%)	12 (12%)	6	28
22	d0	103/113 (91%)	87 (84%)	16 (16%)	3	16
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	11
23	d1	74/74 (100%)	63 (85%)	11 (15%)	4	17
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	92 (84%)	18 (16%)	3	14
25	D3	119/119 (100%)	103 (87%)	16 (13%)	5	22
25	d3	119/119 (100%)	108 (91%)	11 (9%)	11	40
26	D4	112/112 (100%)	103 (92%)	9 (8%)	15	50
26	d4	112/112 (100%)	96 (86%)	16 (14%)	4	19
27	D5	61/88 (69%)	49 (80%)	12 (20%)	1	8
27	d5	61/88 (69%)	52 (85%)	9 (15%)	4	18
28	D6	83/83 (100%)	71 (86%)	12 (14%)	4	19
28	d6	83/83 (100%)	74 (89%)	9 (11%)	8	33
29	D7	70/70 (100%)	64 (91%)	6 (9%)	13	46
29	d7	70/70 (100%)	59 (84%)	11 (16%)	3	15
30	D8	56/59 (95%)	47 (84%)	9 (16%)	3	14
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	15
32	e0	53/53 (100%)	41 (77%)	12 (23%)	1	5
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	31
34	sR	260/261 (100%)	236 (91%)	24 (9%)	11	40
35	SM	97/228 (42%)	82 (84%)	15 (16%)	3	16
35	sM	54/228 (24%)	46 (85%)	8 (15%)	4	18
39	L2	193/195 (99%)	158 (82%)	35 (18%)	2	11
39	l2	192/195 (98%)	156 (81%)	36 (19%)	2	10
40	L3	320/322 (99%)	274 (86%)	46 (14%)	4	19
40	l3	319/322 (99%)	264 (83%)	55 (17%)	2	12
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	14
41	l4	288/288 (100%)	247 (86%)	41 (14%)	4	20
42	L5	244/244 (100%)	203 (83%)	41 (17%)	2	13
42	l5	243/244 (100%)	201 (83%)	42 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	L6	134/152 (88%)	114 (85%)	20 (15%)	4	17
43	l6	135/152 (89%)	115 (85%)	20 (15%)	4	18
44	L7	186/204 (91%)	164 (88%)	22 (12%)	6	29
44	l7	187/204 (92%)	164 (88%)	23 (12%)	6	26
45	L8	187/207 (90%)	160 (86%)	27 (14%)	4	19
45	l8	177/207 (86%)	154 (87%)	23 (13%)	5	24
46	L9	171/171 (100%)	151 (88%)	20 (12%)	7	29
46	l9	171/171 (100%)	142 (83%)	29 (17%)	2	13
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1	8
47	m0	179/186 (96%)	143 (80%)	36 (20%)	1	7
48	M1	147/150 (98%)	124 (84%)	23 (16%)	3	16
48	m1	147/150 (98%)	120 (82%)	27 (18%)	2	10
49	M3	154/158 (98%)	138 (90%)	16 (10%)	9	34
49	m3	154/158 (98%)	132 (86%)	22 (14%)	4	19
50	M4	107/108 (99%)	92 (86%)	15 (14%)	4	20
50	m4	108/108 (100%)	94 (87%)	14 (13%)	5	24
51	M5	175/175 (100%)	153 (87%)	22 (13%)	5	25
51	m5	175/175 (100%)	152 (87%)	23 (13%)	5	24
52	M6	160/161 (99%)	136 (85%)	24 (15%)	3	17
52	m6	160/161 (99%)	134 (84%)	26 (16%)	3	14
53	M7	140/145 (97%)	123 (88%)	17 (12%)	6	27
53	m7	125/145 (86%)	107 (86%)	18 (14%)	4	19
54	M8	150/150 (100%)	136 (91%)	14 (9%)	11	40
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	7
55	M9	153/153 (100%)	132 (86%)	21 (14%)	4	21
55	m9	153/153 (100%)	129 (84%)	24 (16%)	3	15
56	N0	156/156 (100%)	134 (86%)	22 (14%)	4	20
56	n0	156/156 (100%)	135 (86%)	21 (14%)	5	22
57	N1	136/136 (100%)	107 (79%)	29 (21%)	1	6
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	13
58	N2	87/106 (82%)	79 (91%)	8 (9%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	n2	85/106 (80%)	72 (85%)	13 (15%)	3	17
59	N3	104/104 (100%)	90 (86%)	14 (14%)	5	22
59	n3	104/104 (100%)	89 (86%)	15 (14%)	4	19
60	N4	57/129 (44%)	50 (88%)	7 (12%)	6	26
60	n4	100/129 (78%)	88 (88%)	12 (12%)	6	28
61	N5	104/117 (89%)	86 (83%)	18 (17%)	2	12
61	n5	104/117 (89%)	92 (88%)	12 (12%)	7	30
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	12
62	n6	109/109 (100%)	89 (82%)	20 (18%)	2	10
63	N7	115/115 (100%)	104 (90%)	11 (10%)	10	38
63	n7	115/115 (100%)	95 (83%)	20 (17%)	2	12
64	N8	118/118 (100%)	100 (85%)	18 (15%)	3	17
64	n8	118/118 (100%)	100 (85%)	18 (15%)	3	17
65	N9	46/46 (100%)	40 (87%)	6 (13%)	5	24
65	n9	46/46 (100%)	41 (89%)	5 (11%)	8	32
66	O0	81/87 (93%)	70 (86%)	11 (14%)	5	22
66	o0	84/87 (97%)	71 (84%)	13 (16%)	3	16
67	O1	92/96 (96%)	78 (85%)	14 (15%)	3	17
67	o1	94/96 (98%)	76 (81%)	18 (19%)	2	9
68	O2	109/110 (99%)	91 (84%)	18 (16%)	3	14
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	5
69	O3	90/90 (100%)	81 (90%)	9 (10%)	9	36
69	o3	90/90 (100%)	77 (86%)	13 (14%)	4	19
70	O4	95/101 (94%)	84 (88%)	11 (12%)	7	30
70	o4	95/101 (94%)	80 (84%)	15 (16%)	3	15
71	O5	104/104 (100%)	90 (86%)	14 (14%)	5	22
71	o5	103/104 (99%)	90 (87%)	13 (13%)	5	25
72	O6	81/81 (100%)	66 (82%)	15 (18%)	2	10
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	13

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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	11
75	O9	45/45 (100%)	38 (84%)	7 (16%)	3	16
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	7
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	13
76	q0	47/47 (100%)	42 (89%)	5 (11%)	8	34
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	12
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	3	16
78	q2	90/90 (100%)	77 (86%)	13 (14%)	4	19
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	13
79	q3	71/71 (100%)	60 (84%)	11 (16%)	3	16
80	c0	73/98 (74%)	64 (88%)	9 (12%)	6	26
82	p0	105/253 (42%)	94 (90%)	11 (10%)	8	34
85	f	124/133 (93%)	108 (87%)	16 (13%)	5	24
All	All	18850/20374 (92%)	15999 (85%)	2851 (15%)	3	17

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 [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 95th 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 ²)	Q<0.9
1	2	1781/1800 (98%)	0.93	211 (11%) 6 4	60, 99, 172, 210	0
1	6	1795/1800 (99%)	0.61	94 (5%) 31 22	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 1	83, 99, 113, 119	0
3	S1	214/254 (84%)	0.78	33 (15%) 3 2	107, 142, 167, 173	0
3	s1	216/254 (85%)	0.83	30 (13%) 4 3	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 1	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%) 12 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%) 6 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%) 4 3	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%) 2 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%) 11 8	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 ²)	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	1	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%)	28	20	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	1	87, 102, 115, 118	0
20	C8	145/145 (100%)	0.41	8 (5%)	29	21	86, 110, 131, 137	0
20	c8	145/145 (100%)	0.50	5 (3%)	49	39	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%)	2	1	84, 96, 112, 121	0
22	D0	107/120 (89%)	1.89	41 (38%)	0	1	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%)	12	8	88, 111, 122, 128	0
26	d4	134/134 (100%)	0.37	4 (2%)	54	44	68, 92, 105, 108	0
27	D5	70/107 (65%)	0.28	5 (7%)	19	14	119, 131, 137, 138	0
27	d5	69/107 (64%)	0.59	6 (8%)	13	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	1	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	1	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	2	105, 134, 149, 153	0
33	e1	76/76 (100%)	1.55	23 (30%)	1	1	112, 161, 175, 179	0
34	SR	318/318 (100%)	1.65	110 (34%)	0	1	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%)	3	2	56, 109, 181, 186	0
36	1	3149/3396 (92%)	0.63	163 (5%)	31	22	38, 61, 124, 213	0
36	5	3169/3396 (93%)	0.65	118 (3%)	45	35	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%)	87	82	41, 62, 74, 80	0
38	4	158/158 (100%)	0.42	2 (1%)	79	71	47, 64, 94, 125	0
38	8	158/158 (100%)	0.45	3 (1%)	70	60	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%)	14	9	44, 64, 77, 87	0
40	l3	386/386 (100%)	0.43	13 (3%)	49	39	37, 51, 64, 79	0
41	L4	361/361 (100%)	0.57	40 (11%)	7	5	42, 57, 70, 74	0
41	l4	361/361 (100%)	0.77	44 (12%)	5	4	45, 60, 74, 82	0
42	L5	296/296 (100%)	0.46	21 (7%)	19	14	60, 83, 99, 107	0
42	l5	294/296 (99%)	0.36	10 (3%)	49	39	50, 64, 89, 105	0
43	L6	156/175 (89%)	0.48	2 (1%)	79	71	52, 59, 72, 82	0
43	l6	157/175 (89%)	0.50	10 (6%)	23	17	53, 60, 78, 87	0
44	L7	222/243 (91%)	0.55	5 (2%)	64	54	42, 52, 78, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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%) 11 8	70, 86, 109, 117	0
45	l8	231/255 (90%)	0.79	26 (11%) 7 5	73, 86, 106, 114	0
46	L9	191/191 (100%)	0.30	5 (2%) 59 50	62, 72, 83, 92	0
46	l9	191/191 (100%)	0.37	4 (2%) 67 57	47, 57, 72, 82	0
47	M0	211/220 (95%)	0.55	6 (2%) 56 47	47, 61, 88, 110	0
47	m0	213/220 (96%)	0.72	13 (6%) 25 18	45, 64, 88, 97	0
48	M1	169/173 (97%)	0.66	13 (7%) 16 12	70, 88, 99, 102	0
48	m1	169/173 (97%)	0.31	4 (2%) 62 52	54, 71, 79, 83	0
49	M3	193/198 (97%)	1.06	37 (19%) 2 1	43, 68, 93, 114	0
49	m3	194/198 (97%)	0.56	13 (6%) 21 15	44, 71, 100, 112	0
50	M4	136/137 (99%)	0.23	1 (0%) 89 84	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%) 11 8	45, 59, 70, 72	0
51	m5	203/203 (100%)	1.07	32 (15%) 3 2	46, 63, 73, 78	0
52	M6	197/198 (99%)	0.57	7 (3%) 46 37	44, 51, 67, 69	0
52	m6	197/198 (99%)	0.49	8 (4%) 41 31	37, 45, 64, 67	0
53	M7	183/183 (100%)	1.25	26 (14%) 4 3	49, 56, 93, 112	0
53	m7	155/183 (84%)	0.45	7 (4%) 37 28	42, 50, 63, 82	0
54	M8	185/185 (100%)	0.66	11 (5%) 26 18	45, 58, 71, 86	0
54	m8	185/185 (100%)	0.80	18 (9%) 10 7	44, 60, 70, 74	0
55	M9	188/188 (100%)	0.86	21 (11%) 7 5	67, 80, 140, 146	0
55	m9	188/188 (100%)	0.68	14 (7%) 17 13	53, 67, 127, 138	0
56	N0	172/172 (100%)	0.65	6 (3%) 48 38	51, 59, 70, 76	0
56	n0	172/172 (100%)	0.29	1 (0%) 90 86	45, 52, 62, 68	0
57	N1	159/159 (100%)	0.57	5 (3%) 52 43	46, 58, 95, 103	0
57	n1	159/159 (100%)	0.43	4 (2%) 61 51	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%) 26 18	38, 47, 57, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	2.94	38 (38%) 0 1	63, 75, 134, 138	0
60	n4	135/155 (87%)	1.08	19 (14%) 4 3	47, 94, 119, 124	0
61	N5	121/141 (85%)	0.87	12 (9%) 9 7	62, 73, 86, 99	0
61	n5	120/141 (85%)	0.66	9 (7%) 17 12	58, 72, 86, 98	0
62	N6	126/126 (100%)	0.39	3 (2%) 62 52	53, 66, 76, 81	0
62	n6	126/126 (100%)	0.66	6 (4%) 34 26	55, 68, 79, 85	0
63	N7	135/135 (100%)	0.61	12 (8%) 12 8	87, 98, 107, 111	0
63	n7	135/135 (100%)	0.62	15 (11%) 7 5	80, 92, 102, 106	0
64	N8	148/148 (100%)	1.15	19 (12%) 5 3	38, 60, 79, 86	0
64	n8	148/148 (100%)	1.12	24 (16%) 3 2	38, 61, 75, 78	0
65	N9	58/58 (100%)	0.80	6 (10%) 9 6	41, 63, 89, 95	0
65	n9	58/58 (100%)	0.49	3 (5%) 31 22	41, 60, 82, 89	0
66	O0	97/104 (93%)	0.24	2 (2%) 67 57	85, 93, 107, 109	0
66	o0	100/104 (96%)	0.42	5 (5%) 32 24	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%) 11 8	49, 60, 84, 98	0
68	O2	127/129 (98%)	0.53	4 (3%) 52 43	39, 53, 65, 71	0
68	o2	127/129 (98%)	0.48	5 (3%) 43 33	38, 56, 69, 72	0
69	O3	106/106 (100%)	0.85	6 (5%) 27 19	44, 49, 70, 78	0
69	o3	106/106 (100%)	1.11	15 (14%) 4 3	42, 49, 70, 78	0
70	O4	112/119 (94%)	1.26	34 (30%) 1 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%) 87 82	58, 74, 82, 87	0
71	o5	119/119 (100%)	0.20	1 (0%) 87 82	62, 75, 89, 98	0
72	O6	99/99 (100%)	0.19	2 (2%) 68 58	64, 72, 94, 105	0
72	o6	99/99 (100%)	0.30	3 (3%) 54 44	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%) 22 16	86, 97, 109, 114	0
74	o8	77/77 (100%)	0.80	12 (15%) 3 2	80, 91, 101, 103	0
75	O9	50/50 (100%)	1.79	18 (36%) 0 1	55, 60, 64, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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%) 44 34	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%) 55 46	46, 58, 78, 103	0
78	q2	105/105 (100%)	0.65	8 (7%) 17 12	45, 56, 71, 94	0
79	Q3	91/91 (100%)	1.02	17 (18%) 2 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, 95th 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 ²)	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.