



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 06:39 PM UTC

PDB ID : 5DGV / pdb_00005dgv
Title : Complex of yeast 80S ribosome with hypusine-containing/non-modified eIF5A and/or a peptidyl-tRNA analog
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on : 2015-08-28
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

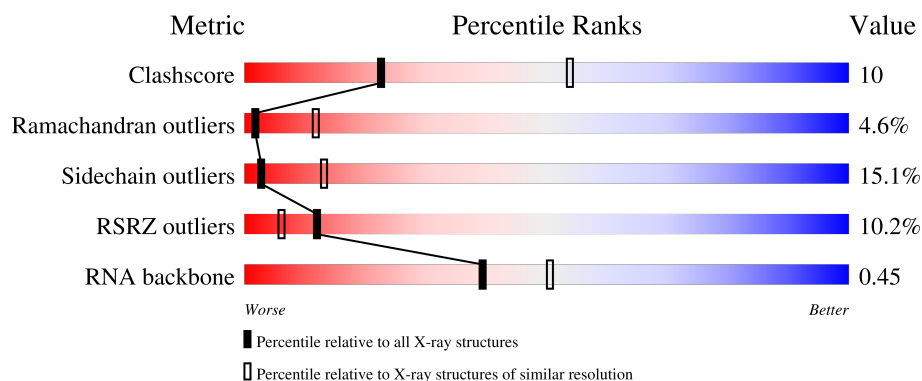
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	6	1800	
2	S0	251	
2	s0	251	

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Mol	Chain	Length	Quality of chain
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	

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Mol	Chain	Length	Quality of chain
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	

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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	263	
35	sM	263	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	

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Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	

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Mol	Chain	Length	Quality of chain
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	

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Mol	Chain	Length	Quality of chain
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	

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Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	
85	C	5	
85	D	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	SPS	C	3401	-	X	-	-
87	SPS	D	3401	-	X	-	-

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O		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
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	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	l3	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	l4	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 (eL8).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

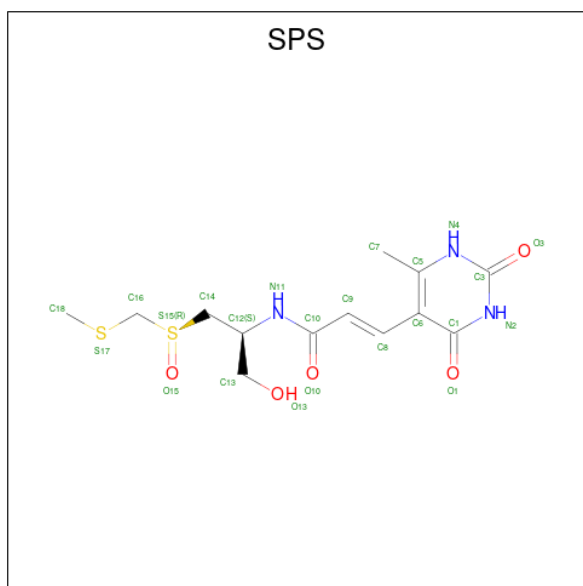
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	D6	1	Total	Zn	0	0
			1	1		
86	D7	1	Total	Zn	0	0
			1	1		
86	D9	1	Total	Zn	0	0
			1	1		
86	E1	1	Total	Zn	0	0
			1	1		
86	O7	1	Total	Zn	0	0
			1	1		
86	Q0	1	Total	Zn	0	0
			1	1		
86	Q2	1	Total	Zn	0	0
			1	1		
86	Q3	1	Total	Zn	0	0
			1	1		
86	d6	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	q3	1	Total	Zn	0	0
			1	1		

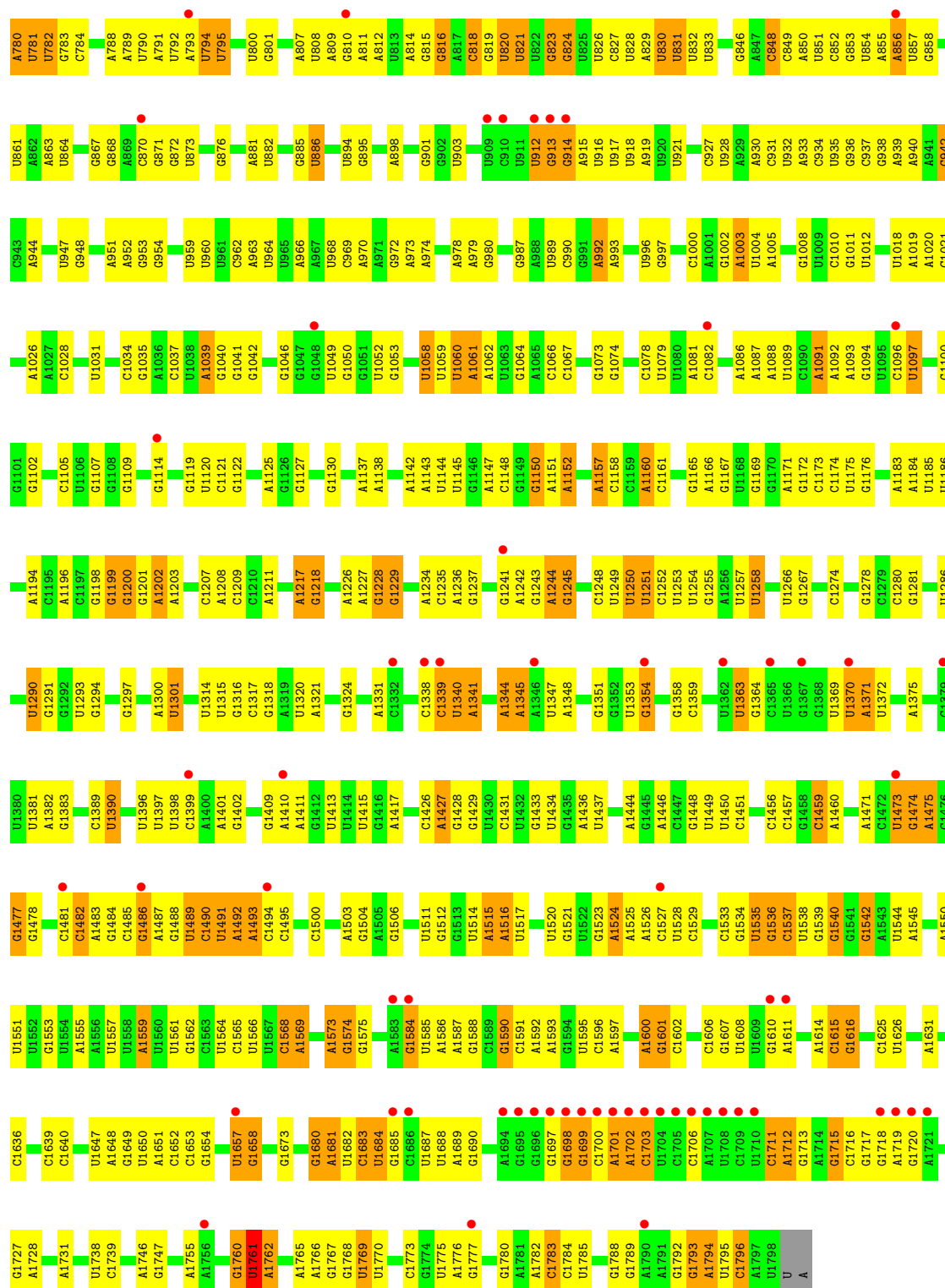
- Molecule 87 is SPARSOMYCIN (CCD ID: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).

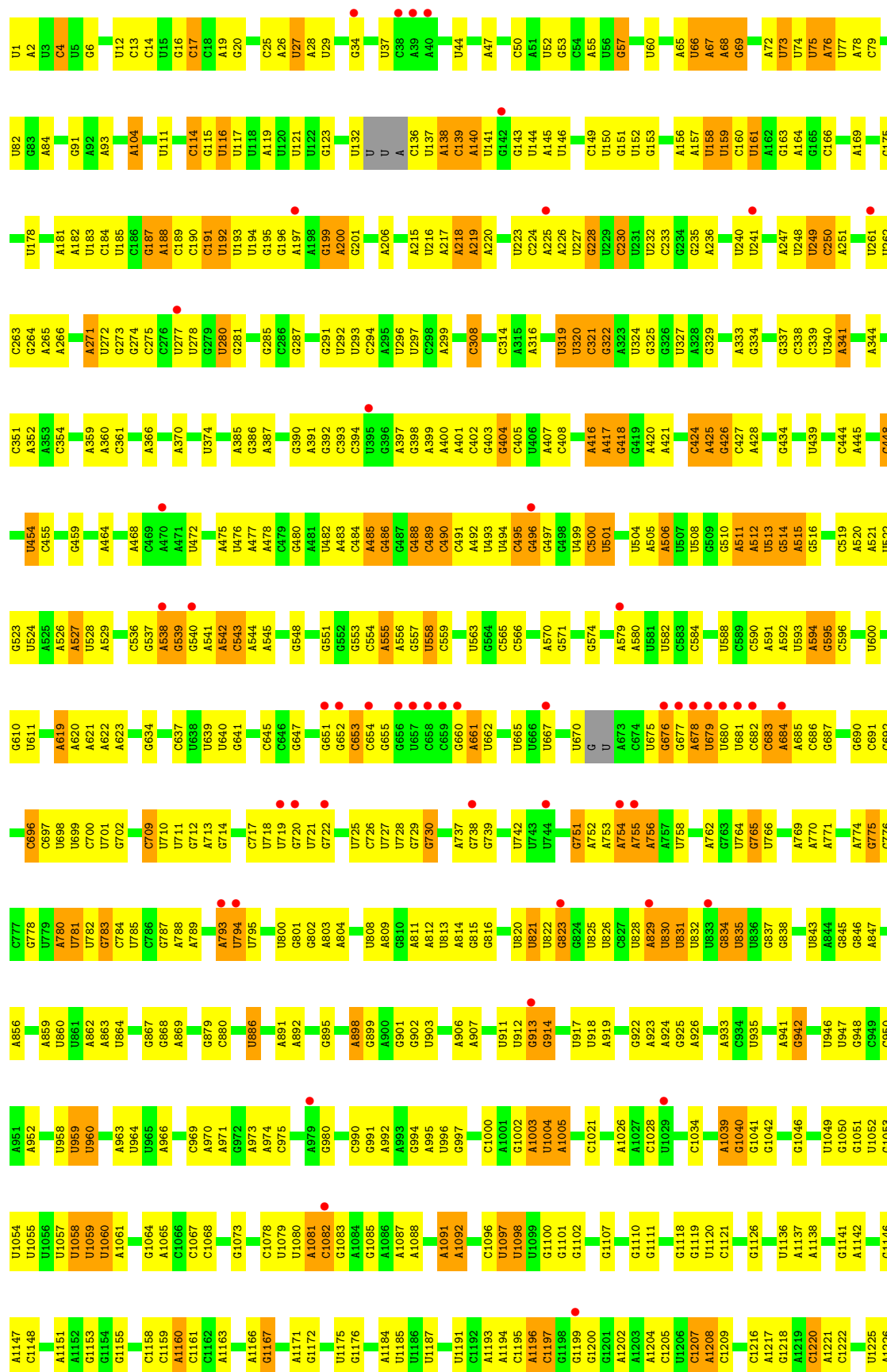


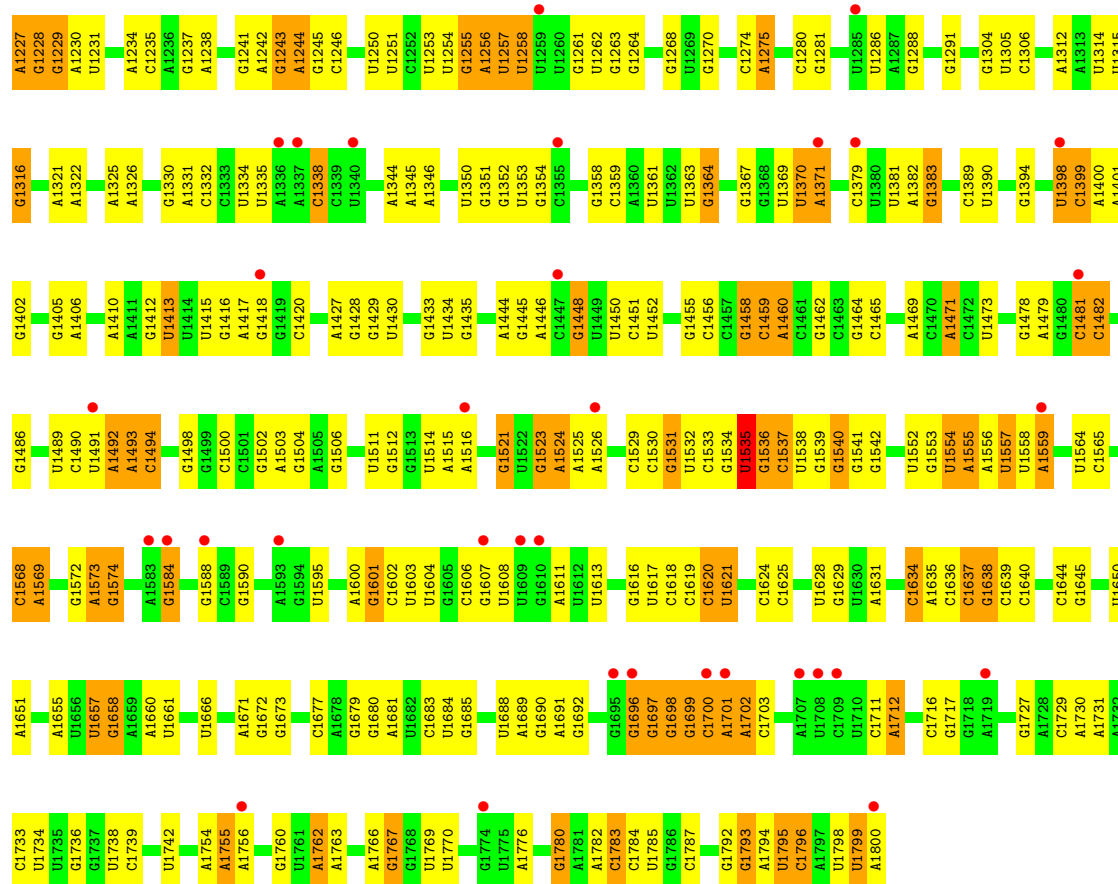
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
87	C	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
87	D	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

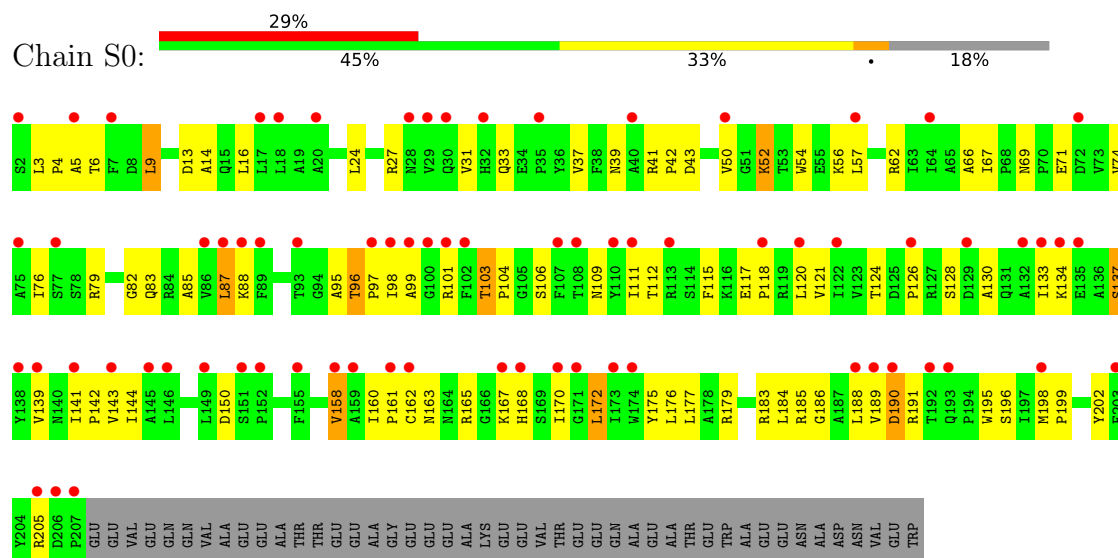
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	C	1	Total	Mg	0	0
			1	1		
88	D	1	Total	Mg	0	0
			1	1		







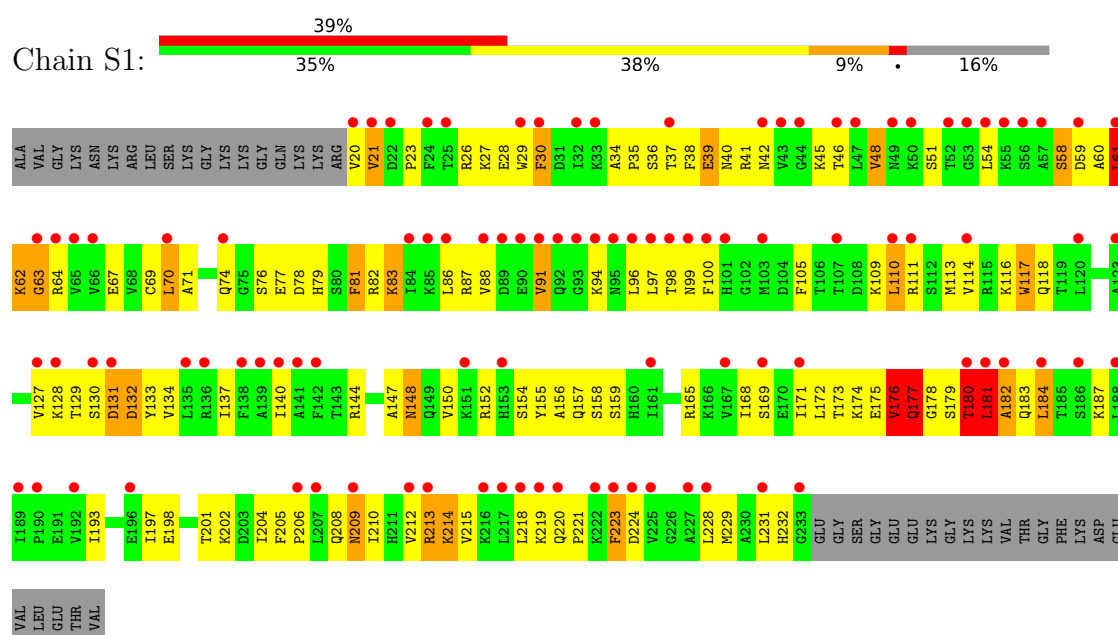
• Molecule 2: 40S ribosomal protein S0-A



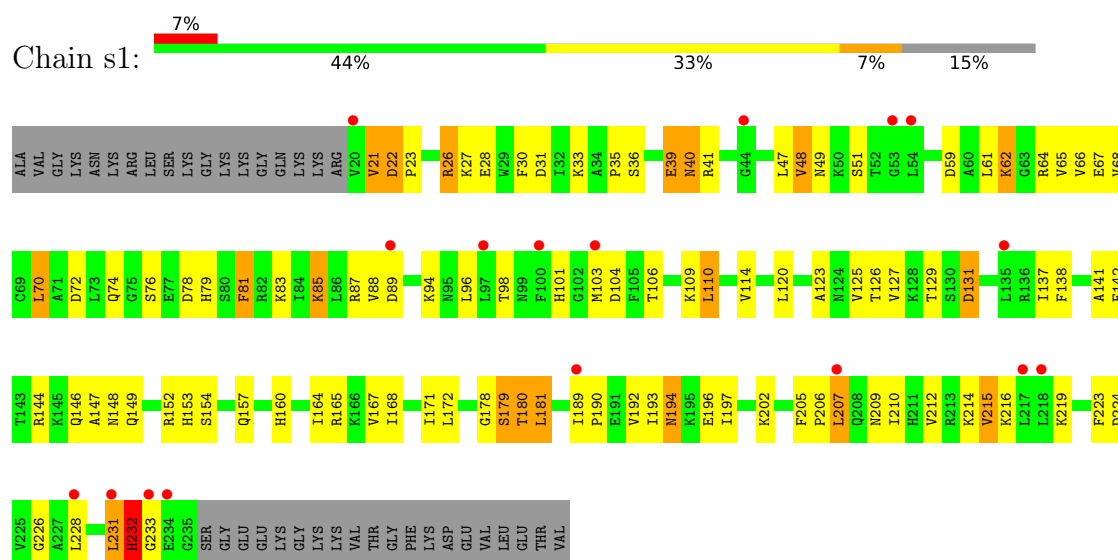
• Molecule 2: 40S ribosomal protein S0-A



- Molecule 3: 40S ribosomal protein S1-A

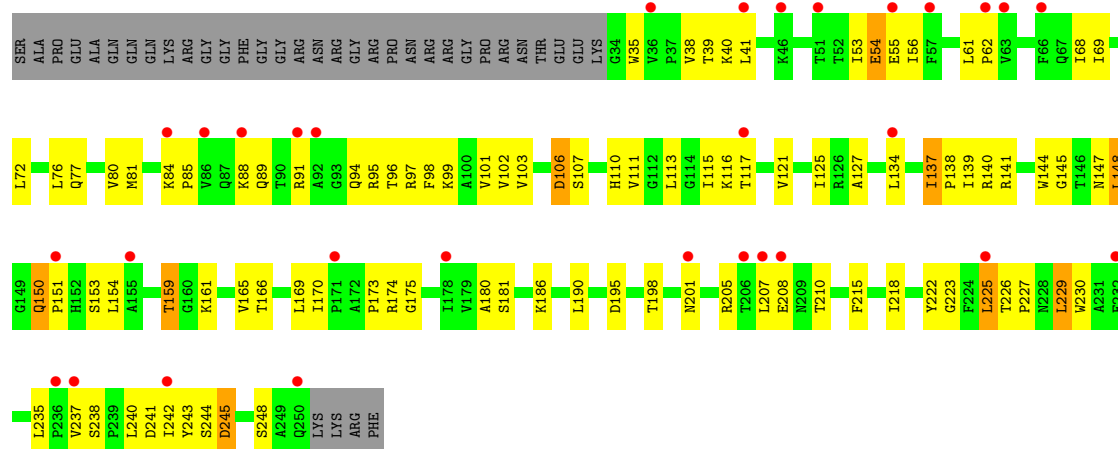


- Molecule 3: 40S ribosomal protein S1-A



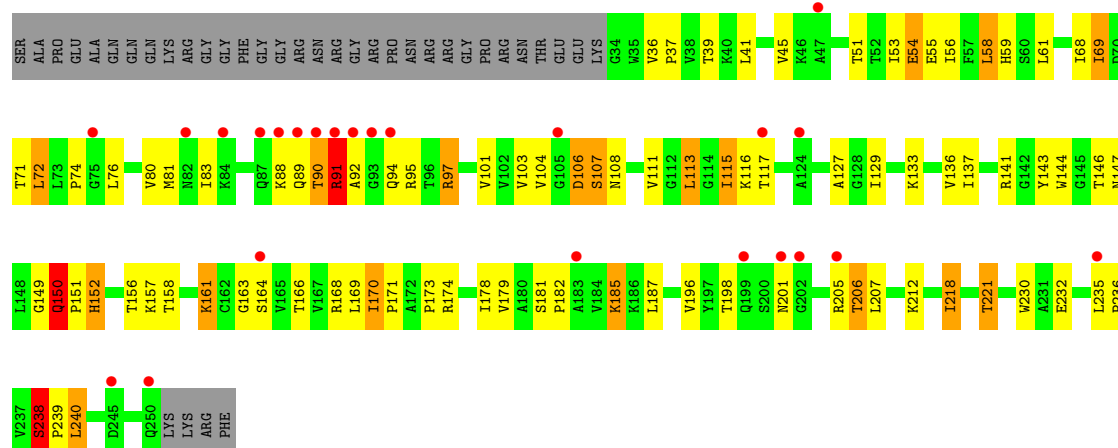
• Molecule 4: 40S ribosomal protein S2

Chain S2: 



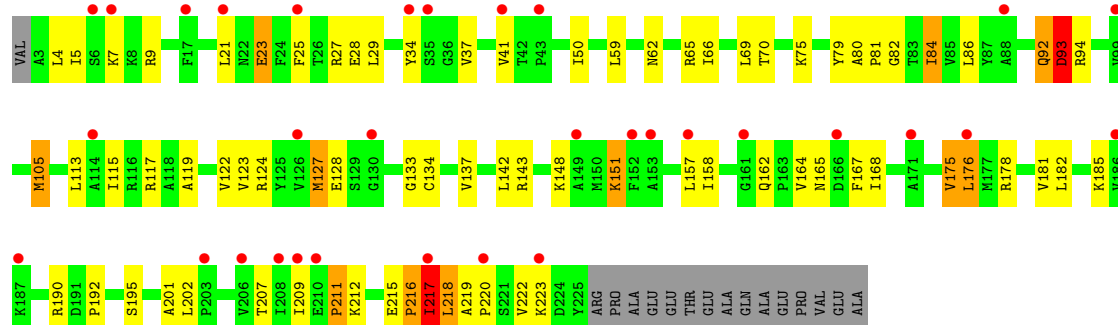
• Molecule 4: 40S ribosomal protein S2

Chain s2: 

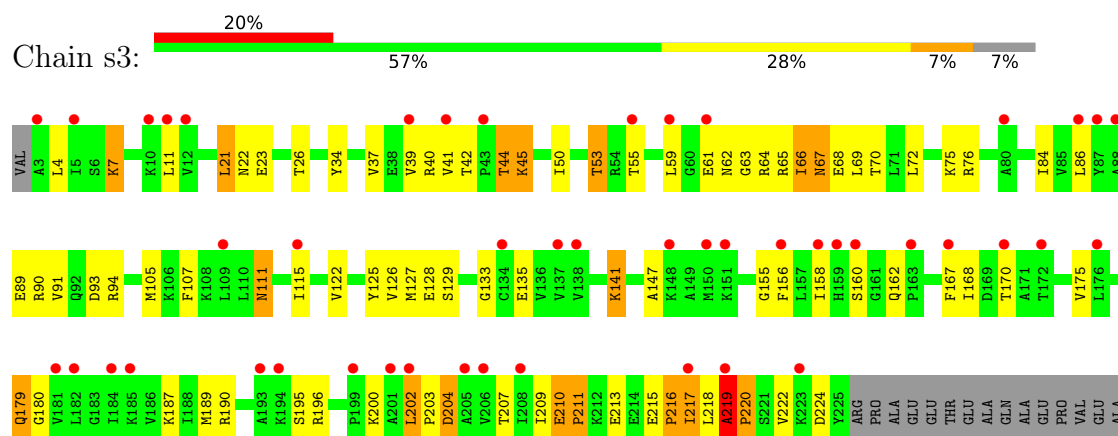


• Molecule 5: 40S ribosomal protein S3

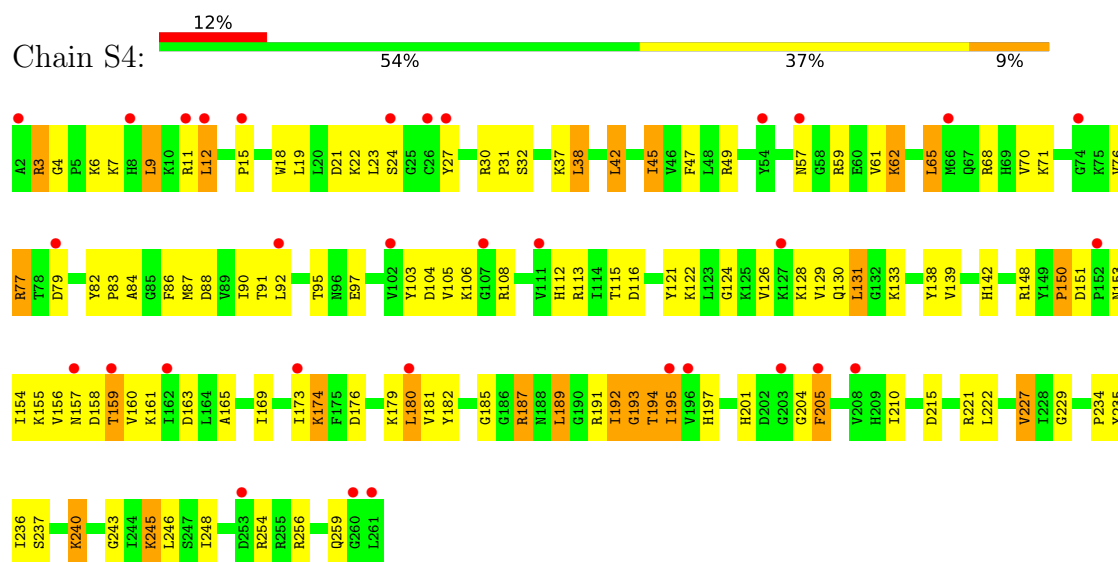
Chain S3: 



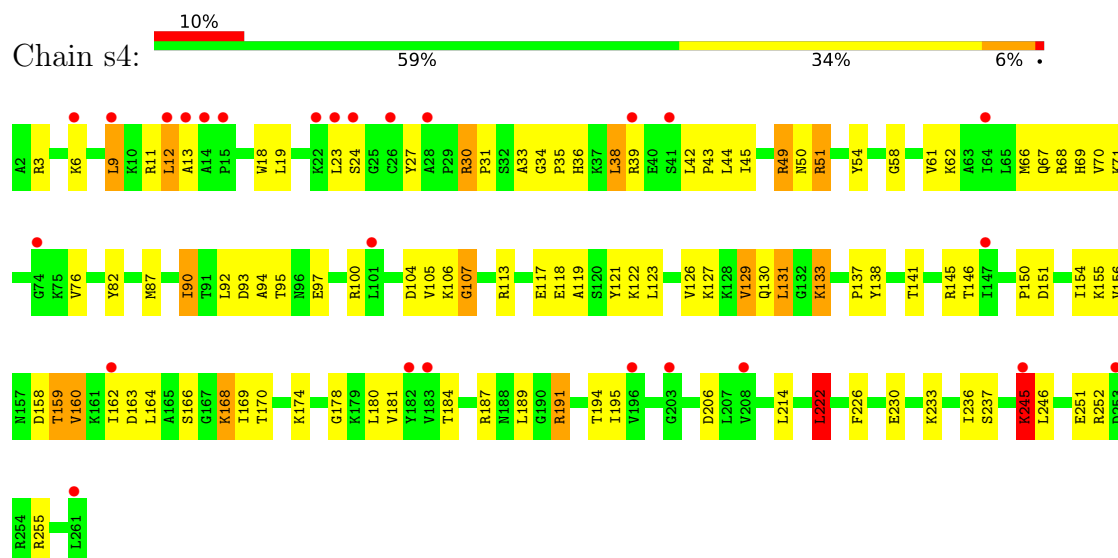
- Molecule 5: 40S ribosomal protein S3



- Molecule 6: 40S ribosomal protein S4-A

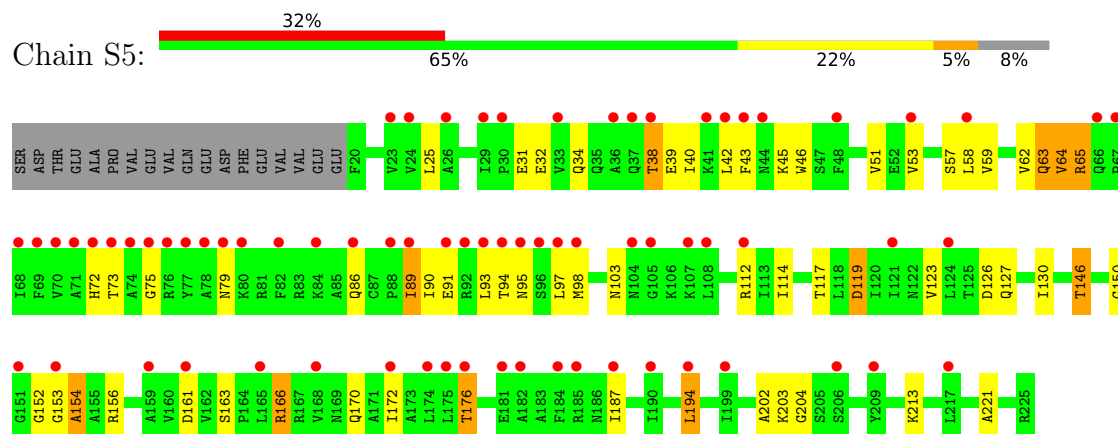


- Molecule 6: 40S ribosomal protein S4-A



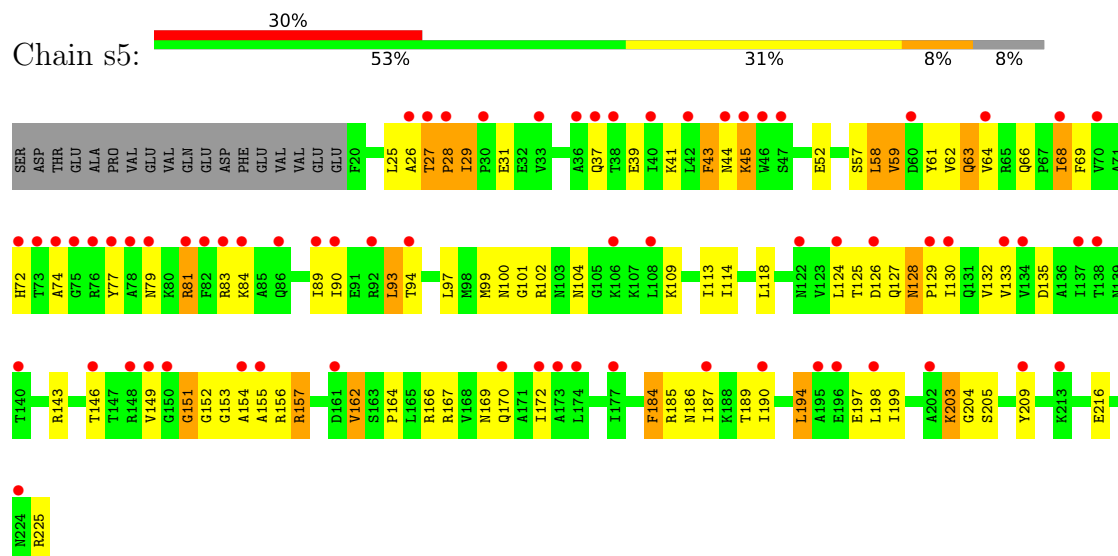
- Molecule 7: 40S ribosomal protein S5

Chain S5:



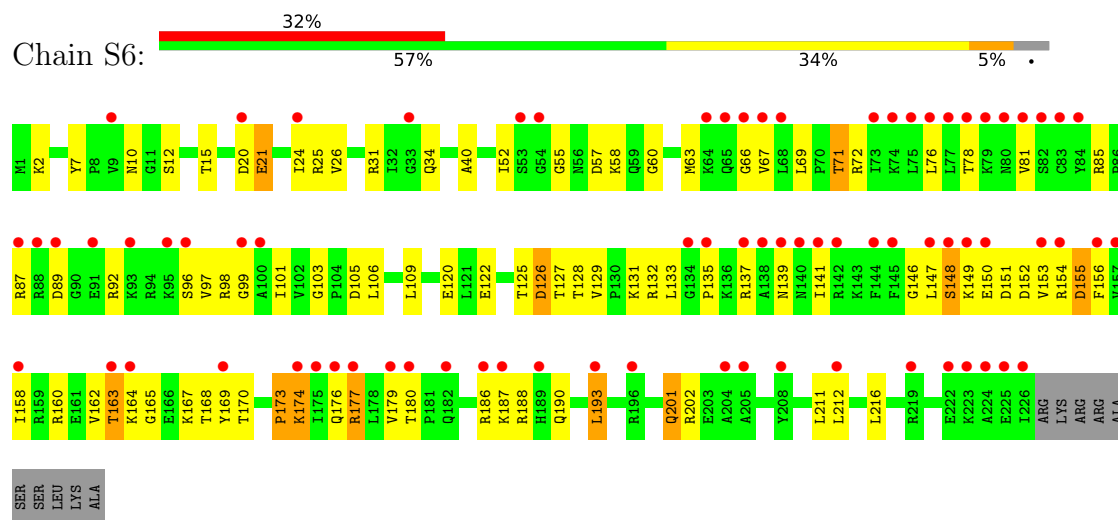
- Molecule 7: 40S ribosomal protein S5

Chain s5:

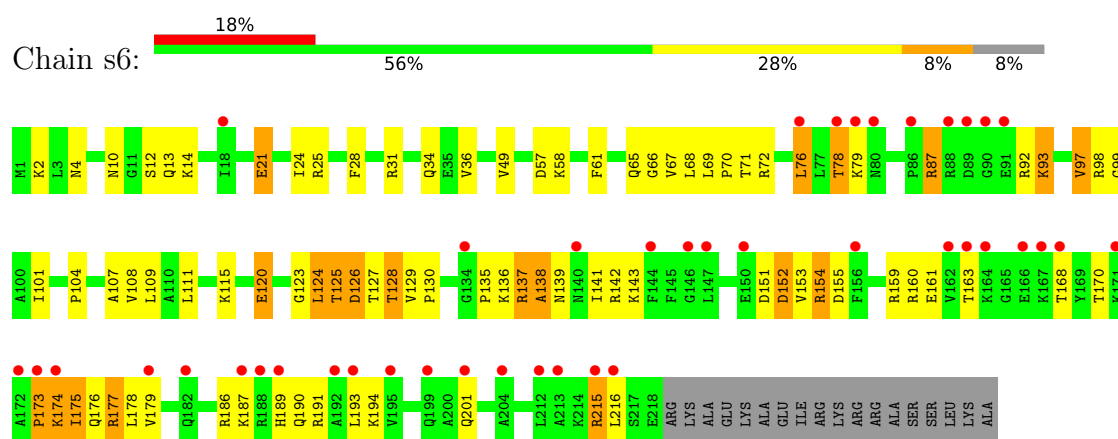


- Molecule 8: 40S ribosomal protein S6-A

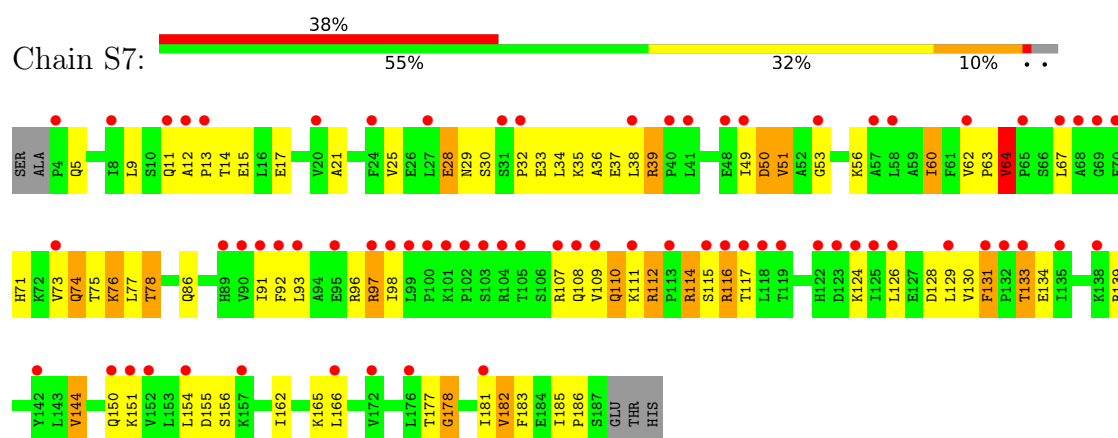
Chain S6:



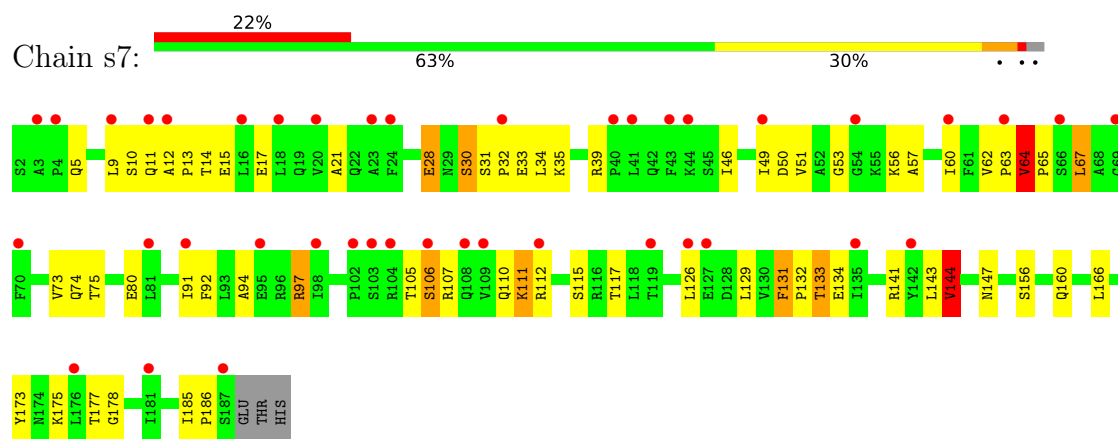
- Molecule 8: 40S ribosomal protein S6-A



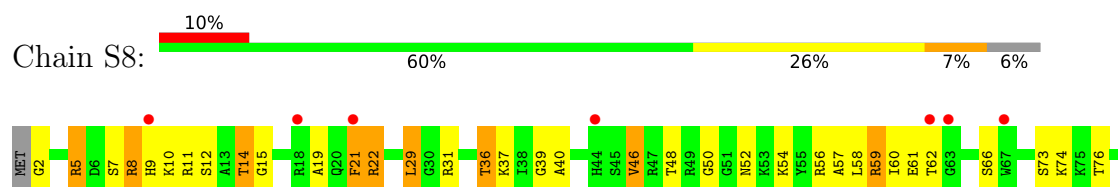
• Molecule 9: 40S ribosomal protein S7-A

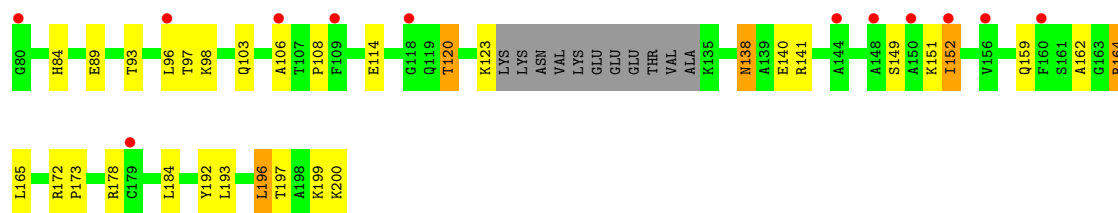


• Molecule 9: 40S ribosomal protein S7-A

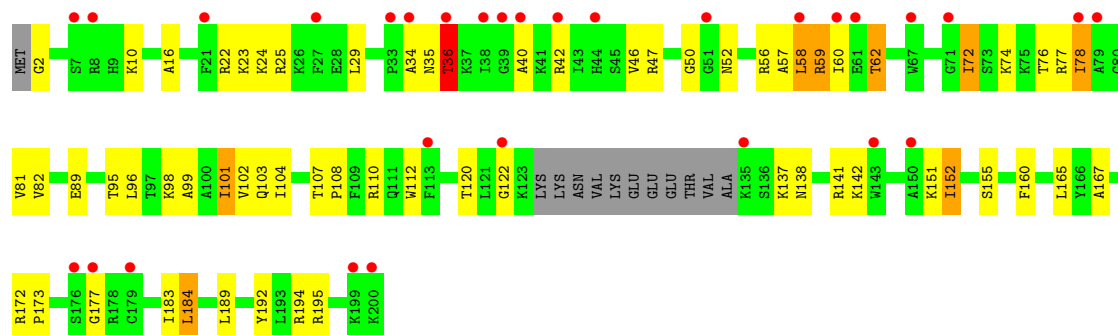


• Molecule 10: 40S ribosomal protein S8-A

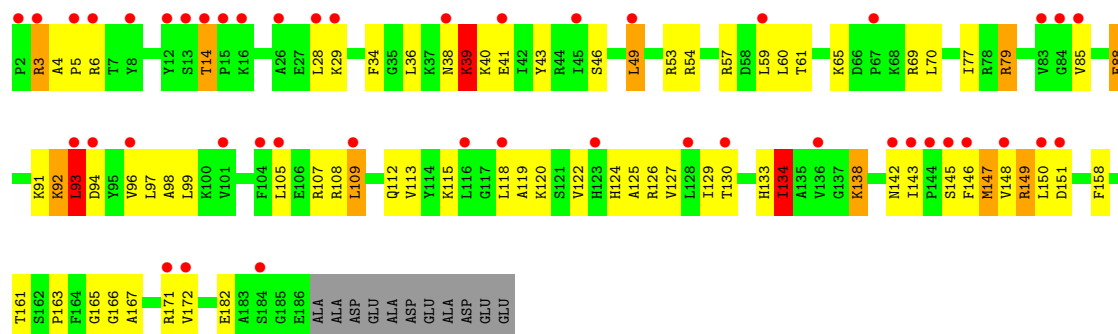




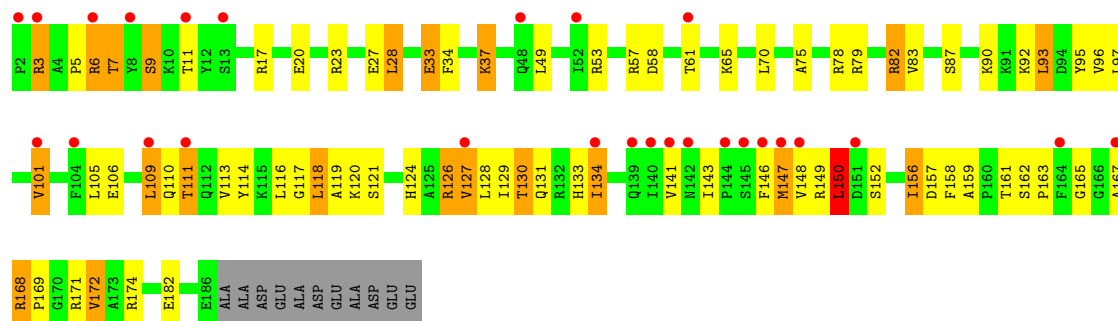
• Molecule 10: 40S ribosomal protein S8-A



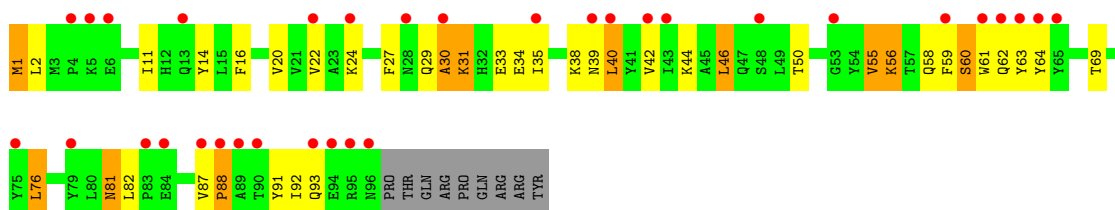
• Molecule 11: 40S ribosomal protein S9-A



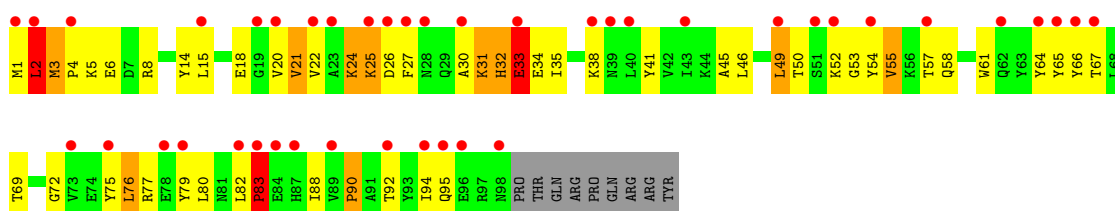
• Molecule 11: 40S ribosomal protein S9-A



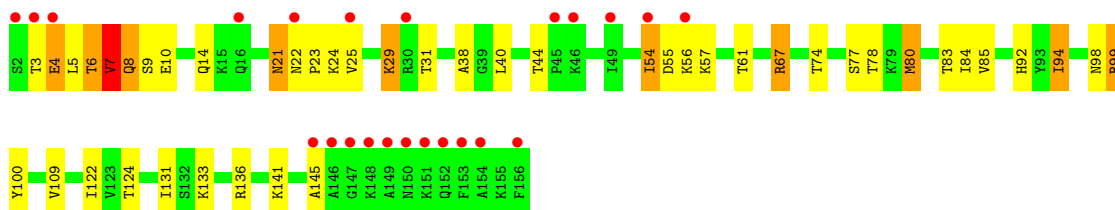
Chain C0:



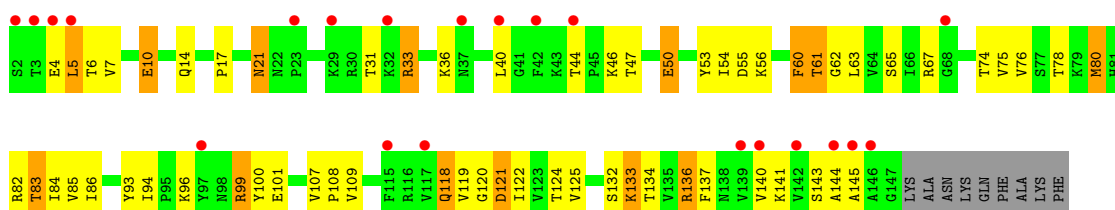
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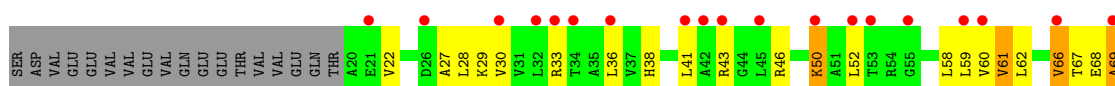
Chain C1:

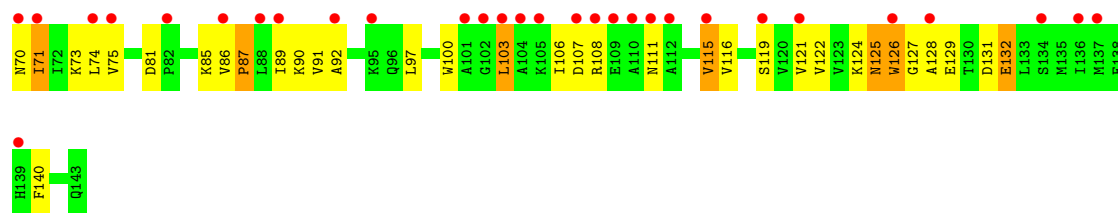


Chain c1:

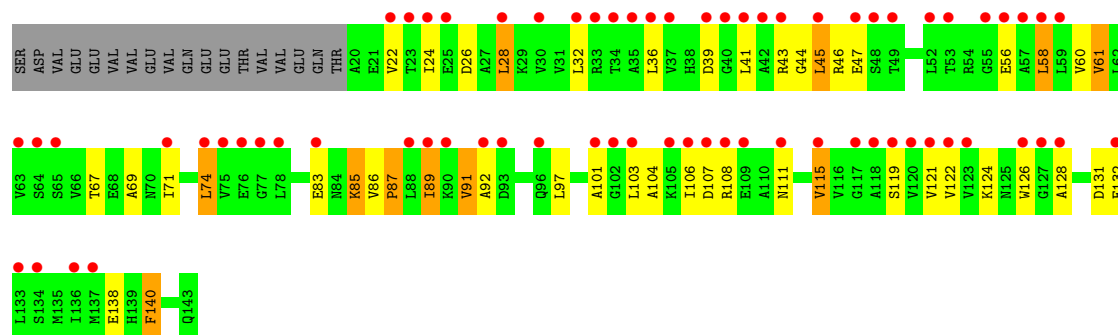


Chain C2:

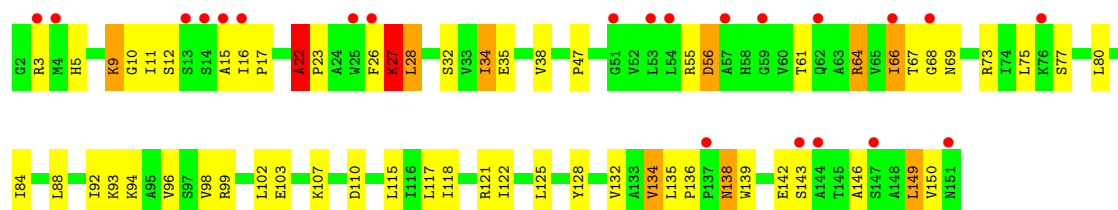




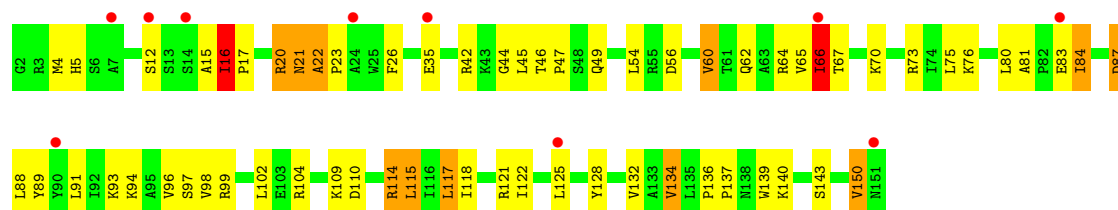
• Molecule 14: 40S ribosomal protein S12



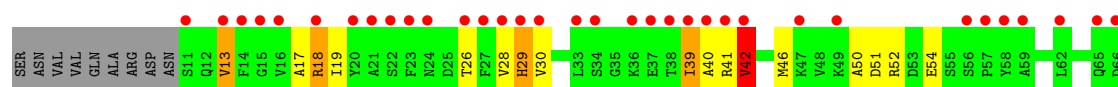
• Molecule 15: 40S ribosomal protein S13

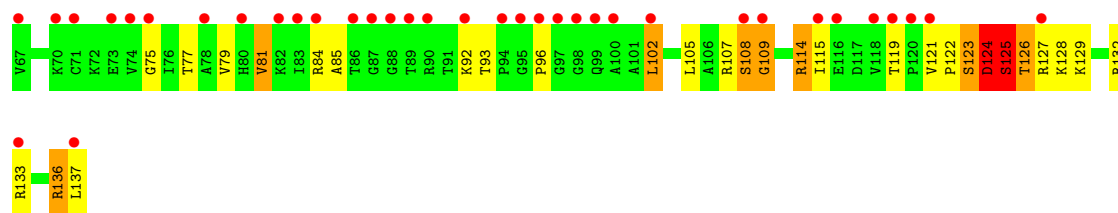


• Molecule 15: 40S ribosomal protein S13

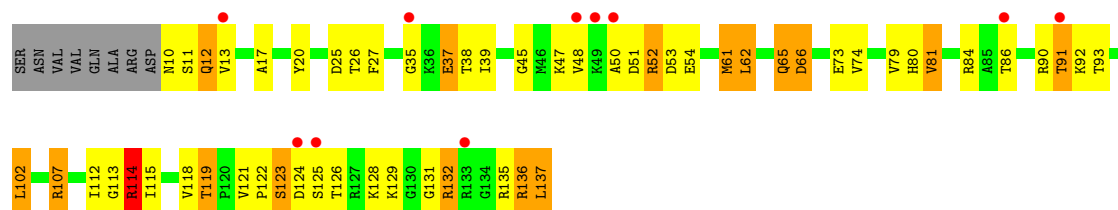


• Molecule 16: 40S ribosomal protein S14-A

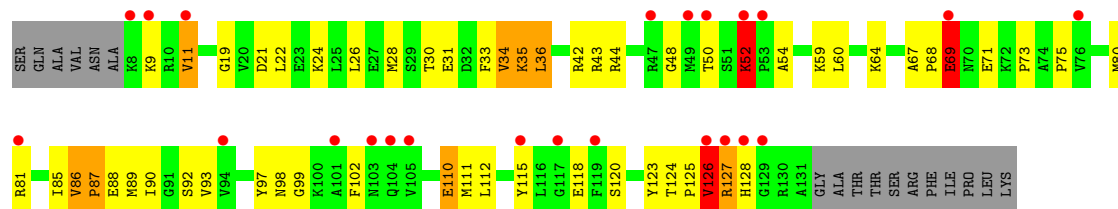




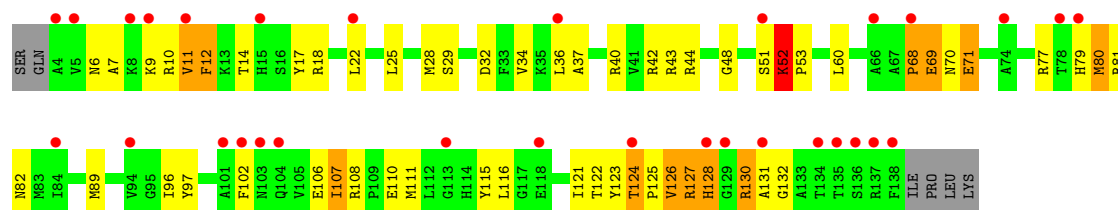
• Molecule 16: 40S ribosomal protein S14-A



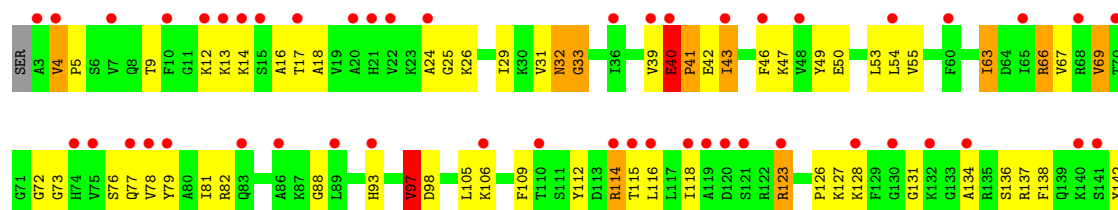
• Molecule 17: 40S ribosomal protein S15



• Molecule 17: 40S ribosomal protein S15

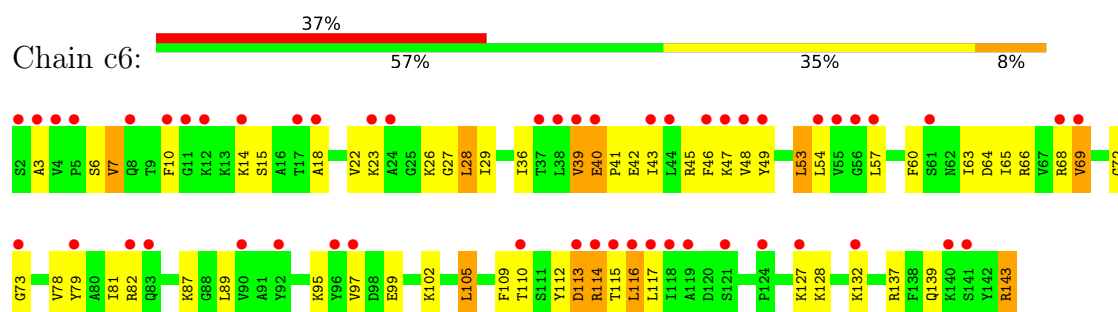


• Molecule 18: 40S ribosomal protein S16-A

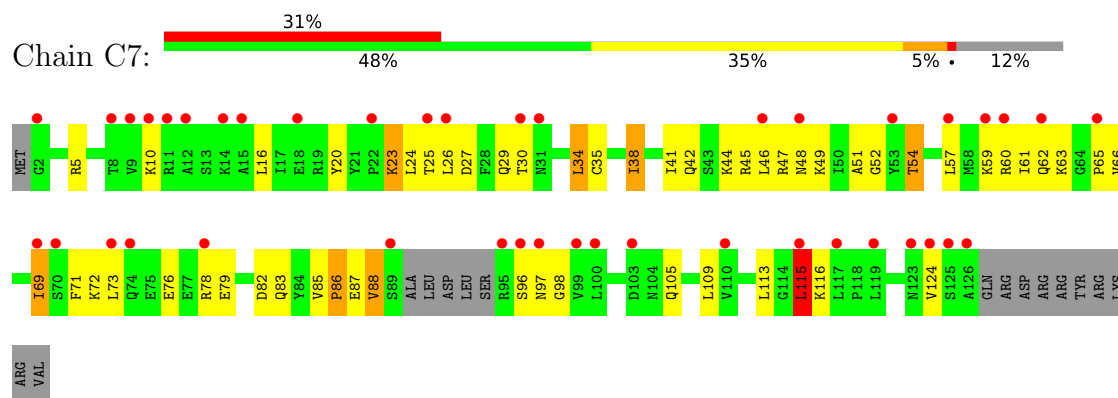




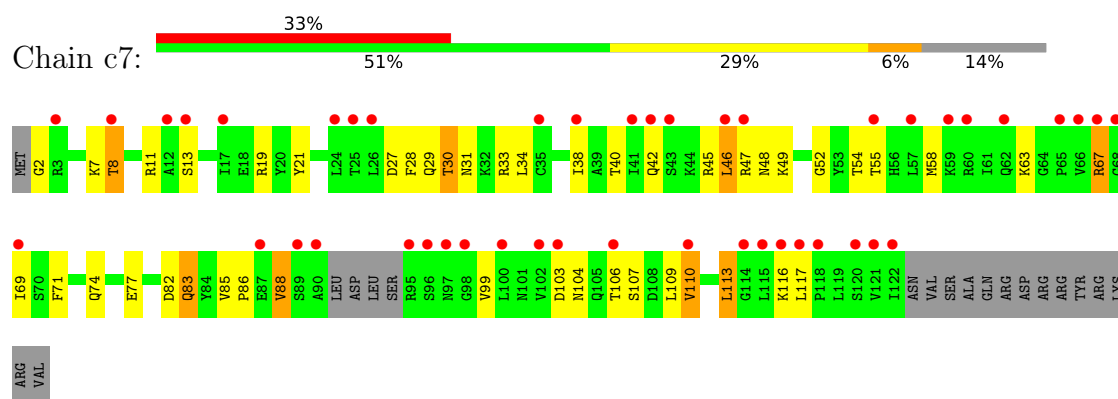
• Molecule 18: 40S ribosomal protein S16-A



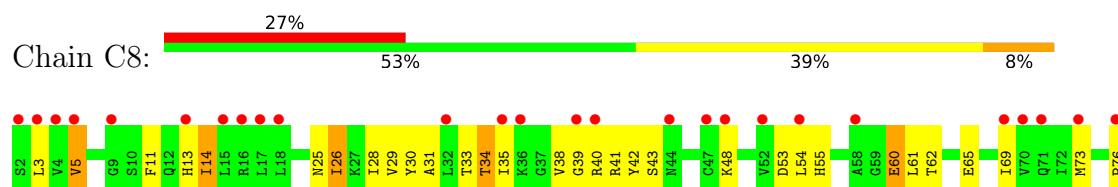
• Molecule 19: 40S ribosomal protein S17-A



• Molecule 19: 40S ribosomal protein S17-A



• Molecule 20: 40S ribosomal protein S18-A

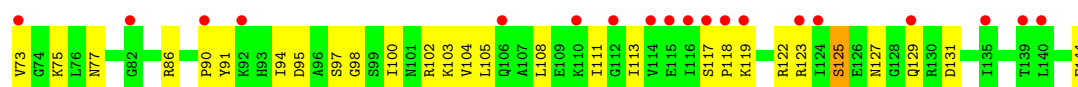
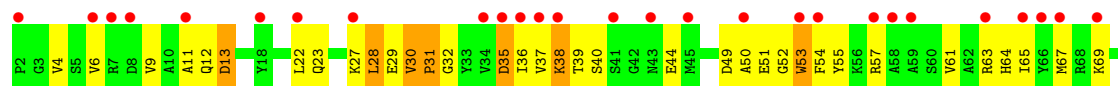




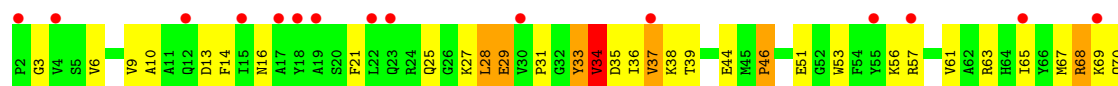
- Molecule 20: 40S ribosomal protein S18-A



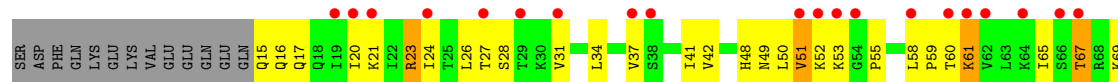
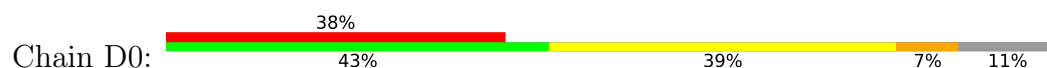
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A

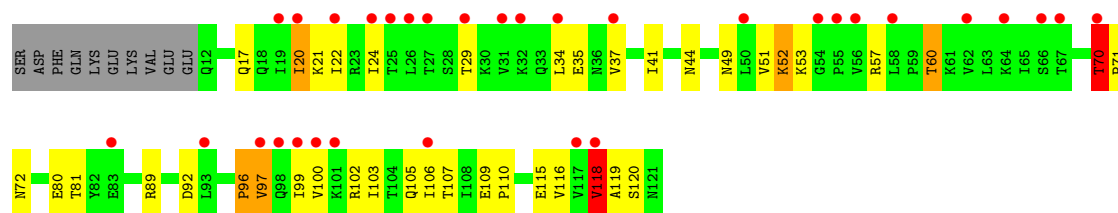


- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20

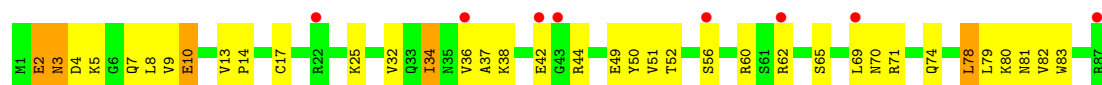




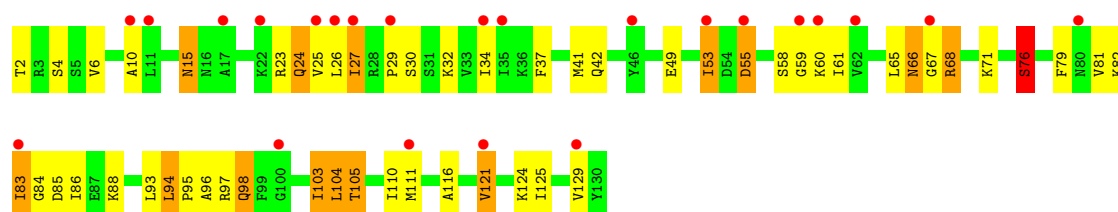
• Molecule 23: 40S ribosomal protein S21-A



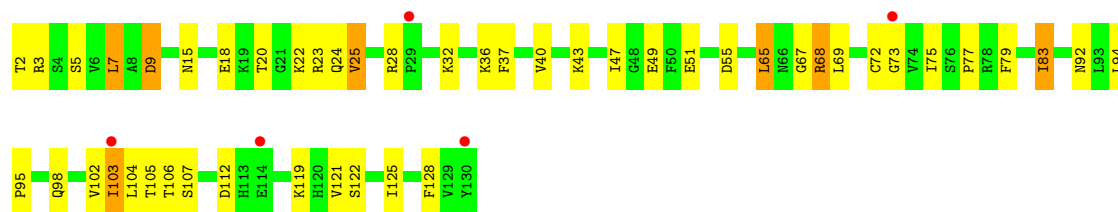
• Molecule 23: 40S ribosomal protein S21-A



• Molecule 24: 40S ribosomal protein S22-A

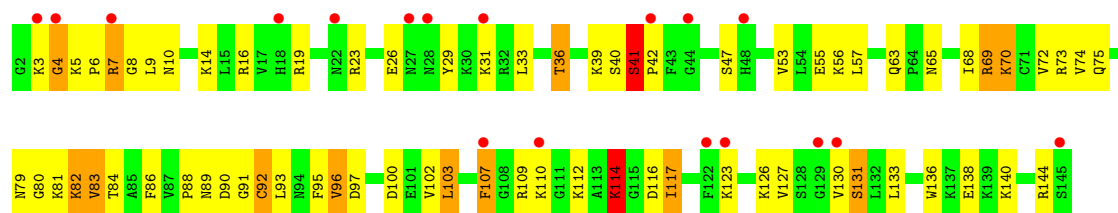


• Molecule 24: 40S ribosomal protein S22-A

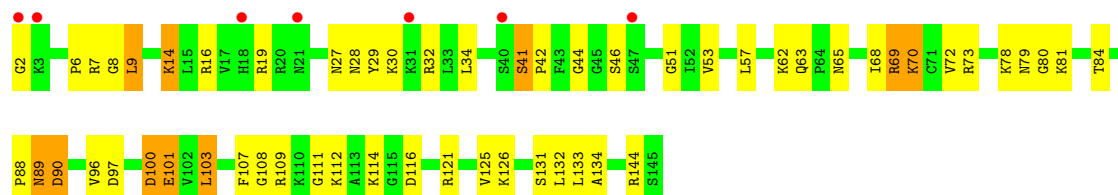


• Molecule 25: 40S ribosomal protein S23-A

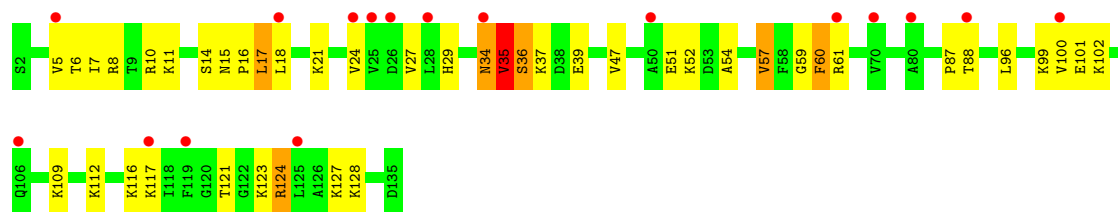




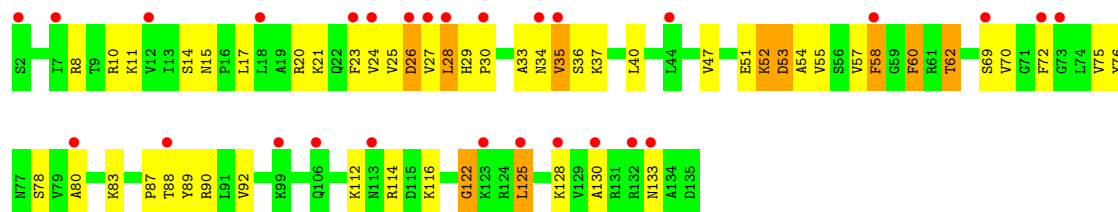
• Molecule 25: 40S ribosomal protein S23-A



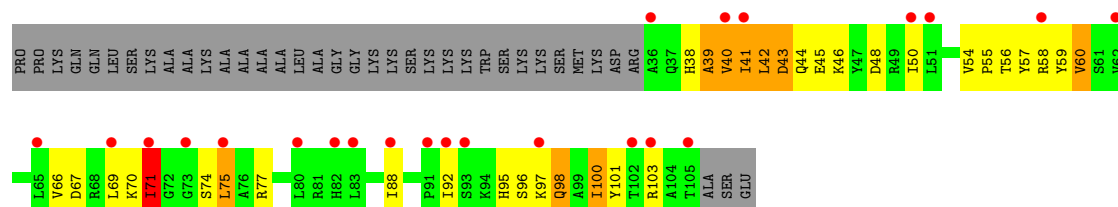
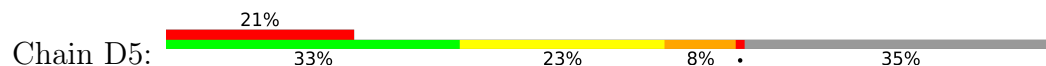
• Molecule 26: 40S ribosomal protein S24-A



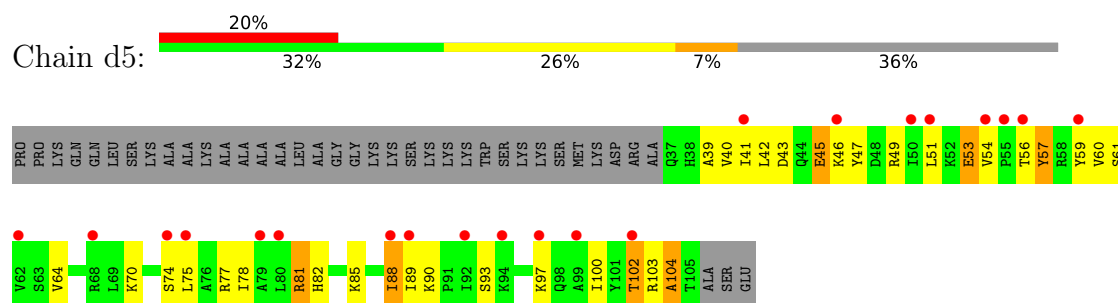
• Molecule 26: 40S ribosomal protein S24-A



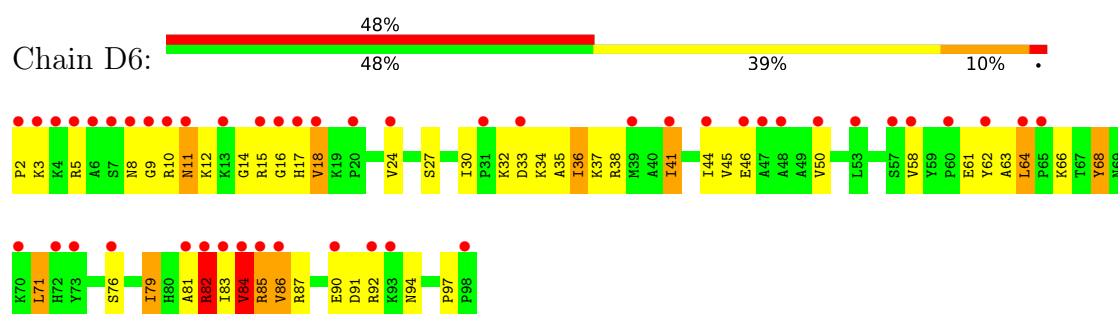
• Molecule 27: 40S ribosomal protein S25-A



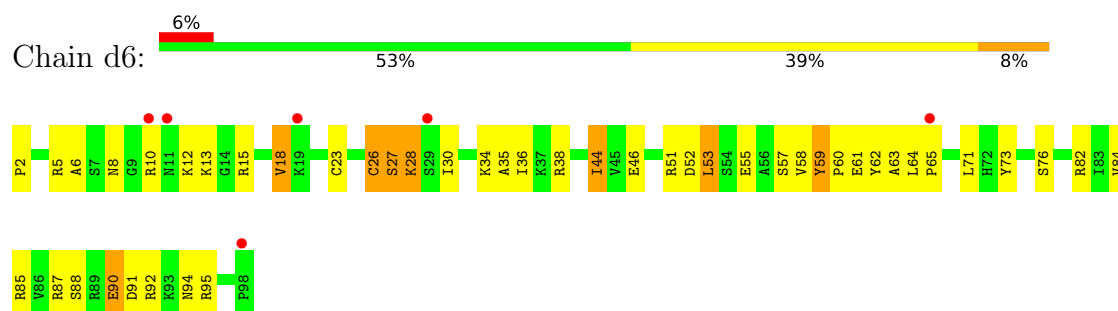
- Molecule 27: 40S ribosomal protein S25-A



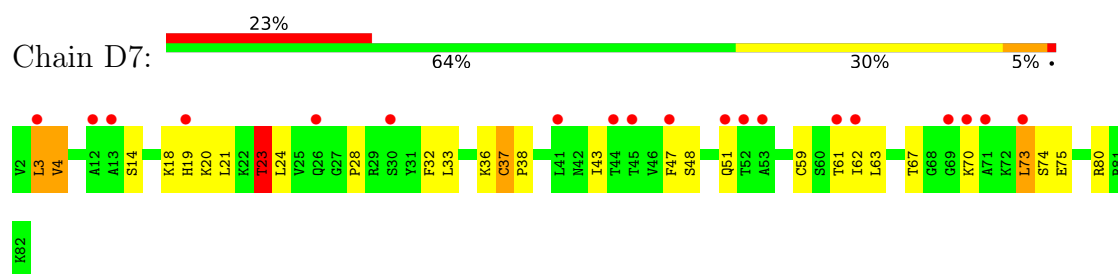
- Molecule 28: 40S ribosomal protein S26-B



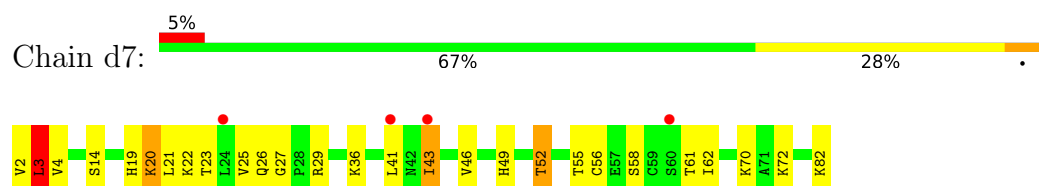
- Molecule 28: 40S ribosomal protein S26-B



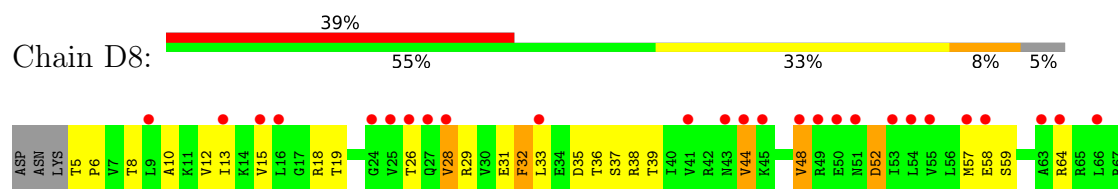
- Molecule 29: 40S ribosomal protein S27-A



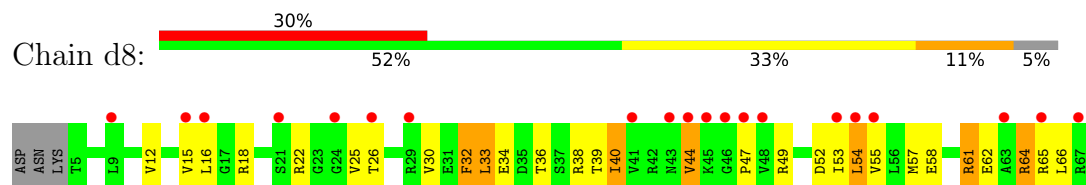
- Molecule 29: 40S ribosomal protein S27-A



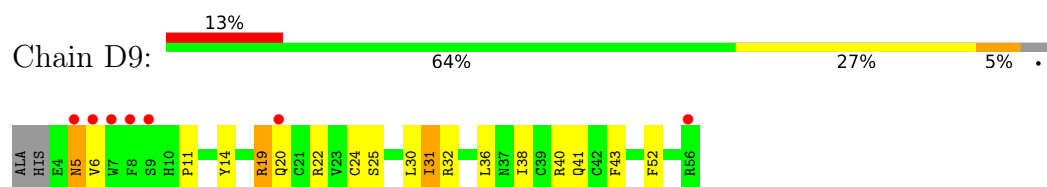
- Molecule 30: 40S ribosomal protein S28-A



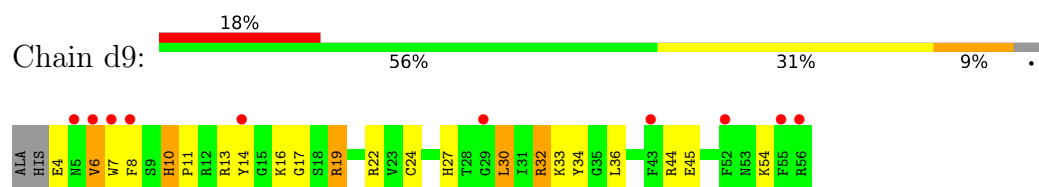
- Molecule 30: 40S ribosomal protein S28-A



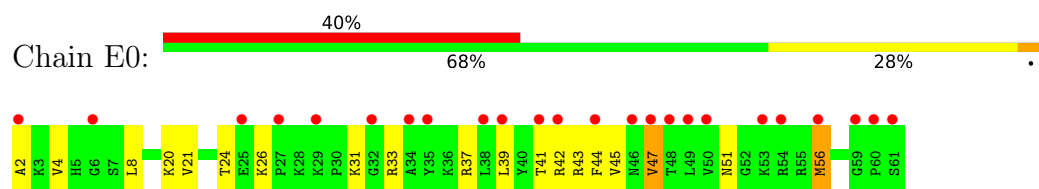
- Molecule 31: 40S ribosomal protein S29-A



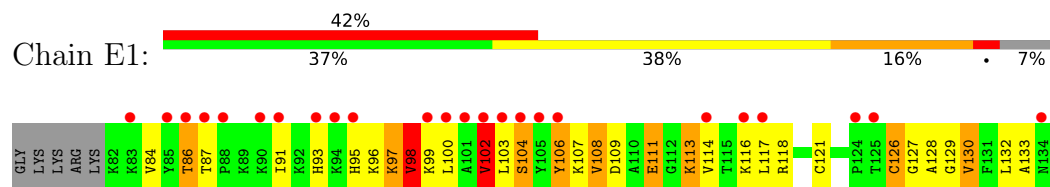
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

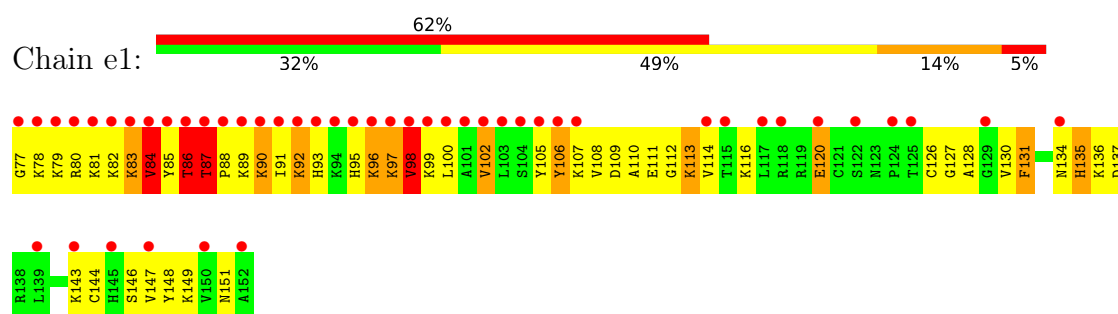


- Molecule 33: Ubiquitin-40S ribosomal protein S31

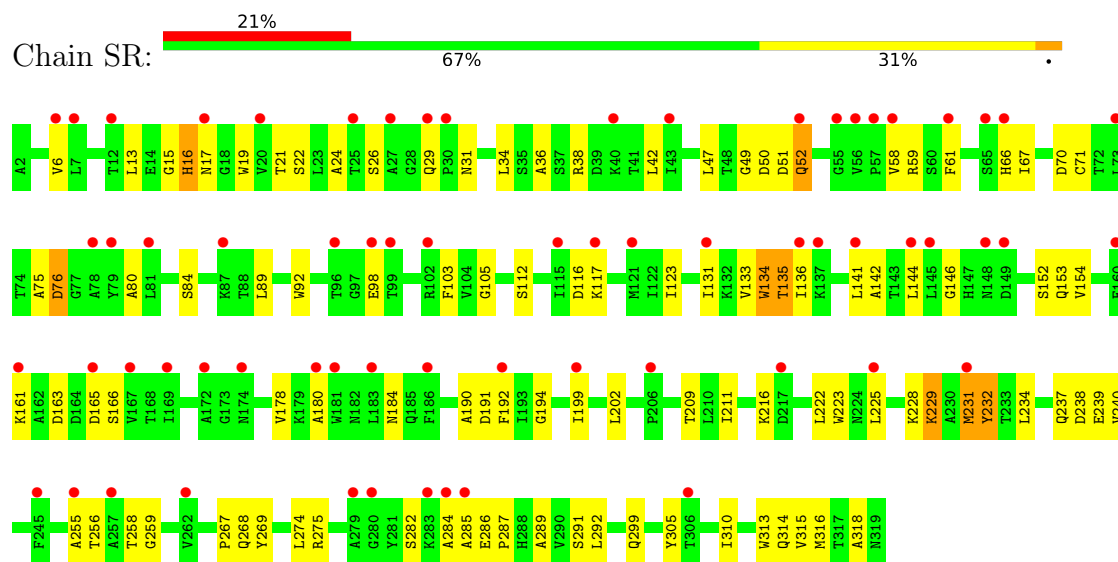


- Molecule 33: Ubiquitin-40S ribosomal protein S31

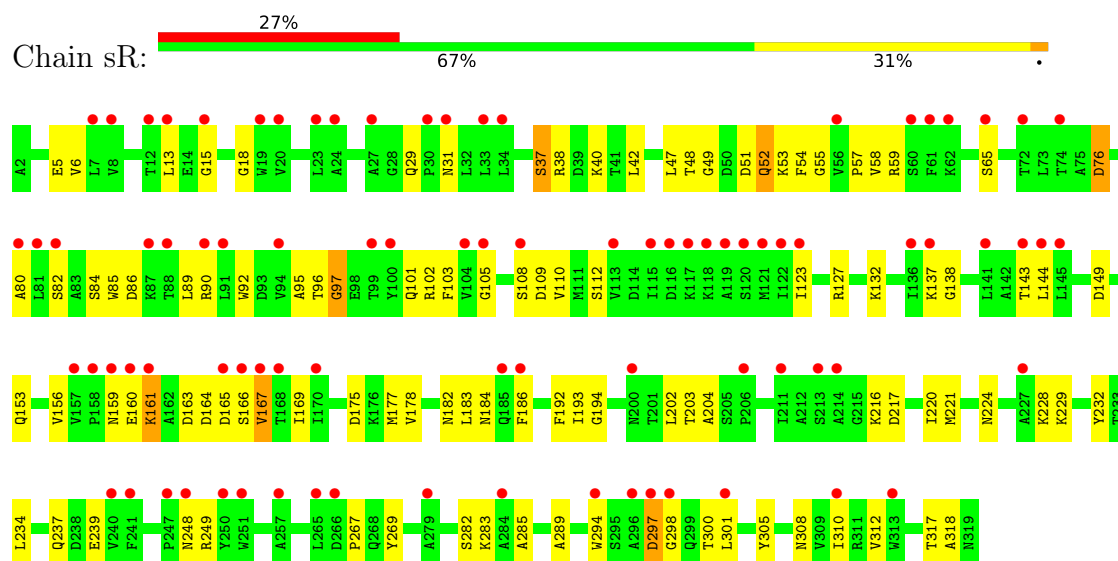




- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



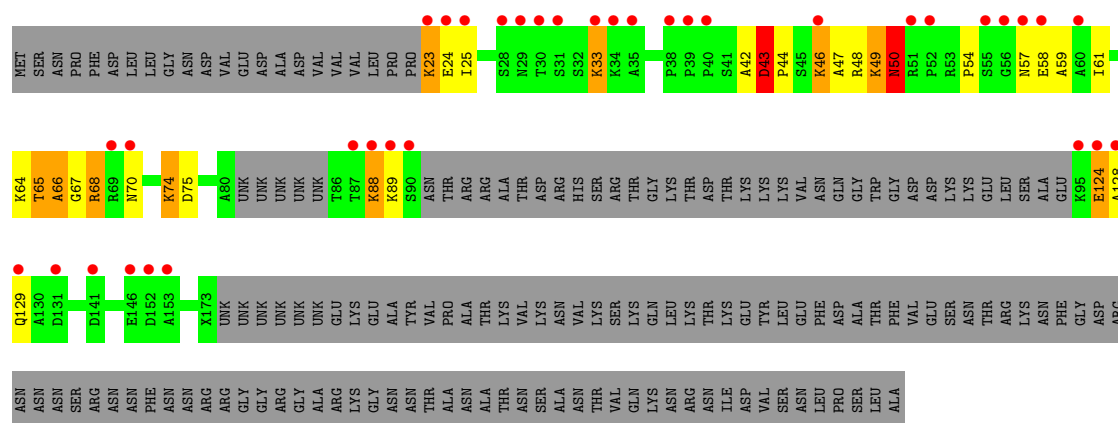
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



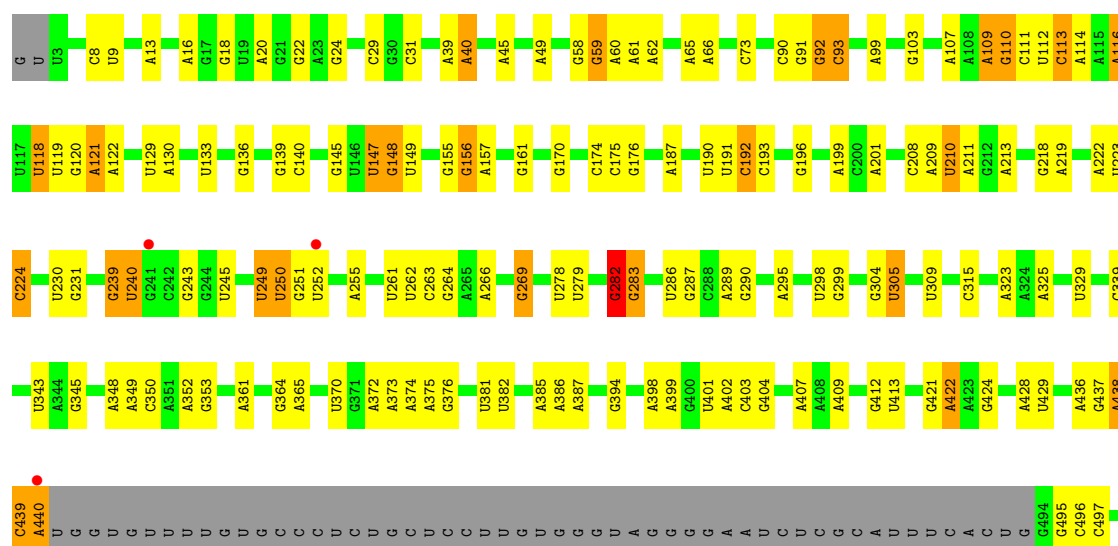
- Molecule 35: Suppressor protein STM1



- Molecule 35: Suppressor protein STM1

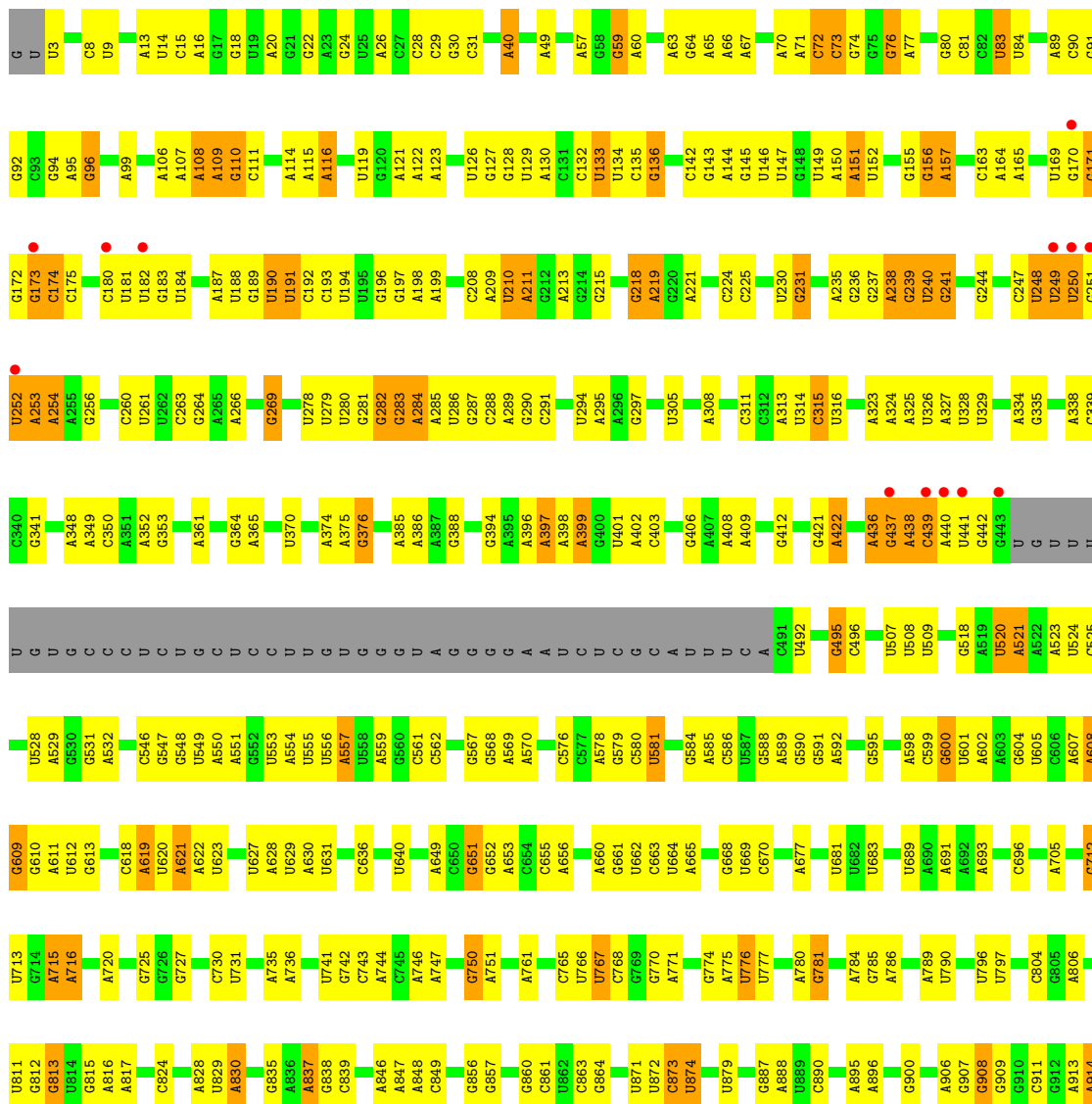


- Molecule 36: 25S ribosomal RNA



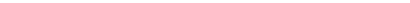
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G1727	C1609	G1522	G1431	A1330	A1244	G1157	C1068	U979	A883	G781	G996	U507
A1729	G1610	U1527	G1432	U1331	A1245	G1158	C1069	A980	U887	A754	G997	U508
G1734	C1615	U1533	A1433	A1332	U1247	A1159	U1071	U981	G887	G785	G999	G517
G1735	U1620	U1537	A1435	U1334	C1248	C1160	G1072	C982	A888	A766	G600	G518
G1736	U1629	G1536	U1437	C1339	G1249	U1168	C1076	A992	U889	G787	U601	A519
U1740	U1630	A1537	U1438	G1340	C1254	G1171	A1079	G993	C890	G788	A602	A520
A1741	U1631	G1538	U1439	U1341	G1255	G1172	U1080	G994	A895	A789	A603	A521
G1742	A1632	U1543	G1443	G1346	C1257	U1173	U1081	U995	U897	G791	G604	A522
G1743	C1633	U1549	A1446	U1347	U1258	C1176	U1082	A996	U898	G792	A607	A523
G1744	G1634	C1550	G1447	U1348	G1261	G1177	G1083	A997	U899	C801	A608	U528
U1746	G1635	U1555	A1450	U1351	G1262	G1178	A1084	A998	G900	C802	G610	A529
G1747	A1638	C1556	G1451	A1352	A1263	A1179	G1090	G1000	G901	G805	A611	A532
G1748	C1639	C1557	U1452	U1353	U1264	U1180	A1091	A1002	A904	A806	G617	G536
A1749	A1643	U1558	A1454	U1354	G1265	U1181	C1092	A1006	G907	A816	C618	U541
G1751	G1654	A1560	A1456	A1355	G1266	A1182	U1094	G1010	G908	A817	C619	G542
A1752	G1655	G1561	A1460	U1356	U1267	C1192	U1095	U1013	C911	C818	U620	C543
C1762	A1656	C1562	A1461	G1357	U1268	A1193	U1096	G1013	G912	U819	A621	C544
U1763	C1657	U1563	G1462	G1358	A1271	G1194	A1098	U1014	A913	A712	A622	U545
U1764	G1658	U1564	A1467	C1359	C1272	A1195	A1099	U1015	A914	U707	G623	C546
G1766	U1659	G1565	A1468	A1360	A1273	C1196	U1100	C1016	A915	U708	G624	G547
C1770	C1660	A1566	U1471	G1367	A1274	C1201	G1101	C1017	U829	A715	G548	U549
C1771	U1672	U1567	U1472	U1368	U1275	A1202	A1102	C1018	A830	A716	U627	A628
G1775	A1683	U1568	G1473	A1369	U1276	A1203	A1103	G1019	G831	G717	A628	A550
G1778	C1685	A1570	A1477	G1370	A1278	U1209	C1107	G1024	A837	G718	C633	A551
G1779	U1686	U1572	G1480	G1382	C1285	U1210	U1108	A1025	U922	U719	G634	G552
G1780	U1687	C1573	A1481	G1383	A1286	A1212	U1109	A1026	C839	G721	G635	A553
C1781	U1688	A1574	A1482	U1386	A1287	G1213	U1110	A1027	C840	C729	C636	A554
G1786	A1696	G1575	G1483	A1387	C1292	U1217	U1111	U1028	A841	C730	U555	U556
A1787	A1697	C1581	U1484	C1391	C1293	A1221	G1112	G1029	A846	G733	C637	A557
G1794	G1700	A1583	G1488	A1394	G1300	G1222	G1117	U1030	A847	U736	C638	U558
U1795	C1701	U1584	A1489	A1395	G1305	A1225	U1120	C1037	A848	C749	U640	A559
A1796	U1797	C1585	G1490	G1400	G1306	G1226	U1121	C1038	C849	A645	U641	C561
A1798	C1710	U1589	G1492	C1403	A1308	C1227	G1126	U1043	G860	A649	U642	C562
A1799	U1715	G1590	U1495	A1407	U1309	G1230	U1127	C1043	C861	A649	U643	U563
G1807	U1716	G1591	C1502	A1408	C1312	A1231	A1128	A1047	U862	C763	G651	A569
A1810	U1717	G1592	A1503	G1412	G1313	C1232	A1129	A1048	C863	U764	A653	C576
A1813	G1718	A1593	A1504	A1414	C1316	G1233	U1130	C1049	C864	C765	C654	C577
A1814	U1719	U1594	C1505	A1419	A1317	U1234	G1131	U1050	G870	U766	A656	A578
A1815	G1720	U1595	C1506	A1419	A1318	U1235	G1134	C958	U871	U767	G579	G579
U1815	U1721	C1597	U1425	U1426	G1319	G1237	A1135	U1051	U872	C768	A660	C580
A1816	G1722	U1598	C1426	U1427	C1320	C1238	U1144	A1054	C873	G774	G661	G590
G1817	A1723	U1603	A1428	A1428	A1326	C1239	G1145	G1063	U874	A775	U662	G591
U1818	U1724	A1603	U1511	U1428	A1327	A1241	C1146	A1064	A876	U776	C670	A592
					C1327			A1065	C877	U778	U671	C593

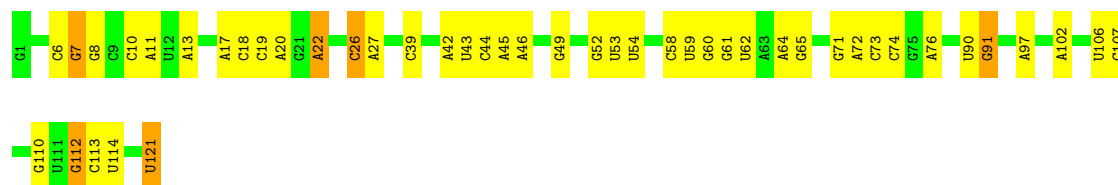
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G2901	C2811	C2812	A2695	G2607	U2516	U	A2352	C2227	C2137	G	U	A1821
U2905	G2814	G2815	A2696	G2610	A2520	U	G2355	A2229	U2137	U	C	G1825
A3005	G2816	G2817	A2704	U2611	G2521	A	A2356	A2242	U2138	A	U	G1830
A3006	G2818	A2817	A2705	U2612	A2522	G	A2363	A2243	U2139	G	U	A1835
U3007	U2915	U2916	G2706	U2613	A2523	A	A2363	A2244	U2140	G	U	C1836
A3012	A2819	G2820	G2714	U2614	G2525	U	A2372	G2249	A2144	C	U	A1839
U3013	G2821	G2822	C2719	C2615	A2529	A	A2373	G2250	C2146	C	U	U1840
U3014	G2823	G2824	U2719	U2617	U2532	G	C2374	G2254	G2150	U	G	A1841
U3023	G2834	G2835	U2723	G2621	G2532	U	G2375	U2254	G2155	U	G	A1842
A3024	U2836	C2837	U2724	C2622	G2533	G	G2385	A2255	G2156	G	C	C1843
C3025	C2838	G2839	U2725	G2623	G2534	G	G2391	A2256	A2158	A	U	C1844
G3028	A2838	G2840	C2726	G2624	A2535	A	G2392	G2261	U2162	G	U	G1845
A3029	G2839	G2841	A2727	G2632	U2537	G	C2393	C2267	C2163	A	U	C1846
U3030	U2842	U2843	G2728	G2633	U2538	C	G2394	U2268	U2169	C	U	A1847
A3033	U2844	C2845	U2736	A2637	A2540	U	A2397	G2272	A2168	G	U	C1848
C3034	U2846	U2847	C2737	A2642	U2541	C	A2400	G2273	U2170	C	U	A1850
U3037	A2848	A2849	A2746	G2645	U2542	G	A	C2278	G2174	G	A	G1851
U3038	G2852	G2853	A2747	C2646	U2543	C	A2402	A2279	U2175	U	G	A1858
G3039	A2854	G2855	A2748	A2647	C2546	G	G2403	A2280	G2176	U	G	G1863
A3040	U2855	G2856	G2749	G2651	A2547	C	A2404	A2281	G2180	U	C	G1866
U3041	U2856	G2857	G2752	U2652	G2548	A	C2405	U2282	G2185	C	U	U1876
C3042	G2858	G2859	U2753	G2655	U2549	G	C2406	G2283	U2186	C	U	A1879
U3043	U2867	U2868	G2754	U2656	C2552	U	C2407	C2284	U2187	C	U	U1880
U3047	U2869	C2870	A2761	G2657	U2553	G	U2408	C2285	A2188	U	A	A1886
A3048	G2871	G2872	U2767	G2658	A2554	A	U2411	G2288	G2193	U	C	A1887
G3053	U2873	U2874	U2768	G2659	G2555	U	U2417	U2294	G2194	A	U	U1895
U3056	U2875	U2876	U2771	G2661	C2560	C	G2418	A2295	A2198	A	G	G1898
U3057	G2877	G2878	C2772	G2662	A2561	A	A2419	U2297	G2203	C	C	A1899
G3059	U2879	U2880	G2776	G2663	A2562	C	U2421	A2298	U2205	G	U	A1900
U3066	G2881	G2882	G2777	G2669	U2565	U	G2424	A2299	G2206	C	C	G1906
C3067	U2883	U2884	A2778	A2674	C2566	A	G2425	G2307	U2207	C	C	A1911
U3068	G2885	G2886	A2779	G2675	C2567	C	U2433	C2308	G2208	C	C	U1912
A3072	U2887	U2888	U2780	A2676	A2569	U	G2435	C2309	A2213	U	U	A1913
C3073	C2889	C2890	U2781	G2677	A2570	U	A2438	U2310	G2215	G	G	G1914
U3077	U2891	U2892	G2784	A2678	U2571	A	A2439	G2311	G2216	C	C	U1915
U3078	G2893	G2894	U2795	A2679	C2572	U	A2443	U2312	G2217	U	U	A1922
U3079	U2895	U2896	U2796	A2680	G2573	G	A2444	G2313	A2218	G	C	U1923
G3080	C2897	C2898	C2797	G2681	G2503	U	G2440	C2331	G2219	C	C	U1924
A3084	U2899	U2900	U2798	U2682	C2507	C	C2444	A2332	A2220	A	U	U1925
G3085	G2901	G2902	G2799	G2683	U2508	A	A2445	G2333	A2223	G	G	G1927
A3086	U2903	U2904	A2799	C2684	C2511	U	U	U2334	A2224	C	C	
U3087	G2905	G2906	A2801	G2685	G2512	G	A	U2335				
G3088	A2907	A2908	A2802	U2688	C2513	G	G	U2336				
	U2996	U2997	G2996	G2690	A2593			C2337				





- Molecule 37: 5S ribosomal RNA

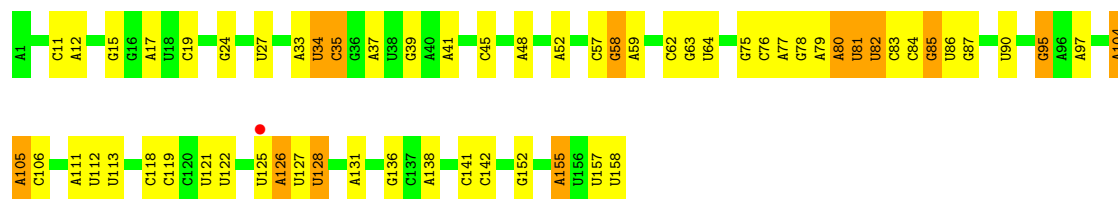
Chain 3:  62% 33% 5%



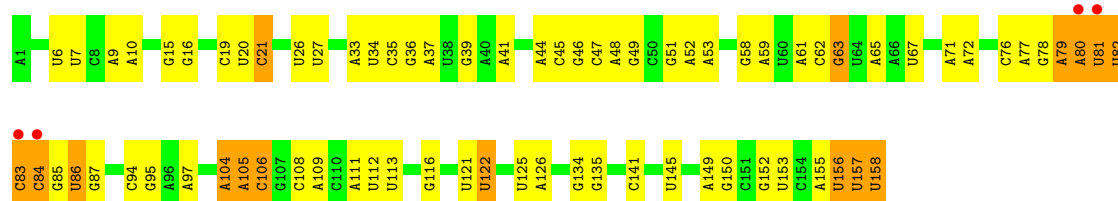
- Molecule 37: 5S ribosomal RNA



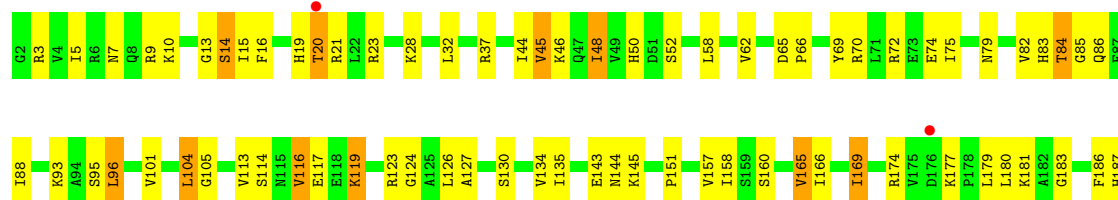
- Molecule 38: 5.8S ribosomal RNA



- Molecule 38: 5.8S ribosomal RNA

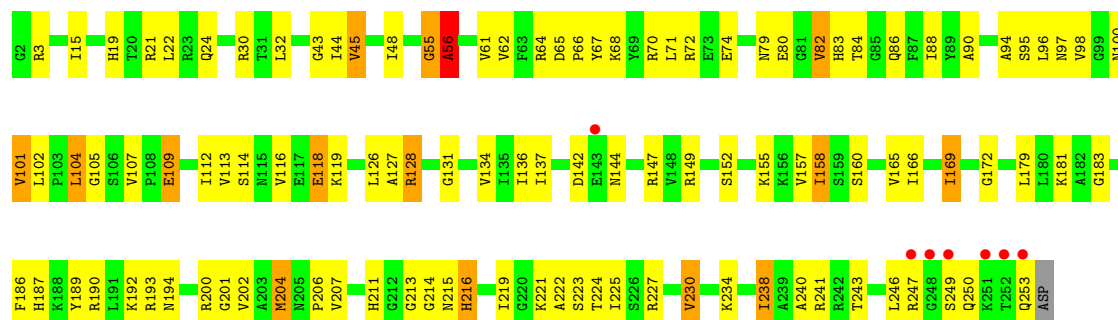


- Molecule 39: 60S ribosomal protein L2-A

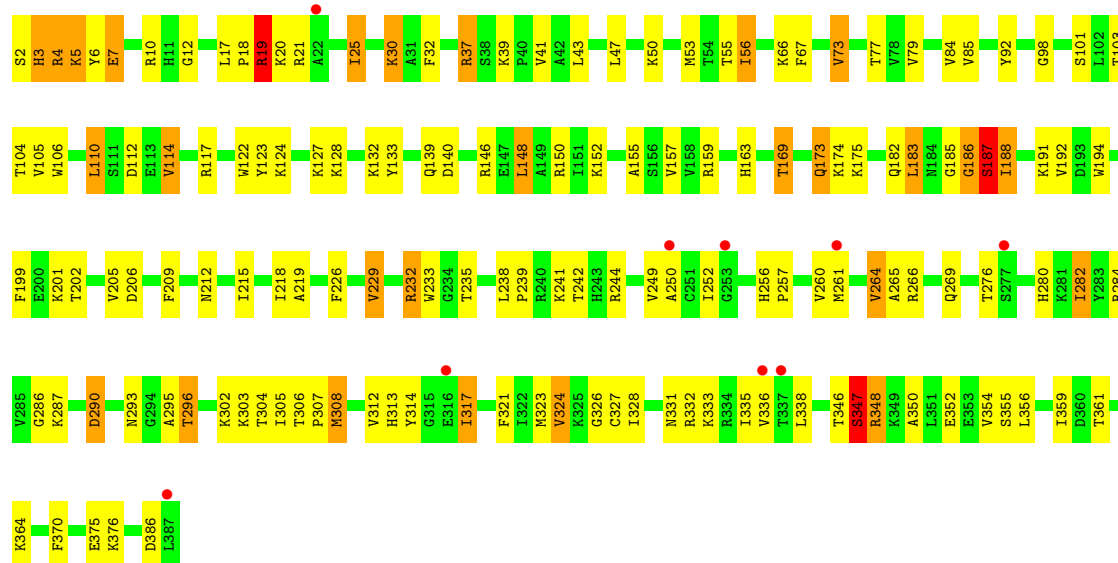




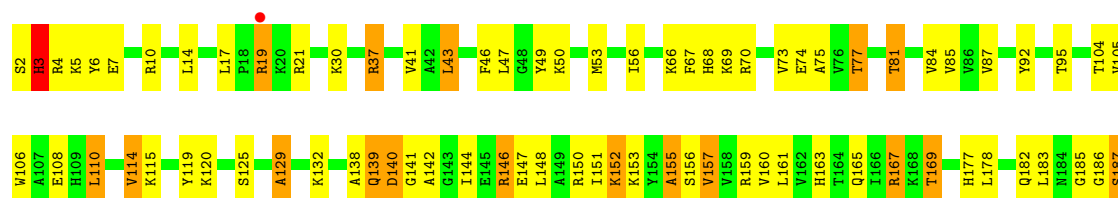
• Molecule 39: 60S ribosomal protein L2-A

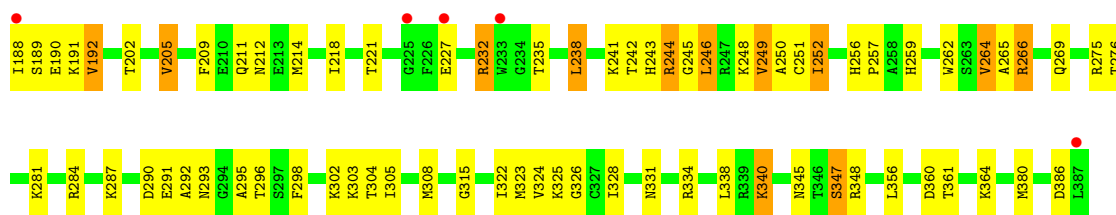


• Molecule 40: 60S ribosomal protein L3

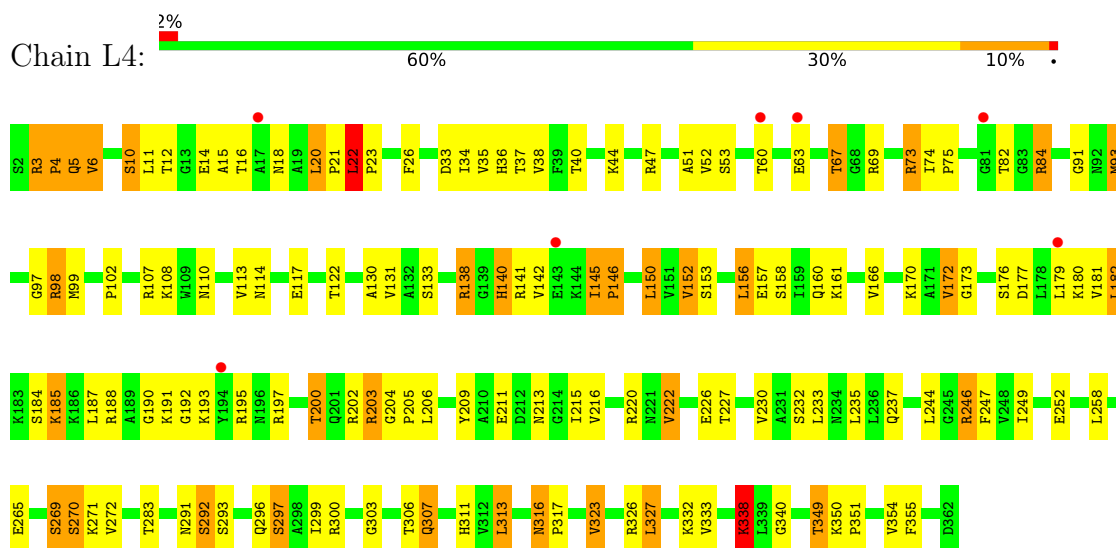


• Molecule 40: 60S ribosomal protein L3

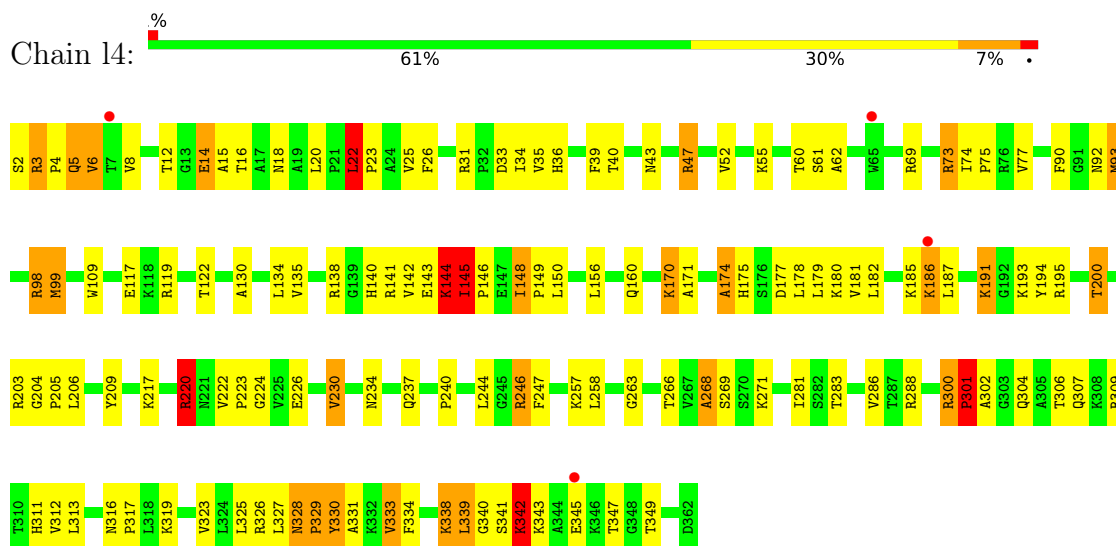




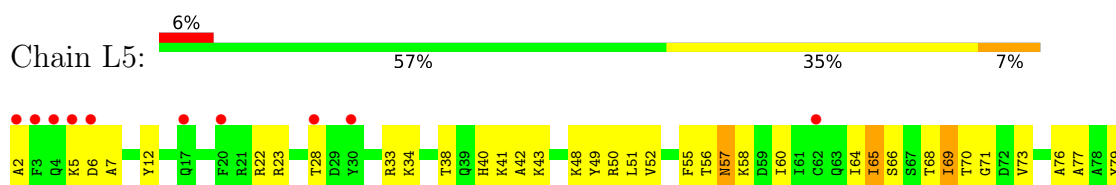
• Molecule 41: 60S ribosomal protein L4-A

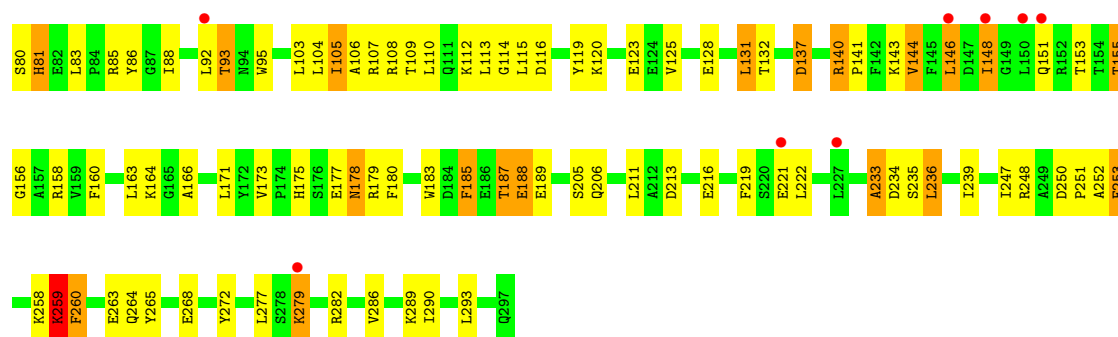


• Molecule 41: 60S ribosomal protein L4-A

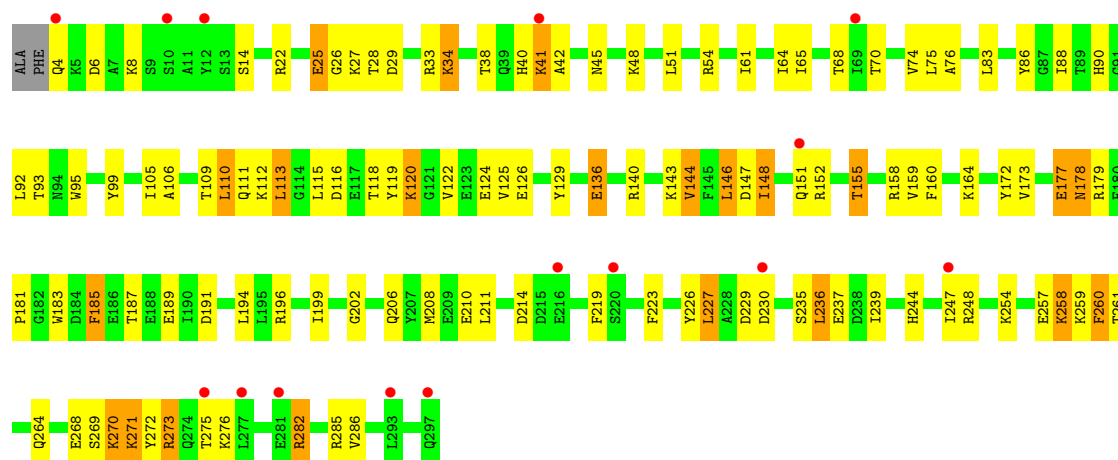


• Molecule 42: 60S ribosomal protein L5

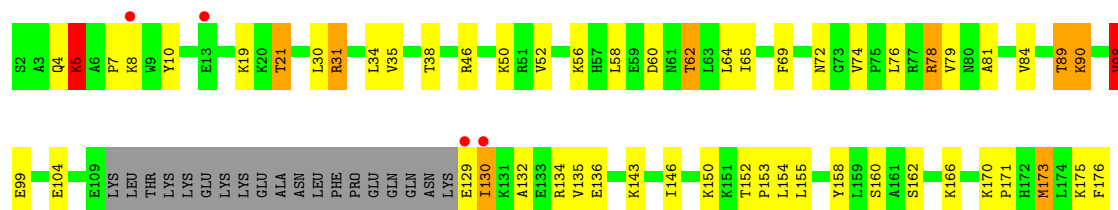




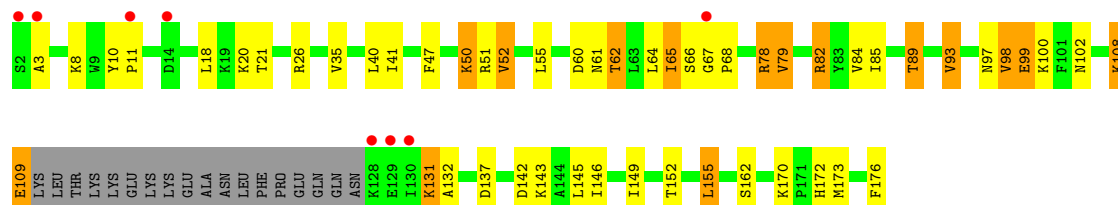
• Molecule 42: 60S ribosomal protein L5



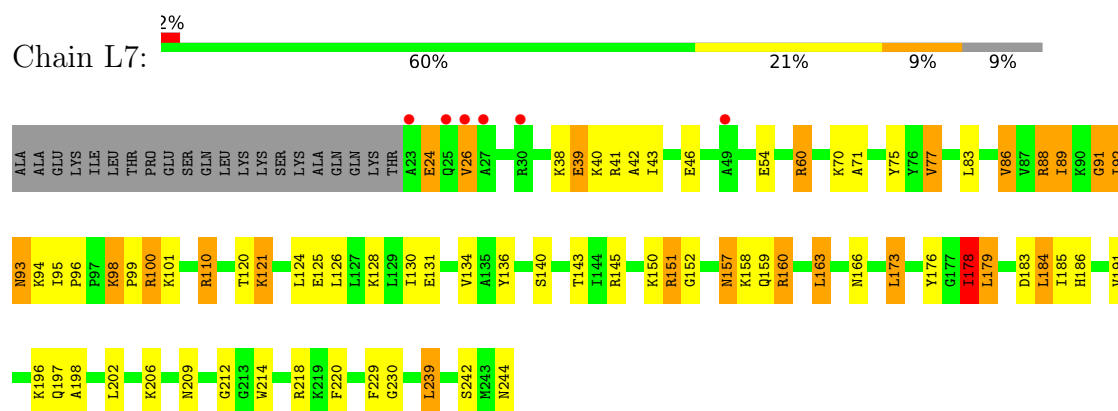
• Molecule 43: 60S ribosomal protein L6-A



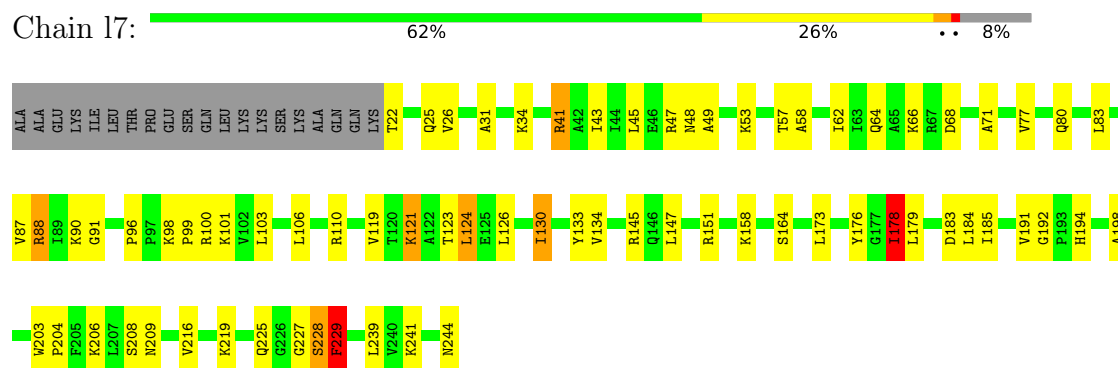
• Molecule 43: 60S ribosomal protein L6-A



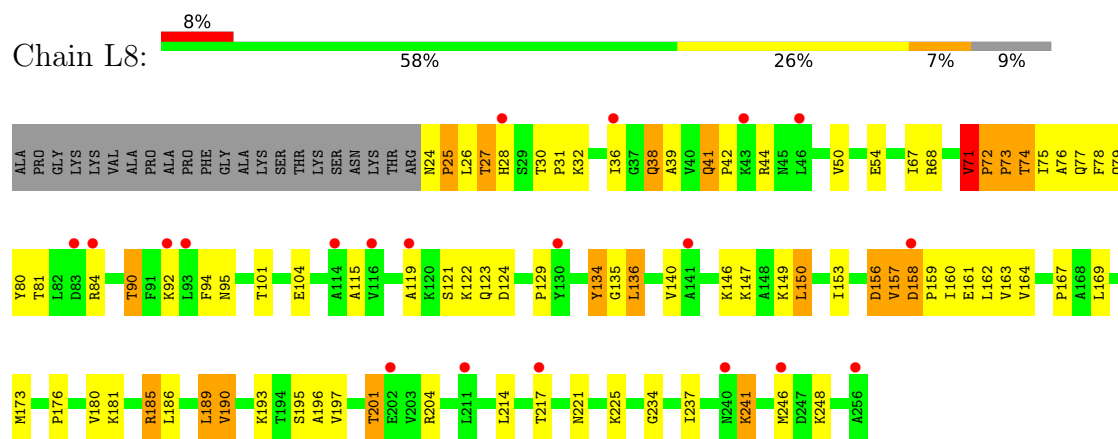
- Molecule 44: 60S ribosomal protein L7-A



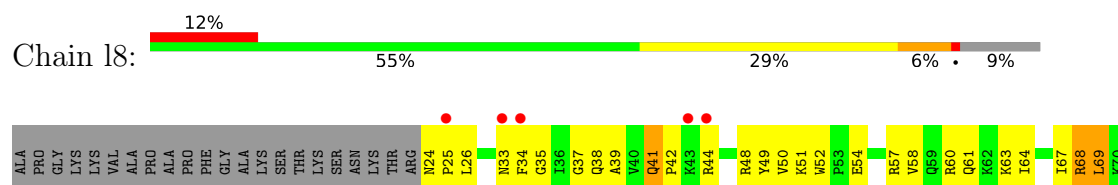
- Molecule 44: 60S ribosomal protein L7-A

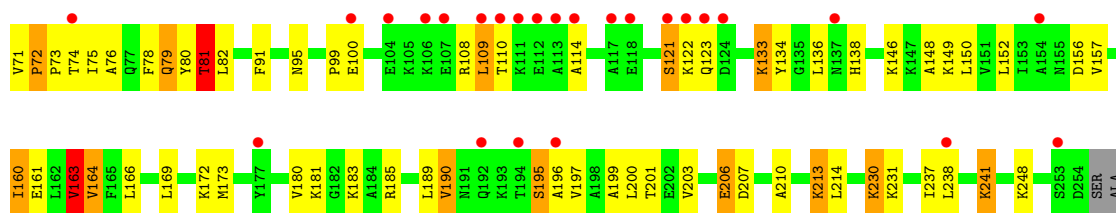


- Molecule 45: 60S ribosomal protein L8-A (eL8)

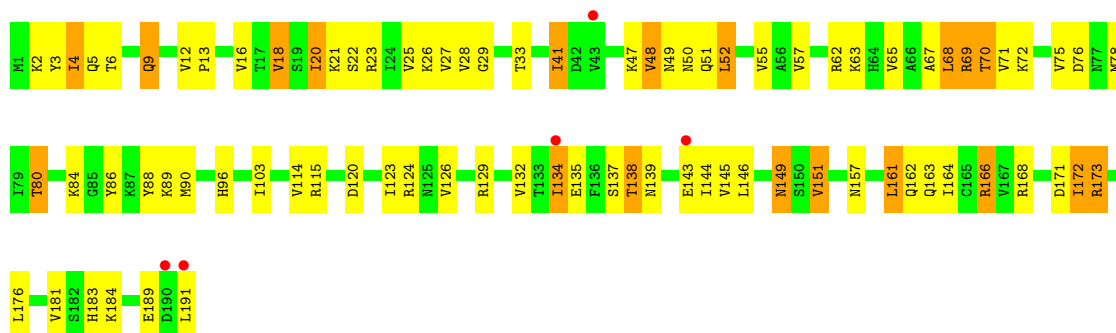


- Molecule 45: 60S ribosomal protein L8-A (eL8)

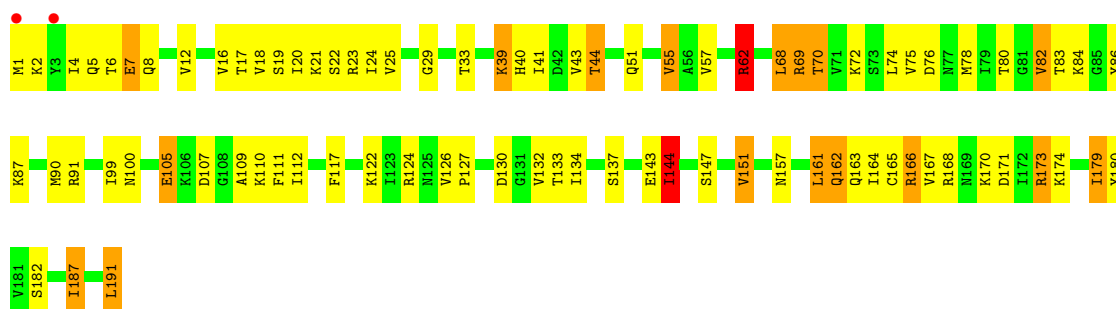




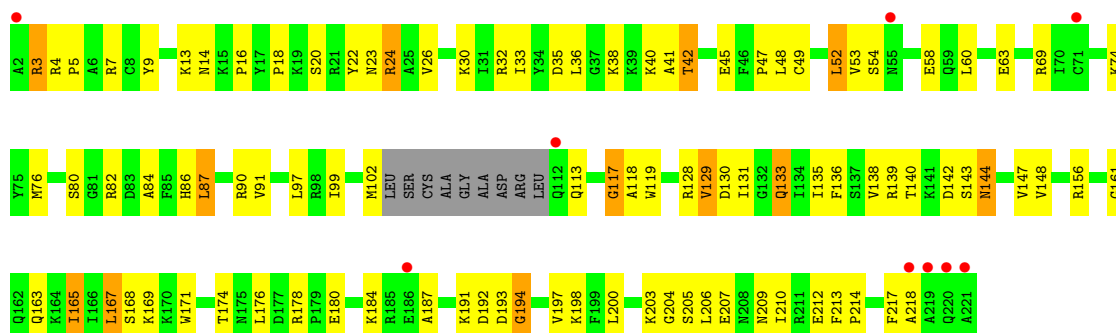
• Molecule 46: 60S ribosomal protein L9-A



• Molecule 46: 60S ribosomal protein L9-A

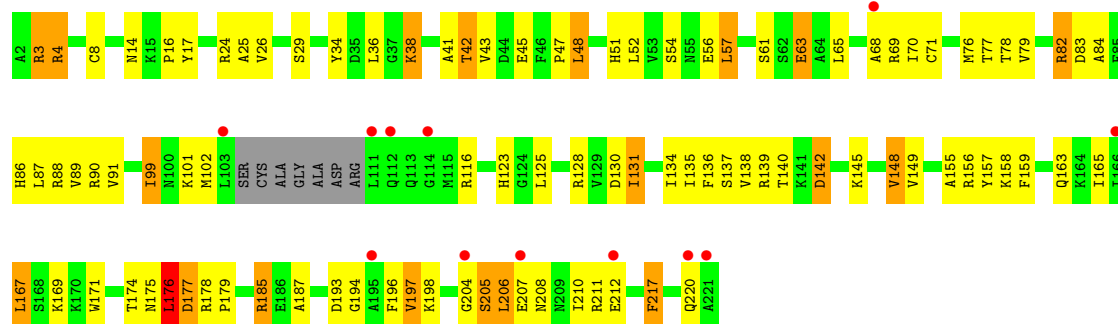


• Molecule 47: 60S ribosomal protein L10



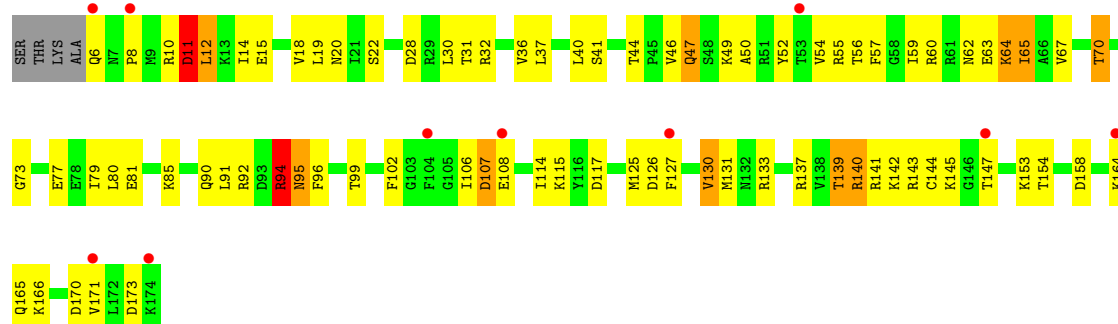
• Molecule 47: 60S ribosomal protein L10

Chain m0: 



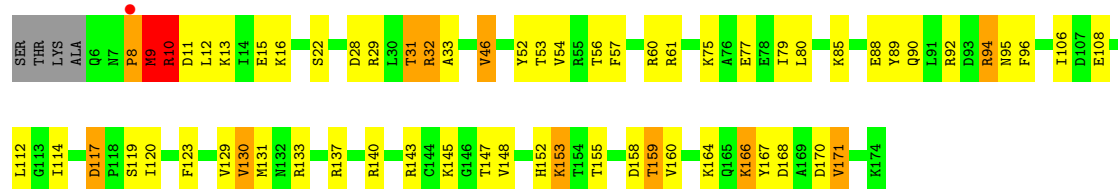
• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 



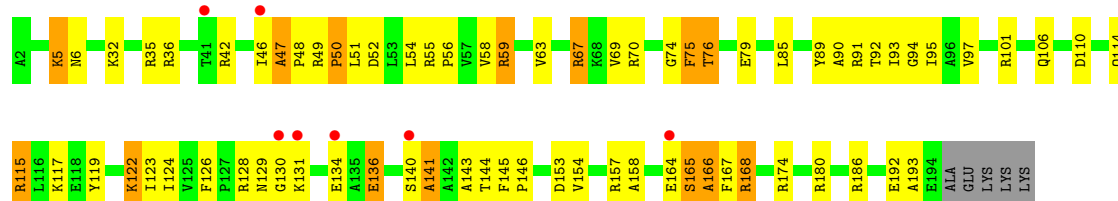
• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 



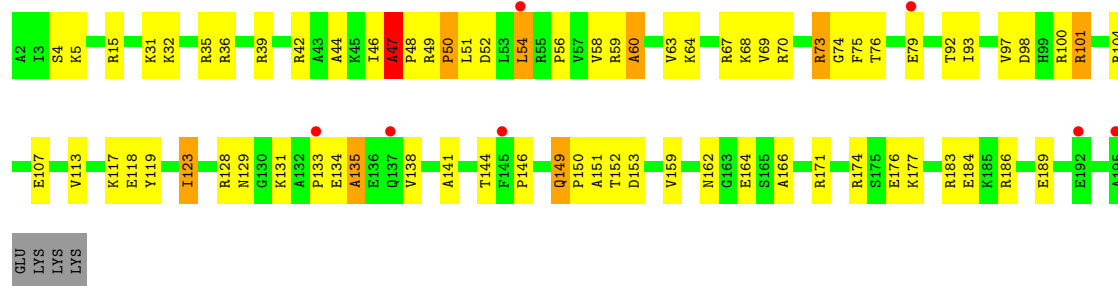
• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 



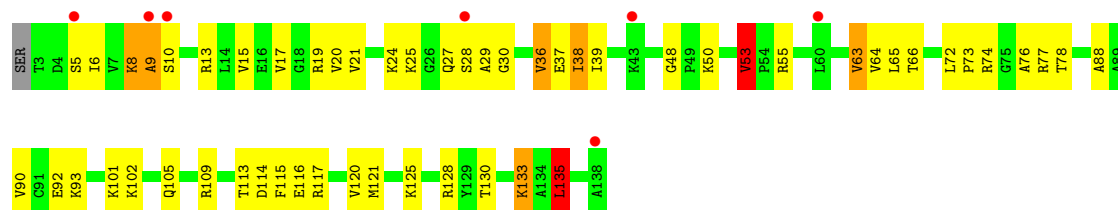
• Molecule 49: 60S ribosomal protein L13-A

Chain m3: 



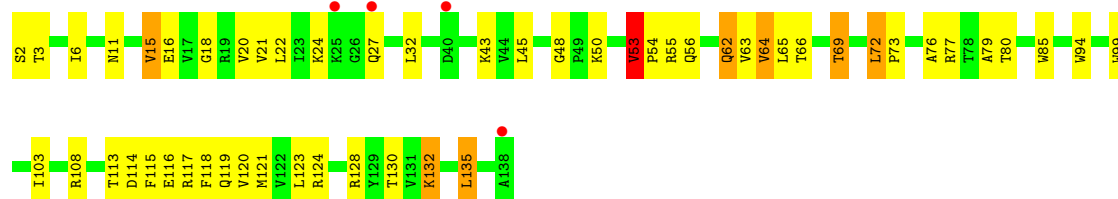
- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 



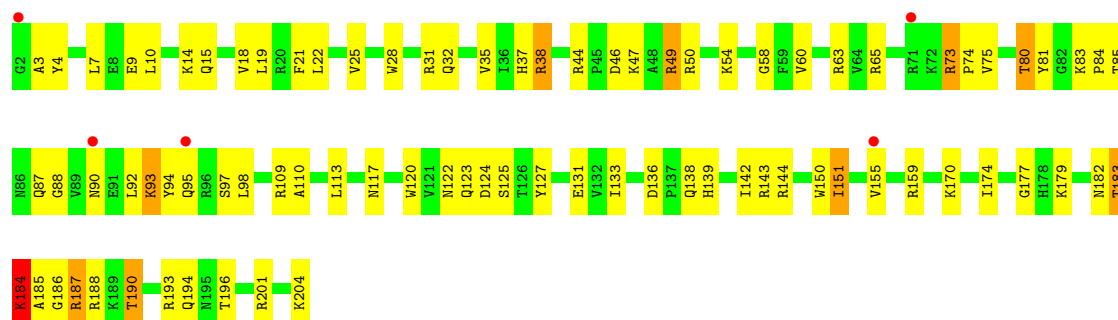
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 

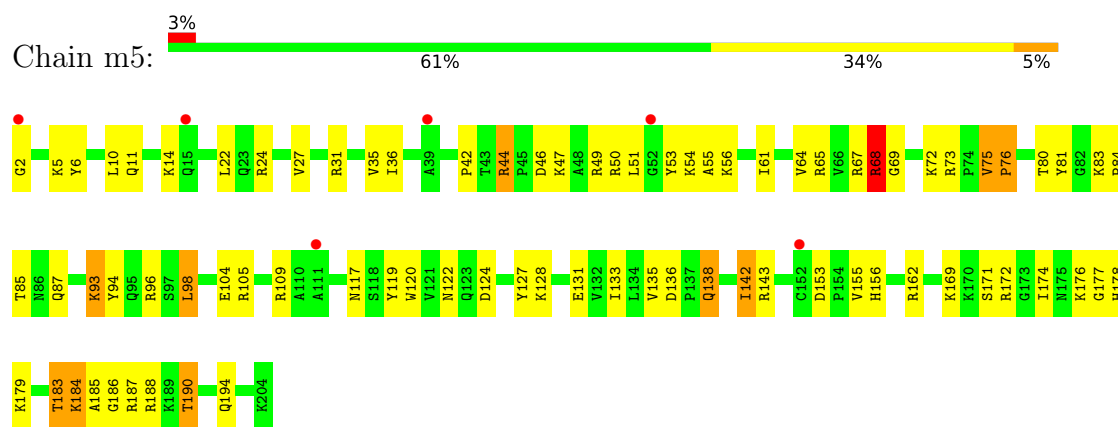


- Molecule 51: 60S ribosomal protein L15-A

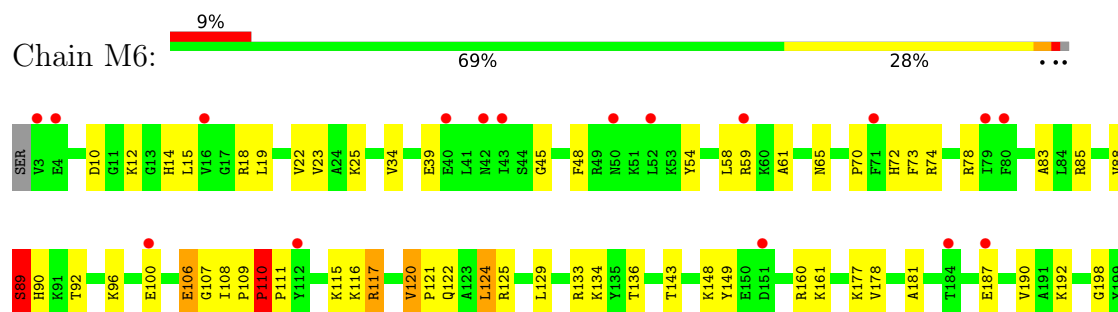
Chain M5: 



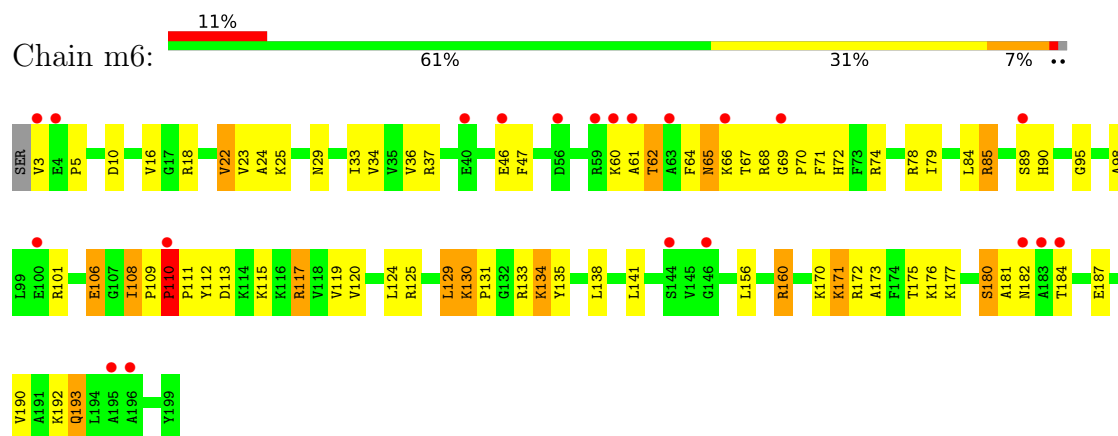
- Molecule 51: 60S ribosomal protein L15-A



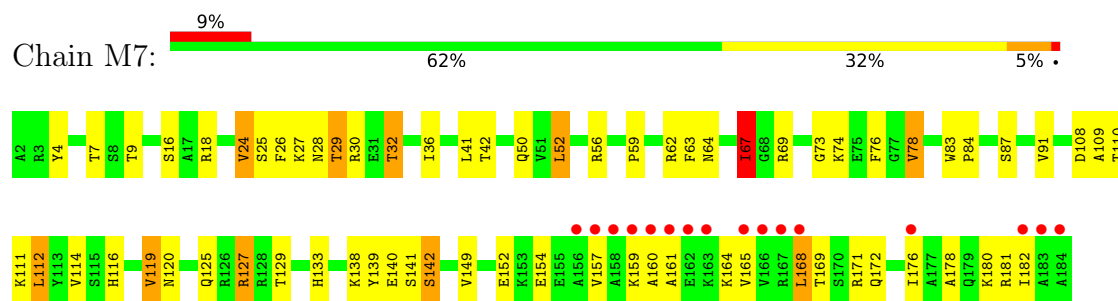
• Molecule 52: 60S ribosomal protein L16-A



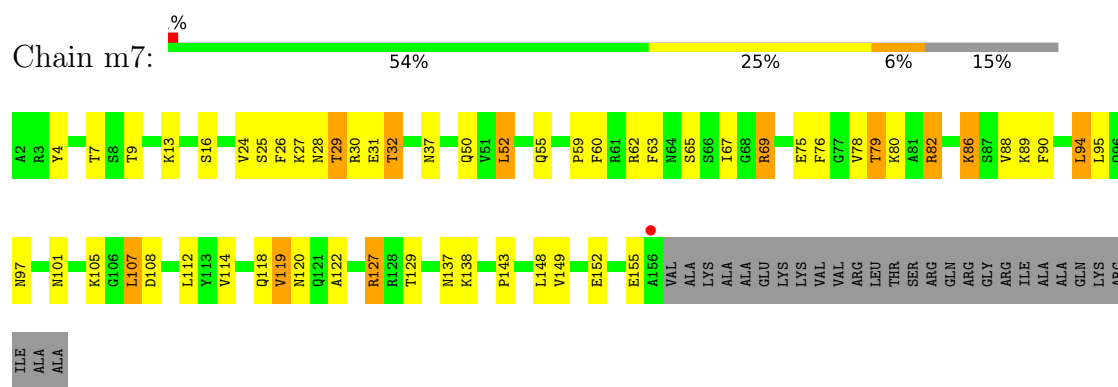
• Molecule 52: 60S ribosomal protein L16-A



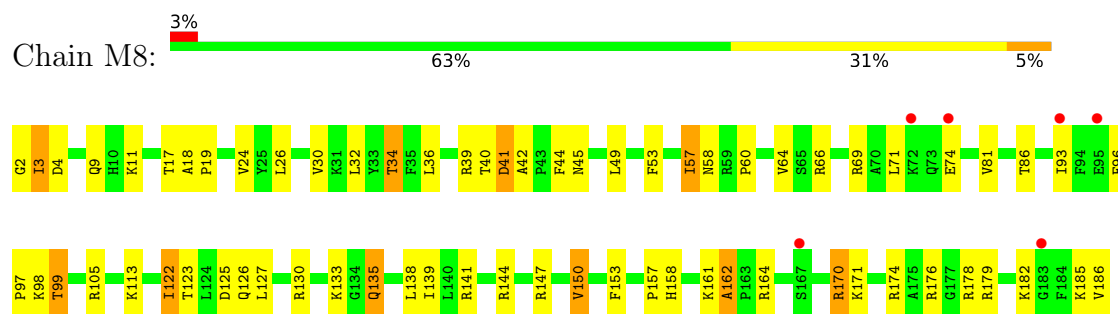
• Molecule 53: 60S ribosomal protein L17-A



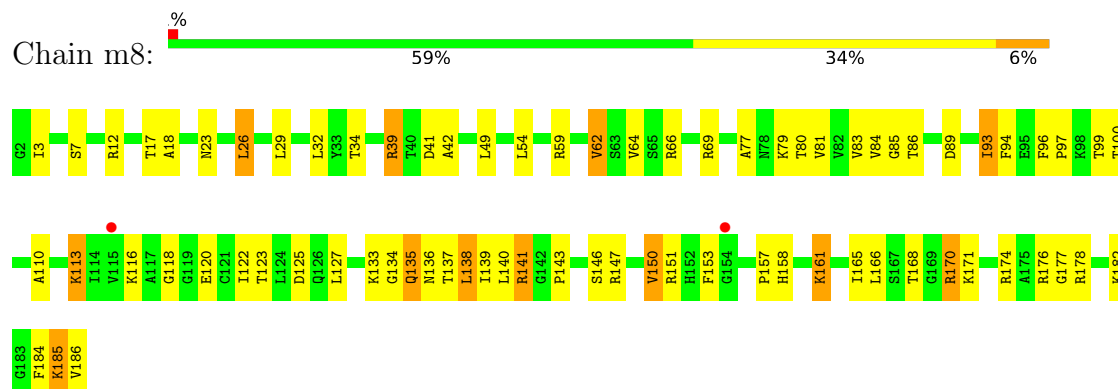
• Molecule 53: 60S ribosomal protein L17-A



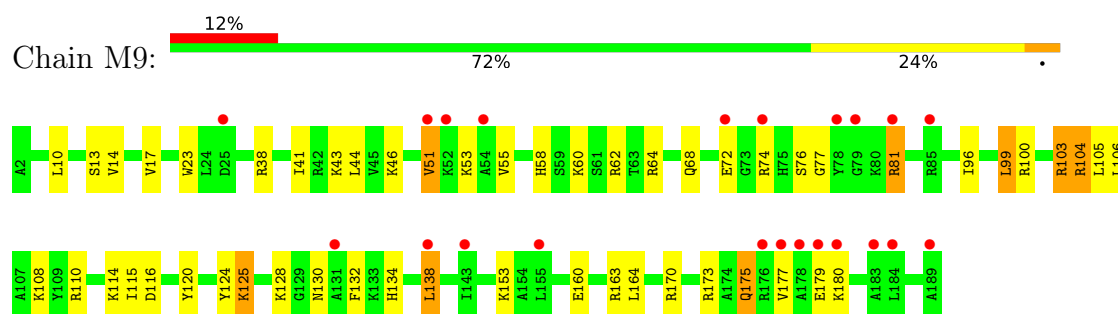
- Molecule 54: 60S ribosomal protein L18-A



- Molecule 54: 60S ribosomal protein L18-A

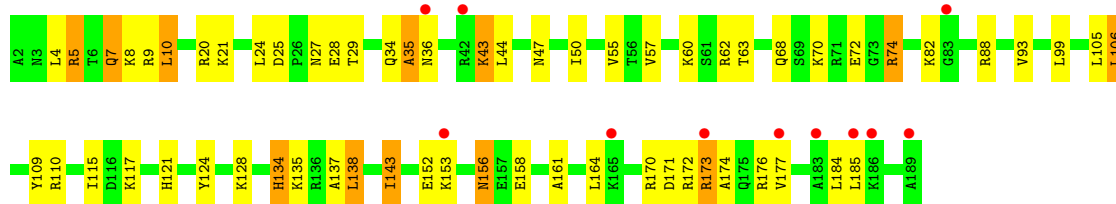


- Molecule 55: 60S ribosomal protein L19-A

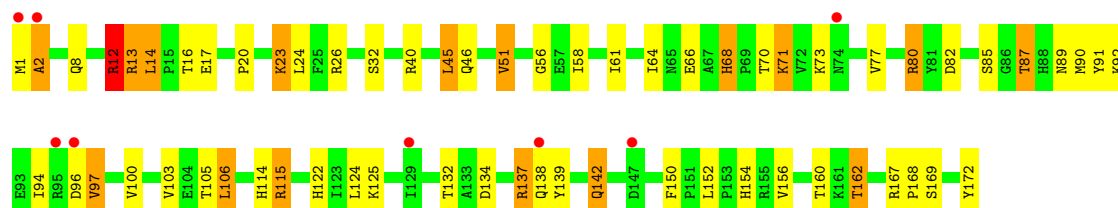


- Molecule 55: 60S ribosomal protein L19-A

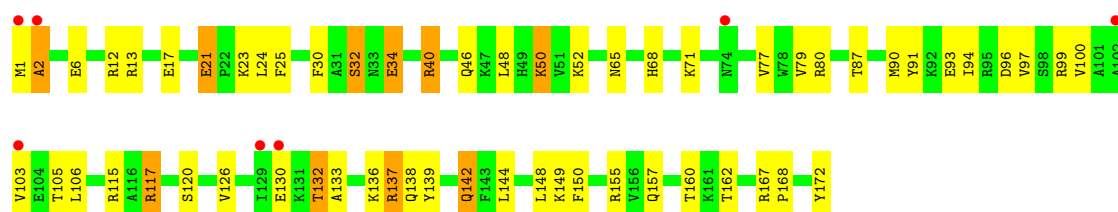




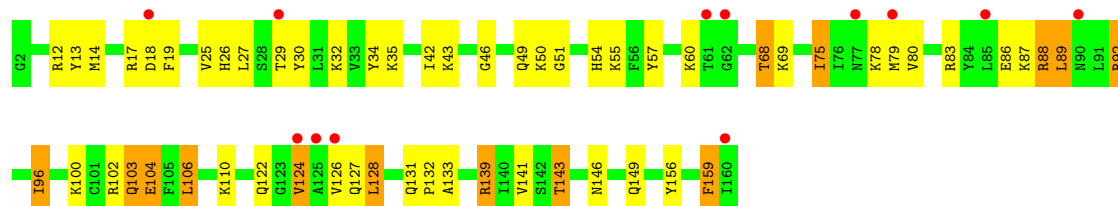
• Molecule 56: 60S ribosomal protein L20-A



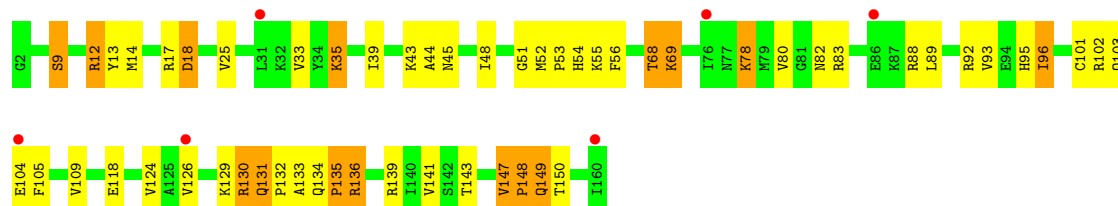
• Molecule 56: 60S ribosomal protein L20-A



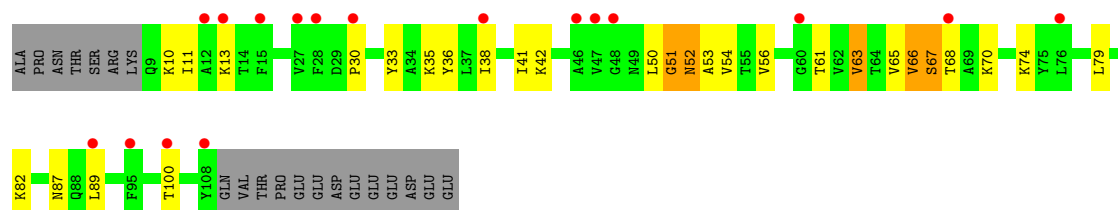
• Molecule 57: 60S ribosomal protein L21-A



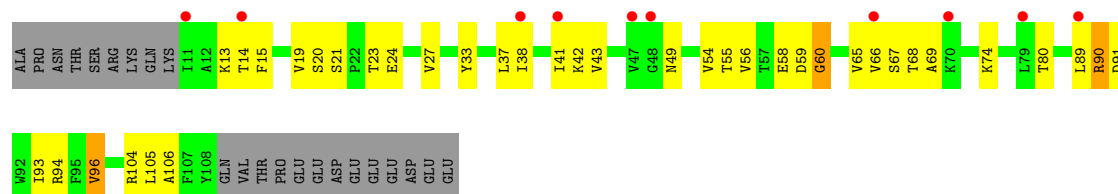
• Molecule 57: 60S ribosomal protein L21-A



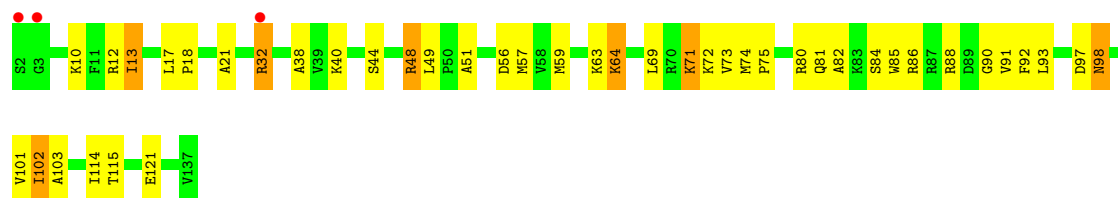
- Molecule 58: 60S ribosomal protein L22-A



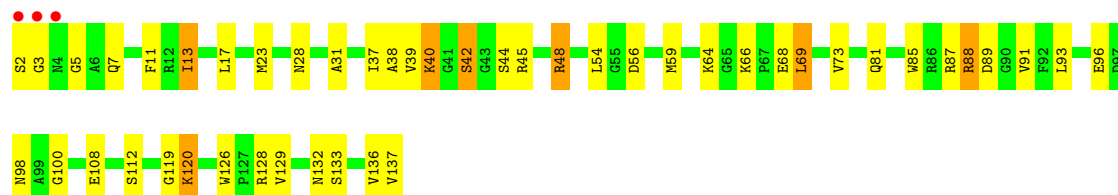
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 59: 60S ribosomal protein L23-A

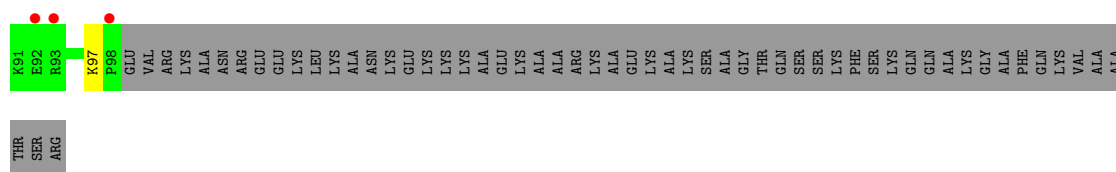


- Molecule 59: 60S ribosomal protein L23-A

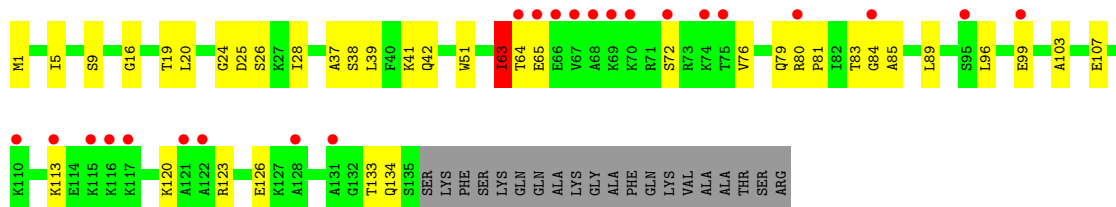


- Molecule 60: 60S ribosomal protein L24-A

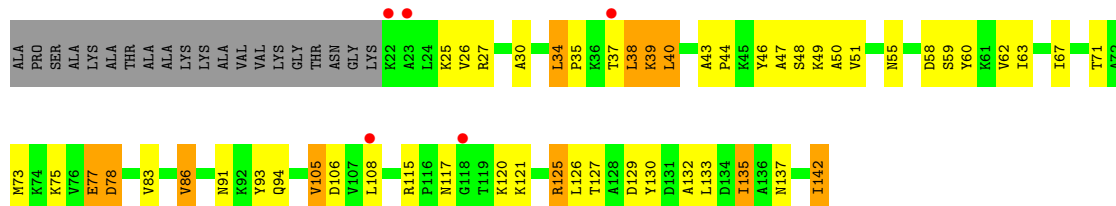




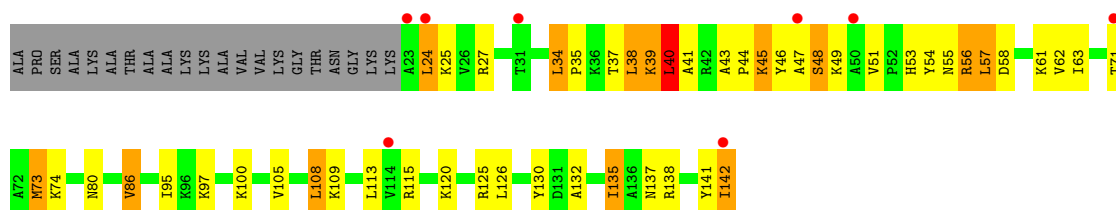
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 61: 60S ribosomal protein L25



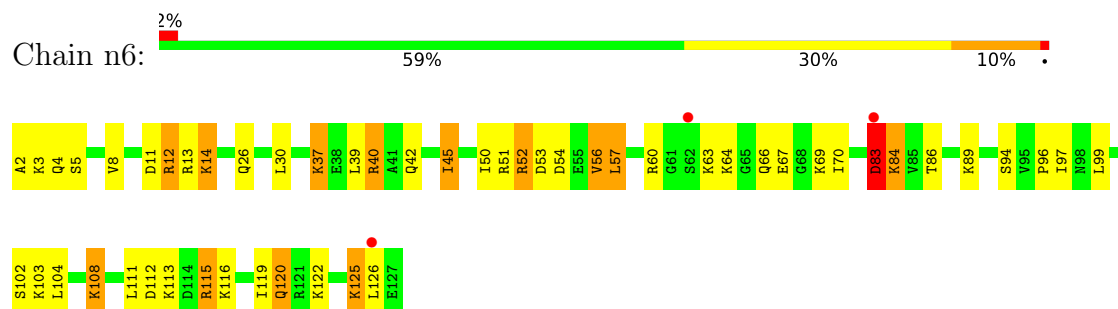
- Molecule 61: 60S ribosomal protein L25



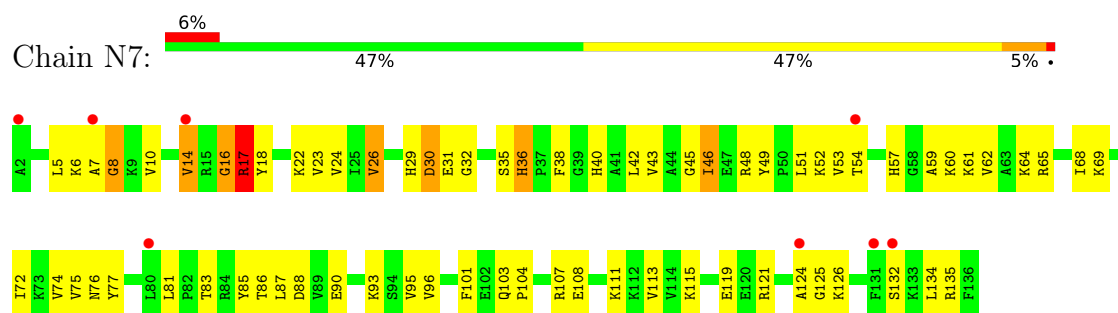
- Molecule 62: 60S ribosomal protein L26-A



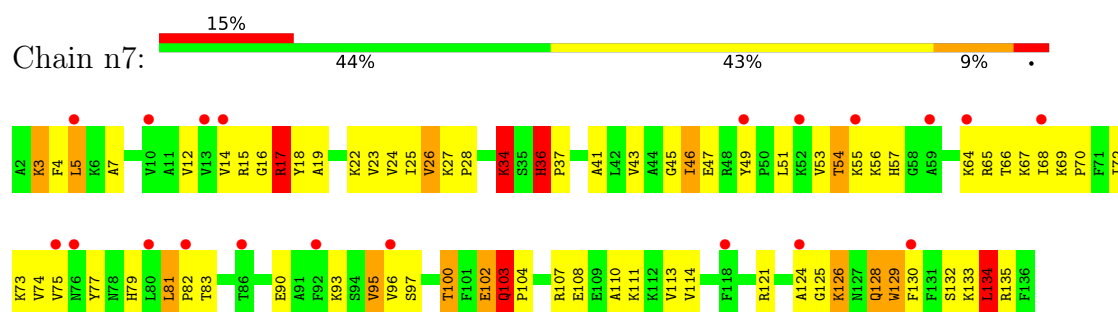
- Molecule 62: 60S ribosomal protein L26-A



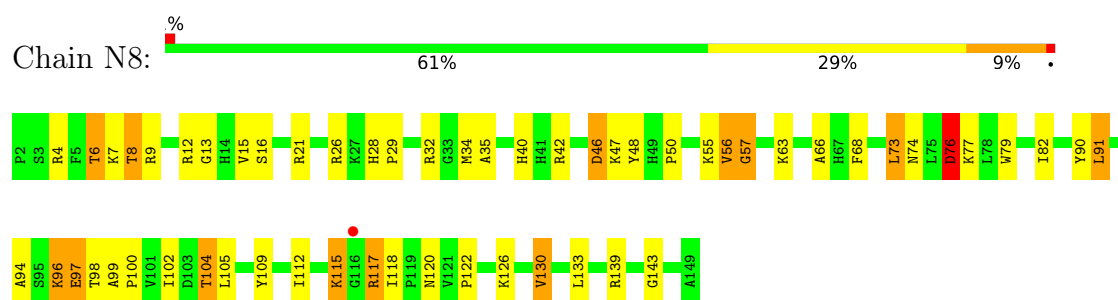
- Molecule 63: 60S ribosomal protein L27-A



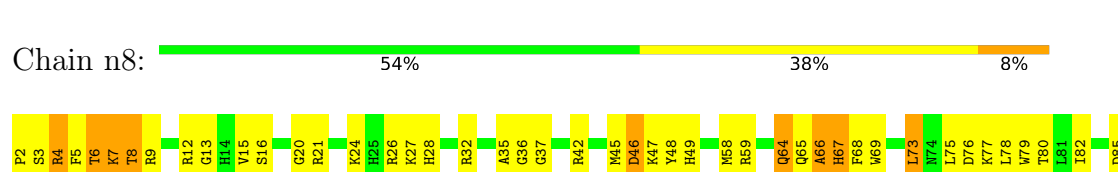
- Molecule 63: 60S ribosomal protein L27-A



- Molecule 64: 60S ribosomal protein L28

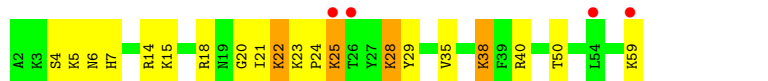


- Molecule 64: 60S ribosomal protein L28

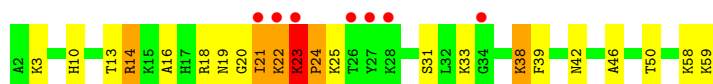




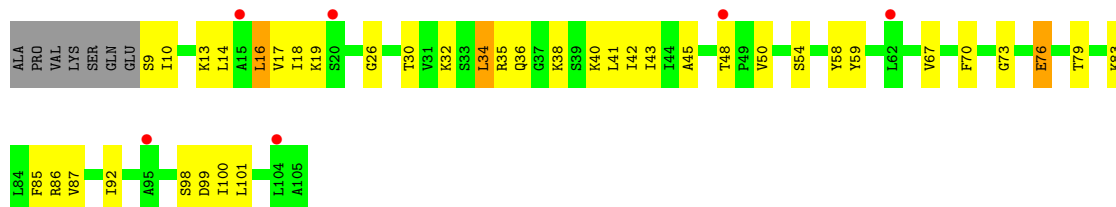
- Molecule 65: 60S ribosomal protein L29



- Molecule 65: 60S ribosomal protein L29



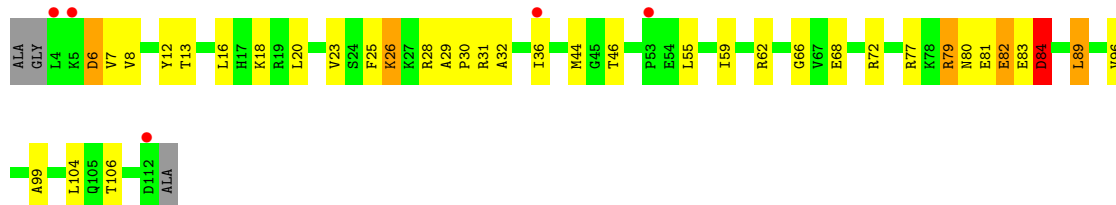
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30

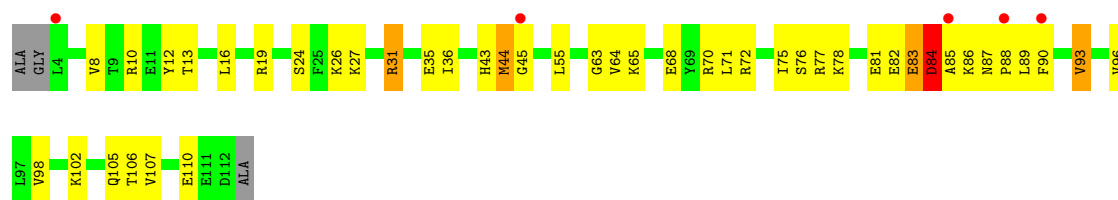


- Molecule 67: 60S ribosomal protein L31-A

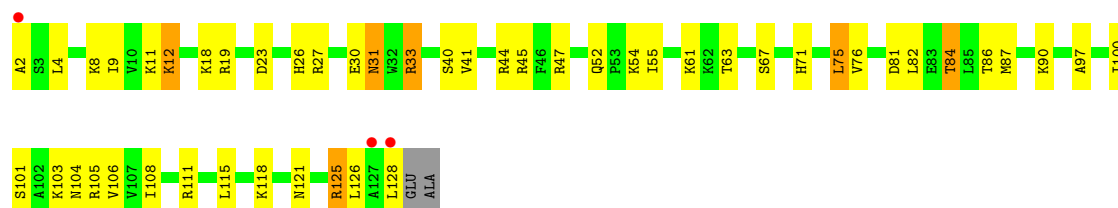


- Molecule 67: 60S ribosomal protein L31-A

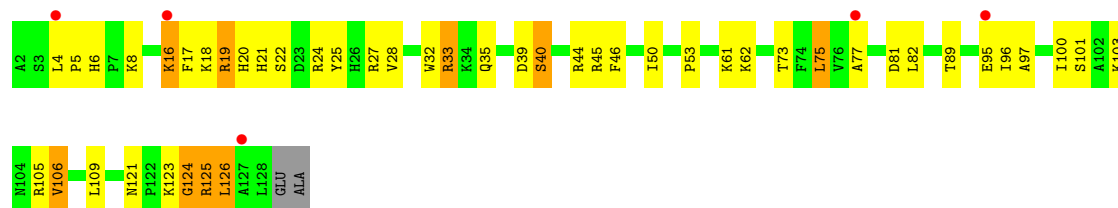




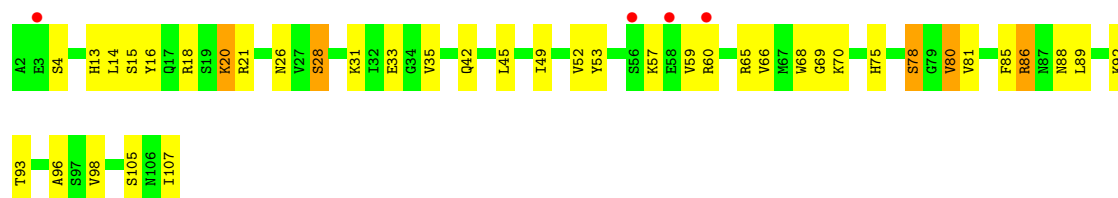
- Molecule 68: 60S ribosomal protein L32



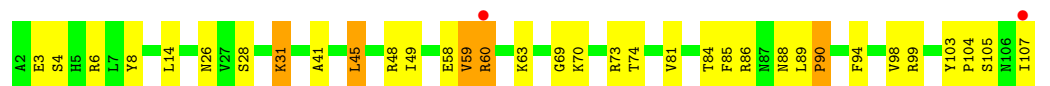
- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A

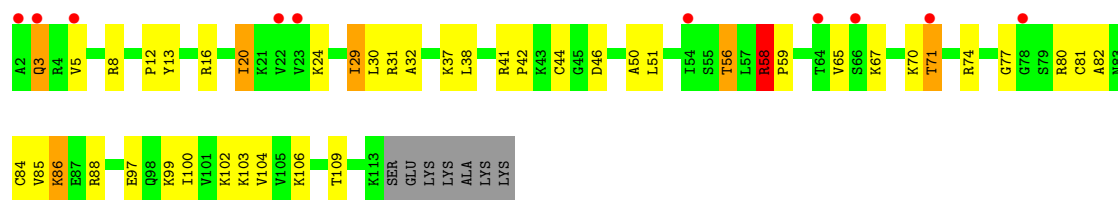


- Molecule 69: 60S ribosomal protein L33-A

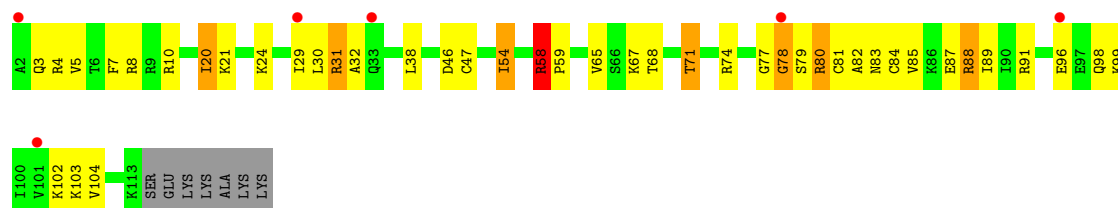


- Molecule 70: 60S ribosomal protein L34-A

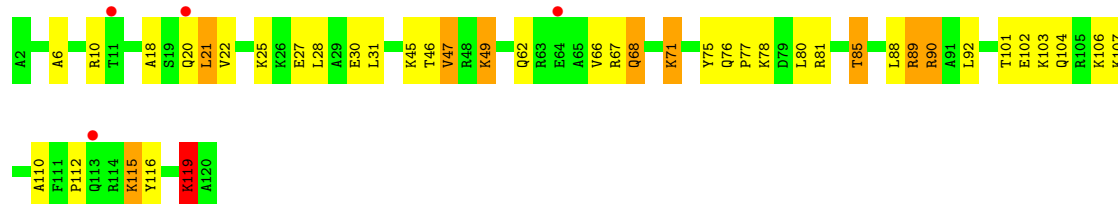




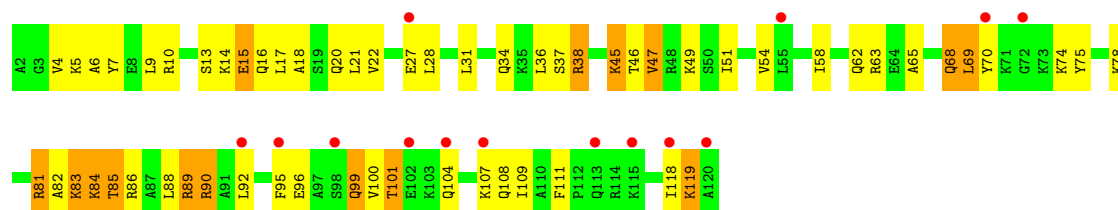
• Molecule 70: 60S ribosomal protein L34-A



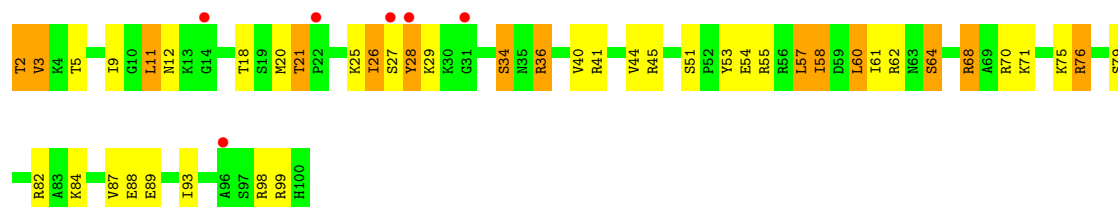
• Molecule 71: 60S ribosomal protein L35-A



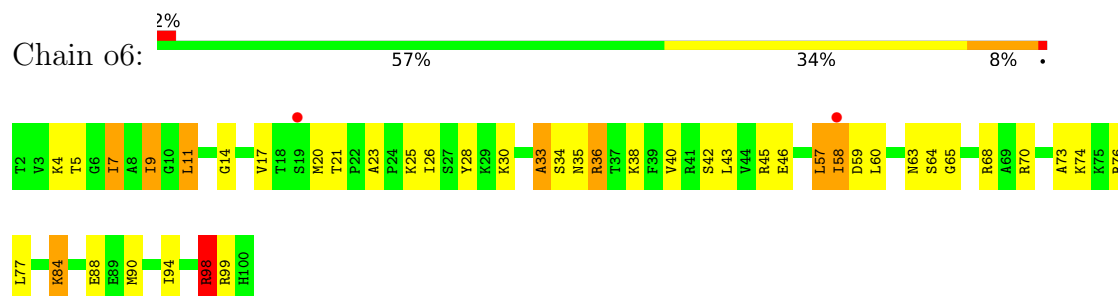
• Molecule 71: 60S ribosomal protein L35-A



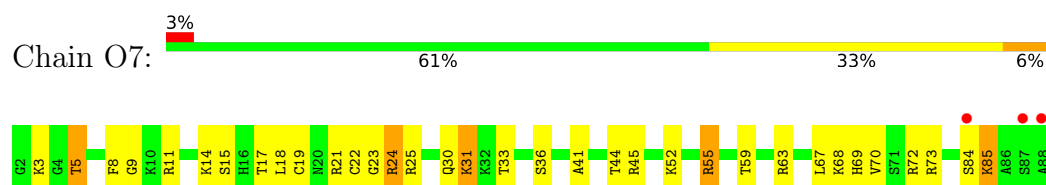
• Molecule 72: 60S ribosomal protein L36-A



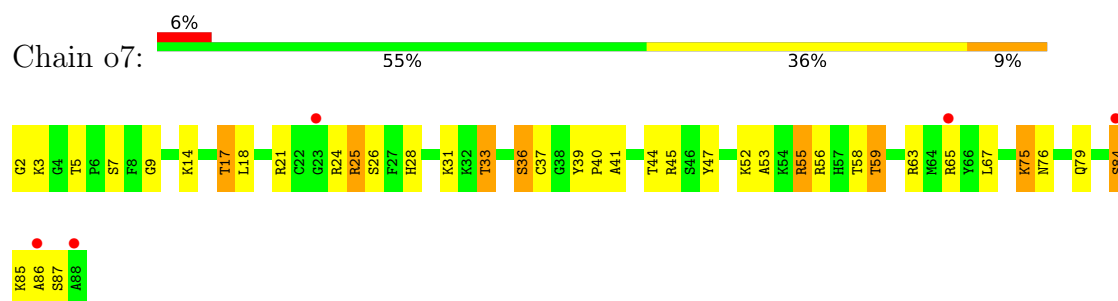
- Molecule 72: 60S ribosomal protein L36-A



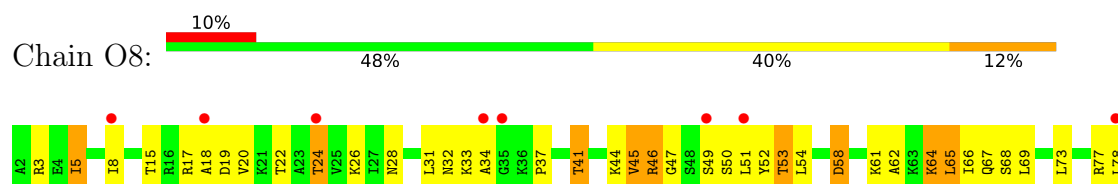
- Molecule 73: 60S ribosomal protein L37-A



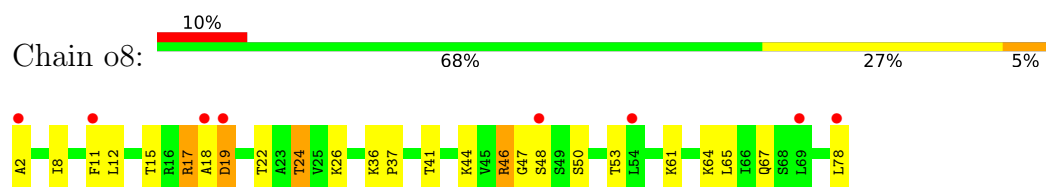
- Molecule 73: 60S ribosomal protein L37-A



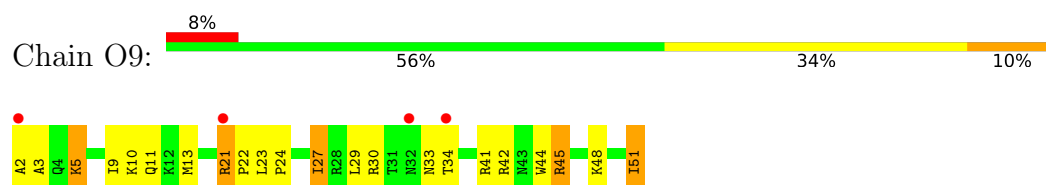
- Molecule 74: 60S ribosomal protein L38



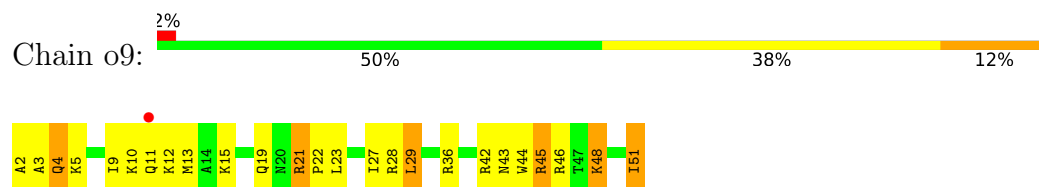
- Molecule 74: 60S ribosomal protein L38



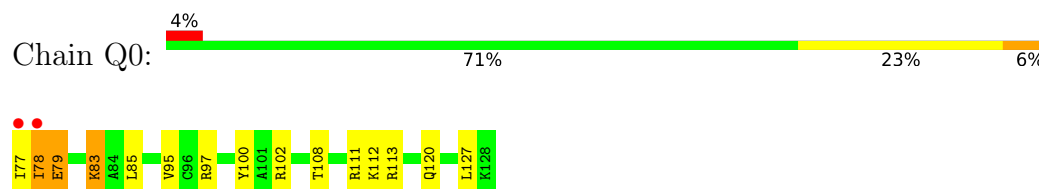
- Molecule 75: 60S ribosomal protein L39



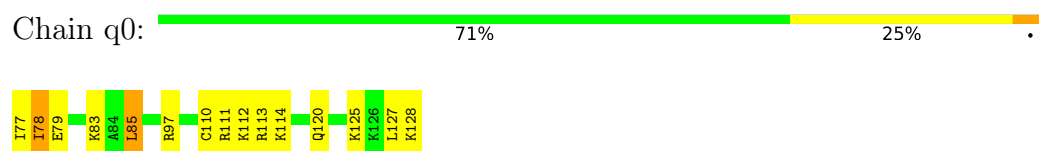
- Molecule 75: 60S ribosomal protein L39



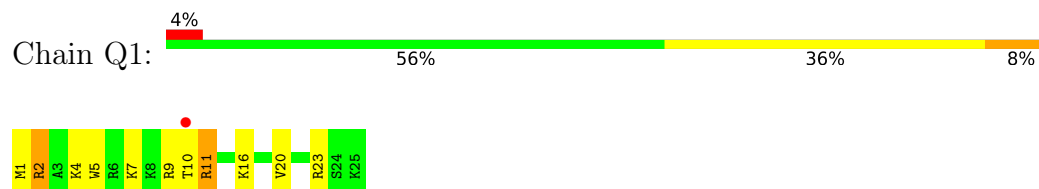
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



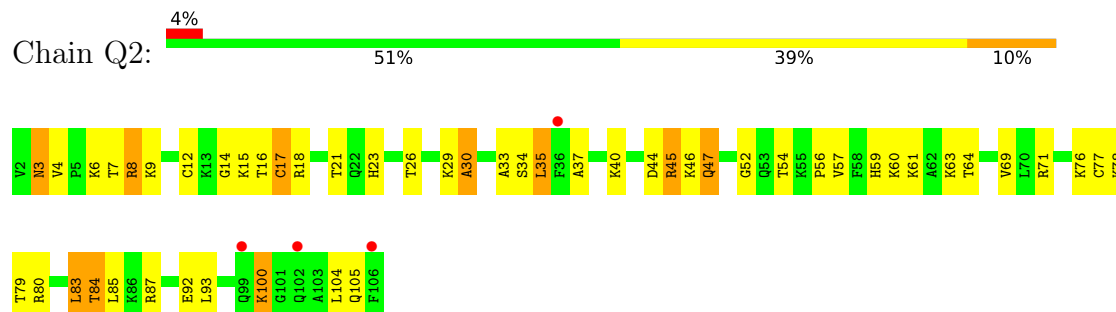
- Molecule 77: 60S ribosomal protein L41-A



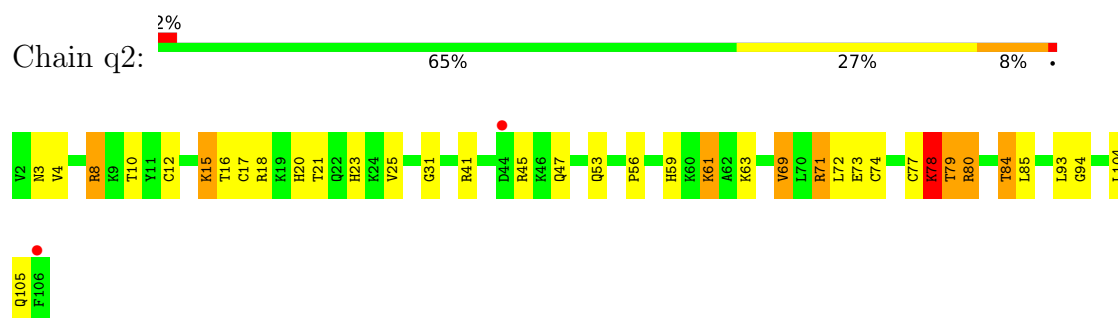
- Molecule 77: 60S ribosomal protein L41-A



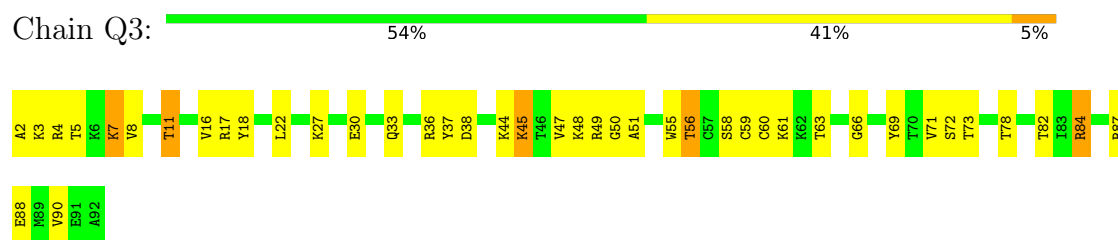
- Molecule 78: 60S ribosomal protein L42-A



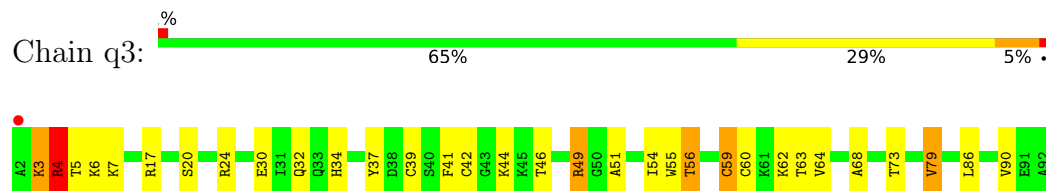
- Molecule 78: 60S ribosomal protein L42-A



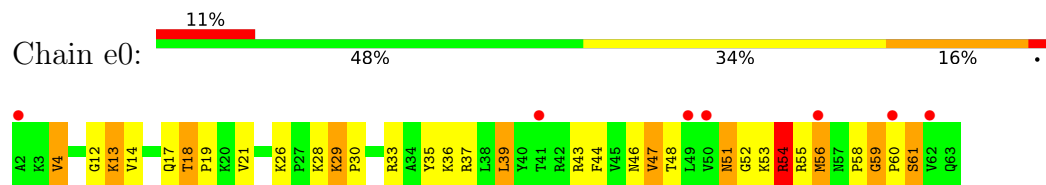
- Molecule 79: 60S ribosomal protein L43-A



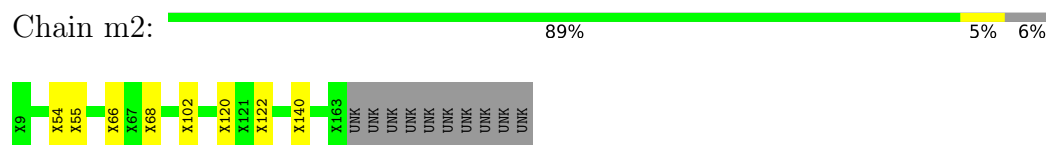
- Molecule 79: 60S ribosomal protein L43-A



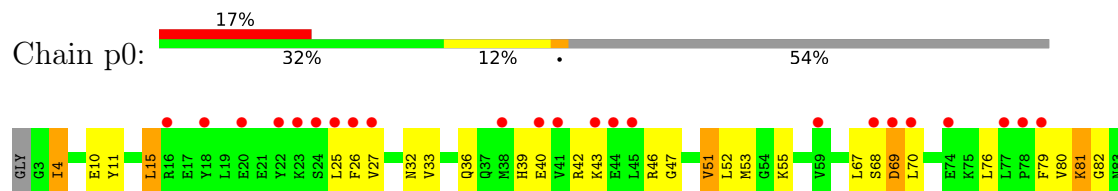
- Molecule 80: 40S ribosomal protein S30-A



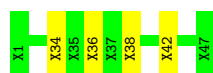
- Molecule 81: 60S ribosomal protein L12-A (uL11)



- Molecule 82: 60S acidic ribosomal protein P0



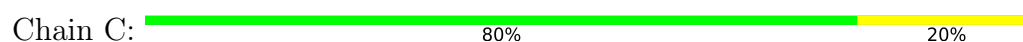
- Molecule 83: 60S ribosomal protein P1 alpha/P2 beta



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	437.14Å 287.91Å 303.85Å 90.00° 98.76° 90.00°	Depositor
Resolution (Å)	149.05 – 3.10 149.05 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (149.05-3.10) 99.9 (149.05-3.10)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.284 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	402683	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

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

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: MG, SPS, ZN, 8AN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.21	0/42467	0.40	1/66169 (0.0%)
1	6	0.23	0/42790	0.42	1/66673 (0.0%)
2	S0	0.36	0/1617	0.87	5/2215 (0.2%)
2	s0	0.39	0/1623	0.90	5/2222 (0.2%)
3	S1	0.33	0/1735	0.80	3/2335 (0.1%)
3	s1	0.38	0/1748	0.85	6/2352 (0.3%)
4	S2	0.38	0/1665	0.82	0/2263
4	s2	0.44	0/1665	0.92	6/2263 (0.3%)
5	S3	0.36	0/1759	0.80	4/2368 (0.2%)
5	s3	0.34	0/1759	0.78	4/2368 (0.2%)
6	S4	0.38	0/2109	0.86	5/2839 (0.2%)
6	s4	0.40	0/2109	0.83	3/2839 (0.1%)
7	S5	0.33	0/1629	0.81	1/2202 (0.0%)
7	s5	0.34	0/1629	0.83	5/2202 (0.2%)
8	S6	0.36	0/1823	0.77	4/2439 (0.2%)
8	s6	0.37	0/1779	0.83	2/2379 (0.1%)
9	S7	0.35	0/1506	0.87	4/2028 (0.2%)
9	s7	0.37	0/1516	0.83	5/2043 (0.2%)
10	S8	0.42	0/1514	0.81	0/2021
10	s8	0.44	0/1514	0.86	4/2021 (0.2%)
11	S9	0.34	0/1519	0.84	4/2035 (0.2%)
11	s9	0.39	0/1519	0.85	3/2035 (0.1%)
12	C0	0.36	0/790	0.83	1/1069 (0.1%)
12	c0	0.33	0/777	0.85	3/1049 (0.3%)
13	C1	0.41	0/1239	0.87	2/1673 (0.1%)
13	c1	0.46	0/1194	0.87	1/1610 (0.1%)
14	C2	0.35	0/900	0.76	0/1224
14	c2	0.32	0/900	0.72	0/1224
15	C3	0.39	0/1215	0.82	3/1638 (0.2%)
15	c3	0.45	0/1215	0.89	5/1638 (0.3%)
16	C4	0.37	0/901	0.87	3/1217 (0.2%)
16	c4	0.42	0/960	0.89	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.38	0/998	0.95	6/1341 (0.4%)
17	c5	0.40	0/1060	0.88	4/1426 (0.3%)
18	C6	0.36	0/1125	0.82	3/1510 (0.2%)
18	c6	0.38	0/1131	0.83	3/1518 (0.2%)
19	C7	0.39	0/935	0.87	0/1254
19	c7	0.35	0/914	0.79	0/1224
20	C8	0.35	0/1211	0.82	3/1628 (0.2%)
20	c8	0.35	0/1211	0.73	0/1628
21	C9	0.36	0/1130	0.81	2/1517 (0.1%)
21	c9	0.38	0/1130	0.85	1/1517 (0.1%)
22	D0	0.36	0/865	0.81	0/1169
22	d0	0.36	0/892	0.85	3/1205 (0.2%)
23	D1	0.35	0/693	0.79	3/935 (0.3%)
23	d1	0.39	0/693	0.80	0/935
24	D2	0.40	0/1038	0.94	5/1395 (0.4%)
24	d2	0.43	0/1038	0.84	1/1395 (0.1%)
25	D3	0.46	0/1139	0.91	3/1518 (0.2%)
25	d3	0.47	0/1139	0.87	4/1518 (0.3%)
26	D4	0.35	0/1087	0.78	0/1449
26	d4	0.38	0/1087	0.90	4/1449 (0.3%)
27	D5	0.38	0/571	0.89	0/768
27	d5	0.33	0/566	0.79	0/761
28	D6	0.41	0/782	0.90	1/1047 (0.1%)
28	d6	0.44	0/782	0.86	0/1047
29	D7	0.36	0/620	0.86	2/838 (0.2%)
29	d7	0.36	0/620	0.86	2/838 (0.2%)
30	D8	0.32	0/499	0.80	0/670
30	d8	0.35	0/499	0.81	0/670
31	D9	0.37	0/452	0.78	0/600
31	d9	0.38	0/452	0.89	2/600 (0.3%)
32	E0	0.37	0/483	0.84	0/643
33	E1	0.40	0/577	0.84	1/770 (0.1%)
33	e1	0.43	0/619	0.94	2/822 (0.2%)
34	SR	0.31	0/2490	0.74	2/3389 (0.1%)
34	sR	0.30	0/2495	0.72	2/3395 (0.1%)
35	SM	0.46	0/984	0.91	6/1323 (0.5%)
35	sM	0.45	0/585	0.80	0/788
36	1	0.30	0/75368	0.50	8/117502 (0.0%)
36	5	0.32	0/75388	0.50	0/117532
37	3	0.25	0/2883	0.41	0/4491
37	7	0.31	0/2883	0.49	0/4491
38	4	0.30	0/3746	0.47	0/5832
38	8	0.27	0/3746	0.45	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.52	0/1948	0.91	2/2617 (0.1%)
39	l2	0.54	0/1946	0.92	5/2614 (0.2%)
40	L3	0.49	0/3146	0.87	1/4228 (0.0%)
40	l3	0.55	0/3146	0.89	1/4228 (0.0%)
41	L4	0.53	0/2800	1.00	13/3790 (0.3%)
41	l4	0.52	0/2800	0.93	9/3790 (0.2%)
42	L5	0.40	0/2425	0.80	2/3271 (0.1%)
42	l5	0.48	0/2408	0.88	4/3248 (0.1%)
43	L6	0.48	0/1260	0.86	2/1694 (0.1%)
43	l6	0.50	0/1269	0.88	0/1705
44	L7	0.53	0/1821	0.88	2/2451 (0.1%)
44	l7	0.54	0/1828	0.94	3/2461 (0.1%)
45	L8	0.42	0/1836	0.92	9/2481 (0.4%)
45	l8	0.41	0/1796	0.86	5/2431 (0.2%)
46	L9	0.46	0/1539	0.83	1/2073 (0.0%)
46	l9	0.50	0/1539	0.88	1/2073 (0.0%)
47	M0	0.47	0/1741	0.84	1/2335 (0.0%)
47	m0	0.52	0/1758	0.88	2/2358 (0.1%)
48	M1	0.39	0/1374	0.83	2/1842 (0.1%)
48	m1	0.47	0/1374	0.87	0/1842
49	M3	0.51	0/1568	0.90	2/2106 (0.1%)
49	m3	0.49	0/1573	0.91	4/2113 (0.2%)
50	M4	0.47	0/1068	0.92	3/1438 (0.2%)
50	m4	0.52	0/1074	0.92	2/1446 (0.1%)
51	M5	0.51	0/1757	0.90	6/2354 (0.3%)
51	m5	0.46	0/1757	0.90	7/2354 (0.3%)
52	M6	0.37	0/1585	0.85	4/2128 (0.2%)
52	m6	0.41	0/1585	0.89	5/2128 (0.2%)
53	M7	0.54	0/1443	0.93	2/1944 (0.1%)
53	m7	0.57	0/1250	0.88	1/1683 (0.1%)
54	M8	0.51	0/1465	0.96	3/1965 (0.2%)
54	m8	0.51	0/1465	0.97	6/1965 (0.3%)
55	M9	0.42	0/1538	0.80	1/2050 (0.0%)
55	m9	0.45	0/1538	0.84	1/2050 (0.0%)
56	N0	0.50	0/1481	0.92	7/1990 (0.4%)
56	n0	0.51	0/1481	0.91	4/1990 (0.2%)
57	N1	0.48	0/1300	0.85	0/1743
57	n1	0.52	0/1300	0.89	4/1743 (0.2%)
58	N2	0.35	0/812	0.78	1/1099 (0.1%)
58	n2	0.35	0/794	0.87	2/1076 (0.2%)
59	N3	0.50	0/1018	0.86	0/1369
59	n3	0.60	0/1018	1.03	6/1369 (0.4%)
60	N4	0.41	0/712	0.95	2/958 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.45	0/1052	0.89	1/1398 (0.1%)
61	N5	0.43	0/979	0.87	2/1321 (0.2%)
61	n5	0.44	0/974	0.88	2/1314 (0.2%)
62	N6	0.47	0/1004	0.93	2/1341 (0.1%)
62	n6	0.47	0/1004	0.84	0/1341
63	N7	0.38	0/1118	0.87	2/1497 (0.1%)
63	n7	0.38	0/1118	0.80	0/1497
64	N8	0.53	0/1204	0.90	1/1612 (0.1%)
64	n8	0.52	0/1204	0.92	4/1612 (0.2%)
65	N9	0.50	0/473	0.82	0/629
65	n9	0.56	0/473	1.24	2/629 (0.3%)
66	O0	0.37	0/751	0.82	0/1008
66	o0	0.38	0/775	0.73	0/1040
67	O1	0.44	0/890	0.82	0/1196
67	o1	0.50	0/897	0.85	0/1205
68	O2	0.53	0/1041	0.92	0/1394
68	o2	0.58	0/1041	0.88	1/1394 (0.1%)
69	O3	0.53	0/868	0.87	2/1168 (0.2%)
69	o3	0.57	0/868	0.97	2/1168 (0.2%)
70	O4	0.46	0/890	0.91	2/1189 (0.2%)
70	o4	0.46	0/890	0.93	2/1189 (0.2%)
71	O5	0.45	0/978	0.87	1/1301 (0.1%)
71	o5	0.40	0/974	0.83	0/1297
72	O6	0.46	0/778	0.87	1/1034 (0.1%)
72	o6	0.41	0/777	0.85	2/1033 (0.2%)
73	O7	0.54	0/696	0.91	2/923 (0.2%)
73	o7	0.53	0/696	0.89	2/923 (0.2%)
74	O8	0.39	0/618	0.80	0/826
74	o8	0.36	0/614	0.74	0/822
75	O9	0.52	0/443	0.85	0/588
75	o9	0.48	0/443	0.82	0/588
76	Q0	0.49	0/423	0.98	2/562 (0.4%)
76	q0	0.54	0/423	0.91	0/562
77	Q1	0.44	0/234	0.87	0/300
77	q1	0.50	0/234	0.89	0/300
78	Q2	0.54	0/860	0.87	0/1136
78	q2	0.52	0/860	0.88	0/1136
79	Q3	0.47	0/701	0.89	0/934
79	q3	0.52	0/701	0.89	0/934
80	e0	0.38	0/499	1.04	6/665 (0.9%)
82	p0	0.34	0/1091	0.84	3/1472 (0.2%)
85	C	0.49	0/54	0.72	0/76
85	D	0.34	0/57	0.57	0/80

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/430695	0.65	349/632350 (0.1%)

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

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

There are no bond length outliers.

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	N4	80	ARG	CA-C-N	11.09	133.71	119.84
60	N4	80	ARG	C-N-CA	11.09	133.71	119.84
65	n9	23	LYS	CA-C-N	-10.49	106.73	119.84
65	n9	23	LYS	C-N-CA	-10.49	106.73	119.84
69	o3	89	LEU	CA-C-N	9.15	131.28	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	L2	19	HIS	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide
22	d0	70	THR	Peptide
52	m6	110	PRO	Peptide

5.2 Too-close contacts [i](#)

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	616	1
1	6	38260	0	19252	611	0
2	S0	1577	0	1567	50	0
2	s0	1583	0	1578	61	0
3	S1	1709	0	1784	83	0
3	s1	1722	0	1793	59	0
4	S2	1635	0	1723	52	0
4	s2	1635	0	1723	43	0
5	S3	1734	0	1817	50	0
5	s3	1734	0	1817	56	0
6	S4	2068	0	2154	69	0
6	s4	2068	0	2154	69	0
7	S5	1609	0	1675	30	0
7	s5	1609	0	1675	52	0
8	S6	1799	0	1879	54	0
8	s6	1755	0	1846	61	0
9	S7	1481	0	1572	49	0
9	s7	1491	0	1578	34	0
10	S8	1489	0	1525	51	0
10	s8	1489	0	1525	41	0
11	S9	1494	0	1573	48	0
11	s9	1494	0	1573	59	0
12	C0	773	0	729	24	0
12	c0	762	0	700	35	0
13	C1	1213	0	1257	30	0
13	c1	1168	0	1233	39	0
14	C2	892	0	891	32	0
14	c2	892	0	891	19	0
15	C3	1192	0	1255	41	0
15	c3	1192	0	1255	41	0
16	C4	891	0	883	36	0
16	c4	949	0	985	40	0
17	C5	977	0	1002	36	0
17	c5	1039	0	1050	36	0
18	C6	1105	0	1166	41	0
18	c6	1111	0	1171	38	0
19	C7	926	0	930	32	0
19	c7	906	0	909	31	0
20	C8	1192	0	1222	50	0
20	c8	1192	0	1222	46	0
21	C9	1112	0	1124	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	c9	1112	0	1124	44	0
22	D0	855	0	917	33	0
22	d0	882	0	939	18	0
23	D1	684	0	672	24	0
23	d1	684	0	672	23	0
24	D2	1021	0	1060	37	0
24	d2	1021	0	1060	35	0
25	D3	1121	0	1196	43	0
25	d3	1121	0	1196	36	0
26	D4	1073	0	1132	27	0
26	d4	1073	0	1132	37	0
27	D5	563	0	603	24	0
27	d5	558	0	598	21	0
28	D6	769	0	814	35	0
28	d6	769	0	814	36	0
29	D7	610	0	630	19	0
29	d7	610	0	631	21	0
30	D8	497	0	535	15	0
30	d8	497	0	535	19	0
31	D9	442	0	428	12	0
31	d9	442	0	428	13	0
32	E0	475	0	525	12	0
33	E1	566	0	602	25	0
33	e1	608	0	657	30	0
34	SR	2437	0	2386	50	0
34	sR	2442	0	2392	56	0
35	SM	1104	0	969	33	0
35	sM	681	0	591	22	0
36	1	67333	0	33838	848	0
36	5	67354	0	33851	852	1
37	3	2579	0	1304	34	0
37	7	2579	0	1304	33	0
38	4	3353	0	1695	38	0
38	8	3353	0	1695	58	0
39	L2	1914	0	1981	64	0
39	l2	1912	0	1976	69	0
40	L3	3075	0	3142	99	0
40	l3	3075	0	3142	90	0
41	L4	2748	0	2859	89	0
41	l4	2748	0	2859	86	0
42	L5	2375	0	2325	84	0
42	l5	2359	0	2311	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	L6	1239	0	1326	35	0
43	l6	1248	0	1339	32	0
44	L7	1784	0	1862	54	0
44	l7	1791	0	1869	44	0
45	L8	1804	0	1875	48	0
45	l8	1764	0	1821	52	0
46	L9	1518	0	1587	61	0
46	l9	1518	0	1587	54	0
47	M0	1705	0	1736	60	0
47	m0	1722	0	1755	62	0
48	M1	1353	0	1383	43	0
48	m1	1353	0	1383	40	0
49	M3	1543	0	1608	46	0
49	m3	1548	0	1613	40	0
50	M4	1053	0	1149	41	0
50	m4	1059	0	1154	34	0
51	M5	1720	0	1779	50	0
51	m5	1720	0	1779	53	0
52	M6	1555	0	1659	32	0
52	m6	1555	0	1659	54	0
53	M7	1420	0	1437	47	0
53	m7	1227	0	1236	36	0
54	M8	1441	0	1543	47	0
54	m8	1441	0	1543	43	0
55	M9	1521	0	1617	32	0
55	m9	1521	0	1617	37	0
56	N0	1445	0	1487	38	0
56	n0	1445	0	1487	29	0
57	N1	1276	0	1323	38	0
57	n1	1276	0	1323	38	0
58	N2	796	0	812	16	0
58	n2	778	0	791	20	0
59	N3	1003	0	1048	28	0
59	n3	1003	0	1048	30	0
60	N4	699	0	640	14	0
60	n4	1038	0	1071	15	0
61	N5	964	0	1025	31	0
61	n5	959	0	1023	29	0
62	N6	993	0	1081	21	0
62	n6	993	0	1081	34	0
63	N7	1092	0	1155	48	0
63	n7	1092	0	1155	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	N8	1173	0	1215	44	0
64	n8	1173	0	1215	44	0
65	N9	462	0	491	14	0
65	n9	462	0	491	14	0
66	O0	743	0	797	21	0
66	o0	767	0	816	17	0
67	O1	876	0	912	17	0
67	o1	883	0	918	19	0
68	O2	1020	0	1090	29	0
68	o2	1020	0	1090	32	0
69	O3	850	0	880	27	0
69	o3	850	0	880	16	0
70	O4	880	0	945	30	0
70	o4	880	0	945	31	0
71	O5	969	0	1078	29	0
71	o5	965	0	1067	46	0
72	O6	771	0	849	24	0
72	o6	770	0	846	22	0
73	O7	681	0	683	25	0
73	o7	681	0	683	30	0
74	O8	612	0	682	22	0
74	o8	608	0	671	10	0
75	O9	436	0	475	18	0
75	o9	436	0	475	22	0
76	Q0	417	0	455	5	0
76	q0	417	0	455	7	0
77	Q1	233	0	284	10	0
77	q1	233	0	284	6	0
78	Q2	847	0	914	24	0
78	q2	847	0	914	30	0
79	Q3	694	0	734	28	0
79	q3	694	0	734	19	0
80	e0	491	0	542	26	0
81	m2	750	0	180	6	0
82	p0	1076	0	1076	19	0
83	p1	235	0	53	2	0
84	p2	230	0	49	1	0
85	C	73	0	48	0	0
85	D	76	0	48	1	0
86	D6	1	0	0	0	0
86	D7	1	0	0	0	0
86	D9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	E1	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
86	d6	1	0	0	0	0
86	d7	1	0	0	0	0
86	d9	1	0	0	0	0
86	e1	1	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q2	1	0	0	0	0
86	q3	1	0	0	0	0
87	C	23	0	18	0	0
87	D	23	0	18	6	0
88	C	1	0	0	0	0
88	D	1	0	0	0	0
All	All	402683	0	297750	7258	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 7258 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:94:ARG:NH2	35:SM:134:ASP:OD1	1.86	1.07
40:l3:296:THR:HG22	40:l3:298:PHE:H	1.31	0.95
1:6:1636:C:H4'	1:6:1637:C:H5'	1.46	0.94
71:O5:85:THR:HG22	71:O5:88:LEU:H	1.33	0.94
36:5:640:U:OP1	64:n8:21:ARG:NH2	2.01	0.94

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	78 (64%)	30 (25%)	14 (12%)	0	1
15	C3	148/150 (99%)	126 (85%)	16 (11%)	6 (4%)	2	13
15	c3	148/150 (99%)	118 (80%)	23 (16%)	7 (5%)	2	11
16	C4	125/136 (92%)	92 (74%)	21 (17%)	12 (10%)	0	3
16	c4	126/136 (93%)	102 (81%)	18 (14%)	6 (5%)	2	11
17	C5	122/141 (86%)	90 (74%)	22 (18%)	10 (8%)	0	4
17	c5	133/141 (94%)	98 (74%)	18 (14%)	17 (13%)	0	1
18	C6	139/142 (98%)	116 (84%)	14 (10%)	9 (6%)	1	6
18	c6	140/142 (99%)	123 (88%)	10 (7%)	7 (5%)	1	11
19	C7	116/136 (85%)	91 (78%)	18 (16%)	7 (6%)	1	7
19	c7	113/136 (83%)	90 (80%)	13 (12%)	10 (9%)	0	3
20	C8	143/145 (99%)	121 (85%)	13 (9%)	9 (6%)	1	6
20	c8	143/145 (99%)	116 (81%)	18 (13%)	9 (6%)	1	6
21	C9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	2	12
21	c9	141/143 (99%)	124 (88%)	13 (9%)	4 (3%)	4	20
22	D0	105/120 (88%)	90 (86%)	11 (10%)	4 (4%)	2	15
22	d0	108/120 (90%)	84 (78%)	18 (17%)	6 (6%)	1	8
23	D1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	8
23	d1	85/87 (98%)	67 (79%)	13 (15%)	5 (6%)	1	8
24	D2	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	30
24	d2	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	47
25	D3	142/144 (99%)	111 (78%)	19 (13%)	12 (8%)	0	4
25	d3	142/144 (99%)	127 (89%)	10 (7%)	5 (4%)	3	16
26	D4	132/134 (98%)	110 (83%)	13 (10%)	9 (7%)	1	5
26	d4	132/134 (98%)	112 (85%)	12 (9%)	8 (6%)	1	7
27	D5	68/107 (64%)	53 (78%)	8 (12%)	7 (10%)	0	2
27	d5	67/107 (63%)	56 (84%)	9 (13%)	2 (3%)	3	19
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	0
28	d6	95/97 (98%)	71 (75%)	18 (19%)	6 (6%)	1	6
29	D7	79/81 (98%)	66 (84%)	11 (14%)	2 (2%)	4	21
29	d7	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	2	15

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	162 (85%)	18 (9%)	11 (6%)	1	8
49	m3	192/198 (97%)	157 (82%)	22 (12%)	13 (7%)	1	5
50	M4	134/137 (98%)	117 (87%)	8 (6%)	9 (7%)	1	6
50	m4	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	3	16
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	3	19
52	M6	195/198 (98%)	182 (93%)	9 (5%)	4 (2%)	5	25
52	m6	195/198 (98%)	181 (93%)	10 (5%)	4 (2%)	5	25
53	M7	181/183 (99%)	151 (83%)	21 (12%)	9 (5%)	1	11
53	m7	153/183 (84%)	141 (92%)	11 (7%)	1 (1%)	18	49
54	M8	183/185 (99%)	164 (90%)	15 (8%)	4 (2%)	5	24
54	m8	183/185 (99%)	162 (88%)	17 (9%)	4 (2%)	5	24
55	M9	186/188 (99%)	169 (91%)	16 (9%)	1 (0%)	24	57
55	m9	186/188 (99%)	168 (90%)	16 (9%)	2 (1%)	11	39
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	4	22
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	10	37
57	N1	157/159 (99%)	140 (89%)	15 (10%)	2 (1%)	9	35
57	n1	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	9	35
58	N2	98/120 (82%)	81 (83%)	15 (15%)	2 (2%)	6	25
58	n2	96/120 (80%)	83 (86%)	12 (12%)	1 (1%)	12	41
59	N3	134/136 (98%)	123 (92%)	10 (8%)	1 (1%)	18	49
59	n3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	18	49
60	N4	96/155 (62%)	80 (83%)	10 (10%)	6 (6%)	1	6
60	n4	133/155 (86%)	110 (83%)	14 (10%)	9 (7%)	1	5
61	N5	119/141 (84%)	107 (90%)	8 (7%)	4 (3%)	3	16
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	4
62	N6	124/126 (98%)	113 (91%)	10 (8%)	1 (1%)	16	47
62	n6	124/126 (98%)	114 (92%)	7 (6%)	3 (2%)	4	22
63	N7	133/135 (98%)	114 (86%)	10 (8%)	9 (7%)	1	5
63	n7	133/135 (98%)	99 (74%)	21 (16%)	13 (10%)	0	3
64	N8	146/148 (99%)	120 (82%)	19 (13%)	7 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	129 (88%)	13 (9%)	4 (3%)	4	20
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	2	16
65	n9	56/58 (97%)	41 (73%)	11 (20%)	4 (7%)	1	5
66	O0	95/104 (91%)	89 (94%)	6 (6%)	0	100	100
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	12	41
67	O1	107/112 (96%)	98 (92%)	3 (3%)	6 (6%)	1	8
67	o1	107/112 (96%)	91 (85%)	11 (10%)	5 (5%)	2	11
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	16	47
68	o2	125/129 (97%)	110 (88%)	11 (9%)	4 (3%)	3	18
69	O3	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
69	o3	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	3	19
70	O4	110/119 (92%)	98 (89%)	11 (10%)	1 (1%)	14	44
70	o4	110/119 (92%)	96 (87%)	11 (10%)	3 (3%)	4	20
71	O5	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	14	44
71	o5	117/119 (98%)	101 (86%)	12 (10%)	4 (3%)	3	16
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	1	10
72	o6	97/99 (98%)	80 (82%)	13 (13%)	4 (4%)	2	13
73	O7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	4	22
73	o7	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	2	11
74	O8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	2	13
74	o8	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	9	35
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	5	25
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	2	13
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	25
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	79 (77%)	21 (20%)	3 (3%)	3	19
78	q2	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	12	41
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3	16
79	q3	89/91 (98%)	82 (92%)	5 (6%)	2 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	38 (63%)	16 (27%)	6 (10%)	0	3
82	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	3	19
All	All	22291/24121 (92%)	18907 (85%)	2362 (11%)	1022 (5%)	2	12

5 of 1022 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	145 (88%)	19 (12%)	5	22
2	s0	165/209 (79%)	139 (84%)	26 (16%)	2	12
3	S1	191/223 (86%)	164 (86%)	27 (14%)	3	15
3	s1	192/223 (86%)	161 (84%)	31 (16%)	2	11
4	S2	176/204 (86%)	145 (82%)	31 (18%)	2	9
4	s2	176/204 (86%)	138 (78%)	38 (22%)	1	5
5	S3	182/194 (94%)	158 (87%)	24 (13%)	4	17
5	s3	182/194 (94%)	155 (85%)	27 (15%)	3	13
6	S4	221/221 (100%)	188 (85%)	33 (15%)	3	13
6	s4	221/221 (100%)	192 (87%)	29 (13%)	4	17
7	S5	173/190 (91%)	158 (91%)	15 (9%)	9	34
7	s5	173/190 (91%)	151 (87%)	22 (13%)	4	18
8	S6	188/201 (94%)	163 (87%)	25 (13%)	4	17
8	s6	187/201 (93%)	159 (85%)	28 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	147 (89%)	18 (11%)	6	24
9	s7	165/169 (98%)	150 (91%)	15 (9%)	9	32
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	14
10	s8	150/161 (93%)	135 (90%)	15 (10%)	7	29
11	S9	158/165 (96%)	134 (85%)	24 (15%)	3	13
11	s9	158/165 (96%)	137 (87%)	21 (13%)	4	17
12	C0	77/98 (79%)	66 (86%)	11 (14%)	3	14
12	c0	73/98 (74%)	62 (85%)	11 (15%)	3	13
13	C1	129/136 (95%)	114 (88%)	15 (12%)	5	22
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	10
14	C2	88/118 (75%)	75 (85%)	13 (15%)	3	13
14	c2	88/118 (75%)	73 (83%)	15 (17%)	2	10
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	11
15	c3	127/127 (100%)	107 (84%)	20 (16%)	2	12
16	C4	81/104 (78%)	65 (80%)	16 (20%)	1	6
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	6
17	C5	101/117 (86%)	89 (88%)	12 (12%)	5	21
17	c5	103/117 (88%)	91 (88%)	12 (12%)	5	22
18	C6	117/118 (99%)	103 (88%)	14 (12%)	5	21
18	c6	118/118 (100%)	105 (89%)	13 (11%)	6	24
19	C7	94/124 (76%)	76 (81%)	18 (19%)	1	7
19	c7	92/124 (74%)	80 (87%)	12 (13%)	4	18
20	C8	128/128 (100%)	111 (87%)	17 (13%)	4	17
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	10
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	9
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	12
22	D0	100/113 (88%)	84 (84%)	16 (16%)	2	12
22	d0	103/113 (91%)	88 (85%)	15 (15%)	3	14
23	D1	74/74 (100%)	64 (86%)	10 (14%)	4	16
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	9
24	D2	110/110 (100%)	90 (82%)	20 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	100 (91%)	10 (9%)	9	32
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	8
25	d3	119/119 (100%)	105 (88%)	14 (12%)	5	21
26	D4	112/112 (100%)	98 (88%)	14 (12%)	4	19
26	d4	112/112 (100%)	104 (93%)	8 (7%)	13	41
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	5
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11
28	D6	83/83 (100%)	68 (82%)	15 (18%)	2	8
28	d6	83/83 (100%)	74 (89%)	9 (11%)	6	25
29	D7	70/70 (100%)	62 (89%)	8 (11%)	5	23
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	5
30	d8	56/59 (95%)	45 (80%)	11 (20%)	1	6
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	10
31	d9	47/48 (98%)	41 (87%)	6 (13%)	4	18
32	E0	51/51 (100%)	44 (86%)	7 (14%)	3	15
33	E1	62/66 (94%)	44 (71%)	18 (29%)	0	1
33	e1	66/66 (100%)	53 (80%)	13 (20%)	1	6
34	SR	259/261 (99%)	240 (93%)	19 (7%)	13	40
34	sR	260/261 (100%)	248 (95%)	12 (5%)	24	55
35	SM	97/193 (50%)	86 (89%)	11 (11%)	5	23
35	sM	54/193 (28%)	47 (87%)	7 (13%)	4	18
39	L2	193/195 (99%)	158 (82%)	35 (18%)	2	8
39	l2	192/195 (98%)	155 (81%)	37 (19%)	1	7
40	L3	321/322 (100%)	266 (83%)	55 (17%)	2	10
40	l3	319/322 (99%)	262 (82%)	57 (18%)	2	9
41	L4	288/288 (100%)	238 (83%)	50 (17%)	2	9
41	l4	288/288 (100%)	241 (84%)	47 (16%)	2	11
42	L5	244/244 (100%)	209 (86%)	35 (14%)	3	14
42	l5	243/244 (100%)	209 (86%)	34 (14%)	3	15
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	9
44	L7	186/204 (91%)	160 (86%)	26 (14%)	3	15
44	l7	187/204 (92%)	166 (89%)	21 (11%)	6	24
45	L8	187/207 (90%)	162 (87%)	25 (13%)	4	17
45	l8	177/207 (86%)	147 (83%)	30 (17%)	2	10
46	L9	171/171 (100%)	143 (84%)	28 (16%)	2	11
46	l9	171/171 (100%)	135 (79%)	36 (21%)	1	5
47	M0	177/186 (95%)	147 (83%)	30 (17%)	2	10
47	m0	179/186 (96%)	148 (83%)	31 (17%)	2	9
48	M1	147/150 (98%)	121 (82%)	26 (18%)	2	9
48	m1	147/150 (98%)	128 (87%)	19 (13%)	4	18
49	M3	154/158 (98%)	134 (87%)	20 (13%)	4	18
49	m3	154/158 (98%)	136 (88%)	18 (12%)	5	22
50	M4	107/108 (99%)	92 (86%)	15 (14%)	3	15
50	m4	108/108 (100%)	91 (84%)	17 (16%)	2	12
51	M5	175/175 (100%)	151 (86%)	24 (14%)	3	15
51	m5	175/175 (100%)	158 (90%)	17 (10%)	8	30
52	M6	160/161 (99%)	147 (92%)	13 (8%)	11	36
52	m6	160/161 (99%)	138 (86%)	22 (14%)	3	15
53	M7	140/145 (97%)	119 (85%)	21 (15%)	3	13
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	9
54	M8	150/150 (100%)	131 (87%)	19 (13%)	4	18
54	m8	150/150 (100%)	122 (81%)	28 (19%)	1	7
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	15
55	m9	153/153 (100%)	128 (84%)	25 (16%)	2	11
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	9
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1	8
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1	7
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	6
58	N2	87/106 (82%)	79 (91%)	8 (9%)	8	31
58	n2	85/106 (80%)	75 (88%)	10 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	91 (88%)	13 (12%)	4	19
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	23
60	N4	57/129 (44%)	52 (91%)	5 (9%)	9	33
60	n4	100/129 (78%)	92 (92%)	8 (8%)	11	37
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	5
61	n5	104/117 (89%)	84 (81%)	20 (19%)	1	7
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	9
62	n6	109/109 (100%)	87 (80%)	22 (20%)	1	5
63	N7	115/115 (100%)	104 (90%)	11 (10%)	8	30
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	6
64	N8	118/118 (100%)	101 (86%)	17 (14%)	3	14
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	8
65	N9	46/46 (100%)	41 (89%)	5 (11%)	6	24
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	6
66	O0	81/87 (93%)	72 (89%)	9 (11%)	6	24
66	o0	84/87 (97%)	73 (87%)	11 (13%)	4	17
67	O1	92/96 (96%)	79 (86%)	13 (14%)	3	15
67	o1	94/96 (98%)	73 (78%)	21 (22%)	1	4
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	11
68	o2	109/110 (99%)	94 (86%)	15 (14%)	3	15
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	12
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	14
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	9
70	o4	95/101 (94%)	80 (84%)	15 (16%)	2	12
71	O5	104/104 (100%)	86 (83%)	18 (17%)	2	9
71	o5	103/104 (99%)	79 (77%)	24 (23%)	1	4
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	5
72	o6	80/81 (99%)	61 (76%)	19 (24%)	1	3
73	O7	70/70 (100%)	62 (89%)	8 (11%)	5	23
73	o7	70/70 (100%)	59 (84%)	11 (16%)	2	12
74	O8	68/68 (100%)	54 (79%)	14 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	7
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	9
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	10
76	q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	9
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1	5
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1	3
78	q2	90/90 (100%)	77 (86%)	13 (14%)	3	14
79	Q3	71/71 (100%)	60 (84%)	11 (16%)	2	12
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	6
80	e0	53/53 (100%)	45 (85%)	8 (15%)	3	13
82	p0	105/253 (42%)	88 (84%)	17 (16%)	2	11
All	All	18727/20169 (93%)	15904 (85%)	2823 (15%)	3	13

5 of 2823 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	d3	100	ASP
49	m3	73	ARG
31	d9	30	LEU
25	d3	84	THR
41	l4	266	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
20	c8	74	GLN
46	l9	96	HIS
22	d0	105	GLN
39	l2	205	ASN
49	m3	99	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1778/1800 (98%)	439 (24%)	50 (2%)
1	6	1792/1800 (99%)	419 (23%)	43 (2%)
36	1	3143/3396 (92%)	621 (19%)	66 (2%)
36	5	3143/3396 (92%)	609 (19%)	63 (2%)
37	3	120/121 (99%)	14 (11%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	0
38	4	157/158 (99%)	33 (21%)	2 (1%)
38	8	157/158 (99%)	31 (19%)	0
85	C	1/5 (20%)	0	0
85	D	1/5 (20%)	0	0
All	All	10412/10960 (95%)	2181 (20%)	225 (2%)

5 of 2181 RNA backbone outliers are listed below:

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

5 of 225 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3377	G
36	5	3317	U
1	6	834	G
36	5	3275	U
36	5	2209	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	8AN	C	76	88,85	21,24,25	1.58	4 (19%)	26,35,38	2.28	10 (38%)
85	8AN	D	76	88,85	21,24,25	1.55	4 (19%)	26,35,38	2.26	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	8AN	C	76	88,85	-	1/7/25/26	0/3/3/3
85	8AN	D	76	88,85	-	1/7/25/26	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	D	76	8AN	C5-C4	4.55	1.47	1.39
85	C	76	8AN	C5-C4	4.51	1.47	1.39
85	C	76	8AN	C5-C6	2.75	1.48	1.41
85	D	76	8AN	C5-N7	-2.62	1.34	1.39
85	C	76	8AN	C8-N7	2.50	1.36	1.31

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	C	76	8AN	C5-C4-N3	-5.95	118.53	126.72
85	D	76	8AN	C5-C4-N3	-5.87	118.63	126.72
85	D	76	8AN	N3-C4-N9	5.00	135.67	127.17
85	C	76	8AN	N3-C4-N9	4.28	134.45	127.17
85	C	76	8AN	C4-C5-N7	-4.04	105.96	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	C	76	8AN	C4'-C5'-O5'-P
85	D	76	8AN	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPS	C	3401	88	20,23,23	3.56	15 (75%)	23,30,30	2.73	12 (52%)
87	SPS	D	3401	88	20,23,23	3.58	14 (70%)	23,30,30	2.98	14 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPS	C	3401	88	-	2/15/18/18	0/1/1/1
87	SPS	D	3401	88	-	5/15/18/18	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	D	3401	SPS	C9-C10	-7.95	1.31	1.48
87	C	3401	SPS	C9-C10	-7.87	1.31	1.48
87	C	3401	SPS	C9-C8	6.61	1.52	1.33
87	D	3401	SPS	C9-C8	6.60	1.52	1.33
87	D	3401	SPS	O13-C13	-5.75	1.18	1.42

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	D	3401	SPS	C7-C5-C6	-5.50	119.35	126.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	C	3401	SPS	C7-C5-C6	-5.45	119.41	126.47
87	C	3401	SPS	C7-C5-N4	5.40	119.70	113.42
87	D	3401	SPS	O15-S15-C14	5.32	113.26	106.12
87	D	3401	SPS	C7-C5-N4	5.25	119.53	113.42

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

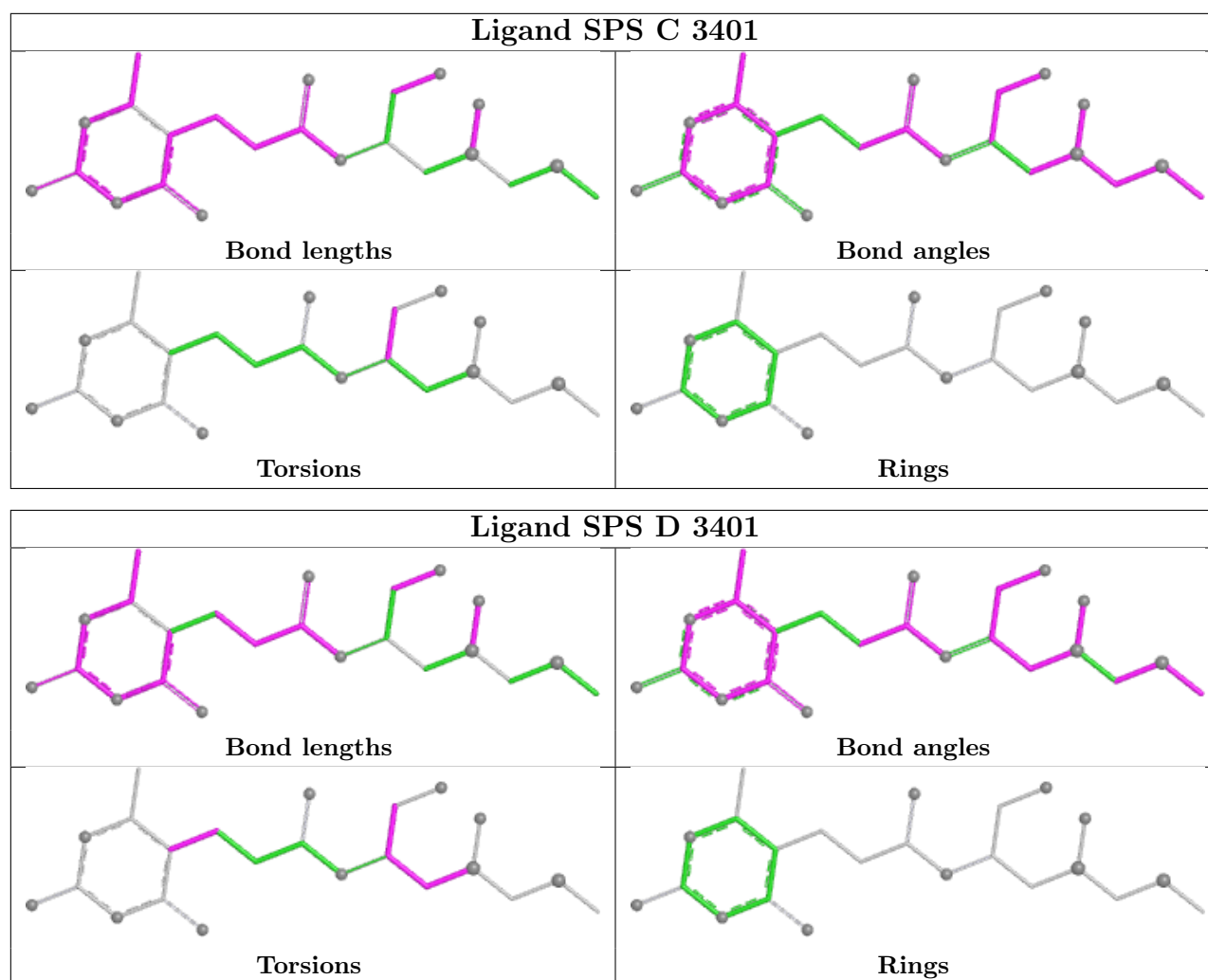
Mol	Chain	Res	Type	Atoms
87	C	3401	SPS	C14-C12-C13-O13
87	D	3401	SPS	C14-C12-C13-O13
87	D	3401	SPS	C12-C14-S15-O15
87	D	3401	SPS	C12-C14-S15-C16
87	C	3401	SPS	N11-C12-C13-O13

There are no ring outliers.

1 monomer is involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
81	m2	2
1	2	2
35	sM	1
35	SM	1
12	c0	1
85	C	1
85	D	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	153:ALA	C	154:UNK	N	39.08
1	SM	141:ALA	C	151:UNK	N	25.76
1	c0	84:GLU	C	87:HIS	N	8.48
1	C	77:PRO	C	78:PRO	N	5.78
1	D	77:PRO	C	78:PRO	N	5.62

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.75	120 (6%) 24 13	35, 88, 194, 293	1 (0%)
1	6	1795/1800 (99%)	0.59	84 (4%) 36 19	28, 78, 178, 271	1 (0%)
2	S0	206/251 (82%)	1.77	73 (35%) 1 0	98, 124, 141, 156	0
2	s0	206/251 (82%)	1.31	34 (16%) 4 2	77, 102, 120, 127	0
3	S1	214/254 (84%)	2.06	100 (46%) 0 0	101, 160, 206, 217	0
3	s1	216/254 (85%)	0.89	17 (7%) 18 10	68, 87, 112, 120	0
4	S2	217/253 (85%)	1.21	30 (13%) 6 4	74, 95, 116, 124	0
4	s2	217/253 (85%)	1.04	24 (11%) 10 5	60, 80, 95, 112	0
5	S3	223/239 (93%)	1.28	32 (14%) 6 3	80, 99, 136, 152	0
5	s3	223/239 (93%)	1.45	47 (21%) 2 1	78, 121, 152, 164	0
6	S4	260/260 (100%)	1.18	32 (12%) 8 5	60, 95, 109, 144	0
6	s4	260/260 (100%)	1.08	26 (10%) 12 6	52, 85, 99, 129	0
7	S5	206/224 (91%)	1.75	72 (34%) 1 0	103, 134, 153, 168	0
7	s5	206/224 (91%)	1.75	68 (33%) 1 0	87, 120, 139, 153	0
8	S6	226/236 (95%)	1.75	76 (33%) 1 0	63, 105, 134, 163	0
8	s6	218/236 (92%)	1.17	42 (19%) 3 1	50, 87, 112, 126	0
9	S7	184/189 (97%)	1.89	71 (38%) 1 0	94, 134, 175, 186	0
9	s7	186/189 (98%)	1.46	41 (22%) 2 1	74, 118, 168, 174	0
10	S8	188/200 (94%)	1.07	19 (10%) 12 6	56, 77, 118, 130	0
10	s8	188/200 (94%)	1.13	30 (15%) 5 2	47, 71, 117, 137	0
11	S9	185/196 (94%)	1.44	46 (24%) 2 1	78, 106, 152, 185	0
11	s9	185/196 (94%)	1.26	27 (14%) 6 3	67, 89, 135, 160	0
12	C0	96/105 (91%)	1.67	33 (34%) 1 0	88, 122, 166, 181	0
12	c0	96/105 (91%)	1.90	42 (43%) 0 0	108, 153, 180, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	1.13	23 (14%)	5	3	61, 74, 133, 148	0
13	c1	146/155 (94%)	1.10	21 (14%)	6	3	52, 69, 101, 130	0
14	C2	124/142 (87%)	1.87	49 (39%)	1	0	162, 188, 207, 214	0
14	c2	124/142 (87%)	2.35	69 (55%)	0	0	211, 238, 259, 264	0
15	C3	150/150 (100%)	1.25	22 (14%)	6	3	70, 89, 114, 119	0
15	c3	150/150 (100%)	0.81	10 (6%)	24	13	56, 74, 96, 99	0
16	C4	127/136 (93%)	2.22	70 (55%)	0	0	68, 155, 181, 187	0
16	c4	128/136 (94%)	0.85	10 (7%)	19	10	48, 90, 104, 109	0
17	C5	124/141 (87%)	1.46	23 (18%)	3	1	82, 102, 124, 162	0
17	c5	135/141 (95%)	1.47	31 (22%)	2	1	73, 105, 118, 128	0
18	C6	141/142 (99%)	1.80	50 (35%)	1	0	83, 118, 125, 128	0
18	c6	142/142 (100%)	1.93	52 (36%)	1	0	74, 113, 131, 136	0
19	C7	120/136 (88%)	1.70	42 (35%)	1	0	91, 114, 151, 157	0
19	c7	117/136 (86%)	1.77	45 (38%)	1	0	80, 106, 135, 150	0
20	C8	145/145 (100%)	1.59	39 (26%)	1	1	77, 114, 154, 160	0
20	c8	145/145 (100%)	1.31	21 (14%)	6	3	87, 102, 141, 147	0
21	C9	143/143 (100%)	1.73	46 (32%)	1	0	87, 114, 133, 142	0
21	c9	143/143 (100%)	1.34	27 (18%)	3	1	81, 103, 127, 136	0
22	D0	107/120 (89%)	1.87	46 (42%)	0	0	74, 120, 154, 157	0
22	d0	110/120 (91%)	1.67	32 (29%)	1	1	75, 132, 171, 177	0
23	D1	87/87 (100%)	1.27	16 (18%)	3	1	98, 107, 135, 144	0
23	d1	87/87 (100%)	0.92	8 (9%)	14	8	75, 89, 116, 124	0
24	D2	129/129 (100%)	1.39	23 (17%)	4	2	70, 88, 96, 104	0
24	d2	129/129 (100%)	0.75	5 (3%)	43	24	58, 71, 78, 87	0
25	D3	144/144 (100%)	0.96	18 (12%)	8	5	61, 67, 77, 101	0
25	d3	144/144 (100%)	0.64	7 (4%)	35	18	50, 56, 71, 91	0
26	D4	134/134 (100%)	1.20	17 (12%)	8	4	73, 107, 120, 134	0
26	d4	134/134 (100%)	1.34	28 (20%)	2	1	61, 92, 108, 118	0
27	D5	70/107 (65%)	1.77	23 (32%)	1	0	130, 149, 160, 161	0
27	d5	69/107 (64%)	1.76	21 (30%)	1	1	106, 132, 148, 150	0
28	D6	97/97 (100%)	2.01	47 (48%)	0	0	72, 89, 178, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.84	6 (6%) 26 14	53, 65, 110, 117	0
29	D7	81/81 (100%)	1.55	19 (23%) 2 1	90, 108, 149, 151	0
29	d7	81/81 (100%)	1.04	4 (4%) 35 18	72, 88, 139, 143	0
30	D8	63/66 (95%)	2.09	26 (41%) 0 0	114, 147, 161, 164	0
30	d8	63/66 (95%)	1.64	20 (31%) 1 1	102, 129, 141, 144	0
31	D9	53/55 (96%)	1.20	7 (13%) 7 4	77, 82, 101, 110	0
31	d9	53/55 (96%)	1.30	10 (18%) 3 1	74, 86, 131, 153	0
32	E0	60/60 (100%)	1.59	24 (40%) 1 0	72, 106, 148, 150	0
33	E1	71/76 (93%)	2.05	32 (45%) 0 0	114, 147, 184, 189	0
33	e1	76/76 (100%)	2.84	47 (61%) 0 0	110, 188, 229, 231	0
34	SR	318/318 (100%)	1.44	66 (20%) 2 1	111, 133, 149, 177	0
34	sR	318/318 (100%)	1.62	86 (27%) 1 1	122, 149, 166, 179	0
35	SM	133/263 (50%)	1.47	40 (30%) 1 1	53, 92, 148, 165	0
35	sM	84/263 (31%)	1.94	36 (42%) 0 0	45, 107, 147, 150	0
36	1	3148/3396 (92%)	0.04	75 (2%) 59 38	29, 49, 128, 262	0
36	5	3149/3396 (92%)	-0.06	66 (2%) 63 42	26, 46, 119, 209	0
37	3	121/121 (100%)	0.17	0 100 100	37, 69, 84, 91	0
37	7	121/121 (100%)	-0.24	1 (0%) 82 65	30, 49, 60, 72	0
38	4	158/158 (100%)	-0.07	1 (0%) 85 70	34, 49, 87, 132	0
38	8	158/158 (100%)	0.08	4 (2%) 58 37	37, 55, 91, 120	0
39	L2	252/253 (99%)	0.37	7 (2%) 55 34	33, 51, 66, 86	0
39	l2	252/253 (99%)	0.36	7 (2%) 55 34	32, 53, 70, 75	0
40	L3	386/386 (100%)	0.42	9 (2%) 61 39	32, 56, 69, 83	0
40	l3	386/386 (100%)	0.17	6 (1%) 70 49	26, 44, 57, 80	0
41	L4	361/361 (100%)	0.22	7 (1%) 66 45	30, 49, 68, 75	0
41	l4	361/361 (100%)	0.34	4 (1%) 78 59	30, 53, 73, 85	0
42	L5	296/296 (100%)	0.86	18 (6%) 27 15	51, 81, 100, 123	0
42	l5	294/296 (99%)	0.55	15 (5%) 33 18	39, 56, 78, 92	0
43	L6	156/175 (89%)	0.32	4 (2%) 57 36	44, 52, 70, 83	0
43	l6	157/175 (89%)	0.46	8 (5%) 33 18	45, 52, 76, 88	0
44	L7	222/243 (91%)	0.11	6 (2%) 56 35	35, 45, 76, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	0.09	0	100	100	32, 42, 82, 119	0
45	L8	233/255 (91%)	0.94	20 (8%)	16	9	61, 75, 118, 126	0
45	l8	231/255 (90%)	1.01	30 (12%)	7	4	67, 81, 112, 123	0
46	L9	191/191 (100%)	0.59	5 (2%)	57	36	52, 65, 79, 94	0
46	l9	191/191 (100%)	0.25	2 (1%)	79	61	40, 52, 72, 82	0
47	M0	211/220 (95%)	0.52	9 (4%)	40	22	39, 61, 96, 108	0
47	m0	213/220 (96%)	0.57	12 (5%)	30	16	33, 54, 75, 96	0
48	M1	169/173 (97%)	0.85	10 (5%)	28	15	63, 84, 99, 104	0
48	m1	169/173 (97%)	0.37	1 (0%)	85	70	42, 60, 72, 78	0
49	M3	193/198 (97%)	0.41	7 (3%)	46	26	33, 58, 97, 118	0
49	m3	194/198 (97%)	0.56	7 (3%)	46	26	36, 64, 106, 125	0
50	M4	136/137 (99%)	0.34	7 (5%)	33	18	49, 55, 69, 80	0
50	m4	137/137 (100%)	0.30	4 (2%)	53	32	44, 50, 66, 87	0
51	M5	203/203 (100%)	0.37	5 (2%)	58	37	31, 48, 58, 62	0
51	m5	203/203 (100%)	0.53	6 (2%)	52	31	35, 53, 66, 69	0
52	M6	197/198 (99%)	0.70	17 (8%)	16	9	35, 42, 57, 59	0
52	m6	197/198 (99%)	0.72	21 (10%)	11	6	30, 36, 55, 58	0
53	M7	183/183 (100%)	0.52	16 (8%)	16	9	36, 47, 115, 160	0
53	m7	155/183 (84%)	0.12	1 (0%)	85	70	33, 41, 58, 78	0
54	M8	185/185 (100%)	0.26	6 (3%)	50	30	37, 49, 66, 79	0
54	m8	185/185 (100%)	0.35	2 (1%)	78	59	36, 52, 62, 67	0
55	M9	188/188 (100%)	0.98	22 (11%)	9	5	51, 67, 166, 188	0
55	m9	188/188 (100%)	0.75	11 (5%)	28	15	46, 60, 154, 171	0
56	N0	172/172 (100%)	0.40	8 (4%)	36	19	43, 53, 68, 72	0
56	n0	172/172 (100%)	0.20	7 (4%)	41	23	37, 45, 58, 67	0
57	N1	159/159 (100%)	0.63	12 (7%)	20	11	37, 52, 95, 105	0
57	n1	159/159 (100%)	0.37	6 (3%)	44	25	32, 42, 77, 85	0
58	N2	100/120 (83%)	1.25	17 (17%)	4	2	86, 104, 112, 116	0
58	n2	98/120 (81%)	1.09	10 (10%)	12	6	74, 91, 101, 106	0
59	N3	136/136 (100%)	0.36	3 (2%)	62	41	40, 52, 66, 76	0
59	n3	136/136 (100%)	0.09	3 (2%)	62	41	30, 42, 55, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	1.41	28 (28%) 1 1	52, 64, 164, 171	0
60	n4	135/155 (87%)	1.02	23 (17%) 4 2	42, 96, 146, 170	0
61	N5	121/141 (85%)	0.59	5 (4%) 41 23	49, 62, 75, 108	0
61	n5	120/141 (85%)	0.69	8 (6%) 24 13	49, 63, 79, 92	0
62	N6	126/126 (100%)	0.33	2 (1%) 70 49	40, 58, 69, 76	0
62	n6	126/126 (100%)	0.49	3 (2%) 59 38	43, 59, 74, 81	0
63	N7	135/135 (100%)	0.77	8 (5%) 28 15	71, 88, 99, 102	0
63	n7	135/135 (100%)	1.13	20 (14%) 5 3	75, 91, 103, 108	0
64	N8	148/148 (100%)	0.31	1 (0%) 84 68	28, 50, 72, 83	0
64	n8	148/148 (100%)	0.31	0 100 100	27, 53, 72, 76	0
65	N9	58/58 (100%)	0.57	4 (6%) 23 12	32, 58, 105, 120	0
65	n9	58/58 (100%)	0.69	7 (12%) 8 5	31, 53, 78, 87	0
66	O0	97/104 (93%)	0.80	6 (6%) 26 14	70, 82, 105, 111	0
66	o0	100/104 (96%)	0.77	7 (7%) 22 12	69, 84, 112, 120	0
67	O1	109/112 (97%)	0.66	5 (4%) 37 20	50, 65, 98, 109	0
67	o1	109/112 (97%)	0.42	5 (4%) 37 20	41, 54, 89, 100	0
68	O2	127/129 (98%)	0.12	3 (2%) 59 38	30, 44, 58, 78	0
68	o2	127/129 (98%)	0.31	5 (3%) 43 24	27, 48, 63, 74	0
69	O3	106/106 (100%)	0.24	4 (3%) 44 25	36, 42, 67, 80	0
69	o3	106/106 (100%)	0.17	2 (1%) 66 45	33, 42, 65, 79	0
70	O4	112/119 (94%)	0.89	10 (8%) 15 8	45, 62, 102, 109	0
70	o4	112/119 (94%)	0.84	6 (5%) 31 17	45, 61, 107, 115	0
71	O5	119/119 (100%)	0.63	4 (3%) 48 28	44, 65, 72, 75	0
71	o5	119/119 (100%)	0.84	14 (11%) 9 5	49, 67, 82, 95	0
72	O6	99/99 (100%)	0.79	6 (6%) 27 15	55, 64, 97, 112	0
72	o6	99/99 (100%)	0.64	2 (2%) 65 44	58, 70, 95, 115	0
73	O7	87/87 (100%)	0.29	3 (3%) 48 28	33, 39, 59, 68	0
73	o7	87/87 (100%)	0.42	5 (5%) 29 16	34, 43, 69, 81	0
74	O8	77/77 (100%)	1.04	8 (10%) 11 6	72, 87, 111, 117	0
74	o8	77/77 (100%)	1.00	8 (10%) 11 6	71, 87, 102, 105	0
75	O9	50/50 (100%)	0.63	4 (8%) 18 10	43, 48, 53, 54	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	0.45	1 (2%) 65 44	43, 49, 57, 59	0
76	Q0	52/52 (100%)	0.44	2 (3%) 44 25	43, 50, 71, 79	0
76	q0	52/52 (100%)	-0.02	0 100 100	34, 39, 54, 57	0
77	Q1	25/25 (100%)	0.73	1 (4%) 42 23	51, 56, 58, 60	0
77	q1	25/25 (100%)	0.44	0 100 100	43, 46, 48, 49	0
78	Q2	105/105 (100%)	0.25	4 (3%) 44 25	34, 51, 76, 103	0
78	q2	105/105 (100%)	0.21	2 (1%) 66 45	35, 46, 64, 97	0
79	Q3	91/91 (100%)	0.36	0 100 100	41, 56, 73, 81	0
79	q3	91/91 (100%)	0.39	1 (1%) 78 59	37, 53, 67, 78	0
80	e0	62/62 (100%)	0.92	7 (11%) 10 5	57, 88, 121, 129	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	1.82	54 (37%) 1 0	98, 131, 238, 246	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
85	C	4/5 (80%)	0.32	0 100 100	34, 36, 37, 37	0
85	D	4/5 (80%)	-0.41	0 100 100	33, 34, 34, 39	0
All	All	33054/35334 (93%)	0.70	3363 (10%) 12 6	26, 68, 150, 293	2 (0%)

The worst 5 of 3363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
73	o7	88	ALA	10.4
60	N4	83	THR	10.0
8	S6	80	ASN	9.3
60	N4	86	SER	9.0
33	e1	89	LYS	8.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
85	8AN	D	76	22/23	0.96	0.08	32,33,34,35	0
85	8AN	C	76	22/23	0.98	0.06	34,34,34,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
86	ZN	D7	101	1/1	0.81	0.14	165,165,165,165	0
86	ZN	d7	101	1/1	0.82	0.14	148,148,148,148	0
88	MG	C	3402	1/1	0.90	0.20	34,34,34,34	0
86	ZN	e1	501	1/1	0.91	0.14	200,200,200,200	0
88	MG	D	3402	1/1	0.91	0.18	33,33,33,33	0
87	SPS	D	3401	23/23	0.92	0.13	29,32,45,48	0
86	ZN	E1	501	1/1	0.93	0.08	155,155,155,155	0
87	SPS	C	3401	23/23	0.96	0.09	29,32,46,48	0
86	ZN	Q2	501	1/1	0.97	0.11	75,75,75,75	0
86	ZN	q2	501	1/1	0.97	0.12	72,72,72,72	0
86	ZN	D6	500	1/1	0.98	0.03	88,88,88,88	0
86	ZN	q0	500	1/1	0.99	0.02	38,38,38,38	0
86	ZN	Q3	501	1/1	0.99	0.04	66,66,66,66	0
86	ZN	q3	501	1/1	0.99	0.05	60,60,60,60	0
86	ZN	d6	500	1/1	0.99	0.03	57,57,57,57	0
86	ZN	Q0	500	1/1	0.99	0.03	46,46,46,46	0
86	ZN	d9	101	1/1	0.99	0.04	85,85,85,85	0
86	ZN	D9	101	1/1	0.99	0.03	85,85,85,85	0
86	ZN	o7	501	1/1	1.00	0.03	46,46,46,46	0
86	ZN	O7	100	1/1	1.00	0.01	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.