



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2026 – 02:09 am BST

PDB ID : 5DGF / pdb_00005dgf
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 : 2015-08-27
Resolution : 3.30 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

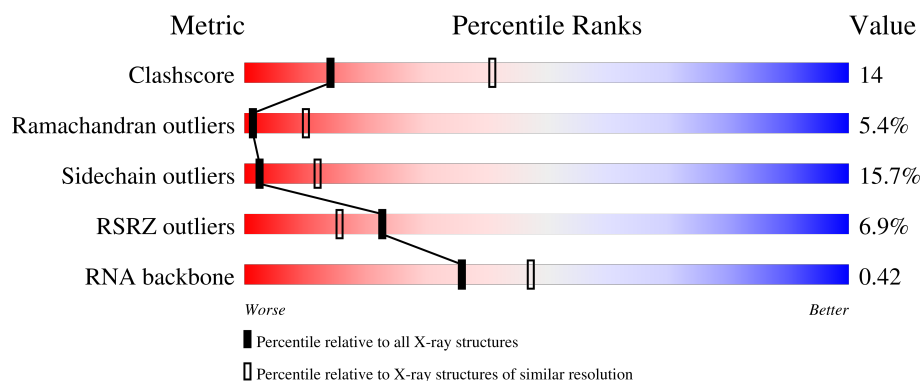
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	

Continued on next page...

Continued from previous page...

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	96	
12	c0	96	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	l3	386	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	M7	183	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
65	n9	58	
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	120	
70	o4	120	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	m2	165	
81	p0	311	
82	p1	47	
82	p2	47	
83	f	157	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 404292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

- 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
			1214	775	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			

- 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 (uS19).

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

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

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

- 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
			1105	653	221	231				
35	sM	104	Total	C	N	O		0	0	0
			680	403	140	137				

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
18	119	ALA	GLY	conflict	UNP P17076

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			1420	882	281	257				
53	m7	155	Total	C	N	O	S	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	S	0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 60S ribosomal protein L12-A (uL11).

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 82 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p1	47	Total	C	N	O		0	0	0
			235	141	47	47				
82	p2	46	Total	C	N	O		0	0	0
			230	138	46	46				

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

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

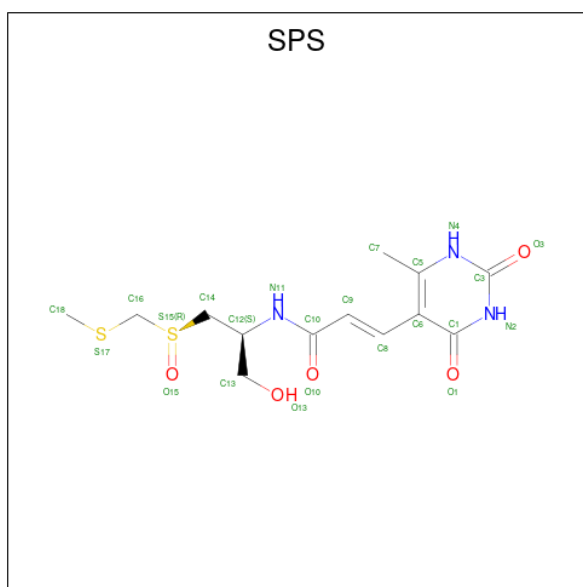
- Molecule 84 is an unknown type called CH-CH-8AN-PRO-PRO.

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

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 86 is SPARSOMYCIN (CCD ID: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).

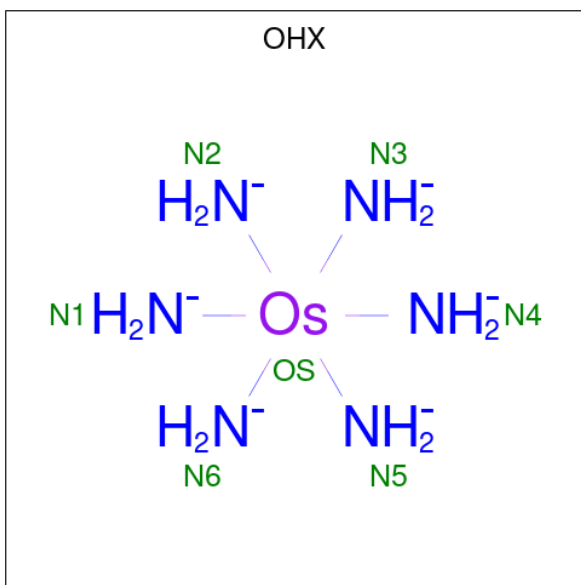


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
86	1	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
86	B	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	1	3	Total	Mg	0	0
			3	3		
87	5	5	Total	Mg	0	0
			5	5		
87	f	2	Total	Mg	0	0
			2	2		
87	B	1	Total	Mg	0	0
			1	1		
87	C	1	Total	Mg	0	0
			1	1		

- Molecule 88 is osmium (III) hexammine (CCD ID: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

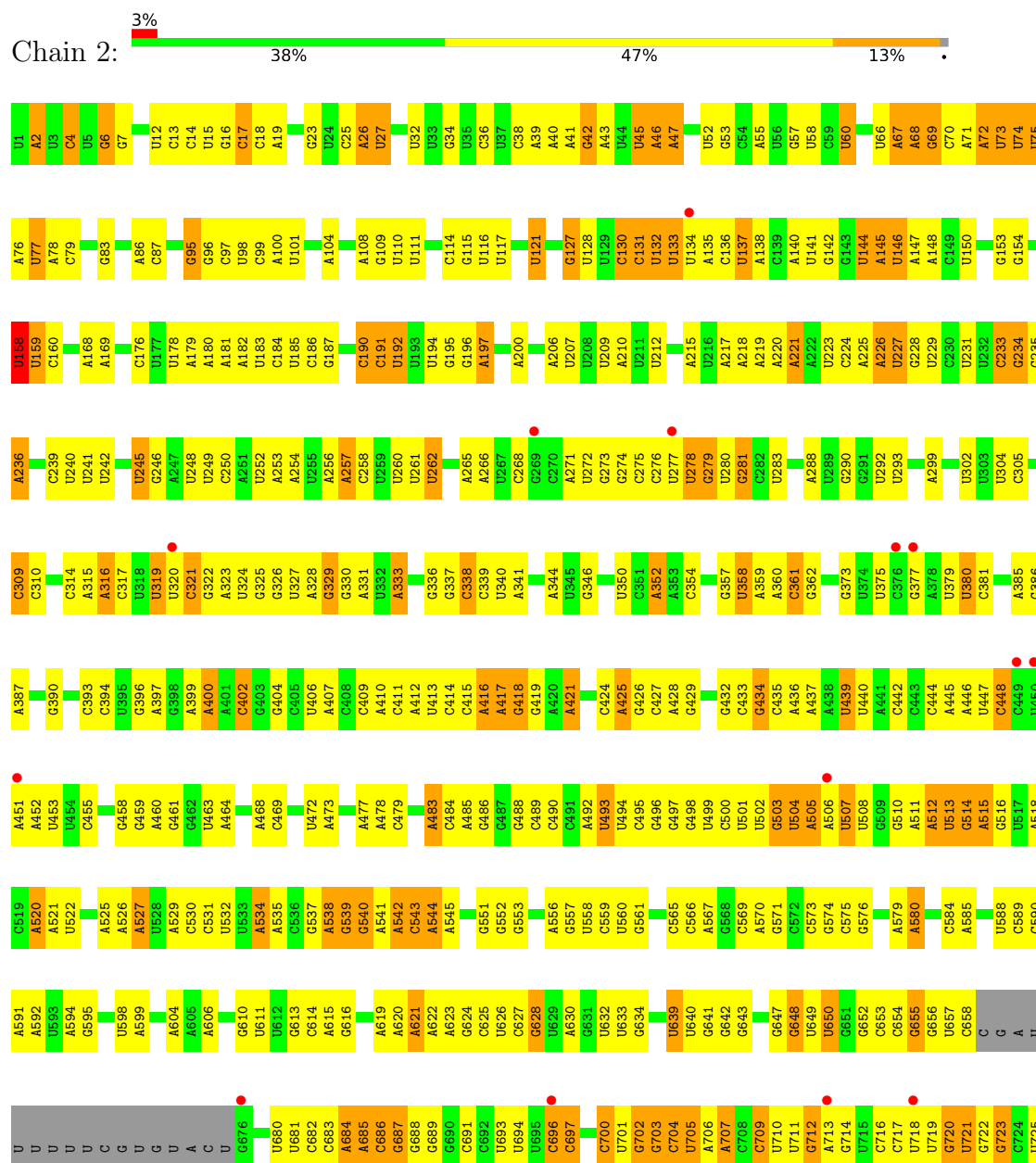
- Molecule 89 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	5	2	Total	O	0	0
			2	2		
89	f	10	Total	O	0	0
			10	10		

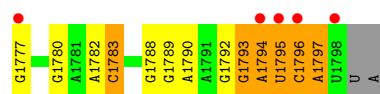
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

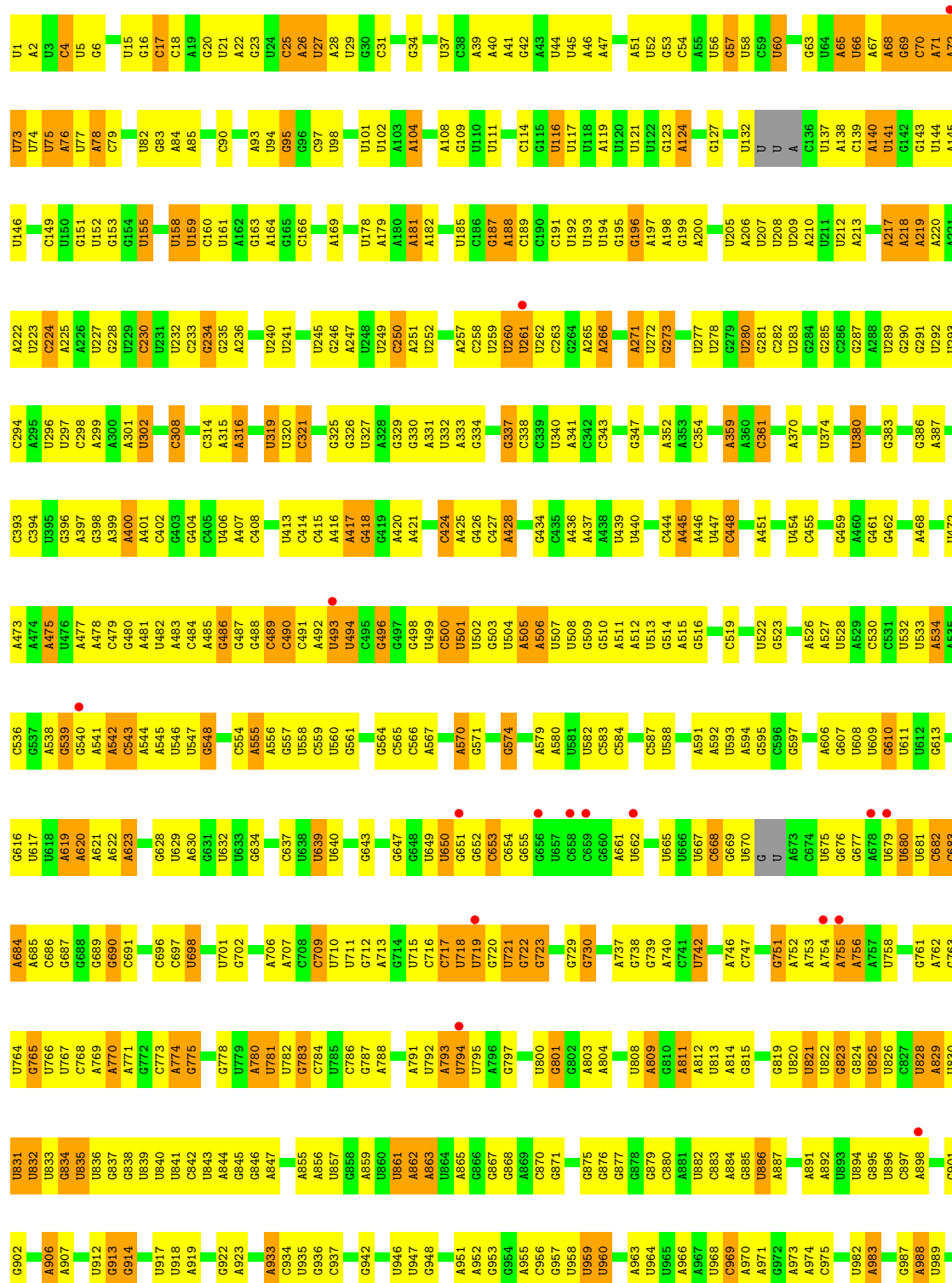
• Molecule 1: 18S ribosomal RNA

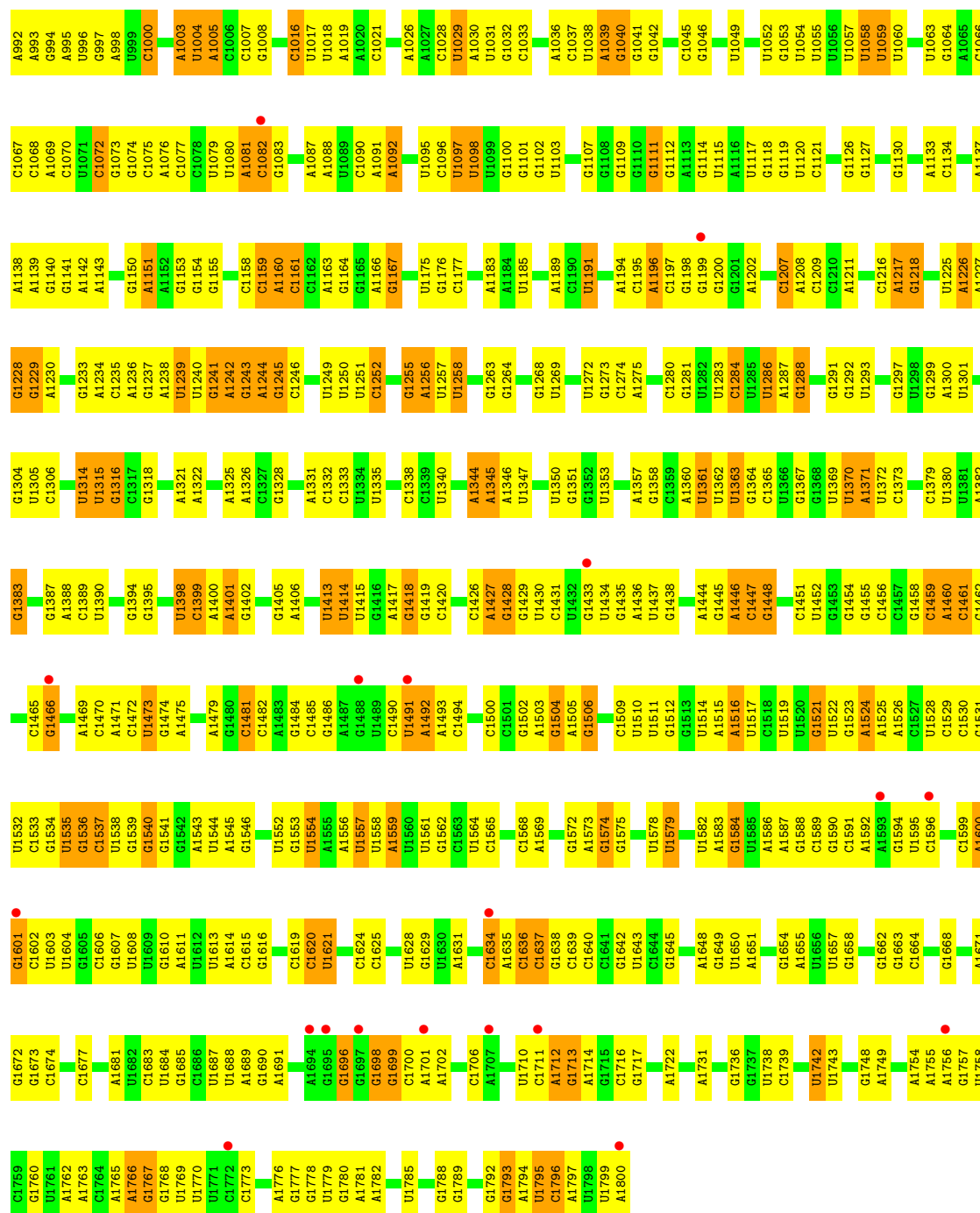


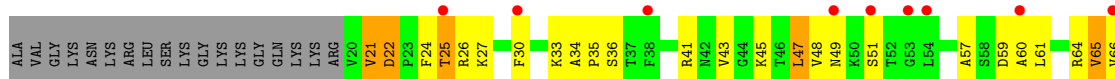
G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	A1712	G1713	A1714	G1718	G1719	G1720	G1727	C1728	A1729	C1730	A1731	G1737	G1738	C1739	G1745	G1746	G1747	C1751	A1752	A1753	A1754	A1755	A1756	G1757	G1758	G761	A762	G763	U764	G765	U766	U767	C768	A769	G772	G773	A774	G775	G776	C777	G778	U779	A780	U781	U782	G783	C784	U785	A788	A789	U790	A862
U1609	G1610	A1611	U1612	C1615	G1616	C1619	C1620	G1621	G1622	C1623	G1624	A1625	G1626	U1627	U1628	G1629	U1630	A1631	A1635	C1636	G1642	U1643	G1649	U1650	A1651	C1652	C1653	G1654	A1655	U1656	U1657	U1585	A1586	A1587	G1588	C1589	G1590	C1591	A1592	A1593	G1594	U1595	C1596	A1597	U1598	C1599	G1600	A1601	C1602	U1603	U1604	G1605	C1606	G1607	A1694	A1695	A1696	A1697	A1698	A1699	A1694	A1695	A1776	
G1541	G1542	G1548	C1549	A1550	U1551	U1552	G1553	U1554	A1555	U1556	U1557	U1558	A1559	U1560	U1561	G1562	C1563	U1564	C1565	U1566	C1567	C1568	A1569	A1573	G1574	G1575	A1576	C1580	C1581	U1582	A1583	U1584	U1585	A1586	A1587	G1588	C1589	G1590	C1591	A1592	A1593	G1594	U1595	C1596	A1597	U1598	C1599	G1600	A1601	C1602	U1603	U1604	G1605	C1606	G1607	A1694	A1695	A1696	A1697	A1698	A1699	A1694	A1695	A1776
A1475	C1476	G1477	A1478	U1479	G1480	C1481	U1482	A1483	G1484	C1485	G1486	U1487	G1488	U1489	C1490	U1491	A1492	C1493	U1494	C1495	G1498	U1499	C1500	A1503	G1504	U1505	C1506	U1511	G1512	U1513	A1514	U1515	A1516	U1517	C1518	U1519	U1520	G1521	U1522	G1523	A1524	U1525	A1526	C1527	U1528	C1529	C1530	C1533	U1534	U1535	U1536	U1537	U1538	U1539	G1540									
A1400	A1401	C1404	U1407	G1408	G1409	A1410	A1411	G1412	U1413	A1414	U1415	A1416	G1417	A1418	C1426	G1427	G1428	G1429	U1430	C1431	U1432	G1433	A1434	U1435	C1436	U1437	U1443	A1444	G1445	A1446	C1447	U1448	U1449	U1450	C1451	U1452	G1453	U1454	G1455	A1456	C1457	G1458	C1459	A1460	C1461	G1462	C1463	U1464	A1469	C1470	A1471	C1472	U1473	G1474										
C1333	U1334	U1335	A1336	U1337	C1338	U1339	A1340	A1341	C1342	U1343	A1344	U1345	A1346	U1347	A1348	G1349	U1350	G1351	C1352	U1353	G1354	C1355	G1358	C1359	A1360	U1361	U1362	U1363	G1364	C1365	G1368	U1369	C1370	A1371	U1372	C1373	C1376	U1377	U1381	A1382	G1383	G1387	A1388	C1389	U1390	A1391	U1392	C1393	G1394	C1395	U1396	U1397	U1398	C1399										
A1244	G1245	U1250	U1251	C1252	U1253	U1254	G1255	U1256	U1257	U1258	G1261	U1266	G1267	A1275	U1276	U1277	G1278	C1279	G1280	U1281	U1282	U1283	C1284	U1285	U1286	U1290	G1291	U1298	U1299	A1300	U1301	G1308	C1309	U1310	U1311	A1312	A1313	U1314	U1315	G1316	C1317	G1318	A1319	U1320	A1321	G1324	A1325	U1326	C1327	C1332														
G1165	A1166	U1167	U1168	G1169	C1173	U1175	U1176	C1177	G1178	U1179	C1180	U1181	A1182	G1183	A1184	U1185	U1186	U1187	G1188	U1191	A1194	C1195	A1196	C1197	G1198	U1199	G1200	A1202	C1207	A1208	U1209	C1210	G1217	U1218	U1219	C1222	A1226	U1227	G1228	C1229	A1230	A1234	C1235	A1236	G1237	U1238	G1241	A1242	G1243															
G1094	U1095	C1096	U1097	U1098	U1099	G1100	G1101	U1104	C1105	U1106	G1107	G1108	G1109	G1110	G1111	G1112	A1113	A1116	G1119	U1120	C1121	G1122	A1125	G1126	A1131	A1132	A1133	U1136	A1137	A1138	U1139	G1140	U1141	A1142	A1143	U1144	U1145	G1146	A1147	U1148	G1149	G1150	A1151	G1155	C1156	A1157	C1158	C1159	A1160	C1161	C1162													
C1028	U1029	U1030	U1031	C1032	G1033	C1034	U1035	A1036	C1037	U1038	A1039	U1040	G1041	G1042	G1046	U1049	G1050	C1051	U1052	G1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	A1061	G1064	A1065	C1066	C1067	C1068	A1069	C1072	G1073	U1074	C1075	A1076	C1077	U1080	A1081	C1082	G1083	A1084	C1085	A1086	U1087	U1088	U1089	C1090	A1091	U1092	A1093										
G942	C943	A944	C947	G948	C950	G951	C952	C954	A951	A952	C954	U956	U957	U958	C959	A970	A971	G972	A973	A974	A979	G980	G986	U987	G988	G989	A992	A993	G994	A995	U996	C997	A998	U999	C1000	U1001	C1002	A1003	U1004	A1005	C1006	U1012	A1013	G1014	C1017	U1018	U1019	C1022	A1026	A1027														
U792	A793	U794	G795	U796	G797	U800	G801	G802	A803	A804	U808	A809	C810	A811	U812	G815	C816	A817	C818	C819	U820	U821	U822	C823	U824	U825	U826	C827	U828	A829	U830	U831	U832	U833	U839	U840	U841	G846	A847	C848	C849	A850	U851	C852	G853	U854	A855	A856	U857	C858	A859	U860	U861	A862										

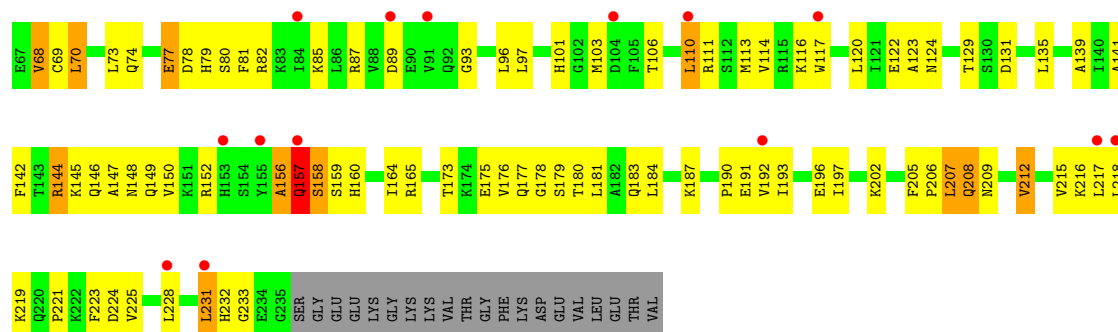


• Molecule 1: 18S ribosomal RNA

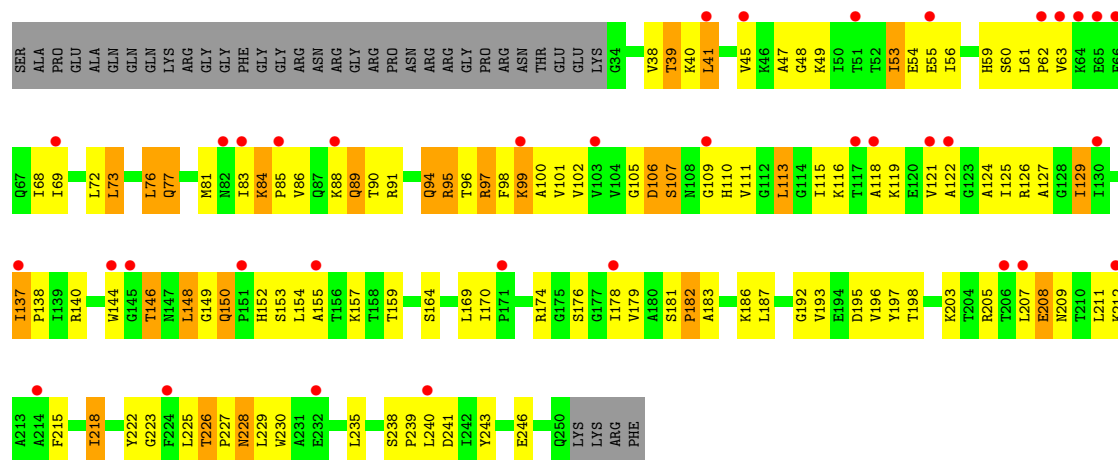




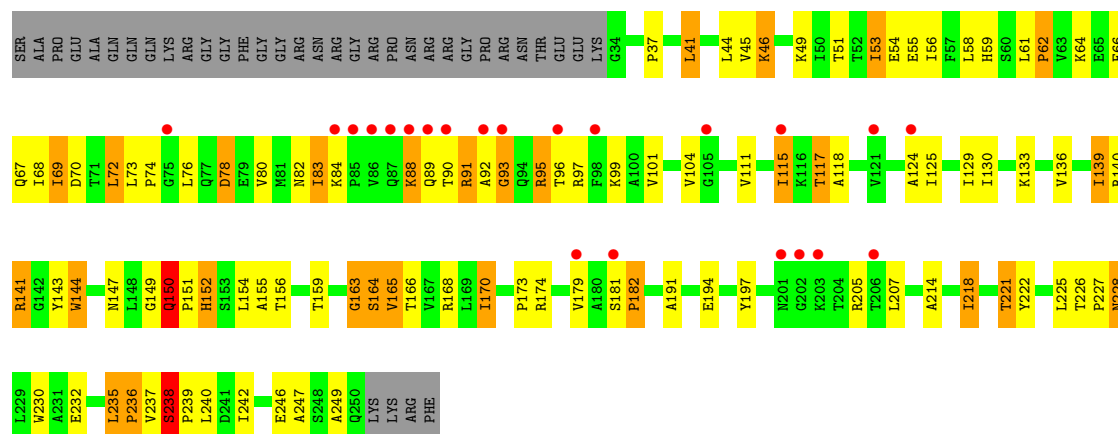




• Molecule 4: 40S ribosomal protein S2

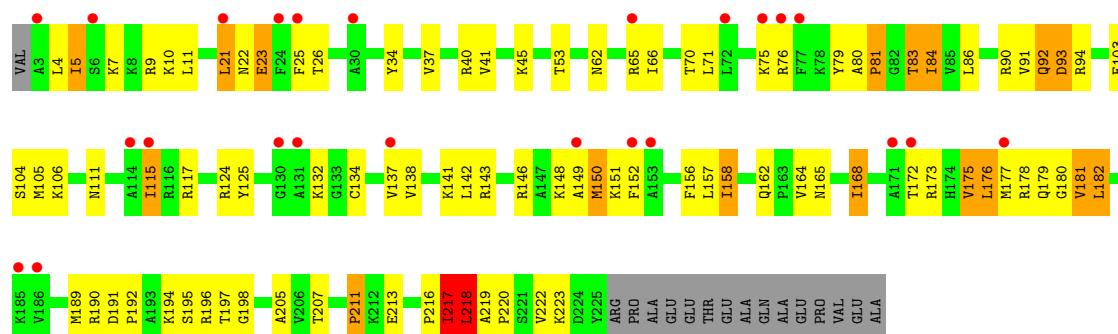


• Molecule 4: 40S ribosomal protein S2

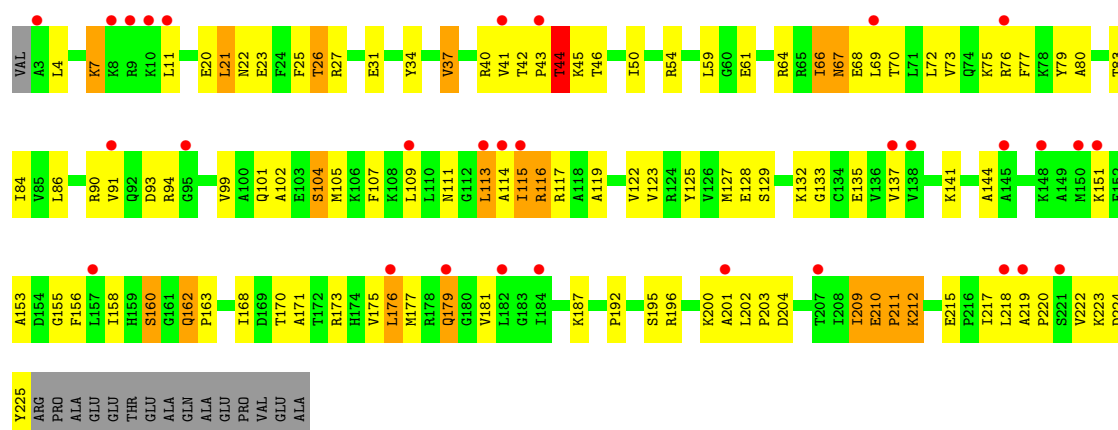


• Molecule 5: 40S ribosomal protein S3

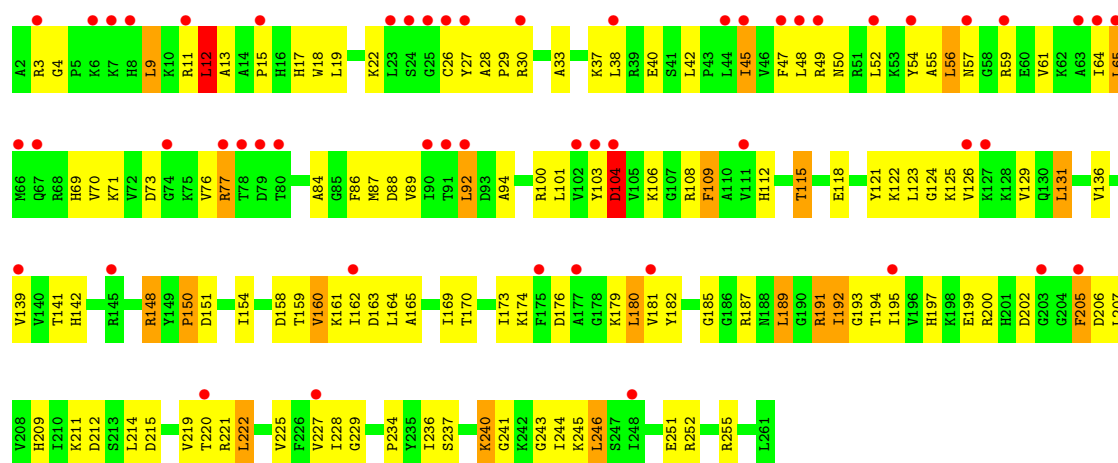




• Molecule 5: 40S ribosomal protein S3

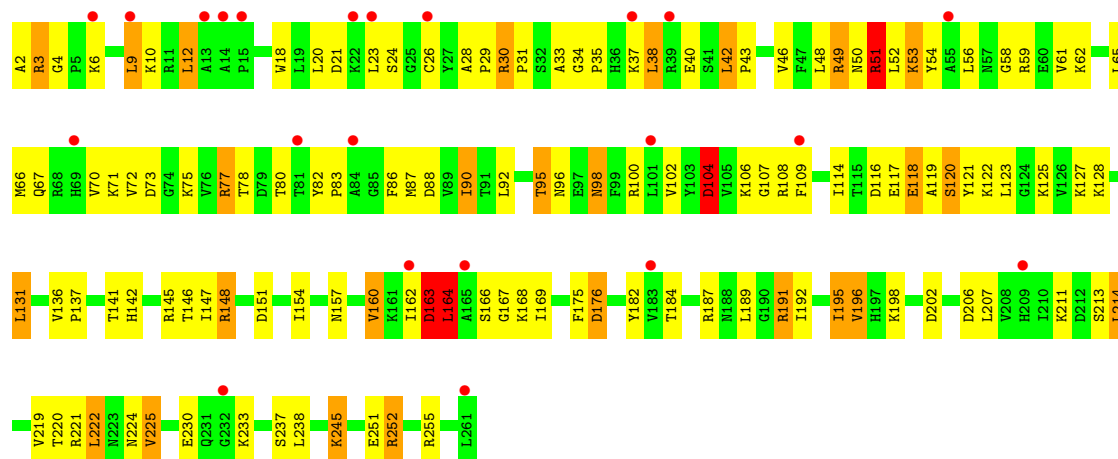


• Molecule 6: 40S ribosomal protein S4-A

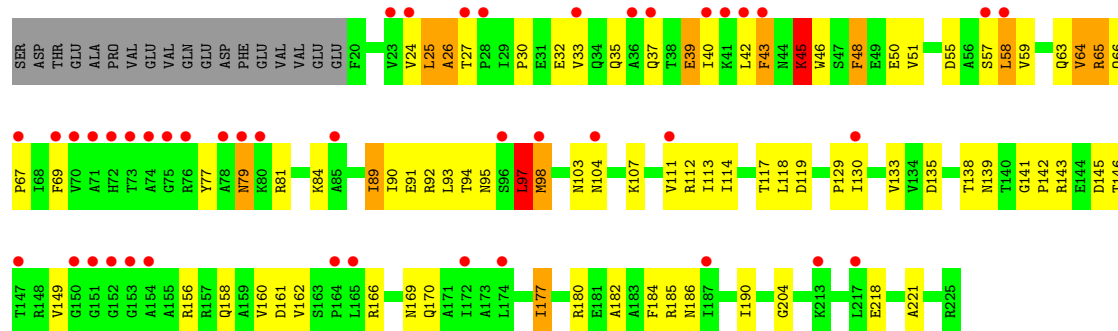


• Molecule 6: 40S ribosomal protein S4-A

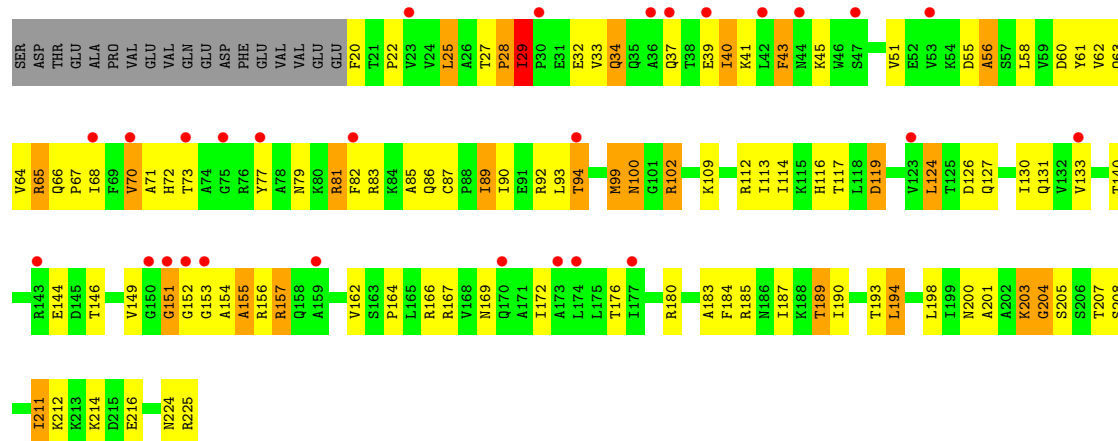




• Molecule 7: 40S ribosomal protein S5

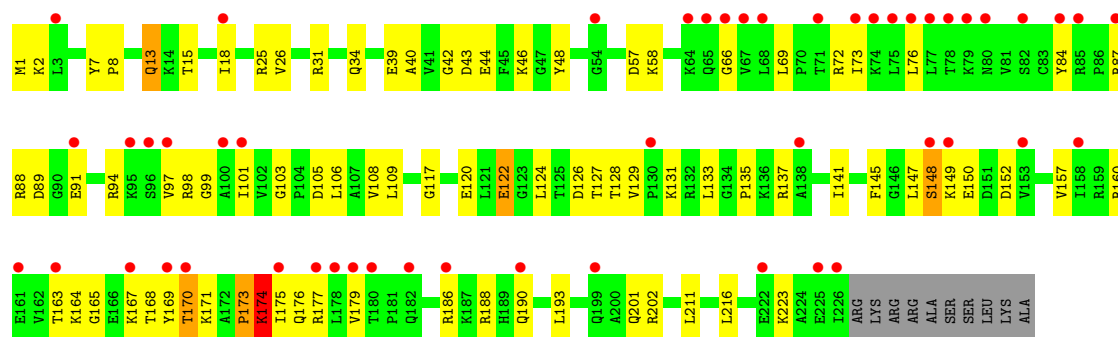


• Molecule 7: 40S ribosomal protein S5

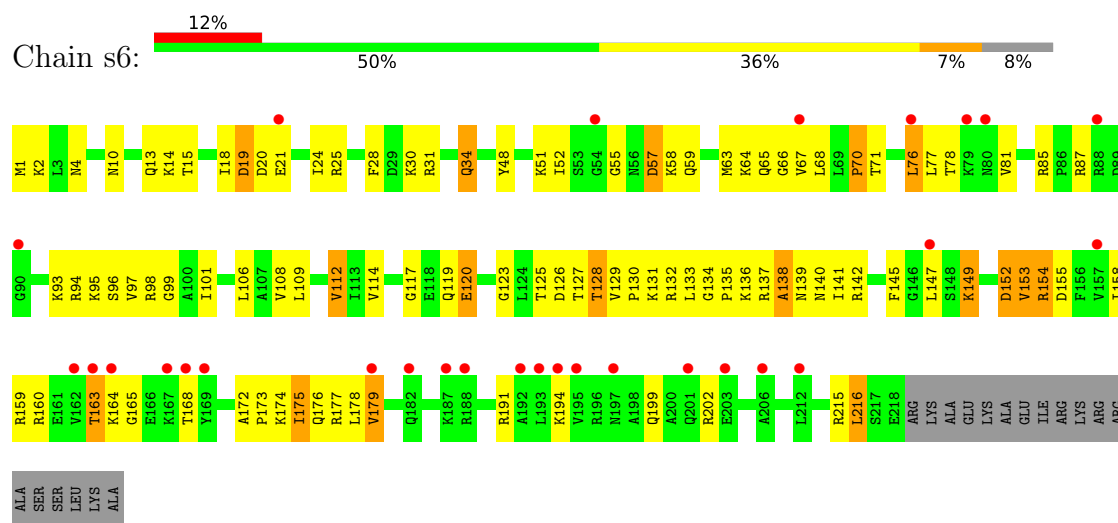


• Molecule 8: 40S ribosomal protein S6-A

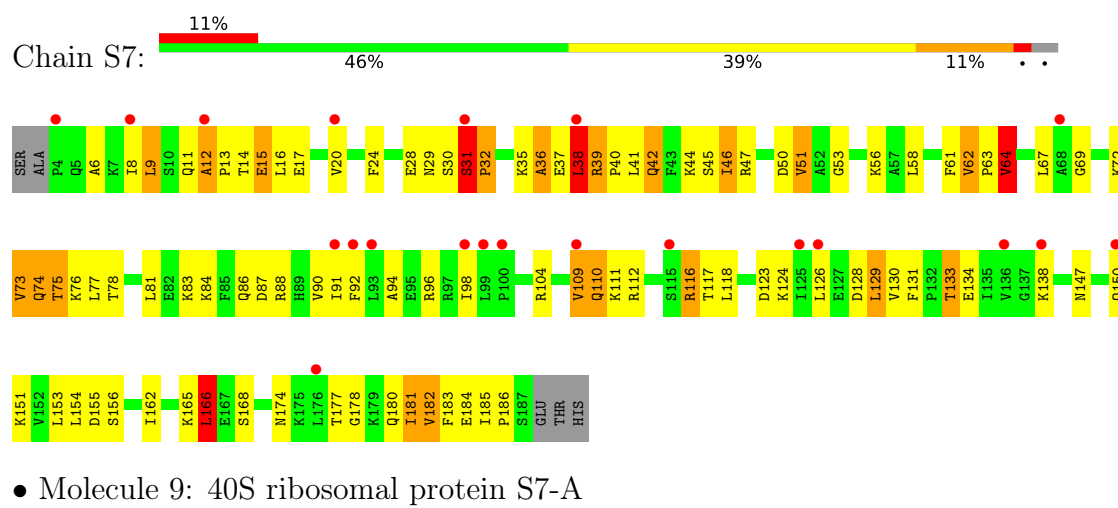




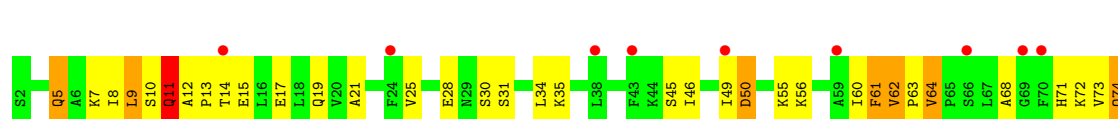
• Molecule 8: 40S ribosomal protein S6-A

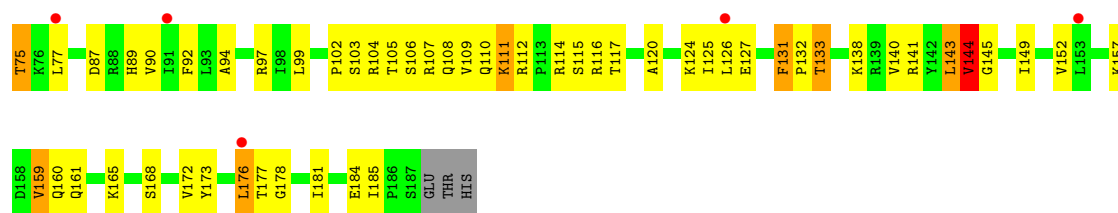


• Molecule 9: 40S ribosomal protein S7-A

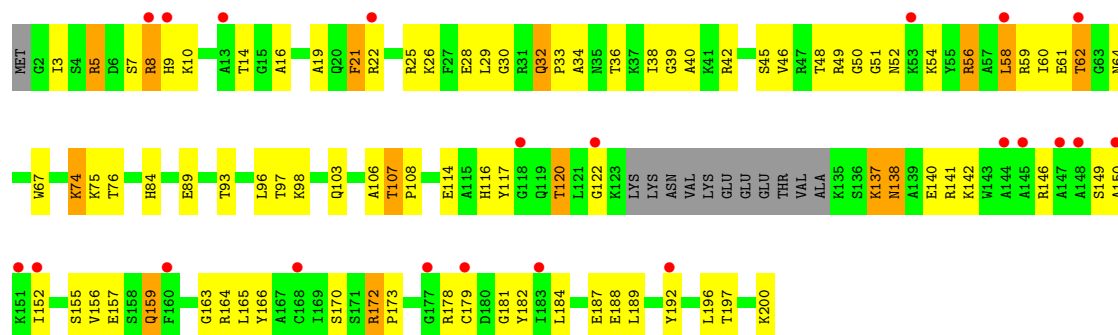


• Molecule 9: 40S ribosomal protein S7-A

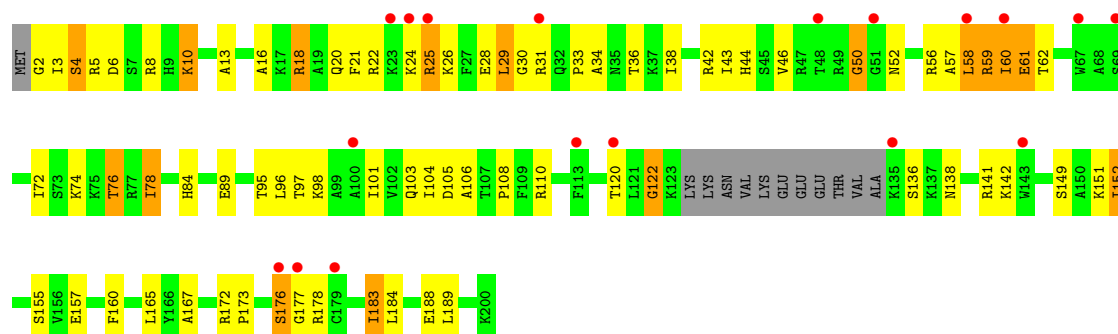




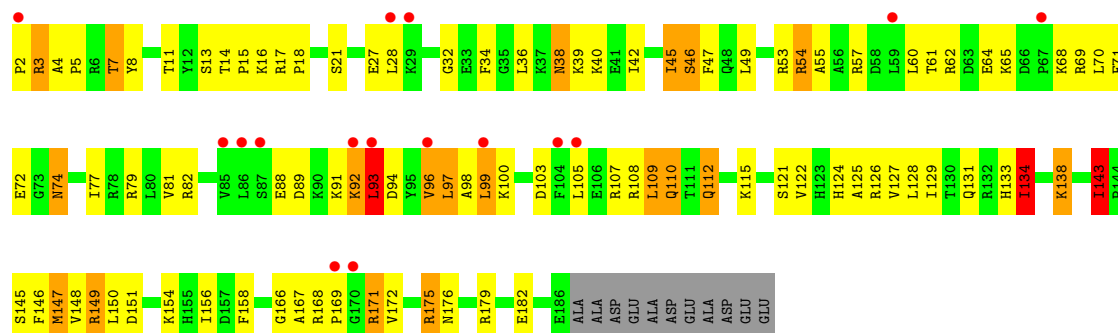
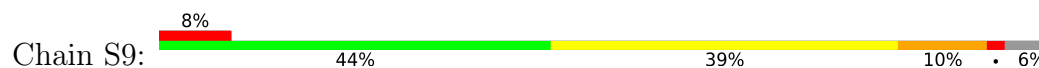
• Molecule 10: 40S ribosomal protein S8-A



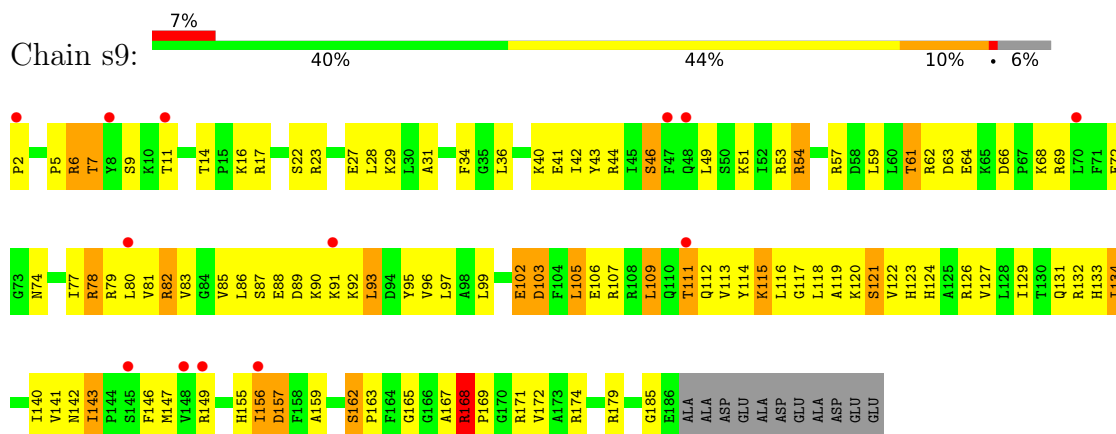
• Molecule 10: 40S ribosomal protein S8-A



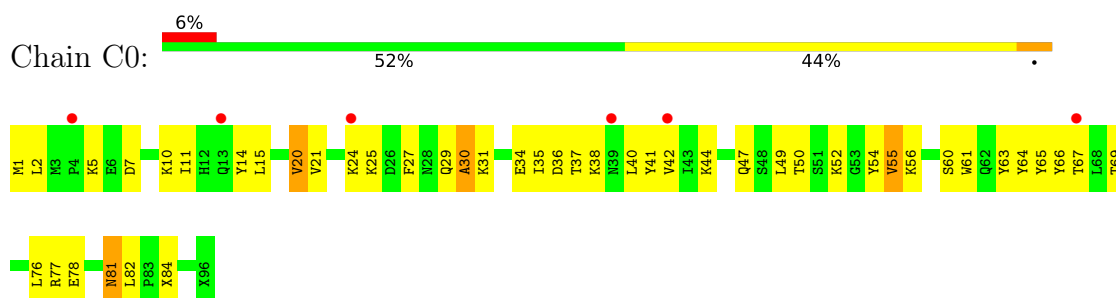
• Molecule 11: 40S ribosomal protein S9-A



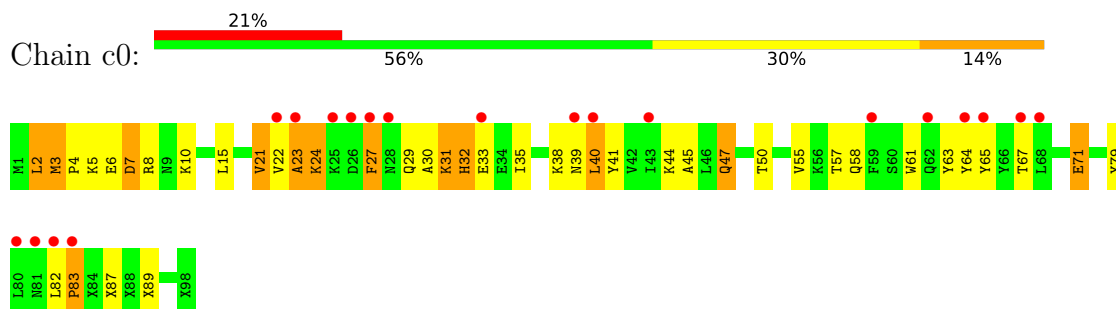
- Molecule 11: 40S ribosomal protein S9-A



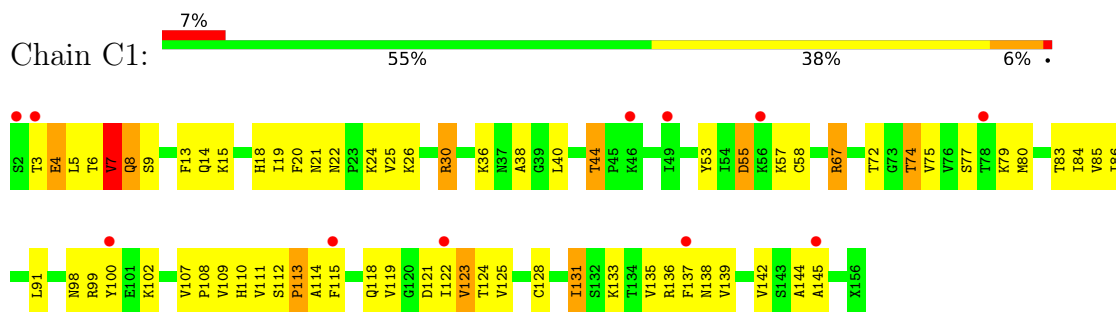
- Molecule 12: 40S ribosomal protein S10-A



- Molecule 12: 40S ribosomal protein S10-A

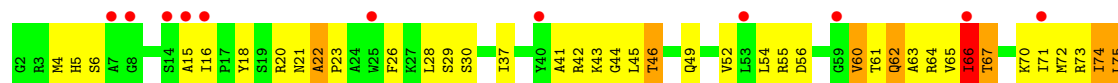


- Molecule 13: 40S ribosomal protein S11-A



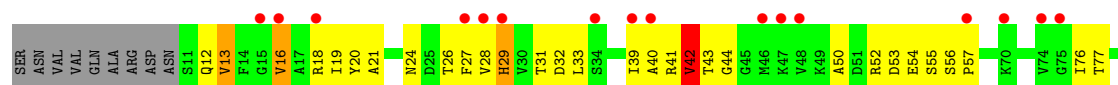
- Molecule 13: 40S ribosomal protein S11-A



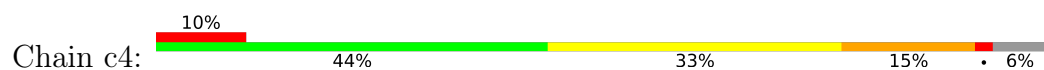




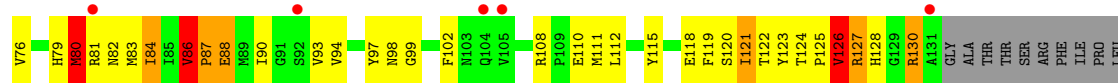
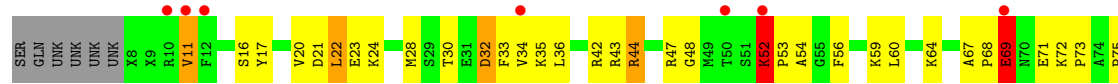
- Molecule 16: 40S ribosomal protein S14-A



- Molecule 16: 40S ribosomal protein S14-A

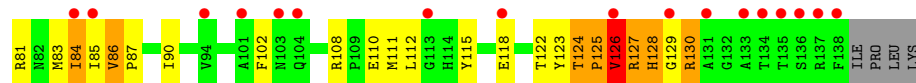
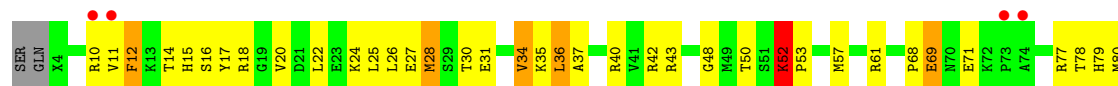


- Molecule 17: 40S ribosomal protein S15 (uS19)

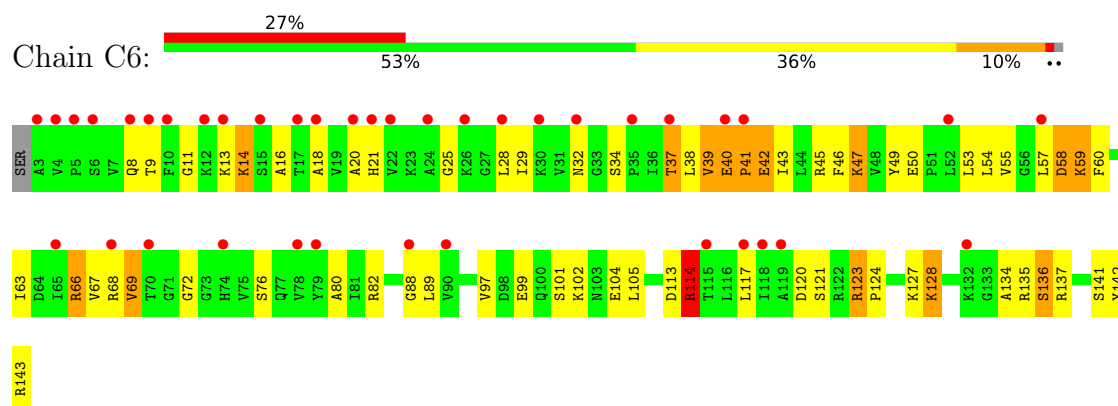


LYS

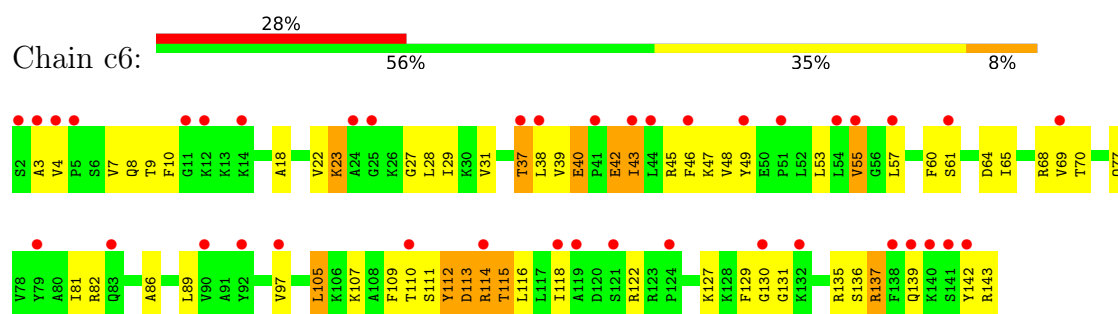
- Molecule 17: 40S ribosomal protein S15 (uS19)



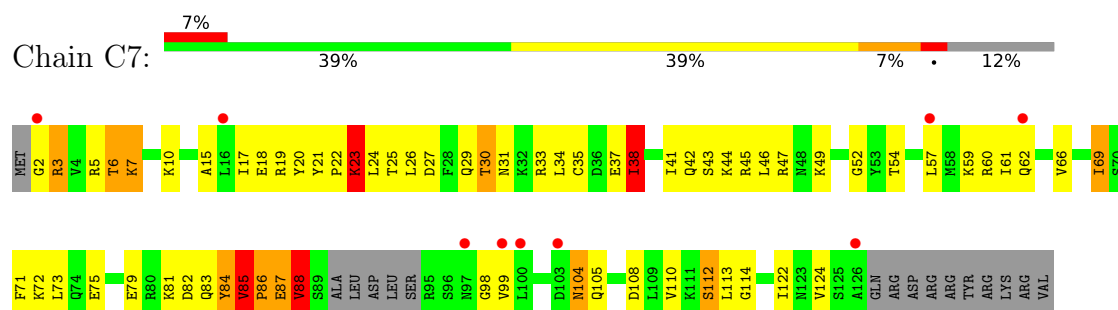
- Molecule 18: 40S ribosomal protein S16-A



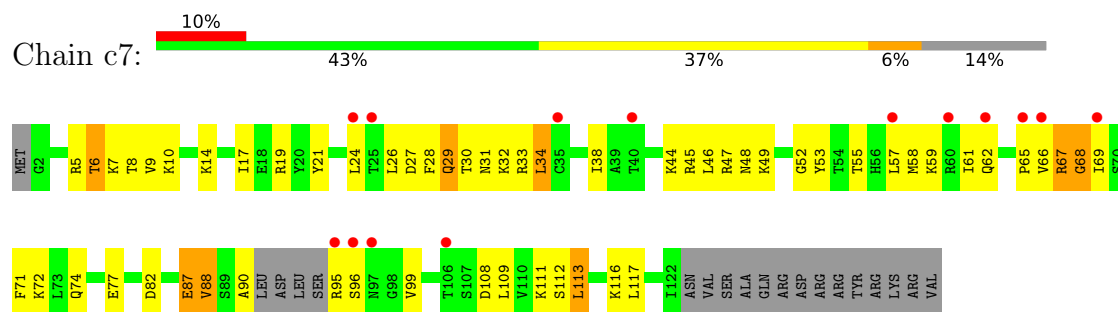
- Molecule 18: 40S ribosomal protein S16-A



- Molecule 19: 40S ribosomal protein S17-A

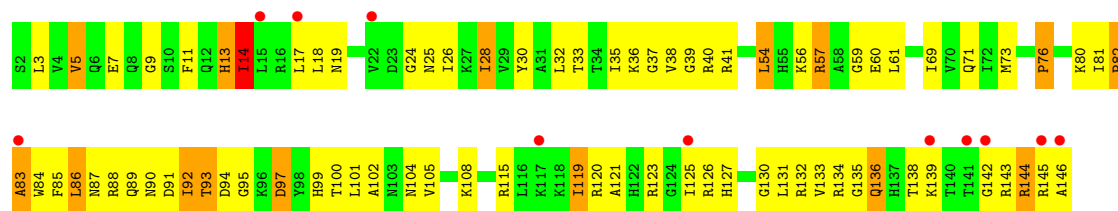


- Molecule 19: 40S ribosomal protein S17-A

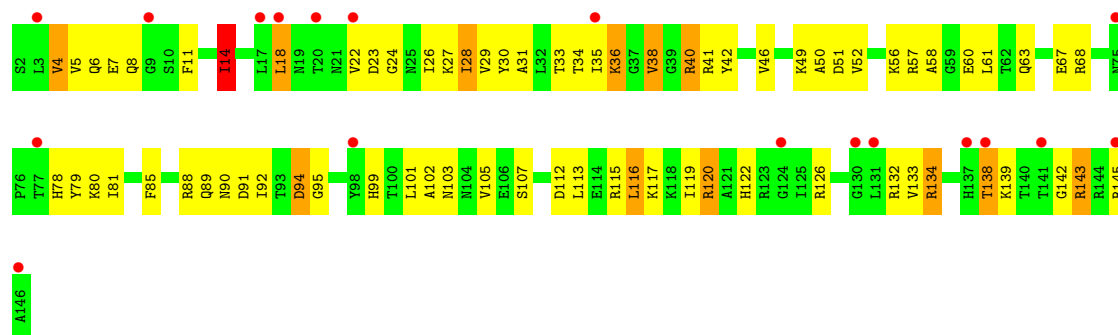


- Molecule 20: 40S ribosomal protein S18-A

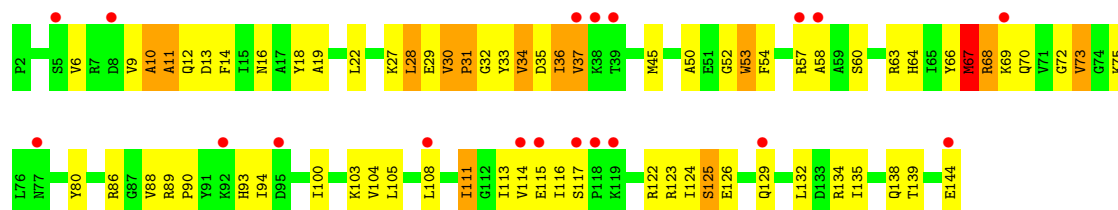




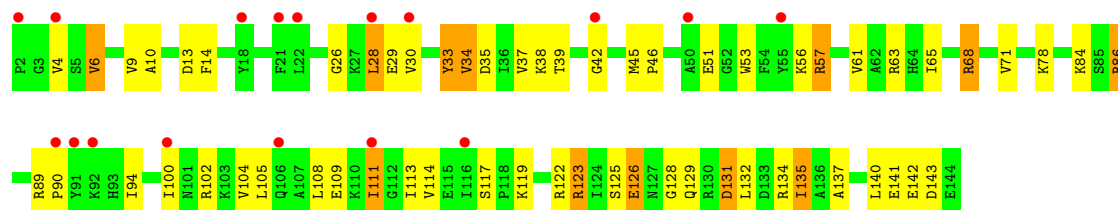
• Molecule 20: 40S ribosomal protein S18-A



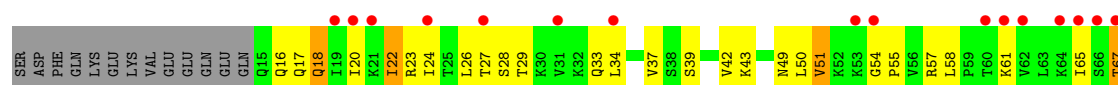
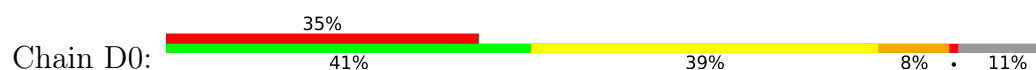
• Molecule 21: 40S ribosomal protein S19-A

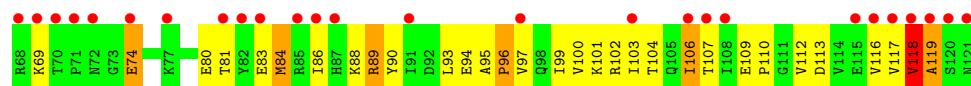


• Molecule 21: 40S ribosomal protein S19-A



• Molecule 22: 40S ribosomal protein S20

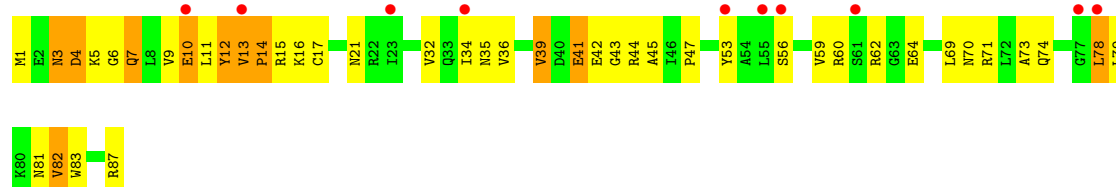




• Molecule 22: 40S ribosomal protein S20



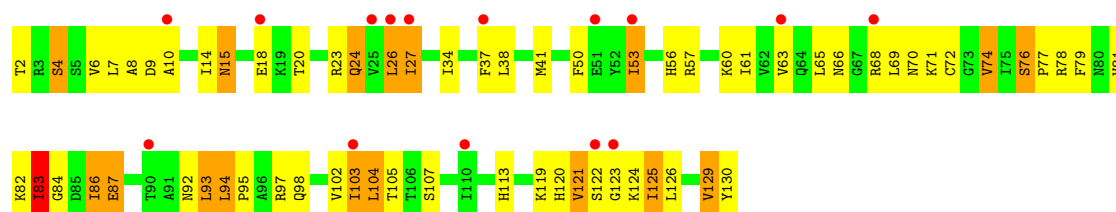
• Molecule 23: 40S ribosomal protein S21-A



• Molecule 23: 40S ribosomal protein S21-A

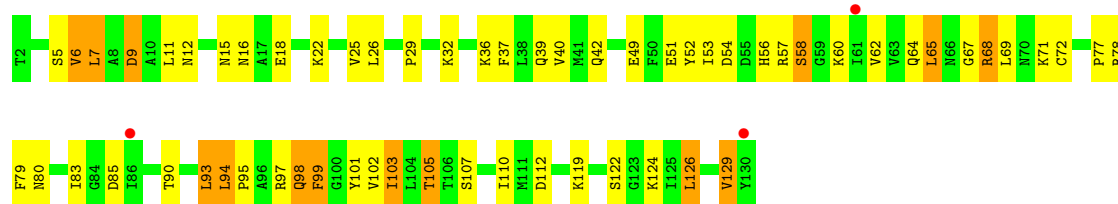


• Molecule 24: 40S ribosomal protein S22-A

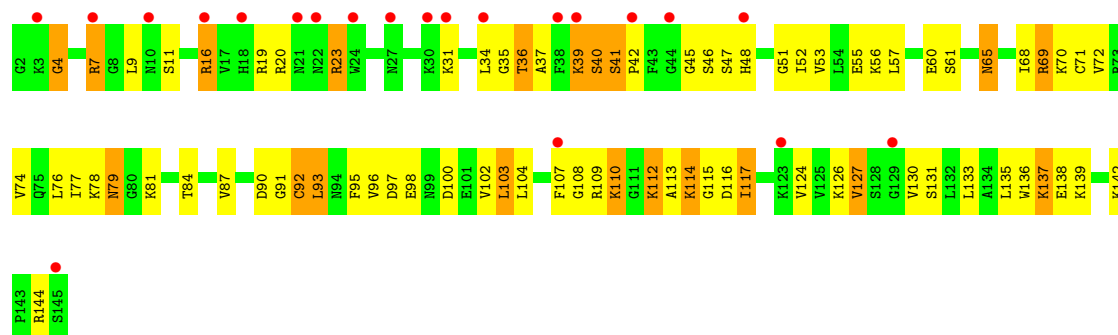


• Molecule 24: 40S ribosomal protein S22-A

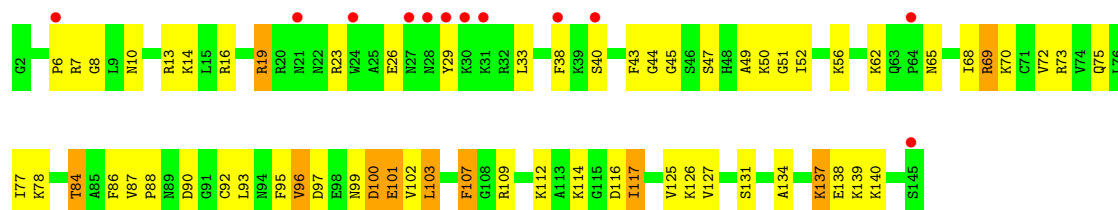




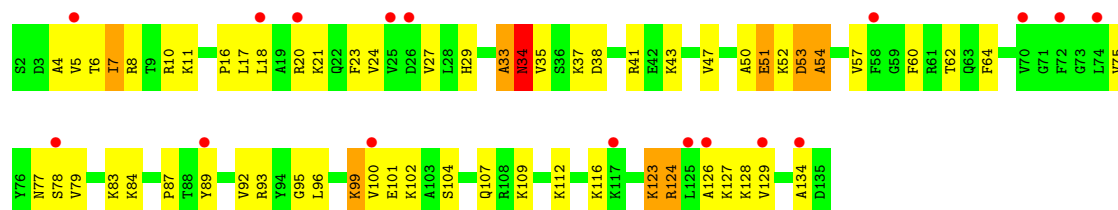
• Molecule 25: 40S ribosomal protein S23-A



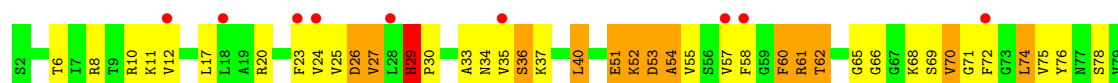
• Molecule 25: 40S ribosomal protein S23-A

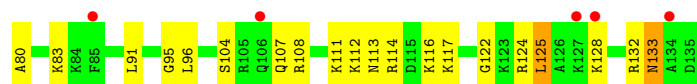


• Molecule 26: 40S ribosomal protein S24-A

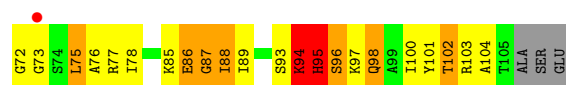
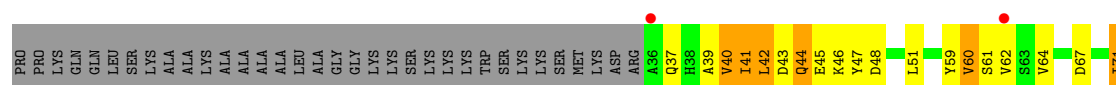
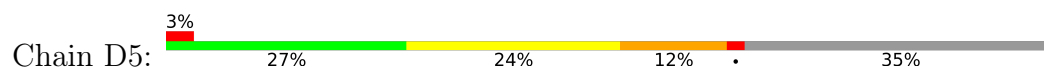


• Molecule 26: 40S ribosomal protein S24-A

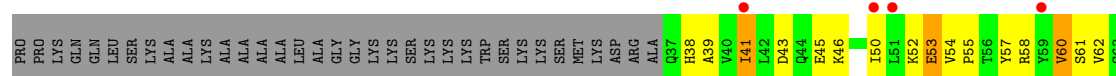
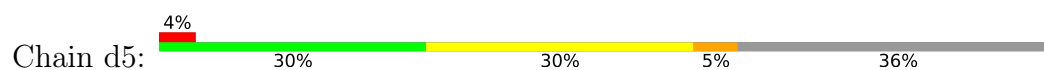




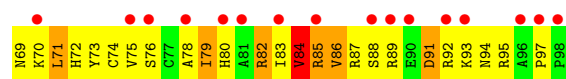
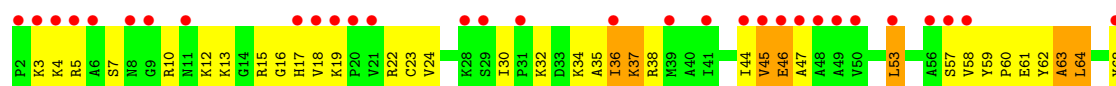
- Molecule 27: 40S ribosomal protein S25-A



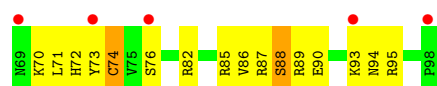
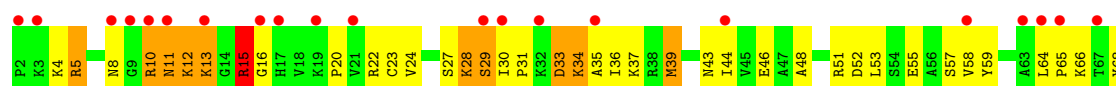
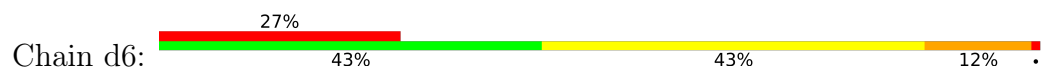
- Molecule 27: 40S ribosomal protein S25-A



- Molecule 28: 40S ribosomal protein S26-B

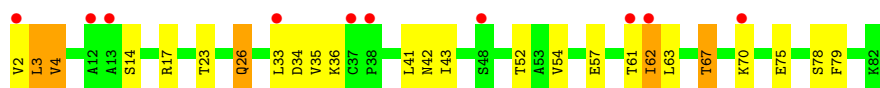


- Molecule 28: 40S ribosomal protein S26-B

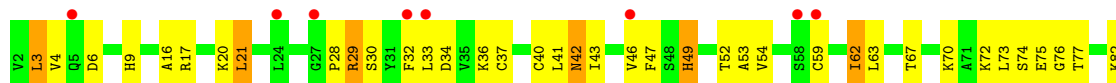


- Molecule 29: 40S ribosomal protein S27-A

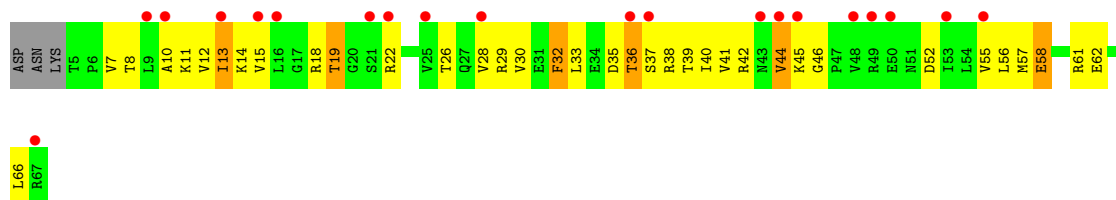




- Molecule 29: 40S ribosomal protein S27-A



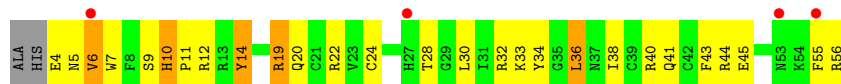
- Molecule 30: 40S ribosomal protein S28-A



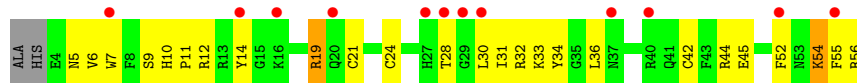
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A

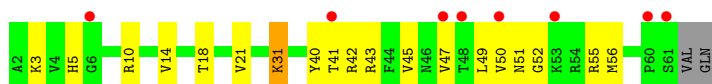


- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

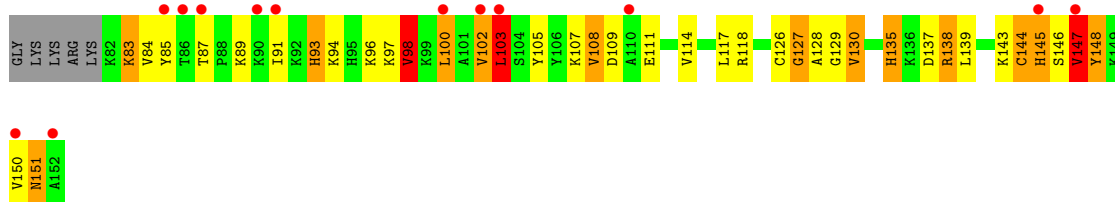




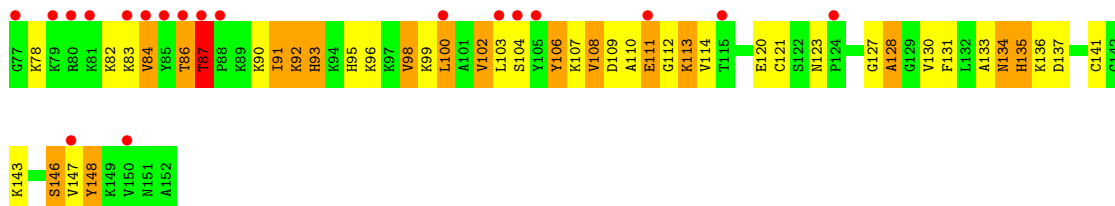
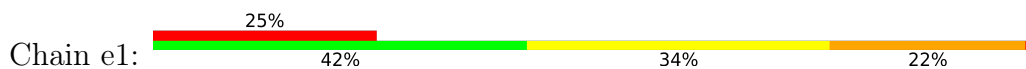
- Molecule 32: 40S ribosomal protein S30-A



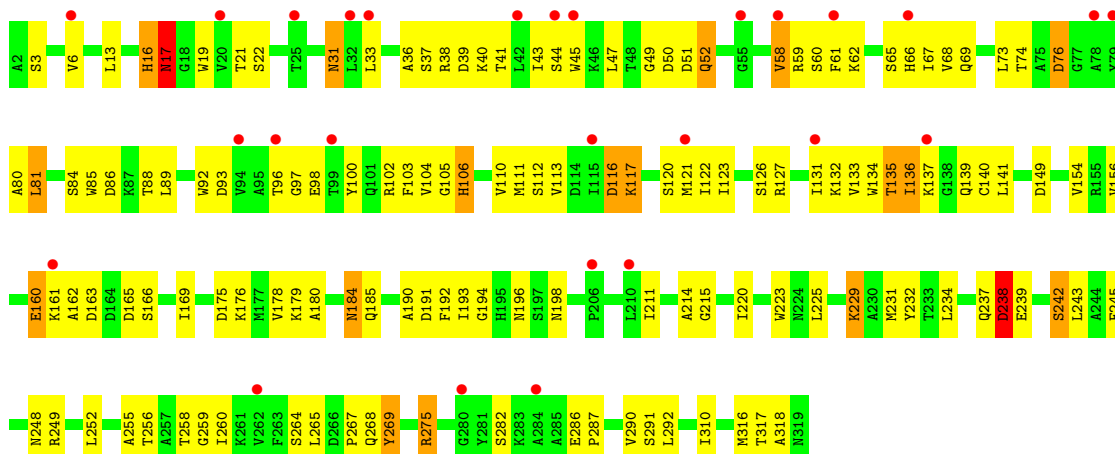
- Molecule 33: Ubiquitin-40S ribosomal protein S31



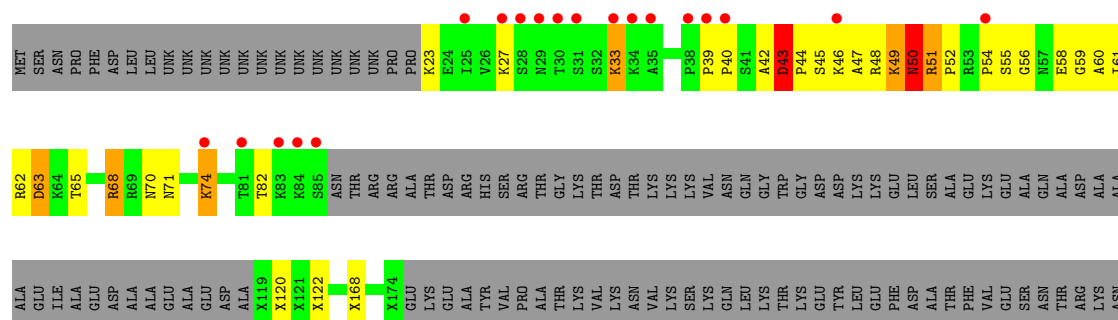
- Molecule 33: Ubiquitin-40S ribosomal protein S31



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



Chain sR:



Chain 1: %



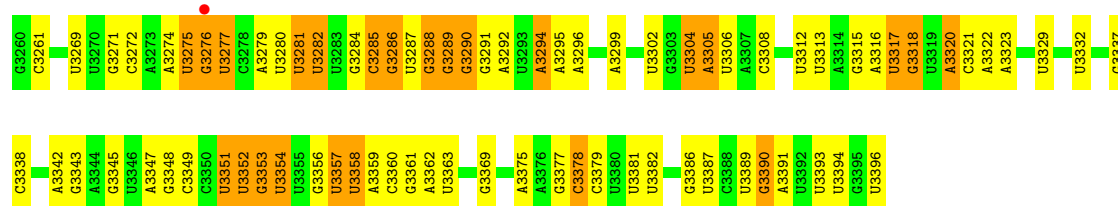


U3237	G3238	U3160	A3163	A3164	A3165	A3166	A3167	A3168	A3169	A3170	A3171	A3172	A3173	A3174	U3175	G3176	A3177	A3178	A3179	A3180	A3181	A3182	A3183	A3187	C3272	A3267	A3268	U3269	U3270	G3271	C3272	U3273	A3274	U3275	U3276	U3277	C3278	A3279	U3280	U3281	U3282	U3283	U3284	U3285	U3286	U3287	U3288	U3289	U3290	U3291	U3292	U3293	U3294	U3295	U3296	U3297	U3298	U3299	U3300	U3301	U3302	U3303	U3304	A3307	C3308	G3309																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C3084	G3085	A3086	A3087	G3088	G3089	U3090	A3091	C3092	C3093	A3094	U3095	A3096	C3097	U3107	G3112	A3113	A3114	C3115	G3116	C3117	C3118	U3119	C3120	U3121	A3122	U3127	A3128	A3129	A3130	U3131	C3132	C3133	A3134	C3137	U3138	A3139	C3140	A3141	A3142	C3143	C3144	C3145	G3146	C3147	A3150	U3151	U3152	U3153	C3154	U3155	U3156	U3157	C3158	A3234	G3309																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U2916	G2917	U2923	C2927	C2928	U2932	A2933	A2934	A2935	A2936	C2937	U2938	G2939	A2940	C2942	C2943	C2944	G2945	A2946	G2947	U2950	U2951	U2955	C2960	A2969	C2970	U2971	G2972	U2974	G2977	U2978	C2983	C2984	C2985	U2986	A2987	G2990	A2991	U2992	G2993	U2996	G2997	A3000	C3002	G3083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A3006	U3007	A3012	U3013	G3015	U3014	G3016	A3017	A3018	U3019	U3023	A3024	C3025	G3028	A3029	G3030	A3035	G3036	U3037	A3040	U3041	U3042	C3043	G3044	G3045	A3046	U3047	A3048	U3049	U3050	G3051	G3052	G3053	U3054	U3055	U3056	G3059	U3066	C3067	G3069	A3070	U3071	C3072	G3074	U3078	U3079	G3080	C3081	G3083																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C3084	G3085	A3086	A3087	G3088	G3089	U3090	A3091	C3092	C3093	A3094	U3095	A3096	C3097	U3107	G3112	A3113	A3114	C3115	G3116	C3117	C3118	U3119	C3120	U3121	A3122	U3127	A3128	A3129	A3130	U3131	C3132	C3133	A3134	C3137	U3138	A3139	C3140	A3141	A3142	C3143	C3144	C3145	G3146	C3147	A3150	U3151	U3152	U3153	C3154	U3155	U3156	U3157	C3158	A3234	G3309																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U2237	G2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2682	A2683	A2684	A2685	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855	A2856	A2857	A2858	A2859	A2860	A2861	A2862	A2863	A2864	A2865	A2866	A2867	A2868	A2869	A2870	A2871	A2872	A2873	A2874	A2875	A2876	A2877	A2878	A2879	A2880	A2881	A2882	A2883	A2884	A2885	A2886	A2887	A2888	A2889	A2890	A2891	A2892	A2893	A2894	A2895	A2896	A2897	A2898	A2899	A2900	A2901	A2902	A2903	A2904	A2905	A2906	A2907	A2908	A2909	A2910	A2911	A2912	A2913	A2914	A2915	A2916	A2917	A2918	A2919	A2920	A2921	A2922	A2923	A2924	A2925	A2926	A2927	A2928	A2929	A2930	A2931	A2932	A2933	A2934	A2935	A2936	A2937	A2938	A2939	A2940	A2941	A2942	A2943	A2944	A2945	A2946	A2947	A2948	A2949	A2950	A2951	A2952	A2953	A2954	A2955	A2956	A2957	A2958	A2959	A2960	A2961	A2962	A2963	A2964	A2965	A2966	A2967	A2968	A2969	A2970	A2971	A2972	A2973	A2974	A2975	A2976	A2977	A2978	A2979	A2980	A2981	A2982	A2983	A2984	A2985	A2986	A2987	A2988	A2989	A2990	A2991	A2992	A2993	A2994	A2995	A2996	A2997	A2998	A2999	A3000	A3001	A3002	A3003	A3004	A3005	A3006	A3007	A3008	A3009	A3010	A3011	A3012	A3013	A3014	A3015	A3016	A3017	A3018	A3019	A3020	A3021	A3022	A3023	A3024	A3025	A3026	A3027	A3028	A3029	A3030	A3031	A3032	A3033	A3034	A3035	A3036	A3037	A3038	A3039	A3040	A3041	A3042	A3043	A3044	A3045	A3046	A3047	A3048	A3049	A3050	A3051	A3052	A3053	A3054	A3055	A3056	A3057	A3058	A3059	A3060	A3061	A3062	A3063	A3064	A3065	A3066	A3067	A3068	A3069	A3070	A3071	A3072	A3073	A3074	A3075	A3076	A3077	A3078	A3079	A3080	A3081	A3082	A3083	A3084	A3085	A3086	A3087	A3088	A3089	A3090	A3091	A3092	A3093	A3094	A3095	A3096	A3097	A3098	A3099	A3100	A3101	A3102	A3103	A3104	A3105	A3106	A3107	A3108	A3109	A3110	A3111	A3112	A3113	A3114	A3115	A3116	A3117	A3118	A3119	A3120	A3121	A3122	A3123	A3124	A3125	A3126	A3127	A3128	A3129	A3130	A3131	A3132	A3133	A3134	A3135	A3136	A3137	A3138	A3139	A3140	A3141	A3142	A3143	A3144	A3145	A3146	A3147	A3148	A3149	A3150	A3151	A3152	A3153	A3154	A3155	A3156	A3157	A3158	A3159	A3160	A3161	A3162	A3163	A3164	A3165	A3166	A3167	A3168	A3169	A3170	A3171	A3172	A3173	A3174	A3175	A3176	A3177	A3178	A3179	A3180	A3181	A3182	A3183	A3184	A3185	A3186	A3187	A3188	A3189	A3190	A3191	A3192	A3193	A3194	A3195	A3196	A3197	A3198	A3199	A3200	A3201	A3202	A3203	A3204	A3205	A3206	A3207	A3208	A3209	A3210	A3211	A3212	A3213	A3214	A3215	A3216	A3217	A3218	A3219	A3220	A3221	A3222	A3223	A3224	A3225	A3226	A3227	A3228	A3229	A3230	A3231	A3232	A3233	A3234	A3235	A3236	A3237	A3238	A3239	A3240	A3241	A3242	A3243	A3244	A3245	A3246	A3247	A3248	A3249	A3250	A3251	A3252	A3253	A3254	A3255	A3256	A3257	A3258	A3259	A3260	A3261	A3262	A3263	A3264	A3265	A3266	A3267	A3268	A3269	A3270	A3271	A3272	A3273	A3274	A3275	A3276	A3277	A3278	A3279	A3280	A3281	A3282	A3283	A3284	A3285	A3286	A3287	A3288	A3289	A3290	A3291	A3292	A3293	A3294	A3295	A3296	A3297	A3298	A3299	A3300	A3301	A3302	A3303	A3304	A3305	A3306	A3307	A3308	A3309	A3310	A3311	A3312

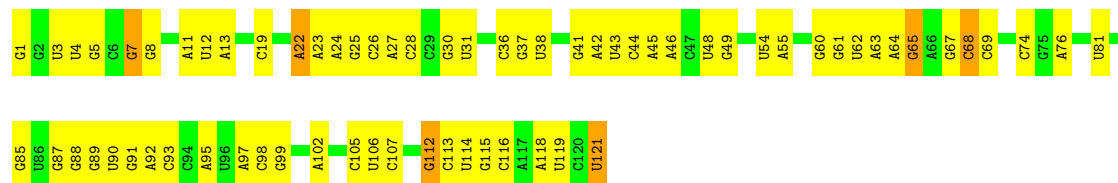




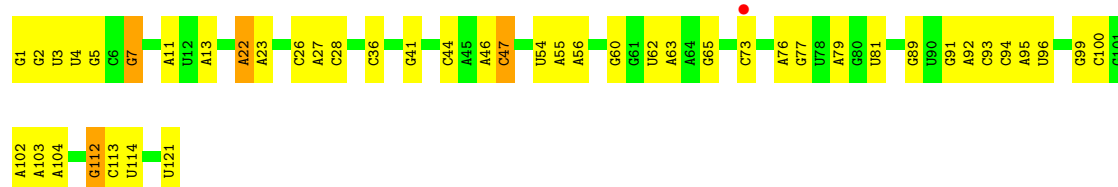
G3182	G3115	U3019	A2941	U2858	C2774	C2699	G2608	G2583	U	G2394	A2214	A2181
A3186	G3116	G3028	C2942	U2859	U2775	G2700	A2609	G2584	G	G2395	A2215	U2132
A3187	G3117	G2943	G2943	U2861	G2776	A2703	G2614	A2535	G	A2396	A2219	C2133
U3192	G3118	A3029	U2944	U2862	G2777	A2704	G2615	A2536	A	A2397	A2220	G2134
C3193	U3119	G3030	G2945	G2863	G2778	A2705	U2617	U2537	G	G2400	A2223	U2135
C3194	U3120		A2946		G2779	G2706	G2618	U2538		A2401	A2224	C2136
C3195	U3121	C3039	G2947	C2867	A2780	C2707	G2619	U2539	C	A2402	A2225	U2137
U3196	A3122	A3040	C2948	U2868	U2781	C2708	G2620	C2540	U	G2403	A2226	A2138
G3197	A3123	U3041	U2949	U2869	U2782	C2709	U2541	U2541	C	A2404	C2227	A2139
U3198	G3124	U3042	G2950	C2870	G2783	C2710	A2626	U2542	G	C2405		
G3199	A3127	G3045	U2954	A2871	A2785	C2711	A2627	U2543	C	C2406		A2144
	A3128	A3046		A2872	G2786	U2712	A2628	U2544	C	C2407		
	A3129	U3047	G2957	U2873		U2713	U2829	C2545		U2408		A2147
	U3130	A3048		U2874	G2794	G2714	C2630	C2546	C	G2409	A2232	U2148
	U3131	A3049	C2960	U2875	U2795	A2715	C2631	A2547	C	U2410	A2233	U2149
	C3132	U3050	G2961	C2796	G2796	A2716	U2632	C2548	A	G2411	A2234	
	C3133	U3051	U2962	C2797	C2797	U2717	U2633	G2549	G	G2412	U2241	G2155
	A3134	G3052	C2963	C2798	C2798		A2634	C2550	U	A2413	A2242	C2156
	U3135	G3053	G2964	U2882	U2799		G2635	A2551	G	G2414	A2243	G2157
			U2965	U2883	G2800	U2722	A2636	C2552	A			
	A3139	U3056	G2966	U2884	G2801	U2723	A2637	U2553	A	G2418	G2245	A2158
	A3142	G3059	A2967	C2885	A2802	U2724	A2643	A2554	A	A2419	G2246	C2163
	C3143	G3060	G2968	U2886		C2726	G2644	C2556	U			
		G3061	A2969	U2887	G2805	U2727	G2645	A2557	A	C2422	G2249	A2168
	G3147	G3062	C2970	U2888		G2728		C2558	C	U2423	G2250	G2169
	U3148	U3063	A2971	C2889	C2810	U2729	G2651	C2559	A	U2424	G2251	U2170
	G3149	C3063	G2972	A2890	C2812	G2730	U2852	C2560	C	A2425	G2252	G2171
	A3150	G3065	U2973	U2891	A2813			U2561	C	U2426	G2253	A2172
	U3151	U3066	U2974	U2892	G2814	C2737	U2655	G2562		U2427	U2254	U2173
	C3152	G3067	U2975	C2893	G2815	A2738	A2656	U2563		U2428	A2255	G2174
	U3153	U3068	C2976	A2900	G2816		A2657	C2564		U2429	A2256	
	C3154	U3069	G2977	G2901	A2817	C2741	G2658	C2565		G2435	C2257	G2177
	U3155	C3072	U2978	U2902	U2818	U2744	G2659	U2566		U2439	U2258	A2178
	U3156	A3073	U2979	U2903	A2819	G2745	G2660	U2567		U2497	U2259	C2179
	G3157	G3074	U2980	U2904		A2746	G2663	U2570		U2498	A2260	G2180
	G3158	G3075	U2981	U2905	U2829	A2747	C2664	U2571		U2499	G2261	C2181
	C3159		U2982	C2906	G2830	A2748	U2665	C2572		G2440	A2262	
	U3160	U3078	U2983	A2911		G2749	G2666	G2573		A2441	A2263	G2187
	C3161	U3079	G2984	G2912	A2833	U2750	C2667	U2574		G2442	U2266	A2188
	C3162	G3080	C2985	C2913	G2834	G2751	A2667	G2575		G2443	U2267	U2189
	A3163		U2986	G2918	U2835	U2752	G2672	G2584		G2444	U2268	
	C3164	G3085	G2987	U2923	C2836	G2753	A2673	G2585		U2446	U2269	C2192
	A3165	A3086	U2988	U2924	A2837	G2754	A2674	G2586		A2447	U2270	U2193
		A3087	G2989	C2925	A2838	C2755	A2675	U2587		G2448	A2271	G2194
	A3168	A3091	U2990	C2926		C2756	A2676	U2588		A2449	G2272	C2197
	U3169	C3092	A3006	U2927	U2843	G2761	A2677	G2589		G2451	G2273	A2198
	A3170		U3007	C2928	C2844	A2762		G2592		U2452	G2276	G2201
	A3171	G3102	A3068	C2931	U2846	U2763	U2688	A2593	G	U	G2277	
	A3172		G3009	U2932	A2847	C2764	A2689	C2594	U	G	A2279	U2205
	U3173	A3106	U3010	A2933	U2848	C2765	G2690	A2595	A	A	A2280	G2206
	U3174	U3107	A3012	A2934	C2849	U2766	A2691	G2599	G	G	A2281	A2207
	G3175		U3013	U2935	G2850			A2524	A	A		A2208
	U3176	U3014	U3014	A2936	A2851	A2769	A2694	C2600	A	A	C2287	U2209
	A3177	G3110	G3015	G2937	C2852	G2770	A2695	A2601	U	U	G2288	G2210
	U3178	U3111	C3016	U2938	A2853	U2771	A2696	G2606	A	A	U2289	U2211
	A3179	G3112	A3017	C2772	U2854	C2772	A2697	G2607	A	A	C2290	C2212
	U3180	A3113	C3018	U2855		C2773	G2698		G	G	A2291	A2213



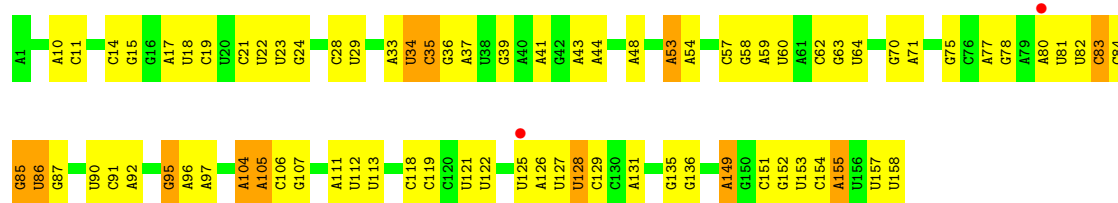
• Molecule 37: 5S ribosomal RNA



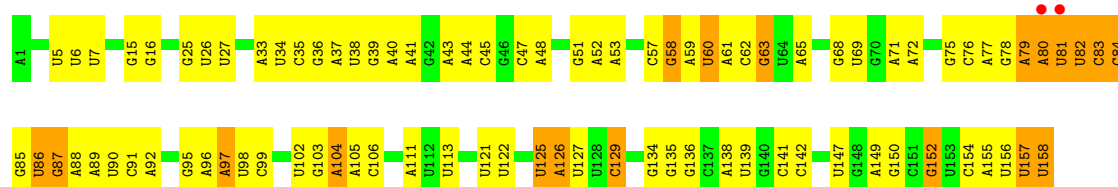
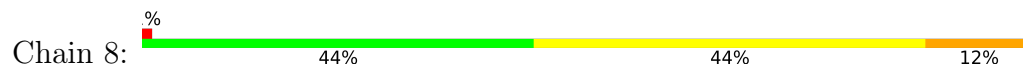
• Molecule 37: 5S ribosomal RNA



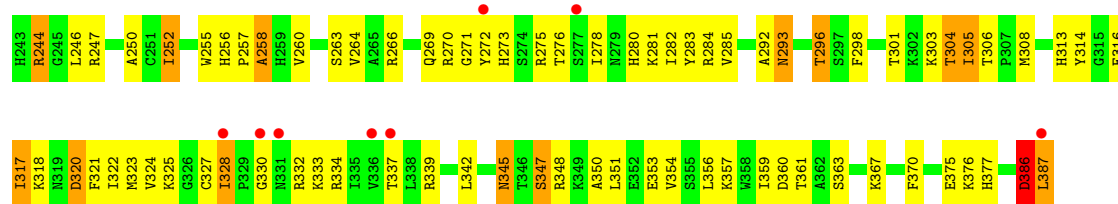
• Molecule 38: 5.8S ribosomal RNA



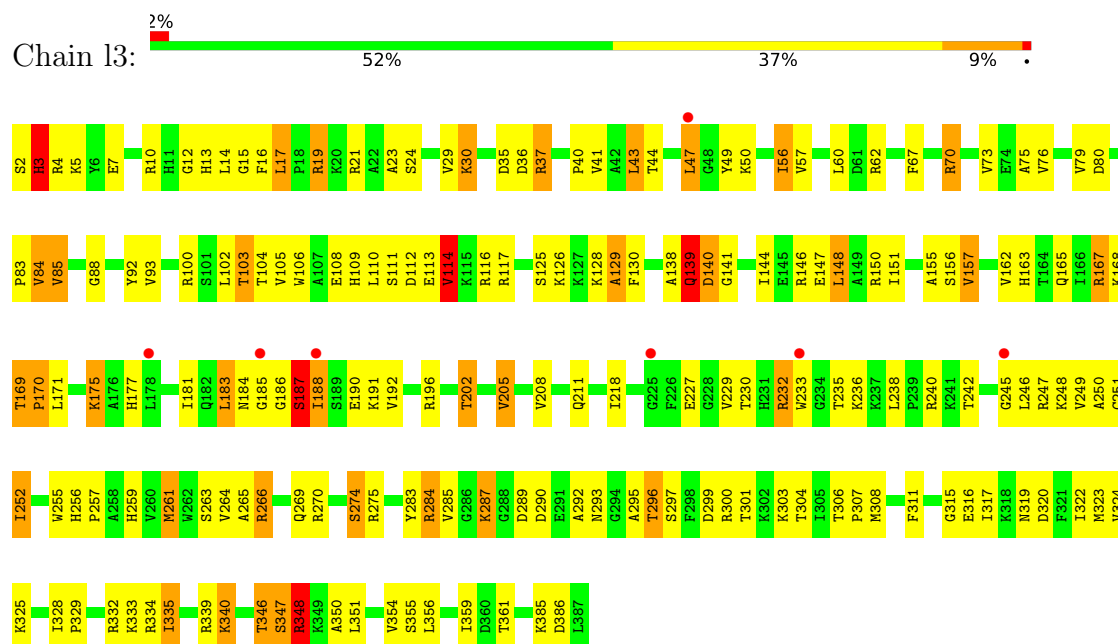
• Molecule 38: 5.8S ribosomal RNA



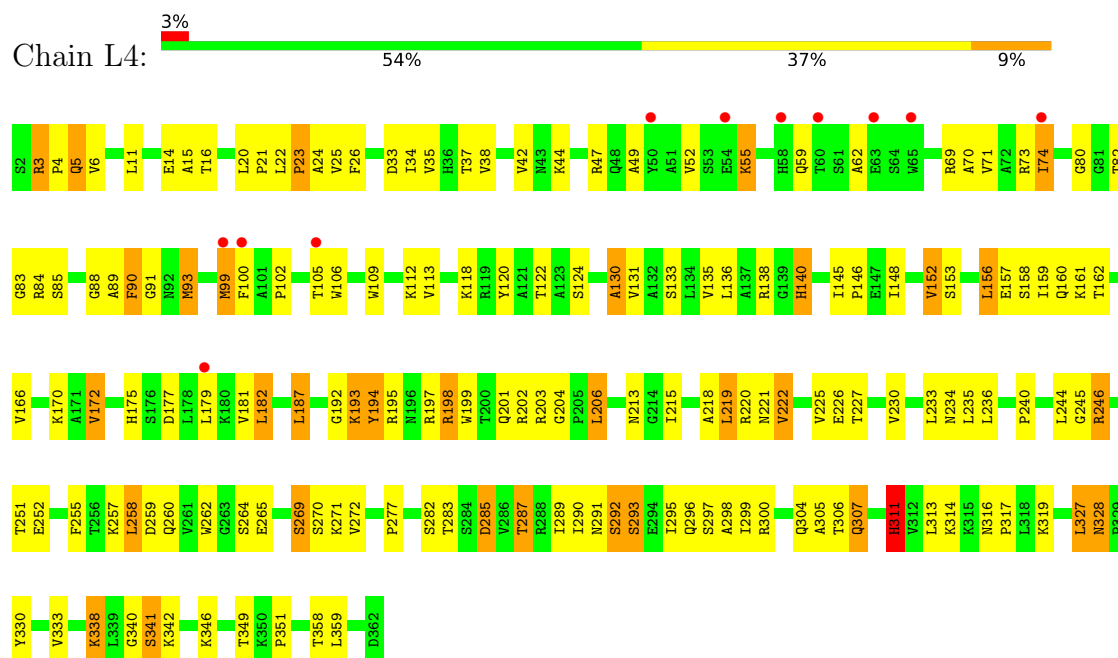
• Molecule 39: 60S ribosomal protein L2-A



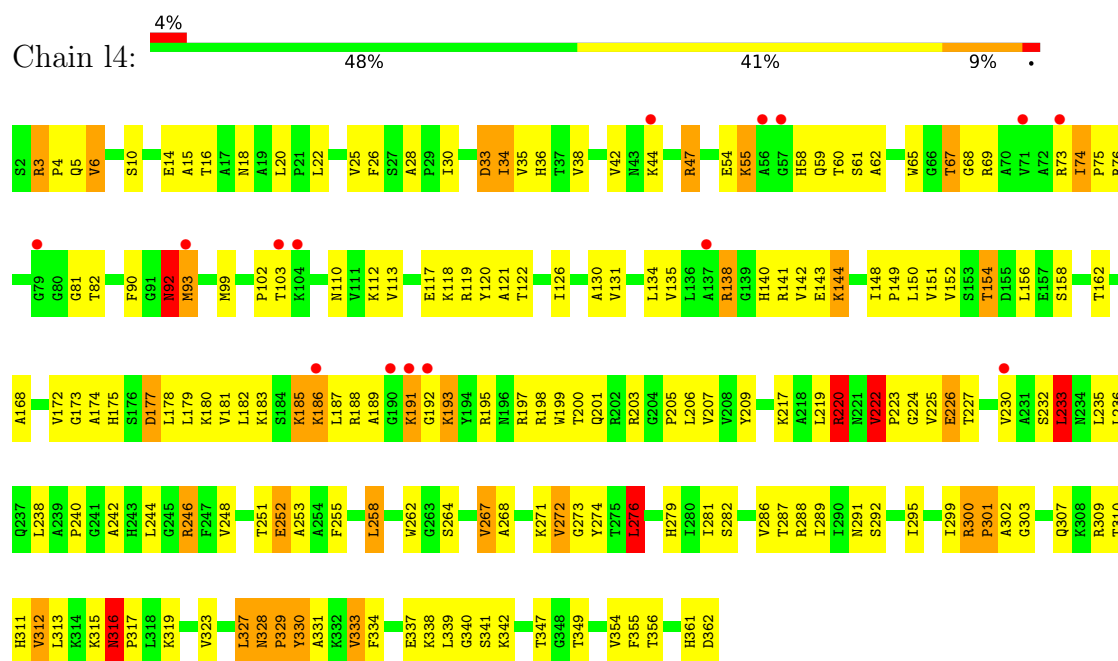
• Molecule 40: 60S ribosomal protein L3



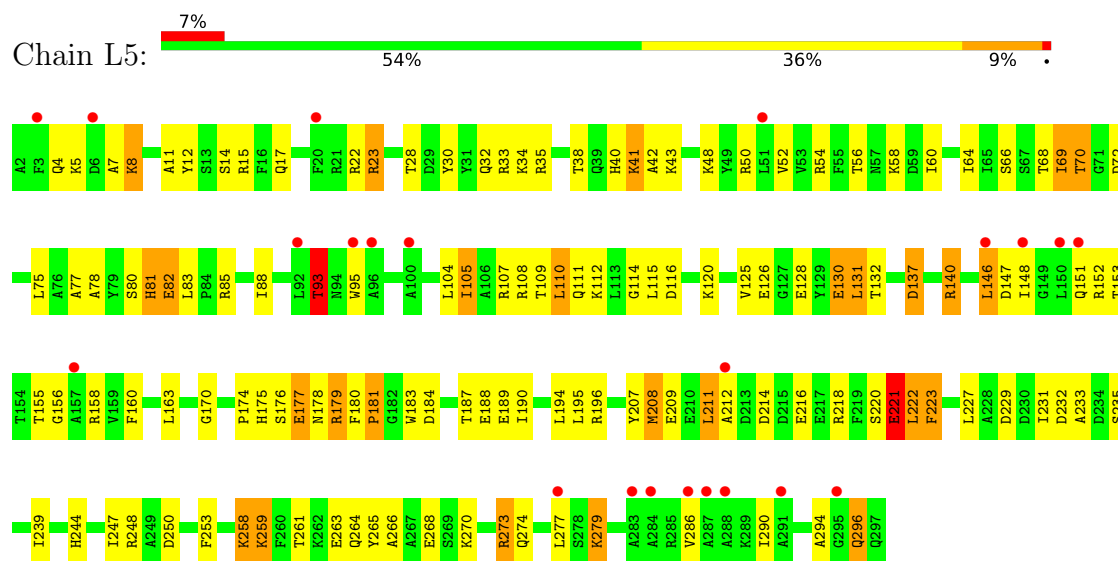
• Molecule 41: 60S ribosomal protein L4-A



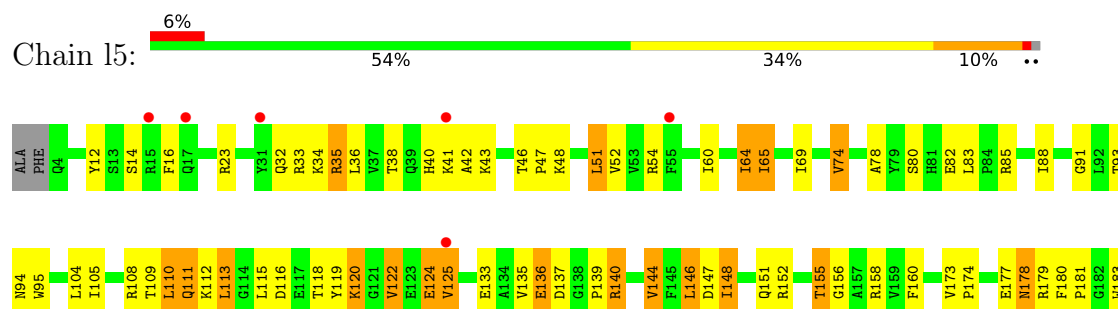
• Molecule 41: 60S ribosomal protein L4-A

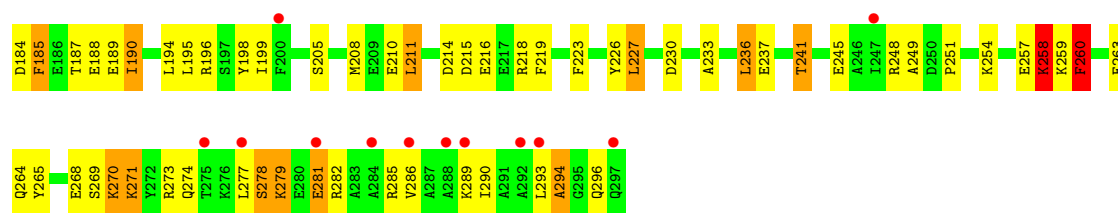


• Molecule 42: 60S ribosomal protein L5

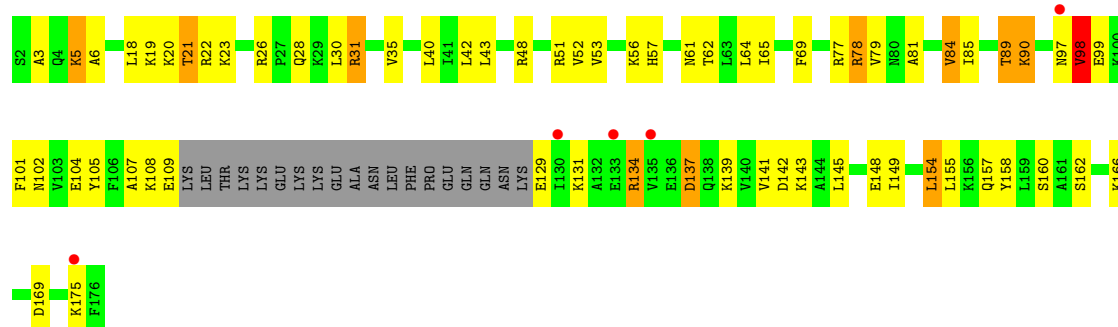


• Molecule 42: 60S ribosomal protein L5

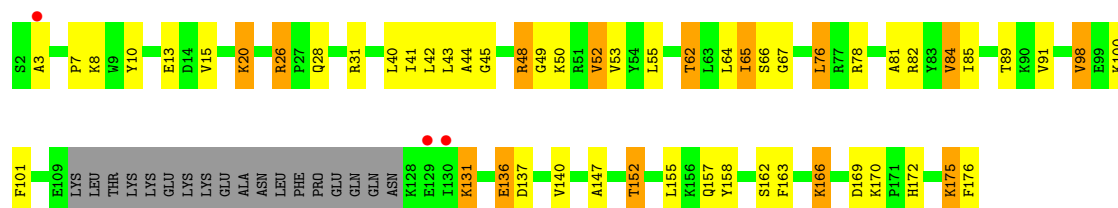




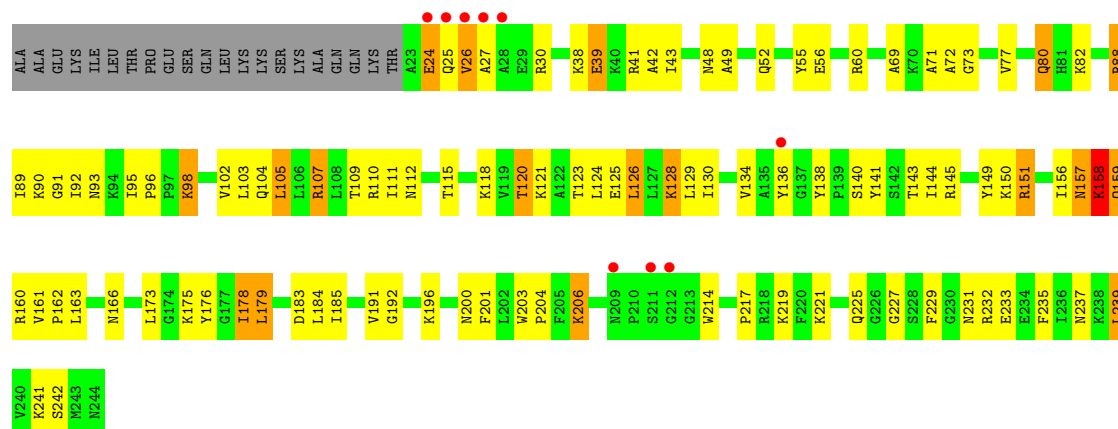
• Molecule 43: 60S ribosomal protein L6-A



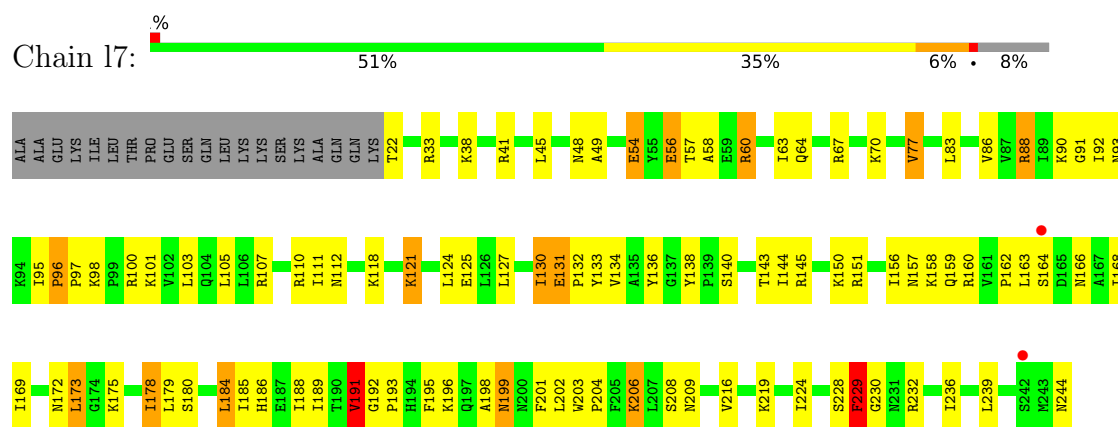
• Molecule 43: 60S ribosomal protein L6-A



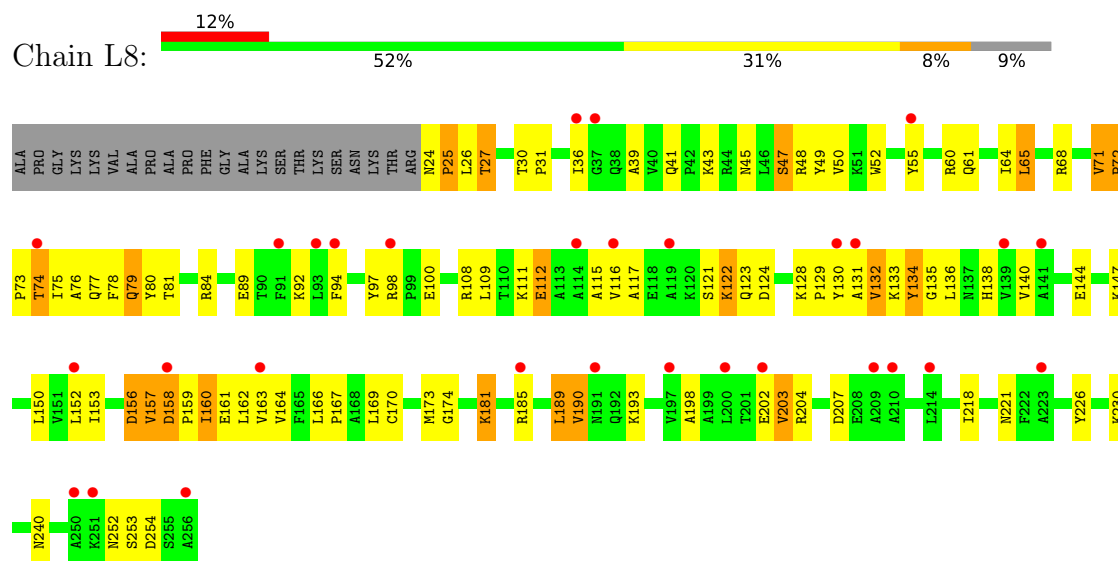
• Molecule 44: 60S ribosomal protein L7-A



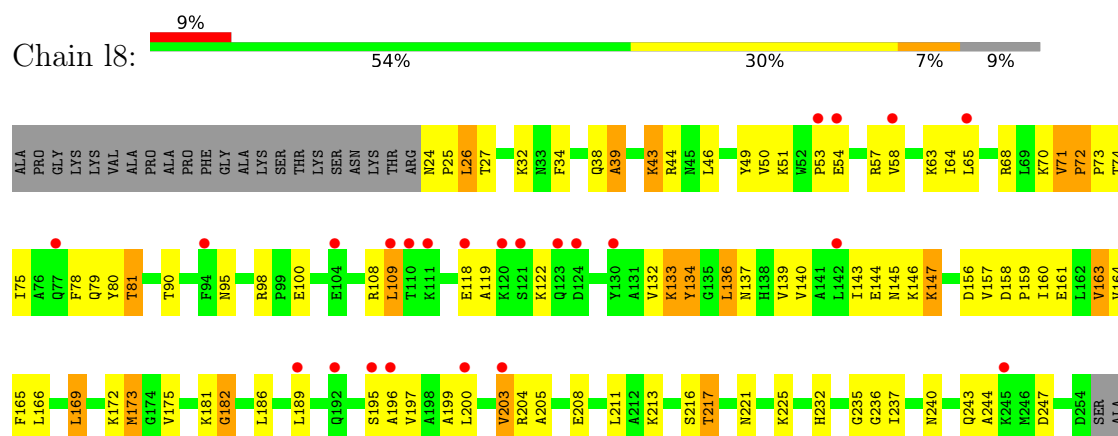
• Molecule 44: 60S ribosomal protein L7-A



• Molecule 45: 60S ribosomal protein L8-A

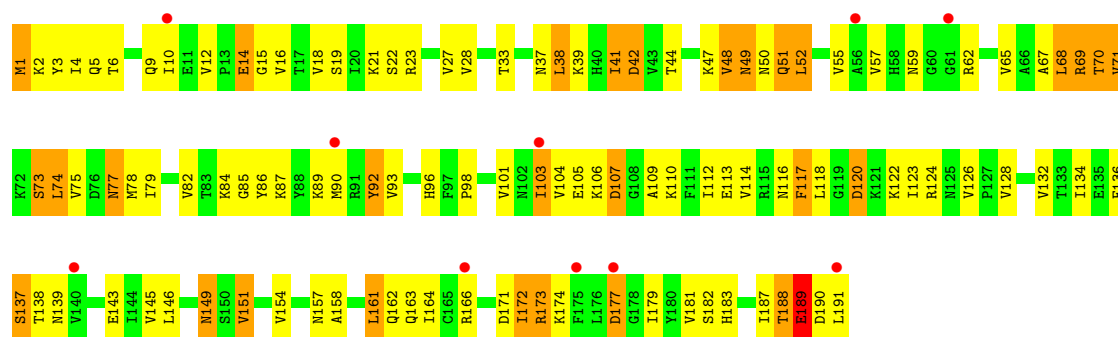


• Molecule 45: 60S ribosomal protein L8-A



• Molecule 46: 60S ribosomal protein L9-A

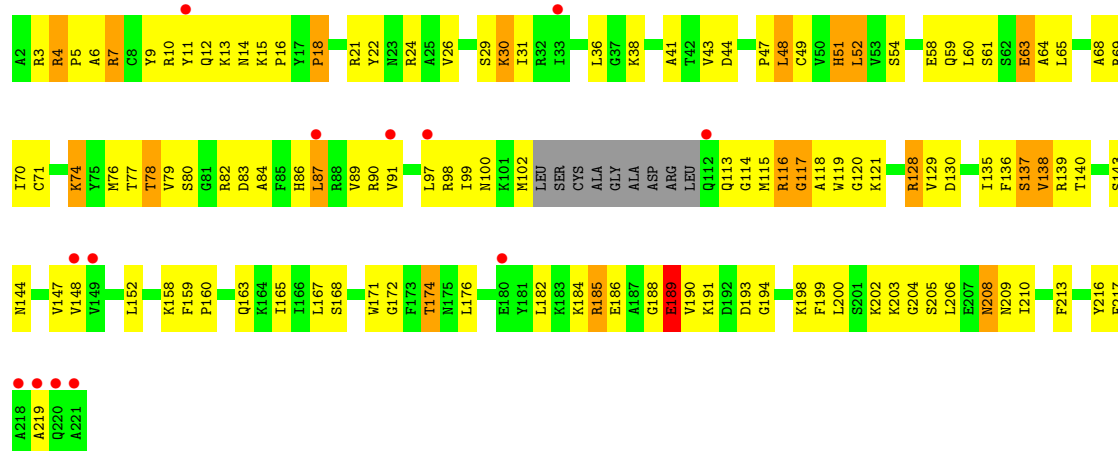
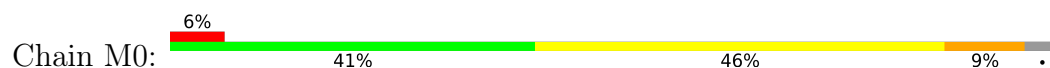




• Molecule 46: 60S ribosomal protein L9-A

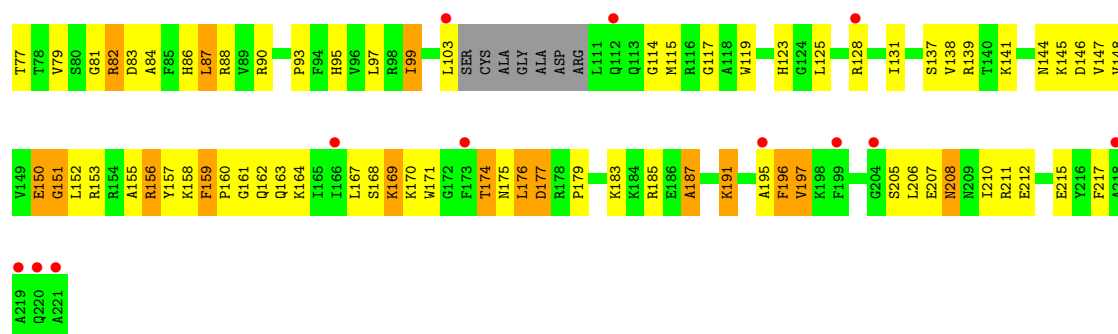


• Molecule 47: 60S ribosomal protein L10

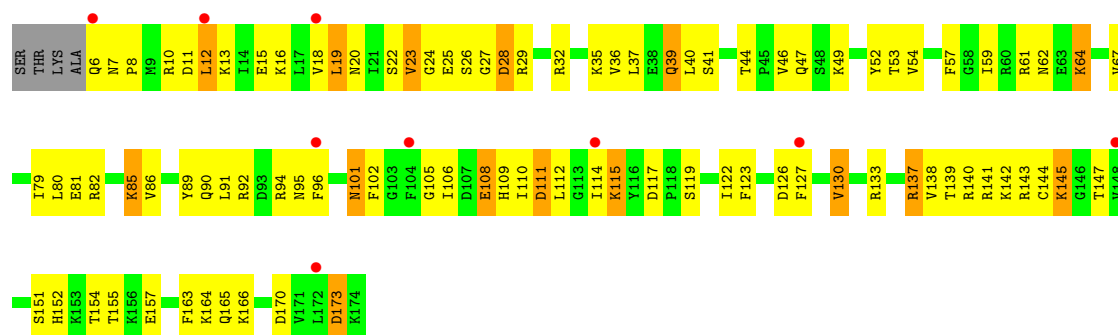


• Molecule 47: 60S ribosomal protein L10

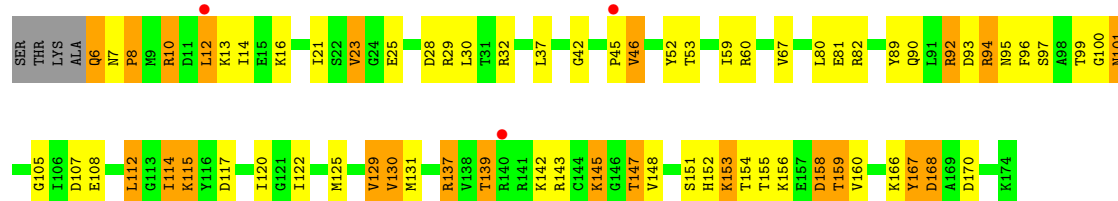




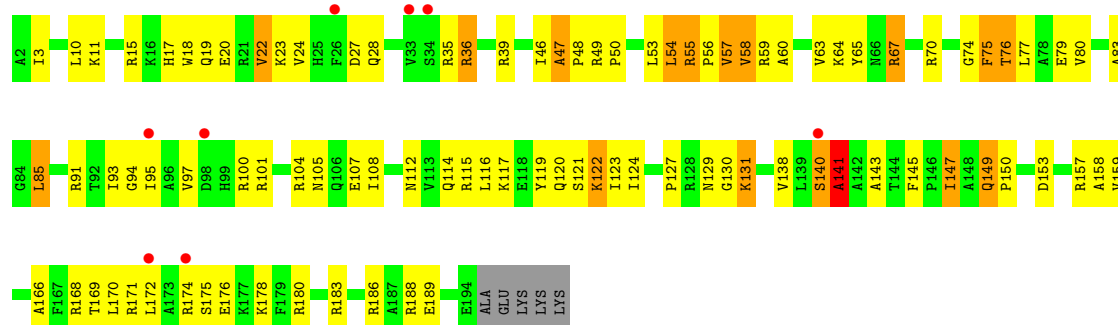
• Molecule 48: 60S ribosomal protein L11-B



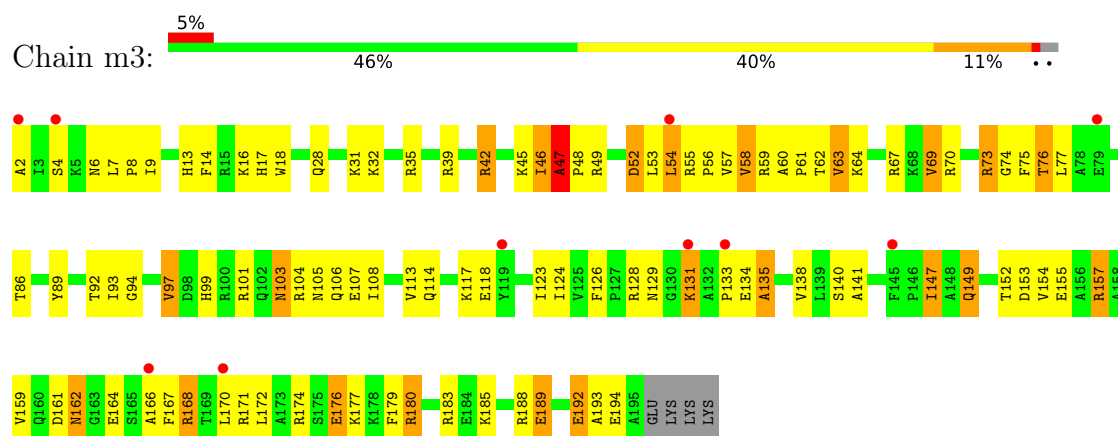
• Molecule 48: 60S ribosomal protein L11-B



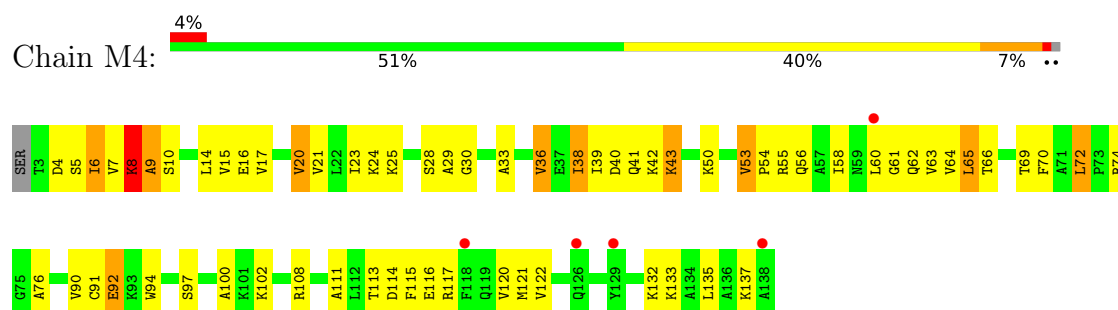
• Molecule 49: 60S ribosomal protein L13-A



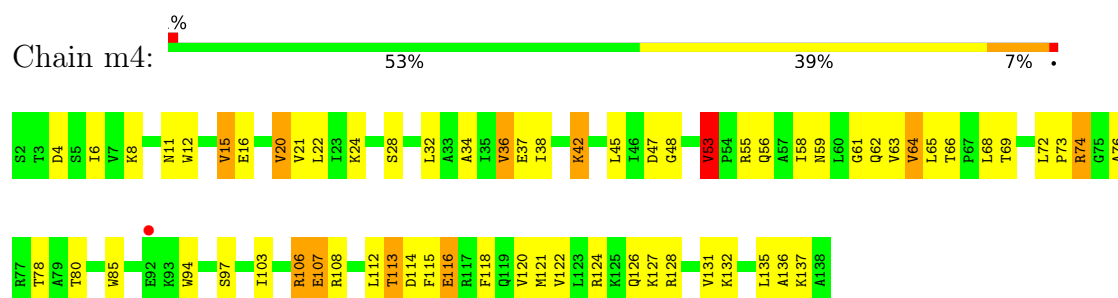
- Molecule 49: 60S ribosomal protein L13-A



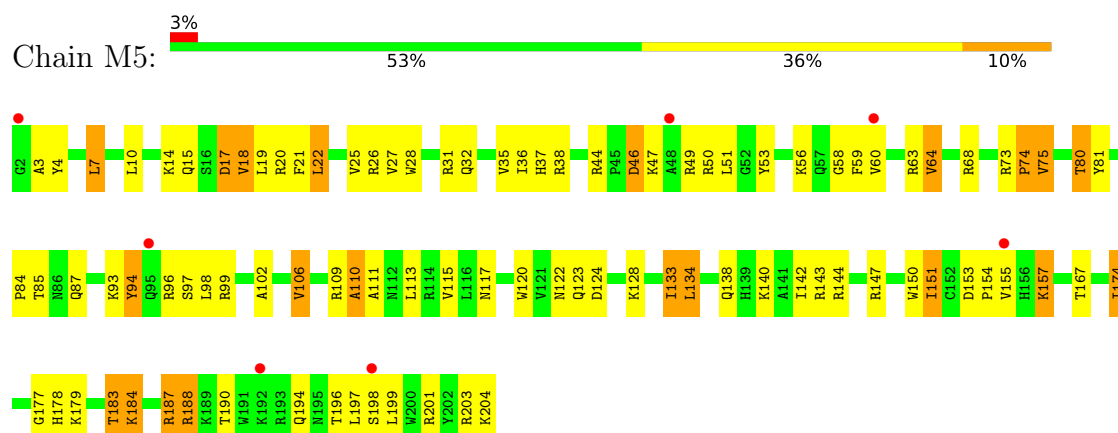
- Molecule 50: 60S ribosomal protein L14-A



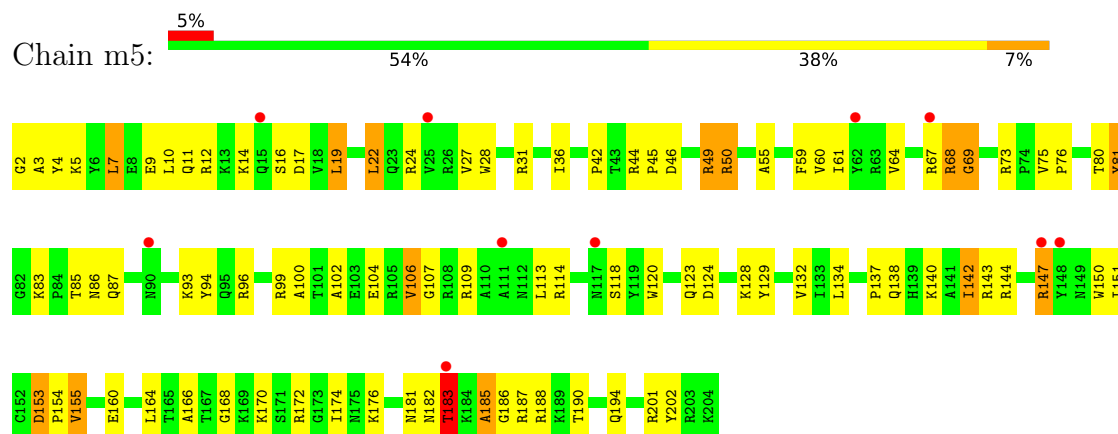
- Molecule 50: 60S ribosomal protein L14-A



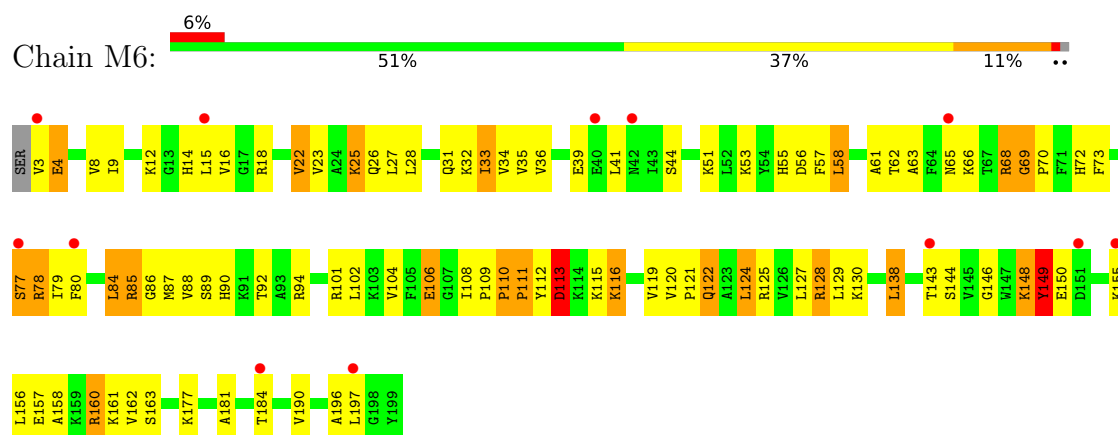
- Molecule 51: 60S ribosomal protein L15-A



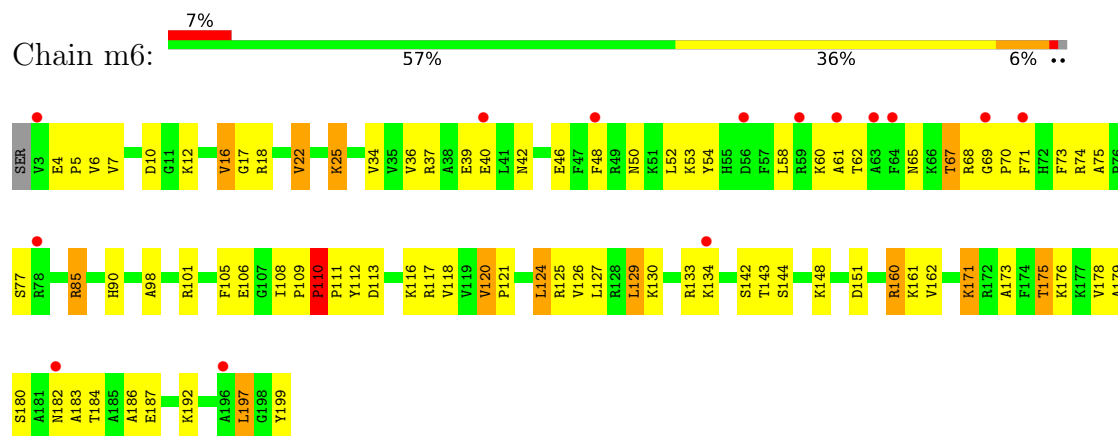
- Molecule 51: 60S ribosomal protein L15-A



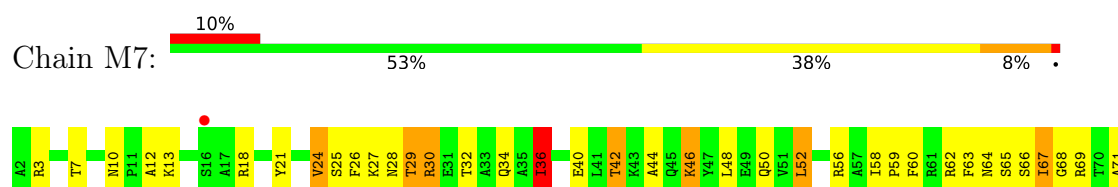
- Molecule 52: 60S ribosomal protein L16-A

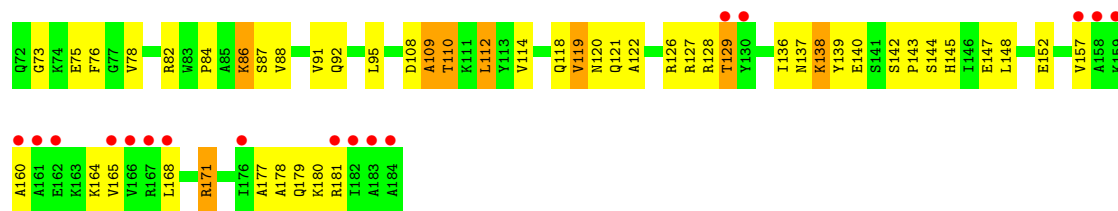


- Molecule 52: 60S ribosomal protein L16-A

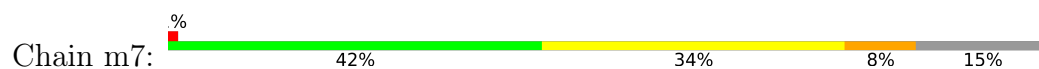


- Molecule 53: 60S ribosomal protein L17-A

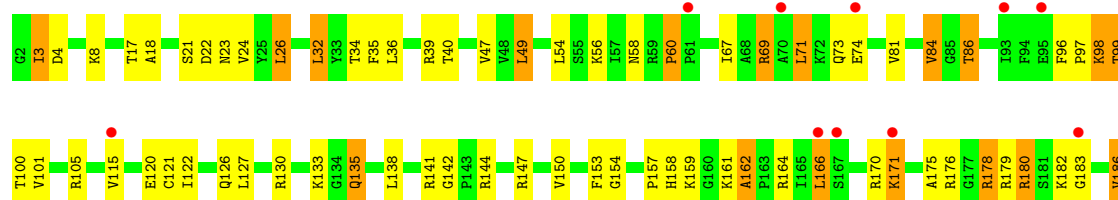




• Molecule 53: 60S ribosomal protein L17-A



• Molecule 54: 60S ribosomal protein L18-A

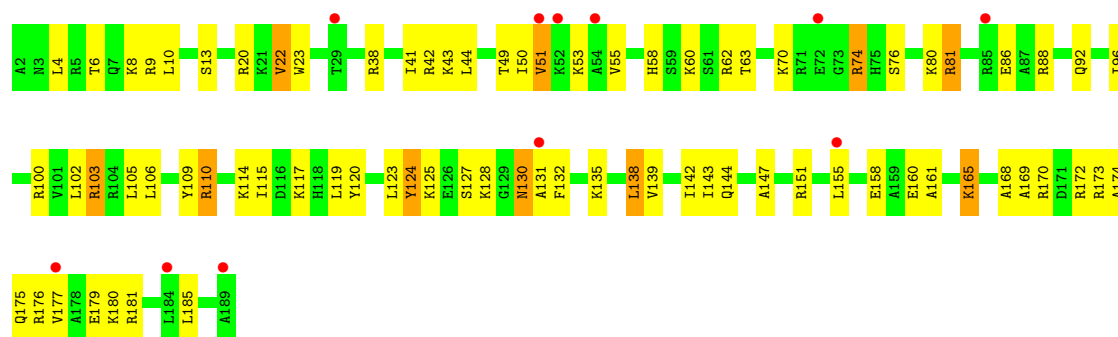


• Molecule 54: 60S ribosomal protein L18-A

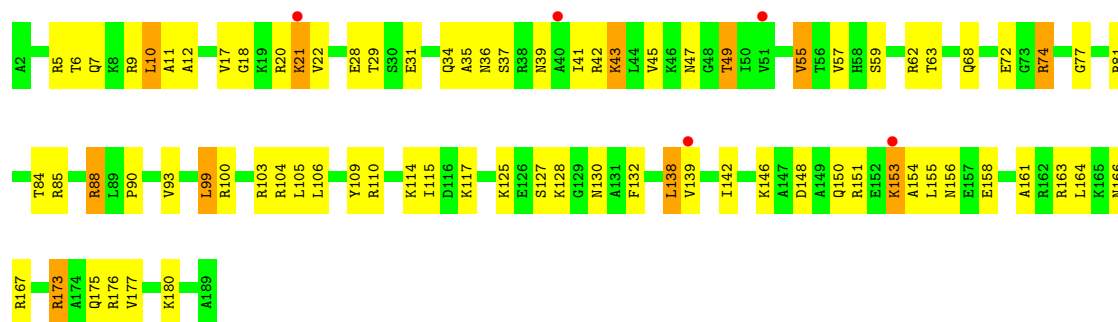


• Molecule 55: 60S ribosomal protein L19-A

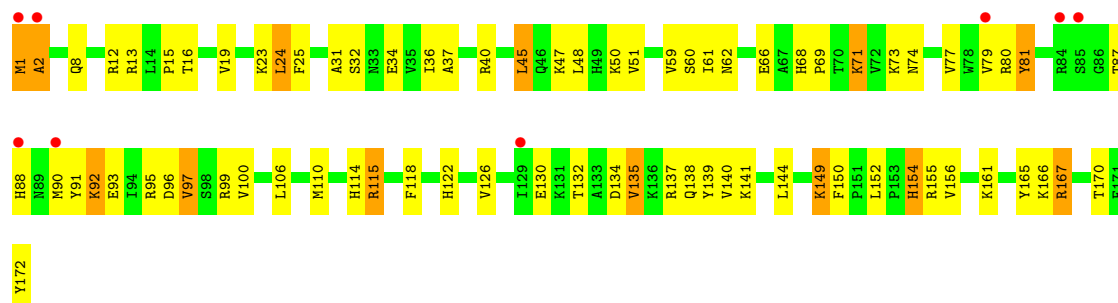




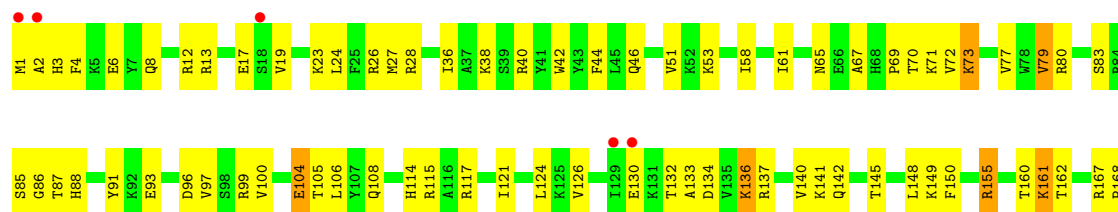
• Molecule 55: 60S ribosomal protein L19-A



• Molecule 56: 60S ribosomal protein L20-A



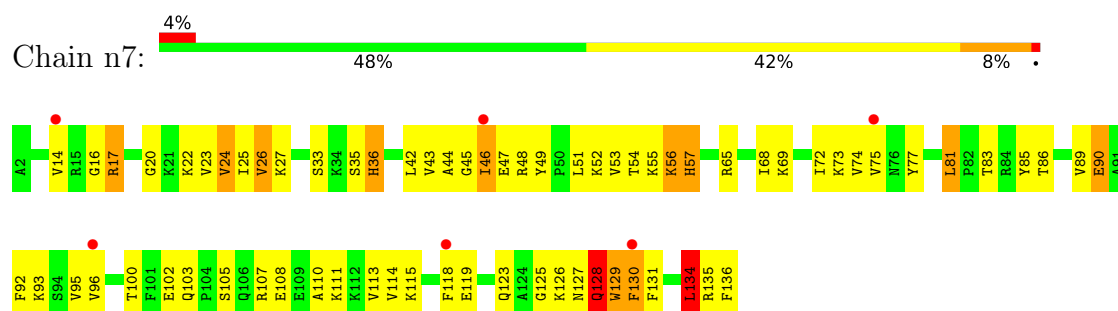
• Molecule 56: 60S ribosomal protein L20-A



Chain N3:



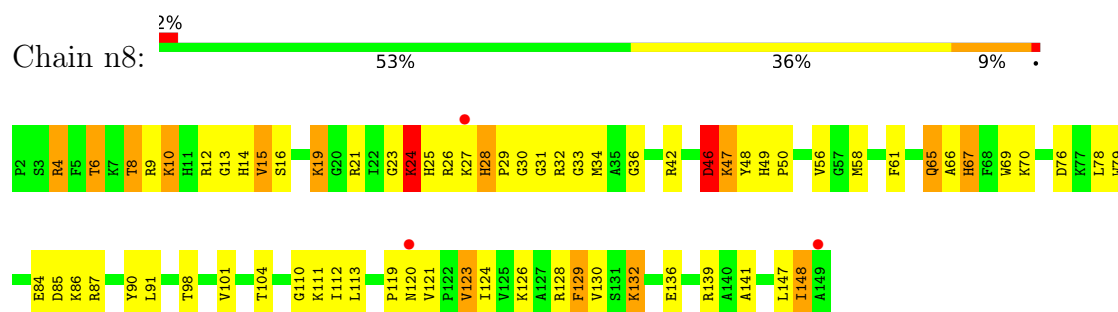
- Molecule 63: 60S ribosomal protein L27-A



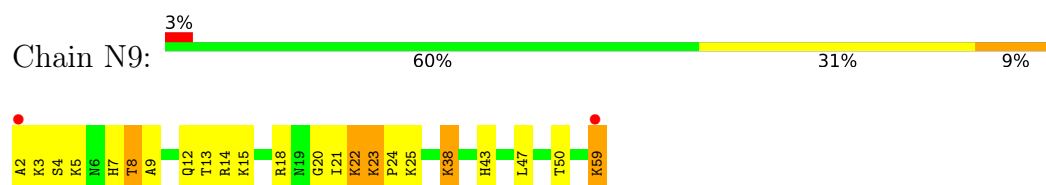
- Molecule 64: 60S ribosomal protein L28



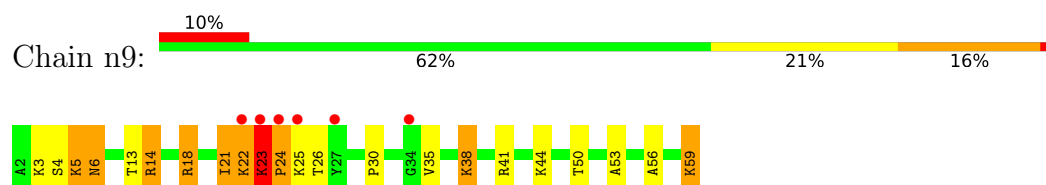
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

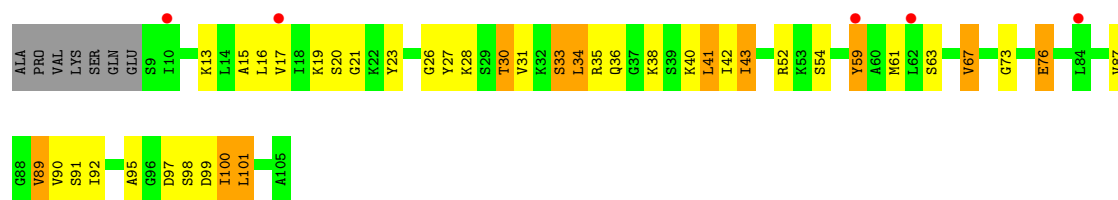


- Molecule 65: 60S ribosomal protein L29

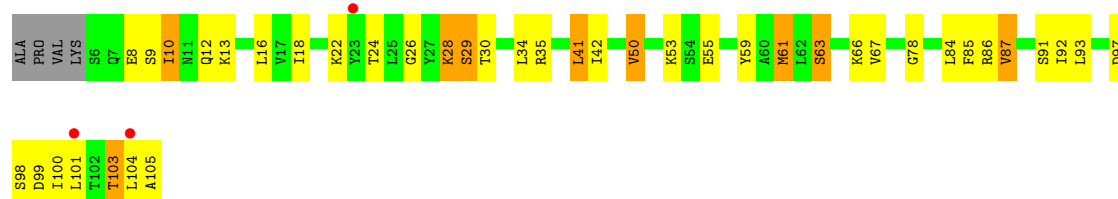


- Molecule 66: 60S ribosomal protein L30

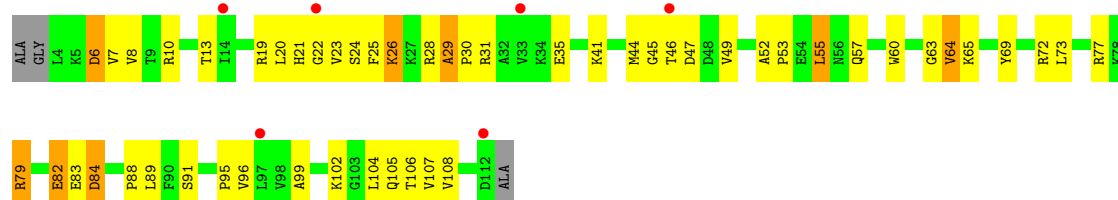




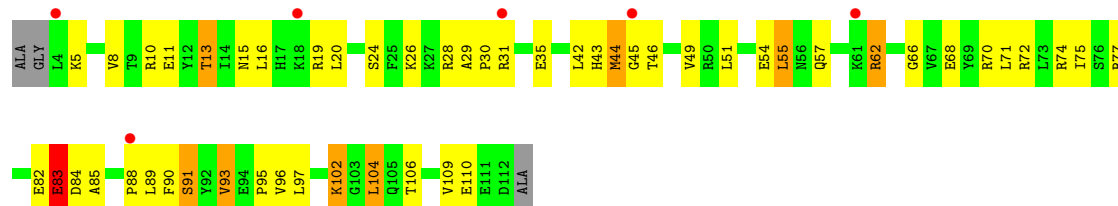
• Molecule 66: 60S ribosomal protein L30



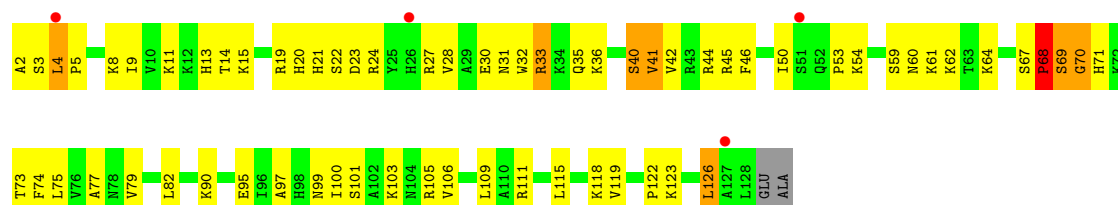
• Molecule 67: 60S ribosomal protein L31-A



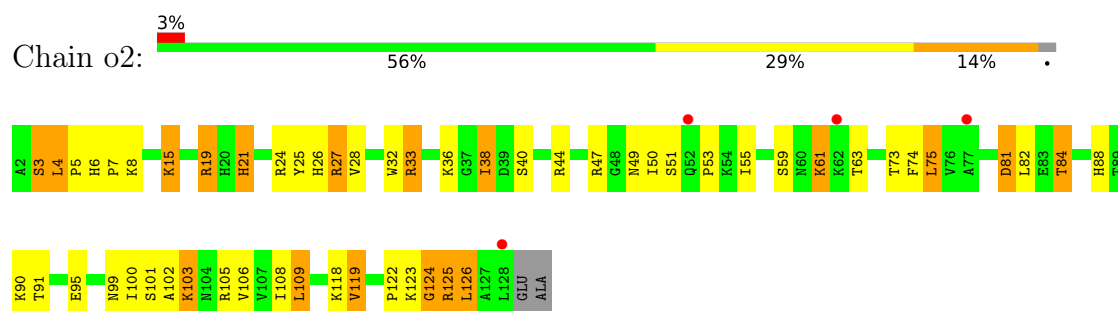
• Molecule 67: 60S ribosomal protein L31-A



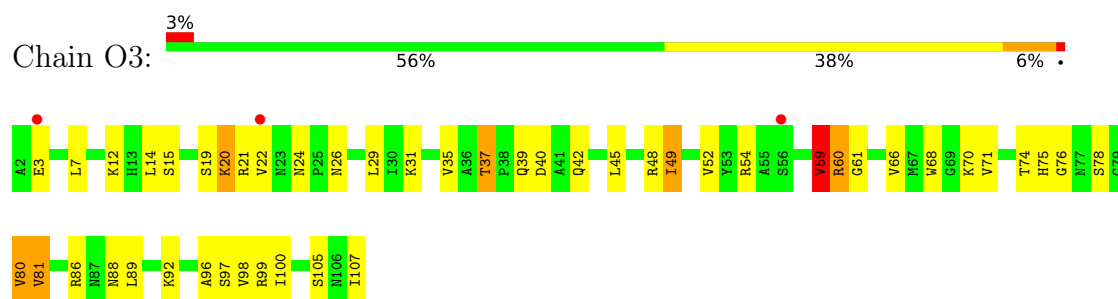
• Molecule 68: 60S ribosomal protein L32



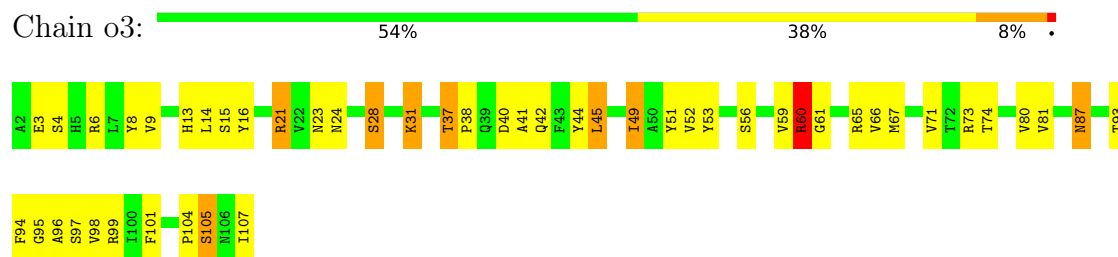
- Molecule 68: 60S ribosomal protein L32



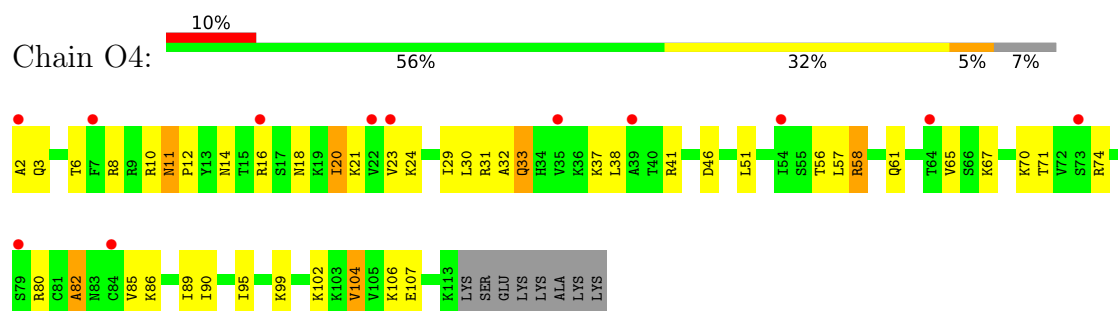
- Molecule 69: 60S ribosomal protein L33-A



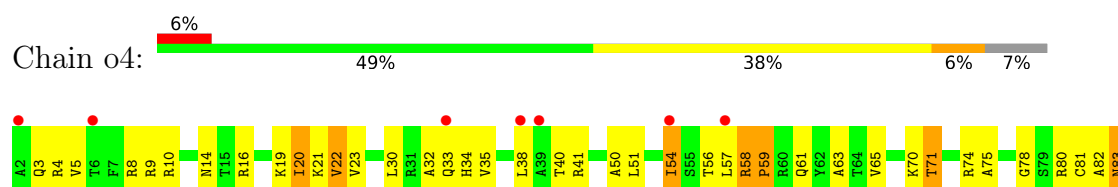
- Molecule 69: 60S ribosomal protein L33-A

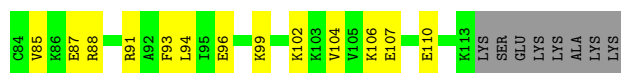


- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A

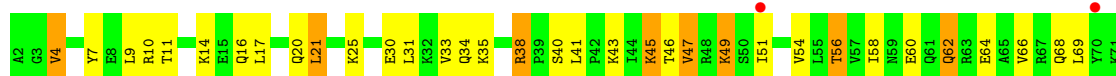




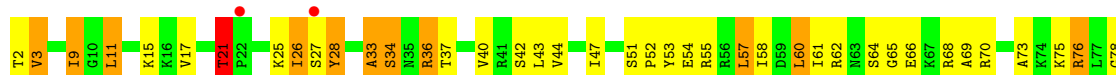
- Molecule 71: 60S ribosomal protein L35-A



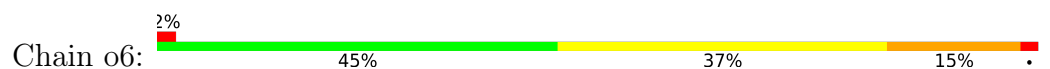
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

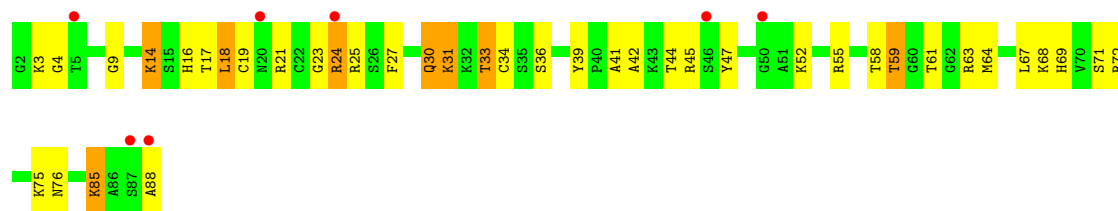


- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A





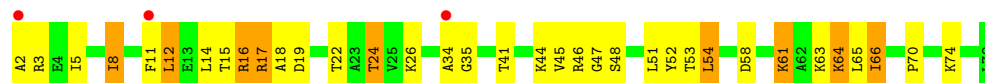
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

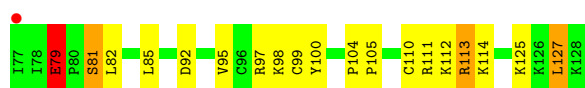


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40

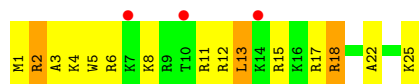




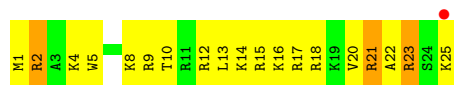
- Molecule 76: Ubiquitin-60S ribosomal protein L40



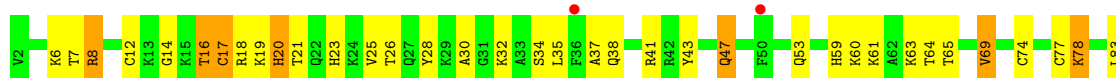
- Molecule 77: 60S ribosomal protein L41-A



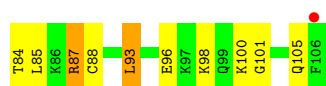
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 82: 60S ribosomal protein P1 alpha/P2 beta

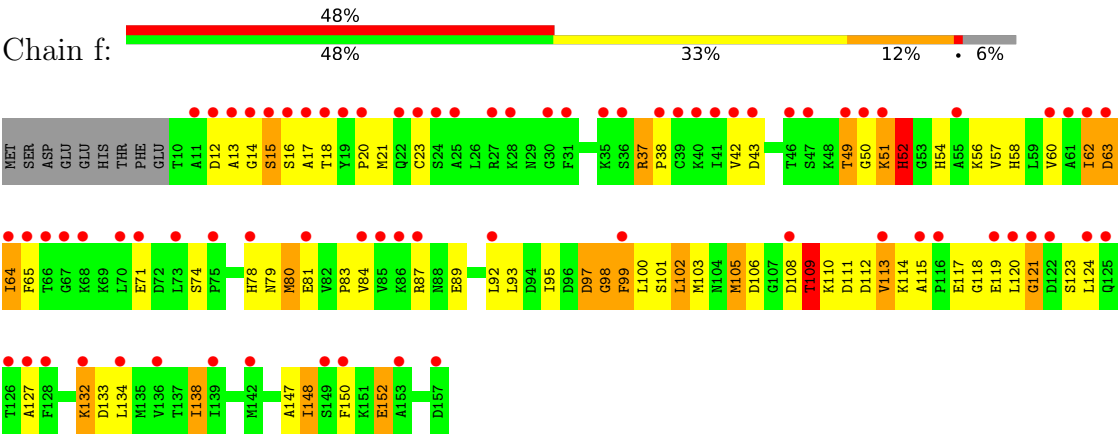
Chain p2:

98%

.



- Molecule 83: Eukaryotic translation initiation factor 5A-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.58Å 287.33Å 303.82Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	99.53 – 3.30 99.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.53-3.30) 99.9 (99.53-3.30)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.310 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	404292	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: 8AN, OHX, CH, SPS, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.21	0/42467	0.39	2/66169 (0.0%)
1	6	0.24	0/42790	0.42	0/66673
2	S0	0.39	0/1617	0.89	7/2215 (0.3%)
2	s0	0.40	0/1623	0.90	2/2222 (0.1%)
3	S1	0.32	0/1735	0.80	3/2335 (0.1%)
3	s1	0.41	0/1748	0.87	7/2352 (0.3%)
4	S2	0.42	0/1665	0.90	6/2263 (0.3%)
4	s2	0.45	0/1665	0.94	6/2263 (0.3%)
5	S3	0.38	0/1759	0.84	4/2368 (0.2%)
5	s3	0.36	0/1759	0.87	6/2368 (0.3%)
6	S4	0.37	0/2109	0.87	4/2839 (0.1%)
6	s4	0.43	0/2109	0.86	4/2839 (0.1%)
7	S5	0.35	0/1629	0.85	2/2202 (0.1%)
7	s5	0.36	0/1629	0.83	4/2202 (0.2%)
8	S6	0.35	0/1823	0.79	0/2439
8	s6	0.40	0/1779	0.83	0/2379
9	S7	0.36	0/1506	0.88	8/2028 (0.4%)
9	s7	0.39	0/1516	0.89	5/2043 (0.2%)
10	S8	0.38	0/1514	0.84	2/2021 (0.1%)
10	s8	0.45	0/1514	0.82	0/2021
11	S9	0.37	0/1519	0.85	5/2035 (0.2%)
11	s9	0.39	0/1519	0.86	4/2035 (0.2%)
12	C0	0.34	0/725	0.71	0/978
12	c0	0.33	0/713	0.82	1/961 (0.1%)
13	C1	0.41	0/1185	0.85	2/1598 (0.1%)
13	c1	0.49	0/1185	0.85	1/1598 (0.1%)
14	C2	0.35	0/819	0.77	0/1109
14	c2	0.31	0/819	0.77	0/1109
15	C3	0.39	0/1215	0.85	3/1638 (0.2%)
15	c3	0.44	0/1215	0.87	2/1638 (0.1%)
16	C4	0.39	0/901	0.89	2/1217 (0.2%)
16	c4	0.39	0/960	0.90	4/1290 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.40	0/988	1.00	8/1327 (0.6%)
17	c5	0.39	0/1030	0.94	4/1384 (0.3%)
18	C6	0.37	0/1125	0.83	3/1510 (0.2%)
18	c6	0.39	0/1131	0.84	0/1518
19	C7	0.42	0/935	0.87	3/1254 (0.2%)
19	c7	0.36	0/914	0.84	0/1224
20	C8	0.37	0/1211	0.79	0/1628
20	c8	0.36	0/1211	0.80	0/1628
21	C9	0.38	0/1130	0.85	2/1517 (0.1%)
21	c9	0.38	0/1130	0.81	0/1517
22	D0	0.40	0/865	0.90	2/1169 (0.2%)
22	d0	0.37	0/892	0.81	0/1205
23	D1	0.38	0/693	0.86	2/935 (0.2%)
23	d1	0.38	0/693	0.84	0/935
24	D2	0.38	0/1038	0.93	4/1395 (0.3%)
24	d2	0.46	0/1038	0.89	2/1395 (0.1%)
25	D3	0.44	0/1139	0.88	4/1518 (0.3%)
25	d3	0.48	0/1139	0.87	1/1518 (0.1%)
26	D4	0.37	0/1087	0.82	0/1449
26	d4	0.40	0/1087	0.90	6/1449 (0.4%)
27	D5	0.39	0/571	0.90	1/768 (0.1%)
27	d5	0.39	0/566	0.89	1/761 (0.1%)
28	D6	0.42	0/782	0.89	3/1047 (0.3%)
28	d6	0.43	0/782	0.85	0/1047
29	D7	0.43	0/620	0.83	0/838
29	d7	0.38	0/620	0.85	0/838
30	D8	0.37	0/499	0.80	0/670
30	d8	0.39	0/499	0.79	0/670
31	D9	0.39	0/452	0.89	3/600 (0.5%)
31	d9	0.38	0/452	0.80	0/600
32	E0	0.39	0/483	0.86	0/643
32	e0	0.40	0/499	1.02	4/665 (0.6%)
33	E1	0.40	0/577	0.89	1/770 (0.1%)
33	e1	0.43	0/619	0.94	4/822 (0.5%)
34	SR	0.35	0/2490	0.78	1/3389 (0.0%)
34	sR	0.32	0/2495	0.73	0/3395
35	SM	0.45	0/925	0.95	4/1240 (0.3%)
35	sM	0.45	0/480	0.93	3/642 (0.5%)
36	1	0.31	0/75394	0.49	2/117545 (0.0%)
36	5	0.33	0/75865	0.50	1/118275 (0.0%)
37	3	0.25	0/2883	0.41	0/4491
37	7	0.31	0/2883	0.47	0/4491
38	4	0.30	0/3746	0.47	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.29	0/3746	0.46	0/5832
39	L2	0.50	0/1948	0.91	2/2617 (0.1%)
39	l2	0.55	0/1946	0.95	2/2614 (0.1%)
40	L3	0.49	0/3146	0.87	3/4228 (0.1%)
40	l3	0.55	0/3146	0.91	6/4228 (0.1%)
41	L4	0.52	0/2800	0.96	9/3790 (0.2%)
41	l4	0.53	0/2800	1.01	16/3790 (0.4%)
42	L5	0.42	0/2425	0.83	2/3271 (0.1%)
42	l5	0.49	0/2408	0.87	1/3248 (0.0%)
43	L6	0.49	0/1260	0.89	2/1694 (0.1%)
43	l6	0.50	0/1269	0.90	3/1705 (0.2%)
44	L7	0.52	0/1821	0.93	4/2451 (0.2%)
44	l7	0.54	0/1828	0.99	13/2461 (0.5%)
45	L8	0.41	0/1836	0.92	8/2481 (0.3%)
45	l8	0.42	0/1796	0.90	6/2431 (0.2%)
46	L9	0.46	0/1539	0.85	0/2073
46	l9	0.52	0/1539	0.87	0/2073
47	M0	0.47	0/1741	0.88	2/2335 (0.1%)
47	m0	0.53	0/1758	0.95	6/2358 (0.3%)
48	M1	0.41	0/1374	0.85	3/1842 (0.2%)
48	m1	0.46	0/1374	0.90	2/1842 (0.1%)
49	M3	0.51	0/1568	0.90	4/2106 (0.2%)
49	m3	0.47	0/1573	0.97	9/2113 (0.4%)
50	M4	0.50	0/1068	0.96	3/1438 (0.2%)
50	m4	0.54	0/1074	0.94	2/1446 (0.1%)
51	M5	0.49	0/1757	0.88	4/2354 (0.2%)
51	m5	0.46	0/1757	0.89	5/2354 (0.2%)
52	M6	0.55	0/1585	0.97	8/2128 (0.4%)
52	m6	0.61	0/1585	1.00	8/2128 (0.4%)
53	M7	0.54	0/1443	0.94	3/1944 (0.2%)
53	m7	0.58	0/1250	0.91	1/1683 (0.1%)
54	M8	0.51	0/1465	1.02	4/1965 (0.2%)
54	m8	0.53	0/1465	0.99	3/1965 (0.2%)
55	M9	0.41	0/1538	0.86	1/2050 (0.0%)
55	m9	0.46	0/1538	0.87	1/2050 (0.0%)
56	N0	0.49	0/1481	0.91	5/1990 (0.3%)
56	n0	0.54	0/1481	0.95	8/1990 (0.4%)
57	N1	0.49	0/1300	0.83	1/1743 (0.1%)
57	n1	0.51	0/1300	0.92	4/1743 (0.2%)
58	N2	0.37	0/812	0.76	0/1099
58	n2	0.36	0/794	0.87	0/1076
59	N3	0.51	0/1018	0.92	1/1369 (0.1%)
59	n3	0.58	0/1018	1.02	3/1369 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.42	0/712	1.13	3/958 (0.3%)
60	n4	0.45	0/1052	0.87	1/1398 (0.1%)
61	N5	0.41	0/979	0.81	0/1321
61	n5	0.44	0/974	0.85	2/1314 (0.2%)
62	N6	0.47	0/1004	0.93	1/1341 (0.1%)
62	n6	0.46	0/1004	0.88	1/1341 (0.1%)
63	N7	0.36	0/1118	0.87	4/1497 (0.3%)
63	n7	0.39	0/1118	0.79	0/1497
64	N8	0.51	0/1204	0.92	1/1612 (0.1%)
64	n8	0.51	0/1204	0.94	4/1612 (0.2%)
65	N9	0.50	0/473	0.93	2/629 (0.3%)
65	n9	0.54	0/473	1.07	1/629 (0.2%)
66	O0	0.38	0/751	0.75	0/1008
66	o0	0.39	0/775	0.83	0/1040
67	O1	0.41	0/890	0.84	2/1196 (0.2%)
67	o1	0.50	0/897	0.87	1/1205 (0.1%)
68	O2	0.54	0/1041	1.04	4/1394 (0.3%)
68	o2	0.55	0/1041	0.96	2/1394 (0.1%)
69	O3	0.57	0/868	0.89	0/1168
69	o3	0.59	0/868	0.88	0/1168
70	O4	0.45	0/890	0.90	2/1189 (0.2%)
70	o4	0.46	0/890	0.95	1/1189 (0.1%)
71	O5	0.46	0/978	0.92	0/1301
71	o5	0.40	0/974	0.86	0/1297
72	O6	0.50	0/778	0.93	2/1034 (0.2%)
72	o6	0.42	0/777	0.82	0/1033
73	O7	0.54	0/696	0.91	1/923 (0.1%)
73	o7	0.52	0/696	0.88	2/923 (0.2%)
74	O8	0.39	0/618	0.85	2/826 (0.2%)
74	o8	0.37	0/614	0.84	0/822
75	O9	0.50	0/443	0.85	0/588
75	o9	0.50	0/443	0.76	0/588
76	Q0	0.51	0/423	0.93	2/562 (0.4%)
76	q0	0.53	0/423	0.78	0/562
77	Q1	0.45	0/234	0.92	1/300 (0.3%)
77	q1	0.55	0/234	0.96	0/300
78	Q2	0.55	0/860	0.91	0/1136
78	q2	0.54	0/860	0.93	1/1136 (0.1%)
79	Q3	0.44	0/701	0.92	1/934 (0.1%)
79	q3	0.52	0/701	0.88	0/934
81	p0	0.32	0/977	0.81	0/1313
83	f	0.52	1/1131 (0.1%)	0.91	2/1522 (0.1%)
84	B	0.31	0/15	0.46	0/20

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
84	C	0.40	0/15	0.70	0/20
All	All	0.37	1/431576 (0.0%)	0.66	379/633602 (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
18	c6	0	1
19	C7	0	1
27	D5	0	1
39	l2	0	1
44	L7	0	1
52	M6	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
83	f	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	f	12	ASP	CA-C	5.52	1.55	1.52

The worst 5 of 379 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	N4	80	ARG	CA-C-N	15.66	139.41	119.84
60	N4	80	ARG	C-N-CA	15.66	139.41	119.84
65	n9	14	ARG	N-CA-C	-9.89	100.48	111.07
54	m8	18	ALA	CA-C-N	-9.52	110.05	120.14
54	m8	18	ALA	C-N-CA	-9.52	110.05	120.14

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
44	L7	157	ASN	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19106	815	0
1	6	38260	0	19252	802	0
2	S0	1577	0	1567	82	0
2	s0	1583	0	1578	77	0
3	S1	1709	0	1784	66	0
3	s1	1722	0	1793	69	0
4	S2	1635	0	1723	78	0
4	s2	1635	0	1723	66	0
5	S3	1734	0	1817	59	0
5	s3	1734	0	1817	68	0
6	S4	2068	0	2154	94	0
6	s4	2068	0	2154	95	0
7	S5	1609	0	1675	63	0
7	s5	1609	0	1675	65	0
8	S6	1799	0	1879	49	0
8	s6	1755	0	1846	72	0
9	S7	1481	0	1572	65	0
9	s7	1491	0	1578	56	0
10	S8	1489	0	1525	64	0
10	s8	1489	0	1525	57	0
11	S9	1494	0	1573	69	0
11	s9	1494	0	1573	88	0
12	C0	773	0	714	34	0
12	c0	762	0	689	25	0
13	C1	1214	0	1237	43	0
13	c1	1168	0	1226	45	0
14	C2	892	0	872	36	0
14	c2	892	0	869	29	0
15	C3	1192	0	1255	43	0
15	c3	1192	0	1255	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C4	891	0	883	43	0
16	c4	949	0	985	52	0
17	C5	977	0	1004	48	0
17	c5	1039	0	1041	40	0
18	C6	1105	0	1166	48	0
18	c6	1111	0	1171	43	0
19	C7	926	0	930	50	0
19	c7	906	0	909	43	0
20	C8	1192	0	1222	59	0
20	c8	1192	0	1222	50	0
21	C9	1112	0	1124	51	0
21	c9	1112	0	1124	44	0
22	D0	855	0	917	42	0
22	d0	882	0	939	33	0
23	D1	684	0	672	40	0
23	d1	684	0	672	37	0
24	D2	1021	0	1060	47	0
24	d2	1021	0	1060	56	0
25	D3	1121	0	1196	58	0
25	d3	1121	0	1196	42	0
26	D4	1073	0	1132	48	0
26	d4	1073	0	1132	45	0
27	D5	563	0	603	25	0
27	d5	558	0	598	29	0
28	D6	769	0	814	45	0
28	d6	769	0	814	40	0
29	D7	610	0	630	14	0
29	d7	610	0	631	27	0
30	D8	497	0	535	28	0
30	d8	497	0	535	16	0
31	D9	442	0	428	20	0
31	d9	442	0	428	13	0
32	E0	475	0	525	12	0
32	e0	491	0	542	19	0
33	E1	566	0	602	26	0
33	e1	608	0	657	24	0
34	SR	2437	0	2386	87	0
34	sR	2442	0	2392	85	1
35	SM	1105	0	959	44	0
35	sM	680	0	542	25	0
36	1	67355	0	33848	1255	1
36	5	67780	0	34065	1218	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	2579	0	1304	64	0
37	7	2579	0	1304	46	0
38	4	3353	0	1695	59	0
38	8	3353	0	1695	71	0
39	L2	1914	0	1981	85	0
39	l2	1912	0	1976	97	0
40	L3	3075	0	3142	140	0
40	l3	3075	0	3142	125	0
41	L4	2748	0	2859	104	0
41	l4	2748	0	2859	133	0
42	L5	2375	0	2325	104	0
42	l5	2359	0	2311	102	0
43	L6	1239	0	1326	49	0
43	l6	1248	0	1339	38	0
44	L7	1784	0	1862	73	0
44	l7	1791	0	1869	73	0
45	L8	1804	0	1875	70	0
45	l8	1764	0	1821	50	0
46	L9	1518	0	1587	78	0
46	l9	1518	0	1587	52	0
47	M0	1705	0	1736	85	0
47	m0	1722	0	1755	77	0
48	M1	1353	0	1383	45	0
48	m1	1353	0	1383	42	0
49	M3	1543	0	1608	76	0
49	m3	1548	0	1613	73	0
50	M4	1053	0	1149	45	0
50	m4	1059	0	1154	46	0
51	M5	1720	0	1779	73	0
51	m5	1720	0	1779	75	0
52	M6	1555	0	1659	64	0
52	m6	1555	0	1659	48	0
53	M7	1420	0	1437	56	0
53	m7	1227	0	1236	57	0
54	M8	1441	0	1543	51	0
54	m8	1441	0	1543	66	0
55	M9	1521	0	1617	62	0
55	m9	1521	0	1617	52	0
56	N0	1445	0	1487	50	0
56	n0	1445	0	1487	55	0
57	N1	1276	0	1323	46	0
57	n1	1276	0	1323	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	N2	796	0	812	26	0
58	n2	778	0	791	17	0
59	N3	1003	0	1048	41	0
59	n3	1003	0	1048	39	0
60	N4	699	0	640	24	0
60	n4	1038	0	1071	36	0
61	N5	964	0	1025	44	0
61	n5	959	0	1023	36	0
62	N6	993	0	1081	40	0
62	n6	993	0	1081	42	0
63	N7	1092	0	1155	58	0
63	n7	1092	0	1155	46	0
64	N8	1173	0	1215	66	0
64	n8	1173	0	1215	53	0
65	N9	462	0	491	19	0
65	n9	462	0	491	18	0
66	O0	743	0	797	26	0
66	o0	767	0	816	28	0
67	O1	876	0	912	35	0
67	o1	883	0	918	28	0
68	O2	1020	0	1090	43	0
68	o2	1020	0	1090	40	0
69	O3	850	0	880	36	0
69	o3	850	0	880	33	0
70	O4	880	0	945	32	0
70	o4	880	0	945	36	0
71	O5	969	0	1078	37	0
71	o5	965	0	1067	59	0
72	O6	771	0	849	39	0
72	o6	770	0	846	35	0
73	O7	681	0	683	35	0
73	o7	681	0	683	19	0
74	O8	612	0	682	20	0
74	o8	608	0	671	22	0
75	O9	436	0	475	18	0
75	o9	436	0	475	22	0
76	Q0	417	0	455	10	0
76	q0	417	0	455	14	0
77	Q1	233	0	284	14	0
77	q1	233	0	284	11	0
78	Q2	847	0	914	28	0
78	q2	847	0	914	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	Q3	694	0	734	29	0
79	q3	694	0	734	28	0
80	m2	750	0	185	10	0
81	p0	1077	0	1012	29	0
82	p1	235	0	53	2	0
82	p2	230	0	52	0	0
83	f	1116	0	1108	49	0
84	B	76	0	49	3	0
84	C	73	0	49	4	0
85	D6	1	0	0	0	0
85	D7	1	0	0	0	0
85	D9	1	0	0	0	0
85	E1	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q0	1	0	0	0	0
85	Q2	1	0	0	0	0
85	Q3	1	0	0	0	0
85	d6	1	0	0	0	0
85	d7	1	0	0	0	0
85	d9	1	0	0	0	0
85	e1	1	0	0	0	0
85	o7	1	0	0	0	0
85	q0	1	0	0	0	0
85	q2	1	0	0	0	0
85	q3	1	0	0	0	0
86	1	23	0	18	3	0
86	B	23	0	18	2	0
87	1	3	0	0	0	0
87	5	5	0	0	0	0
87	B	1	0	0	0	0
87	C	1	0	0	0	0
87	f	2	0	0	0	0
88	1	14	0	0	0	0
88	5	7	0	0	0	0
89	5	2	0	0	0	0
89	f	10	0	0	0	0
All	All	404292	0	298868	9867	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 14.

The worst 5 of 9867 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)
78:Q2:17:CYS:SG	78:Q2:77:CYS:SG	2.32	1.28
83:f:110:LYS:NZ	83:f:112:ASP:OD1	1.85	1.09
83:f:99:PHE:HA	83:f:100:LEU:HB2	1.45	0.98
1:6:514:G:HO2'	1:6:515:A:H8	1.13	0.97
1:6:104:A:H61	1:6:308:C:H5'	1.29	0.96

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)
36:1:3153:U:O4	34:sR:79:TYR:OH[2_656]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	151 (74%)	30 (15%)	23 (11%)	0	2
2	s0	204/251 (81%)	164 (80%)	25 (12%)	15 (7%)	1	6
3	S1	212/254 (84%)	152 (72%)	38 (18%)	22 (10%)	0	2
3	s1	214/254 (84%)	168 (78%)	33 (15%)	13 (6%)	1	9
4	S2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1	8
4	s2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1	8
5	S3	221/239 (92%)	187 (85%)	26 (12%)	8 (4%)	2	17
5	s3	221/239 (92%)	176 (80%)	35 (16%)	10 (4%)	2	13
6	S4	258/260 (99%)	202 (78%)	46 (18%)	10 (4%)	2	16
6	s4	258/260 (99%)	189 (73%)	53 (20%)	16 (6%)	1	9
7	S5	204/224 (91%)	155 (76%)	37 (18%)	12 (6%)	1	9
7	s5	204/224 (91%)	160 (78%)	29 (14%)	15 (7%)	1	6
8	S6	224/236 (95%)	193 (86%)	22 (10%)	9 (4%)	2	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	s6	216/236 (92%)	182 (84%)	22 (10%)	12 (6%)	1	9
9	S7	182/189 (96%)	134 (74%)	27 (15%)	21 (12%)	0	2
9	s7	184/189 (97%)	152 (83%)	20 (11%)	12 (6%)	1	8
10	S8	184/200 (92%)	151 (82%)	24 (13%)	9 (5%)	1	12
10	s8	184/200 (92%)	157 (85%)	20 (11%)	7 (4%)	2	16
11	S9	183/196 (93%)	149 (81%)	23 (13%)	11 (6%)	1	9
11	s9	183/196 (93%)	147 (80%)	27 (15%)	9 (5%)	1	12
12	C0	82/96 (85%)	71 (87%)	8 (10%)	3 (4%)	2	17
12	c0	82/96 (85%)	56 (68%)	16 (20%)	10 (12%)	0	1
13	C1	143/155 (92%)	116 (81%)	18 (13%)	9 (6%)	1	8
13	c1	143/155 (92%)	115 (80%)	21 (15%)	7 (5%)	1	12
14	C2	107/142 (75%)	70 (65%)	27 (25%)	10 (9%)	0	3
14	c2	107/142 (75%)	75 (70%)	22 (21%)	10 (9%)	0	3
15	C3	148/150 (99%)	124 (84%)	20 (14%)	4 (3%)	4	22
15	c3	148/150 (99%)	116 (78%)	23 (16%)	9 (6%)	1	9
16	C4	125/136 (92%)	81 (65%)	33 (26%)	11 (9%)	0	4
16	c4	126/136 (93%)	96 (76%)	15 (12%)	15 (12%)	0	1
17	C5	121/141 (86%)	95 (78%)	12 (10%)	14 (12%)	0	2
17	c5	128/141 (91%)	98 (77%)	19 (15%)	11 (9%)	0	4
18	C6	139/142 (98%)	116 (84%)	14 (10%)	9 (6%)	1	8
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	1	8
19	C7	116/136 (85%)	82 (71%)	23 (20%)	11 (10%)	0	3
19	c7	113/136 (83%)	93 (82%)	13 (12%)	7 (6%)	1	9
20	C8	143/145 (99%)	116 (81%)	17 (12%)	10 (7%)	1	7
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	1	12
21	C9	141/143 (99%)	115 (82%)	18 (13%)	8 (6%)	1	9
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	2	14
22	D0	105/120 (88%)	89 (85%)	9 (9%)	7 (7%)	1	7
22	d0	108/120 (90%)	89 (82%)	14 (13%)	5 (5%)	2	13
23	D1	85/87 (98%)	66 (78%)	11 (13%)	8 (9%)	0	3
23	d1	85/87 (98%)	63 (74%)	17 (20%)	5 (6%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	D2	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	24
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	4	24
25	D3	142/144 (99%)	109 (77%)	21 (15%)	12 (8%)	0	4
25	d3	142/144 (99%)	117 (82%)	20 (14%)	5 (4%)	3	18
26	D4	132/134 (98%)	109 (83%)	13 (10%)	10 (8%)	1	6
26	d4	132/134 (98%)	110 (83%)	15 (11%)	7 (5%)	1	10
27	D5	68/107 (64%)	48 (71%)	13 (19%)	7 (10%)	0	2
27	d5	67/107 (63%)	51 (76%)	15 (22%)	1 (2%)	8	32
28	D6	95/97 (98%)	56 (59%)	21 (22%)	18 (19%)	0	0
28	d6	95/97 (98%)	66 (70%)	20 (21%)	9 (10%)	0	3
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	2	16
29	d7	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	1	11
30	D8	61/66 (92%)	50 (82%)	9 (15%)	2 (3%)	3	19
30	d8	61/66 (92%)	47 (77%)	11 (18%)	3 (5%)	1	12
31	D9	51/55 (93%)	39 (76%)	9 (18%)	3 (6%)	1	9
31	d9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	2	16
32	E0	58/62 (94%)	46 (79%)	10 (17%)	2 (3%)	3	18
32	e0	60/62 (97%)	40 (67%)	12 (20%)	8 (13%)	0	1
33	E1	69/76 (91%)	35 (51%)	17 (25%)	17 (25%)	0	0
33	e1	74/76 (97%)	36 (49%)	21 (28%)	17 (23%)	0	0
34	SR	316/318 (99%)	263 (83%)	36 (11%)	17 (5%)	1	10
34	sR	316/318 (99%)	252 (80%)	53 (17%)	11 (4%)	3	18
35	SM	120/273 (44%)	91 (76%)	18 (15%)	11 (9%)	0	3
35	sM	61/273 (22%)	42 (69%)	11 (18%)	8 (13%)	0	1
39	L2	250/253 (99%)	213 (85%)	27 (11%)	10 (4%)	2	15
39	l2	250/253 (99%)	205 (82%)	30 (12%)	15 (6%)	1	9
40	L3	384/386 (100%)	316 (82%)	49 (13%)	19 (5%)	1	12
40	l3	384/386 (100%)	330 (86%)	39 (10%)	15 (4%)	2	16
41	L4	359/361 (99%)	291 (81%)	46 (13%)	22 (6%)	1	9
41	l4	359/361 (99%)	296 (82%)	43 (12%)	20 (6%)	1	9
42	L5	294/296 (99%)	232 (79%)	44 (15%)	18 (6%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	248 (85%)	38 (13%)	6 (2%)	5	26
43	L6	152/175 (87%)	122 (80%)	27 (18%)	3 (2%)	6	27
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	4	23
44	L7	220/243 (90%)	185 (84%)	24 (11%)	11 (5%)	1	11
44	l7	221/243 (91%)	192 (87%)	21 (10%)	8 (4%)	2	17
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	2	12
45	l8	229/255 (90%)	174 (76%)	40 (18%)	15 (7%)	1	7
46	L9	189/191 (99%)	145 (77%)	29 (15%)	15 (8%)	1	5
46	l9	189/191 (99%)	158 (84%)	24 (13%)	7 (4%)	2	17
47	M0	207/220 (94%)	161 (78%)	37 (18%)	9 (4%)	2	14
47	m0	209/220 (95%)	169 (81%)	29 (14%)	11 (5%)	1	10
48	M1	167/173 (96%)	128 (77%)	27 (16%)	12 (7%)	1	6
48	m1	167/173 (96%)	145 (87%)	9 (5%)	13 (8%)	1	5
49	M3	191/198 (96%)	153 (80%)	30 (16%)	8 (4%)	2	14
49	m3	192/198 (97%)	152 (79%)	27 (14%)	13 (7%)	1	7
50	M4	134/137 (98%)	116 (87%)	12 (9%)	6 (4%)	2	13
50	m4	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	5	26
51	M5	201/203 (99%)	175 (87%)	20 (10%)	6 (3%)	3	20
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	4	23
52	M6	195/198 (98%)	174 (89%)	12 (6%)	9 (5%)	2	13
52	m6	195/198 (98%)	172 (88%)	20 (10%)	3 (2%)	8	32
53	M7	181/183 (99%)	151 (83%)	25 (14%)	5 (3%)	4	21
53	m7	153/183 (84%)	137 (90%)	14 (9%)	2 (1%)	9	35
54	M8	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	2	16
54	m8	183/185 (99%)	154 (84%)	21 (12%)	8 (4%)	2	13
55	M9	186/188 (99%)	164 (88%)	17 (9%)	5 (3%)	4	22
55	m9	186/188 (99%)	164 (88%)	20 (11%)	2 (1%)	11	39
56	N0	170/172 (99%)	151 (89%)	15 (9%)	4 (2%)	4	24
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	10	37
57	N1	157/159 (99%)	131 (83%)	20 (13%)	6 (4%)	2	16
57	n1	157/159 (99%)	138 (88%)	16 (10%)	3 (2%)	6	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	N2	98/120 (82%)	73 (74%)	20 (20%)	5 (5%)	1	11
58	n2	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	3	20
59	N3	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	2	17
59	n3	134/136 (98%)	122 (91%)	4 (3%)	8 (6%)	1	9
60	N4	96/155 (62%)	66 (69%)	21 (22%)	9 (9%)	0	3
60	n4	133/155 (86%)	102 (77%)	23 (17%)	8 (6%)	1	9
61	N5	119/141 (84%)	103 (87%)	12 (10%)	4 (3%)	3	18
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	0	4
62	N6	124/126 (98%)	104 (84%)	19 (15%)	1 (1%)	16	45
62	n6	124/126 (98%)	102 (82%)	17 (14%)	5 (4%)	2	15
63	N7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	7
63	n7	133/135 (98%)	100 (75%)	26 (20%)	7 (5%)	1	10
64	N8	146/148 (99%)	113 (77%)	26 (18%)	7 (5%)	2	12
64	n8	146/148 (99%)	110 (75%)	25 (17%)	11 (8%)	1	6
65	N9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	2	17
65	n9	56/58 (97%)	41 (73%)	9 (16%)	6 (11%)	0	2
66	O0	95/104 (91%)	83 (87%)	11 (12%)	1 (1%)	11	39
66	o0	98/104 (94%)	86 (88%)	10 (10%)	2 (2%)	6	27
67	O1	107/112 (96%)	96 (90%)	6 (6%)	5 (5%)	2	12
67	o1	107/112 (96%)	85 (79%)	15 (14%)	7 (6%)	1	8
68	O2	125/129 (97%)	110 (88%)	11 (9%)	4 (3%)	3	19
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	3	19
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	6	28
69	o3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	6	28
70	O4	110/120 (92%)	96 (87%)	11 (10%)	3 (3%)	4	22
70	o4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	2	17
71	O5	117/119 (98%)	95 (81%)	12 (10%)	10 (8%)	0	4
71	o5	117/119 (98%)	94 (80%)	21 (18%)	2 (2%)	7	30
72	O6	97/99 (98%)	76 (78%)	12 (12%)	9 (9%)	0	3
72	o6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	2
73	O7	85/87 (98%)	69 (81%)	14 (16%)	2 (2%)	4	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	o7	85/87 (98%)	70 (82%)	14 (16%)	1 (1%)	10	37
74	O8	75/77 (97%)	66 (88%)	7 (9%)	2 (3%)	4	22
74	o8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	7
75	O9	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	1	8
75	o9	48/50 (96%)	39 (81%)	9 (19%)	0	100	100
76	Q0	50/52 (96%)	43 (86%)	6 (12%)	1 (2%)	6	27
76	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	27
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	14
78	Q2	103/105 (98%)	85 (82%)	13 (13%)	5 (5%)	1	12
78	q2	103/105 (98%)	88 (85%)	9 (9%)	6 (6%)	1	9
79	Q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	1	7
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	11	39
81	p0	117/311 (38%)	97 (83%)	14 (12%)	6 (5%)	1	11
83	f	146/157 (93%)	91 (62%)	35 (24%)	20 (14%)	0	1
All	All	22316/24284 (92%)	18108 (81%)	2992 (13%)	1216 (5%)	1	10

5 of 1216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	95	ALA
2	S0	158	VAL
2	S0	190	ASP
2	S0	192	THR
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%)	143 (87%)	21 (13%)	4	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	s0	165/209 (79%)	141 (86%)	24 (14%)	3	14
3	S1	191/223 (86%)	165 (86%)	26 (14%)	3	16
3	s1	192/223 (86%)	165 (86%)	27 (14%)	3	14
4	S2	176/204 (86%)	149 (85%)	27 (15%)	3	13
4	s2	176/204 (86%)	134 (76%)	42 (24%)	1	4
5	S3	182/194 (94%)	152 (84%)	30 (16%)	2	11
5	s3	182/194 (94%)	157 (86%)	25 (14%)	3	16
6	S4	221/221 (100%)	193 (87%)	28 (13%)	4	18
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	10
7	S5	173/190 (91%)	157 (91%)	16 (9%)	8	30
7	s5	173/190 (91%)	143 (83%)	30 (17%)	2	9
8	S6	188/201 (94%)	163 (87%)	25 (13%)	4	17
8	s6	187/201 (93%)	160 (86%)	27 (14%)	3	14
9	S7	165/169 (98%)	145 (88%)	20 (12%)	5	20
9	s7	165/169 (98%)	150 (91%)	15 (9%)	9	31
10	S8	150/161 (93%)	133 (89%)	17 (11%)	5	21
10	s8	150/161 (93%)	129 (86%)	21 (14%)	3	15
11	S9	158/165 (96%)	129 (82%)	29 (18%)	1	7
11	s9	158/165 (96%)	132 (84%)	26 (16%)	2	11
12	C0	77/77 (100%)	70 (91%)	7 (9%)	9	31
12	c0	73/77 (95%)	63 (86%)	10 (14%)	3	16
13	C1	129/129 (100%)	117 (91%)	12 (9%)	8	30
13	c1	129/129 (100%)	109 (84%)	20 (16%)	2	12
14	C2	88/106 (83%)	71 (81%)	17 (19%)	1	6
14	c2	88/106 (83%)	77 (88%)	11 (12%)	4	19
15	C3	127/127 (100%)	108 (85%)	19 (15%)	3	13
15	c3	127/127 (100%)	107 (84%)	20 (16%)	2	12
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1	5
16	c4	97/104 (93%)	79 (81%)	18 (19%)	1	7
17	C5	101/113 (89%)	84 (83%)	17 (17%)	2	11
17	c5	103/113 (91%)	85 (82%)	18 (18%)	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	101 (86%)	16 (14%)	3	16
18	c6	118/118 (100%)	104 (88%)	14 (12%)	5	20
19	C7	94/124 (76%)	77 (82%)	17 (18%)	2	8
19	c7	92/124 (74%)	82 (89%)	10 (11%)	6	23
20	C8	128/128 (100%)	105 (82%)	23 (18%)	2	8
20	c8	128/128 (100%)	109 (85%)	19 (15%)	3	13
21	C9	115/115 (100%)	96 (84%)	19 (16%)	2	11
21	c9	115/115 (100%)	99 (86%)	16 (14%)	3	15
22	D0	100/113 (88%)	87 (87%)	13 (13%)	4	17
22	d0	103/113 (91%)	88 (85%)	15 (15%)	3	14
23	D1	74/74 (100%)	66 (89%)	8 (11%)	6	23
23	d1	74/74 (100%)	69 (93%)	5 (7%)	14	42
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	7
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	18
25	D3	119/119 (100%)	104 (87%)	15 (13%)	4	18
25	d3	119/119 (100%)	105 (88%)	14 (12%)	5	20
26	D4	112/112 (100%)	101 (90%)	11 (10%)	7	28
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4	19
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	5
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	6
28	D6	83/83 (100%)	71 (86%)	12 (14%)	3	14
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	12
29	D7	70/70 (100%)	62 (89%)	8 (11%)	5	21
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	10
30	D8	56/59 (95%)	48 (86%)	8 (14%)	3	14
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	8
31	D9	47/48 (98%)	40 (85%)	7 (15%)	3	13
31	d9	47/48 (98%)	38 (81%)	9 (19%)	1	7
32	E0	51/53 (96%)	46 (90%)	5 (10%)	7	28
32	e0	53/53 (100%)	38 (72%)	15 (28%)	0	2
33	E1	62/66 (94%)	48 (77%)	14 (23%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e1	66/66 (100%)	52 (79%)	14 (21%)	1	5
34	SR	259/261 (99%)	228 (88%)	31 (12%)	5	20
34	sR	260/261 (100%)	239 (92%)	21 (8%)	11	36
35	SM	97/183 (53%)	82 (84%)	15 (16%)	2	12
35	sM	54/183 (30%)	46 (85%)	8 (15%)	3	13
39	L2	193/195 (99%)	162 (84%)	31 (16%)	2	12
39	l2	192/195 (98%)	158 (82%)	34 (18%)	2	8
40	L3	319/322 (99%)	263 (82%)	56 (18%)	2	9
40	l3	319/322 (99%)	253 (79%)	66 (21%)	1	6
41	L4	288/288 (100%)	244 (85%)	44 (15%)	3	13
41	l4	288/288 (100%)	236 (82%)	52 (18%)	2	8
42	L5	244/244 (100%)	209 (86%)	35 (14%)	3	14
42	l5	243/244 (100%)	194 (80%)	49 (20%)	1	6
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	14
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	8
44	L7	186/204 (91%)	163 (88%)	23 (12%)	4	19
44	l7	187/204 (92%)	162 (87%)	25 (13%)	4	16
45	L8	187/207 (90%)	163 (87%)	24 (13%)	4	18
45	l8	177/207 (86%)	151 (85%)	26 (15%)	3	14
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	5
46	l9	171/171 (100%)	141 (82%)	30 (18%)	2	9
47	M0	177/186 (95%)	146 (82%)	31 (18%)	2	9
47	m0	179/186 (96%)	146 (82%)	33 (18%)	1	7
48	M1	147/150 (98%)	119 (81%)	28 (19%)	1	7
48	m1	147/150 (98%)	123 (84%)	24 (16%)	2	11
49	M3	154/158 (98%)	132 (86%)	22 (14%)	3	14
49	m3	154/158 (98%)	128 (83%)	26 (17%)	2	10
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	11
50	m4	108/108 (100%)	89 (82%)	19 (18%)	2	9
51	M5	175/175 (100%)	148 (85%)	27 (15%)	2	12
51	m5	175/175 (100%)	152 (87%)	23 (13%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	M6	160/161 (99%)	132 (82%)	28 (18%)	2	9
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	9
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	6
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	9
54	M8	150/150 (100%)	130 (87%)	20 (13%)	4	17
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	6
55	M9	153/153 (100%)	134 (88%)	19 (12%)	4	19
55	m9	153/153 (100%)	130 (85%)	23 (15%)	3	13
56	N0	156/156 (100%)	132 (85%)	24 (15%)	2	12
56	n0	156/156 (100%)	134 (86%)	22 (14%)	3	14
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	4
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	6
58	N2	87/106 (82%)	78 (90%)	9 (10%)	7	25
58	n2	85/106 (80%)	74 (87%)	11 (13%)	4	17
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	12
59	n3	104/104 (100%)	86 (83%)	18 (17%)	2	9
60	N4	57/129 (44%)	53 (93%)	4 (7%)	14	41
60	n4	100/129 (78%)	94 (94%)	6 (6%)	17	46
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	5
61	n5	104/117 (89%)	87 (84%)	17 (16%)	2	11
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	5
62	n6	109/109 (100%)	89 (82%)	20 (18%)	2	7
63	N7	115/115 (100%)	98 (85%)	17 (15%)	3	13
63	n7	115/115 (100%)	97 (84%)	18 (16%)	2	12
64	N8	118/118 (100%)	103 (87%)	15 (13%)	4	18
64	n8	118/118 (100%)	98 (83%)	20 (17%)	2	10
65	N9	46/46 (100%)	40 (87%)	6 (13%)	4	17
65	n9	46/46 (100%)	39 (85%)	7 (15%)	3	13
66	O0	81/87 (93%)	66 (82%)	15 (18%)	1	7
66	o0	84/87 (97%)	72 (86%)	12 (14%)	3	14
67	O1	92/96 (96%)	79 (86%)	13 (14%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	7
68	O2	109/110 (99%)	94 (86%)	15 (14%)	3	15
68	o2	109/110 (99%)	83 (76%)	26 (24%)	1	4
69	O3	90/90 (100%)	72 (80%)	18 (20%)	1	6
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	8
70	O4	95/102 (93%)	82 (86%)	13 (14%)	3	16
70	o4	95/102 (93%)	81 (85%)	14 (15%)	3	14
71	O5	104/104 (100%)	94 (90%)	10 (10%)	8	29
71	o5	103/104 (99%)	86 (84%)	17 (16%)	2	11
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	5
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	2
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2	12
73	o7	70/70 (100%)	61 (87%)	9 (13%)	4	17
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	5
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3	13
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	17
75	o9	45/45 (100%)	41 (91%)	4 (9%)	9	32
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	10
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4	17
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
79	q3	71/71 (100%)	60 (84%)	11 (16%)	2	12
81	p0	105/232 (45%)	94 (90%)	11 (10%)	6	25
83	f	124/133 (93%)	102 (82%)	22 (18%)	2	8
All	All	18849/20177 (93%)	15893 (84%)	2956 (16%)	2	12

5 of 2956 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	c9	135	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	l8	134	TYR
26	d4	40	LEU
21	c9	131	ASP
40	l3	84	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
20	c8	25	ASN
46	l9	58	HIS
25	d3	22	ASN
40	l3	211	GLN
50	m4	59	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	456 (25%)	40 (2%)
1	6	1791/1800 (99%)	447 (24%)	29 (1%)
36	1	3145/3396 (92%)	677 (21%)	53 (1%)
36	5	3163/3396 (93%)	651 (20%)	52 (1%)
37	3	120/121 (99%)	11 (9%)	0
37	7	120/121 (99%)	13 (10%)	0
38	4	157/158 (99%)	32 (20%)	3 (1%)
38	8	157/158 (99%)	34 (21%)	0
All	All	10430/10950 (95%)	2321 (22%)	177 (1%)

5 of 2321 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	6	G
1	2	17	C
1	2	23	G

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	6	1097	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	5	1331	U
1	6	1481	C
36	5	916	G
36	5	1816	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 28 are monoatomic - leaving 5 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
86	SPS	1	3401	-	20,23,23	3.57	14 (70%)	24,30,30	2.66	9 (37%)
86	SPS	B	3401	87	20,23,23	3.57	13 (65%)	24,30,30	2.39	11 (45%)
88	OHX	5	3406	-	0,6,6	-	-	-	-	-
88	OHX	1	3405	-	0,6,6	-	-	-	-	-
88	OHX	1	3406	-	0,6,6	-	-	-	-	-

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
86	SPS	B	3401	87	-	3/15/18/18	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPS	1	3401	-	-	3/15/18/18	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	3401	SPS	C9-C10	-8.24	1.31	1.48
86	B	3401	SPS	C9-C10	-7.97	1.31	1.48
86	B	3401	SPS	C9-C8	6.68	1.53	1.33
86	1	3401	SPS	C9-C8	6.42	1.52	1.33
86	B	3401	SPS	O13-C13	-5.45	1.19	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	3401	SPS	C7-C5-N4	6.16	120.77	113.45
86	1	3401	SPS	C7-C5-C6	-5.75	118.29	126.69
86	1	3401	SPS	C5-N4-C3	-4.59	120.13	123.71
86	B	3401	SPS	C7-C5-C6	-4.41	120.25	126.69
86	B	3401	SPS	C18-S17-C16	3.98	111.12	100.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	B	3401	SPS	N11-C12-C13-O13
86	1	3401	SPS	C14-C12-C13-O13
86	B	3401	SPS	C14-C12-C13-O13
86	1	3401	SPS	N11-C12-C13-O13
86	B	3401	SPS	C5-C6-C8-C9

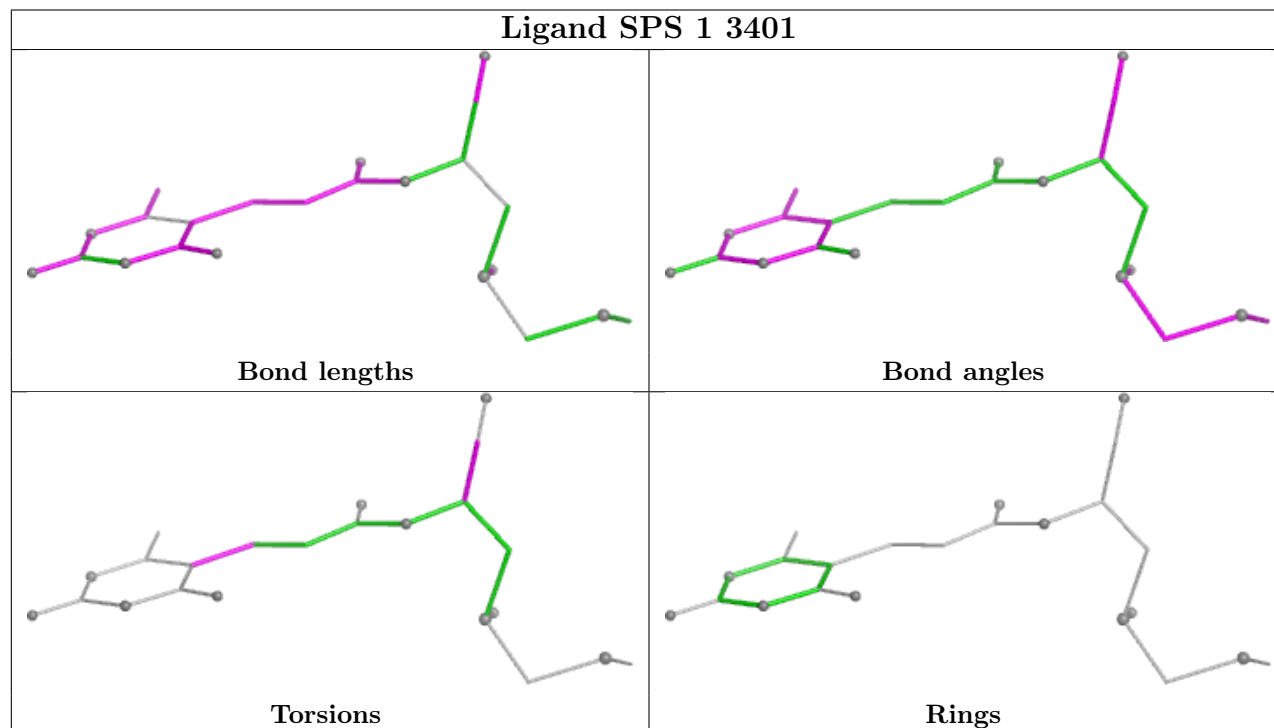
There are no ring outliers.

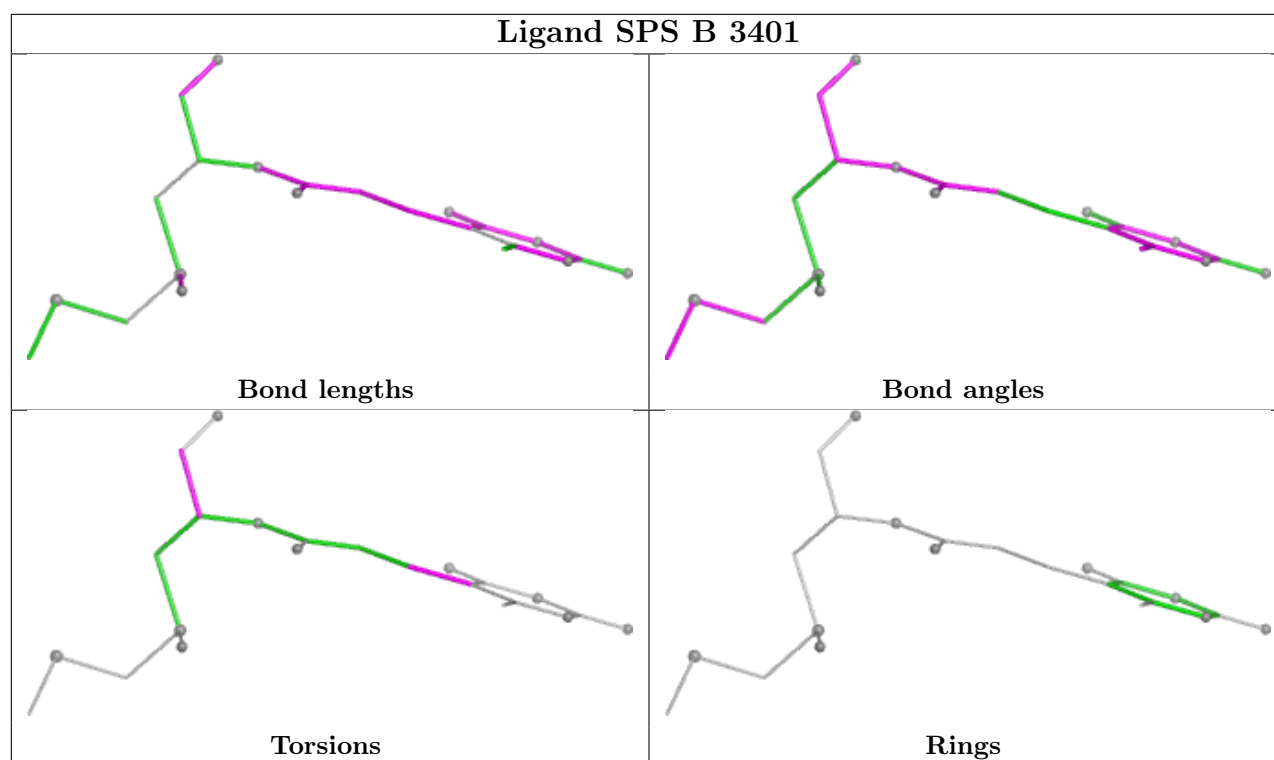
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3401	SPS	3	0
86	B	3401	SPS	2	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](#)

10 such 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	$\# Z > 2$
84	CH	B	75	84,87	16,21,22	0.73	0	20,30,33	1.91	2 (10%)
84	CH	C	74	84	16,18,22	0.92	1 (6%)	20,26,33	1.75	2 (10%)
84	CH	C	75	84,87	16,21,22	0.96	2 (12%)	20,30,33	1.91	2 (10%)
84	8AN	C	76	84,87	22,24,25	1.48	4 (18%)	26,35,38	2.31	9 (34%)
84	CH	B	74	84	16,21,22	1.02	1 (6%)	20,30,33	1.81	2 (10%)
84	8AN	B	76	84,87	22,24,25	1.49	3 (13%)	26,35,38	2.32	9 (34%)

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
84	CH	B	75	84,87	-	0/5/25/26	0/2/2/2
84	CH	C	74	84	-	2/4/22/26	0/2/2/2
84	CH	C	75	84,87	-	1/5/25/26	0/2/2/2
84	8AN	C	76	84,87	-	3/7/25/26	0/3/3/3
84	CH	B	74	84	-	0/5/25/26	0/2/2/2
84	8AN	B	76	84,87	-	3/7/25/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	B	76	8AN	C5-C4	4.72	1.47	1.39
84	C	76	8AN	C5-C4	4.34	1.47	1.39
84	B	74	CH	C4-N3	-2.99	1.33	1.37
84	C	74	CH	C4-N3	-2.79	1.33	1.37
84	B	76	8AN	C5-C6	2.62	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	B	74	CH	C5-C4-N3	7.27	122.18	118.04
84	C	75	CH	C5-C4-N3	7.25	122.17	118.04
84	C	76	8AN	C5-C4-N3	-6.33	118.50	126.75
84	B	76	8AN	C5-C4-N3	-6.19	118.67	126.75
84	B	75	CH	C5-C4-N3	6.07	121.50	118.04

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	C	74	CH	C3'-C4'-C5'-O5'
84	C	74	CH	O4'-C4'-C5'-O5'
84	C	76	8AN	C3'-C4'-C5'-O5'
84	B	76	8AN	C3'-C4'-C5'-O5'
84	C	76	8AN	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	B	75	CH	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	C	74	CH	3	0
84	C	75	CH	1	0
84	B	74	CH	1	0
84	B	76	8AN	1	0

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
80	m2	2
35	sM	1
35	SM	1
12	c0	1
36	5	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	38.68
1	SM	141:ALA	C	151:UNK	N	26.53
1	c0	84:UNK	C	87:UNK	N	8.84
1	2	1716:C	O3'	1717:G	P	5.83
1	5	2437:G	O3'	2438:A	P	4.00

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%)	0.42	49 (2%) 55 36	41, 98, 170, 210	1 (0%)
1	6	1795/1800 (99%)	0.25	35 (1%) 66 48	34, 86, 157, 204	1 (0%)
2	S0	206/251 (82%)	1.09	29 (14%) 6 5	100, 112, 123, 128	0
2	s0	206/251 (82%)	0.78	14 (6%) 23 16	80, 97, 111, 117	0
3	S1	214/254 (84%)	1.24	45 (21%) 2 2	110, 145, 169, 175	0
3	s1	216/254 (85%)	0.94	23 (10%) 11 9	80, 96, 114, 123	0
4	S2	217/253 (85%)	1.24	36 (16%) 4 4	83, 96, 109, 113	0
4	s2	217/253 (85%)	0.88	22 (10%) 12 10	68, 79, 93, 108	0
5	S3	223/239 (93%)	1.07	24 (10%) 11 9	91, 100, 123, 128	0
5	s3	223/239 (93%)	1.11	31 (13%) 6 5	86, 112, 131, 137	0
6	S4	260/260 (100%)	1.35	53 (20%) 3 2	77, 99, 107, 124	0
6	s4	260/260 (100%)	0.95	22 (8%) 16 13	60, 82, 92, 119	0
7	S5	206/224 (91%)	1.43	44 (21%) 2 2	104, 124, 131, 134	0
7	s5	206/224 (91%)	1.13	28 (13%) 7 6	87, 108, 123, 130	0
8	S6	226/236 (95%)	1.40	50 (22%) 2 2	77, 105, 126, 132	0
8	s6	218/236 (92%)	1.05	29 (13%) 7 6	60, 89, 106, 114	0
9	S7	184/189 (97%)	1.07	21 (11%) 10 8	102, 121, 136, 142	0
9	s7	186/189 (98%)	0.81	14 (7%) 20 15	77, 104, 130, 134	0
10	S8	188/200 (94%)	0.94	22 (11%) 9 8	70, 86, 119, 129	0
10	s8	188/200 (94%)	0.83	18 (9%) 13 11	56, 73, 113, 130	0
11	S9	185/196 (94%)	1.03	16 (8%) 16 12	89, 106, 130, 141	0
11	s9	185/196 (94%)	0.79	13 (7%) 22 15	71, 88, 115, 126	0
12	C0	83/96 (86%)	0.81	6 (7%) 21 15	94, 112, 122, 126	0
12	c0	83/96 (86%)	1.50	20 (24%) 2 1	103, 131, 145, 149	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	144/155 (92%)	1.01	11 (7%) 20 14	73, 83, 101, 113	0
13	c1	144/155 (92%)	0.93	16 (11%) 10 9	59, 70, 91, 113	0
14	C2	108/142 (76%)	1.21	20 (18%) 3 3	137, 145, 150, 152	0
14	c2	108/142 (76%)	1.48	32 (29%) 1 1	167, 183, 196, 199	0
15	C3	150/150 (100%)	1.12	17 (11%) 10 8	82, 95, 111, 115	0
15	c3	150/150 (100%)	0.78	14 (9%) 14 11	66, 79, 95, 100	0
16	C4	127/136 (93%)	1.36	27 (21%) 2 2	84, 142, 156, 161	0
16	c4	128/136 (94%)	0.94	13 (10%) 12 10	67, 101, 113, 116	0
17	C5	122/141 (86%)	1.12	12 (9%) 13 10	88, 99, 111, 117	0
17	c5	129/141 (91%)	1.14	21 (16%) 4 4	86, 103, 113, 119	0
18	C6	141/142 (99%)	1.53	39 (27%) 1 1	91, 112, 117, 120	0
18	c6	142/142 (100%)	1.50	40 (28%) 1 1	83, 102, 115, 126	0
19	C7	120/136 (88%)	0.95	9 (7%) 20 15	97, 109, 125, 129	0
19	c7	117/136 (86%)	0.83	14 (11%) 9 7	88, 101, 115, 119	0
20	C8	145/145 (100%)	0.86	11 (7%) 20 14	85, 110, 131, 138	0
20	c8	145/145 (100%)	1.00	18 (12%) 8 6	86, 101, 116, 126	0
21	C9	143/143 (100%)	1.13	19 (13%) 7 6	96, 112, 122, 126	0
21	c9	143/143 (100%)	0.83	17 (11%) 9 7	85, 97, 112, 118	0
22	D0	107/120 (89%)	2.03	42 (39%) 1 1	86, 112, 123, 125	0
22	d0	110/120 (91%)	1.24	12 (10%) 10 9	84, 114, 138, 147	0
23	D1	87/87 (100%)	0.90	10 (11%) 9 8	96, 104, 119, 127	0
23	d1	87/87 (100%)	0.42	1 (1%) 78 60	76, 88, 104, 112	0
24	D2	129/129 (100%)	1.23	15 (11%) 9 8	83, 95, 101, 109	0
24	d2	129/129 (100%)	0.54	3 (2%) 61 42	64, 74, 81, 87	0
25	D3	144/144 (100%)	1.05	21 (14%) 6 5	69, 77, 86, 96	0
25	d3	144/144 (100%)	0.80	12 (8%) 17 13	56, 61, 71, 79	0
26	D4	134/134 (100%)	1.10	17 (12%) 8 6	86, 107, 118, 129	0
26	d4	134/134 (100%)	0.92	14 (10%) 11 9	68, 90, 105, 110	0
27	D5	70/107 (65%)	0.89	3 (4%) 40 25	119, 130, 139, 140	0
27	d5	69/107 (64%)	0.80	4 (5%) 29 19	99, 113, 123, 125	0
28	D6	97/97 (100%)	2.17	47 (48%) 0 0	88, 106, 154, 159	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	1.46	26 (26%) 1 1	70, 87, 116, 123	0
29	D7	81/81 (100%)	1.21	10 (12%) 8 7	98, 110, 135, 141	0
29	d7	81/81 (100%)	1.03	8 (9%) 13 10	80, 93, 121, 128	0
30	D8	63/66 (95%)	1.65	20 (31%) 1 1	111, 127, 139, 143	0
30	d8	63/66 (95%)	1.23	9 (14%) 6 5	104, 116, 127, 129	0
31	D9	53/55 (96%)	0.89	4 (7%) 20 15	84, 91, 107, 112	0
31	d9	53/55 (96%)	1.23	12 (22%) 2 2	82, 92, 128, 139	0
32	E0	60/62 (96%)	1.03	8 (13%) 7 6	78, 107, 129, 134	0
32	e0	62/62 (100%)	0.81	9 (14%) 6 5	63, 88, 109, 122	0
33	E1	71/76 (93%)	1.29	13 (18%) 3 3	107, 133, 145, 148	0
33	e1	76/76 (100%)	1.57	19 (25%) 2 1	112, 158, 170, 175	0
34	SR	318/318 (100%)	0.90	27 (8%) 16 13	109, 120, 132, 146	0
34	sR	318/318 (100%)	1.14	45 (14%) 6 5	110, 126, 140, 150	0
35	SM	121/273 (44%)	1.13	21 (17%) 4 4	59, 94, 111, 116	0
35	sM	63/273 (23%)	1.70	19 (30%) 1 1	55, 105, 111, 112	0
36	1	3149/3396 (92%)	-0.02	29 (0%) 81 65	35, 59, 123, 212	0
36	5	3169/3396 (93%)	-0.08	45 (1%) 73 55	35, 54, 124, 188	0
37	3	121/121 (100%)	-0.14	0 100 100	43, 76, 90, 96	0
37	7	121/121 (100%)	-0.28	1 (0%) 82 68	39, 59, 70, 75	0
38	4	158/158 (100%)	-0.04	2 (1%) 75 56	43, 61, 91, 130	0
38	8	158/158 (100%)	-0.01	2 (1%) 75 56	43, 63, 96, 120	0
39	L2	252/253 (99%)	0.80	23 (9%) 15 11	42, 61, 77, 82	0
39	l2	252/253 (99%)	0.44	10 (3%) 42 28	43, 59, 74, 83	0
40	L3	386/386 (100%)	0.42	15 (3%) 43 29	42, 63, 77, 85	0
40	l3	386/386 (100%)	0.15	7 (1%) 67 49	34, 49, 62, 77	0
41	L4	361/361 (100%)	0.35	11 (3%) 52 35	40, 54, 70, 71	0
41	l4	361/361 (100%)	0.45	15 (4%) 40 26	40, 57, 73, 88	0
42	L5	296/296 (100%)	0.73	22 (7%) 20 15	58, 81, 97, 111	0
42	l5	294/296 (99%)	0.45	18 (6%) 27 18	49, 60, 84, 93	0
43	L6	156/175 (89%)	0.34	5 (3%) 50 34	49, 57, 72, 79	0
43	l6	157/175 (89%)	0.35	3 (1%) 66 48	49, 57, 75, 85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	0.21	9 (4%) 41 27	40, 49, 73, 106	0
44	l7	223/243 (91%)	0.21	2 (0%) 81 65	39, 49, 80, 107	0
45	L8	233/255 (91%)	0.94	30 (12%) 7 6	67, 81, 104, 112	0
45	l8	231/255 (90%)	0.86	24 (10%) 11 9	73, 84, 106, 114	0
46	L9	191/191 (100%)	0.72	10 (5%) 33 22	60, 70, 82, 93	0
46	l9	191/191 (100%)	0.21	2 (1%) 79 63	44, 55, 71, 81	0
47	M0	211/220 (95%)	0.57	13 (6%) 26 18	45, 63, 92, 106	0
47	m0	213/220 (96%)	0.52	12 (5%) 30 20	40, 55, 80, 90	0
48	M1	169/173 (97%)	0.62	9 (5%) 32 22	68, 84, 94, 98	0
48	m1	169/173 (97%)	0.37	3 (1%) 67 49	52, 67, 77, 82	0
49	M3	193/198 (97%)	0.41	8 (4%) 41 27	39, 64, 92, 113	0
49	m3	194/198 (97%)	0.62	10 (5%) 33 22	41, 69, 100, 111	0
50	M4	136/137 (99%)	0.34	5 (3%) 45 31	54, 61, 73, 83	0
50	m4	137/137 (100%)	0.25	1 (0%) 84 70	48, 54, 69, 82	0
51	M5	203/203 (100%)	0.49	7 (3%) 48 32	41, 56, 66, 69	0
51	m5	203/203 (100%)	0.58	10 (4%) 35 23	44, 60, 71, 76	0
52	M6	197/198 (99%)	0.53	12 (6%) 27 18	42, 49, 65, 68	0
52	m6	197/198 (99%)	0.40	14 (7%) 22 15	34, 42, 64, 66	0
53	M7	183/183 (100%)	0.63	18 (9%) 13 10	47, 55, 98, 116	0
53	m7	155/183 (84%)	0.10	1 (0%) 85 73	39, 46, 59, 77	0
54	M8	185/185 (100%)	0.47	10 (5%) 31 21	43, 55, 69, 88	0
54	m8	185/185 (100%)	0.43	5 (2%) 56 37	42, 57, 66, 70	0
55	M9	188/188 (100%)	0.78	11 (5%) 28 19	65, 77, 135, 140	0
55	m9	188/188 (100%)	0.51	5 (2%) 56 37	51, 65, 121, 134	0
56	N0	172/172 (100%)	0.42	8 (4%) 36 24	49, 57, 69, 74	0
56	n0	172/172 (100%)	0.18	5 (2%) 53 35	43, 49, 59, 66	0
57	N1	159/159 (100%)	0.41	4 (2%) 58 39	42, 56, 93, 101	0
57	n1	159/159 (100%)	0.47	5 (3%) 51 35	40, 49, 83, 87	0
58	N2	100/120 (83%)	0.90	11 (11%) 10 9	93, 104, 120, 122	0
58	n2	98/120 (81%)	0.79	9 (9%) 14 11	75, 88, 94, 97	0
59	N3	136/136 (100%)	0.54	10 (7%) 20 15	51, 60, 70, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	0.21	3 (2%) 62 43	36, 45, 55, 58	0
60	N4	98/155 (63%)	1.35	23 (23%) 2 2	62, 72, 134, 147	0
60	n4	135/155 (87%)	0.89	17 (12%) 8 6	46, 91, 115, 116	0
61	N5	121/141 (85%)	0.66	10 (8%) 17 13	58, 69, 84, 95	0
61	n5	120/141 (85%)	0.75	7 (5%) 29 19	56, 68, 85, 93	0
62	N6	126/126 (100%)	0.35	3 (2%) 59 40	50, 62, 74, 79	0
62	n6	126/126 (100%)	0.44	3 (2%) 59 40	51, 64, 77, 83	0
63	N7	135/135 (100%)	0.58	5 (3%) 45 31	82, 94, 103, 109	0
63	n7	135/135 (100%)	0.51	6 (4%) 39 25	76, 91, 102, 105	0
64	N8	148/148 (100%)	0.35	1 (0%) 84 70	35, 56, 74, 82	0
64	n8	148/148 (100%)	0.39	3 (2%) 65 46	34, 59, 74, 77	0
65	N9	58/58 (100%)	0.46	2 (3%) 48 32	38, 61, 95, 106	0
65	n9	58/58 (100%)	0.65	6 (10%) 12 10	38, 58, 78, 85	0
66	O0	97/104 (93%)	0.69	5 (5%) 33 22	81, 89, 101, 102	0
66	o0	100/104 (96%)	0.63	3 (3%) 52 35	75, 82, 102, 108	0
67	O1	109/112 (97%)	0.77	6 (5%) 30 21	61, 72, 91, 103	0
67	o1	109/112 (97%)	0.46	6 (5%) 30 21	47, 58, 81, 90	0
68	O2	127/129 (98%)	0.26	4 (3%) 51 35	36, 49, 62, 68	0
68	o2	127/129 (98%)	0.34	4 (3%) 51 35	35, 52, 63, 71	0
69	O3	106/106 (100%)	0.35	3 (2%) 55 36	42, 47, 71, 78	0
69	o3	106/106 (100%)	0.31	0 100 100	40, 46, 69, 75	0
70	O4	112/120 (93%)	0.97	12 (10%) 11 9	57, 75, 101, 107	0
70	o4	112/120 (93%)	0.80	7 (6%) 26 17	50, 68, 99, 103	0
71	O5	119/119 (100%)	0.71	7 (5%) 28 19	55, 70, 78, 82	0
71	o5	119/119 (100%)	0.71	9 (7%) 20 14	59, 71, 87, 96	0
72	O6	99/99 (100%)	0.39	2 (2%) 65 46	60, 68, 91, 102	0
72	o6	99/99 (100%)	0.43	2 (2%) 65 46	64, 72, 88, 103	0
73	O7	87/87 (100%)	0.78	7 (8%) 18 14	43, 50, 65, 71	0
73	o7	87/87 (100%)	0.58	3 (3%) 48 32	41, 50, 73, 84	0
74	O8	77/77 (100%)	0.57	3 (3%) 43 29	83, 93, 108, 113	0
74	o8	77/77 (100%)	0.65	3 (3%) 43 29	77, 86, 94, 98	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	0.73	6 (12%) 9 7	52, 57, 59, 60	0
75	o9	50/50 (100%)	0.55	4 (8%) 18 14	50, 55, 63, 63	0
76	Q0	52/52 (100%)	0.25	1 (1%) 66 48	53, 59, 74, 79	0
76	q0	52/52 (100%)	-0.08	0 100 100	41, 45, 55, 58	0
77	Q1	25/25 (100%)	0.89	3 (12%) 9 7	62, 66, 73, 74	0
77	q1	25/25 (100%)	0.66	1 (4%) 42 28	50, 56, 58, 58	0
78	Q2	105/105 (100%)	0.33	3 (2%) 53 35	41, 56, 76, 91	0
78	q2	105/105 (100%)	0.29	3 (2%) 53 35	44, 56, 70, 93	0
79	Q3	91/91 (100%)	0.86	7 (7%) 19 14	54, 65, 80, 85	0
79	q3	91/91 (100%)	0.52	3 (3%) 49 33	46, 59, 72, 84	0
80	m2	0/165	-	-	-	-
81	p0	120/311 (38%)	1.33	30 (25%) 2 1	101, 124, 144, 152	0
82	p1	0/47	-	-	-	-
82	p2	0/47	-	-	-	-
83	f	148/157 (94%)	2.12	75 (50%) 0 0	44, 82, 144, 147	75 (50%)
All	All	33080/35493 (93%)	0.55	2267 (6%) 23 16	34, 74, 132, 212	77 (0%)

The worst 5 of 2267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	d0	64	LYS	9.9
7	S5	152	GLY	9.6
60	N4	86	SER	8.6
47	m0	221	ALA	8.5
1	2	1756[A]	A	8.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
85	ZN	D7	101	1/1	0.84	0.11	141,141,141,141	0
85	ZN	d7	101	1/1	0.84	0.10	131,131,131,131	0
87	MG	5	3402	1/1	0.84	0.12	45,45,45,45	0
87	MG	5	3404	1/1	0.84	0.26	36,36,36,36	0
87	MG	C	101	1/1	0.85	0.26	49,49,49,49	0
87	MG	5	3405	1/1	0.86	0.32	42,42,42,42	0
87	MG	1	3402	1/1	0.88	0.45	21,21,21,21	0
87	MG	B	3402	1/1	0.90	0.25	40,40,40,40	0
87	MG	1	3404	1/1	0.91	0.26	29,29,29,29	0
85	ZN	E1	501	1/1	0.93	0.06	136,136,136,136	0
87	MG	5	3401	1/1	0.94	0.17	41,41,41,41	0
85	ZN	e1	501	1/1	0.94	0.09	164,164,164,164	0
87	MG	1	3403	1/1	0.95	0.18	45,45,45,45	0
86	SPS	1	3401	23/23	0.95	0.10	40,43,57,59	0
86	SPS	B	3401	23/23	0.96	0.11	37,40,54,56	0
85	ZN	d6	500	1/1	0.97	0.07	87,87,87,87	0
85	ZN	D6	500	1/1	0.97	0.10	105,105,105,105	0
88	OHX	1	3405	7/7	0.97	0.14	91,91,91,91	0
85	ZN	Q2	501	1/1	0.98	0.11	76,76,76,76	0
85	ZN	q2	501	1/1	0.98	0.10	77,77,77,77	0
88	OHX	5	3406	7/7	0.98	0.14	95,95,95,95	0
85	ZN	D9	101	1/1	0.99	0.06	88,88,88,88	0
87	MG	f	1002	1/1	0.99	0.04	66,66,66,66	0
85	ZN	d9	101	1/1	0.99	0.03	94,94,94,94	0
85	ZN	Q3	501	1/1	0.99	0.03	77,77,77,77	0
87	MG	5	3403	1/1	0.99	0.36	23,23,23,23	0
88	OHX	1	3406	7/7	0.99	0.06	73,73,73,73	0
85	ZN	Q0	500	1/1	0.99	0.03	57,57,57,57	0
85	ZN	q3	501	1/1	1.00	0.04	69,69,69,69	0
85	ZN	o7	501	1/1	1.00	0.02	51,51,51,51	0
85	ZN	q0	500	1/1	1.00	0.02	42,42,42,42	0
87	MG	f	1001	1/1	1.00	0.21	52,52,52,52	0
85	ZN	O7	100	1/1	1.00	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.