



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2016 – 07:23 PM EST

PDB ID : 5DGF
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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

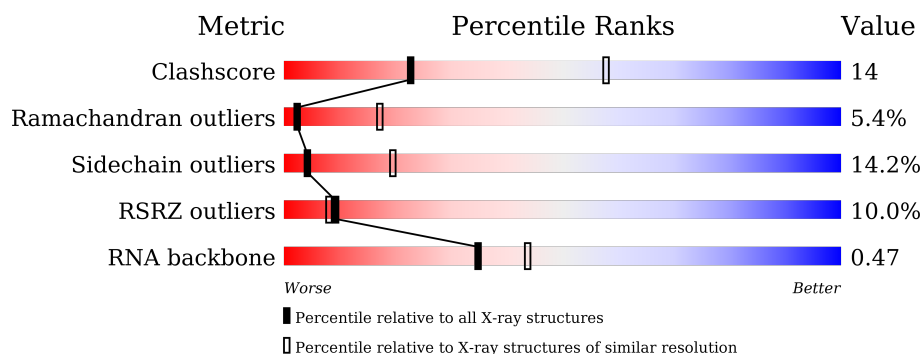
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	<div> <div>5%</div> <div>38% 47% 14%</div> <div>..</div> </div>
1	6	1800	<div> <div>3%</div> <div>40% 45% 14%</div> <div>.</div> </div>
2	S0	251	<div> <div>20%</div> <div>27% 41% 14% 18%</div> </div>
2	s0	251	<div> <div>20%</div> <div>67% 15% 18%</div> </div>
3	S1	254	<div> <div>30%</div> <div>26% 47% 10% 16%</div> <div>.</div> </div>
3	s1	254	<div> <div>17%</div> <div>69% 15% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	96	
12	c0	96	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	




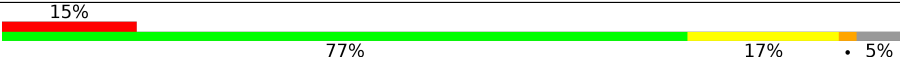
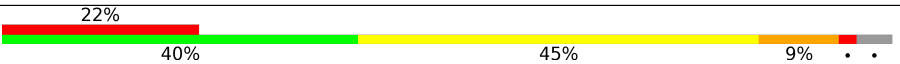


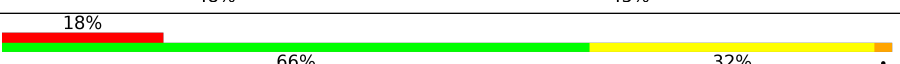
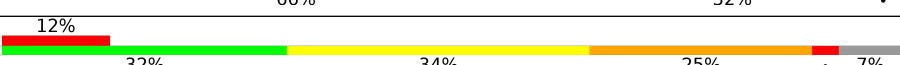
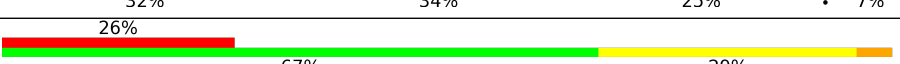
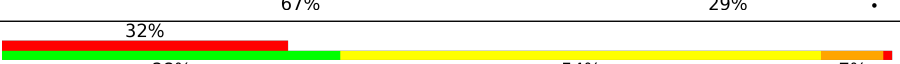
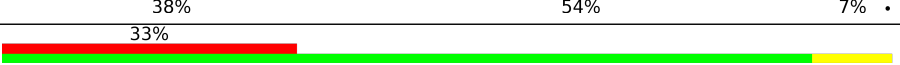
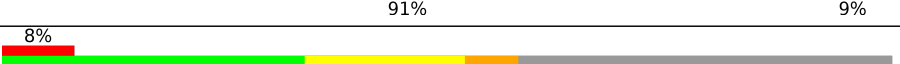



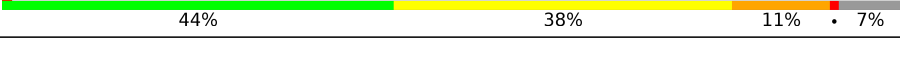
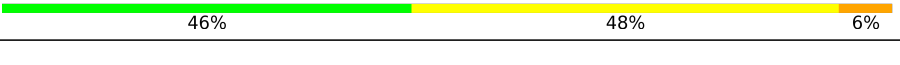


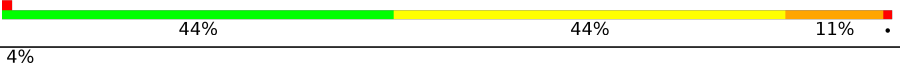
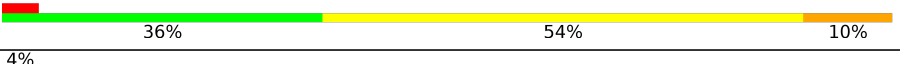



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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134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

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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	

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Mol	Chain	Length	Quality of chain
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	

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Mol	Chain	Length	Quality of chain
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	

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Mol	Chain	Length	Quality of chain
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	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	
78	Q2	105	
78	q2	105	

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Mol	Chain	Length	Quality of chain
79	Q3	91	
79	q3	91	
80	m2	165	
81	p0	311	
82	p1	47	
82	p2	47	
83	f	157	
84	B	5	
84	C	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	SPS	B	3401	-	-	-	X
87	MG	5	3401	-	-	-	X
87	MG	5	3404	-	-	-	X
87	MG	5	3405	-	-	-	X

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			

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

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

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

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

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

- 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			

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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	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

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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			

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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			

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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			

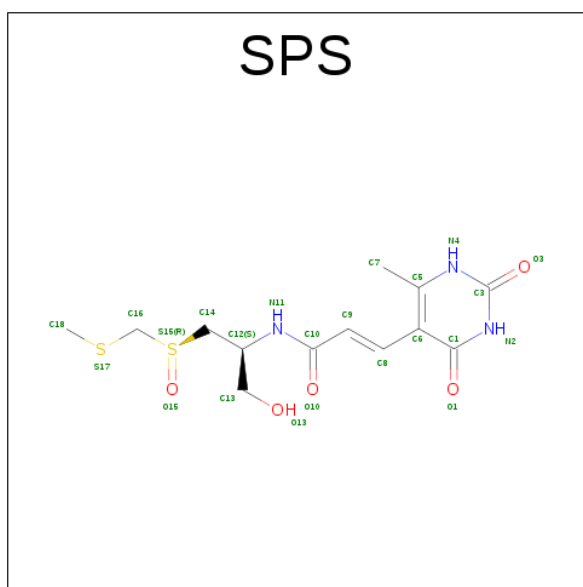
- Molecule 84 is a protein called CH-CH-8AN-PRO-PRO.

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

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 86 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).

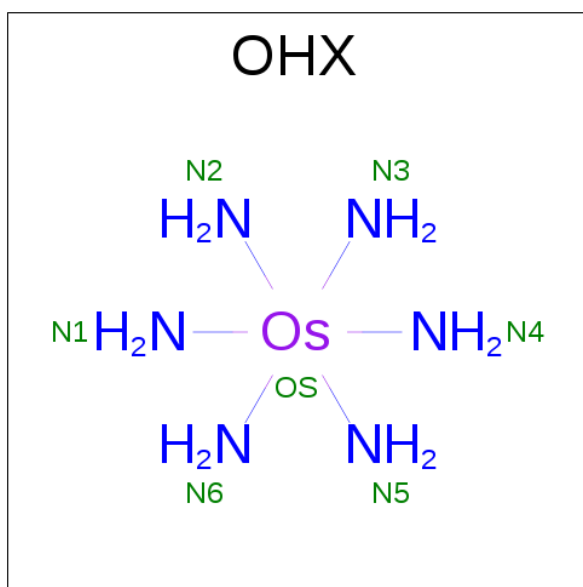


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
86	1	1	Total	C	N	O	S	0	0
			23	13	3	5	2		
86	B	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 88 is osmium (III) hexammine (three-letter code: 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		

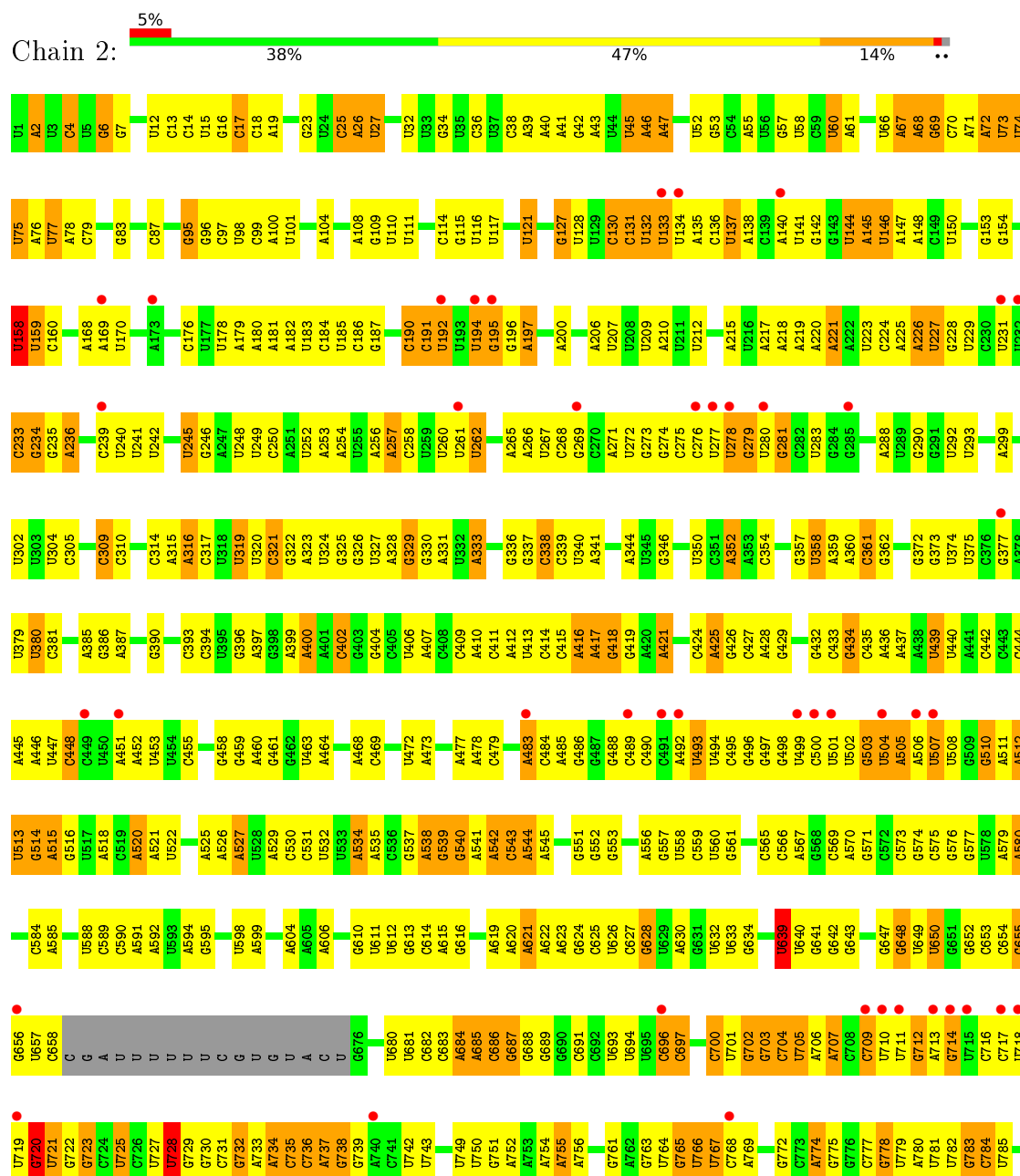
- Molecule 89 is water.

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

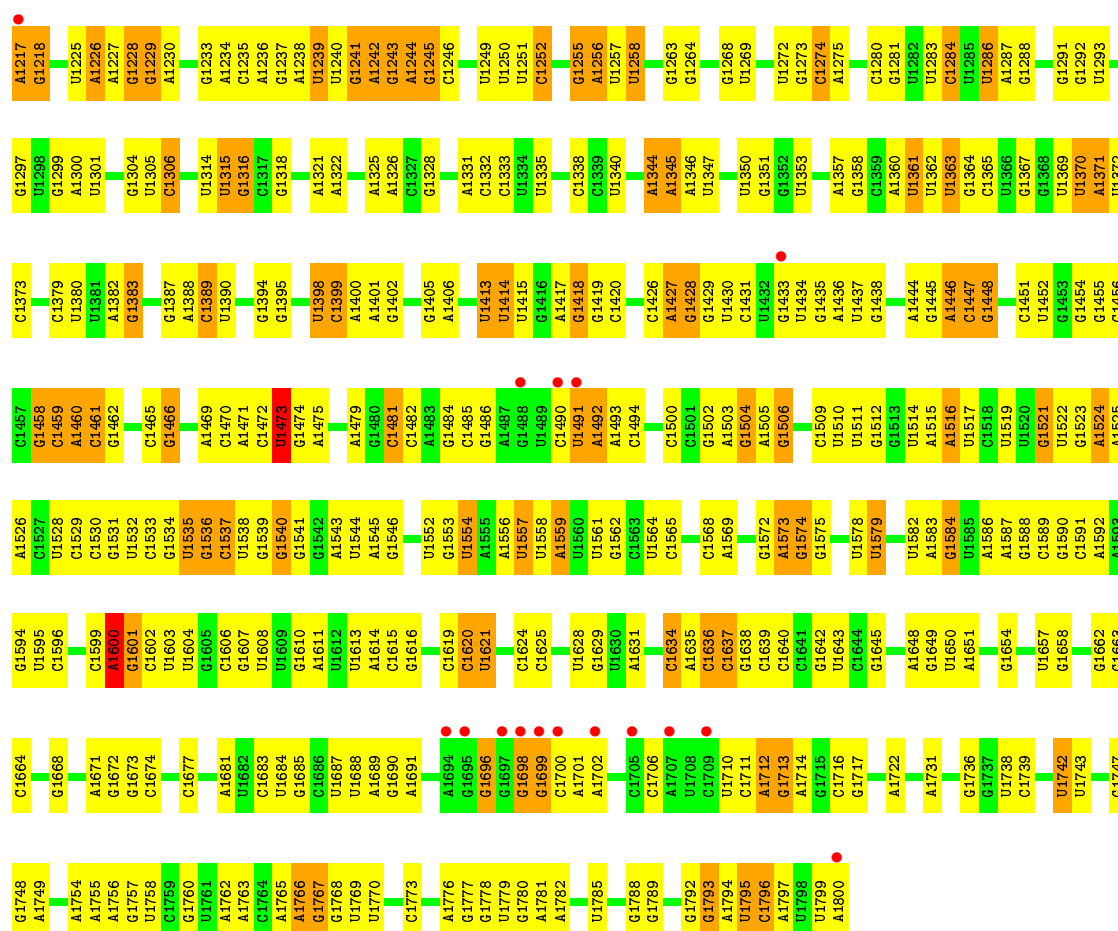
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 18S ribosomal RNA





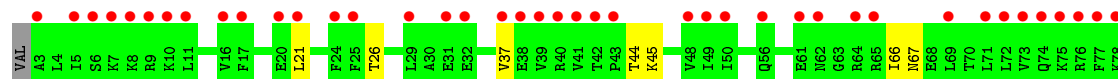
A1133	A1137	A1138	A1139	G1140	A1141	A1142	A1143	G1150	A1151	A1152	G1153	G1154	G1155	C1158	C1159	C1160	C1161	G1162	A1163	G1164	G1165	G1166	G1167	U1175	G1176	G1177	A1183	A1184	U1185	U1186	A1189	C1190	U1191	A1194	C1195	C1196	C1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U1063	A1064	A1065	C1066	C1067	C1068	C1069	C1070	U1071	U1072	G1073	G1074	C1075	A1076	C1077	C1078	C1079	C1080	A1081	C1082	G1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	U1095	C1096	U1097	U1098	U1099	G1100	G1101	G1102	U1103	G1107	G1108	G1109	G1110	G1111	G1112	A1113	G1114	G1115	A1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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• Molecule 2: 40S ribosomal protein S0-A

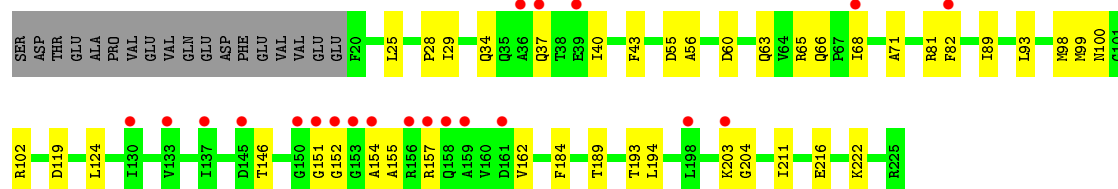
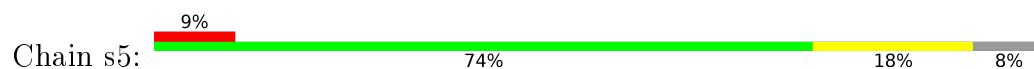




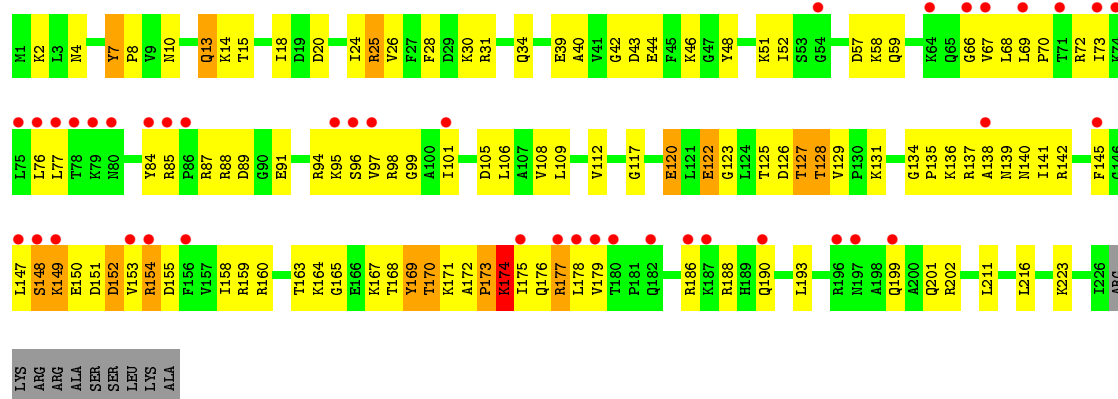




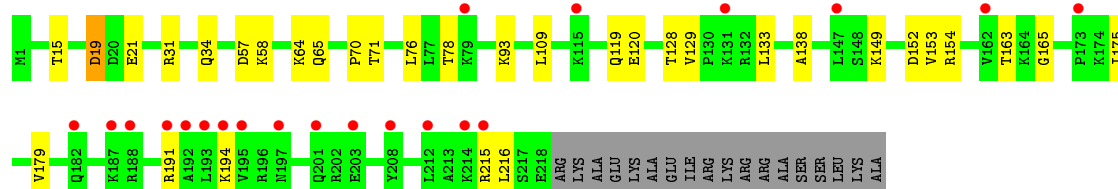
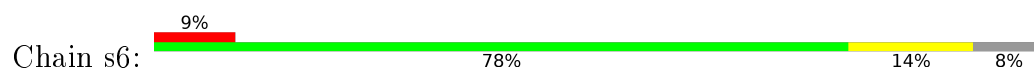
• Molecule 7: 40S ribosomal protein S5



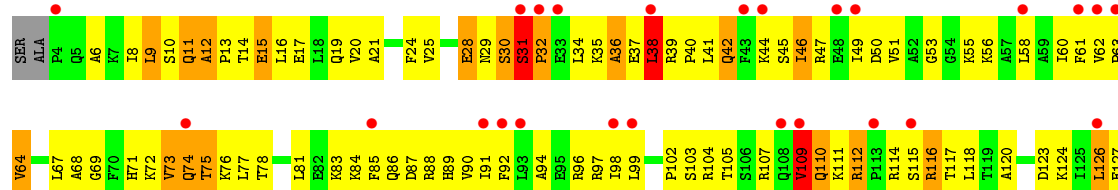
• Molecule 8: 40S ribosomal protein S6-A

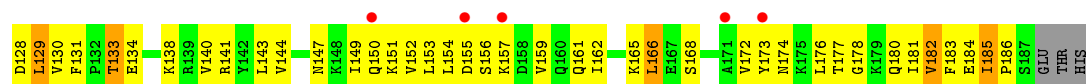


• Molecule 8: 40S ribosomal protein S6-A

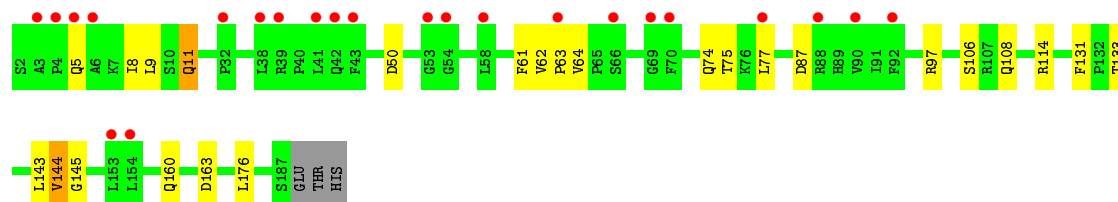
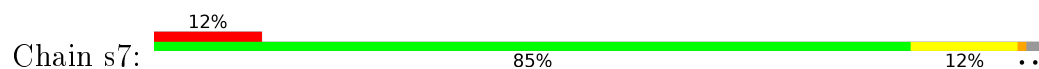


• Molecule 9: 40S ribosomal protein S7-A

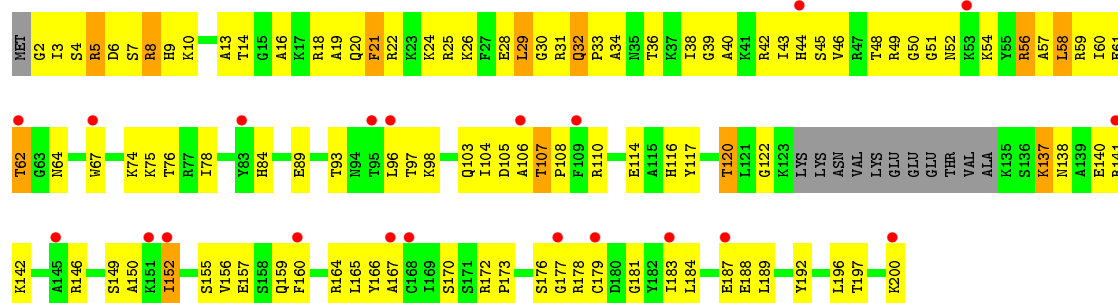
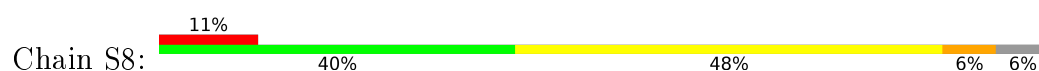




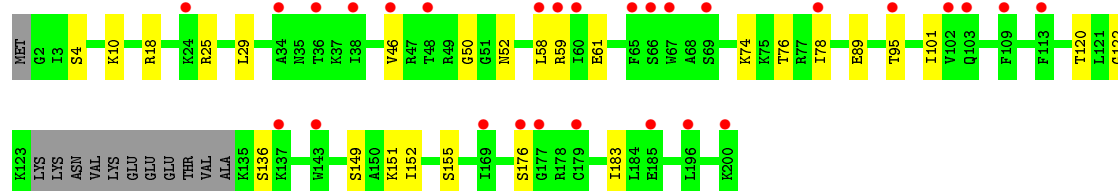
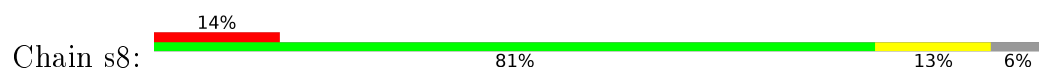
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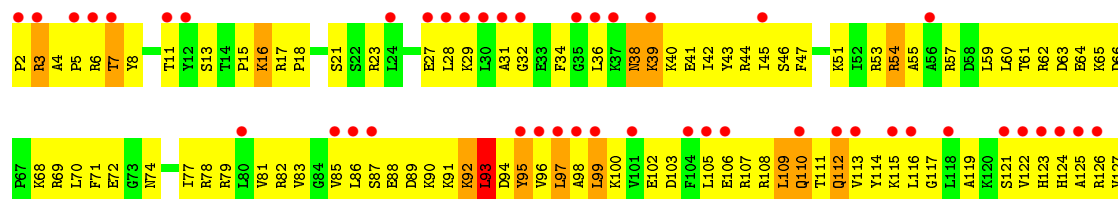
• Molecule 10: 40S ribosomal protein S8-A

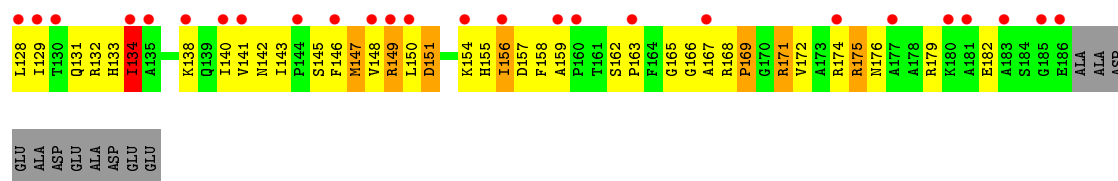


• Molecule 10: 40S ribosomal protein S8-A

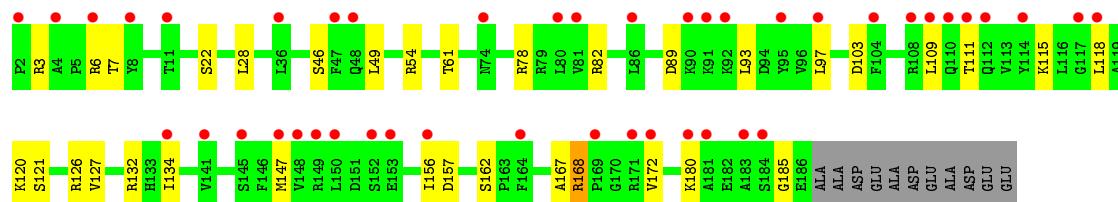
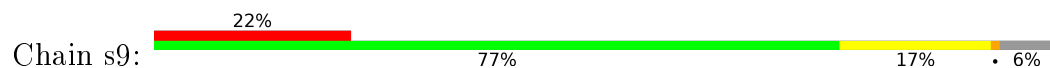


• Molecule 11: 40S ribosomal protein S9-A

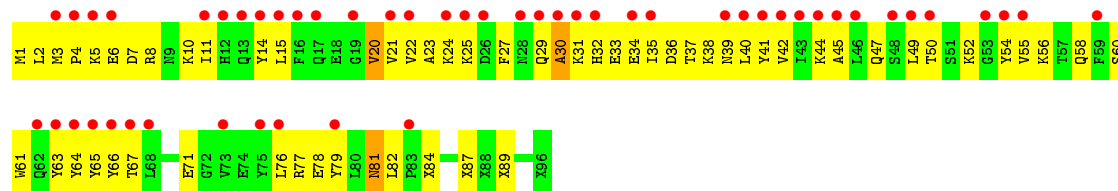




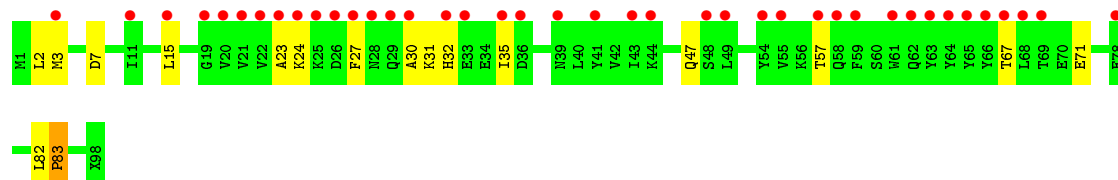
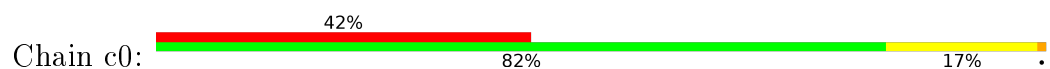
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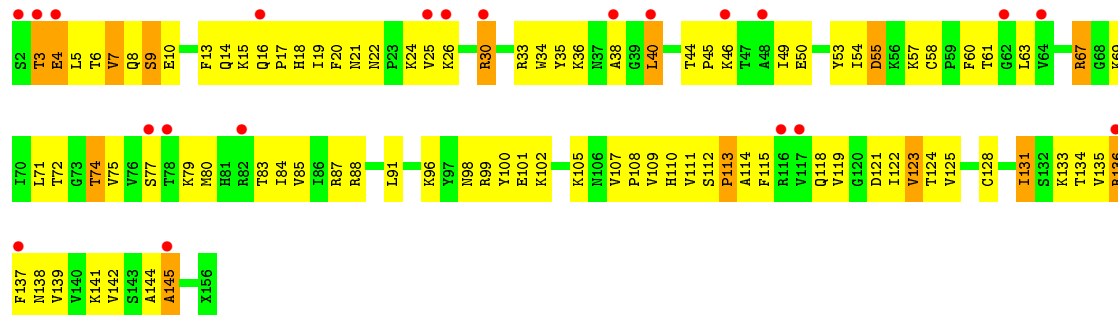
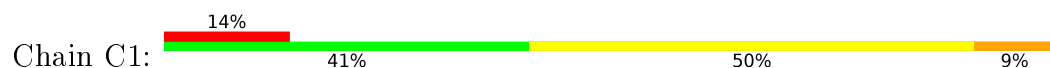
• Molecule 12: 40S ribosomal protein S10-A



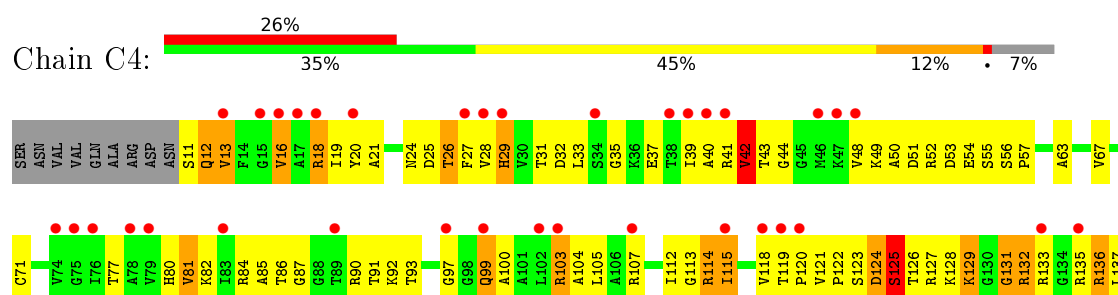
• Molecule 12: 40S ribosomal protein S10-A



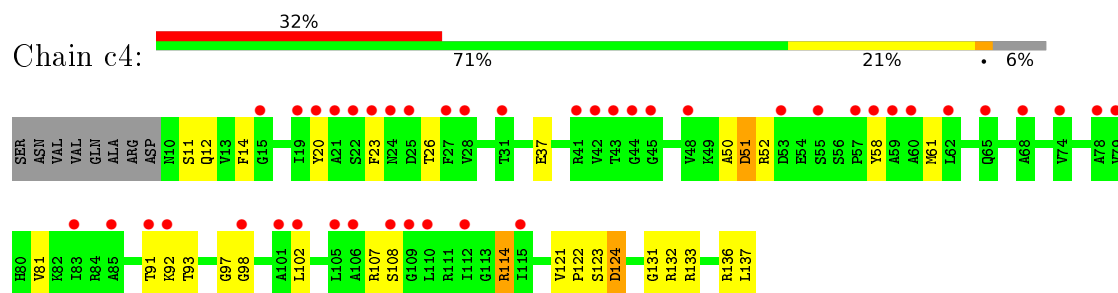
• Molecule 13: 40S ribosomal protein S11-A



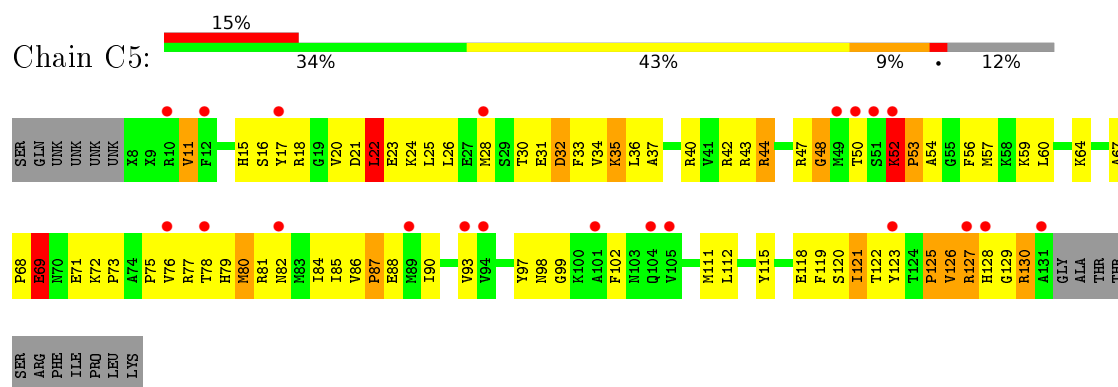
- Molecule 16: 40S ribosomal protein S14-A



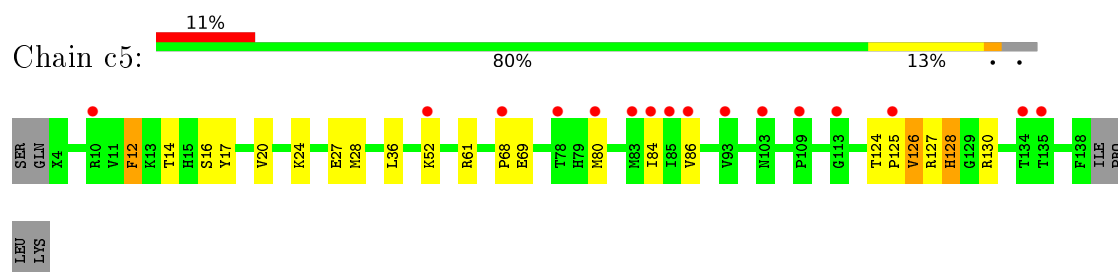
- Molecule 16: 40S ribosomal protein S14-A



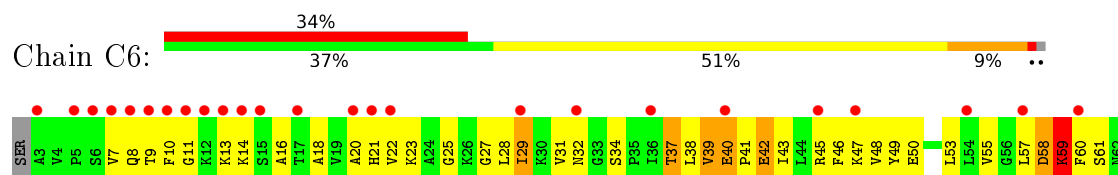
- Molecule 17: 40S ribosomal protein S15 (uS19)

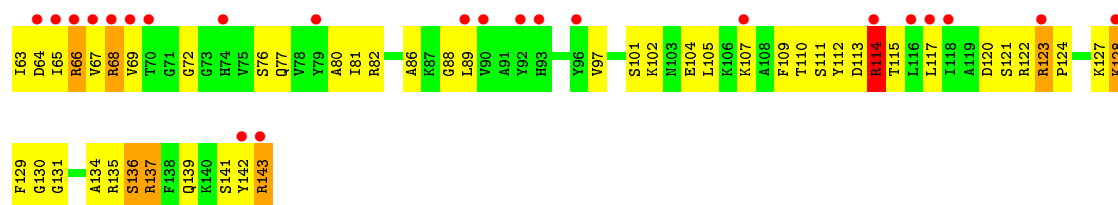


- Molecule 17: 40S ribosomal protein S15 (uS19)

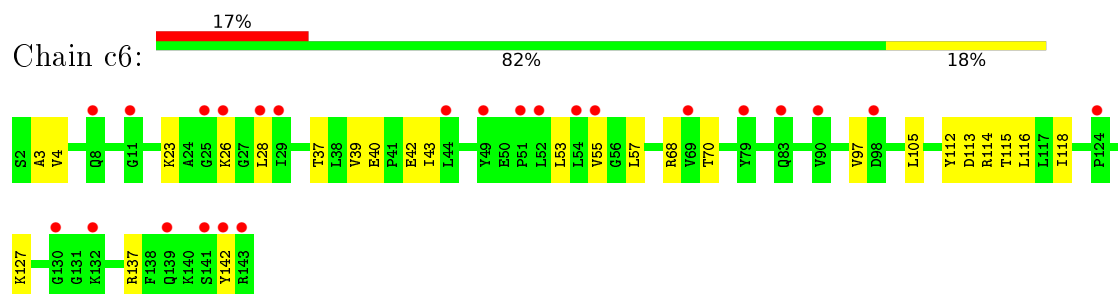


- Molecule 18: 40S ribosomal protein S16-A

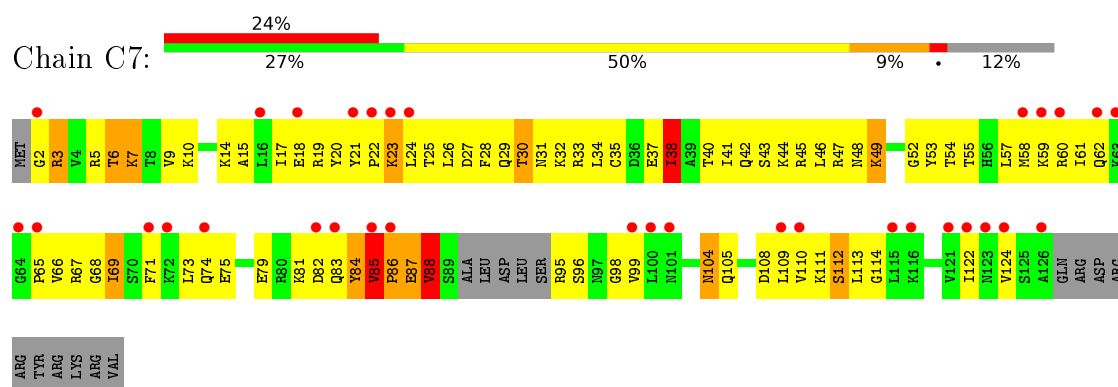




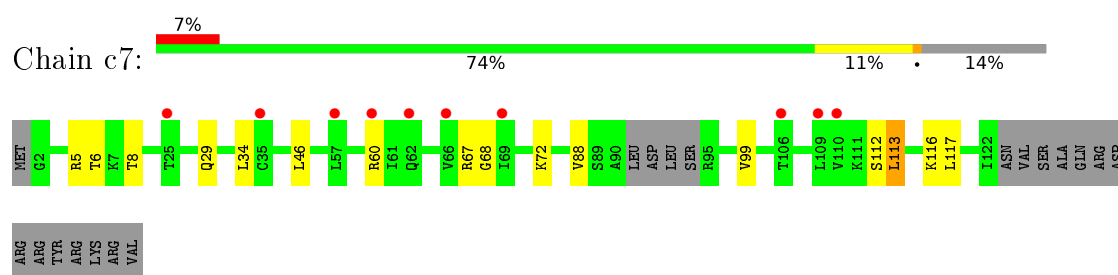
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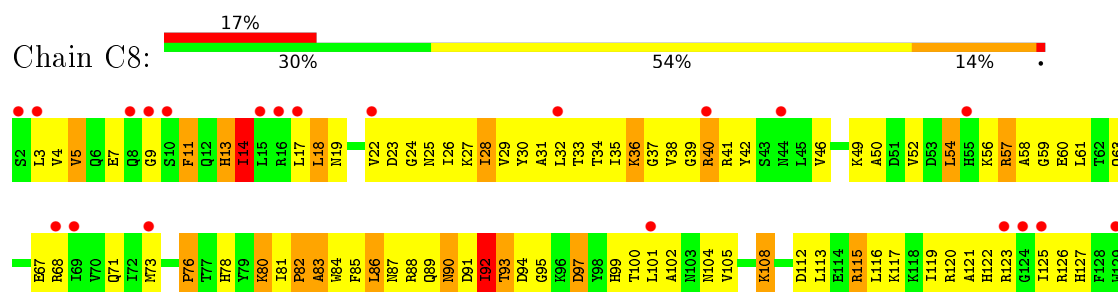
• Molecule 19: 40S ribosomal protein S17-A

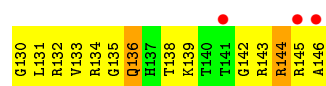


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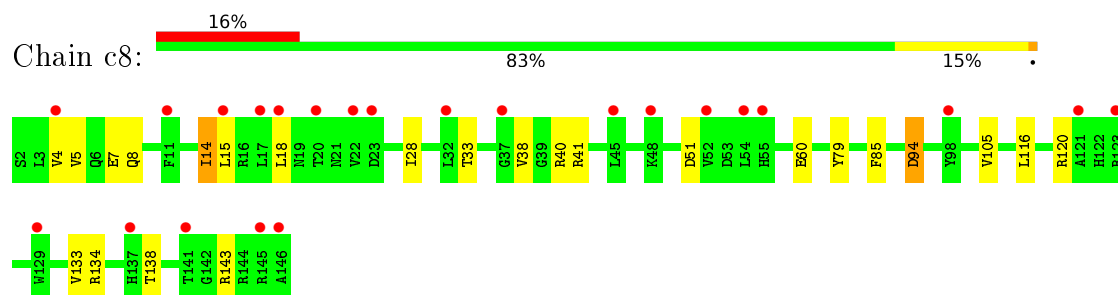


• Molecule 20: 40S ribosomal protein S18-A

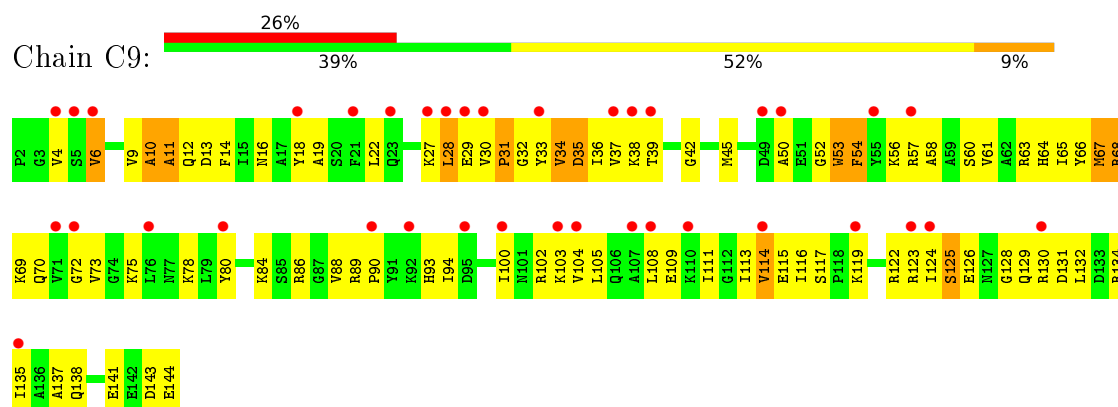




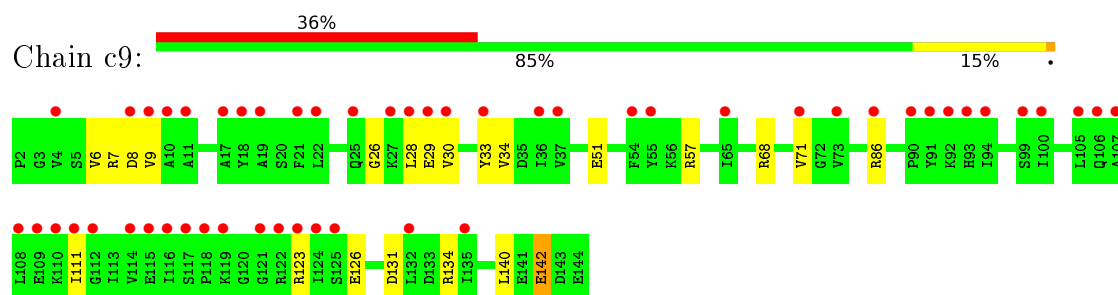
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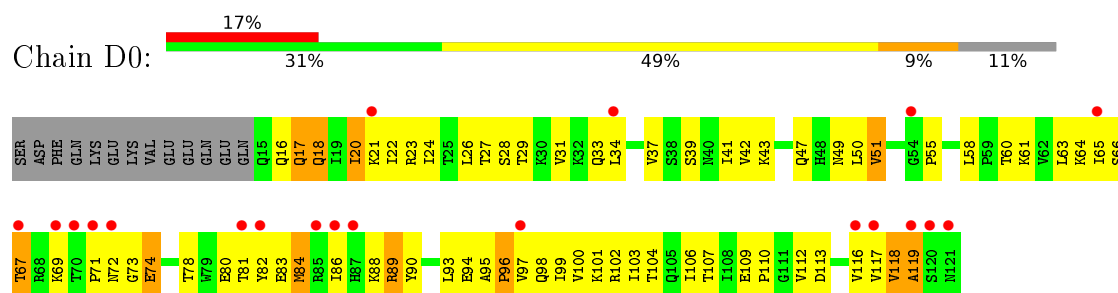
- Molecule 21: 40S ribosomal protein S19-A



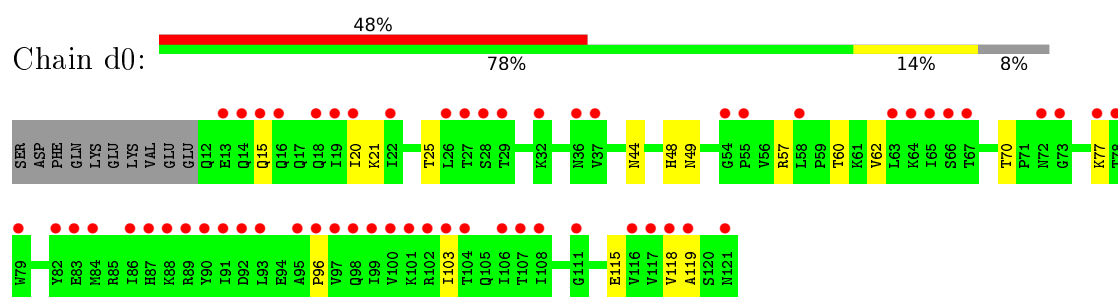
- Molecule 21: 40S ribosomal protein S19-A



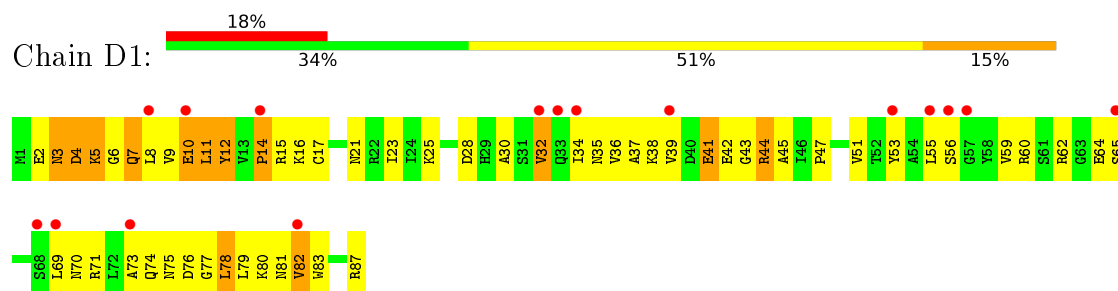
- Molecule 22: 40S ribosomal protein S20



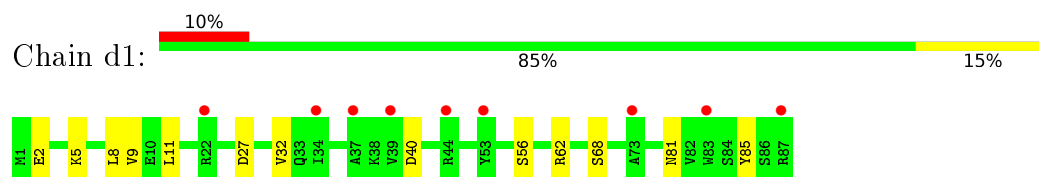
- Molecule 22: 40S ribosomal protein S20



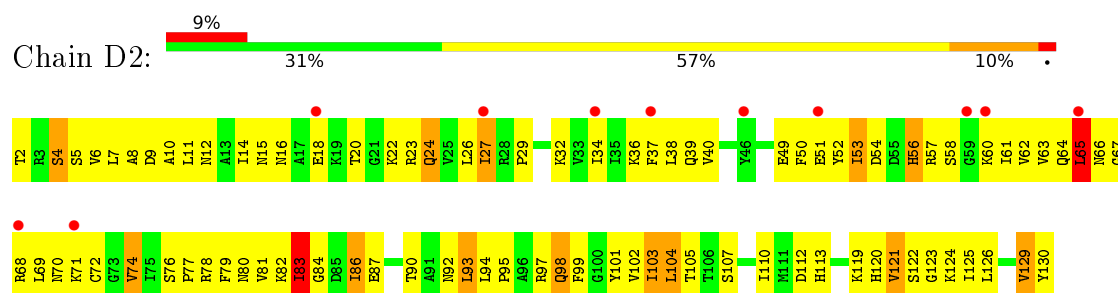
- Molecule 23: 40S ribosomal protein S21-A



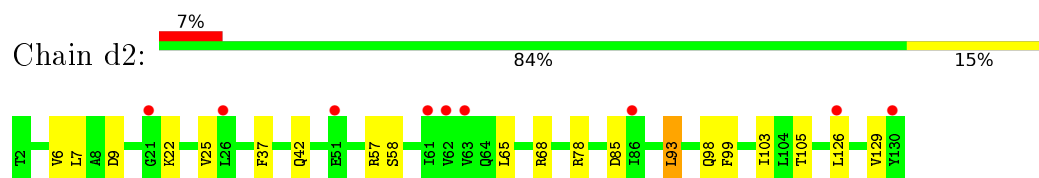
- Molecule 23: 40S ribosomal protein S21-A



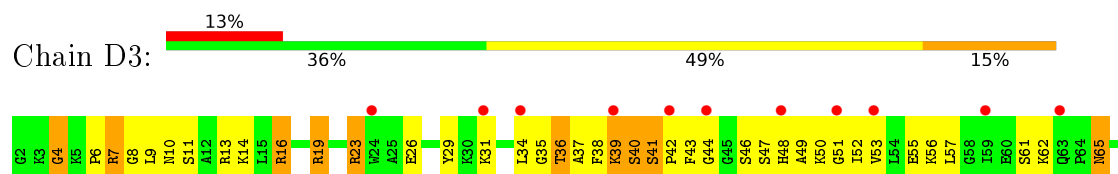
- Molecule 24: 40S ribosomal protein S22-A

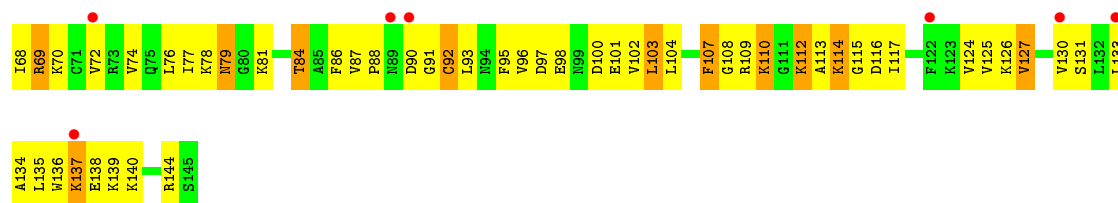


- Molecule 24: 40S ribosomal protein S22-A

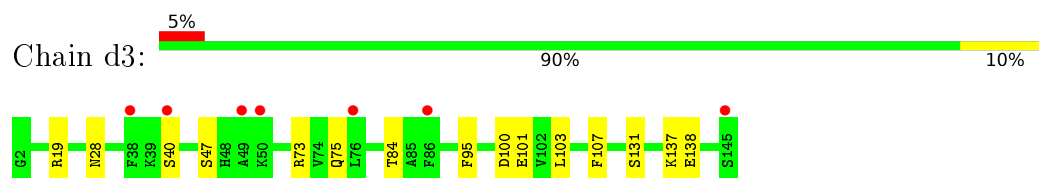


- Molecule 25: 40S ribosomal protein S23-A

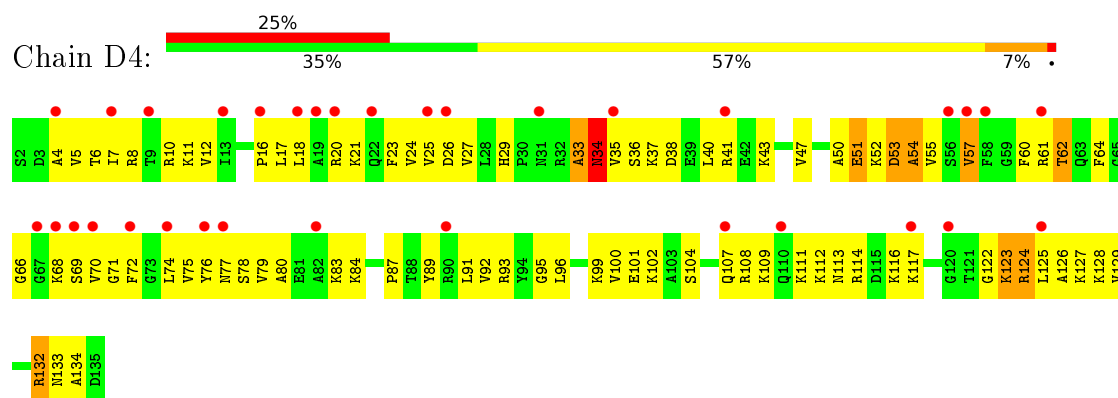




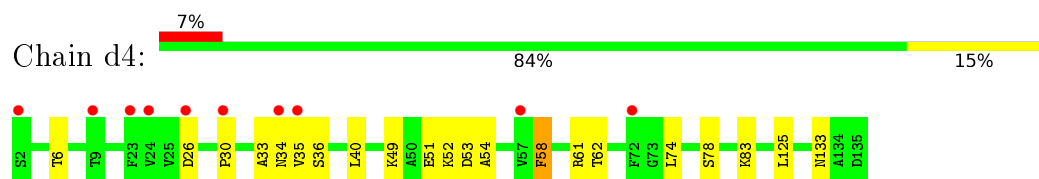
- Molecule 25: 40S ribosomal protein S23-A



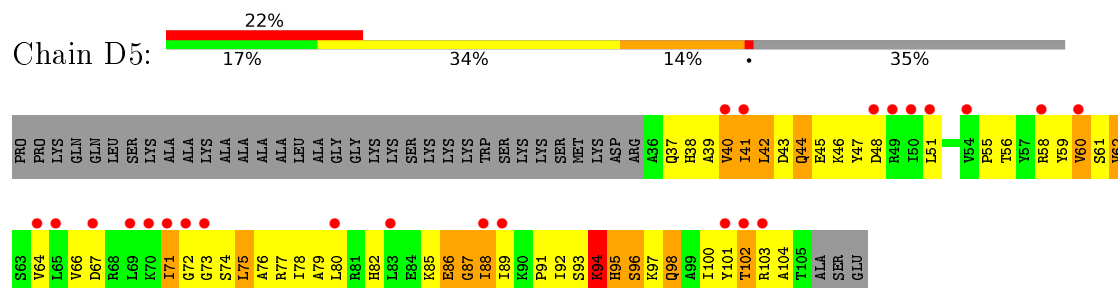
- Molecule 26: 40S ribosomal protein S24-A



- Molecule 26: 40S ribosomal protein S24-A

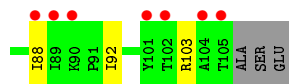


- Molecule 27: 40S ribosomal protein S25-A

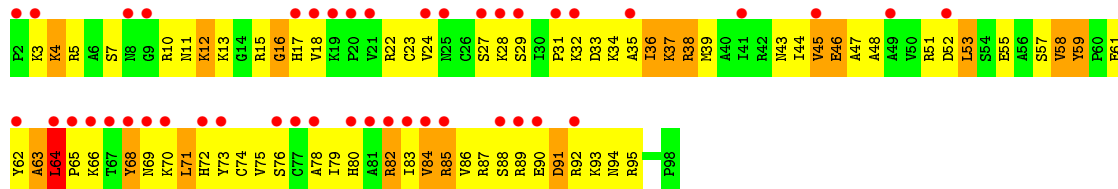


- Molecule 27: 40S ribosomal protein S25-A

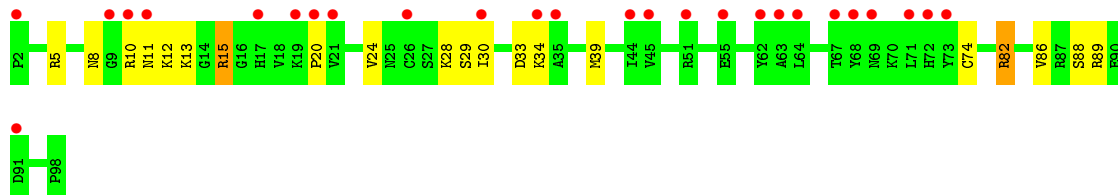




- Molecule 28: 40S ribosomal protein S26-B



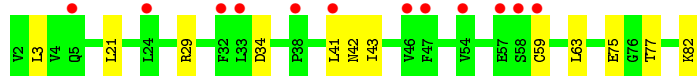
- Molecule 28: 40S ribosomal protein S26-B



- Molecule 29: 40S ribosomal protein S27-A

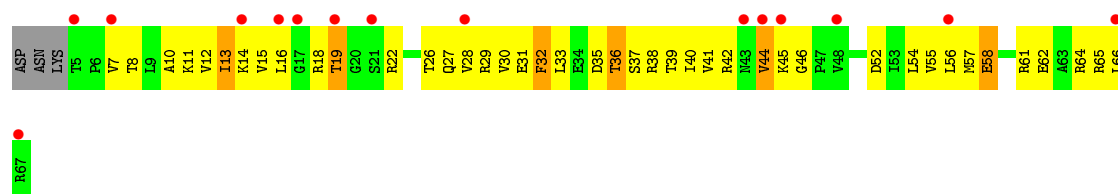


- Molecule 29: 40S ribosomal protein S27-A

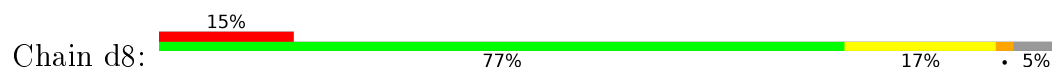


- Molecule 30: 40S ribosomal protein S28-A





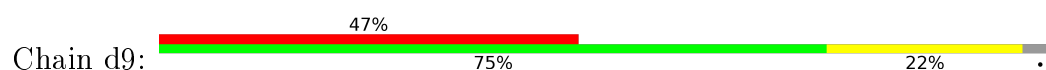
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

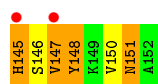


- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: Ubiquitin-40S ribosomal protein S31





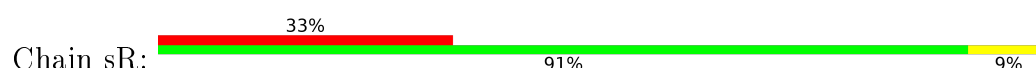
- Molecule 33: Ubiquitin-40S ribosomal protein S31



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



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



- Molecule 35: Suppressor protein STM1

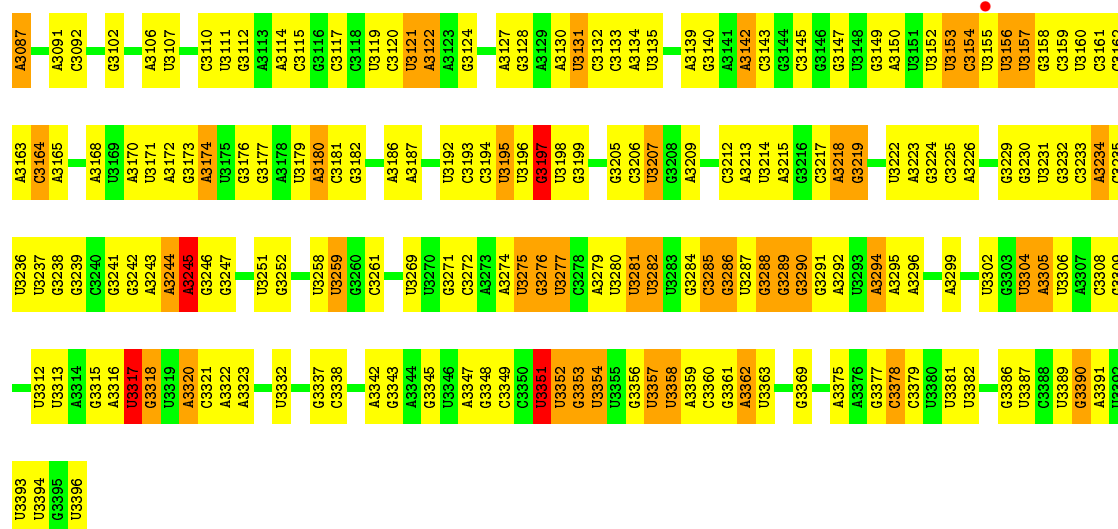
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C1596	G1507	G1340	G1262	A1182	U1096	A926	G754	C675	G595	A521	G395
C1597	C1508	U1341	A1263	C1185	G1097	C927	G760	C676	C596	A522	A396
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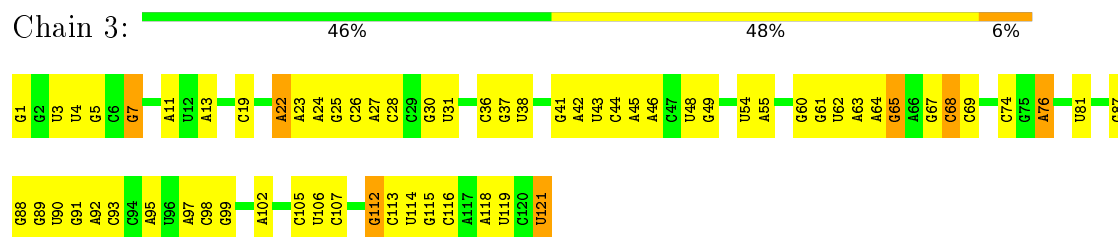




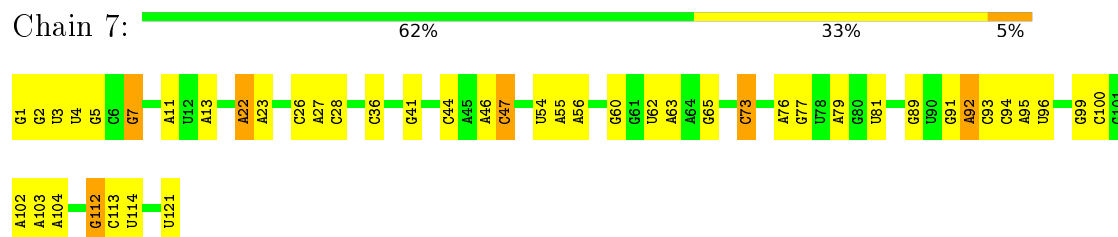
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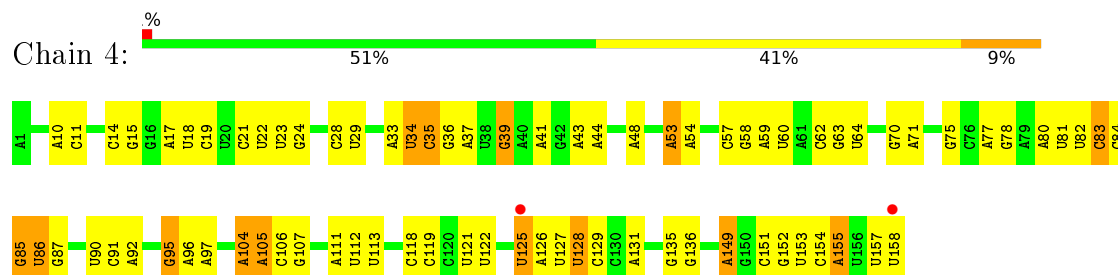
• Molecule 37: 5S ribosomal RNA



• Molecule 37: 5S ribosomal RNA

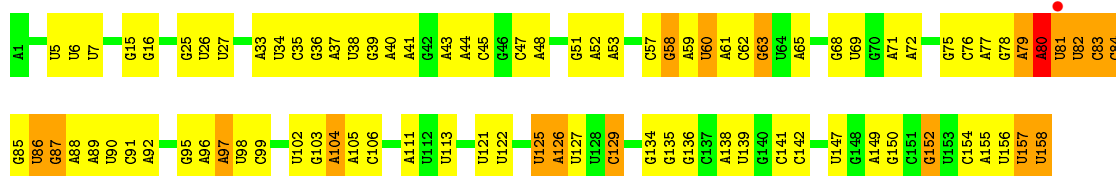


• Molecule 38: 5.8S ribosomal RNA

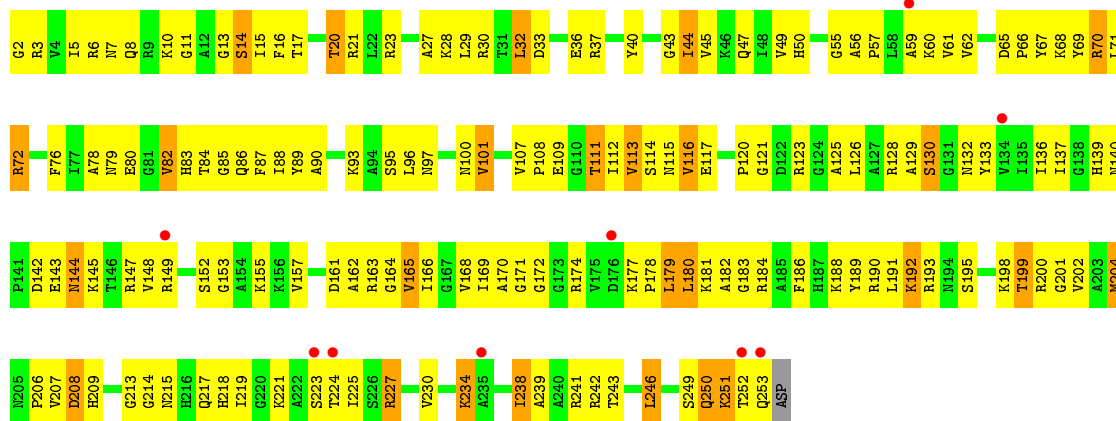


• Molecule 38: 5.8S ribosomal RNA

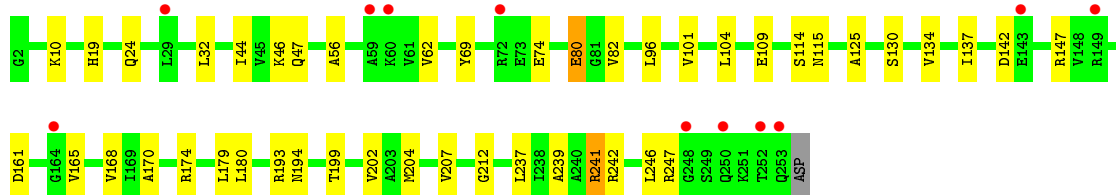
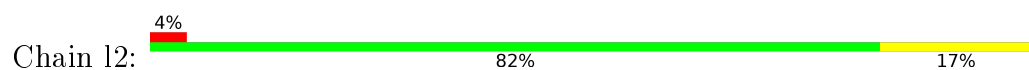




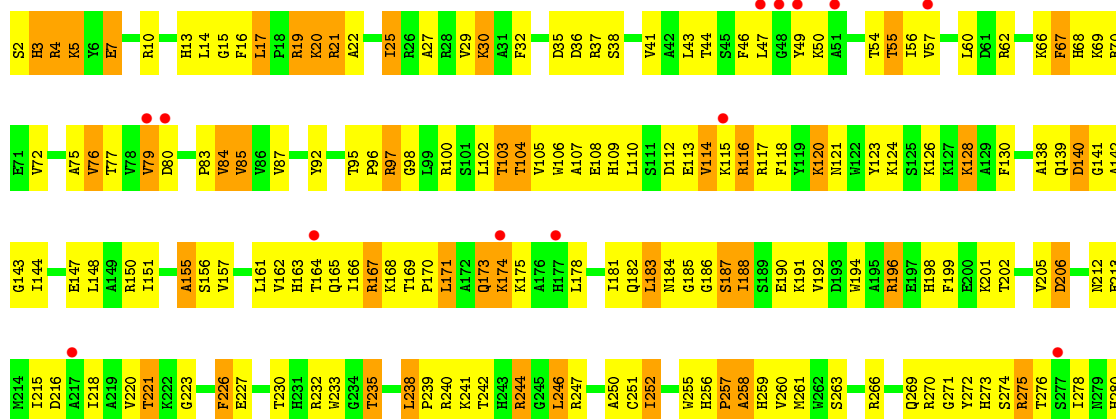
• Molecule 39: 60S ribosomal protein L2-A

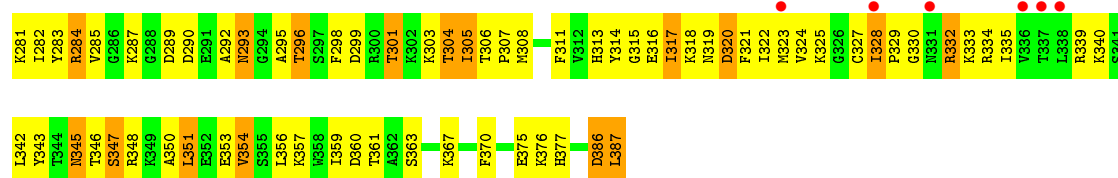


• Molecule 39: 60S ribosomal protein L2-A

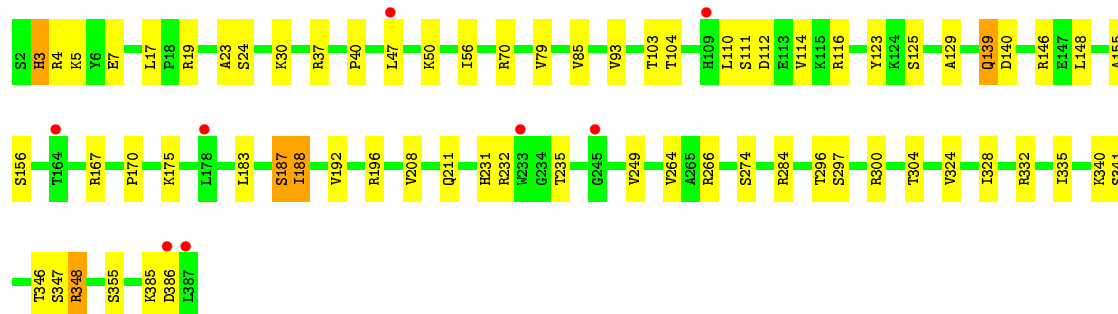
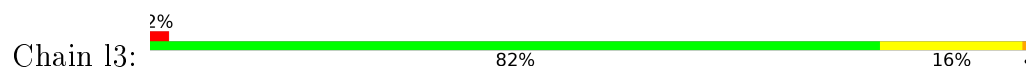


• Molecule 40: 60S ribosomal protein L3

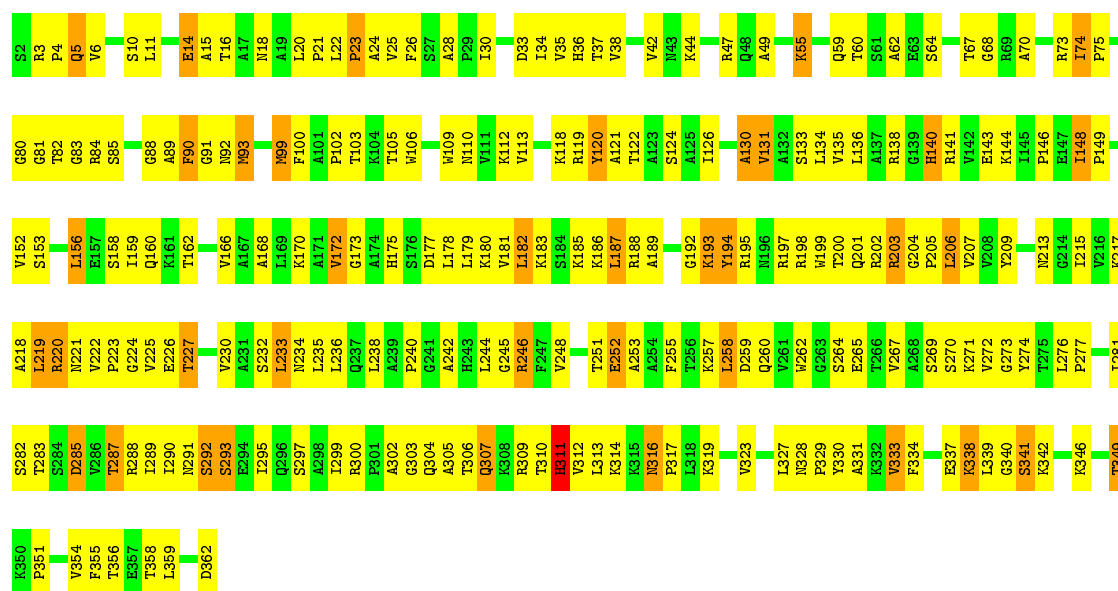




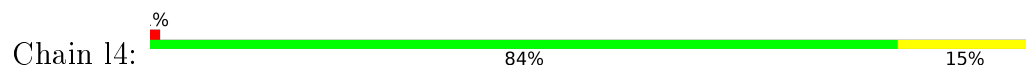
• Molecule 40: 60S ribosomal protein L3

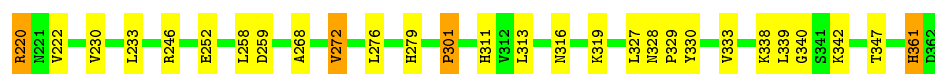


• Molecule 41: 60S ribosomal protein L4-A

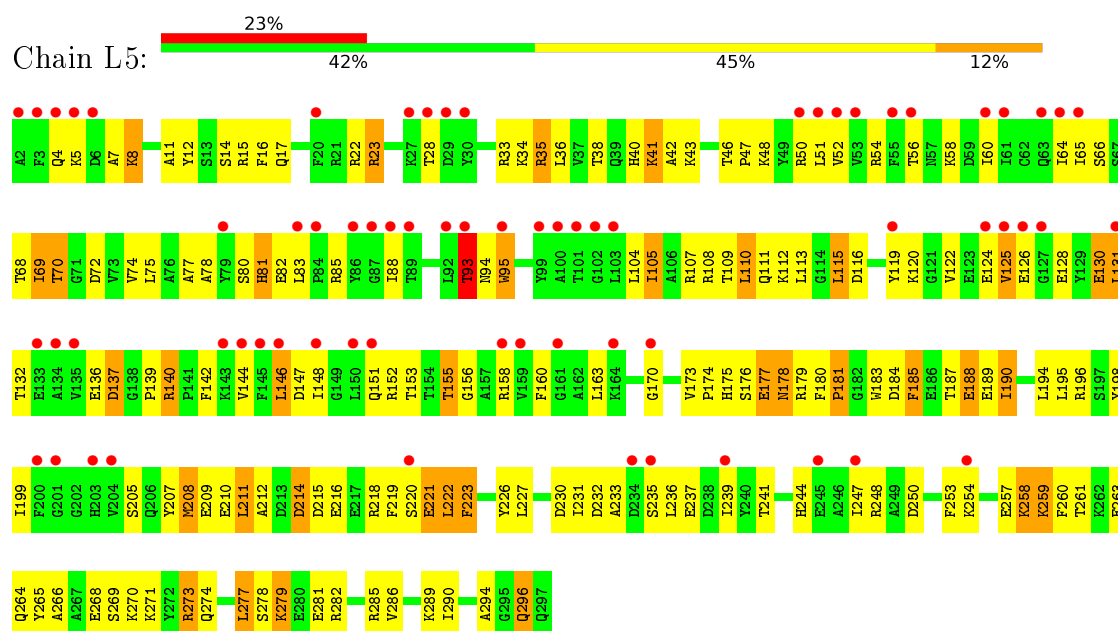


• Molecule 41: 60S ribosomal protein L4-A

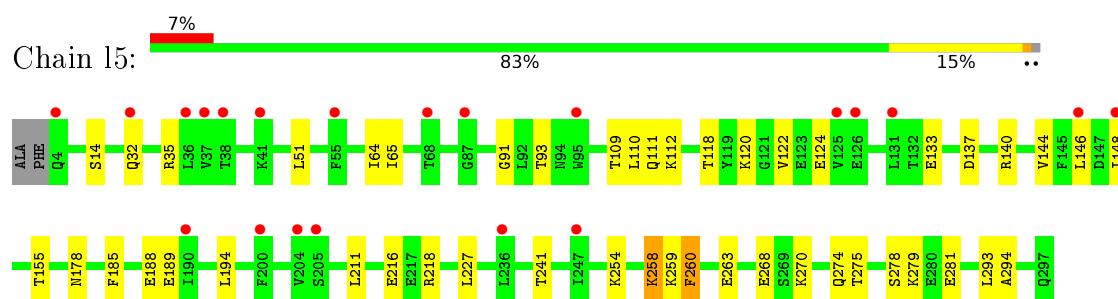




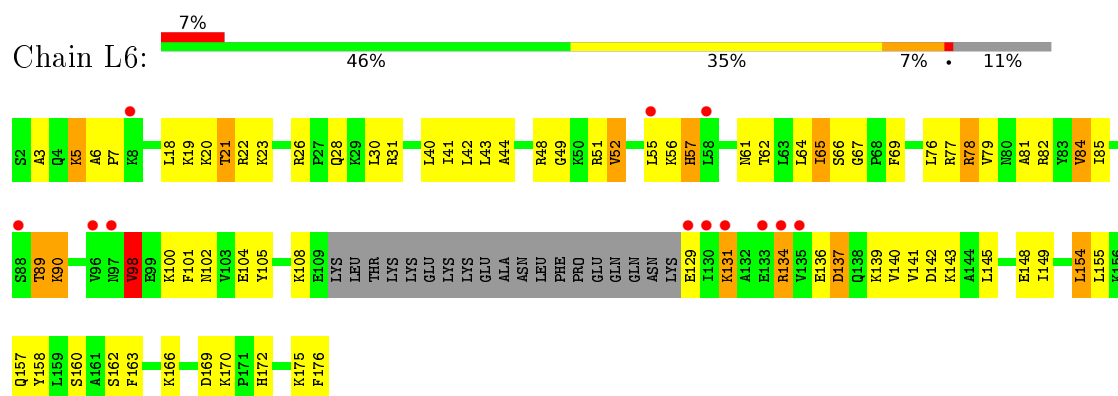
• Molecule 42: 60S ribosomal protein L5



• Molecule 42: 60S ribosomal protein L5

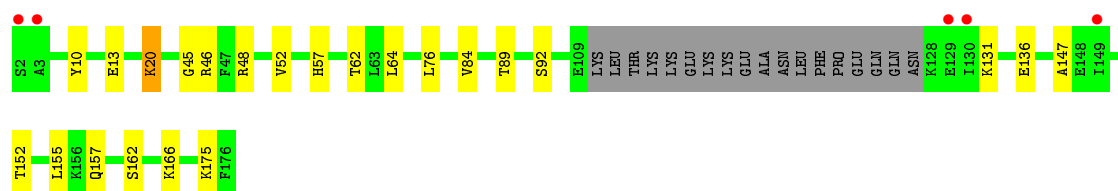


• Molecule 43: 60S ribosomal protein L6-A

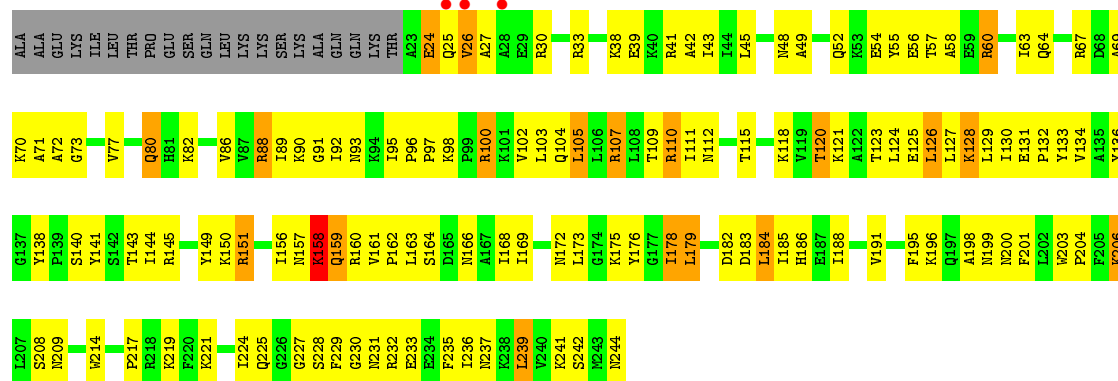


• Molecule 43: 60S ribosomal protein L6-A

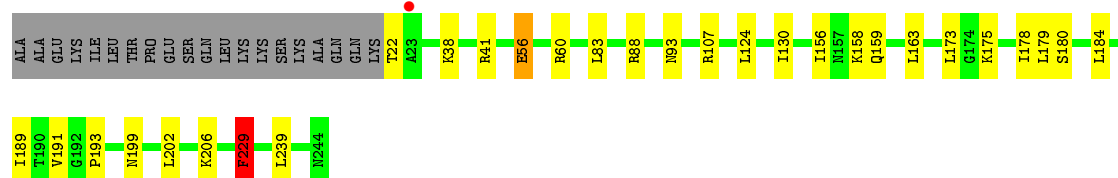
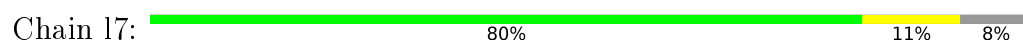




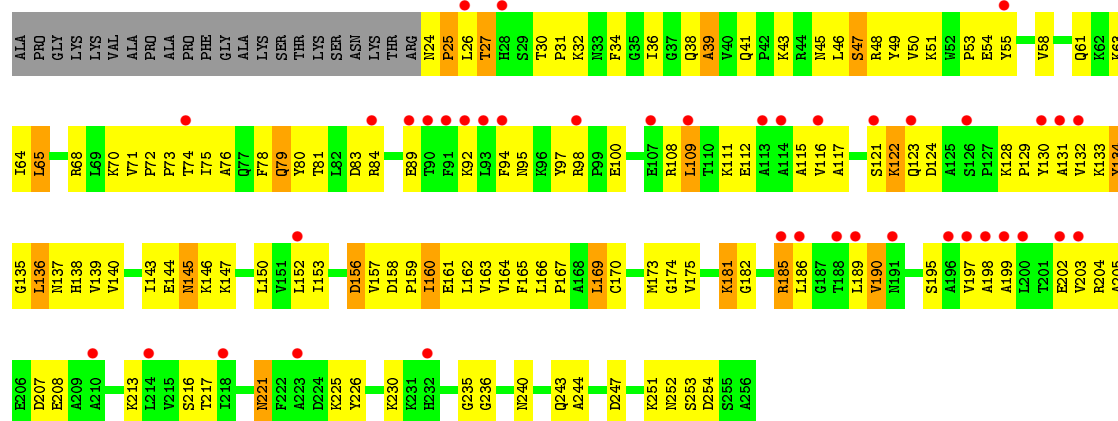
• Molecule 44: 60S ribosomal protein L7-A



• Molecule 44: 60S ribosomal protein L7-A

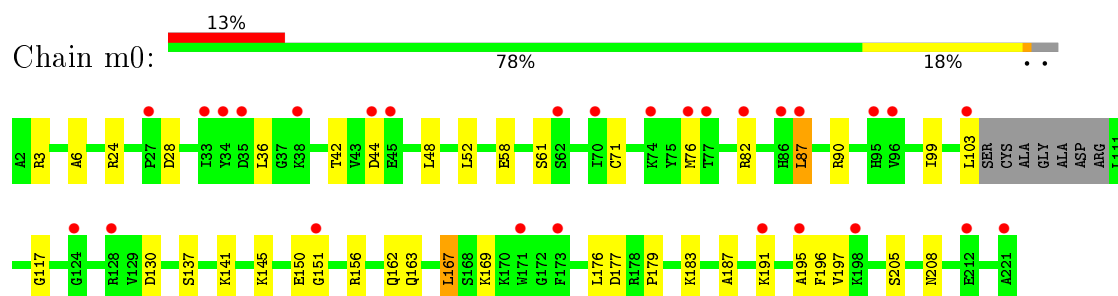


• Molecule 45: 60S ribosomal protein L8-A

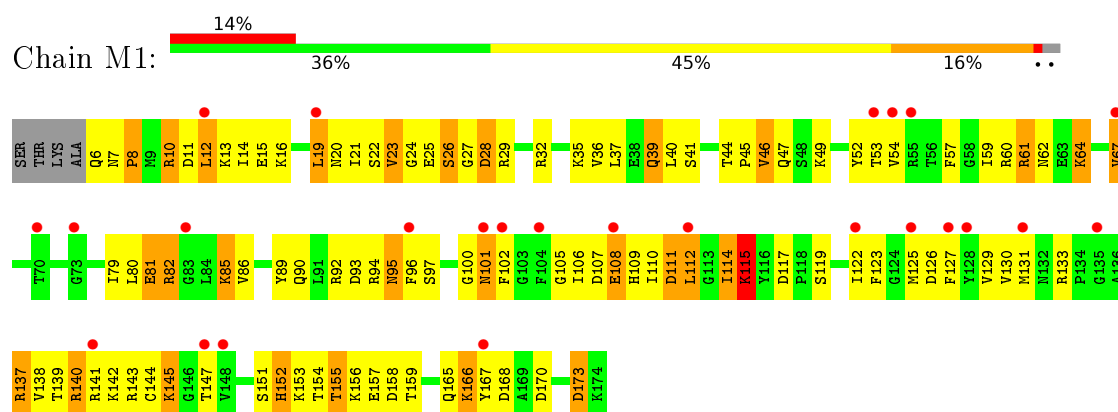


• Molecule 45: 60S ribosomal protein L8-A

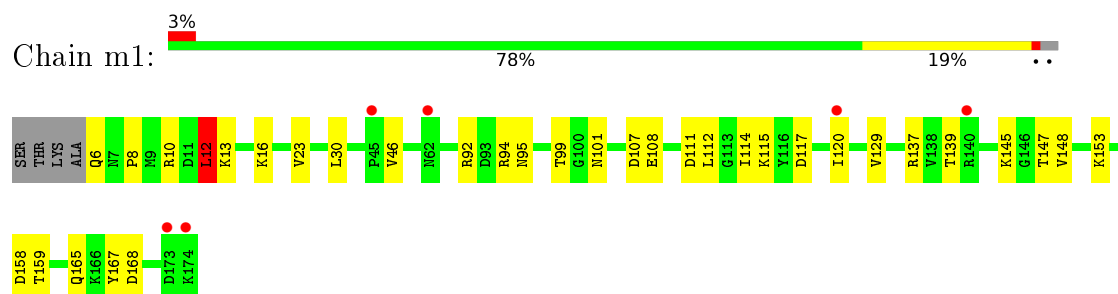
- Molecule 47: 60S ribosomal protein L10



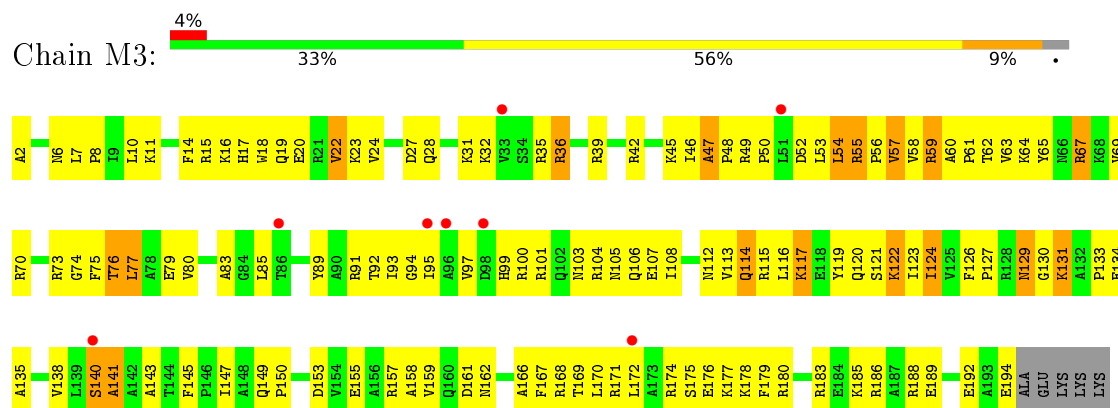
- Molecule 48: 60S ribosomal protein L11-B



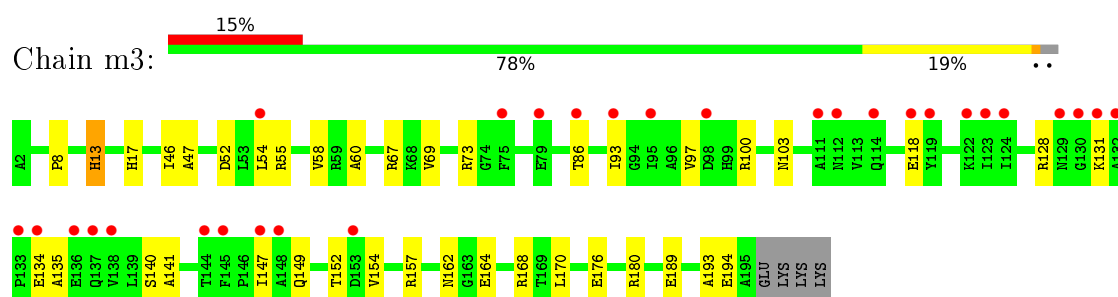
- Molecule 48: 60S ribosomal protein L11-B



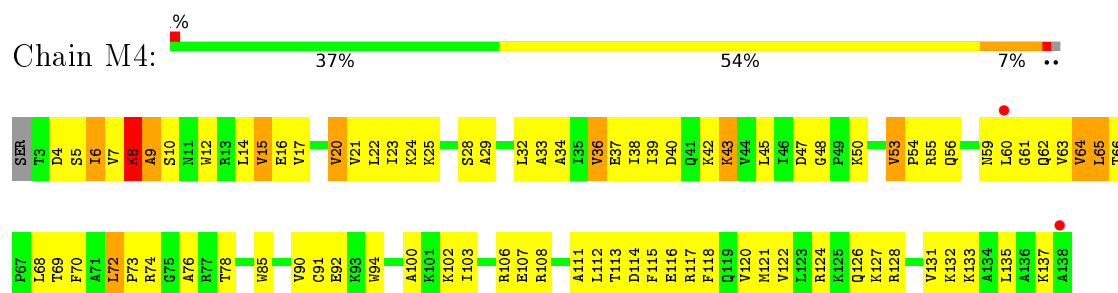
- Molecule 49: 60S ribosomal protein L13-A



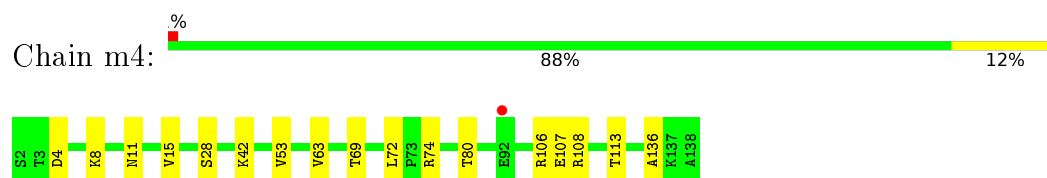
- Molecule 49: 60S ribosomal protein L13-A



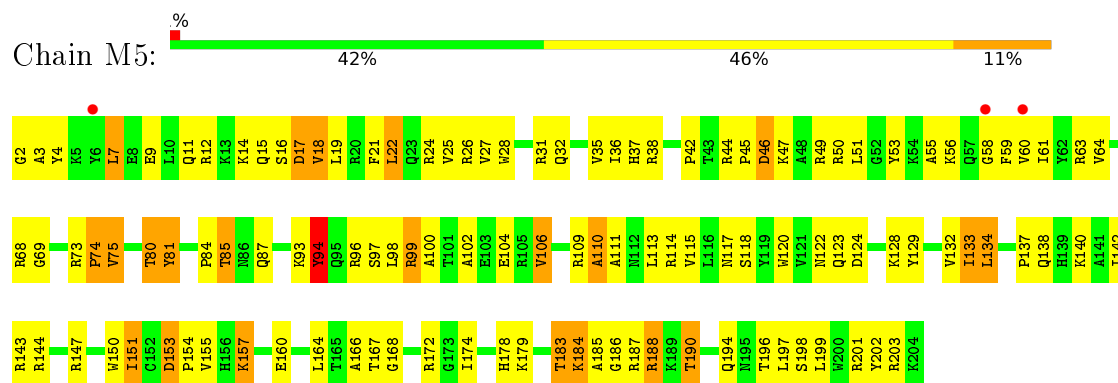
- Molecule 50: 60S ribosomal protein L14-A



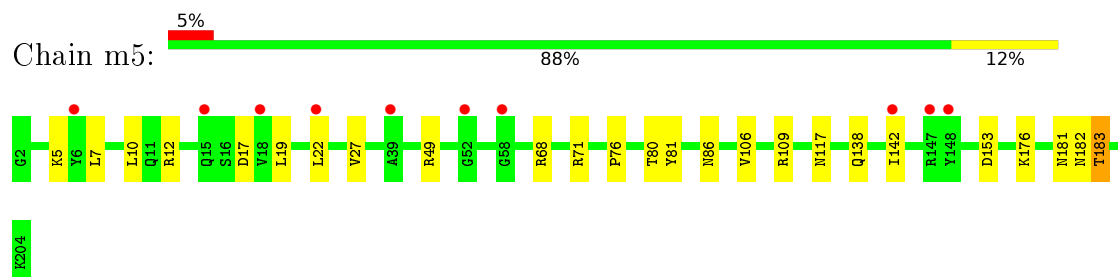
- Molecule 50: 60S ribosomal protein L14-A



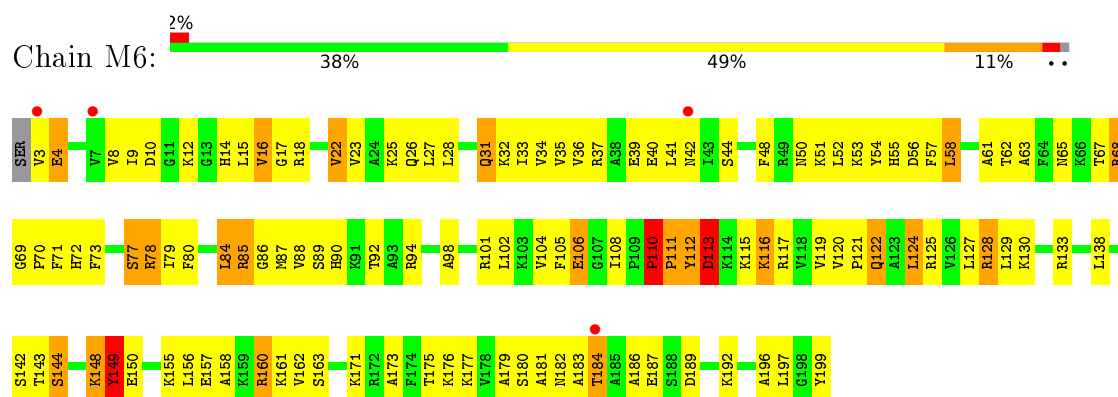
- Molecule 51: 60S ribosomal protein L15-A



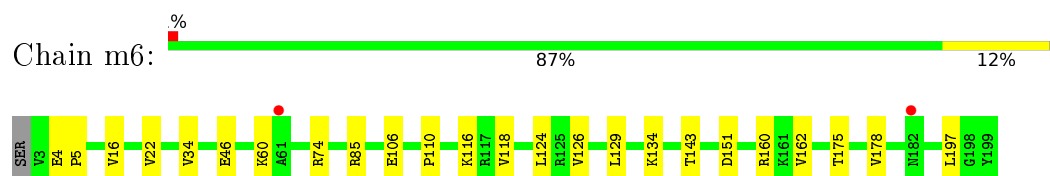
- Molecule 51: 60S ribosomal protein L15-A



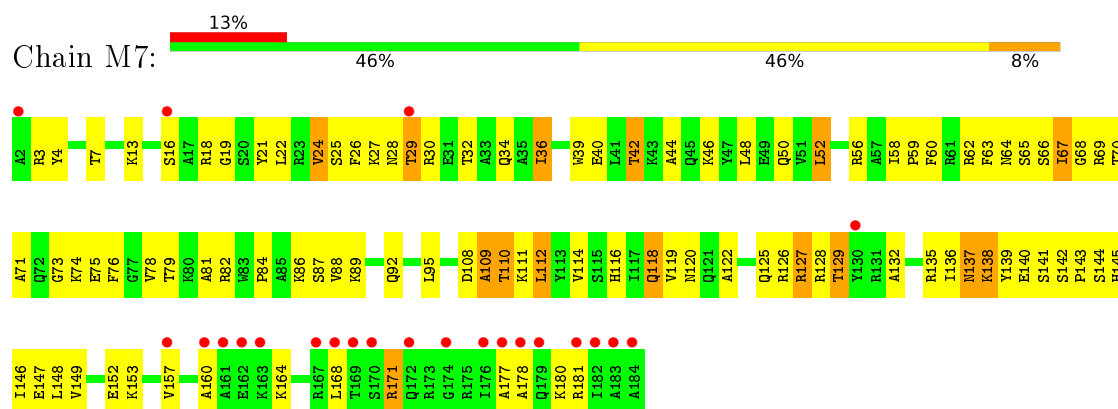
- Molecule 52: 60S ribosomal protein L16-A



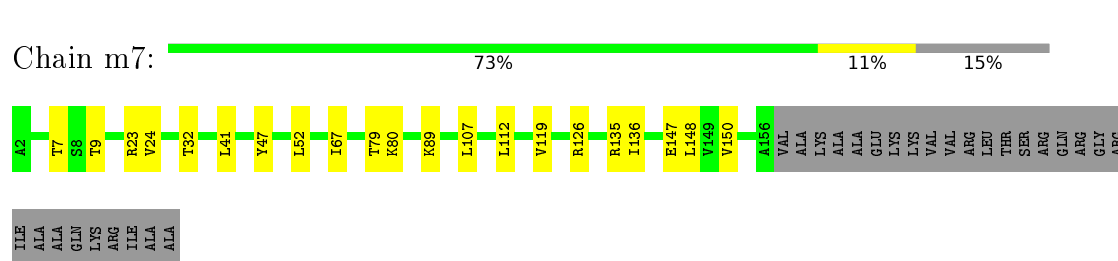
• Molecule 52: 60S ribosomal protein L16-A



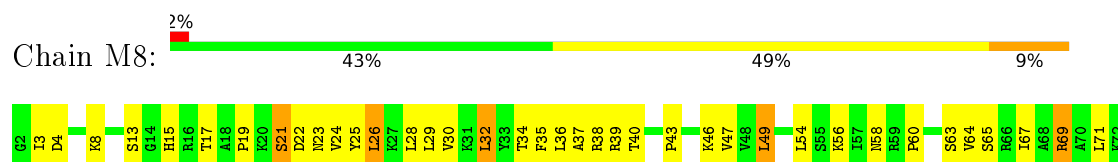
• Molecule 53: 60S ribosomal protein L17-A

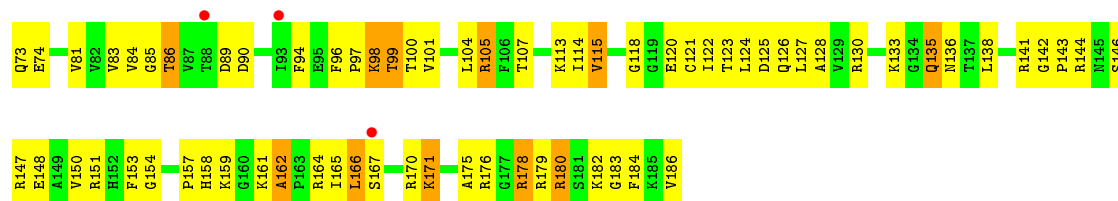


• Molecule 53: 60S ribosomal protein L17-A



• Molecule 54: 60S ribosomal protein L18-A





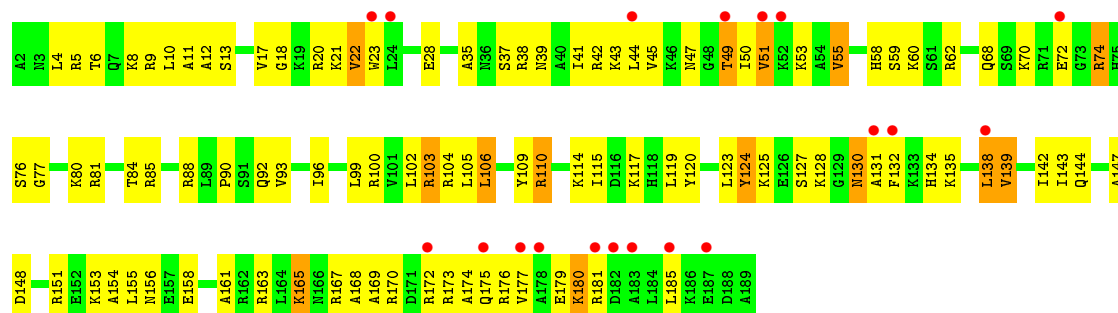
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 83% 16%



• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 10% 45% 48% 7%



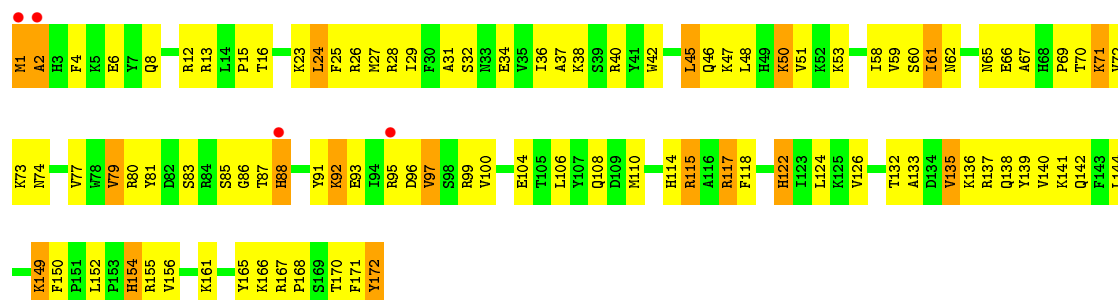
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 6% 88% 12%

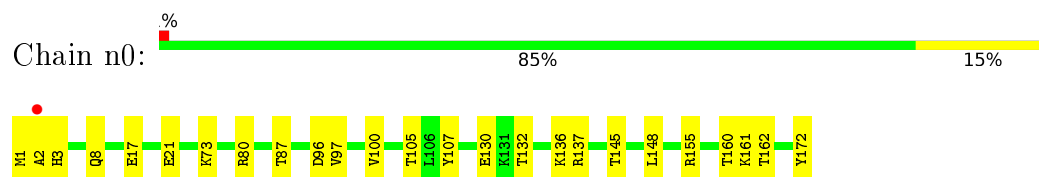


• Molecule 56: 60S ribosomal protein L20-A

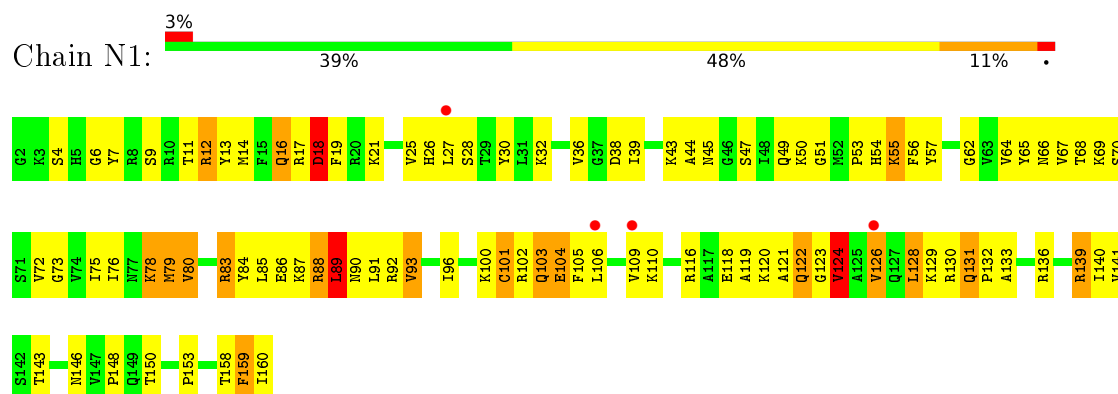
Chain N0: 2% 43% 47% 10%



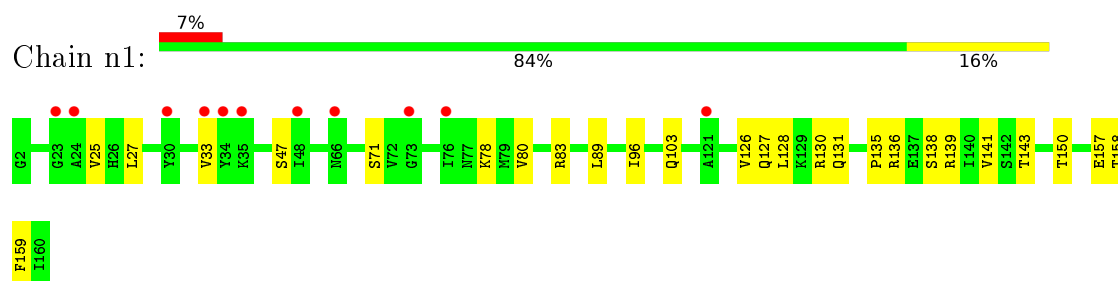
- Molecule 56: 60S ribosomal protein L20-A



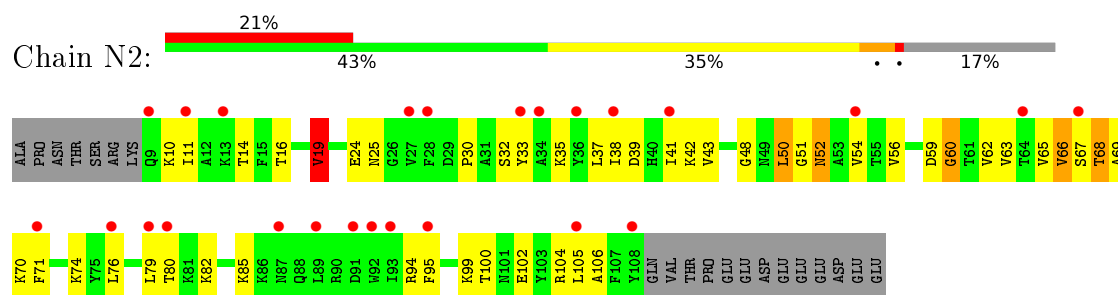
- Molecule 57: 60S ribosomal protein L21-A



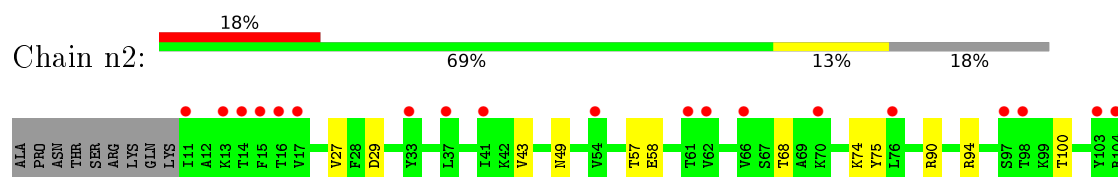
- Molecule 57: 60S ribosomal protein L21-A

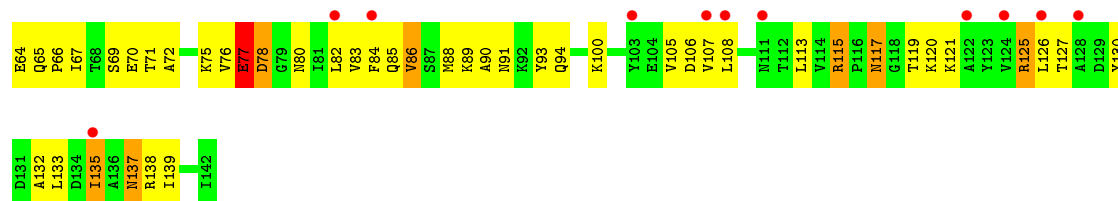


- Molecule 58: 60S ribosomal protein L22-A

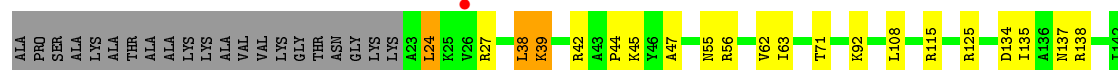


- Molecule 58: 60S ribosomal protein L22-A

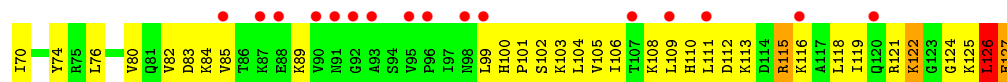
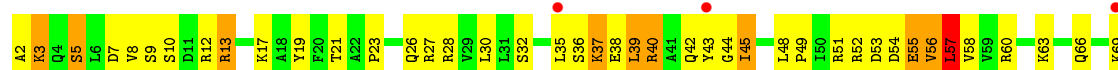
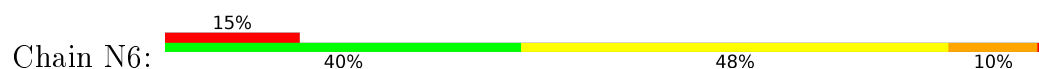




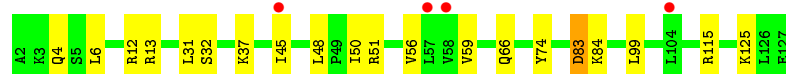
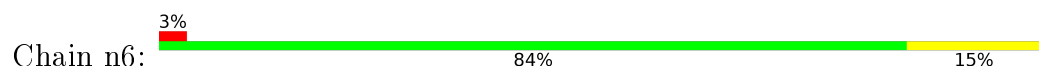
- Molecule 61: 60S ribosomal protein L25



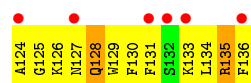
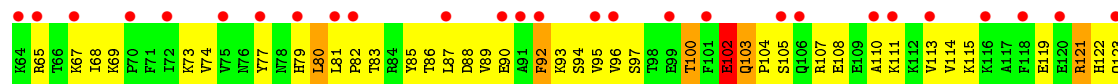
- Molecule 62: 60S ribosomal protein L26-A



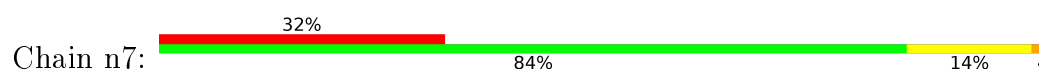
- Molecule 62: 60S ribosomal protein L26-A

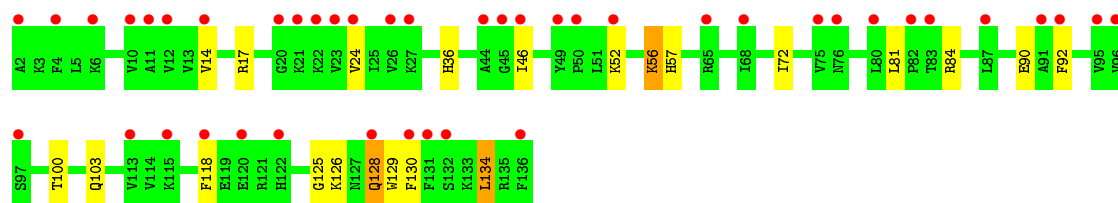


- Molecule 63: 60S ribosomal protein L27-A

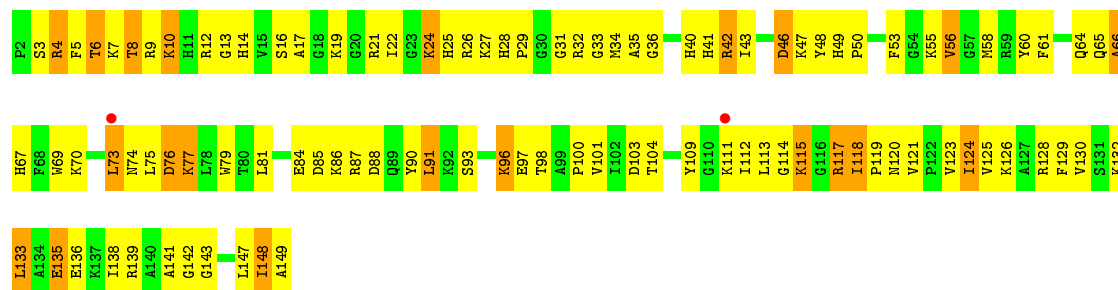


- Molecule 63: 60S ribosomal protein L27-A

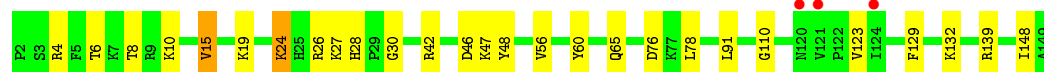
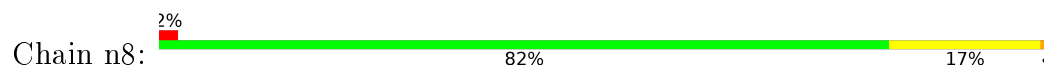




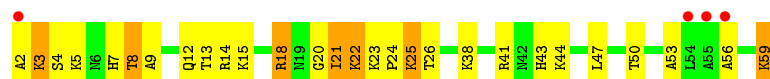
• Molecule 64: 60S ribosomal protein L28



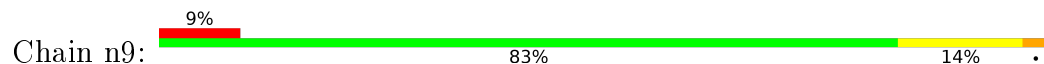
• Molecule 64: 60S ribosomal protein L28



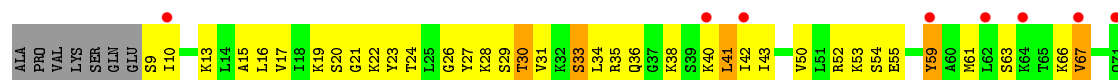
• Molecule 65: 60S ribosomal protein L29

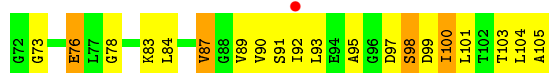


• Molecule 65: 60S ribosomal protein L29

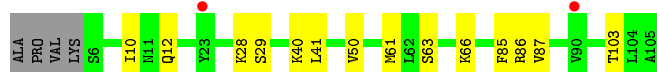
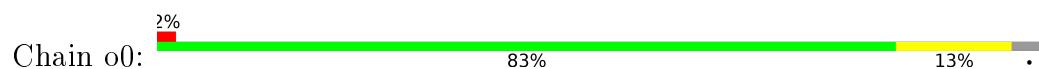


• Molecule 66: 60S ribosomal protein L30

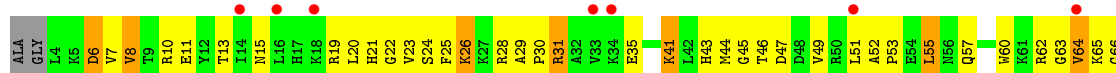
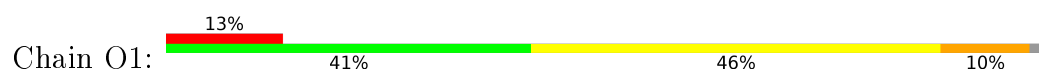




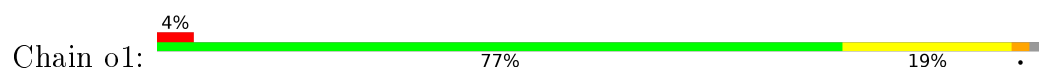
- Molecule 66: 60S ribosomal protein L30



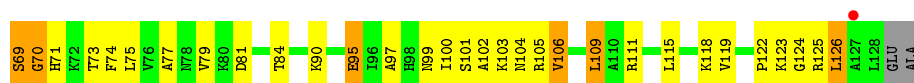
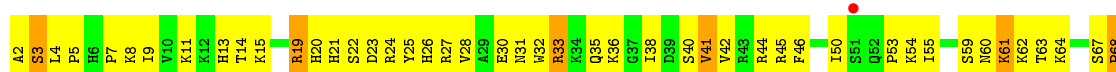
- Molecule 67: 60S ribosomal protein L31-A



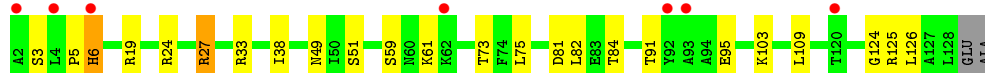
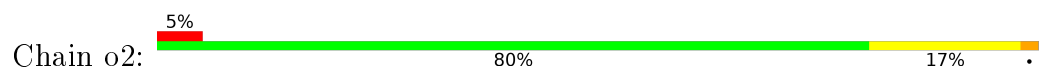
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32

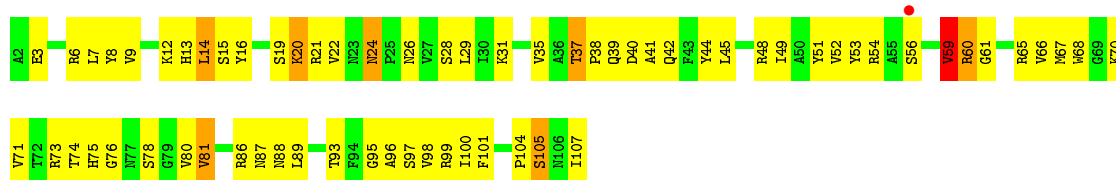


- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A





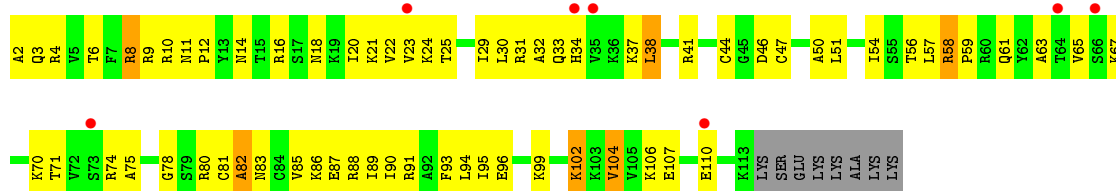
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 85% 15%



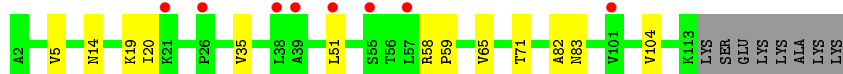
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 6% 38% 51% 5% 7%



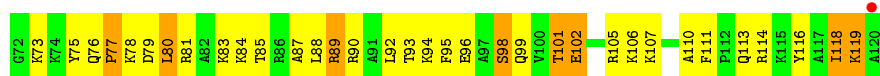
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 7% 83% 11% 7%



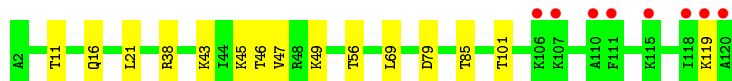
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 5% 38% 50% 13%

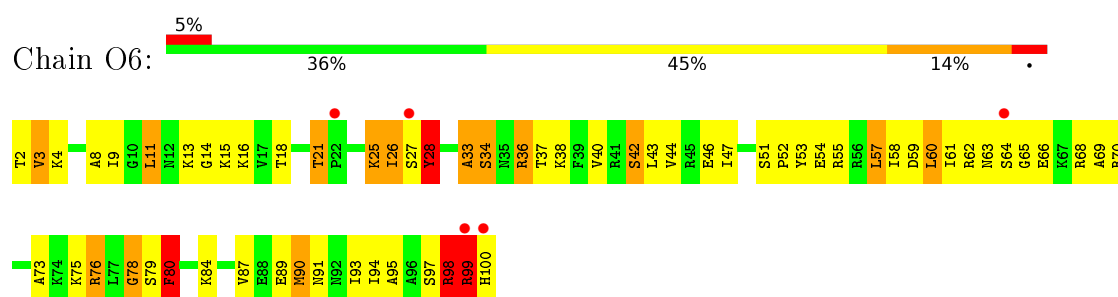


- Molecule 71: 60S ribosomal protein L35-A

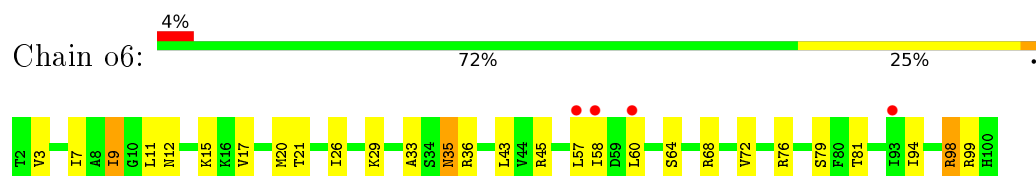
Chain o5: 7% 87% 13%



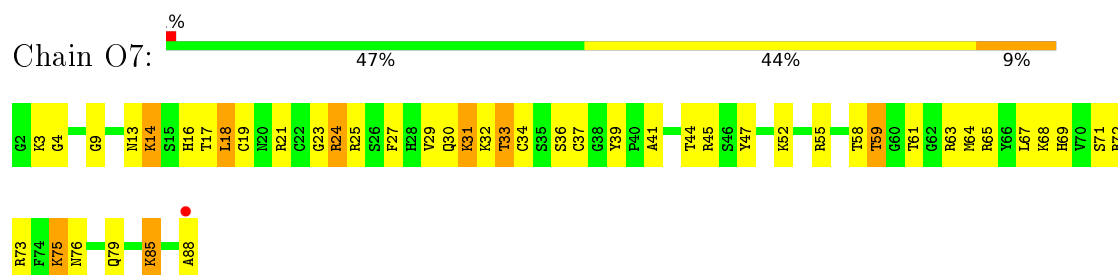
- Molecule 72: 60S ribosomal protein L36-A



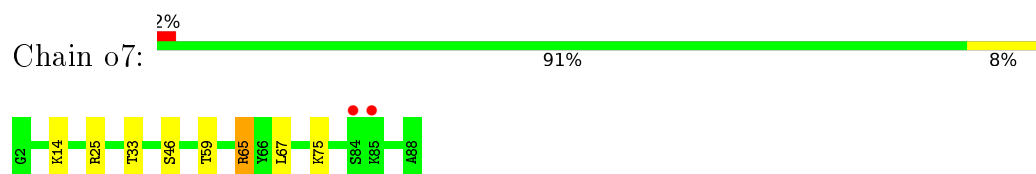
- Molecule 72: 60S ribosomal protein L36-A



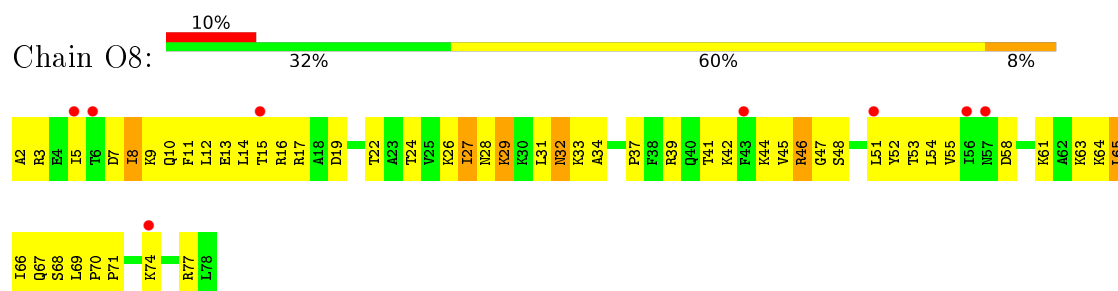
- Molecule 73: 60S ribosomal protein L37-A



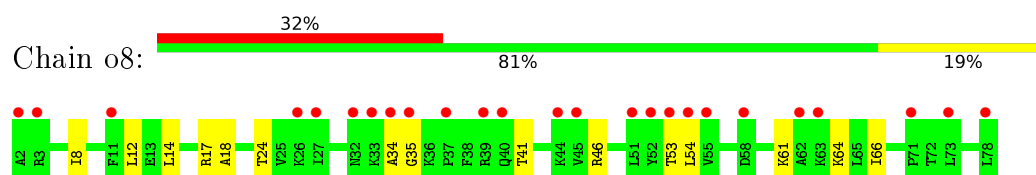
- Molecule 73: 60S ribosomal protein L37-A



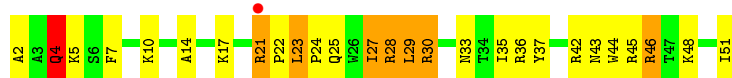
- Molecule 74: 60S ribosomal protein L38



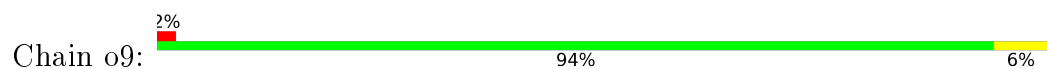
- Molecule 74: 60S ribosomal protein L38



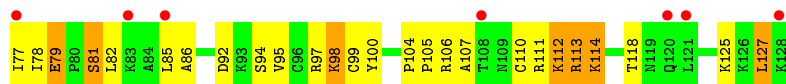
- Molecule 75: 60S ribosomal protein L39



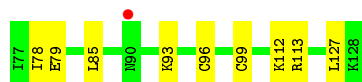
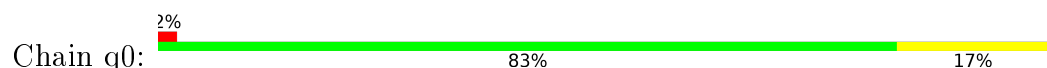
- Molecule 75: 60S ribosomal protein L39



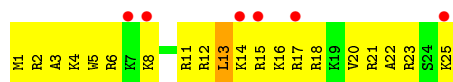
- Molecule 76: Ubiquitin-60S ribosomal protein L40



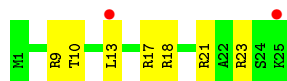
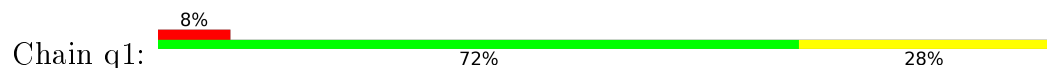
- Molecule 76: Ubiquitin-60S ribosomal protein L40



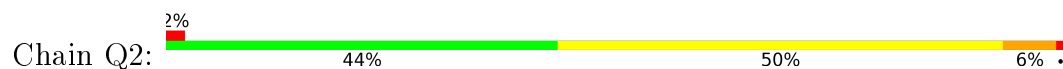
- Molecule 77: 60S ribosomal protein L41-A

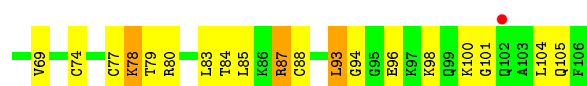


- Molecule 77: 60S ribosomal protein L41-A

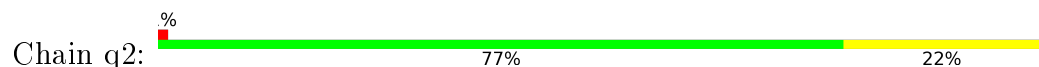


- Molecule 78: 60S ribosomal protein L42-A

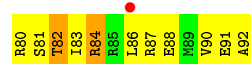
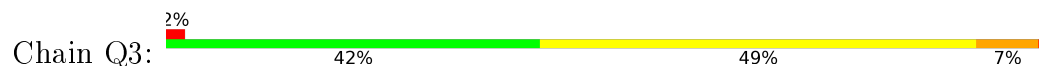




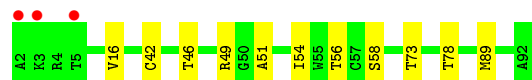
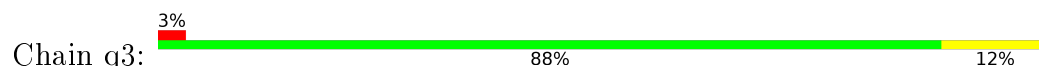
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



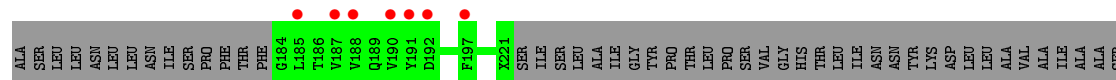
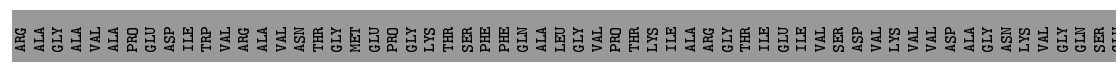
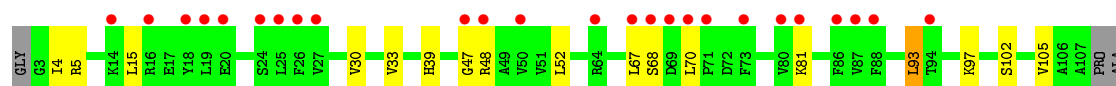
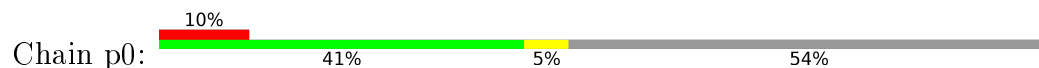
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 60S ribosomal protein L12-A (uL11)



- Molecule 81: 60S acidic ribosomal protein P0



TYR	HIS	TYR	PRO	GLU	ILE	GLU	ASP	LEU	VAL	ASP	ARG	ILE	GLU	ASN	PRO	GLU	LYS	TYR	ALA	ALA	ALA	ALA	ALA	PRO	ALA	ALA	THR	SER	ALA	SER	GLY	ASP	ALA	ALA	PRO	ALA	GLU	GLU	ALA	ALA	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	ASP	ASP	MET	GLY	PHE	GLY	LEU	PHE	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain p1:  100%


There are no outlier residues recorded for this chain.

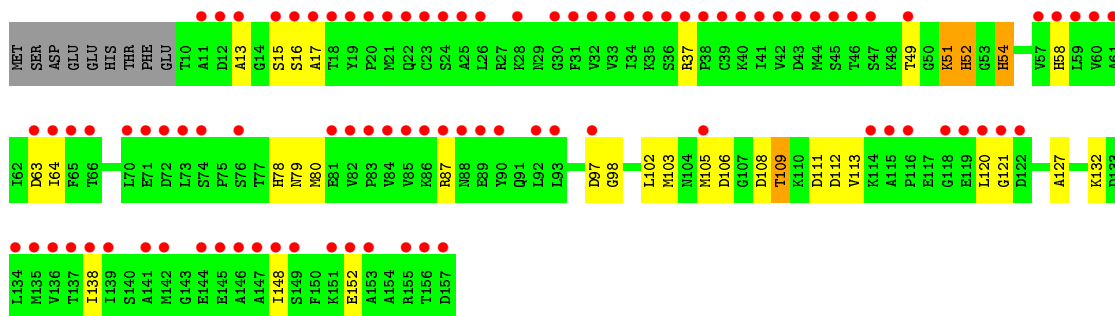
- Molecule 82: 60S ribosomal protein P1 alpha/P2 beta

Chain p2:  98%



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

Chain f:  59% 73% 19% 6%



- Molecule 84: CH-CH-8AN-PRO-PRO

Chain B:  40% 60%



- Molecule 84: CH-CH-8AN-PRO-PRO

Chain C:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.58 Å 287.33 Å 303.82 Å 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 3.33 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.310 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 74.2	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: ZN, CH, SPS, MG, OHX, 8AN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.36	0/42467	0.89	42/66169 (0.1%)
1	6	0.43	0/42790	0.93	50/66673 (0.1%)
2	S0	0.28	0/1617	0.50	0/2215
2	s0	0.29	0/1623	0.51	0/2222
3	S1	0.26	0/1735	0.50	0/2335
3	s1	0.32	0/1748	0.53	0/2352
4	S2	0.30	0/1665	0.52	0/2263
4	s2	0.33	0/1665	0.55	1/2263 (0.0%)
5	S3	0.29	0/1759	0.47	0/2368
5	s3	0.27	0/1759	0.47	0/2368
6	S4	0.29	0/2109	0.53	0/2839
6	s4	0.34	0/2109	0.55	0/2839
7	S5	0.27	0/1629	0.50	0/2202
7	s5	0.28	0/1629	0.48	0/2202
8	S6	0.29	0/1823	0.47	0/2439
8	s6	0.33	0/1779	0.53	0/2379
9	S7	0.28	0/1506	0.53	1/2028 (0.0%)
9	s7	0.29	0/1516	0.52	0/2043
10	S8	0.30	0/1514	0.51	0/2021
10	s8	0.34	0/1514	0.52	0/2021
11	S9	0.29	0/1519	0.48	0/2035
11	s9	0.31	0/1519	0.50	0/2035
12	C0	0.28	0/725	0.44	0/978
12	c0	0.27	0/713	0.51	1/961 (0.1%)
13	C1	0.31	0/1185	0.50	0/1598
13	c1	0.36	0/1185	0.55	0/1598
14	C2	0.26	0/819	0.49	0/1109
14	c2	0.22	0/819	0.47	0/1109
15	C3	0.31	0/1215	0.52	1/1638 (0.1%)
15	c3	0.33	0/1215	0.51	0/1638
16	C4	0.26	0/901	0.51	0/1217
16	c4	0.30	0/960	0.54	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.31	0/988	0.54	0/1327
17	c5	0.29	0/1030	0.52	0/1384
18	C6	0.29	0/1125	0.54	2/1510 (0.1%)
18	c6	0.29	0/1131	0.51	0/1518
19	C7	0.30	0/935	0.52	0/1254
19	c7	0.27	0/914	0.50	0/1224
20	C8	0.30	0/1211	0.51	0/1628
20	c8	0.28	0/1211	0.49	0/1628
21	C9	0.29	0/1130	0.48	0/1517
21	c9	0.29	0/1130	0.47	0/1517
22	D0	0.30	0/865	0.52	0/1169
22	d0	0.29	0/892	0.49	0/1205
23	D1	0.29	0/693	0.49	0/935
23	d1	0.31	0/693	0.50	0/935
24	D2	0.30	0/1038	0.55	1/1395 (0.1%)
24	d2	0.35	0/1038	0.56	1/1395 (0.1%)
25	D3	0.35	0/1139	0.55	0/1518
25	d3	0.38	0/1139	0.57	0/1518
26	D4	0.29	0/1087	0.47	0/1449
26	d4	0.31	0/1087	0.51	0/1449
27	D5	0.26	0/571	0.55	0/768
27	d5	0.26	0/566	0.47	0/761
28	D6	0.29	0/782	0.53	0/1047
28	d6	0.34	0/782	0.53	0/1047
29	D7	0.29	0/620	0.51	0/838
29	d7	0.28	0/620	0.49	0/838
30	D8	0.27	0/499	0.47	0/670
30	d8	0.28	0/499	0.49	0/670
31	D9	0.32	0/452	0.55	1/600 (0.2%)
31	d9	0.33	0/452	0.50	0/600
32	E0	0.28	0/483	0.48	0/643
32	e0	0.32	0/499	0.54	0/665
33	E1	0.29	0/577	0.56	0/770
33	e1	0.29	0/619	0.58	0/822
34	SR	0.26	0/2490	0.49	0/3389
34	sR	0.25	0/2495	0.44	0/3395
35	SM	0.31	0/925	0.54	1/1240 (0.1%)
35	sM	0.31	0/480	0.53	0/642
36	1	0.56	0/75394	1.03	115/117545 (0.1%)
36	5	0.59	2/75865 (0.0%)	1.05	143/118275 (0.1%)
37	3	0.46	0/2883	0.91	0/4491
37	7	0.55	0/2883	1.00	2/4491 (0.0%)
38	4	0.53	0/3746	1.00	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.52	0/3746	0.97	2/5832 (0.0%)
39	L2	0.37	0/1948	0.57	0/2617
39	l2	0.40	0/1946	0.62	0/2614
40	L3	0.39	0/3146	0.56	0/4228
40	l3	0.45	0/3146	0.58	0/4228
41	L4	0.41	0/2800	0.61	0/3790
41	l4	0.41	1/2800 (0.0%)	0.63	2/3790 (0.1%)
42	L5	0.35	0/2425	0.53	0/3271
42	l5	0.42	0/2408	0.55	0/3248
43	L6	0.39	0/1260	0.55	0/1694
43	l6	0.41	0/1269	0.57	0/1705
44	L7	0.42	0/1821	0.59	0/2451
44	l7	0.43	0/1828	0.62	2/2461 (0.1%)
45	L8	0.31	0/1836	0.53	0/2481
45	l8	0.32	0/1796	0.51	0/2431
46	L9	0.36	0/1539	0.56	0/2073
46	l9	0.40	0/1539	0.57	0/2073
47	M0	0.40	1/1741 (0.1%)	0.55	0/2335
47	m0	0.43	0/1758	0.61	2/2358 (0.1%)
48	M1	0.31	0/1374	0.50	0/1842
48	m1	0.38	0/1374	0.59	1/1842 (0.1%)
49	M3	0.40	0/1568	0.59	0/2106
49	m3	0.37	0/1573	0.57	0/2113
50	M4	0.40	0/1068	0.54	0/1438
50	m4	0.41	0/1074	0.57	0/1446
51	M5	0.38	0/1757	0.56	0/2354
51	m5	0.36	0/1757	0.55	0/2354
52	M6	0.44	0/1585	0.59	0/2128
52	m6	0.50	0/1585	0.61	0/2128
53	M7	0.41	0/1443	0.58	0/1944
53	m7	0.44	0/1250	0.59	0/1683
54	M8	0.39	0/1465	0.60	0/1965
54	m8	0.39	0/1465	0.60	0/1965
55	M9	0.31	0/1538	0.49	0/2050
55	m9	0.34	0/1538	0.51	0/2050
56	N0	0.39	0/1481	0.56	0/1990
56	n0	0.44	0/1481	0.59	0/1990
57	N1	0.40	0/1300	0.56	1/1743 (0.1%)
57	n1	0.43	0/1300	0.55	0/1743
58	N2	0.30	0/812	0.48	0/1099
58	n2	0.32	0/794	0.52	0/1076
59	N3	0.39	0/1018	0.57	0/1369
59	n3	0.45	0/1018	0.61	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.31	0/712	0.50	0/958
60	n4	0.35	0/1052	0.51	0/1398
61	N5	0.33	0/979	0.55	0/1321
61	n5	0.36	0/974	0.57	0/1314
62	N6	0.35	0/1004	0.62	2/1341 (0.1%)
62	n6	0.35	0/1004	0.57	0/1341
63	N7	0.30	0/1118	0.50	0/1497
63	n7	0.31	0/1118	0.51	0/1497
64	N8	0.41	0/1204	0.62	0/1612
64	n8	0.40	0/1204	0.61	0/1612
65	N9	0.38	0/473	0.60	0/629
65	n9	0.43	0/473	0.67	0/629
66	O0	0.30	0/751	0.47	0/1008
66	o0	0.31	0/775	0.52	0/1040
67	O1	0.34	0/890	0.52	0/1196
67	o1	0.41	0/897	0.60	0/1205
68	O2	0.43	0/1041	0.63	0/1394
68	o2	0.44	0/1041	0.62	0/1394
69	O3	0.48	0/868	0.56	0/1168
69	o3	0.48	0/868	0.58	0/1168
70	O4	0.34	0/890	0.54	0/1189
70	o4	0.34	0/890	0.58	0/1189
71	O5	0.37	0/978	0.57	0/1301
71	o5	0.34	0/974	0.53	0/1297
72	O6	0.37	0/778	0.60	0/1034
72	o6	0.34	0/777	0.54	0/1033
73	O7	0.42	0/696	0.61	0/923
73	o7	0.40	0/696	0.59	0/923
74	O8	0.30	0/618	0.47	0/826
74	o8	0.31	0/614	0.54	0/822
75	O9	0.39	0/443	0.58	0/588
75	o9	0.39	0/443	0.53	0/588
76	Q0	0.43	0/423	0.60	0/562
76	q0	0.45	0/423	0.55	0/562
77	Q1	0.36	0/234	0.59	0/300
77	q1	0.43	0/234	0.62	0/300
78	Q2	0.53	1/860 (0.1%)	0.63	0/1136
78	q2	0.52	1/860 (0.1%)	0.63	1/1136 (0.1%)
79	Q3	0.37	0/701	0.59	0/934
79	q3	0.43	0/701	0.56	0/934
81	p0	0.27	0/977	0.48	0/1313
83	f	0.34	0/1131	0.58	0/1522
84	B	0.31	0/15	0.54	0/20

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
84	C	0.41	0/15	0.80	0/20
All	All	0.46	6/431576 (0.0%)	0.85	380/633602 (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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	8.77	1.97	1.82
78	Q2	17	CYS	CB-SG	7.99	1.95	1.82
36	5	1152	G	N9-C4	-5.86	1.33	1.38
36	5	942	U	C4-O4	5.25	1.27	1.23
47	M0	8	CYS	CB-SG	-5.03	1.73	1.81

The worst 5 of 380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-11.60	119.04	126.00
36	5	1152	G	N3-C4-C5	11.31	134.25	128.60
36	5	2726	C	C6-N1-C2	-9.68	116.43	120.30
36	5	1152	G	C2-N3-C4	-9.61	107.10	111.90
36	1	406	G	O4'-C1'-N9	9.54	115.83	108.20

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
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	823	0
1	6	38260	0	19252	792	0
2	S0	1577	0	1567	142	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	128	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	138	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	116	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	182	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	118	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	109	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	114	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	114	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	151	0
11	s9	1494	0	1573	0	0
12	C0	773	0	714	57	0
12	c0	762	0	689	0	0
13	C1	1214	0	1237	85	0
13	c1	1168	0	1226	0	0
14	C2	892	0	872	64	0
14	c2	892	0	869	0	0
15	C3	1192	0	1255	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	c3	1192	0	1255	0	0
16	C4	891	0	883	78	0
16	c4	949	0	985	0	0
17	C5	977	0	1004	82	0
17	c5	1039	0	1041	0	0
18	C6	1105	0	1166	85	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	85	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	100	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	86	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	71	0
22	d0	882	0	939	0	0
23	D1	684	0	672	75	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	97	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	90	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	91	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	52	0
27	d5	558	0	598	0	0
28	D6	769	0	814	80	0
28	d6	769	0	814	0	0
29	D7	610	0	630	41	0
29	d7	610	0	631	0	0
30	D8	497	0	535	43	0
30	d8	497	0	535	0	0
31	D9	442	0	428	32	0
31	d9	442	0	428	0	0
32	E0	475	0	525	29	0
32	e0	491	0	542	0	0
33	E1	566	0	602	49	0
33	e1	608	0	657	0	0
34	SR	2437	0	2386	150	0
34	sR	2442	0	2392	0	1
35	SM	1105	0	959	67	0
35	sM	680	0	542	0	0
36	1	67355	0	33848	1240	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	67780	0	34065	1205	0
37	3	2579	0	1304	61	0
37	7	2579	0	1304	46	0
38	4	3353	0	1695	59	0
38	8	3353	0	1695	70	0
39	L2	1914	0	1981	172	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	240	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	219	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	188	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	79	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	131	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	114	0
45	l8	1764	0	1821	0	0
46	L9	1518	0	1587	120	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	146	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	81	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	137	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	82	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	139	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	106	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	100	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	108	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	112	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	98	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	n1	1276	0	1323	0	0
58	N2	796	0	812	38	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	72	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	43	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	71	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	79	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	93	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	108	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	34	0
65	n9	462	0	491	0	0
66	O0	743	0	797	51	0
66	o0	767	0	816	0	0
67	O1	876	0	912	60	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	76	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	64	0
69	o3	850	0	880	0	0
70	O4	880	0	945	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	92	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	69	0
72	o6	770	0	846	0	0
73	O7	681	0	683	53	0
73	o7	681	0	683	0	0
74	O8	612	0	682	42	0
74	o8	608	0	671	0	0
75	O9	436	0	475	33	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	23	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	22	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	q2	847	0	914	0	0
79	Q3	694	0	734	56	0
79	q3	694	0	734	0	0
80	m2	750	0	185	0	0
81	p0	1077	0	1012	0	0
82	p1	235	0	53	0	0
82	p2	230	0	52	0	0
83	f	1116	0	1108	0	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	2	0
86	B	23	0	18	3	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	9280	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 9280 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)
1:6:104:A:H61	1:6:308:C:H5'	1.29	0.96
1:2:1456:C:H5''	1:2:1457:C:H5''	1.49	0.94
34:SR:82:SER:HG	34:SR:92:TRP:HE1	2.15	0.94
36:5:438:A:N1	36:5:621:A:N6	2.17	0.92
36:5:3274:A:H3'	36:5:3275:U:H5''	1.51	0.92

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	3
2	s0	204/251 (81%)	164 (80%)	25 (12%)	15 (7%)	1	10
3	S1	212/254 (84%)	152 (72%)	38 (18%)	22 (10%)	1	4
3	s1	214/254 (84%)	168 (78%)	33 (15%)	13 (6%)	2	14
4	S2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1	13
4	s2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1	13
5	S3	221/239 (92%)	187 (85%)	26 (12%)	8 (4%)	4	28
5	s3	221/239 (92%)	176 (80%)	35 (16%)	10 (4%)	3	21
6	S4	258/260 (99%)	202 (78%)	46 (18%)	10 (4%)	4	25
6	s4	258/260 (99%)	189 (73%)	53 (20%)	16 (6%)	2	14
7	S5	204/224 (91%)	155 (76%)	37 (18%)	12 (6%)	2	15
7	s5	204/224 (91%)	160 (78%)	29 (14%)	15 (7%)	1	10
8	S6	224/236 (95%)	193 (86%)	22 (10%)	9 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	s6	216/236 (92%)	182 (84%)	22 (10%)	12 (6%)	2	16
9	S7	182/189 (96%)	134 (74%)	27 (15%)	21 (12%)	0	3
9	s7	184/189 (97%)	152 (83%)	20 (11%)	12 (6%)	1	13
10	S8	184/200 (92%)	151 (82%)	24 (13%)	9 (5%)	3	19
10	s8	184/200 (92%)	157 (85%)	20 (11%)	7 (4%)	4	26
11	S9	183/196 (93%)	149 (81%)	23 (13%)	11 (6%)	2	15
11	s9	183/196 (93%)	147 (80%)	27 (15%)	9 (5%)	3	19
12	C0	82/96 (85%)	71 (87%)	8 (10%)	3 (4%)	4	27
12	c0	82/96 (85%)	56 (68%)	16 (20%)	10 (12%)	0	2
13	C1	143/155 (92%)	116 (81%)	18 (13%)	9 (6%)	2	13
13	c1	143/155 (92%)	115 (80%)	21 (15%)	7 (5%)	3	19
14	C2	107/142 (75%)	70 (65%)	27 (25%)	10 (9%)	1	6
14	c2	107/142 (75%)	75 (70%)	22 (21%)	10 (9%)	1	6
15	C3	148/150 (99%)	124 (84%)	20 (14%)	4 (3%)	6	35
15	c3	148/150 (99%)	116 (78%)	23 (16%)	9 (6%)	2	14
16	C4	125/136 (92%)	81 (65%)	33 (26%)	11 (9%)	1	7
16	c4	126/136 (93%)	96 (76%)	15 (12%)	15 (12%)	0	3
17	C5	121/141 (86%)	95 (78%)	12 (10%)	14 (12%)	0	3
17	c5	128/141 (91%)	98 (77%)	19 (15%)	11 (9%)	1	7
18	C6	139/142 (98%)	116 (84%)	14 (10%)	9 (6%)	1	13
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	2	13
19	C7	116/136 (85%)	82 (71%)	23 (20%)	11 (10%)	1	6
19	c7	113/136 (83%)	93 (82%)	13 (12%)	7 (6%)	2	14
20	C8	143/145 (99%)	116 (81%)	17 (12%)	10 (7%)	1	11
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	3	19
21	C9	141/143 (99%)	115 (82%)	18 (13%)	8 (6%)	2	16
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	3	23
22	D0	105/120 (88%)	89 (85%)	9 (9%)	7 (7%)	1	12
22	d0	108/120 (90%)	89 (82%)	14 (13%)	5 (5%)	3	21
23	D1	85/87 (98%)	66 (78%)	11 (13%)	8 (9%)	1	6
23	d1	85/87 (98%)	63 (74%)	17 (20%)	5 (6%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	D2	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	7	38
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	7	38
25	D3	142/144 (99%)	109 (77%)	21 (15%)	12 (8%)	1	7
25	d3	142/144 (99%)	117 (82%)	20 (14%)	5 (4%)	4	29
26	D4	132/134 (98%)	109 (83%)	13 (10%)	10 (8%)	1	9
26	d4	132/134 (98%)	110 (83%)	15 (11%)	7 (5%)	2	17
27	D5	68/107 (64%)	48 (71%)	13 (19%)	7 (10%)	1	4
27	d5	67/107 (63%)	51 (76%)	15 (22%)	1 (2%)	13	49
28	D6	95/97 (98%)	56 (59%)	21 (22%)	18 (19%)	0	1
28	d6	95/97 (98%)	66 (70%)	20 (21%)	9 (10%)	1	6
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	4	26
29	d7	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	2	19
30	D8	61/66 (92%)	50 (82%)	9 (15%)	2 (3%)	5	30
30	d8	61/66 (92%)	47 (77%)	11 (18%)	3 (5%)	3	19
31	D9	51/55 (93%)	39 (76%)	9 (18%)	3 (6%)	2	15
31	d9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	4	25
32	E0	58/62 (94%)	46 (79%)	10 (17%)	2 (3%)	5	29
32	e0	60/62 (97%)	40 (67%)	12 (20%)	8 (13%)	0	2
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%)	2	17
34	sR	316/318 (99%)	252 (80%)	53 (17%)	11 (4%)	4	29
35	SM	120/273 (44%)	91 (76%)	18 (15%)	11 (9%)	1	6
35	sM	61/273 (22%)	42 (69%)	11 (18%)	8 (13%)	0	2
39	L2	250/253 (99%)	213 (85%)	27 (11%)	10 (4%)	4	24
39	l2	250/253 (99%)	205 (82%)	30 (12%)	15 (6%)	2	15
40	L3	384/386 (100%)	316 (82%)	49 (13%)	19 (5%)	3	19
40	l3	384/386 (100%)	330 (86%)	39 (10%)	15 (4%)	4	25
41	L4	359/361 (99%)	291 (81%)	46 (13%)	22 (6%)	2	14
41	l4	359/361 (99%)	296 (82%)	43 (12%)	20 (6%)	2	16
42	L5	294/296 (99%)	232 (79%)	44 (15%)	18 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	248 (85%)	38 (13%)	6 (2%)	9	42
43	L6	152/175 (87%)	122 (80%)	27 (18%)	3 (2%)	9	43
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	7	36
44	L7	220/243 (90%)	185 (84%)	24 (11%)	11 (5%)	3	19
44	l7	221/243 (91%)	192 (87%)	21 (10%)	8 (4%)	4	28
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	3	20
45	l8	229/255 (90%)	174 (76%)	40 (18%)	15 (7%)	1	12
46	L9	189/191 (99%)	145 (77%)	29 (15%)	15 (8%)	1	8
46	l9	189/191 (99%)	158 (84%)	24 (13%)	7 (4%)	4	27
47	M0	207/220 (94%)	161 (78%)	37 (18%)	9 (4%)	3	23
47	m0	209/220 (95%)	169 (81%)	29 (14%)	11 (5%)	2	17
48	M1	167/173 (96%)	128 (77%)	27 (16%)	12 (7%)	1	11
48	m1	167/173 (96%)	145 (87%)	9 (5%)	13 (8%)	1	9
49	M3	191/198 (96%)	153 (80%)	30 (16%)	8 (4%)	3	23
49	m3	192/198 (97%)	152 (79%)	27 (14%)	13 (7%)	1	12
50	M4	134/137 (98%)	116 (87%)	12 (9%)	6 (4%)	3	21
50	m4	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	8	41
51	M5	201/203 (99%)	175 (87%)	20 (10%)	6 (3%)	5	33
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	7	37
52	M6	195/198 (98%)	174 (89%)	12 (6%)	9 (5%)	3	21
52	m6	195/198 (98%)	172 (88%)	20 (10%)	3 (2%)	13	49
53	M7	181/183 (99%)	151 (83%)	25 (14%)	5 (3%)	6	34
53	m7	153/183 (84%)	137 (90%)	14 (9%)	2 (1%)	15	52
54	M8	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	4	26
54	m8	183/185 (99%)	154 (84%)	21 (12%)	8 (4%)	3	22
55	M9	186/188 (99%)	164 (88%)	17 (9%)	5 (3%)	6	35
55	m9	186/188 (99%)	164 (88%)	20 (11%)	2 (1%)	17	57
56	N0	170/172 (99%)	151 (89%)	15 (9%)	4 (2%)	7	38
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	16	54
57	N1	157/159 (99%)	131 (83%)	20 (13%)	6 (4%)	4	26
57	n1	157/159 (99%)	138 (88%)	16 (10%)	3 (2%)	10	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	N2	98/120 (82%)	73 (74%)	20 (20%)	5 (5%)	2	19
58	n2	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	5	32
59	N3	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	4	27
59	n3	134/136 (98%)	122 (91%)	4 (3%)	8 (6%)	2	15
60	N4	96/155 (62%)	66 (69%)	21 (22%)	9 (9%)	1	6
60	n4	133/155 (86%)	102 (77%)	23 (17%)	8 (6%)	2	15
61	N5	119/141 (84%)	103 (87%)	12 (10%)	4 (3%)	5	29
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	1	7
62	N6	124/126 (98%)	104 (84%)	19 (15%)	1 (1%)	24	62
62	n6	124/126 (98%)	102 (82%)	17 (14%)	5 (4%)	4	24
63	N7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	12
63	n7	133/135 (98%)	100 (75%)	26 (20%)	7 (5%)	2	17
64	N8	146/148 (99%)	113 (77%)	26 (18%)	7 (5%)	3	20
64	n8	146/148 (99%)	110 (75%)	25 (17%)	11 (8%)	1	10
65	N9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	4	28
65	n9	56/58 (97%)	41 (73%)	9 (16%)	6 (11%)	0	4
66	O0	95/104 (91%)	83 (87%)	11 (12%)	1 (1%)	17	57
66	o0	98/104 (94%)	86 (88%)	10 (10%)	2 (2%)	9	43
67	O1	107/112 (96%)	96 (90%)	6 (6%)	5 (5%)	3	20
67	o1	107/112 (96%)	85 (79%)	15 (14%)	7 (6%)	1	13
68	O2	125/129 (97%)	110 (88%)	11 (9%)	4 (3%)	5	31
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	5	31
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	10	45
69	o3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	10	45
70	O4	110/120 (92%)	96 (87%)	11 (10%)	3 (3%)	6	35
70	o4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	4	28
71	O5	117/119 (98%)	95 (81%)	12 (10%)	10 (8%)	1	7
71	o5	117/119 (98%)	94 (80%)	21 (18%)	2 (2%)	11	47
72	O6	97/99 (98%)	76 (78%)	12 (12%)	9 (9%)	1	6
72	o6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	1	4
73	O7	85/87 (98%)	69 (81%)	14 (16%)	2 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	o7	85/87 (98%)	70 (82%)	14 (16%)	1 (1%)	16	54
74	O8	75/77 (97%)	66 (88%)	7 (9%)	2 (3%)	6	35
74	o8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	12
75	O9	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	2	13
75	o9	48/50 (96%)	39 (81%)	9 (19%)	0	100	100
76	Q0	50/52 (96%)	43 (86%)	6 (12%)	1 (2%)	9	43
76	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	9	43
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	3	23
78	Q2	103/105 (98%)	85 (82%)	13 (13%)	5 (5%)	3	19
78	q2	103/105 (98%)	88 (85%)	9 (9%)	6 (6%)	2	15
79	Q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	1	12
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	17	57
81	p0	117/311 (38%)	97 (83%)	14 (12%)	6 (5%)	2	19
83	f	146/157 (93%)	91 (62%)	35 (24%)	20 (14%)	0	2
All	All	22316/24284 (92%)	18108 (81%)	2992 (13%)	1216 (5%)	2	17

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%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	s0	165/209 (79%)	140 (85%)	25 (15%)	3	16
3	S1	191/223 (86%)	169 (88%)	22 (12%)	7	29
3	s1	192/223 (86%)	164 (85%)	28 (15%)	4	18
4	S2	176/204 (86%)	155 (88%)	21 (12%)	6	27
4	s2	176/204 (86%)	141 (80%)	35 (20%)	1	7
5	S3	182/194 (94%)	157 (86%)	25 (14%)	4	20
5	s3	182/194 (94%)	162 (89%)	20 (11%)	8	31
6	S4	221/221 (100%)	192 (87%)	29 (13%)	5	22
6	s4	221/221 (100%)	188 (85%)	33 (15%)	4	17
7	S5	173/190 (91%)	157 (91%)	16 (9%)	11	40
7	s5	173/190 (91%)	147 (85%)	26 (15%)	3	17
8	S6	188/201 (94%)	165 (88%)	23 (12%)	6	26
8	s6	187/201 (93%)	165 (88%)	22 (12%)	6	27
9	S7	165/169 (98%)	145 (88%)	20 (12%)	6	26
9	s7	165/169 (98%)	150 (91%)	15 (9%)	12	41
10	S8	150/161 (93%)	136 (91%)	14 (9%)	11	40
10	s8	150/161 (93%)	131 (87%)	19 (13%)	5	24
11	S9	158/165 (96%)	133 (84%)	25 (16%)	3	15
11	s9	158/165 (96%)	132 (84%)	26 (16%)	3	14
12	C0	77/77 (100%)	71 (92%)	6 (8%)	16	50
12	c0	73/77 (95%)	66 (90%)	7 (10%)	10	38
13	C1	129/129 (100%)	117 (91%)	12 (9%)	11	40
13	c1	129/129 (100%)	113 (88%)	16 (12%)	6	25
14	C2	88/106 (83%)	73 (83%)	15 (17%)	2	12
14	c2	88/106 (83%)	80 (91%)	8 (9%)	12	41
15	C3	127/127 (100%)	110 (87%)	17 (13%)	5	21
15	c3	127/127 (100%)	110 (87%)	17 (13%)	5	21
16	C4	81/104 (78%)	67 (83%)	14 (17%)	2	11
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	7
17	C5	101/113 (89%)	91 (90%)	10 (10%)	10	37
17	c5	103/113 (91%)	89 (86%)	14 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	C6	117/118 (99%)	103 (88%)	14 (12%)	6	27
18	c6	118/118 (100%)	102 (86%)	16 (14%)	5	21
19	C7	94/124 (76%)	79 (84%)	15 (16%)	3	14
19	c7	92/124 (74%)	82 (89%)	10 (11%)	8	32
20	C8	128/128 (100%)	104 (81%)	24 (19%)	2	8
20	c8	128/128 (100%)	109 (85%)	19 (15%)	4	17
21	C9	115/115 (100%)	99 (86%)	16 (14%)	4	20
21	c9	115/115 (100%)	98 (85%)	17 (15%)	4	17
22	D0	100/113 (88%)	91 (91%)	9 (9%)	12	42
22	d0	103/113 (91%)	91 (88%)	12 (12%)	7	28
23	D1	74/74 (100%)	65 (88%)	9 (12%)	6	26
23	d1	74/74 (100%)	66 (89%)	8 (11%)	8	32
24	D2	110/110 (100%)	94 (86%)	16 (14%)	4	18
24	d2	110/110 (100%)	93 (84%)	17 (16%)	3	16
25	D3	119/119 (100%)	105 (88%)	14 (12%)	6	27
25	d3	119/119 (100%)	109 (92%)	10 (8%)	14	46
26	D4	112/112 (100%)	103 (92%)	9 (8%)	15	49
26	d4	112/112 (100%)	97 (87%)	15 (13%)	5	21
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	5
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	14
28	D6	83/83 (100%)	73 (88%)	10 (12%)	6	27
28	d6	83/83 (100%)	70 (84%)	13 (16%)	3	15
29	D7	70/70 (100%)	62 (89%)	8 (11%)	7	29
29	d7	70/70 (100%)	62 (89%)	8 (11%)	7	29
30	D8	56/59 (95%)	48 (86%)	8 (14%)	4	19
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	10
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	12
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/53 (96%)	47 (92%)	4 (8%)	16	50
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	2
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e1	66/66 (100%)	55 (83%)	11 (17%)	3	13
34	SR	259/261 (99%)	227 (88%)	32 (12%)	6	25
34	sR	260/261 (100%)	243 (94%)	17 (6%)	21	59
35	SM	97/183 (53%)	79 (81%)	18 (19%)	2	9
35	sM	54/183 (30%)	46 (85%)	8 (15%)	4	17
39	L2	193/195 (99%)	166 (86%)	27 (14%)	4	20
39	l2	192/195 (98%)	161 (84%)	31 (16%)	3	14
40	L3	319/322 (99%)	267 (84%)	52 (16%)	3	14
40	l3	319/322 (99%)	261 (82%)	58 (18%)	2	9
41	L4	288/288 (100%)	252 (88%)	36 (12%)	6	24
41	l4	288/288 (100%)	248 (86%)	40 (14%)	4	20
42	L5	244/244 (100%)	208 (85%)	36 (15%)	4	17
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2	10
43	L6	134/152 (88%)	116 (87%)	18 (13%)	5	21
43	l6	135/152 (89%)	115 (85%)	20 (15%)	4	17
44	L7	186/204 (91%)	162 (87%)	24 (13%)	5	23
44	l7	187/204 (92%)	164 (88%)	23 (12%)	6	25
45	L8	187/207 (90%)	165 (88%)	22 (12%)	6	27
45	l8	177/207 (86%)	153 (86%)	24 (14%)	5	21
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	143 (84%)	28 (16%)	3	14
47	M0	177/186 (95%)	144 (81%)	33 (19%)	2	9
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	13
48	M1	147/150 (98%)	117 (80%)	30 (20%)	1	6
48	m1	147/150 (98%)	125 (85%)	22 (15%)	3	17
49	M3	154/158 (98%)	133 (86%)	21 (14%)	5	21
49	m3	154/158 (98%)	127 (82%)	27 (18%)	2	11
50	M4	107/108 (99%)	93 (87%)	14 (13%)	5	22
50	m4	108/108 (100%)	94 (87%)	14 (13%)	5	22
51	M5	175/175 (100%)	151 (86%)	24 (14%)	4	20
51	m5	175/175 (100%)	154 (88%)	21 (12%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	M6	160/161 (99%)	134 (84%)	26 (16%)	3	14
52	m6	160/161 (99%)	139 (87%)	21 (13%)	5	22
53	M7	140/145 (97%)	120 (86%)	20 (14%)	4	19
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	16
54	M8	150/150 (100%)	132 (88%)	18 (12%)	6	27
54	m8	150/150 (100%)	126 (84%)	24 (16%)	3	14
55	M9	153/153 (100%)	136 (89%)	17 (11%)	8	31
55	m9	153/153 (100%)	133 (87%)	20 (13%)	5	22
56	N0	156/156 (100%)	132 (85%)	24 (15%)	3	16
56	n0	156/156 (100%)	133 (85%)	23 (15%)	4	18
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	6
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	12
58	N2	87/106 (82%)	79 (91%)	8 (9%)	11	40
58	n2	85/106 (80%)	73 (86%)	12 (14%)	4	20
59	N3	104/104 (100%)	90 (86%)	14 (14%)	5	21
59	n3	104/104 (100%)	91 (88%)	13 (12%)	6	24
60	N4	57/129 (44%)	52 (91%)	5 (9%)	12	44
60	n4	100/129 (78%)	95 (95%)	5 (5%)	30	68
61	N5	104/117 (89%)	83 (80%)	21 (20%)	1	6
61	n5	104/117 (89%)	90 (86%)	14 (14%)	5	21
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	11
62	n6	109/109 (100%)	93 (85%)	16 (15%)	4	18
63	N7	115/115 (100%)	99 (86%)	16 (14%)	4	20
63	n7	115/115 (100%)	97 (84%)	18 (16%)	3	15
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	12
64	n8	118/118 (100%)	101 (86%)	17 (14%)	4	19
65	N9	46/46 (100%)	40 (87%)	6 (13%)	5	22
65	n9	46/46 (100%)	41 (89%)	5 (11%)	8	32
66	O0	81/87 (93%)	69 (85%)	12 (15%)	4	17
66	o0	84/87 (97%)	72 (86%)	12 (14%)	4	19
67	O1	92/96 (96%)	80 (87%)	12 (13%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	o1	94/96 (98%)	76 (81%)	18 (19%)	2	8
68	O2	109/110 (99%)	94 (86%)	15 (14%)	4	20
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	6
69	O3	90/90 (100%)	75 (83%)	15 (17%)	3	13
69	o3	90/90 (100%)	76 (84%)	14 (16%)	3	16
70	O4	95/102 (93%)	84 (88%)	11 (12%)	7	29
70	o4	95/102 (93%)	86 (90%)	9 (10%)	11	38
71	O5	104/104 (100%)	95 (91%)	9 (9%)	13	45
71	o5	103/104 (99%)	90 (87%)	13 (13%)	5	24
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1	7
72	o6	80/81 (99%)	59 (74%)	21 (26%)	0	2
73	O7	70/70 (100%)	59 (84%)	11 (16%)	3	15
73	o7	70/70 (100%)	62 (89%)	8 (11%)	7	29
74	O8	68/68 (100%)	56 (82%)	12 (18%)	2	10
74	o8	67/68 (98%)	57 (85%)	10 (15%)	4	17
75	O9	45/45 (100%)	38 (84%)	7 (16%)	3	16
75	o9	45/45 (100%)	42 (93%)	3 (7%)	20	58
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	12
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	5	22
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	10
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	6
79	Q3	71/71 (100%)	60 (84%)	11 (16%)	3	16
79	q3	71/71 (100%)	61 (86%)	10 (14%)	4	20
81	p0	105/232 (45%)	93 (89%)	12 (11%)	7	29
83	f	124/133 (93%)	107 (86%)	17 (14%)	4	20
84	B	2/2 (100%)	2 (100%)	0	100	100
84	C	2/2 (100%)	2 (100%)	0	100	100
All	All	18853/20181 (93%)	16183 (86%)	2670 (14%)	4	19

5 of 2670 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	104	VAL
9	s7	50	ASP
65	n9	38	LYS
73	O7	85	LYS
3	s1	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
57	N1	26	HIS
9	s7	71	HIS
64	n8	25	HIS
4	s2	94	GLN
9	s7	74	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	455 (25%)	40 (2%)
1	6	1791/1800 (99%)	447 (24%)	29 (1%)
36	1	3145/3396 (92%)	672 (21%)	53 (1%)
36	5	3163/3396 (93%)	649 (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	10429/10950 (95%)	2313 (22%)	177 (1%)

5 of 2313 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
36	1	2585	G

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Mol	Chain	Res	Type
1	6	187	G
36	5	2513	U
36	1	2817	A
36	1	3350	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
84	CH	B	74	84	14,21,22	0.82	0	18,30,33	0.49	0
84	CH	B	75	87,84	14,21,22	0.66	0	18,30,33	0.82	0
84	8AN	B	76	87,84	18,24,25	1.11	1 (5%)	10,35,38	2.14	2 (20%)
84	CH	C	74	84	15,18,22	0.79	1 (6%)	18,26,33	0.75	0
84	CH	C	75	87,84	14,21,22	0.74	0	18,30,33	0.54	0
84	8AN	C	76	87,84	18,24,25	1.14	1 (5%)	10,35,38	2.12	1 (10%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	C	74	CH	C6-C5	-2.03	1.33	1.38
84	C	76	8AN	C5-C4	2.93	1.47	1.40
84	B	76	8AN	C5-C4	3.25	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	C	76	8AN	N3-C2-N1	-5.83	124.30	128.87
84	B	76	8AN	N3-C2-N1	-5.71	124.39	128.87
84	B	76	8AN	N6-C6-N1	2.18	122.18	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	19,23,23	3.50	10 (52%)	16,30,30	2.99	7 (43%)
88	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	SPS	B	3401	87	19,23,23	3.49	11 (57%)	16,30,30	3.14	8 (50%)

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	1	3401	-	-	0/15/18/18	0/1/1/1
88	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3406	-	-	0/0/0/0	0/0/0/0
86	SPS	B	3401	87	-	0/15/18/18	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	3401	SPS	C9-C10	-8.75	1.31	1.48
86	B	3401	SPS	C9-C10	-8.45	1.31	1.48
86	B	3401	SPS	O13-C13	-5.31	1.19	1.42
86	1	3401	SPS	O13-C13	-5.20	1.19	1.42
86	B	3401	SPS	O10-C10	-2.99	1.18	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	B	3401	SPS	N2-C3-N4	-5.15	119.01	127.69
86	1	3401	SPS	C7-C5-C6	-4.46	118.29	123.63
86	1	3401	SPS	N2-C3-N4	-4.33	120.39	127.69
86	B	3401	SPS	C7-C5-C6	-2.82	120.25	123.63
86	1	3401	SPS	C6-C8-C9	-2.77	118.07	127.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3401	SPS	2	0
86	B	3401	SPS	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	m2	2
1	2	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%)	0.48	91 (5%) 32 25	60, 98, 170, 210	0
1	6	1795/1800 (99%)	0.27	58 (3%) 51 44	44, 86, 157, 204	0
2	S0	206/251 (82%)	1.22	49 (23%) 1 1	100, 112, 123, 128	0
2	s0	206/251 (82%)	1.16	50 (24%) 1 1	80, 97, 111, 117	0
3	S1	214/254 (84%)	1.60	77 (35%) 0 1	110, 145, 169, 175	0
3	s1	216/254 (85%)	1.03	44 (20%) 1 1	80, 96, 114, 123	0
4	S2	217/253 (85%)	0.73	30 (13%) 4 3	83, 96, 109, 113	0
4	s2	217/253 (85%)	0.45	9 (4%) 41 34	68, 79, 93, 108	0
5	S3	223/239 (93%)	0.67	26 (11%) 6 5	91, 100, 123, 128	0
5	s3	223/239 (93%)	1.46	72 (32%) 1 1	86, 112, 131, 137	0
6	S4	260/260 (100%)	1.31	67 (25%) 1 1	77, 99, 107, 124	0
6	s4	260/260 (100%)	1.20	60 (23%) 1 1	60, 82, 92, 119	0
7	S5	206/224 (91%)	1.21	41 (19%) 1 1	104, 124, 131, 134	0
7	s5	206/224 (91%)	0.62	21 (10%) 9 7	87, 108, 123, 130	0
8	S6	226/236 (95%)	0.85	41 (18%) 2 1	77, 105, 126, 132	0
8	s6	218/236 (92%)	0.49	21 (9%) 10 9	60, 89, 106, 114	0
9	S7	184/189 (97%)	0.90	30 (16%) 2 2	102, 121, 136, 142	0
9	s7	186/189 (98%)	0.67	23 (12%) 5 4	77, 104, 130, 134	0
10	S8	188/200 (94%)	0.78	21 (11%) 7 5	70, 86, 119, 129	0
10	s8	188/200 (94%)	1.01	28 (14%) 3 2	56, 73, 113, 130	0
11	S9	185/196 (94%)	1.69	71 (38%) 0 1	89, 106, 130, 141	0
11	s9	185/196 (94%)	1.21	44 (23%) 1 1	71, 88, 115, 126	0
12	C0	83/96 (86%)	2.34	51 (61%) 0 0	94, 112, 122, 126	0
12	c0	83/96 (86%)	2.04	40 (48%) 0 0	103, 131, 145, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	144/155 (92%)	1.04	21 (14%) 3 3	73, 83, 101, 113	0
13	c1	144/155 (92%)	0.84	9 (6%) 23 19	59, 70, 91, 113	0
14	C2	108/142 (76%)	0.52	14 (12%) 5 3	137, 145, 150, 152	0
14	c2	108/142 (76%)	0.82	16 (14%) 3 3	167, 183, 196, 199	0
15	C3	150/150 (100%)	0.59	16 (10%) 8 6	82, 95, 111, 115	0
15	c3	150/150 (100%)	0.14	5 (3%) 50 43	67, 79, 95, 100	0
16	C4	127/136 (93%)	1.42	35 (27%) 1 1	84, 142, 156, 161	0
16	c4	128/136 (94%)	1.53	43 (33%) 0 1	67, 101, 113, 116	0
17	C5	122/141 (86%)	0.94	21 (17%) 2 2	88, 99, 111, 117	0
17	c5	129/141 (91%)	0.67	16 (12%) 5 4	86, 103, 113, 119	0
18	C6	141/142 (99%)	1.70	48 (34%) 0 1	91, 112, 117, 120	0
18	c6	142/142 (100%)	0.82	24 (16%) 2 2	83, 102, 115, 126	0
19	C7	120/136 (88%)	1.44	33 (27%) 1 1	97, 109, 125, 129	0
19	c7	117/136 (86%)	0.38	10 (8%) 13 10	88, 101, 115, 119	0
20	C8	145/145 (100%)	0.95	24 (16%) 2 2	85, 110, 131, 138	0
20	c8	145/145 (100%)	0.80	23 (15%) 3 2	86, 101, 116, 126	0
21	C9	143/143 (100%)	1.40	37 (25%) 1 1	96, 112, 122, 126	0
21	c9	143/143 (100%)	1.63	52 (36%) 0 1	85, 97, 112, 118	0
22	D0	107/120 (89%)	0.98	20 (18%) 2 1	86, 112, 123, 125	0
22	d0	110/120 (91%)	2.37	58 (52%) 0 0	84, 114, 138, 147	0
23	D1	87/87 (100%)	0.91	16 (18%) 2 1	96, 104, 119, 127	0
23	d1	87/87 (100%)	0.70	9 (10%) 9 7	76, 88, 104, 112	0
24	D2	129/129 (100%)	0.64	11 (8%) 13 10	83, 95, 101, 109	0
24	d2	129/129 (100%)	0.46	9 (6%) 19 16	64, 74, 81, 87	0
25	D3	144/144 (100%)	0.81	18 (12%) 5 4	69, 77, 86, 96	0
25	d3	144/144 (100%)	0.60	7 (4%) 33 27	56, 61, 71, 79	0
26	D4	134/134 (100%)	1.30	33 (24%) 1 1	86, 107, 118, 129	0
26	d4	134/134 (100%)	0.36	10 (7%) 17 14	68, 90, 105, 110	0
27	D5	70/107 (65%)	1.51	24 (34%) 0 1	119, 130, 139, 140	0
27	d5	69/107 (64%)	1.51	19 (27%) 1 1	99, 113, 123, 125	0
28	D6	97/97 (100%)	2.01	44 (45%) 0 0	88, 106, 154, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
28	d6	97/97 (100%)	1.37	26 (26%)	1	1	70, 87, 116, 123	0
29	D7	81/81 (100%)	1.23	17 (20%)	1	1	98, 110, 135, 141	0
29	d7	81/81 (100%)	0.94	12 (14%)	3	3	80, 93, 121, 128	0
30	D8	63/66 (95%)	1.21	15 (23%)	1	1	111, 127, 139, 143	0
30	d8	63/66 (95%)	1.06	10 (15%)	3	2	104, 116, 127, 129	0
31	D9	53/55 (96%)	1.26	12 (22%)	1	1	84, 91, 107, 112	0
31	d9	53/55 (96%)	2.26	26 (49%)	0	0	82, 92, 128, 139	0
32	E0	60/62 (96%)	1.84	21 (35%)	0	1	78, 107, 129, 134	0
32	e0	62/62 (100%)	0.83	11 (17%)	2	1	63, 88, 109, 122	0
33	E1	71/76 (93%)	0.66	9 (12%)	5	4	107, 133, 145, 148	0
33	e1	76/76 (100%)	1.09	20 (26%)	1	1	112, 158, 170, 175	0
34	SR	318/318 (100%)	1.49	102 (32%)	1	1	109, 120, 132, 146	0
34	sR	318/318 (100%)	1.56	105 (33%)	0	1	110, 126, 140, 150	0
35	SM	121/273 (44%)	0.86	22 (18%)	2	1	59, 94, 111, 116	0
35	sM	63/273 (23%)	1.60	21 (33%)	0	1	55, 105, 111, 112	0
36	1	3149/3396 (92%)	0.18	48 (1%)	76	71	35, 59, 123, 212	0
36	5	3169/3396 (93%)	0.21	48 (1%)	76	71	35, 54, 124, 188	0
37	3	121/121 (100%)	-0.00	0	100	100	43, 76, 90, 96	0
37	7	121/121 (100%)	-0.09	0	100	100	39, 59, 70, 75	0
38	4	158/158 (100%)	0.12	2 (1%)	79	74	43, 61, 91, 130	0
38	8	158/158 (100%)	0.11	1 (0%)	90	88	43, 63, 96, 120	0
39	L2	252/253 (99%)	0.36	9 (3%)	46	39	42, 61, 77, 82	0
39	l2	252/253 (99%)	0.41	11 (4%)	38	31	43, 59, 74, 83	0
40	L3	386/386 (100%)	0.45	19 (4%)	33	27	42, 63, 77, 85	0
40	l3	386/386 (100%)	0.33	8 (2%)	67	60	34, 49, 62, 77	0
41	L4	361/361 (100%)	-0.03	0	100	100	40, 54, 70, 71	0
41	l4	361/361 (100%)	0.14	2 (0%)	90	88	40, 57, 73, 88	0
42	L5	296/296 (100%)	1.15	68 (22%)	1	1	58, 81, 97, 111	0
42	l5	294/296 (99%)	0.61	21 (7%)	19	15	49, 60, 84, 93	0
43	L6	156/175 (89%)	0.59	12 (7%)	16	13	49, 57, 72, 79	0
43	l6	157/175 (89%)	0.19	5 (3%)	51	44	49, 57, 75, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	0.19	3 (1%) 78 73	40, 49, 73, 106	0
44	l7	223/243 (91%)	-0.05	1 (0%) 93 92	39, 49, 80, 107	0
45	L8	233/255 (91%)	0.94	41 (17%) 2 1	67, 81, 104, 112	0
45	l8	231/255 (90%)	1.04	41 (17%) 2 1	73, 84, 106, 114	0
46	L9	191/191 (100%)	0.21	9 (4%) 35 29	60, 70, 82, 93	0
46	l9	191/191 (100%)	0.08	1 (0%) 91 90	44, 55, 71, 81	0
47	M0	211/220 (95%)	1.09	40 (18%) 2 1	45, 63, 92, 106	0
47	m0	213/220 (96%)	0.96	28 (13%) 5 3	40, 55, 80, 90	0
48	M1	169/173 (97%)	1.03	25 (14%) 3 3	68, 84, 94, 98	0
48	m1	169/173 (97%)	0.38	6 (3%) 46 39	52, 67, 77, 82	0
49	M3	193/198 (97%)	0.40	8 (4%) 41 34	39, 64, 92, 113	0
49	m3	194/198 (97%)	0.77	29 (14%) 3 2	41, 69, 100, 111	0
50	M4	136/137 (99%)	-0.04	2 (1%) 76 71	54, 61, 73, 83	0
50	m4	137/137 (100%)	-0.03	1 (0%) 89 86	48, 54, 69, 82	0
51	M5	203/203 (100%)	0.27	3 (1%) 76 71	41, 56, 66, 69	0
51	m5	203/203 (100%)	0.47	10 (4%) 33 27	44, 60, 71, 76	0
52	M6	197/198 (99%)	0.27	4 (2%) 68 62	42, 49, 65, 68	0
52	m6	197/198 (99%)	0.08	2 (1%) 84 80	34, 42, 64, 66	0
53	M7	183/183 (100%)	0.87	23 (12%) 5 4	47, 55, 98, 116	0
53	m7	155/183 (84%)	0.17	0 100 100	39, 46, 59, 77	0
54	M8	185/185 (100%)	0.22	3 (1%) 74 69	43, 55, 69, 88	0
54	m8	185/185 (100%)	0.11	0 100 100	42, 57, 66, 70	0
55	M9	188/188 (100%)	0.55	19 (10%) 9 8	65, 77, 135, 140	0
55	m9	188/188 (100%)	0.49	12 (6%) 23 19	51, 65, 121, 134	0
56	N0	172/172 (100%)	0.18	4 (2%) 64 57	49, 57, 69, 74	0
56	n0	172/172 (100%)	0.02	1 (0%) 90 88	43, 49, 59, 66	0
57	N1	159/159 (100%)	0.44	4 (2%) 61 54	42, 56, 93, 101	0
57	n1	159/159 (100%)	0.57	11 (6%) 20 16	40, 49, 83, 87	0
58	N2	100/120 (83%)	1.06	25 (25%) 1 1	93, 104, 120, 122	0
58	n2	98/120 (81%)	1.04	21 (21%) 1 1	75, 88, 94, 97	0
59	N3	136/136 (100%)	0.67	11 (8%) 15 11	51, 60, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	0.41	3 (2%) 65 59	36, 45, 55, 58	0
60	N4	98/155 (63%)	1.83	28 (28%) 1 1	62, 72, 134, 147	0
60	n4	135/155 (87%)	0.74	19 (14%) 4 3	46, 91, 115, 116	0
61	N5	121/141 (85%)	0.80	13 (10%) 8 6	58, 69, 84, 95	0
61	n5	120/141 (85%)	0.27	1 (0%) 87 84	56, 68, 85, 93	0
62	N6	126/126 (100%)	0.84	19 (15%) 3 2	50, 62, 74, 79	0
62	n6	126/126 (100%)	0.42	4 (3%) 51 44	51, 64, 77, 83	0
63	N7	135/135 (100%)	1.78	49 (36%) 0 1	82, 94, 103, 109	0
63	n7	135/135 (100%)	1.44	43 (31%) 1 1	76, 91, 102, 105	0
64	N8	148/148 (100%)	0.36	2 (1%) 78 73	35, 56, 74, 82	0
64	n8	148/148 (100%)	0.16	3 (2%) 68 62	34, 59, 74, 77	0
65	N9	58/58 (100%)	0.54	4 (6%) 20 16	38, 61, 95, 106	0
65	n9	58/58 (100%)	0.36	5 (8%) 13 10	38, 58, 78, 85	0
66	O0	97/104 (93%)	0.64	9 (9%) 11 9	81, 89, 101, 102	0
66	o0	100/104 (96%)	0.44	2 (2%) 68 62	75, 82, 102, 108	0
67	O1	109/112 (97%)	0.97	14 (12%) 5 4	61, 72, 91, 103	0
67	o1	109/112 (97%)	0.45	4 (3%) 45 38	47, 58, 81, 90	0
68	O2	127/129 (98%)	0.16	2 (1%) 74 69	36, 49, 62, 68	0
68	o2	127/129 (98%)	0.54	7 (5%) 29 23	35, 52, 63, 71	0
69	O3	106/106 (100%)	0.31	1 (0%) 85 82	42, 47, 71, 78	0
69	o3	106/106 (100%)	0.14	0 100 100	40, 46, 69, 75	0
70	O4	112/120 (93%)	0.60	7 (6%) 23 19	57, 75, 101, 107	0
70	o4	112/120 (93%)	0.66	8 (7%) 19 15	50, 68, 99, 103	0
71	O5	119/119 (100%)	0.32	6 (5%) 32 26	55, 70, 78, 82	0
71	o5	119/119 (100%)	0.59	8 (6%) 21 17	59, 71, 87, 96	0
72	O6	99/99 (100%)	0.63	5 (5%) 32 25	60, 68, 91, 102	0
72	o6	99/99 (100%)	0.40	4 (4%) 42 34	64, 72, 88, 103	0
73	O7	87/87 (100%)	0.13	1 (1%) 82 78	43, 50, 65, 71	0
73	o7	87/87 (100%)	0.21	2 (2%) 64 57	41, 50, 73, 84	0
74	O8	77/77 (100%)	0.86	8 (10%) 8 7	83, 93, 108, 113	0
74	o8	77/77 (100%)	1.51	25 (32%) 1 1	77, 86, 94, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	0.49	1 (2%) 68 62	52, 57, 59, 60	0
75	o9	50/50 (100%)	0.27	1 (2%) 68 62	50, 55, 63, 63	0
76	Q0	52/52 (100%)	0.86	7 (13%) 4 3	53, 59, 74, 79	0
76	q0	52/52 (100%)	0.37	1 (1%) 70 63	41, 45, 55, 58	0
77	Q1	25/25 (100%)	1.26	6 (24%) 1 1	62, 66, 73, 74	0
77	q1	25/25 (100%)	0.99	2 (8%) 15 12	50, 56, 58, 58	0
78	Q2	105/105 (100%)	0.12	2 (1%) 70 63	41, 56, 76, 91	0
78	q2	105/105 (100%)	0.26	1 (0%) 84 80	44, 56, 71, 93	0
79	Q3	91/91 (100%)	0.21	2 (2%) 65 59	54, 65, 80, 85	0
79	q3	91/91 (100%)	0.38	3 (3%) 50 43	46, 59, 72, 84	0
80	m2	0/165	-	-	-	-
81	p0	120/311 (38%)	1.26	32 (26%) 1 1	101, 124, 144, 152	0
82	p1	0/47	-	-	-	-
82	p2	0/47	-	-	-	-
83	f	148/157 (94%)	2.86	92 (62%) 0 0	55, 96, 150, 153	75 (50%)
84	B	2/5 (40%)	0.21	0 100 100	43, 43, 43, 44	0
84	C	2/5 (40%)	0.25	0 100 100	49, 49, 49, 49	0
All	All	33084/35503 (93%)	0.60	3317 (10%) 9 8	34, 74, 132, 212	75 (0%)

The worst 5 of 3317 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	13.9
1	2	1699	G	13.8
53	M7	161	ALA	12.0
1	2	1696	G	12.0
1	2	1697	G	11.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
84	CH	B	75	20/21	0.95	0.21	-	44,44,50,51	0
84	CH	C	74	17/21	0.90	0.21	-	47,48,55,57	0
84	CH	C	75	20/21	0.98	0.17	-	46,47,51,51	0
84	8AN	B	76	22/23	0.96	0.22	-	42,44,45,45	0
84	8AN	C	76	22/23	0.96	0.20	-	47,47,47,47	0
84	CH	B	74	20/21	0.96	0.25	-	47,50,62,62	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3405	1/1	0.96	0.74	14.49	42,42,42,42	0
87	MG	5	3404	1/1	0.95	0.47	11.33	36,36,36,36	0
87	MG	5	3401	1/1	0.95	0.37	8.09	41,41,41,41	0
86	SPS	B	3401	23/23	0.96	0.31	2.09	37,40,54,56	0
85	ZN	q3	501	1/1	1.00	0.17	0.18	69,69,69,69	0
86	SPS	1	3401	23/23	0.94	0.24	-0.37	40,43,57,59	0
85	ZN	o7	501	1/1	0.99	0.21	-0.50	51,51,51,51	0
85	ZN	D7	101	1/1	0.81	0.21	-1.08	141,141,141,141	0
85	ZN	e1	501	1/1	0.79	0.08	-1.26	164,164,164,164	0
85	ZN	E1	501	1/1	0.97	0.05	-1.29	136,136,136,136	0
85	ZN	O7	100	1/1	0.99	0.14	-1.41	52,52,52,52	0
85	ZN	Q3	501	1/1	0.98	0.11	-1.45	77,77,77,77	0
85	ZN	q0	500	1/1	0.99	0.13	-1.76	42,42,42,42	0
85	ZN	Q0	500	1/1	0.98	0.10	-1.90	57,57,57,57	0
85	ZN	D9	101	1/1	0.98	0.08	-1.93	88,88,88,88	0
85	ZN	q2	501	1/1	0.97	0.05	-2.00	77,77,77,77	0
85	ZN	d9	101	1/1	0.99	0.09	-2.06	94,94,94,94	0
85	ZN	d7	101	1/1	0.82	0.15	-2.26	131,131,131,131	0
85	ZN	d6	500	1/1	0.97	0.06	-2.31	87,87,87,87	0
85	ZN	D6	500	1/1	0.94	0.07	-2.46	105,105,105,105	0
85	ZN	Q2	501	1/1	0.91	0.05	-3.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3406	7/7	0.99	0.14	-4.40	73,73,73,73	0
88	OHX	5	3406	7/7	0.98	0.09	-4.49	95,95,95,95	0
88	OHX	1	3405	7/7	0.98	0.09	-6.82	91,91,91,91	0
87	MG	1	3402	1/1	0.93	0.65	-	21,21,21,21	0
87	MG	f	1001	1/1	0.97	0.33	-	52,52,52,52	0
87	MG	B	3402	1/1	0.96	0.32	-	40,40,40,40	0
87	MG	C	101	1/1	0.94	0.31	-	49,49,49,49	0
87	MG	5	3402	1/1	0.84	0.36	-	45,45,45,45	0
87	MG	f	1002	1/1	0.93	0.08	-	66,66,66,66	0
87	MG	1	3404	1/1	0.94	0.65	-	29,29,29,29	0
87	MG	1	3403	1/1	0.89	0.38	-	45,45,45,45	0
87	MG	5	3403	1/1	0.98	0.54	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.