wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 11:25 am BST

PDB ID	:	5NDG
Title	:	Crystal structure of geneticin (G418) bound to the yeast 80S ribosome
Authors	:	Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2017-03-08
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

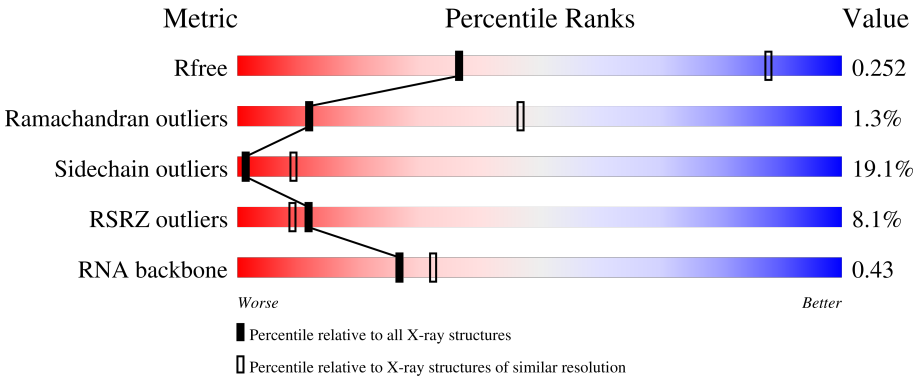
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
R_{free}	130704	1049 (3.88-3.52)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 64% 25% · 6%
1	6	1800	2% 66% 26% · 6%
2	S0	206	7% 82% 17%
2	s0	206	10% 83% 16% ·
3	S1	216	18% 75% 22% ··

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Mol	Chain	Length	Quality of chain
3	s1	216	19% 83% 17%
4	S2	217	% 79% 21%
4	s2	217	4% 83% 17%
5	S3	223	3% 83% 17%
5	s3	223	6% 79% 19%
6	S4	260	21% 83% 16%
6	s4	260	9% 87% 13%
7	S5	206	11% 81% 19%
7	s5	206	28% 82% 17%
8	S6	236	16% 79% 17%
8	s6	236	11% 78% 14% 8%
9	S7	185	18% 78% 19%
9	s7	185	14% 77% 21%
10	S8	200	26% 82% 12% 6%
10	s8	200	10% 80% 14% 6%
11	S9	185	36% 82% 17%
11	s9	185	42% 87% 13%
12	C0	105	20% 72% 14% 12%
12	c0	105	39% 70% 16% 12%
13	C1	156	11% 79% 12% 9%
13	c1	156	4% 77% 15% 6%
14	C2	143	31% 64% 16% 16%
14	c2	143	55% 63% 23% 13%
15	C3	150	3% 85% 15%
15	c3	150	2% 80% 19%

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Mol	Chain	Length	Quality of chain
16	C4	128	4% 81% 16%
16	c4	128	5% 84% 16%
17	C5	141	5% 70% 16% 13%
17	c5	141	14% 70% 15% 16%
18	C6	141	16% 79% 19%
18	c6	141	56% 84% 16%
19	C7	136	12% 70% 15% 14%
19	c7	136	6% 72% 12% 14%
20	C8	145	6% 77% 21%
20	c8	145	19% 81% 19%
21	C9	143	11% 83% 16%
21	c9	143	43% 84% 15%
22	D0	107	19% 79% 19%
22	d0	107	25% 77% 16% 6%
23	D1	87	5% 82% 17%
23	d1	87	3% 84% 16%
24	D2	129	9% 85% 13%
24	d2	129	5% 87% 12%
25	D3	144	2% 80% 20%
25	d3	144	92% 8%
26	D4	134	22% 81% 17%
26	d4	134	11% 81% 19%
27	D5	70	20% 67% 30%
27	d5	70	36% 86% 13%
28	D6	97	5% 65% 31%

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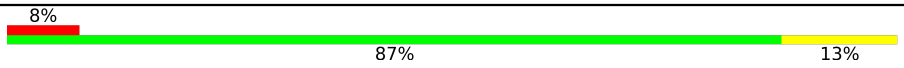
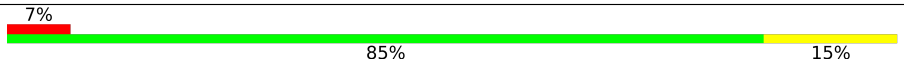
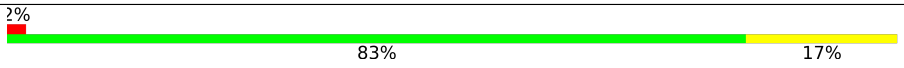
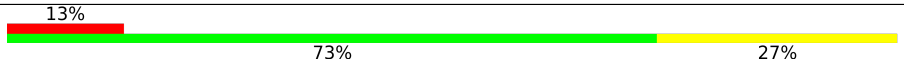
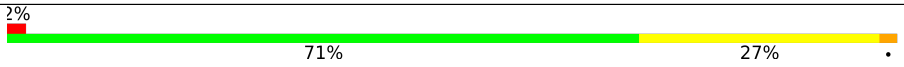
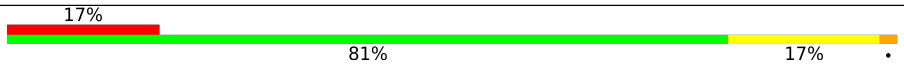
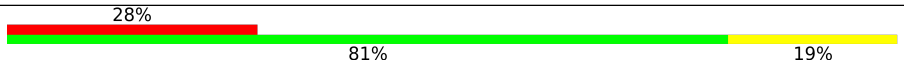
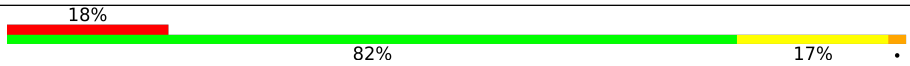
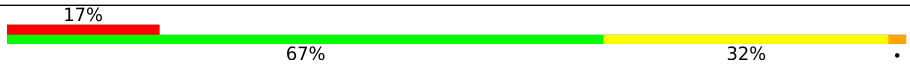
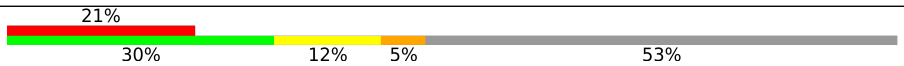
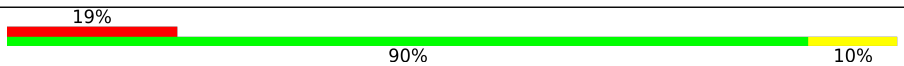
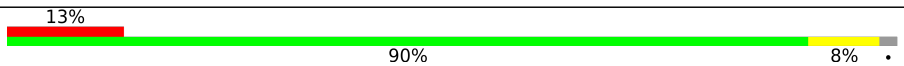
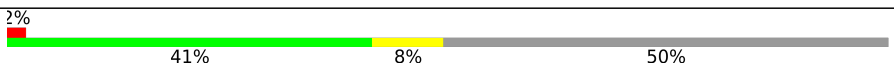
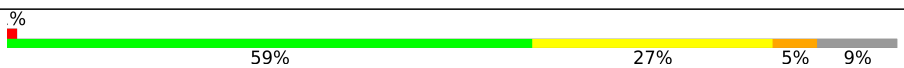
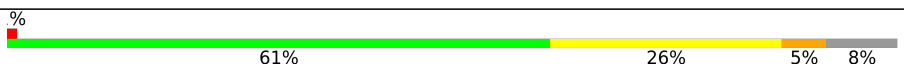
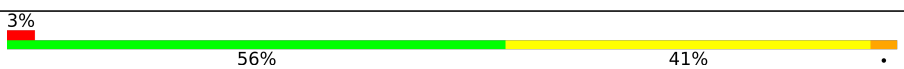
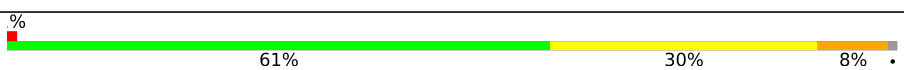
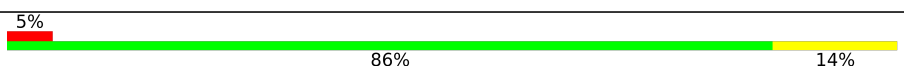
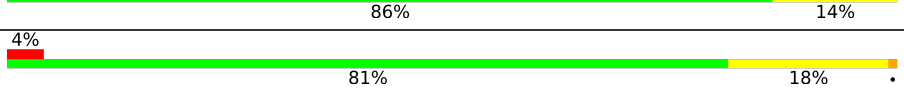
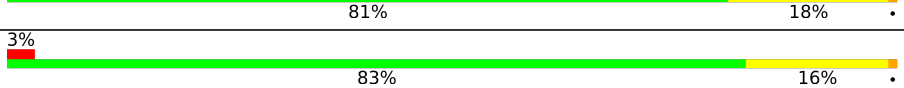
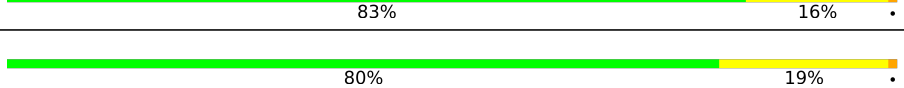
Mol	Chain	Length	Quality of chain
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	60	
32	e0	60	
33	E1	152	
33	e1	152	
34	SR	318	
34	sR	318	
35	SM	272	
35	sM	272	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	

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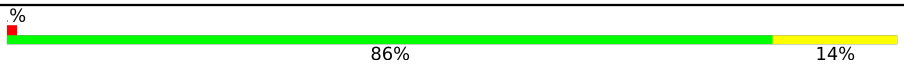
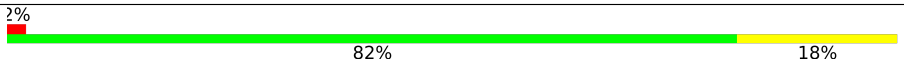
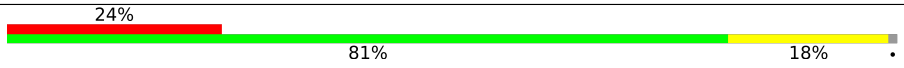
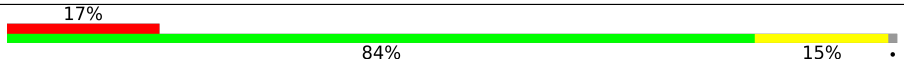
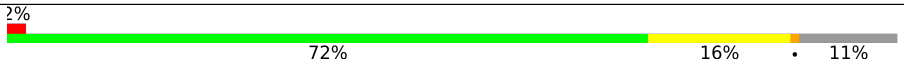
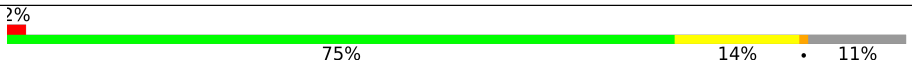
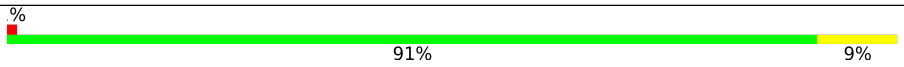
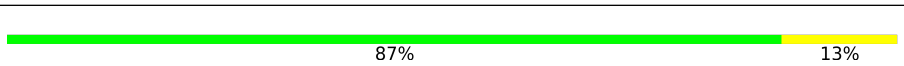
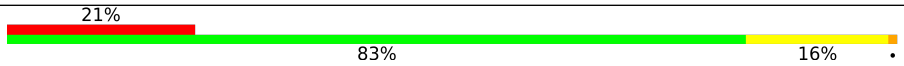
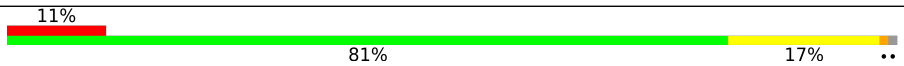
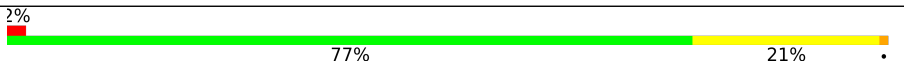
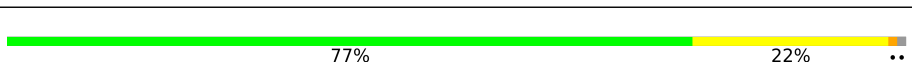
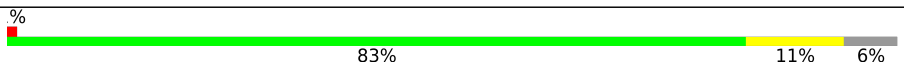
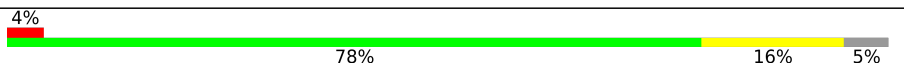
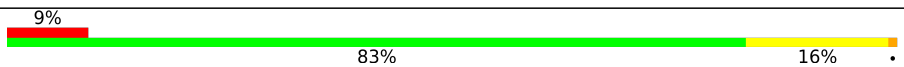
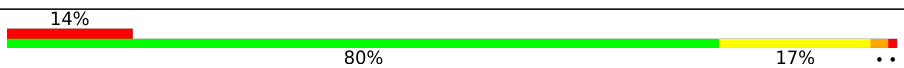
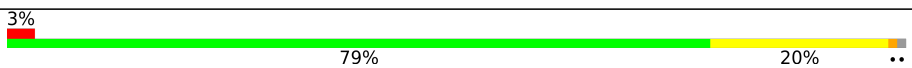
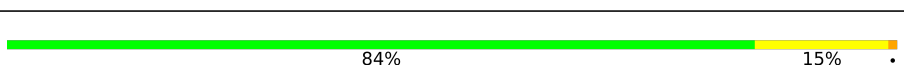
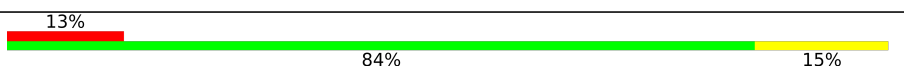
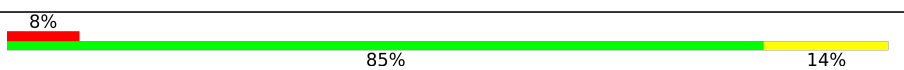
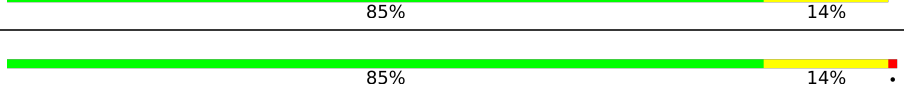
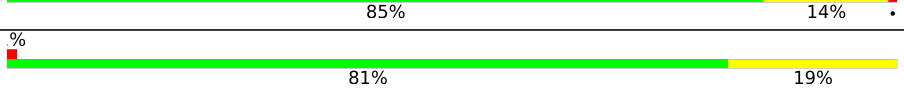
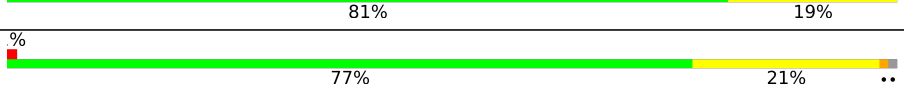
Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	176	
43	l6	176	
44	L7	223	
44	l7	223	
45	L8	233	
45	l8	233	
46	L9	191	
46	l9	191	
47	M0	221	
47	m0	221	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	184	

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Mol	Chain	Length	Quality of chain
53	m7	184	2% 75% 20% 5%
54	M8	185	4% 86% 14%
54	m8	185	% 86% 14%
55	M9	188	11% 80% 20%
55	m9	188	10% 77% 20%
56	N0	172	81% 16%
56	n0	172	81% 19%
57	N1	159	16% 82% 17%
57	n1	159	5% 82% 18%
58	N2	98	23% 88% 12%
58	n2	98	9% 83% 17%
59	N3	135	12% 89% 11%
59	n3	135	2% 88% 10%
60	N4	155	11% 70% 9% 21%
60	n4	155	12% 68% 8% 24%
61	N5	121	11% 82% 18%
61	n5	121	2% 82% 17%
62	N6	126	24% 81% 18%
62	n6	126	12% 79% 19%
63	N7	135	35% 84% 14%
63	n7	135	18% 79% 19%
64	N8	148	11% 80% 19%
64	n8	148	% 82% 17%
65	N9	58	17% 86% 14%
65	n9	58	14% 84% 16%

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Mol	Chain	Length	Quality of chain
66	O0	100	18% 77% 19%
66	o0	100	5% 87% 13%
67	O1	109	15% 81% 18%
67	o1	109	8% 80% 18%
68	O2	127	5% 87% 13%
68	o2	127	86% 14%
69	O3	106	2% 86% 14%
69	o3	106	2% 82% 18%
70	O4	112	11% 79% 21%
70	o4	112	6% 84% 16%
71	O5	119	4% 82% 18%
71	o5	119	3% 82% 18%
72	O6	99	14% 75% 24%
72	o6	99	7% 77% 22%
73	O7	84	76% 24%
73	o7	84	82% 14%
74	O8	77	19% 81% 19%
74	o8	77	21% 83% 16%
75	O9	50	80% 18%
75	o9	50	84% 16%
76	Q0	52	4% 79% 21%
76	q0	52	4% 81% 19%
77	Q1	25	12% 88% 12%
77	q1	25	4% 60% 40%
78	Q2	105	23% 80% 20%

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Mol	Chain	Length	Quality of chain
78	q2	105	12% 88% 12%
79	Q3	91	2% 86% 14%
79	q3	91	81% 19%
80	p0	312	24% 39% 5% 56%

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
81	MG	1	3404	-	-	-	X
81	MG	1	3423	-	-	-	X
81	MG	1	3425	-	-	-	X
81	MG	1	3429	-	-	-	X
81	MG	1	3431	-	-	-	X
81	MG	1	3441	-	-	-	X
81	MG	1	3485	-	-	-	X
81	MG	1	3486	-	-	-	X
81	MG	1	3487	-	-	-	X
81	MG	1	3505	-	-	-	X
81	MG	1	3523	-	-	-	X
81	MG	1	3540	-	-	-	X
81	MG	1	3543	-	-	-	X
81	MG	1	3547	-	-	-	X
81	MG	1	3553	-	-	-	X
81	MG	1	3565	-	-	-	X
81	MG	1	3578	-	-	-	X
81	MG	1	3579	-	-	-	X
81	MG	1	3582	-	-	-	X
81	MG	1	3609	-	-	-	X
81	MG	1	3612	-	-	-	X
81	MG	1	3620	-	-	-	X
81	MG	1	3630	-	-	-	X
81	MG	1	3634	-	-	-	X
81	MG	1	3635	-	-	-	X
81	MG	1	3641	-	-	-	X
81	MG	1	3643	-	-	-	X
81	MG	1	3645	-	-	-	X
81	MG	1	3659	-	-	-	X
81	MG	1	3660	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3663	-	-	-	X
81	MG	1	3668	-	-	-	X
81	MG	1	3673	-	-	-	X
81	MG	1	3676	-	-	-	X
81	MG	1	3687	-	-	-	X
81	MG	1	3688	-	-	-	X
81	MG	1	3690	-	-	-	X
81	MG	1	3692	-	-	-	X
81	MG	1	3693	-	-	-	X
81	MG	1	3695	-	-	-	X
81	MG	1	3700	-	-	-	X
81	MG	1	3704	-	-	-	X
81	MG	1	3712	-	-	-	X
81	MG	1	3720	-	-	-	X
81	MG	1	3721	-	-	-	X
81	MG	1	3723	-	-	-	X
81	MG	1	3724	-	-	-	X
81	MG	1	3725	-	-	-	X
81	MG	1	3726	-	-	-	X
81	MG	1	3727	-	-	-	X
81	MG	1	3733	-	-	-	X
81	MG	1	3744	-	-	-	X
81	MG	1	3745	-	-	-	X
81	MG	1	3748	-	-	-	X
81	MG	1	3761	-	-	-	X
81	MG	1	3762	-	-	-	X
81	MG	1	3763	-	-	-	X
81	MG	1	3769	-	-	-	X
81	MG	1	3771	-	-	-	X
81	MG	1	3773	-	-	-	X
81	MG	1	3780	-	-	-	X
81	MG	1	3781	-	-	-	X
81	MG	1	3782	-	-	-	X
81	MG	1	3783	-	-	-	X
81	MG	1	3784	-	-	-	X
81	MG	1	3785	-	-	-	X
81	MG	1	3788	-	-	-	X
81	MG	1	3789	-	-	-	X
81	MG	1	3791	-	-	-	X
81	MG	1	3792	-	-	-	X
81	MG	1	3795	-	-	-	X
81	MG	1	3800	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3801	-	-	-	X
81	MG	1	3802	-	-	-	X
81	MG	1	3804	-	-	-	X
81	MG	1	3806	-	-	-	X
81	MG	2	1904	-	-	-	X
81	MG	2	1907	-	-	-	X
81	MG	2	1915	-	-	-	X
81	MG	2	1921	-	-	-	X
81	MG	2	1928	-	-	-	X
81	MG	2	1937	-	-	-	X
81	MG	2	1951	-	-	-	X
81	MG	2	1953	-	-	-	X
81	MG	2	1967	-	-	-	X
81	MG	2	1970	-	-	-	X
81	MG	2	1972	-	-	-	X
81	MG	2	1985	-	-	-	X
81	MG	2	1986	-	-	-	X
81	MG	2	1989	-	-	-	X
81	MG	2	1990	-	-	-	X
81	MG	2	1995	-	-	-	X
81	MG	2	1999	-	-	-	X
81	MG	2	2006	-	-	-	X
81	MG	3	201	-	-	-	X
81	MG	3	202	-	-	-	X
81	MG	3	205	-	-	-	X
81	MG	4	202	-	-	-	X
81	MG	4	206	-	-	-	X
81	MG	4	208	-	-	-	X
81	MG	4	210	-	-	-	X
81	MG	4	211	-	-	-	X
81	MG	4	215	-	-	-	X
81	MG	4	216	-	-	-	X
81	MG	4	222	-	-	-	X
81	MG	5	3412	-	-	-	X
81	MG	5	3426	-	-	-	X
81	MG	5	3465	-	-	-	X
81	MG	5	3488	-	-	-	X
81	MG	5	3491	-	-	-	X
81	MG	5	3493	-	-	-	X
81	MG	5	3500	-	-	-	X
81	MG	5	3514	-	-	-	X
81	MG	5	3516	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3549	-	-	-	X
81	MG	5	3555	-	-	-	X
81	MG	5	3558	-	-	-	X
81	MG	5	3566	-	-	-	X
81	MG	5	3567	-	-	-	X
81	MG	5	3594	-	-	-	X
81	MG	5	3601	-	-	-	X
81	MG	5	3606	-	-	-	X
81	MG	5	3617	-	-	-	X
81	MG	5	3634	-	-	-	X
81	MG	5	3636	-	-	-	X
81	MG	5	3638	-	-	-	X
81	MG	5	3643	-	-	-	X
81	MG	5	3647	-	-	-	X
81	MG	5	3648	-	-	-	X
81	MG	5	3660	-	-	-	X
81	MG	5	3667	-	-	-	X
81	MG	5	3669	-	-	-	X
81	MG	5	3672	-	-	-	X
81	MG	5	3675	-	-	-	X
81	MG	5	3676	-	-	-	X
81	MG	5	3677	-	-	-	X
81	MG	5	3684	-	-	-	X
81	MG	5	3693	-	-	-	X
81	MG	5	3708	-	-	-	X
81	MG	5	3710	-	-	-	X
81	MG	5	3712	-	-	-	X
81	MG	5	3713	-	-	-	X
81	MG	5	3716	-	-	-	X
81	MG	5	3722	-	-	-	X
81	MG	5	3724	-	-	-	X
81	MG	5	3726	-	-	-	X
81	MG	5	3728	-	-	-	X
81	MG	5	3740	-	-	-	X
81	MG	5	3743	-	-	-	X
81	MG	5	3745	-	-	-	X
81	MG	5	3750	-	-	-	X
81	MG	5	3754	-	-	-	X
81	MG	5	3758	-	-	-	X
81	MG	5	3759	-	-	-	X
81	MG	5	3761	-	-	-	X
81	MG	5	3762	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3765	-	-	-	X
81	MG	5	3771	-	-	-	X
81	MG	5	3779	-	-	-	X
81	MG	5	3787	-	-	-	X
81	MG	5	3788	-	-	-	X
81	MG	5	3789	-	-	-	X
81	MG	5	3790	-	-	-	X
81	MG	5	3792	-	-	-	X
81	MG	5	3793	-	-	-	X
81	MG	5	3794	-	-	-	X
81	MG	5	3800	-	-	-	X
81	MG	5	3803	-	-	-	X
81	MG	5	3806	-	-	-	X
81	MG	5	3807	-	-	-	X
81	MG	5	3811	-	-	-	X
81	MG	5	3812	-	-	-	X
81	MG	5	3818	-	-	-	X
81	MG	5	3819	-	-	-	X
81	MG	5	3820	-	-	-	X
81	MG	5	3822	-	-	-	X
81	MG	5	3823	-	-	-	X
81	MG	5	3825	-	-	-	X
81	MG	5	3826	-	-	-	X
81	MG	5	3832	-	-	-	X
81	MG	5	3833	-	-	-	X
81	MG	5	3834	-	-	-	X
81	MG	5	3837	-	-	-	X
81	MG	5	3838	-	-	-	X
81	MG	5	3839	-	-	-	X
81	MG	5	3840	-	-	-	X
81	MG	5	3841	-	-	-	X
81	MG	5	3842	-	-	-	X
81	MG	6	1910	-	-	-	X
81	MG	6	1911	-	-	-	X
81	MG	6	1916	-	-	-	X
81	MG	6	1918	-	-	-	X
81	MG	6	1919	-	-	-	X
81	MG	6	1922	-	-	-	X
81	MG	6	1939	-	-	-	X
81	MG	6	1952	-	-	-	X
81	MG	6	1958	-	-	-	X
81	MG	6	1972	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	6	1978	-	-	-	X
81	MG	6	1980	-	-	-	X
81	MG	6	1985	-	-	-	X
81	MG	6	1997	-	-	-	X
81	MG	6	2000	-	-	-	X
81	MG	6	2003	-	-	-	X
81	MG	6	2006	-	-	-	X
81	MG	6	2008	-	-	-	X
81	MG	6	2009	-	-	-	X
81	MG	6	2011	-	-	-	X
81	MG	6	2012	-	-	-	X
81	MG	7	206	-	-	-	X
81	MG	7	207	-	-	-	X
81	MG	8	204	-	-	-	X
81	MG	8	205	-	-	-	X
81	MG	8	206	-	-	-	X
81	MG	8	210	-	-	-	X
81	MG	8	213	-	-	-	X
81	MG	M6	201	-	-	-	X
81	MG	M7	201	-	-	-	X
81	MG	M7	205	-	-	-	X
81	MG	N8	202	-	-	-	X
81	MG	O2	202	-	-	-	X
81	MG	O3	201	-	-	-	X
81	MG	O9	101	-	-	-	X
81	MG	S1	301	-	-	-	X
81	MG	S8	301	-	-	-	X
81	MG	d3	201	-	-	-	X
81	MG	l2	301	-	-	-	X
81	MG	l3	403	-	-	-	X
81	MG	m6	201	-	-	-	X
81	MG	n0	201	-	-	-	X
81	MG	n0	202	-	-	-	X
81	MG	n5	201	-	-	-	X
81	MG	o2	202	-	-	-	X
81	MG	o3	201	-	-	-	X
81	MG	o3	203	-	-	-	X
81	MG	o5	201	-	-	-	X
81	MG	o7	505	-	-	-	X
81	MG	q2	503	-	-	-	X
81	MG	q2	504	-	-	-	X
81	MG	s8	302	-	-	-	X

2 Entry composition (i)

There are 84 unique types of molecules in this entry. The entry contains 397710 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	1688	Total	C	N	O	P	0	0	0
			35985	16089	6386	11822	1688			
1	6	1700	Total	C	N	O	P	0	0	0
			36234	16201	6426	11907	1700			

- 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	185	Total	C	N	O	0	0	0
			1486	954	266	266			

- 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	92	Total	C	N	O	S	0	0	0
			752	487	122	141	2			
12	c0	92	Total	C	N	O	S	0	0	0
			741	478	121	140	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	142	Total	C	N	O	S	0	0	0
			1146	735	217	191	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	120	Total	C	N	O	S	0	0	0
			870	548	152	168	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	122	Total	C	N	O	S	0	0	0
			967	616	180	164	7			
17	c5	119	Total	C	N	O	S	0	0	0
			939	595	176	161	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	141	Total	C	N	O	0	0	0
			1105	708	203	194			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	117	Total	C	N	O	S	0	0	0
			911	568	174	167	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	105	Total	C	N	O	S	0	0	0
			837	529	152	155	1			
22	d0	101	Total	C	N	O	S	0	0	0
			805	512	145	147	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 1073	C 676	N 208	O 189	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	45	Total	C	N	O	S	0	0	0
			352	222	66	60	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	313	Total	C	N	O	S	0	0	0
			2403	1521	411	463	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011
sR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	135	Total	C	N	O	0	0	0
			985	581	197	207			
35	sM	115	Total	C	N	O	0	0	0
			874	514	177	183			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3078	Total	C	N	O	P	0	0	0
			65838	29408	11870	21482	3078			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	5	3127	Total	C	N	O	P	0	0	0
			66891	29878	12066	21820	3127			

- 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	157	Total	C	N	O	P	0	0	0
			3333	1491	584	1101	157			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	294	Total	C	N	O	S	0	0	0
			2357	1491	410	454	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	190	Total	C	N	O	S	0	0	0
			1510	957	273	276	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	208	Total	C	N	O	S	0	0	0
			1690	1074	319	291	6			
47	m0	209	Total	C	N	O	S	0	0	0
			1696	1077	321	293	5			

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

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	0	0	0
			1420	882	281	257			
53	m7	175	Total	C	N	O	0	0	0
			1378	856	273	249			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	m9	183	Total	C	N	O	0	0	0
			1482	911	320	251			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	170	Total	C	N	O	S	0	0	0
			1432	922	265	242	3			
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	98	Total	C	N	O	0	0	0
			778	505	127	146			
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	135	Total	C	N	O	S	0	0	0
			997	625	188	177	7			
59	n3	134	Total	C	N	O	S	0	0	0
			993	623	187	176	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	122	Total	C	N	O	S	0	0	0
			925	582	184	158	1			
60	n4	118	Total	C	N	O	S	0	0	0
			946	597	188	160	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	124	Total	C	N	O	0	0	0
			976	614	190	172			

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

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

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

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

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

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

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

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

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

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

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

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

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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	84	Total	C	N	O	S	0	0	0
			665	405	145	110	5			
73	o7	82	Total	C	N	O	S	0	0	0
			650	396	142	107	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	49	Total	C	N	O	S	0	0	0
			431	269	96	64	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 694	C 429	N 138	O 121	S 6	0	0	0
79	q3	91	Total 694	C 429	N 138	O 121	S 6	0	0	0

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	p0	138	Total 1052	C 672	N 187	O 190	S 3	0	0	0

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	2	111	Total 111	Mg 111	0	0
81	S1	1	Total 1	Mg 1	0	0
81	S8	1	Total 1	Mg 1	0	0
81	C0	1	Total 1	Mg 1	0	0
81	C4	2	Total 2	Mg 2	0	0
81	C8	1	Total 1	Mg 1	0	0
81	D2	2	Total 2	Mg 2	0	0
81	D9	1	Total 1	Mg 1	0	0
81	SM	1	Total 1	Mg 1	0	0
81	1	407	Total 407	Mg 407	0	0
81	3	9	Total 9	Mg 9	0	0
81	4	25	Total 25	Mg 25	1	0
81	L2	3	Total 3	Mg 3	0	0
81	L3	2	Total 2	Mg 2	0	0
81	L5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	L6	1	Total Mg 1 1	0	0
81	L8	1	Total Mg 1 1	0	0
81	M0	2	Total Mg 2 2	0	0
81	M4	1	Total Mg 1 1	0	0
81	M5	1	Total Mg 1 1	0	0
81	M6	1	Total Mg 1 1	0	0
81	M7	6	Total Mg 6 6	0	0
81	N2	1	Total Mg 1 1	0	0
81	N7	1	Total Mg 1 1	0	0
81	N8	2	Total Mg 2 2	0	0
81	O2	3	Total Mg 3 3	0	0
81	O3	2	Total Mg 2 2	0	0
81	O5	1	Total Mg 1 1	0	0
81	O6	2	Total Mg 2 2	0	0
81	O7	1	Total Mg 1 1	0	0
81	O8	1	Total Mg 1 1	0	0
81	O9	1	Total Mg 1 1	0	0
81	Q2	1	Total Mg 1 1	0	0
81	6	112	Total Mg 112 112	0	0
81	s8	2	Total Mg 2 2	0	0
81	c3	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	d3	2	Total Mg 2 2	0	0
81	sM	1	Total Mg 1 1	0	0
81	5	443	Total Mg 443 443	1	0
81	7	8	Total Mg 8 8	0	0
81	8	14	Total Mg 14 14	0	0
81	l2	4	Total Mg 4 4	0	0
81	l3	4	Total Mg 4 4	0	0
81	l4	1	Total Mg 1 1	0	0
81	l7	2	Total Mg 2 2	0	0
81	l9	1	Total Mg 1 1	0	0
81	m0	1	Total Mg 1 1	0	0
81	m6	1	Total Mg 1 1	0	0
81	m7	5	Total Mg 5 5	0	0
81	n0	2	Total Mg 2 2	0	0
81	n3	2	Total Mg 2 2	0	0
81	n4	1	Total Mg 1 1	0	0
81	n5	1	Total Mg 1 1	0	0
81	n7	1	Total Mg 1 1	0	0
81	o2	2	Total Mg 2 2	0	0
81	o3	3	Total Mg 3 3	0	0
81	o5	1	Total Mg 1 1	0	0

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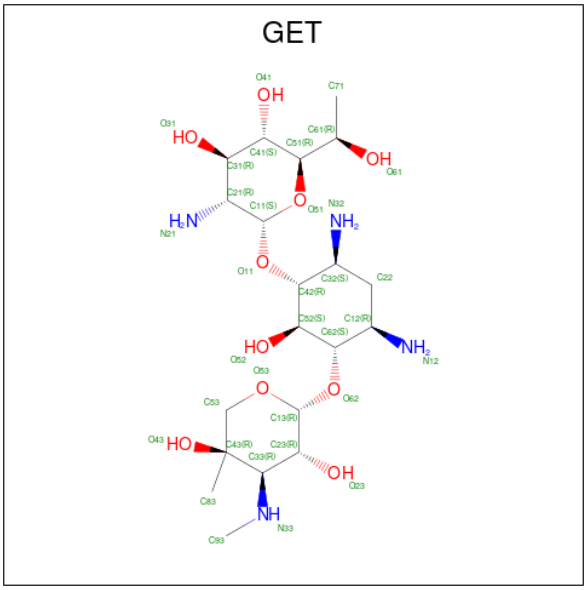
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	o7	5	Total Mg 5 5	0	0
81	q2	4	Total Mg 4 4	0	0

- Molecule 82 is GENETICIN (three-letter code: GET) (formula: $C_{20}H_{40}N_4O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	2	1	Total C N O 34 20 4 10	0	0
82	2	1	Total C N O 34 20 4 10	0	0
82	2	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	6	1	Total C N O 34 20 4 10	0	0
82	6	1	Total C N O 34 20 4 10	0	0
82	6	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	5	1	Total C N O 34 20 4 10	0	0
82	n6	1	Total C N O 34 20 4 10	0	0

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	D6	1	Total Zn 1 1	0	0
83	D7	1	Total Zn 1 1	0	0
83	D9	1	Total Zn 1 1	0	0
83	E1	1	Total Zn 1 1	0	0
83	O4	1	Total Zn 1 1	0	0
83	O7	1	Total Zn 1 1	0	0
83	Q0	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	Q2	1	Total Zn 1 1	0	0
83	Q3	1	Total Zn 1 1	0	0
83	d6	1	Total Zn 1 1	0	0
83	d7	1	Total Zn 1 1	0	0
83	d9	1	Total Zn 1 1	0	0
83	e1	1	Total Zn 1 1	0	0
83	o4	1	Total Zn 1 1	0	0
83	o7	1	Total Zn 1 1	0	0
83	q0	1	Total Zn 1 1	0	0
83	q2	1	Total Zn 1 1	0	0
83	q3	1	Total Zn 1 1	0	0

- Molecule 84 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	2	99	Total O 99 99	0	0
84	S4	1	Total O 1 1	0	0
84	C1	1	Total O 1 1	0	0
84	C3	1	Total O 1 1	0	0
84	C6	1	Total O 1 1	0	0
84	C9	2	Total O 2 2	0	0
84	D3	1	Total O 1 1	0	0
84	D9	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	SM	1	Total O 1 1	0	0
84	1	367	Total O 367 367	2	0
84	3	18	Total O 18 18	0	0
84	4	7	Total O 7 7	0	0
84	L2	1	Total O 1 1	0	0
84	L3	1	Total O 1 1	0	0
84	L4	1	Total O 1 1	0	0
84	M0	2	Total O 2 2	0	0
84	M5	1	Total O 1 1	0	0
84	M6	2	Total O 2 2	0	0
84	M7	4	Total O 4 4	0	0
84	N1	3	Total O 3 3	0	0
84	N3	3	Total O 3 3	0	0
84	N5	1	Total O 1 1	0	0
84	N8	1	Total O 1 1	0	0
84	O1	2	Total O 2 2	0	0
84	O2	2	Total O 2 2	0	0
84	6	111	Total O 111 111	0	0
84	c3	1	Total O 1 1	0	0
84	c8	1	Total O 1 1	0	0
84	c9	2	Total O 2 2	0	0

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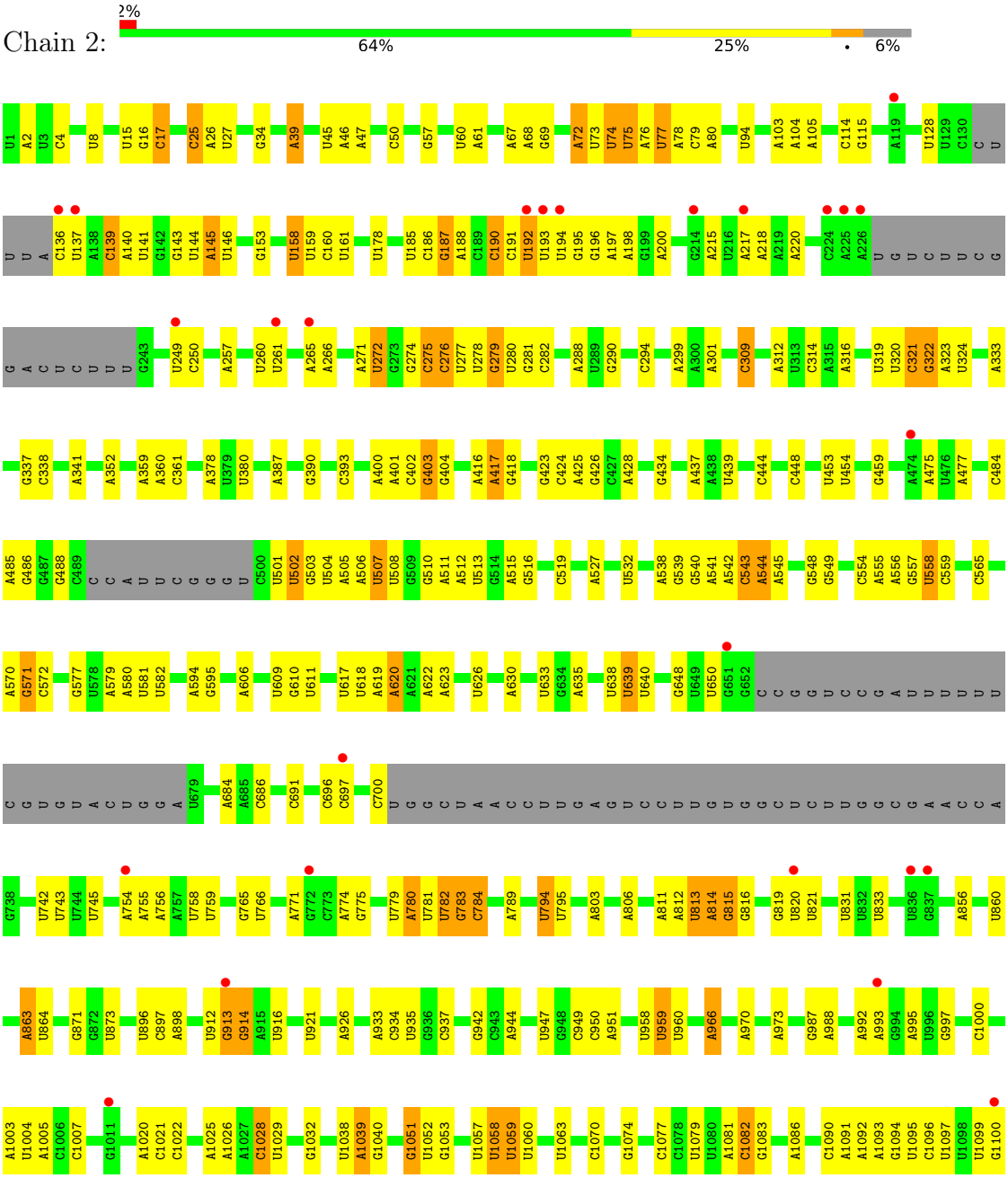
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	d3	2	Total O 2 2	0	0
84	5	365	Total O 365 365	1	0
84	7	11	Total O 11 11	0	0
84	8	7	Total O 7 7	0	0
84	l2	1	Total O 1 1	0	0
84	l3	4	Total O 4 4	0	0
84	l4	2	Total O 2 2	0	0
84	l9	1	Total O 1 1	0	0
84	m0	1	Total O 1 1	0	0
84	m5	3	Total O 3 3	0	0
84	m6	1	Total O 1 1	0	0
84	m7	2	Total O 2 2	0	0
84	m9	2	Total O 2 2	0	0
84	n1	3	Total O 3 3	0	0
84	n3	3	Total O 3 3	0	0
84	o2	3	Total O 3 3	0	0
84	o4	2	Total O 2 2	0	0
84	o7	1	Total O 1 1	0	0
84	q2	1	Total O 1 1	0	0

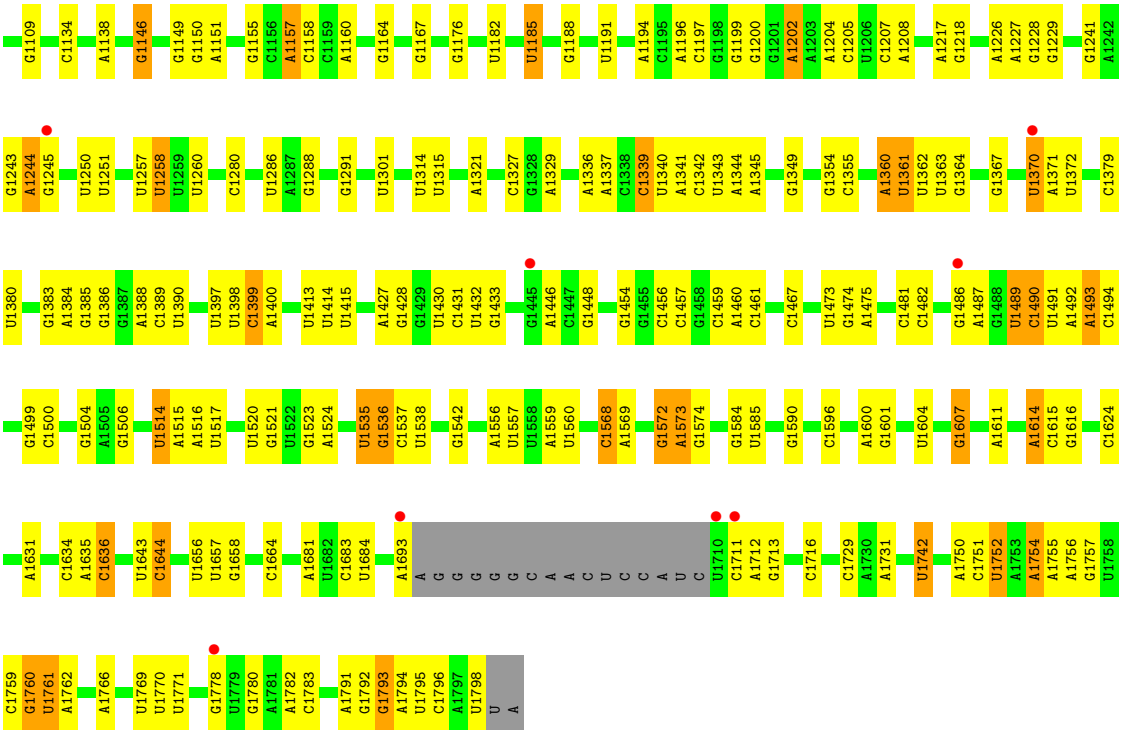
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

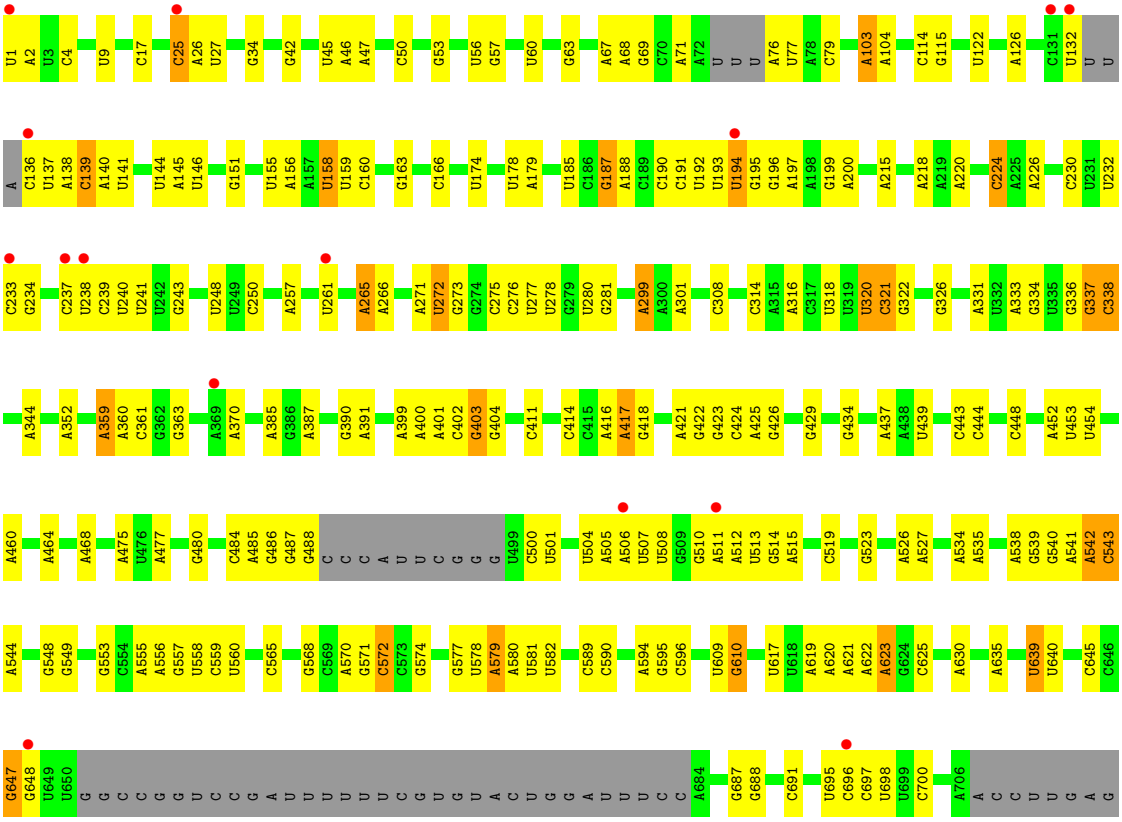
Chain 2:

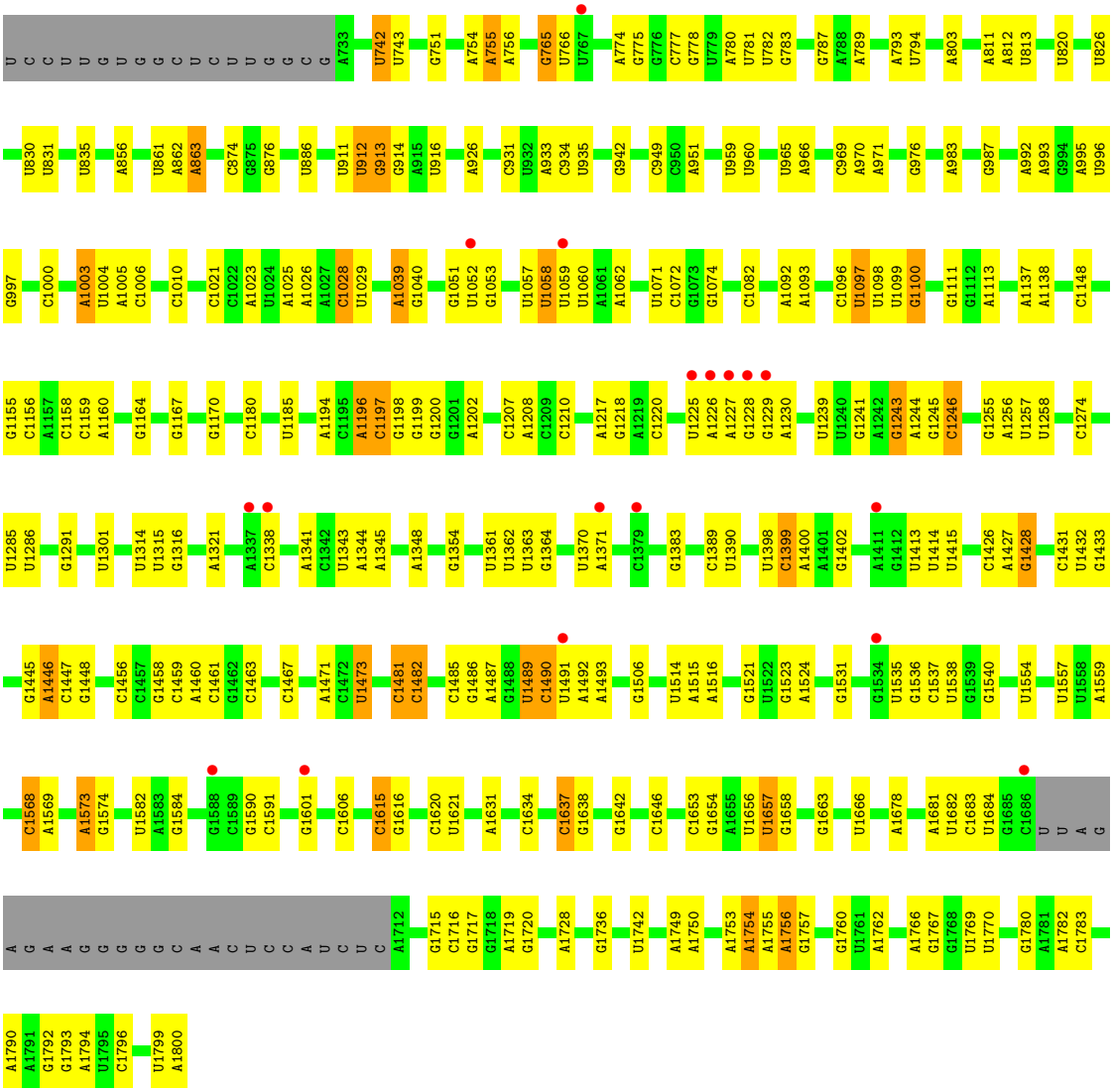




• Molecule 1: 18S ribosomal RNA

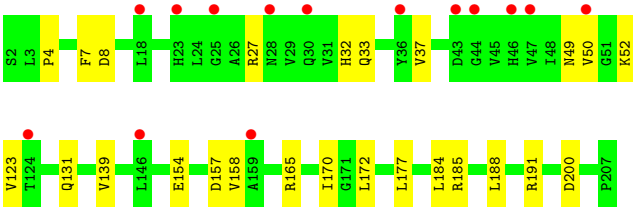
Chain 6:





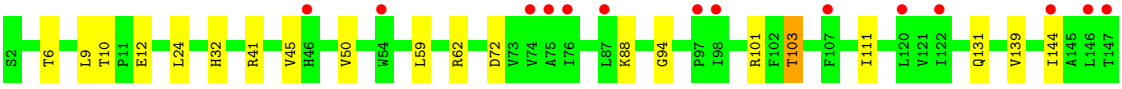
• Molecule 2: 40S ribosomal protein S0-A

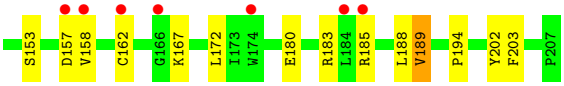
Chain S0:



• Molecule 2: 40S ribosomal protein S0-A

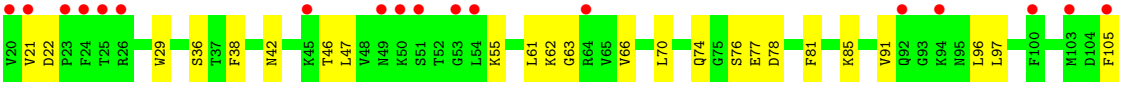
Chain s0:

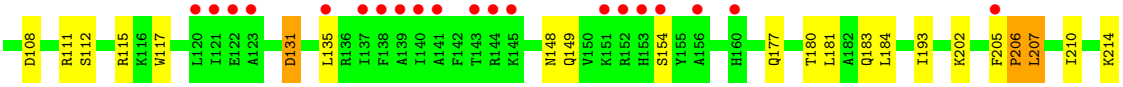


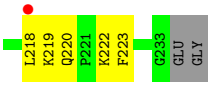


• Molecule 3: 40S ribosomal protein S1-A

Chain S1:

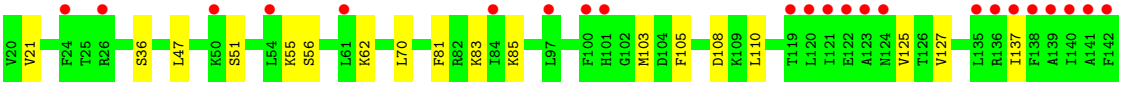


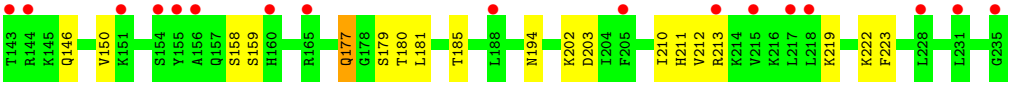




• Molecule 3: 40S ribosomal protein S1-A

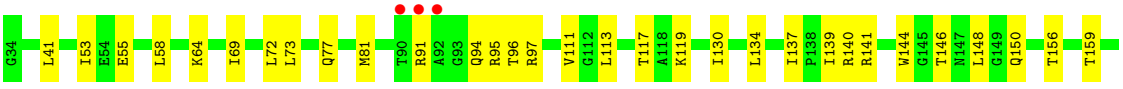
Chain s1:

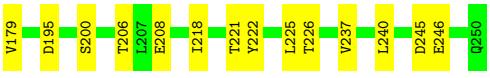




• Molecule 4: 40S ribosomal protein S2

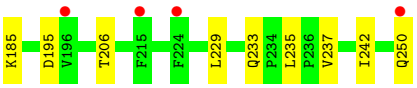
Chain S2:





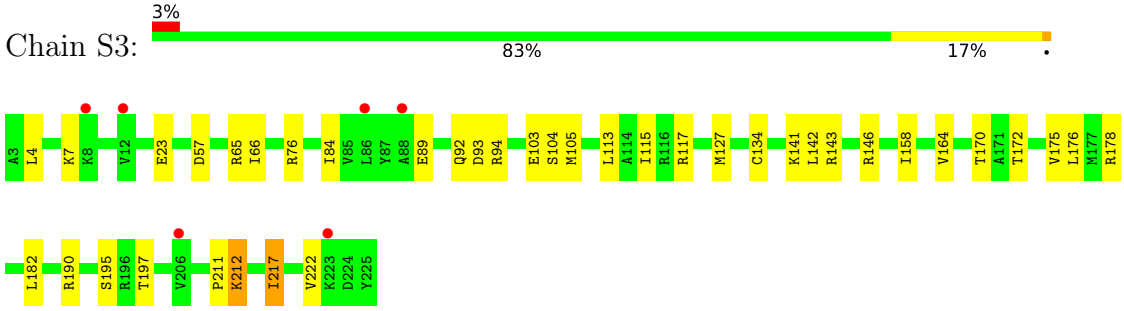
• Molecule 4: 40S ribosomal protein S2

Chain s2:



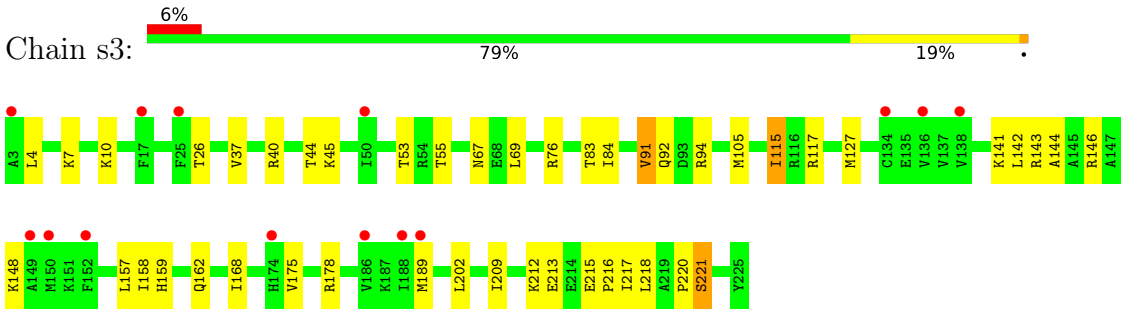
• Molecule 5: 40S ribosomal protein S3

Chain S3:



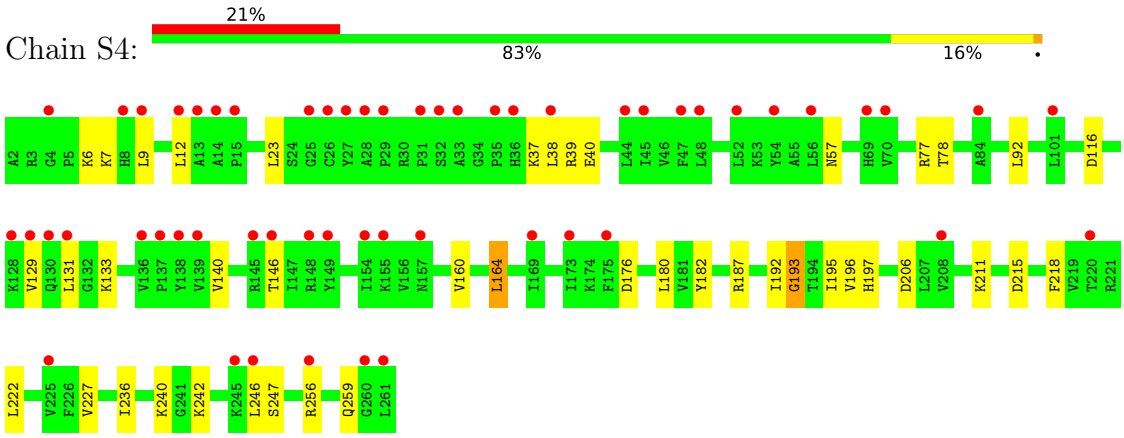
• Molecule 5: 40S ribosomal protein S3

Chain s3:



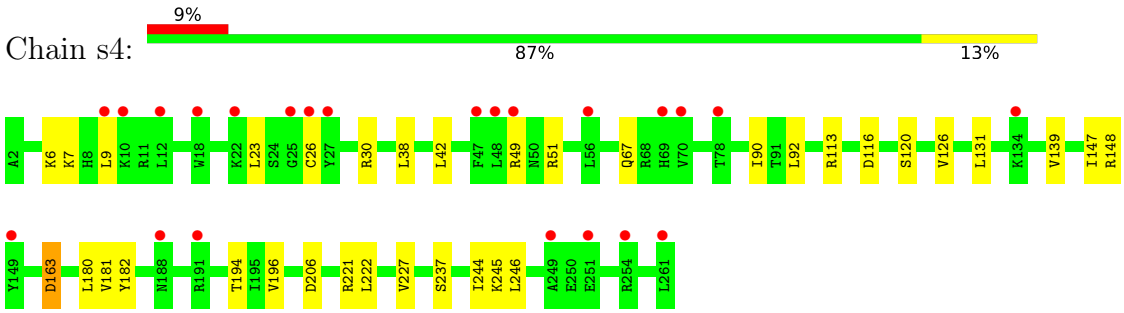
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



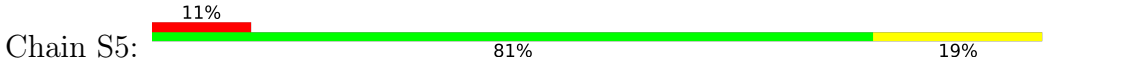
• Molecule 6: 40S ribosomal protein S4-A

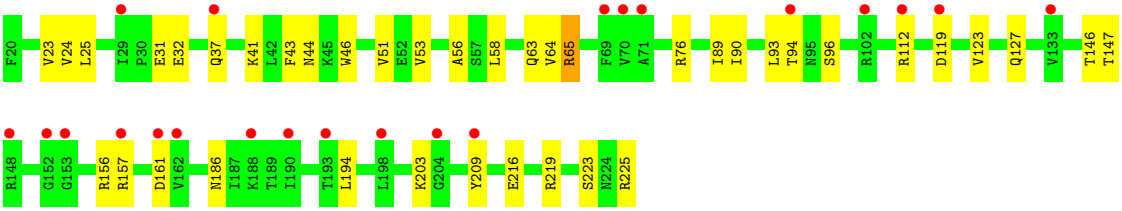
Chain s4:



• Molecule 7: 40S ribosomal protein S5

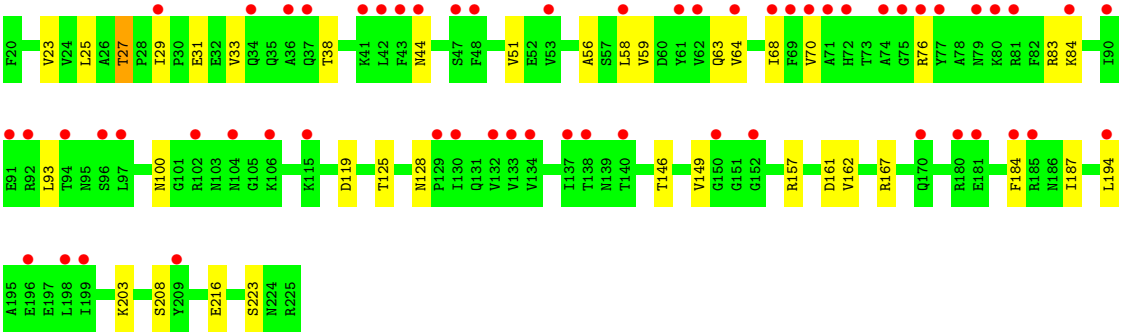
Chain S5:





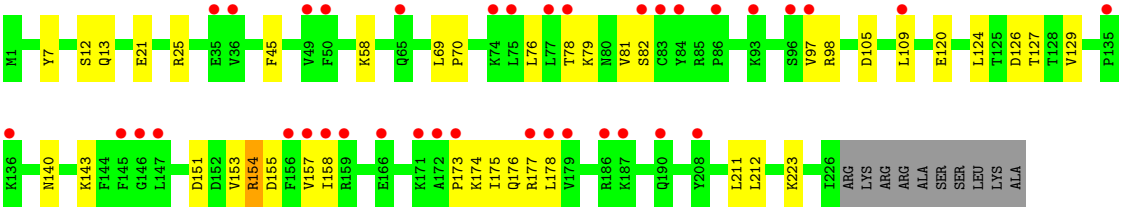
• Molecule 7: 40S ribosomal protein S5

Chain s5:



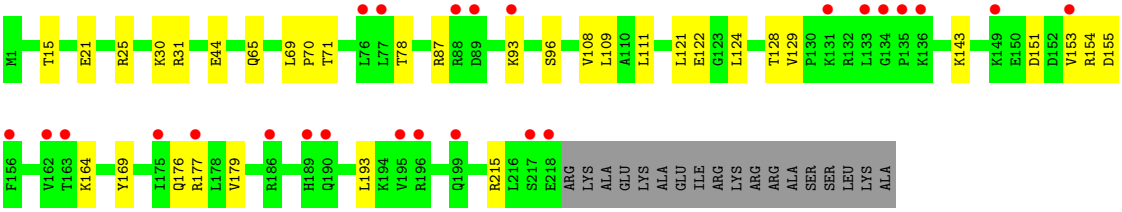
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



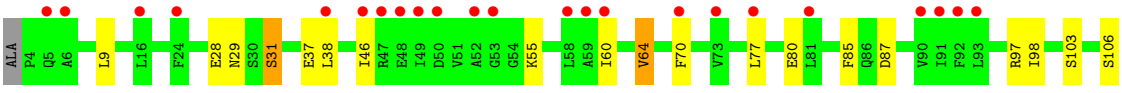
• Molecule 8: 40S ribosomal protein S6-A

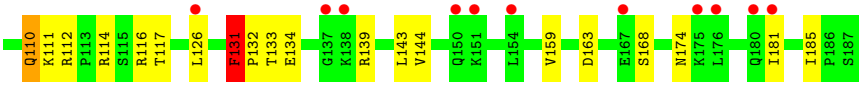
Chain s6:



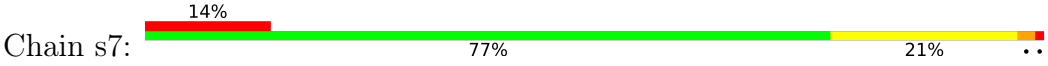
• Molecule 9: 40S ribosomal protein S7-A

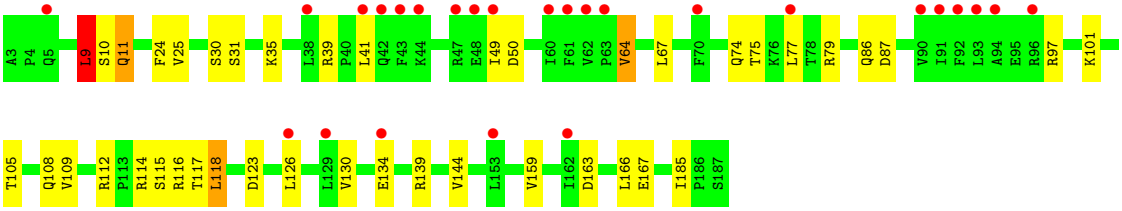
Chain S7:



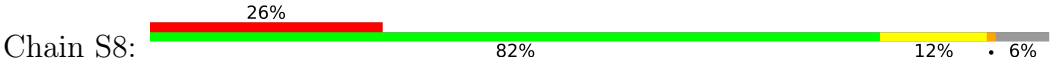


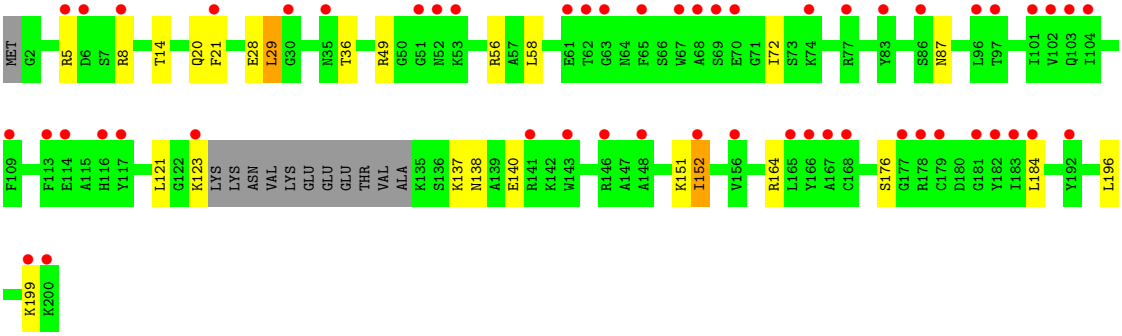
• Molecule 9: 40S ribosomal protein S7-A



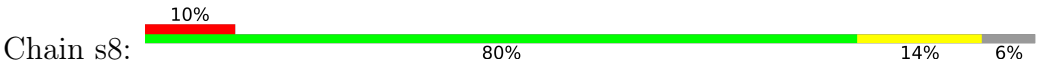


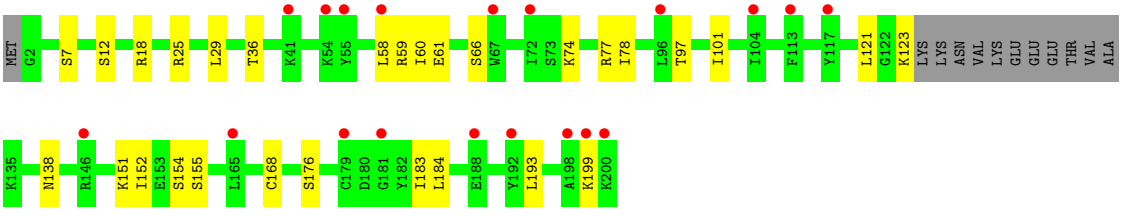
• Molecule 10: 40S ribosomal protein S8-A



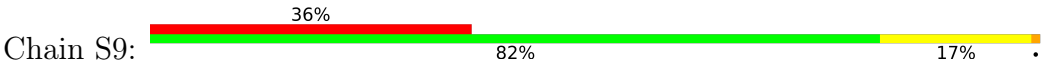


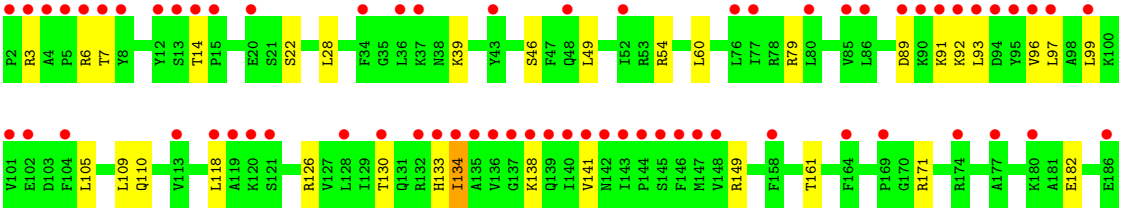
• Molecule 10: 40S ribosomal protein S8-A





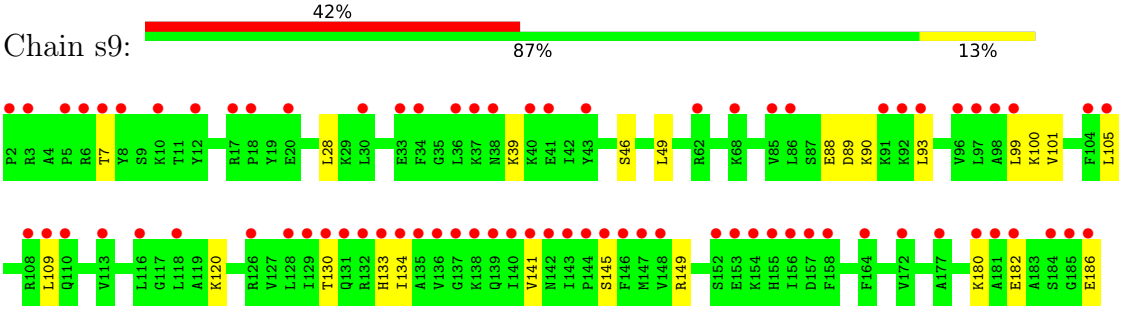
• Molecule 11: 40S ribosomal protein S9-A





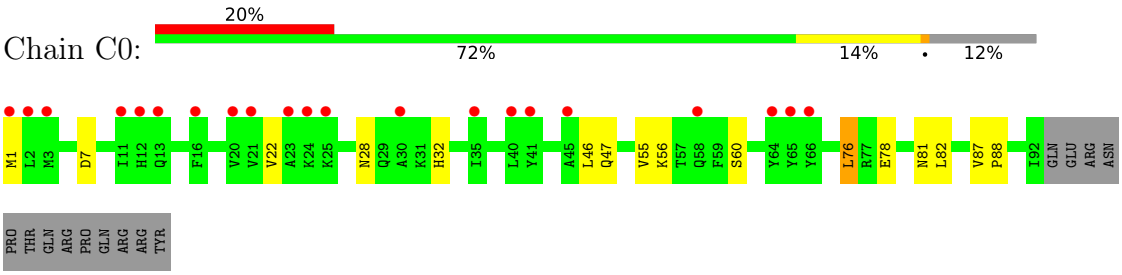
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



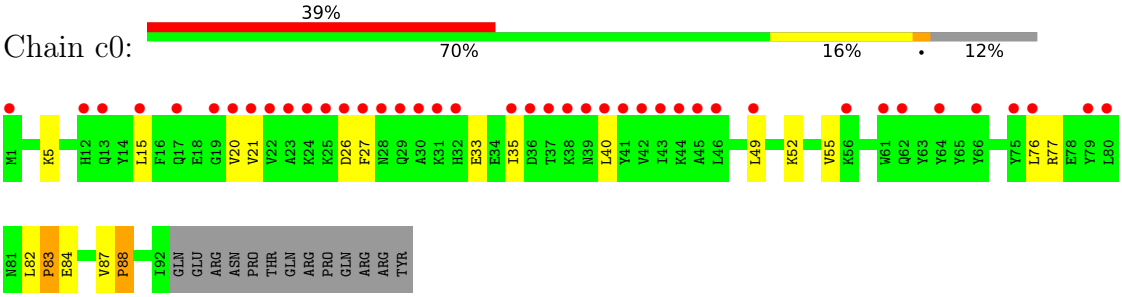
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



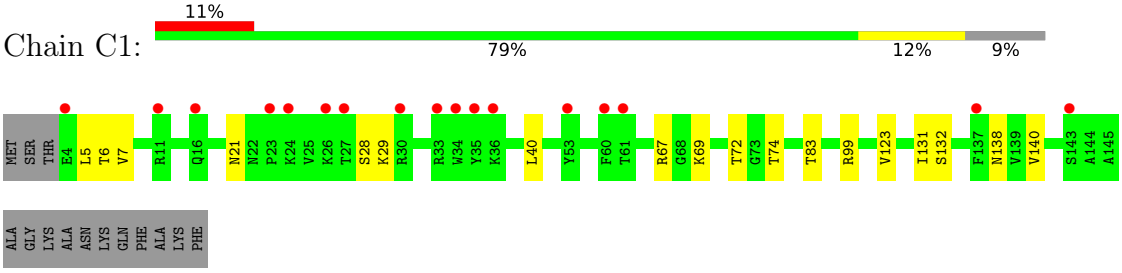
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



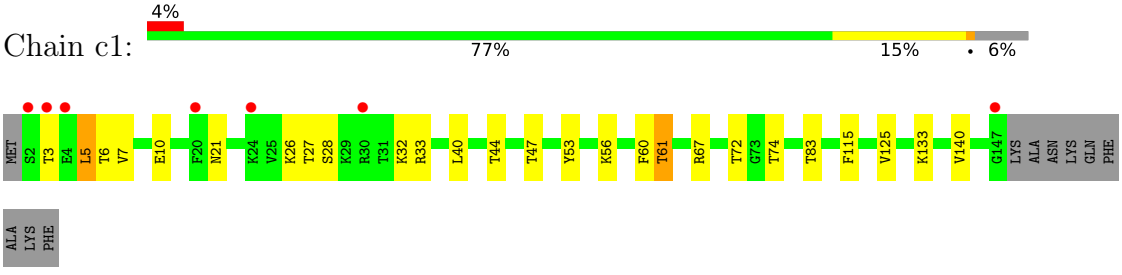
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



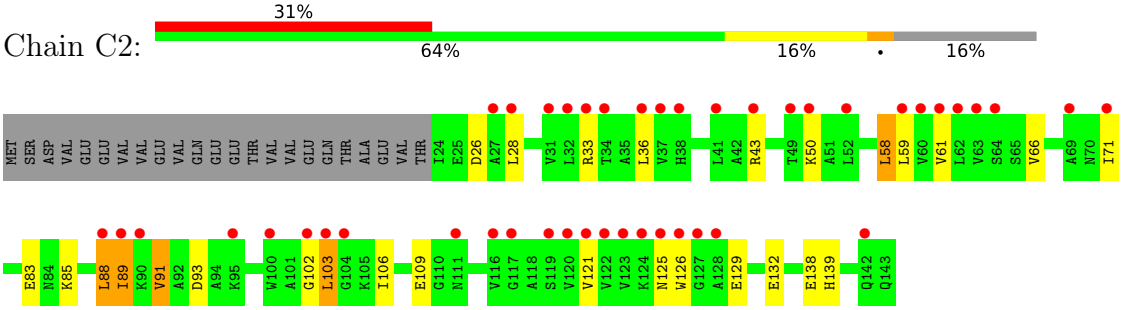
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



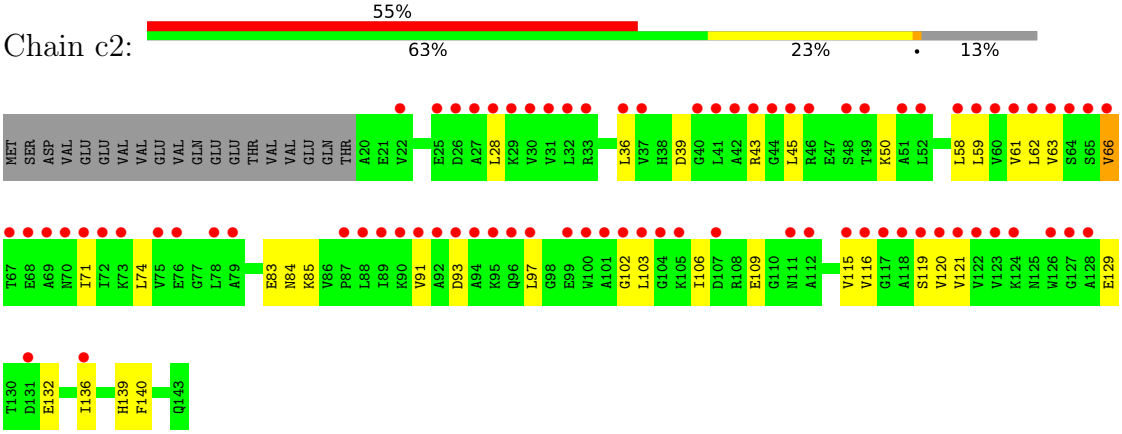
• Molecule 14: 40S ribosomal protein S12

Chain C2:



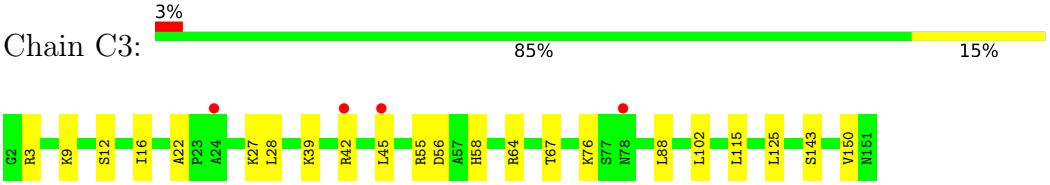
• Molecule 14: 40S ribosomal protein S12

Chain c2:



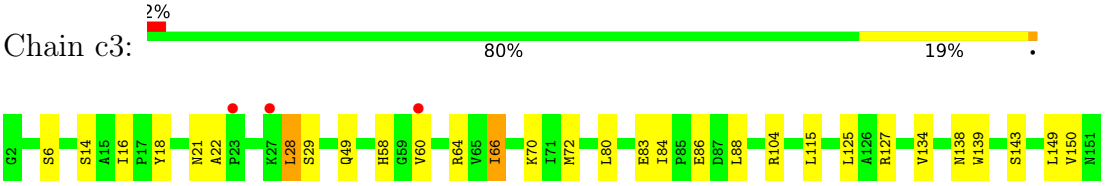
• Molecule 15: 40S ribosomal protein S13

Chain C3:



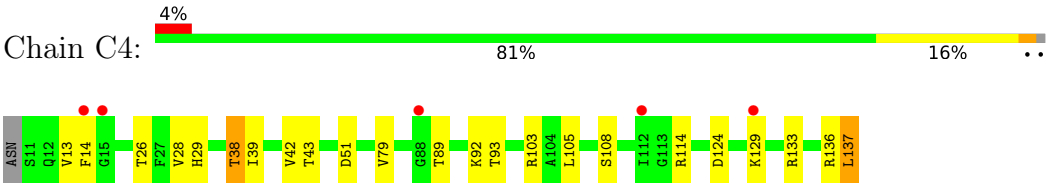
• Molecule 15: 40S ribosomal protein S13

Chain c3:



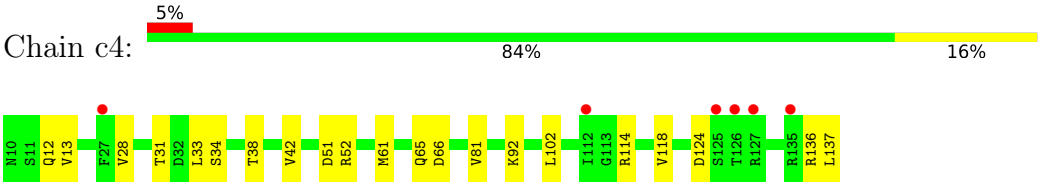
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



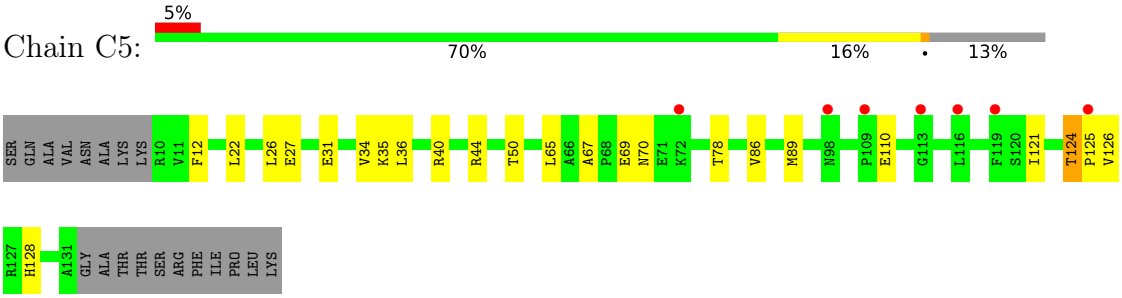
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



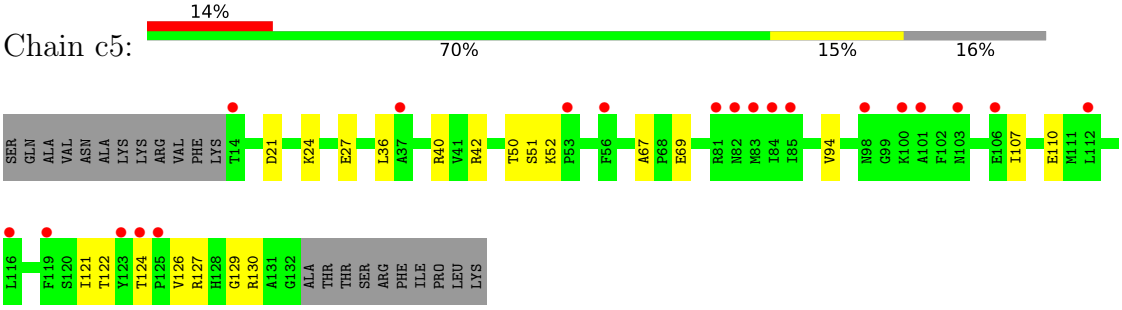
• Molecule 17: 40S ribosomal protein S15

Chain C5:



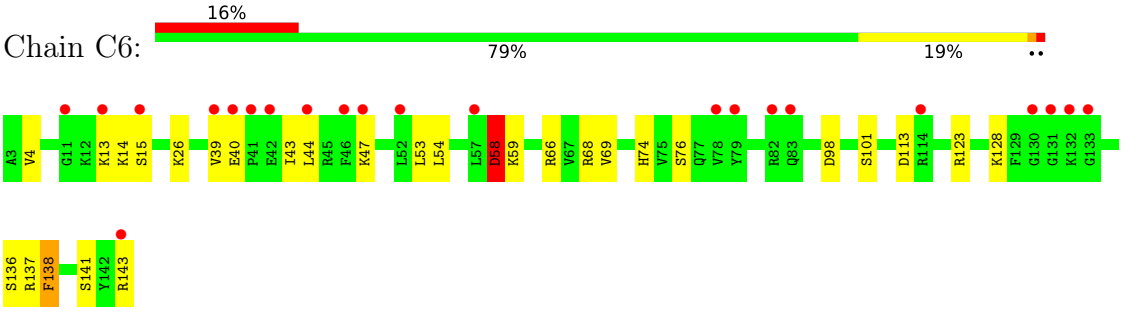
• Molecule 17: 40S ribosomal protein S15

Chain c5:



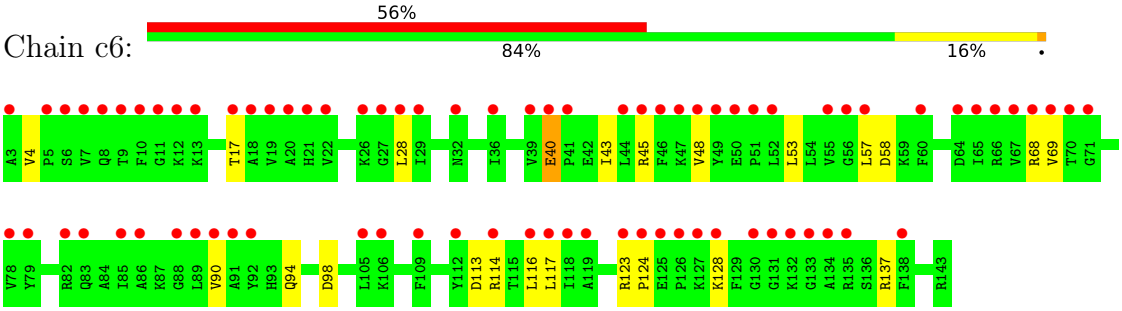
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



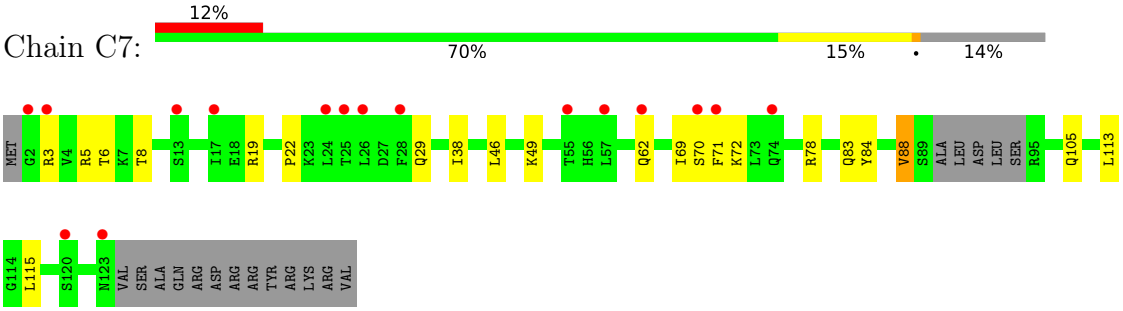
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



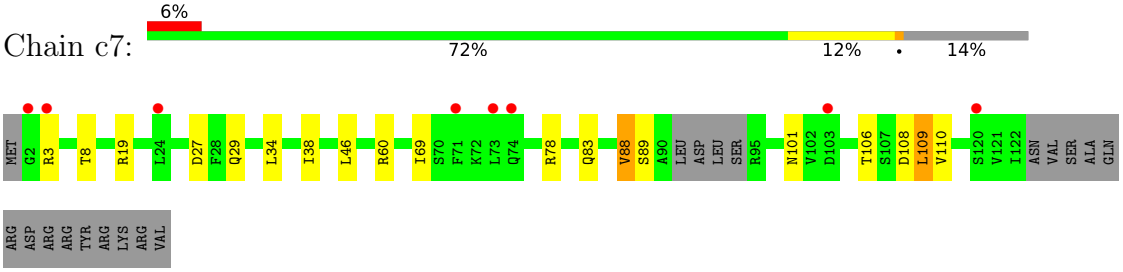
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



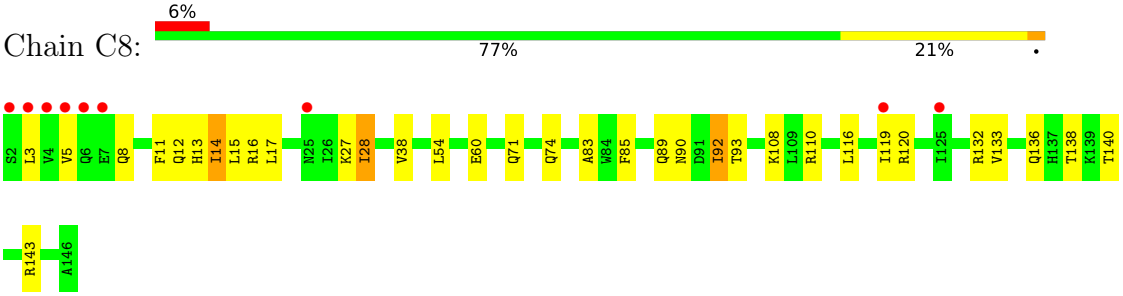
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



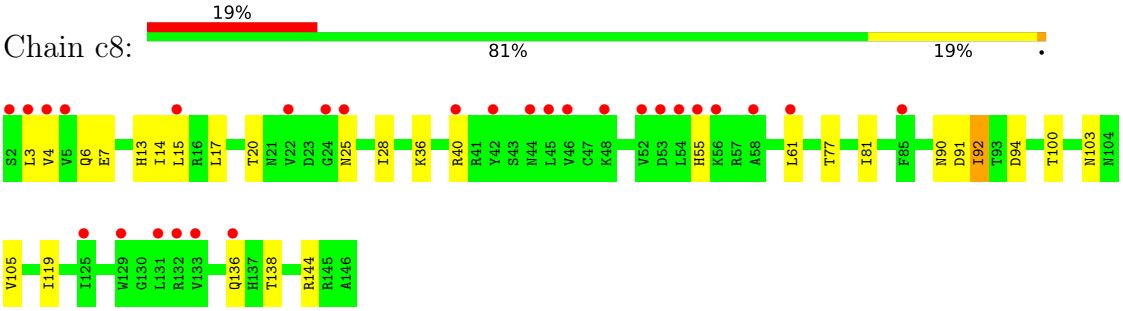
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



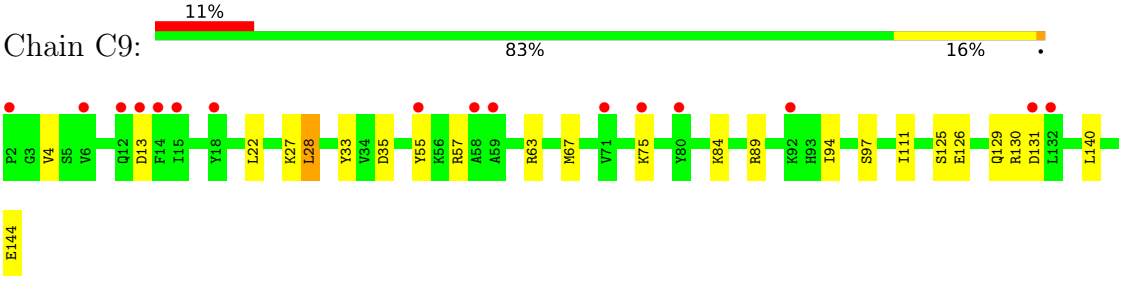
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



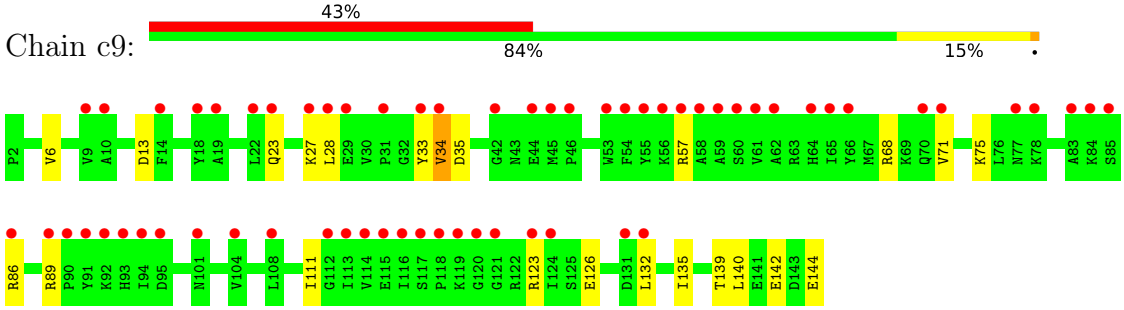
• Molecule 21: 40S ribosomal protein S19-A

Chain C9:



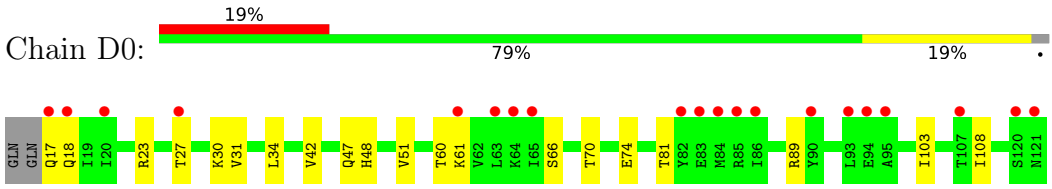
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



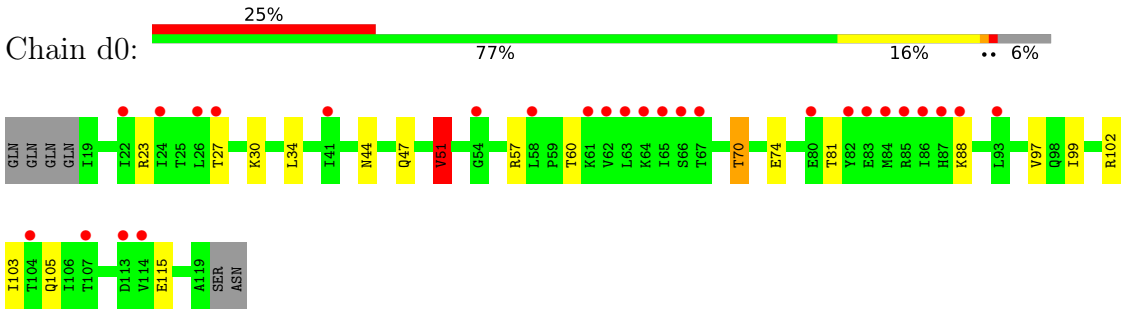
• Molecule 22: 40S ribosomal protein S20

Chain D0:



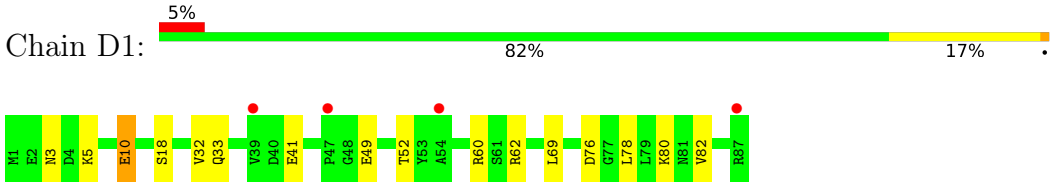
• Molecule 22: 40S ribosomal protein S20

Chain d0:



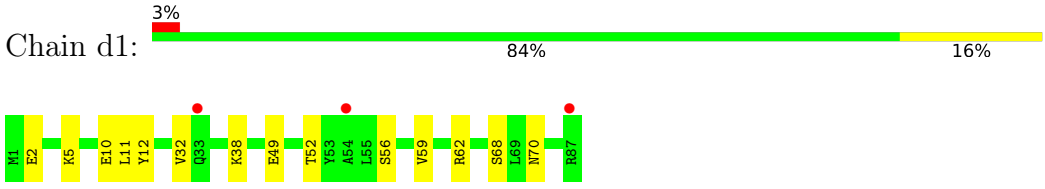
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



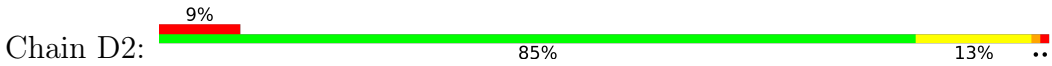
• Molecule 23: 40S ribosomal protein S21-A

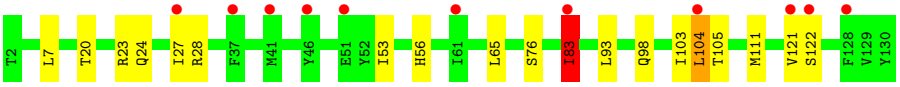
Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

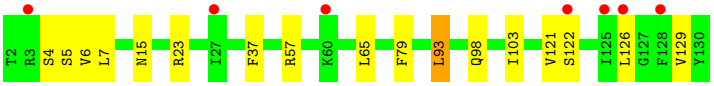
Chain D2:





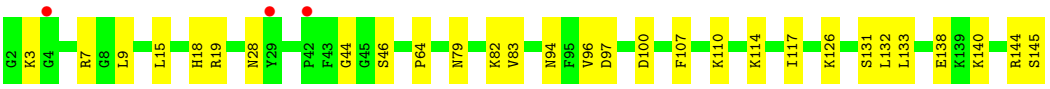
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



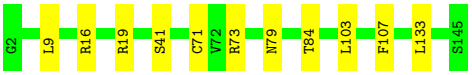
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



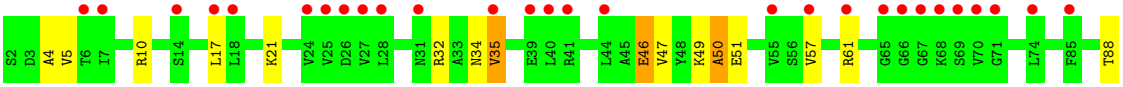
• Molecule 25: 40S ribosomal protein S23-A

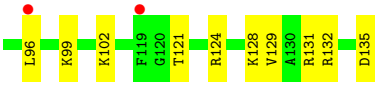
Chain d3:



• Molecule 26: 40S ribosomal protein S24-A

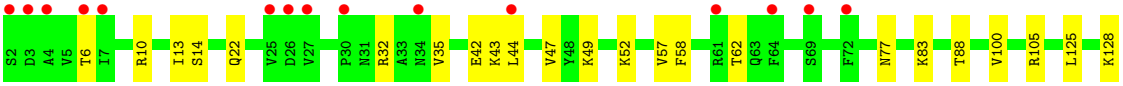
Chain D4:

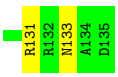




• Molecule 26: 40S ribosomal protein S24-A

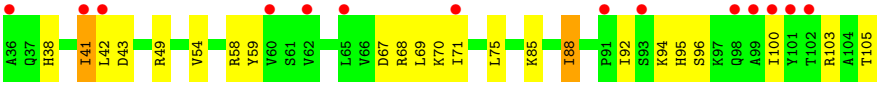
Chain d4:





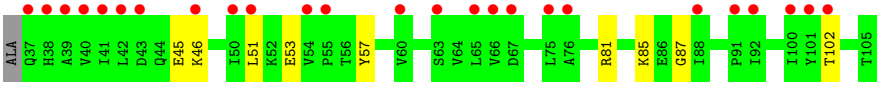
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



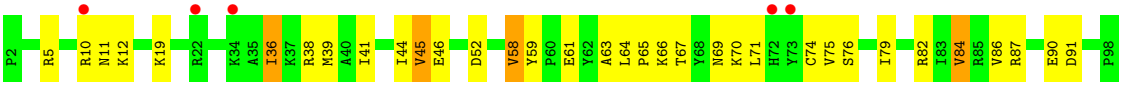
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



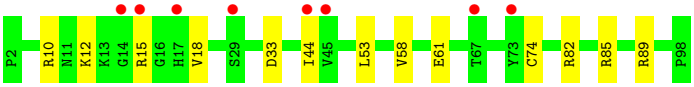
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



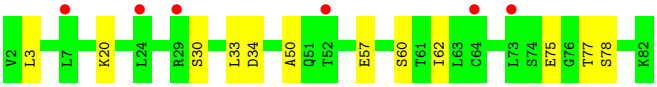
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



• Molecule 29: 40S ribosomal protein S27-A

Chain D7:

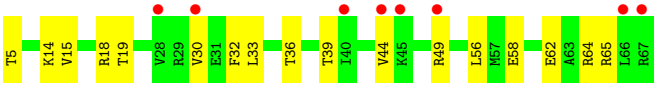


• Molecule 29: 40S ribosomal protein S27-A

Chain d7:

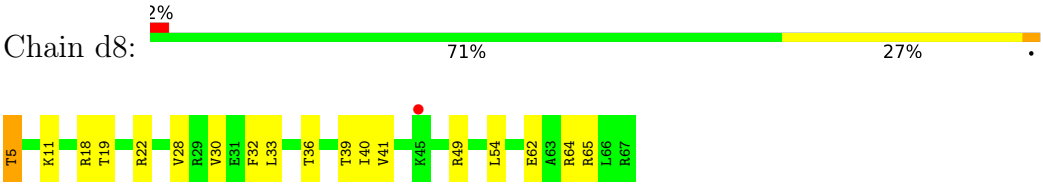
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



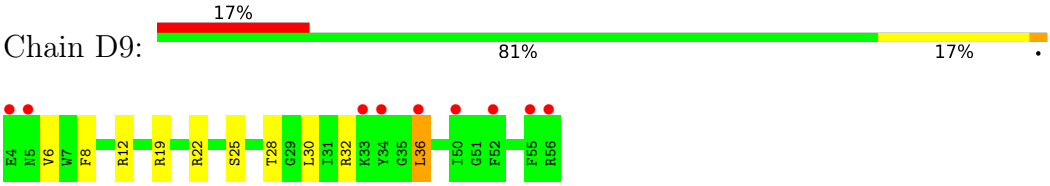
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



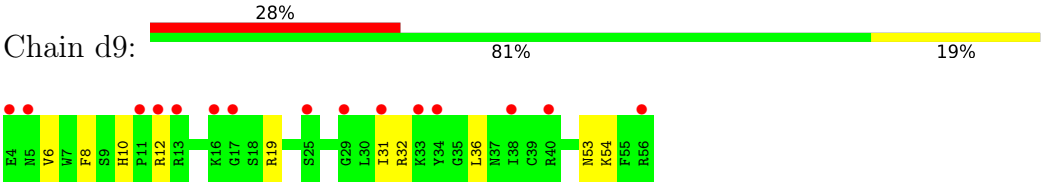
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



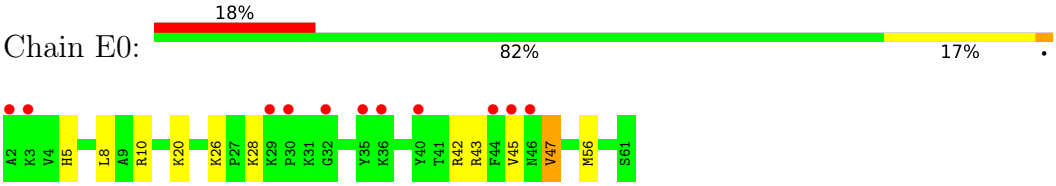
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



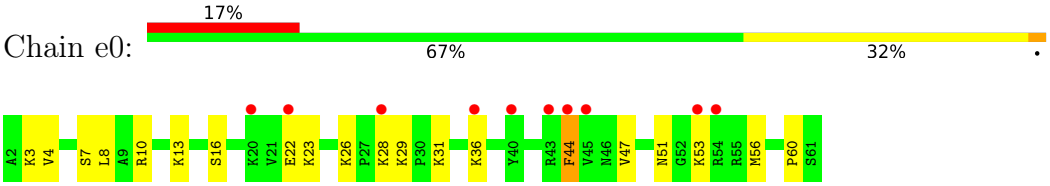
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



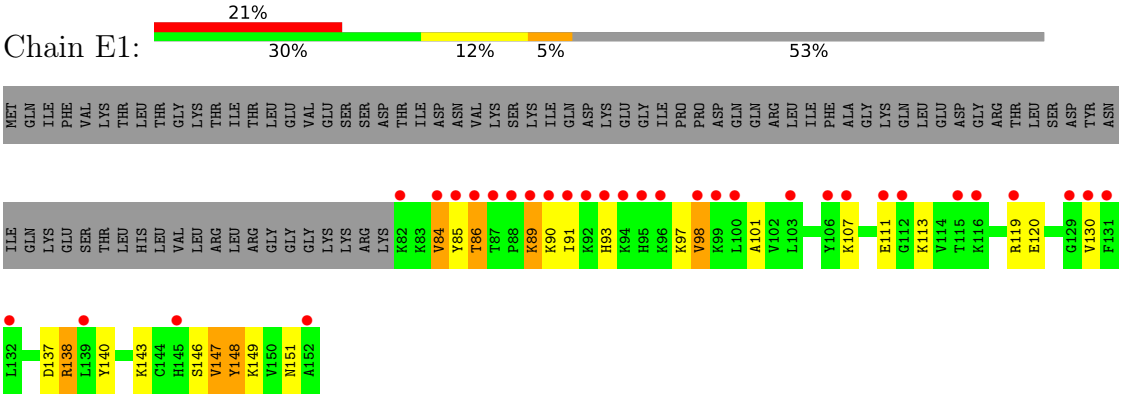
• Molecule 32: 40S ribosomal protein S30-A

Chain e0:



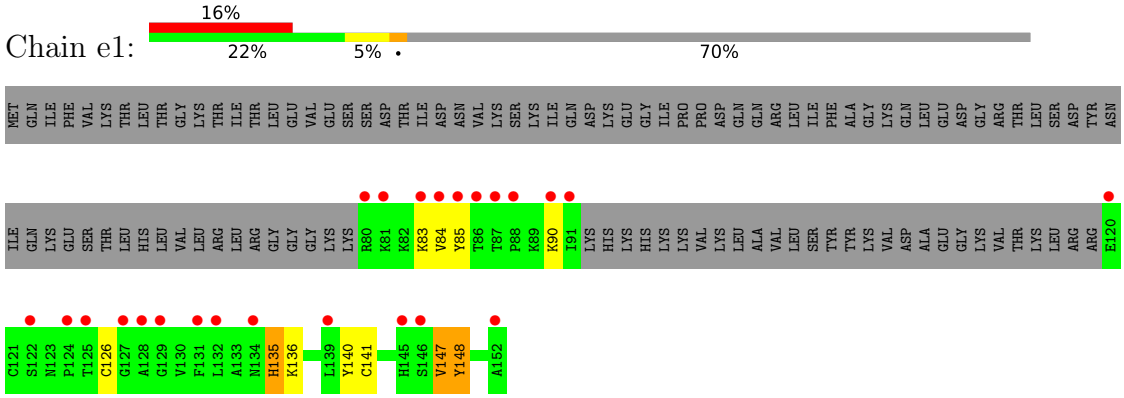
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



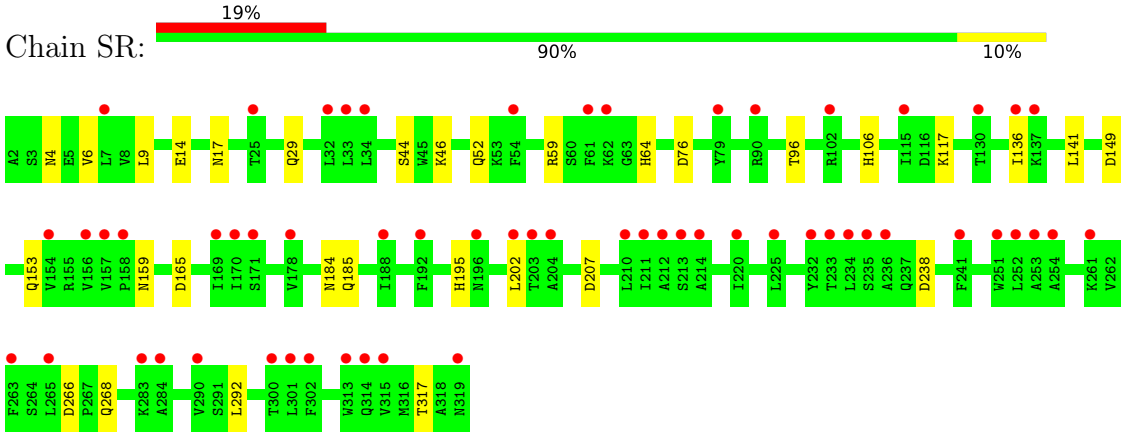
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



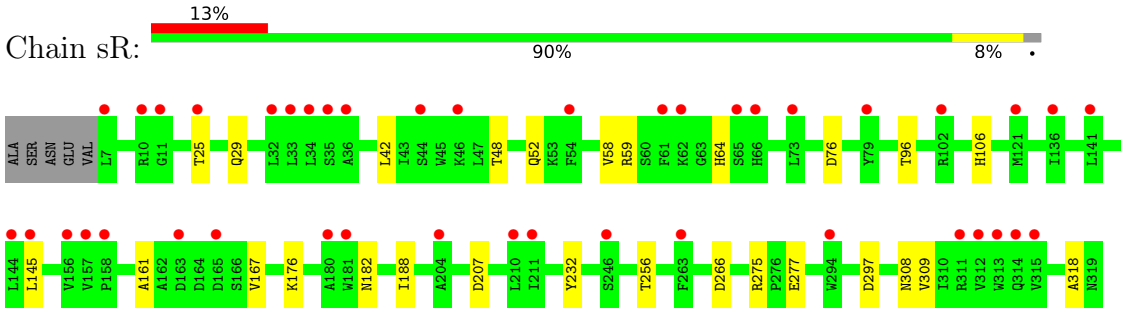
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



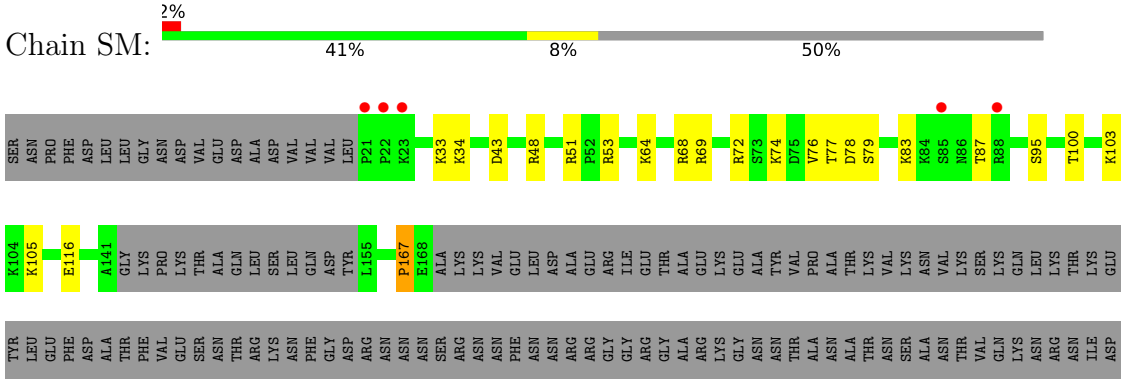
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



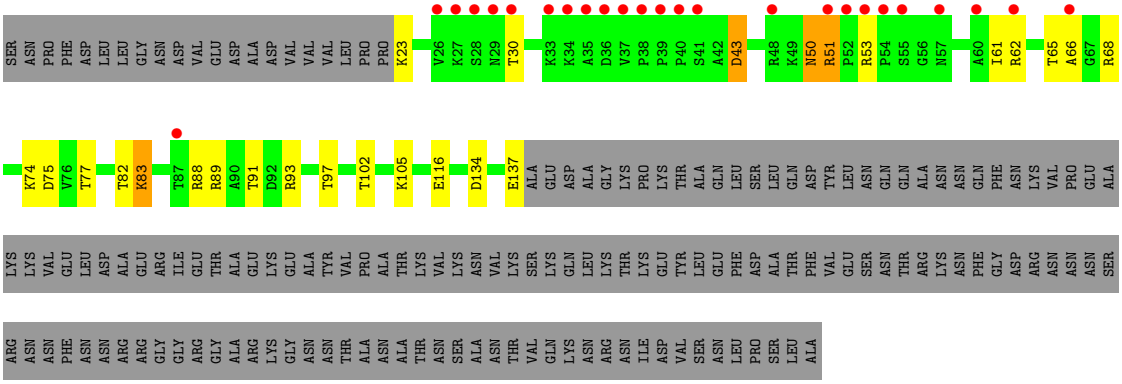
• Molecule 35: Suppressor protein STM1

Chain SM:



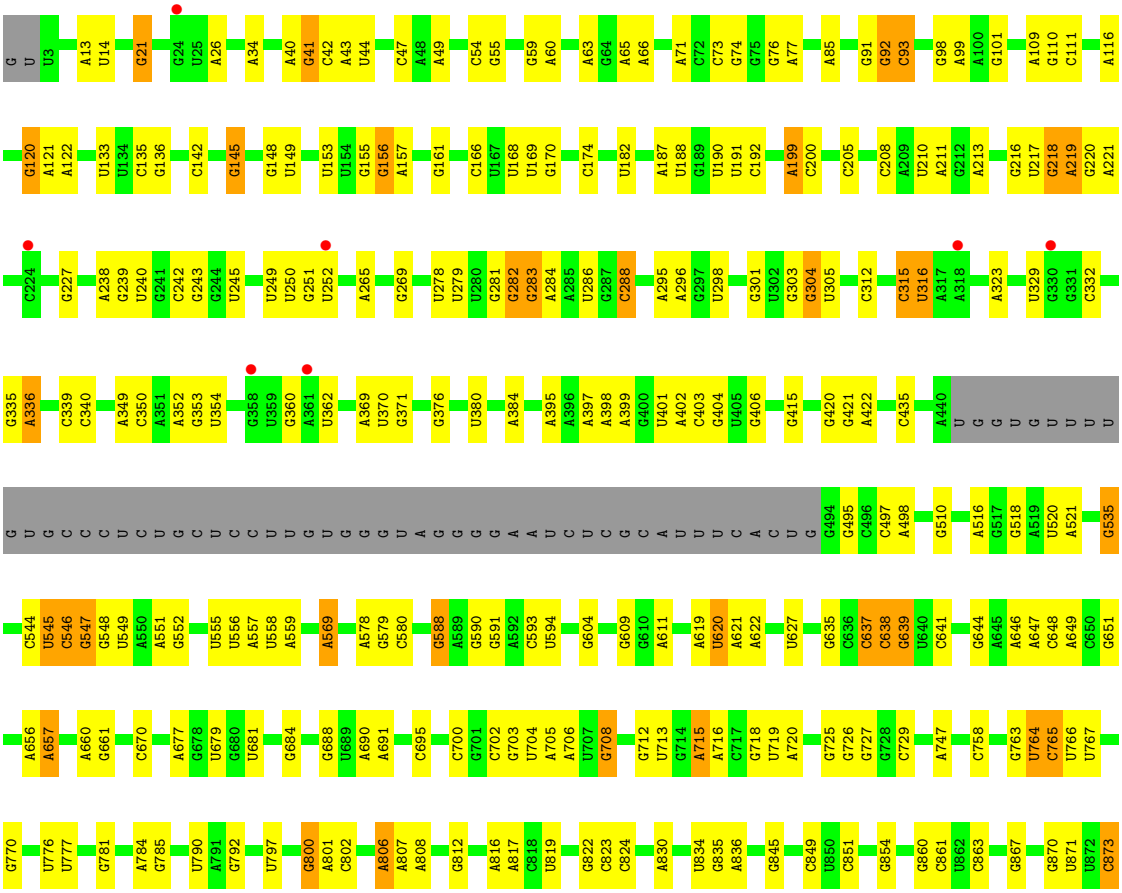
• Molecule 35: Suppressor protein STM1

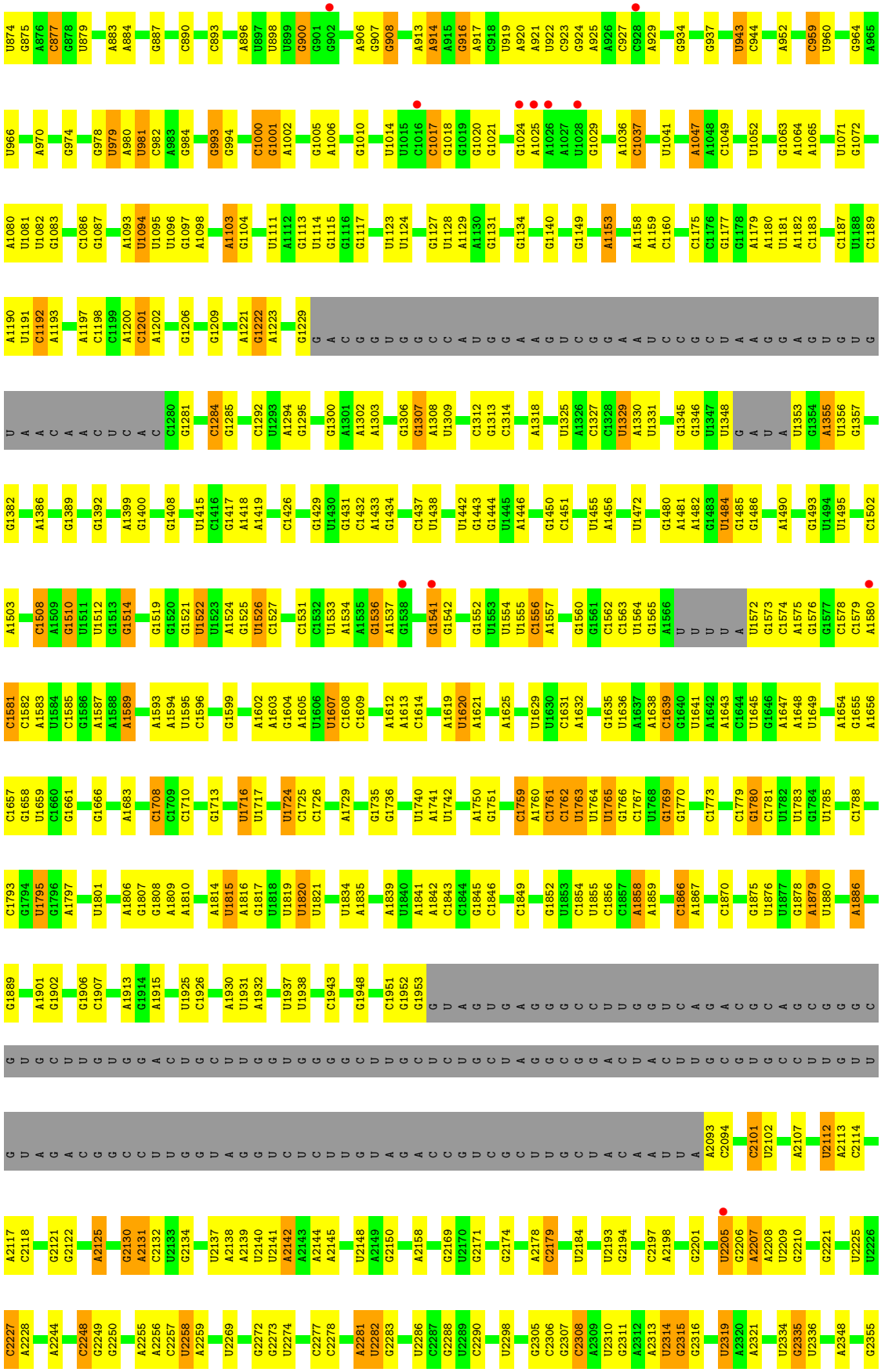
Chain sM:

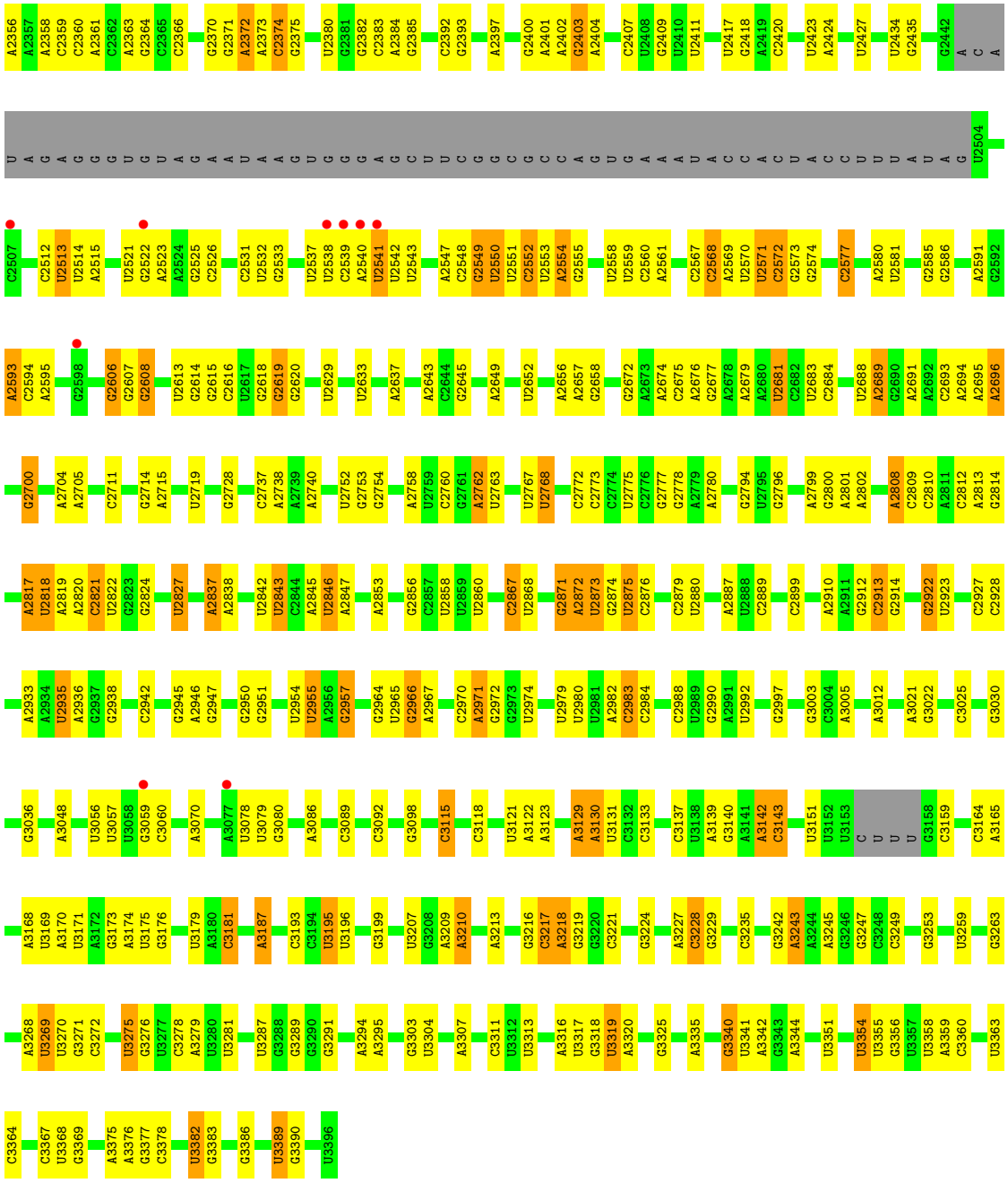


• Molecule 36: 25S ribosomal RNA

Chain 1:

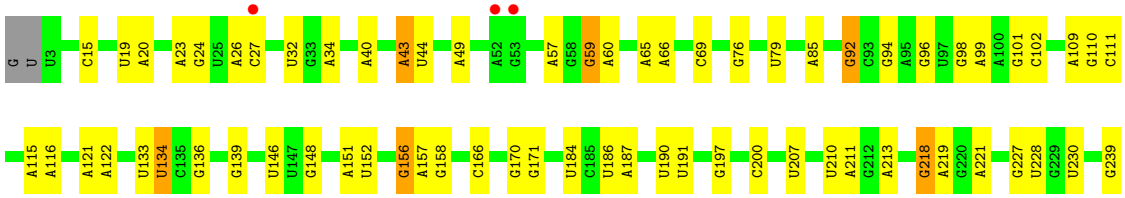


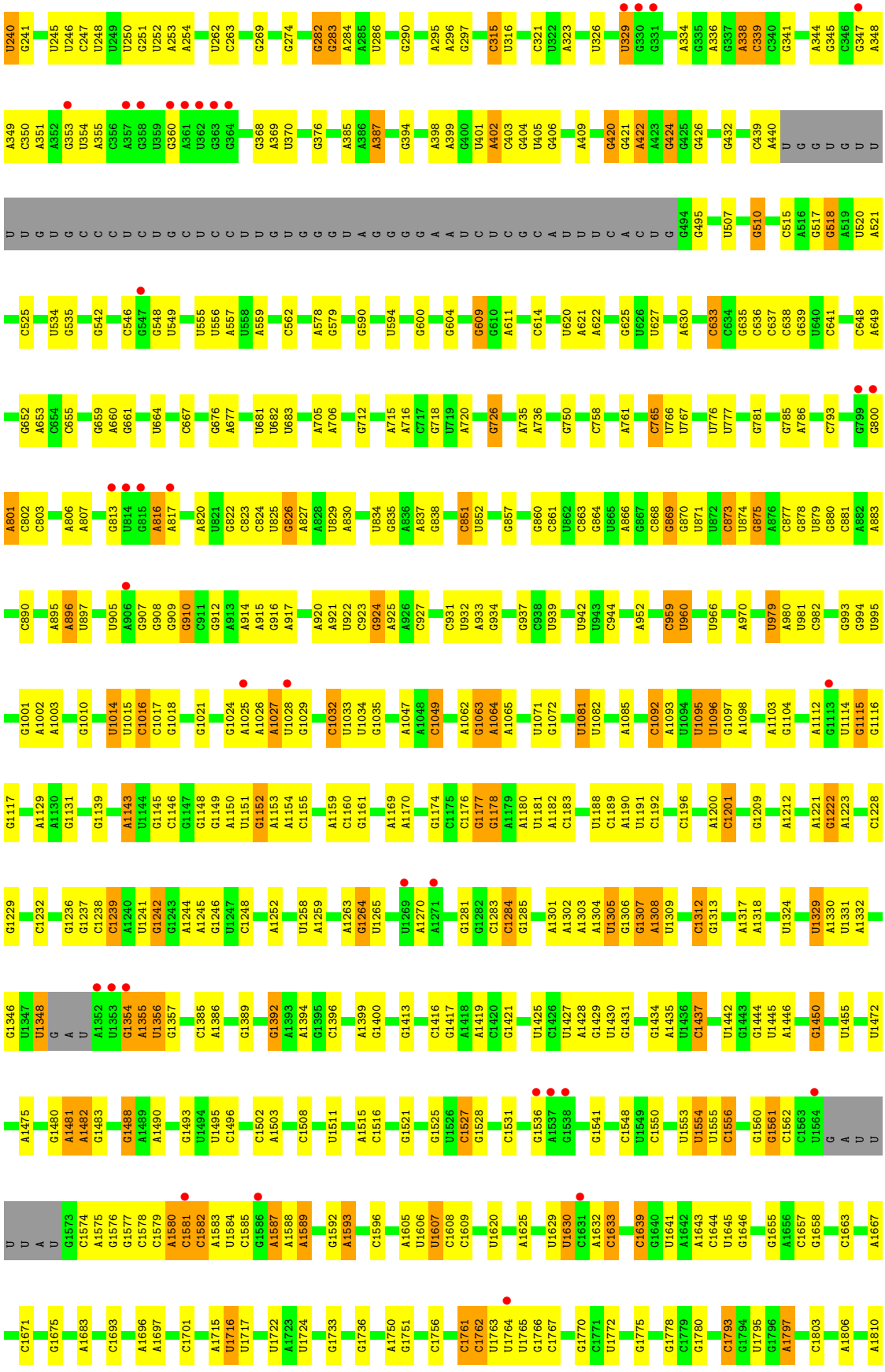




• Molecule 36: 25S ribosomal RNA

Chain 5:

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A349 C350 A351 A352 G353 U354 A355 C356 A357 G358 U359 G360 A361 U362 G363 G364 G368 A369 U370 G376 A385 A386 A387 G394 A398 A399 G400 U401 A402 C403 G404 U405 G406 A409 G420 G421 A422 A423 G424 G425 G426 G432 C439 A440 U G G U G U
U U U G U G C C C U U U C U U C C C U U G U U G C A U U U C A C U G G494 G495 U507 G510 C515 A516 G517 G518 A519 U520 A521
C525 U534 G535 G542 C546 G547 G548 U549 U555 U556 A557 U558 A559 C562 A578 G579 G590 U594 G600 G604 G609 G610 A611 C614 U620 A621 A622 G625 U626 U627 A630 C633 C634 G635 C636 C637 C638 G639 U640 C641 C648 A649
G652 A653 C654 C655 G659 A660 C661 U664 C667 G676 A677 U681 U682 U683 A705 A706 G712 A715 A716 C717 G718 U719 A720 G726 A735 A736 G750 C758 A761 C765 U766 U767 U776 U777 G781 G785 A786 C793 G799 G800
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C890 A895 A896 U897 U905 A906 G907 G908 G909 G910 C911 G912 A913 A914 A915 G916 A917 A920 A921 U922 C923 G924 A925 A926 C927 C931 U932 A933 G934 G937 C938 U939 U942 U943 C944 A952 C959 U960 U966 A970 U979 A980 U981 C982 G993 G994 U995
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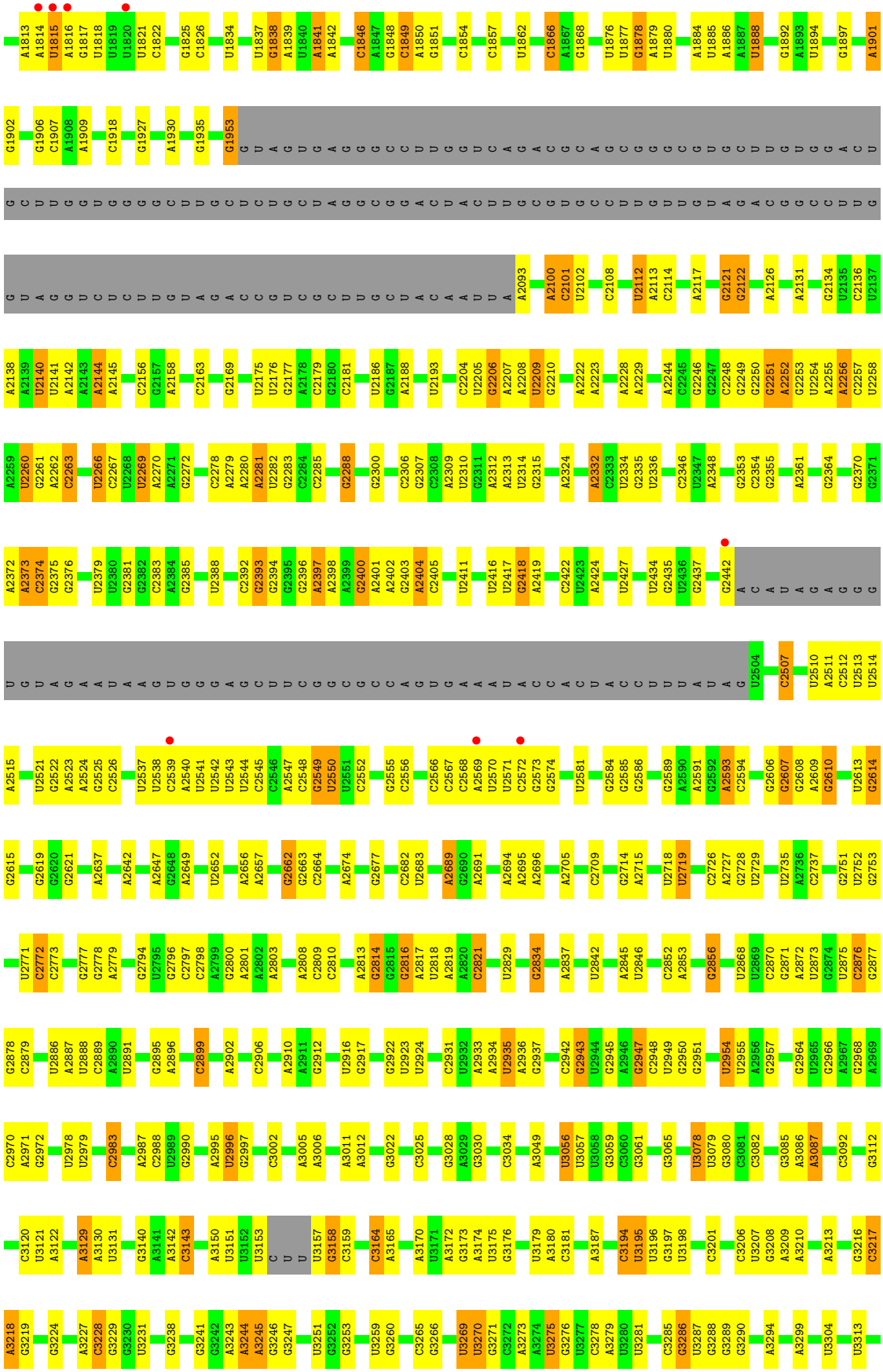
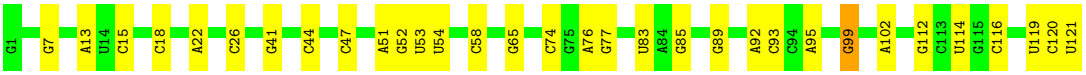


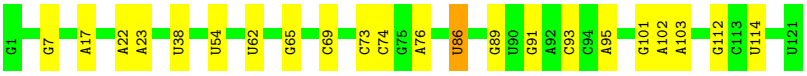
• Molecule 37: 5S ribosomal RNA

Chain 3:



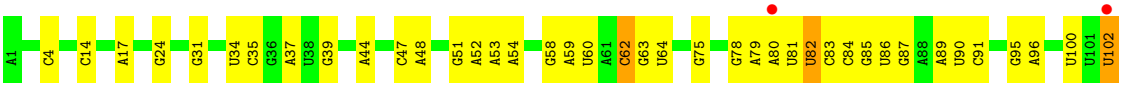
• Molecule 37: 5S ribosomal RNA

Chain 7:



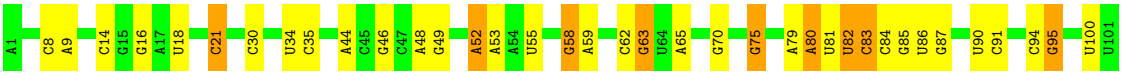
• Molecule 38: 5.8S ribosomal RNA

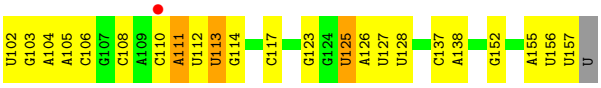
Chain 4:



• Molecule 38: 5.8S ribosomal RNA

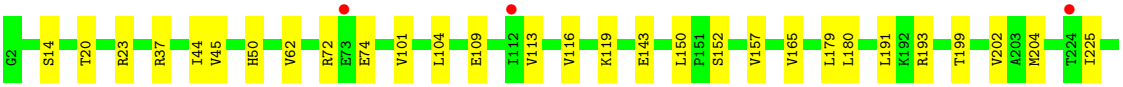
Chain 8:

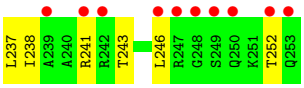




• Molecule 39: 60S ribosomal protein L2-A

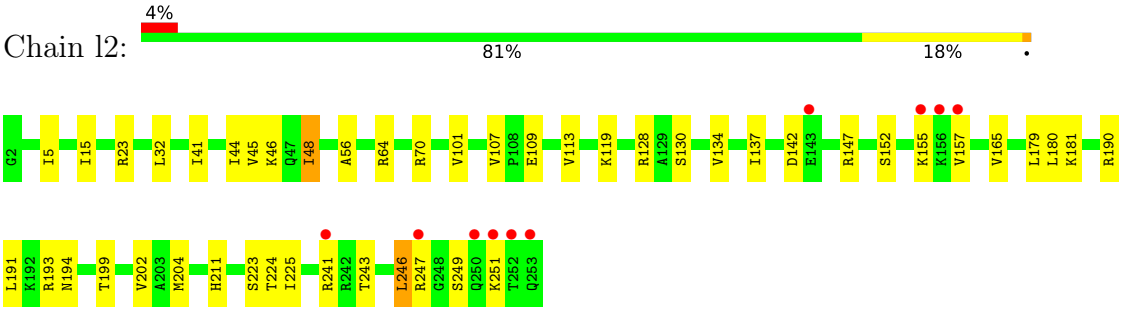
Chain L2:





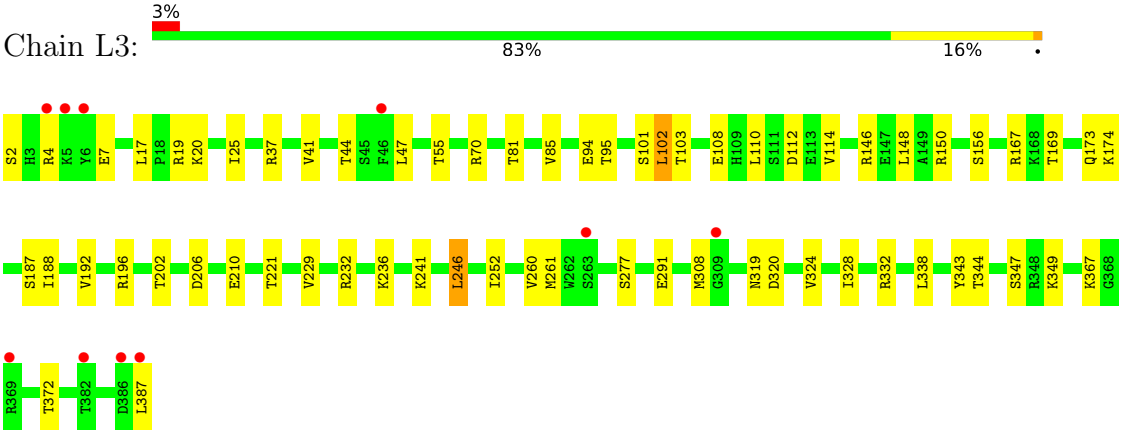
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



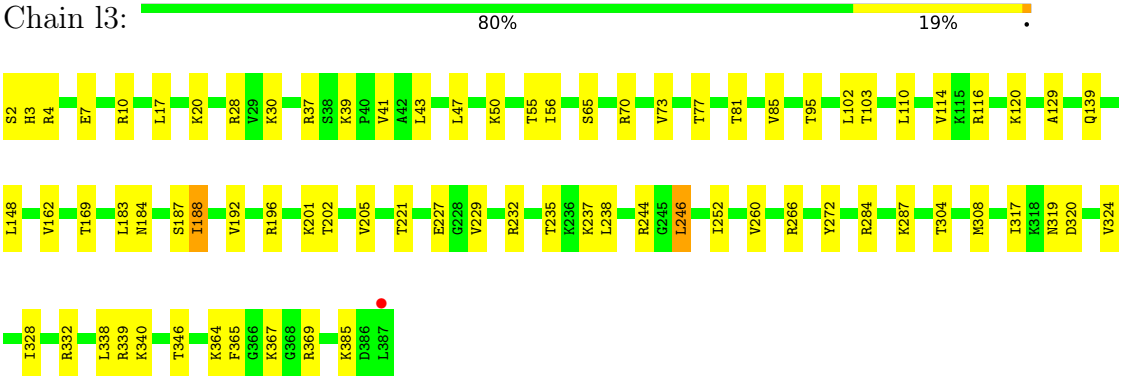
• Molecule 40: 60S ribosomal protein L3

Chain L3:



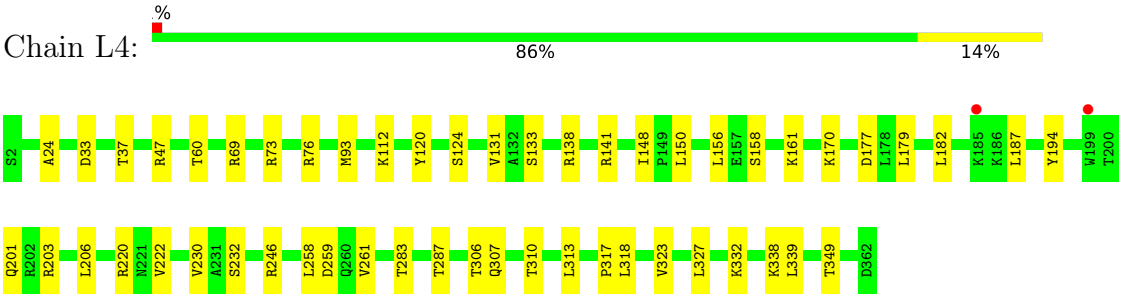
• Molecule 40: 60S ribosomal protein L3

Chain l3:



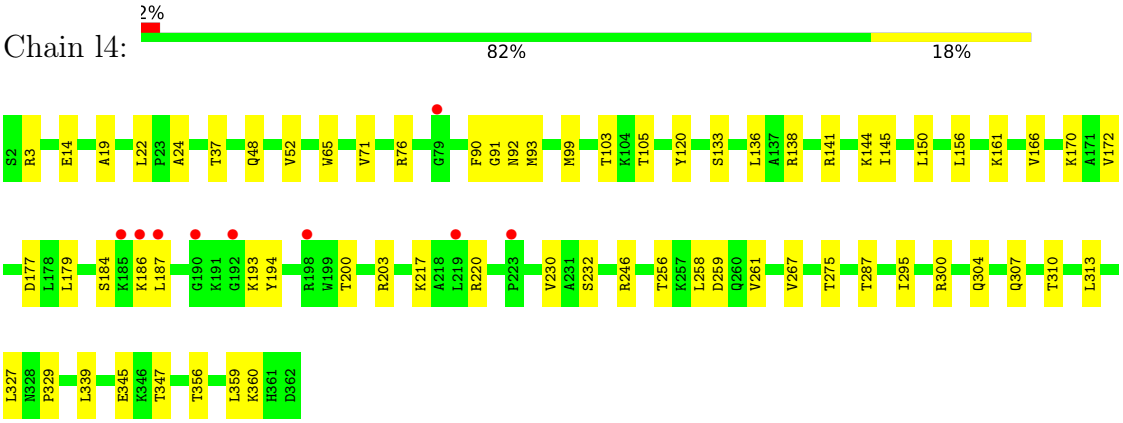
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



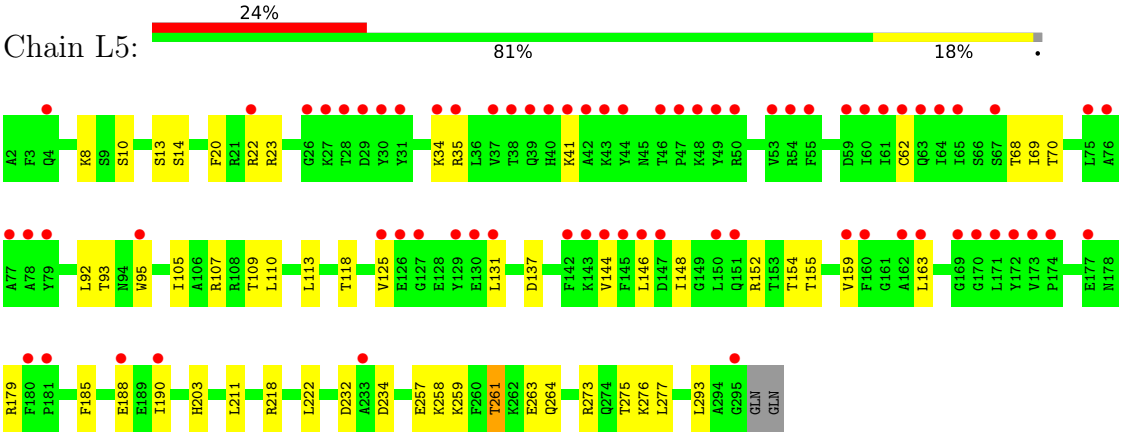
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



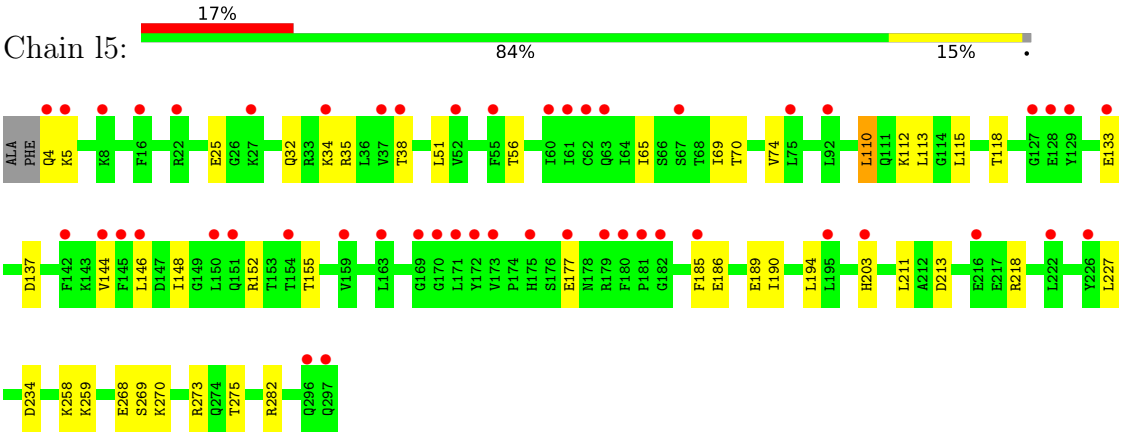
• Molecule 42: 60S ribosomal protein L5

Chain L5:



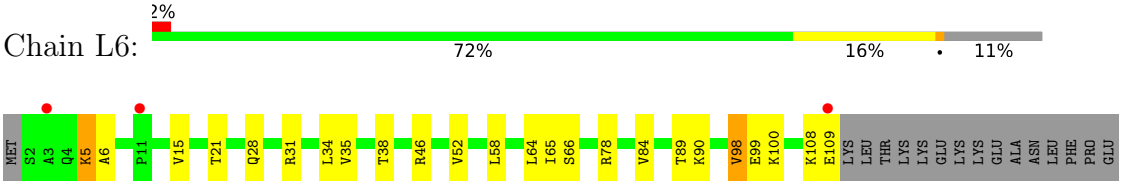
• Molecule 42: 60S ribosomal protein L5

Chain l5:



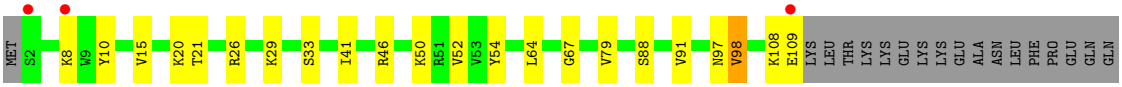
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



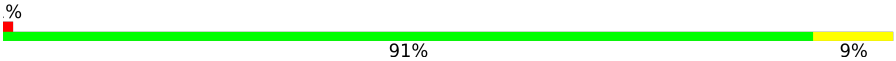
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



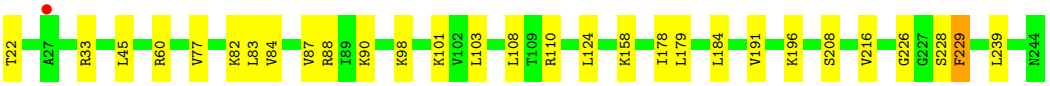
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



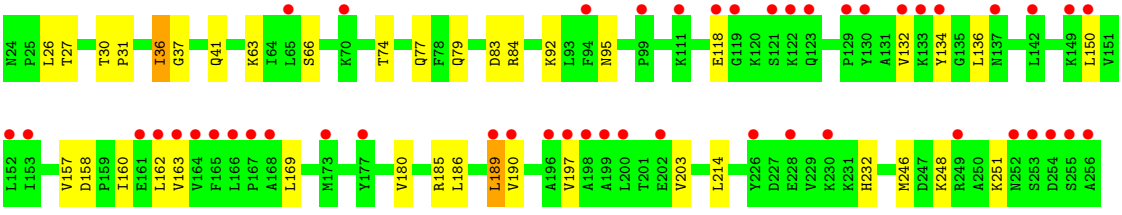
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



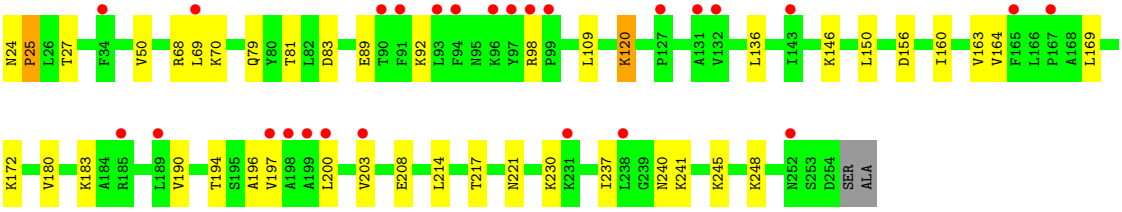
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



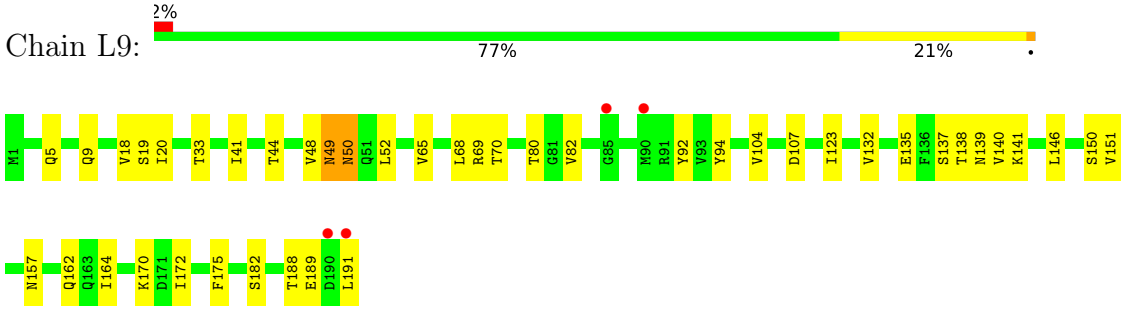
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



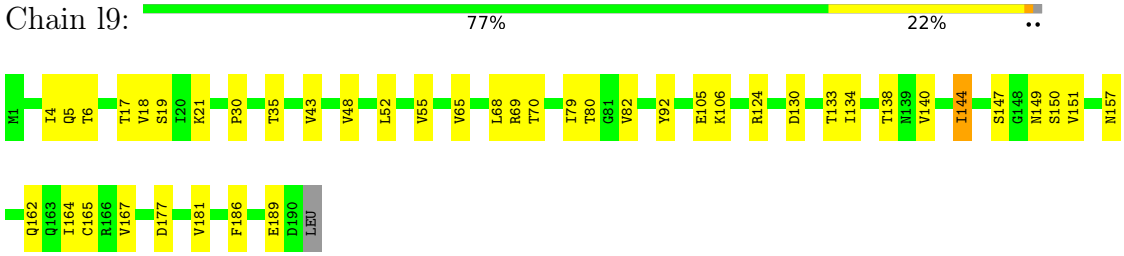
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



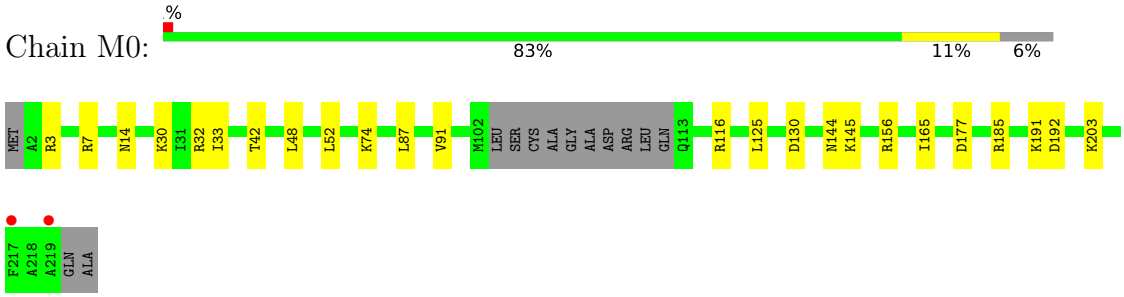
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



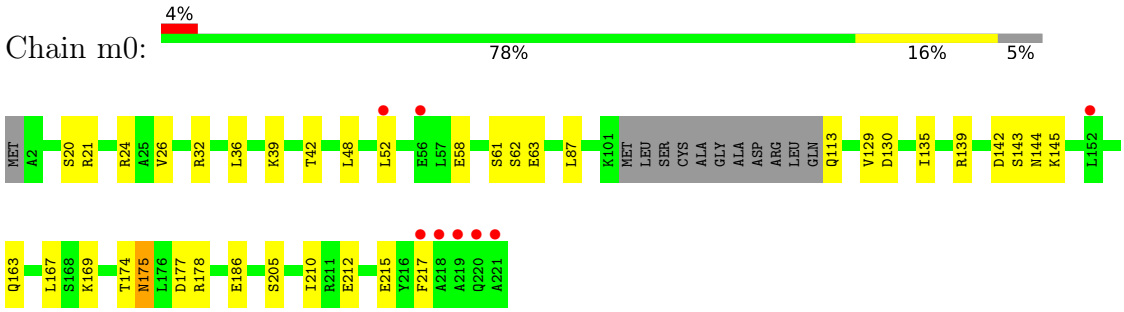
• Molecule 47: 60S ribosomal protein L10

Chain M0:



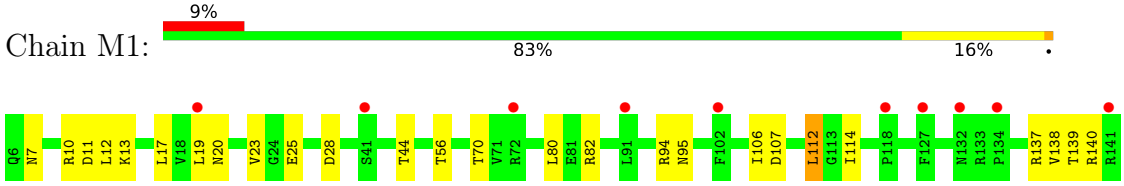
• Molecule 47: 60S ribosomal protein L10

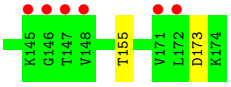
Chain m0:



• Molecule 48: 60S ribosomal protein L11-A

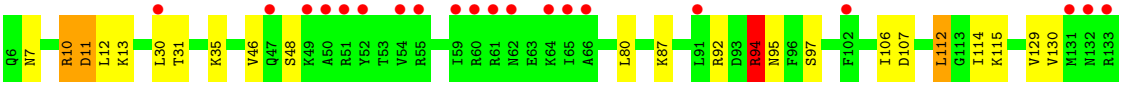
Chain M1:

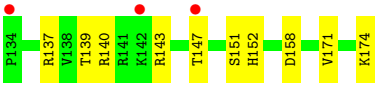




• Molecule 48: 60S ribosomal protein L11-A

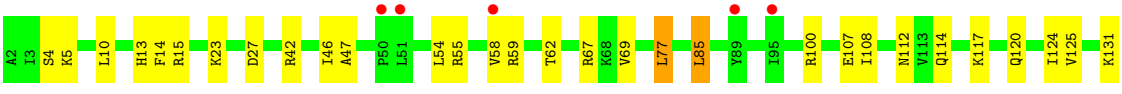
Chain m1:

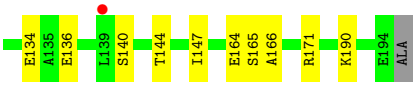




• Molecule 49: 60S ribosomal protein L13-A

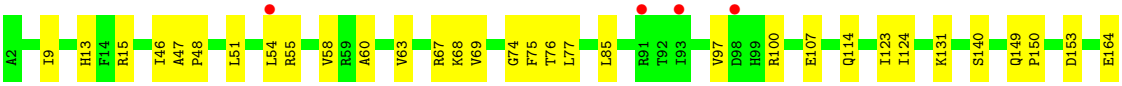
Chain M3:

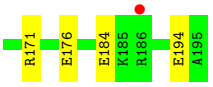




• Molecule 49: 60S ribosomal protein L13-A

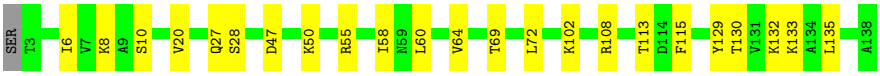
Chain m3:





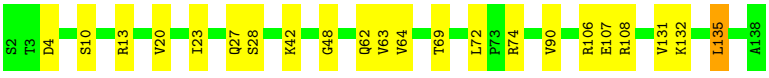
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



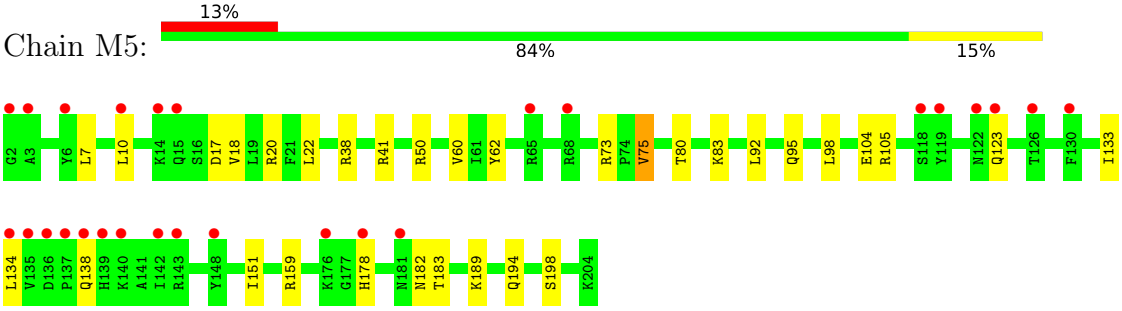
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



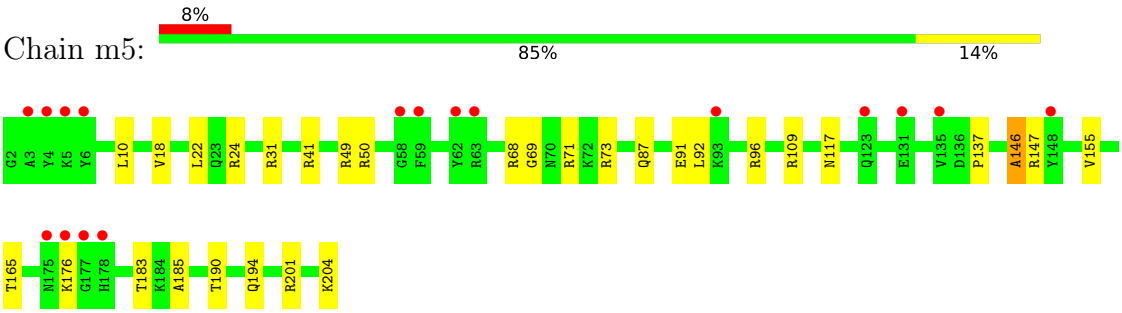
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



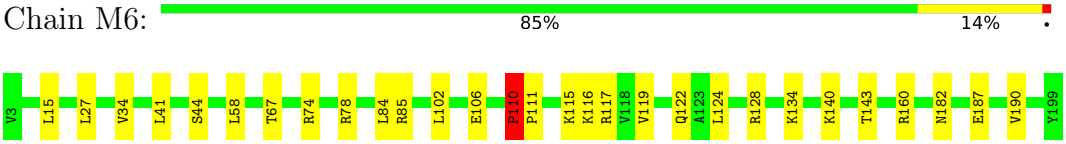
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



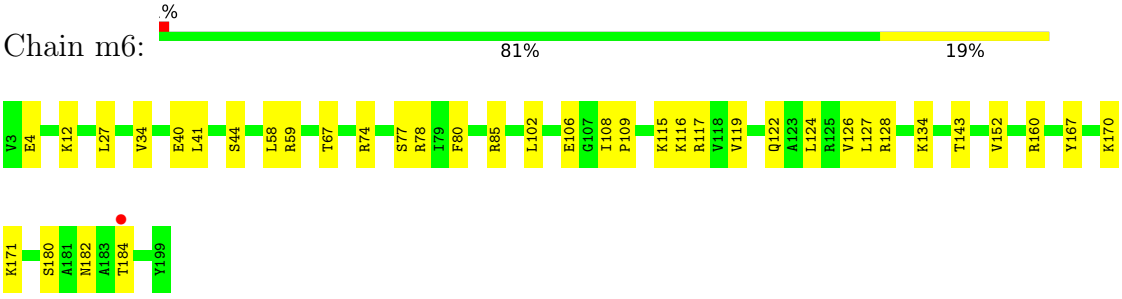
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



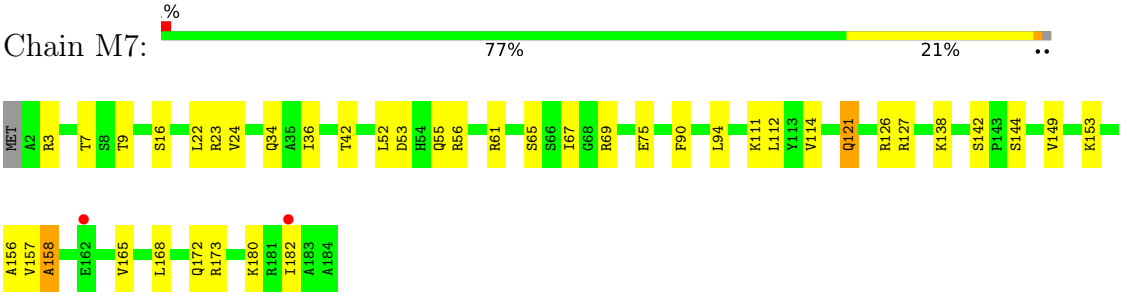
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



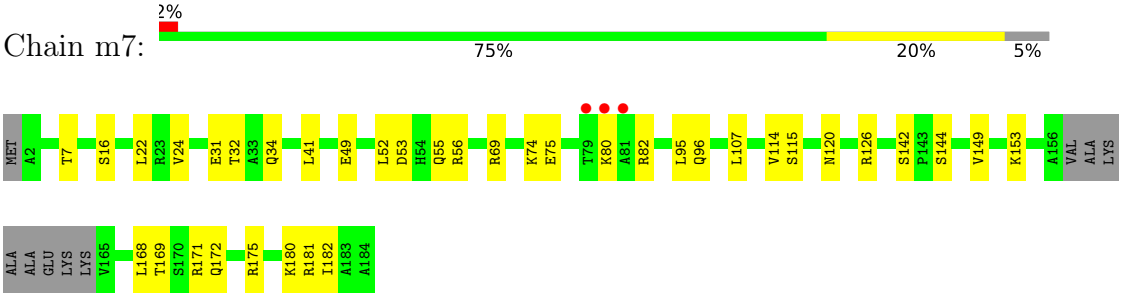
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



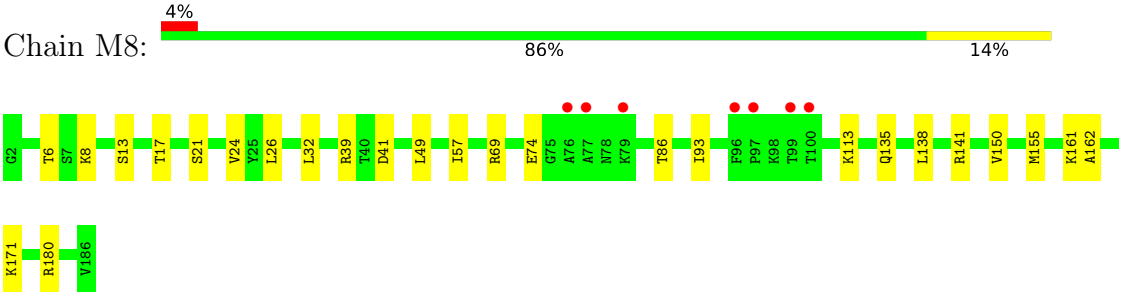
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



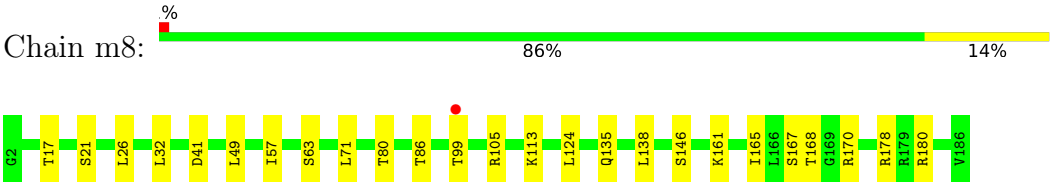
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



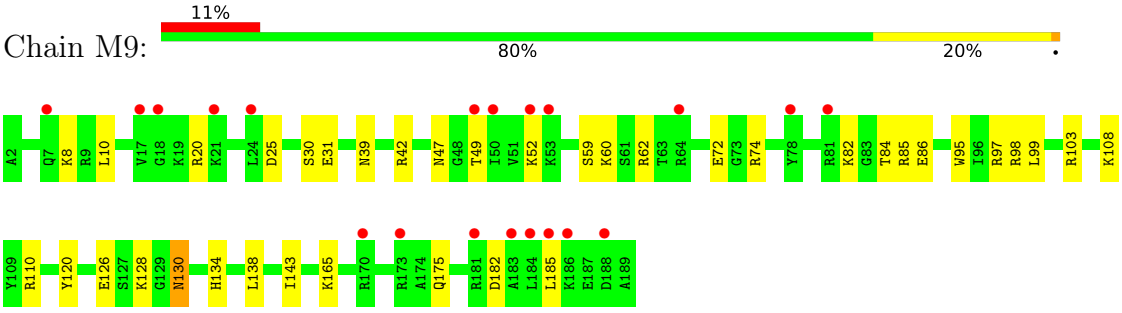
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



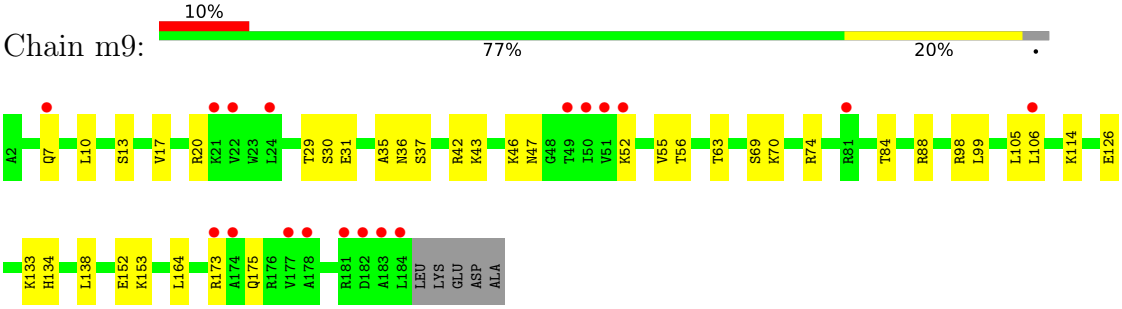
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



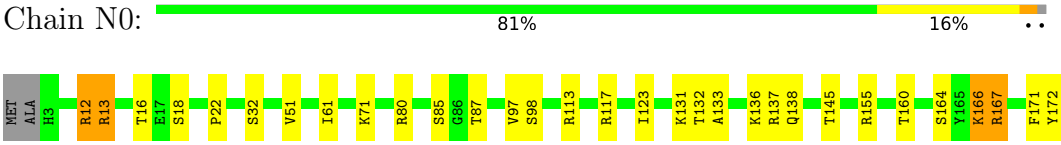
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



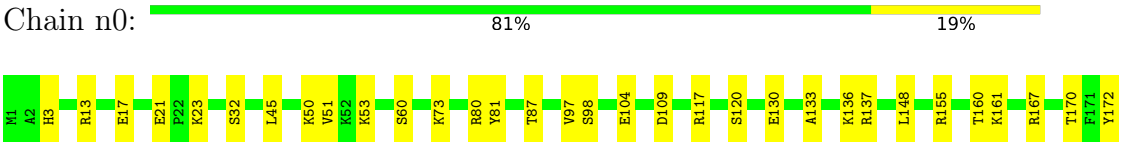
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



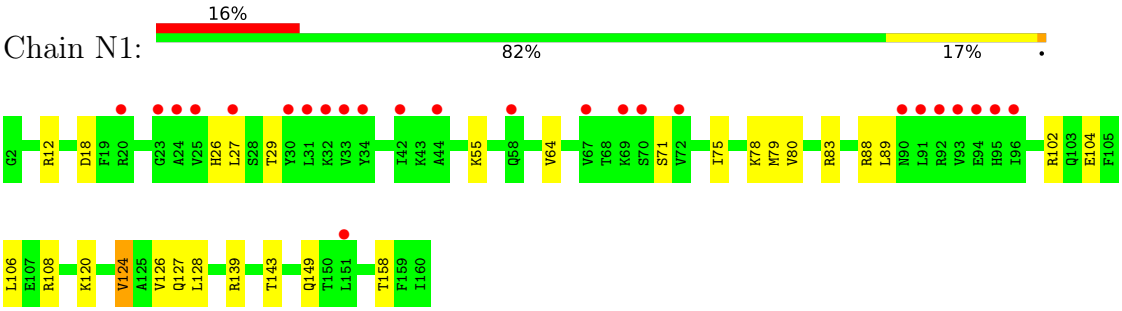
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



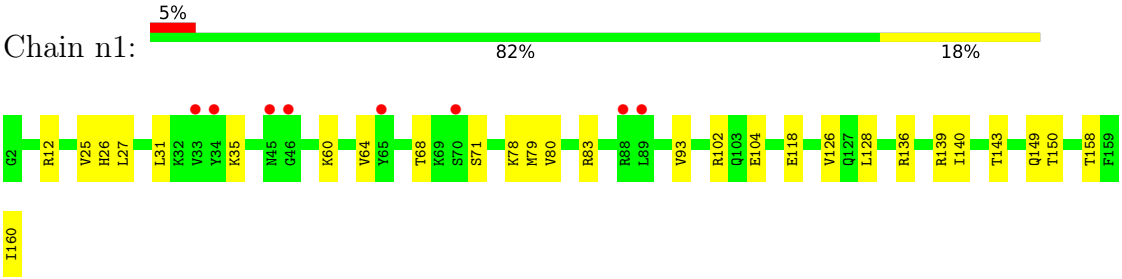
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



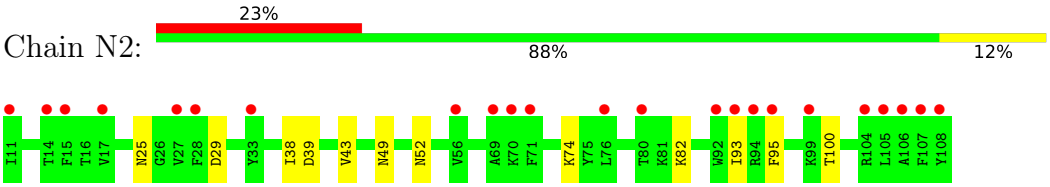
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



• Molecule 58: 60S ribosomal protein L22-A

Chain N2:

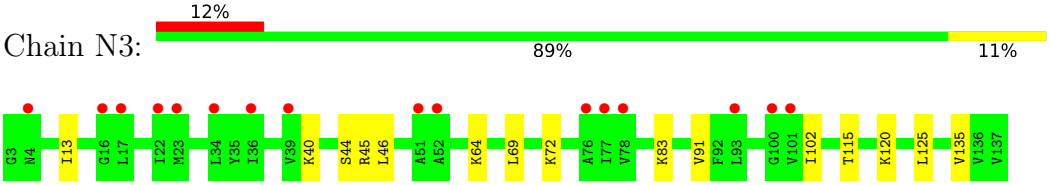


• Molecule 58: 60S ribosomal protein L22-A

Chain n2:

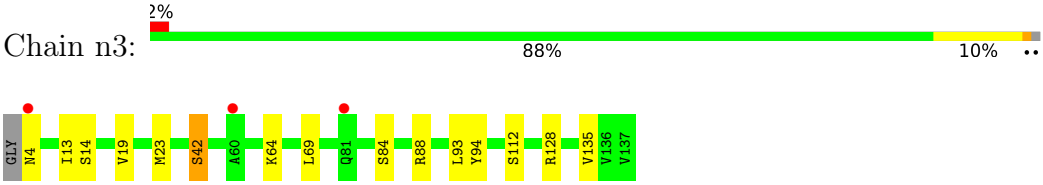
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



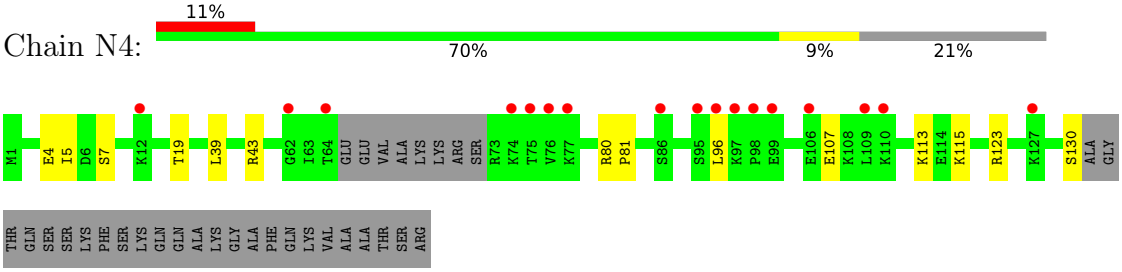
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



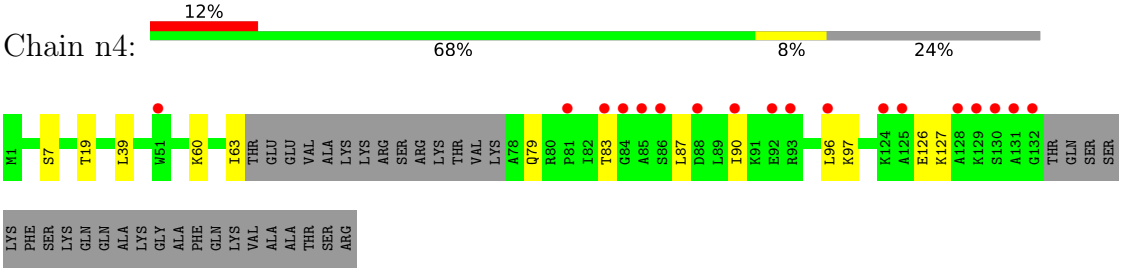
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



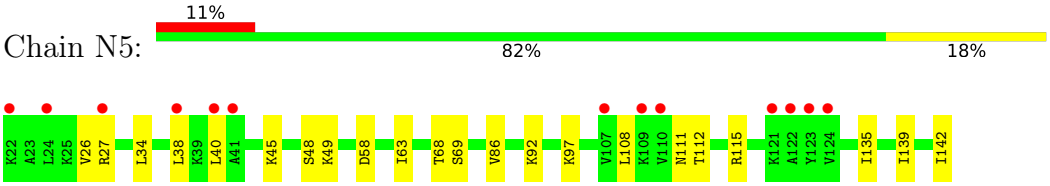
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



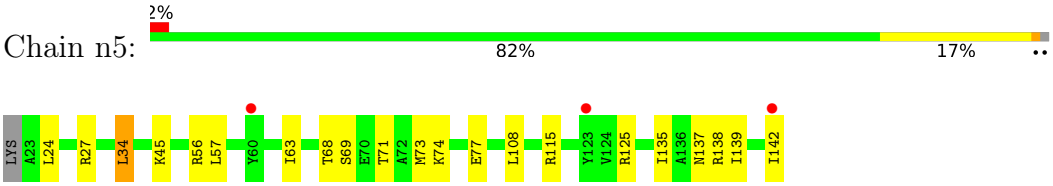
• Molecule 61: 60S ribosomal protein L25

Chain N5:



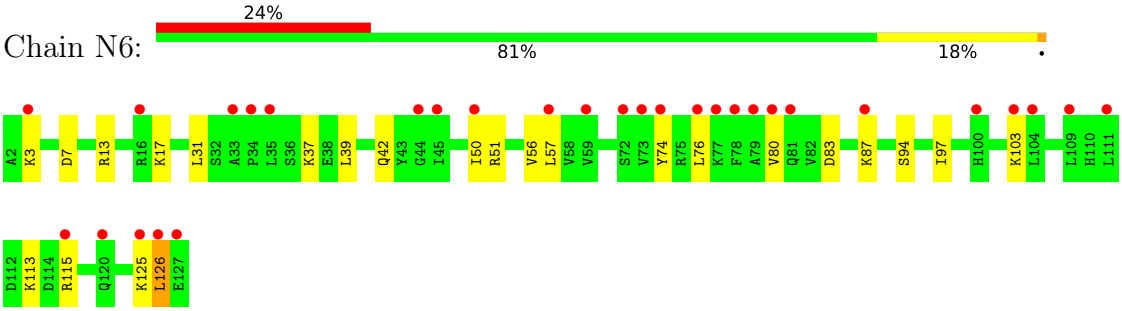
• Molecule 61: 60S ribosomal protein L25

Chain n5:



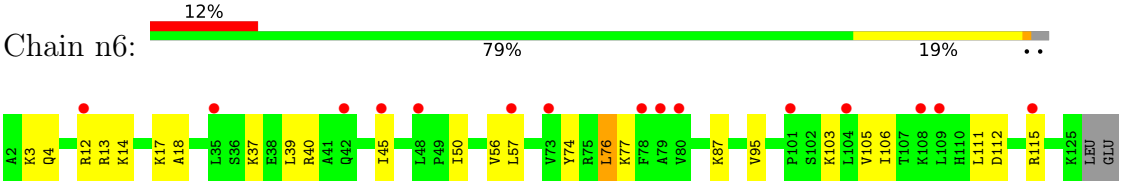
• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



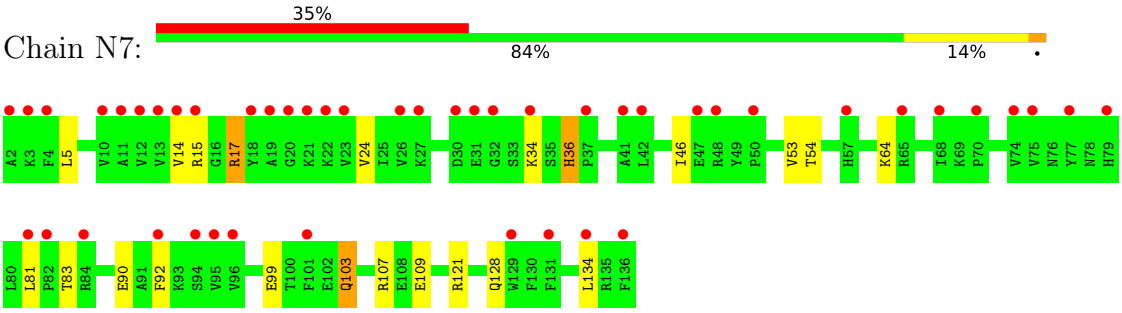
• Molecule 62: 60S ribosomal protein L26-A

Chain n6:



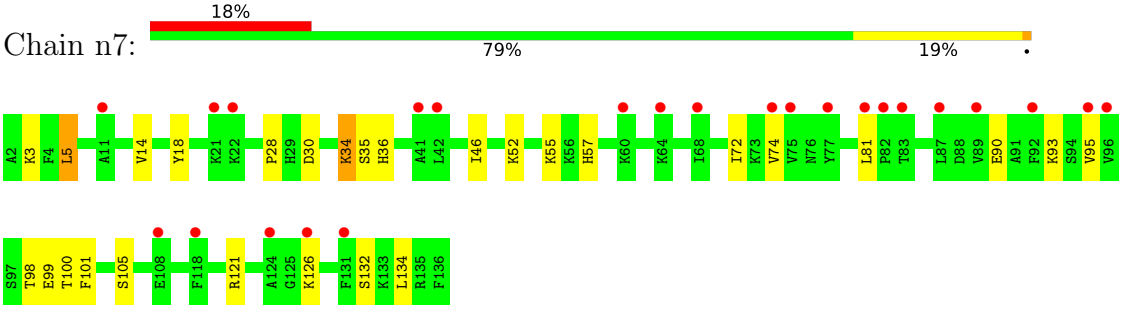
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



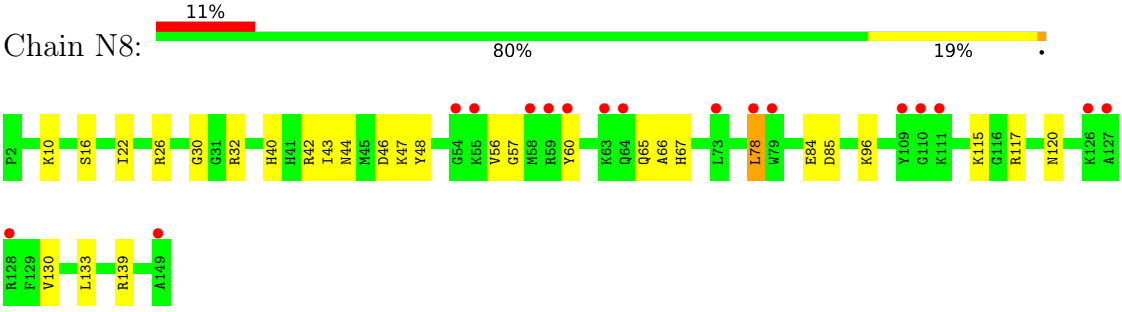
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



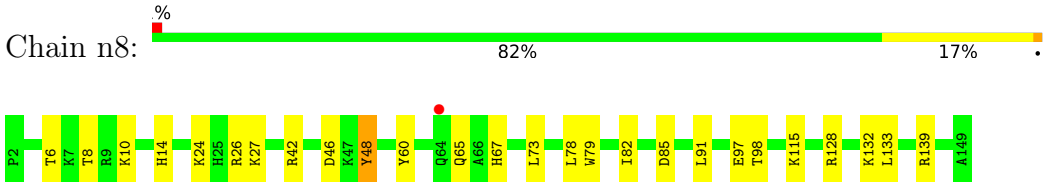
• Molecule 64: 60S ribosomal protein L28

Chain N8:



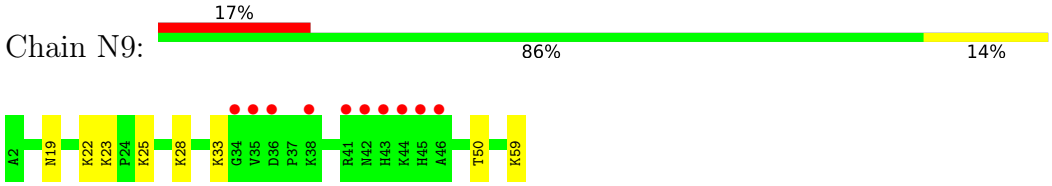
• Molecule 64: 60S ribosomal protein L28

Chain n8:



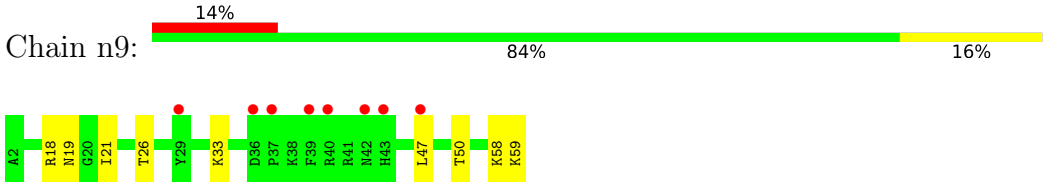
• Molecule 65: 60S ribosomal protein L29

Chain N9:



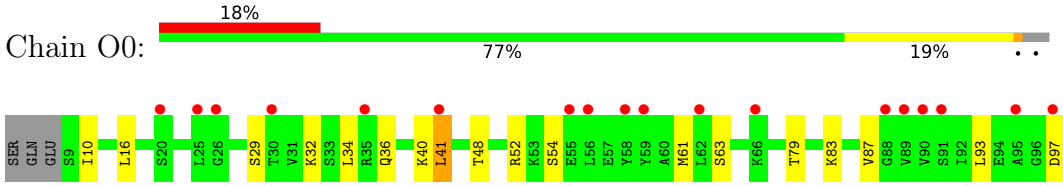
• Molecule 65: 60S ribosomal protein L29

Chain n9:



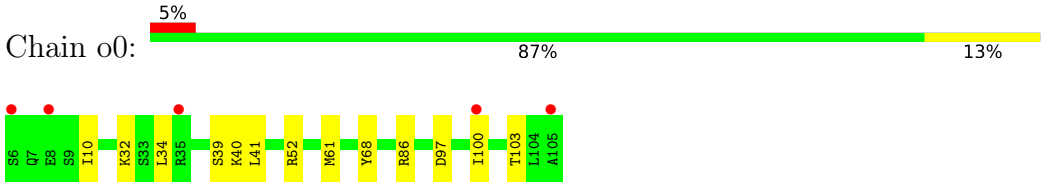
• Molecule 66: 60S ribosomal protein L30

Chain O0:



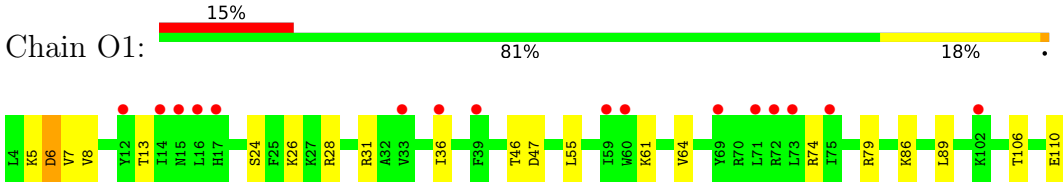
• Molecule 66: 60S ribosomal protein L30

Chain o0:



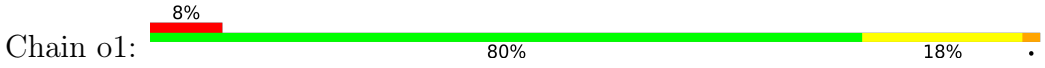
• Molecule 67: 60S ribosomal protein L31-A

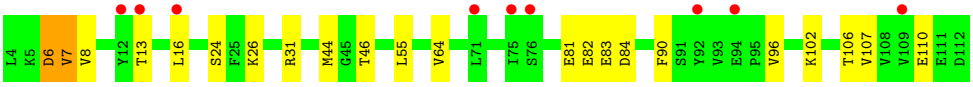
Chain O1:



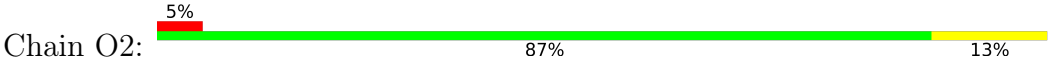
• Molecule 67: 60S ribosomal protein L31-A

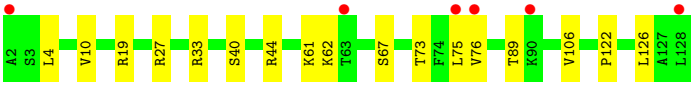
Chain o1:



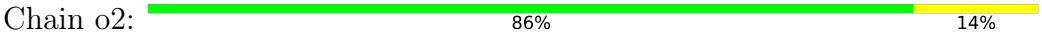


• Molecule 68: 60S ribosomal protein L32

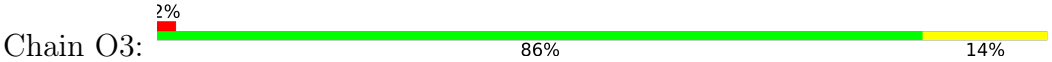


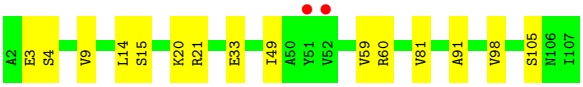


• Molecule 68: 60S ribosomal protein L32

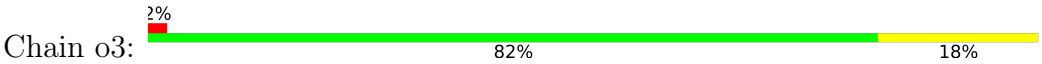


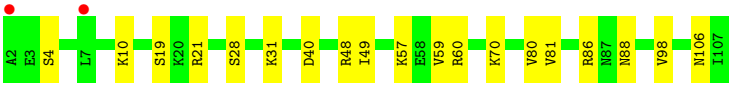
• Molecule 69: 60S ribosomal protein L33-A



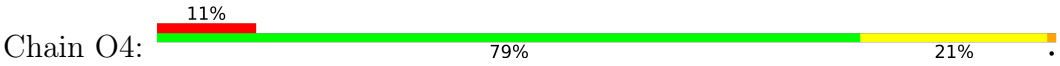


• Molecule 69: 60S ribosomal protein L33-A

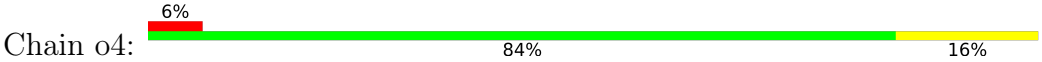


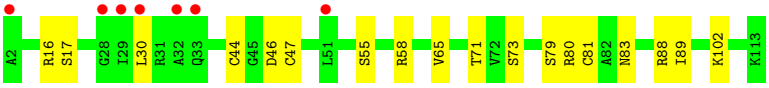


• Molecule 70: 60S ribosomal protein L34-A



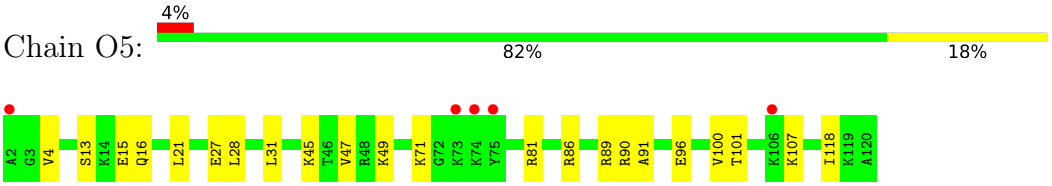
• Molecule 70: 60S ribosomal protein L34-A





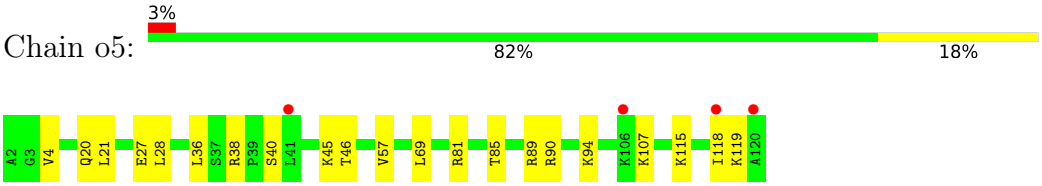
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



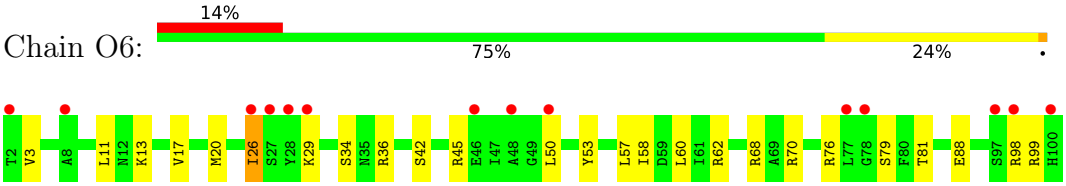
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



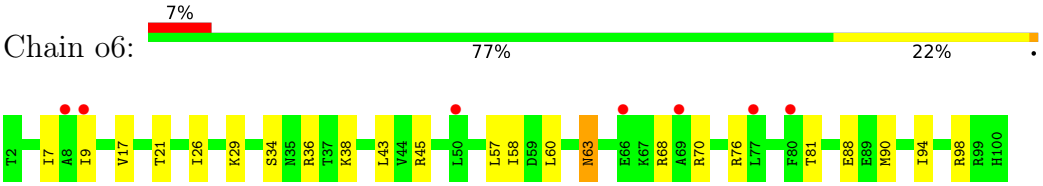
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



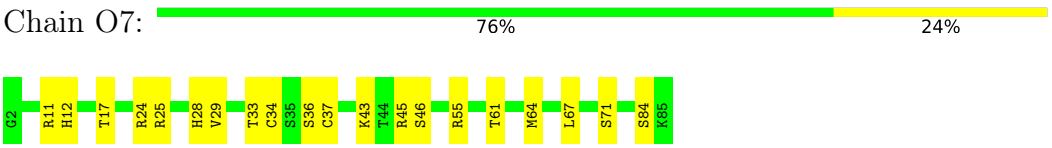
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



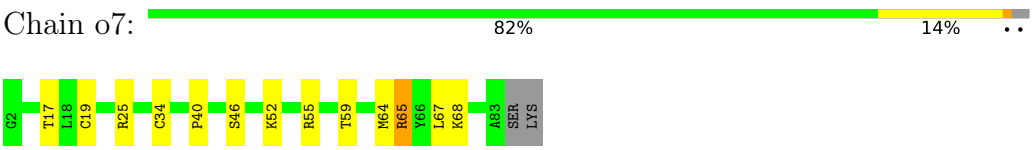
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



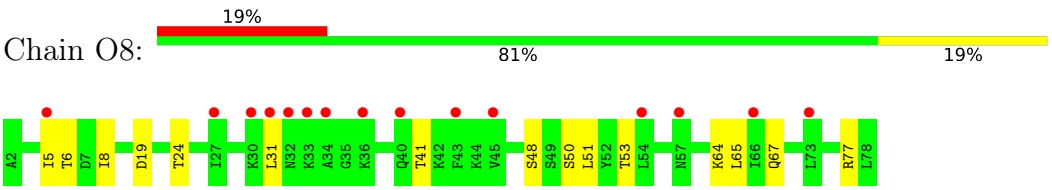
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



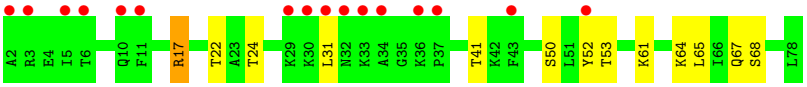
• Molecule 74: 60S ribosomal protein L38

Chain O8:



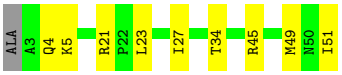
• Molecule 74: 60S ribosomal protein L38

Chain o8:



• Molecule 75: 60S ribosomal protein L39

Chain O9:

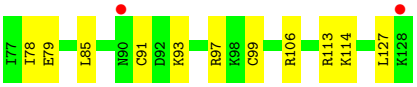


• Molecule 75: 60S ribosomal protein L39

Chain o9:

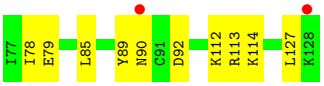
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



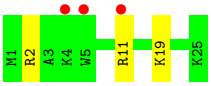
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:

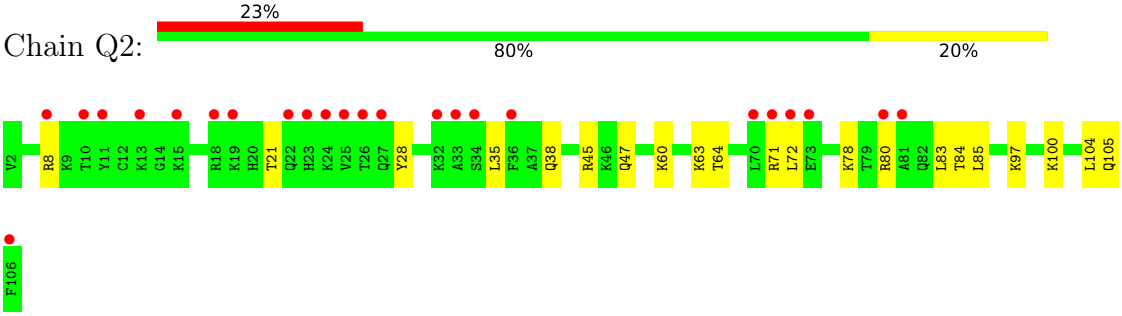


• Molecule 77: 60S ribosomal protein L41-A

Chain q1:

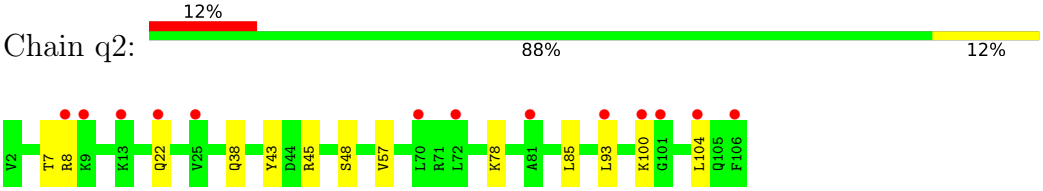
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



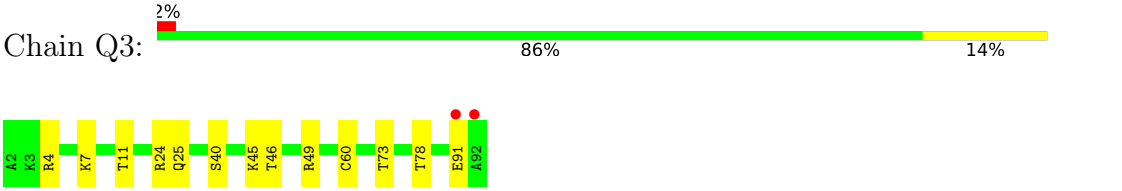
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



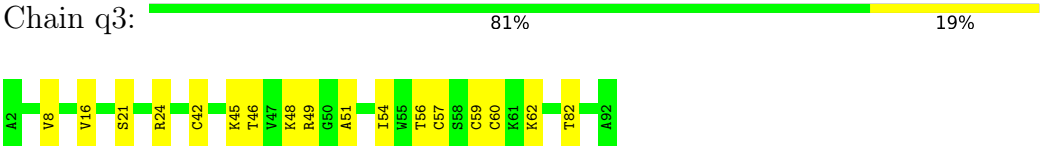
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



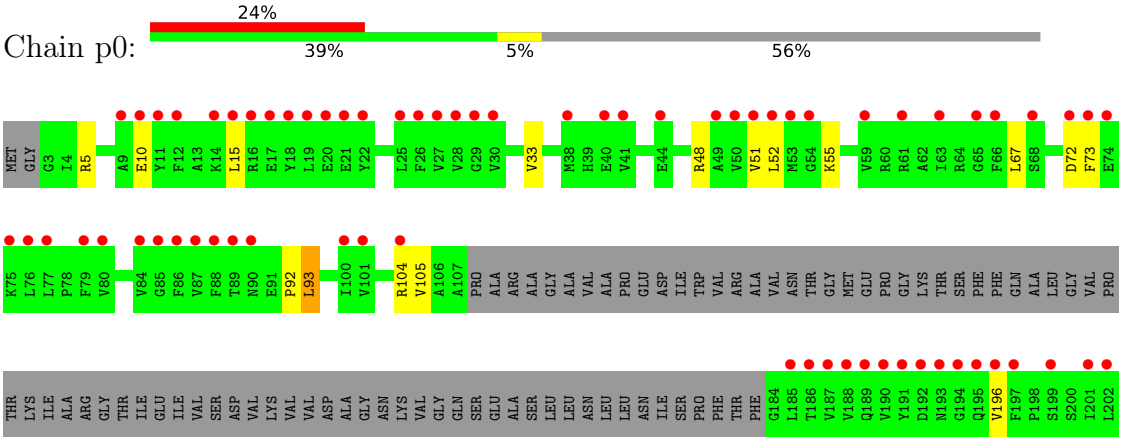
• Molecule 79: 60S ribosomal protein L43-A

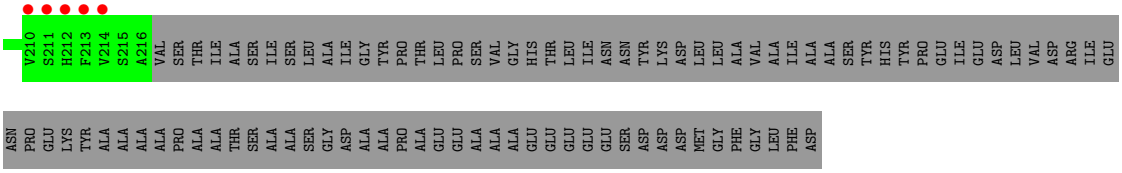
Chain q3:



• Molecule 80: 60S acidic ribosomal protein P0

Chain p0:




V210
S211
H212
F213
V214
S215
A216
VAL SER THR ILE ALA SER ILE SER LEU ALA ILE GLY TYR PRO THR LEU PRO SER VAL GLY HIS THR LEU ILE ASN ASN TYR LYS ASP LEU LEU ALA VAL ALA ILE ALA ALA SER TYR HIS TYR PRO GLU ILE GLU ASP LEU VAL ASP ARG ILE GLU
ASN PRO GLU LYS TYR ALA ALA ALA PRO ALA ALA THR SER ALA ALA SER GLY ASP ALA ALA PRO ALA GLU GLU ALA ALA ALA GLU GLU GLU GLU SER ASP ASP ASP MET GLY PHE GLY LEU PHE ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	443.59Å 297.32Å 300.15Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	91.75 – 3.70 101.93 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (91.75-3.70) 89.5 (101.93-3.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.253 0.210 , 0.252	Depositor DCC
R_{free} test set	16296 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	120.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 113.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	397710	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GET

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	0.58	1/40250 (0.0%)	1.19	219/62707 (0.3%)
1	6	0.60	8/40528 (0.0%)	1.18	200/63141 (0.3%)
2	S0	0.36	0/1617	0.61	0/2215
2	s0	0.35	0/1623	0.60	0/2222
3	S1	0.34	0/1735	0.68	2/2335 (0.1%)
3	s1	0.34	0/1748	0.59	0/2352
4	S2	0.37	0/1665	0.65	1/2263 (0.0%)
4	s2	0.39	0/1665	0.65	1/2263 (0.0%)
5	S3	0.42	0/1759	0.61	0/2368
5	s3	0.36	0/1759	0.61	0/2368
6	S4	0.37	0/2109	0.64	3/2839 (0.1%)
6	s4	0.41	1/2109 (0.0%)	0.66	0/2839
7	S5	0.35	0/1629	0.59	0/2202
7	s5	0.34	0/1629	0.60	0/2202
8	S6	0.36	0/1823	0.56	0/2439
8	s6	0.40	0/1779	0.61	0/2379
9	S7	0.38	0/1506	0.64	0/2028
9	s7	0.39	0/1511	0.70	2/2036 (0.1%)
10	S8	0.40	0/1514	0.64	2/2021 (0.1%)
10	s8	0.47	0/1514	0.65	0/2021
11	S9	0.36	0/1519	0.62	0/2035
11	s9	0.39	0/1519	0.61	1/2035 (0.0%)
12	C0	0.37	0/769	0.71	1/1039 (0.1%)
12	c0	0.36	0/757	0.73	1/1022 (0.1%)
13	C1	0.40	0/1172	0.69	1/1580 (0.1%)
13	c1	0.47	0/1194	0.68	1/1610 (0.1%)
14	C2	0.33	0/878	0.71	3/1192 (0.3%)
14	c2	0.32	0/898	0.70	0/1220
15	C3	0.39	0/1215	0.65	0/1638
15	c3	0.40	0/1215	0.63	1/1638 (0.1%)
16	C4	0.37	0/901	0.65	1/1217 (0.1%)
16	c4	0.34	0/960	0.63	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.50	1/988 (0.1%)	0.69	0/1327
17	c5	0.40	0/959	0.67	0/1288
18	C6	0.43	0/1125	0.65	0/1510
18	c6	0.68	2/1125 (0.2%)	0.62	0/1510
19	C7	0.35	0/920	0.61	0/1233
19	c7	0.34	0/915	0.64	1/1227 (0.1%)
20	C8	0.40	0/1211	0.68	0/1628
20	c8	0.35	0/1211	0.63	0/1628
21	C9	0.45	0/1130	0.65	1/1517 (0.1%)
21	c9	0.37	0/1130	0.64	0/1517
22	D0	0.41	0/847	0.64	0/1145
22	d0	0.37	0/815	0.58	0/1102
23	D1	0.40	0/693	0.66	0/935
23	d1	0.37	0/693	0.61	0/935
24	D2	0.37	0/1038	0.70	2/1395 (0.1%)
24	d2	0.40	0/1038	0.64	1/1395 (0.1%)
25	D3	0.46	0/1139	0.73	1/1518 (0.1%)
25	d3	0.48	0/1139	0.68	0/1518
26	D4	0.32	0/1087	0.59	1/1449 (0.1%)
26	d4	0.39	0/1087	0.66	0/1449
27	D5	0.37	0/571	0.72	0/768
27	d5	0.34	0/566	0.58	0/761
28	D6	0.70	1/782 (0.1%)	0.73	1/1047 (0.1%)
28	d6	0.36	0/782	0.64	0/1047
29	D7	0.33	0/620	0.62	0/838
29	d7	0.36	0/620	0.68	0/838
30	D8	1.18	1/499 (0.2%)	0.61	0/670
30	d8	0.84	1/499 (0.2%)	0.61	0/670
31	D9	0.49	0/452	0.77	1/600 (0.2%)
31	d9	0.44	0/452	0.64	0/600
32	E0	0.42	0/483	0.68	0/643
32	e0	0.43	0/483	0.72	0/643
33	E1	0.44	0/577	0.89	0/770
33	e1	0.37	0/358	0.68	0/477
34	SR	0.31	0/2490	0.56	0/3389
34	sR	0.32	0/2456	0.57	0/3343
35	SM	0.41	0/994	0.70	1/1335 (0.1%)
35	sM	0.43	0/882	0.65	0/1180
36	1	0.76	18/73692 (0.0%)	1.39	806/114882 (0.7%)
36	5	0.79	25/74873 (0.0%)	1.40	785/116727 (0.7%)
37	3	0.64	0/2883	1.23	21/4491 (0.5%)
37	7	0.60	0/2883	1.11	9/4491 (0.2%)
38	4	0.74	0/3746	1.38	36/5832 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	8	0.80	0/3724	1.47	46/5798 (0.8%)
39	L2	0.45	0/1948	0.71	2/2617 (0.1%)
39	l2	0.53	1/1946 (0.1%)	0.77	1/2614 (0.0%)
40	L3	0.51	0/3146	0.70	2/4228 (0.0%)
40	l3	0.56	0/3146	0.72	1/4228 (0.0%)
41	L4	0.46	0/2800	0.71	3/3790 (0.1%)
41	l4	0.54	2/2800 (0.1%)	0.72	1/3790 (0.0%)
42	L5	0.42	0/2407	0.65	0/3247
42	l5	0.37	0/2408	0.58	1/3248 (0.0%)
43	L6	0.51	0/1260	0.70	0/1694
43	l6	0.58	0/1269	0.73	0/1705
44	L7	0.51	0/1821	0.66	0/2451
44	l7	0.52	0/1828	0.68	0/2461
45	L8	0.44	1/1836 (0.1%)	0.62	1/2481 (0.0%)
45	l8	0.43	1/1795 (0.1%)	0.65	1/2429 (0.0%)
46	L9	0.48	0/1539	0.66	0/2073
46	l9	0.49	0/1531	0.71	0/2062
47	M0	0.51	0/1726	0.68	0/2314
47	m0	0.47	0/1732	0.72	0/2323
48	M1	0.42	0/1374	0.66	1/1842 (0.1%)
48	m1	0.37	0/1374	0.62	1/1842 (0.1%)
49	M3	0.46	1/1568 (0.1%)	0.68	1/2106 (0.0%)
49	m3	0.47	0/1573	0.71	0/2113
50	M4	0.48	0/1068	0.68	0/1438
50	m4	0.55	0/1074	0.74	1/1446 (0.1%)
51	M5	0.46	0/1757	0.68	0/2354
51	m5	0.50	0/1757	0.75	1/2354 (0.0%)
52	M6	0.59	0/1585	0.74	2/2128 (0.1%)
52	m6	0.62	0/1585	0.76	1/2128 (0.0%)
53	M7	0.53	0/1443	0.72	1/1944 (0.1%)
53	m7	0.56	0/1400	0.77	1/1882 (0.1%)
54	M8	0.40	0/1465	0.62	0/1965
54	m8	0.45	0/1465	0.69	2/1965 (0.1%)
55	M9	0.40	0/1538	0.60	0/2050
55	m9	0.43	0/1499	0.61	0/1998
56	N0	0.51	0/1468	0.68	0/1973
56	n0	0.52	0/1481	0.70	0/1990
57	N1	0.48	0/1300	0.67	0/1743
57	n1	0.43	0/1300	0.61	0/1743
58	N2	0.40	0/794	0.63	0/1076
58	n2	0.39	0/794	0.57	0/1076
59	N3	0.49	0/1012	0.71	1/1361 (0.1%)
59	n3	0.58	0/1008	0.79	0/1356

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	N4	0.44	0/937	0.56	0/1243
60	n4	0.47	1/959 (0.1%)	0.66	2/1267 (0.2%)
61	N5	0.44	0/979	0.72	0/1321
61	n5	0.53	0/974	0.78	1/1314 (0.1%)
62	N6	0.45	0/1004	0.75	2/1341 (0.1%)
62	n6	0.48	0/987	0.82	2/1318 (0.2%)
63	N7	0.47	1/1118 (0.1%)	0.63	0/1497
63	n7	0.49	0/1118	0.63	1/1497 (0.1%)
64	N8	0.43	0/1204	0.73	1/1612 (0.1%)
64	n8	0.47	0/1204	0.72	1/1612 (0.1%)
65	N9	0.41	0/473	0.60	0/629
65	n9	0.44	0/473	0.72	0/629
66	O0	0.40	0/751	0.61	1/1008 (0.1%)
66	o0	0.45	0/775	0.62	0/1040
67	O1	0.47	0/890	0.71	0/1196
67	o1	0.52	0/897	0.71	1/1205 (0.1%)
68	O2	0.50	0/1041	0.72	0/1394
68	o2	0.53	0/1041	0.73	0/1394
69	O3	0.56	0/868	0.72	0/1168
69	o3	0.59	0/868	0.79	1/1168 (0.1%)
70	O4	0.43	0/890	0.71	1/1189 (0.1%)
70	o4	0.48	0/890	0.73	1/1189 (0.1%)
71	O5	0.44	0/978	0.66	0/1301
71	o5	0.51	0/974	0.69	0/1297
72	O6	0.45	1/778 (0.1%)	0.70	1/1034 (0.1%)
72	o6	0.43	0/777	0.67	0/1033
73	O7	0.54	1/680 (0.1%)	0.75	0/901
73	o7	0.63	0/665	0.84	1/882 (0.1%)
74	O8	0.38	0/618	0.60	0/826
74	o8	0.42	0/614	0.62	0/822
75	O9	0.45	0/438	0.66	0/581
75	o9	0.52	0/443	0.67	0/588
76	Q0	0.55	0/423	0.78	0/562
76	q0	0.66	0/423	0.76	0/562
77	Q1	0.41	0/234	0.67	0/300
77	q1	0.48	0/234	0.74	0/300
78	Q2	0.48	0/860	0.67	0/1136
78	q2	0.47	0/860	0.68	0/1136
79	Q3	0.45	0/701	0.62	0/934
79	q3	0.43	0/701	0.68	0/934
80	p0	0.34	0/1067	0.58	1/1439 (0.1%)
All	All	0.62	69/423555 (0.0%)	1.11	2197/621249 (0.4%)

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
2	S0	0	1
2	s0	0	1
3	S1	0	4
4	S2	0	1
4	s2	0	2
5	s3	0	1
6	S4	0	1
7	S5	0	3
7	s5	0	4
8	s6	0	1
9	S7	0	4
9	s7	0	6
11	s9	0	2
12	c0	0	1
13	C1	0	1
14	C2	0	3
14	c2	0	1
15	c3	0	1
16	C4	0	1
17	C5	0	2
17	c5	0	4
18	C6	0	3
18	c6	0	1
19	C7	0	1
20	C8	0	3
20	c8	0	1
22	d0	0	2
24	D2	0	1
25	D3	0	1
26	D4	0	2
27	D5	0	2
27	d5	0	2
28	D6	0	2
29	D7	0	1
32	e0	0	2
33	E1	0	5
33	e1	0	3
34	SR	0	1
34	sR	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	sM	0	1
39	l2	0	2
40	L3	0	2
40	l3	0	1
41	l4	0	1
42	L5	0	3
42	l5	0	2
43	L6	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
45	l8	0	3
46	L9	0	1
48	m1	0	1
49	m3	0	2
50	m4	0	1
51	M5	0	1
51	m5	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	2
56	N0	0	4
56	n0	0	2
58	n2	0	1
60	N4	0	2
62	N6	0	1
63	n7	0	2
64	N8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	2
69	O3	0	1
70	o4	0	1
71	O5	0	1
71	o5	0	1
72	O6	0	1
72	o6	0	1
79	q3	0	2
80	p0	0	1
All	All	0	141

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D8	5	THR	C-N	25.28	1.82	1.34
18	c6	4	VAL	C-N	18.52	1.69	1.34
30	d8	5	THR	C-N	17.27	1.67	1.34
28	D6	59	TYR	C-N	16.33	1.65	1.34
17	C5	67	ALA	C-N	9.82	1.52	1.34

The worst 5 of 2197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	C4-N9-C1'	-16.36	105.24	126.50
36	5	1152	G	N3-C4-N9	-16.24	116.26	126.00
36	5	1152	G	C8-N9-C1'	15.84	147.59	127.00
36	5	1152	G	N3-C4-C5	14.71	135.96	128.60
36	1	2392	C	C6-N1-C2	13.33	125.63	120.30

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	94	GLY	Peptide
3	S1	131	ASP	Peptide
3	S1	205	PHE	Peptide
3	S1	206	PRO	Peptide
3	S1	36	SER	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	204/206 (99%)	174 (85%)	26 (13%)	4 (2%)	7 39
2	s0	204/206 (99%)	176 (86%)	23 (11%)	5 (2%)	5 35
3	S1	212/216 (98%)	162 (76%)	45 (21%)	5 (2%)	6 35
3	s1	214/216 (99%)	195 (91%)	15 (7%)	4 (2%)	8 40
4	S2	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	17 54
4	s2	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29 66
5	S3	221/223 (99%)	202 (91%)	15 (7%)	4 (2%)	8 41
5	s3	221/223 (99%)	195 (88%)	18 (8%)	8 (4%)	3 29
6	S4	258/260 (99%)	226 (88%)	30 (12%)	2 (1%)	19 56
6	s4	258/260 (99%)	234 (91%)	21 (8%)	3 (1%)	13 48
7	S5	204/206 (99%)	178 (87%)	21 (10%)	5 (2%)	5 35
7	s5	204/206 (99%)	183 (90%)	18 (9%)	3 (2%)	10 44
8	S6	224/236 (95%)	209 (93%)	9 (4%)	6 (3%)	5 33
8	s6	216/236 (92%)	196 (91%)	17 (8%)	3 (1%)	11 45
9	S7	182/185 (98%)	154 (85%)	20 (11%)	8 (4%)	2 24
9	s7	183/185 (99%)	157 (86%)	23 (13%)	3 (2%)	9 43
10	S8	184/200 (92%)	160 (87%)	23 (12%)	1 (0%)	29 66
10	s8	184/200 (92%)	171 (93%)	11 (6%)	2 (1%)	14 50
11	S9	183/185 (99%)	162 (88%)	20 (11%)	1 (0%)	29 66
11	s9	183/185 (99%)	169 (92%)	14 (8%)	0	100 100
12	C0	90/105 (86%)	77 (86%)	10 (11%)	3 (3%)	4 31
12	c0	90/105 (86%)	65 (72%)	19 (21%)	6 (7%)	1 16
13	C1	140/156 (90%)	128 (91%)	10 (7%)	2 (1%)	11 45
13	c1	144/156 (92%)	130 (90%)	11 (8%)	3 (2%)	7 38
14	C2	118/143 (82%)	87 (74%)	27 (23%)	4 (3%)	3 30
14	c2	122/143 (85%)	89 (73%)	25 (20%)	8 (7%)	1 16
15	C3	148/150 (99%)	134 (90%)	12 (8%)	2 (1%)	11 45
15	c3	148/150 (99%)	129 (87%)	16 (11%)	3 (2%)	7 39
16	C4	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19 56
16	c4	126/128 (98%)	111 (88%)	15 (12%)	0	100 100
17	C5	120/141 (85%)	100 (83%)	18 (15%)	2 (2%)	9 42
17	c5	117/141 (83%)	99 (85%)	14 (12%)	4 (3%)	3 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	C6	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	4 32
18	c6	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22 59
19	C7	113/136 (83%)	100 (88%)	12 (11%)	1 (1%)	17 54
19	c7	115/136 (85%)	104 (90%)	10 (9%)	1 (1%)	17 54
20	C8	143/145 (99%)	123 (86%)	17 (12%)	3 (2%)	7 38
20	c8	143/145 (99%)	122 (85%)	18 (13%)	3 (2%)	7 38
21	C9	141/143 (99%)	125 (89%)	16 (11%)	0	100 100
21	c9	141/143 (99%)	128 (91%)	12 (8%)	1 (1%)	22 59
22	D0	103/107 (96%)	98 (95%)	5 (5%)	0	100 100
22	d0	99/107 (92%)	88 (89%)	9 (9%)	2 (2%)	7 39
23	D1	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	6 35
23	d1	85/87 (98%)	75 (88%)	10 (12%)	0	100 100
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19 56
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19 56
25	D3	142/144 (99%)	119 (84%)	19 (13%)	4 (3%)	5 33
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100 100
26	D4	132/134 (98%)	121 (92%)	8 (6%)	3 (2%)	6 36
26	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	10 44
27	D5	68/70 (97%)	52 (76%)	14 (21%)	2 (3%)	4 32
27	d5	67/70 (96%)	61 (91%)	6 (9%)	0	100 100
28	D6	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0 6
28	d6	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	14 50
29	D7	79/81 (98%)	69 (87%)	9 (11%)	1 (1%)	12 47
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12 47
30	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100 100
30	d8	61/63 (97%)	52 (85%)	9 (15%)	0	100 100
31	D9	51/53 (96%)	49 (96%)	2 (4%)	0	100 100
31	d9	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	3 27
32	E0	58/60 (97%)	51 (88%)	4 (7%)	3 (5%)	2 21
32	e0	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2 21
33	E1	69/152 (45%)	44 (64%)	19 (28%)	6 (9%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	e1	41/152 (27%)	31 (76%)	8 (20%)	2 (5%)	2 22
34	SR	316/318 (99%)	298 (94%)	18 (6%)	0	100 100
34	sR	311/318 (98%)	291 (94%)	19 (6%)	1 (0%)	41 74
35	SM	131/272 (48%)	116 (88%)	12 (9%)	3 (2%)	6 36
35	sM	113/272 (42%)	94 (83%)	13 (12%)	6 (5%)	2 21
39	L2	250/252 (99%)	235 (94%)	15 (6%)	0	100 100
39	l2	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	34 69
40	L3	384/386 (100%)	352 (92%)	30 (8%)	2 (0%)	29 66
40	l3	384/386 (100%)	361 (94%)	19 (5%)	4 (1%)	15 51
41	L4	359/361 (99%)	321 (89%)	35 (10%)	3 (1%)	19 56
41	l4	359/361 (99%)	322 (90%)	31 (9%)	6 (2%)	9 42
42	L5	292/296 (99%)	264 (90%)	23 (8%)	5 (2%)	9 42
42	l5	292/296 (99%)	276 (94%)	16 (6%)	0	100 100
43	L6	152/176 (86%)	142 (93%)	6 (4%)	4 (3%)	5 34
43	l6	153/176 (87%)	139 (91%)	11 (7%)	3 (2%)	7 39
44	L7	220/223 (99%)	205 (93%)	15 (7%)	0	100 100
44	l7	221/223 (99%)	210 (95%)	9 (4%)	2 (1%)	17 54
45	L8	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	9 42
45	l8	229/233 (98%)	201 (88%)	23 (10%)	5 (2%)	6 37
46	L9	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	29 66
46	l9	188/191 (98%)	176 (94%)	9 (5%)	3 (2%)	9 43
47	M0	204/221 (92%)	193 (95%)	11 (5%)	0	100 100
47	m0	205/221 (93%)	186 (91%)	18 (9%)	1 (0%)	29 66
48	M1	167/169 (99%)	136 (81%)	29 (17%)	2 (1%)	13 48
48	m1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	3 29
49	M3	191/194 (98%)	172 (90%)	14 (7%)	5 (3%)	5 34
49	m3	192/194 (99%)	162 (84%)	25 (13%)	5 (3%)	5 34
50	M4	134/137 (98%)	123 (92%)	9 (7%)	2 (2%)	10 44
50	m4	135/137 (98%)	127 (94%)	8 (6%)	0	100 100
51	M5	201/203 (99%)	181 (90%)	18 (9%)	2 (1%)	15 51
51	m5	201/203 (99%)	185 (92%)	13 (6%)	3 (2%)	10 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	M6	195/197 (99%)	182 (93%)	11 (6%)	2 (1%)	15 51
52	m6	195/197 (99%)	185 (95%)	10 (5%)	0	100 100
53	M7	181/184 (98%)	168 (93%)	11 (6%)	2 (1%)	14 50
53	m7	171/184 (93%)	159 (93%)	12 (7%)	0	100 100
54	M8	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	29 66
54	m8	183/185 (99%)	171 (93%)	12 (7%)	0	100 100
55	M9	186/188 (99%)	174 (94%)	10 (5%)	2 (1%)	14 50
55	m9	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	25 62
56	N0	168/172 (98%)	154 (92%)	12 (7%)	2 (1%)	13 48
56	n0	170/172 (99%)	165 (97%)	5 (3%)	0	100 100
57	N1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	25 62
57	n1	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25 62
58	N2	96/98 (98%)	86 (90%)	10 (10%)	0	100 100
58	n2	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	15 51
59	N3	133/135 (98%)	128 (96%)	5 (4%)	0	100 100
59	n3	132/135 (98%)	128 (97%)	3 (2%)	1 (1%)	19 56
60	N4	118/155 (76%)	110 (93%)	8 (7%)	0	100 100
60	n4	114/155 (74%)	106 (93%)	8 (7%)	0	100 100
61	N5	119/121 (98%)	109 (92%)	10 (8%)	0	100 100
61	n5	118/121 (98%)	102 (86%)	15 (13%)	1 (1%)	19 56
62	N6	124/126 (98%)	116 (94%)	8 (6%)	0	100 100
62	n6	122/126 (97%)	116 (95%)	4 (3%)	2 (2%)	9 43
63	N7	133/135 (98%)	120 (90%)	11 (8%)	2 (2%)	10 44
63	n7	133/135 (98%)	117 (88%)	14 (10%)	2 (2%)	10 44
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	3 30
64	n8	146/148 (99%)	128 (88%)	16 (11%)	2 (1%)	11 45
65	N9	56/58 (97%)	50 (89%)	6 (11%)	0	100 100
65	n9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3 29
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100 100
66	o0	98/100 (98%)	93 (95%)	5 (5%)	0	100 100
67	O1	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	5 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
67	o1	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	8 40
68	O2	125/127 (98%)	117 (94%)	8 (6%)	0	100 100
68	o2	125/127 (98%)	112 (90%)	13 (10%)	0	100 100
69	O3	104/106 (98%)	98 (94%)	6 (6%)	0	100 100
69	o3	104/106 (98%)	93 (89%)	11 (11%)	0	100 100
70	O4	110/112 (98%)	102 (93%)	6 (6%)	2 (2%)	8 41
70	o4	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17 54
71	O5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	9 42
71	o5	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17 54
72	O6	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15 51
72	o6	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15 51
73	O7	82/84 (98%)	76 (93%)	5 (6%)	1 (1%)	13 48
73	o7	80/84 (95%)	74 (92%)	5 (6%)	1 (1%)	12 47
74	O8	75/77 (97%)	67 (89%)	8 (11%)	0	100 100
74	o8	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12 47
75	O9	47/50 (94%)	43 (92%)	4 (8%)	0	100 100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	7 38
76	Q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7 39
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7 39
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
77	q1	23/25 (92%)	23 (100%)	0	0	100 100
78	Q2	103/105 (98%)	89 (86%)	14 (14%)	0	100 100
78	q2	103/105 (98%)	99 (96%)	4 (4%)	0	100 100
79	Q3	89/91 (98%)	80 (90%)	9 (10%)	0	100 100
79	q3	89/91 (98%)	82 (92%)	7 (8%)	0	100 100
80	p0	134/312 (43%)	121 (90%)	12 (9%)	1 (1%)	22 59
All	All	22212/23608 (94%)	19993 (90%)	1922 (9%)	297 (1%)	12 47

5 of 297 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	207	LEU
8	S6	153	VAL

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Mol	Chain	Res	Type
9	S7	111	LYS
12	C0	87	VAL
12	C0	88	PRO

5.3.2 Protein sidechains (i)

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	164/173 (95%)	131 (80%)	33 (20%)	1 8
2	s0	165/173 (95%)	135 (82%)	30 (18%)	1 11
3	S1	191/192 (100%)	148 (78%)	43 (22%)	1 6
3	s1	192/192 (100%)	158 (82%)	34 (18%)	2 12
4	S2	176/176 (100%)	135 (77%)	41 (23%)	1 6
4	s2	176/176 (100%)	141 (80%)	35 (20%)	1 8
5	S3	182/182 (100%)	145 (80%)	37 (20%)	1 8
5	s3	182/182 (100%)	142 (78%)	40 (22%)	1 6
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2 12
6	s4	221/221 (100%)	189 (86%)	32 (14%)	3 18
7	S5	173/173 (100%)	140 (81%)	33 (19%)	1 9
7	s5	173/173 (100%)	142 (82%)	31 (18%)	2 11
8	S6	188/201 (94%)	153 (81%)	35 (19%)	1 10
8	s6	187/201 (93%)	157 (84%)	30 (16%)	2 15
9	S7	165/165 (100%)	133 (81%)	32 (19%)	1 9
9	s7	165/165 (100%)	129 (78%)	36 (22%)	1 6
10	S8	150/161 (93%)	126 (84%)	24 (16%)	2 15
10	s8	150/161 (93%)	123 (82%)	27 (18%)	1 11
11	S9	158/158 (100%)	125 (79%)	33 (21%)	1 7
11	s9	158/158 (100%)	137 (87%)	21 (13%)	4 22
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2 12
13	C1	127/137 (93%)	113 (89%)	14 (11%)	6 29
13	c1	129/137 (94%)	105 (81%)	24 (19%)	1 10
14	C2	88/119 (74%)	65 (74%)	23 (26%)	0 4
14	c2	88/119 (74%)	62 (70%)	26 (30%)	0 2
15	C3	127/127 (100%)	107 (84%)	20 (16%)	2 16
15	c3	127/127 (100%)	100 (79%)	27 (21%)	1 7
16	C4	81/97 (84%)	59 (73%)	22 (27%)	0 3
16	c4	97/97 (100%)	76 (78%)	21 (22%)	1 7
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1 8
17	c5	98/117 (84%)	85 (87%)	13 (13%)	4 22
18	C6	117/117 (100%)	92 (79%)	25 (21%)	1 7
18	c6	117/117 (100%)	97 (83%)	20 (17%)	2 13
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1 6
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1 7
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0 5
20	c8	128/128 (100%)	103 (80%)	25 (20%)	1 9
21	C9	115/115 (100%)	91 (79%)	24 (21%)	1 7
21	c9	115/115 (100%)	92 (80%)	23 (20%)	1 8
22	D0	98/100 (98%)	78 (80%)	20 (20%)	1 8
22	d0	94/100 (94%)	76 (81%)	18 (19%)	1 9
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1 8
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1 9
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2 15
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3 18
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1 9
25	d3	119/119 (100%)	108 (91%)	11 (9%)	9 36
26	D4	112/112 (100%)	89 (80%)	23 (20%)	1 7
26	d4	112/112 (100%)	89 (80%)	23 (20%)	1 7
27	D5	61/61 (100%)	40 (66%)	21 (34%)	0 1
27	d5	61/61 (100%)	54 (88%)	7 (12%)	5 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	D6	83/83 (100%)	59 (71%)	24 (29%)	0 2
28	d6	83/83 (100%)	71 (86%)	12 (14%)	3 18
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3 19
29	d7	70/70 (100%)	57 (81%)	13 (19%)	1 10
30	D8	56/56 (100%)	40 (71%)	16 (29%)	0 2
30	d8	56/56 (100%)	38 (68%)	18 (32%)	0 1
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1 7
31	d9	47/47 (100%)	39 (83%)	8 (17%)	2 13
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2 12
32	e0	51/51 (100%)	35 (69%)	16 (31%)	0 1
33	E1	62/135 (46%)	41 (66%)	21 (34%)	0 1
33	e1	39/135 (29%)	30 (77%)	9 (23%)	1 6
34	SR	259/260 (100%)	229 (88%)	30 (12%)	5 27
34	sR	255/260 (98%)	230 (90%)	25 (10%)	8 33
35	SM	97/227 (43%)	77 (79%)	20 (21%)	1 7
35	sM	93/227 (41%)	70 (75%)	23 (25%)	0 5
39	L2	193/194 (100%)	160 (83%)	33 (17%)	2 13
39	l2	192/194 (99%)	148 (77%)	44 (23%)	1 6
40	L3	320/322 (99%)	260 (81%)	60 (19%)	1 10
40	l3	318/322 (99%)	246 (77%)	72 (23%)	1 6
41	L4	288/288 (100%)	242 (84%)	46 (16%)	2 15
41	l4	288/288 (100%)	232 (81%)	56 (19%)	1 9
42	L5	242/244 (99%)	194 (80%)	48 (20%)	1 8
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2 12
43	L6	134/153 (88%)	108 (81%)	26 (19%)	1 9
43	l6	135/153 (88%)	113 (84%)	22 (16%)	2 15
44	L7	186/187 (100%)	166 (89%)	20 (11%)	6 29
44	l7	187/187 (100%)	161 (86%)	26 (14%)	3 20
45	L8	187/191 (98%)	154 (82%)	33 (18%)	2 12
45	l8	177/191 (93%)	143 (81%)	34 (19%)	1 9
46	L9	171/171 (100%)	128 (75%)	43 (25%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	l9	170/171 (99%)	129 (76%)	41 (24%)	0 5
47	M0	177/187 (95%)	153 (86%)	24 (14%)	3 21
47	m0	177/187 (95%)	140 (79%)	37 (21%)	1 7
48	M1	147/147 (100%)	121 (82%)	26 (18%)	2 12
48	m1	147/147 (100%)	117 (80%)	30 (20%)	1 8
49	M3	154/154 (100%)	119 (77%)	35 (23%)	1 6
49	m3	154/154 (100%)	125 (81%)	29 (19%)	1 10
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1 9
50	m4	108/108 (100%)	87 (81%)	21 (19%)	1 9
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2 13
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3 19
52	M6	160/160 (100%)	134 (84%)	26 (16%)	2 15
52	m6	160/160 (100%)	124 (78%)	36 (22%)	1 6
53	M7	140/146 (96%)	102 (73%)	38 (27%)	0 3
53	m7	139/146 (95%)	103 (74%)	36 (26%)	0 4
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2 14
54	m8	150/150 (100%)	127 (85%)	23 (15%)	2 17
55	M9	153/153 (100%)	116 (76%)	37 (24%)	0 5
55	m9	149/153 (97%)	112 (75%)	37 (25%)	0 5
56	N0	155/156 (99%)	126 (81%)	29 (19%)	1 10
56	n0	156/156 (100%)	126 (81%)	30 (19%)	1 9
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1 7
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1 8
58	N2	85/85 (100%)	73 (86%)	12 (14%)	3 20
58	n2	85/85 (100%)	70 (82%)	15 (18%)	2 12
59	N3	103/103 (100%)	89 (86%)	14 (14%)	3 21
59	n3	103/103 (100%)	88 (85%)	15 (15%)	3 18
60	N4	85/129 (66%)	73 (86%)	12 (14%)	3 20
60	n4	97/129 (75%)	85 (88%)	12 (12%)	4 24
61	N5	104/105 (99%)	82 (79%)	22 (21%)	1 7
61	n5	104/105 (99%)	84 (81%)	20 (19%)	1 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1 8
62	n6	107/109 (98%)	85 (79%)	22 (21%)	1 7
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1 9
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1 7
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1 10
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1 8
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3 17
65	n9	46/46 (100%)	40 (87%)	6 (13%)	4 22
66	O0	81/84 (96%)	61 (75%)	20 (25%)	0 5
66	o0	84/84 (100%)	71 (84%)	13 (16%)	2 17
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1 9
67	o1	94/96 (98%)	75 (80%)	19 (20%)	1 8
68	O2	109/109 (100%)	92 (84%)	17 (16%)	2 17
68	o2	109/109 (100%)	91 (84%)	18 (16%)	2 14
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2 17
69	o3	90/90 (100%)	72 (80%)	18 (20%)	1 8
70	O4	95/95 (100%)	73 (77%)	22 (23%)	1 6
70	o4	95/95 (100%)	80 (84%)	15 (16%)	2 16
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1 10
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1 10
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0 2
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0 3
73	O7	69/69 (100%)	51 (74%)	18 (26%)	0 4
73	o7	67/69 (97%)	55 (82%)	12 (18%)	2 11
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1 6
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1 9
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1 8
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2 17
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1 7
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1 9
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0 0
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1 6
78	q2	90/90 (100%)	77 (86%)	13 (14%)	3 19
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	1 10
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1 7
80	p0	105/254 (41%)	91 (87%)	14 (13%)	4 22
All	All	18730/19834 (94%)	15159 (81%)	3571 (19%)	1 9

5 of 3571 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	s1	127	VAL
79	q3	42	CYS
20	c8	20	THR
75	o9	51	ILE
57	n1	79	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
12	c0	32	HIS
68	o2	35	GLN
39	l2	19	HIS
68	o2	13	HIS
57	n1	146	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1680/1800 (93%)	462 (27%)	67 (3%)
1	6	1695/1800 (94%)	427 (25%)	51 (3%)
36	1	3071/3396 (90%)	760 (24%)	101 (3%)
36	5	3120/3396 (91%)	739 (23%)	109 (3%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	48 (30%)	6 (3%)
38	8	156/158 (98%)	41 (26%)	8 (5%)
All	All	10119/10950 (92%)	2512 (24%)	344 (3%)

5 of 2512 RNA backbone outliers are listed below:

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

5 of 344 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	369	A
36	5	2101	C
36	5	735	A
36	5	1238	C
36	5	2374	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1260 ligands modelled in this entry, 1239 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
82	GET	1	3812	-	33,36,36	0.31	0	43,55,55	1.18	3 (6%)
82	GET	1	3810	-	33,36,36	0.32	0	43,55,55	1.57	7 (16%)
82	GET	6	2014	-	33,36,36	0.17	0	43,55,55	1.08	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
82	GET	6	2013	-	33,36,36	0.24	0	43,55,55	0.69	1 (2%)
82	GET	1	3813	-	33,36,36	0.42	0	43,55,55	1.83	9 (20%)
82	GET	5	3849	-	33,36,36	0.42	0	43,55,55	1.25	3 (6%)
82	GET	2	2014	-	33,36,36	0.39	0	43,55,55	1.29	5 (11%)
82	GET	5	3850	-	33,36,36	0.30	0	43,55,55	1.18	4 (9%)
82	GET	1	3808	-	33,36,36	0.34	0	43,55,55	1.62	7 (16%)
82	GET	n6	201	-	33,36,36	0.22	0	43,55,55	1.11	4 (9%)
82	GET	5	3844	-	33,36,36	0.24	0	43,55,55	1.50	7 (16%)
82	GET	5	3847	-	33,36,36	0.40	0	43,55,55	1.50	6 (13%)
82	GET	2	2012	-	33,36,36	0.30	0	43,55,55	0.98	2 (4%)
82	GET	5	3846	-	33,36,36	0.26	0	43,55,55	1.13	2 (4%)
82	GET	1	3809	-	33,36,36	0.28	0	43,55,55	1.04	5 (11%)
82	GET	2	2013	-	33,36,36	0.16	0	43,55,55	0.94	3 (6%)
82	GET	5	3851	-	33,36,36	0.21	0	43,55,55	0.66	1 (2%)
82	GET	1	3811	-	33,36,36	0.20	0	43,55,55	0.62	1 (2%)
82	GET	5	3848	-	33,36,36	0.26	0	43,55,55	1.76	3 (6%)
82	GET	5	3845	-	33,36,36	0.27	0	43,55,55	0.91	2 (4%)
82	GET	6	2015	-	33,36,36	1.93	8 (24%)	43,55,55	2.93	21 (48%)

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
82	GET	1	3812	-	-	6/13/74/74	0/3/3/3
82	GET	1	3810	-	-	2/13/74/74	0/3/3/3
82	GET	6	2014	-	-	6/13/74/74	0/3/3/3
82	GET	6	2013	-	-	1/13/74/74	0/3/3/3
82	GET	1	3813	-	-	7/13/74/74	0/3/3/3
82	GET	5	3849	-	-	4/13/74/74	0/3/3/3
82	GET	2	2014	-	-	5/13/74/74	1/3/3/3
82	GET	5	3850	-	-	6/13/74/74	0/3/3/3
82	GET	1	3808	-	-	9/13/74/74	0/3/3/3
82	GET	n6	201	-	-	6/13/74/74	0/3/3/3
82	GET	5	3844	-	-	5/13/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GET	5	3847	-	-	8/13/74/74	0/3/3/3
82	GET	2	2012	-	-	2/13/74/74	1/3/3/3
82	GET	5	3846	-	-	6/13/74/74	0/3/3/3
82	GET	1	3809	-	-	10/13/74/74	0/3/3/3
82	GET	2	2013	-	-	6/13/74/74	0/3/3/3
82	GET	5	3851	-	-	6/13/74/74	0/3/3/3
82	GET	1	3811	-	-	1/13/74/74	0/3/3/3
82	GET	5	3848	-	-	3/13/74/74	0/3/3/3
82	GET	5	3845	-	-	1/13/74/74	0/3/3/3
82	GET	6	2015	-	-	5/13/74/74	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	6	2015	GET	C23-C33	5.14	1.64	1.53
82	6	2015	GET	C22-C12	3.63	1.61	1.53
82	6	2015	GET	C41-C31	3.54	1.61	1.52
82	6	2015	GET	C22-C32	2.91	1.60	1.53
82	6	2015	GET	C51-C61	2.68	1.56	1.52

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	5	3848	GET	C23-C33-N33	-7.62	90.62	110.84
82	6	2015	GET	C11-C21-N21	7.35	123.45	110.20
82	6	2015	GET	O31-C31-C21	-7.02	97.61	110.22
82	1	3810	GET	O11-C11-C21	6.48	119.38	108.22
82	6	2015	GET	C31-C21-N21	-5.66	99.46	111.05

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	2	2012	GET	C23-C33-N33-C93
82	2	2013	GET	C41-C51-C61-O61
82	2	2013	GET	C41-C51-C61-C71
82	2	2013	GET	O51-C51-C61-O61
82	2	2013	GET	C23-C33-N33-C93

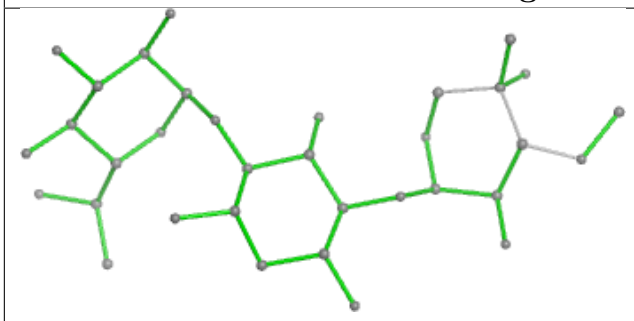
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	2	2012	GET	C13-C23-C33-C43-C53-O53
82	2	2014	GET	C11-C21-C31-C41-C51-O51

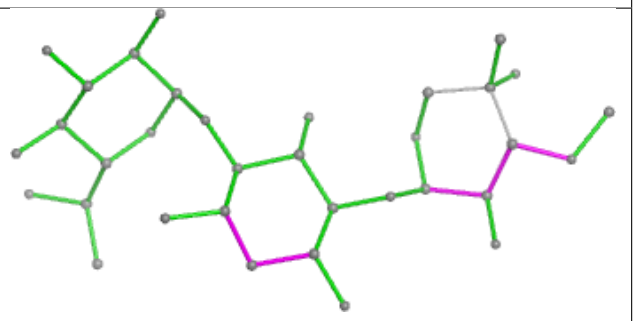
No monomer is involved in short contacts.

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

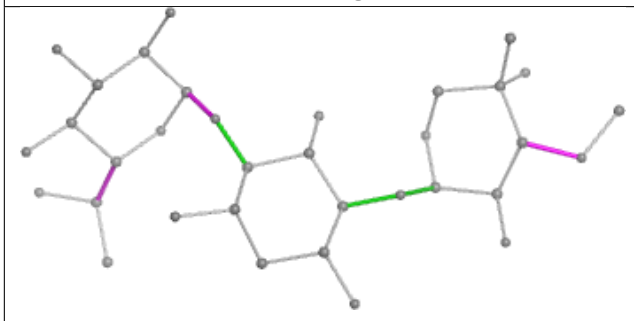
Ligand GET 1 3812



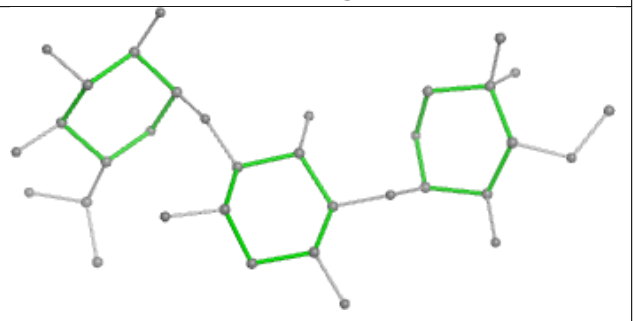
Bond lengths



Bond angles

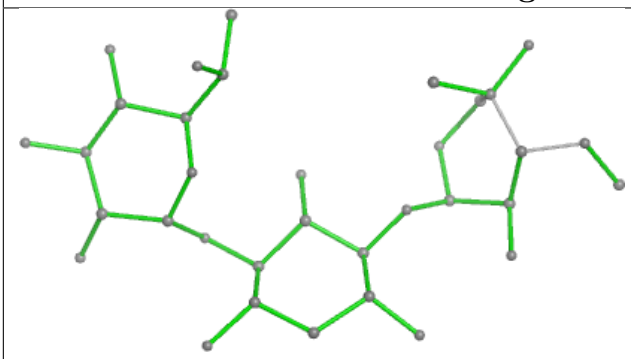


Torsions

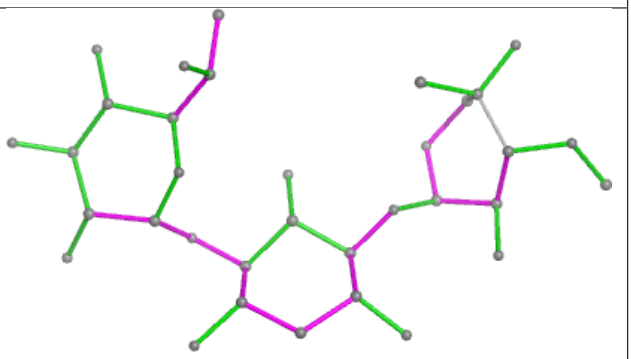


Rings

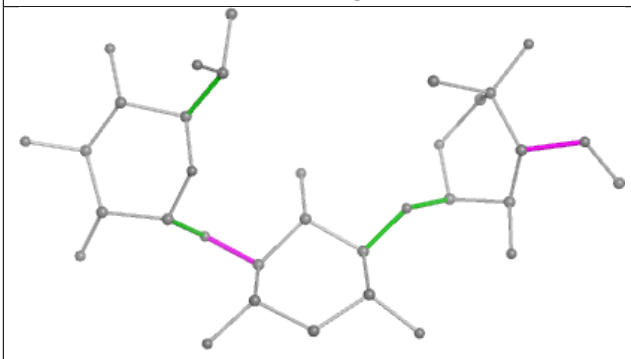
Ligand GET 1 3810



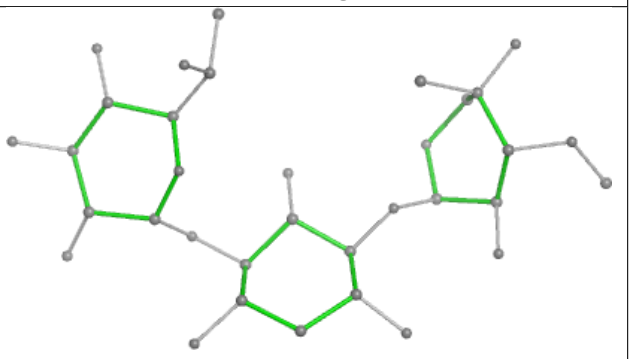
Bond lengths



Bond angles

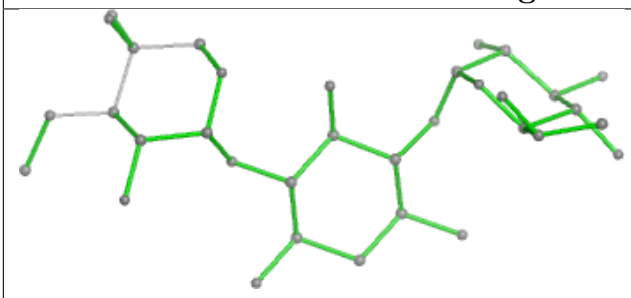


Torsions

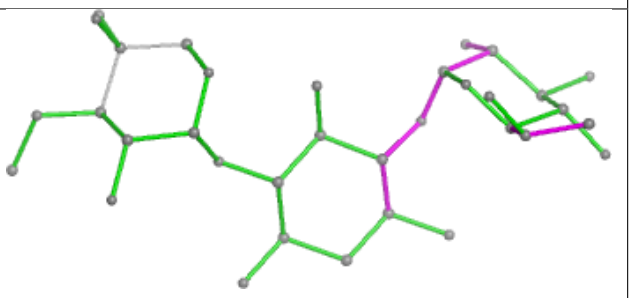


Rings

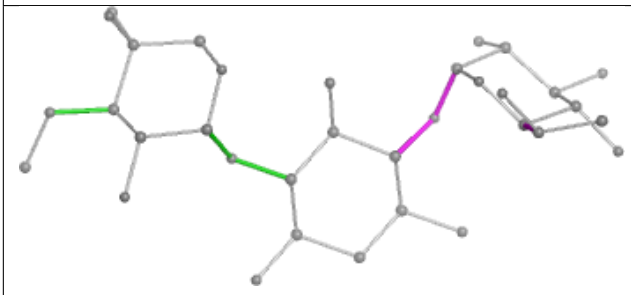
Ligand GET 6 2014



Bond lengths



Bond angles



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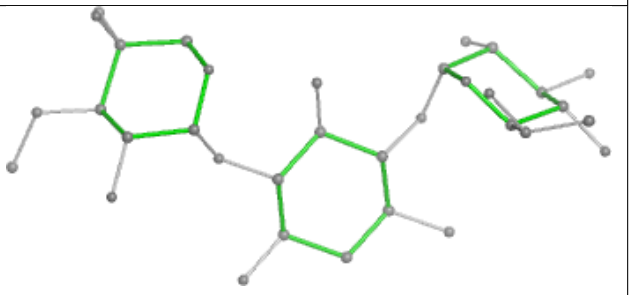
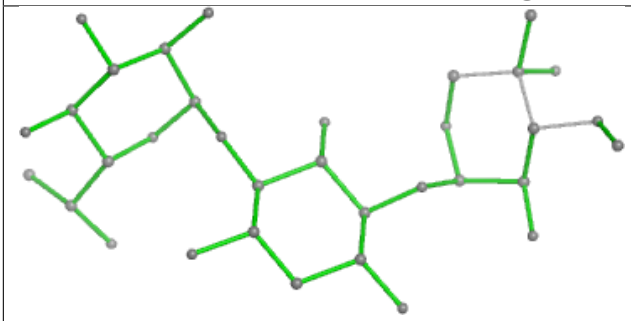
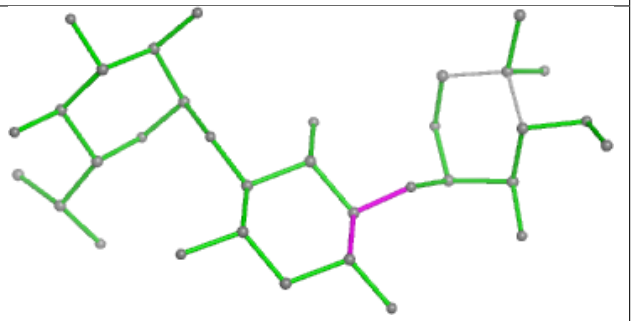


Rings

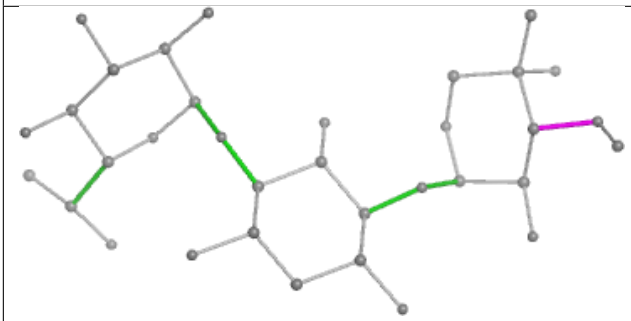
Ligand GET 6 2013



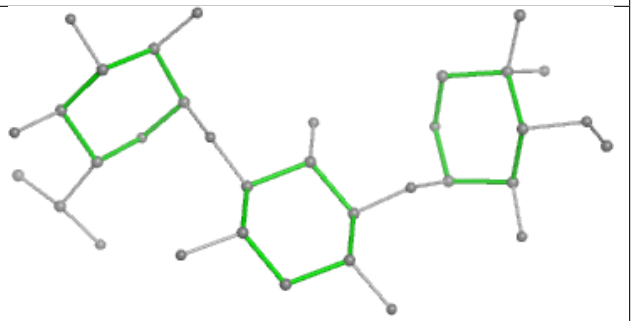
Bond lengths



Bond angles

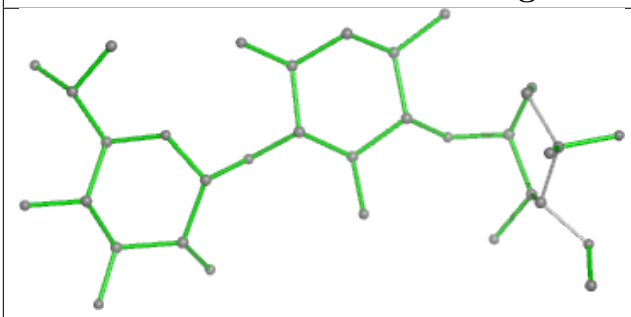


Torsions

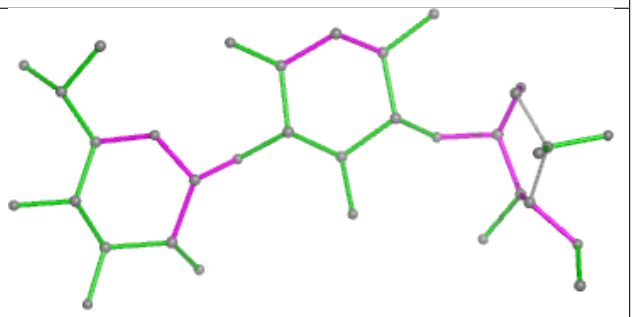


Rings

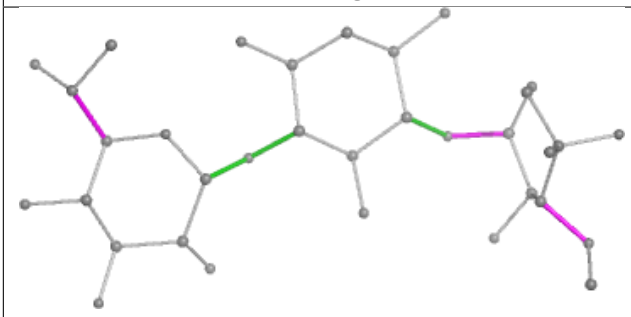
Ligand GET 1 3813



Bond lengths



Bond angles



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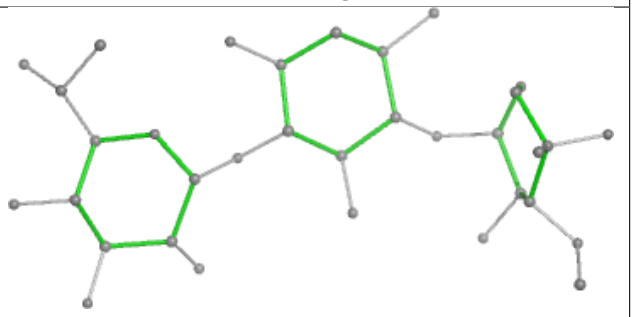
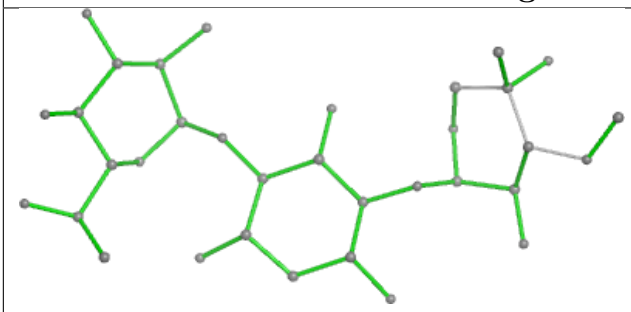


Rings

Ligand GET 5 3849



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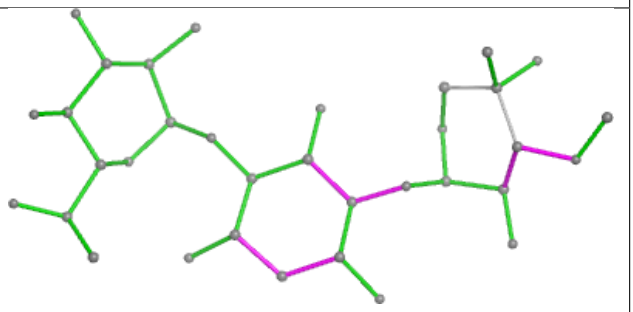
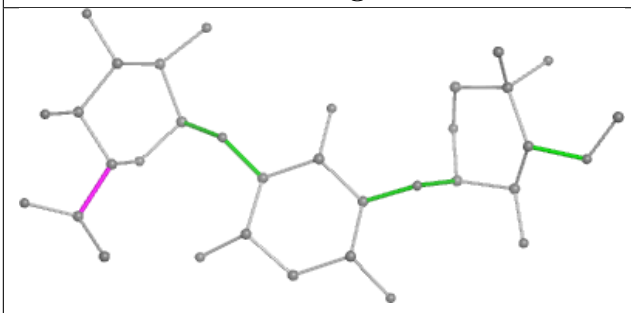


Bond angles



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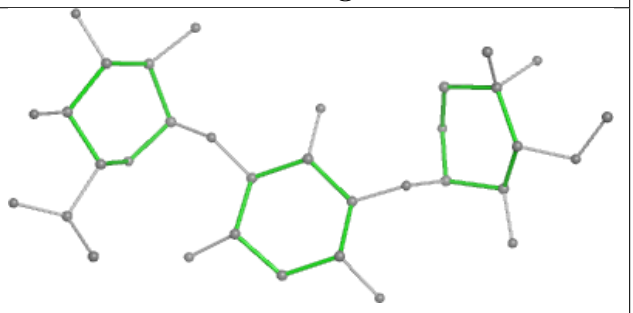
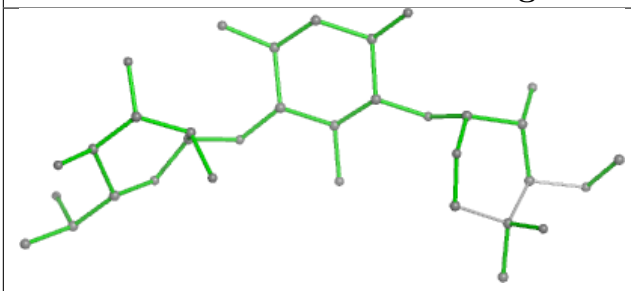


Rings

Ligand GET 2 2014



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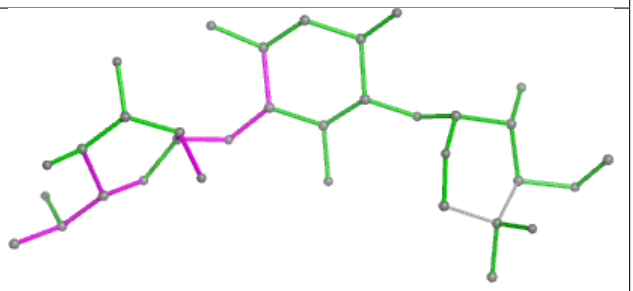
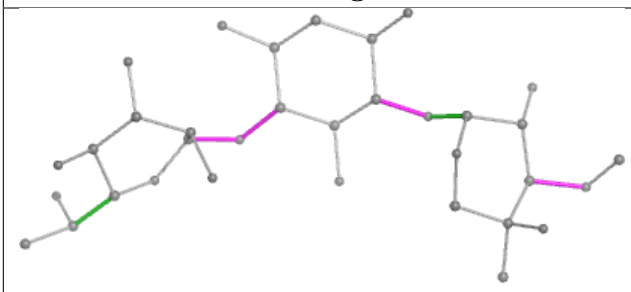


Bond angles



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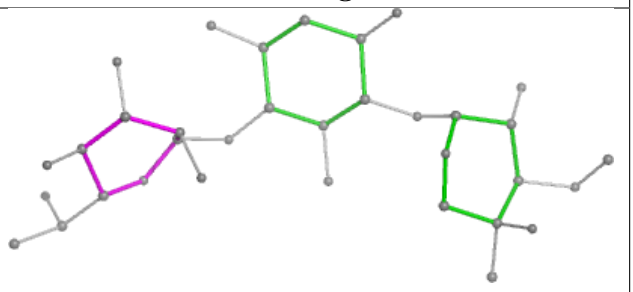
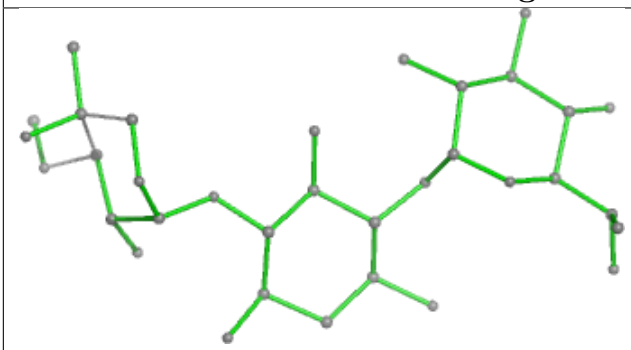


Rings

Ligand GET 5 3850



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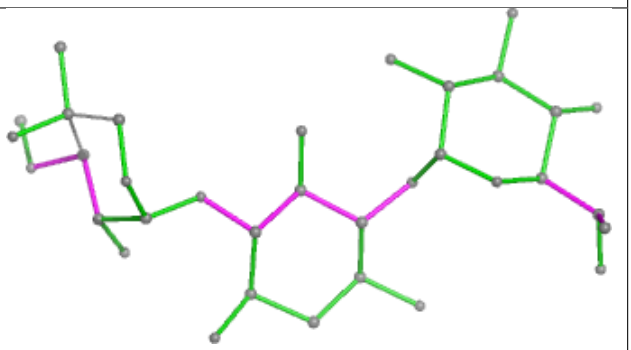

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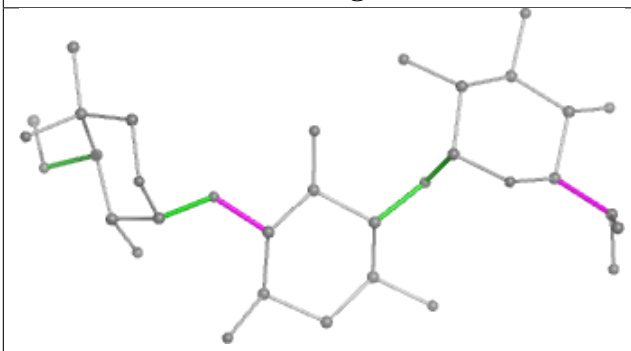

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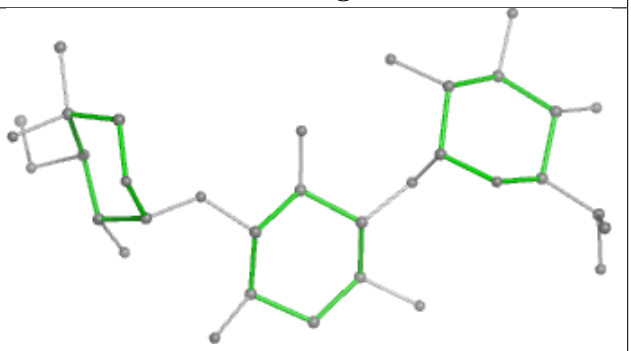
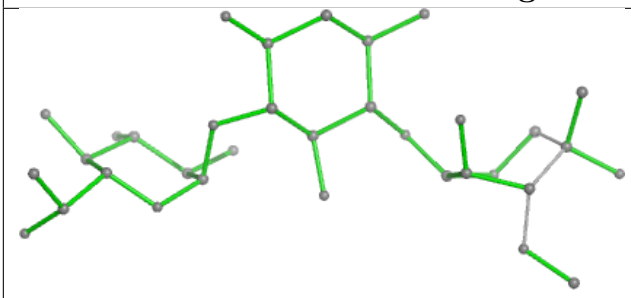


Rings

Ligand GET 1 3808



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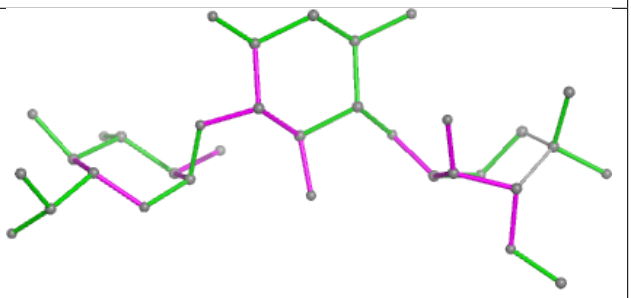
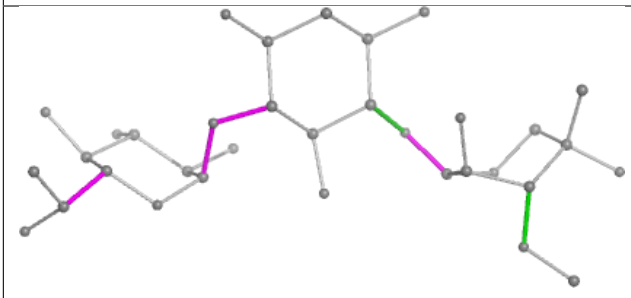
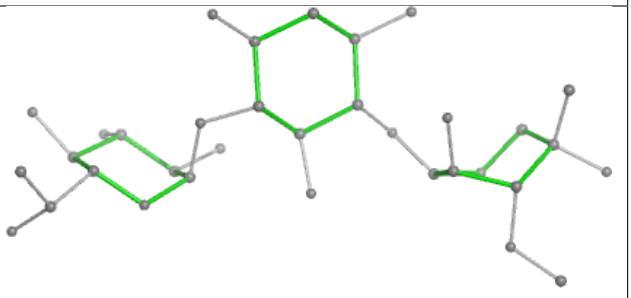


Bond angles

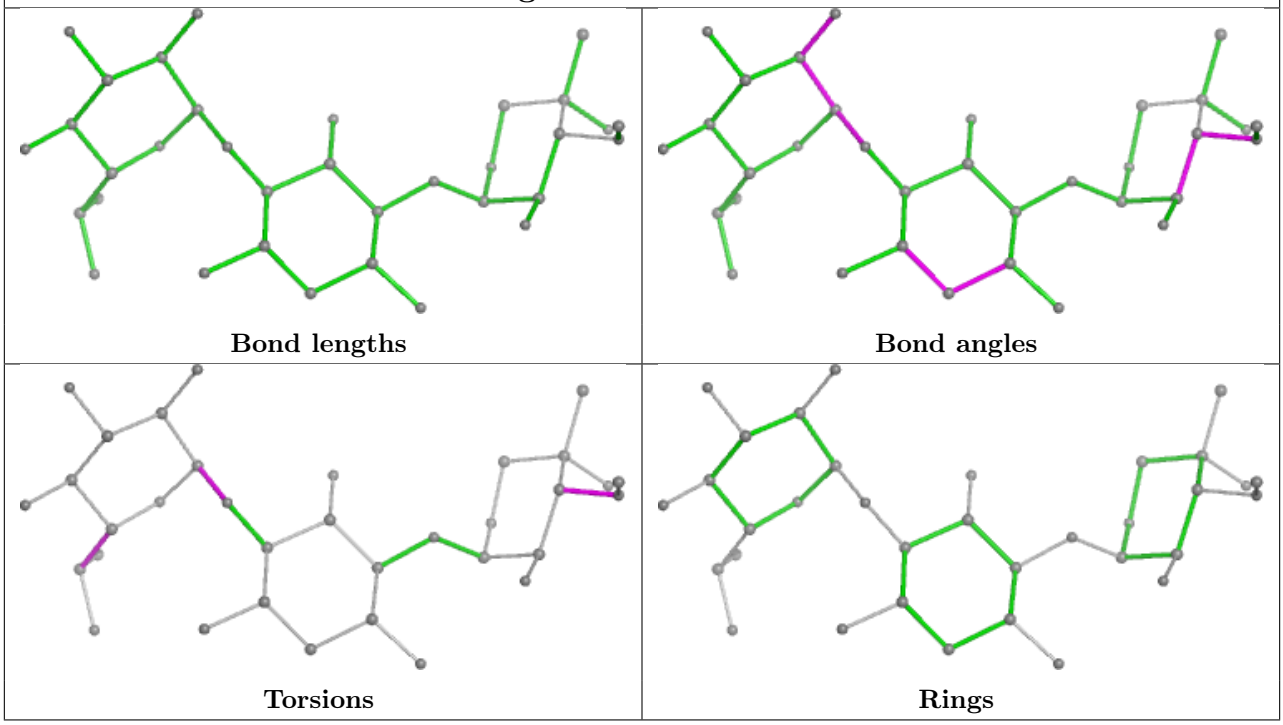


Torsions

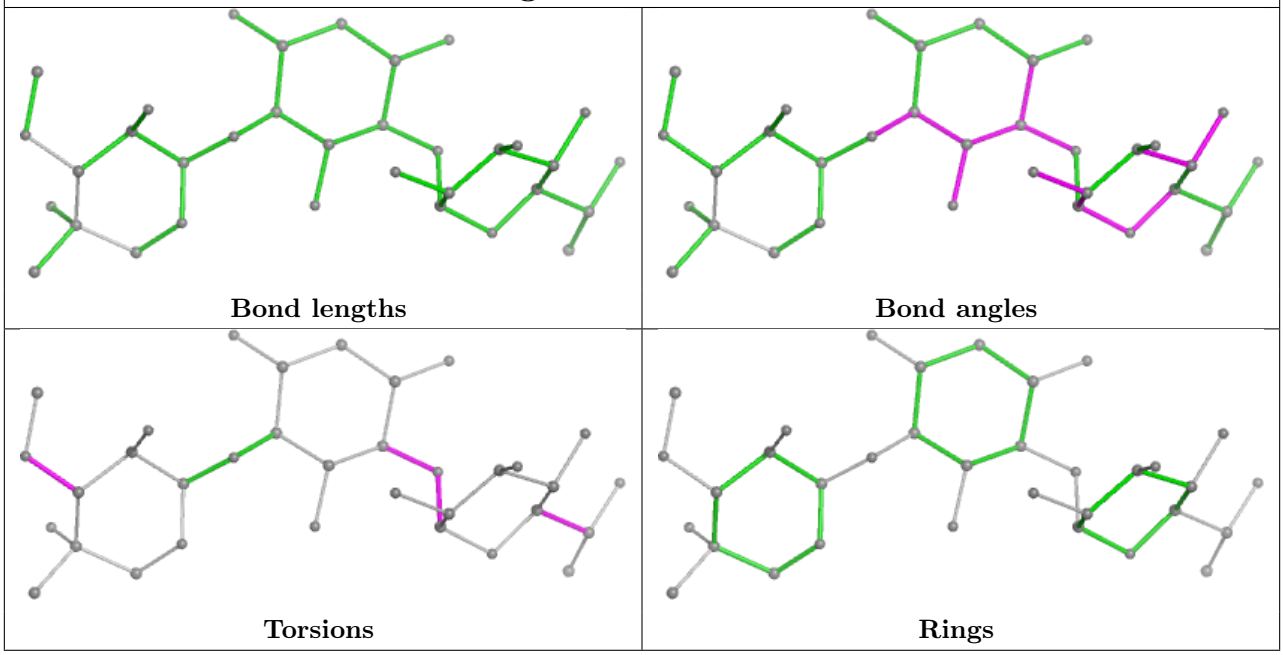


Rings

Ligand GET n6 201



Ligand GET 5 3844



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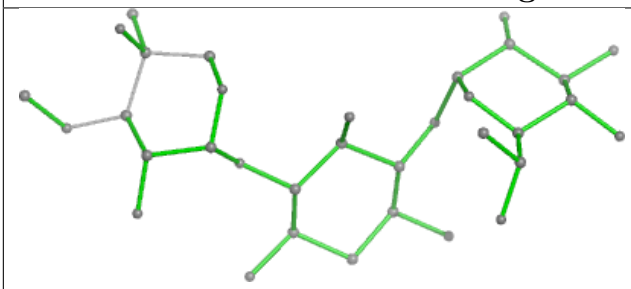
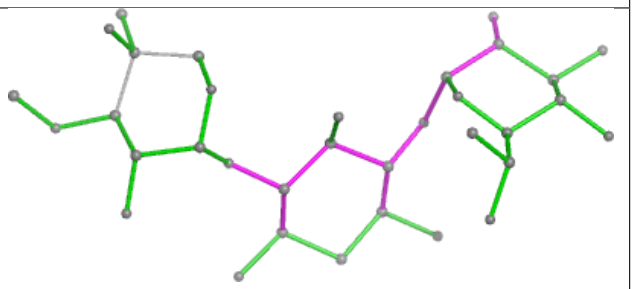
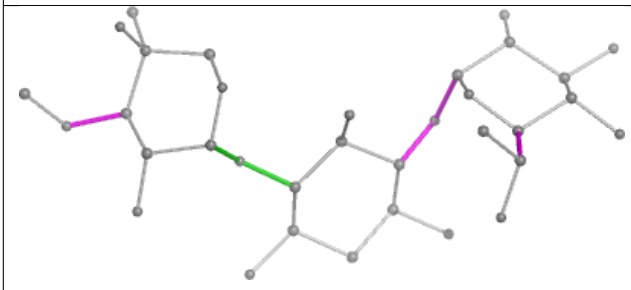


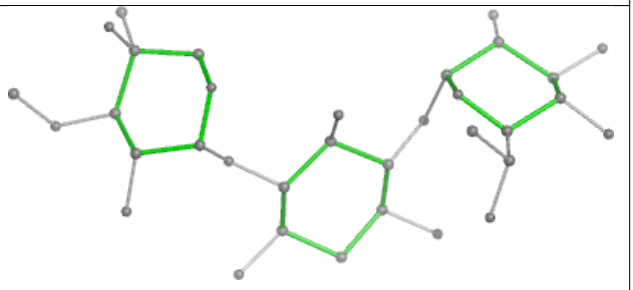
Bond lengths



Bond angles

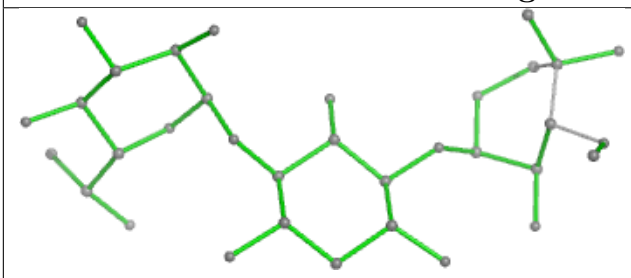


Torsions



Rings

Ligand GET 2 2012



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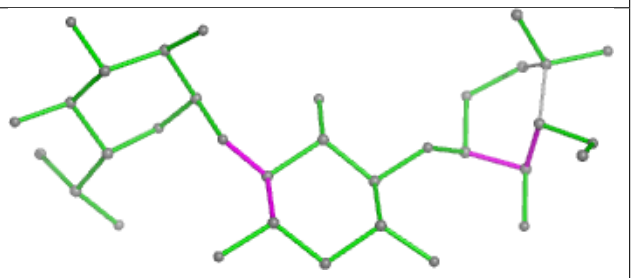
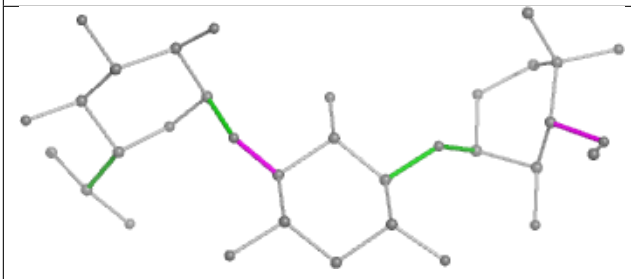
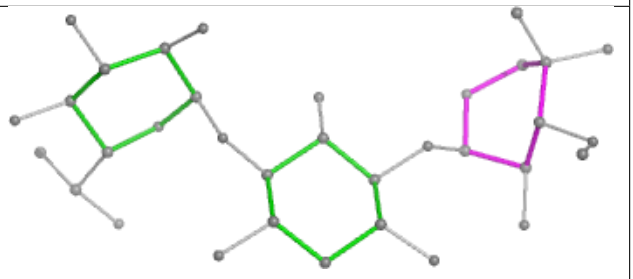


Bond angles

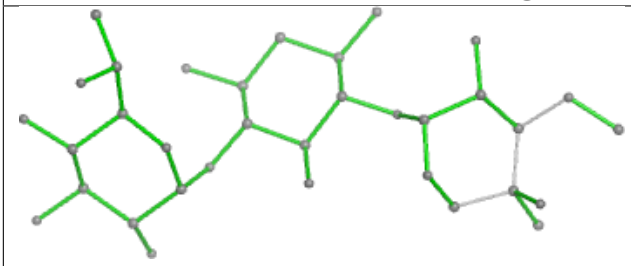


Torsions

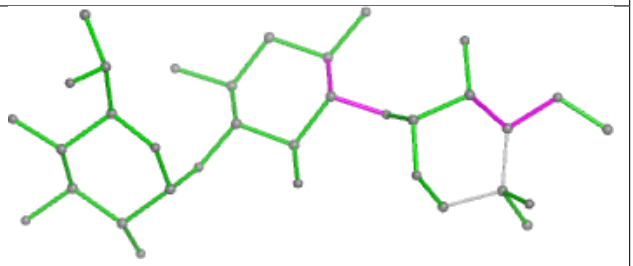


Rings

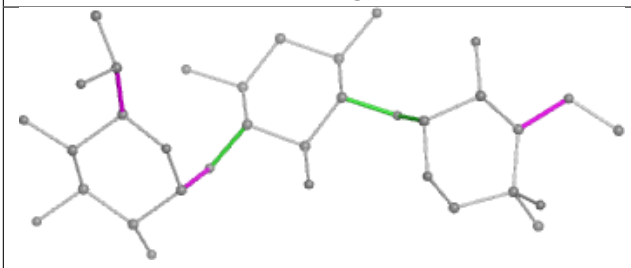
Ligand GET 5 3846



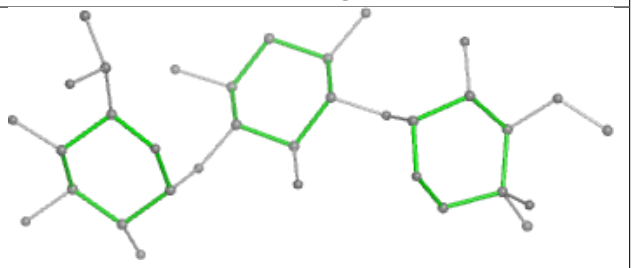
Bond lengths



Bond angles

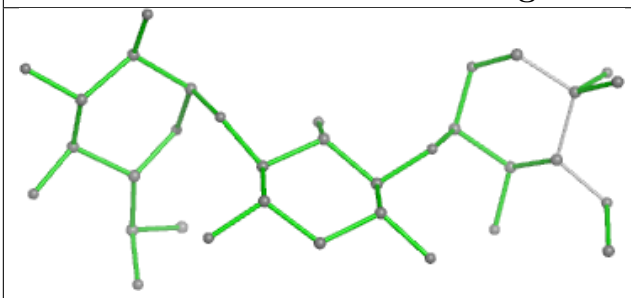


Torsions

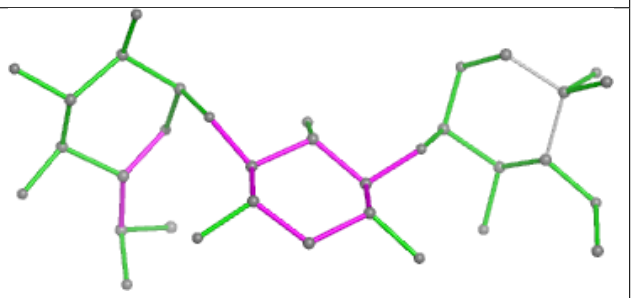


Rings

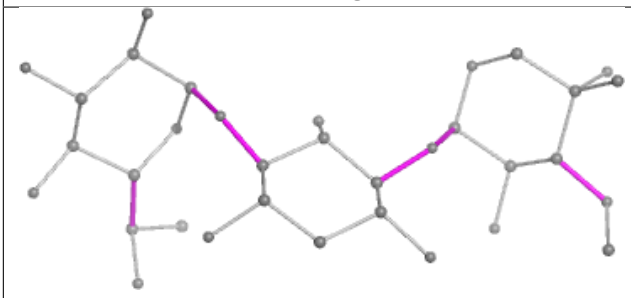
Ligand GET 1 3809



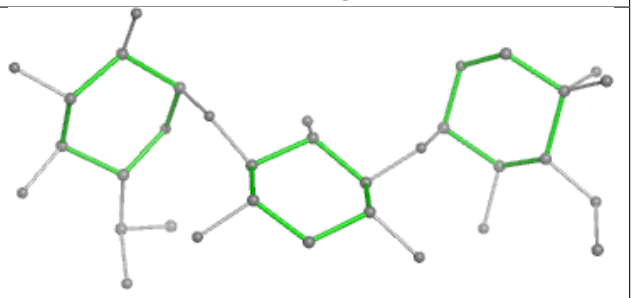
Bond lengths



Bond angles

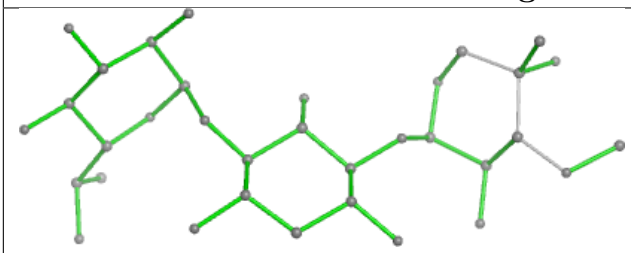


Torsions

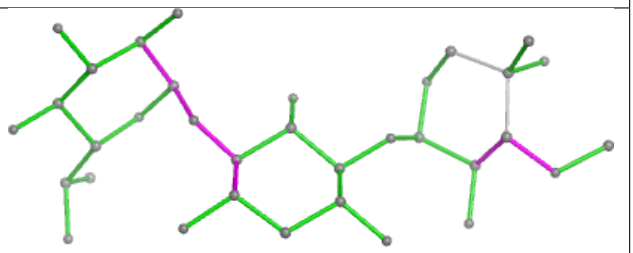


Rings

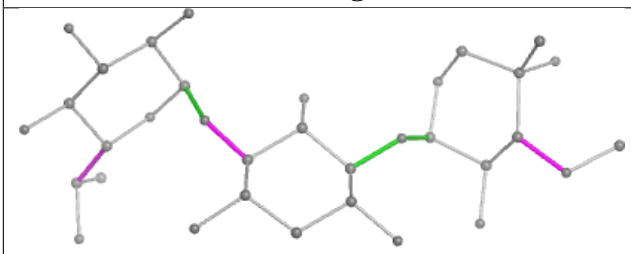
Ligand GET 2 2013



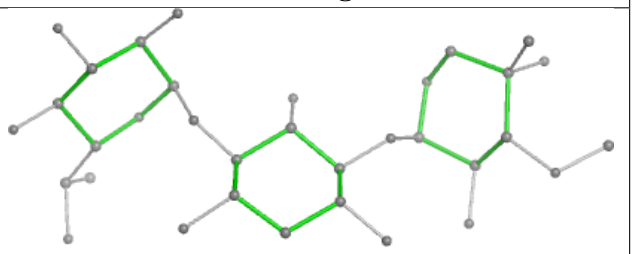
Bond lengths



Bond angles

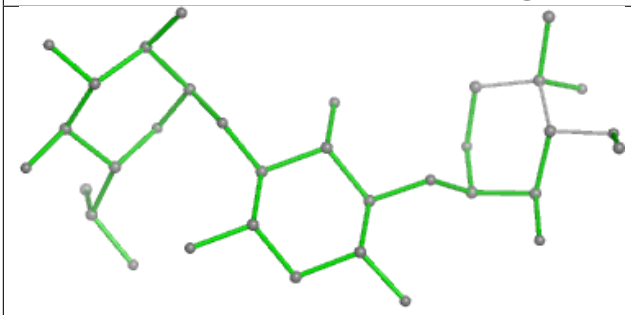


Torsions

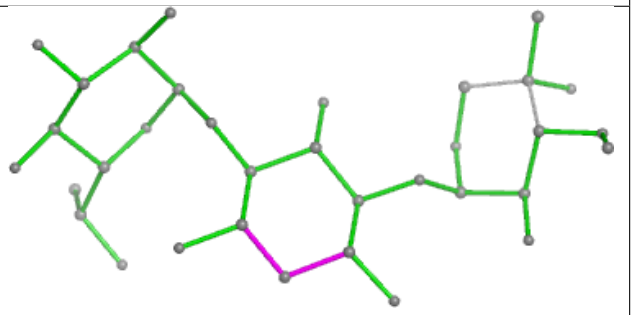


Rings

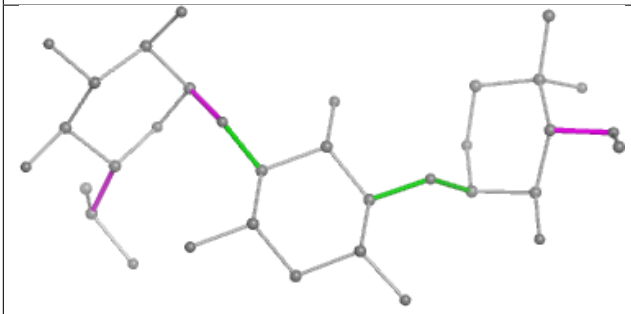
Ligand GET 5 3851



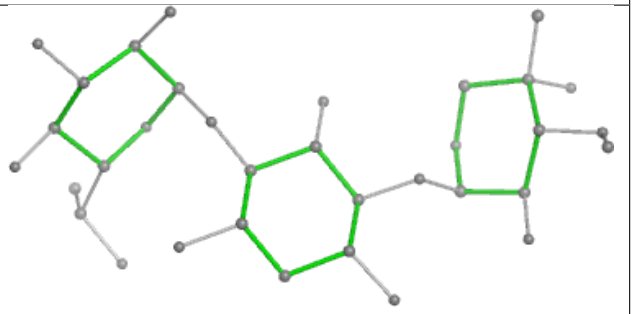
Bond lengths



Bond angles

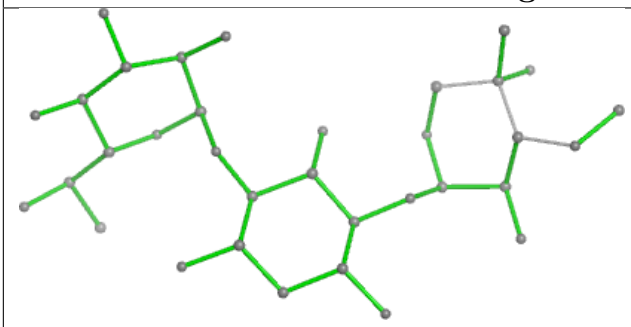


Torsions

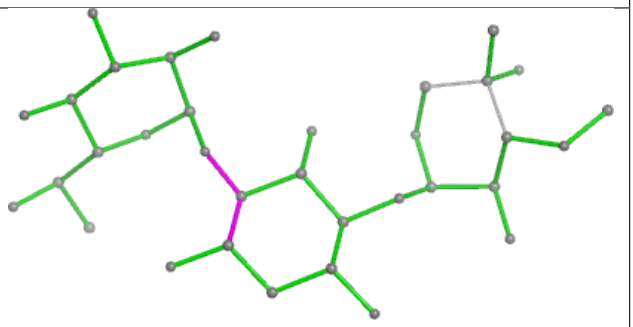


Rings

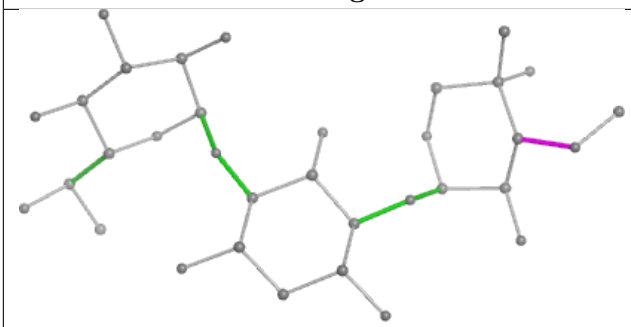
Ligand GET 1 3811



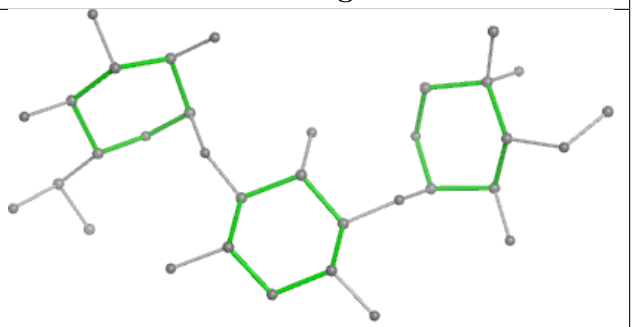
Bond lengths



Bond angles

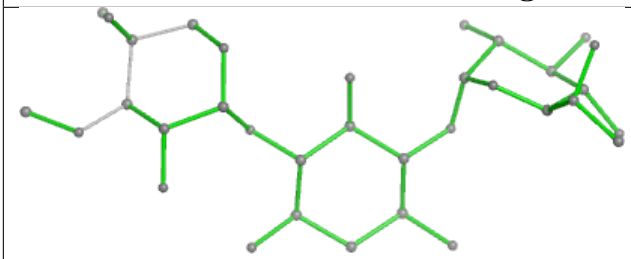


Torsions

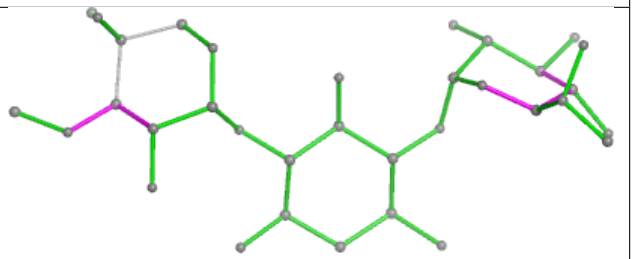


Rings

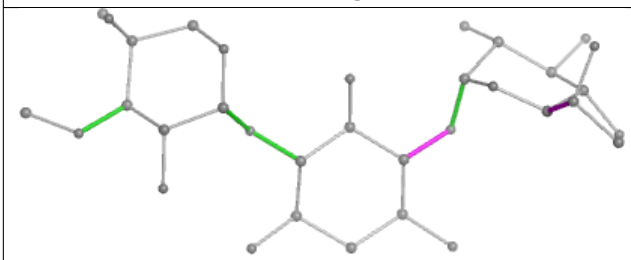
Ligand GET 5 3848



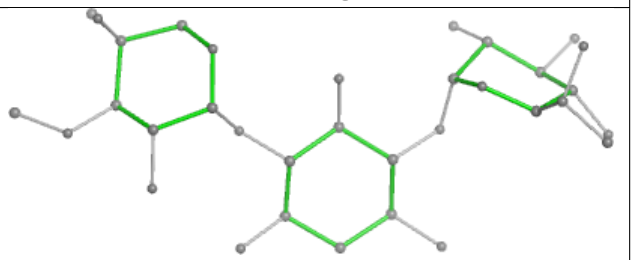
Bond lengths



Bond angles

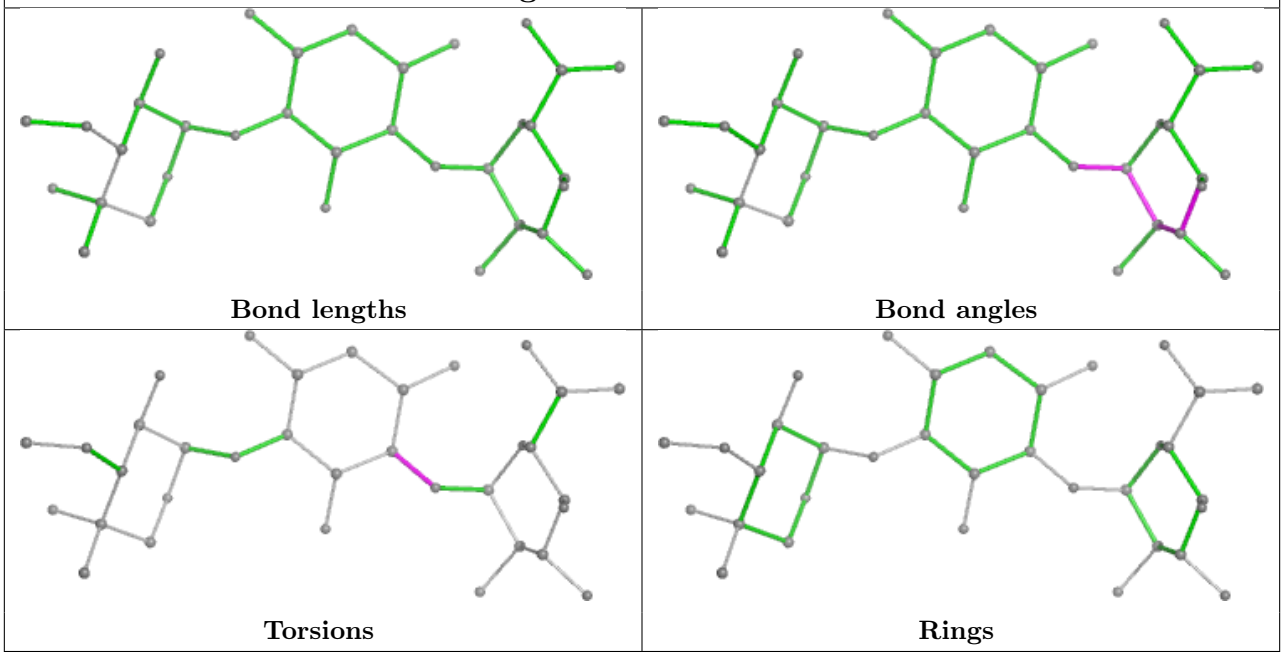


Torsions

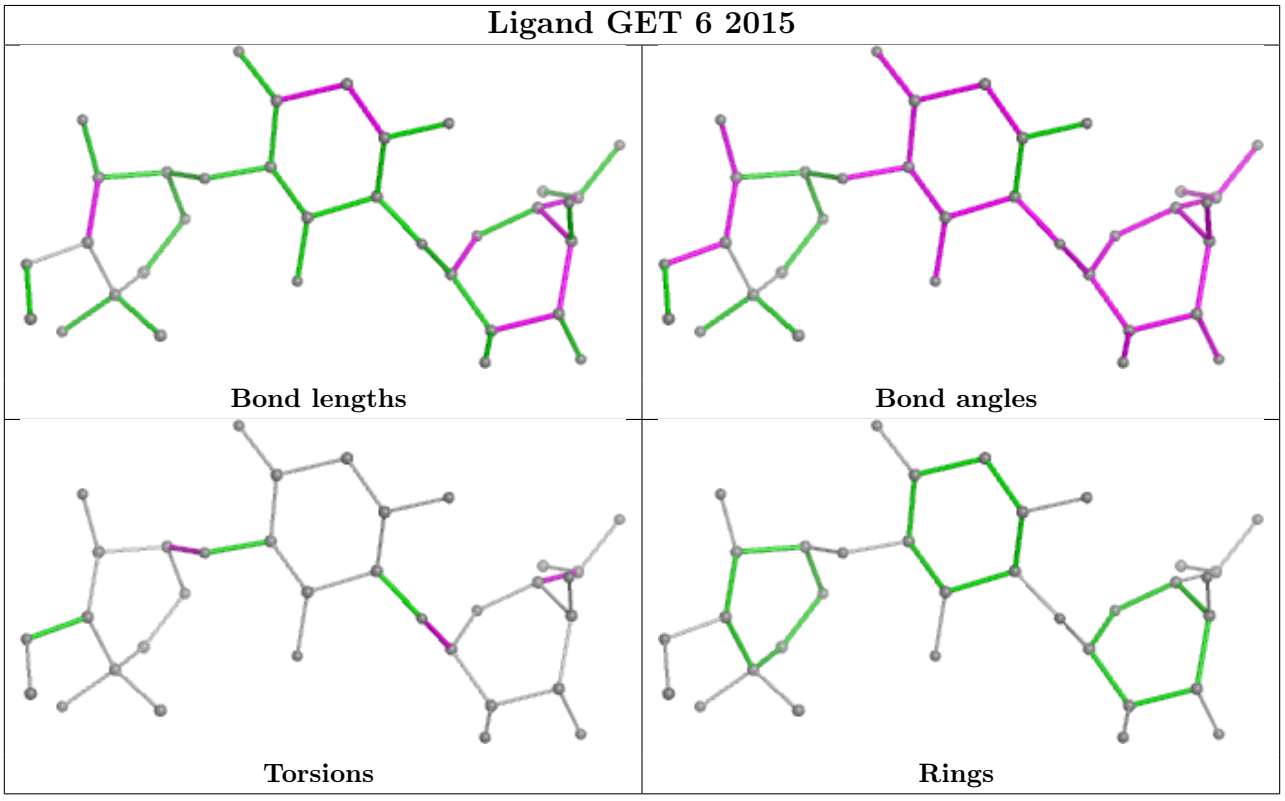


Rings

Ligand GET 5 3845



Ligand GET 6 2015



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1
30	D8	1
18	c6	1
30	d8	1
28	D6	1
39	l2	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	3.84
1	D8	5:THR	C	6:PRO	N	1.82
1	c6	4:VAL	C	5:PRO	N	1.69
1	d8	5:THR	C	6:PRO	N	1.67
1	D6	59:TYR	C	60:PRO	N	1.65

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, 95^{th} 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	1688/1800 (93%)	0.09	34 (2%)	65	53	109, 170, 289, 329	0
1	6	1700/1800 (94%)	0.11	33 (1%)	66	55	101, 171, 254, 295	0
2	S0	206/206 (100%)	0.43	15 (7%)	15	11	173, 208, 229, 240	0
2	s0	206/206 (100%)	0.56	21 (10%)	6	5	171, 192, 212, 220	0
3	S1	214/216 (99%)	0.80	39 (18%)	1	1	194, 239, 265, 270	0
3	s1	216/216 (100%)	0.75	40 (18%)	1	1	171, 207, 229, 241	0
4	S2	217/217 (100%)	0.15	3 (1%)	75	64	147, 178, 199, 213	0
4	s2	217/217 (100%)	0.37	9 (4%)	37	27	144, 169, 192, 211	0
5	S3	223/223 (100%)	0.18	6 (2%)	54	42	133, 156, 222, 235	0
5	s3	223/223 (100%)	0.37	14 (6%)	20	13	168, 198, 240, 247	0
6	S4	260/260 (100%)	1.02	55 (21%)	0	0	175, 227, 242, 258	0
6	s4	260/260 (100%)	0.50	23 (8%)	10	7	126, 174, 193, 231	0
7	S5	206/206 (100%)	0.59	22 (10%)	6	5	153, 185, 199, 206	0
7	s5	206/206 (100%)	1.24	58 (28%)	0	0	199, 217, 245, 248	0
8	S6	226/236 (95%)	0.71	37 (16%)	1	1	166, 211, 269, 303	0
8	s6	218/236 (92%)	0.57	25 (11%)	4	4	128, 177, 205, 214	0
9	S7	184/185 (99%)	1.00	34 (18%)	1	1	209, 268, 310, 313	0
9	s7	185/185 (100%)	0.74	26 (14%)	2	2	166, 204, 230, 235	0
10	S8	188/200 (94%)	1.42	53 (28%)	0	0	160, 200, 261, 281	0
10	s8	188/200 (94%)	0.85	19 (10%)	7	5	124, 153, 209, 238	0
11	S9	185/185 (100%)	1.80	67 (36%)	0	0	162, 210, 238, 253	0
11	s9	185/185 (100%)	1.84	77 (41%)	0	0	151, 188, 220, 261	0
12	C0	92/105 (87%)	1.14	21 (22%)	0	0	141, 170, 190, 194	0
12	c0	92/105 (87%)	2.00	41 (44%)	0	0	197, 228, 244, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	142/156 (91%)	0.94	17 (11%) 4 4	161, 194, 232, 265	0
13	c1	146/156 (93%)	0.30	7 (4%) 30 22	128, 142, 181, 197	0
14	C2	120/143 (83%)	1.64	44 (36%) 0 0	212, 235, 252, 258	0
14	c2	124/143 (86%)	2.76	79 (63%) 0 0	275, 290, 306, 315	0
15	C3	150/150 (100%)	0.29	4 (2%) 54 42	167, 208, 244, 247	0
15	c3	150/150 (100%)	0.20	3 (2%) 65 53	138, 161, 184, 191	0
16	C4	127/128 (99%)	0.20	5 (3%) 39 28	147, 201, 230, 236	0
16	c4	128/128 (100%)	0.25	6 (4%) 31 23	136, 198, 216, 223	0
17	C5	122/141 (86%)	0.39	7 (5%) 23 16	134, 163, 182, 196	0
17	c5	119/141 (84%)	0.81	20 (16%) 1 1	179, 214, 233, 237	0
18	C6	141/141 (100%)	0.94	22 (15%) 2 1	133, 170, 188, 197	0
18	c6	141/141 (100%)	2.59	79 (56%) 0 0	177, 226, 241, 246	0
19	C7	117/136 (86%)	0.71	16 (13%) 3 3	162, 195, 242, 247	0
19	c7	117/136 (86%)	0.33	8 (6%) 17 12	190, 206, 225, 229	0
20	C8	145/145 (100%)	0.28	9 (6%) 20 14	133, 172, 206, 215	0
20	c8	145/145 (100%)	0.74	28 (19%) 1 1	175, 221, 248, 254	0
21	C9	143/143 (100%)	0.80	16 (11%) 5 4	138, 163, 181, 198	0
21	c9	143/143 (100%)	2.11	62 (43%) 0 0	197, 234, 253, 259	0
22	D0	105/107 (98%)	0.84	20 (19%) 1 1	125, 164, 196, 202	0
22	d0	101/107 (94%)	1.29	27 (26%) 0 0	171, 227, 255, 261	0
23	D1	87/87 (100%)	0.33	4 (4%) 32 24	182, 200, 226, 237	0
23	d1	87/87 (100%)	0.33	3 (3%) 45 34	170, 179, 208, 215	0
24	D2	129/129 (100%)	0.48	11 (8%) 10 8	176, 195, 212, 224	0
24	d2	129/129 (100%)	0.40	7 (5%) 25 19	142, 159, 172, 186	0
25	D3	144/144 (100%)	0.12	3 (2%) 63 52	130, 139, 163, 169	0
25	d3	144/144 (100%)	0.13	0 100 100	122, 131, 147, 164	0
26	D4	134/134 (100%)	1.01	30 (22%) 0 0	186, 230, 242, 250	0
26	d4	134/134 (100%)	0.42	15 (11%) 5 4	146, 190, 211, 227	0
27	D5	70/70 (100%)	1.24	14 (20%) 1 0	175, 202, 214, 217	0
27	d5	69/70 (98%)	1.58	25 (36%) 0 0	223, 244, 254, 258	0
28	D6	97/97 (100%)	0.26	5 (5%) 27 20	145, 167, 227, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.41	8 (8%) 11 9	140, 154, 218, 222	0
29	D7	81/81 (100%)	0.34	6 (7%) 14 10	196, 233, 277, 288	0
29	d7	81/81 (100%)	0.44	2 (2%) 57 45	161, 181, 221, 225	0
30	D8	63/63 (100%)	0.52	8 (12%) 3 4	169, 197, 216, 226	0
30	d8	63/63 (100%)	-0.16	1 (1%) 72 61	187, 211, 225, 229	0
31	D9	53/53 (100%)	0.72	9 (16%) 1 1	125, 132, 160, 170	0
31	d9	53/53 (100%)	1.45	15 (28%) 0 0	180, 191, 224, 249	0
32	E0	60/60 (100%)	0.80	11 (18%) 1 1	137, 178, 205, 210	0
32	e0	60/60 (100%)	0.82	10 (16%) 1 1	141, 182, 208, 215	0
33	E1	71/152 (46%)	2.02	32 (45%) 0 0	157, 207, 238, 244	0
33	e1	45/152 (29%)	2.04	24 (53%) 0 0	198, 263, 280, 283	0
34	SR	318/318 (100%)	0.99	59 (18%) 1 1	189, 218, 242, 262	0
34	sR	313/318 (98%)	0.65	42 (13%) 3 3	221, 240, 258, 318	0
35	SM	135/272 (49%)	0.07	5 (3%) 41 30	133, 155, 230, 255	0
35	sM	115/272 (42%)	0.67	25 (21%) 0 0	154, 179, 231, 293	0
36	1	3078/3396 (90%)	0.05	27 (0%) 84 76	82, 131, 236, 350	0
36	5	3127/3396 (92%)	0.09	47 (1%) 73 63	83, 121, 213, 304	0
37	3	121/121 (100%)	-0.21	0 100 100	92, 159, 191, 204	0
37	7	121/121 (100%)	-0.16	0 100 100	95, 170, 205, 211	0
38	4	158/158 (100%)	0.17	5 (3%) 47 35	100, 159, 221, 285	0
38	8	157/158 (99%)	0.23	1 (0%) 89 83	96, 132, 183, 217	0
39	L2	252/252 (100%)	0.31	13 (5%) 27 20	104, 154, 189, 209	0
39	l2	252/252 (100%)	0.20	10 (3%) 38 28	97, 127, 152, 170	0
40	L3	386/386 (100%)	0.09	10 (2%) 56 43	84, 121, 147, 180	0
40	l3	386/386 (100%)	-0.01	1 (0%) 94 90	83, 111, 131, 164	0
41	L4	361/361 (100%)	0.01	2 (0%) 89 83	94, 144, 170, 183	0
41	l4	361/361 (100%)	0.19	9 (2%) 57 45	91, 125, 147, 160	0
42	L5	294/296 (99%)	0.97	71 (24%) 0 0	127, 188, 205, 210	0
42	l5	294/296 (99%)	0.83	50 (17%) 1 1	141, 197, 221, 235	0
43	L6	156/176 (88%)	0.12	3 (1%) 66 55	109, 127, 147, 163	0
43	l6	157/176 (89%)	0.20	4 (2%) 57 45	105, 118, 143, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	L7	222/223 (99%)	0.05	2 (0%) 84 76	95, 123, 164, 193	0
44	l7	223/223 (100%)	-0.06	1 (0%) 92 88	96, 114, 149, 189	0
45	L8	233/233 (100%)	1.02	48 (20%) 1 0	188, 228, 265, 283	0
45	l8	231/233 (99%)	0.63	26 (11%) 5 4	152, 178, 213, 223	0
46	L9	191/191 (100%)	0.20	4 (2%) 63 52	113, 131, 146, 172	0
46	l9	190/191 (99%)	0.04	0 100 100	110, 125, 145, 154	0
47	M0	208/221 (94%)	-0.12	2 (0%) 82 73	97, 115, 162, 181	0
47	m0	209/221 (94%)	0.24	8 (3%) 40 30	102, 125, 180, 194	0
48	M1	169/169 (100%)	0.60	16 (9%) 8 6	151, 165, 173, 175	0
48	m1	169/169 (100%)	0.78	23 (13%) 3 3	171, 191, 201, 204	0
49	M3	193/194 (99%)	0.16	6 (3%) 49 36	109, 185, 219, 232	0
49	m3	194/194 (100%)	0.16	5 (2%) 56 43	102, 156, 197, 209	0
50	M4	136/137 (99%)	-0.21	0 100 100	118, 129, 144, 153	0
50	m4	137/137 (100%)	-0.13	0 100 100	113, 121, 146, 176	0
51	M5	203/203 (100%)	0.92	27 (13%) 3 3	117, 163, 193, 205	0
51	m5	203/203 (100%)	0.59	17 (8%) 11 8	106, 133, 154, 163	0
52	M6	197/197 (100%)	-0.09	0 100 100	83, 97, 140, 150	0
52	m6	197/197 (100%)	-0.13	1 (0%) 91 85	85, 97, 139, 147	0
53	M7	183/184 (99%)	0.14	2 (1%) 80 71	92, 108, 159, 196	0
53	m7	175/184 (95%)	0.15	3 (1%) 70 59	91, 104, 140, 157	0
54	M8	185/185 (100%)	0.22	7 (3%) 40 30	103, 149, 173, 180	0
54	m8	185/185 (100%)	0.20	1 (0%) 91 85	102, 131, 147, 155	0
55	M9	188/188 (100%)	0.43	20 (10%) 6 5	137, 167, 298, 318	0
55	m9	183/188 (97%)	0.47	18 (9%) 7 6	114, 135, 212, 223	0
56	N0	170/172 (98%)	0.07	0 100 100	104, 121, 143, 156	0
56	n0	172/172 (100%)	-0.07	0 100 100	100, 116, 137, 154	0
57	N1	159/159 (100%)	0.75	25 (15%) 2 1	100, 136, 196, 205	0
57	n1	159/159 (100%)	0.35	8 (5%) 28 21	110, 134, 182, 186	0
58	N2	98/98 (100%)	1.41	23 (23%) 0 0	186, 205, 216, 219	0
58	n2	98/98 (100%)	0.34	9 (9%) 9 6	159, 174, 187, 190	0
59	N3	135/135 (100%)	0.69	16 (11%) 4 4	95, 117, 129, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
59	n3	134/135 (99%)	0.35	3 (2%) 62 50	89, 104, 116, 128	0
60	N4	122/155 (78%)	0.82	17 (13%) 2 3	123, 163, 280, 283	0
60	n4	118/155 (76%)	0.66	18 (15%) 2 1	103, 136, 235, 242	0
61	N5	121/121 (100%)	0.53	13 (10%) 6 5	143, 176, 210, 245	0
61	n5	120/121 (99%)	0.26	3 (2%) 57 45	119, 143, 165, 189	0
62	N6	126/126 (100%)	1.33	30 (23%) 0 0	130, 150, 177, 192	0
62	n6	124/126 (98%)	0.98	15 (12%) 4 4	113, 138, 166, 177	0
63	N7	135/135 (100%)	1.53	47 (34%) 0 0	209, 238, 257, 269	0
63	n7	135/135 (100%)	1.14	24 (17%) 1 1	155, 177, 193, 203	0
64	N8	148/148 (100%)	0.59	17 (11%) 4 4	92, 165, 197, 210	0
64	n8	148/148 (100%)	0.24	1 (0%) 87 81	92, 144, 169, 173	0
65	N9	58/58 (100%)	0.75	10 (17%) 1 1	93, 154, 197, 203	0
65	n9	58/58 (100%)	0.68	8 (13%) 2 3	96, 150, 197, 206	0
66	O0	97/100 (97%)	0.92	18 (18%) 1 1	197, 217, 237, 241	0
66	o0	100/100 (100%)	0.20	5 (5%) 28 21	151, 166, 186, 197	0
67	O1	109/109 (100%)	0.77	16 (14%) 2 2	116, 141, 173, 183	0
67	o1	109/109 (100%)	0.78	9 (8%) 11 9	105, 132, 166, 186	0
68	O2	127/127 (100%)	0.49	6 (4%) 31 23	89, 118, 134, 153	0
68	o2	127/127 (100%)	0.15	0 100 100	88, 111, 124, 154	0
69	O3	106/106 (100%)	0.17	2 (1%) 66 55	88, 103, 119, 122	0
69	o3	106/106 (100%)	0.33	2 (1%) 66 55	89, 101, 116, 123	0
70	O4	112/112 (100%)	0.86	12 (10%) 6 5	138, 186, 249, 258	0
70	o4	112/112 (100%)	0.25	7 (6%) 20 13	113, 144, 201, 211	0
71	O5	119/119 (100%)	0.25	5 (4%) 36 27	162, 182, 210, 218	0
71	o5	119/119 (100%)	0.34	4 (3%) 45 34	129, 152, 174, 182	0
72	O6	99/99 (100%)	0.76	14 (14%) 2 2	170, 194, 221, 241	0
72	o6	99/99 (100%)	0.70	7 (7%) 16 11	150, 162, 186, 207	0
73	O7	84/84 (100%)	-0.04	0 100 100	103, 129, 178, 189	0
73	o7	82/84 (97%)	0.21	0 100 100	94, 111, 140, 153	0
74	O8	77/77 (100%)	1.02	15 (19%) 1 1	194, 216, 228, 229	0
74	o8	77/77 (100%)	1.14	16 (20%) 1 0	154, 174, 185, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	O9	49/50 (98%)	0.30	0 100 100	122, 135, 142, 146	0
75	o9	50/50 (100%)	0.09	0 100 100	106, 117, 127, 129	0
76	Q0	52/52 (100%)	0.60	2 (3%) 40 30	100, 107, 147, 156	0
76	q0	52/52 (100%)	0.42	2 (3%) 40 30	101, 111, 138, 145	0
77	Q1	25/25 (100%)	1.16	3 (12%) 4 4	113, 125, 130, 132	0
77	q1	25/25 (100%)	0.62	1 (4%) 38 28	113, 121, 125, 126	0
78	Q2	105/105 (100%)	0.99	24 (22%) 0 0	113, 143, 167, 178	0
78	q2	105/105 (100%)	0.51	13 (12%) 4 4	109, 144, 170, 189	0
79	Q3	91/91 (100%)	-0.14	2 (2%) 62 50	118, 158, 189, 203	0
79	q3	91/91 (100%)	-0.04	0 100 100	102, 129, 153, 167	0
80	p0	138/312 (44%)	2.34	74 (53%) 0 0	202, 229, 270, 271	0
All	All	32690/34558 (94%)	0.42	2661 (8%) 12 9	82, 159, 244, 350	0

The worst 5 of 2661 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	c6	20	ALA	12.2
45	L8	199	ALA	11.8
31	d9	4	GLU	10.9
60	n4	132	GLY	9.5
6	s4	261	LEU	9.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.