wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2024 – 12:56 am BST

PDB ID	:	5NDW
Title	:	Crystal structure of aminoglycoside TC007 bound to the yeast 80S ribosome
Authors	:	Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2017-03-09
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:

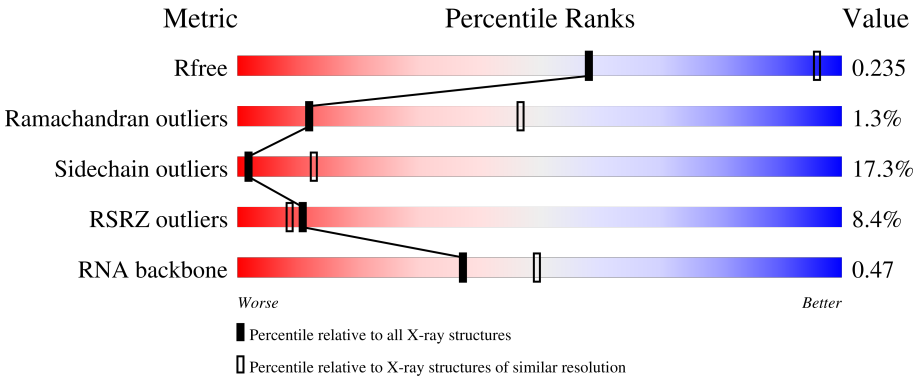
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	1	3396	57% 28% 6% 9%
1	5	3396	59% 27% . 9%
2	2	1800	3% 64% 29% 6% .
2	6	1800	% 66% 25% 5% .
3	3	121	67% 31% .

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Mol	Chain	Length	Quality of chain
3	7	121	79% 20%
4	4	158	% 64% 31% 5%
4	8	158	2% 64% 32%
5	C0	105	32% 76% 14% 9%
5	c0	105	19% 68% 20% 11%
6	C1	156	30% 87% 11%
6	c1	156	13% 74% 19% 6%
7	C2	143	39% 62% 20% 17%
7	c2	143	38% 65% 21% 13%
8	C3	150	5% 83% 17%
8	c3	150	9% 84% 15%
9	C4	128	5% 79% 19%
9	c4	128	21% 84% 16%
10	C5	141	10% 70% 17% 12%
10	c5	141	13% 74% 13% 11%
11	C6	141	33% 78% 21%
11	c6	141	30% 80% 18%
12	C7	136	15% 71% 14% 12%
12	c7	136	5% 76% 12% 11%
13	C8	145	11% 77% 20%
13	c8	145	10% 81% 17%
14	C9	143	10% 87% 12%
14	c9	143	8% 85% 14%
15	D0	107	37% 77% 20%
15	d0	107	9% 74% 21%

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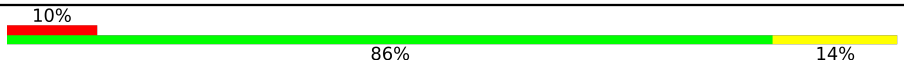
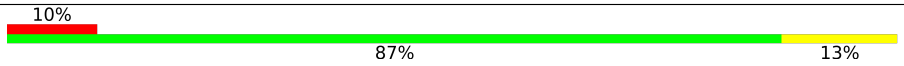
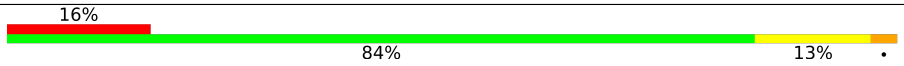
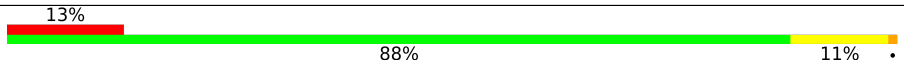
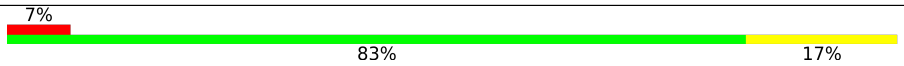
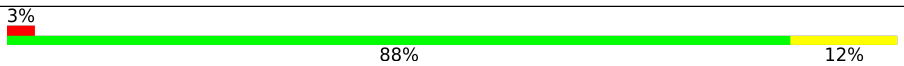
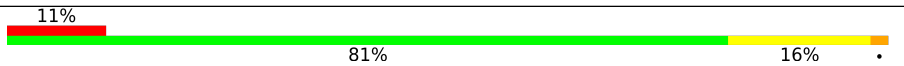
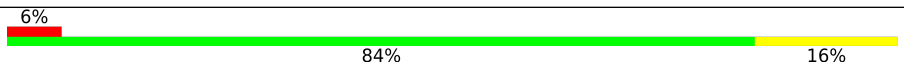
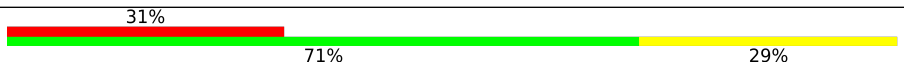
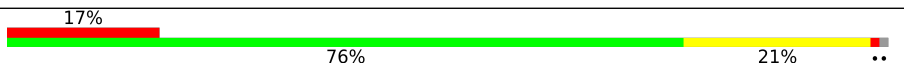
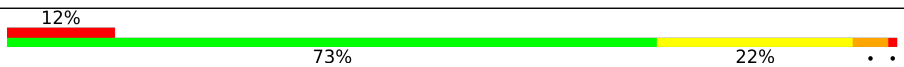
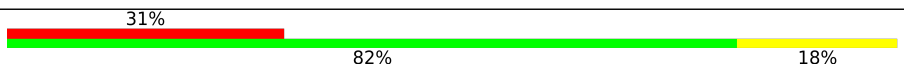
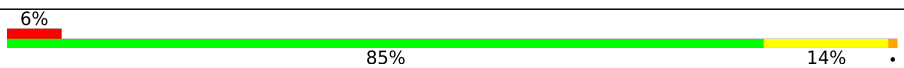
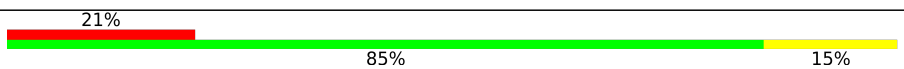
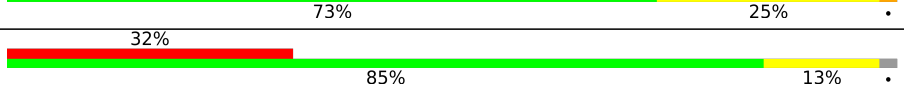
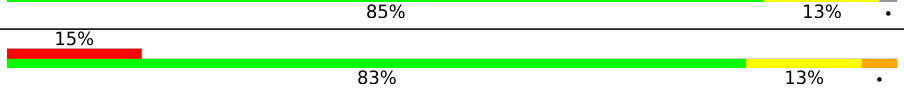
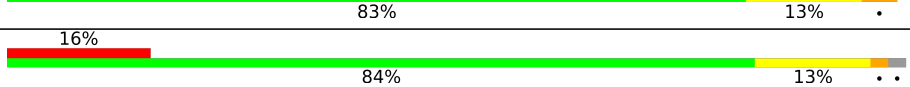
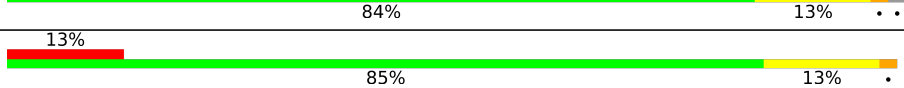
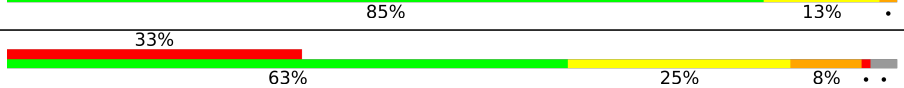
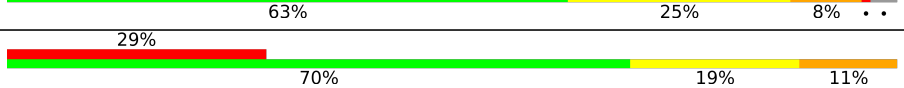
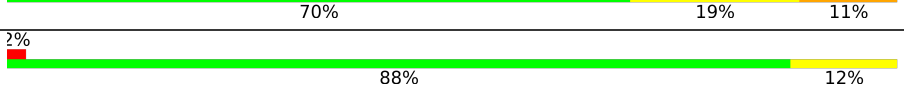
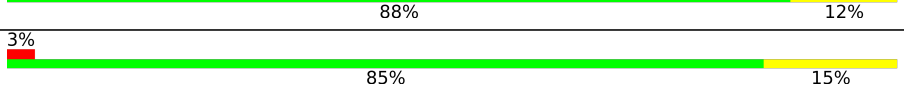
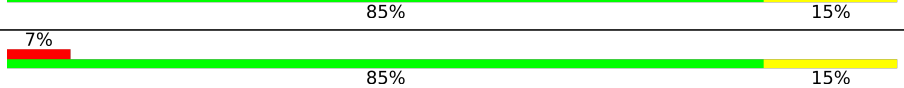
Mol	Chain	Length	Quality of chain
16	D1	87	
16	d1	87	
17	D2	129	
17	d2	129	
18	D3	144	
18	d3	144	
19	D4	134	
19	d4	134	
20	D5	70	
20	d5	70	
21	D6	97	
21	d6	97	
22	D7	81	
22	d7	81	
23	D8	63	
23	d8	63	
24	D9	53	
24	d9	53	
25	E0	61	
25	e0	61	
26	E1	73	
26	e1	73	
27	L2	252	
27	l2	252	
28	L3	386	

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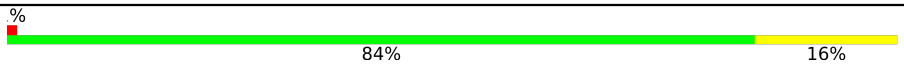
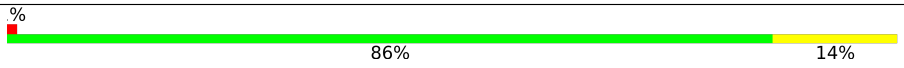
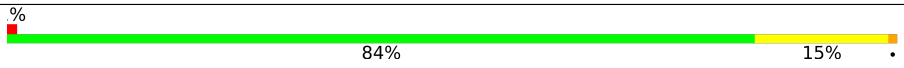
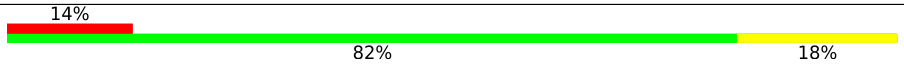
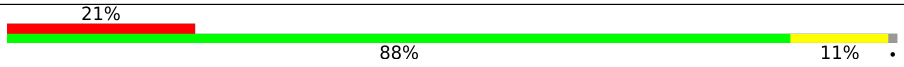
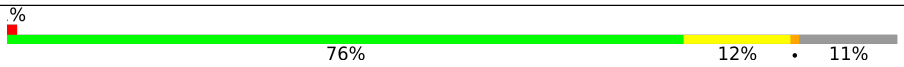
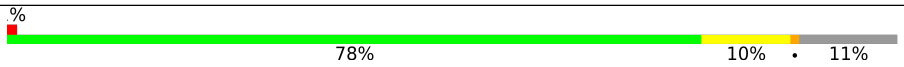
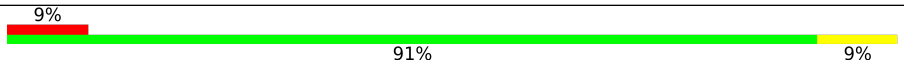
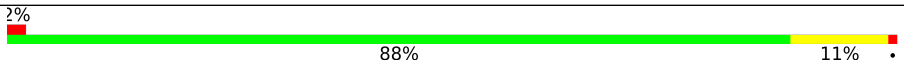
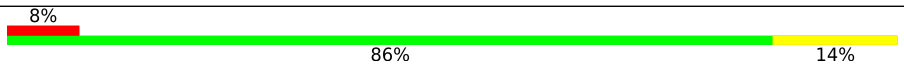
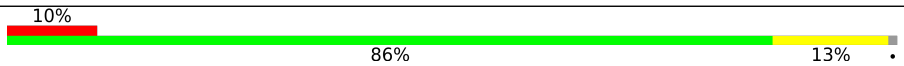
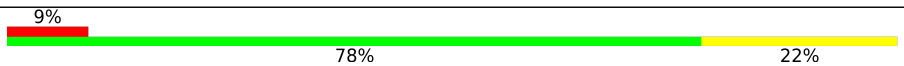
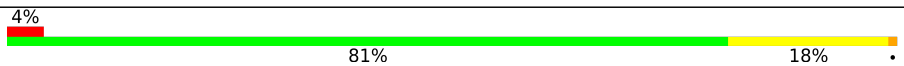
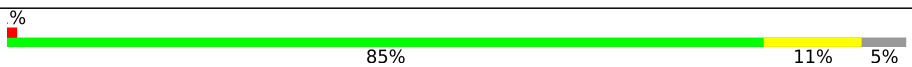
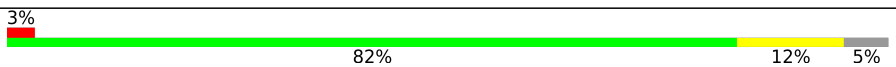
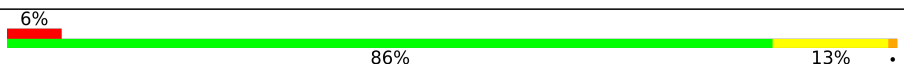
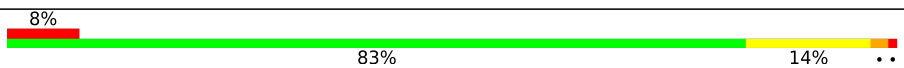
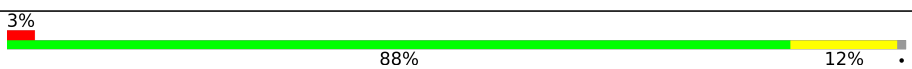
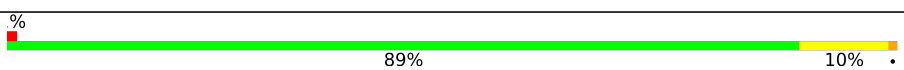
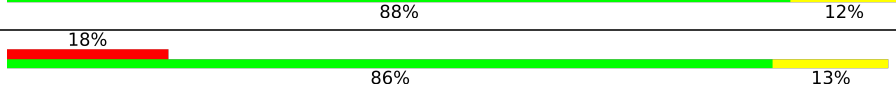
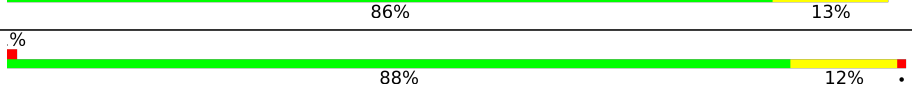
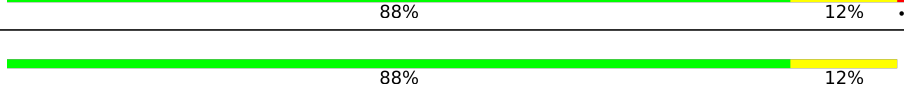
Mol	Chain	Length	Quality of chain
28	l3	386	
29	L4	361	
29	l4	361	
30	L5	296	
30	l5	296	
31	L6	176	
31	l6	176	
32	L7	223	
32	l7	223	
33	L8	233	
33	l8	233	
34	L9	191	
34	l9	191	
35	M0	221	
35	m0	221	
36	M1	169	
36	m1	169	
37	M3	194	
37	m3	194	
38	M4	137	
38	m4	137	
39	M5	203	
39	m5	203	
40	M6	197	
40	m6	197	

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Mol	Chain	Length	Quality of chain
41	M7	184	2% 83% 16%
41	m7	184	2% 85% 14%
42	M8	185	13% 88% 12%
42	m8	185	15% 90% 10%
43	M9	188	5% 88% 12%
43	m9	188	6% 83% 15%
44	N0	172	11% 81% 17%
44	n0	172	4% 85% 15%
45	N1	159	20% 77% 23%
45	n1	159	30% 85% 15%
46	N2	100	12% 82% 18%
46	n2	100	13% 81% 16%
47	N3	136	4% 90% 10%
47	n3	136	2% 93% 7%
48	N4	155	16% 77% 7% 16%
48	n4	155	12% 77% 5% 16%
49	N5	121	7% 84% 15%
49	n5	121	29% 74% 26%
50	N6	126	3% 84% 13%
50	n6	126	8% 80% 17%
51	N7	135	19% 84% 13%
51	n7	135	11% 82% 16%
52	N8	148	7% 89% 11%
52	n8	148	12% 87% 13%
53	N9	58	24% 81% 19%

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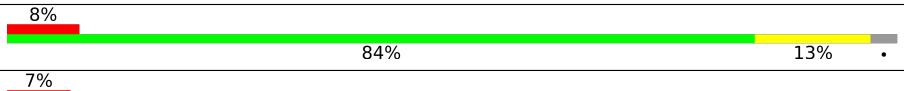
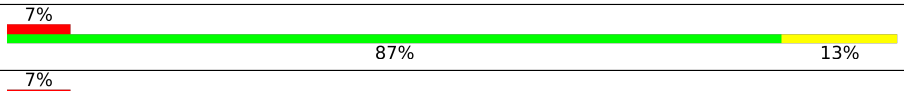
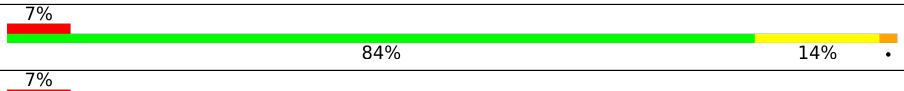
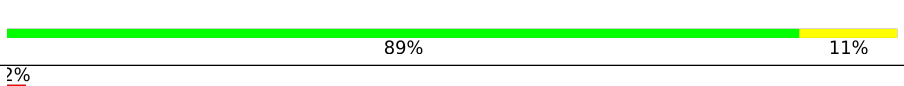
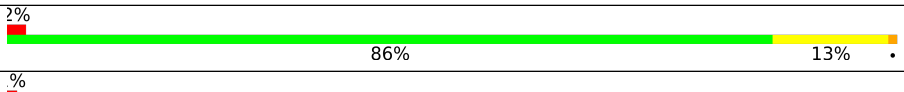
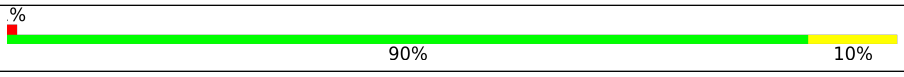
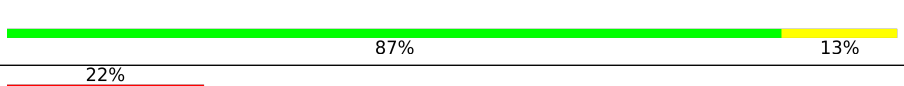
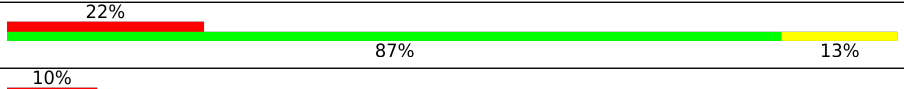
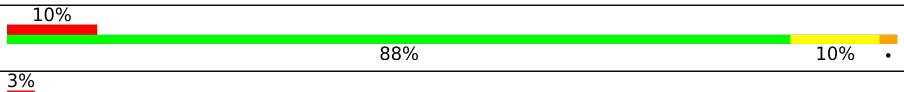
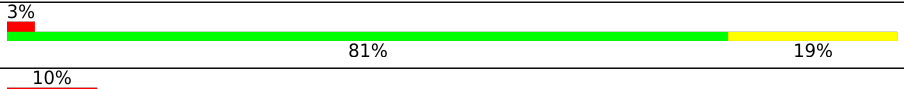
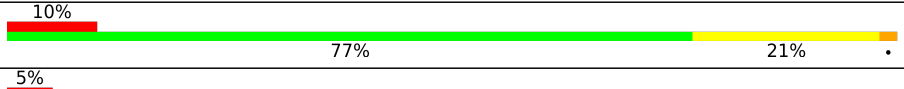
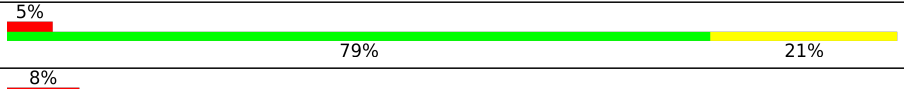
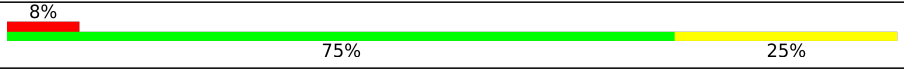
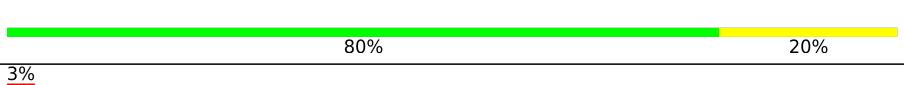
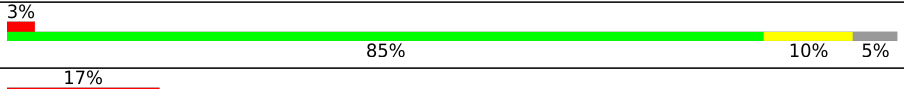
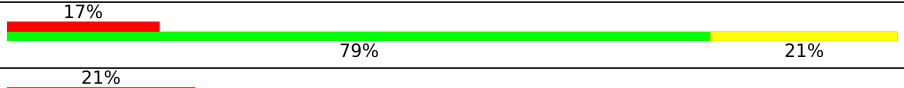
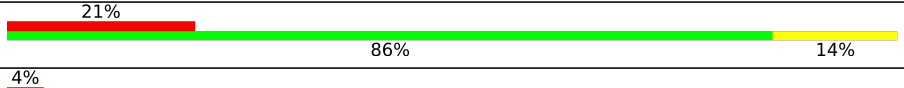
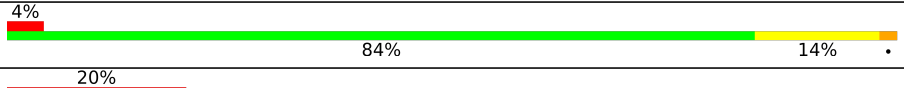
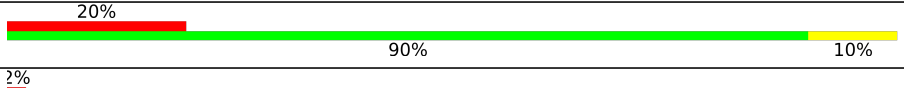
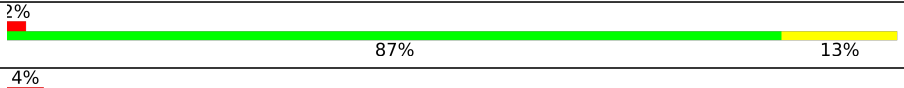
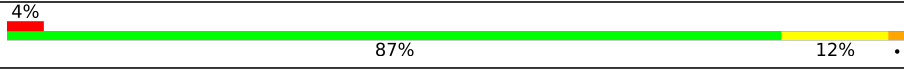
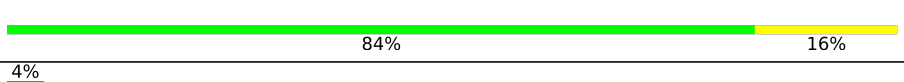
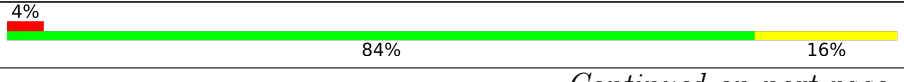
Mol	Chain	Length	Quality of chain
53	n9	58	
54	O0	100	
54	o0	100	
55	O1	109	
55	o1	109	
56	O2	127	
56	o2	127	
57	O3	106	
57	o3	106	
58	O4	112	
58	o4	112	
59	O5	119	
59	o5	119	
60	O6	99	
60	o6	99	
61	O7	87	
61	o7	87	
62	O8	77	
62	o8	77	
63	O9	50	
63	o9	50	
64	Q0	52	
64	q0	52	
65	Q1	25	
65	q1	25	

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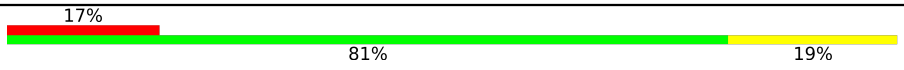
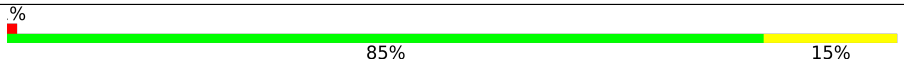
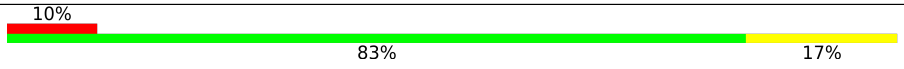
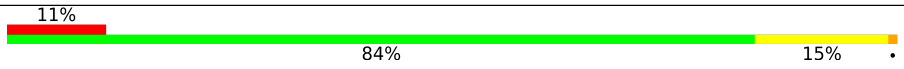
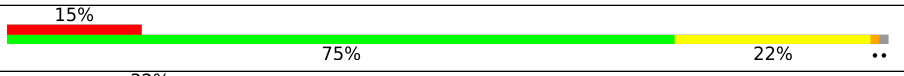
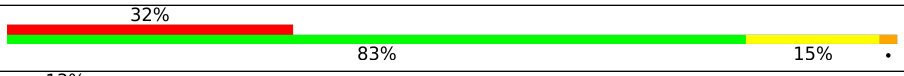
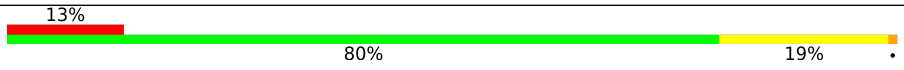
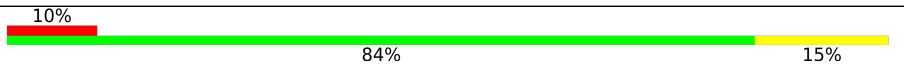
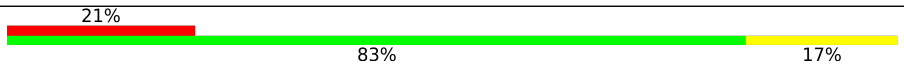
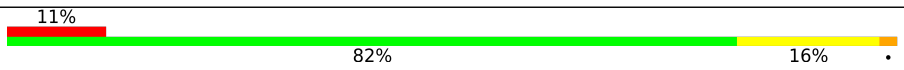
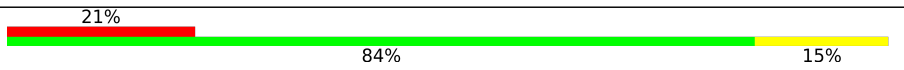
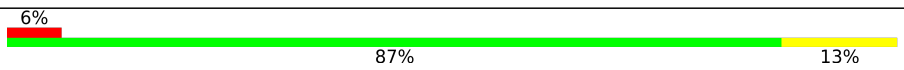
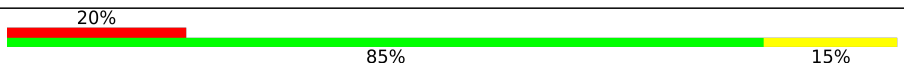
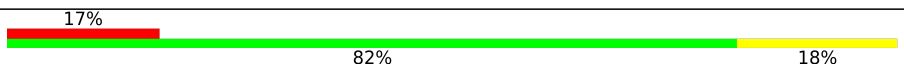
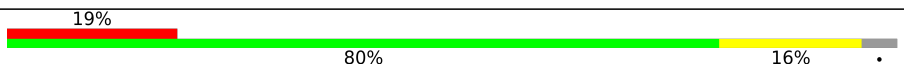
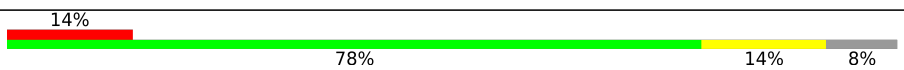
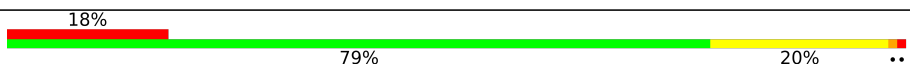
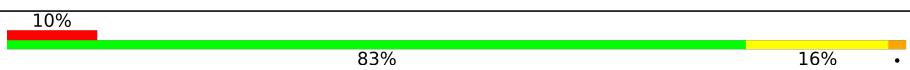
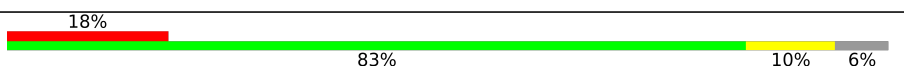
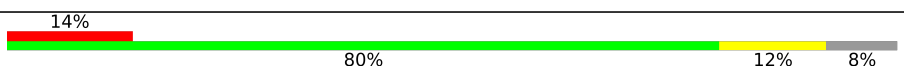
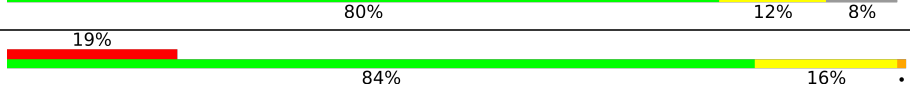
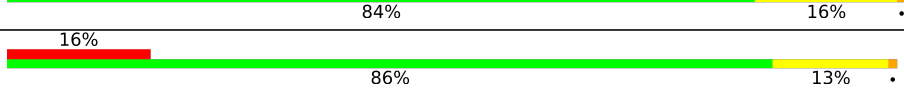
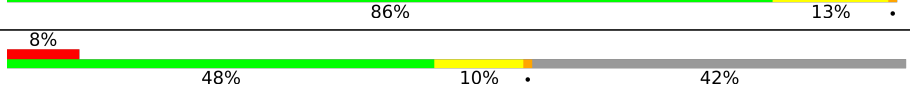
Mol	Chain	Length	Quality of chain
66	Q2	105	
66	q2	105	
67	Q3	91	
67	q3	91	
68	S0	206	
68	s0	206	
69	S1	216	
69	s1	216	
70	S2	217	
70	s2	217	
71	S3	223	
71	s3	223	
72	S4	260	
72	s4	260	
73	S5	206	
73	s5	206	
74	S6	236	
74	s6	236	
75	S7	184	
75	s7	184	
76	S8	200	
76	s8	200	
77	S9	185	
77	s9	185	
78	SM	272	

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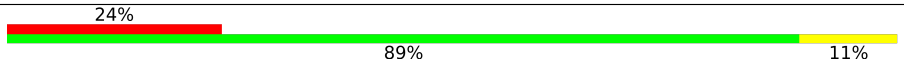
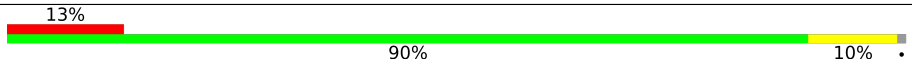
Mol	Chain	Length	Quality of chain
78	sM	272	
79	SR	318	
79	sR	318	

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
80	MG	1	3413	-	-	-	X
80	MG	1	3418	-	-	-	X
80	MG	1	3431	-	-	-	X
80	MG	1	3441	-	-	-	X
80	MG	1	3448	-	-	-	X
80	MG	1	3461	-	-	-	X
80	MG	1	3480	-	-	-	X
80	MG	1	3492	-	-	-	X
80	MG	1	3498	-	-	-	X
80	MG	1	3504	-	-	-	X
80	MG	1	3505	-	-	-	X
80	MG	1	3515	-	-	-	X
80	MG	1	3517	-	-	-	X
80	MG	1	3523	-	-	-	X
80	MG	1	3544	-	-	-	X
80	MG	1	3548	-	-	-	X
80	MG	1	3550	-	-	-	X
80	MG	1	3551	-	-	-	X
80	MG	1	3552	-	-	-	X
80	MG	1	3559	-	-	-	X
80	MG	1	3564	-	-	-	X
80	MG	1	3567	-	-	-	X
80	MG	1	3569	-	-	-	X
80	MG	1	3571	-	-	-	X
80	MG	1	3576	-	-	-	X
80	MG	1	3580	-	-	-	X
80	MG	1	3590	-	-	-	X
80	MG	1	3598	-	-	-	X
80	MG	1	3608	-	-	-	X
80	MG	1	3609	-	-	-	X
80	MG	1	3623	-	-	-	X
80	MG	1	3658	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	1	3659	-	-	-	X
80	MG	1	3664	-	-	-	X
80	MG	1	3667	-	-	-	X
80	MG	1	3674	-	-	-	X
80	MG	1	3687	-	-	-	X
80	MG	1	3690	-	-	-	X
80	MG	1	3699	-	-	-	X
80	MG	1	3706	-	-	-	X
80	MG	1	3708	-	-	-	X
80	MG	1	3709	-	-	-	X
80	MG	1	3712	-	-	-	X
80	MG	1	3713	-	-	-	X
80	MG	1	3737	-	-	-	X
80	MG	1	3739	-	-	-	X
80	MG	1	3740	-	-	-	X
80	MG	1	3741	-	-	-	X
80	MG	1	3744	-	-	-	X
80	MG	1	3761	-	-	-	X
80	MG	1	3763	-	-	-	X
80	MG	1	3775	-	-	-	X
80	MG	1	3829	-	-	-	X
80	MG	1	3841	-	-	-	X
80	MG	1	3842	-	-	-	X
80	MG	1	3853	-	-	-	X
80	MG	1	3854	-	-	-	X
80	MG	1	3856	-	-	-	X
80	MG	1	3858	-	-	-	X
80	MG	1	3860	-	-	-	X
80	MG	1	3862	-	-	-	X
80	MG	1	3864	-	-	-	X
80	MG	1	3867	-	-	-	X
80	MG	1	3868	-	-	-	X
80	MG	1	3876	-	-	-	X
80	MG	1	3877	-	-	-	X
80	MG	1	3880	-	-	-	X
80	MG	2	1908	-	-	-	X
80	MG	2	1944	-	-	-	X
80	MG	2	1947	-	-	-	X
80	MG	2	1968	-	-	-	X
80	MG	2	1973	-	-	-	X
80	MG	2	1977	-	-	-	X
80	MG	2	2022	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	2	2026	-	-	-	X
80	MG	2	2027	-	-	-	X
80	MG	3	201	-	-	-	X
80	MG	4	202	-	-	-	X
80	MG	4	203	-	-	-	X
80	MG	4	206	-	-	-	X
80	MG	4	207	-	-	-	X
80	MG	4	214	-	-	-	X
80	MG	5	3426	-	-	-	X
80	MG	5	3430	-	-	-	X
80	MG	5	3431	-	-	-	X
80	MG	5	3437	-	-	-	X
80	MG	5	3445	-	-	-	X
80	MG	5	3457	-	-	-	X
80	MG	5	3459	-	-	-	X
80	MG	5	3463	-	-	-	X
80	MG	5	3464	-	-	-	X
80	MG	5	3466	-	-	-	X
80	MG	5	3471	-	-	-	X
80	MG	5	3480	-	-	-	X
80	MG	5	3481	-	-	-	X
80	MG	5	3488	-	-	-	X
80	MG	5	3491	-	-	-	X
80	MG	5	3493	-	-	-	X
80	MG	5	3506	-	-	-	X
80	MG	5	3513	-	-	-	X
80	MG	5	3516	-	-	-	X
80	MG	5	3543	-	-	-	X
80	MG	5	3556	-	-	-	X
80	MG	5	3565	-	-	-	X
80	MG	5	3588	-	-	-	X
80	MG	5	3595	-	-	-	X
80	MG	5	3598	-	-	-	X
80	MG	5	3601	-	-	-	X
80	MG	5	3603	-	-	-	X
80	MG	5	3614	-	-	-	X
80	MG	5	3619	-	-	-	X
80	MG	5	3627	-	-	-	X
80	MG	5	3635	-	-	-	X
80	MG	5	3640	-	-	-	X
80	MG	5	3650	-	-	-	X
80	MG	5	3664	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	5	3667	-	-	-	X
80	MG	5	3694	-	-	-	X
80	MG	5	3696	-	-	-	X
80	MG	5	3697	-	-	-	X
80	MG	5	3698	-	-	-	X
80	MG	5	3701	-	-	-	X
80	MG	5	3702	-	-	-	X
80	MG	5	3705	-	-	-	X
80	MG	5	3707	-	-	-	X
80	MG	5	3713	-	-	-	X
80	MG	5	3725	-	-	-	X
80	MG	5	3728	-	-	-	X
80	MG	5	3731	-	-	-	X
80	MG	5	3735	-	-	-	X
80	MG	5	3736	-	-	-	X
80	MG	5	3738	-	-	-	X
80	MG	5	3740	-	-	-	X
80	MG	5	3750	-	-	-	X
80	MG	5	3764	-	-	-	X
80	MG	5	3768	-	-	-	X
80	MG	5	3800	-	-	-	X
80	MG	5	3822	-	-	-	X
80	MG	5	3829	-	-	-	X
80	MG	5	3832	-	-	-	X
80	MG	5	3834	-	-	-	X
80	MG	5	3843	-	-	-	X
80	MG	5	3846	-	-	-	X
80	MG	5	3847	-	-	-	X
80	MG	6	1901	-	-	-	X
80	MG	6	1904	-	-	-	X
80	MG	6	1908	-	-	-	X
80	MG	6	1913	-	-	-	X
80	MG	6	1915	-	-	-	X
80	MG	6	1921	-	-	-	X
80	MG	6	1939	-	-	-	X
80	MG	6	1940	-	-	-	X
80	MG	6	1965	-	-	-	X
80	MG	6	1967	-	-	-	X
80	MG	6	1979	-	-	-	X
80	MG	6	1981	-	-	-	X
80	MG	6	1995	-	-	-	X
80	MG	6	1996	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	6	2009	-	-	-	X
80	MG	6	2033	-	-	-	X
80	MG	6	2038	-	-	-	X
80	MG	6	2041	-	-	-	X
80	MG	6	2046	-	-	-	X
80	MG	6	2047	-	-	-	X
80	MG	6	2050	-	-	-	X
80	MG	6	2054	-	-	-	X
80	MG	6	2060	-	-	-	X
80	MG	8	203	-	-	-	X
80	MG	8	206	-	-	-	X
80	MG	C4	202	-	-	-	X
80	MG	M6	201	-	-	-	X
80	MG	N0	201	-	-	-	X
80	MG	O1	201	-	-	-	X
80	MG	O1	202	-	-	-	X
80	MG	O3	202	-	-	-	X
80	MG	O4	502	-	-	-	X
80	MG	c1	201	-	-	-	X
80	MG	c1	202	-	-	-	X
80	MG	d2	201	-	-	-	X
80	MG	d3	201	-	-	-	X
80	MG	l3	401	-	-	-	X
80	MG	l5	301	-	-	-	X
80	MG	m6	201	-	-	-	X
80	MG	n1	201	-	-	-	X
80	MG	n6	201	-	-	-	X
80	MG	n8	201	-	-	-	X
80	MG	o3	201	-	-	-	X
80	MG	q2	503	-	-	-	X
80	MG	q2	504	-	-	-	X

2 Entry composition (i)

There are 83 unique types of molecules in this entry. The entry contains 400111 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3090	Total	C	N	O	P	0	0	0
			66081	29518	11903	21570	3090			
1	5	3080	Total	C	N	O	P	0	0	0
			65880	29427	11878	21495	3080			

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	1770	Total	C	N	O	P	0	0	0
			37692	16850	6663	12409	1770			
2	6	1736	Total	C	N	O	P	0	0	0
			36971	16529	6541	12165	1736			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 4 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 5 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
5	c0	93	Total	C	N	O	S	0	0	0
			746	481	122	141	2			

- Molecule 6 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C1	154	Total	C	N	O	S	0	0	0
			1207	771	229	204	3			
6	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 7 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C2	119	Total	C	N	O	S	0	0	0
			865	545	151	167	2			
7	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 8 is a protein called 40S ribosomal protein S13.

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

- Molecule 9 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	c5	125	Total 987	C 627	N 186	O 167	S 7	0	0	0

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	C6	141	Total 1105	C 708	N 203	O 194	0	0	0
11	c6	141	Total 1105	C 708	N 203	O 194	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C7	120	Total 926	C 577	N 177	O 170	S 2	0	0	0
12	c7	121	Total 926	C 575	N 178	O 171	S 2	0	0	0

- Molecule 13 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	d0	104	Total 828	C 524	N 150	O 153	S 1	0	0	0
15	D0	105	Total 841	C 532	N 153	O 155	S 1	0	0	0

- Molecule 16 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 17 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 19 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 20 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 21 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 22 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 23 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
24	D9	52	Total	C	N	O	S	0	0	0
			433	269	91	69	4			

- Molecule 25 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	e0	61	Total	C	N	O	S	0	0	0
			482	304	99	78	1			
25	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

- Molecule 26 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	e1	73	Total	C	N	O	S	0	0	0
			586	374	112	96	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

- Molecule 27 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L3.

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

- Molecule 29 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			
30	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 31 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			
31	L6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 32 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	l8	231	Total	C	N	O	S	0	0	0
			1764	1130	316	315	3			
33	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 34 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
34	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 35 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	m0	209	Total	C	N	O	S	0	0	0
			1696	1077	321	293	5			
35	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 36 is a protein called 60S ribosomal protein L11-B.

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

- Molecule 37 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 40 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	m7	183	Total	C	N	O	0	0	0
			1420	882	281	257			
41	M7	183	Total	C	N	O	0	0	0
			1420	882	281	257			

- Molecule 42 is a protein called 60S ribosomal protein L18-A.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	m9	184	Total	C	N	O	0	0	0
			1490	917	321	252			
43	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 44 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	n0	171	Total	C	N	O	S	0	0	0
			1437	925	266	243	3			
44	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 45 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 46 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 47 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	n3	135	Total	C	N	O	S	0	0	0
			997	625	188	177	7			
47	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 48 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	n4	130	Total	C	N	O	S	0	0	0
			1007	634	200	172	1			
48	N4	130	Total	C	N	O	S	0	0	0
			965	606	192	166	1			

- Molecule 49 is a protein called 60S ribosomal protein L25.

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

- Molecule 50 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	n6	122	Total	C	N	O	0	0	0
			963	606	187	170			
50	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 51 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L28.

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

- Molecule 53 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	n9	56	Total 444	C 277	N 96	O 71	0	0	0
53	N9	58	Total 462	C 289	N 100	O 73	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L30.

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

- Molecule 55 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 56 is a protein called 60S ribosomal protein L32.

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

- Molecule 57 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 58 is a protein called 60S ribosomal protein L34-A.

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

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

- Molecule 59 is a protein called 60S ribosomal protein L35-A.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	o7	83	Total 656	C 399	N 143	O 109	S 5	0	0	0
61	O7	87	Total 681	C 414	N 148	O 114	S 5	0	0	0

- Molecule 62 is a protein called 60S ribosomal protein L38.

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

- Molecule 63 is a protein called 60S ribosomal protein L39.

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

- Molecule 64 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 65 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 66 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	q2	104	Total	C	N	O	S	0	0	0
			836	525	169	137	5			
66	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 67 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

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

- Molecule 71 is a protein called 40S ribosomal protein S3.

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

- Molecule 72 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S5.

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

- Molecule 74 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 75 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
75	s7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
75	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			

- Molecule 76 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	s8	185	Total	C	N	O	S	0	0	0
			1466	910	293	261	2			
76	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 77 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 78 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
78	sM	131	Total	C	N	O	0	0	0
			958	564	193	201			
78	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	sR	316	Total	C	N	O	S	0	0	0
			2427	1535	415	469	8			
79	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
80	1	485	Total Mg 485 485	0	0
80	2	128	Total Mg 128 128	0	0
80	3	13	Total Mg 13 13	0	0
80	4	19	Total Mg 19 19	1	0
80	5	449	Total Mg 449 449	1	0
80	6	160	Total Mg 160 160	0	0
80	7	8	Total Mg 8 8	0	0
80	8	10	Total Mg 10 10	0	0
80	c1	2	Total Mg 2 2	0	0
80	c3	1	Total Mg 1 1	0	0
80	C4	3	Total Mg 3 3	0	0
80	C6	1	Total Mg 1 1	0	0
80	c7	1	Total Mg 1 1	0	0
80	C8	1	Total Mg 1 1	0	0
80	c8	2	Total Mg 2 2	0	0
80	C9	1	Total Mg 1 1	0	0
80	c9	1	Total Mg 1 1	0	0
80	d2	1	Total Mg 1 1	0	0
80	D2	1	Total Mg 1 1	0	0
80	d3	1	Total Mg 1 1	0	0
80	d9	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
80	l2	2	Total Mg 2 2	0	0
80	L2	2	Total Mg 2 2	0	0
80	l3	3	Total Mg 3 3	0	0
80	L3	2	Total Mg 2 2	0	0
80	l4	1	Total Mg 1 1	0	0
80	l5	1	Total Mg 1 1	0	0
80	L6	3	Total Mg 3 3	0	0
80	l7	1	Total Mg 1 1	0	0
80	L7	2	Total Mg 2 2	0	0
80	L9	1	Total Mg 1 1	0	0
80	m0	2	Total Mg 2 2	0	0
80	M0	2	Total Mg 2 2	0	0
80	m5	1	Total Mg 1 1	0	0
80	M5	3	Total Mg 3 3	0	0
80	m6	1	Total Mg 1 1	0	0
80	M6	1	Total Mg 1 1	0	0
80	m7	2	Total Mg 2 2	0	0
80	M7	4	Total Mg 4 4	0	0
80	M8	1	Total Mg 1 1	0	0
80	N0	1	Total Mg 1 1	0	0
80	n1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
80	n3	1	Total Mg 1 1	0	0
80	N3	1	Total Mg 1 1	0	0
80	n6	1	Total Mg 1 1	0	0
80	N6	1	Total Mg 1 1	0	0
80	n7	1	Total Mg 1 1	0	0
80	N7	1	Total Mg 1 1	0	0
80	n8	1	Total Mg 1 1	0	0
80	N8	1	Total Mg 1 1	0	0
80	O1	2	Total Mg 2 2	0	0
80	o2	2	Total Mg 2 2	0	0
80	O2	1	Total Mg 1 1	0	0
80	o3	2	Total Mg 2 2	0	0
80	O3	2	Total Mg 2 2	0	0
80	o4	1	Total Mg 1 1	0	0
80	O4	1	Total Mg 1 1	0	0
80	O5	1	Total Mg 1 1	0	0
80	O6	1	Total Mg 1 1	0	0
80	o7	2	Total Mg 2 2	0	0
80	O7	2	Total Mg 2 2	0	0
80	q2	3	Total Mg 3 3	0	0
80	Q2	1	Total Mg 1 1	0	0

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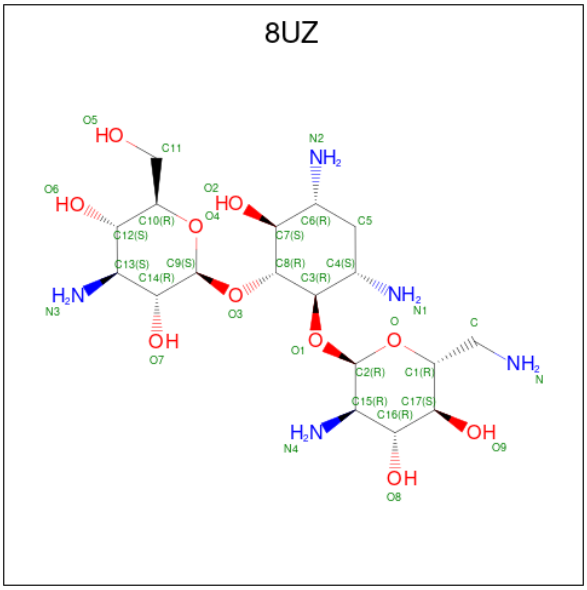
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
80	s0	1	Total Mg 1 1	0	0
80	S1	1	Total Mg 1 1	0	0
80	S4	1	Total Mg 1 1	0	0
80	s4	1	Total Mg 1 1	0	0
80	S6	1	Total Mg 1 1	0	0
80	s6	1	Total Mg 1 1	0	0
80	s8	1	Total Mg 1 1	0	0
80	SM	2	Total Mg 2 2	0	0

- Molecule 81 is TC007 (three-letter code: 8UZ) (formula: $C_{18}H_{37}N_5O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	1	1	Total C N O 33 18 5 10	0	0
81	2	1	Total C N O 33 18 5 10	0	0
81	2	1	Total C N O 33 18 5 10	0	0
81	2	1	Total C N O 33 18 5 10	0	0
81	3	1	Total C N O 33 18 5 10	0	0
81	4	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	5	1	Total C N O 33 18 5 10	0	0
81	6	1	Total C N O 33 18 5 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	7	1	Total C N O 33 18 5 10	0	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	d6	1	Total Zn 1 1	0	0
82	D6	1	Total Zn 1 1	0	0
82	D7	1	Total Zn 1 1	0	0
82	d9	1	Total Zn 1 1	0	0
82	D9	1	Total Zn 1 1	0	0
82	e1	1	Total Zn 1 1	0	0
82	E1	1	Total Zn 1 1	0	0
82	o4	1	Total Zn 1 1	0	0
82	O4	1	Total Zn 1 1	0	0
82	o7	1	Total Zn 1 1	0	0
82	O7	1	Total Zn 1 1	0	0
82	q0	1	Total Zn 1 1	0	0
82	Q0	1	Total Zn 1 1	0	0
82	q2	1	Total Zn 1 1	0	0
82	Q2	1	Total Zn 1 1	0	0
82	q3	1	Total Zn 1 1	0	0
82	Q3	1	Total Zn 1 1	0	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	1	597	Total O 597 597	3	0
83	2	154	Total O 154 154	0	0
83	3	23	Total O 23 23	0	0
83	4	7	Total O 7 7	0	0
83	5	556	Total O 556 556	0	0
83	6	204	Total O 204 204	0	0
83	7	19	Total O 19 19	0	0
83	8	10	Total O 10 10	0	0
83	C3	2	Total O 2 2	0	0
83	C4	1	Total O 1 1	0	0
83	c4	1	Total O 1 1	0	0
83	C6	1	Total O 1 1	0	0
83	c6	1	Total O 1 1	0	0
83	C7	1	Total O 1 1	0	0
83	c8	1	Total O 1 1	0	0
83	C9	3	Total O 3 3	0	0
83	c9	4	Total O 4 4	0	0
83	D0	1	Total O 1 1	0	0
83	d3	1	Total O 1 1	0	0
83	D3	2	Total O 2 2	0	0
83	d6	3	Total O 3 3	0	0
83	D6	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	d9	2	Total O 2 2	0	0
83	l2	4	Total O 4 4	0	0
83	L2	3	Total O 3 3	0	0
83	l3	4	Total O 4 4	0	0
83	L3	1	Total O 1 1	0	0
83	l4	3	Total O 3 3	0	0
83	L4	1	Total O 1 1	0	0
83	l5	3	Total O 3 3	0	0
83	L5	2	Total O 2 2	0	0
83	l9	2	Total O 2 2	0	0
83	M0	2	Total O 2 2	0	0
83	M3	3	Total O 3 3	0	0
83	m5	3	Total O 3 3	0	0
83	M5	1	Total O 1 1	0	0
83	M6	3	Total O 3 3	0	0
83	m7	3	Total O 3 3	0	0
83	M7	4	Total O 4 4	0	0
83	m8	1	Total O 1 1	0	0
83	m9	5	Total O 5 5	0	0
83	M9	2	Total O 2 2	0	0
83	n1	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	N1	3	Total O 3 3	0	0
83	n3	3	Total O 3 3	0	0
83	N3	3	Total O 3 3	0	0
83	N5	1	Total O 1 1	0	0
83	N6	3	Total O 3 3	0	0
83	n8	3	Total O 3 3	0	0
83	N8	1	Total O 1 1	0	0
83	o1	3	Total O 3 3	0	0
83	O1	5	Total O 5 5	0	0
83	o2	5	Total O 5 5	0	0
83	O2	3	Total O 3 3	0	0
83	o4	4	Total O 4 4	0	0
83	O4	1	Total O 1 1	0	0
83	O5	1	Total O 1 1	0	0
83	o6	3	Total O 3 3	0	0
83	o7	1	Total O 1 1	0	0
83	O7	4	Total O 4 4	0	0
83	O9	2	Total O 2 2	0	0
83	q0	1	Total O 1 1	0	0
83	q2	1	Total O 1 1	0	0
83	Q2	1	Total O 1 1	0	0

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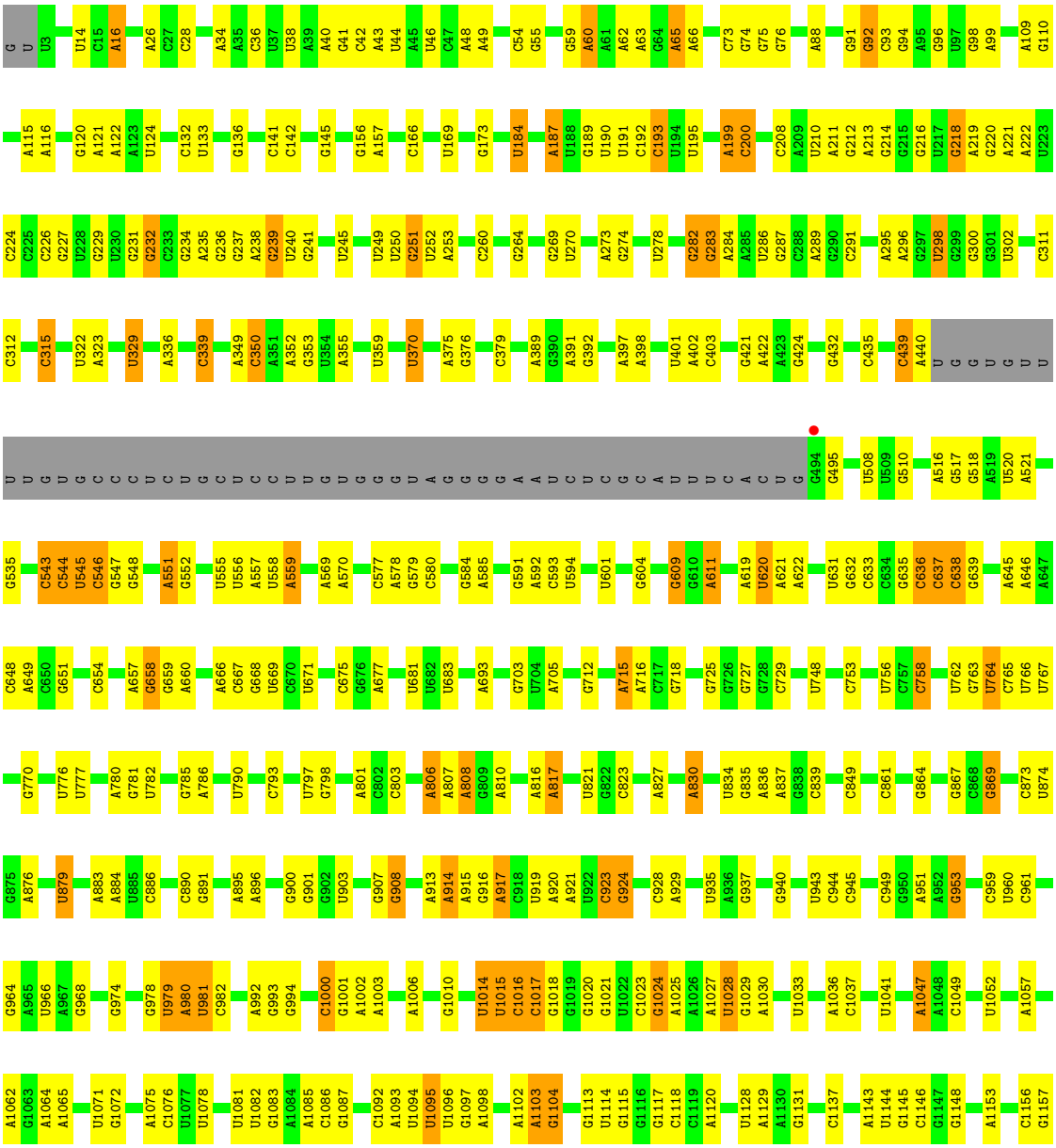
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	S6	1	Total O 1 1	0	0
83	S9	1	Total O 1 1	0	0
83	sM	3	Total O 3 3	0	0
83	SM	1	Total O 1 1	0	0

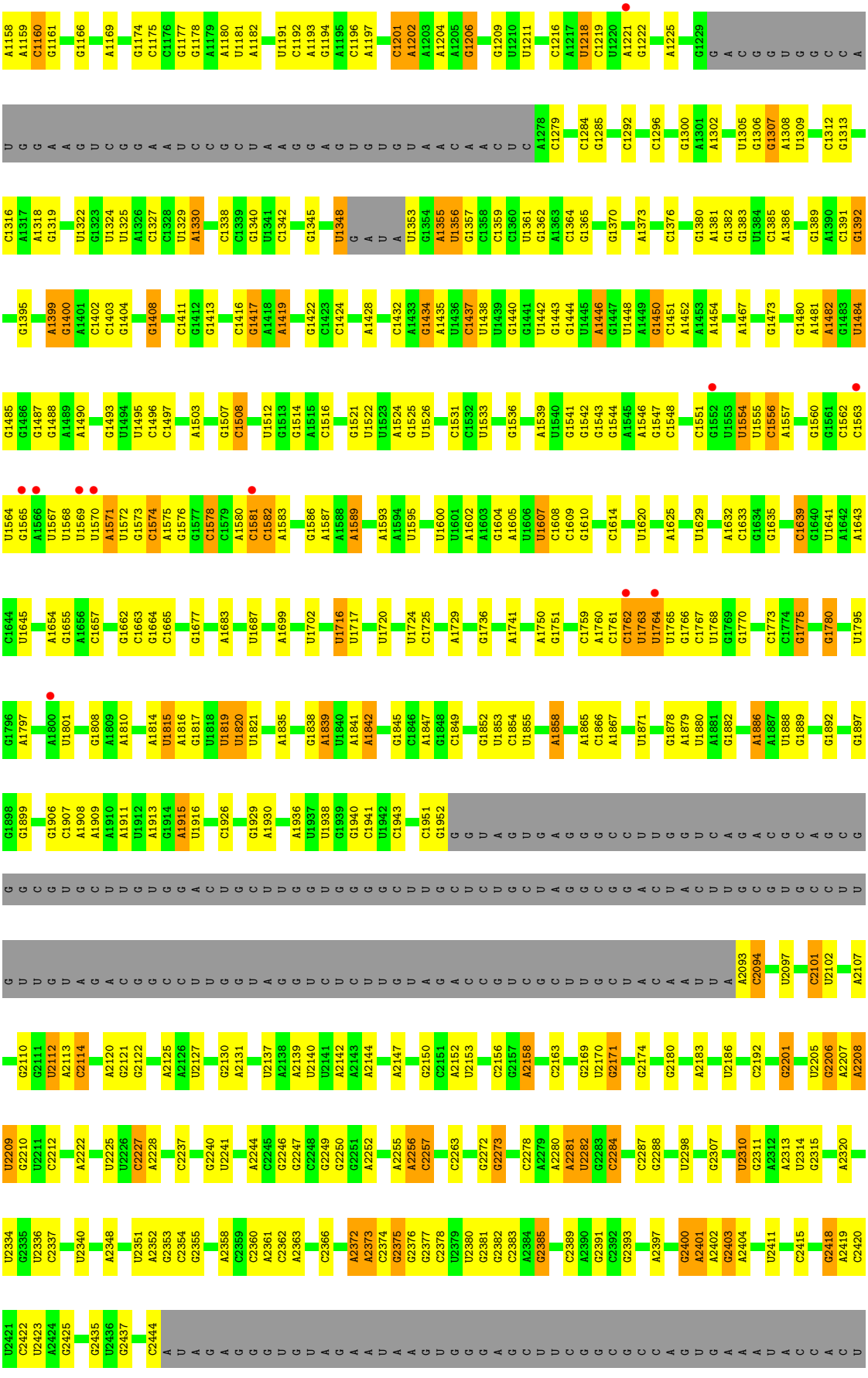
3 Residue-property plots (i)

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: 25S ribosomal RNA

Chain 1:

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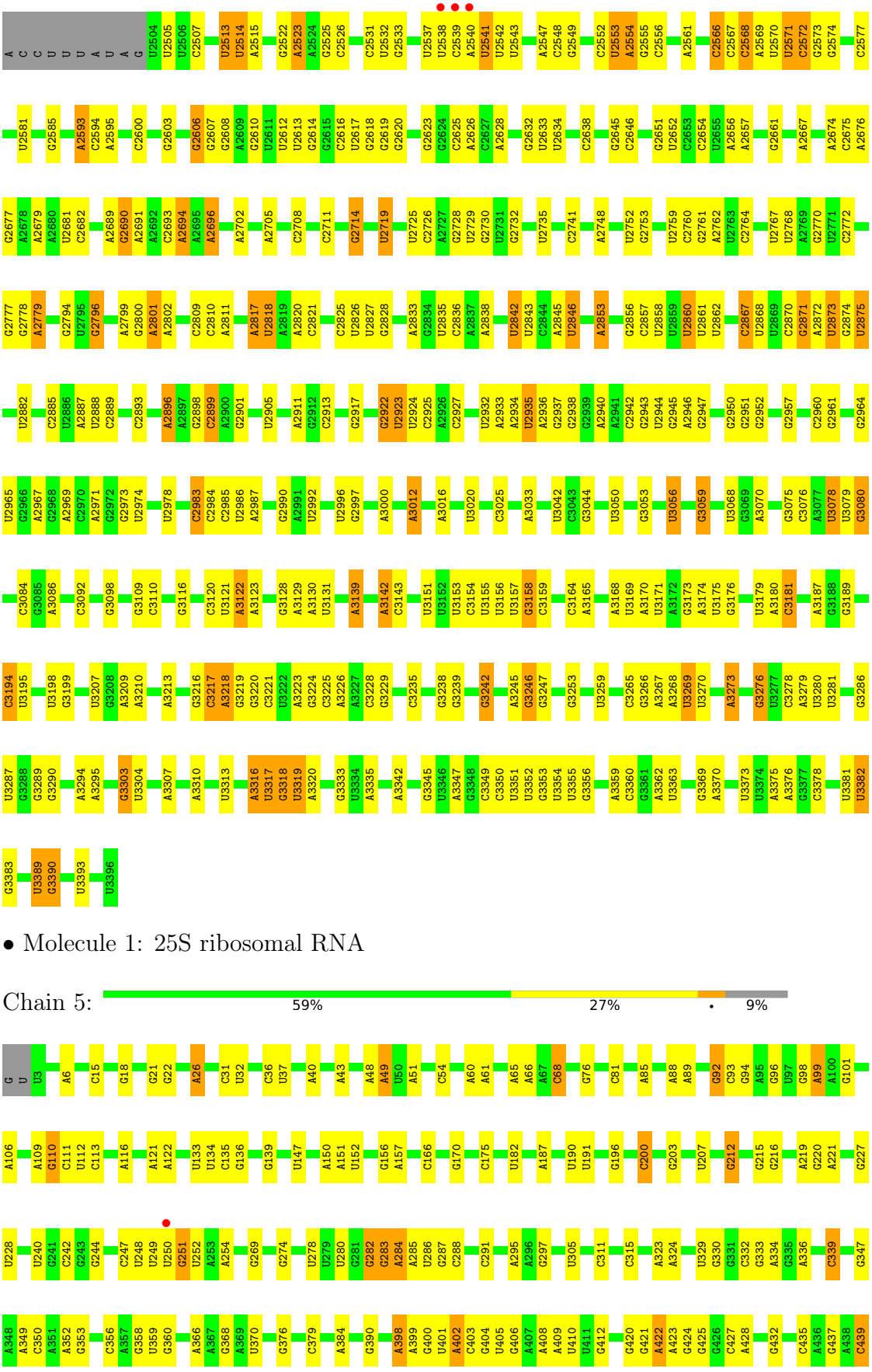
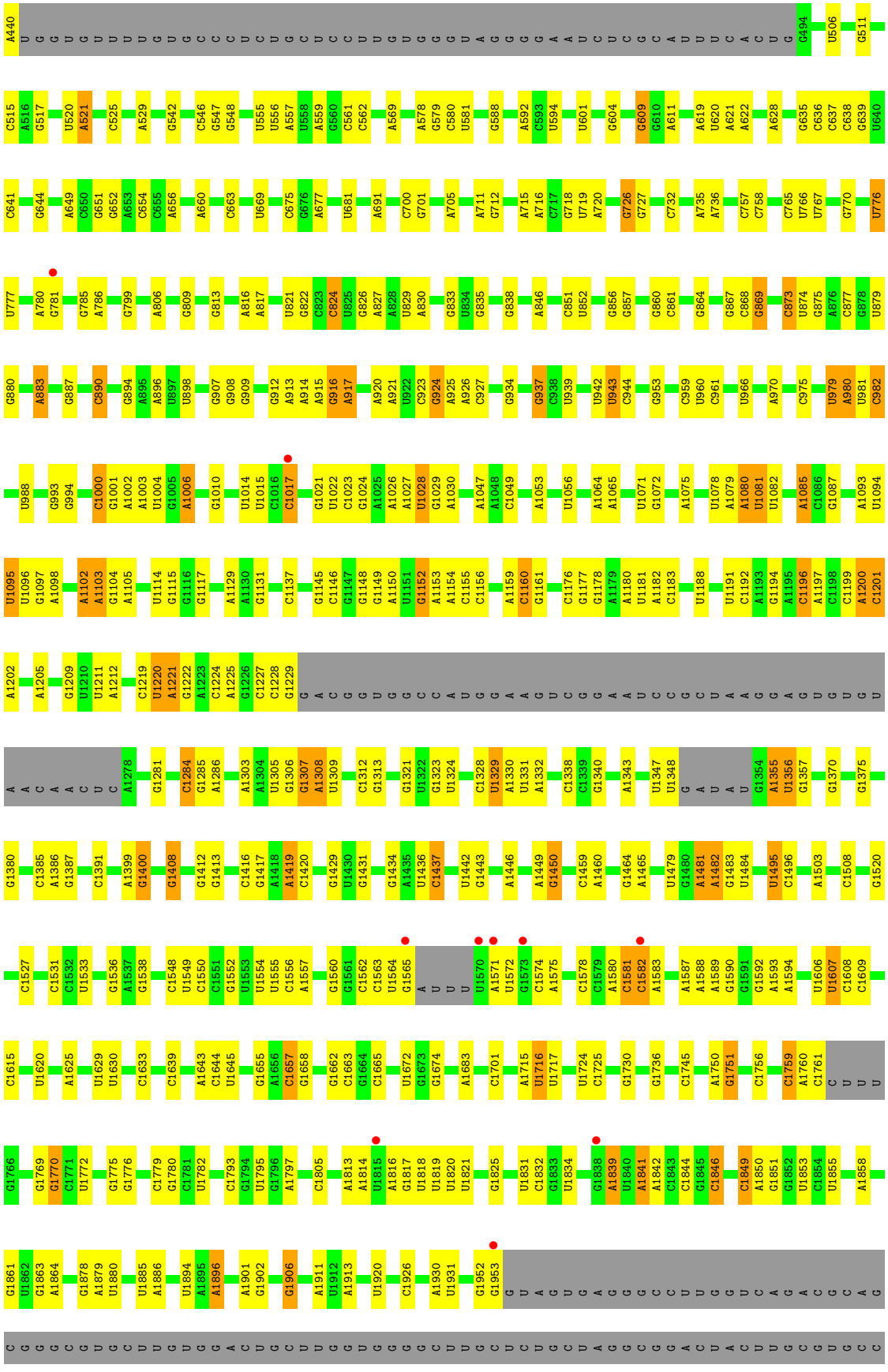
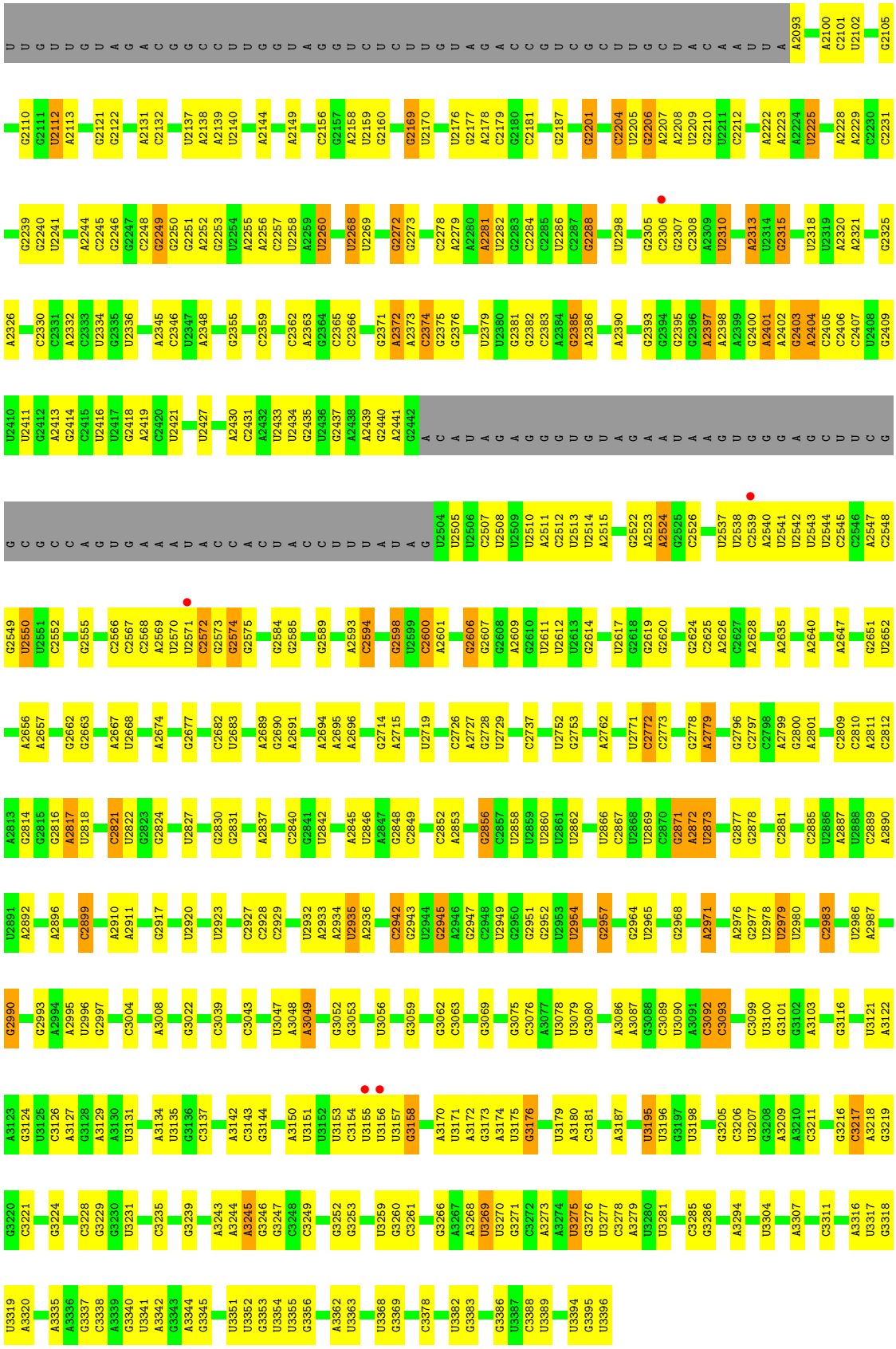


• Molecule 1: 25S ribosomal RNA

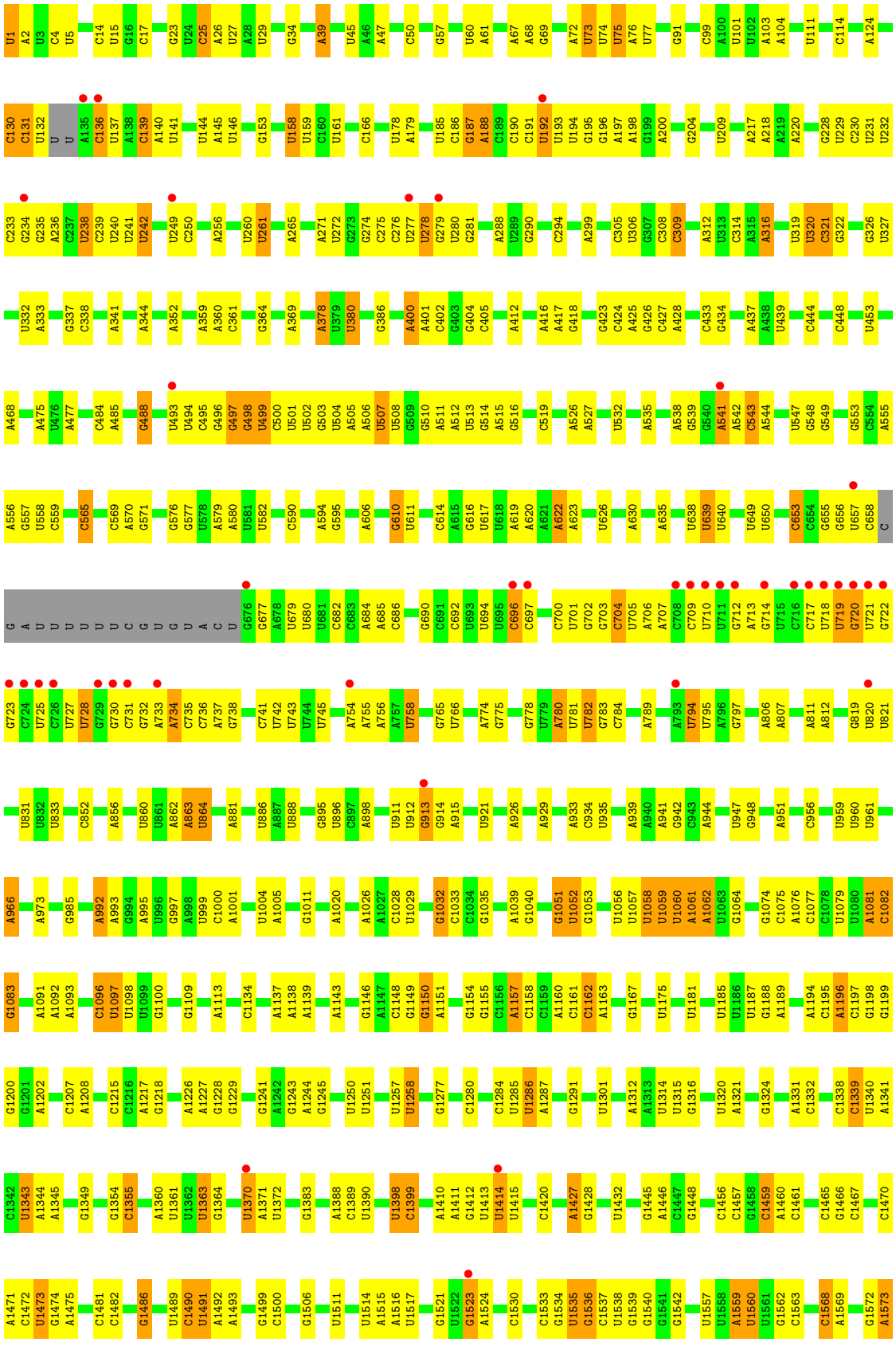
Chain 5:

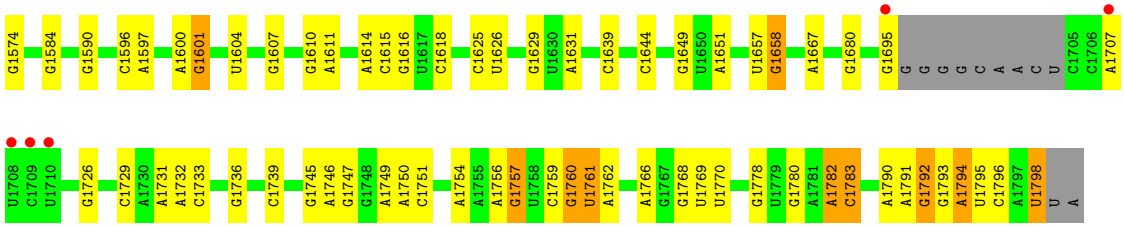




• Molecule 2: 18S ribosomal RNA

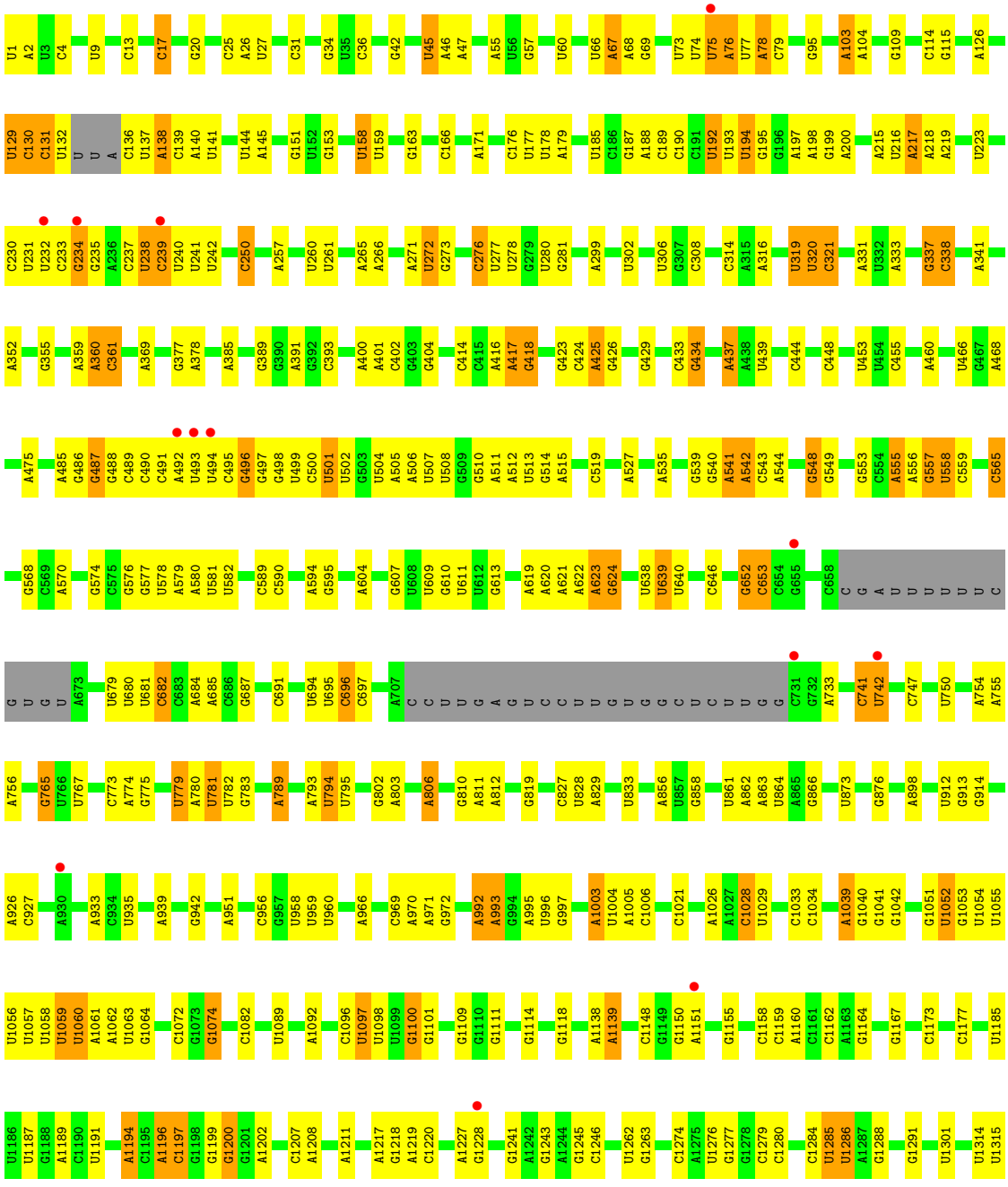
Chain 2:

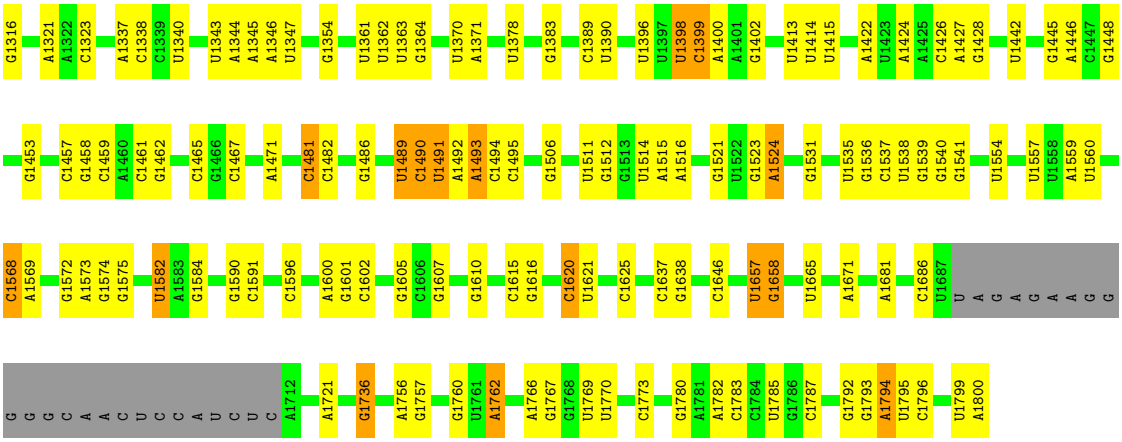




• Molecule 2: 18S ribosomal RNA

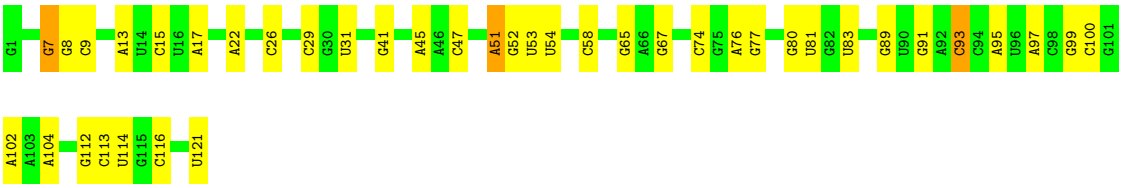
Chain 6:





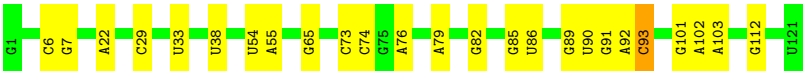
• Molecule 3: 5S ribosomal RNA

Chain 3:



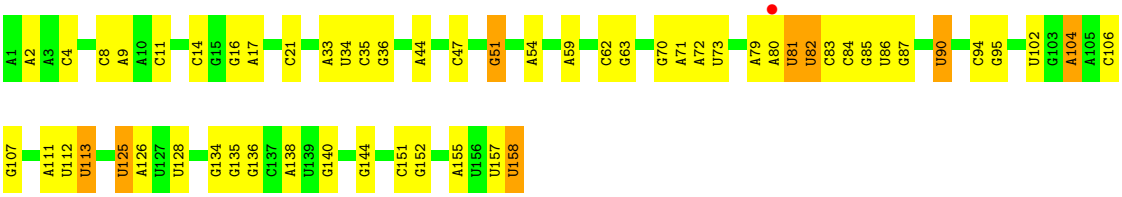
• Molecule 3: 5S ribosomal RNA

Chain 7:



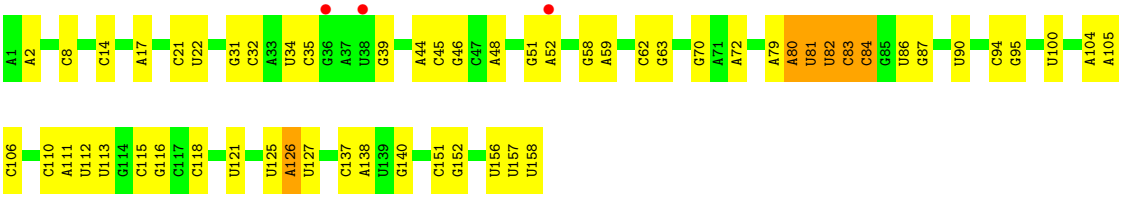
• Molecule 4: 5.8S ribosomal RNA

Chain 4:



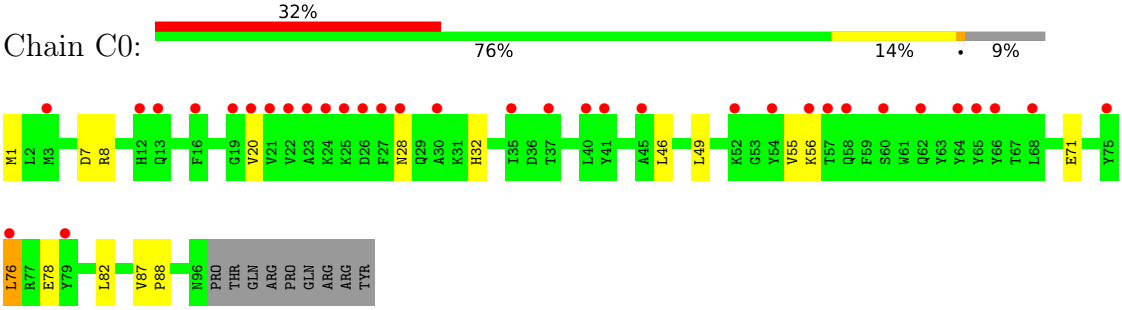
• Molecule 4: 5.8S ribosomal RNA

Chain 8:



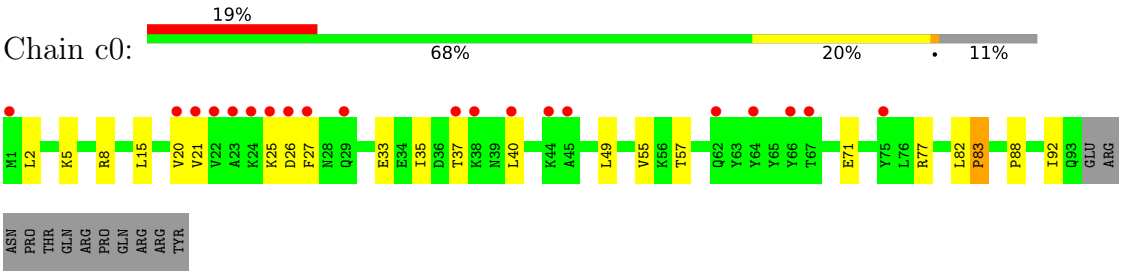
• Molecule 5: 40S ribosomal protein S10-A

Chain C0:



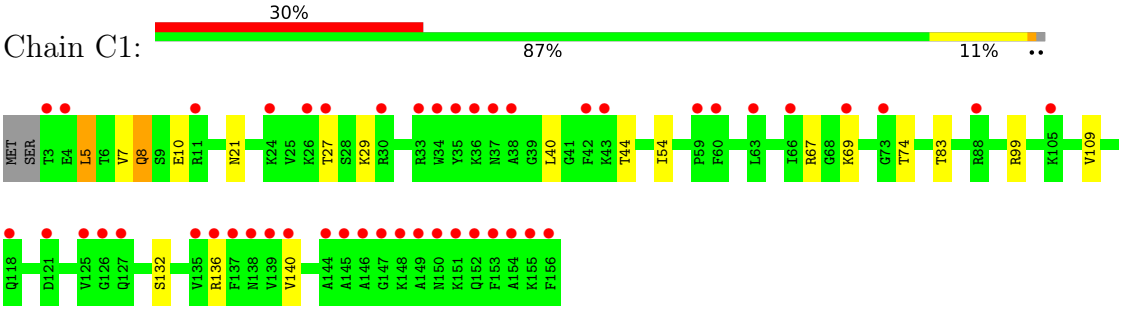
• Molecule 5: 40S ribosomal protein S10-A

Chain c0:



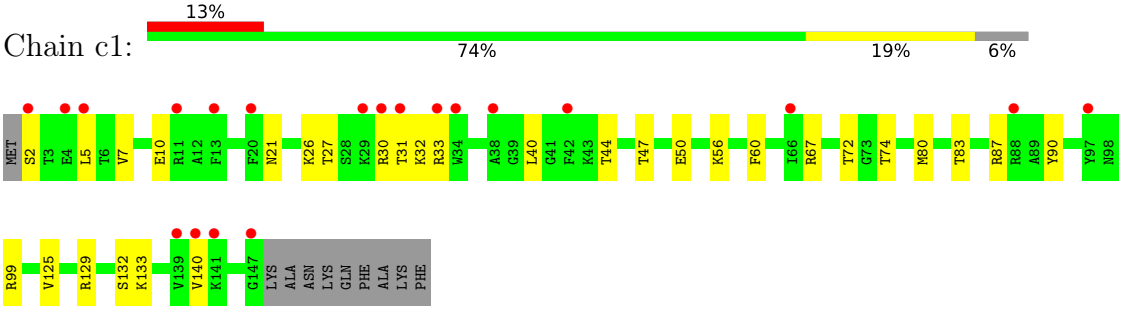
• Molecule 6: 40S ribosomal protein S11-A

Chain C1:



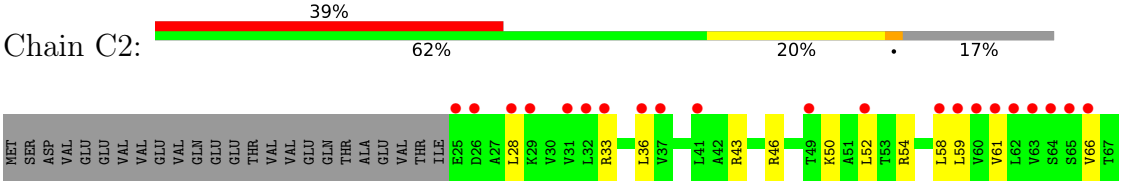
• Molecule 6: 40S ribosomal protein S11-A

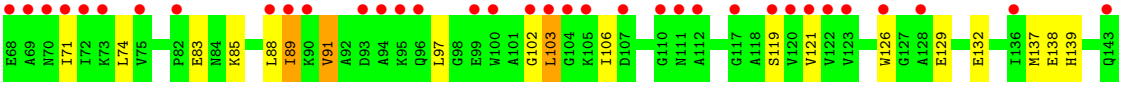
Chain c1:



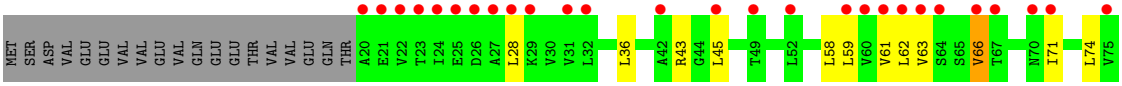
• Molecule 7: 40S ribosomal protein S12

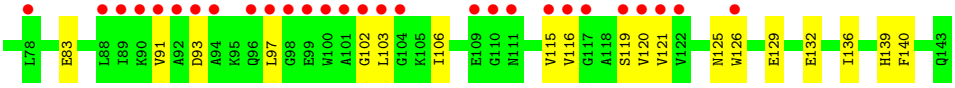
Chain C2:



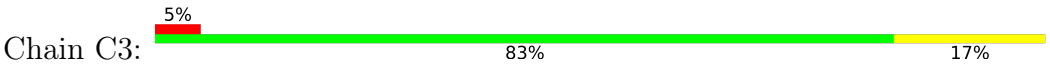


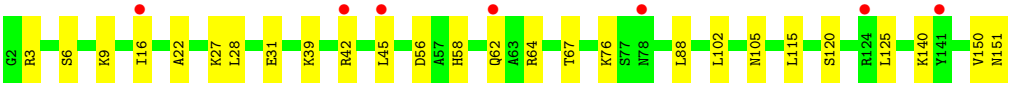
• Molecule 7: 40S ribosomal protein S12



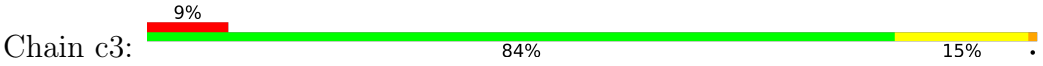


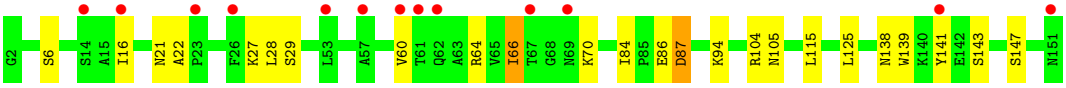
• Molecule 8: 40S ribosomal protein S13



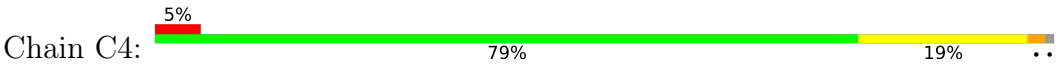


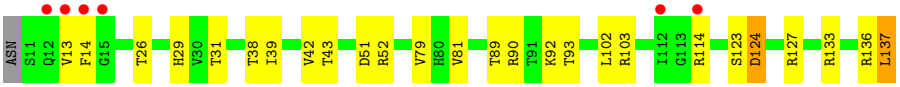
• Molecule 8: 40S ribosomal protein S13



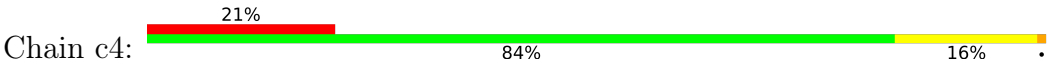


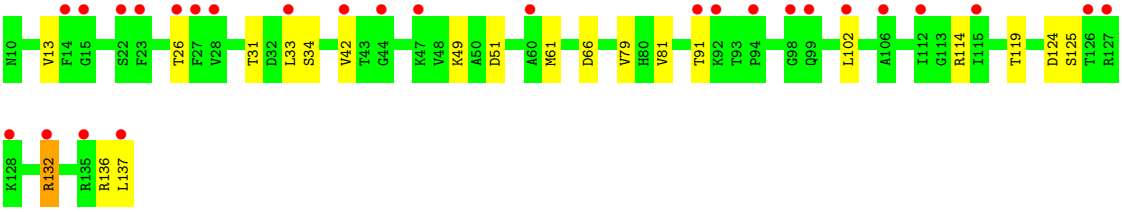
• Molecule 9: 40S ribosomal protein S14-B





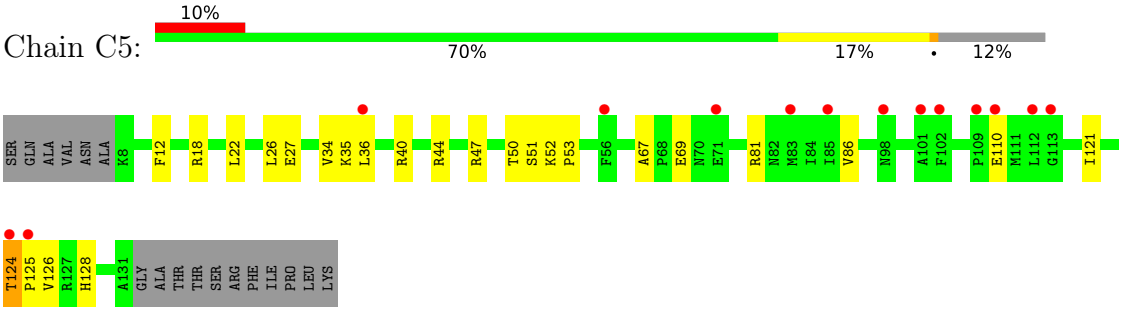
• Molecule 9: 40S ribosomal protein S14-B





• Molecule 10: 40S ribosomal protein S15

Chain C5:



• Molecule 10: 40S ribosomal protein S15

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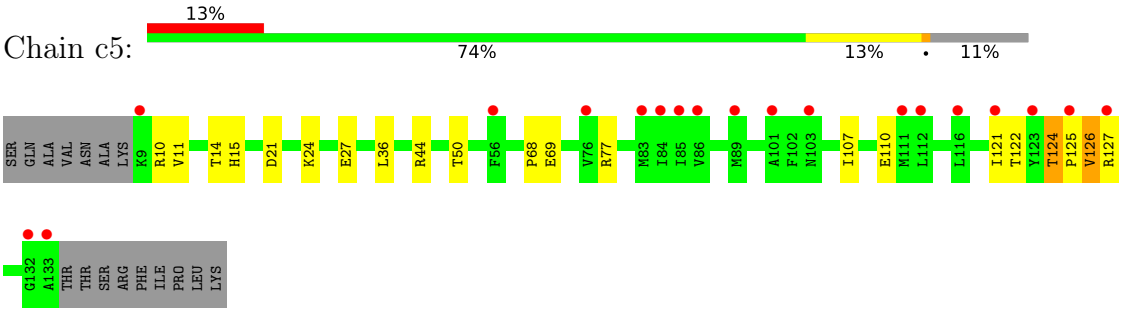
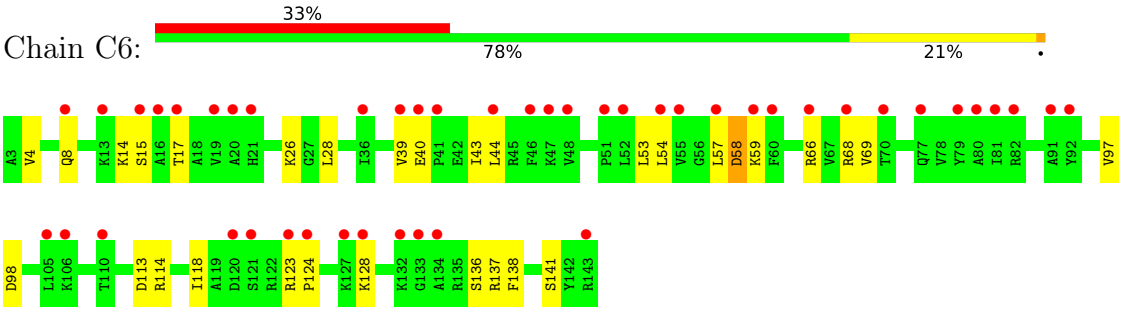


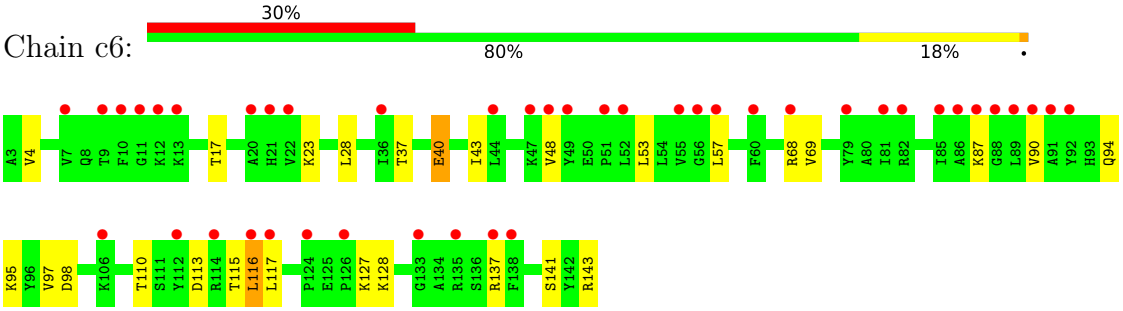
• Molecule 11: 40S ribosomal protein S16-A

Chain C6:



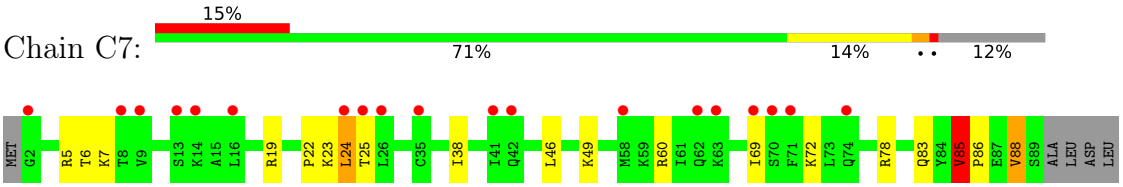
• Molecule 11: 40S ribosomal protein S16-A

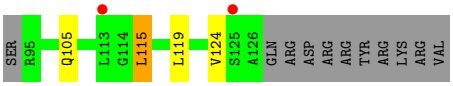
Chain c6:



• Molecule 12: 40S ribosomal protein S17-A

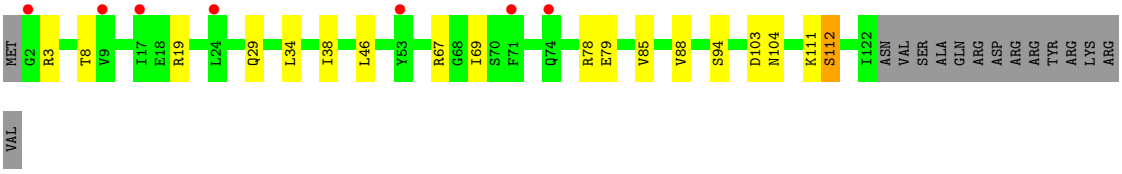
Chain C7:





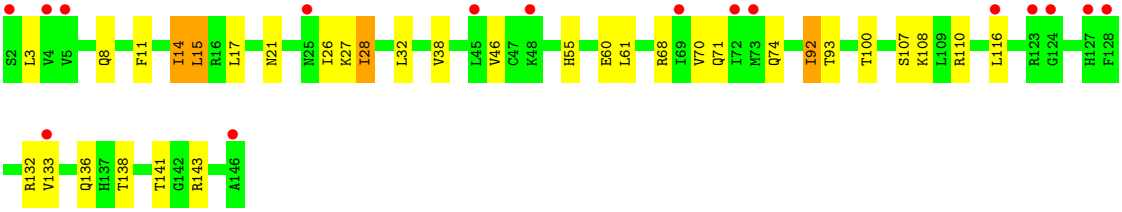
• Molecule 12: 40S ribosomal protein S17-A

Chain c7:



• Molecule 13: 40S ribosomal protein S18-A

Chain C8:

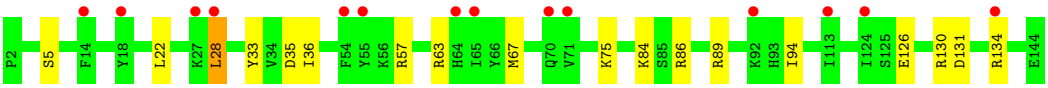


• Molecule 13: 40S ribosomal protein S18-A

Chain c8:

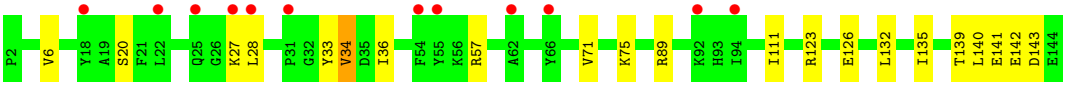
• Molecule 14: 40S ribosomal protein S19-A

Chain C9:



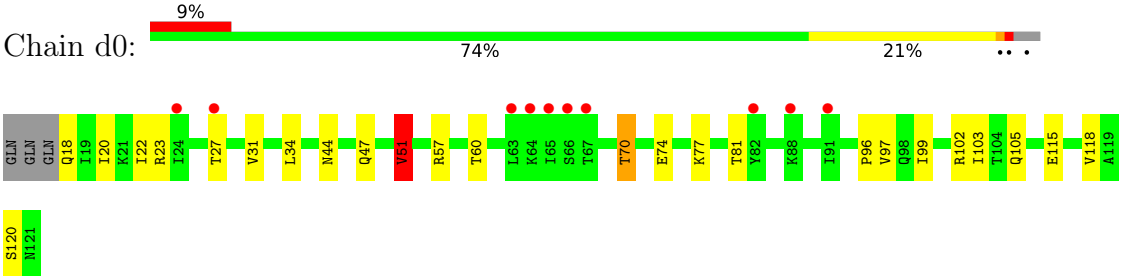
• Molecule 14: 40S ribosomal protein S19-A

Chain c9:



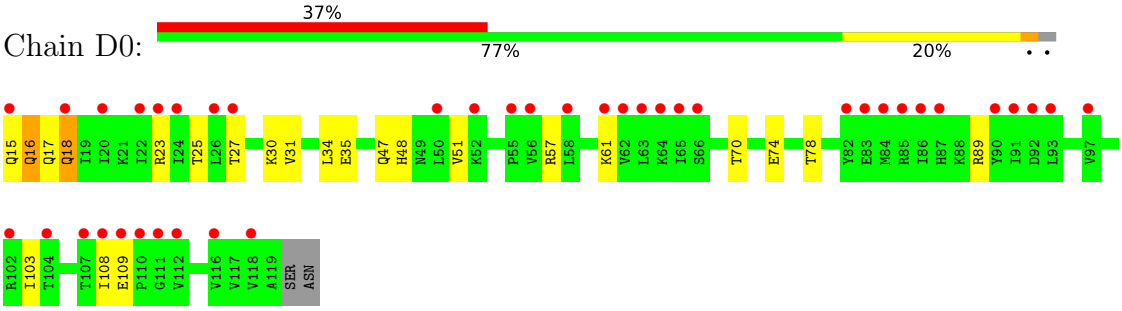
• Molecule 15: 40S ribosomal protein S20

Chain d0:



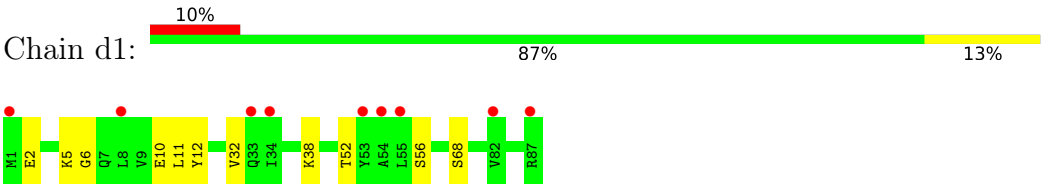
• Molecule 15: 40S ribosomal protein S20

Chain D0:



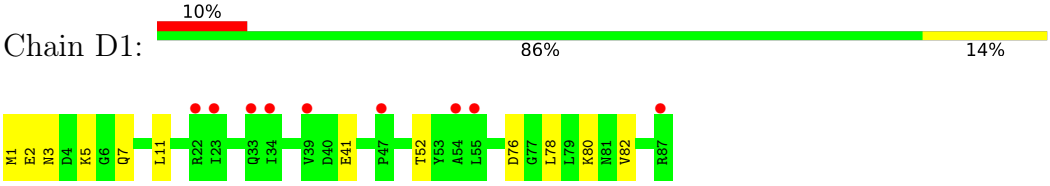
• Molecule 16: 40S ribosomal protein S21-A

Chain d1:



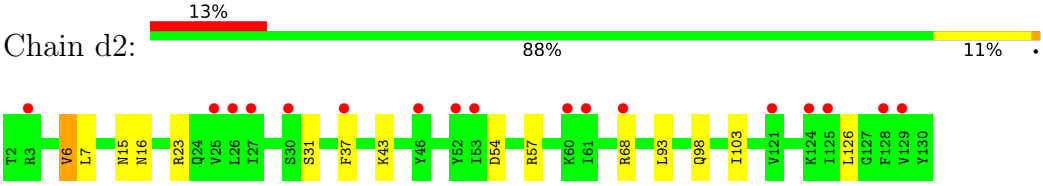
• Molecule 16: 40S ribosomal protein S21-A

Chain D1:



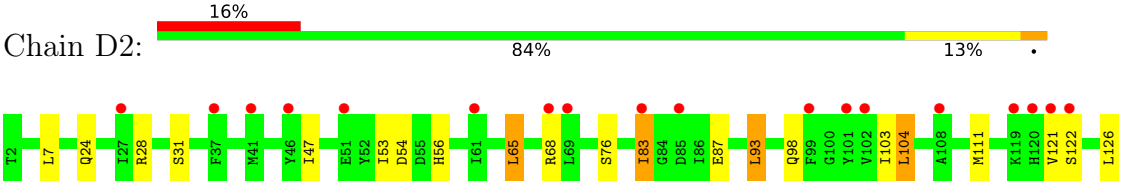
• Molecule 17: 40S ribosomal protein S22-A

Chain d2:



• Molecule 17: 40S ribosomal protein S22-A

Chain D2:

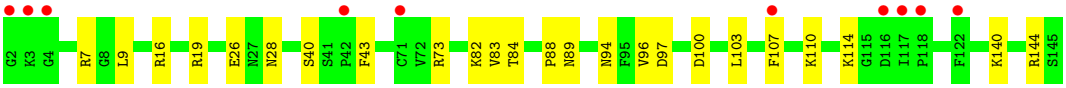


• Molecule 18: 40S ribosomal protein S23-A

Chain d3:

• Molecule 18: 40S ribosomal protein S23-A

Chain D3:



• Molecule 19: 40S ribosomal protein S24-A

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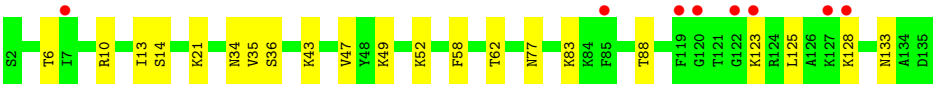
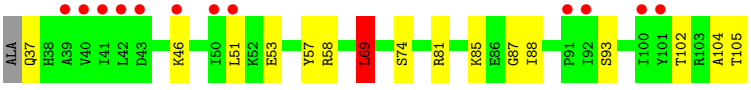


• Molecule 19: 40S ribosomal protein S24-A

Chain D4:

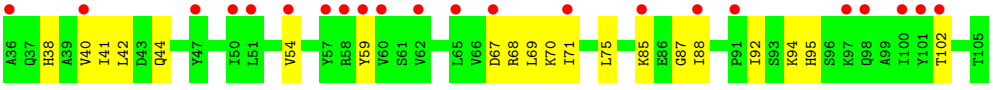
• Molecule 20: 40S ribosomal protein S25-A

Chain d5:



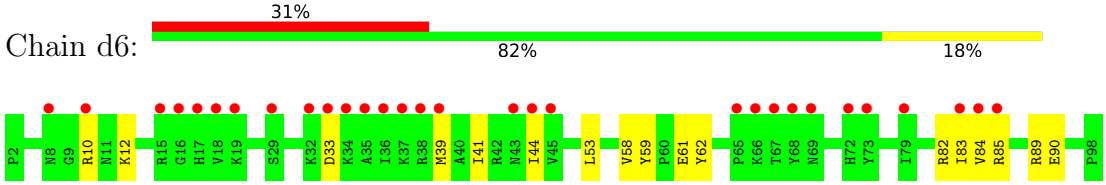
• Molecule 20: 40S ribosomal protein S25-A

Chain D5:



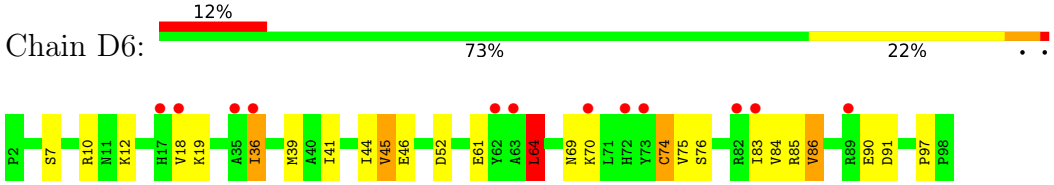
• Molecule 21: 40S ribosomal protein S26-B

Chain d6:



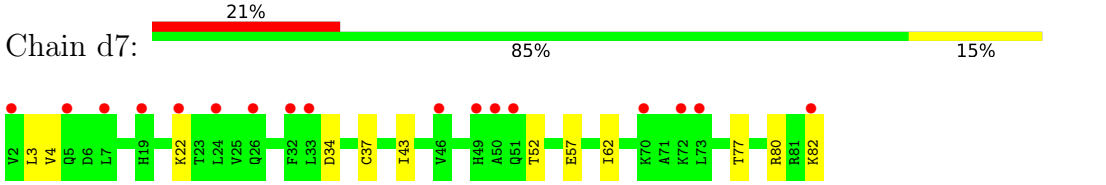
• Molecule 21: 40S ribosomal protein S26-B

Chain D6:



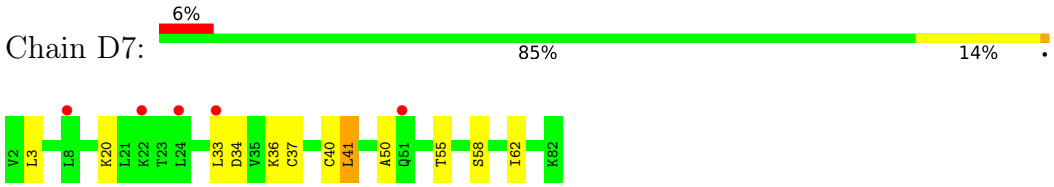
• Molecule 22: 40S ribosomal protein S27-A

Chain d7:



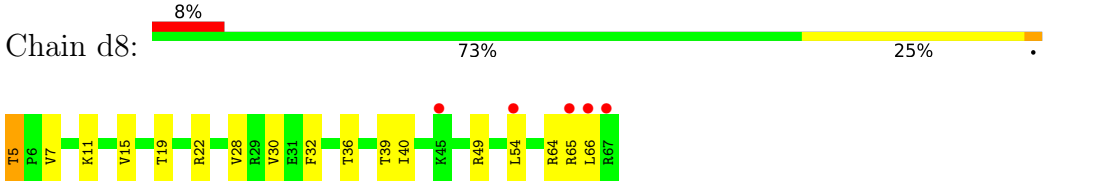
• Molecule 22: 40S ribosomal protein S27-A

Chain D7:



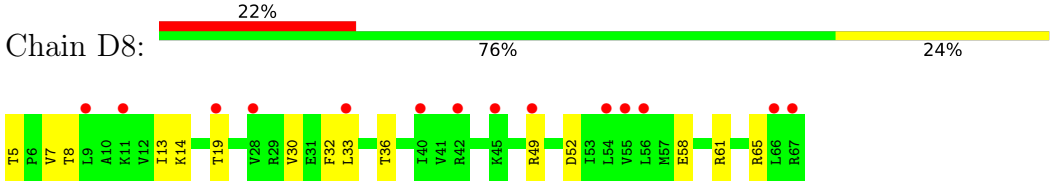
• Molecule 23: 40S ribosomal protein S28-A

Chain d8:



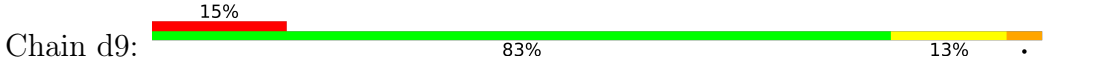
• Molecule 23: 40S ribosomal protein S28-A

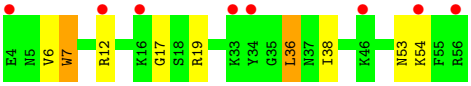
Chain D8:



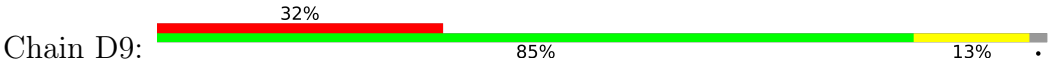
• Molecule 24: 40S ribosomal protein S29-A

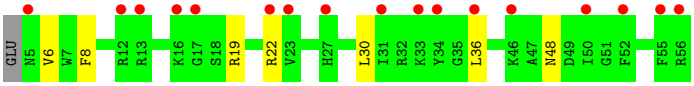
Chain d9:



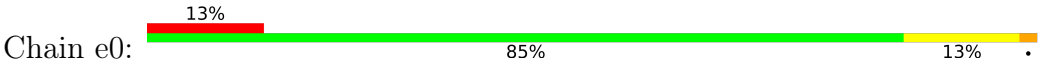


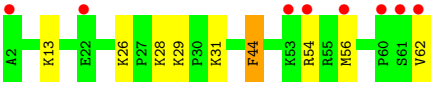
• Molecule 24: 40S ribosomal protein S29-A



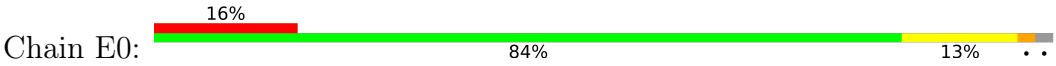


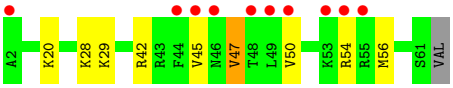
• Molecule 25: 40S ribosomal protein S30-A



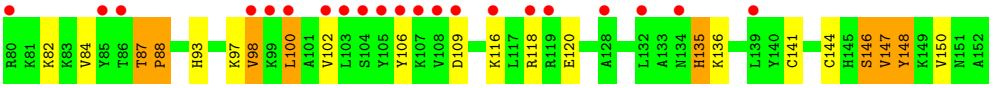


• Molecule 25: 40S ribosomal protein S30-A

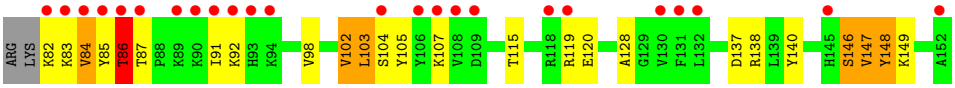




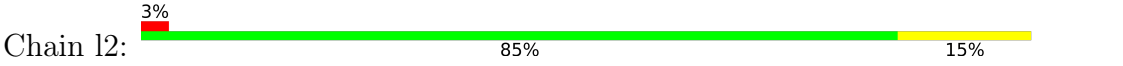
• Molecule 26: Ubiquitin-40S ribosomal protein S31

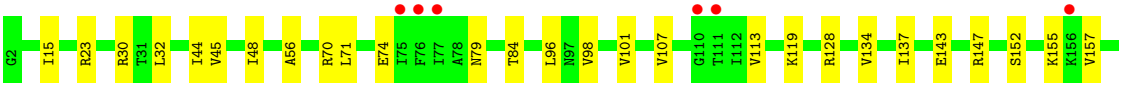


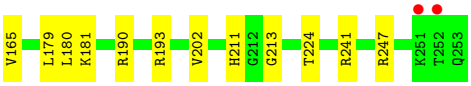
• Molecule 26: Ubiquitin-40S ribosomal protein S31



• Molecule 27: 60S ribosomal protein L2-A

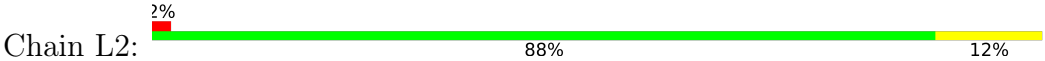


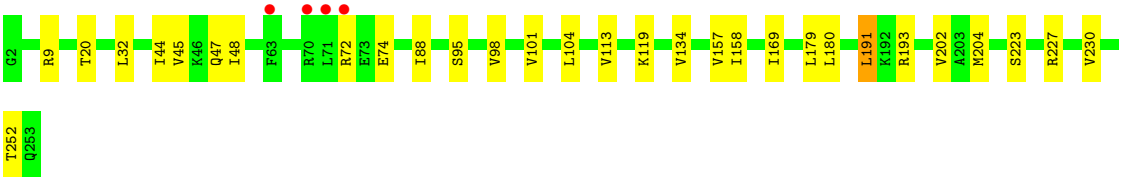




• Molecule 27: 60S ribosomal protein L2-A

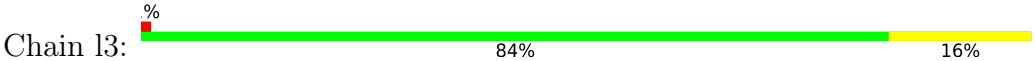
Chain L2:

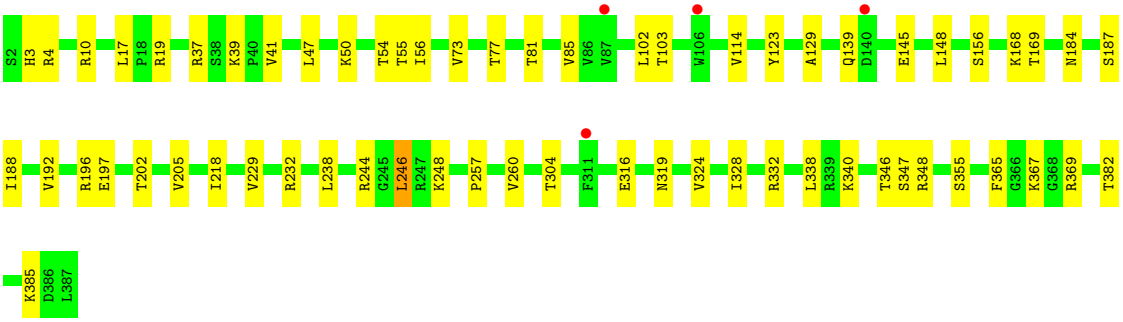




• Molecule 28: 60S ribosomal protein L3

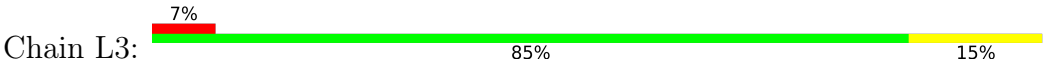
Chain l3:

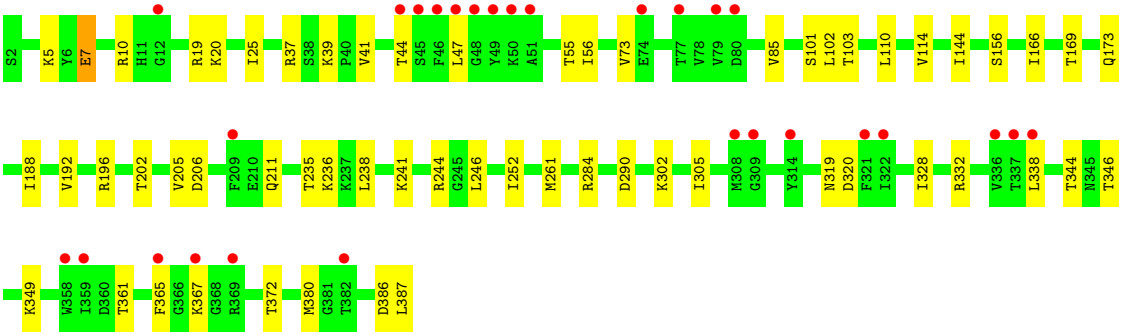




• Molecule 28: 60S ribosomal protein L3

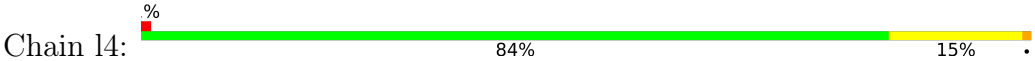
Chain L3:

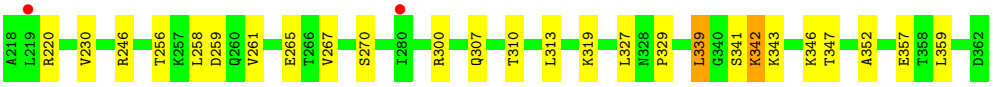




• Molecule 29: 60S ribosomal protein L4-A

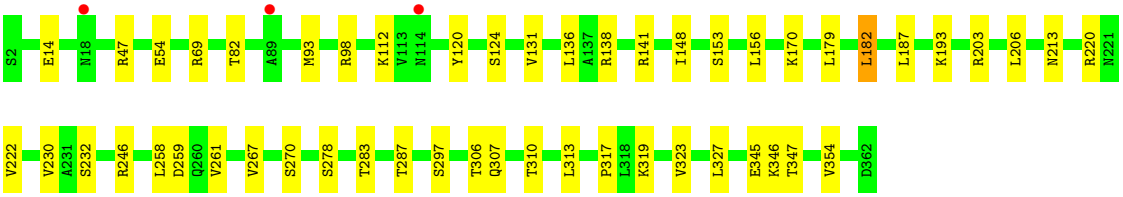
Chain l4:





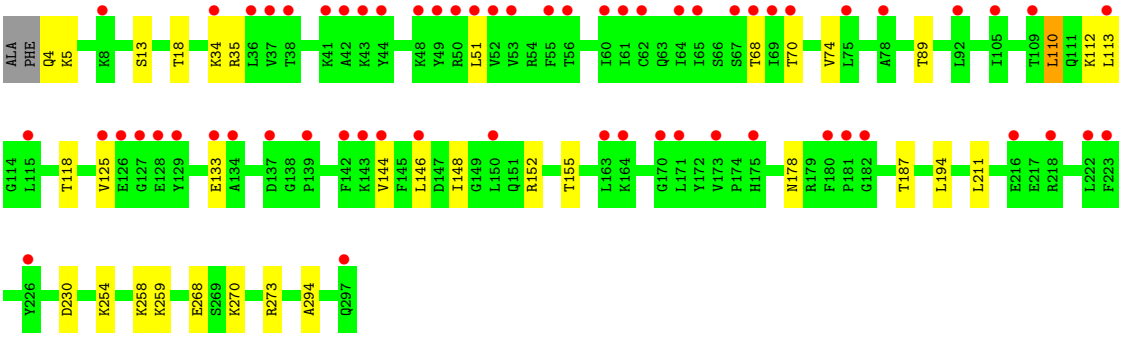
• Molecule 29: 60S ribosomal protein L4-A

Chain L4:



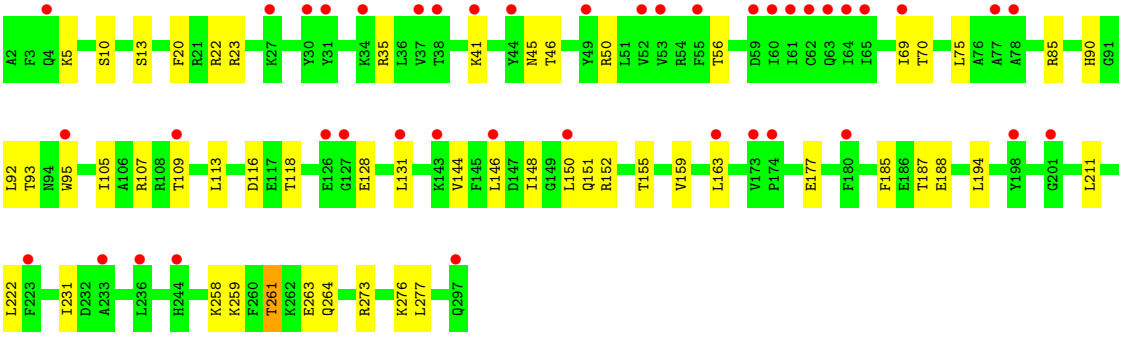
• Molecule 30: 60S ribosomal protein L5

Chain l5:



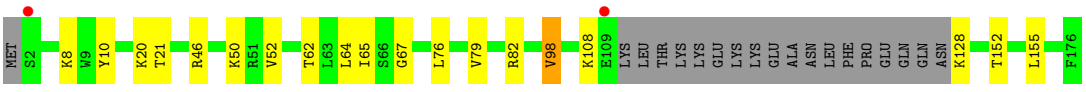
• Molecule 30: 60S ribosomal protein L5

Chain L5:



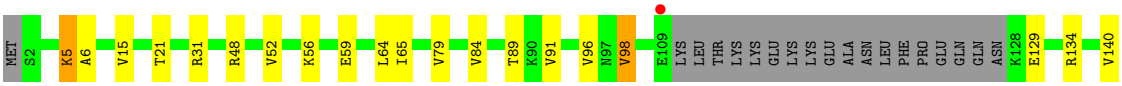
• Molecule 31: 60S ribosomal protein L6-A

Chain l6:



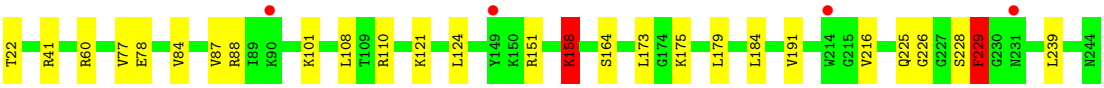
• Molecule 31: 60S ribosomal protein L6-A

Chain L6:



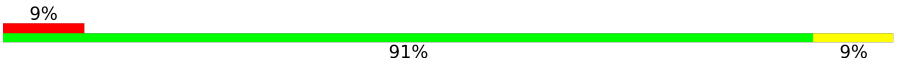
• Molecule 32: 60S ribosomal protein L7-A

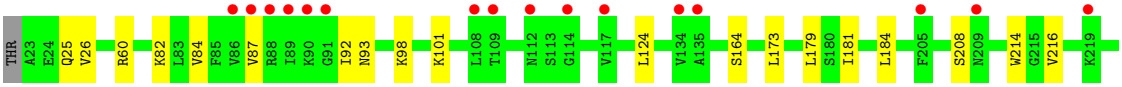
Chain l7:

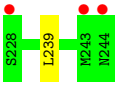


• Molecule 32: 60S ribosomal protein L7-A

Chain L7:

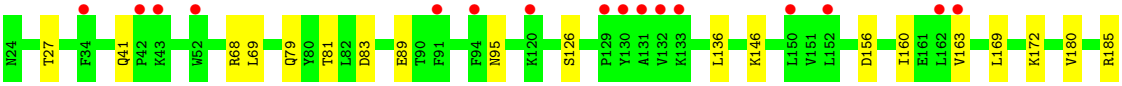


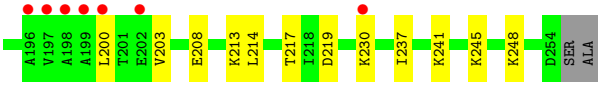




• Molecule 33: 60S ribosomal protein L8-A

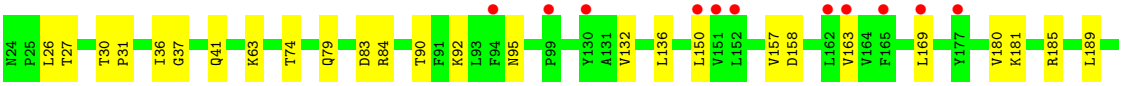
Chain l8:

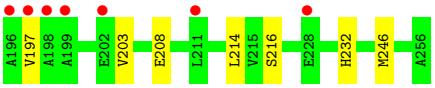




• Molecule 33: 60S ribosomal protein L8-A

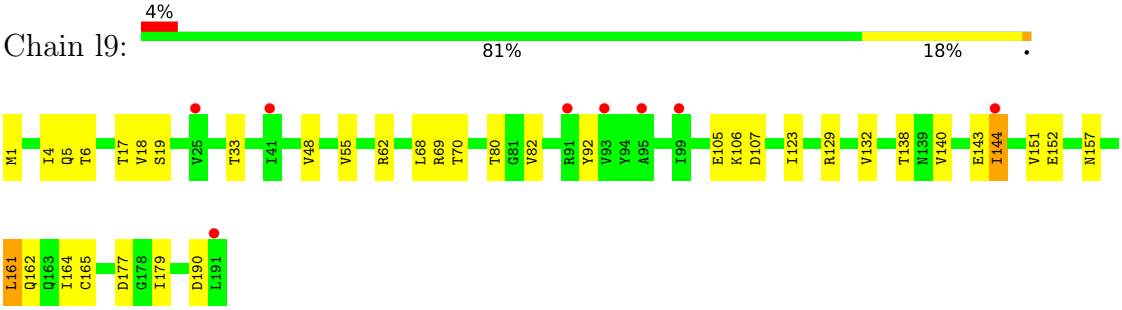
Chain L8:





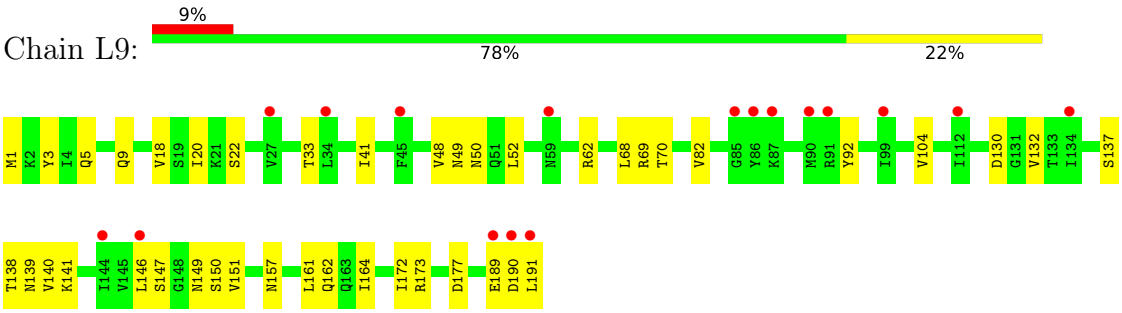
• Molecule 34: 60S ribosomal protein L9-A

Chain l9:



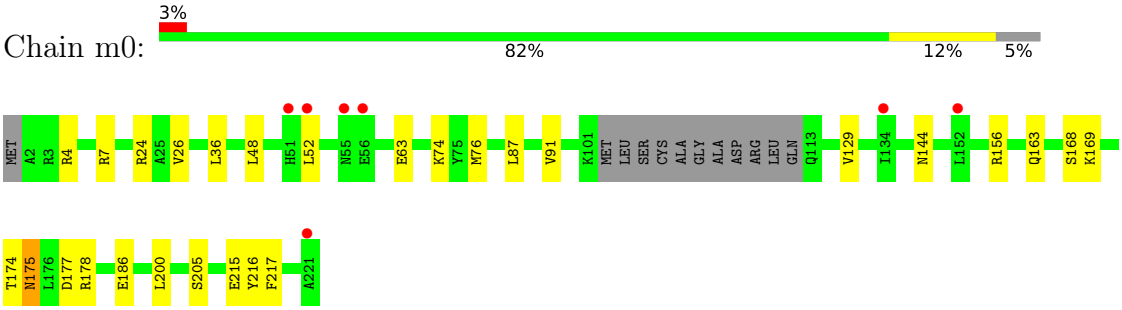
• Molecule 34: 60S ribosomal protein L9-A

Chain L9:



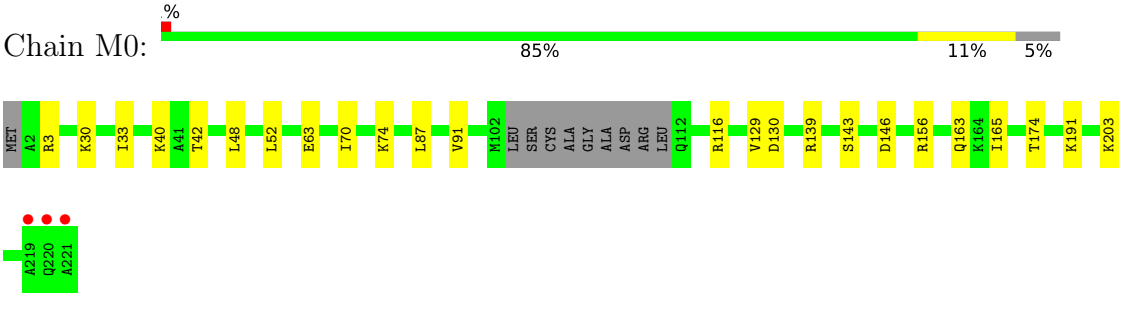
• Molecule 35: 60S ribosomal protein L10

Chain m0:



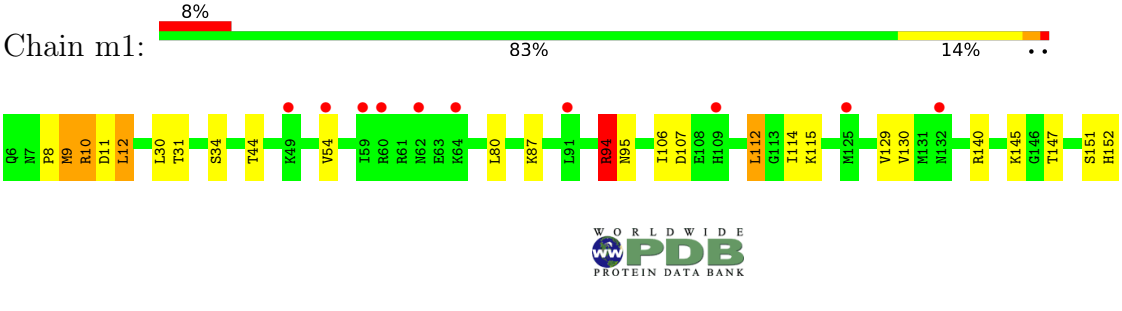
• Molecule 35: 60S ribosomal protein L10

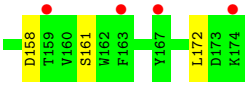
Chain M0:



• Molecule 36: 60S ribosomal protein L11-B

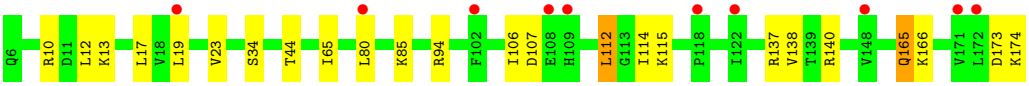
Chain m1:





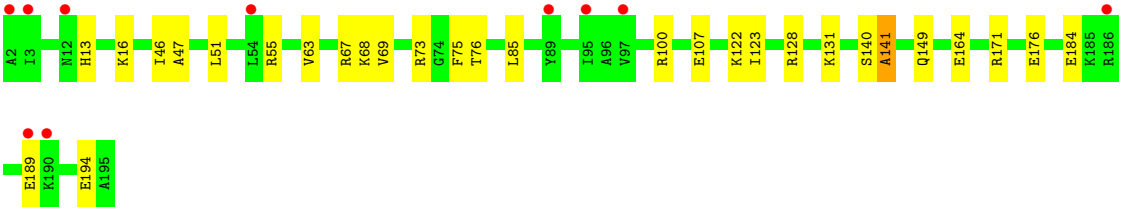
• Molecule 36: 60S ribosomal protein L11-B

Chain M1:



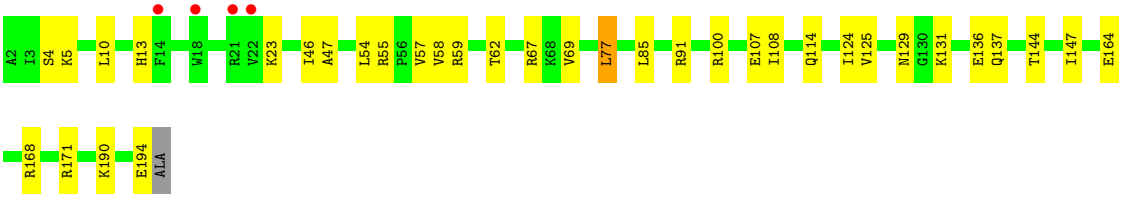
• Molecule 37: 60S ribosomal protein L13-A

Chain m3:



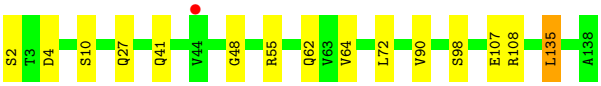
• Molecule 37: 60S ribosomal protein L13-A

Chain M3:



• Molecule 38: 60S ribosomal protein L14-A

Chain m4:

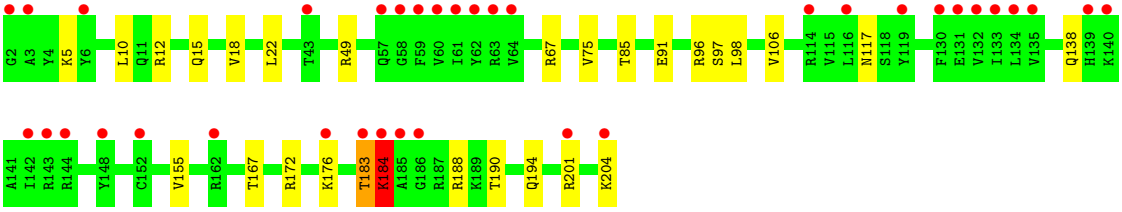


• Molecule 38: 60S ribosomal protein L14-A

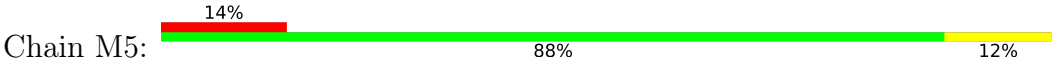
Chain M4:

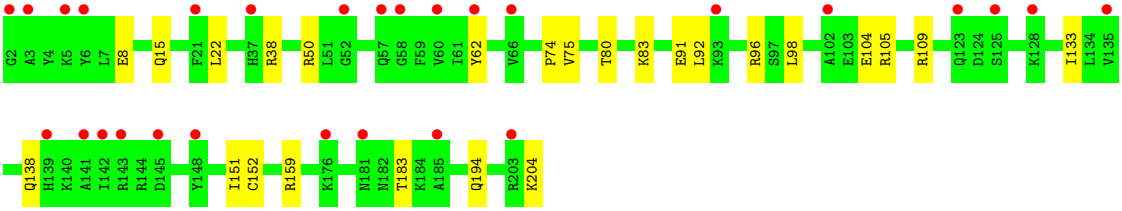
• Molecule 39: 60S ribosomal protein L15-A

Chain m5:

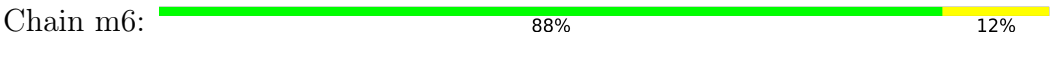


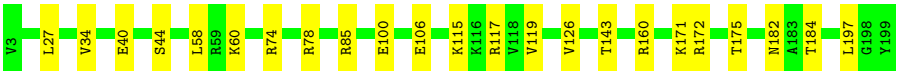
• Molecule 39: 60S ribosomal protein L15-A



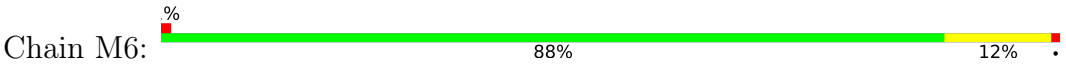


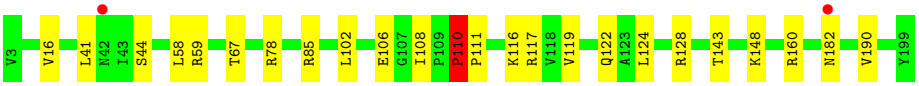
• Molecule 40: 60S ribosomal protein L16-A



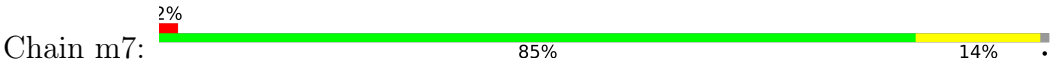


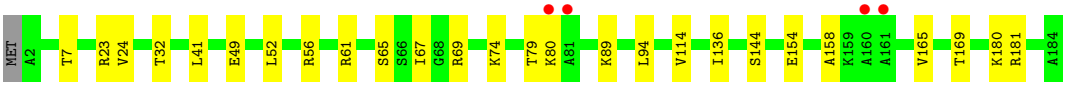
• Molecule 40: 60S ribosomal protein L16-A



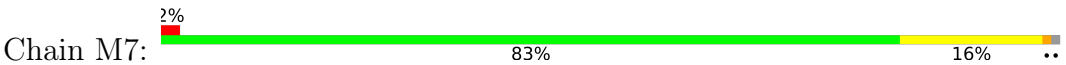


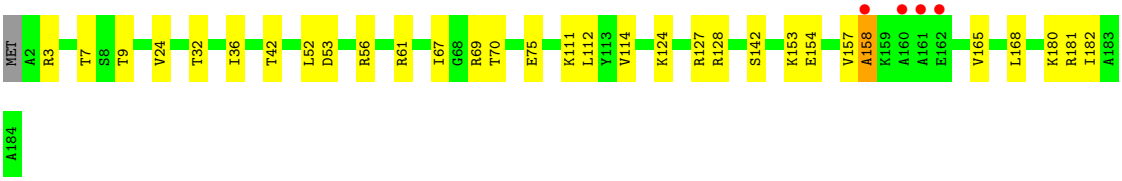
• Molecule 41: 60S ribosomal protein L17-A





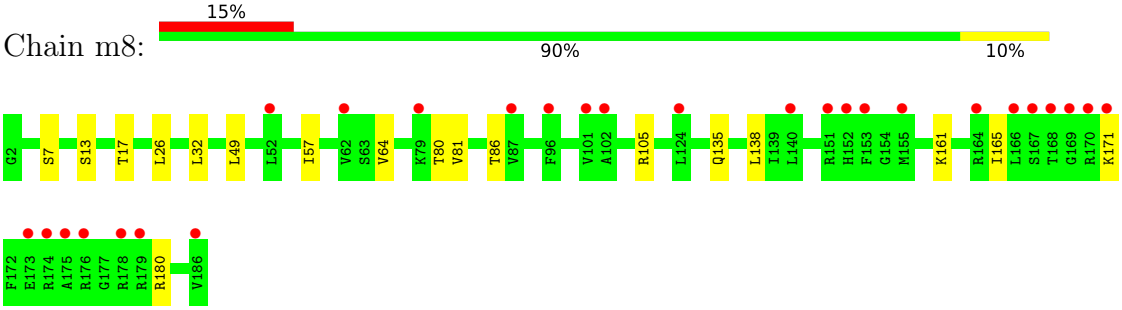
• Molecule 41: 60S ribosomal protein L17-A





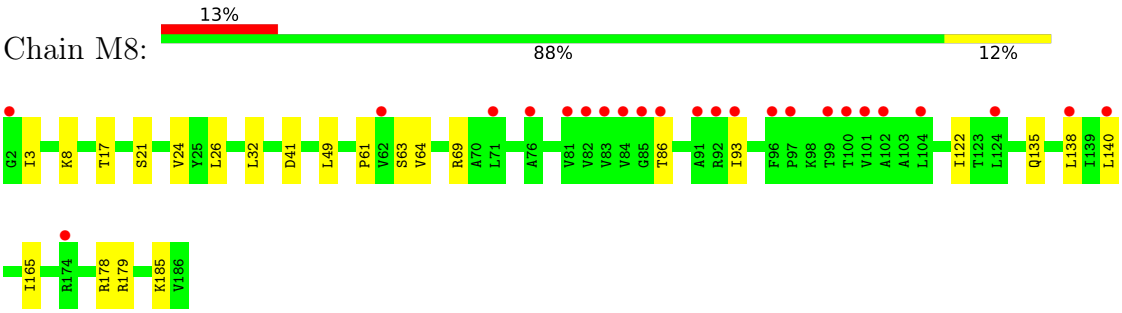
• Molecule 42: 60S ribosomal protein L18-A

Chain m8:



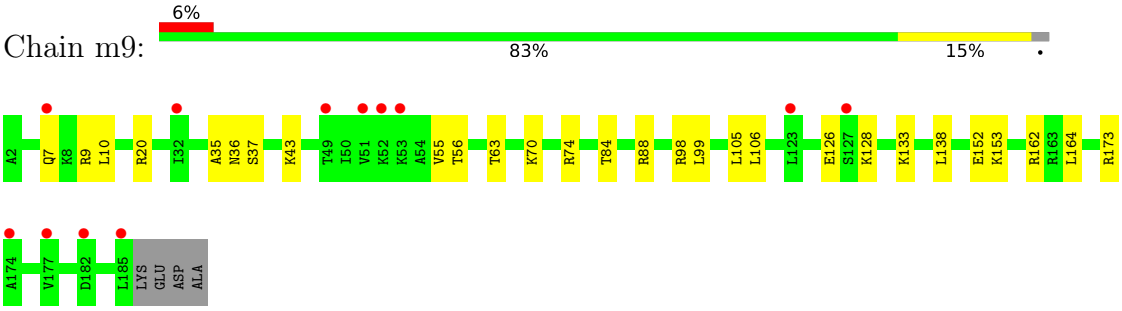
• Molecule 42: 60S ribosomal protein L18-A

Chain M8:



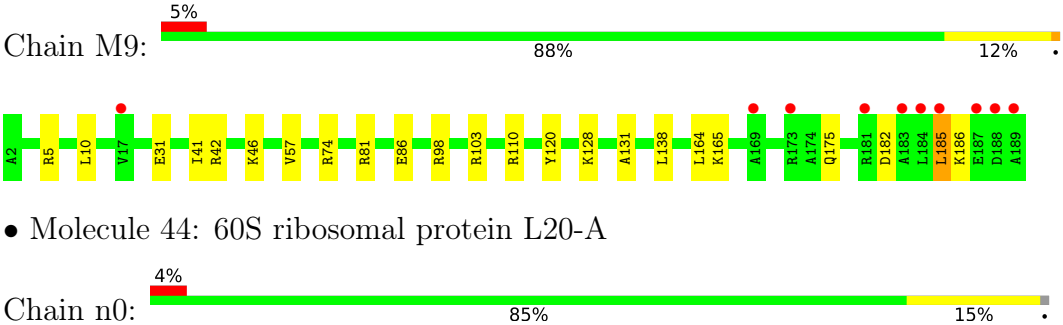
• Molecule 43: 60S ribosomal protein L19-A

Chain m9:



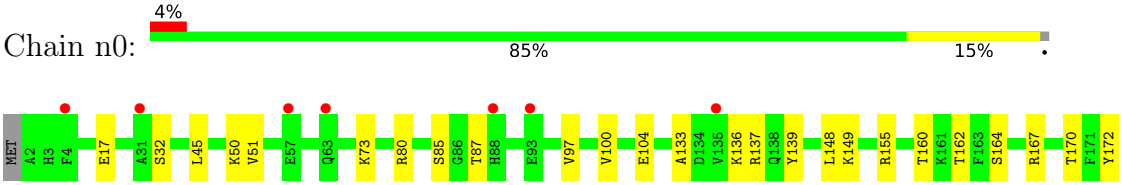
• Molecule 43: 60S ribosomal protein L19-A

Chain M9:



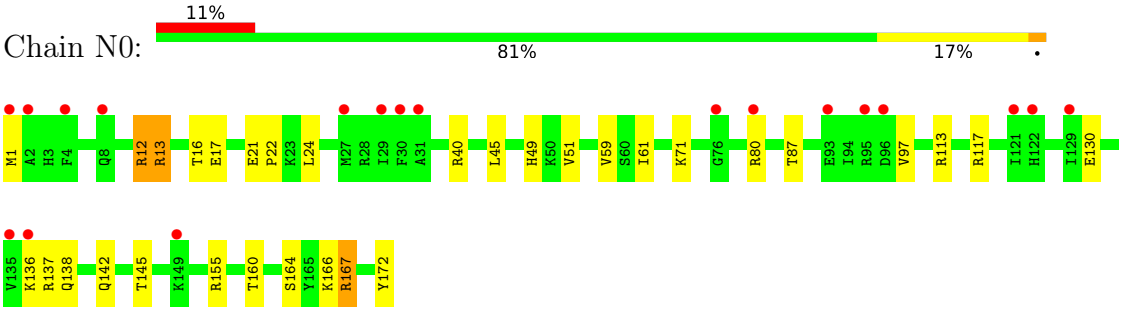
• Molecule 44: 60S ribosomal protein L20-A

Chain n0:



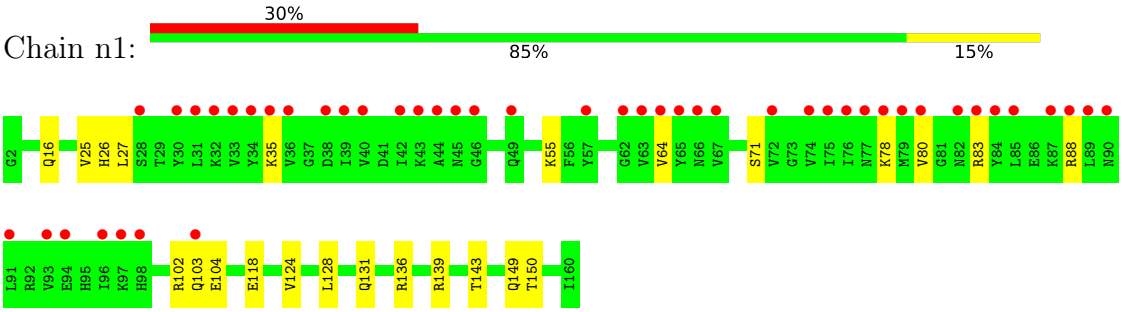
• Molecule 44: 60S ribosomal protein L20-A

Chain N0:



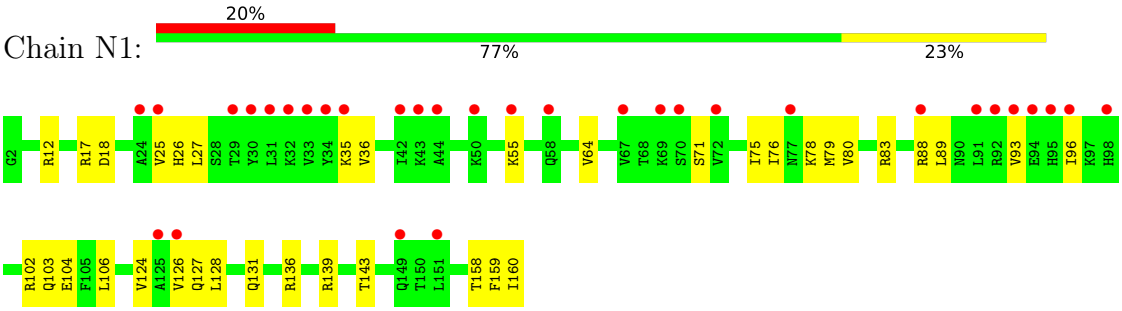
• Molecule 45: 60S ribosomal protein L21-A

Chain n1:



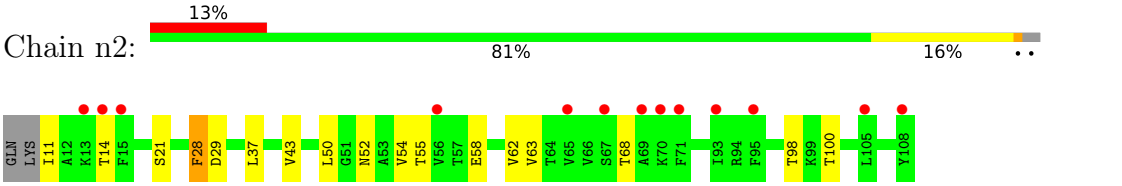
• Molecule 45: 60S ribosomal protein L21-A

Chain N1:



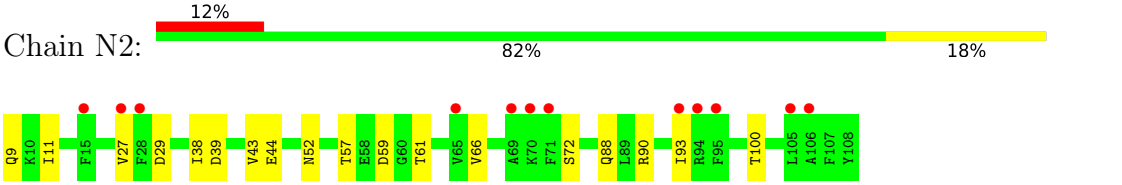
• Molecule 46: 60S ribosomal protein L22-A

Chain n2:



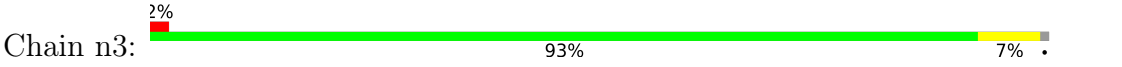
• Molecule 46: 60S ribosomal protein L22-A

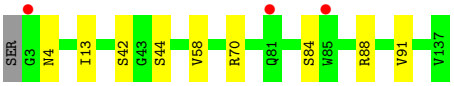
Chain N2:



• Molecule 47: 60S ribosomal protein L23-A

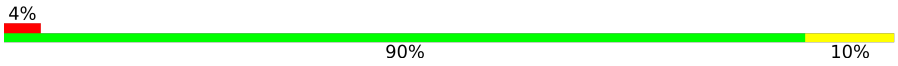
Chain n3:

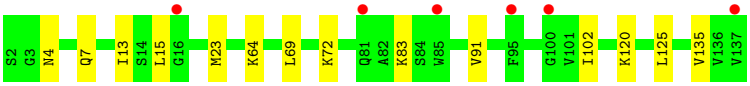




• Molecule 47: 60S ribosomal protein L23-A

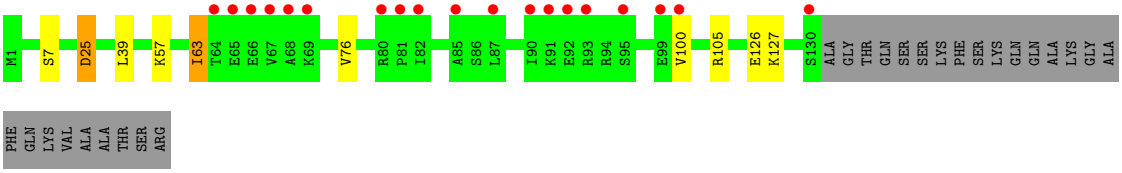
Chain N3:





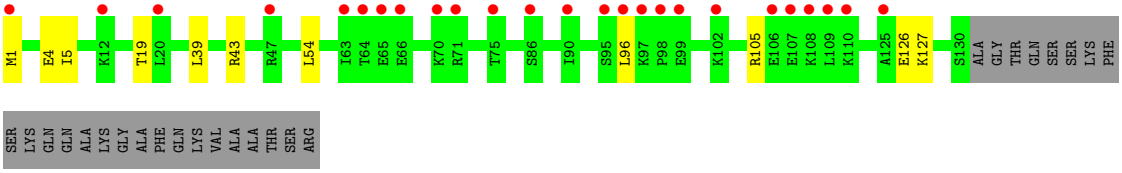
• Molecule 48: 60S ribosomal protein L24-A

Chain n4:



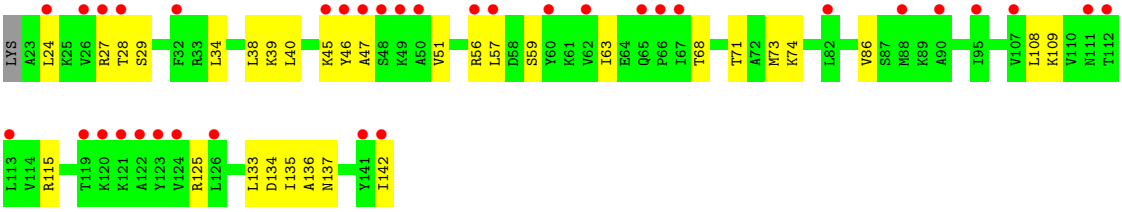
• Molecule 48: 60S ribosomal protein L24-A

Chain N4:



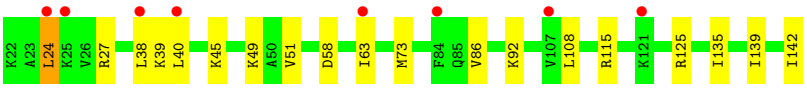
• Molecule 49: 60S ribosomal protein L25

Chain n5:



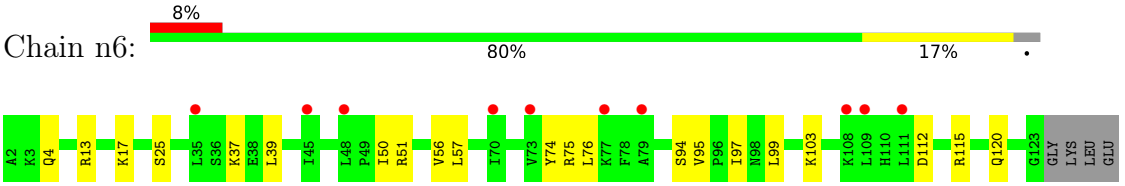
• Molecule 49: 60S ribosomal protein L25

Chain N5:



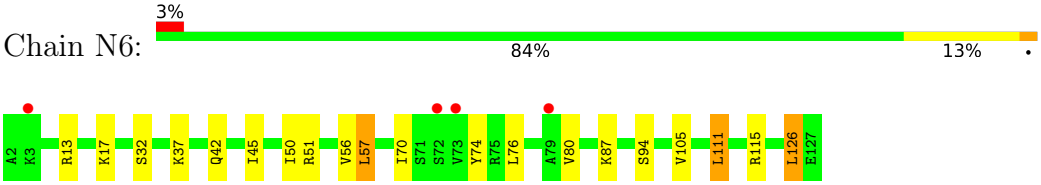
• Molecule 50: 60S ribosomal protein L26-A

Chain n6:



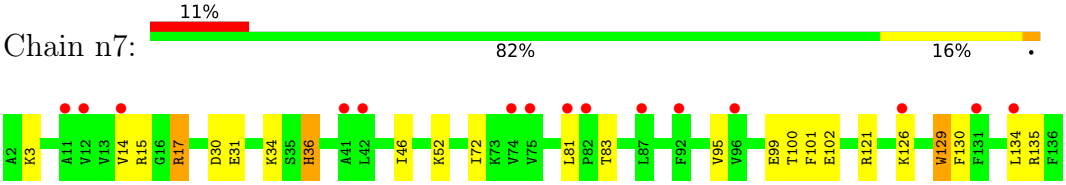
• Molecule 50: 60S ribosomal protein L26-A

Chain N6:



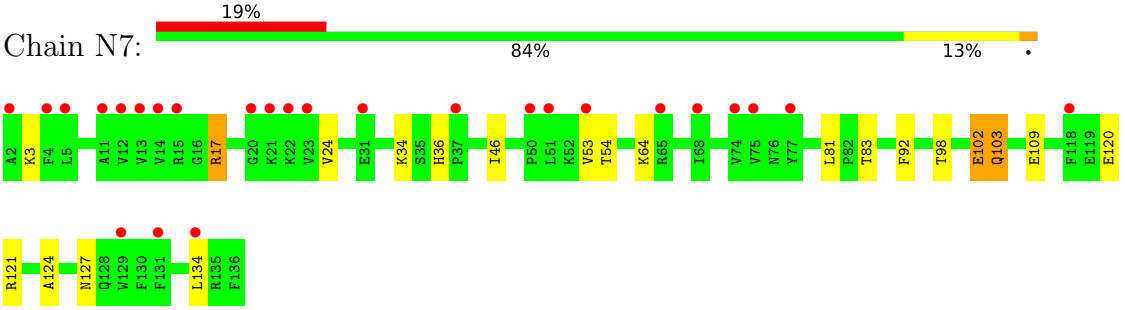
• Molecule 51: 60S ribosomal protein L27-A

Chain n7:



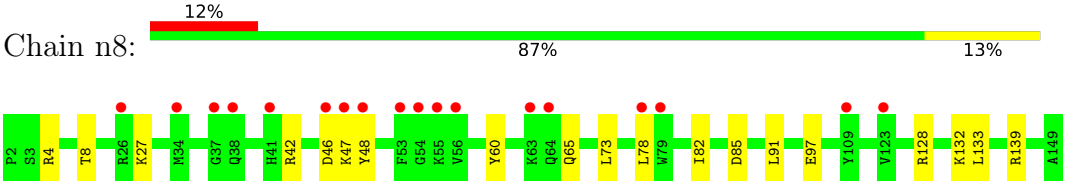
• Molecule 51: 60S ribosomal protein L27-A

Chain N7:



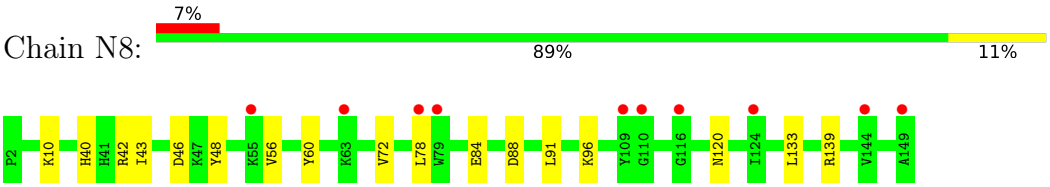
• Molecule 52: 60S ribosomal protein L28

Chain n8:



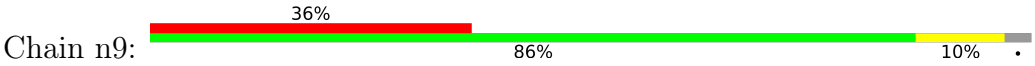
• Molecule 52: 60S ribosomal protein L28

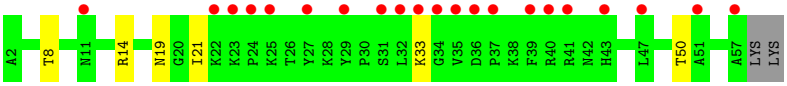
Chain N8:



• Molecule 53: 60S ribosomal protein L29

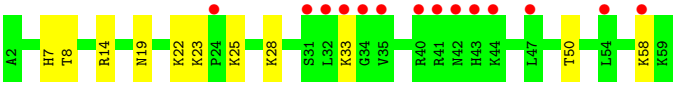
Chain n9:





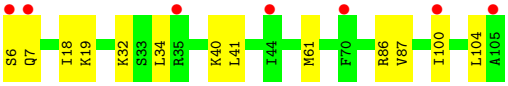
• Molecule 53: 60S ribosomal protein L29

Chain N9:



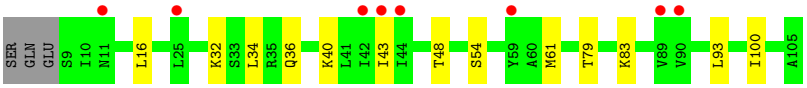
• Molecule 54: 60S ribosomal protein L30

Chain o0:



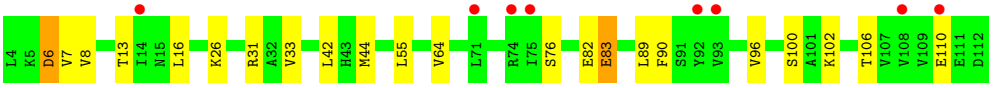
• Molecule 54: 60S ribosomal protein L30

Chain O0:



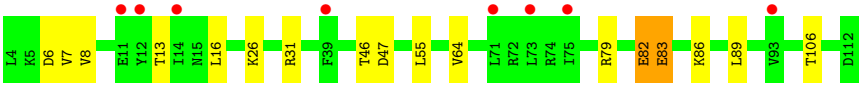
• Molecule 55: 60S ribosomal protein L31-A

Chain o1:



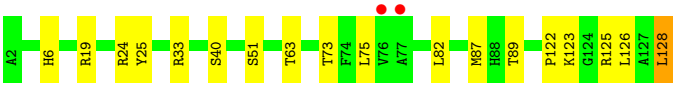
• Molecule 55: 60S ribosomal protein L31-A

Chain O1:



• Molecule 56: 60S ribosomal protein L32

Chain o2:

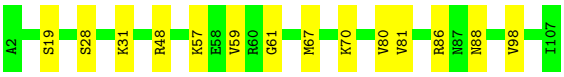


• Molecule 56: 60S ribosomal protein L32

Chain O2:

• Molecule 57: 60S ribosomal protein L33-A

Chain o3:

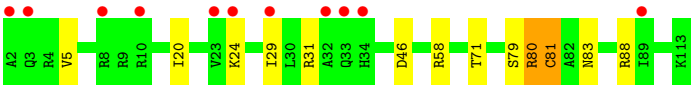


• Molecule 57: 60S ribosomal protein L33-A

Chain O3:

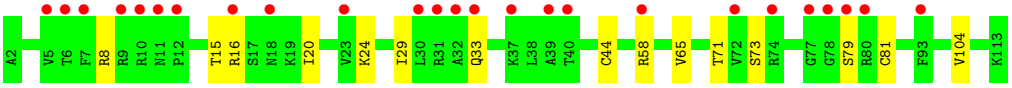
• Molecule 58: 60S ribosomal protein L34-A

Chain o4:



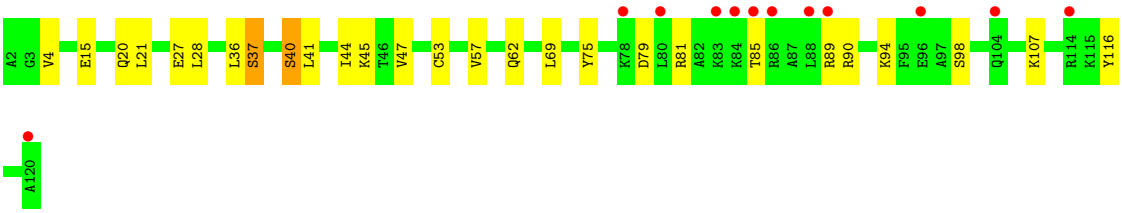
• Molecule 58: 60S ribosomal protein L34-A

Chain O4:



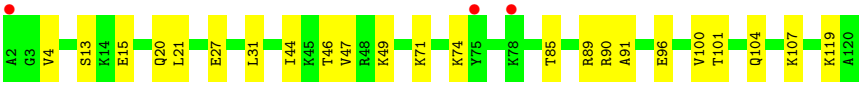
• Molecule 59: 60S ribosomal protein L35-A

Chain o5:



• Molecule 59: 60S ribosomal protein L35-A

Chain O5:

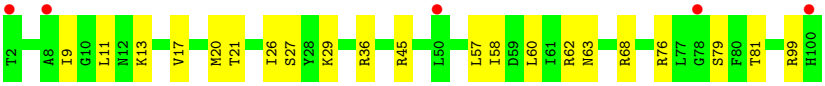


• Molecule 60: 60S ribosomal protein L36-A

Chain o6:

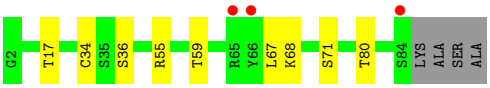
• Molecule 60: 60S ribosomal protein L36-A

Chain O6:



• Molecule 61: 60S ribosomal protein L37-A

Chain o7:

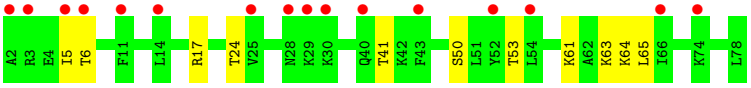


• Molecule 61: 60S ribosomal protein L37-A

Chain O7:

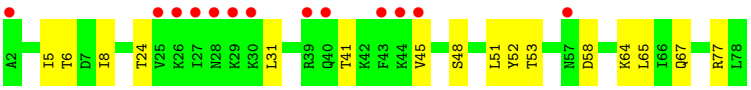
• Molecule 62: 60S ribosomal protein L38

Chain o8:



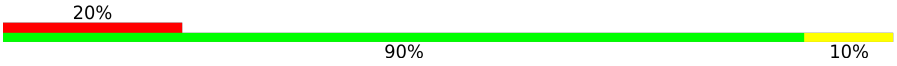
• Molecule 62: 60S ribosomal protein L38

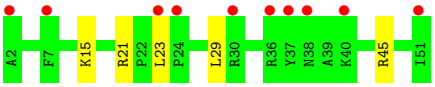
Chain O8:



• Molecule 63: 60S ribosomal protein L39

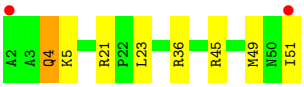
Chain o9:





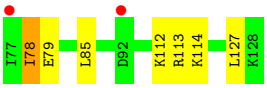
• Molecule 63: 60S ribosomal protein L39

Chain O9:



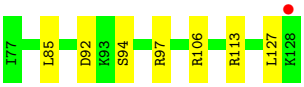
• Molecule 64: Ubiquitin-60S ribosomal protein L40

Chain q0:



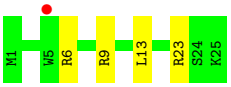
• Molecule 64: Ubiquitin-60S ribosomal protein L40

Chain Q0:



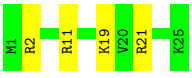
• Molecule 65: 60S ribosomal protein L41-A

Chain q1:



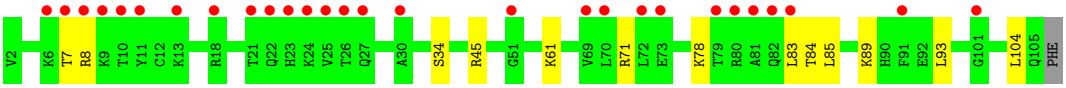
• Molecule 65: 60S ribosomal protein L41-A

Chain Q1:



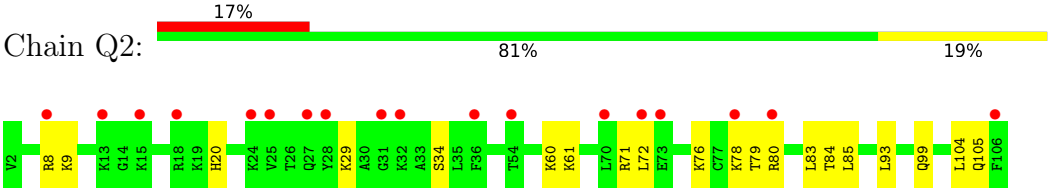
• Molecule 66: 60S ribosomal protein L42-A

Chain q2:



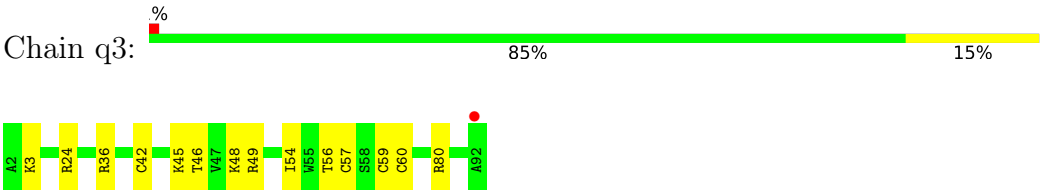
• Molecule 66: 60S ribosomal protein L42-A

Chain Q2:



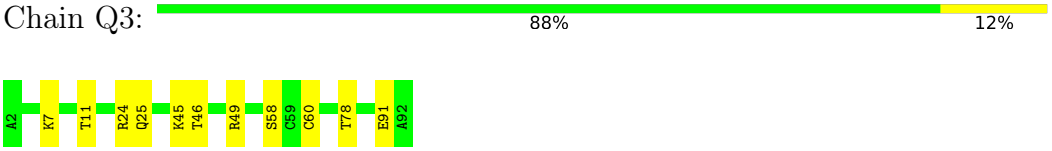
• Molecule 67: 60S ribosomal protein L43-A

Chain q3:



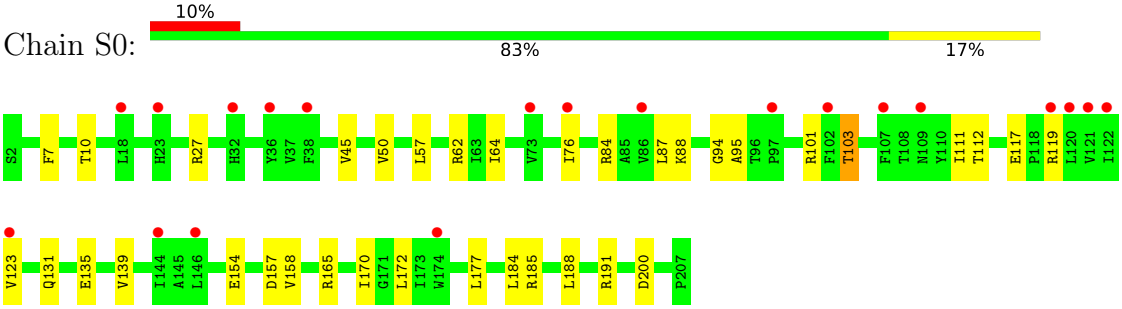
• Molecule 67: 60S ribosomal protein L43-A

Chain Q3:



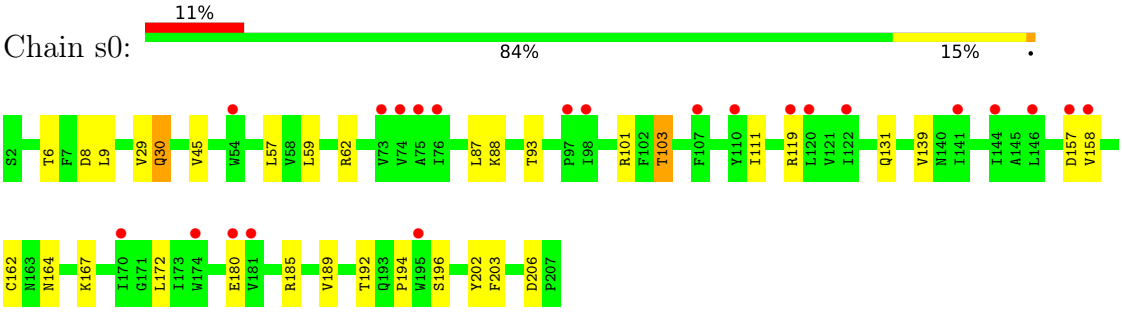
• Molecule 68: 40S ribosomal protein S0-A

Chain S0:



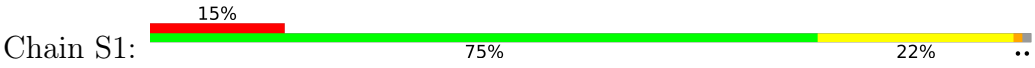
• Molecule 68: 40S ribosomal protein S0-A

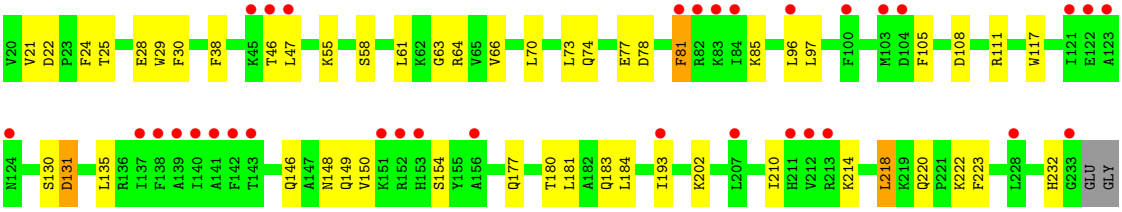
Chain s0:



• Molecule 69: 40S ribosomal protein S1-A

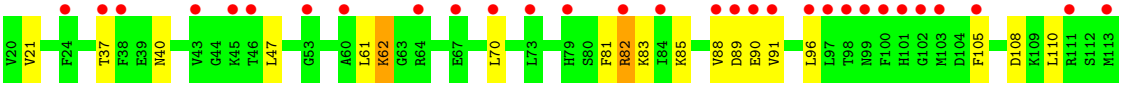
Chain S1:

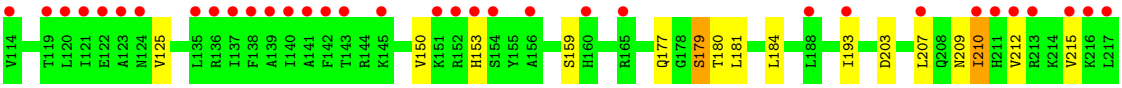




• Molecule 69: 40S ribosomal protein S1-A

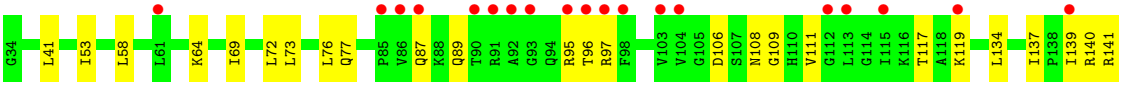
Chain s1:

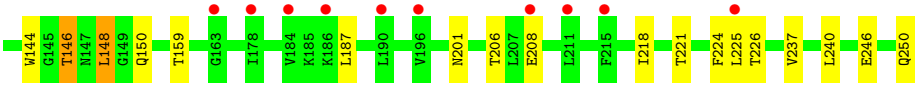




• Molecule 70: 40S ribosomal protein S2

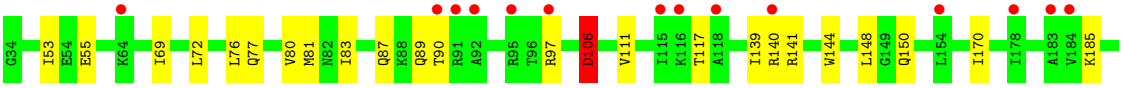
Chain S2:

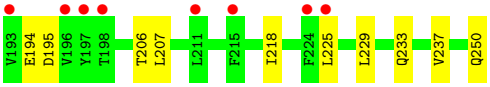




• Molecule 70: 40S ribosomal protein S2

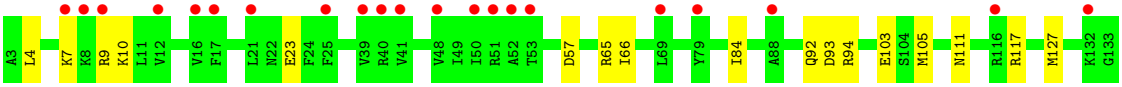
Chain s2:

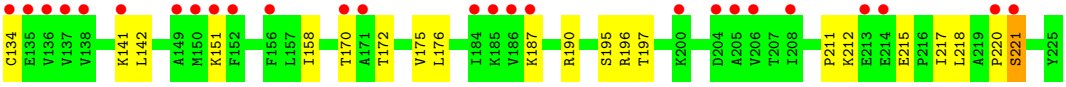




• Molecule 71: 40S ribosomal protein S3

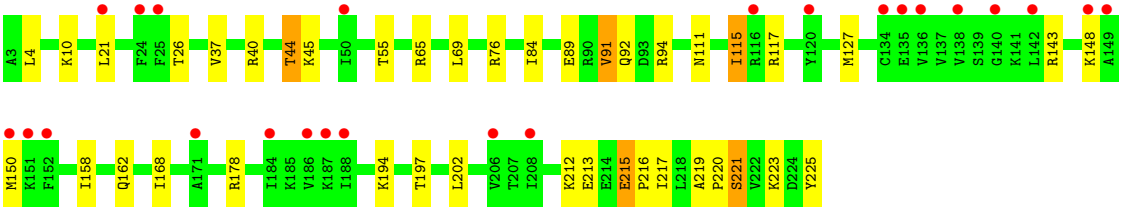
Chain S3:





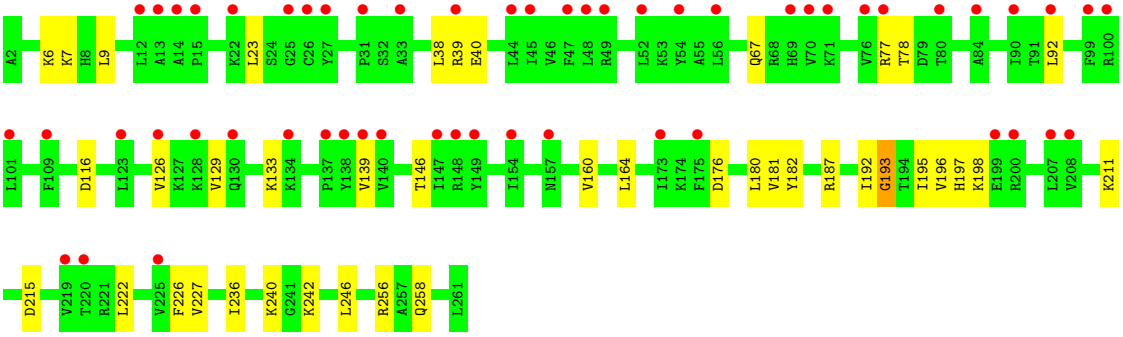
• Molecule 71: 40S ribosomal protein S3

Chain s3:



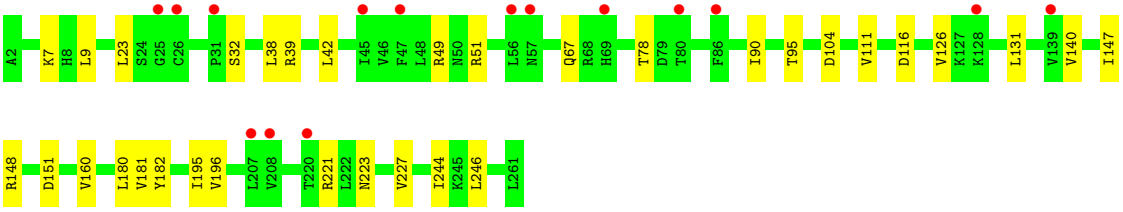
• Molecule 72: 40S ribosomal protein S4-A

Chain S4:



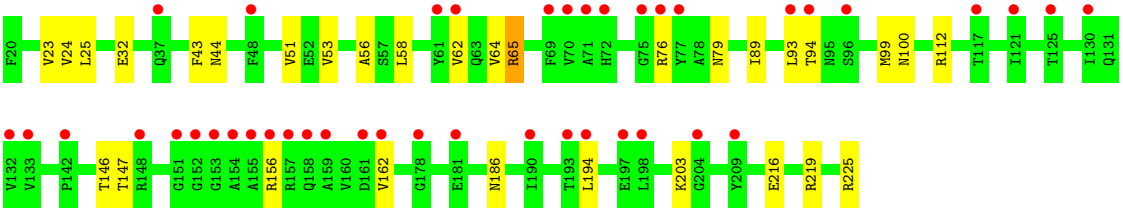
• Molecule 72: 40S ribosomal protein S4-A

Chain s4:



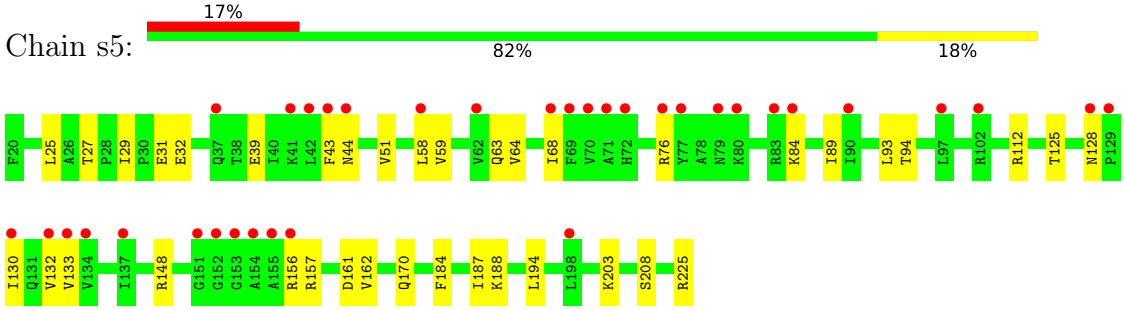
• Molecule 73: 40S ribosomal protein S5

Chain S5:



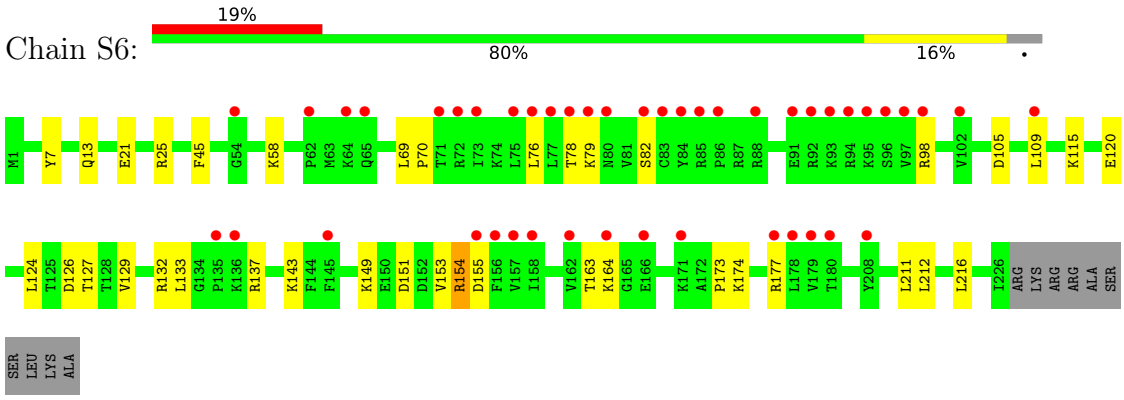
• Molecule 73: 40S ribosomal protein S5

Chain s5:



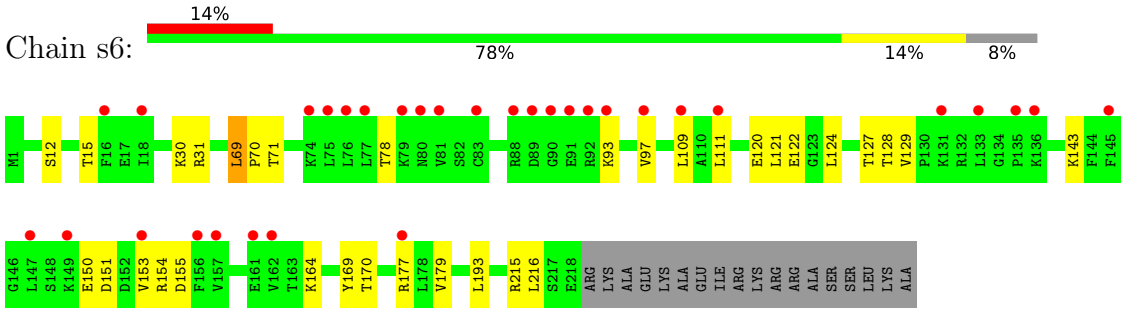
• Molecule 74: 40S ribosomal protein S6-A

Chain S6:



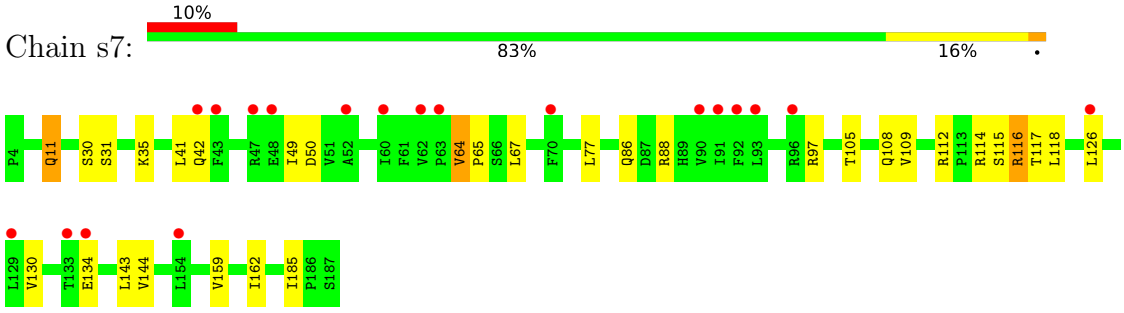
• Molecule 74: 40S ribosomal protein S6-A

Chain s6:



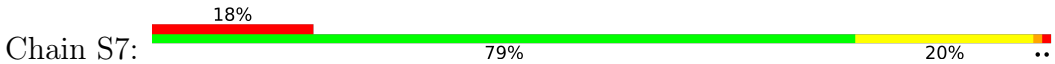
• Molecule 75: 40S ribosomal protein S7-A

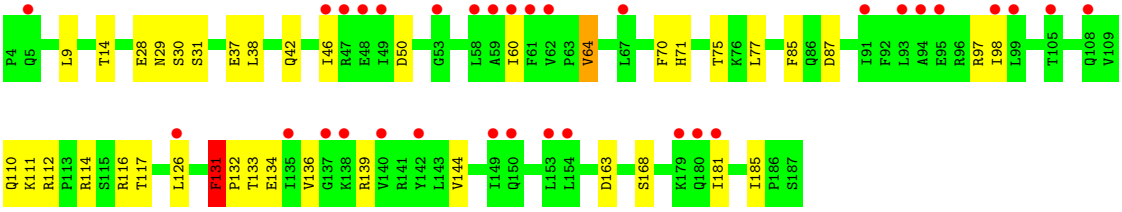
Chain s7:



• Molecule 75: 40S ribosomal protein S7-A

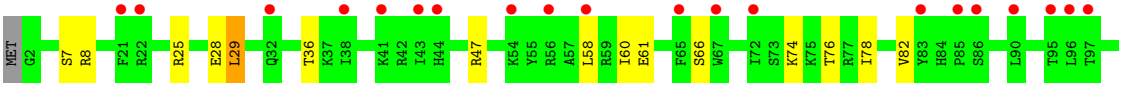
Chain S7:

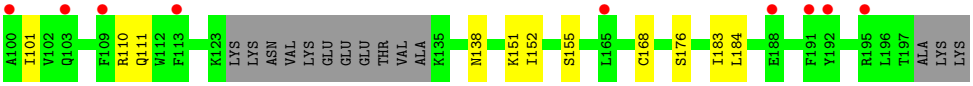




• Molecule 76: 40S ribosomal protein S8-A

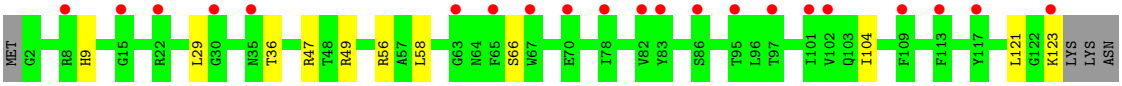
Chain s8:

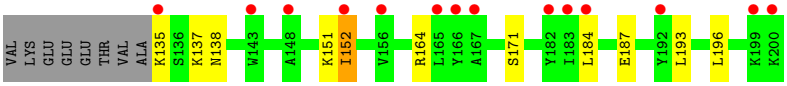




• Molecule 76: 40S ribosomal protein S8-A

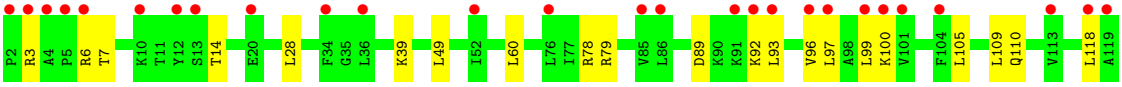
Chain S8:

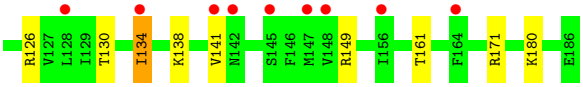




• Molecule 77: 40S ribosomal protein S9-A

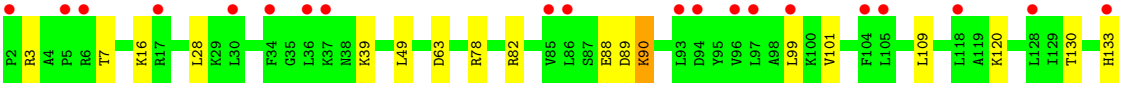
Chain S9:

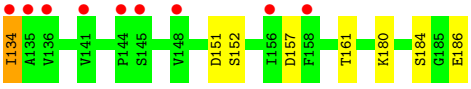




• Molecule 77: 40S ribosomal protein S9-A

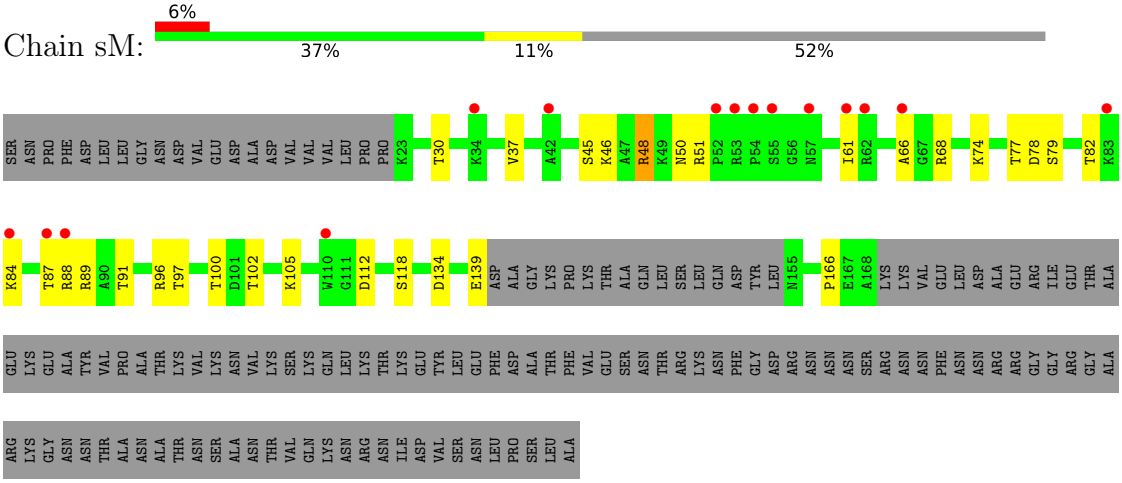
Chain s9:





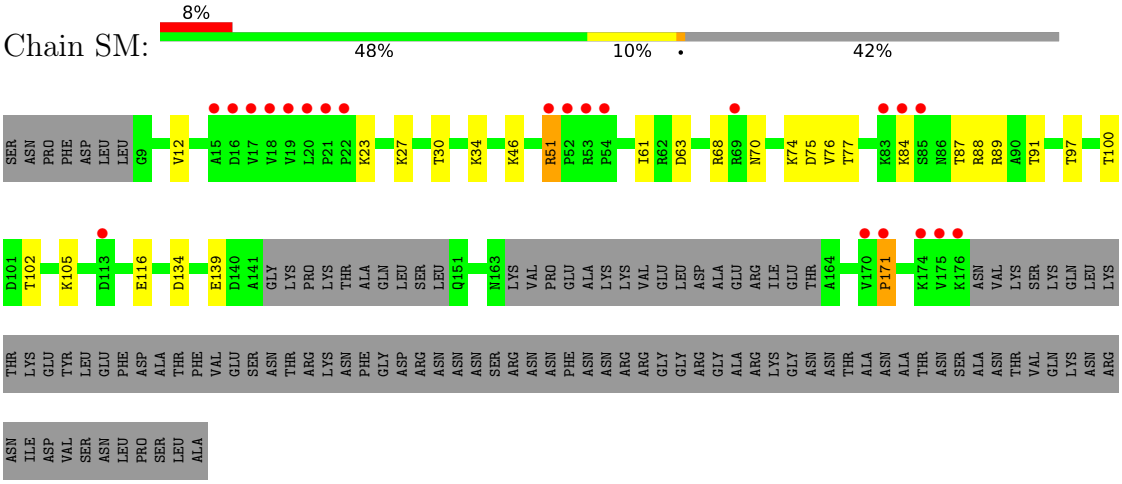
• Molecule 78: Suppressor protein STM1

Chain sM:



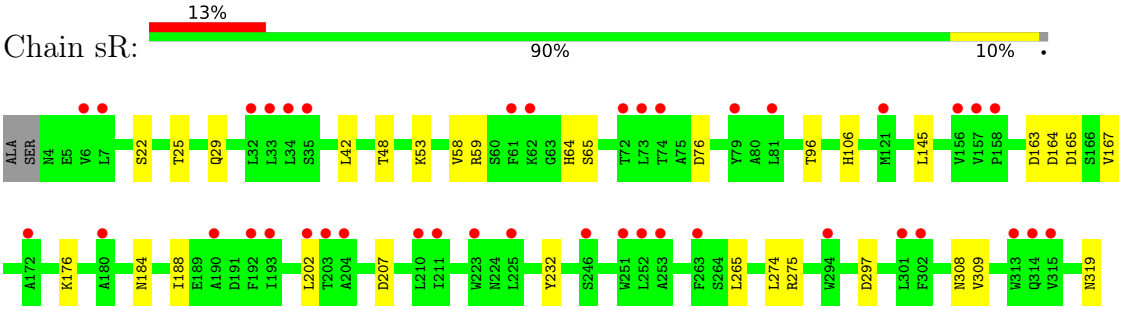
• Molecule 78: Suppressor protein STM1

Chain SM:



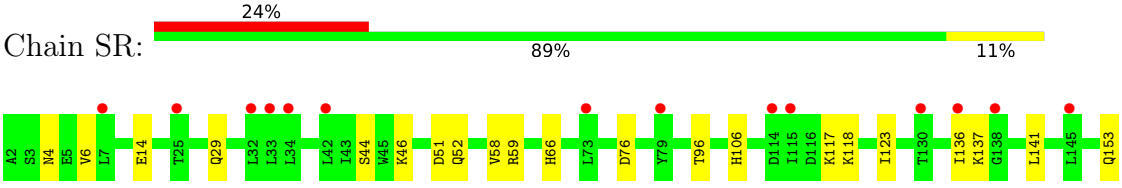
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

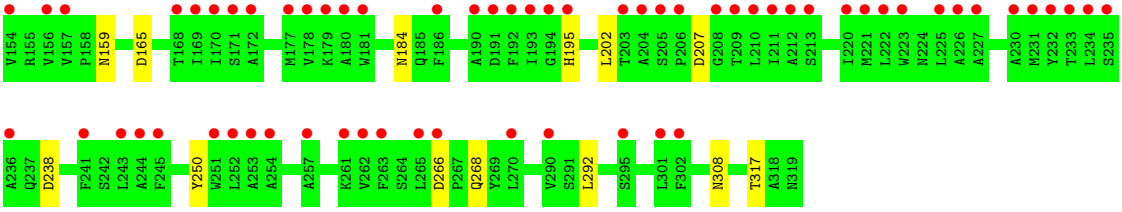
Chain sR:



• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:




V154 R155 V156 V157 P158 N159 D165 T168 I169 I170 S171 A172 M177 V178 K179 A180 W181 N184 Q185 F186 A190 D191 F192 I193 G194 H195 L202 T203 A204 S205 P206 D207 G208 T209 L210 I211 A212 S213 I220 M221 L222 W223 N224 L225 A226 A227 A230 M231 Y232 T233 L234 S235
A236 Q237 D238 F241 S242 L243 A244 F245 Y250 W251 L252 A253 A254 A257 K261 V262 F263 S264 L265 D266 P267 Q268 Y269 L270 V290 S291 L292 S295 L301 F302 N308 T317 A318 N319

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	442.14Å 298.76Å 299.77Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	147.83 – 3.70 147.83 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.83-3.70) 92.7 (147.83-3.70)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.235 0.192 , 0.235	Depositor DCC
R_{free} test set	16291 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	118.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 98.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	400111	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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, 8UZ, MG

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	1	0.92	42/73963 (0.1%)	1.53	1261/115306 (1.1%)
1	5	0.84	20/73738 (0.0%)	1.45	984/114951 (0.9%)
2	2	0.68	6/42154 (0.0%)	1.30	354/65680 (0.5%)
2	6	0.68	4/41349 (0.0%)	1.29	326/64423 (0.5%)
3	3	0.81	0/2883	1.42	33/4491 (0.7%)
3	7	0.66	0/2883	1.16	10/4491 (0.2%)
4	4	0.84	0/3746	1.47	52/5832 (0.9%)
4	8	0.81	0/3746	1.44	41/5832 (0.7%)
5	C0	0.39	0/789	0.66	1/1067 (0.1%)
5	c0	0.35	0/762	0.68	2/1029 (0.2%)
6	C1	0.51	0/1233	0.69	1/1665 (0.1%)
6	c1	0.49	0/1194	0.69	0/1610
7	C2	0.36	0/873	0.71	1/1185 (0.1%)
7	c2	0.35	0/898	0.67	0/1220
8	C3	0.46	0/1215	0.66	0/1638
8	c3	0.44	0/1215	0.60	0/1638
9	C4	0.41	0/901	0.71	2/1217 (0.2%)
9	c4	0.37	0/960	0.61	0/1290
10	C5	0.48	1/998 (0.1%)	0.63	0/1341
10	c5	0.42	0/1008	0.68	0/1353
11	C6	0.49	1/1125 (0.1%)	0.66	1/1510 (0.1%)
11	c6	0.56	1/1125 (0.1%)	0.64	0/1510
12	C7	0.40	0/935	0.73	2/1254 (0.2%)
12	c7	0.40	0/935	0.62	0/1255
13	C8	0.45	0/1211	0.71	1/1628 (0.1%)
13	c8	0.43	0/1211	0.69	1/1628 (0.1%)
14	C9	0.41	0/1130	0.63	1/1517 (0.1%)
14	c9	0.42	0/1130	0.60	0/1517
15	D0	0.42	0/851	0.64	1/1150 (0.1%)
15	d0	0.40	0/838	0.62	0/1133
16	D1	0.50	0/693	0.66	0/935
16	d1	0.46	0/693	0.63	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	D2	0.44	0/1038	0.70	4/1395 (0.3%)
17	d2	0.44	0/1038	0.65	1/1395 (0.1%)
18	D3	0.52	0/1139	0.73	0/1518
18	d3	0.48	0/1139	0.70	0/1518
19	D4	0.41	0/1087	0.63	1/1449 (0.1%)
19	d4	0.42	0/1087	0.68	0/1449
20	D5	0.41	0/571	0.71	0/768
20	d5	0.35	0/566	0.63	1/761 (0.1%)
21	D6	0.50	0/782	0.82	2/1047 (0.2%)
21	d6	0.42	0/782	0.63	0/1047
22	D7	0.36	0/620	0.65	1/838 (0.1%)
22	d7	0.40	0/620	0.66	0/838
23	D8	0.40	0/499	0.63	0/670
23	d8	0.68	1/499 (0.2%)	0.66	1/670 (0.1%)
24	D9	0.57	0/443	0.70	0/588
24	d9	0.54	0/452	0.72	1/600 (0.2%)
25	E0	0.43	0/483	0.66	0/643
25	e0	0.45	0/490	0.67	0/653
26	E1	0.46	0/577	0.88	3/770 (0.4%)
26	e1	0.42	0/597	0.81	1/795 (0.1%)
27	L2	0.53	0/1948	0.73	1/2617 (0.0%)
27	l2	0.55	0/1946	0.71	0/2614
28	L3	0.60	2/3146 (0.1%)	0.71	0/4228
28	l3	0.58	0/3146	0.71	1/4228 (0.0%)
29	L4	0.57	0/2800	0.75	0/3790
29	l4	0.53	0/2800	0.71	1/3790 (0.0%)
30	L5	0.50	0/2425	0.65	0/3271
30	l5	0.38	0/2408	0.55	1/3248 (0.0%)
31	L6	0.59	0/1269	0.72	0/1705
31	l6	0.59	0/1269	0.70	0/1705
32	L7	0.57	1/1821 (0.1%)	0.67	0/2451
32	l7	0.55	0/1828	0.67	1/2461 (0.0%)
33	L8	0.47	1/1836 (0.1%)	0.62	0/2481
33	l8	0.41	0/1796	0.61	1/2430 (0.0%)
34	L9	0.54	0/1539	0.70	1/2073 (0.0%)
34	l9	0.54	0/1539	0.70	1/2073 (0.0%)
35	M0	0.59	0/1741	0.74	0/2335
35	m0	0.53	0/1732	0.69	0/2323
36	M1	0.46	0/1374	0.69	1/1842 (0.1%)
36	m1	0.37	0/1374	0.61	1/1842 (0.1%)
37	M3	0.54	1/1568 (0.1%)	0.70	0/2106
37	m3	0.49	0/1573	0.68	1/2113 (0.0%)
38	M4	0.50	0/1068	0.64	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	m4	0.53	0/1074	0.68	1/1446 (0.1%)
39	M5	0.58	2/1757 (0.1%)	0.70	0/2354
39	m5	0.51	0/1757	0.71	0/2354
40	M6	0.66	0/1585	0.69	0/2128
40	m6	0.70	0/1585	0.74	1/2128 (0.0%)
41	M7	0.59	0/1443	0.76	0/1944
41	m7	0.59	0/1443	0.75	0/1944
42	M8	0.50	0/1465	0.71	0/1965
42	m8	0.45	0/1465	0.65	0/1965
43	M9	0.48	0/1538	0.65	1/2050 (0.0%)
43	m9	0.45	0/1507	0.60	0/2009
44	N0	0.57	0/1481	0.69	1/1990 (0.1%)
44	n0	0.56	0/1473	0.66	0/1980
45	N1	0.51	0/1300	0.65	0/1743
45	n1	0.49	0/1300	0.60	0/1743
46	N2	0.46	0/812	0.64	0/1099
46	n2	0.41	0/794	0.57	1/1076 (0.1%)
47	N3	0.62	0/1018	0.73	1/1369 (0.1%)
47	n3	0.60	0/1012	0.75	0/1361
48	N4	0.50	0/978	0.60	0/1302
48	n4	0.49	0/1021	0.60	0/1356
49	N5	0.48	0/979	0.69	0/1321
49	n5	0.48	0/974	0.72	0/1314
50	N6	0.55	0/1004	0.76	3/1341 (0.2%)
50	n6	0.57	1/974 (0.1%)	0.73	0/1302
51	N7	0.47	1/1118 (0.1%)	0.60	0/1497
51	n7	0.77	1/1118 (0.1%)	0.62	0/1497
52	N8	0.54	0/1204	0.74	0/1612
52	n8	0.49	0/1204	0.71	0/1612
53	N9	0.52	0/473	0.65	0/629
53	n9	0.43	0/455	0.68	0/607
54	O0	0.46	0/751	0.63	0/1008
54	o0	0.41	0/775	0.62	1/1040 (0.1%)
55	O1	0.58	0/890	0.70	0/1196
55	o1	0.56	0/897	0.69	0/1205
56	O2	0.57	0/1041	0.74	0/1394
56	o2	0.56	0/1041	0.74	1/1394 (0.1%)
57	O3	0.62	0/868	0.78	0/1168
57	o3	0.66	0/868	0.76	1/1168 (0.1%)
58	O4	0.48	0/890	0.64	0/1189
58	o4	0.45	0/890	0.62	0/1189
59	O5	0.52	0/978	0.66	0/1301
59	o5	0.56	2/974 (0.2%)	0.65	0/1297

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	O6	0.48	0/778	0.66	0/1034
60	o6	0.46	0/777	0.65	0/1033
61	O7	0.65	2/696 (0.3%)	0.79	0/923
61	o7	0.60	0/671	0.76	0/890
62	O8	0.44	0/618	0.59	0/826
62	o8	0.42	0/614	0.59	0/822
63	O9	0.56	0/443	0.75	0/588
63	o9	0.51	0/443	0.64	0/588
64	Q0	0.60	0/423	0.78	0/562
64	q0	0.59	0/423	0.77	0/562
65	Q1	0.59	0/234	0.77	0/300
65	q1	0.55	0/234	0.69	0/300
66	Q2	0.54	0/860	0.75	0/1136
66	q2	0.45	0/848	0.61	0/1120
67	Q3	0.59	0/701	0.68	0/934
67	q3	0.48	0/701	0.70	0/934
68	S0	0.42	0/1617	0.61	0/2215
68	s0	0.42	1/1623 (0.1%)	0.62	0/2222
69	S1	0.39	0/1735	0.68	2/2335 (0.1%)
69	s1	0.36	0/1748	0.62	0/2352
70	S2	0.44	0/1665	0.66	0/2263
70	s2	0.43	0/1665	0.63	0/2263
71	S3	0.45	0/1759	0.60	0/2368
71	s3	0.42	0/1759	0.62	0/2368
72	S4	0.41	0/2109	0.66	1/2839 (0.0%)
72	s4	0.43	0/2109	0.67	0/2839
73	S5	0.38	0/1629	0.58	0/2202
73	s5	0.42	0/1629	0.60	0/2202
74	S6	0.40	0/1823	0.57	0/2439
74	s6	0.43	0/1779	0.61	0/2379
75	S7	0.42	0/1506	0.68	1/2028 (0.0%)
75	s7	0.39	0/1506	0.68	1/2028 (0.0%)
76	S8	0.44	0/1514	0.65	1/2021 (0.0%)
76	s8	0.46	0/1491	0.65	1/1992 (0.1%)
77	S9	0.41	0/1519	0.61	0/2035
77	s9	0.42	0/1519	0.61	1/2035 (0.0%)
78	SM	0.44	0/1113	0.70	2/1502 (0.1%)
78	sM	0.43	0/964	0.67	2/1291 (0.2%)
79	SR	0.33	0/2490	0.57	0/3389
79	sR	0.37	0/2480	0.59	1/3376 (0.0%)
All	All	0.70	91/425229 (0.0%)	1.19	3127/623929 (0.5%)

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
5	c0	0	1
7	C2	0	2
7	c2	0	1
9	C4	0	2
9	c4	0	1
10	C5	0	1
10	c5	0	3
11	C6	0	2
11	c6	0	1
12	C7	0	3
12	c7	0	3
13	C8	0	1
13	c8	0	1
15	d0	0	3
17	D2	0	1
17	d2	0	1
18	D3	0	1
19	D4	0	2
20	D5	0	3
20	d5	0	2
21	D6	0	3
22	D7	0	1
24	d9	0	1
25	e0	0	1
26	E1	0	4
26	e1	0	6
27	l2	0	3
28	L3	0	3
28	l3	0	1
29	L4	0	1
29	l4	0	3
30	L5	0	1
30	l5	0	2
31	l6	0	1
32	l7	0	2
33	L8	0	1
34	L9	0	1
36	m1	0	3
37	M3	0	1
37	m3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	m4	0	1
39	m5	0	2
40	M6	0	1
41	M7	0	2
43	M9	0	1
44	N0	0	3
44	n0	0	2
48	n4	0	1
50	n6	0	1
51	N7	0	2
51	n7	0	1
53	N9	0	1
53	n9	0	1
55	O1	0	1
55	o1	0	2
56	o2	0	1
58	o4	0	2
59	O5	0	1
60	O6	0	1
66	Q2	0	1
67	q3	0	1
68	S0	0	2
69	S1	0	2
70	S2	0	2
70	s2	0	2
71	S3	0	1
71	s3	0	4
72	S4	0	1
73	S5	0	4
73	s5	0	1
74	s6	0	1
75	S7	0	4
75	s7	0	4
77	s9	0	3
78	SM	0	1
79	SR	0	1
All	All	0	137

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	n7	36	HIS	C-N	20.49	1.73	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d8	5	THR	C-N	12.69	1.58	1.34
11	c6	4	VAL	C-N	10.62	1.54	1.34
1	5	1103	A	N9-C4	9.38	1.43	1.37
1	1	2093	A	N9-C4	8.68	1.43	1.37

The worst 5 of 3127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1059	U	O5'-P-OP2	-30.24	74.41	110.70
2	2	1059	U	OP1-P-OP2	17.12	145.28	119.60
2	2	1059	U	O5'-P-OP1	-16.80	90.55	110.70
2	2	1058	U	OP2-P-O3'	-13.98	74.45	105.20
1	5	1152	G	N3-C4-C5	13.14	135.17	128.60

There are no chirality outliers.

5 of 137 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C2	102	GLY	Peptide
7	C2	88	LEU	Peptide
9	C4	90	ARG	Peptide
5	c0	25	LYS	Peptide
7	c2	102	GLY	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
5	C0	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	7 38
5	c0	91/105 (87%)	68 (75%)	19 (21%)	4 (4%)	2 24
6	C1	152/156 (97%)	136 (90%)	14 (9%)	2 (1%)	12 47
6	c1	144/156 (92%)	130 (90%)	12 (8%)	2 (1%)	11 45
7	C2	117/143 (82%)	87 (74%)	26 (22%)	4 (3%)	3 30
7	c2	122/143 (85%)	95 (78%)	22 (18%)	5 (4%)	3 26
8	C3	148/150 (99%)	135 (91%)	11 (7%)	2 (1%)	11 45
8	c3	148/150 (99%)	134 (90%)	10 (7%)	4 (3%)	5 33
9	C4	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	9 43
9	c4	126/128 (98%)	112 (89%)	13 (10%)	1 (1%)	19 56
10	C5	122/141 (86%)	102 (84%)	15 (12%)	5 (4%)	3 26
10	c5	123/141 (87%)	104 (85%)	16 (13%)	3 (2%)	6 35
11	C6	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	3 29
11	c6	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22 59
12	C7	116/136 (85%)	98 (84%)	14 (12%)	4 (3%)	3 30
12	c7	119/136 (88%)	104 (87%)	13 (11%)	2 (2%)	9 42
13	C8	143/145 (99%)	125 (87%)	15 (10%)	3 (2%)	7 38
13	c8	143/145 (99%)	126 (88%)	13 (9%)	4 (3%)	5 33
14	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100 100
14	c9	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	22 59
15	D0	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	15 51
15	d0	102/107 (95%)	87 (85%)	12 (12%)	3 (3%)	4 32
16	D1	85/87 (98%)	70 (82%)	14 (16%)	1 (1%)	13 48
16	d1	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13 48
17	D2	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9 43
17	d2	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19 56
18	D3	142/144 (99%)	120 (84%)	18 (13%)	4 (3%)	5 33
18	d3	142/144 (99%)	134 (94%)	8 (6%)	0	100 100
19	D4	132/134 (98%)	119 (90%)	10 (8%)	3 (2%)	6 36
19	d4	132/134 (98%)	115 (87%)	15 (11%)	2 (2%)	10 44
20	D5	68/70 (97%)	53 (78%)	14 (21%)	1 (2%)	10 44
20	d5	67/70 (96%)	61 (91%)	5 (8%)	1 (2%)	10 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	D6	95/97 (98%)	66 (70%)	22 (23%)	7 (7%)	1 13
21	d6	95/97 (98%)	76 (80%)	17 (18%)	2 (2%)	7 38
22	D7	79/81 (98%)	74 (94%)	5 (6%)	0	100 100
22	d7	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	12 47
23	D8	61/63 (97%)	53 (87%)	8 (13%)	0	100 100
23	d8	61/63 (97%)	53 (87%)	8 (13%)	0	100 100
24	D9	50/53 (94%)	47 (94%)	3 (6%)	0	100 100
24	d9	51/53 (96%)	46 (90%)	3 (6%)	2 (4%)	3 27
25	E0	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9 42
25	e0	59/61 (97%)	54 (92%)	5 (8%)	0	100 100
26	E1	69/73 (94%)	39 (56%)	20 (29%)	10 (14%)	0 3
26	e1	71/73 (97%)	43 (61%)	21 (30%)	7 (10%)	0 8
27	L2	250/252 (99%)	235 (94%)	15 (6%)	0	100 100
27	l2	250/252 (99%)	231 (92%)	18 (7%)	1 (0%)	34 69
28	L3	384/386 (100%)	354 (92%)	30 (8%)	0	100 100
28	l3	384/386 (100%)	367 (96%)	15 (4%)	2 (0%)	29 66
29	L4	359/361 (99%)	321 (89%)	36 (10%)	2 (1%)	25 62
29	l4	359/361 (99%)	328 (91%)	27 (8%)	4 (1%)	14 50
30	L5	294/296 (99%)	261 (89%)	28 (10%)	5 (2%)	9 42
30	l5	292/296 (99%)	280 (96%)	11 (4%)	1 (0%)	41 74
31	L6	153/176 (87%)	144 (94%)	5 (3%)	4 (3%)	5 34
31	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	12 47
32	L7	220/223 (99%)	206 (94%)	13 (6%)	1 (0%)	29 66
32	l7	221/223 (99%)	206 (93%)	11 (5%)	4 (2%)	8 41
33	L8	231/233 (99%)	208 (90%)	19 (8%)	4 (2%)	9 42
33	l8	229/233 (98%)	201 (88%)	26 (11%)	2 (1%)	17 54
34	L9	189/191 (99%)	176 (93%)	12 (6%)	1 (0%)	29 66
34	l9	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	29 66
35	M0	207/221 (94%)	195 (94%)	11 (5%)	1 (0%)	29 66
35	m0	205/221 (93%)	192 (94%)	12 (6%)	1 (0%)	29 66
36	M1	167/169 (99%)	142 (85%)	23 (14%)	2 (1%)	13 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	m1	167/169 (99%)	147 (88%)	12 (7%)	8 (5%)	2 22
37	M3	191/194 (98%)	171 (90%)	18 (9%)	2 (1%)	15 51
37	m3	192/194 (99%)	167 (87%)	22 (12%)	3 (2%)	9 43
38	M4	134/137 (98%)	124 (92%)	8 (6%)	2 (2%)	10 44
38	m4	135/137 (98%)	132 (98%)	3 (2%)	0	100 100
39	M5	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	15 51
39	m5	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	15 51
40	M6	195/197 (99%)	187 (96%)	6 (3%)	2 (1%)	15 51
40	m6	195/197 (99%)	188 (96%)	7 (4%)	0	100 100
41	M7	181/184 (98%)	171 (94%)	9 (5%)	1 (1%)	25 62
41	m7	181/184 (98%)	171 (94%)	9 (5%)	1 (1%)	25 62
42	M8	183/185 (99%)	171 (93%)	12 (7%)	0	100 100
42	m8	183/185 (99%)	172 (94%)	11 (6%)	0	100 100
43	M9	186/188 (99%)	177 (95%)	8 (4%)	1 (0%)	29 66
43	m9	182/188 (97%)	177 (97%)	4 (2%)	1 (0%)	29 66
44	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	13 48
44	n0	169/172 (98%)	166 (98%)	3 (2%)	0	100 100
45	N1	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25 62
45	n1	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25 62
46	N2	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	15 51
46	n2	96/100 (96%)	89 (93%)	7 (7%)	0	100 100
47	N3	134/136 (98%)	129 (96%)	5 (4%)	0	100 100
47	n3	133/136 (98%)	130 (98%)	2 (2%)	1 (1%)	19 56
48	N4	128/155 (83%)	116 (91%)	12 (9%)	0	100 100
48	n4	128/155 (83%)	115 (90%)	10 (8%)	3 (2%)	6 36
49	N5	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	19 56
49	n5	118/121 (98%)	106 (90%)	10 (8%)	2 (2%)	9 42
50	N6	124/126 (98%)	118 (95%)	6 (5%)	0	100 100
50	n6	120/126 (95%)	116 (97%)	4 (3%)	0	100 100
51	N7	133/135 (98%)	122 (92%)	9 (7%)	2 (2%)	10 44
51	n7	133/135 (98%)	114 (86%)	16 (12%)	3 (2%)	6 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	N8	146/148 (99%)	132 (90%)	13 (9%)	1 (1%)	22 59
52	n8	146/148 (99%)	133 (91%)	10 (7%)	3 (2%)	7 38
53	N9	56/58 (97%)	52 (93%)	4 (7%)	0	100 100
53	n9	54/58 (93%)	46 (85%)	7 (13%)	1 (2%)	8 40
54	O0	95/100 (95%)	90 (95%)	5 (5%)	0	100 100
54	o0	98/100 (98%)	92 (94%)	6 (6%)	0	100 100
55	O1	107/109 (98%)	100 (94%)	4 (4%)	3 (3%)	5 33
55	o1	107/109 (98%)	99 (92%)	4 (4%)	4 (4%)	3 28
56	O2	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	19 56
56	o2	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	19 56
57	O3	104/106 (98%)	100 (96%)	4 (4%)	0	100 100
57	o3	104/106 (98%)	97 (93%)	6 (6%)	1 (1%)	15 51
58	O4	110/112 (98%)	105 (96%)	5 (4%)	0	100 100
58	o4	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	17 54
59	O5	117/119 (98%)	105 (90%)	11 (9%)	1 (1%)	17 54
59	o5	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	17 54
60	O6	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15 51
60	o6	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	4 32
61	O7	85/87 (98%)	78 (92%)	7 (8%)	0	100 100
61	o7	81/87 (93%)	74 (91%)	7 (9%)	0	100 100
62	O8	75/77 (97%)	69 (92%)	6 (8%)	0	100 100
62	o8	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12 47
63	O9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	7 38
63	o9	48/50 (96%)	47 (98%)	1 (2%)	0	100 100
64	Q0	50/52 (96%)	47 (94%)	3 (6%)	0	100 100
64	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7 39
65	Q1	23/25 (92%)	23 (100%)	0	0	100 100
65	q1	23/25 (92%)	23 (100%)	0	0	100 100
66	Q2	103/105 (98%)	91 (88%)	12 (12%)	0	100 100
66	q2	102/105 (97%)	97 (95%)	5 (5%)	0	100 100
67	Q3	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	q3	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
68	S0	204/206 (99%)	172 (84%)	27 (13%)	5 (2%)	5	35
68	s0	204/206 (99%)	176 (86%)	21 (10%)	7 (3%)	3	30
69	S1	212/216 (98%)	167 (79%)	42 (20%)	3 (1%)	11	45
69	s1	214/216 (99%)	190 (89%)	19 (9%)	5 (2%)	6	36
70	S2	215/217 (99%)	192 (89%)	19 (9%)	4 (2%)	8	40
70	s2	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29	66
71	S3	221/223 (99%)	201 (91%)	15 (7%)	5 (2%)	6	36
71	s3	221/223 (99%)	198 (90%)	15 (7%)	8 (4%)	3	29
72	S4	258/260 (99%)	233 (90%)	23 (9%)	2 (1%)	19	56
72	s4	258/260 (99%)	232 (90%)	24 (9%)	2 (1%)	19	56
73	S5	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	44
73	s5	204/206 (99%)	181 (89%)	20 (10%)	3 (2%)	10	44
74	S6	224/236 (95%)	208 (93%)	9 (4%)	7 (3%)	4	32
74	s6	216/236 (92%)	198 (92%)	15 (7%)	3 (1%)	11	45
75	S7	182/184 (99%)	151 (83%)	24 (13%)	7 (4%)	3	27
75	s7	182/184 (99%)	153 (84%)	25 (14%)	4 (2%)	6	37
76	S8	184/200 (92%)	160 (87%)	22 (12%)	2 (1%)	14	50
76	s8	181/200 (90%)	171 (94%)	8 (4%)	2 (1%)	14	50
77	S9	183/185 (99%)	159 (87%)	22 (12%)	2 (1%)	14	50
77	s9	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	29	66
78	SM	155/272 (57%)	125 (81%)	27 (17%)	3 (2%)	8	40
78	sM	125/272 (46%)	105 (84%)	17 (14%)	3 (2%)	6	35
79	SR	316/318 (99%)	293 (93%)	23 (7%)	0	100	100
79	sR	314/318 (99%)	290 (92%)	24 (8%)	0	100	100
All	All	22224/23150 (96%)	20097 (90%)	1833 (8%)	294 (1%)	12	47

5 of 294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C0	88	PRO
7	c2	91	VAL
10	c5	11	VAL

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Mol	Chain	Res	Type
10	c5	126	VAL
11	C6	58	ASP

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
5	C0	77/98 (79%)	63 (82%)	14 (18%)	1 11
5	c0	73/98 (74%)	57 (78%)	16 (22%)	1 6
6	C1	128/137 (93%)	110 (86%)	18 (14%)	3 20
6	c1	129/137 (94%)	101 (78%)	28 (22%)	1 7
7	C2	88/119 (74%)	61 (69%)	27 (31%)	0 2
7	c2	88/119 (74%)	62 (70%)	26 (30%)	0 2
8	C3	127/127 (100%)	103 (81%)	24 (19%)	1 9
8	c3	127/127 (100%)	105 (83%)	22 (17%)	2 12
9	C4	81/97 (84%)	59 (73%)	22 (27%)	0 3
9	c4	97/97 (100%)	77 (79%)	20 (21%)	1 7
10	C5	101/117 (86%)	82 (81%)	19 (19%)	1 10
10	c5	102/117 (87%)	85 (83%)	17 (17%)	2 14
11	C6	117/117 (100%)	94 (80%)	23 (20%)	1 8
11	c6	117/117 (100%)	90 (77%)	27 (23%)	1 6
12	C7	94/124 (76%)	75 (80%)	19 (20%)	1 8
12	c7	92/124 (74%)	78 (85%)	14 (15%)	3 17
13	C8	128/128 (100%)	96 (75%)	32 (25%)	0 4
13	c8	128/128 (100%)	104 (81%)	24 (19%)	1 10
14	C9	115/115 (100%)	97 (84%)	18 (16%)	2 16
14	c9	115/115 (100%)	94 (82%)	21 (18%)	1 10
15	D0	98/100 (98%)	75 (76%)	23 (24%)	1 5
15	d0	97/100 (97%)	75 (77%)	22 (23%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	D1	74/74 (100%)	63 (85%)	11 (15%)	3 18
16	d1	74/74 (100%)	64 (86%)	10 (14%)	4 21
17	D2	110/110 (100%)	92 (84%)	18 (16%)	2 15
17	d2	110/110 (100%)	97 (88%)	13 (12%)	5 26
18	D3	119/119 (100%)	100 (84%)	19 (16%)	2 15
18	d3	119/119 (100%)	102 (86%)	17 (14%)	3 19
19	D4	112/112 (100%)	90 (80%)	22 (20%)	1 9
19	d4	112/112 (100%)	93 (83%)	19 (17%)	2 13
20	D5	61/61 (100%)	45 (74%)	16 (26%)	0 4
20	d5	61/61 (100%)	47 (77%)	14 (23%)	1 6
21	D6	83/83 (100%)	63 (76%)	20 (24%)	0 5
21	d6	83/83 (100%)	68 (82%)	15 (18%)	1 11
22	D7	70/70 (100%)	59 (84%)	11 (16%)	2 16
22	d7	70/70 (100%)	59 (84%)	11 (16%)	2 16
23	D8	56/56 (100%)	41 (73%)	15 (27%)	0 3
23	d8	56/56 (100%)	40 (71%)	16 (29%)	0 2
24	D9	46/47 (98%)	39 (85%)	7 (15%)	3 17
24	d9	47/47 (100%)	40 (85%)	7 (15%)	3 18
25	E0	51/52 (98%)	42 (82%)	9 (18%)	2 12
25	e0	52/52 (100%)	43 (83%)	9 (17%)	2 12
26	E1	62/64 (97%)	46 (74%)	16 (26%)	0 4
26	e1	64/64 (100%)	48 (75%)	16 (25%)	0 4
27	L2	193/194 (100%)	163 (84%)	30 (16%)	2 17
27	l2	192/194 (99%)	157 (82%)	35 (18%)	1 11
28	L3	320/322 (99%)	264 (82%)	56 (18%)	2 12
28	l3	319/322 (99%)	260 (82%)	59 (18%)	1 10
29	L4	288/288 (100%)	239 (83%)	49 (17%)	2 13
29	l4	288/288 (100%)	237 (82%)	51 (18%)	2 12
30	L5	244/244 (100%)	196 (80%)	48 (20%)	1 8
30	l5	243/244 (100%)	212 (87%)	31 (13%)	4 23
31	L6	135/153 (88%)	114 (84%)	21 (16%)	2 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	l6	135/153 (88%)	118 (87%)	17 (13%)	4 23
32	L7	186/187 (100%)	168 (90%)	18 (10%)	8 33
32	l7	187/187 (100%)	163 (87%)	24 (13%)	4 23
33	L8	187/191 (98%)	160 (86%)	27 (14%)	3 19
33	l8	178/191 (93%)	150 (84%)	28 (16%)	2 16
34	L9	171/171 (100%)	132 (77%)	39 (23%)	1 6
34	l9	171/171 (100%)	134 (78%)	37 (22%)	1 7
35	M0	177/187 (95%)	154 (87%)	23 (13%)	4 22
35	m0	177/187 (95%)	149 (84%)	28 (16%)	2 16
36	M1	147/147 (100%)	124 (84%)	23 (16%)	2 17
36	m1	147/147 (100%)	124 (84%)	23 (16%)	2 17
37	M3	154/154 (100%)	122 (79%)	32 (21%)	1 7
37	m3	154/154 (100%)	129 (84%)	25 (16%)	2 15
38	M4	107/108 (99%)	93 (87%)	14 (13%)	4 22
38	m4	108/108 (100%)	94 (87%)	14 (13%)	4 22
39	M5	175/175 (100%)	154 (88%)	21 (12%)	5 25
39	m5	175/175 (100%)	148 (85%)	27 (15%)	2 17
40	M6	160/160 (100%)	137 (86%)	23 (14%)	3 19
40	m6	160/160 (100%)	138 (86%)	22 (14%)	3 21
41	M7	140/146 (96%)	111 (79%)	29 (21%)	1 7
41	m7	140/146 (96%)	115 (82%)	25 (18%)	2 11
42	M8	150/150 (100%)	127 (85%)	23 (15%)	2 17
42	m8	150/150 (100%)	132 (88%)	18 (12%)	5 25
43	M9	153/153 (100%)	132 (86%)	21 (14%)	3 21
43	m9	150/153 (98%)	123 (82%)	27 (18%)	1 11
44	N0	156/156 (100%)	127 (81%)	29 (19%)	1 10
44	n0	155/156 (99%)	132 (85%)	23 (15%)	3 18
45	N1	136/136 (100%)	101 (74%)	35 (26%)	0 4
45	n1	136/136 (100%)	113 (83%)	23 (17%)	2 13
46	N2	87/87 (100%)	70 (80%)	17 (20%)	1 9
46	n2	85/87 (98%)	68 (80%)	17 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	N3	104/104 (100%)	91 (88%)	13 (12%)	4 23
47	n3	103/104 (99%)	95 (92%)	8 (8%)	12 42
48	N4	85/129 (66%)	74 (87%)	11 (13%)	4 22
48	n4	97/129 (75%)	89 (92%)	8 (8%)	11 41
49	N5	104/105 (99%)	85 (82%)	19 (18%)	1 10
49	n5	104/105 (99%)	75 (72%)	29 (28%)	0 2
50	N6	109/109 (100%)	89 (82%)	20 (18%)	1 10
50	n6	106/109 (97%)	87 (82%)	19 (18%)	2 11
51	N7	115/115 (100%)	96 (84%)	19 (16%)	2 14
51	n7	115/115 (100%)	93 (81%)	22 (19%)	1 9
52	N8	118/118 (100%)	102 (86%)	16 (14%)	3 21
52	n8	118/118 (100%)	102 (86%)	16 (14%)	3 21
53	N9	46/46 (100%)	36 (78%)	10 (22%)	1 7
53	n9	44/46 (96%)	40 (91%)	4 (9%)	9 36
54	O0	81/84 (96%)	68 (84%)	13 (16%)	2 15
54	o0	84/84 (100%)	72 (86%)	12 (14%)	3 19
55	O1	92/96 (96%)	77 (84%)	15 (16%)	2 15
55	o1	94/96 (98%)	76 (81%)	18 (19%)	1 9
56	O2	109/109 (100%)	96 (88%)	13 (12%)	5 25
56	o2	109/109 (100%)	93 (85%)	16 (15%)	3 18
57	O3	90/90 (100%)	79 (88%)	11 (12%)	5 24
57	o3	90/90 (100%)	78 (87%)	12 (13%)	4 22
58	O4	95/95 (100%)	80 (84%)	15 (16%)	2 16
58	o4	95/95 (100%)	83 (87%)	12 (13%)	4 23
59	O5	104/104 (100%)	83 (80%)	21 (20%)	1 8
59	o5	103/104 (99%)	77 (75%)	26 (25%)	0 4
60	O6	81/81 (100%)	62 (76%)	19 (24%)	1 5
60	o6	80/81 (99%)	58 (72%)	22 (28%)	0 3
61	O7	70/70 (100%)	54 (77%)	16 (23%)	1 6
61	o7	68/70 (97%)	59 (87%)	9 (13%)	4 22
62	O8	68/68 (100%)	52 (76%)	16 (24%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	o8	67/68 (98%)	57 (85%)	10 (15%)	3 18
63	O9	45/45 (100%)	37 (82%)	8 (18%)	2 12
63	o9	45/45 (100%)	40 (89%)	5 (11%)	6 28
64	Q0	47/47 (100%)	40 (85%)	7 (15%)	3 18
64	q0	47/47 (100%)	40 (85%)	7 (15%)	3 18
65	Q1	23/23 (100%)	19 (83%)	4 (17%)	2 12
65	q1	23/23 (100%)	19 (83%)	4 (17%)	2 12
66	Q2	90/90 (100%)	71 (79%)	19 (21%)	1 7
66	q2	89/90 (99%)	76 (85%)	13 (15%)	3 18
67	Q3	71/71 (100%)	61 (86%)	10 (14%)	3 20
67	q3	71/71 (100%)	58 (82%)	13 (18%)	1 10
68	S0	164/173 (95%)	134 (82%)	30 (18%)	1 10
68	s0	165/173 (95%)	138 (84%)	27 (16%)	2 15
69	S1	191/192 (100%)	144 (75%)	47 (25%)	0 5
69	s1	192/192 (100%)	156 (81%)	36 (19%)	1 10
70	S2	176/176 (100%)	137 (78%)	39 (22%)	1 6
70	s2	176/176 (100%)	143 (81%)	33 (19%)	1 10
71	S3	182/182 (100%)	149 (82%)	33 (18%)	1 11
71	s3	182/182 (100%)	148 (81%)	34 (19%)	1 10
72	S4	221/221 (100%)	183 (83%)	38 (17%)	2 13
72	s4	221/221 (100%)	190 (86%)	31 (14%)	3 20
73	S5	173/173 (100%)	148 (86%)	25 (14%)	3 18
73	s5	173/173 (100%)	139 (80%)	34 (20%)	1 8
74	S6	188/201 (94%)	156 (83%)	32 (17%)	2 13
74	s6	187/201 (93%)	157 (84%)	30 (16%)	2 15
75	S7	165/165 (100%)	135 (82%)	30 (18%)	1 11
75	s7	165/165 (100%)	139 (84%)	26 (16%)	2 16
76	S8	150/161 (93%)	130 (87%)	20 (13%)	4 22
76	s8	148/161 (92%)	124 (84%)	24 (16%)	2 15
77	S9	158/158 (100%)	129 (82%)	29 (18%)	1 10
77	s9	158/158 (100%)	135 (85%)	23 (15%)	3 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	SM	97/227 (43%)	73 (75%)	24 (25%)	0 5
78	sM	94/227 (41%)	68 (72%)	26 (28%)	0 2
79	SR	259/261 (99%)	226 (87%)	33 (13%)	4 23
79	sR	258/261 (99%)	228 (88%)	30 (12%)	5 27
All	All	18669/19450 (96%)	15436 (83%)	3233 (17%)	2 12

5 of 3233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	N1	18	ASP
59	o5	94	LYS
79	sR	319	ASN
46	N2	43	VAL
45	N1	12	ARG

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

Mol	Chain	Res	Type
47	N3	98	ASN
79	SR	288	HIS
53	N9	45	HIS
79	SR	195	HIS
74	s6	80	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3084/3396 (90%)	644 (20%)	99 (3%)
1	5	3071/3396 (90%)	615 (20%)	70 (2%)
2	2	1767/1800 (98%)	481 (27%)	62 (3%)
2	6	1731/1800 (96%)	411 (23%)	55 (3%)
3	3	120/121 (99%)	17 (14%)	1 (0%)
3	7	120/121 (99%)	15 (12%)	1 (0%)
4	4	157/158 (99%)	32 (20%)	4 (2%)
4	8	157/158 (99%)	33 (21%)	4 (2%)
All	All	10207/10950 (93%)	2248 (22%)	296 (2%)

5 of 2248 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	14	U
1	1	16	A
1	1	26	A
1	1	40	A
1	1	43	A

5 of 296 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	3317	U
2	6	1573	A
2	6	76	A
2	6	555	A
1	1	3375	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1407 ligands modelled in this entry, 1382 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
81	8UZ	2	2029	-	35,35,35	0.36	0	49,52,52	1.36	6 (12%)
81	8UZ	1	3892	-	35,35,35	0.44	0	49,52,52	1.35	4 (8%)
81	8UZ	5	3855	-	35,35,35	0.35	0	49,52,52	1.28	8 (16%)
81	8UZ	2	2030	-	35,35,35	0.26	0	49,52,52	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
81	8UZ	6	2061	-	35,35,35	0.36	0	49,52,52	1.51	7 (14%)
81	8UZ	5	3856	-	35,35,35	0.28	0	49,52,52	1.45	7 (14%)
81	8UZ	5	3851	-	35,35,35	0.25	0	49,52,52	1.12	5 (10%)
81	8UZ	2	2031	-	35,35,35	0.37	0	49,52,52	1.02	3 (6%)
81	8UZ	5	3850	-	35,35,35	0.31	0	49,52,52	1.08	3 (6%)
81	8UZ	1	3895	-	35,35,35	0.34	0	49,52,52	1.27	7 (14%)
81	8UZ	1	3886	-	35,35,35	0.37	0	49,52,52	1.28	5 (10%)
81	8UZ	1	3891	-	35,35,35	0.36	0	49,52,52	1.37	7 (14%)
81	8UZ	1	3893	-	35,35,35	0.54	0	49,52,52	0.96	3 (6%)
81	8UZ	1	3887	-	35,35,35	0.42	0	49,52,52	1.30	3 (6%)
81	8UZ	7	209	-	35,35,35	0.43	0	49,52,52	1.21	6 (12%)
81	8UZ	5	3853	-	35,35,35	0.31	0	49,52,52	1.23	6 (12%)
81	8UZ	1	3894	-	35,35,35	0.34	0	49,52,52	1.41	5 (10%)
81	8UZ	5	3854	-	35,35,35	0.34	0	49,52,52	1.79	6 (12%)
81	8UZ	5	3857	-	35,35,35	0.36	0	49,52,52	0.96	3 (6%)
81	8UZ	1	3888	-	35,35,35	0.33	0	49,52,52	1.05	3 (6%)
81	8UZ	5	3852	-	35,35,35	0.36	0	49,52,52	1.23	3 (6%)
81	8UZ	1	3890	-	35,35,35	0.35	0	49,52,52	1.32	4 (8%)
81	8UZ	4	220	-	35,35,35	0.54	0	49,52,52	1.56	8 (16%)
81	8UZ	1	3889	-	35,35,35	0.19	0	49,52,52	0.80	2 (4%)
81	8UZ	3	214	-	35,35,35	0.44	0	49,52,52	1.58	7 (14%)

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
81	8UZ	2	2029	-	-	10/12/72/72	0/3/3/3
81	8UZ	1	3892	-	-	4/12/72/72	0/3/3/3
81	8UZ	5	3855	-	-	6/12/72/72	0/3/3/3
81	8UZ	2	2030	-	-	5/12/72/72	0/3/3/3
81	8UZ	6	2061	-	-	5/12/72/72	0/3/3/3
81	8UZ	5	3856	-	-	5/12/72/72	0/3/3/3
81	8UZ	5	3851	-	-	4/12/72/72	0/3/3/3
81	8UZ	2	2031	-	-	3/12/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	8UZ	5	3850	-	-	3/12/72/72	0/3/3/3
81	8UZ	1	3895	-	-	7/12/72/72	0/3/3/3
81	8UZ	1	3886	-	-	4/12/72/72	0/3/3/3
81	8UZ	1	3891	-	-	8/12/72/72	0/3/3/3
81	8UZ	1	3893	-	-	4/12/72/72	0/3/3/3
81	8UZ	1	3887	-	-	9/12/72/72	0/3/3/3
81	8UZ	7	209	-	-	7/12/72/72	0/3/3/3
81	8UZ	5	3853	-	-	6/12/72/72	0/3/3/3
81	8UZ	1	3894	-	-	3/12/72/72	0/3/3/3
81	8UZ	5	3854	-	-	5/12/72/72	0/3/3/3
81	8UZ	5	3857	-	-	7/12/72/72	0/3/3/3
81	8UZ	1	3888	-	-	7/12/72/72	0/3/3/3
81	8UZ	5	3852	-	-	3/12/72/72	0/3/3/3
81	8UZ	1	3890	-	-	6/12/72/72	0/3/3/3
81	8UZ	4	220	-	-	6/12/72/72	0/3/3/3
81	8UZ	1	3889	-	-	1/12/72/72	0/3/3/3
81	8UZ	3	214	-	-	4/12/72/72	0/3/3/3

There are no bond length outliers.

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	5	3854	8UZ	C2-C15-N4	7.37	123.48	110.20
81	5	3854	8UZ	C14-C13-C12	-6.83	96.24	111.06
81	6	2061	8UZ	C2-C15-N4	6.73	122.33	110.20
81	1	3894	8UZ	C2-C15-N4	5.79	120.64	110.20
81	3	214	8UZ	O1-C2-C15	5.52	117.72	108.22

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

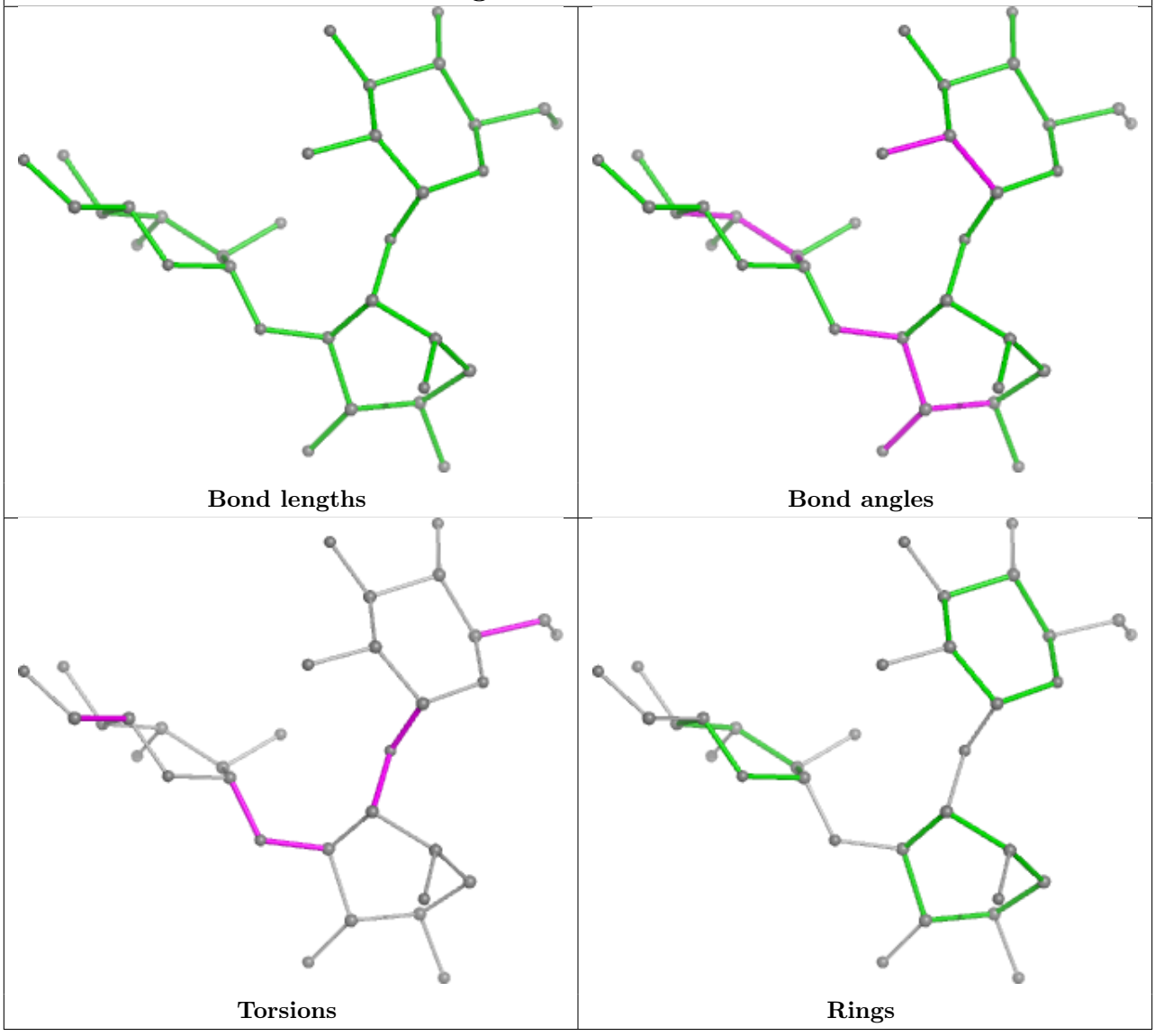
Mol	Chain	Res	Type	Atoms
81	1	3886	8UZ	C14-C9-O3-C8
81	1	3887	8UZ	N-C-C1-C17
81	1	3887	8UZ	N-C-C1-O
81	1	3887	8UZ	C15-C2-O1-C3
81	1	3888	8UZ	N-C-C1-O

There are no ring outliers.

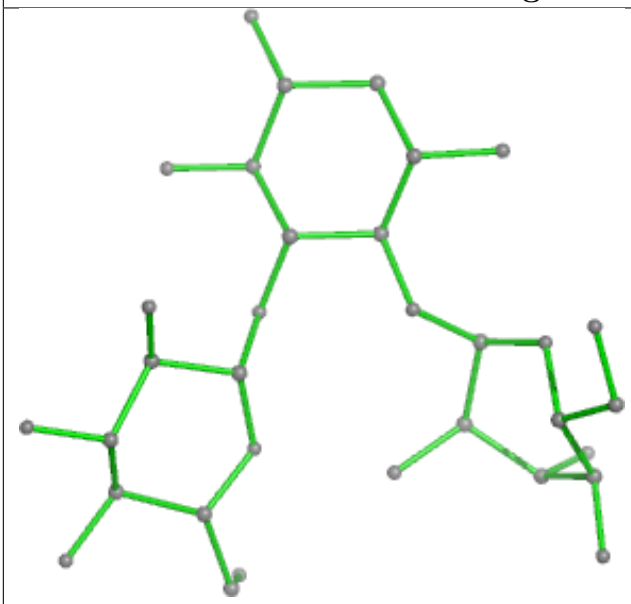
No monomer is involved in short contacts.

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.

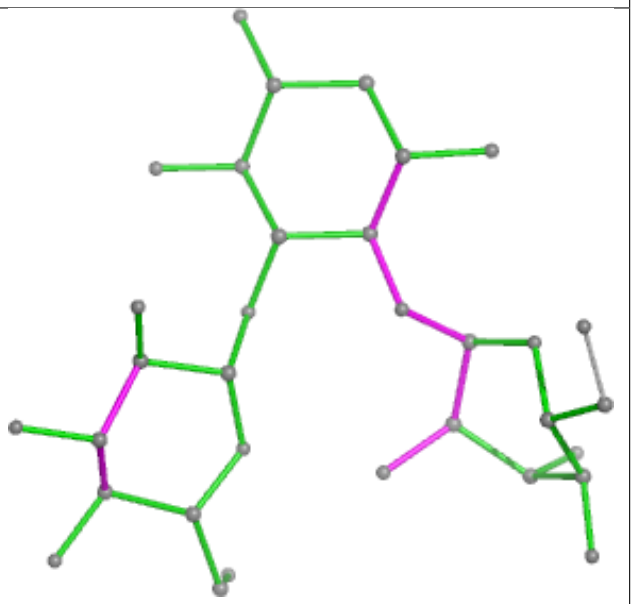
Ligand 8UZ 2 2029



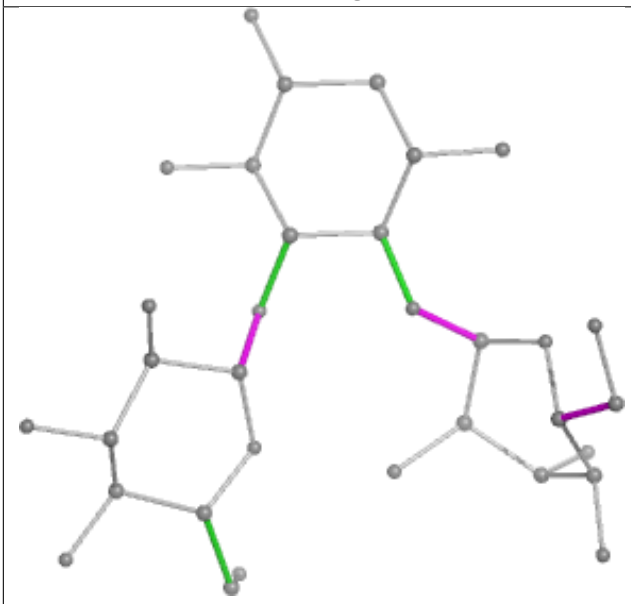
Ligand 8UZ 1 3892



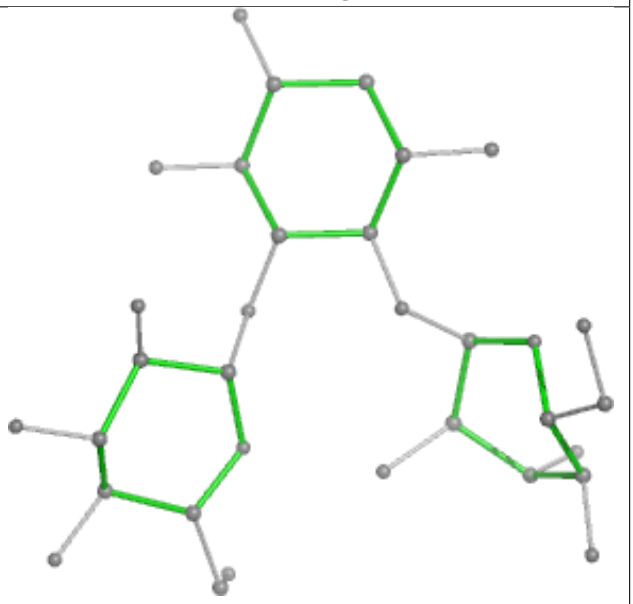
Bond lengths



Bond angles

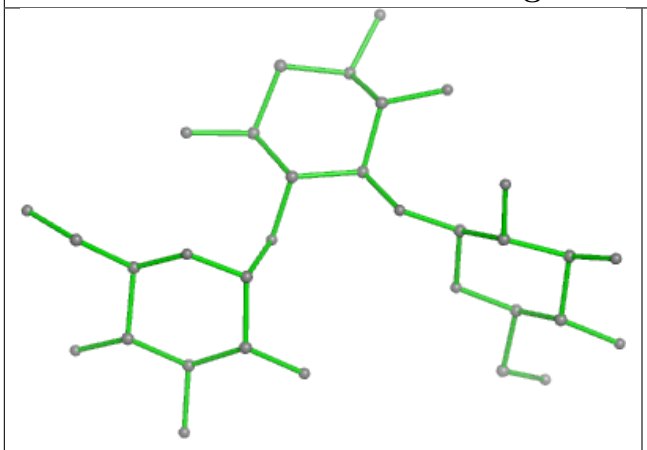


Torsions



Rings

Ligand 8UZ 5 3855



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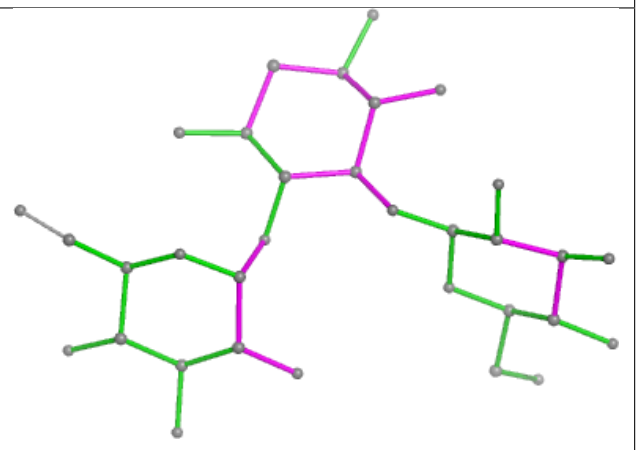
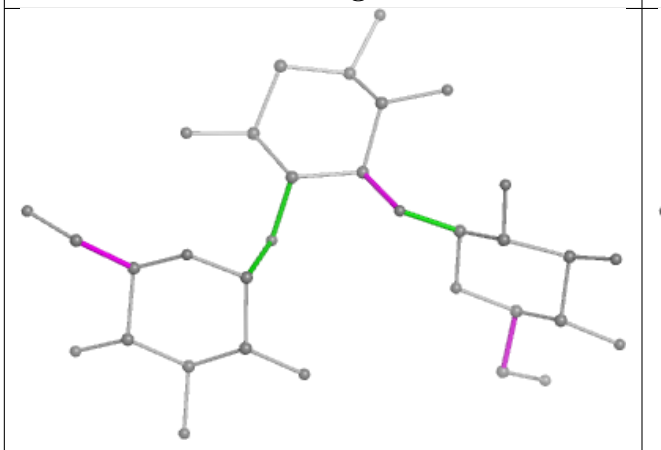


Bond angles



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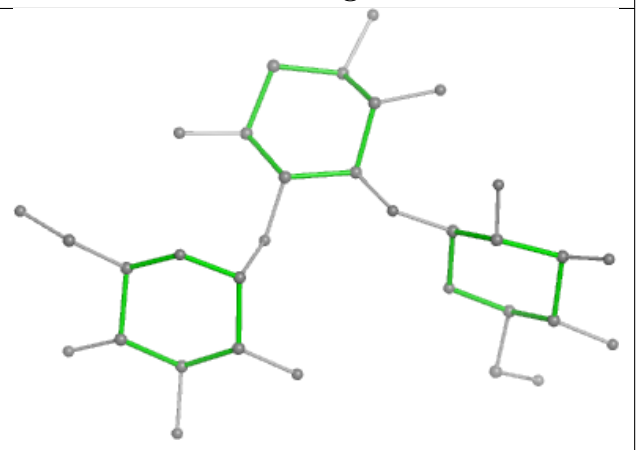
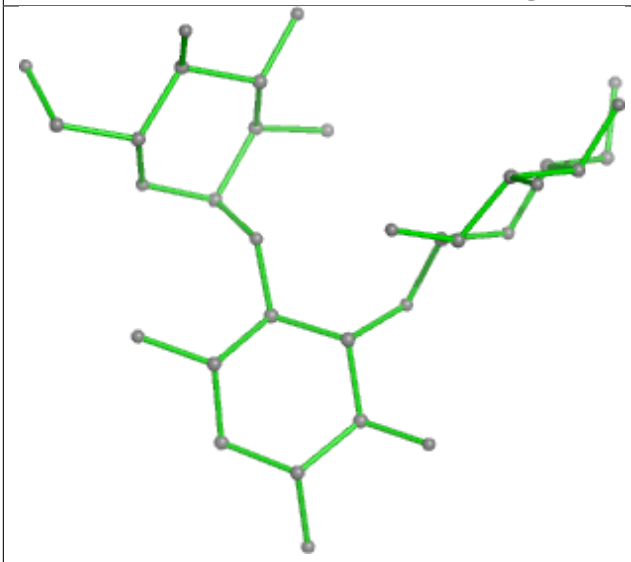
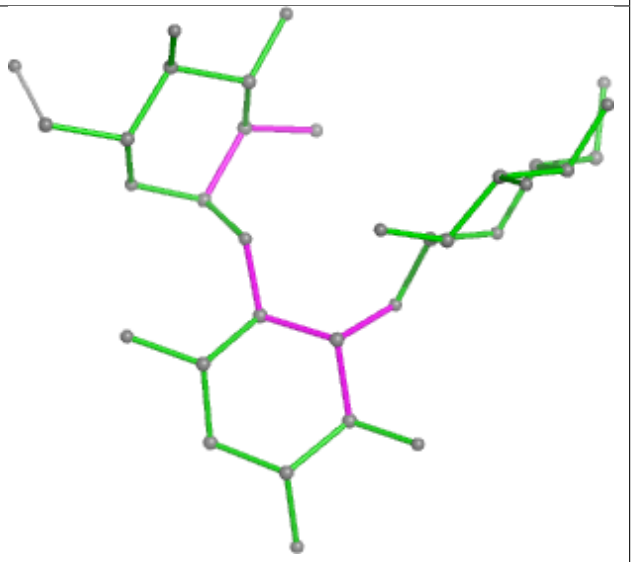


Rings

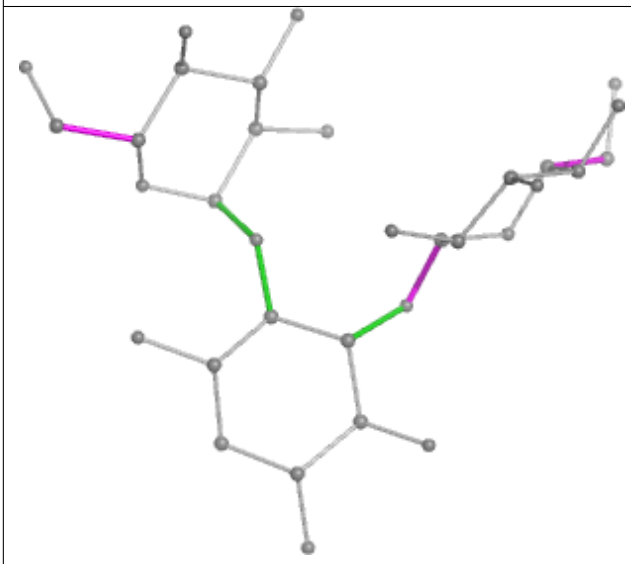
Ligand 8UZ 2 2030



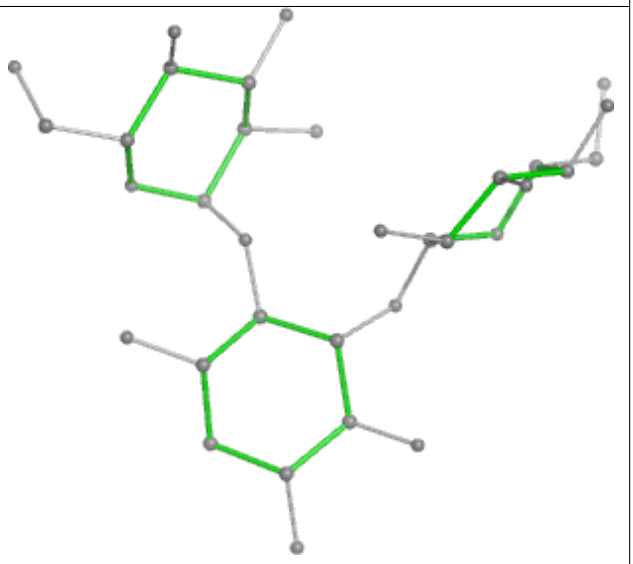
Bond lengths



Bond angles

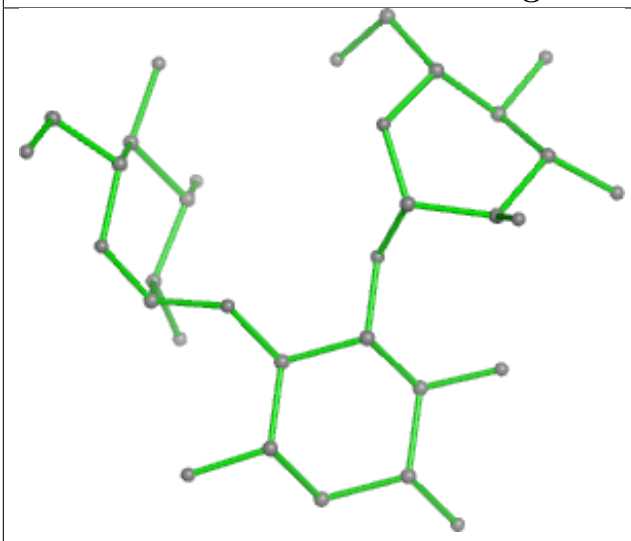


Torsions



Rings

Ligand 8UZ 6 2061



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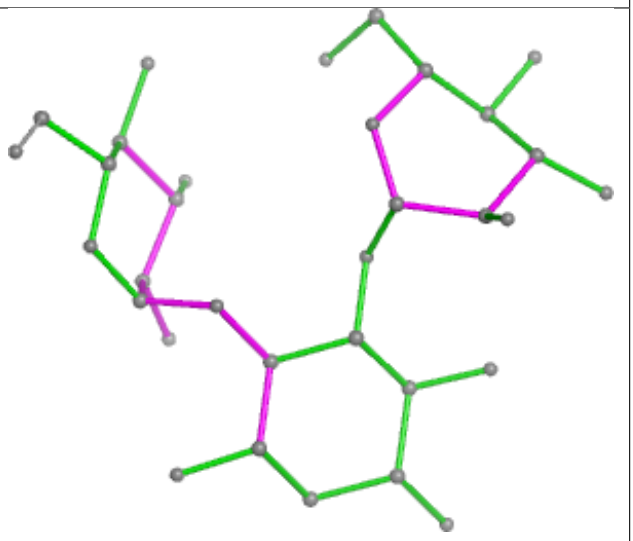
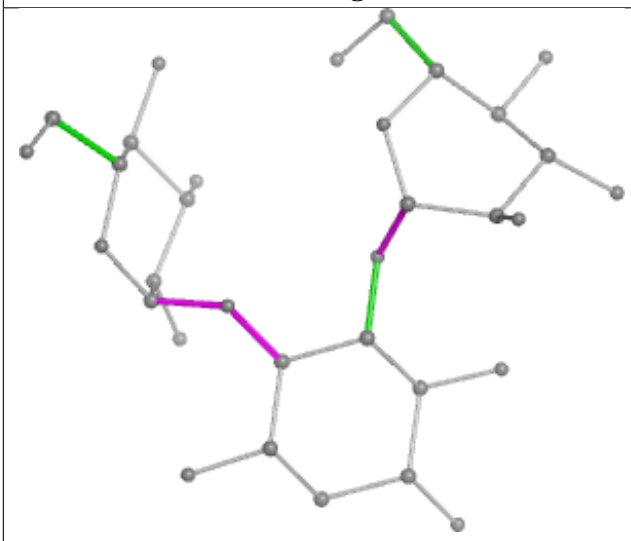
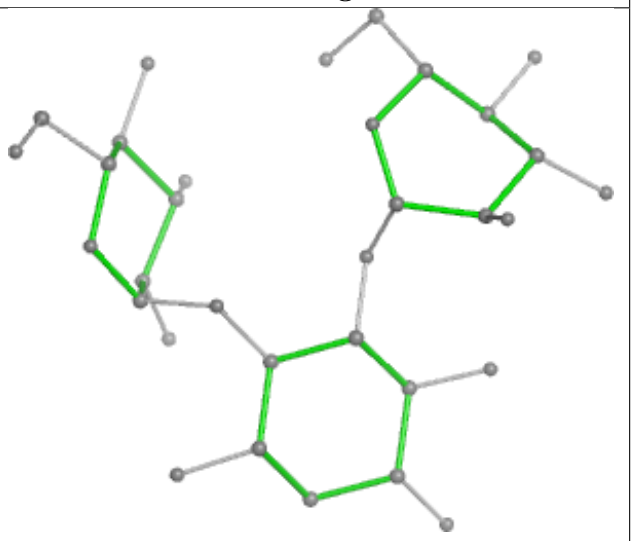


Bond angles

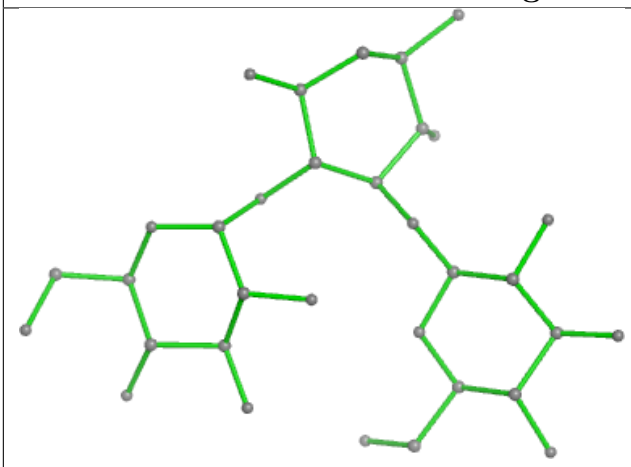


Torsions



Rings

Ligand 8UZ 5 3856



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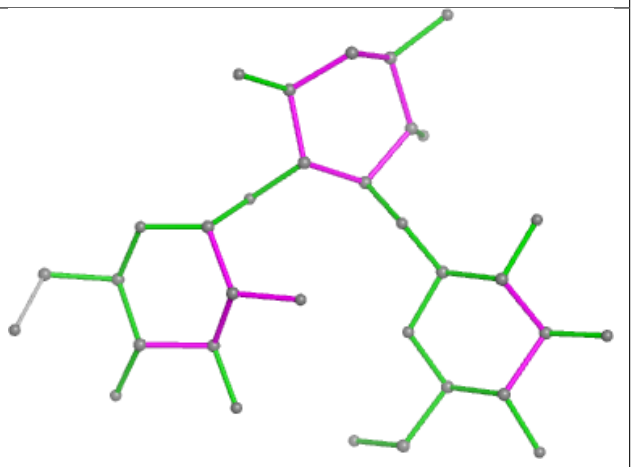
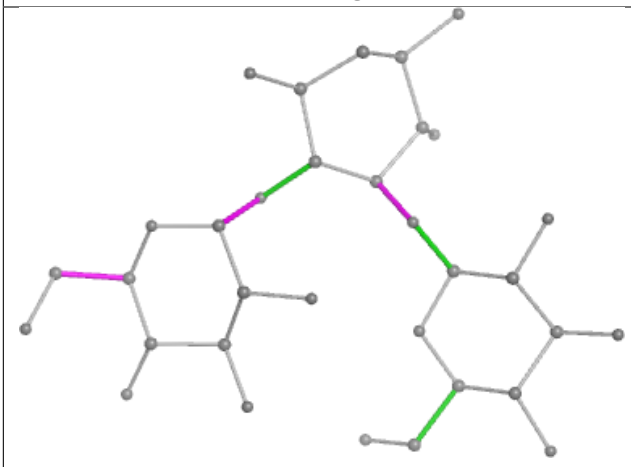


Bond angles



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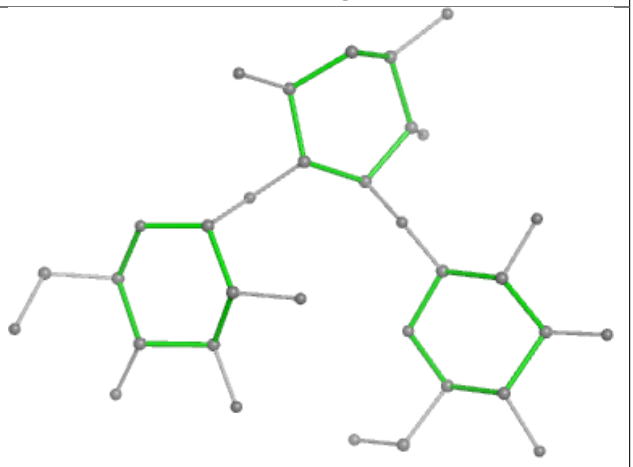
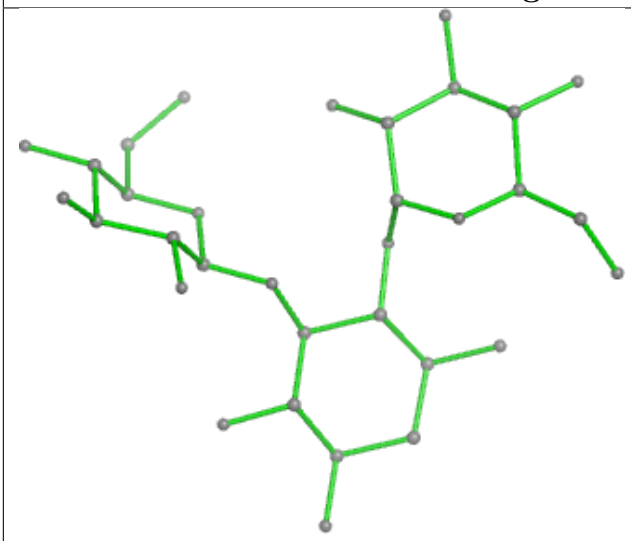


Rings

Ligand 8UZ 5 3851



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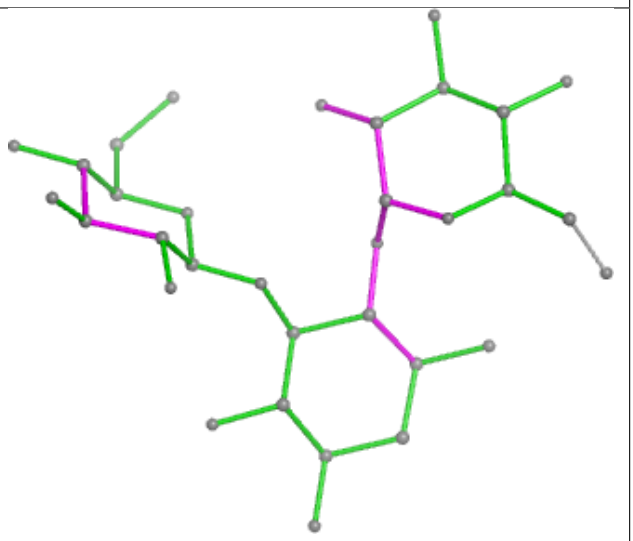

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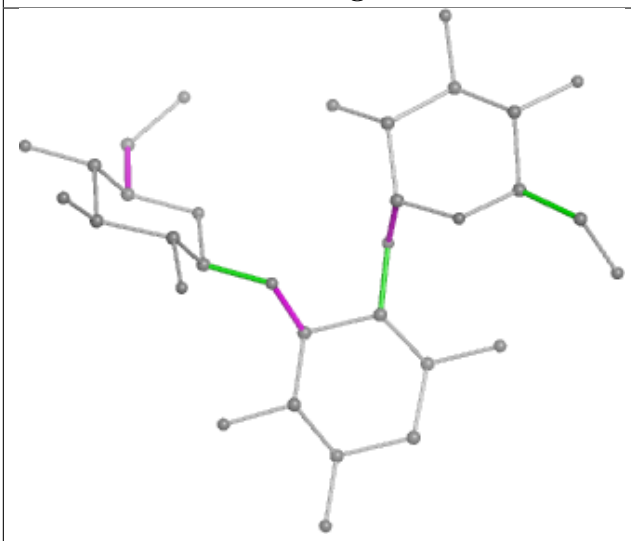

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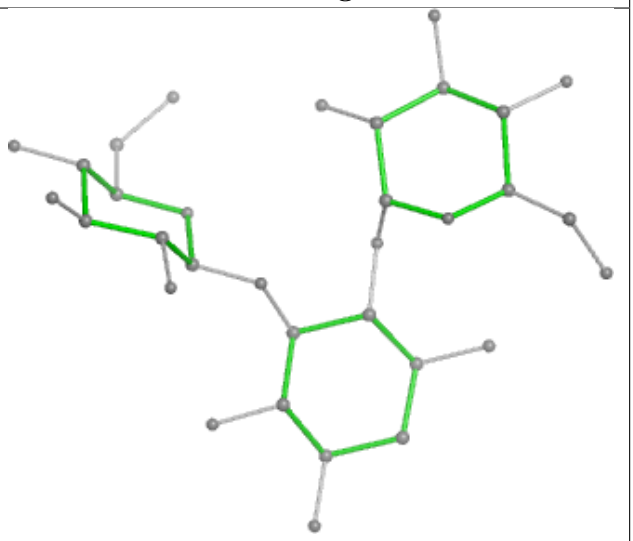
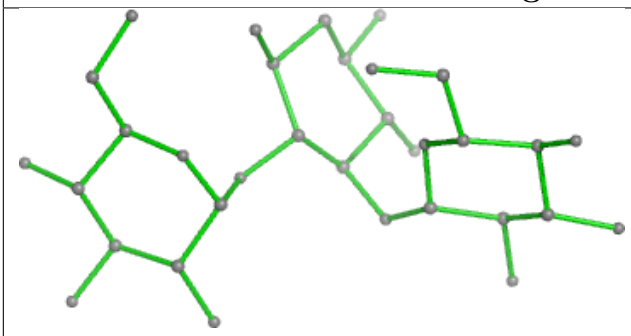


Rings

Ligand 8UZ 2 2031



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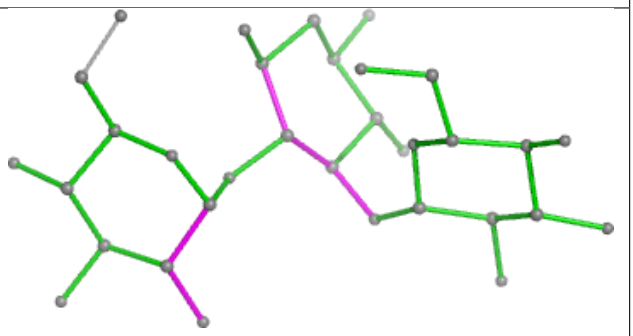
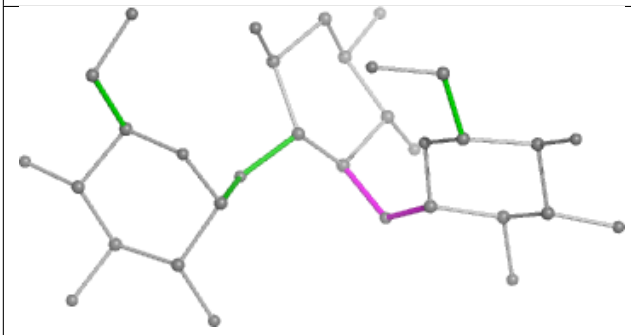


Bond angles



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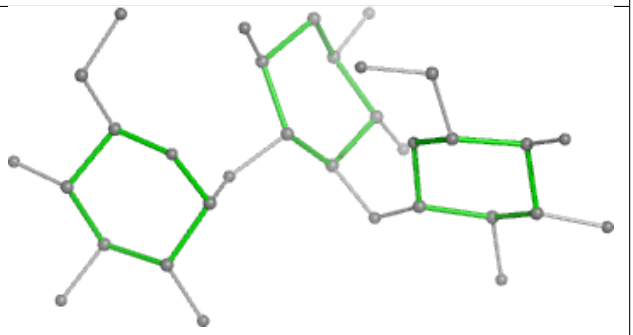
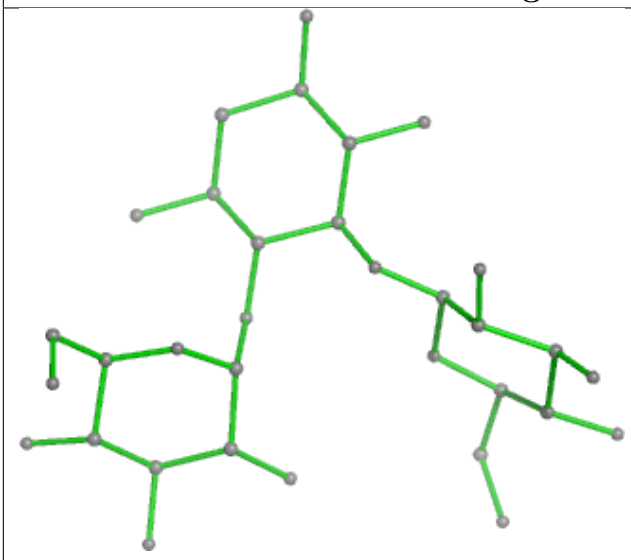


Rings

Ligand 8UZ 5 3850



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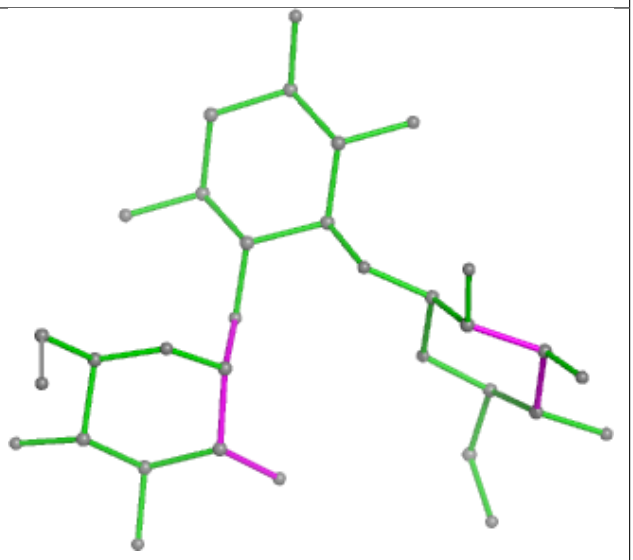

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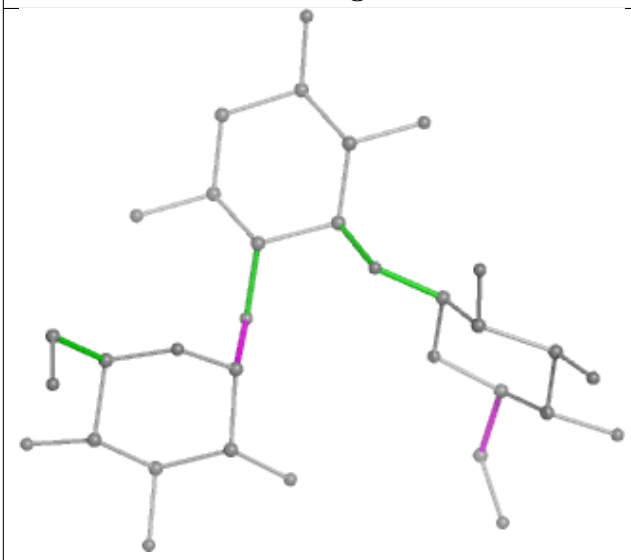

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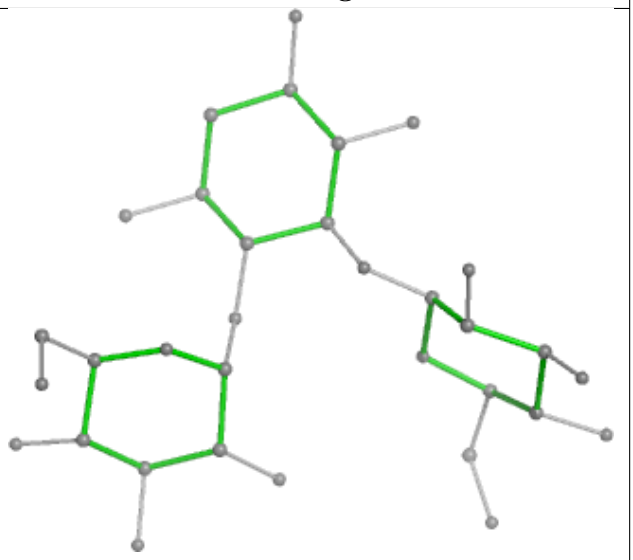
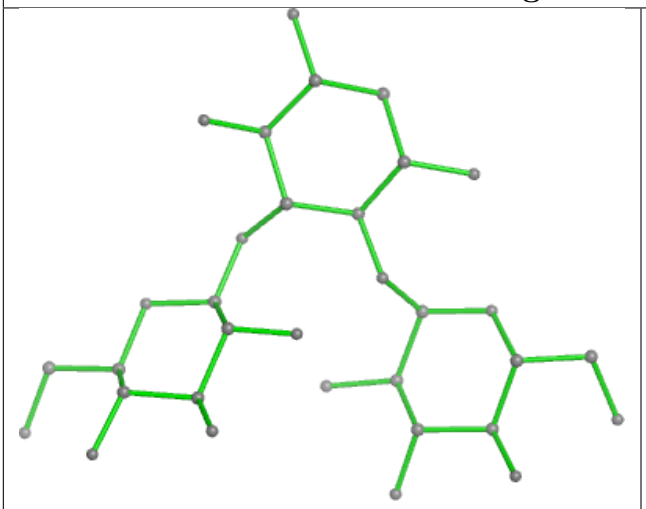


Rings

Ligand 8UZ 1 3895



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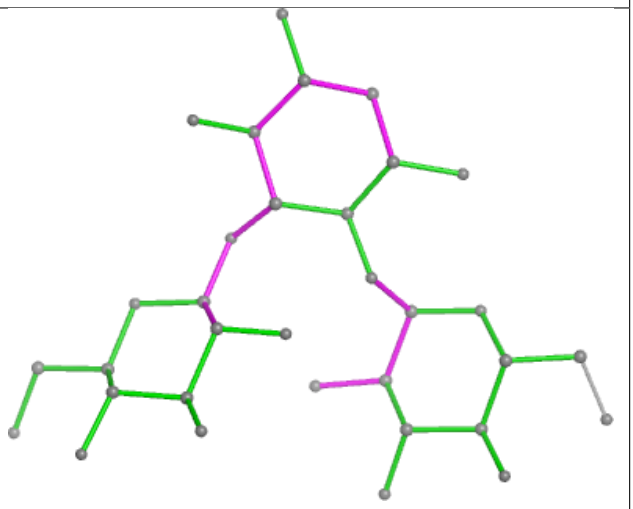
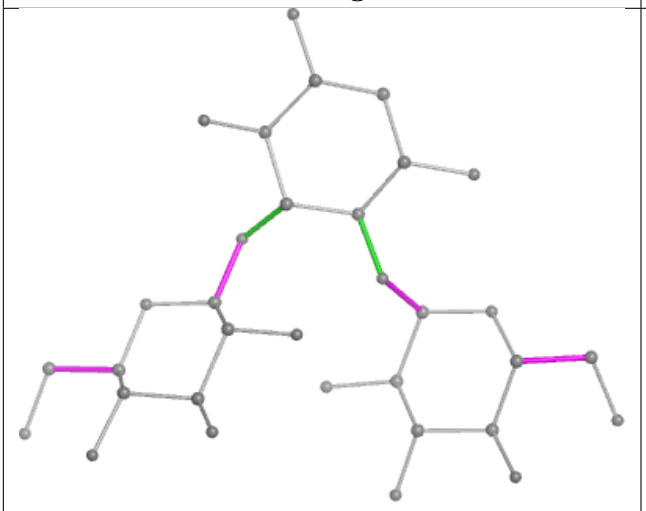
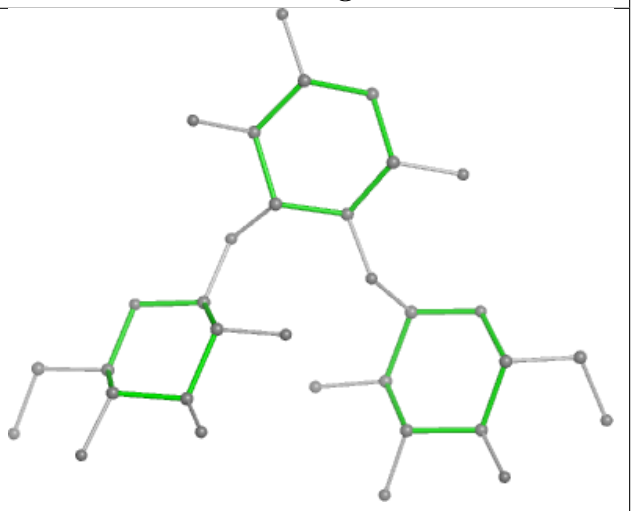


Bond angles

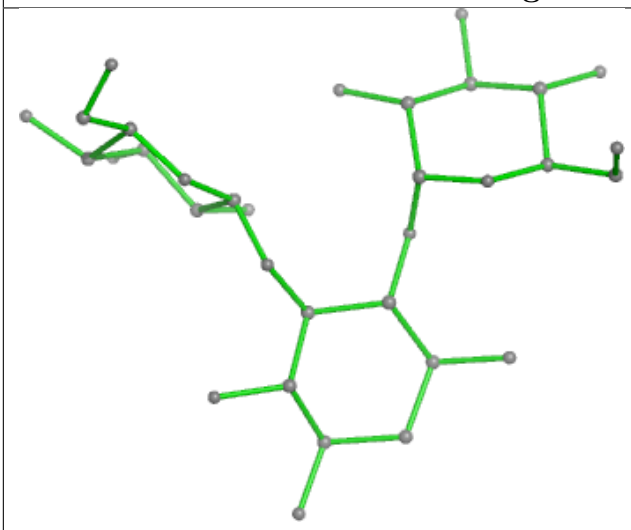


Torsions



Rings

Ligand 8UZ 1 3886



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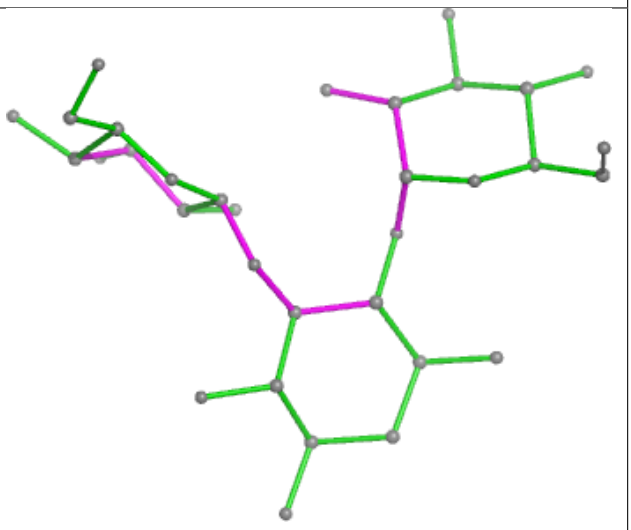

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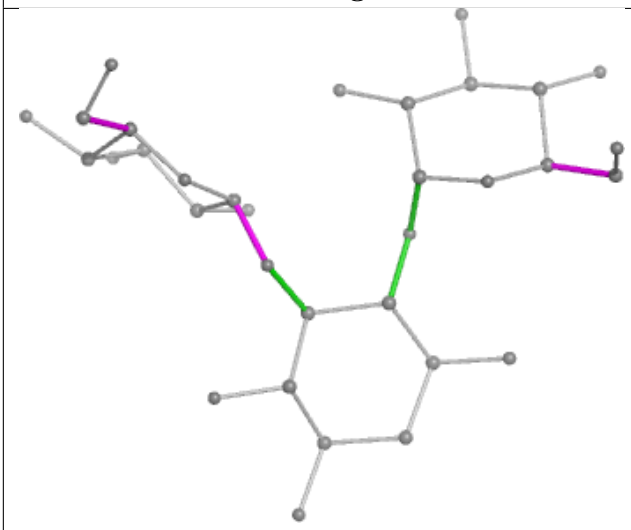

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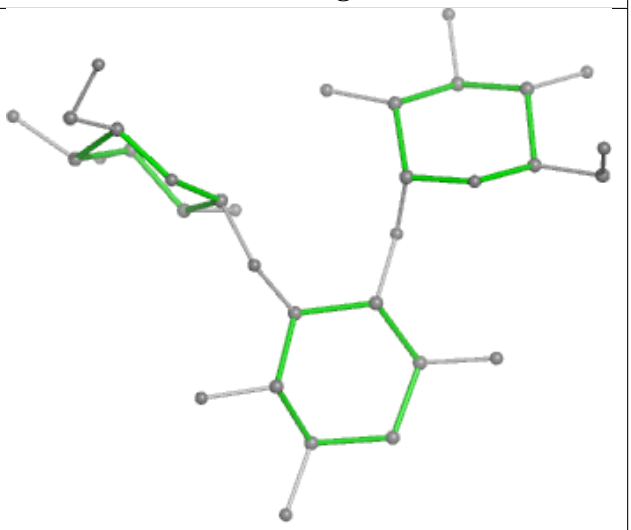
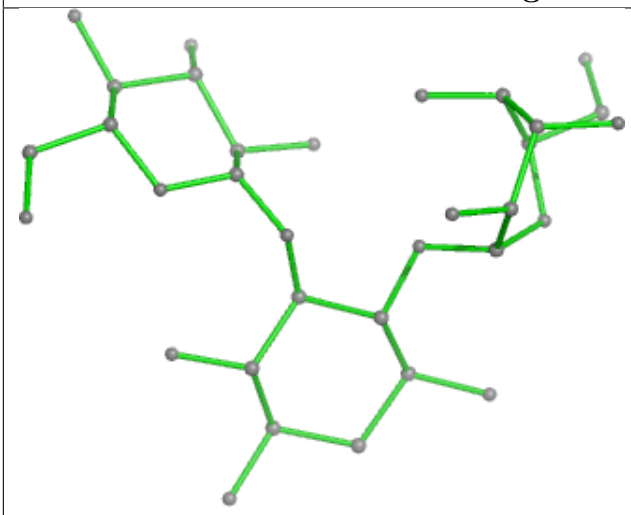


Rings

Ligand 8UZ 1 3891



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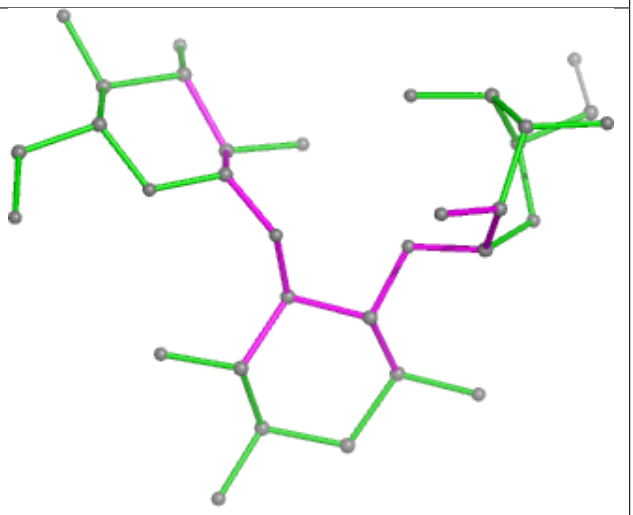

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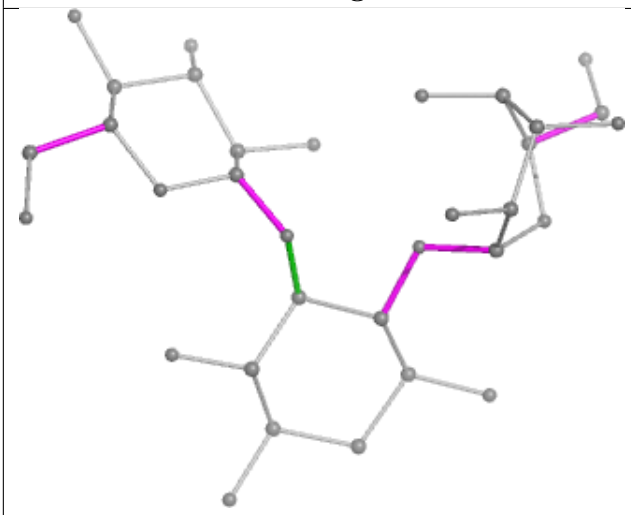

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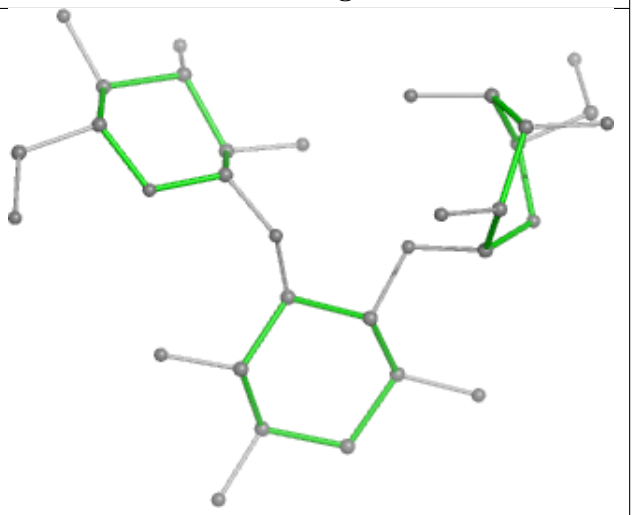
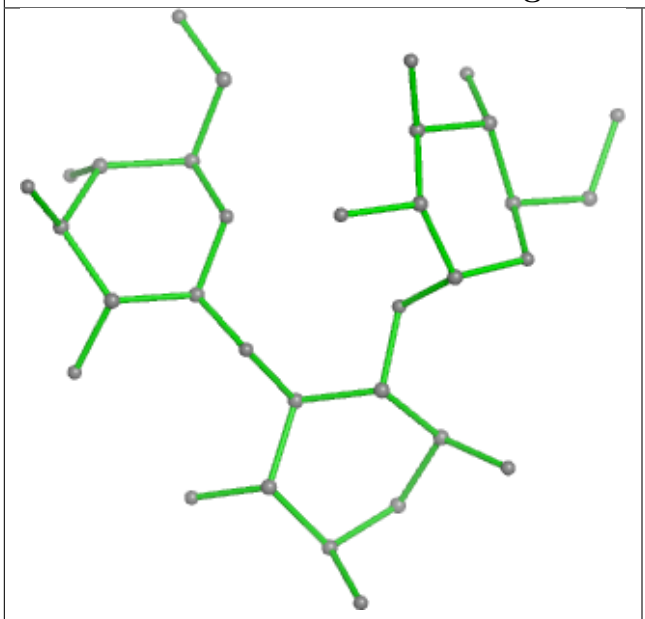


Rings

Ligand 8UZ 1 3893



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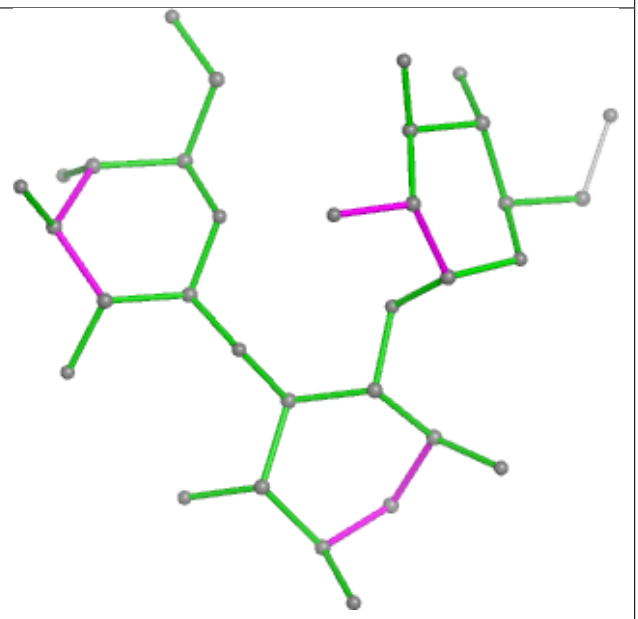
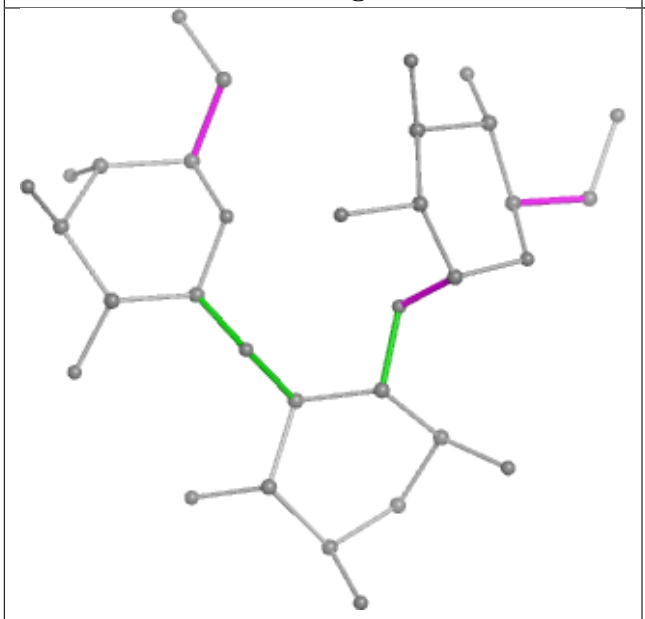


Bond angles



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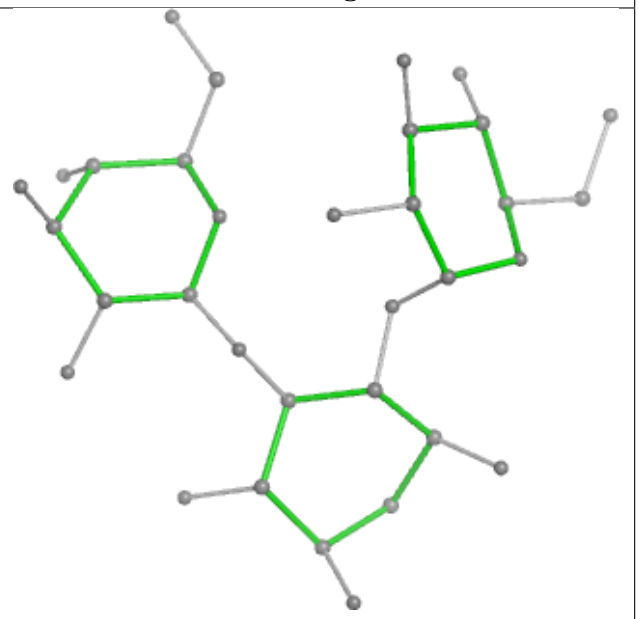
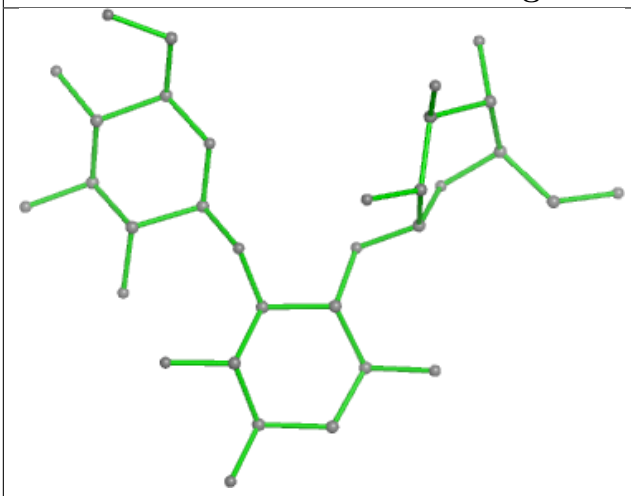


Rings

Ligand 8UZ 1 3887



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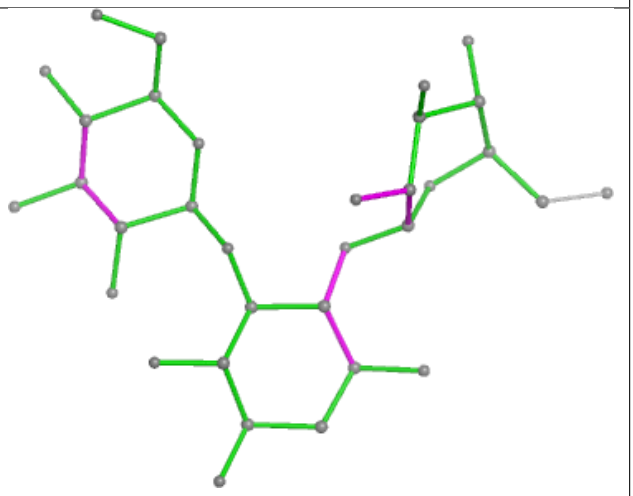
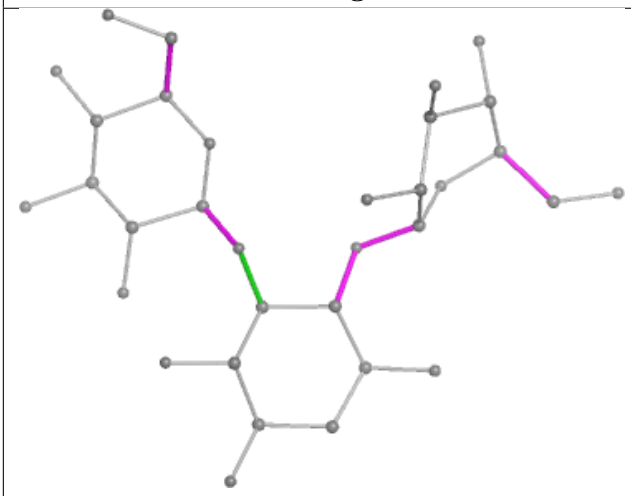


Bond angles



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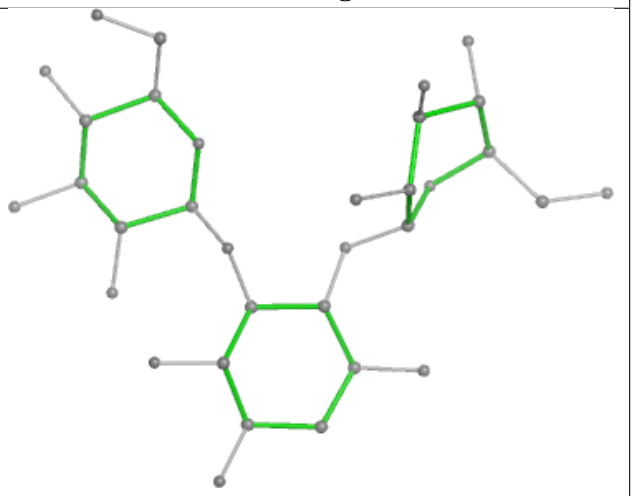
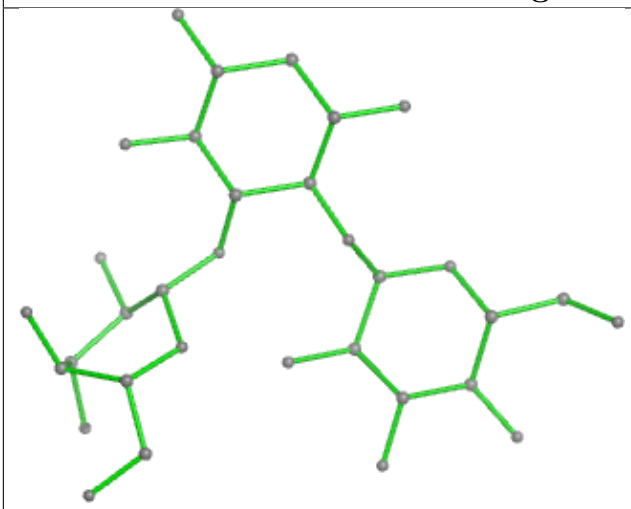


Rings

Ligand 8UZ 7 209



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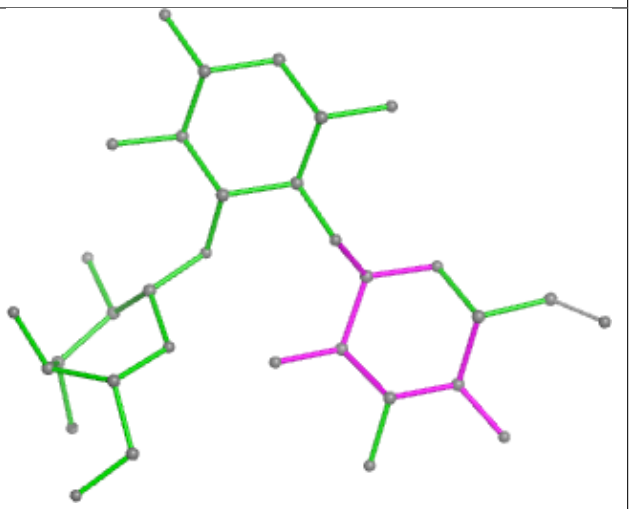
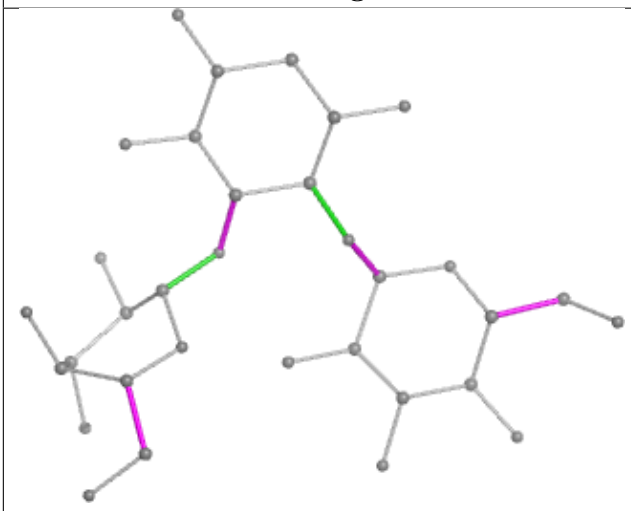
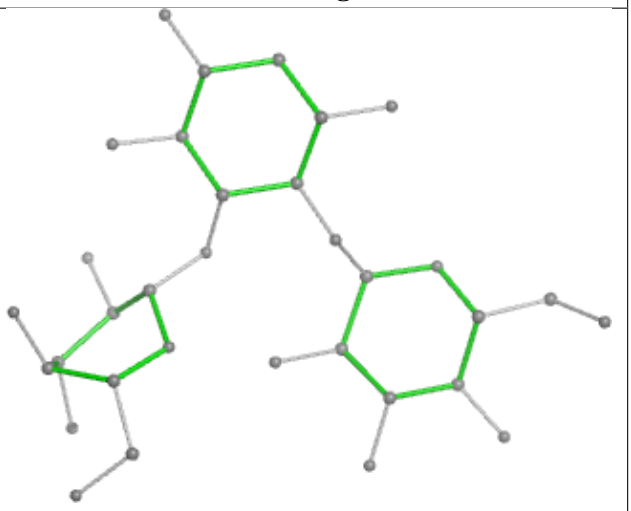


Bond angles

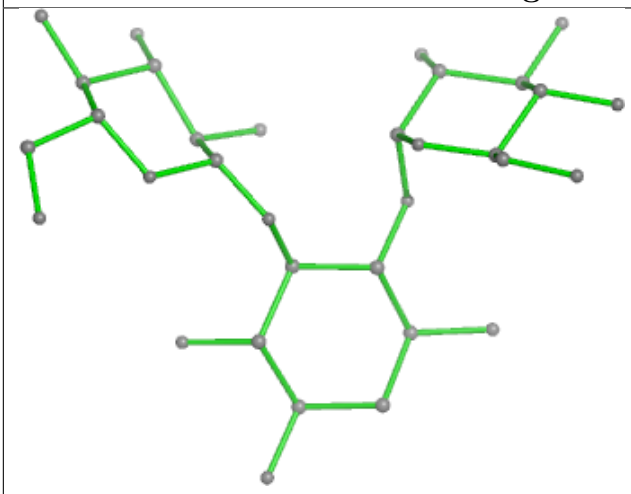


Torsions

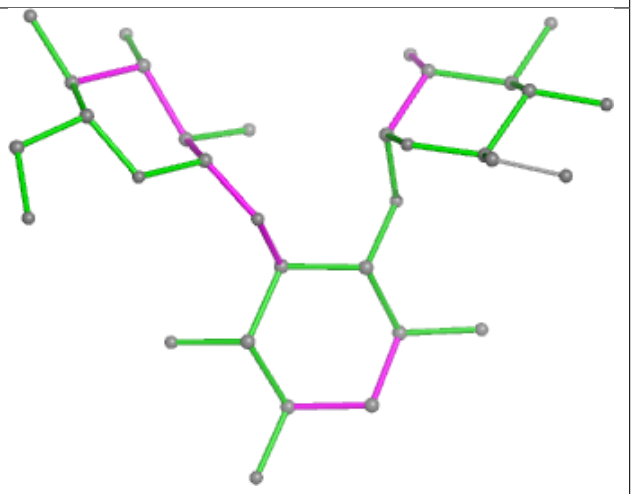


Rings

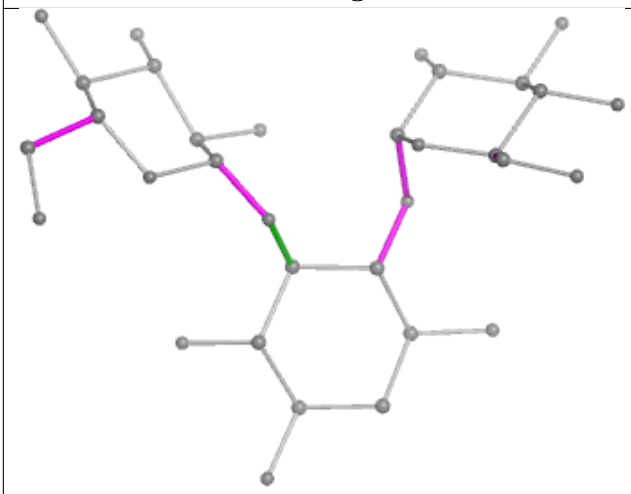
Ligand 8UZ 5 3853



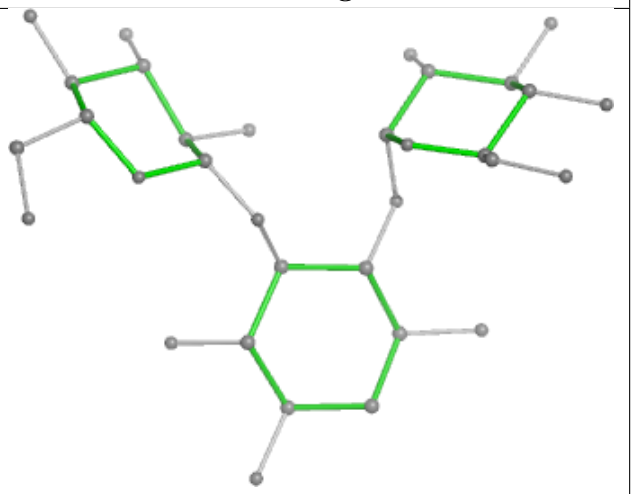
Bond lengths



Bond angles

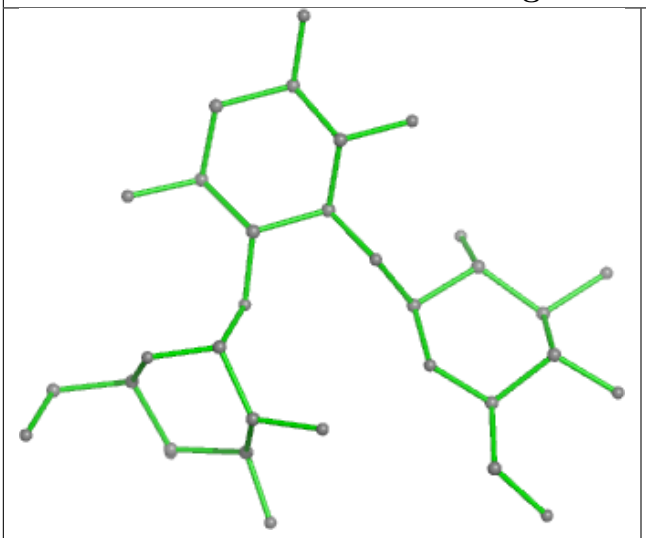


Torsions

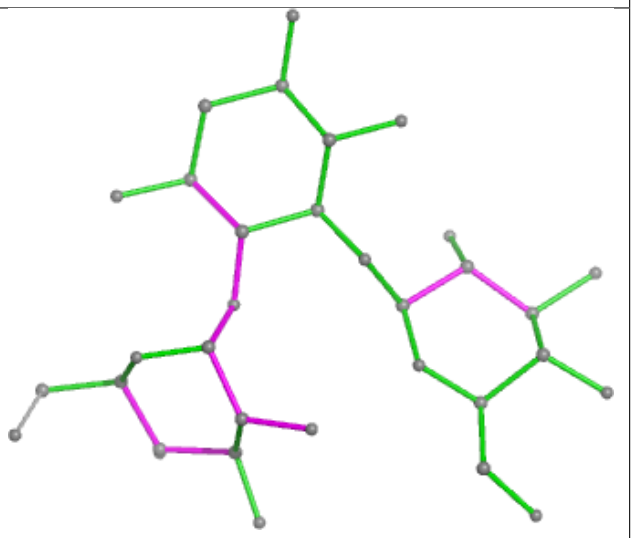


Rings

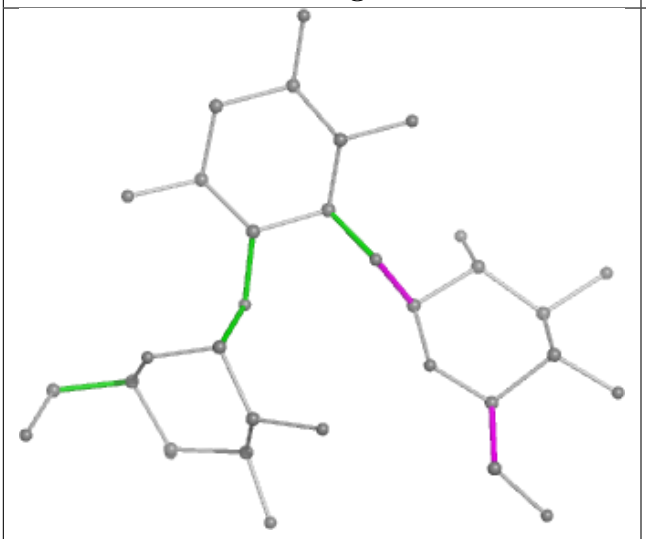
Ligand 8UZ 1 3894



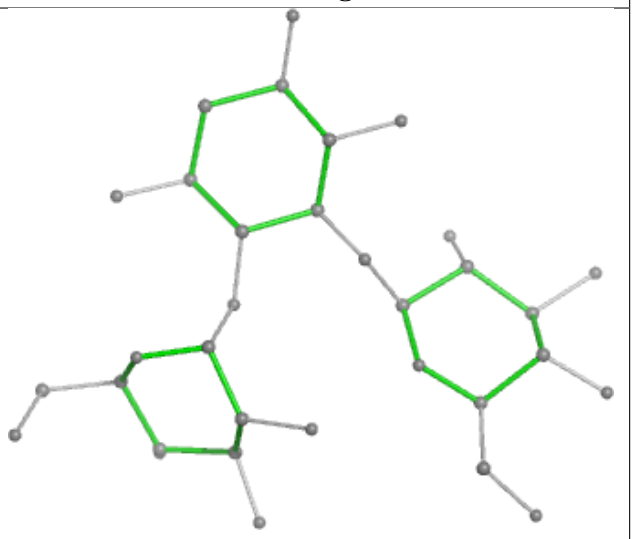
Bond lengths



Bond angles

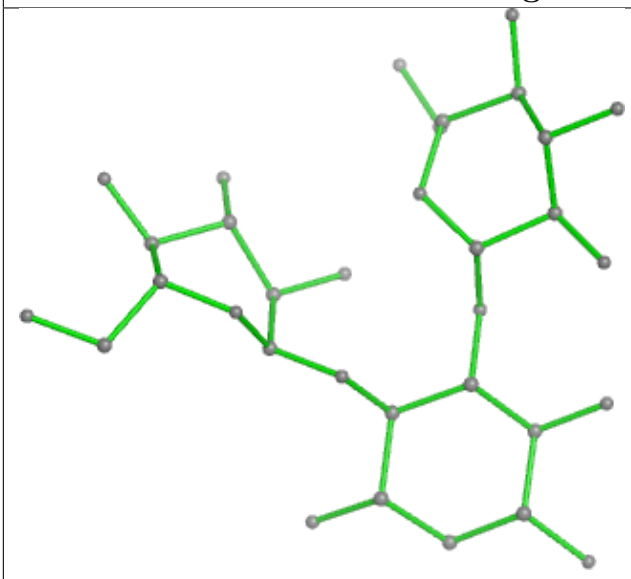


Torsions

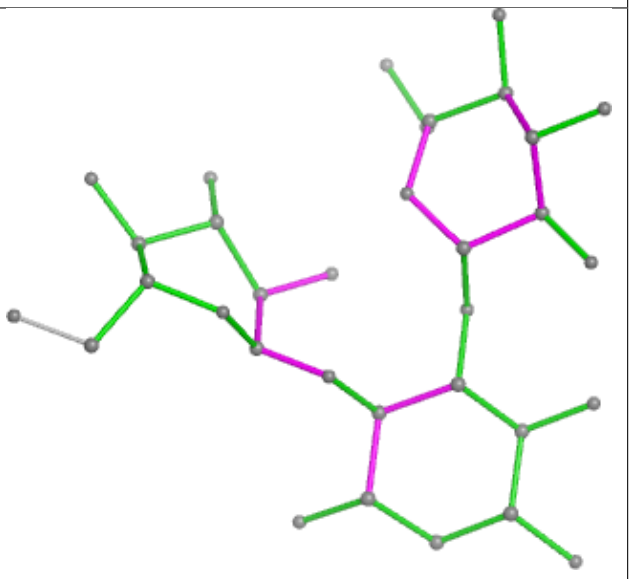


Rings

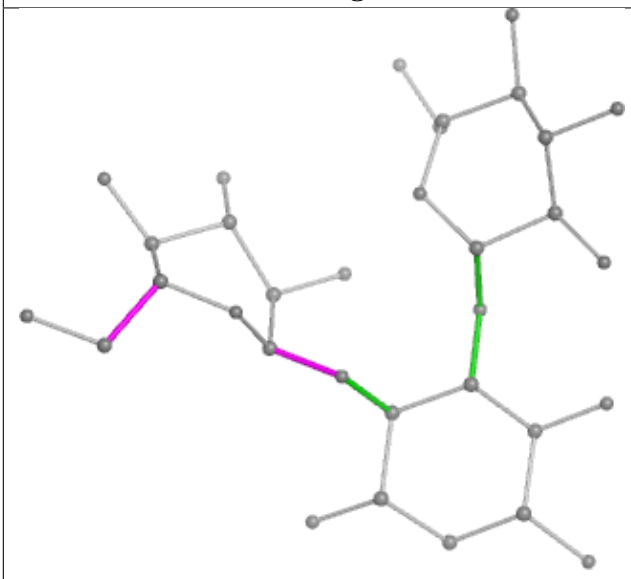
Ligand 8UZ 5 3854



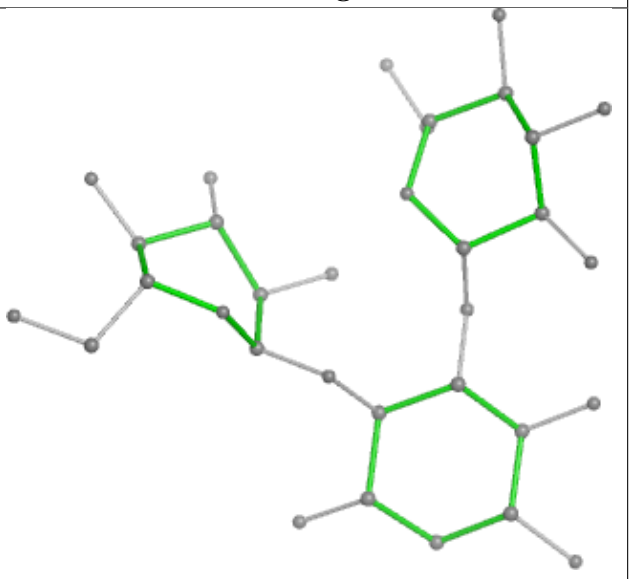
Bond lengths



Bond angles

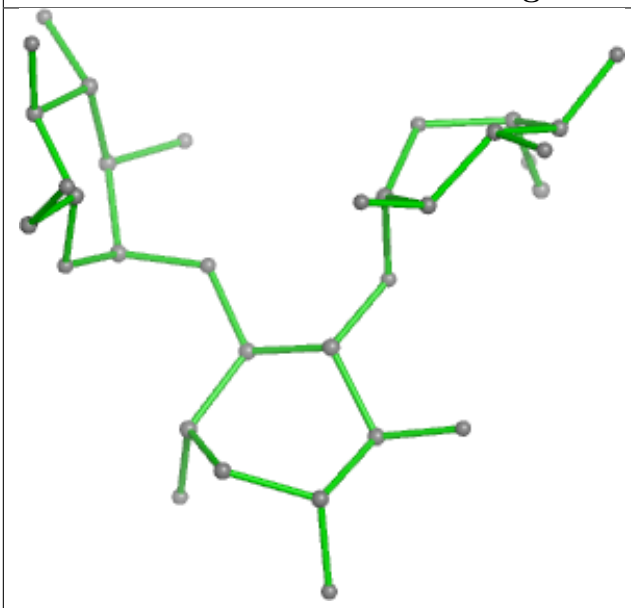


Torsions

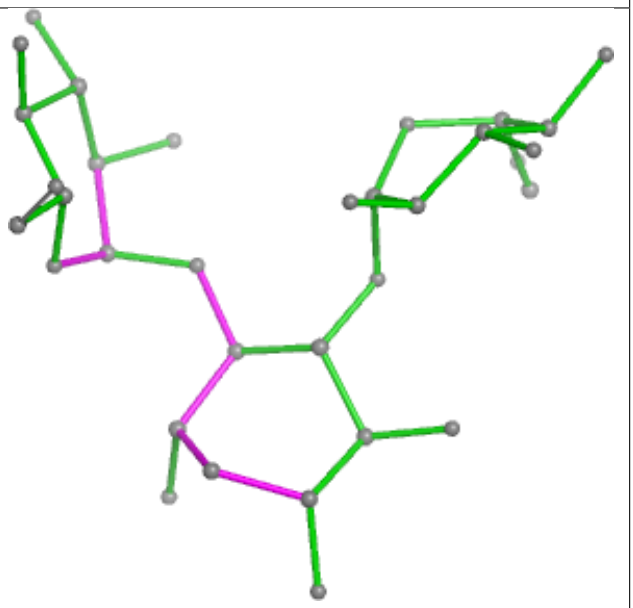


Rings

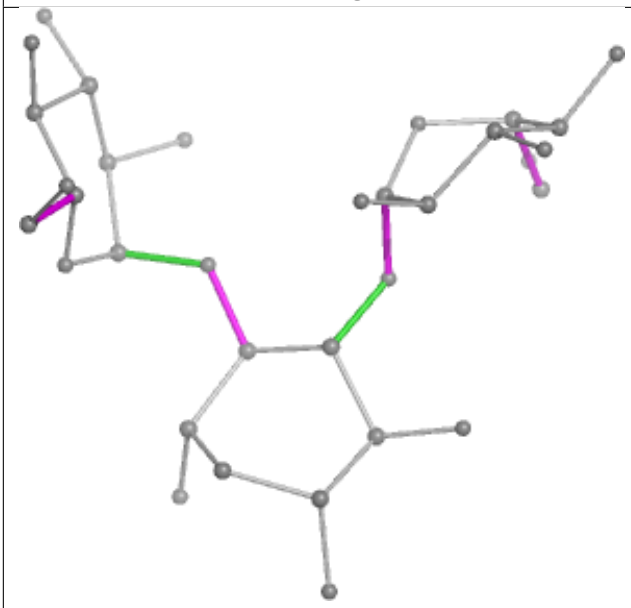
Ligand 8UZ 5 3857



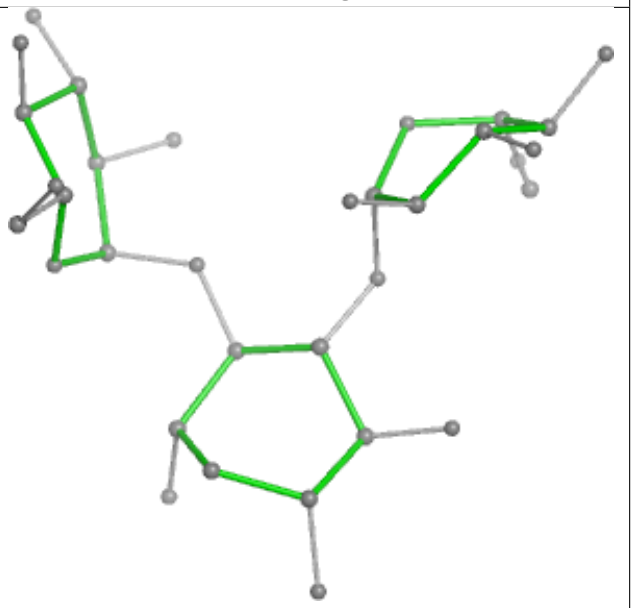
Bond lengths



Bond angles

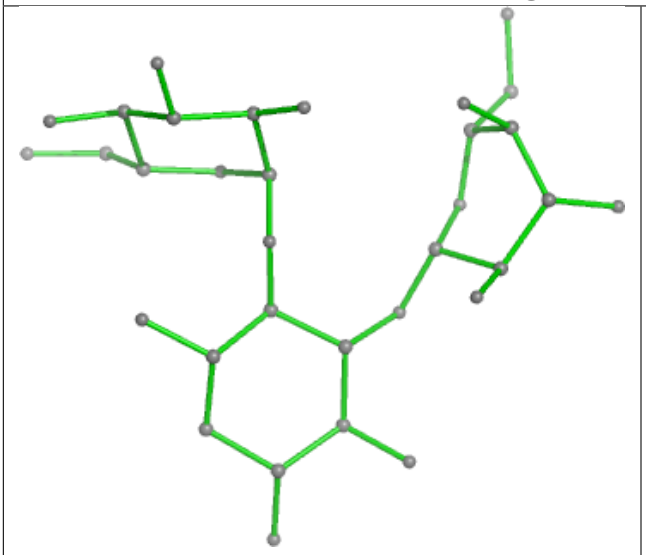


Torsions

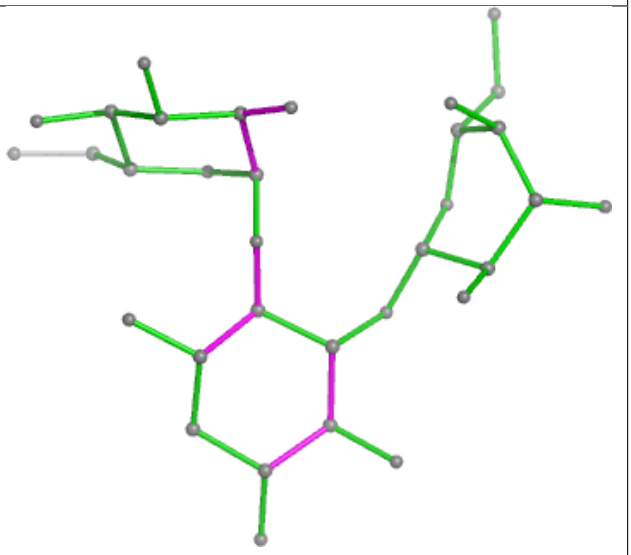


Rings

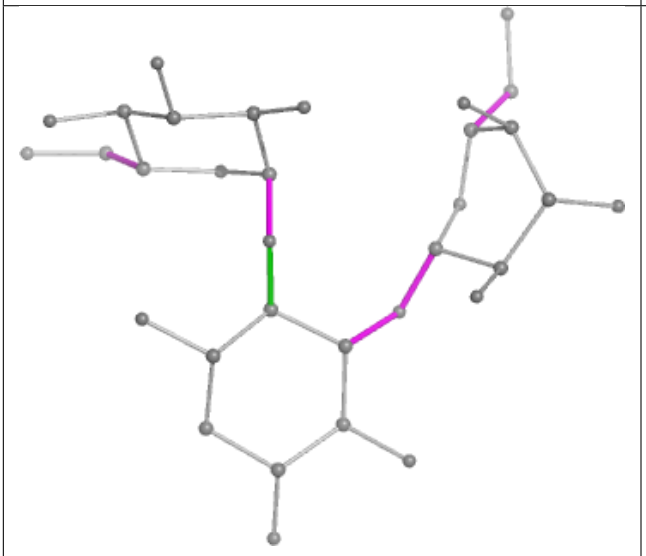
Ligand 8UZ 1 3888



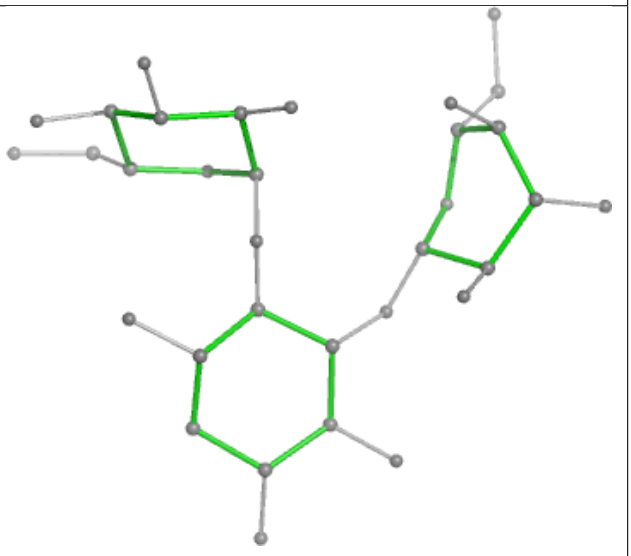
Bond lengths



Bond angles

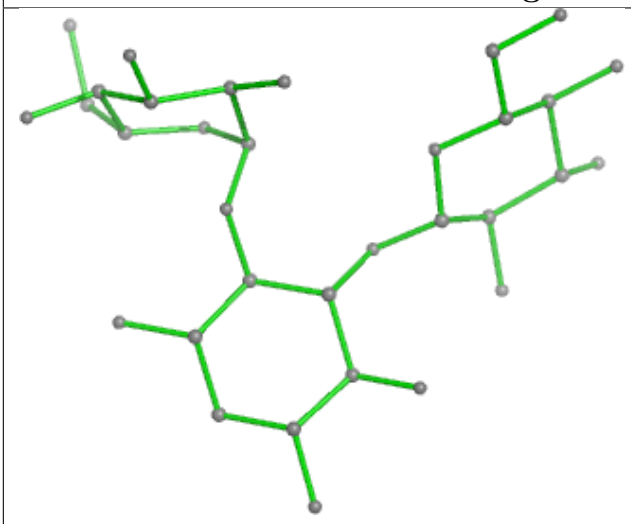


Torsions

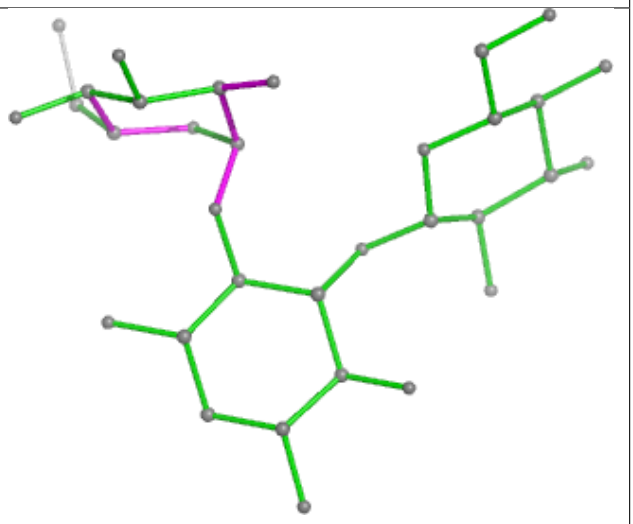


Rings

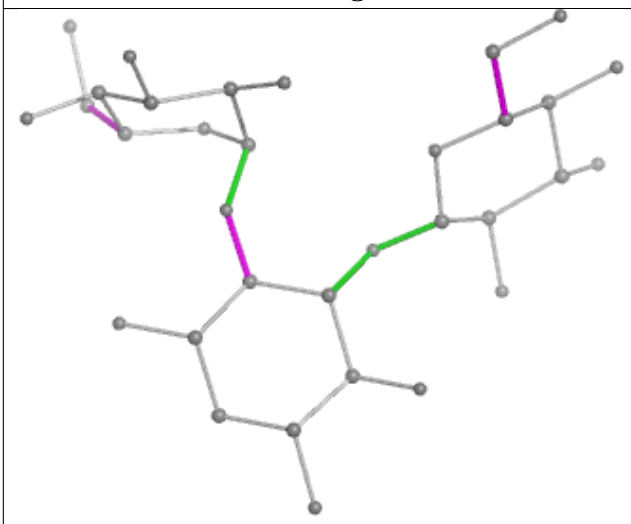
Ligand 8UZ 5 3852



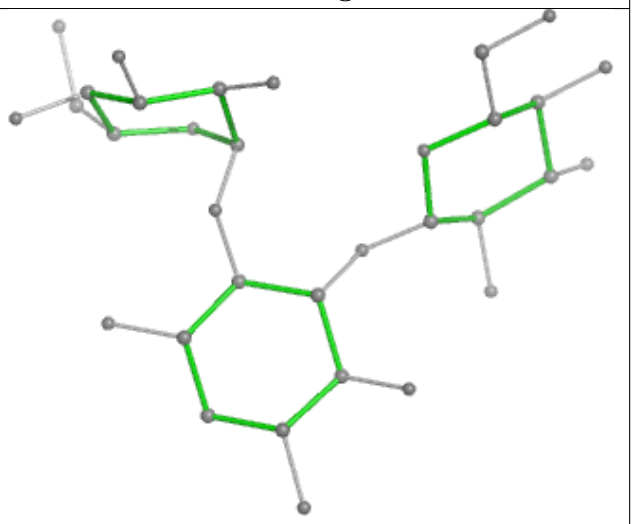
Bond lengths



Bond angles

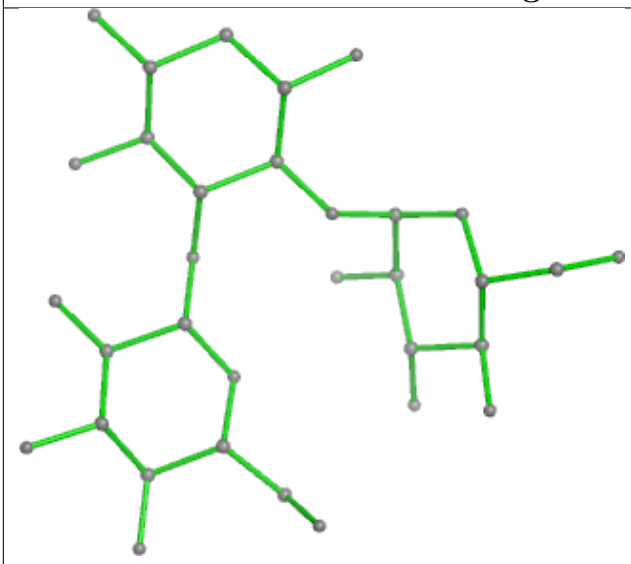


Torsions

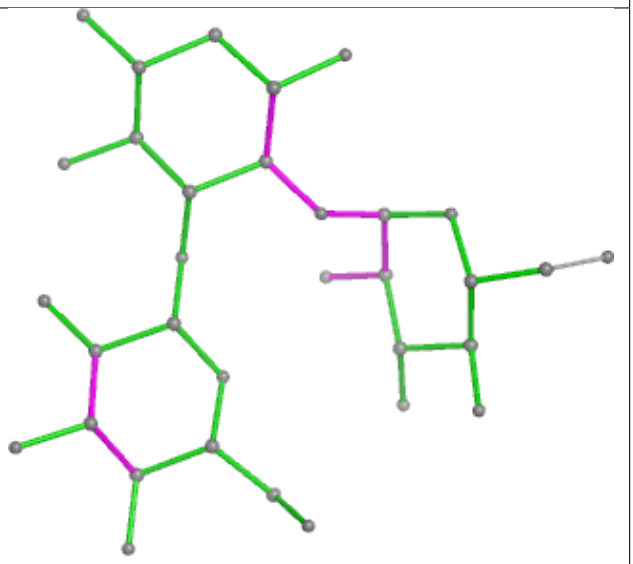


Rings

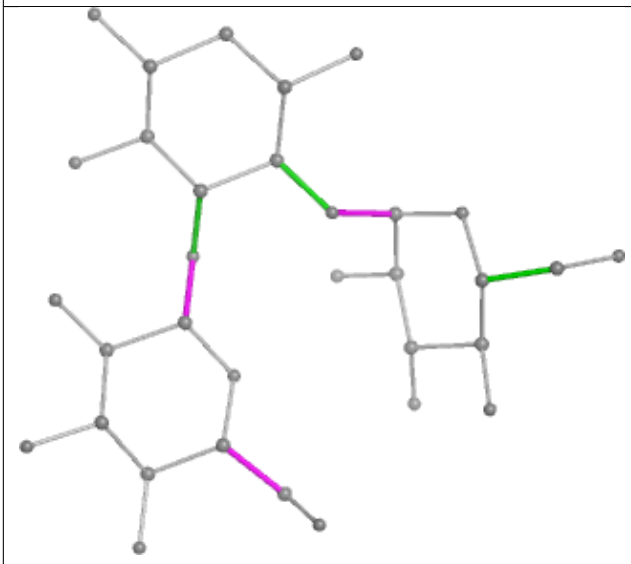
Ligand 8UZ 1 3890



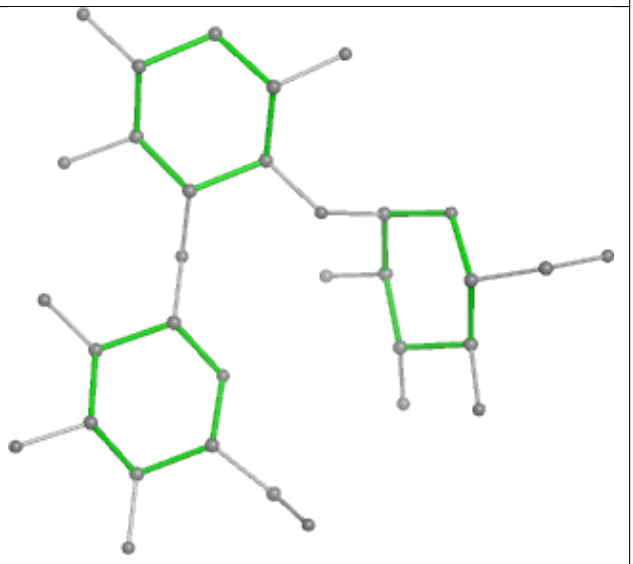
Bond lengths



Bond angles

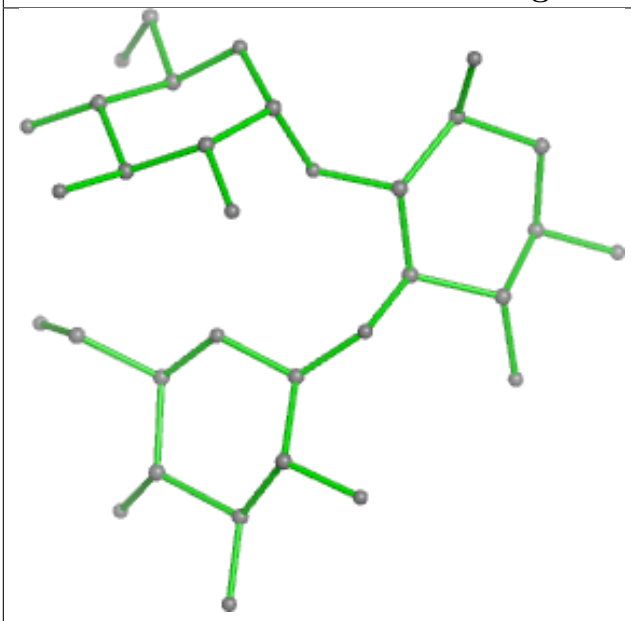


Torsions

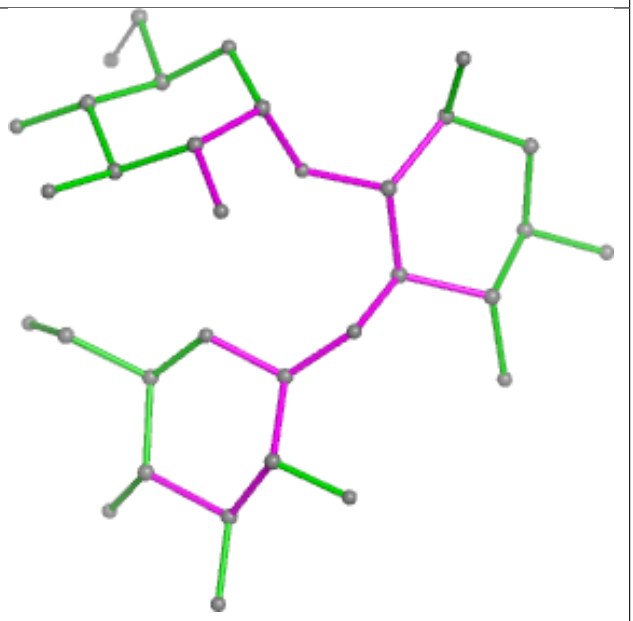


Rings

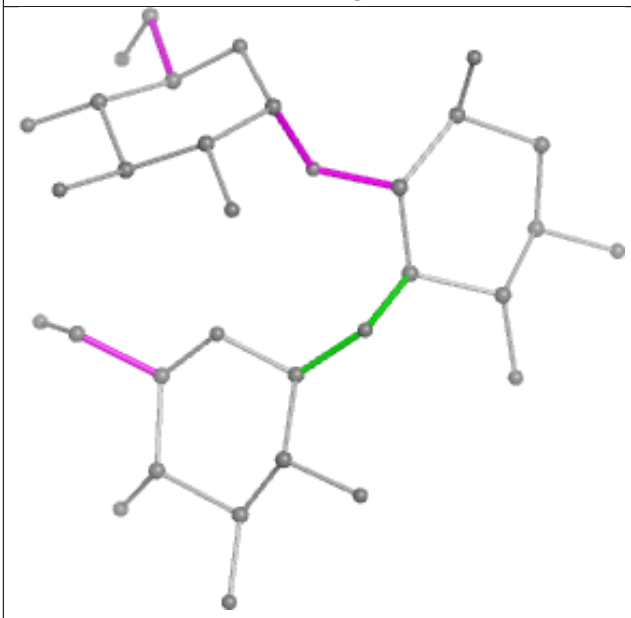
Ligand 8UZ 4 220



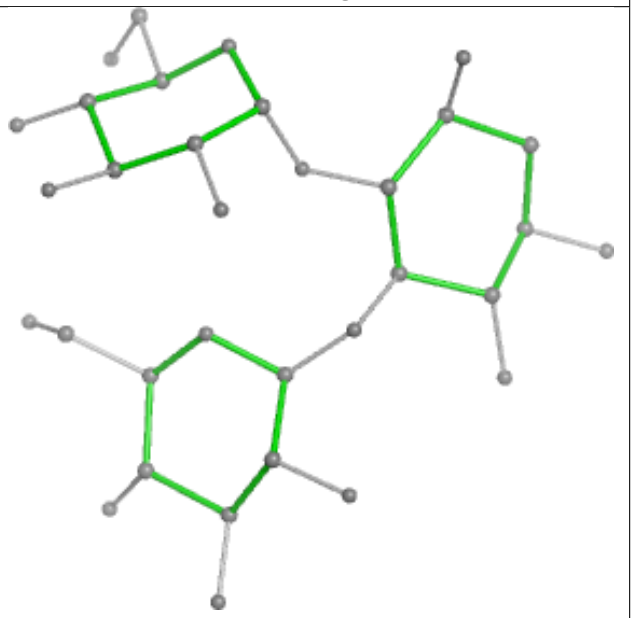
Bond lengths



Bond angles

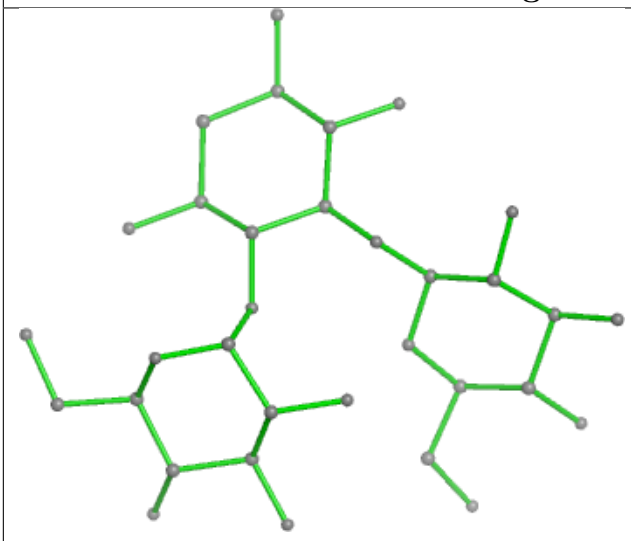


Torsions

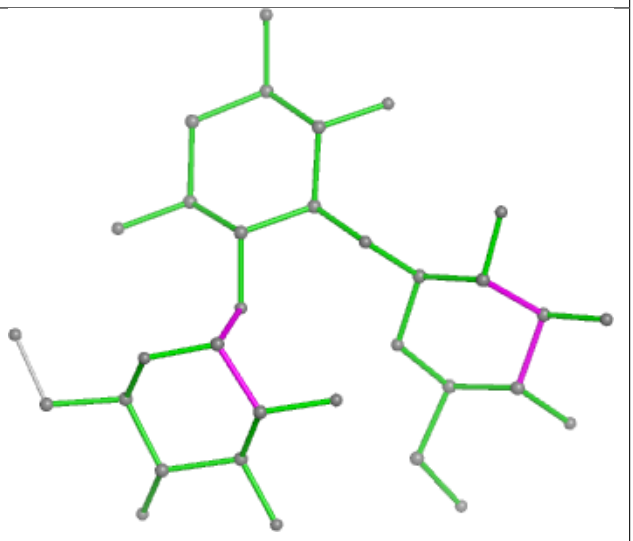


Rings

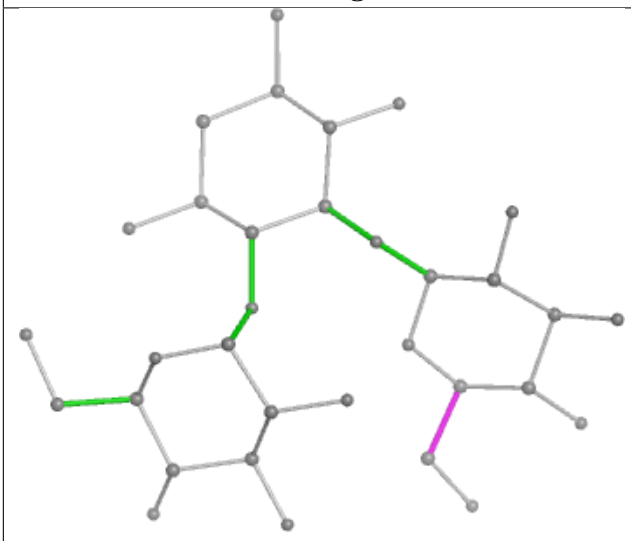
Ligand 8UZ 1 3889



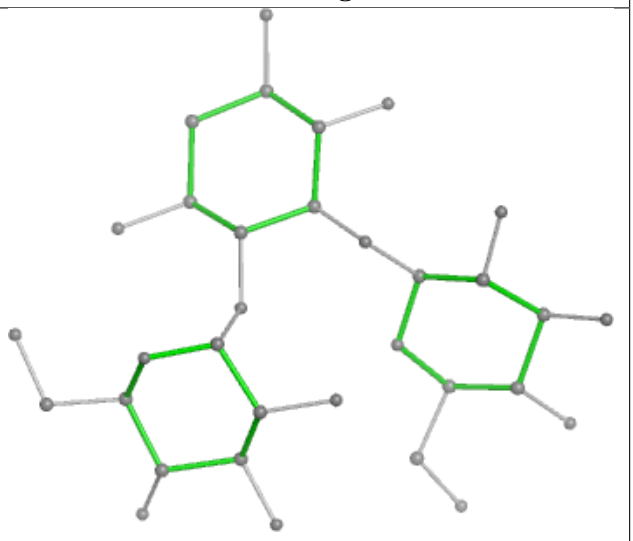
Bond lengths



Bond angles

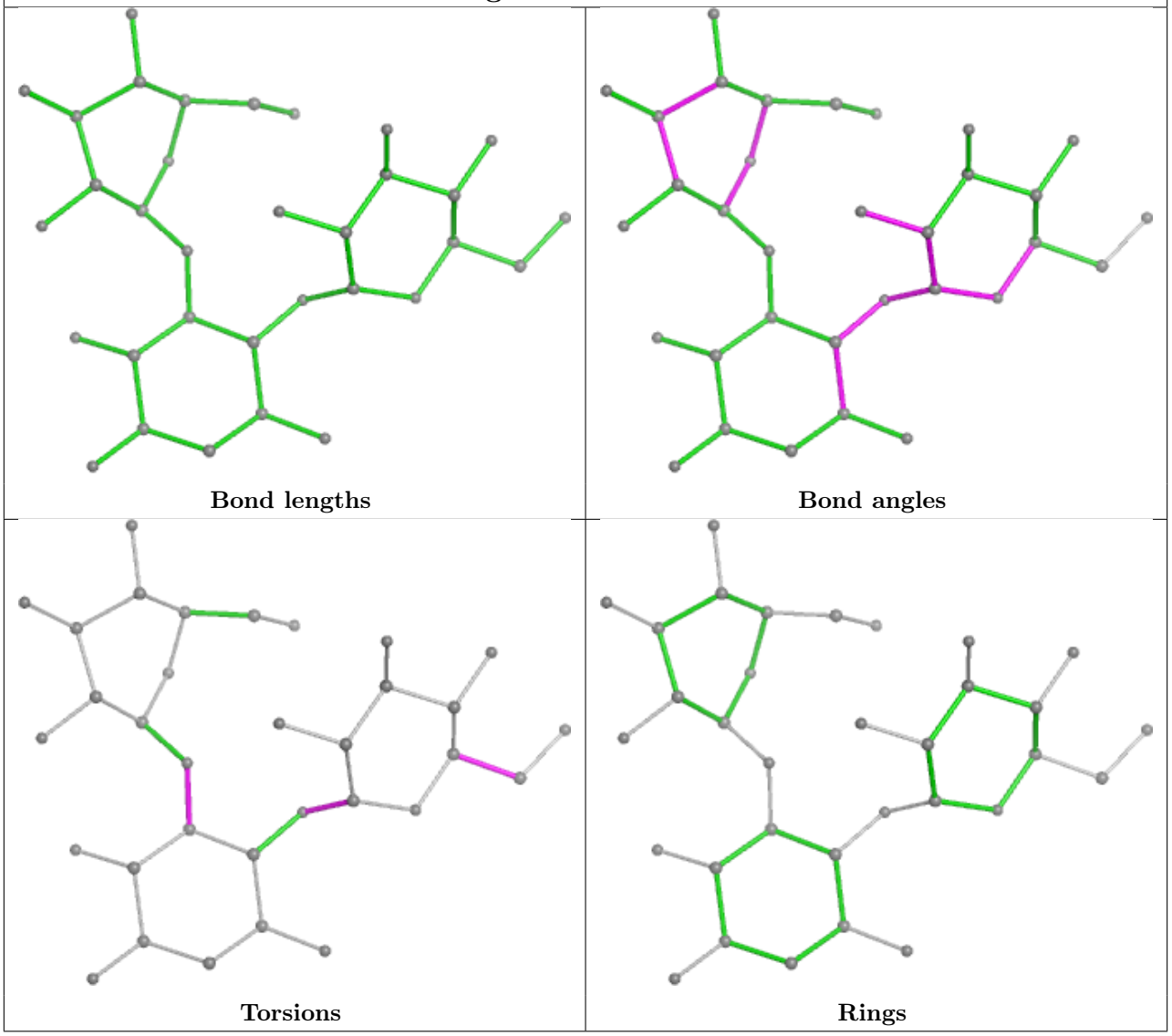


Torsions



Rings

Ligand 8UZ 3 214



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	5	1
78	sM	1
51	n7	1
37	M3	1

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Mol	Chain	Number of breaks
50	n6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1017:C	O3'	1018:G	P	6.05
1	sM	50:ASN	C	51:ARG	N	3.56
1	n7	36:HIS	C	37:PRO	N	1.73
1	M3	125:VAL	C	126:PHE	N	1.18
1	n6	99:LEU	C	100:HIS	N	1.17

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	1	3090/3396 (90%)	-0.01	15 (0%) 91 85	73, 114, 221, 384	0
1	5	3080/3396 (90%)	-0.04	16 (0%) 91 85	75, 122, 223, 357	0
2	2	1770/1800 (98%)	-0.13	46 (2%) 56 43	91, 158, 320, 453	0
2	6	1736/1800 (96%)	-0.26	13 (0%) 87 81	95, 154, 275, 374	0
3	3	121/121 (100%)	-0.51	0 100 100	88, 150, 179, 215	0
3	7	121/121 (100%)	-0.54	0 100 100	90, 171, 210, 226	0
4	4	158/158 (100%)	-0.11	1 (0%) 89 83	82, 126, 196, 327	0
4	8	158/158 (100%)	-0.06	3 (1%) 66 55	88, 138, 203, 271	0
5	C0	96/105 (91%)	1.54	34 (35%) 0 0	138, 198, 247, 261	0
5	c0	93/105 (88%)	0.80	20 (21%) 0 0	161, 209, 265, 317	0
6	C1	154/156 (98%)	1.47	47 (30%) 0 0	114, 150, 268, 325	0
6	c1	146/156 (93%)	0.91	20 (13%) 3 3	103, 137, 199, 244	0
7	C2	119/143 (83%)	2.08	56 (47%) 0 0	207, 274, 323, 343	0
7	c2	124/143 (86%)	1.98	55 (44%) 0 0	215, 274, 321, 343	0
8	C3	150/150 (100%)	0.39	7 (4%) 31 23	120, 171, 208, 232	0
8	c3	150/150 (100%)	0.74	13 (8%) 10 7	117, 157, 195, 229	0
9	C4	127/128 (99%)	0.12	6 (4%) 31 23	111, 171, 218, 250	0
9	c4	128/128 (100%)	1.01	27 (21%) 1 0	126, 185, 232, 278	0
10	C5	124/141 (87%)	0.76	14 (11%) 5 4	139, 185, 244, 296	0
10	c5	125/141 (88%)	0.55	19 (15%) 2 2	132, 180, 239, 260	0
11	C6	141/141 (100%)	1.39	46 (32%) 0 0	113, 175, 232, 275	0
11	c6	141/141 (100%)	1.20	43 (30%) 0 0	124, 171, 219, 243	0
12	C7	120/136 (88%)	0.74	21 (17%) 1 1	127, 192, 251, 284	0
12	c7	121/136 (88%)	0.24	7 (5%) 23 16	135, 186, 246, 340	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C8	145/145 (100%)	0.65	16 (11%) 5 4	127, 194, 255, 283	0
13	c8	145/145 (100%)	0.48	15 (10%) 6 5	133, 175, 221, 248	0
14	C9	143/143 (100%)	0.51	14 (9%) 7 6	128, 175, 216, 241	0
14	c9	143/143 (100%)	0.53	12 (8%) 11 8	137, 175, 210, 252	0
15	D0	105/107 (98%)	1.46	40 (38%) 0 0	117, 174, 261, 277	0
15	d0	104/107 (97%)	0.51	10 (9%) 8 6	133, 188, 257, 300	0
16	D1	87/87 (100%)	0.66	9 (10%) 6 5	137, 174, 221, 251	0
16	d1	87/87 (100%)	0.67	9 (10%) 6 5	132, 168, 212, 238	0
17	D2	129/129 (100%)	1.09	20 (15%) 2 1	114, 154, 185, 229	0
17	d2	129/129 (100%)	0.77	17 (13%) 3 3	112, 145, 171, 199	0
18	D3	144/144 (100%)	0.49	10 (6%) 16 11	101, 132, 166, 191	0
18	d3	144/144 (100%)	0.50	5 (3%) 44 33	96, 127, 154, 192	0
19	D4	134/134 (100%)	0.50	15 (11%) 5 4	144, 199, 233, 275	0
19	d4	134/134 (100%)	0.25	8 (5%) 21 15	122, 174, 224, 254	0
20	D5	70/70 (100%)	1.36	22 (31%) 0 0	146, 212, 265, 290	0
20	d5	69/70 (98%)	0.68	12 (17%) 1 1	159, 205, 240, 250	0
21	D6	97/97 (100%)	0.77	12 (12%) 4 4	108, 149, 225, 242	0
21	d6	97/97 (100%)	1.32	30 (30%) 0 0	108, 151, 241, 257	0
22	D7	81/81 (100%)	0.32	5 (6%) 20 14	119, 192, 254, 273	0
22	d7	81/81 (100%)	1.01	17 (20%) 1 0	130, 170, 251, 277	0
23	D8	63/63 (100%)	0.99	14 (22%) 0 0	137, 199, 263, 293	0
23	d8	63/63 (100%)	0.55	5 (7%) 12 9	144, 195, 229, 255	0
24	D9	52/53 (98%)	1.32	17 (32%) 0 0	121, 148, 181, 242	0
24	d9	53/53 (100%)	0.67	8 (15%) 2 2	131, 155, 201, 270	0
25	E0	60/61 (98%)	0.80	10 (16%) 1 1	127, 175, 237, 256	0
25	e0	61/61 (100%)	0.57	8 (13%) 3 3	118, 172, 231, 265	0
26	E1	71/73 (97%)	1.71	24 (33%) 0 0	184, 254, 297, 331	0
26	e1	73/73 (100%)	1.50	21 (28%) 0 0	194, 252, 323, 356	0
27	L2	252/252 (100%)	0.29	4 (1%) 72 61	70, 117, 155, 210	0
27	l2	252/252 (100%)	0.29	8 (3%) 47 35	85, 129, 167, 268	0
28	L3	386/386 (100%)	0.47	28 (7%) 15 11	71, 106, 143, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	l3	386/386 (100%)	0.14	4 (1%) 82 73	71, 103, 141, 238	0
29	L4	361/361 (100%)	0.18	3 (0%) 86 78	77, 120, 160, 215	0
29	l4	361/361 (100%)	0.10	4 (1%) 80 71	83, 129, 171, 207	0
30	L5	296/296 (100%)	0.73	42 (14%) 2 2	101, 165, 219, 253	0
30	l5	294/296 (99%)	0.99	62 (21%) 1 0	130, 193, 248, 273	0
31	L6	157/176 (89%)	-0.09	1 (0%) 89 83	87, 119, 160, 180	0
31	l6	157/176 (89%)	0.04	2 (1%) 77 67	82, 112, 171, 222	0
32	L7	222/223 (99%)	0.47	19 (8%) 10 8	83, 113, 169, 245	0
32	l7	223/223 (100%)	0.22	4 (1%) 68 57	77, 113, 161, 269	0
33	L8	233/233 (100%)	0.54	18 (7%) 13 10	124, 171, 236, 295	0
33	l8	231/233 (99%)	0.51	23 (9%) 7 5	134, 182, 244, 323	0
34	L9	191/191 (100%)	0.46	17 (8%) 9 7	85, 123, 158, 208	0
34	l9	191/191 (100%)	0.53	8 (4%) 36 27	82, 116, 147, 226	0
35	M0	211/221 (95%)	0.05	3 (1%) 75 64	82, 111, 181, 250	0
35	m0	209/221 (94%)	0.27	7 (3%) 46 35	89, 118, 180, 278	0
36	M1	169/169 (100%)	0.36	10 (5%) 22 15	123, 155, 188, 203	0
36	m1	169/169 (100%)	0.61	14 (8%) 11 9	136, 183, 219, 250	0
37	M3	193/194 (99%)	-0.04	4 (2%) 63 52	79, 144, 187, 263	0
37	m3	194/194 (100%)	0.28	10 (5%) 27 20	106, 162, 211, 286	0
38	M4	136/137 (99%)	0.24	4 (2%) 51 39	96, 123, 157, 191	0
38	m4	137/137 (100%)	0.05	1 (0%) 87 81	87, 111, 137, 182	0
39	M5	203/203 (100%)	1.06	28 (13%) 2 3	88, 124, 150, 166	0
39	m5	203/203 (100%)	1.11	36 (17%) 1 1	96, 140, 170, 183	0
40	M6	197/197 (100%)	0.17	2 (1%) 82 73	67, 97, 140, 196	0
40	m6	197/197 (100%)	0.09	0 100 100	67, 94, 138, 166	0
41	M7	183/184 (99%)	0.13	4 (2%) 62 50	75, 99, 184, 250	0
41	m7	183/184 (99%)	0.45	4 (2%) 62 50	76, 105, 176, 253	0
42	M8	185/185 (100%)	0.75	24 (12%) 3 3	89, 121, 149, 183	0
42	m8	185/185 (100%)	0.67	27 (14%) 2 2	93, 138, 166, 194	0
43	M9	188/188 (100%)	0.16	10 (5%) 26 20	92, 134, 244, 336	0
43	m9	184/188 (97%)	0.32	12 (6%) 18 12	101, 137, 218, 301	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	N0	172/172 (100%)	0.88	19 (11%) 5 4	88, 115, 150, 188	0
44	n0	171/172 (99%)	0.43	7 (4%) 37 27	80, 108, 139, 189	0
45	N1	159/159 (100%)	1.13	32 (20%) 1 0	94, 126, 187, 212	0
45	n1	159/159 (100%)	1.18	47 (29%) 0 0	100, 136, 187, 244	0
46	N2	100/100 (100%)	0.60	12 (12%) 4 4	126, 172, 211, 237	0
46	n2	98/100 (98%)	0.38	13 (13%) 3 3	139, 180, 223, 247	0
47	N3	136/136 (100%)	0.52	6 (4%) 34 25	69, 105, 149, 254	0
47	n3	135/136 (99%)	0.37	3 (2%) 62 50	72, 100, 135, 178	0
48	N4	130/155 (83%)	1.18	25 (19%) 1 1	88, 171, 291, 313	0
48	n4	130/155 (83%)	0.70	19 (14%) 2 2	93, 180, 259, 294	0
49	N5	121/121 (100%)	0.50	8 (6%) 18 12	105, 138, 175, 245	0
49	n5	120/121 (99%)	1.37	35 (29%) 0 0	113, 150, 191, 229	0
50	N6	126/126 (100%)	0.55	4 (3%) 47 35	96, 127, 164, 209	0
50	n6	122/126 (96%)	0.68	10 (8%) 11 9	104, 144, 177, 183	0
51	N7	135/135 (100%)	0.96	26 (19%) 1 1	143, 184, 224, 242	0
51	n7	135/135 (100%)	0.77	15 (11%) 5 4	137, 187, 227, 253	0
52	N8	148/148 (100%)	0.77	10 (6%) 17 12	79, 123, 170, 199	0
52	n8	148/148 (100%)	0.65	18 (12%) 4 4	90, 144, 188, 213	0
53	N9	58/58 (100%)	1.33	14 (24%) 0 0	82, 135, 196, 215	0
53	n9	56/58 (96%)	1.65	21 (37%) 0 0	91, 158, 203, 245	0
54	O0	97/100 (97%)	0.52	8 (8%) 11 9	138, 162, 212, 221	0
54	o0	100/100 (100%)	0.37	7 (7%) 16 11	128, 165, 222, 241	0
55	O1	109/109 (100%)	0.61	8 (7%) 15 11	81, 119, 186, 224	0
55	o1	109/109 (100%)	0.59	8 (7%) 15 11	89, 124, 204, 257	0
56	O2	127/127 (100%)	0.17	0 100 100	77, 100, 133, 192	0
56	o2	127/127 (100%)	0.35	2 (1%) 72 61	75, 108, 139, 200	0
57	O3	106/106 (100%)	0.16	1 (0%) 84 76	74, 97, 130, 145	0
57	o3	106/106 (100%)	0.30	0 100 100	76, 95, 123, 162	0
58	O4	112/112 (100%)	1.21	25 (22%) 0 0	102, 143, 228, 286	0
58	o4	112/112 (100%)	0.50	11 (9%) 7 6	109, 150, 203, 243	0
59	O5	119/119 (100%)	0.30	3 (2%) 57 45	109, 146, 190, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
59	o5	119/119 (100%)	0.73	12 (10%) 7 5	126, 157, 193, 207	0
60	O6	99/99 (100%)	0.38	5 (5%) 28 21	126, 151, 195, 302	0
60	o6	99/99 (100%)	0.35	8 (8%) 12 9	128, 169, 209, 289	0
61	O7	87/87 (100%)	0.06	0 100 100	80, 104, 186, 209	0
61	o7	83/87 (95%)	0.23	3 (3%) 42 32	91, 119, 150, 202	0
62	O8	77/77 (100%)	0.83	13 (16%) 1 1	132, 168, 205, 227	0
62	o8	77/77 (100%)	1.24	16 (20%) 1 0	150, 180, 220, 227	0
63	O9	50/50 (100%)	0.61	2 (4%) 38 28	94, 117, 133, 144	0
63	o9	50/50 (100%)	1.44	10 (20%) 1 0	108, 125, 145, 152	0
64	Q0	52/52 (100%)	0.07	1 (1%) 66 55	92, 110, 155, 190	0
64	q0	52/52 (100%)	0.30	2 (3%) 40 30	83, 106, 135, 148	0
65	Q1	25/25 (100%)	0.45	0 100 100	96, 115, 136, 144	0
65	q1	25/25 (100%)	0.30	1 (4%) 38 28	102, 117, 148, 156	0
66	Q2	105/105 (100%)	0.88	18 (17%) 1 1	86, 132, 166, 258	0
66	q2	104/105 (99%)	1.14	28 (26%) 0 0	111, 156, 199, 215	0
67	Q3	91/91 (100%)	0.01	0 100 100	88, 127, 175, 217	0
67	q3	91/91 (100%)	0.18	1 (1%) 80 71	79, 131, 176, 210	0
68	S0	206/206 (100%)	0.56	20 (9%) 7 6	128, 178, 224, 271	0
68	s0	206/206 (100%)	0.39	22 (10%) 6 5	133, 174, 214, 262	0
69	S1	214/216 (99%)	0.75	33 (15%) 2 1	138, 201, 253, 279	0
69	s1	216/216 (100%)	1.30	69 (31%) 0 0	139, 202, 254, 312	0
70	S2	217/217 (100%)	0.79	29 (13%) 3 3	120, 161, 202, 244	0
70	s2	217/217 (100%)	0.57	22 (10%) 7 5	114, 155, 195, 226	0
71	S3	223/223 (100%)	1.13	47 (21%) 1 0	113, 166, 236, 306	0
71	s3	223/223 (100%)	0.53	24 (10%) 5 4	137, 174, 236, 267	0
72	S4	260/260 (100%)	1.02	55 (21%) 0 0	131, 181, 213, 254	0
72	s4	260/260 (100%)	0.45	15 (5%) 23 16	109, 159, 203, 253	0
73	S5	206/206 (100%)	1.16	42 (20%) 1 0	125, 189, 236, 278	0
73	s5	206/206 (100%)	0.98	35 (16%) 1 1	145, 185, 230, 264	0
74	S6	226/236 (95%)	0.84	45 (19%) 1 0	125, 186, 246, 272	0
74	s6	218/236 (92%)	0.63	32 (14%) 2 2	111, 162, 216, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
75	S7	184/184 (100%)	0.83	33 (17%)	1	1	154, 208, 268, 305	0
75	s7	184/184 (100%)	0.46	19 (10%)	6	5	133, 195, 250, 297	0
76	S8	188/200 (94%)	1.01	35 (18%)	1	1	113, 154, 219, 291	0
76	s8	185/200 (92%)	0.87	29 (15%)	2	1	101, 142, 204, 250	0
77	S9	185/185 (100%)	0.98	36 (19%)	1	1	129, 186, 240, 279	0
77	s9	185/185 (100%)	0.87	29 (15%)	2	1	119, 169, 223, 263	0
78	SM	159/272 (58%)	0.51	22 (13%)	2	3	117, 185, 279, 371	0
78	sM	131/272 (48%)	0.38	15 (11%)	4	4	129, 182, 270, 311	0
79	SR	318/318 (100%)	1.13	77 (24%)	0	0	164, 221, 281, 318	0
79	sR	316/318 (99%)	0.58	40 (12%)	3	4	143, 199, 251, 293	0
All	All	32778/34100 (96%)	0.41	2743 (8%)	11	8	67, 147, 242, 453	0

The worst 5 of 2743 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
78	SM	19	VAL	12.3
34	l9	191	LEU	12.0
1	5	1565	G	11.1
54	o0	6	SER	10.7
78	SM	18	VAL	9.3

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.