



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 08:11 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

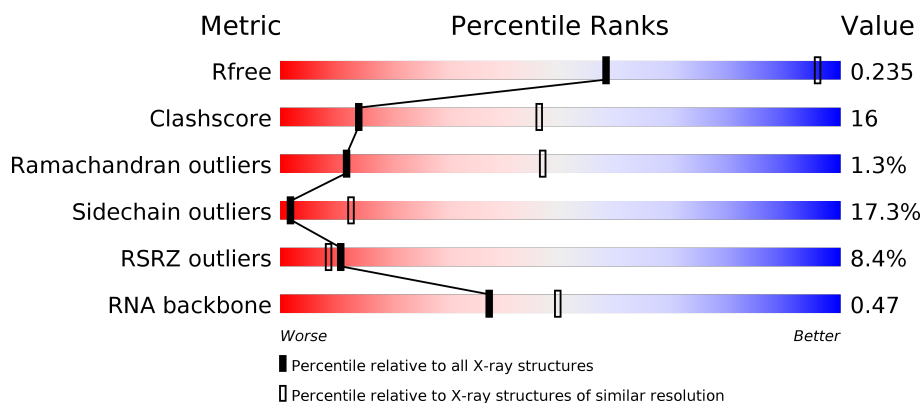
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.





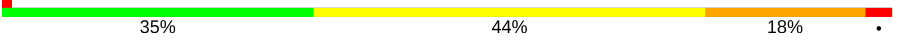
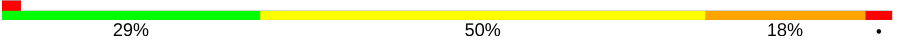


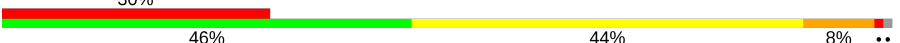

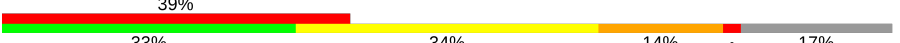

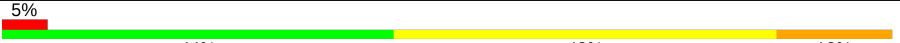

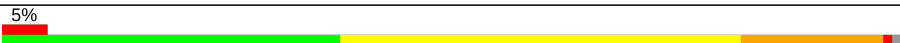

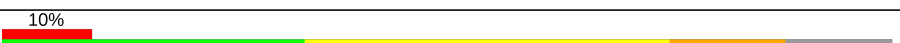

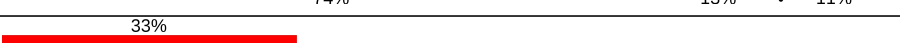
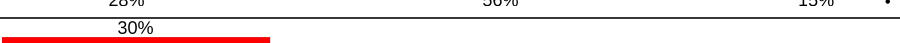
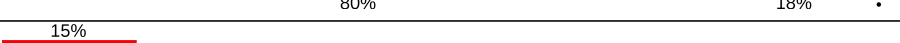
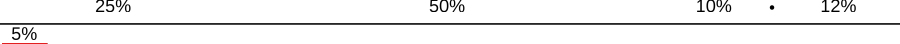
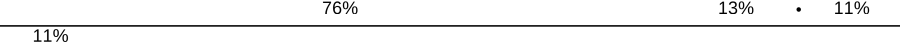
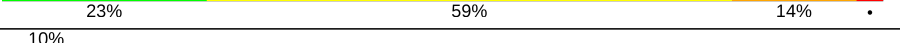

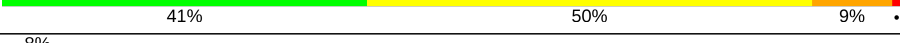

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	
1	5	3396	
2	2	1800	
2	6	1800	

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Mol	Chain	Length	Quality of chain
3	3	121	
3	7	121	
4	4	158	
4	8	158	
5	C0	105	
5	c0	105	
6	C1	156	
6	c1	156	
7	C2	143	
7	c2	143	
8	C3	150	
8	c3	150	
9	C4	128	
9	c4	128	
10	C5	141	
10	c5	141	
11	C6	141	
11	c6	141	
12	C7	136	
12	c7	136	
13	C8	145	
13	c8	145	
14	C9	143	
14	c9	143	
15	D0	107	

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Mol	Chain	Length	Quality of chain
15	d0	107	
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	

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Mol	Chain	Length	Quality of chain
28	L3	386	
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	

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Mol	Chain	Length	Quality of chain
40	m6	197	
41	M7	184	
41	m7	184	
42	M8	185	
42	m8	185	
43	M9	188	
43	m9	188	
44	N0	172	
44	n0	172	
45	N1	159	
45	n1	159	
46	N2	100	
46	n2	100	
47	N3	136	
47	n3	136	
48	N4	155	
48	n4	155	
49	N5	121	
49	n5	121	
50	N6	126	
50	n6	126	
51	N7	135	
51	n7	135	
52	N8	148	
52	n8	148	

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Mol	Chain	Length	Quality of chain
53	N9	58	
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	

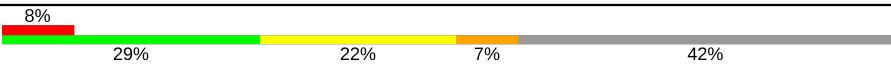

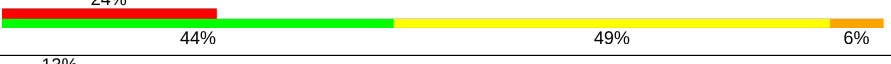
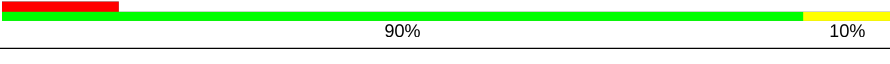
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Mol	Chain	Length	Quality of chain
65	q1	25	
66	Q2	105	
66	q2	105	
67	Q3	91	
67	q3	91	
68	S0	206	
68	s0	206	
69	S1	216	
69	s1	216	
70	S2	217	
70	s2	217	
71	S3	223	
71	s3	223	
72	S4	260	
72	s4	260	
73	S5	206	
73	s5	206	
74	S6	236	
74	s6	236	
75	S7	184	
75	s7	184	
76	S8	200	
76	s8	200	
77	S9	185	
77	s9	185	

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Mol	Chain	Length	Quality of chain
78	SM	272	
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	1	3623	-	-	-	X
80	MG	1	3658	-	-	-	X
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	2	1977	-	-	-	X
80	MG	2	2022	-	-	-	X
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	5	3650	-	-	-	X
80	MG	5	3664	-	-	-	X
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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	MG	6	1995	-	-	-	X
80	MG	6	1996	-	-	-	X
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	C	N	O	S	0	0	0
			987	627	186	167	7			

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

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

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

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

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

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

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

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

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

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

- 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	17	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	18	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	19	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	C	N	O	0	0	0
			444	277	96	71			
53	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	0	0	0
			1481	951	265	265				
75	S7	184	Total	C	N	O	S	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	S	0	0	0
			958	564	193	201				
78	SM	159	Total	C	N	O	S	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	L7	2	Total 2	Mg 2	0	0
80	s0	1	Total 1	Mg 1	0	0
80	n8	1	Total 1	Mg 1	0	0
80	s8	1	Total 1	Mg 1	0	0
80	O2	1	Total 1	Mg 1	0	0
80	N0	1	Total 1	Mg 1	0	0
80	o2	2	Total 2	Mg 2	0	0
80	6	160	Total 160	Mg 160	0	0
80	D2	1	Total 1	Mg 1	0	0
80	O4	1	Total 1	Mg 1	0	0
80	m5	1	Total 1	Mg 1	0	0
80	l3	3	Total 3	Mg 3	0	0
80	C8	1	Total 1	Mg 1	0	0
80	O3	2	Total 2	Mg 2	0	0
80	S6	1	Total 1	Mg 1	0	0
80	c9	1	Total 1	Mg 1	0	0
80	l7	1	Total 1	Mg 1	0	0
80	M5	3	Total 3	Mg 3	0	0
80	N7	1	Total 1	Mg 1	0	0
80	C4	3	Total 3	Mg 3	0	0
80	N6	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
80	d2	1	Total 1	Mg 1	0	0
80	SM	2	Total 2	Mg 2	0	0
80	o4	1	Total 1	Mg 1	0	0
80	s4	1	Total 1	Mg 1	0	0
80	M0	2	Total 2	Mg 2	0	0
80	c1	2	Total 2	Mg 2	0	0
80	5	449	Total 449	Mg 449	1	0
80	n1	1	Total 1	Mg 1	0	0
80	c8	2	Total 2	Mg 2	0	0
80	O7	2	Total 2	Mg 2	0	0
80	s6	1	Total 1	Mg 1	0	0
80	l4	1	Total 1	Mg 1	0	0
80	C9	1	Total 1	Mg 1	0	0
80	1	485	Total 485	Mg 485	0	0
80	S1	1	Total 1	Mg 1	0	0
80	L9	1	Total 1	Mg 1	0	0
80	M8	1	Total 1	Mg 1	0	0
80	Q2	1	Total 1	Mg 1	0	0
80	d3	1	Total 1	Mg 1	0	0
80	o3	2	Total 2	Mg 2	0	0
80	N3	1	Total 1	Mg 1	0	0

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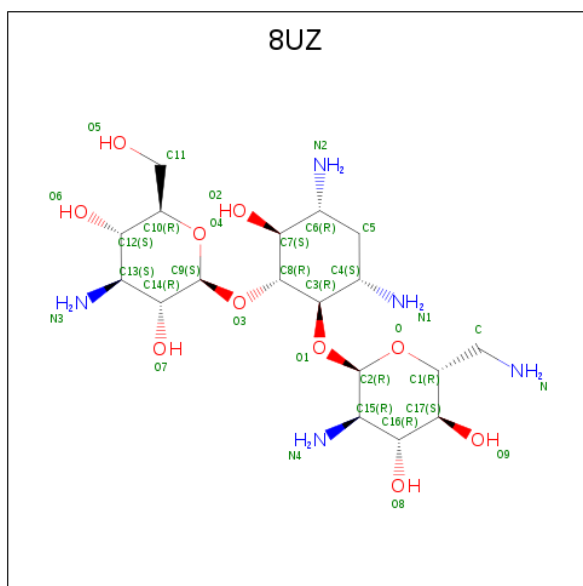
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
80	N8	1	Total 1	Mg 1	0	0
80	4	19	Total 19	Mg 19	1	0
80	n6	1	Total 1	Mg 1	0	0
80	S4	1	Total 1	Mg 1	0	0
80	L2	2	Total 2	Mg 2	0	0
80	O6	1	Total 1	Mg 1	0	0
80	o7	2	Total 2	Mg 2	0	0
80	l5	1	Total 1	Mg 1	0	0
80	m7	2	Total 2	Mg 2	0	0
80	M7	4	Total 4	Mg 4	0	0
80	L6	3	Total 3	Mg 3	0	0
80	n7	1	Total 1	Mg 1	0	0
80	m6	1	Total 1	Mg 1	0	0
80	O1	2	Total 2	Mg 2	0	0
80	q2	3	Total 3	Mg 3	0	0
80	C6	1	Total 1	Mg 1	0	0
80	d9	2	Total 2	Mg 2	0	0
80	c7	1	Total 1	Mg 1	0	0
80	7	8	Total 8	Mg 8	0	0
80	n3	1	Total 1	Mg 1	0	0
80	L3	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
80	O5	1	Total	Mg	0	0
			1	1		
80	2	128	Total	Mg	0	0
			128	128		
80	12	2	Total	Mg	0	0
			2	2		
80	8	10	Total	Mg	0	0
			10	10		
80	m0	2	Total	Mg	0	0
			2	2		
80	M6	1	Total	Mg	0	0
			1	1		
80	c3	1	Total	Mg	0	0
			1	1		
80	3	13	Total	Mg	0	0
			13	13		

- 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	0	0
			33	18	5	10		
81	1	1	Total	C	N	O	0	0
			33	18	5	10		
81	1	1	Total	C	N	O	0	0
			33	18	5	10		

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

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

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

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

- 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 2	O 2	0	0
83	l2	4	Total 4	O 4	0	0
83	L2	3	Total 3	O 3	0	0
83	l3	4	Total 4	O 4	0	0
83	L3	1	Total 1	O 1	0	0
83	l4	3	Total 3	O 3	0	0
83	L4	1	Total 1	O 1	0	0
83	l5	3	Total 3	O 3	0	0
83	L5	2	Total 2	O 2	0	0
83	l9	2	Total 2	O 2	0	0
83	M0	2	Total 2	O 2	0	0
83	M3	3	Total 3	O 3	0	0
83	m5	3	Total 3	O 3	0	0
83	M5	1	Total 1	O 1	0	0
83	M6	3	Total 3	O 3	0	0
83	m7	3	Total 3	O 3	0	0
83	M7	4	Total 4	O 4	0	0
83	m8	1	Total 1	O 1	0	0
83	m9	5	Total 5	O 5	0	0
83	M9	2	Total 2	O 2	0	0
83	n1	2	Total 2	O 2	0	0

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

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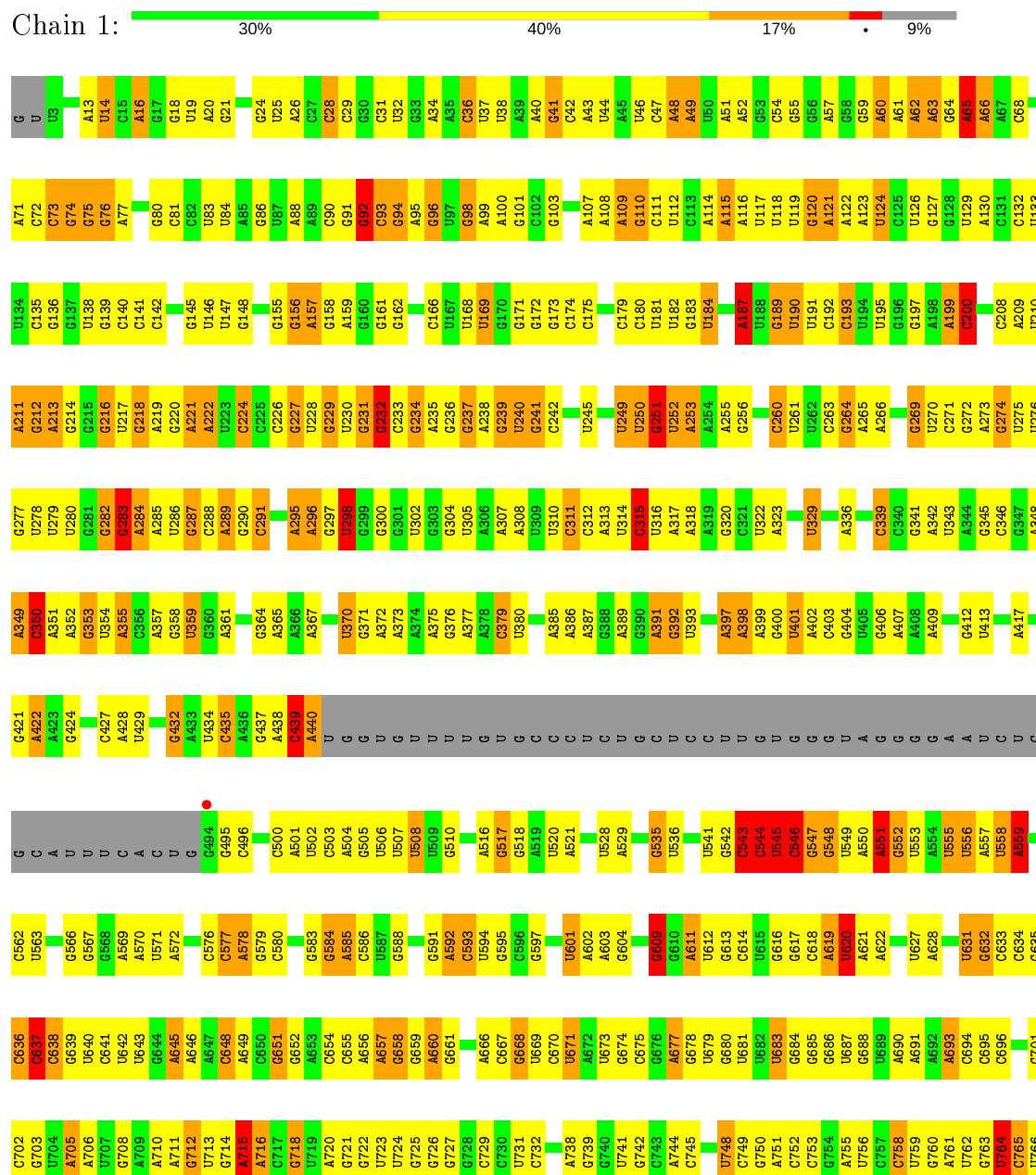
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	S6	1	Total 1	O 1	0	0
83	S9	1	Total 1	O 1	0	0
83	sM	3	Total 3	O 3	0	0
83	SM	1	Total 1	O 1	0	0

3 Residue-property plots

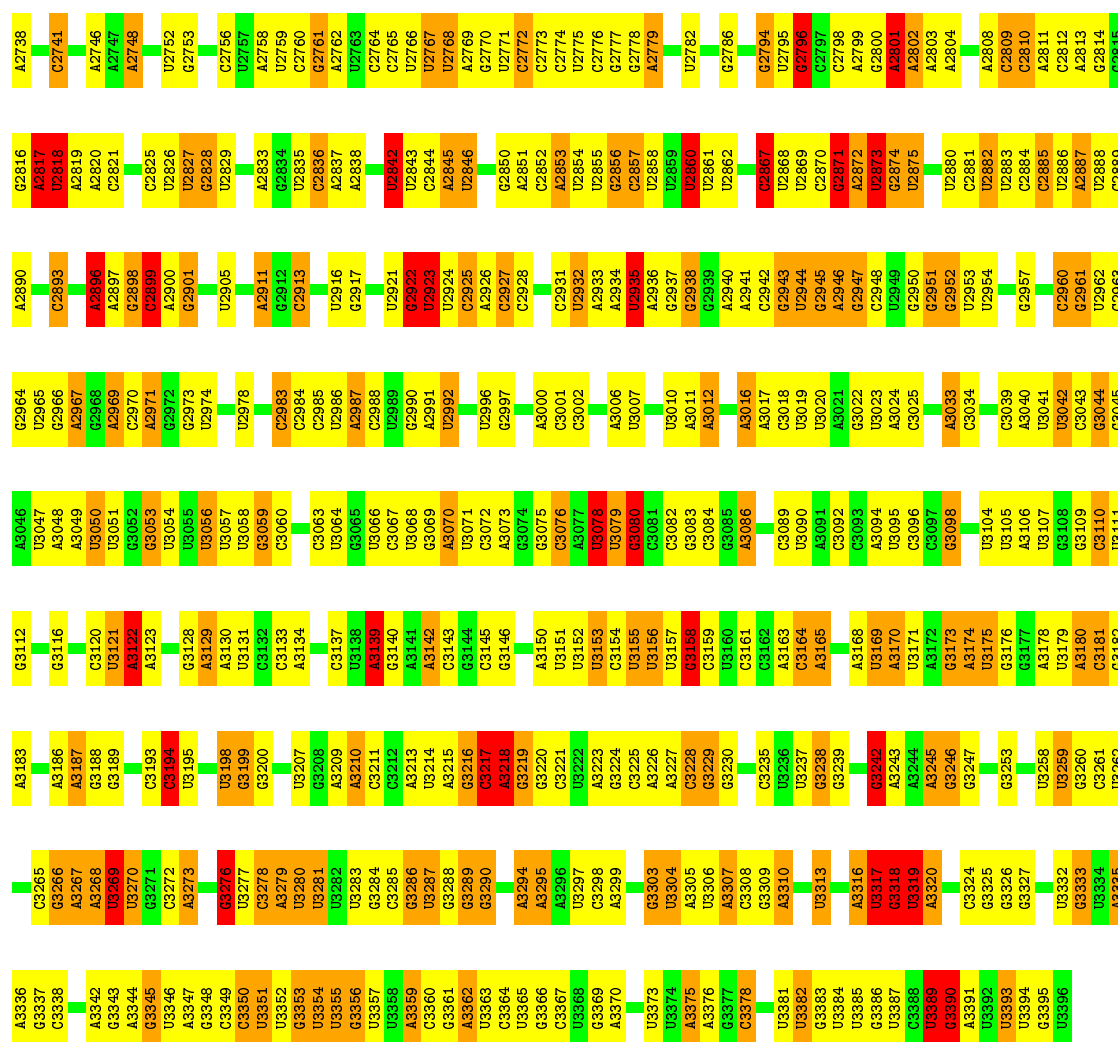
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



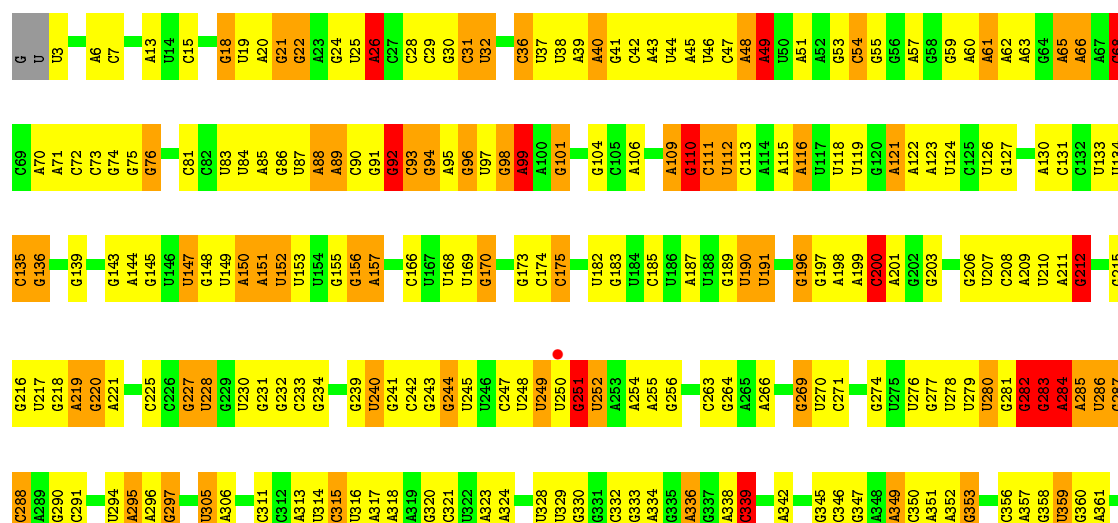
U1645	C1581	A1515	U1448	U1384	U1318	U	A1190	U1114	A1047	C975	G968	U767
A1648	C1582	C1516	A1449	C1385	G1319	C	U1191	G1115	A1043	U976	G909	C768
U1649	A1583	G1517	A1450	A1386	C1320	G	C1192	G1116	C1049	C977	G910	C769
G1650	U1584	C1451	C1451	G1389	G1321	C	A1193	G1117	U1050	G978	C911	A771
G1651	C1585	U1521	A1452	A1390	G1322	U	G1194	C1118	U1051	U979	A912	A837
G1652	A1587	U1523	A1454	C1391	U1324	U	A1195	C1119	U1052	A980	A913	G838
G1653	A1588	A1524	U1455	G1392	U1325	A	C1196	A1120	A1053	U981	A914	C839
A1654	A1589	G1525	A1456	A1393	A1326	G	C1197	U1125	A1054	C982	A915	U776
G1655	U1590	U1526	U1457	G1394	C1327	G	C1198	G1126	A1055	G986	G916	U777
G1656	A1591	C1531	U1458	A1395	C1328	A	U1127	G1127	U1056	U987	A917	U778
G1657	U1592	U1532	C1459	C1396	U1329	G	C1201	U1128	A1062	A992	U919	A780
A1658	A1593	U1533	A1460	U1398	A1330	U	A1202	A1129	A1063	G993	A920	A781
U1659	A1594	C1534	U1463	A1399	U1334	G	A1203	A1130	G1063	G994	A921	U782
C1660	U1595	A1535	C1464	A1400	C1335	U	A1205	G1131	A1064	G995	U922	A784
G1661	C1596	G1536	A1467	A1401	U1336	U	G1206	C1132	A1065	U996	C923	G854
G1662	C1597	A1537	C1468	A1402	A1337	A	G1209	A1133	G1066	A996	A925	A786
C1663	G1598	A1538	U1470	C1403	C1338	U	U1210	C1137	U1071	G999	A926	G787
G1664	U1600	A1539	U1471	G1404	C1339	A	U1211	G1138	G1072	C1000	C927	C788
G1665	U1601	U1540	U1472	U1405	G1340	C	A1212	U1139	U1073	G1001	C928	A789
A1667	A1602	G1541	G1473	A1406	U1341	A	G1213	G1143	U1074	A1002	A929	G791
G1668	A1603	G1542	A1474	A1407	C1342	C	C1216	U1144	A1075	A1003	U930	G792
	G1604	G1543	A1475	G1408	A1343	U	G1217	G1145	C1076	U1004	U935	C793
G1674	A1605	G1544	G1476	C1411	G1344	C	U1218	C1146	U1077	G1005	U936	U794
G1675	U1606	A1545	A1477	G1412	G1345	A	C1219	C1147	U1078	A1006	U937	G795
A1676	U1607	A1546	G1480	G1413	U1346	U	C1220	G1148	A1079	U1007	A936	U796
G1677	C1608	G1547	A1481	A1414	U1347	U	G1221	G1149	U1080	U1008	U937	G797
G1680	C1609	C1548	A1482	C1416	U1348	G	G1222	A1153	U1081	A1009	C938	G798
U1681	G1610	C1551	G1483	G1417	A	U	A1223	A1154	U1082	G1010	U939	G799
U1682	A1613	G1552	U1484	A1418	U	A	G1224	C1155	G1083	G940	G940	G800
A1683	C1614	U1553	G1485	A1419	A	U	A1225	C1156	A1084	G1013	G941	A801
	C1615	U1554	G1486	A1420	U1353	A	G1226	G1157	U1015	U1014	U942	G875
U1686	G1616	U1555	G1487	G1421	G1354	U	C1227	A1158	C1086	A876	U943	C803
U1687	G1617	C1556	G1488	G1422	A1355	U	G1228	A1159	C1016	C877	C944	C804
U1688	G1618	A1557	A1489	C1423	U1356	U	G1229	G1160	C1017	G878	C945	G805
U1689	A1619	A1558	A1490	C1424	G1357	U	C1292	G1161	G1018	U879	A806	A806
A1690	U1620	A1559	A1491	U1427	C1358	U	A	G1164	G1019	G880	A807	A807
U1691	A1621	G1560	G1492	A1428	C1359	C	C1293	A1165	C1020	C881	C949	A808
U1692	U1622	G1561	G1493	A1429	C1360	G	G1295	G1166	G1021	A882	G950	G809
C1693		C1562	U1494	U1430	U1361	U	C1296	U1167	U1022	A883	A951	A810
U1694	A1625	C1563	U1495	G1431	G1362	U	G1300	U1168	C1023	A884	U811	U811
U1695	U1629	U1564	C1496	A1432	C1363	U	A1301	A1169	G1024	U885	G812	G812
A1696	U1630	A1566	C1497	A1433	C1364	G	G1302	A1170	A1025	C886	U955	G813
C1697	C1631	U1567	A1498	G1434	G1365	C	C1303	G1174	A1026	C890	U956	U814
A1699	C1632	U1568	U1503	A1435	G1366	U	A1304	C1175	A1027	G891	U957	G815
G1700	C1633	U1569	A1504	U1436	U1367	A	U1305	G1176	G1028	U892	C956	A816
C1701	G1634	U1570	C1505	C1437	U1368	G	G1306	C1177	A1029	A895	C959	A817
U1702	G1635	A1571	C1506	U1438	G1370	U	G1307	G1178	A1030	C1031	U960	C818
	U1636	U1572	A1507	U1439	A1373	A	A1308	G1179	A1031	C1032	C961	U821
C1709	A1638	C1573	G1507	G1441	U1376	U	A	A1180	U1033	U897	A962	G822
G1712	U1639	U1574	C1508	G1442	C1376	C	G	U1181	A1036	G900	G964	G823
G1713	C1640	A1575	U1509	G1443	U1380	U	U	A1182	C1037	A896	G901	G826
	U1641	G1576	U1510	G1444	G1381	C	C	A1185	C1038	G902	U966	A828
U1716	A1642	C1577	U1511	U1445	G1382	G	G	C1186	U1039	A967	U968	U829
U1717	A1643	U1578	U1512	G1446	G1383	A	A	C1189	A1041	A906	G974	A830
G1718	C1644	A1580	G1514	G1447	A1317	A	A					G931

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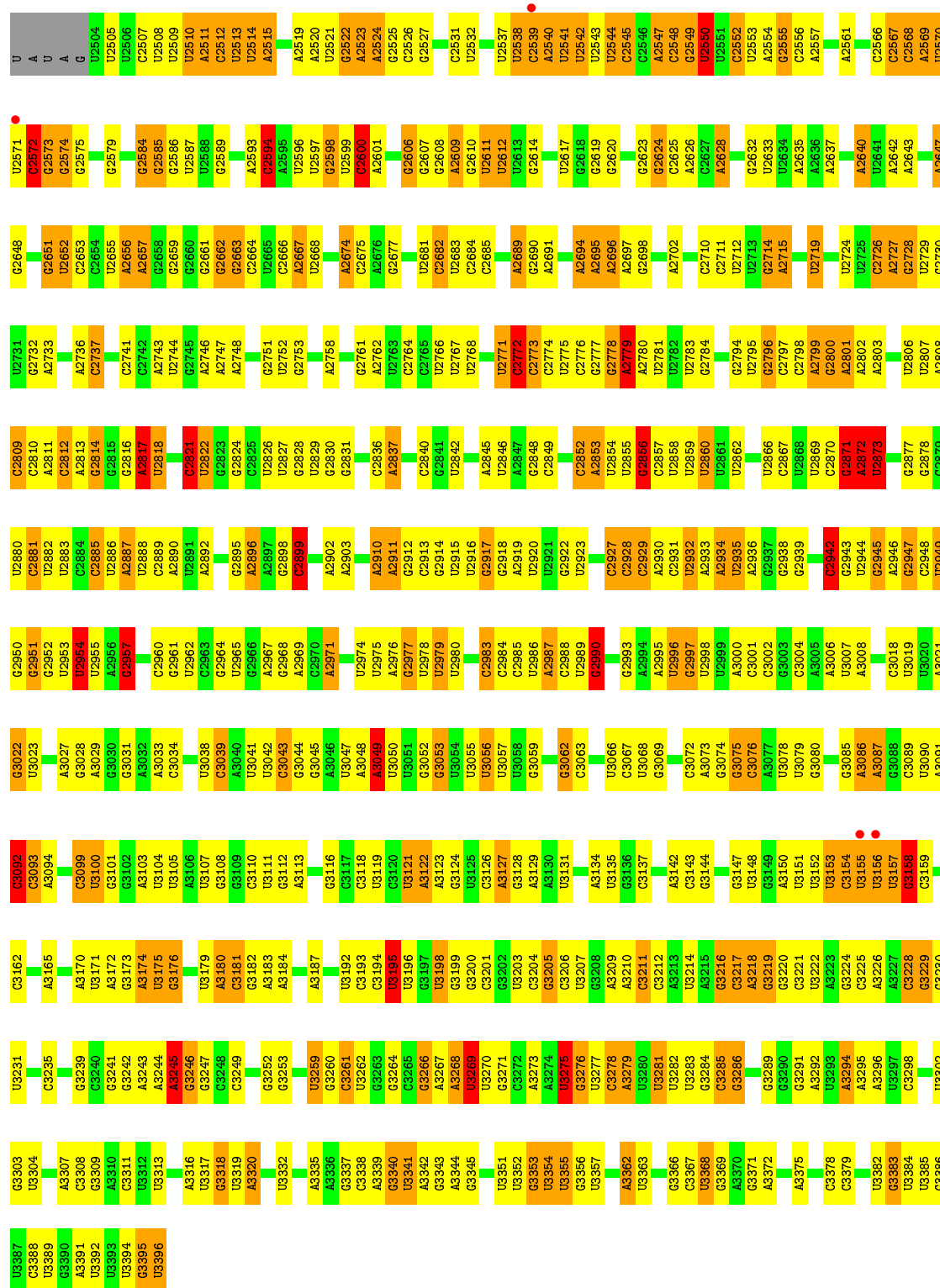
• Molecule 1: 25S ribosomal RNA

Chain 5: 33% 39% 16% 9%





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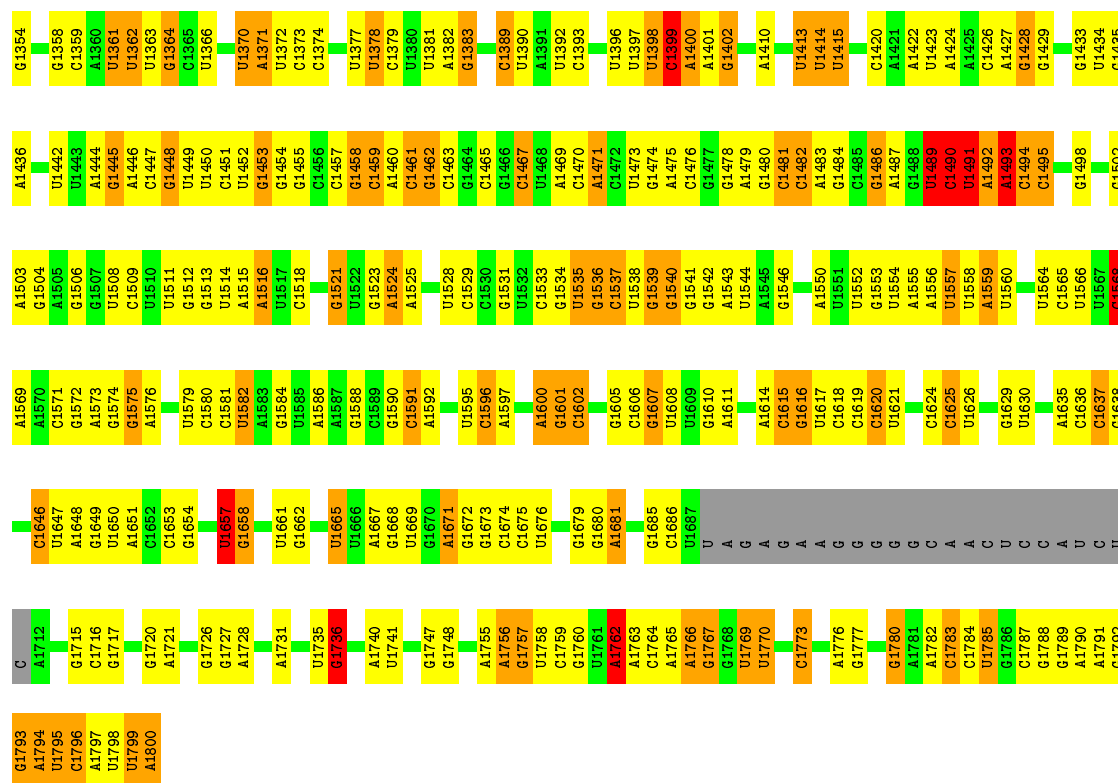


• Molecule 2: 18S ribosomal RNA



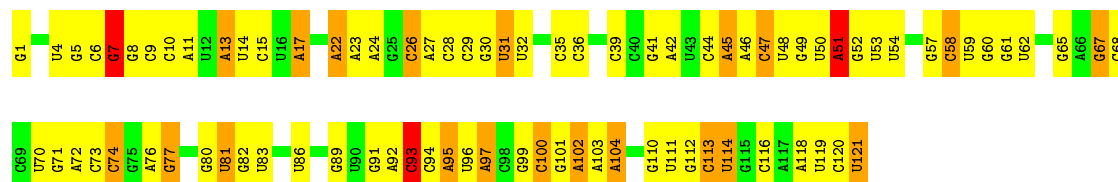
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	C943	U873	U795	U727	U	G595	C519	A445	G373	A301	G235	C160	U159	C4
U1017	A944	C874	A796	U728	U	U600	A520	U446	U374	U302	C237	U161	G91	U5
U1018	U945		G797	G729	U	U603	A521	U447	U375	U303	U238	A182	A92	G6
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	G948	C880	G802	G732	U	A605	A451	A452	U380	U306	U241	C166	U94	U15
	C949	A881	A803	A733	U	A606	A453	U454	C381	G307	U242	U167	G95	G16
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A1027	A951	C883	A805	C735	A	U609	U522	C455	G385	C309	U244	A169	C97	C17
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	A971		U828	A754		G624	G549	A478	G403	U327	G264	C190	U117	U44
C1045	A972		U831	A755		U625	G552	C479	G404	U328	A265	C191	U45	U45
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G1073	G1072		G866	A788		G658	U582	A511	C435		C294	U229	U152	A78
C1074			G867	U789		C		A512	A436	G364		G230	G153	C79
C1075			G868	U790		G	C950	U513	A437				U154	A80
A1076			G869	G722		A	A591	G514	A438		U297	U231		
C1077				G723										





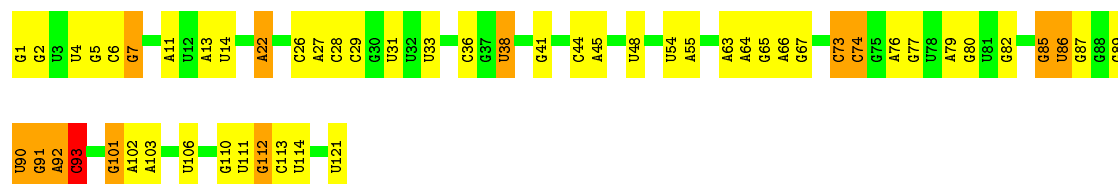
• Molecule 3: 5S ribosomal RNA

Chain 3: 31% 50% 17%



• Molecule 3: 5S ribosomal RNA

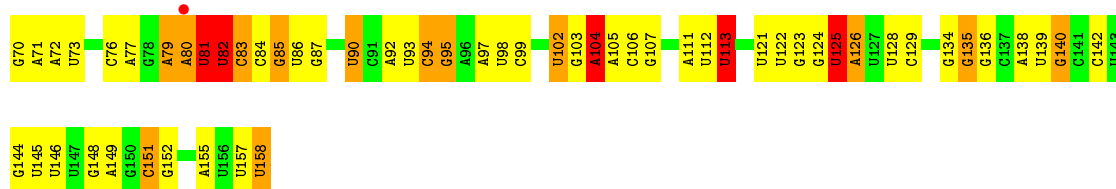
Chain 7: 55% 34% 10%



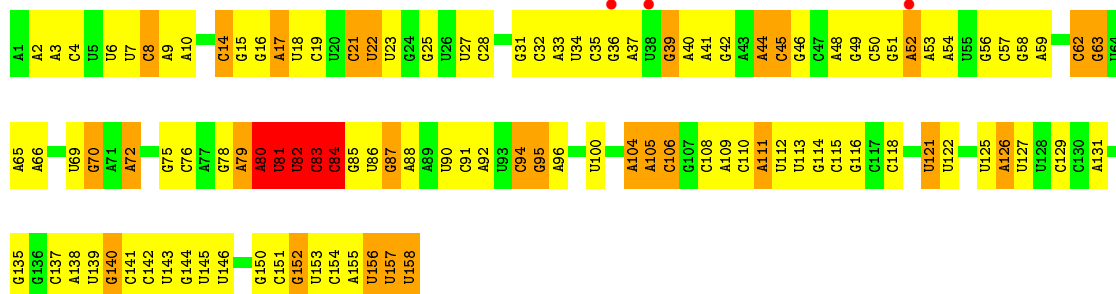
• Molecule 4: 5.8S ribosomal RNA

Chain 4: 35% 44% 18%

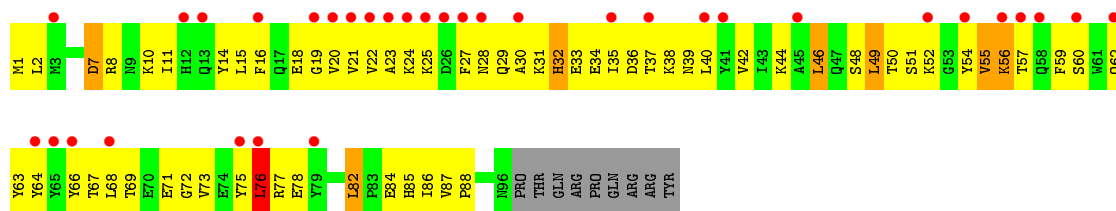




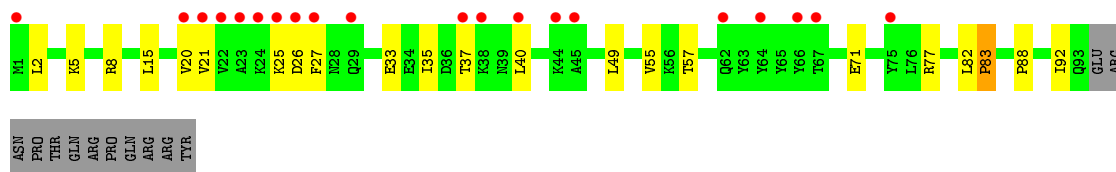
• Molecule 4: 5.8S ribosomal RNA



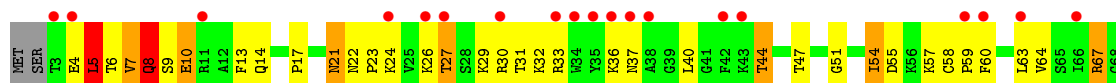
• Molecule 5: 40S ribosomal protein S10-A



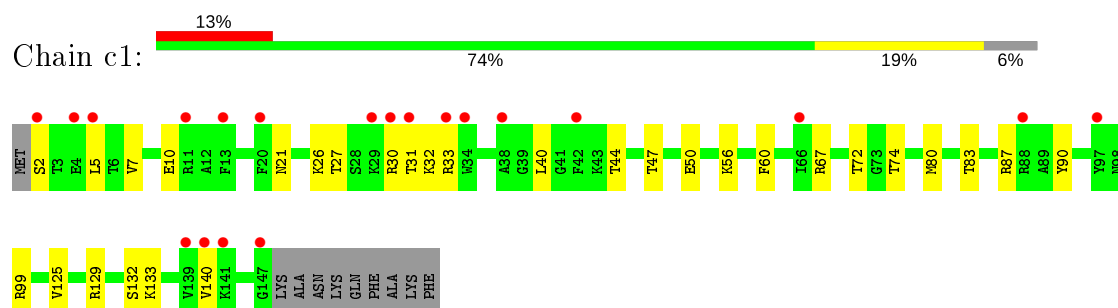
• Molecule 5: 40S ribosomal protein S10-A



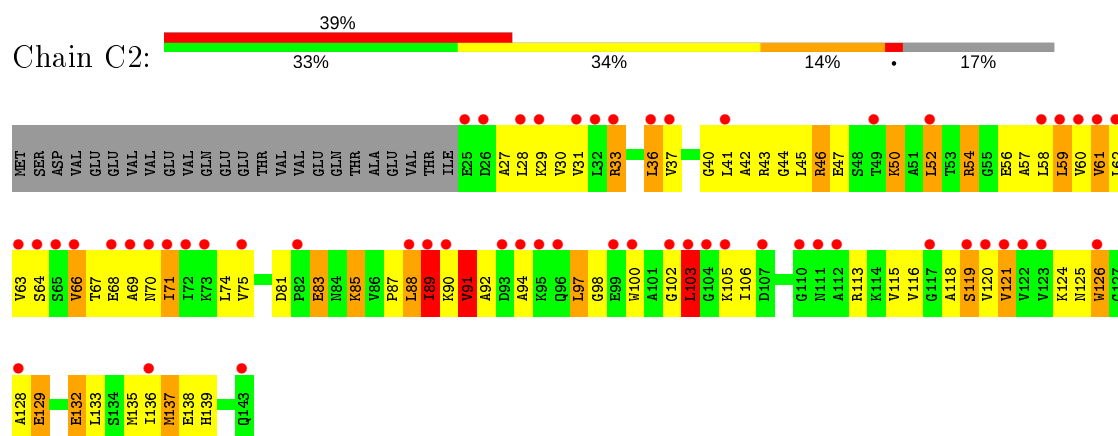
• Molecule 6: 40S ribosomal protein S11-A



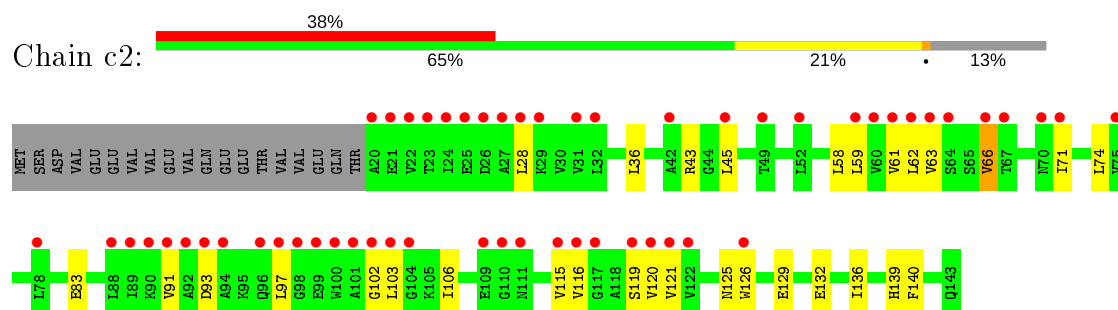
- Molecule 6: 40S ribosomal protein S11-A



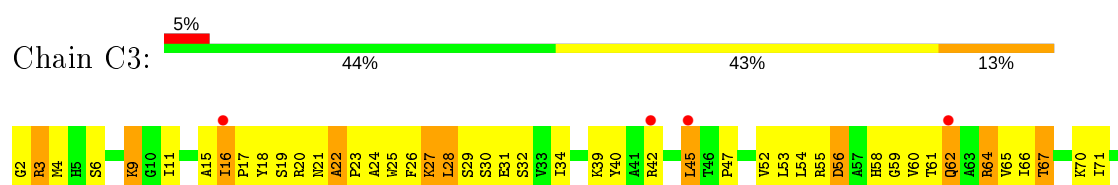
- Molecule 7: 40S ribosomal protein S12

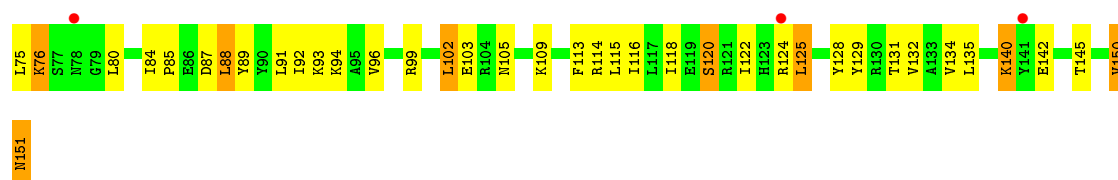


- Molecule 7: 40S ribosomal protein S12

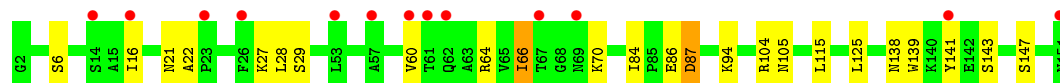
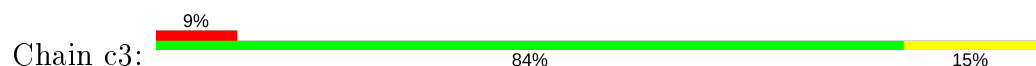


- Molecule 8: 40S ribosomal protein S13





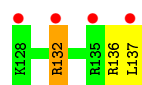
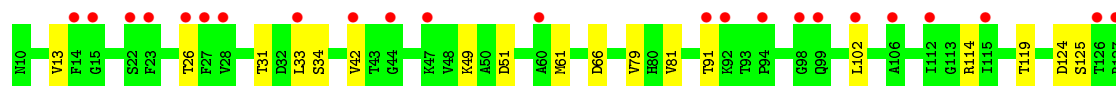
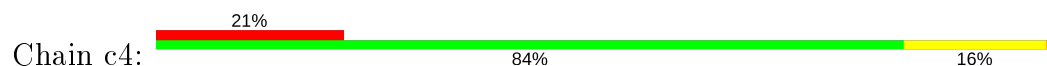
- Molecule 8: 40S ribosomal protein S13



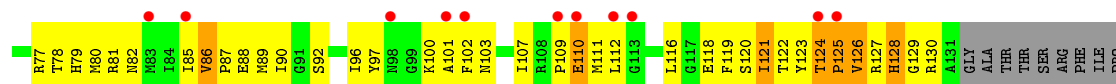
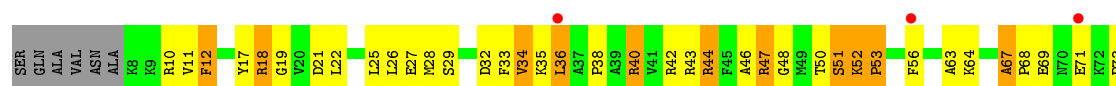
- Molecule 9: 40S ribosomal protein S14-B



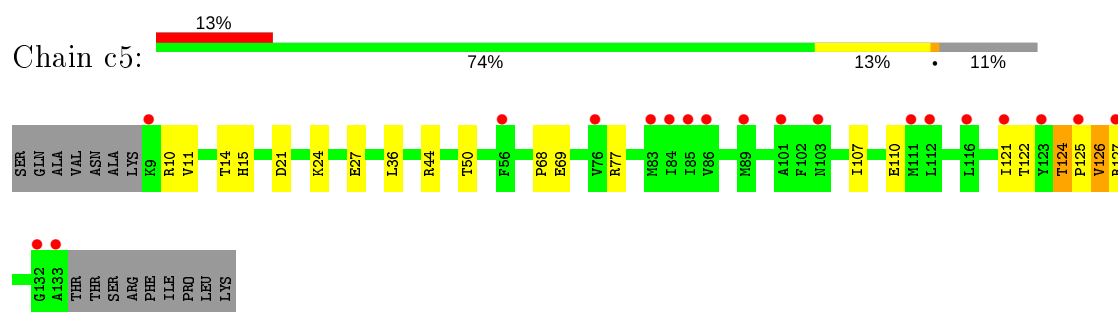
- Molecule 9: 40S ribosomal protein S14-B



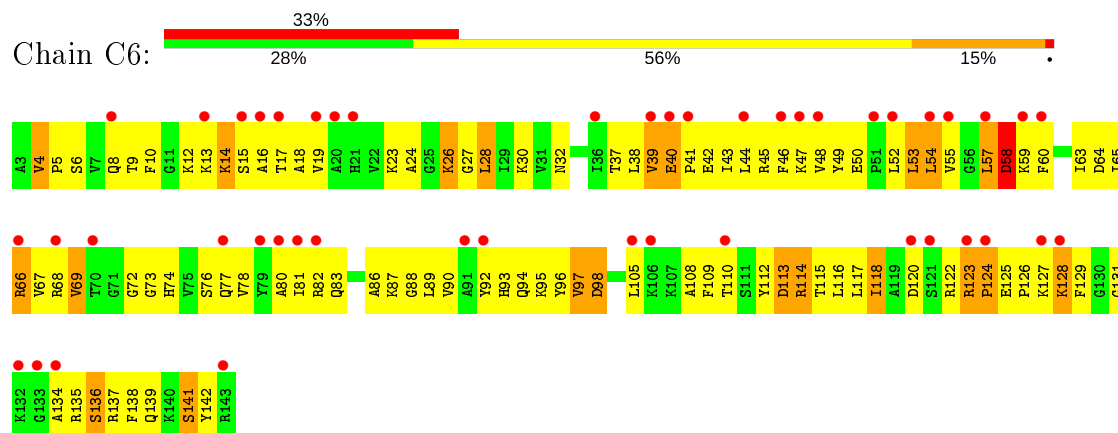
- Molecule 10: 40S ribosomal protein S15



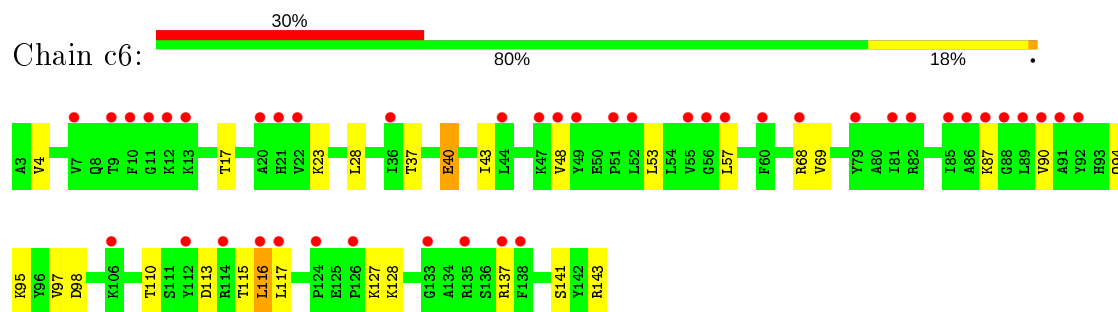
- Molecule 10: 40S ribosomal protein S15



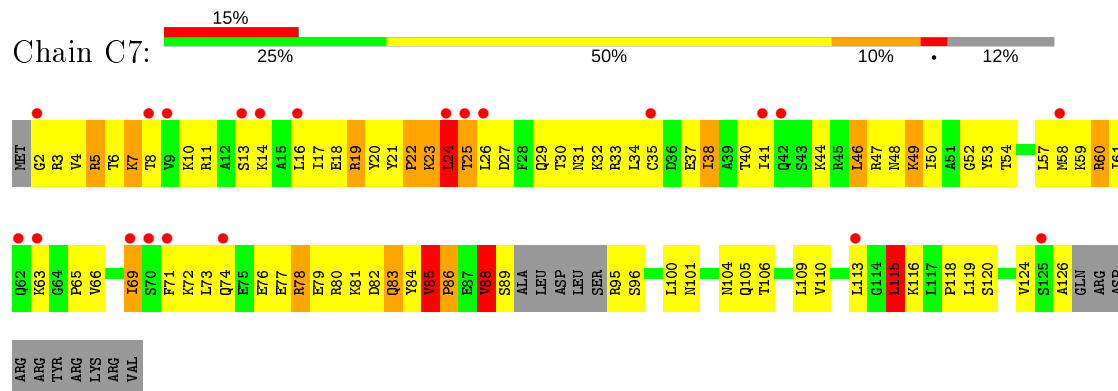
- Molecule 11: 40S ribosomal protein S16-A



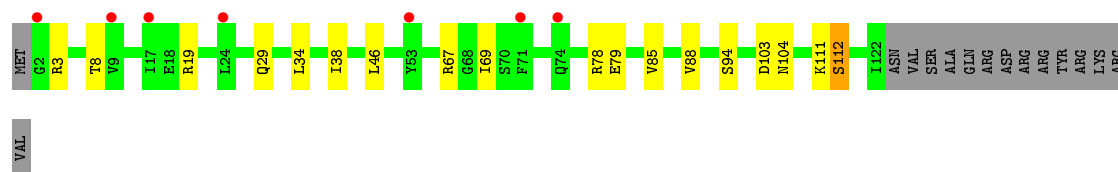
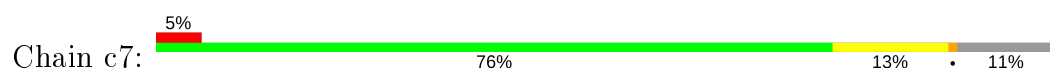
- Molecule 11: 40S ribosomal protein S16-A



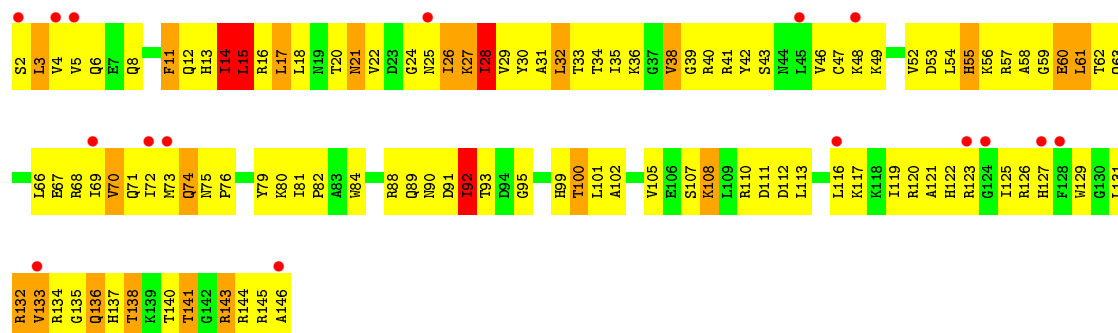
- Molecule 12: 40S ribosomal protein S17-A



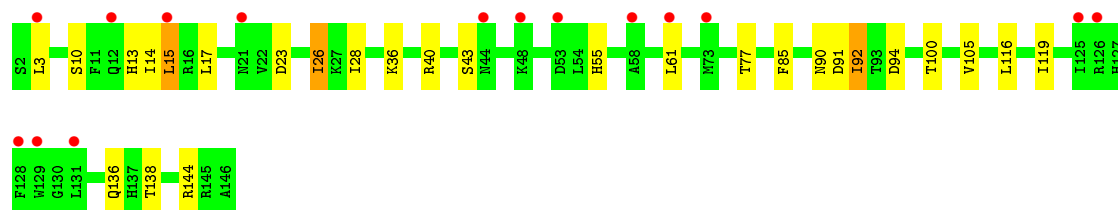
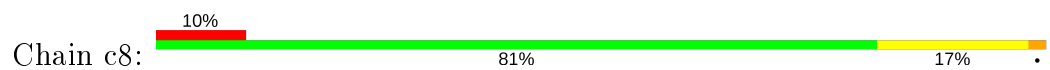
- Molecule 12: 40S ribosomal protein S17-A



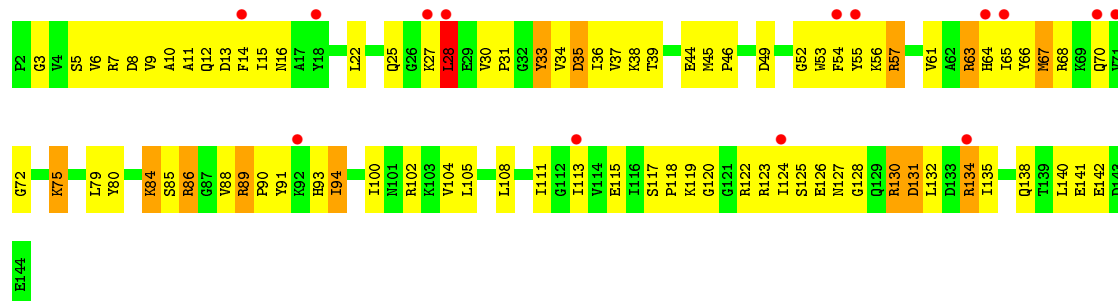
- Molecule 13: 40S ribosomal protein S18-A



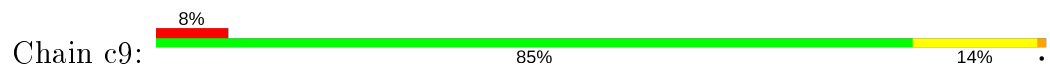
- Molecule 13: 40S ribosomal protein S18-A

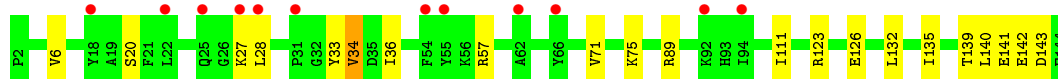


- Molecule 14: 40S ribosomal protein S19-A

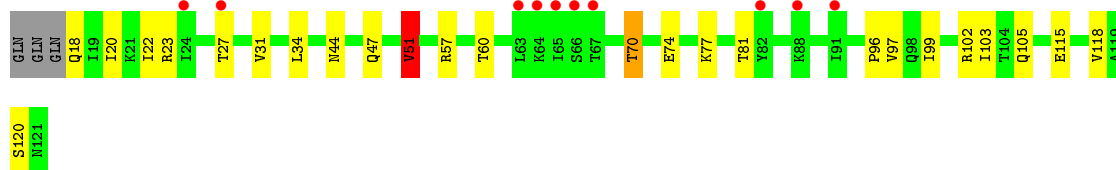
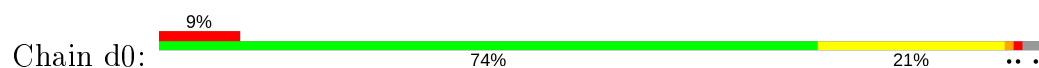


- Molecule 14: 40S ribosomal protein S19-A

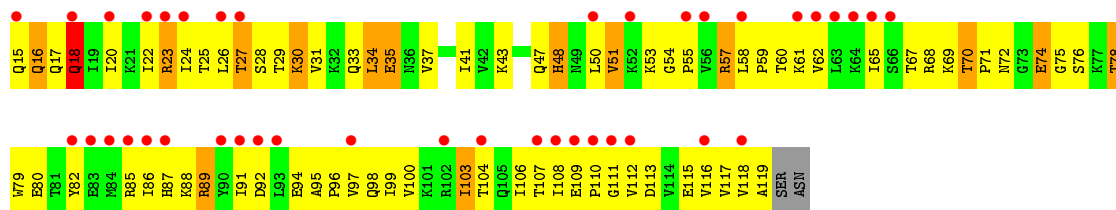




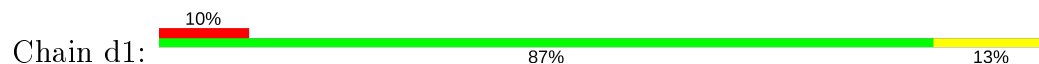
- Molecule 15: 40S ribosomal protein S20



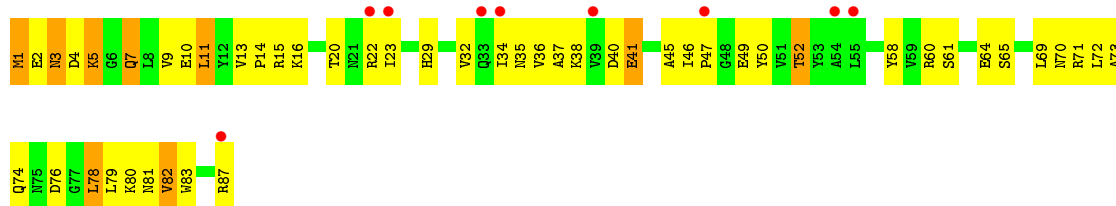
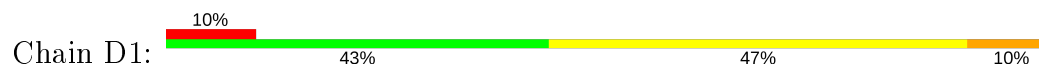
- Molecule 15: 40S ribosomal protein S20



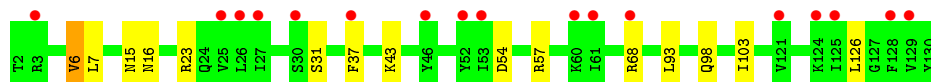
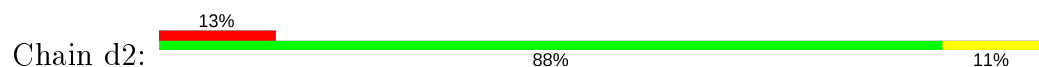
- Molecule 16: 40S ribosomal protein S21-A



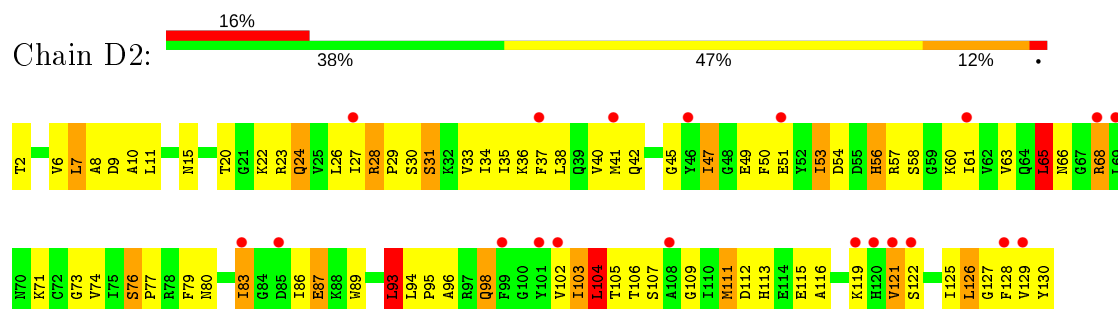
- Molecule 16: 40S ribosomal protein S21-A



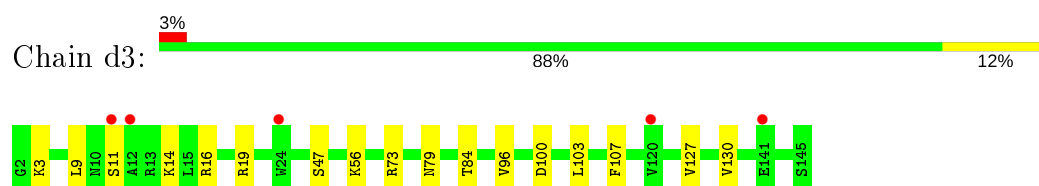
- Molecule 17: 40S ribosomal protein S22-A



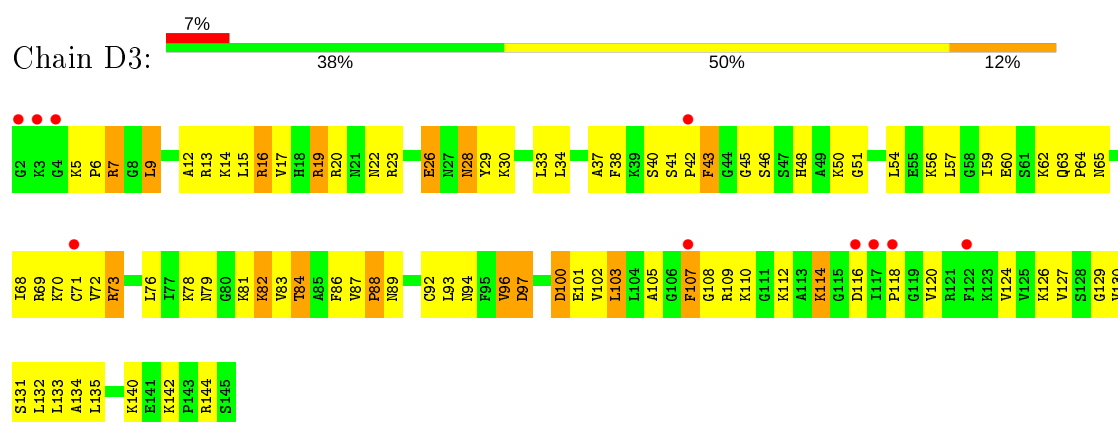
- Molecule 17: 40S ribosomal protein S22-A



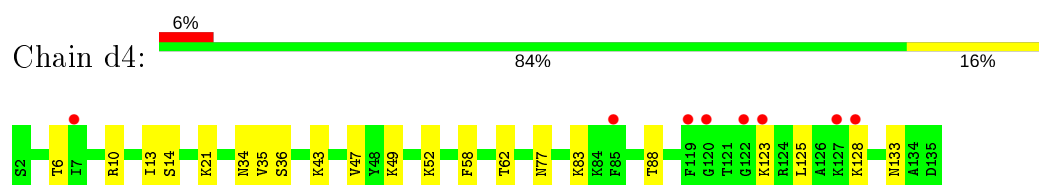
- Molecule 18: 40S ribosomal protein S23-A



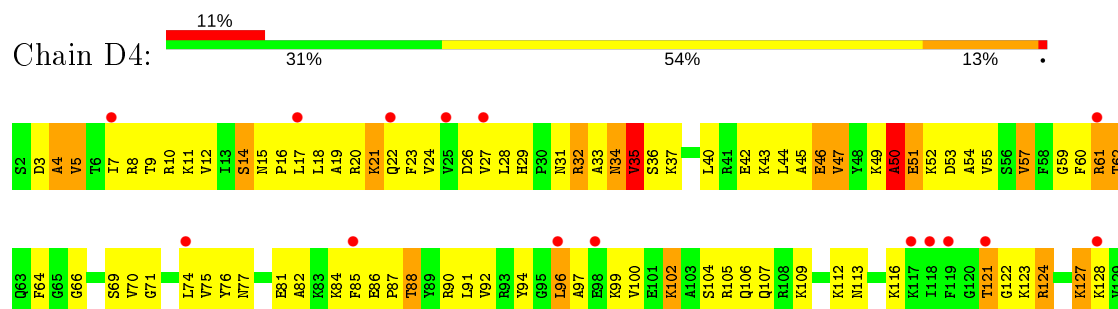
- Molecule 18: 40S ribosomal protein S23-A



- Molecule 19: 40S ribosomal protein S24-A

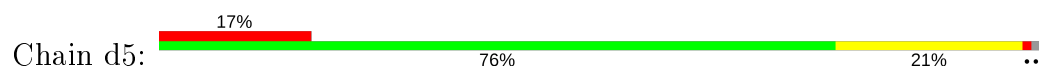


- Molecule 19: 40S ribosomal protein S24-A

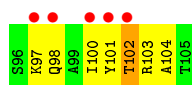
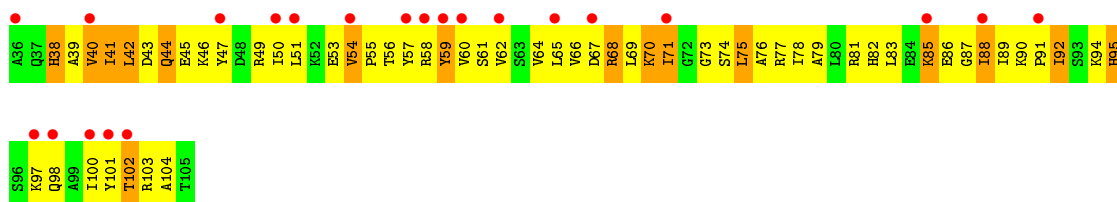




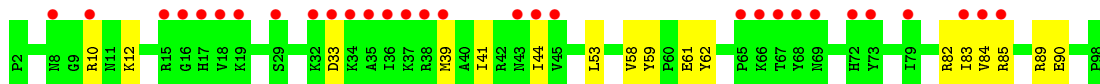
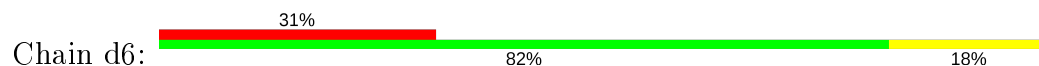
- Molecule 20: 40S ribosomal protein S25-A



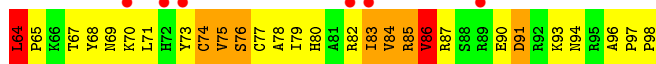
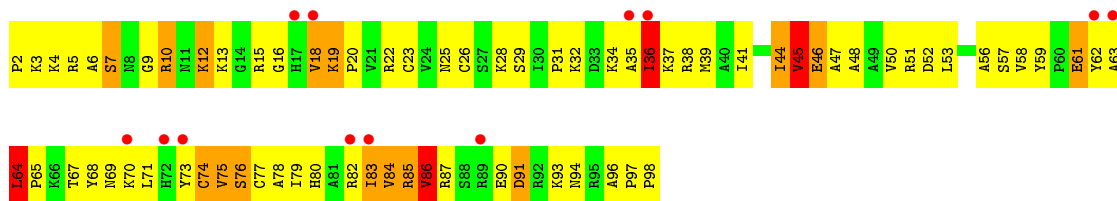
- Molecule 20: 40S ribosomal protein S25-A



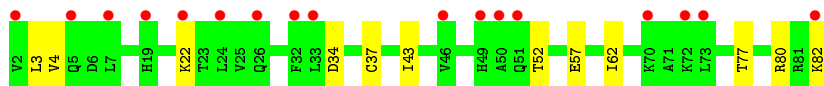
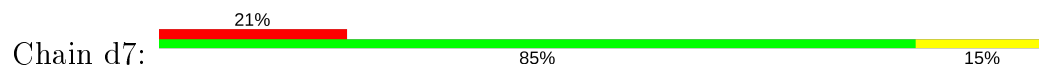
- Molecule 21: 40S ribosomal protein S26-B



- Molecule 21: 40S ribosomal protein S26-B

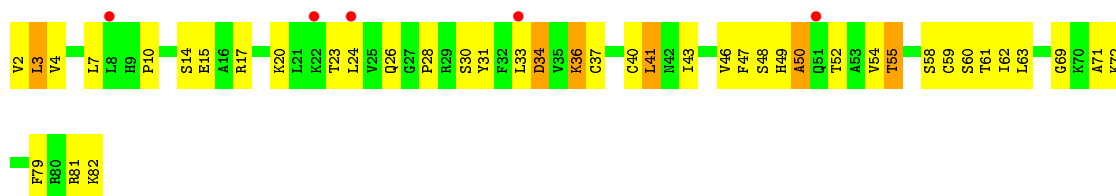


- Molecule 22: 40S ribosomal protein S27-A

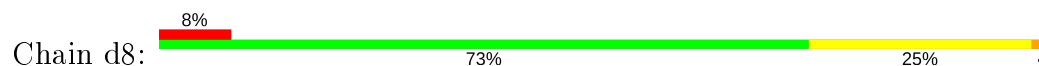


- Molecule 22: 40S ribosomal protein S27-A





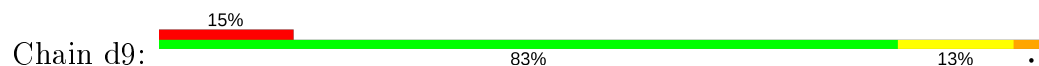
- Molecule 23: 40S ribosomal protein S28-A



- Molecule 23: 40S ribosomal protein S28-A



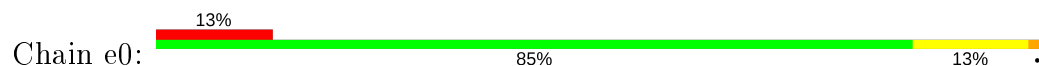
- Molecule 24: 40S ribosomal protein S29-A



- Molecule 24: 40S ribosomal protein S29-A



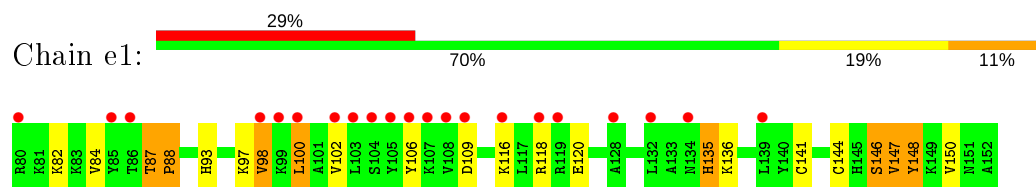
- Molecule 25: 40S ribosomal protein S30-A



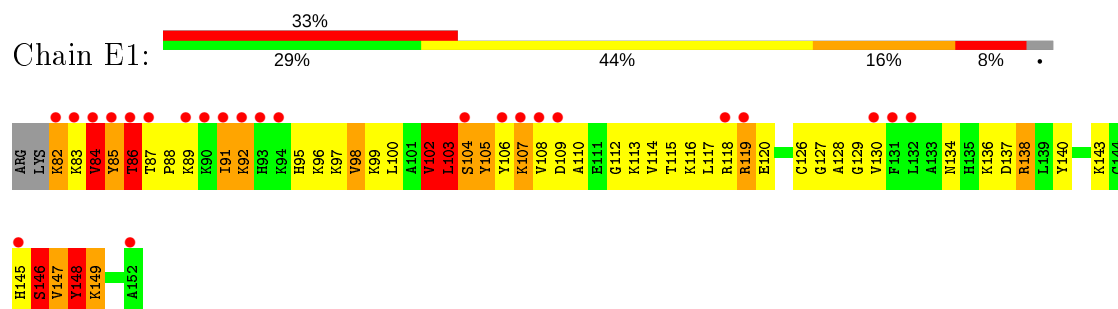
- Molecule 25: 40S ribosomal protein S30-A



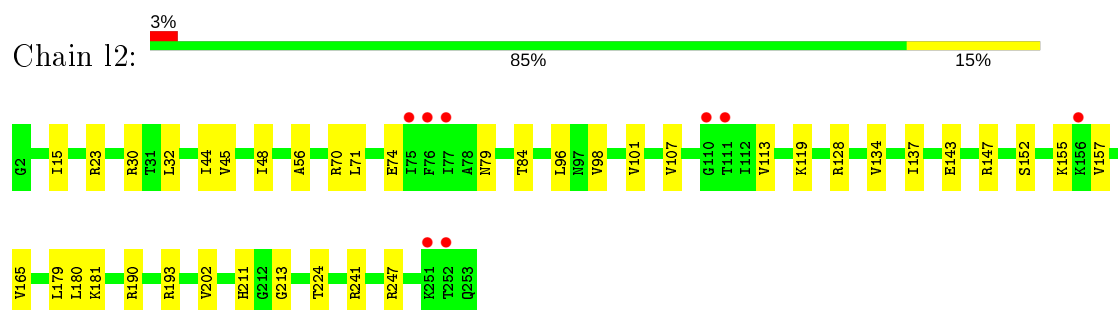
- Molecule 26: Ubiquitin-40S ribosomal protein S31



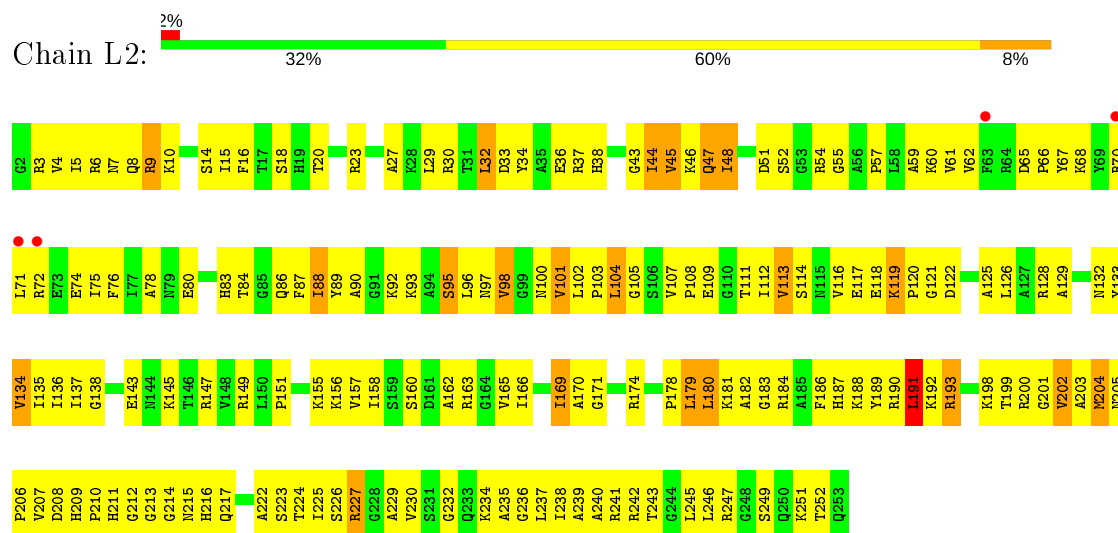
- Molecule 26: Ubiquitin-40S ribosomal protein S31



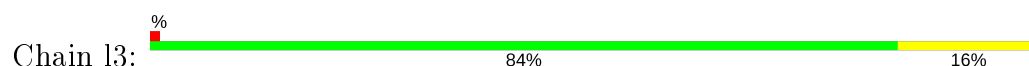
- Molecule 27: 60S ribosomal protein L2-A

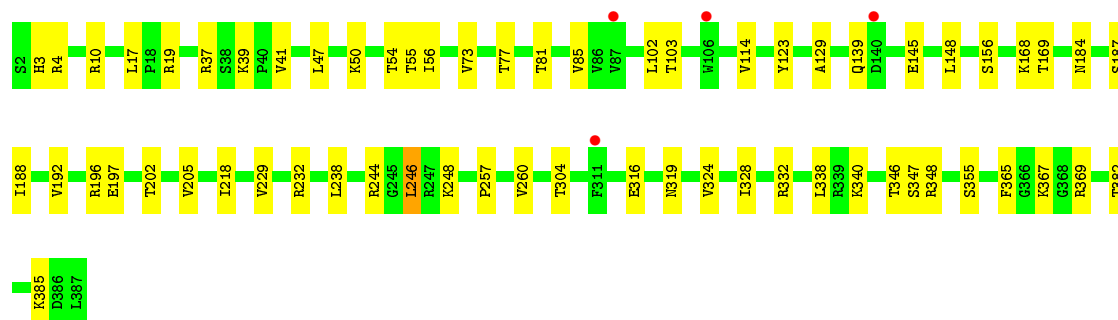


- Molecule 27: 60S ribosomal protein L2-A



- Molecule 28: 60S ribosomal protein L3

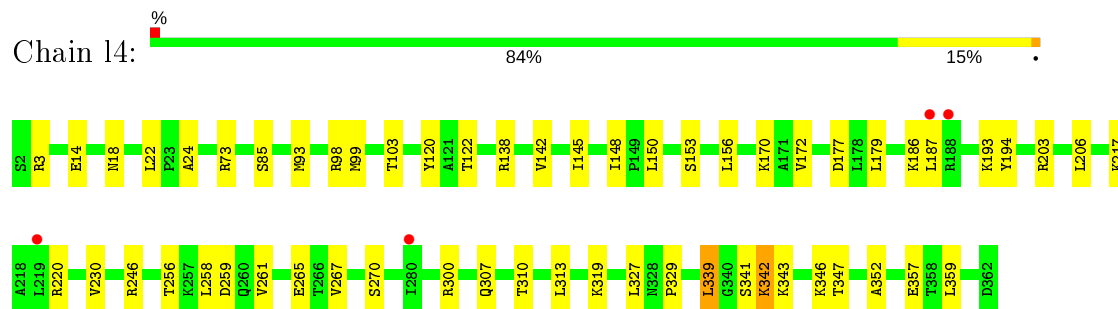




• Molecule 28: 60S ribosomal protein L3

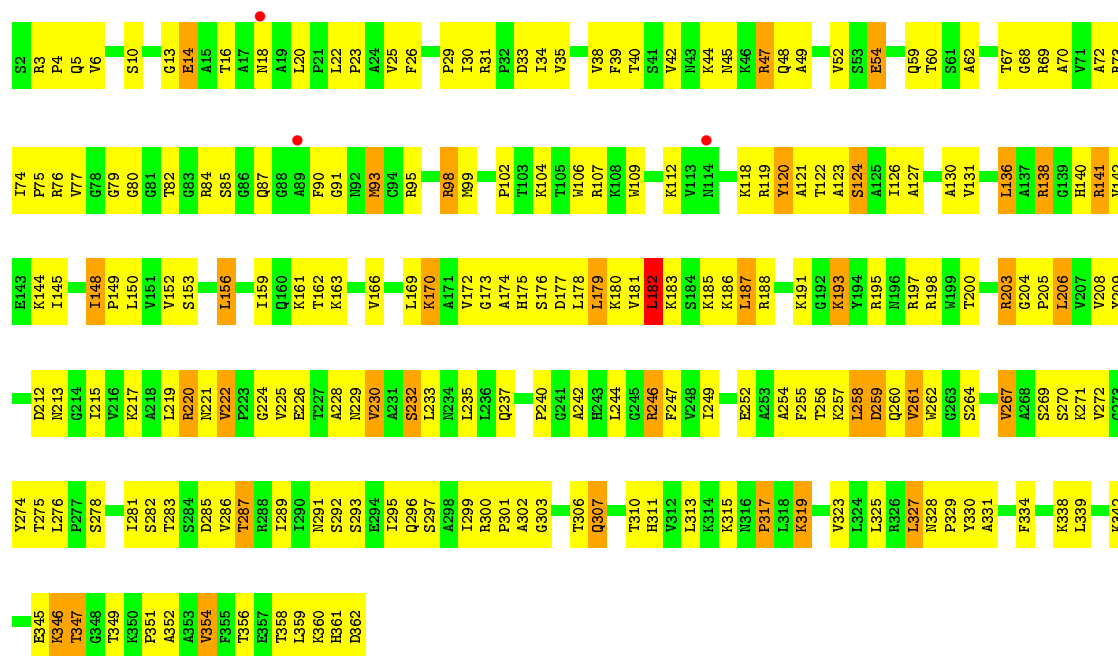


• Molecule 29: 60S ribosomal protein L4-A

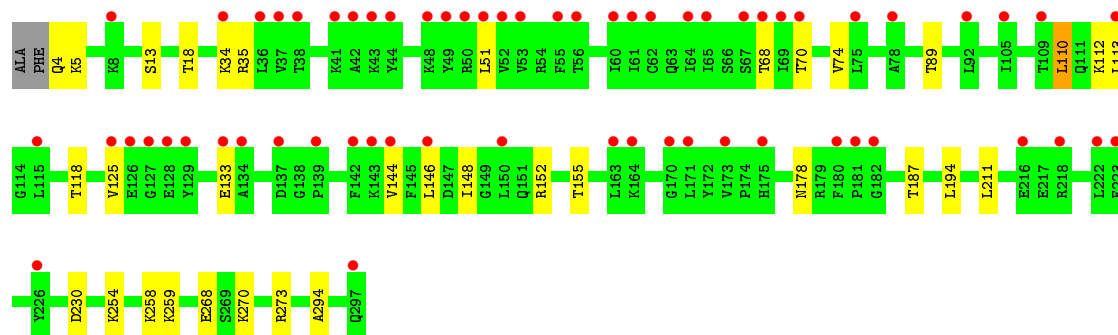
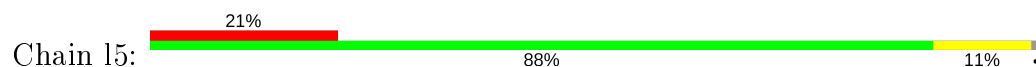


• Molecule 29: 60S ribosomal protein L4-A

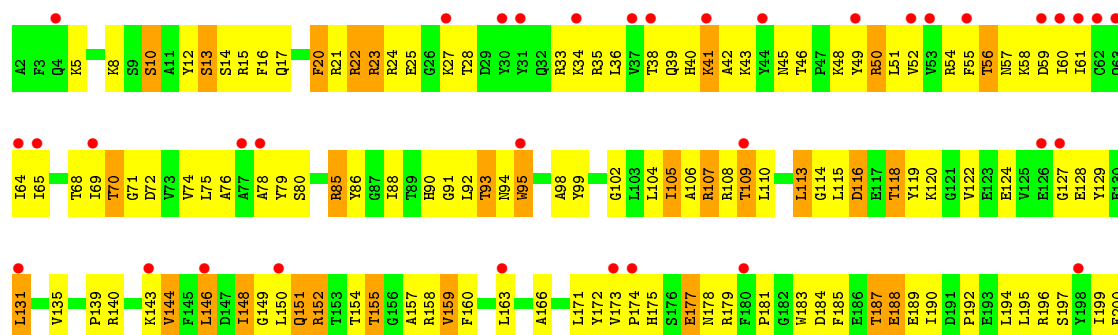


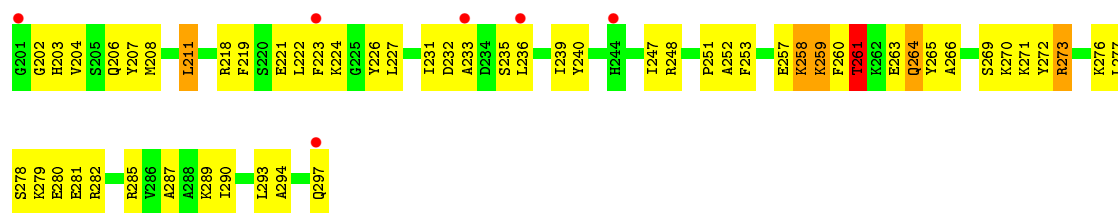


• Molecule 30: 60S ribosomal protein L5

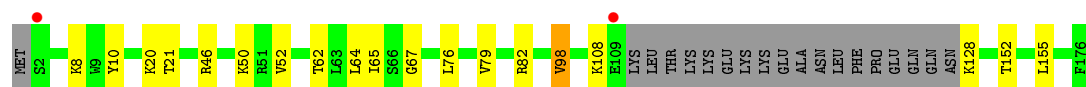
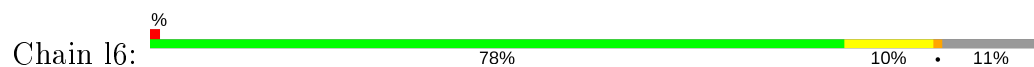


• Molecule 30: 60S ribosomal protein L5

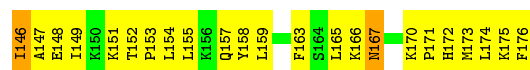




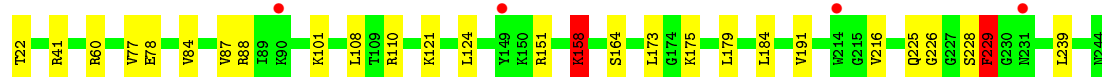
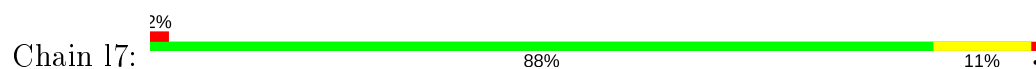
• Molecule 31: 60S ribosomal protein L6-A



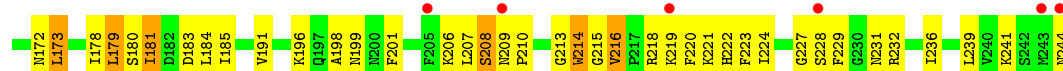
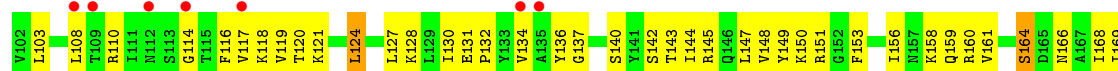
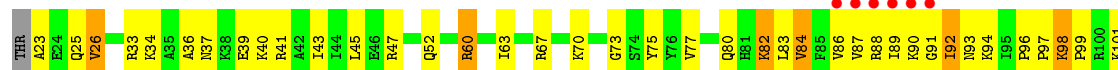
• Molecule 31: 60S ribosomal protein L6-A



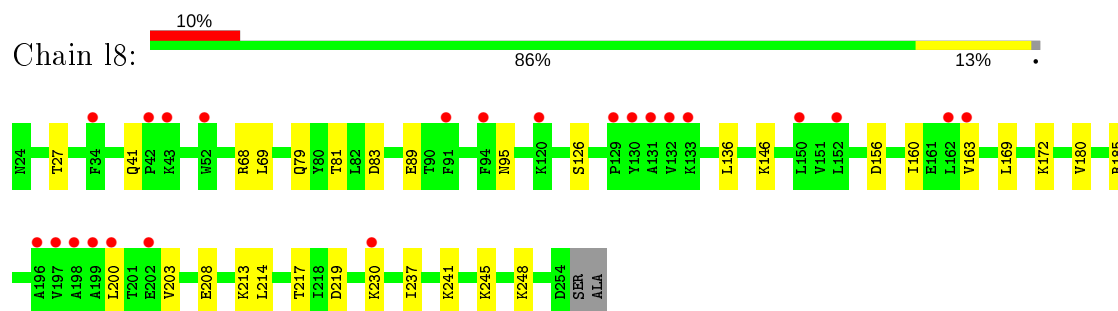
• Molecule 32: 60S ribosomal protein L7-A



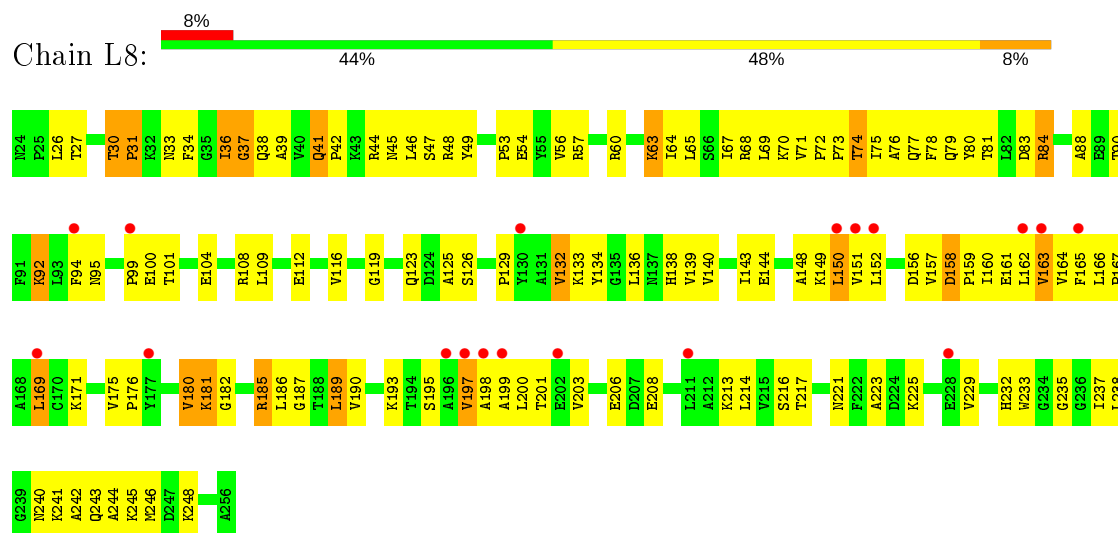
• Molecule 32: 60S ribosomal protein L7-A



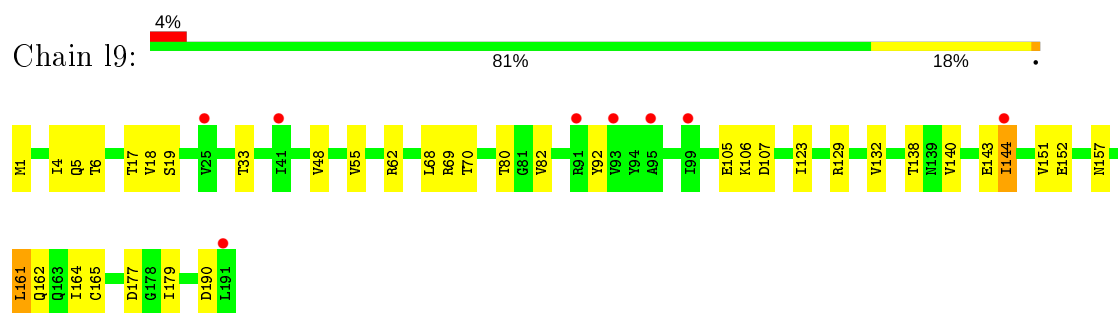
- Molecule 33: 60S ribosomal protein L8-A



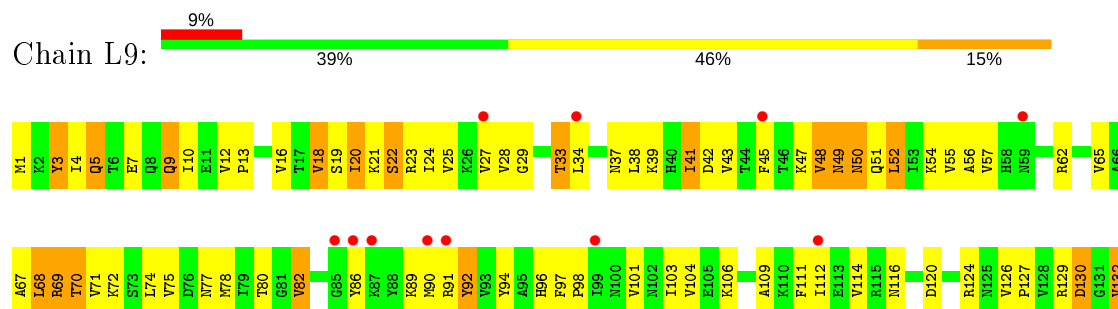
- Molecule 33: 60S ribosomal protein L8-A

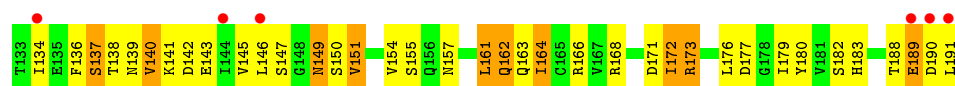


- Molecule 34: 60S ribosomal protein L9-A

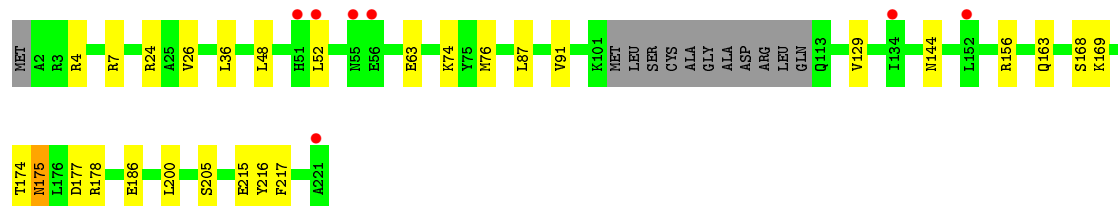
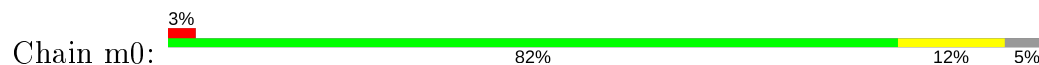


- Molecule 34: 60S ribosomal protein L9-A

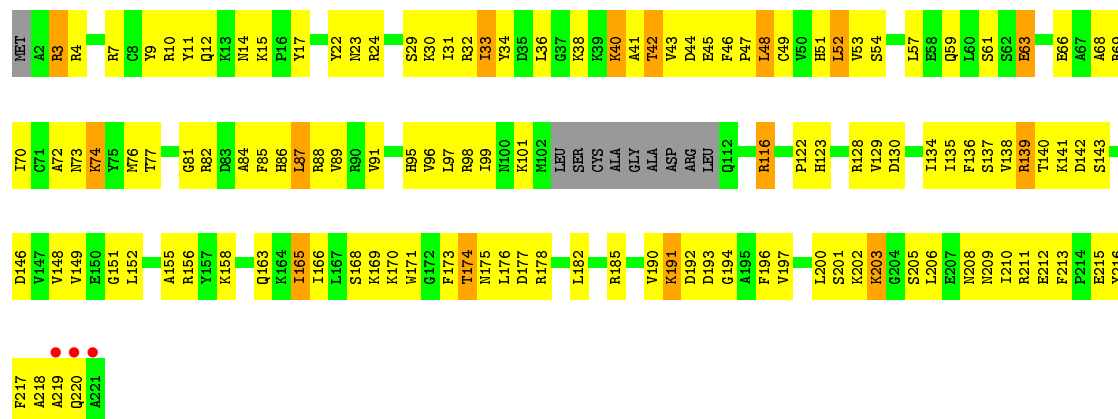




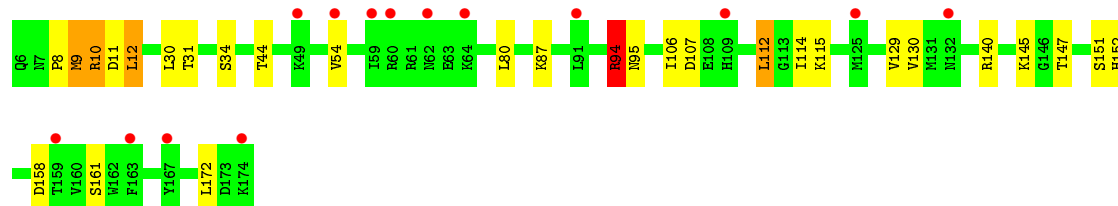
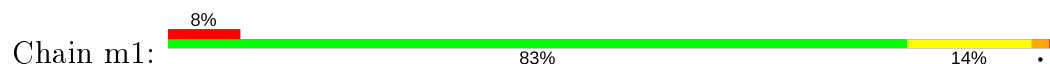
- Molecule 35: 60S ribosomal protein L10



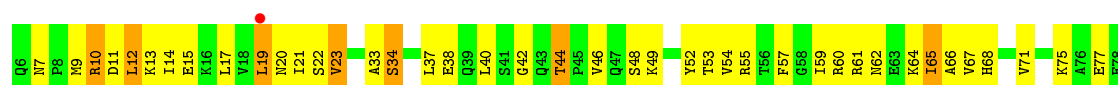
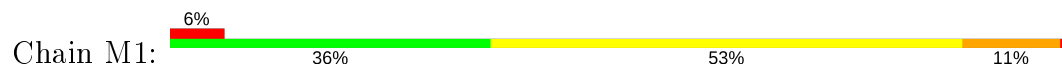
- Molecule 35: 60S ribosomal protein L10

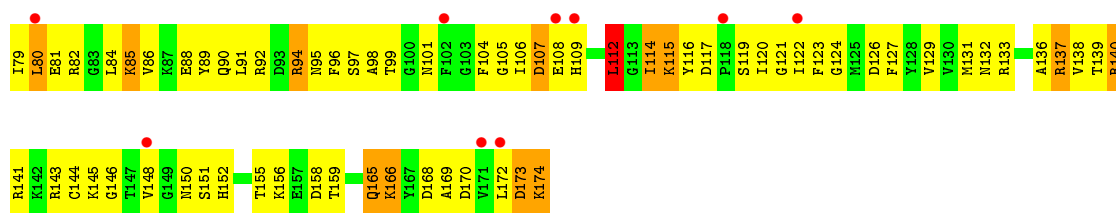


- Molecule 36: 60S ribosomal protein L11-B

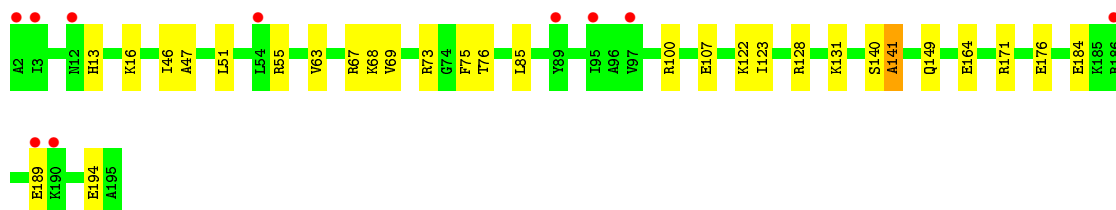
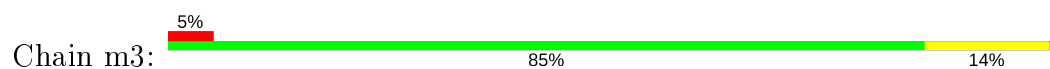


- Molecule 36: 60S ribosomal protein L11-B

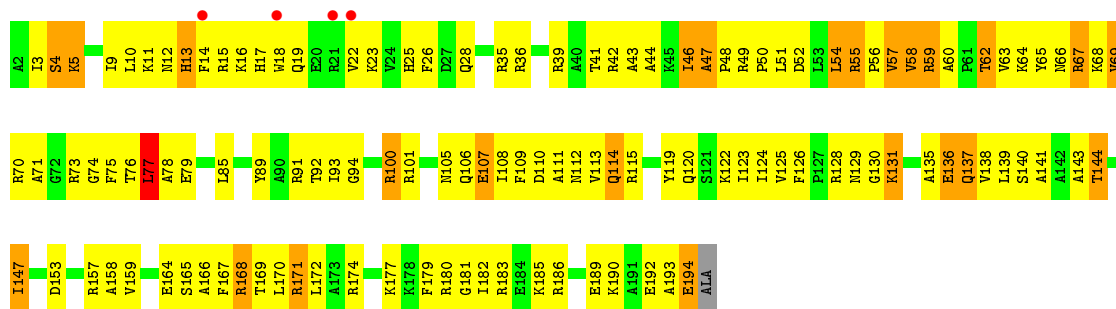




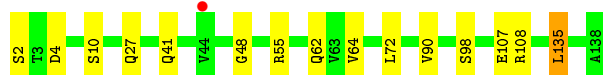
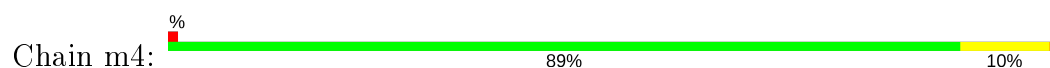
• Molecule 37: 60S ribosomal protein L13-A



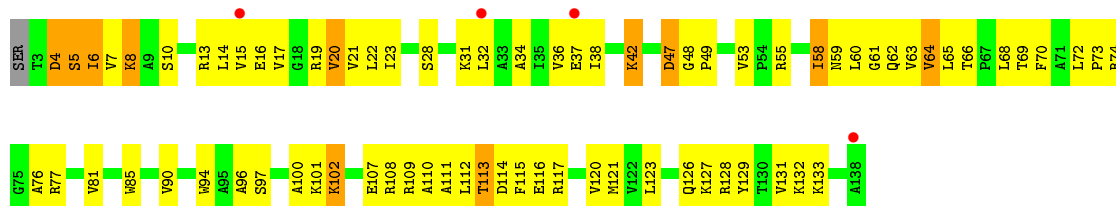
• Molecule 37: 60S ribosomal protein L13-A



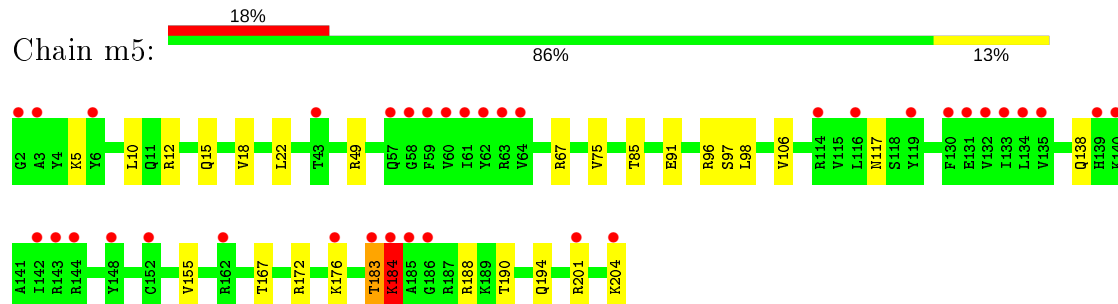
• Molecule 38: 60S ribosomal protein L14-A



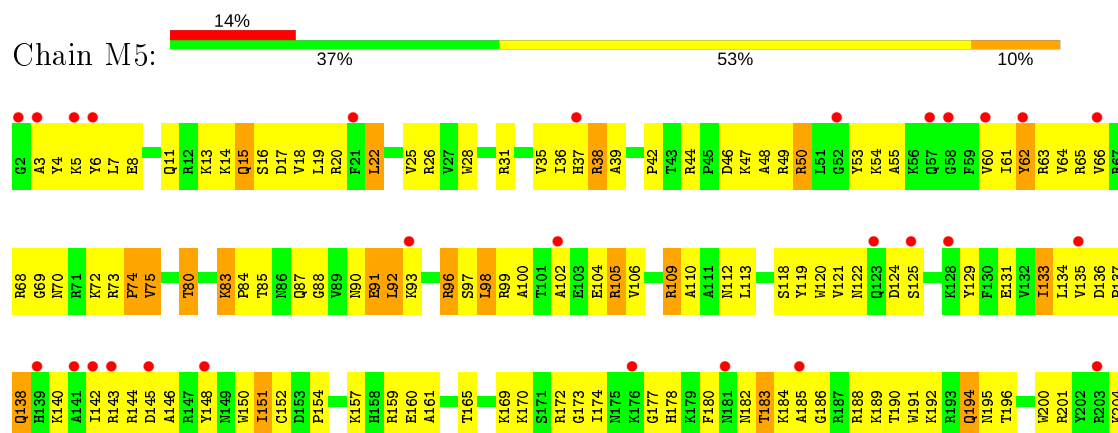
• Molecule 38: 60S ribosomal protein L14-A



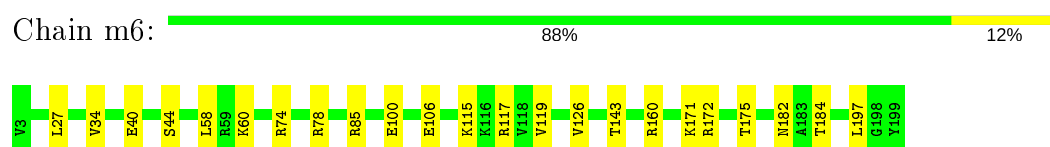
- Molecule 39: 60S ribosomal protein L15-A



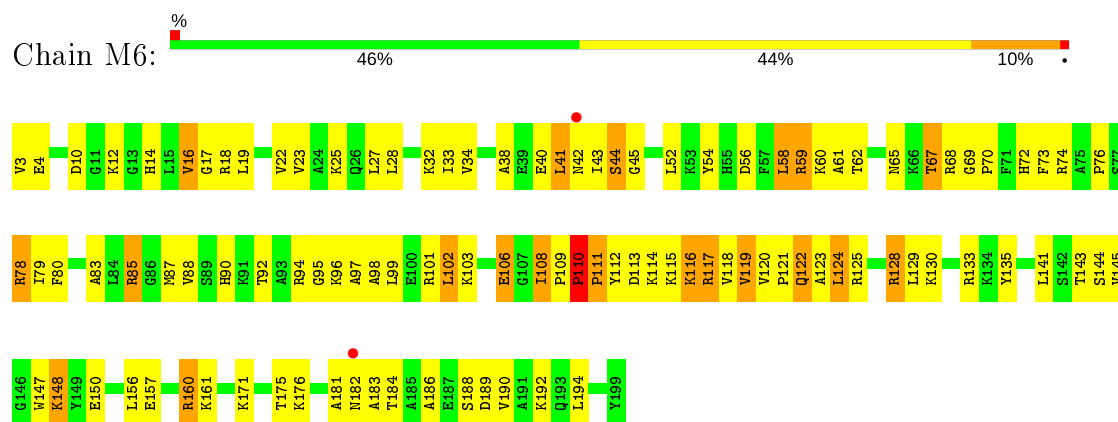
- Molecule 39: 60S ribosomal protein L15-A



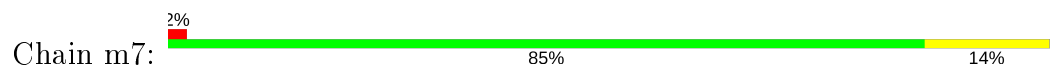
- Molecule 40: 60S ribosomal protein L16-A

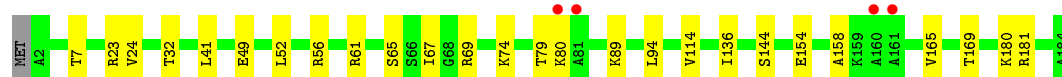


- Molecule 40: 60S ribosomal protein L16-A

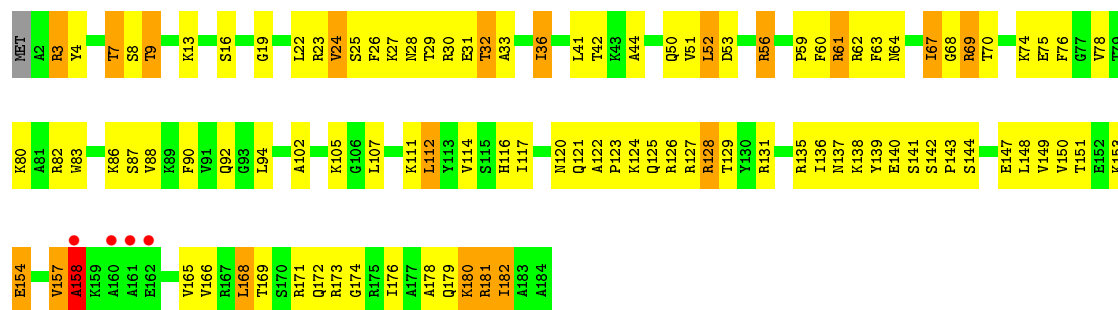


- Molecule 41: 60S ribosomal protein L17-A

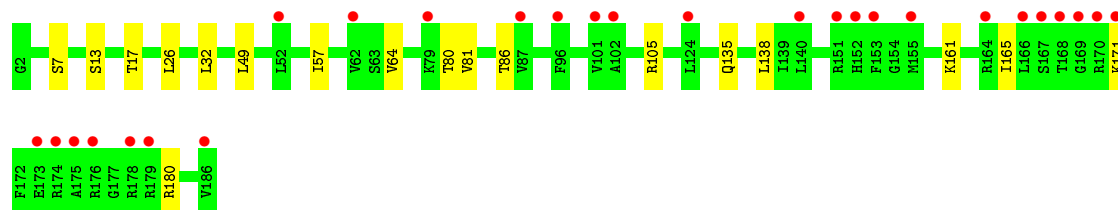
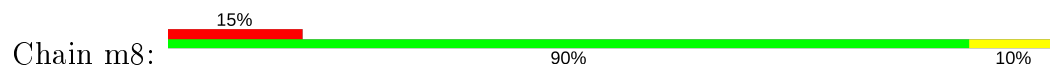




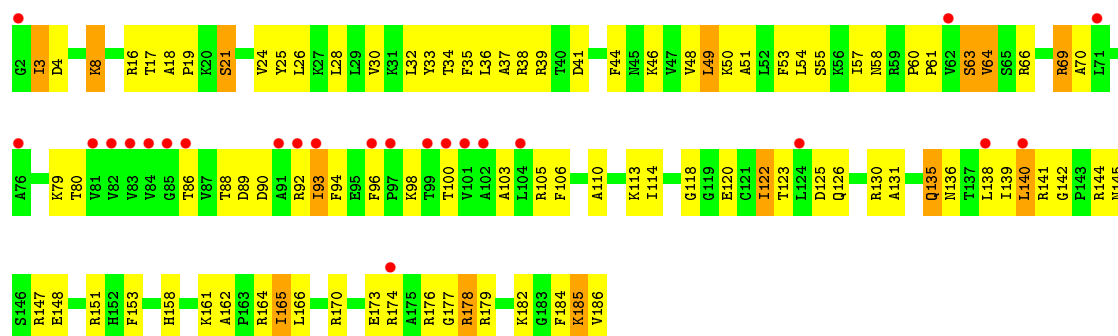
- Molecule 41: 60S ribosomal protein L17-A



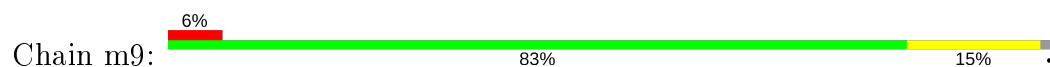
- Molecule 42: 60S ribosomal protein L18-A

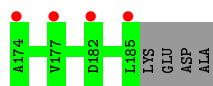


- Molecule 42: 60S ribosomal protein L18-A

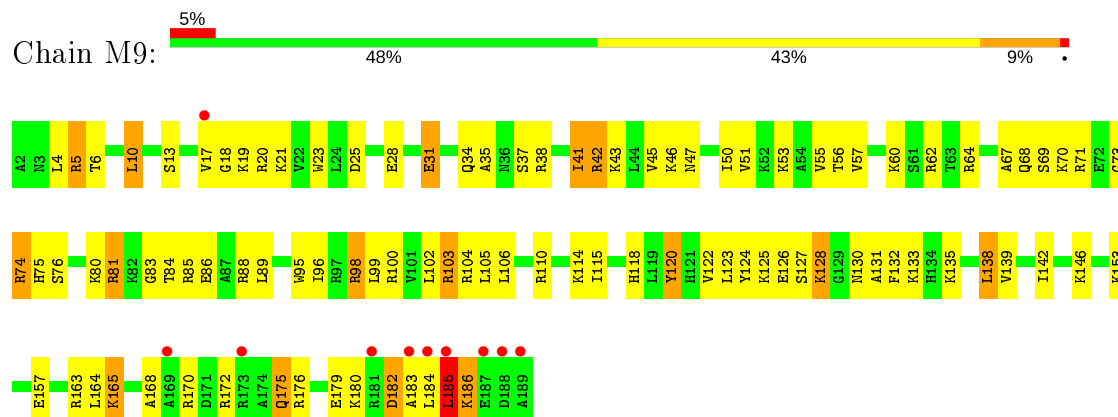


- Molecule 43: 60S ribosomal protein L19-A

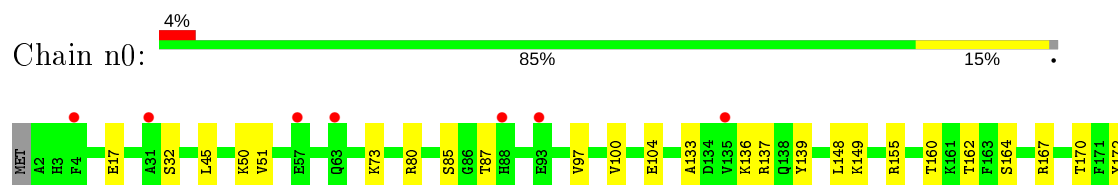




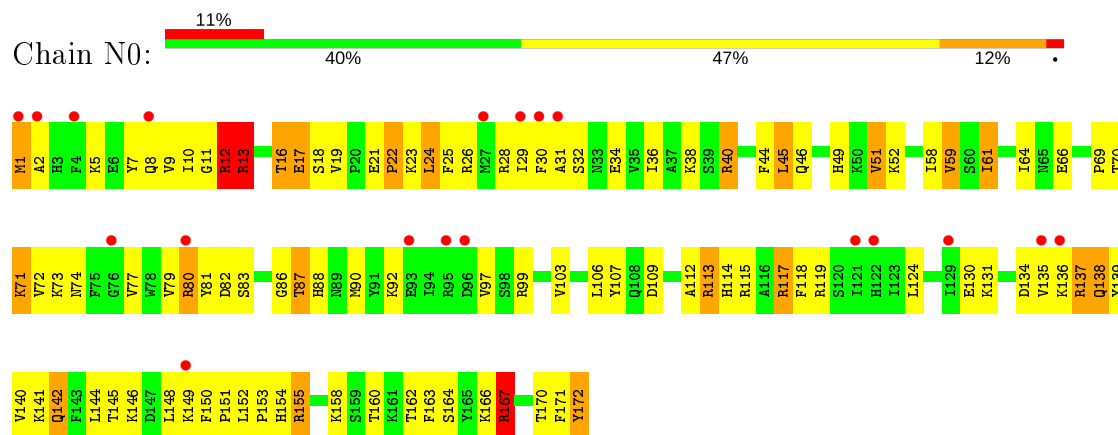
• Molecule 43: 60S ribosomal protein L19-A



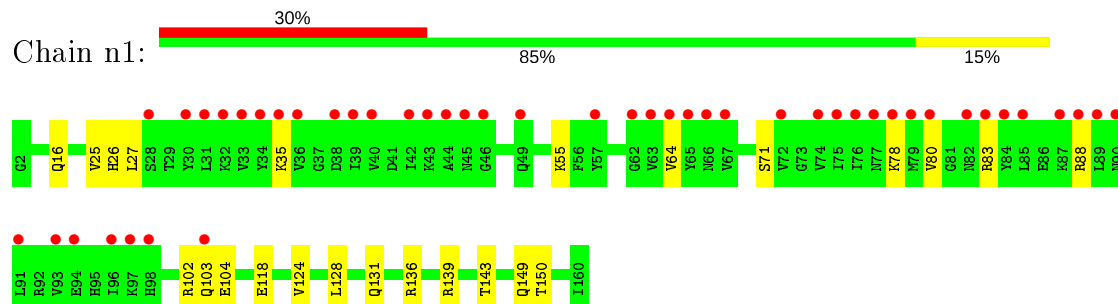
• Molecule 44: 60S ribosomal protein L20-A



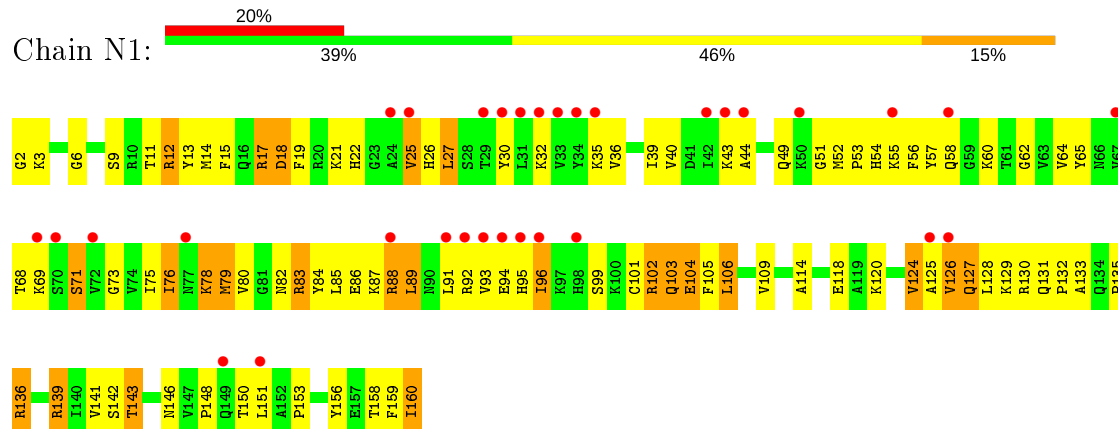
• Molecule 44: 60S ribosomal protein L20-A



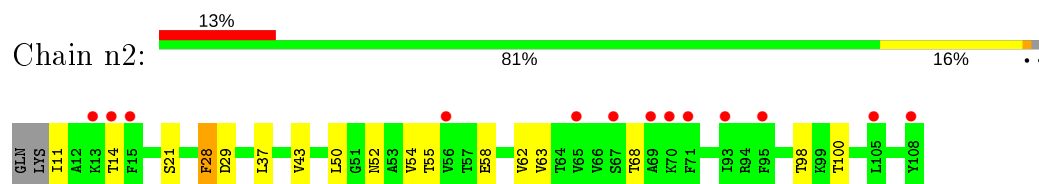
• Molecule 45: 60S ribosomal protein L21-A



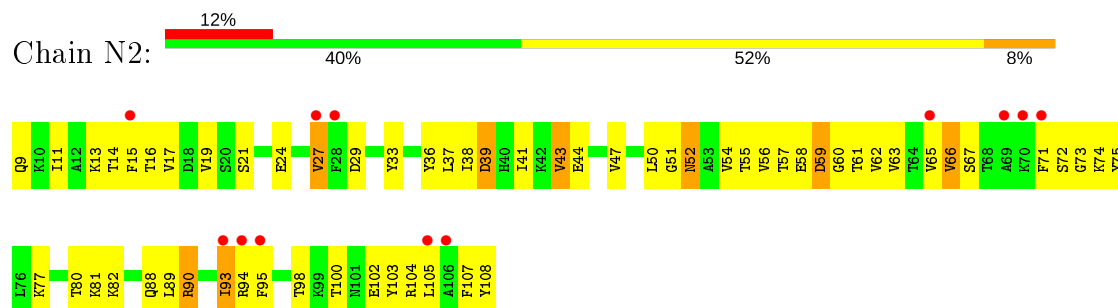
- Molecule 45: 60S ribosomal protein L21-A



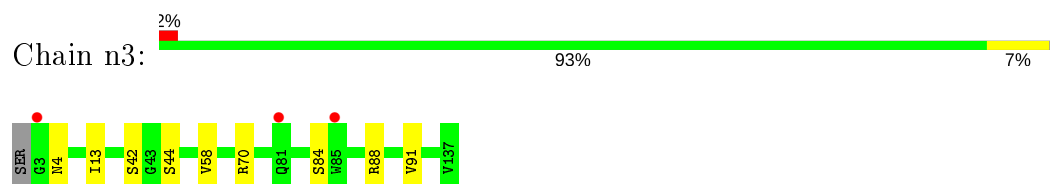
- Molecule 46: 60S ribosomal protein L22-A



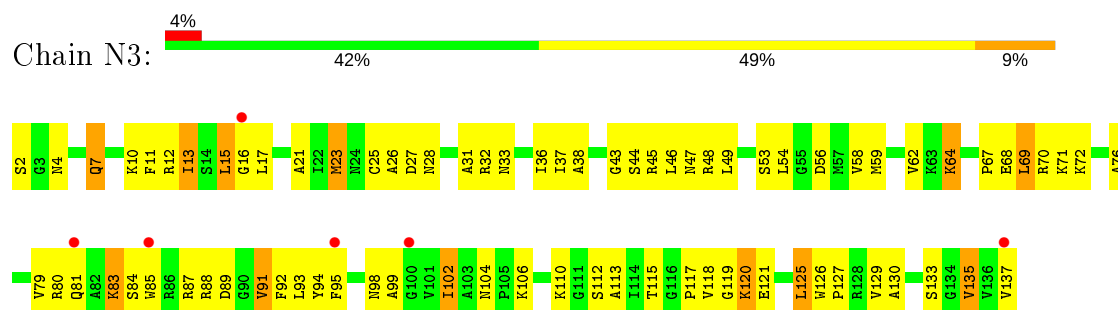
- Molecule 46: 60S ribosomal protein L22-A



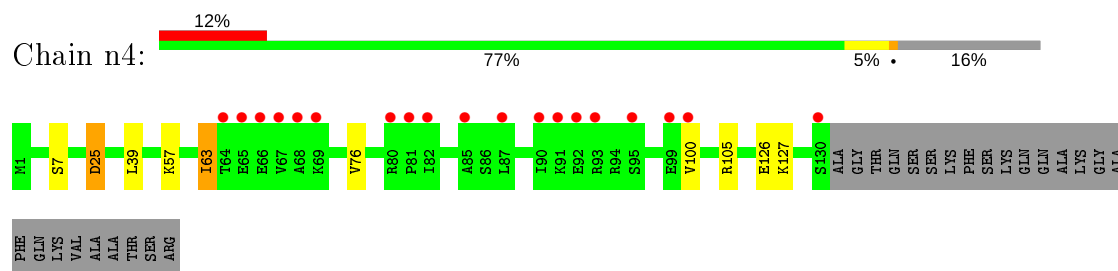
- Molecule 47: 60S ribosomal protein L23-A



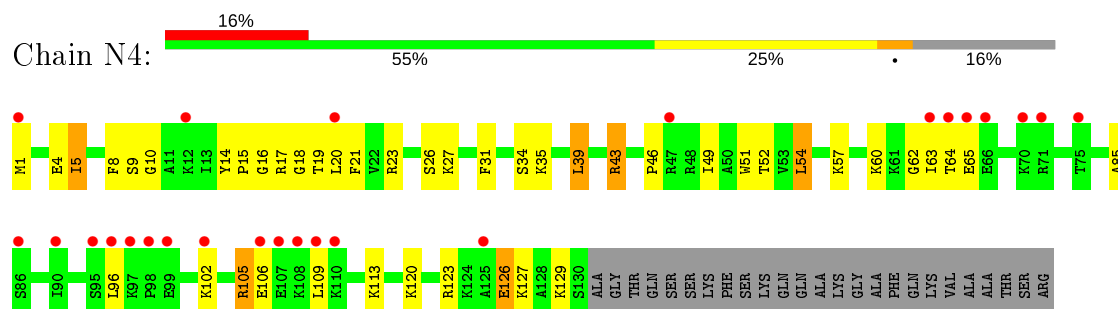
- Molecule 47: 60S ribosomal protein L23-A



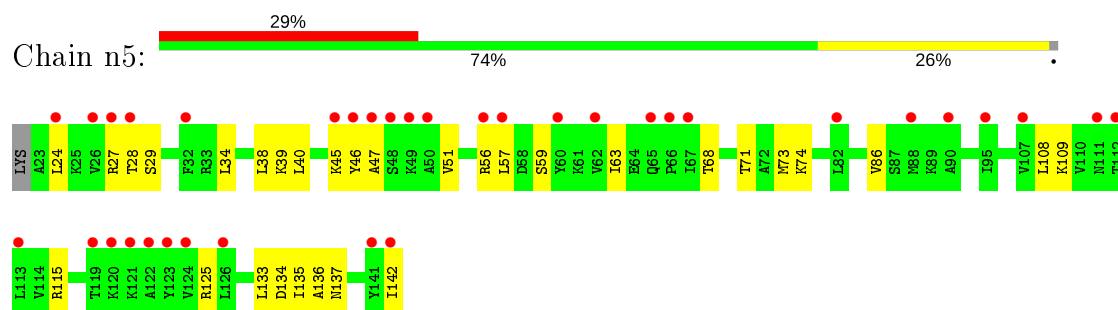
- Molecule 48: 60S ribosomal protein L24-A



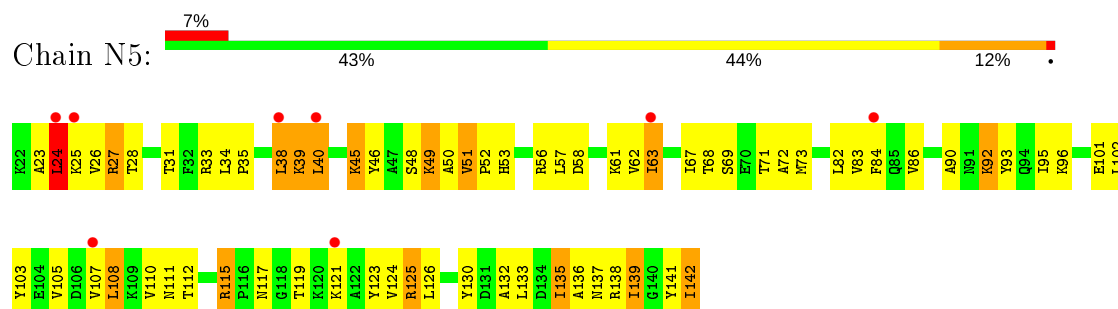
- Molecule 48: 60S ribosomal protein L24-A



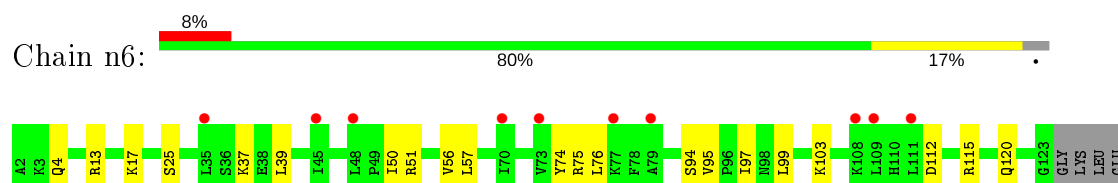
- Molecule 49: 60S ribosomal protein L25



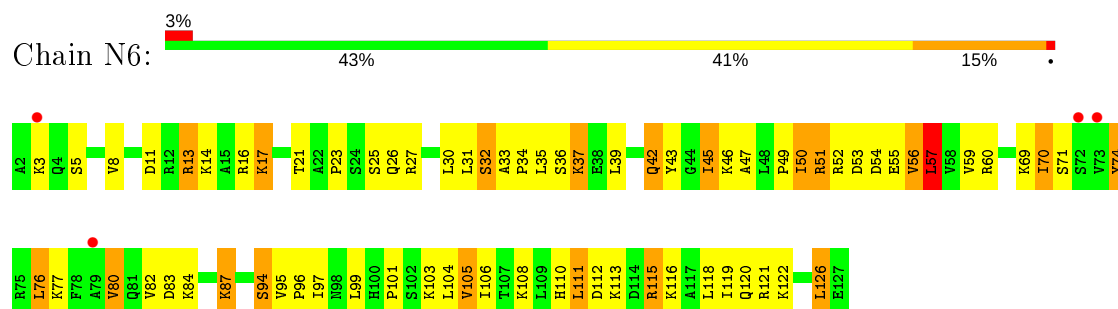
- Molecule 49: 60S ribosomal protein L25



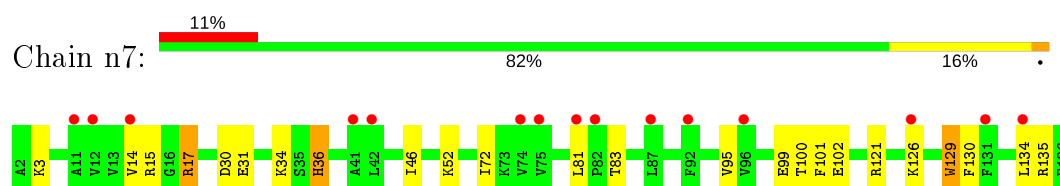
- Molecule 50: 60S ribosomal protein L26-A



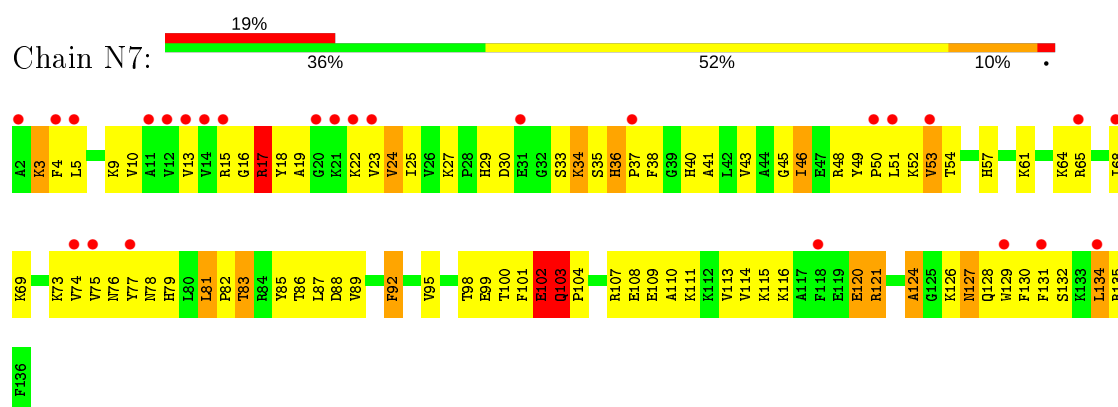
- Molecule 50: 60S ribosomal protein L26-A



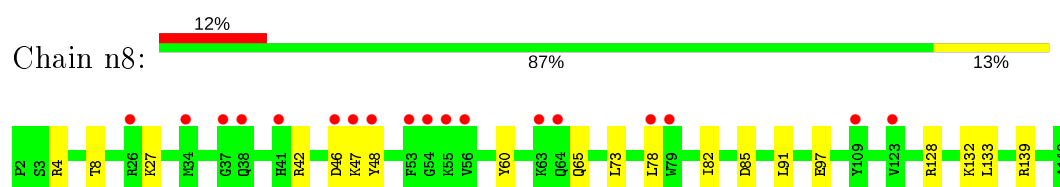
- Molecule 51: 60S ribosomal protein L27-A



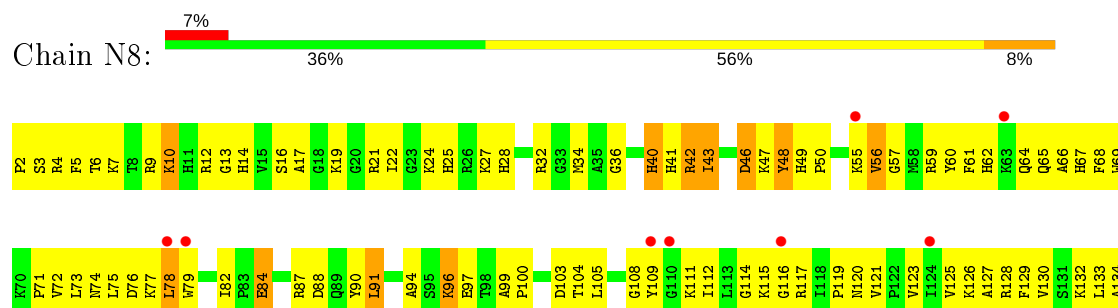
- Molecule 51: 60S ribosomal protein L27-A

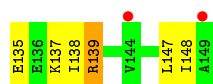


- Molecule 52: 60S ribosomal protein L28

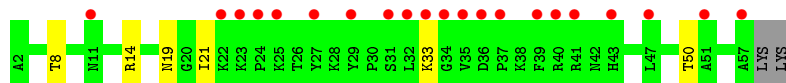
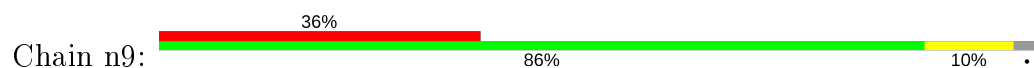


- Molecule 52: 60S ribosomal protein L28

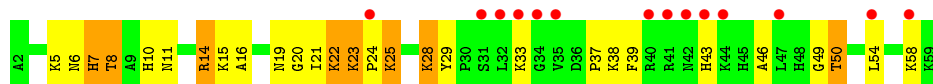




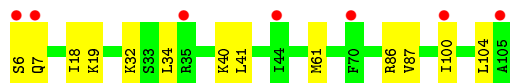
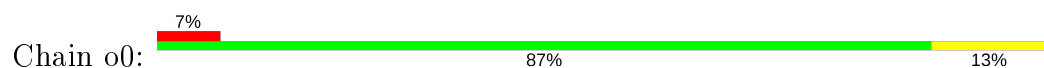
- Molecule 53: 60S ribosomal protein L29



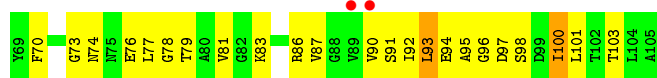
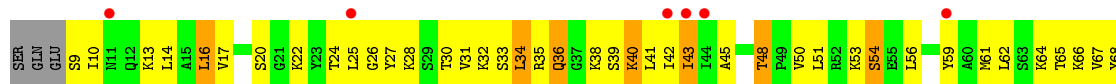
- Molecule 53: 60S ribosomal protein L29



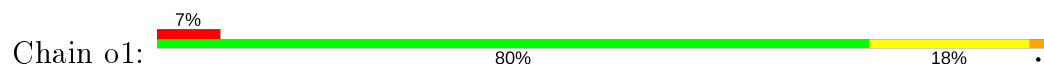
- Molecule 54: 60S ribosomal protein L30



- Molecule 54: 60S ribosomal protein L30

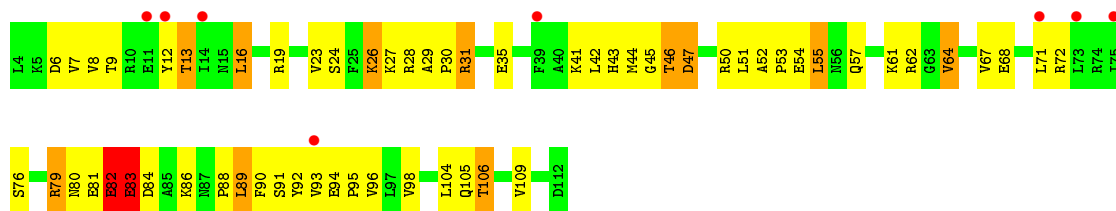


- Molecule 55: 60S ribosomal protein L31-A

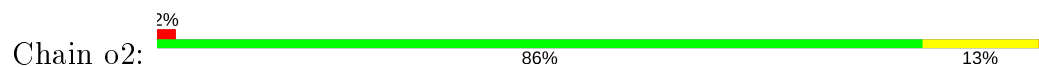


- Molecule 55: 60S ribosomal protein L31-A

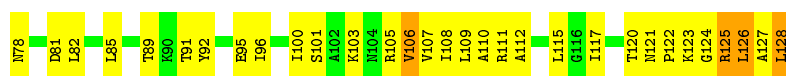




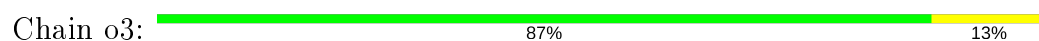
- Molecule 56: 60S ribosomal protein L32



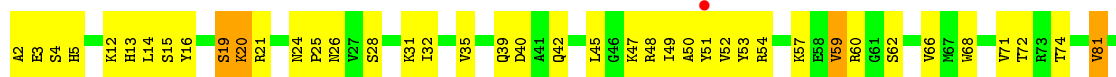
- Molecule 56: 60S ribosomal protein L32



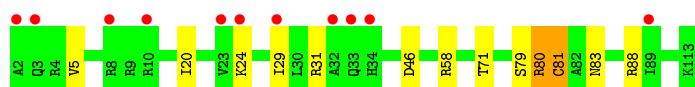
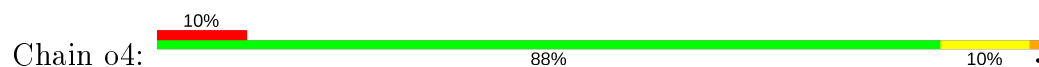
- Molecule 57: 60S ribosomal protein L33-A



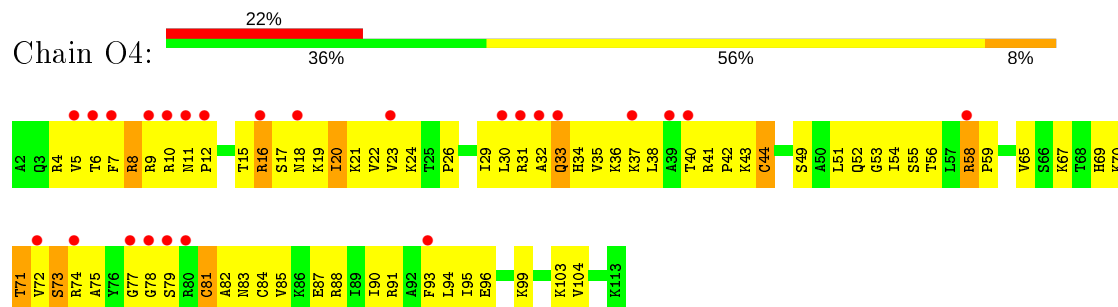
- Molecule 57: 60S ribosomal protein L33-A



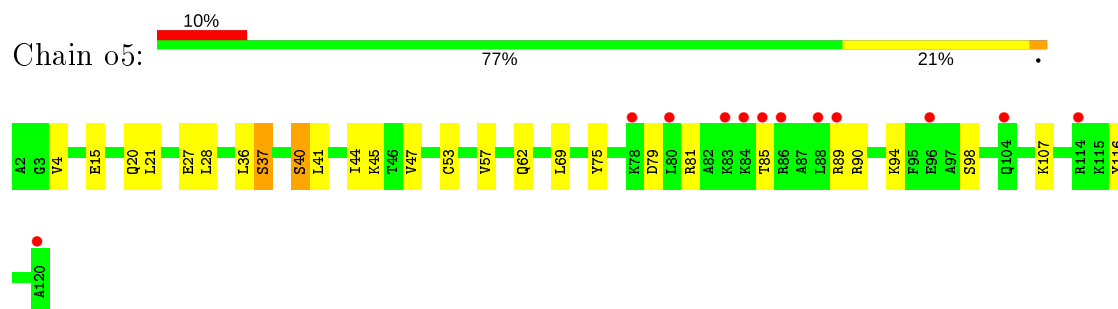
- Molecule 58: 60S ribosomal protein L34-A



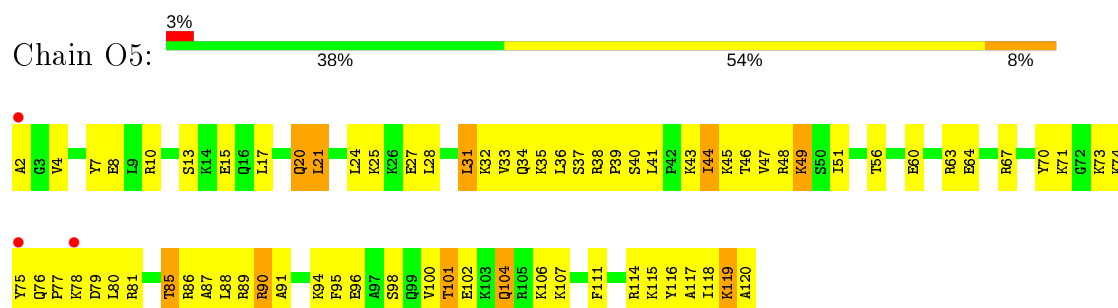
- Molecule 58: 60S ribosomal protein L34-A



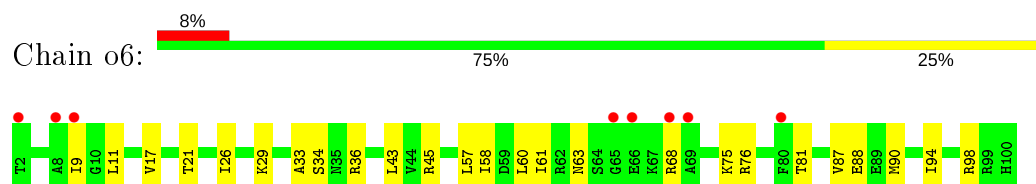
- Molecule 59: 60S ribosomal protein L35-A



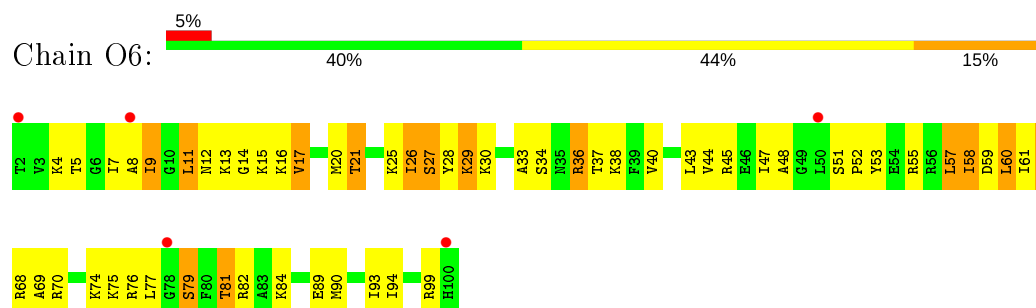
- Molecule 59: 60S ribosomal protein L35-A



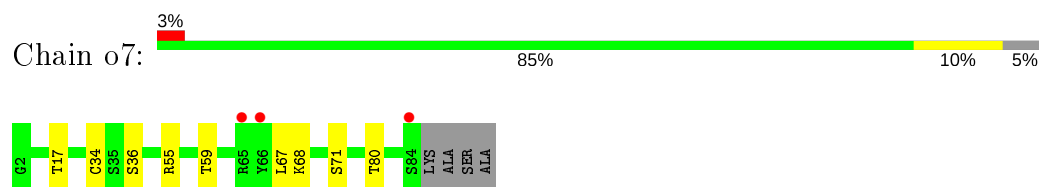
- Molecule 60: 60S ribosomal protein L36-A



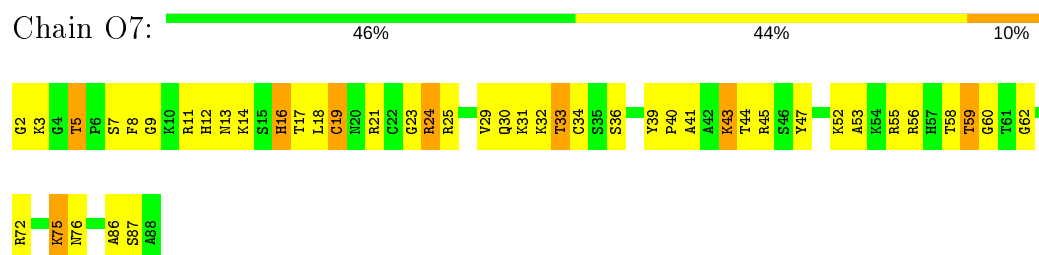
- Molecule 60: 60S ribosomal protein L36-A



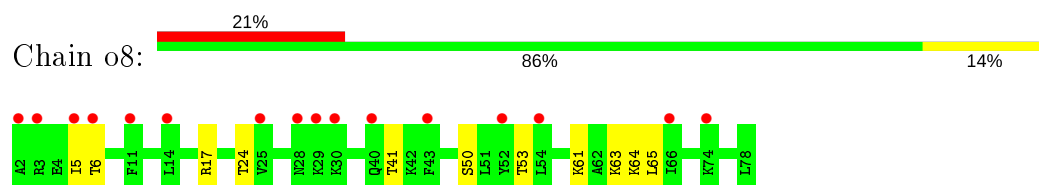
- Molecule 61: 60S ribosomal protein L37-A



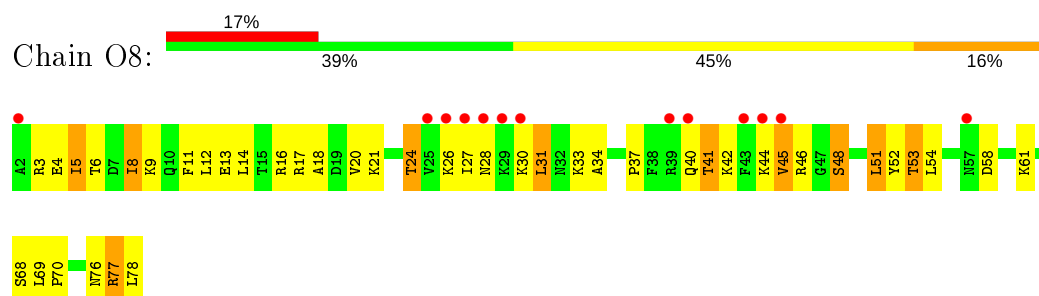
- Molecule 61: 60S ribosomal protein L37-A



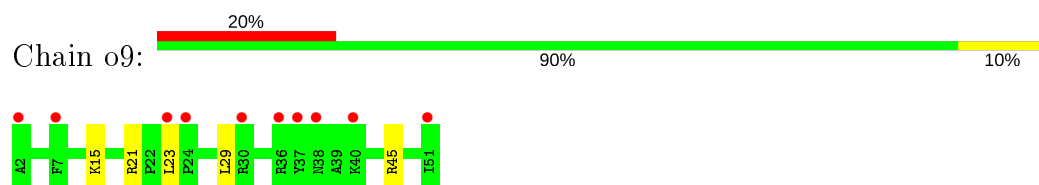
- Molecule 62: 60S ribosomal protein L38



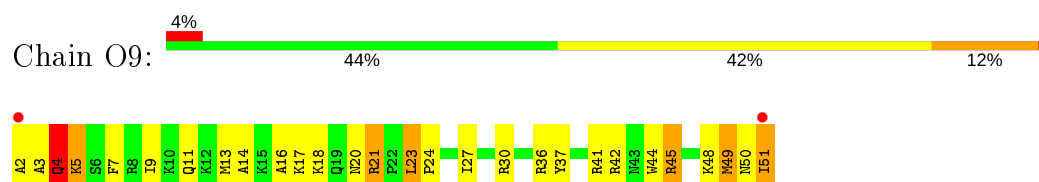
- Molecule 62: 60S ribosomal protein L38



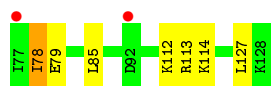
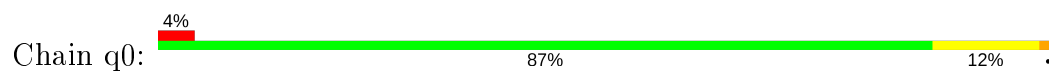
- Molecule 63: 60S ribosomal protein L39



- Molecule 63: 60S ribosomal protein L39



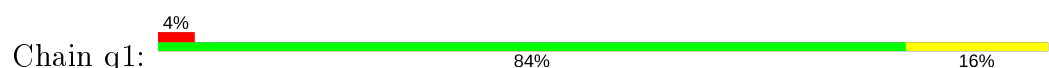
- Molecule 64: Ubiquitin-60S ribosomal protein L40



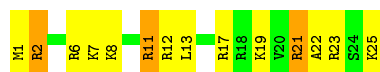
- Molecule 64: Ubiquitin-60S ribosomal protein L40



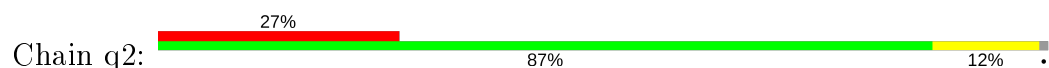
- Molecule 65: 60S ribosomal protein L41-A



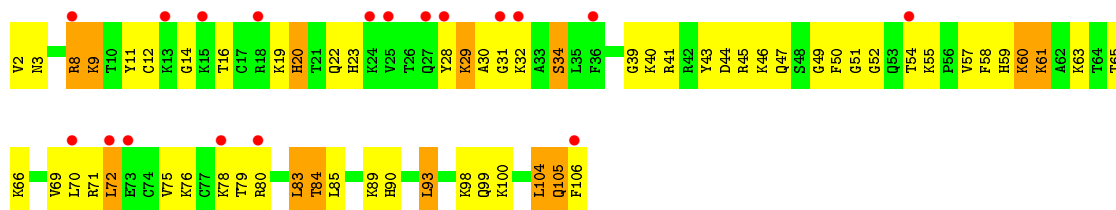
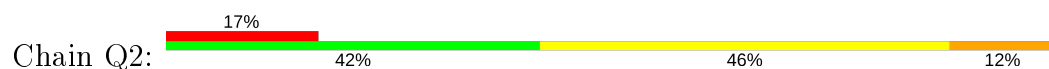
- Molecule 65: 60S ribosomal protein L41-A



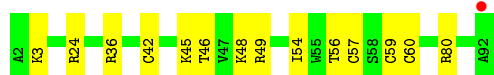
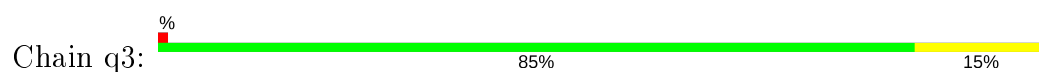
- Molecule 66: 60S ribosomal protein L42-A



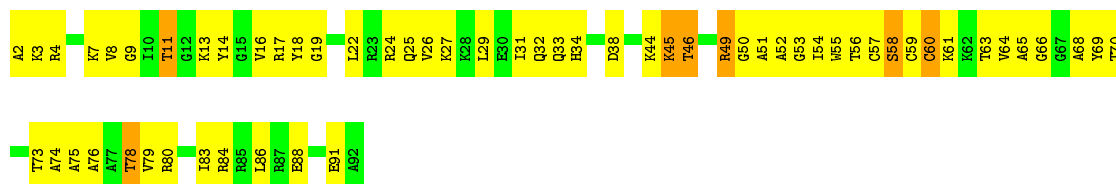
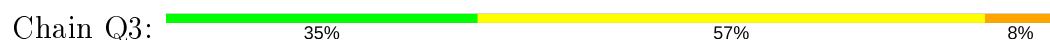
- Molecule 66: 60S ribosomal protein L42-A



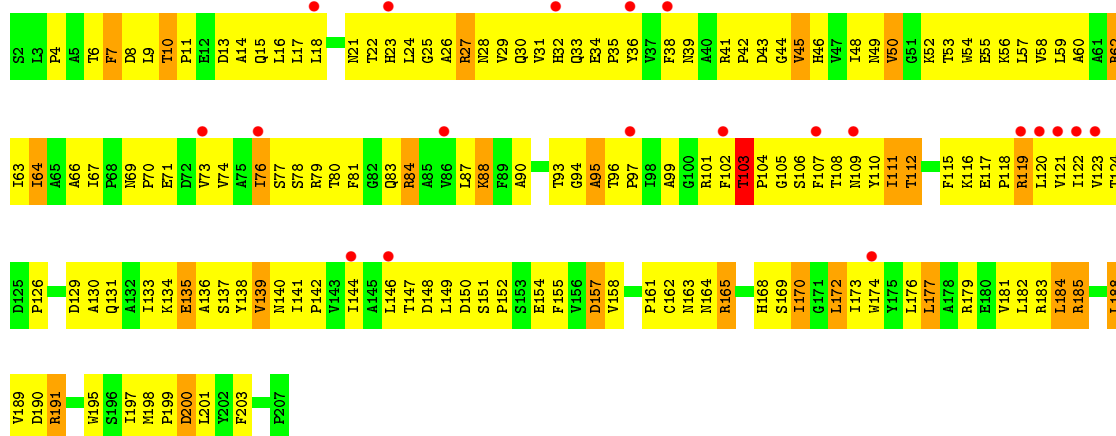
- Molecule 67: 60S ribosomal protein L43-A



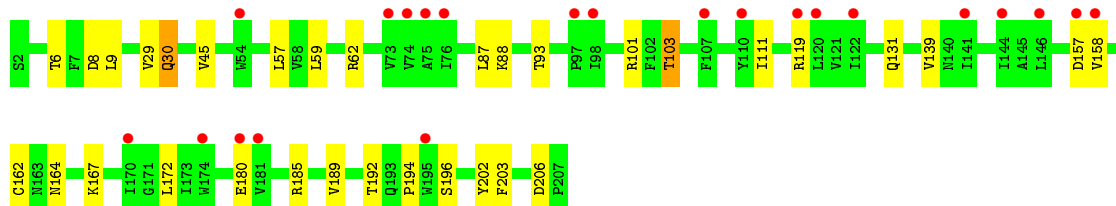
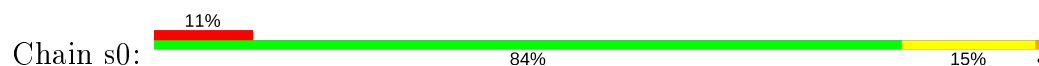
- Molecule 67: 60S ribosomal protein L43-A



- Molecule 68: 40S ribosomal protein S0-A

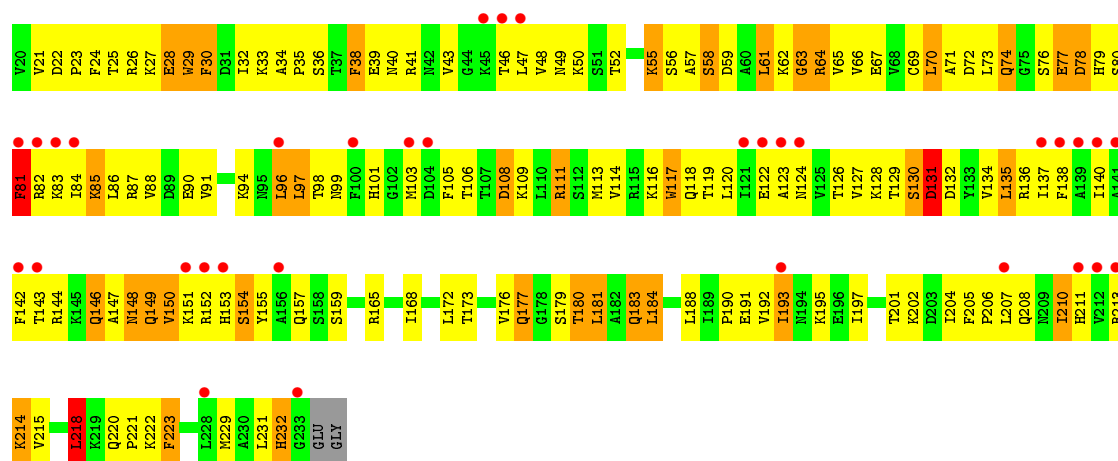


- Molecule 68: 40S ribosomal protein S0-A

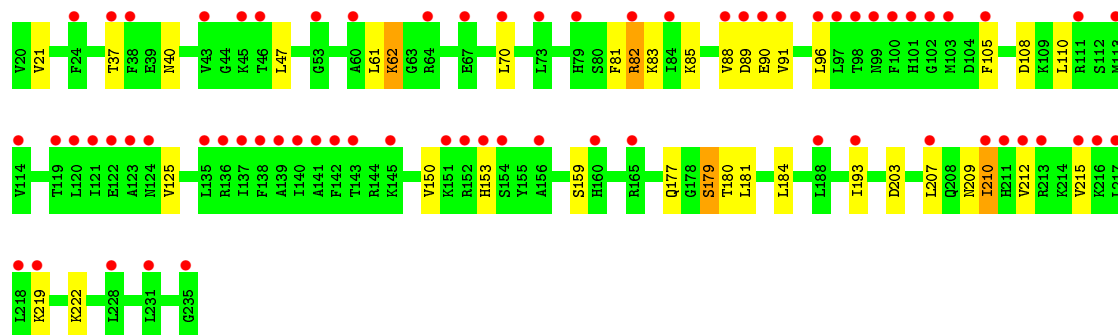
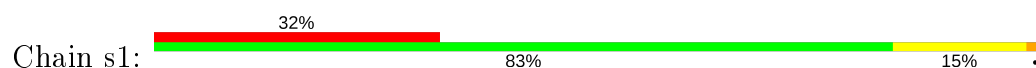


- Molecule 69: 40S ribosomal protein S1-A

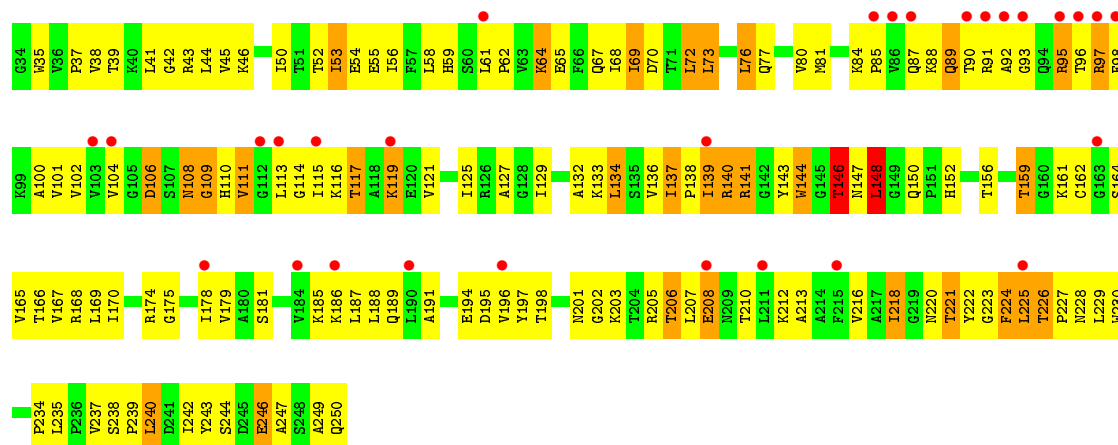




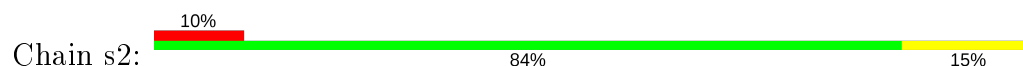
• Molecule 69: 40S ribosomal protein S1-A

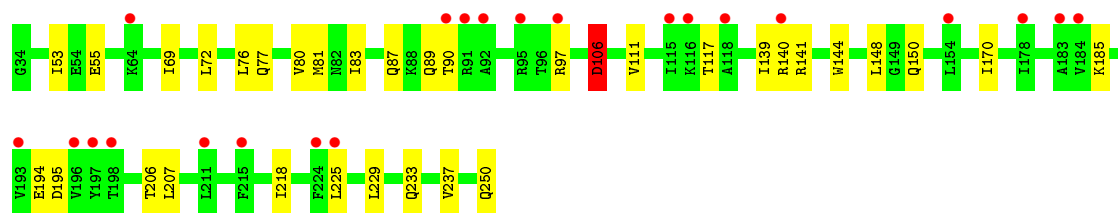


• Molecule 70: 40S ribosomal protein S2

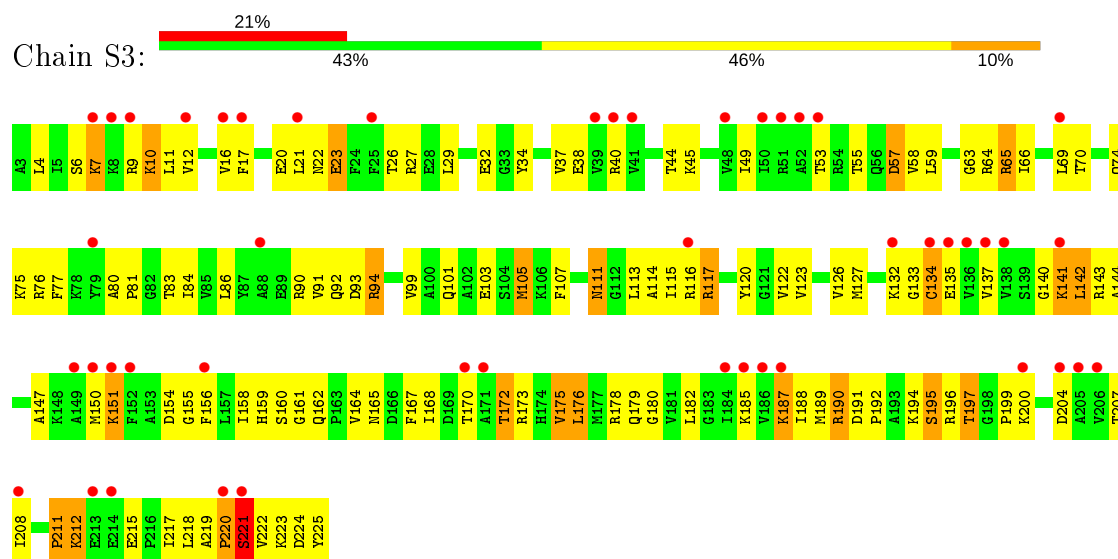


• Molecule 70: 40S ribosomal protein S2

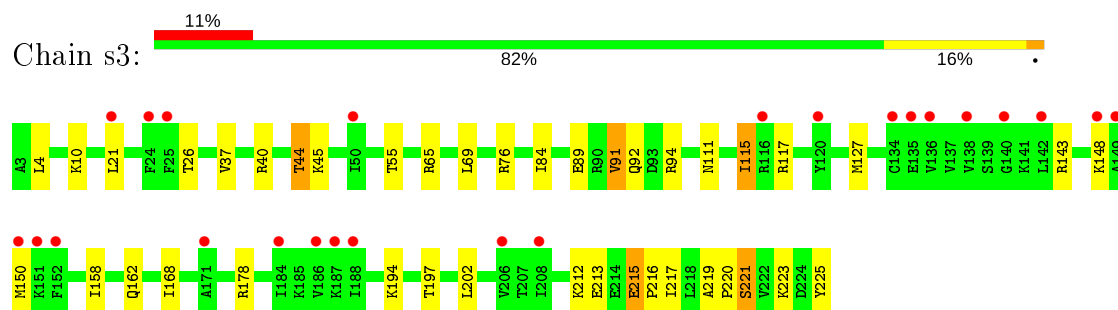




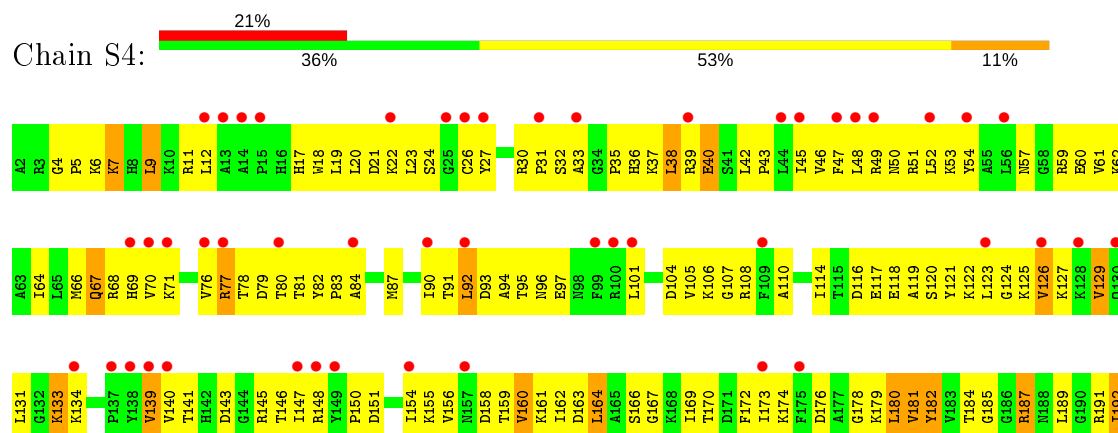
• Molecule 71: 40S ribosomal protein S3



• Molecule 71: 40S ribosomal protein S3

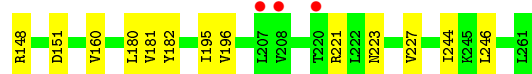
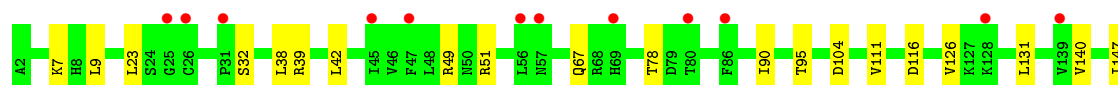
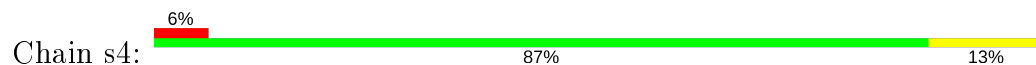


• Molecule 72: 40S ribosomal protein S4-A

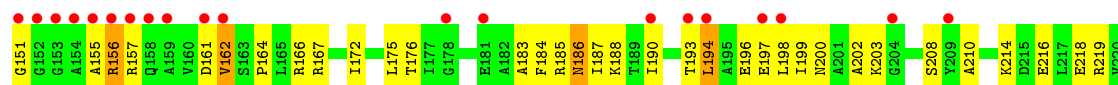
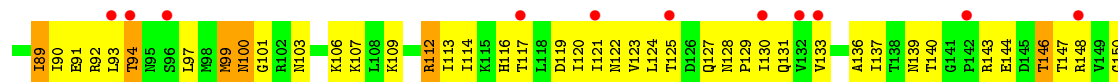
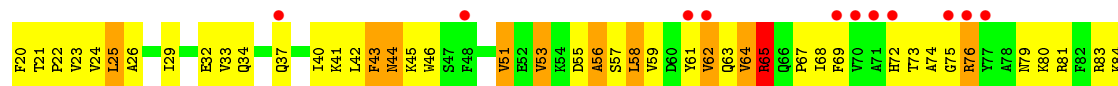




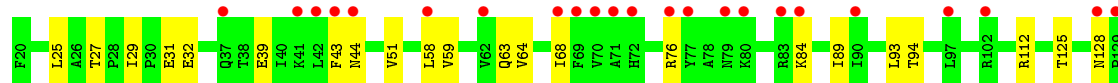
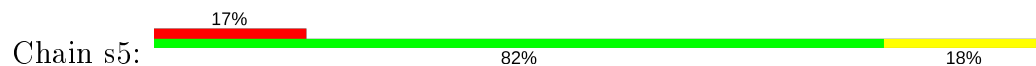
• Molecule 72: 40S ribosomal protein S4-A



• Molecule 73: 40S ribosomal protein S5

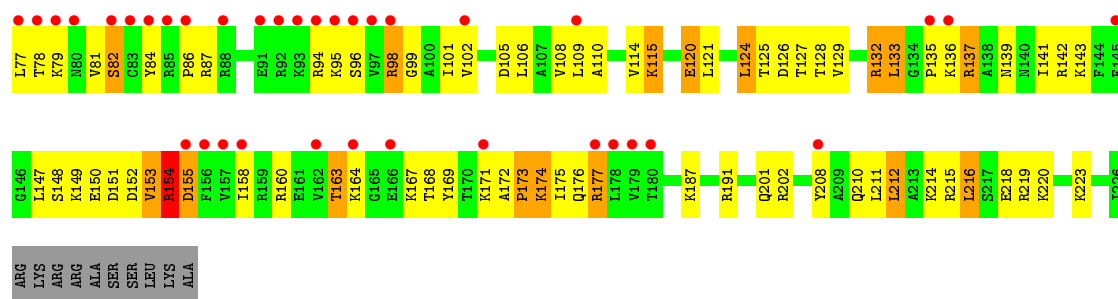


• Molecule 73: 40S ribosomal protein S5

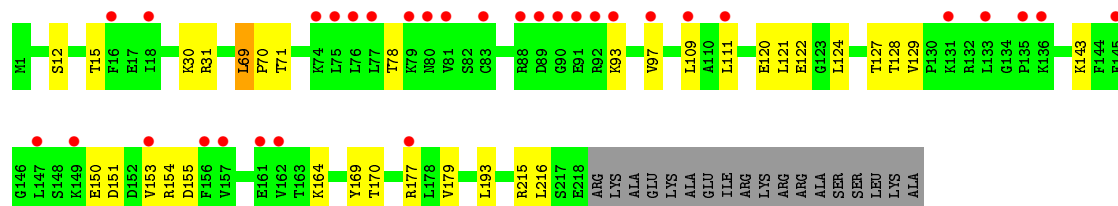
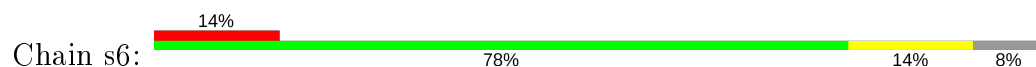


• Molecule 74: 40S ribosomal protein S6-A

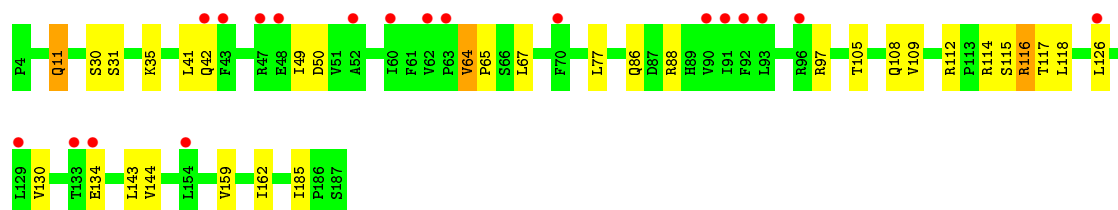
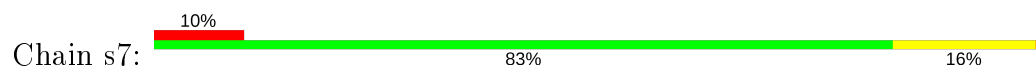




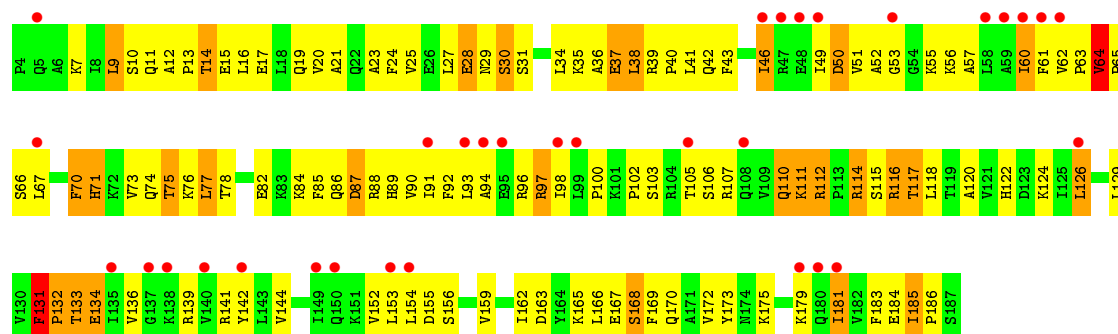
- Molecule 74: 40S ribosomal protein S6-A



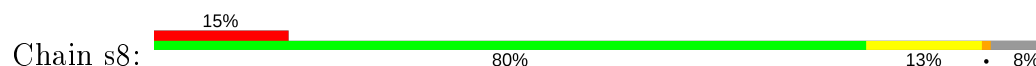
- Molecule 75: 40S ribosomal protein S7-A

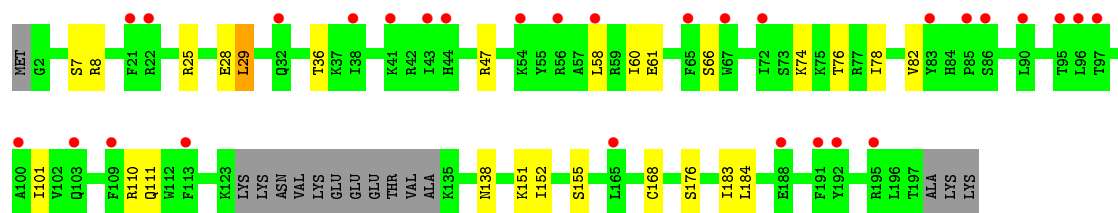


- Molecule 75: 40S ribosomal protein S7-A

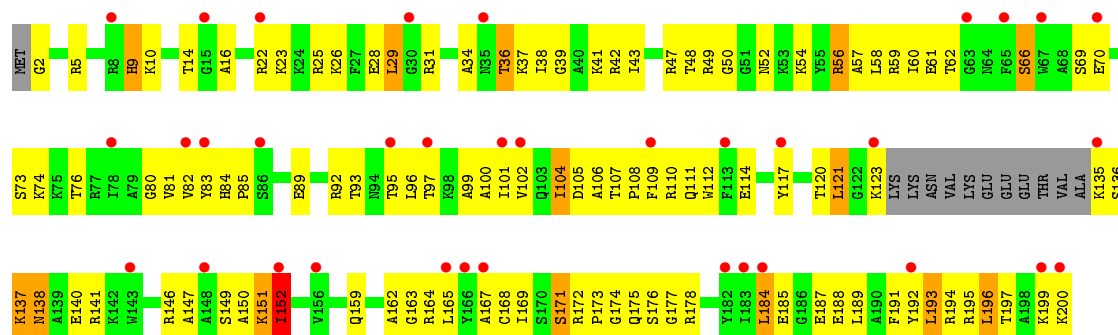


- Molecule 76: 40S ribosomal protein S8-A

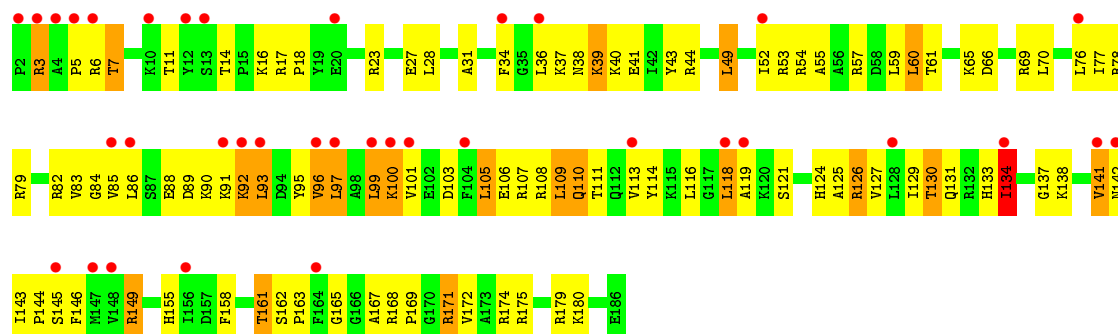
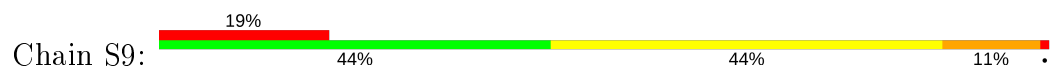




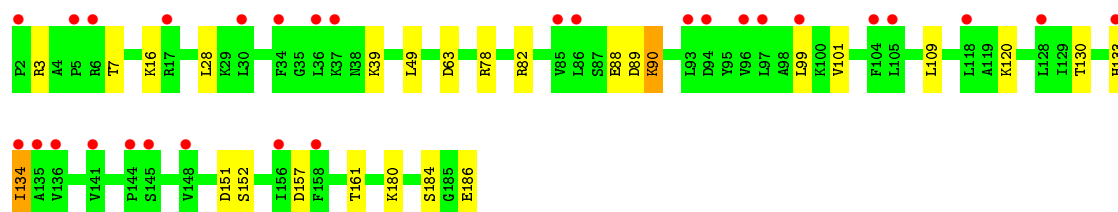
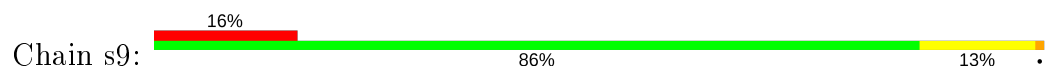
• Molecule 76: 40S ribosomal protein S8-A



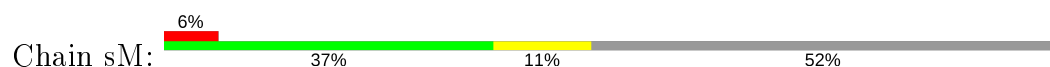
• Molecule 77: 40S ribosomal protein S9-A

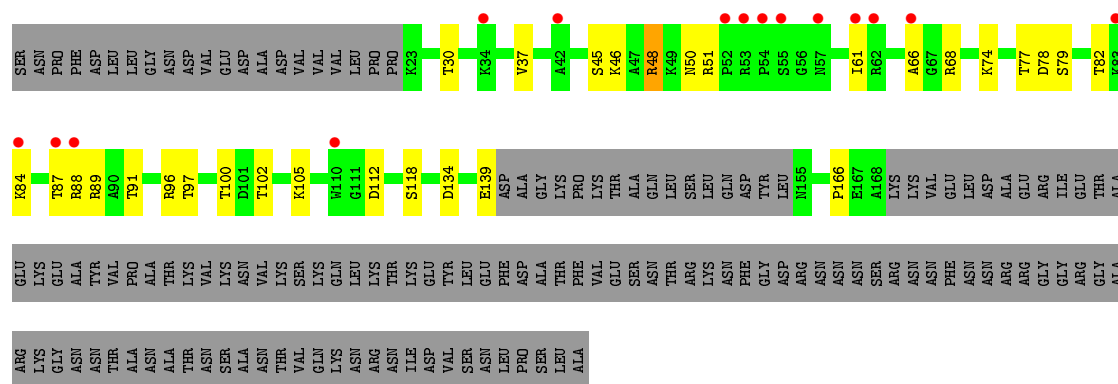


• Molecule 77: 40S ribosomal protein S9-A

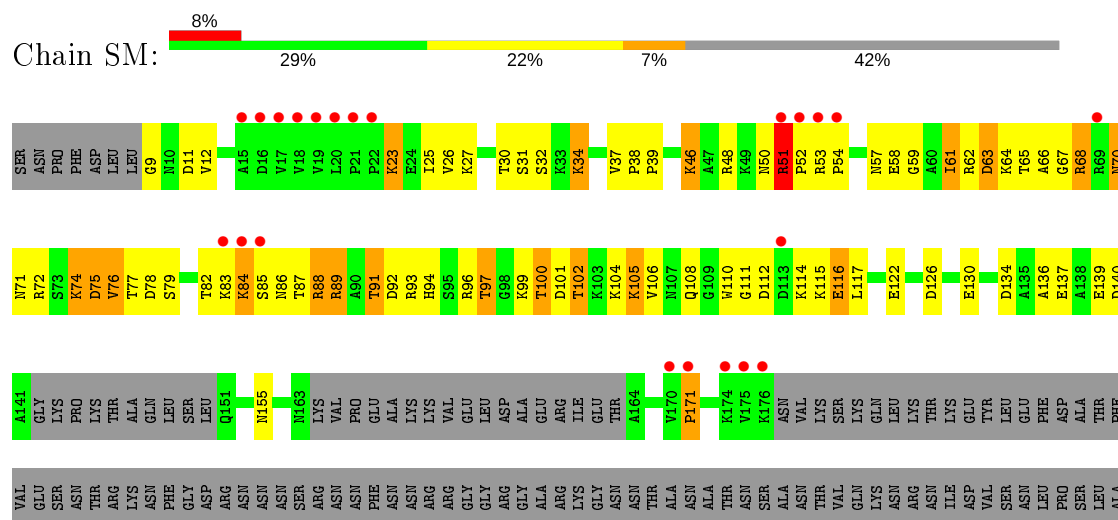


• Molecule 78: Suppressor protein STM1

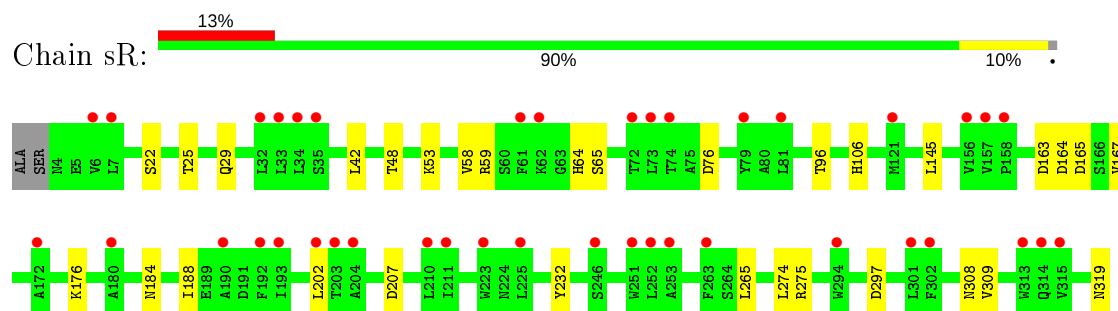




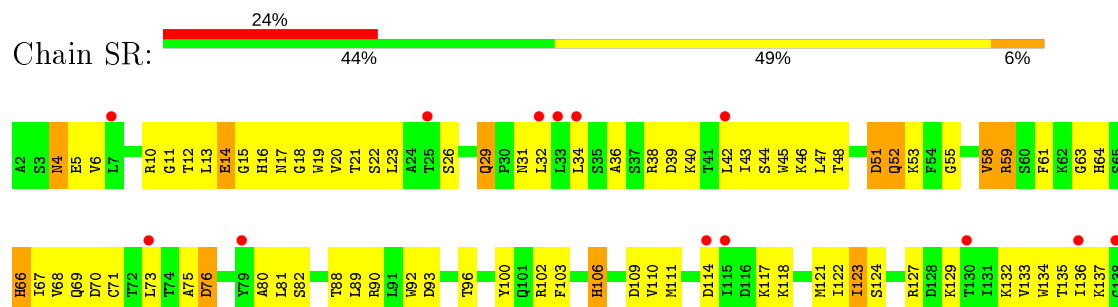
- Molecule 78: Suppressor protein STM1

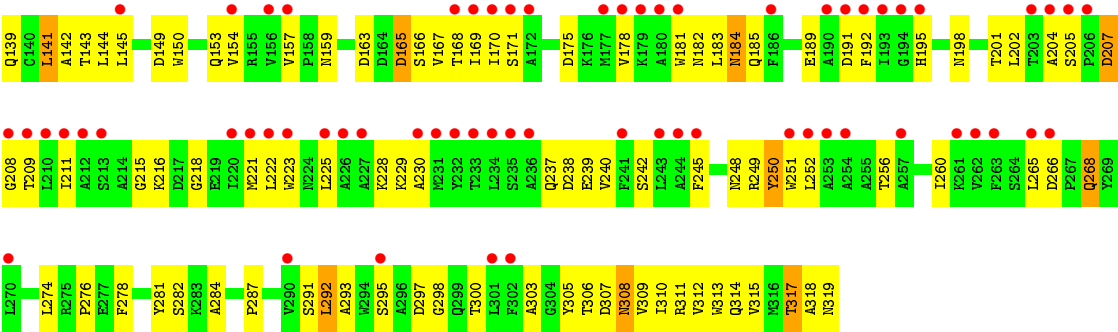


- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	442.14 Å 298.76 Å 299.77 Å 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
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 3.67 Å)	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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 8UZ

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(°)	Ideal(°)
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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	66081	0	33208	1565	0
1	5	65880	0	33109	1448	1
2	2	37692	0	18964	969	1
2	6	36971	0	18603	851	0
3	3	2579	0	1303	77	0
3	7	2579	0	1304	55	0
4	4	3353	0	1695	91	0
4	8	3353	0	1695	100	0
5	C0	772	0	727	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	c0	746	0	693	0	0
6	C1	1207	0	1252	83	0
6	c1	1168	0	1233	0	0
7	C2	865	0	874	58	0
7	c2	890	0	887	0	0
8	C3	1192	0	1255	90	0
8	c3	1192	0	1255	0	0
9	C4	891	0	883	103	0
9	c4	949	0	985	0	0
10	C5	977	0	1002	81	0
10	c5	987	0	1019	0	0
11	C6	1105	0	1166	108	0
11	c6	1105	0	1166	0	0
12	C7	926	0	930	108	0
12	c7	926	0	918	0	0
13	C8	1192	0	1222	158	0
13	c8	1192	0	1221	0	0
14	C9	1112	0	1124	97	0
14	c9	1112	0	1124	0	0
15	D0	841	0	906	80	0
15	d0	828	0	893	0	0
16	D1	684	0	672	70	0
16	d1	684	0	672	0	0
17	D2	1021	0	1060	77	0
17	d2	1021	0	1060	0	0
18	D3	1121	0	1196	99	0
18	d3	1121	0	1196	0	0
19	D4	1073	0	1132	87	0
19	d4	1073	0	1132	0	0
20	D5	563	0	603	87	0
20	d5	558	0	598	0	0
21	D6	769	0	814	101	0
21	d6	769	0	814	0	0
22	D7	610	0	632	34	0
22	d7	610	0	633	0	0
23	D8	497	0	535	43	0
23	d8	497	0	535	0	0
24	D9	433	0	422	34	0
24	d9	442	0	428	0	0
25	E0	475	0	525	51	0
25	e0	482	0	534	0	0
26	E1	566	0	604	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	e1	586	0	629	0	0
27	L2	1914	0	1981	211	0
27	l2	1912	0	1976	0	0
28	L3	3075	0	3142	262	0
28	l3	3075	0	3142	0	0
29	L4	2748	0	2859	229	0
29	l4	2748	0	2859	0	0
30	L5	2375	0	2324	219	0
30	l5	2359	0	2311	0	0
31	L6	1248	0	1339	95	0
31	l6	1248	0	1339	0	0
32	L7	1784	0	1862	132	0
32	l7	1791	0	1869	0	0
33	L8	1804	0	1877	129	0
33	l8	1764	0	1822	0	0
34	L9	1518	0	1587	127	0
34	l9	1518	0	1587	0	0
35	M0	1705	0	1736	145	0
35	m0	1696	0	1731	0	0
36	M1	1353	0	1383	113	0
36	m1	1353	0	1383	0	0
37	M3	1543	0	1607	155	0
37	m3	1548	0	1613	0	0
38	M4	1053	0	1149	93	0
38	m4	1059	0	1154	0	0
39	M5	1720	0	1779	146	0
39	m5	1720	0	1779	0	0
40	M6	1555	0	1659	110	0
40	m6	1555	0	1659	0	0
41	M7	1420	0	1437	115	0
41	m7	1420	0	1437	0	0
42	M8	1441	0	1543	96	0
42	m8	1441	0	1543	0	0
43	M9	1521	0	1617	105	0
43	m9	1490	0	1589	0	0
44	N0	1445	0	1487	109	0
44	n0	1437	0	1475	0	0
45	N1	1276	0	1323	98	0
45	n1	1276	0	1323	0	0
46	N2	796	0	812	44	0
46	n2	778	0	791	0	0
47	N3	1003	0	1048	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	n3	997	0	1043	0	0
48	N4	965	0	953	34	0
48	n4	1007	0	1043	0	0
49	N5	964	0	1025	75	0
49	n5	959	0	1023	0	0
50	N6	993	0	1081	77	0
50	n6	963	0	1047	0	0
51	N7	1092	0	1155	101	0
51	n7	1092	0	1155	0	0
52	N8	1173	0	1215	140	0
52	n8	1173	0	1215	0	0
53	N9	462	0	491	30	0
53	n9	444	0	465	0	0
54	O0	743	0	797	71	0
54	o0	767	0	816	0	0
55	O1	876	0	912	61	0
55	o1	883	0	918	0	0
56	O2	1020	0	1090	64	0
56	o2	1020	0	1090	0	0
57	O3	850	0	880	63	0
57	o3	850	0	880	0	0
58	O4	880	0	944	86	0
58	o4	880	0	944	0	0
59	O5	969	0	1078	76	0
59	o5	965	0	1067	0	0
60	O6	771	0	849	61	0
60	o6	770	0	846	0	0
61	O7	681	0	683	57	0
61	o7	656	0	655	0	0
62	O8	612	0	682	38	0
62	o8	608	0	671	0	0
63	O9	436	0	475	45	0
63	o9	436	0	475	0	0
64	Q0	417	0	455	31	0
64	q0	417	0	455	0	0
65	Q1	233	0	284	16	0
65	q1	233	0	284	0	0
66	Q2	847	0	917	54	0
66	q2	836	0	908	0	0
67	Q3	694	0	735	73	0
67	q3	694	0	735	0	0
68	S0	1577	0	1567	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	s0	1583	0	1578	0	0
69	S1	1709	0	1784	157	0
69	s1	1722	0	1793	0	0
70	S2	1635	0	1723	162	0
70	s2	1635	0	1723	0	0
71	S3	1734	0	1817	126	0
71	s3	1734	0	1817	0	0
72	S4	2068	0	2154	155	0
72	s4	2068	0	2154	0	0
73	S5	1609	0	1675	150	0
73	s5	1609	0	1675	0	0
74	S6	1799	0	1879	111	0
74	s6	1755	0	1845	0	0
75	S7	1481	0	1572	126	0
75	s7	1481	0	1572	0	0
76	S8	1489	0	1525	128	0
76	s8	1466	0	1494	0	0
77	S9	1494	0	1572	135	0
77	s9	1494	0	1573	0	0
78	SM	1104	0	999	110	0
78	sM	958	0	917	0	0
79	SR	2437	0	2386	139	0
79	sR	2427	0	2371	0	0
80	1	485	0	0	0	0
80	2	128	0	0	0	0
80	3	13	0	0	0	0
80	4	19	0	0	0	0
80	5	449	0	0	0	0
80	6	160	0	0	0	0
80	7	8	0	0	0	0
80	8	10	0	0	0	0
80	C4	3	0	0	0	0
80	C6	1	0	0	1	0
80	C8	1	0	0	0	0
80	C9	1	0	0	0	0
80	D2	1	0	0	0	0
80	L2	2	0	0	0	0
80	L3	2	0	0	0	0
80	L6	3	0	0	0	0
80	L7	2	0	0	0	0
80	L9	1	0	0	0	0
80	M0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	M5	3	0	0	0	0
80	M6	1	0	0	0	0
80	M7	4	0	0	0	0
80	M8	1	0	0	1	0
80	N0	1	0	0	0	0
80	N3	1	0	0	0	0
80	N6	1	0	0	0	0
80	N7	1	0	0	0	0
80	N8	1	0	0	0	0
80	O1	2	0	0	0	0
80	O2	1	0	0	0	0
80	O3	2	0	0	0	0
80	O4	1	0	0	0	0
80	O5	1	0	0	0	0
80	O6	1	0	0	0	0
80	O7	2	0	0	0	0
80	Q2	1	0	0	0	0
80	S1	1	0	0	0	0
80	S4	1	0	0	0	0
80	S6	1	0	0	0	0
80	SM	2	0	0	0	0
80	c1	2	0	0	0	0
80	c3	1	0	0	0	0
80	c7	1	0	0	0	0
80	c8	2	0	0	0	0
80	c9	1	0	0	0	0
80	d2	1	0	0	0	0
80	d3	1	0	0	0	0
80	d9	2	0	0	0	0
80	l2	2	0	0	0	0
80	l3	3	0	0	0	0
80	l4	1	0	0	0	0
80	l5	1	0	0	0	0
80	l7	1	0	0	0	0
80	m0	2	0	0	0	0
80	m5	1	0	0	0	0
80	m6	1	0	0	0	0
80	m7	2	0	0	0	0
80	n1	1	0	0	0	0
80	n3	1	0	0	0	0
80	n6	1	0	0	0	0
80	n7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	n8	1	0	0	0	0
80	o2	2	0	0	0	0
80	o3	2	0	0	0	0
80	o4	1	0	0	0	0
80	o7	2	0	0	0	0
80	q2	3	0	0	0	0
80	s0	1	0	0	0	0
80	s4	1	0	0	0	0
80	s6	1	0	0	0	0
80	s8	1	0	0	0	0
81	1	330	0	0	20	0
81	2	99	0	0	5	0
81	3	33	0	0	6	0
81	4	33	0	0	2	0
81	5	264	0	0	12	0
81	6	33	0	0	1	0
81	7	33	0	0	2	0
82	D6	1	0	0	0	0
82	D7	1	0	0	0	0
82	D9	1	0	0	0	0
82	E1	1	0	0	0	0
82	O4	1	0	0	0	0
82	O7	1	0	0	0	0
82	Q0	1	0	0	0	0
82	Q2	1	0	0	0	0
82	Q3	1	0	0	0	0
82	d6	1	0	0	0	0
82	d9	1	0	0	0	0
82	e1	1	0	0	0	0
82	o4	1	0	0	0	0
82	o7	1	0	0	0	0
82	q0	1	0	0	0	0
82	q2	1	0	0	0	0
82	q3	1	0	0	0	0
83	1	597	0	0	37	0
83	2	154	0	0	13	0
83	3	23	0	0	1	0
83	4	7	0	0	0	0
83	5	556	0	0	36	0
83	6	204	0	0	12	0
83	7	19	0	0	2	0
83	8	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	C3	2	0	0	0	0
83	C4	1	0	0	0	0
83	C6	1	0	0	0	0
83	C7	1	0	0	0	0
83	C9	3	0	0	0	0
83	D0	1	0	0	0	0
83	D3	2	0	0	1	0
83	D6	1	0	0	1	0
83	L2	3	0	0	3	0
83	L3	1	0	0	1	0
83	L4	1	0	0	0	0
83	L5	2	0	0	0	0
83	M0	2	0	0	0	0
83	M3	3	0	0	0	0
83	M5	1	0	0	0	0
83	M6	3	0	0	0	0
83	M7	4	0	0	0	0
83	M9	2	0	0	0	0
83	N1	3	0	0	0	0
83	N3	3	0	0	1	0
83	N5	1	0	0	0	0
83	N6	3	0	0	0	0
83	N8	1	0	0	0	0
83	O1	5	0	0	0	0
83	O2	3	0	0	1	0
83	O4	1	0	0	1	0
83	O5	1	0	0	0	0
83	O7	4	0	0	2	0
83	O9	2	0	0	0	0
83	Q2	1	0	0	0	0
83	S6	1	0	0	0	0
83	S9	1	0	0	0	0
83	SM	1	0	0	1	0
83	c4	1	0	0	0	0
83	c6	1	0	0	0	0
83	c8	1	0	0	0	0
83	c9	4	0	0	0	0
83	d3	1	0	0	0	0
83	d6	3	0	0	0	0
83	d9	2	0	0	0	0
83	l2	4	0	0	0	0
83	l3	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	l4	3	0	0	0	0
83	l5	3	0	0	0	0
83	l9	2	0	0	0	0
83	m5	3	0	0	0	0
83	m7	3	0	0	0	0
83	m8	1	0	0	0	0
83	m9	5	0	0	0	0
83	n1	2	0	0	0	0
83	n3	3	0	0	0	0
83	n8	3	0	0	0	0
83	o1	3	0	0	0	0
83	o2	5	0	0	0	0
83	o4	4	0	0	0	0
83	o6	3	0	0	0	0
83	o7	1	0	0	0	0
83	q0	1	0	0	0	0
83	q2	1	0	0	0	0
83	sM	3	0	0	0	0
All	All	400111	0	294576	10587	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 10587 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:N7:36:HIS:C	51:N7:37:PRO:N	1.44	1.39
28:L3:41:VAL:HA	28:L3:185:GLY:HA3	1.51	1.15
2:6:780:A:H4'	2:6:781:U:H5'	1.28	1.14
2:6:1636:C:H4'	2:6:1637:C:H5'	1.32	1.07
2:2:1585:U:H3	2:2:1611:A:H2	1.04	0.99

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1355:C:O3'	1:5:3221:C:O2'[2_546]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
10	c5	126	VAL
11	C6	58	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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
37	m3	73	ARG
44	N0	61	ILE
75	s7	126	LEU
37	M3	147	ILE
41	m7	65	SER

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

Mol	Chain	Res	Type
39	M5	138	GLN
52	n8	28	HIS
79	sR	182	ASN
42	m8	58	ASN
47	N3	98	ASN

5.3.3 RNA ⓘ

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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
2	2	755	A
4	4	125	U
2	6	1097	U
2	2	913	G
2	2	1344	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 carbohydrates 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	1	3894	-	35,35,35	0.34	0	49,52,52	1.41	5 (10%)
81	8UZ	1	3892	-	35,35,35	0.44	0	49,52,52	1.35	4 (8%)
81	8UZ	5	3851	-	35,35,35	0.25	0	49,52,52	1.12	5 (10%)
81	8UZ	6	2061	-	35,35,35	0.36	0	49,52,52	1.51	7 (14%)
81	8UZ	5	3853	-	35,35,35	0.31	0	49,52,52	1.23	6 (12%)
81	8UZ	2	2030	-	35,35,35	0.26	0	49,52,52	1.21	4 (8%)
81	8UZ	1	3886	-	35,35,35	0.37	0	49,52,52	1.28	5 (10%)
81	8UZ	5	3857	-	35,35,35	0.36	0	49,52,52	0.96	3 (6%)
81	8UZ	5	3854	-	35,35,35	0.34	0	49,52,52	1.79	6 (12%)
81	8UZ	2	2031	-	35,35,35	0.37	0	49,52,52	1.02	3 (6%)
81	8UZ	1	3895	-	35,35,35	0.34	0	49,52,52	1.27	7 (14%)
81	8UZ	5	3855	-	35,35,35	0.35	0	49,52,52	1.28	8 (16%)
81	8UZ	1	3887	-	35,35,35	0.42	0	49,52,52	1.30	3 (6%)
81	8UZ	2	2029	-	35,35,35	0.36	0	49,52,52	1.36	6 (12%)
81	8UZ	7	209	-	35,35,35	0.43	0	49,52,52	1.21	6 (12%)
81	8UZ	4	220	-	35,35,35	0.54	0	49,52,52	1.56	8 (16%)
81	8UZ	3	214	-	35,35,35	0.44	0	49,52,52	1.58	7 (14%)
81	8UZ	1	3893	-	35,35,35	0.54	0	49,52,52	0.96	3 (6%)
81	8UZ	1	3890	-	35,35,35	0.35	0	49,52,52	1.32	4 (8%)
81	8UZ	1	3889	-	35,35,35	0.19	0	49,52,52	0.80	2 (4%)
81	8UZ	5	3850	-	35,35,35	0.31	0	49,52,52	1.08	3 (6%)
81	8UZ	1	3891	-	35,35,35	0.36	0	49,52,52	1.37	7 (14%)
81	8UZ	1	3888	-	35,35,35	0.33	0	49,52,52	1.05	3 (6%)
81	8UZ	5	3856	-	35,35,35	0.28	0	49,52,52	1.45	7 (14%)
81	8UZ	5	3852	-	35,35,35	0.36	0	49,52,52	1.23	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	8UZ	1	3894	-	-	3/12/72/72	0/3/3/3
81	8UZ	1	3892	-	-	4/12/72/72	0/3/3/3
81	8UZ	5	3851	-	-	4/12/72/72	0/3/3/3
81	8UZ	6	2061	-	-	5/12/72/72	0/3/3/3
81	8UZ	5	3853	-	-	6/12/72/72	0/3/3/3
81	8UZ	2	2030	-	-	5/12/72/72	0/3/3/3
81	8UZ	1	3886	-	-	4/12/72/72	0/3/3/3
81	8UZ	5	3857	-	-	7/12/72/72	0/3/3/3
81	8UZ	5	3854	-	-	5/12/72/72	0/3/3/3
81	8UZ	2	2031	-	-	3/12/72/72	0/3/3/3
81	8UZ	1	3895	-	-	7/12/72/72	0/3/3/3
81	8UZ	5	3855	-	-	6/12/72/72	0/3/3/3
81	8UZ	1	3887	-	-	9/12/72/72	0/3/3/3
81	8UZ	2	2029	-	-	10/12/72/72	0/3/3/3
81	8UZ	7	209	-	-	7/12/72/72	0/3/3/3
81	8UZ	4	220	-	-	6/12/72/72	0/3/3/3
81	8UZ	3	214	-	-	4/12/72/72	0/3/3/3
81	8UZ	1	3893	-	-	4/12/72/72	0/3/3/3
81	8UZ	1	3890	-	-	6/12/72/72	0/3/3/3
81	8UZ	1	3889	-	-	1/12/72/72	0/3/3/3
81	8UZ	5	3850	-	-	3/12/72/72	0/3/3/3
81	8UZ	1	3891	-	-	8/12/72/72	0/3/3/3
81	8UZ	1	3888	-	-	7/12/72/72	0/3/3/3
81	8UZ	5	3856	-	-	5/12/72/72	0/3/3/3
81	8UZ	5	3852	-	-	3/12/72/72	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(°)	Ideal(°)
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	3	214	8UZ	N-C-C1-O
81	3	214	8UZ	C15-C2-O1-C3
81	2	2029	8UZ	N-C-C1-C17
81	2	2029	8UZ	N-C-C1-O
81	2	2029	8UZ	C15-C2-O1-C3

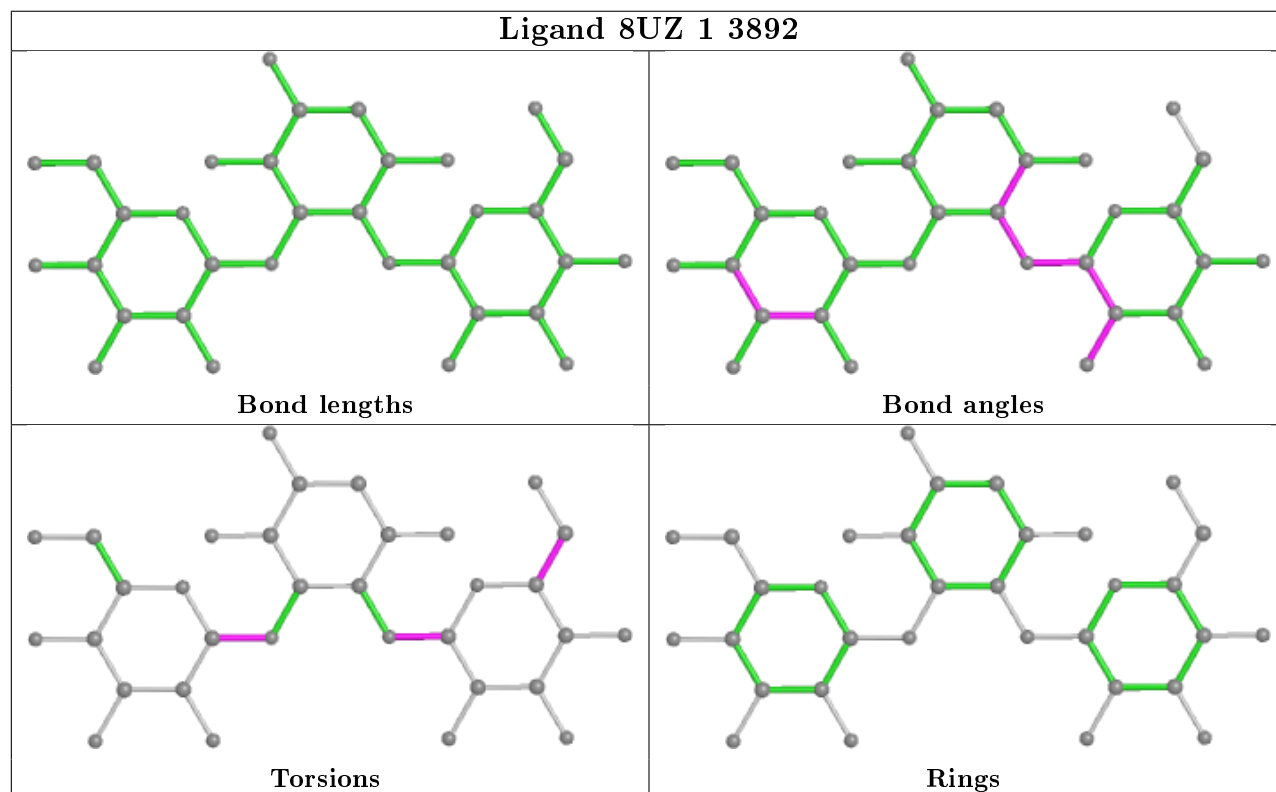
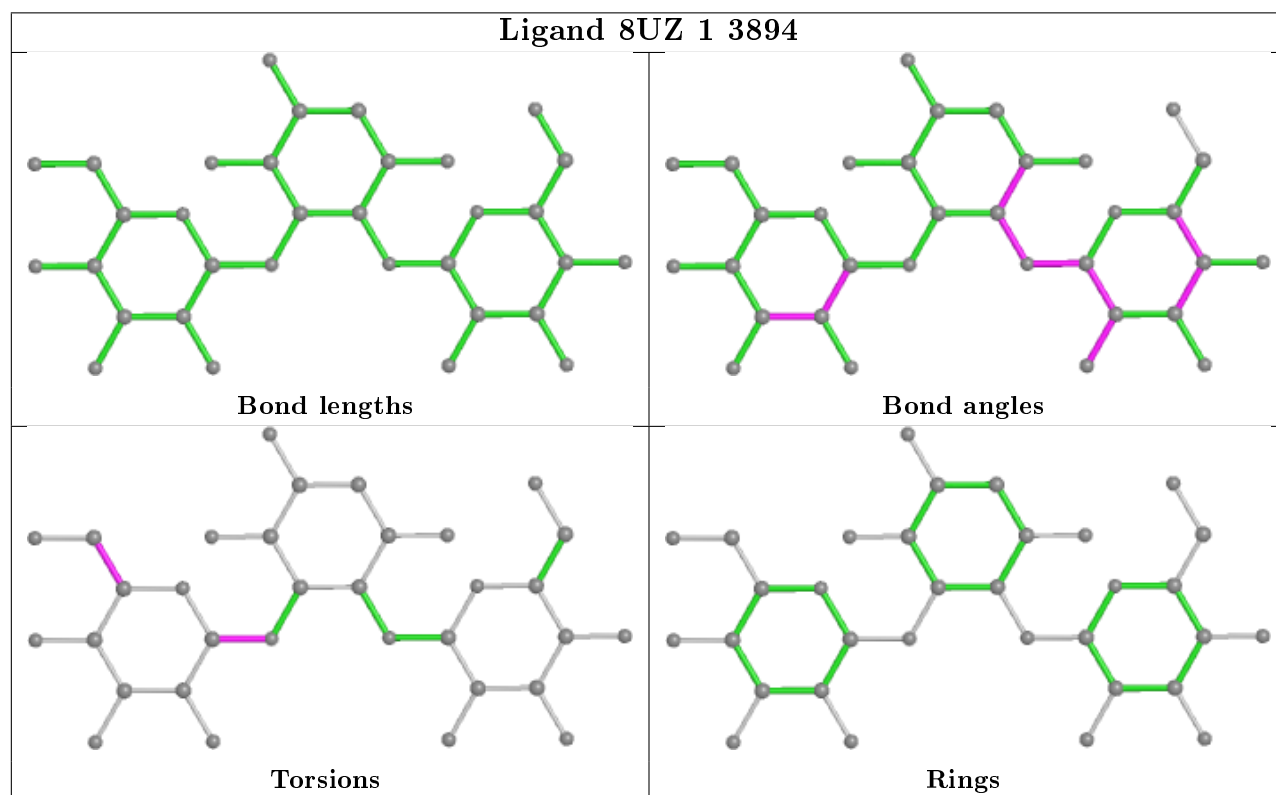
There are no ring outliers.

21 monomers are involved in 48 short contacts:

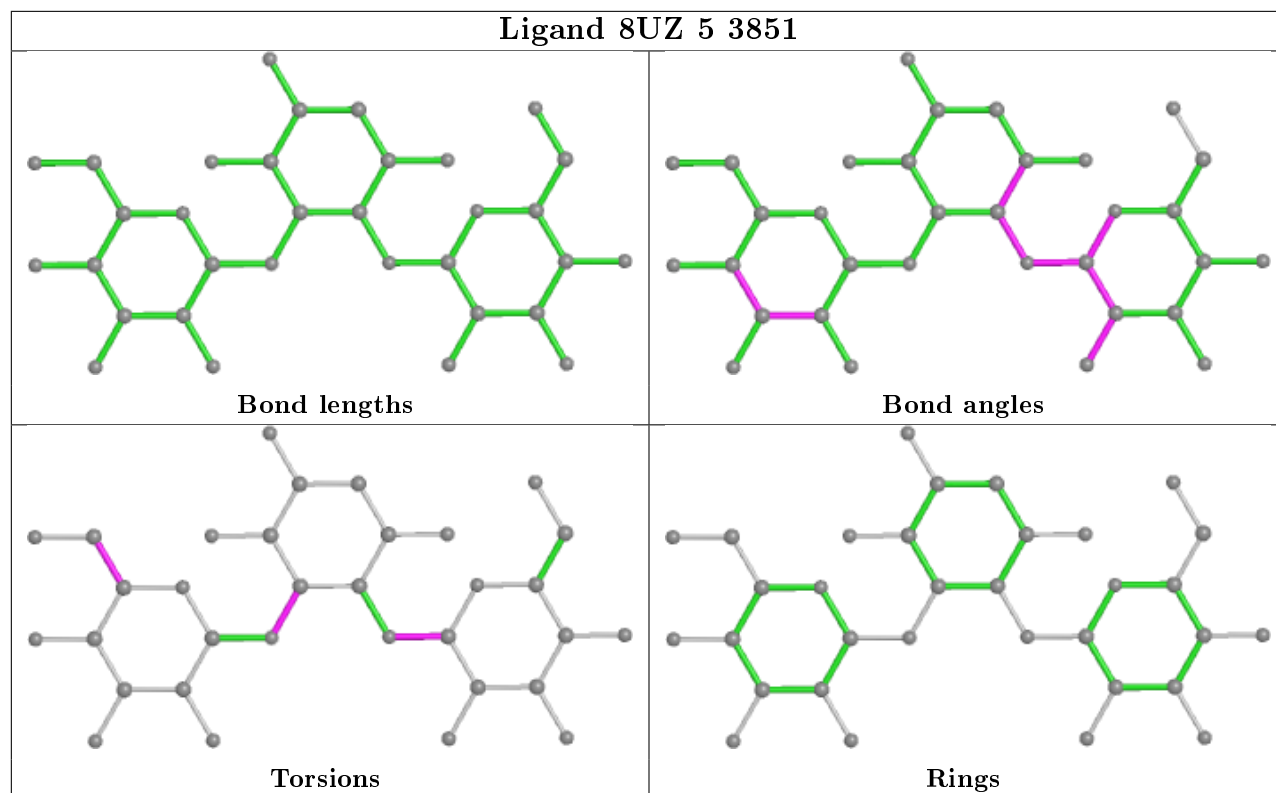
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	1	3894	8UZ	2	0
81	1	3892	8UZ	2	0
81	5	3851	8UZ	2	0
81	6	2061	8UZ	1	0
81	5	3853	8UZ	2	0
81	2	2030	8UZ	3	0
81	1	3886	8UZ	1	0
81	5	3857	8UZ	1	0
81	5	3854	8UZ	1	0
81	1	3895	8UZ	2	0
81	5	3855	8UZ	5	0
81	1	3887	8UZ	3	0
81	2	2029	8UZ	2	0
81	7	209	8UZ	2	0
81	4	220	8UZ	2	0
81	3	214	8UZ	6	0
81	1	3893	8UZ	4	0
81	1	3890	8UZ	1	0
81	1	3889	8UZ	1	0
81	1	3888	8UZ	4	0
81	5	3852	8UZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

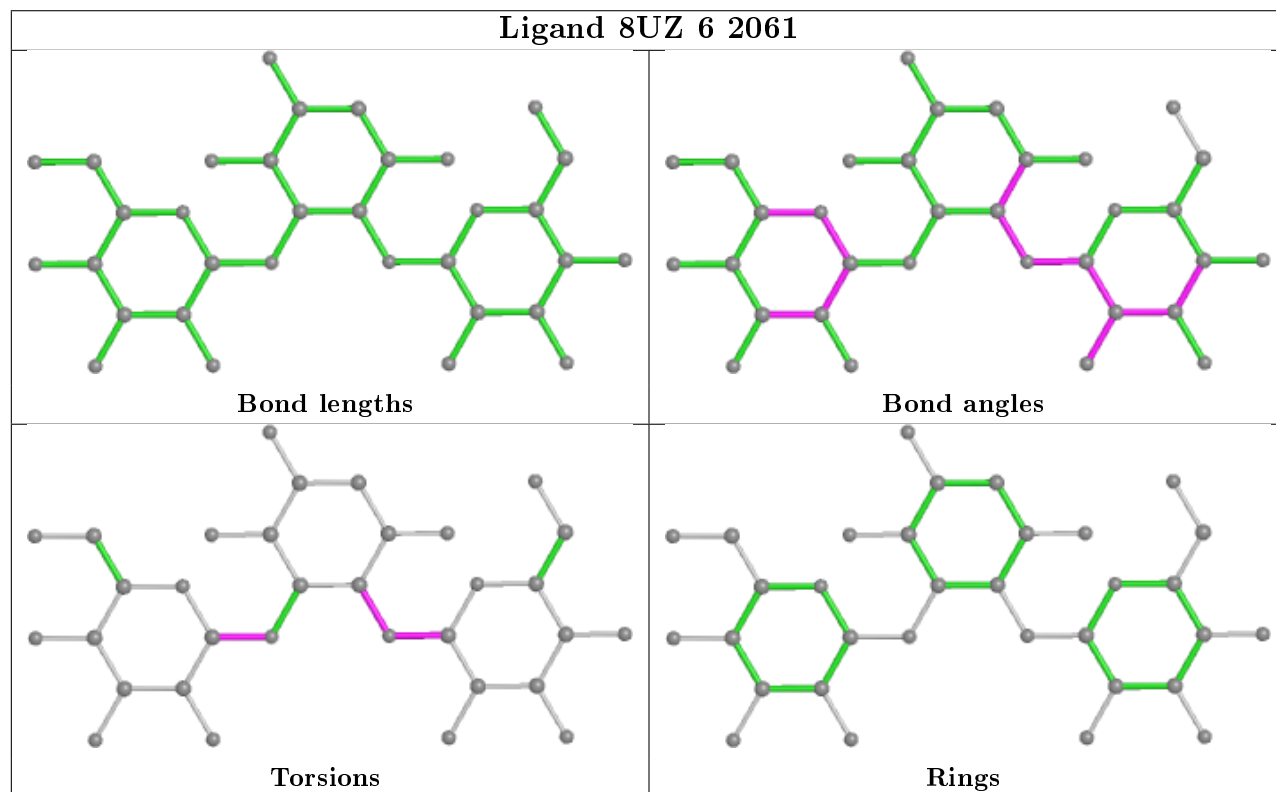
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

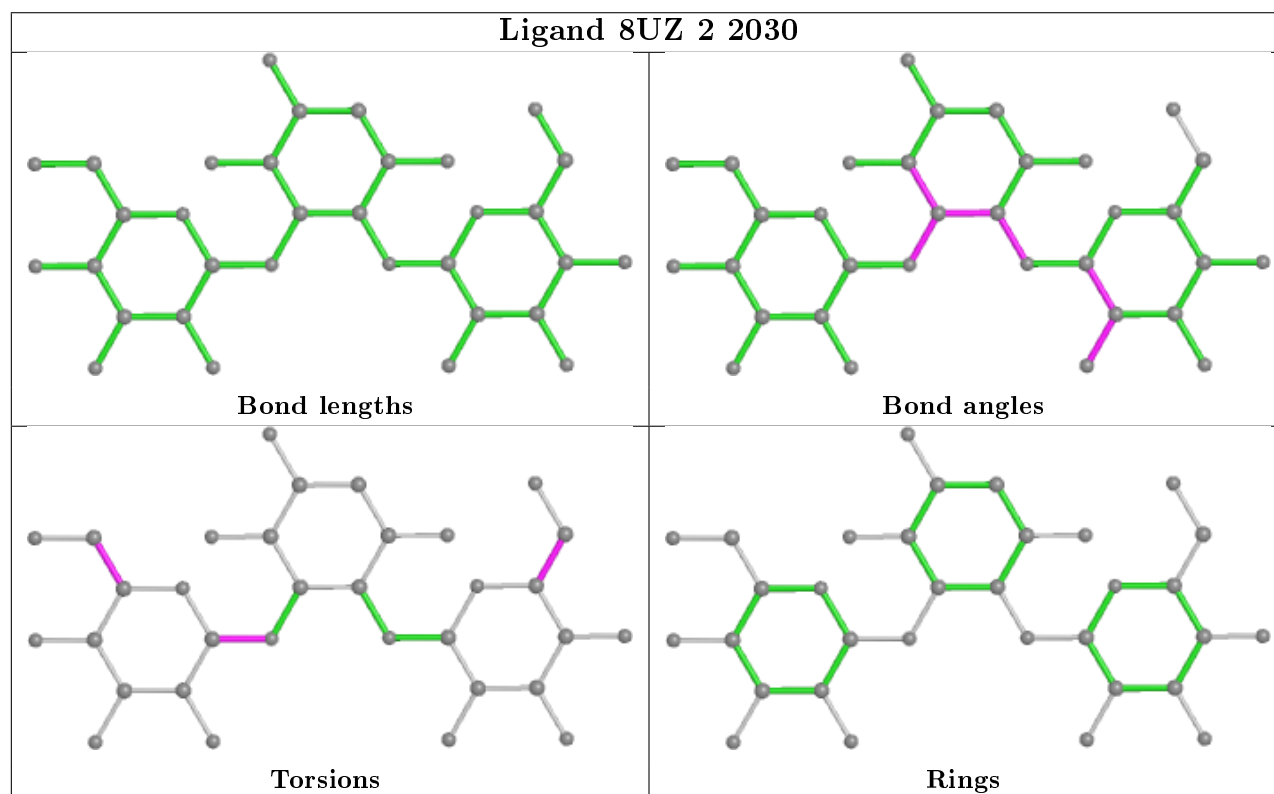
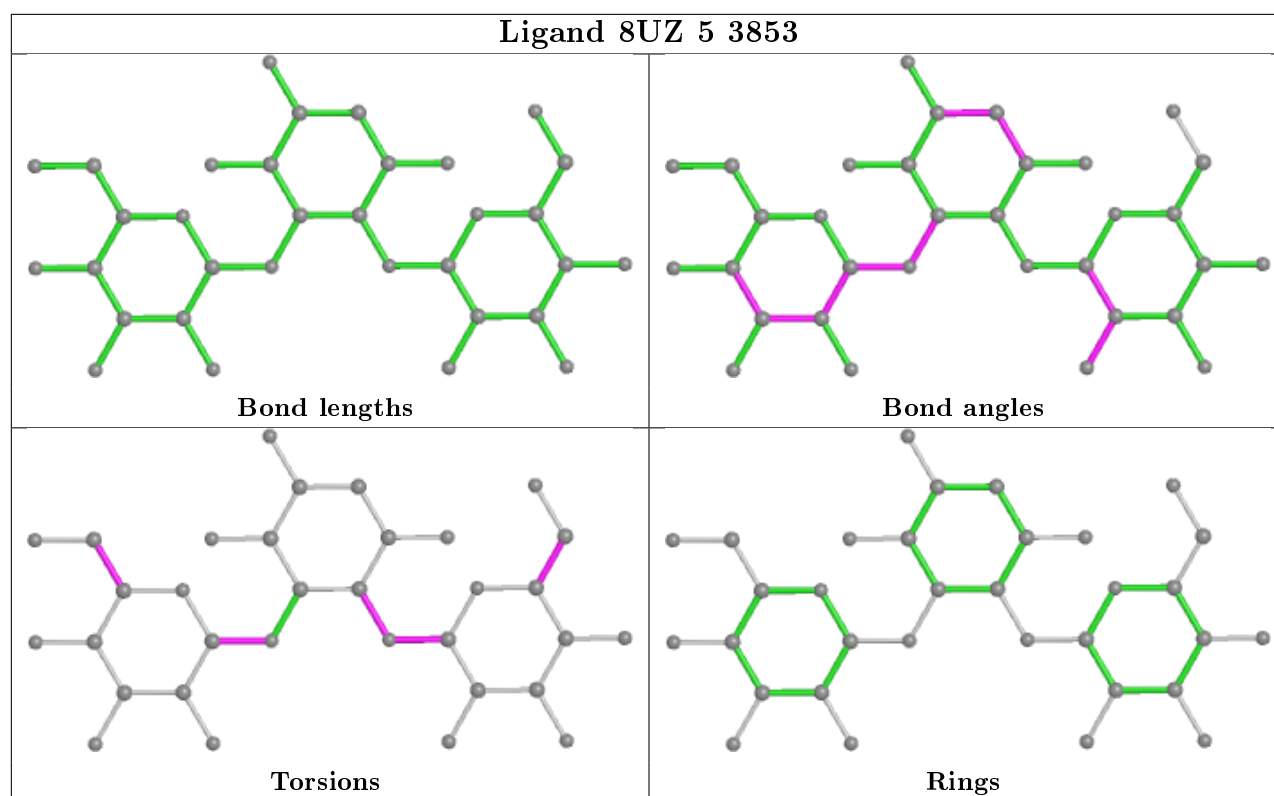


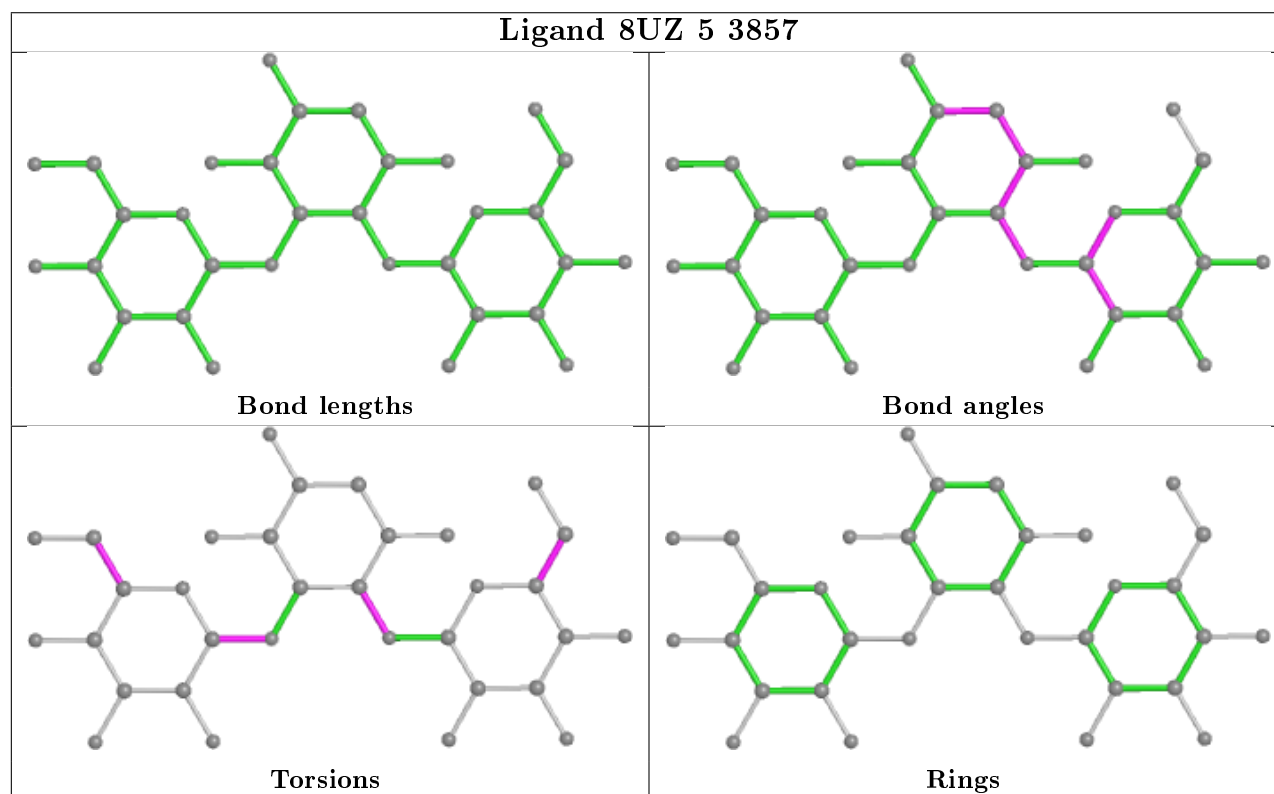
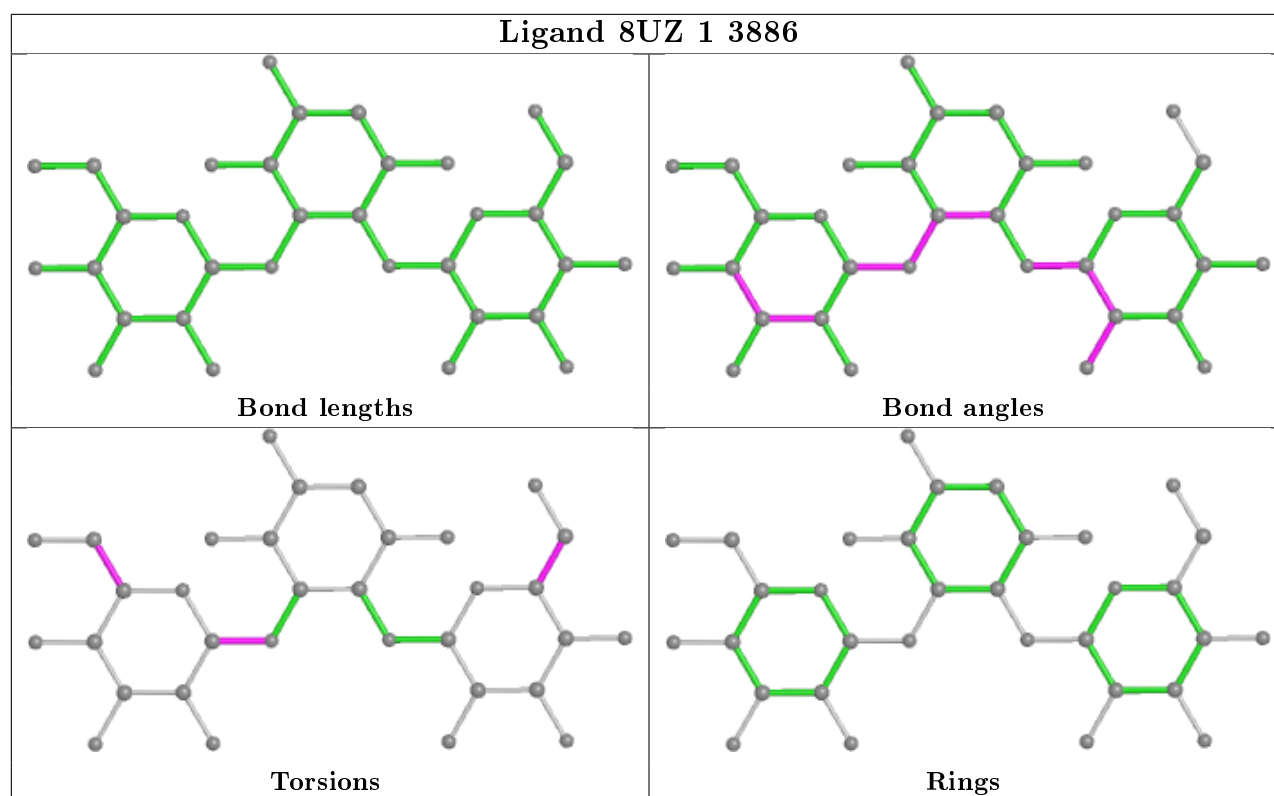
Ligand 8UZ 5 3851

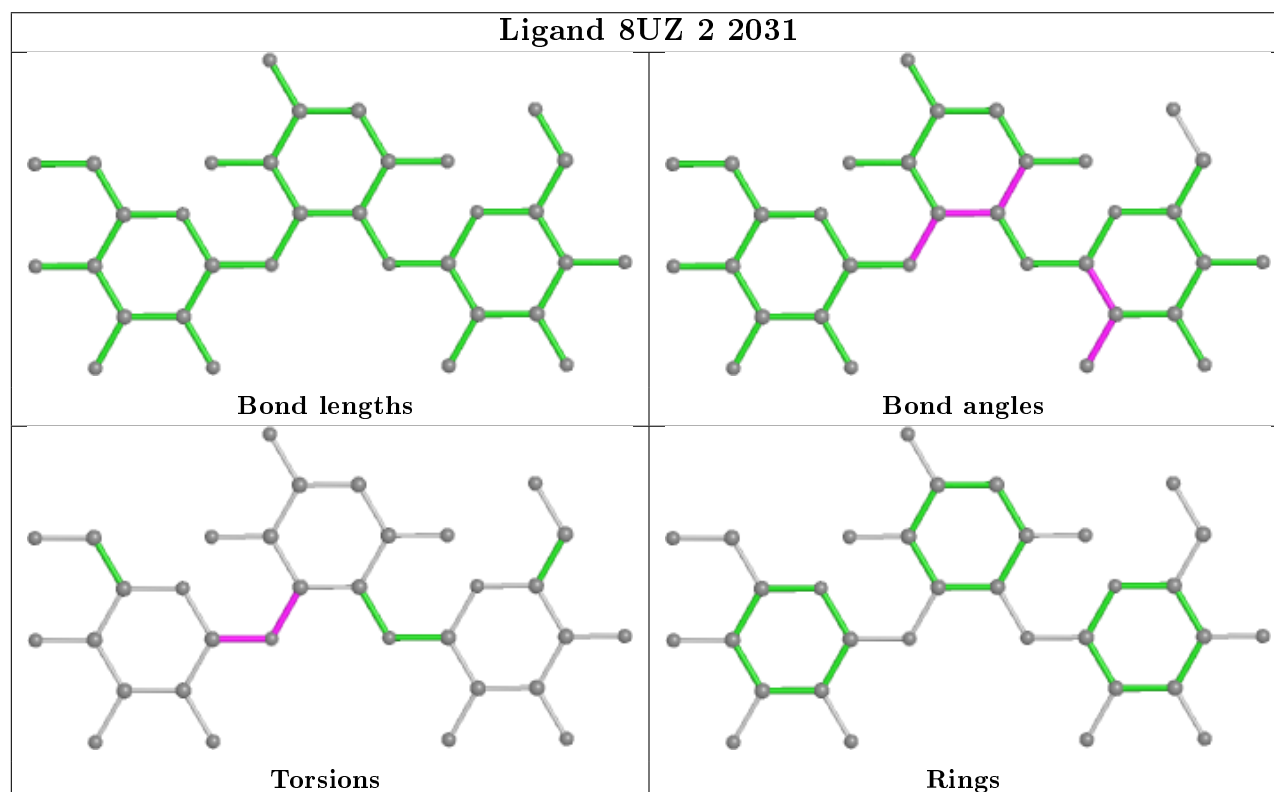
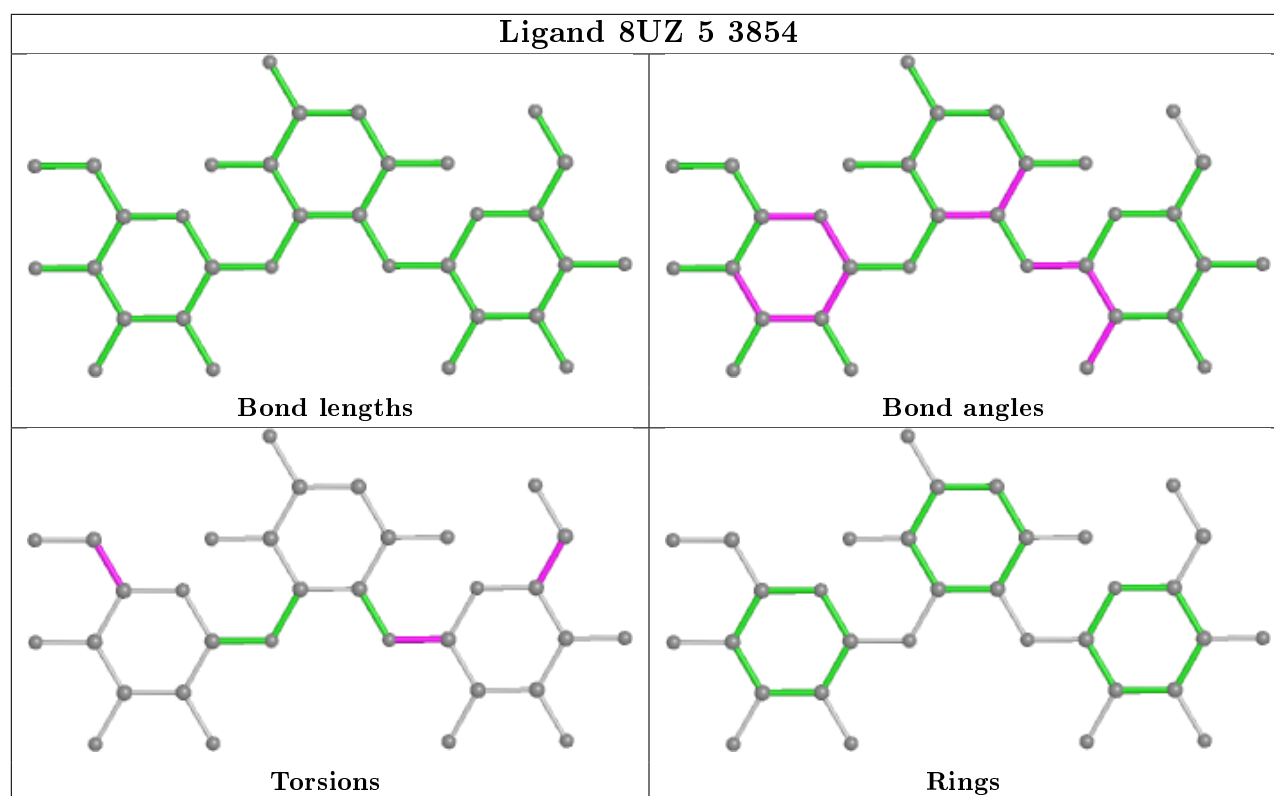


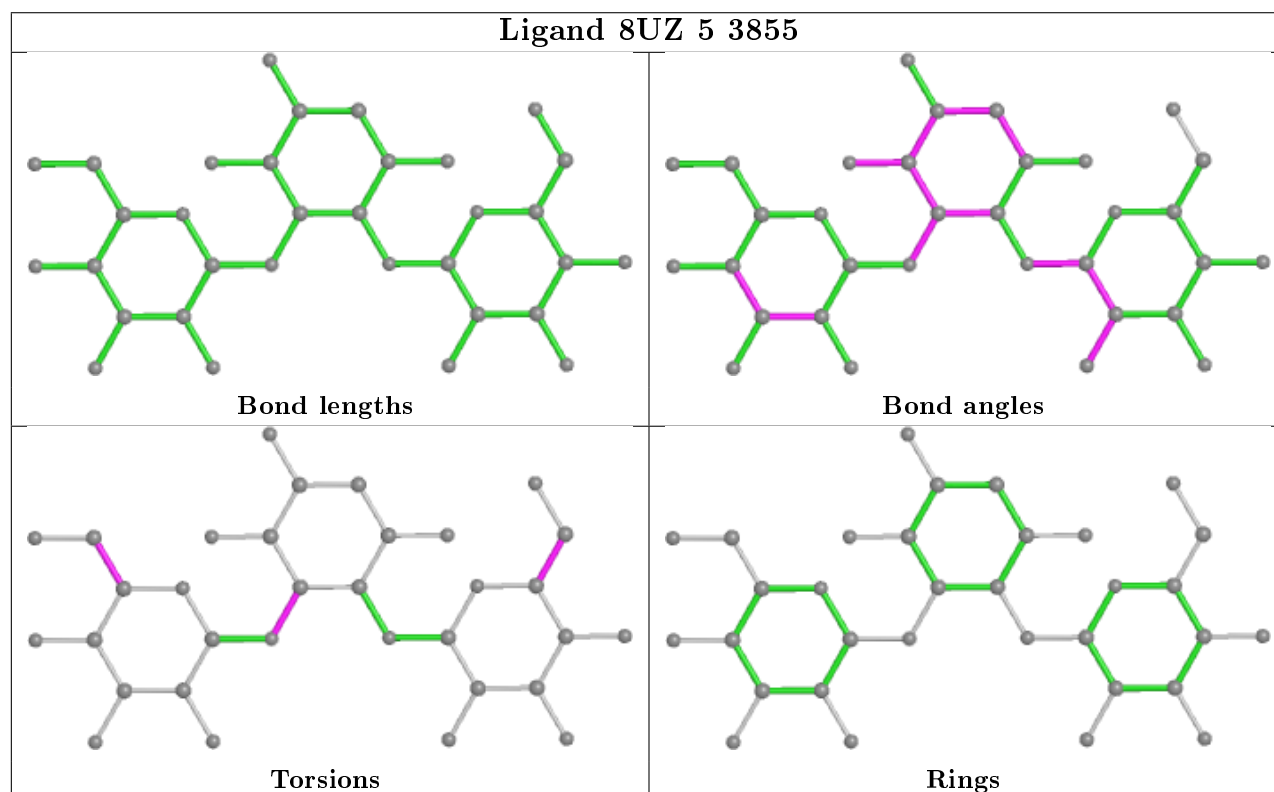
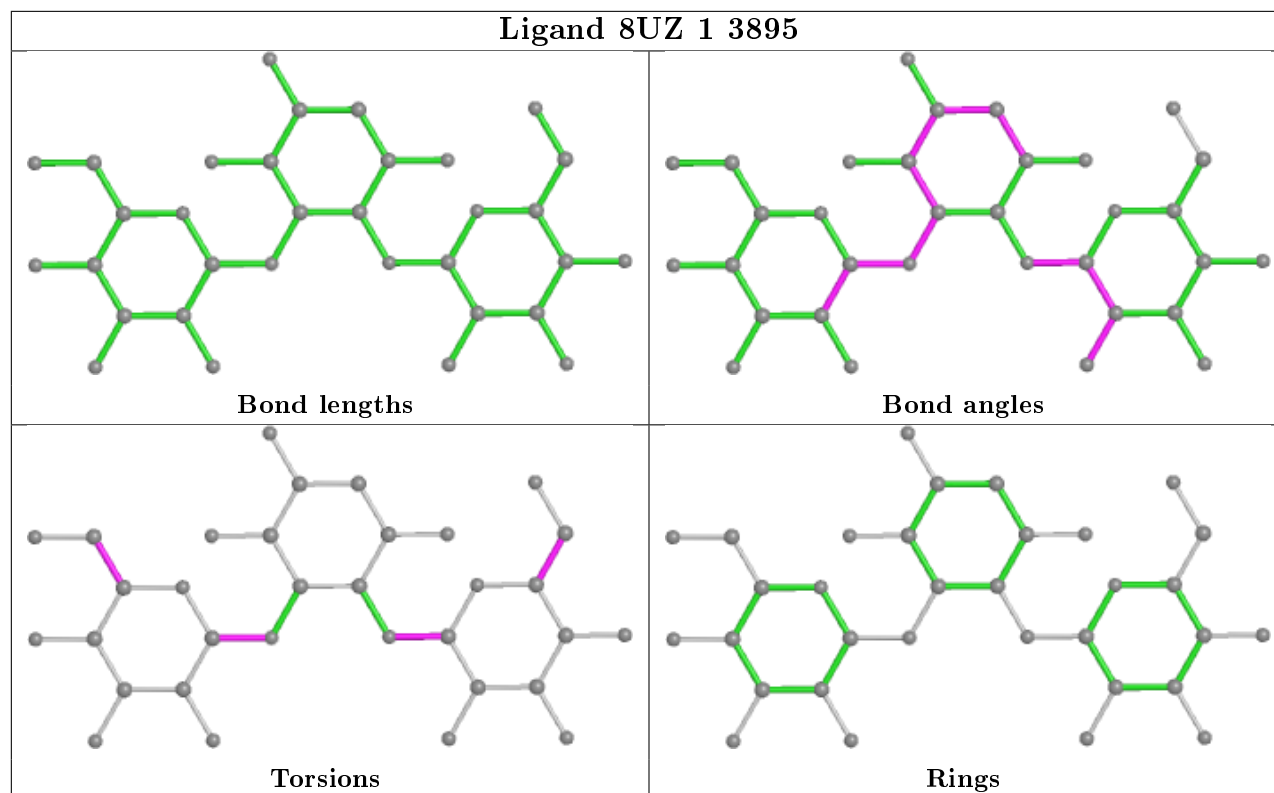
Ligand 8UZ 6 2061

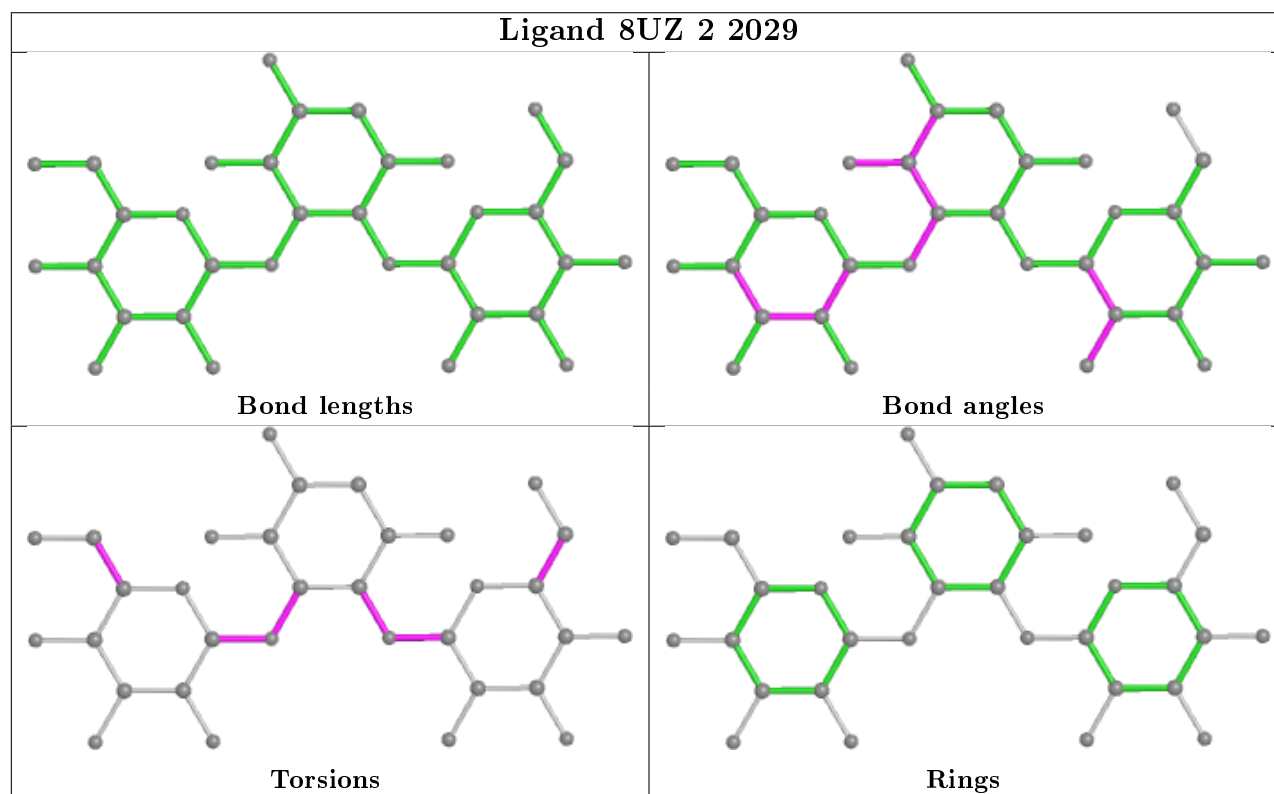
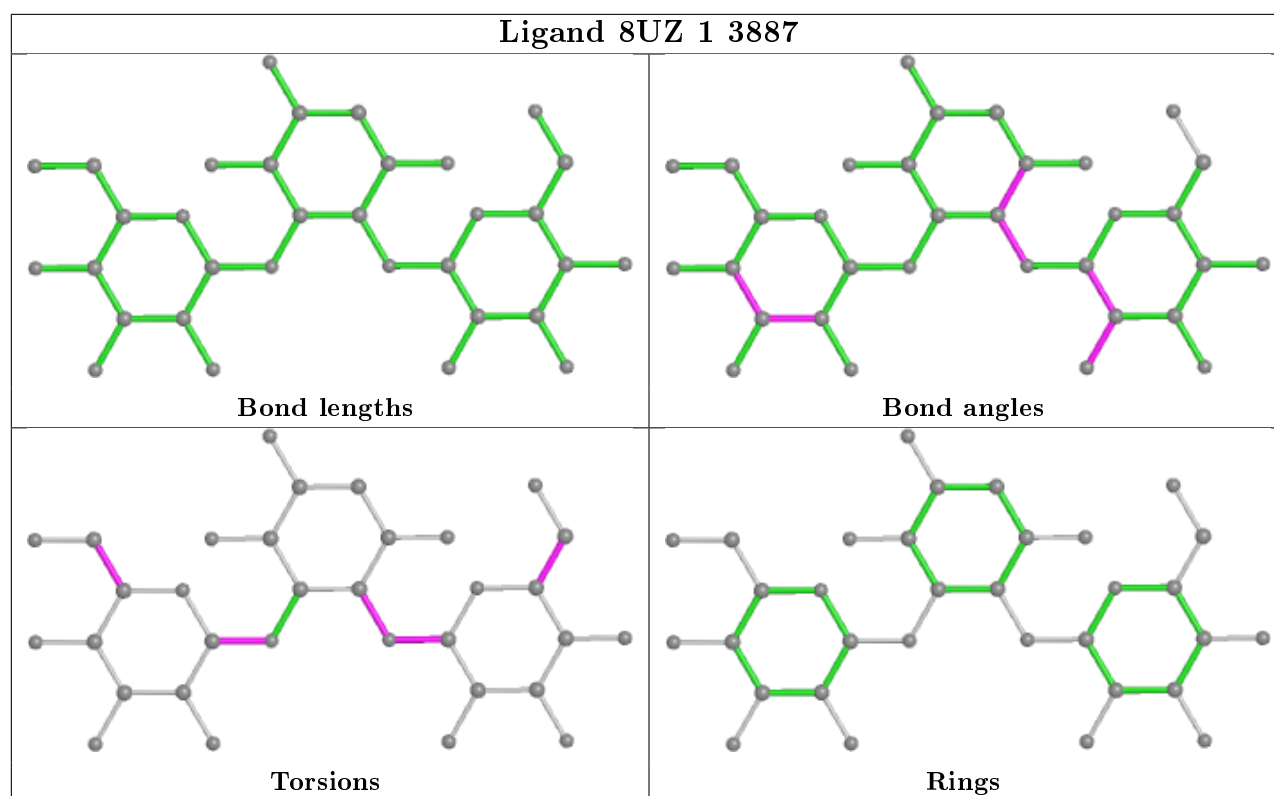




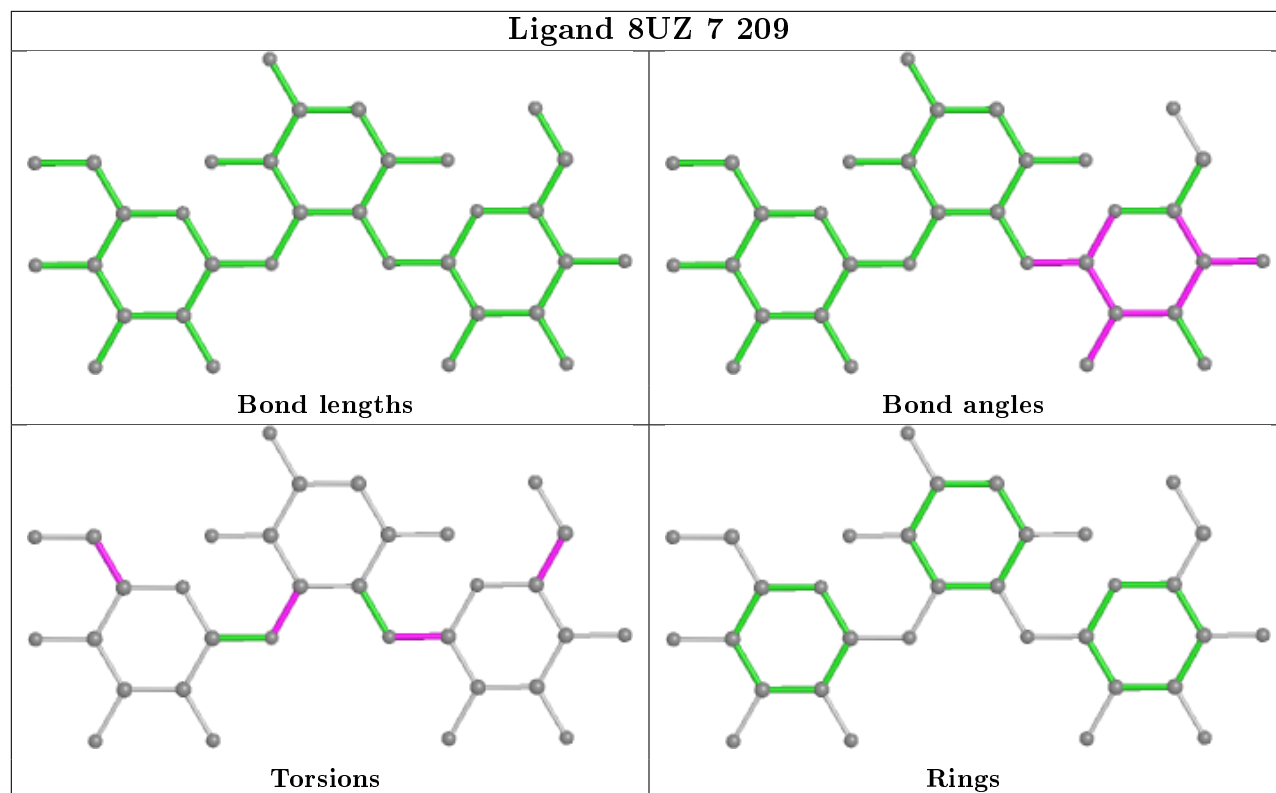




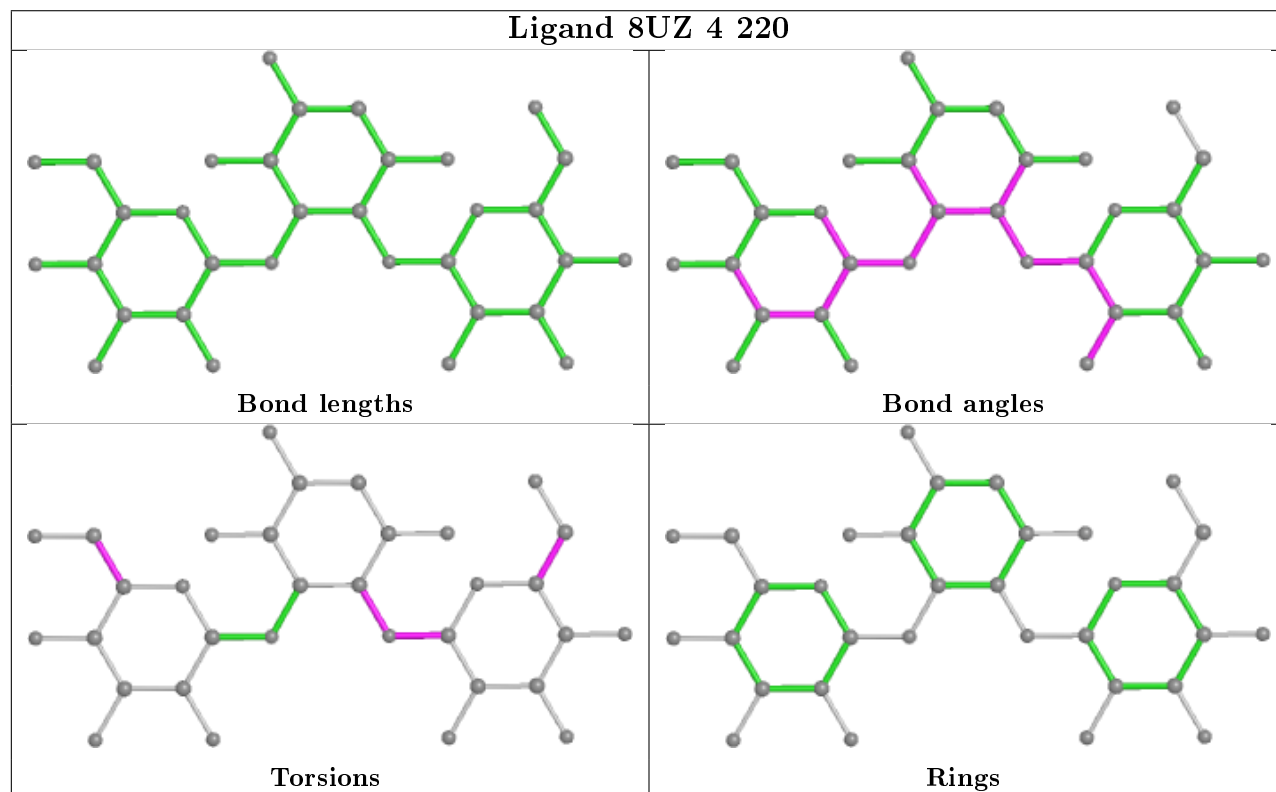




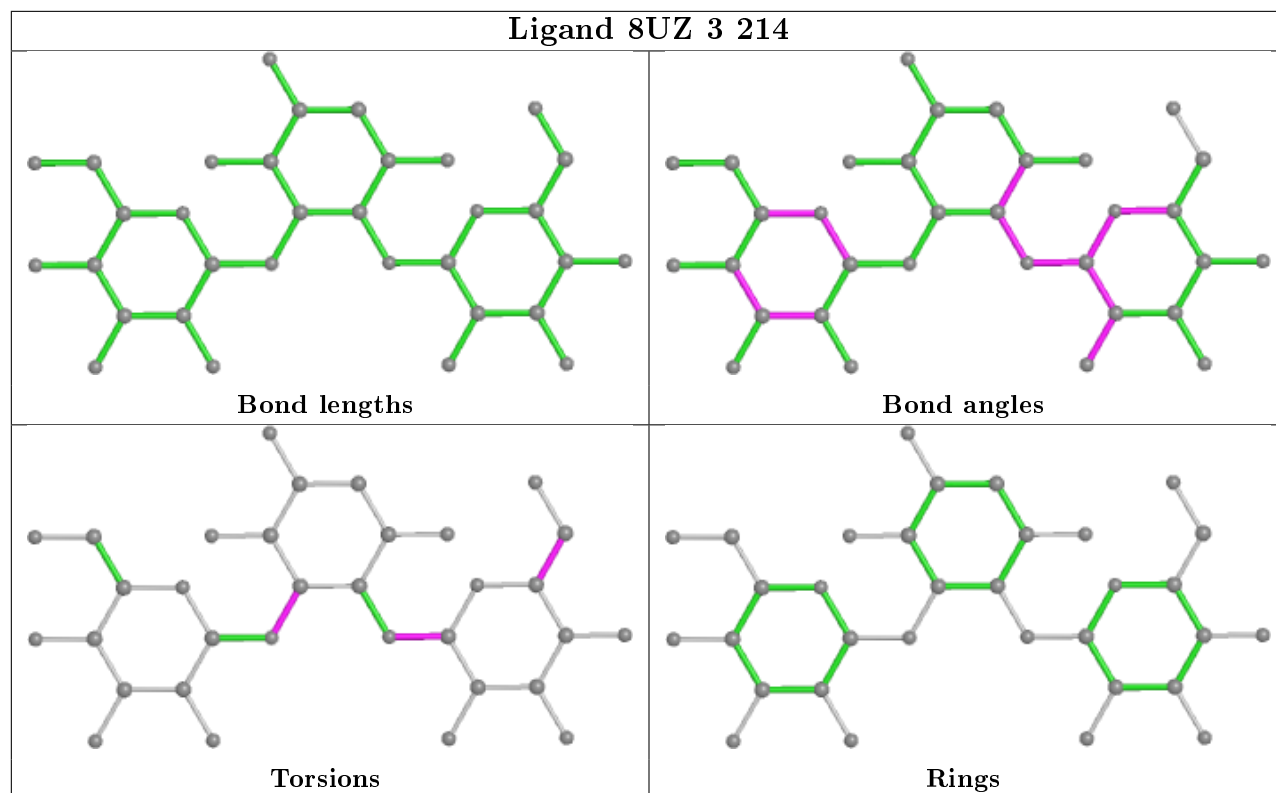
Ligand 8UZ 7 209



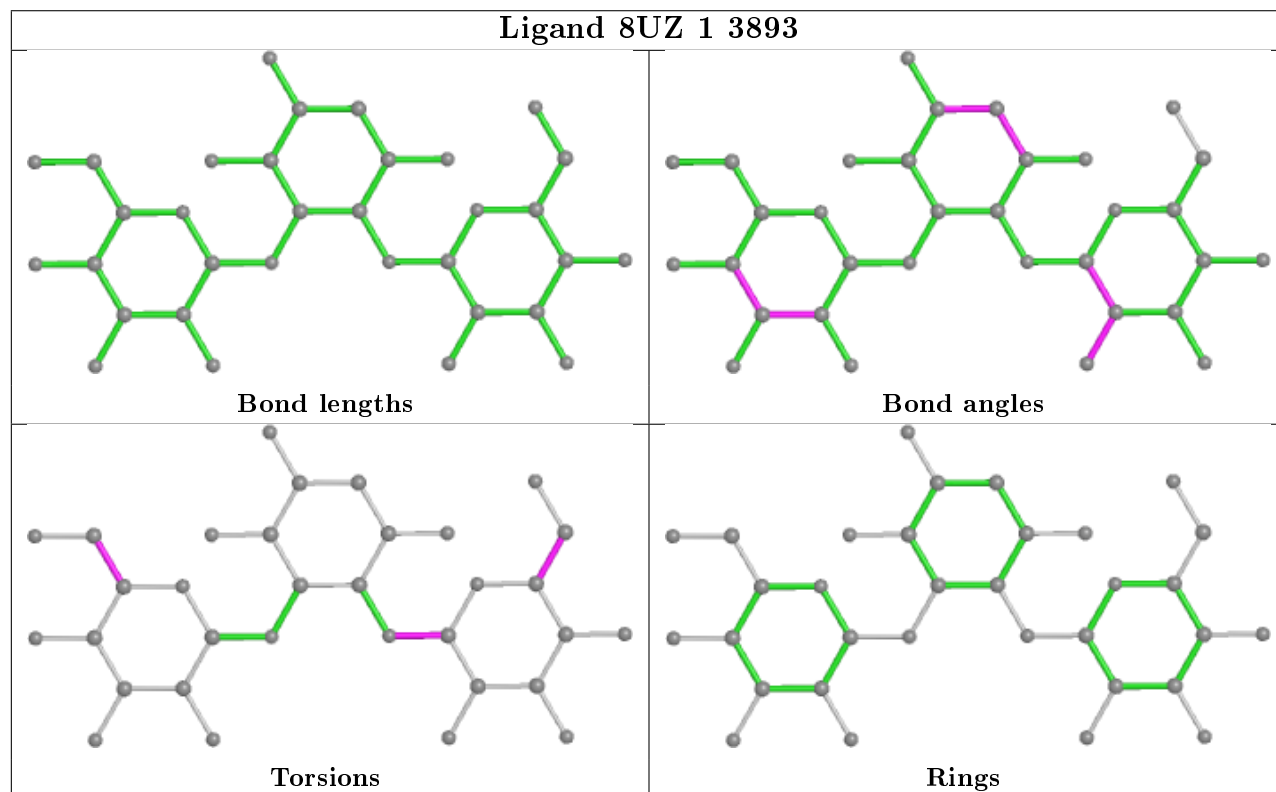
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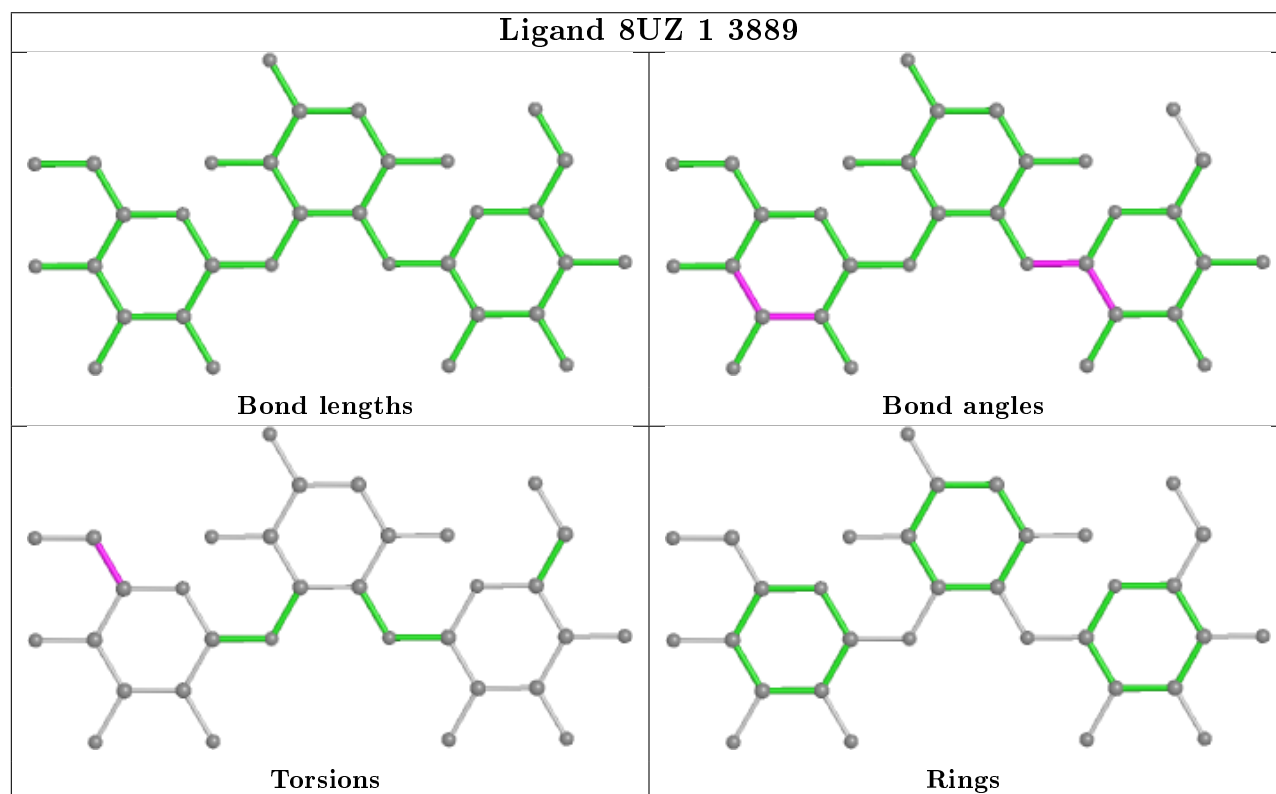
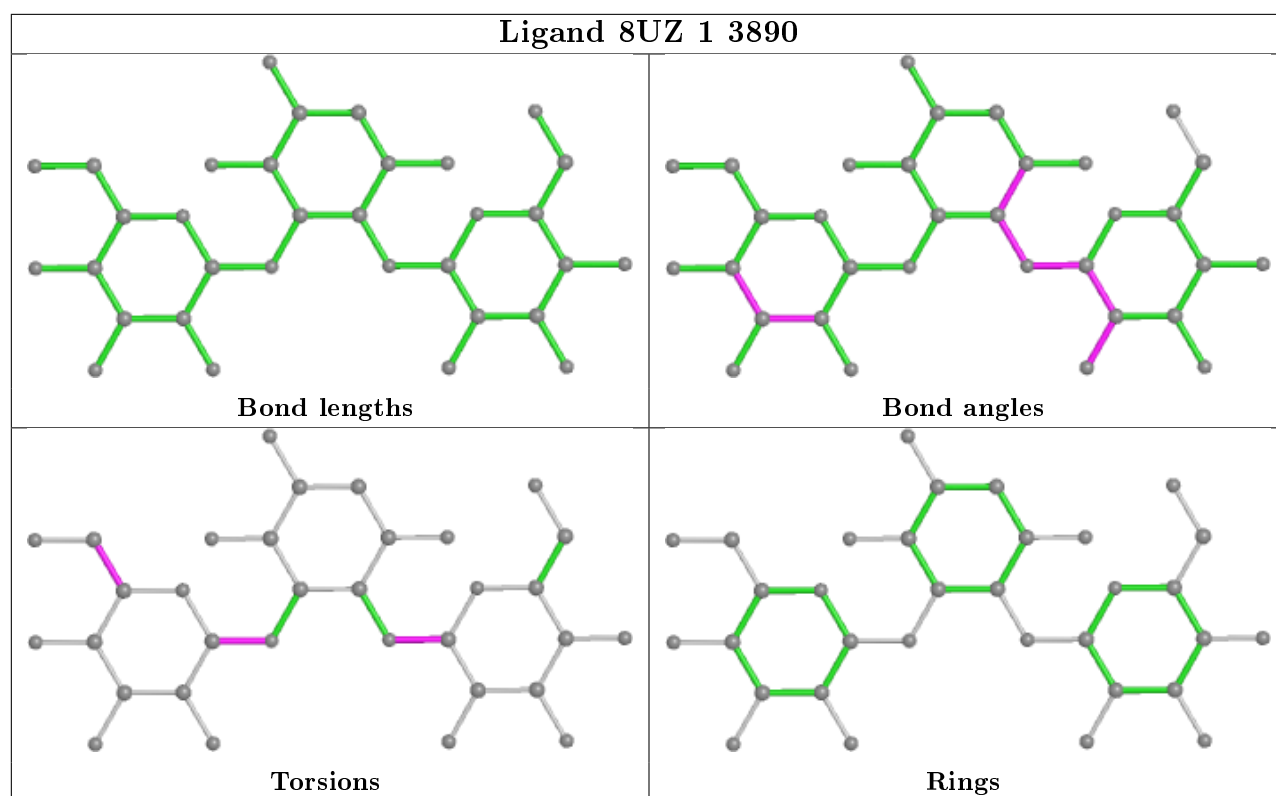


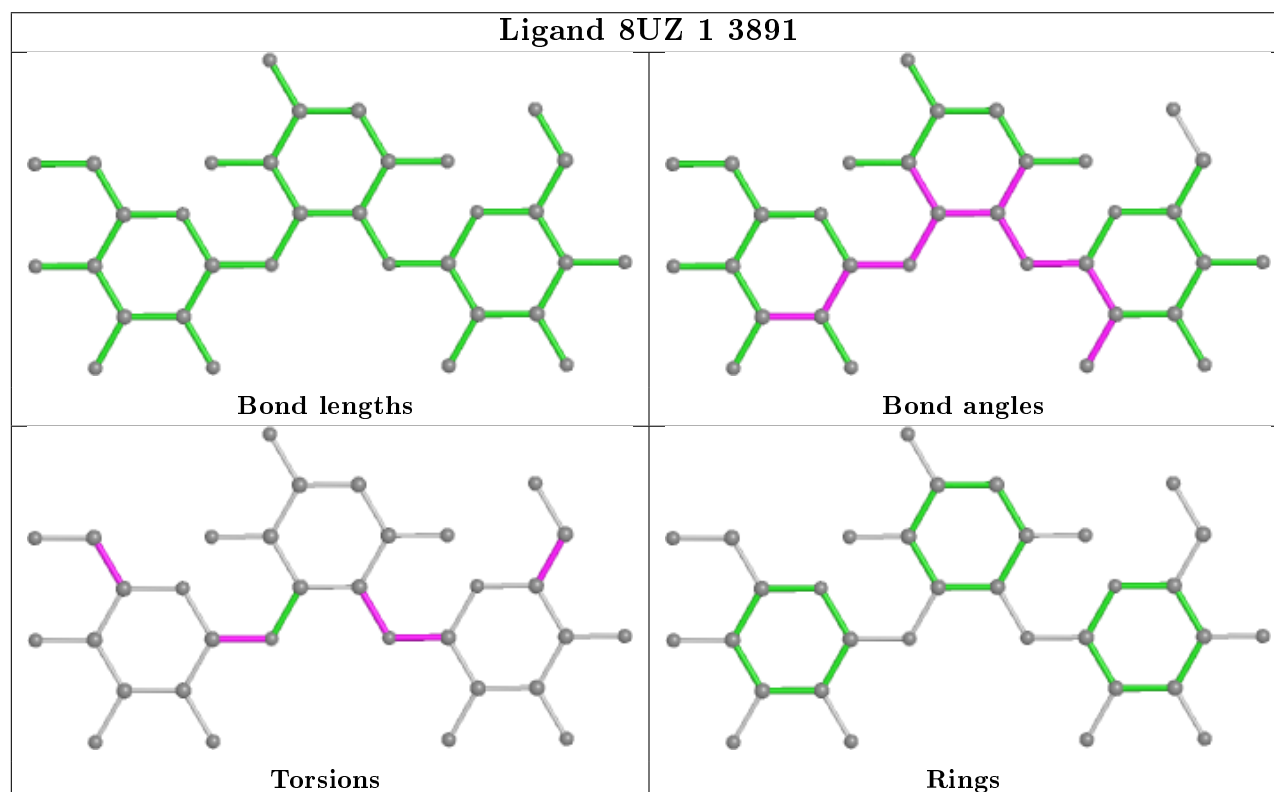
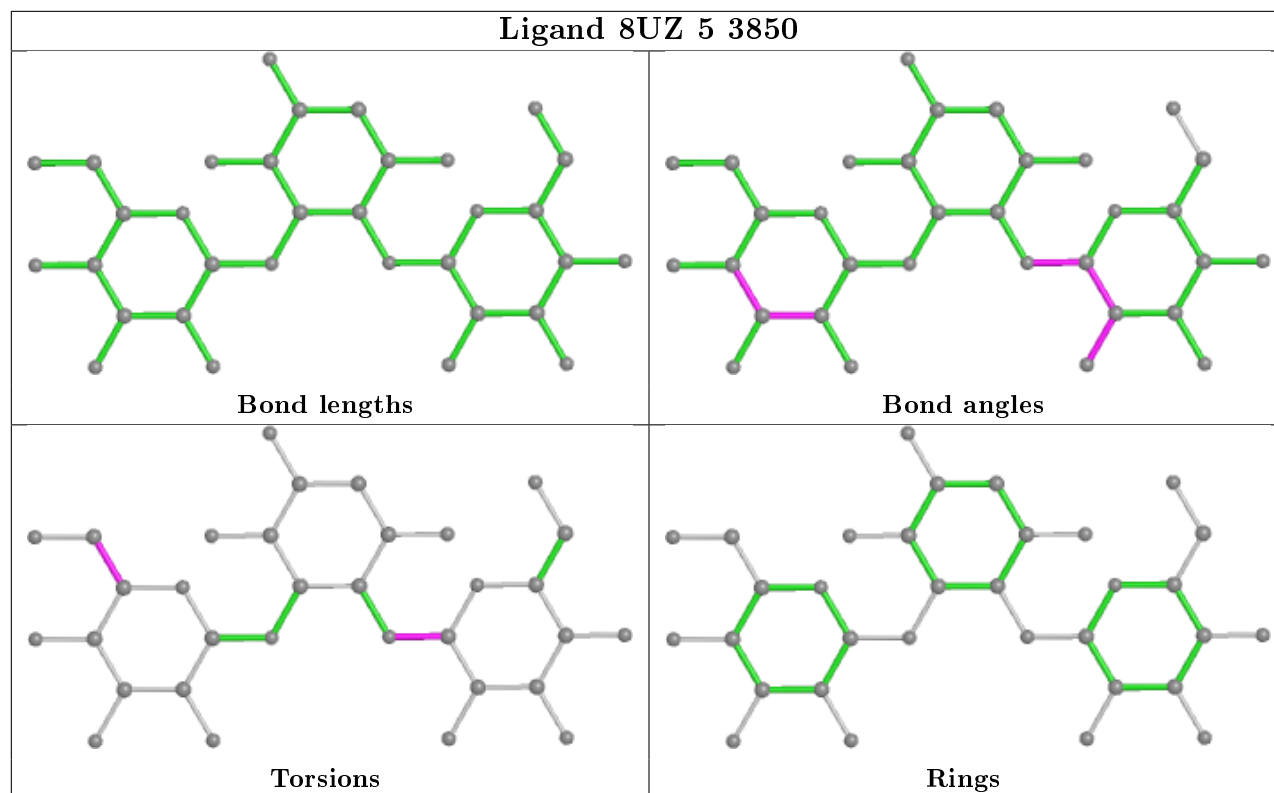
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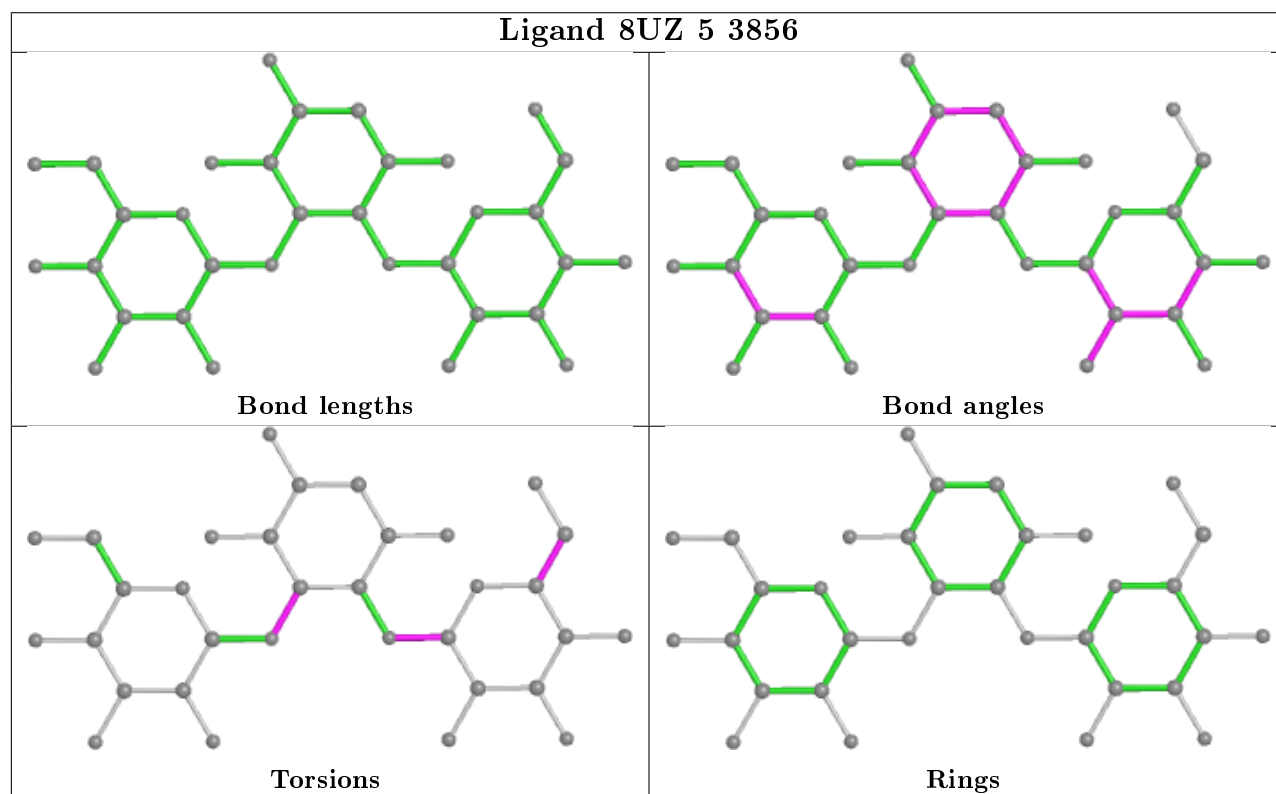
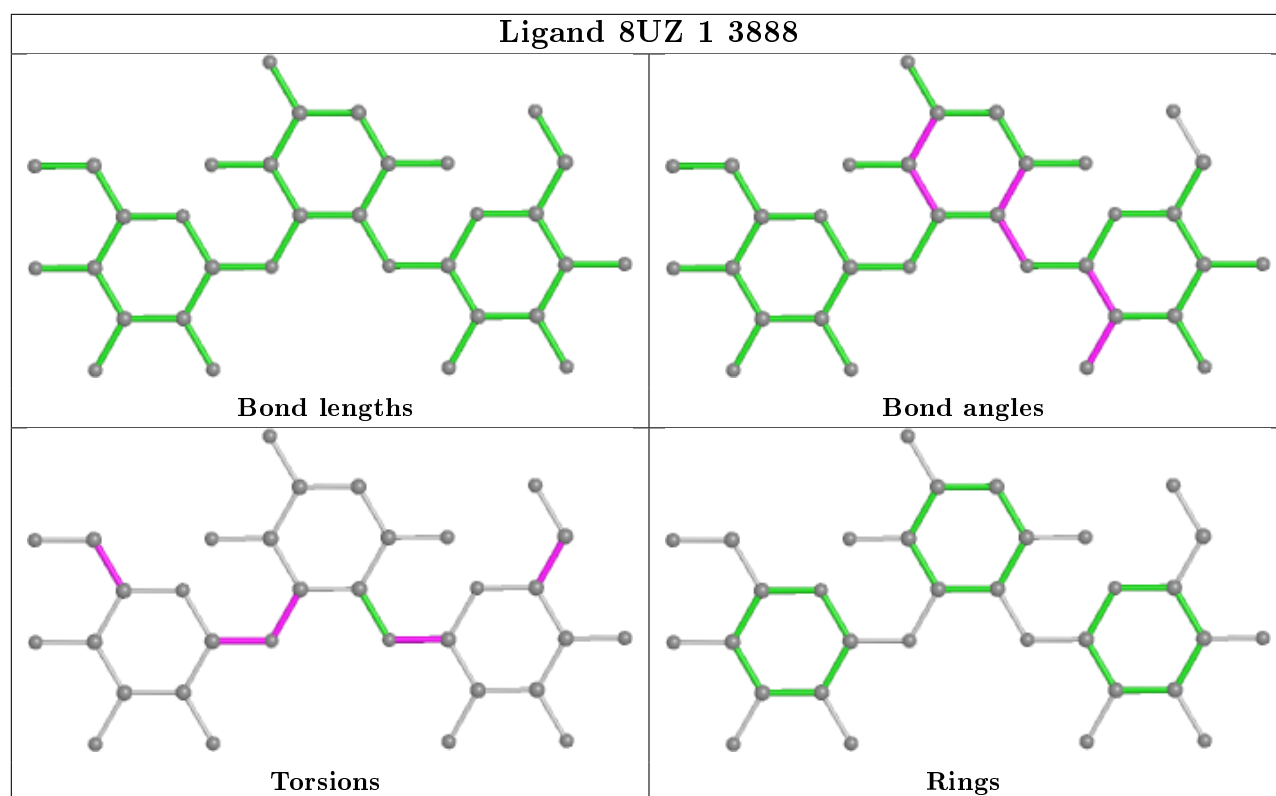


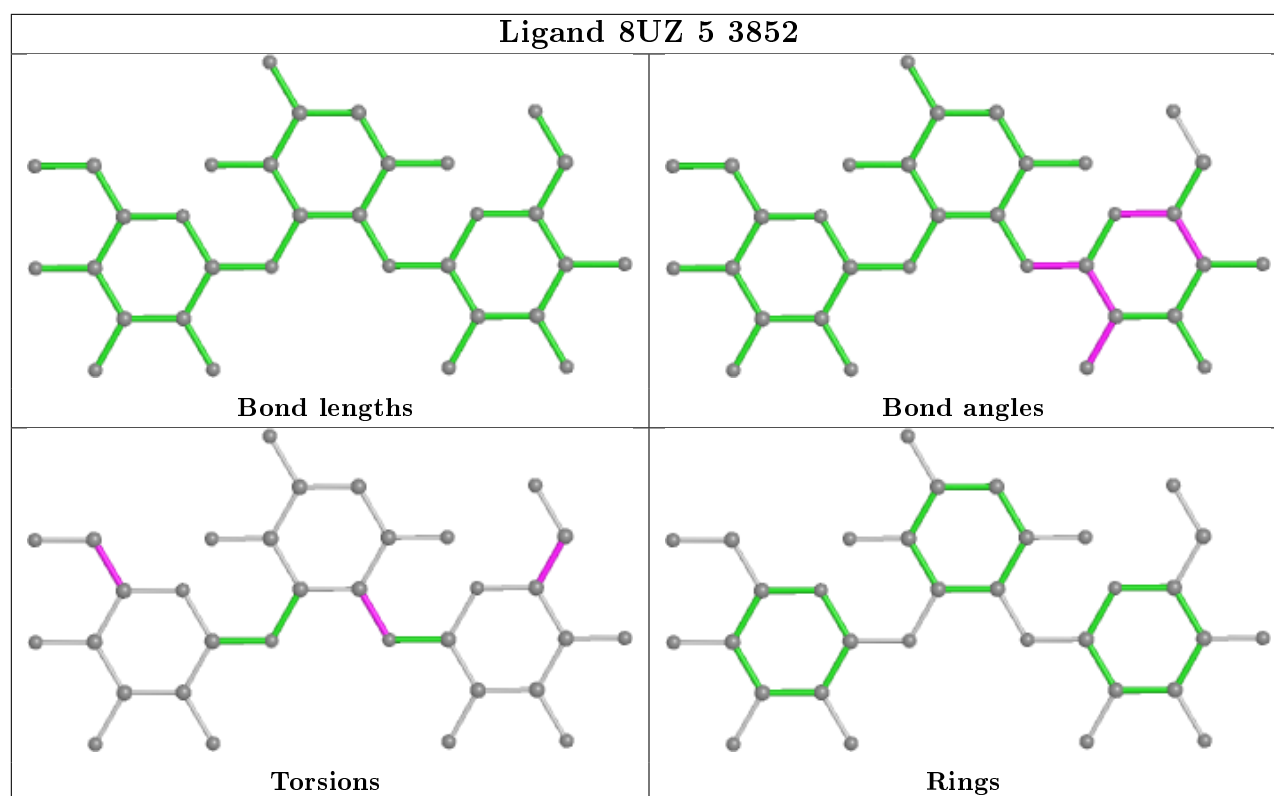
Ligand 8UZ 1 3893











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
78	sM	1
50	n6	1
37	M3	1
51	n7	1
1	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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, 251	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, 125, 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	81, 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, 101, 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, 153	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	6	2054	1/1	0.19	0.42	153,153,153,153	0
80	MG	1	3469	1/1	0.24	0.29	104,104,104,104	0
80	MG	1	3737	1/1	0.27	1.02	121,121,121,121	0
80	MG	6	1921	1/1	0.34	0.55	128,128,128,128	0
80	MG	1	3703	1/1	0.35	0.33	108,108,108,108	0
80	MG	5	3598	1/1	0.35	0.51	95,95,95,95	0
80	MG	8	205	1/1	0.42	0.29	102,102,102,102	0
80	MG	5	3603	1/1	0.46	0.53	112,112,112,112	0
80	MG	4	203	1/1	0.47	0.67	108,108,108,108	0
80	MG	7	205	1/1	0.53	0.09	170,170,170,170	0
80	MG	O2	201	1/1	0.54	0.38	84,84,84,84	0
80	MG	1	3441	1/1	0.54	0.86	142,142,142,142	0
80	MG	2	1999	1/1	0.56	0.13	150,150,150,150	0
80	MG	1	3431	1/1	0.56	0.85	87,87,87,87	0
80	MG	1	3856	1/1	0.56	0.41	94,94,94,94	0
80	MG	1	3761	1/1	0.57	0.67	80,80,80,80	0
80	MG	5	3843	1/1	0.58	0.77	89,89,89,89	0
80	MG	6	1989	1/1	0.59	0.35	131,131,131,131	0
80	MG	5	3431	1/1	0.62	1.06	79,79,79,79	0
80	MG	6	1972	1/1	0.62	0.17	134,134,134,134	0
80	MG	2	1989	1/1	0.64	0.23	150,150,150,150	0
80	MG	2	2017	1/1	0.65	0.18	165,165,165,165	0
80	MG	1	3664	1/1	0.66	0.47	102,102,102,102	0
80	MG	4	206	1/1	0.69	0.78	82,82,82,82	0
80	MG	2	1995	1/1	0.69	0.24	126,126,126,126	0
80	MG	5	3650	1/1	0.70	0.78	92,92,92,92	0
80	MG	2	1944	1/1	0.70	1.09	96,96,96,96	0
80	MG	1	3713	1/1	0.70	0.56	96,96,96,96	0
80	MG	6	1968	1/1	0.71	0.09	150,150,150,150	0
80	MG	1	3461	1/1	0.71	0.80	96,96,96,96	0
80	MG	1	3814	1/1	0.71	0.28	104,104,104,104	0
80	MG	1	3544	1/1	0.75	1.17	79,79,79,79	0
80	MG	5	3829	1/1	0.75	1.48	88,88,88,88	0
80	MG	5	3697	1/1	0.77	1.23	98,98,98,98	0
80	MG	1	3808	1/1	0.79	0.27	112,112,112,112	1
82	ZN	e1	501	1/1	0.79	0.06	268,268,268,268	0
80	MG	5	3473	1/1	0.80	0.14	139,139,139,139	0
80	MG	5	3445	1/1	0.80	0.62	77,77,77,77	0
80	MG	1	3609	1/1	0.80	1.07	98,98,98,98	0
80	MG	2	1988	1/1	0.80	0.12	148,148,148,148	0
80	MG	5	3820	1/1	0.81	0.19	130,130,130,130	0
80	MG	1	3655	1/1	0.81	0.25	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3605	1/1	0.81	0.17	136,136,136,136	0
80	MG	1	3685	1/1	0.82	0.62	77,77,77,77	0
80	MG	1	3524	1/1	0.82	0.28	114,114,114,114	0
80	MG	6	1973	1/1	0.82	0.12	136,136,136,136	0
80	MG	6	1988	1/1	0.82	0.13	130,130,130,130	0
80	MG	1	3669	1/1	0.82	0.23	115,115,115,115	0
80	MG	5	3778	1/1	0.82	0.19	134,134,134,134	1
80	MG	2	2005	1/1	0.83	0.39	145,145,145,145	0
80	MG	5	3621	1/1	0.83	0.37	81,81,81,81	0
80	MG	L3	401	1/1	0.83	0.31	74,74,74,74	0
80	MG	5	3439	1/1	0.83	0.41	86,86,86,86	0
80	MG	1	3800	1/1	0.83	0.24	107,107,107,107	1
80	MG	1	3718	1/1	0.83	0.49	82,82,82,82	0
80	MG	6	2042	1/1	0.84	0.24	119,119,119,119	0
80	MG	2	1994	1/1	0.84	0.06	174,174,174,174	0
80	MG	6	2051	1/1	0.84	0.11	163,163,163,163	0
80	MG	6	2010	1/1	0.84	0.28	166,166,166,166	0
80	MG	1	3751	1/1	0.85	0.57	71,71,71,71	0
80	MG	5	3737	1/1	0.85	0.26	102,102,102,102	0
80	MG	1	3711	1/1	0.85	0.44	82,82,82,82	0
80	MG	1	3783	1/1	0.85	0.30	95,95,95,95	0
80	MG	3	206	1/1	0.85	0.22	123,123,123,123	0
80	MG	5	3760	1/1	0.85	0.34	96,96,96,96	0
80	MG	5	3519	1/1	0.85	0.66	111,111,111,111	0
80	MG	5	3613	1/1	0.85	0.14	144,144,144,144	0
80	MG	6	2016	1/1	0.85	0.20	137,137,137,137	0
80	MG	1	3822	1/1	0.86	0.12	95,95,95,95	1
80	MG	2	1916	1/1	0.86	0.41	121,121,121,121	0
80	MG	C4	203	1/1	0.86	0.42	107,107,107,107	0
80	MG	5	3654	1/1	0.86	0.56	96,96,96,96	0
80	MG	1	3663	1/1	0.86	0.66	102,102,102,102	0
80	MG	2	1945	1/1	0.86	0.22	117,117,117,117	0
80	MG	5	3833	1/1	0.86	0.30	145,145,145,145	0
80	MG	4	218	1/1	0.86	0.65	122,122,122,122	0
80	MG	6	2023	1/1	0.86	0.25	131,131,131,131	0
80	MG	6	1947	1/1	0.87	0.21	110,110,110,110	0
80	MG	5	3544	1/1	0.87	0.26	121,121,121,121	0
80	MG	6	2021	1/1	0.87	0.20	146,146,146,146	0
80	MG	5	3470	1/1	0.88	0.11	147,147,147,147	0
80	MG	6	2003	1/1	0.88	0.23	173,173,173,173	0
80	MG	5	3676	1/1	0.88	0.31	96,96,96,96	0
80	MG	5	3477	1/1	0.88	0.16	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3628	1/1	0.89	0.28	111,111,111,111	0
80	MG	1	3774	1/1	0.89	0.47	95,95,95,95	1
80	MG	6	1969	1/1	0.89	0.17	134,134,134,134	0
80	MG	2	1917	1/1	0.90	0.09	124,124,124,124	0
80	MG	6	2040	1/1	0.90	0.11	117,117,117,117	0
80	MG	1	3732	1/1	0.90	0.65	79,79,79,79	0
80	MG	1	3549	1/1	0.90	0.72	73,73,73,73	0
80	MG	2	1961	1/1	0.90	0.16	131,131,131,131	0
80	MG	2	1991	1/1	0.90	0.30	156,156,156,156	0
80	MG	1	3416	1/1	0.90	0.53	84,84,84,84	0
80	MG	s6	301	1/1	0.90	0.13	119,119,119,119	0
80	MG	5	3567	1/1	0.91	0.46	95,95,95,95	0
80	MG	5	3549	1/1	0.91	0.26	118,118,118,118	0
80	MG	1	3624	1/1	0.91	0.38	91,91,91,91	1
80	MG	4	211	1/1	0.91	0.19	102,102,102,102	0
80	MG	1	3508	1/1	0.91	0.40	120,120,120,120	0
80	MG	5	3680	1/1	0.91	0.12	106,106,106,106	1
80	MG	1	3575	1/1	0.91	0.53	82,82,82,82	0
80	MG	m5	301	1/1	0.91	0.21	125,125,125,125	0
80	MG	6	2043	1/1	0.91	0.26	117,117,117,117	0
80	MG	5	3507	1/1	0.91	0.64	82,82,82,82	0
80	MG	5	3639	1/1	0.92	0.20	109,109,109,109	0
80	MG	2	1950	1/1	0.92	0.30	129,129,129,129	0
80	MG	6	2045	1/1	0.92	0.37	105,105,105,105	0
80	MG	6	2025	1/1	0.92	0.34	115,115,115,115	0
80	MG	5	3596	1/1	0.92	0.30	96,96,96,96	0
80	MG	l3	402	1/1	0.92	0.29	77,77,77,77	0
80	MG	1	3440	1/1	0.92	0.42	105,105,105,105	0
80	MG	6	1926	1/1	0.92	0.16	118,118,118,118	1
81	8UZ	7	209	33/33	0.93	0.18	109,109,109,109	0
80	MG	5	3789	1/1	0.93	0.26	95,95,95,95	0
80	MG	1	3578	1/1	0.93	0.23	102,102,102,102	0
80	MG	6	1934	1/1	0.93	0.41	106,106,106,106	0
80	MG	L2	302	1/1	0.93	0.38	78,78,78,78	0
80	MG	5	3644	1/1	0.93	0.22	96,96,96,96	0
80	MG	6	2059	1/1	0.93	0.39	141,141,141,141	0
81	8UZ	5	3856	33/33	0.94	0.14	121,121,121,121	0
80	MG	2	2004	1/1	0.94	0.17	112,112,112,112	1
80	MG	1	3409	1/1	0.94	0.35	88,88,88,88	0
80	MG	1	3734	1/1	0.94	0.28	85,85,85,85	0
80	MG	2	1954	1/1	0.94	0.36	100,100,100,100	0
80	MG	1	3755	1/1	0.94	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3596	1/1	0.94	0.16	98,98,98,98	0
80	MG	1	3495	1/1	0.95	0.28	83,83,83,83	0
80	MG	2	1942	1/1	0.95	0.11	115,115,115,115	0
80	MG	1	3828	1/1	0.95	0.44	83,83,83,83	1
80	MG	1	3619	1/1	0.95	0.42	76,76,76,76	0
80	MG	6	2056	1/1	0.95	0.14	157,157,157,157	0
80	MG	5	3583	1/1	0.95	0.23	97,97,97,97	0
80	MG	5	3612	1/1	0.95	0.13	137,137,137,137	0
80	MG	1	3650	1/1	0.95	0.36	81,81,81,81	0
80	MG	5	3662	1/1	0.95	0.32	95,95,95,95	0
80	MG	1	3560	1/1	0.95	0.35	189,189,189,189	0
80	MG	5	3714	1/1	0.95	0.15	101,101,101,101	0
80	MG	5	3806	1/1	0.95	0.64	97,97,97,97	1
80	MG	1	3459	1/1	0.96	0.09	103,103,103,103	0
80	MG	1	3509	1/1	0.96	0.15	111,111,111,111	0
80	MG	5	3529	1/1	0.96	0.27	82,82,82,82	0
80	MG	1	3746	1/1	0.96	0.20	113,113,113,113	0
80	MG	5	3423	1/1	0.96	0.30	86,86,86,86	0
80	MG	1	3642	1/1	0.96	0.35	79,79,79,79	0
80	MG	5	3510	1/1	0.96	0.33	96,96,96,96	0
80	MG	5	3409	1/1	0.96	0.17	87,87,87,87	0
80	MG	5	3695	1/1	0.96	0.23	86,86,86,86	0
80	MG	1	3512	1/1	0.96	0.57	97,97,97,97	0
80	MG	1	3793	1/1	0.96	0.43	89,89,89,89	1
80	MG	1	3425	1/1	0.96	0.10	117,117,117,117	1
80	MG	5	3805	1/1	0.96	0.08	143,143,143,143	0
80	MG	5	3436	1/1	0.97	0.30	95,95,95,95	1
80	MG	2	1940	1/1	0.97	0.24	115,115,115,115	0
80	MG	1	3638	1/1	0.97	0.50	77,77,77,77	0
80	MG	N3	201	1/1	0.97	0.25	81,81,81,81	0
80	MG	c8	201	1/1	0.97	0.14	145,145,145,145	0
80	MG	1	3636	1/1	0.97	0.27	80,80,80,80	0
80	MG	5	3617	1/1	0.97	0.20	129,129,129,129	0
80	MG	5	3550	1/1	0.97	0.22	127,127,127,127	0
80	MG	1	3633	1/1	0.97	0.27	77,77,77,77	0
80	MG	1	3641	1/1	0.97	0.26	77,77,77,77	0
80	MG	5	3570	1/1	0.97	0.30	91,91,91,91	0
80	MG	1	3802	1/1	0.97	0.27	104,104,104,104	0
80	MG	6	1961	1/1	0.97	0.10	125,125,125,125	0
80	MG	5	3773	1/1	0.97	0.44	83,83,83,83	0
80	MG	5	3557	1/1	0.97	0.29	108,108,108,108	0
80	MG	1	3644	1/1	0.97	0.34	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	6	1909	1/1	0.97	0.20	109,109,109,109	0
80	MG	5	3761	1/1	0.97	0.14	110,110,110,110	1
80	MG	6	2036	1/1	0.98	0.21	108,108,108,108	0
80	MG	1	3455	1/1	0.98	0.21	97,97,97,97	0
82	ZN	Q3	501	1/1	0.98	0.12	131,131,131,131	0
80	MG	1	3566	1/1	0.98	0.23	95,95,95,95	0
80	MG	5	3734	1/1	0.98	0.17	112,112,112,112	1
80	MG	5	3535	1/1	0.98	0.14	105,105,105,105	0
80	MG	5	3711	1/1	0.98	0.28	106,106,106,106	0
80	MG	6	1945	1/1	0.98	0.08	143,143,143,143	1
80	MG	1	3530	1/1	0.98	0.34	88,88,88,88	0
80	MG	5	3443	1/1	0.98	0.36	82,82,82,82	0
80	MG	2	1922	1/1	0.98	0.46	118,118,118,118	0
80	MG	4	210	1/1	0.99	0.29	89,89,89,89	0
80	MG	5	3794	1/1	0.99	0.30	95,95,95,95	0
80	MG	1	3496	1/1	0.99	0.15	93,93,93,93	1
80	MG	1	3547	1/1	0.99	0.21	81,81,81,81	0
80	MG	5	3636	1/1	-	-	116,116,116,116	1
80	MG	6	1979	1/1	-0.01	0.45	128,128,128,128	0
80	MG	1	3864	1/1	0.10	0.49	107,107,107,107	0
80	MG	1	3867	1/1	0.16	0.74	107,107,107,107	0
80	MG	2	2022	1/1	0.26	0.90	110,110,110,110	0
80	MG	1	3690	1/1	0.29	0.72	89,89,89,89	0
80	MG	O1	202	1/1	0.34	0.41	123,123,123,123	0
80	MG	1	3792	1/1	0.36	0.12	151,151,151,151	0
80	MG	5	3601	1/1	0.38	0.97	130,130,130,130	0
80	MG	O5	201	1/1	0.45	0.16	123,123,123,123	0
80	MG	5	3566	1/1	0.47	0.28	117,117,117,117	0
80	MG	5	3481	1/1	0.47	0.67	101,101,101,101	0
80	MG	q2	503	1/1	0.48	0.46	111,111,111,111	0
80	MG	1	3851	1/1	0.51	0.22	100,100,100,100	1
80	MG	1	3854	1/1	0.52	0.50	96,96,96,96	0
80	MG	2	2027	1/1	0.52	0.47	107,107,107,107	0
80	MG	n8	201	1/1	0.52	0.79	93,93,93,93	0
80	MG	1	3571	1/1	0.53	0.65	97,97,97,97	0
80	MG	s4	301	1/1	0.54	0.33	135,135,135,135	0
80	MG	1	3699	1/1	0.54	0.67	80,80,80,80	0
80	MG	2	1977	1/1	0.55	0.70	120,120,120,120	0
80	MG	s0	301	1/1	0.55	0.27	112,112,112,112	0
80	MG	5	3696	1/1	0.56	0.77	83,83,83,83	0
80	MG	1	3551	1/1	0.56	0.79	80,80,80,80	0
80	MG	1	3775	1/1	0.57	0.48	106,106,106,106	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3632	1/1	0.57	0.24	125,125,125,125	0
80	MG	d2	201	1/1	0.58	0.71	110,110,110,110	0
80	MG	6	1922	1/1	0.60	0.10	168,168,168,168	0
80	MG	1	3559	1/1	0.60	1.04	104,104,104,104	0
80	MG	5	3725	1/1	0.60	0.44	86,86,86,86	0
80	MG	5	3456	1/1	0.62	0.40	99,99,99,99	0
80	MG	n1	201	1/1	0.62	0.52	110,110,110,110	0
80	MG	5	3721	1/1	0.62	0.35	101,101,101,101	0
80	MG	4	216	1/1	0.62	0.19	134,134,134,134	0
80	MG	m6	201	1/1	0.63	0.59	84,84,84,84	0
80	MG	l5	301	1/1	0.64	0.45	134,134,134,134	0
80	MG	5	3743	1/1	0.64	0.21	144,144,144,144	1
80	MG	1	3740	1/1	0.64	0.52	84,84,84,84	0
80	MG	5	3437	1/1	0.65	1.17	90,90,90,90	0
80	MG	1	3413	1/1	0.67	0.48	87,87,87,87	0
80	MG	5	3614	1/1	0.67	0.81	106,106,106,106	0
80	MG	1	3590	1/1	0.67	0.51	94,94,94,94	0
80	MG	6	1920	1/1	0.67	0.17	133,133,133,133	0
80	MG	2	1929	1/1	0.68	0.27	143,143,143,143	0
80	MG	1	3841	1/1	0.68	0.75	111,111,111,111	0
80	MG	5	3602	1/1	0.69	0.32	145,145,145,145	0
80	MG	6	1915	1/1	0.69	0.50	99,99,99,99	0
80	MG	6	2009	1/1	0.69	0.49	167,167,167,167	0
80	MG	5	3759	1/1	0.69	0.20	118,118,118,118	0
80	MG	1	3817	1/1	0.70	0.21	102,102,102,102	1
80	MG	1	3880	1/1	0.70	0.53	84,84,84,84	0
80	MG	5	3702	1/1	0.70	1.31	99,99,99,99	0
80	MG	6	2033	1/1	0.71	0.63	101,101,101,101	1
80	MG	1	3744	1/1	0.71	0.74	96,96,96,96	0
80	MG	C4	202	1/1	0.72	1.11	129,129,129,129	0
80	MG	5	3573	1/1	0.73	0.23	105,105,105,105	0
80	MG	1	3668	1/1	0.73	0.24	118,118,118,118	0
80	MG	2	1968	1/1	0.73	0.42	123,123,123,123	0
80	MG	6	1904	1/1	0.74	0.68	119,119,119,119	0
80	MG	6	2047	1/1	0.74	0.76	106,106,106,106	0
80	MG	6	2046	1/1	0.74	0.71	108,108,108,108	0
80	MG	1	3623	1/1	0.74	0.42	93,93,93,93	0
80	MG	1	3667	1/1	0.75	0.41	87,87,87,87	0
80	MG	6	1959	1/1	0.75	0.15	140,140,140,140	0
80	MG	1	3728	1/1	0.75	0.23	84,84,84,84	1
80	MG	5	3748	1/1	0.75	0.39	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3832	1/1	0.76	0.41	109,109,109,109	0
80	MG	5	3826	1/1	0.76	0.37	82,82,82,82	0
80	MG	7	208	1/1	0.77	0.28	99,99,99,99	1
80	MG	2	1996	1/1	0.77	0.27	142,142,142,142	0
80	MG	5	3781	1/1	0.77	0.25	95,95,95,95	1
80	MG	5	3459	1/1	0.77	0.79	89,89,89,89	0
80	MG	1	3603	1/1	0.77	0.14	113,113,113,113	1
80	MG	5	3660	1/1	0.78	0.13	149,149,149,149	0
80	MG	2	2001	1/1	0.78	0.23	143,143,143,143	0
80	MG	1	3798	1/1	0.78	0.16	114,114,114,114	0
80	MG	1	3468	1/1	0.78	0.24	105,105,105,105	0
80	MG	6	1967	1/1	0.79	0.82	112,112,112,112	0
81	8UZ	5	3852	33/33	0.79	0.33	125,125,125,125	33
80	MG	5	3839	1/1	0.79	0.34	84,84,84,84	0
80	MG	1	3853	1/1	0.79	0.42	90,90,90,90	0
80	MG	1	3525	1/1	0.79	0.23	114,114,114,114	0
80	MG	1	3450	1/1	0.79	0.16	101,101,101,101	1
80	MG	1	3877	1/1	0.80	0.67	90,90,90,90	0
80	MG	1	3780	1/1	0.80	0.37	90,90,90,90	0
80	MG	2	1924	1/1	0.80	0.11	161,161,161,161	0
80	MG	6	1946	1/1	0.80	0.26	111,111,111,111	0
80	MG	2	2023	1/1	0.80	0.24	169,169,169,169	0
80	MG	4	205	1/1	0.80	0.72	89,89,89,89	0
80	MG	1	3861	1/1	0.81	0.22	97,97,97,97	0
80	MG	1	3812	1/1	0.81	0.32	108,108,108,108	1
80	MG	o2	202	1/1	0.81	0.29	94,94,94,94	0
80	MG	5	3744	1/1	0.81	0.49	138,138,138,138	0
81	8UZ	5	3855	33/33	0.81	0.30	138,138,138,138	0
80	MG	5	3797	1/1	0.82	0.42	116,116,116,116	0
80	MG	5	3518	1/1	0.82	0.31	112,112,112,112	0
80	MG	5	3703	1/1	0.82	0.89	83,83,83,83	0
80	MG	1	3456	1/1	0.82	0.72	104,104,104,104	0
80	MG	1	3587	1/1	0.82	0.29	95,95,95,95	0
80	MG	6	2000	1/1	0.82	0.18	139,139,139,139	0
80	MG	1	3446	1/1	0.82	0.36	81,81,81,81	0
80	MG	2	1904	1/1	0.83	0.94	101,101,101,101	0
80	MG	5	3819	1/1	0.83	0.57	92,92,92,92	0
80	MG	6	1982	1/1	0.83	0.23	171,171,171,171	1
80	MG	2	2011	1/1	0.83	0.09	136,136,136,136	0
80	MG	2	1937	1/1	0.83	0.30	116,116,116,116	0
80	MG	5	3638	1/1	0.83	0.25	106,106,106,106	0
80	MG	1	3729	1/1	0.83	0.40	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	6	2037	1/1	0.83	0.33	109,109,109,109	0
80	MG	1	3872	1/1	0.84	0.21	122,122,122,122	0
80	MG	6	1963	1/1	0.84	0.71	115,115,115,115	0
80	MG	1	3462	1/1	0.84	0.60	143,143,143,143	0
80	MG	5	3840	1/1	0.84	0.44	95,95,95,95	0
80	MG	5	3708	1/1	0.84	1.03	91,91,91,91	0
80	MG	1	3785	1/1	0.84	0.17	104,104,104,104	1
80	MG	1	3848	1/1	0.84	0.27	93,93,93,93	0
80	MG	M7	204	1/1	0.84	0.44	81,81,81,81	0
81	8UZ	5	3857	33/33	0.85	0.18	133,133,133,133	0
80	MG	5	3688	1/1	0.85	0.23	111,111,111,111	0
80	MG	5	3802	1/1	0.85	0.15	119,119,119,119	0
80	MG	5	3784	1/1	0.85	0.39	106,106,106,106	0
80	MG	6	2039	1/1	0.85	0.11	120,120,120,120	0
80	MG	1	3483	1/1	0.85	0.76	68,68,68,68	0
80	MG	M7	201	1/1	0.85	0.38	75,75,75,75	0
80	MG	5	3559	1/1	0.86	2.05	63,63,63,63	0
80	MG	1	3563	1/1	0.86	0.66	122,122,122,122	0
80	MG	2	2010	1/1	0.86	0.37	114,114,114,114	0
80	MG	1	3589	1/1	0.86	0.39	94,94,94,94	0
80	MG	2	1976	1/1	0.86	0.48	101,101,101,101	0
80	MG	1	3526	1/1	0.86	0.66	84,84,84,84	0
80	MG	6	1950	1/1	0.86	0.40	102,102,102,102	0
80	MG	C8	201	1/1	0.86	0.12	166,166,166,166	0
80	MG	1	3599	1/1	0.87	0.26	165,165,165,165	0
80	MG	1	3720	1/1	0.87	0.41	79,79,79,79	0
80	MG	O7	102	1/1	0.87	0.16	124,124,124,124	0
80	MG	1	3677	1/1	0.87	0.28	76,76,76,76	0
80	MG	5	3593	1/1	0.87	0.95	77,77,77,77	0
80	MG	5	3546	1/1	0.87	0.61	109,109,109,109	0
80	MG	5	3785	1/1	0.87	0.25	103,103,103,103	0
80	MG	5	3751	1/1	0.87	0.98	101,101,101,101	0
80	MG	2	1901	1/1	0.88	0.50	121,121,121,121	0
80	MG	1	3617	1/1	0.88	0.27	93,93,93,93	0
80	MG	5	3512	1/1	0.88	0.34	92,92,92,92	0
80	MG	1	3477	1/1	0.88	0.46	78,78,78,78	0
80	MG	5	3606	1/1	0.88	0.13	142,142,142,142	0
80	MG	5	3678	1/1	0.88	0.71	108,108,108,108	0
80	MG	1	3745	1/1	0.88	0.30	105,105,105,105	0
80	MG	1	3428	1/1	0.88	0.26	103,103,103,103	0
80	MG	1	3610	1/1	0.88	0.11	99,99,99,99	1
80	MG	5	3845	1/1	0.89	0.30	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3484	1/1	0.89	0.38	99,99,99,99	0
80	MG	5	3715	1/1	0.89	0.30	93,93,93,93	0
81	8UZ	2	2030	33/33	0.89	0.27	148,149,149,149	0
80	MG	c3	200	1/1	0.89	0.47	117,117,117,117	0
80	MG	6	2044	1/1	0.89	0.43	129,129,129,129	0
80	MG	6	1985	1/1	0.89	0.22	134,134,134,134	0
80	MG	5	3670	1/1	0.89	0.36	98,98,98,98	0
80	MG	1	3806	1/1	0.90	0.29	93,93,93,93	0
80	MG	2	2028	1/1	0.90	0.06	174,174,174,174	0
80	MG	5	3812	1/1	0.90	0.21	96,96,96,96	0
80	MG	1	3620	1/1	0.90	0.13	116,116,116,116	0
80	MG	5	3562	1/1	0.90	0.22	128,128,128,128	0
80	MG	5	3706	1/1	0.90	0.65	85,85,85,85	0
80	MG	1	3661	1/1	0.90	0.57	93,93,93,93	0
80	MG	1	3561	1/1	0.90	0.27	109,109,109,109	0
80	MG	1	3760	1/1	0.90	0.33	89,89,89,89	0
81	8UZ	1	3893	33/33	0.90	0.24	105,105,105,105	0
80	MG	2	1915	1/1	0.90	0.15	130,130,130,130	0
80	MG	5	3438	1/1	0.90	0.32	88,88,88,88	0
81	8UZ	1	3889	33/33	0.90	0.23	119,119,119,119	0
80	MG	5	3787	1/1	0.90	0.20	109,109,109,109	0
80	MG	1	3847	1/1	0.90	0.27	90,90,90,90	0
80	MG	1	3611	1/1	0.90	0.50	95,95,95,95	0
80	MG	5	3555	1/1	0.91	0.13	130,130,130,130	0
80	MG	1	3879	1/1	0.91	0.24	165,165,165,165	0
80	MG	5	3758	1/1	0.91	0.21	100,100,100,100	1
80	MG	5	3641	1/1	0.91	0.11	117,117,117,117	0
80	MG	2	1993	1/1	0.91	0.12	164,164,164,164	0
80	MG	1	3482	1/1	0.91	0.38	74,74,74,74	0
80	MG	5	3538	1/1	0.91	0.15	115,115,115,115	0
80	MG	1	3675	1/1	0.91	0.06	117,117,117,117	1
80	MG	5	3476	1/1	0.91	0.22	132,132,132,132	0
80	MG	1	3436	1/1	0.91	0.34	88,88,88,88	0
80	MG	5	3526	1/1	0.91	0.32	87,87,87,87	0
81	8UZ	6	2061	33/33	0.92	0.27	135,135,135,135	0
80	MG	1	3582	1/1	0.92	0.14	126,126,126,126	0
80	MG	5	3548	1/1	0.92	0.12	127,127,127,127	0
81	8UZ	5	3850	33/33	0.92	0.22	114,114,114,114	0
80	MG	1	3749	1/1	0.92	0.33	79,79,79,79	0
80	MG	1	3757	1/1	0.92	0.20	87,87,87,87	0
80	MG	2	1990	1/1	0.92	0.57	114,114,114,114	0
80	MG	5	3824	1/1	0.92	0.09	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	6	1978	1/1	0.92	0.09	146,146,146,146	0
80	MG	5	3658	1/1	0.92	0.23	103,103,103,103	1
80	MG	2	2016	1/1	0.93	0.42	124,124,124,124	0
80	MG	2	1941	1/1	0.93	0.36	111,111,111,111	0
80	MG	1	3805	1/1	0.93	0.62	89,89,89,89	1
80	MG	5	3765	1/1	0.93	0.34	99,99,99,99	0
80	MG	6	1910	1/1	0.93	0.24	109,109,109,109	0
80	MG	1	3784	1/1	0.93	0.24	102,102,102,102	0
80	MG	5	3769	1/1	0.93	0.23	98,98,98,98	0
80	MG	6	1938	1/1	0.93	0.13	107,107,107,107	0
81	8UZ	5	3851	33/33	0.93	0.17	125,125,125,125	0
80	MG	5	3817	1/1	0.93	0.29	108,108,108,108	1
80	MG	6	1955	1/1	0.93	1.12	89,89,89,89	0
80	MG	6	1994	1/1	0.93	0.12	144,144,144,144	0
80	MG	o7	502	1/1	0.93	0.32	98,98,98,98	0
80	MG	1	3773	1/1	0.93	0.27	92,92,92,92	0
80	MG	14	401	1/1	0.93	0.26	114,114,114,114	1
80	MG	1	3795	1/1	0.94	0.30	103,103,103,103	0
81	8UZ	1	3886	33/33	0.94	0.13	123,123,123,123	0
80	MG	1	3579	1/1	0.94	0.25	129,129,129,129	0
80	MG	1	3528	1/1	0.94	0.48	90,90,90,90	0
80	MG	m0	302	1/1	0.94	0.19	94,94,94,94	0
80	MG	2	1913	1/1	0.94	0.11	125,125,125,125	0
80	MG	5	3541	1/1	0.94	0.16	115,115,115,115	0
80	MG	1	3639	1/1	0.94	0.17	82,82,82,82	0
80	MG	5	3498	1/1	0.94	0.52	99,99,99,99	0
80	MG	6	1993	1/1	0.94	0.10	136,136,136,136	0
80	MG	5	3497	1/1	0.94	0.23	100,100,100,100	0
80	MG	1	3683	1/1	0.94	0.23	81,81,81,81	0
80	MG	5	3757	1/1	0.94	0.12	107,107,107,107	0
80	MG	6	2008	1/1	0.94	0.07	160,160,160,160	0
80	MG	6	2030	1/1	0.94	0.23	130,130,130,130	0
80	MG	1	3444	1/1	0.94	0.27	82,82,82,82	0
80	MG	5	3780	1/1	0.94	0.45	94,94,94,94	1
80	MG	6	2013	1/1	0.94	0.14	130,130,130,130	0
80	MG	2	1914	1/1	0.94	0.15	128,128,128,128	0
80	MG	5	3616	1/1	0.94	0.15	132,132,132,132	0
80	MG	6	1917	1/1	0.95	0.38	128,128,128,128	0
80	MG	n7	201	1/1	0.95	0.20	148,148,148,148	0
80	MG	5	3753	1/1	0.95	0.22	92,92,92,92	0
80	MG	6	2032	1/1	0.95	0.12	145,145,145,145	0
80	MG	1	3605	1/1	0.95	0.20	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3682	1/1	0.95	0.23	80,80,80,80	0
80	MG	2	1969	1/1	0.95	0.25	118,118,118,118	0
80	MG	2	1943	1/1	0.95	0.21	112,112,112,112	0
80	MG	5	3496	1/1	0.95	0.43	93,93,93,93	0
80	MG	1	3769	1/1	0.95	0.22	93,93,93,93	0
80	MG	2	1953	1/1	0.95	0.24	113,113,113,113	0
80	MG	1	3420	1/1	0.95	0.36	90,90,90,90	0
80	MG	2	1955	1/1	0.95	0.17	109,109,109,109	0
80	MG	1	3863	1/1	0.95	0.11	99,99,99,99	0
80	MG	2	1981	1/1	0.95	0.12	136,136,136,136	0
80	MG	1	3499	1/1	0.95	0.09	107,107,107,107	0
80	MG	6	1905	1/1	0.95	0.19	122,122,122,122	0
80	MG	1	3447	1/1	0.95	0.23	82,82,82,82	0
80	MG	5	3461	1/1	0.95	0.29	95,95,95,95	0
80	MG	5	3552	1/1	0.96	0.12	139,139,139,139	0
80	MG	5	3486	1/1	0.96	0.14	106,106,106,106	0
80	MG	5	3747	1/1	0.96	0.24	97,97,97,97	0
80	MG	5	3568	1/1	0.96	0.31	98,98,98,98	0
80	MG	1	3666	1/1	0.96	0.27	78,78,78,78	0
80	MG	4	213	1/1	0.96	0.25	105,105,105,105	0
80	MG	2	1956	1/1	0.96	0.21	152,152,152,152	0
80	MG	5	3651	1/1	0.96	0.24	86,86,86,86	1
80	MG	4	208	1/1	0.96	0.26	88,88,88,88	0
80	MG	5	3841	1/1	0.96	0.17	120,120,120,120	0
80	MG	1	3427	1/1	0.96	0.19	110,110,110,110	0
80	MG	1	3421	1/1	0.96	0.24	94,94,94,94	0
80	MG	2	1906	1/1	0.96	0.10	144,144,144,144	0
80	MG	6	1916	1/1	0.96	0.13	113,113,113,113	0
80	MG	5	3419	1/1	0.96	0.30	87,87,87,87	0
80	MG	6	1991	1/1	0.96	0.27	138,138,138,138	0
80	MG	5	3533	1/1	0.96	0.16	91,91,91,91	0
80	MG	4	204	1/1	0.96	0.11	127,127,127,127	0
80	MG	M5	301	1/1	0.96	0.25	88,88,88,88	0
80	MG	1	3411	1/1	0.96	0.30	92,92,92,92	0
80	MG	1	3738	1/1	0.96	0.22	93,93,93,93	0
80	MG	M8	201	1/1	0.96	0.64	97,97,97,97	0
80	MG	6	1935	1/1	0.96	0.12	109,109,109,109	0
80	MG	1	3434	1/1	0.96	0.31	80,80,80,80	0
80	MG	3	212	1/1	0.96	0.42	121,121,121,121	1
80	MG	7	201	1/1	0.96	0.05	147,147,147,147	1
80	MG	1	3452	1/1	0.97	0.29	95,95,95,95	0
80	MG	8	202	1/1	0.97	0.12	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3524	1/1	0.97	0.48	85,85,85,85	0
80	MG	5	3682	1/1	0.97	0.08	113,113,113,113	0
80	MG	5	3404	1/1	0.97	0.38	82,82,82,82	0
80	MG	5	3504	1/1	0.97	0.35	94,94,94,94	0
80	MG	1	3766	1/1	0.97	0.15	159,159,159,159	0
80	MG	2	1963	1/1	0.97	0.18	128,128,128,128	0
80	MG	1	3630	1/1	0.97	0.24	82,82,82,82	0
80	MG	2	1909	1/1	0.97	0.11	133,133,133,133	0
80	MG	o7	503	1/1	0.97	0.19	126,126,126,126	1
80	MG	4	215	1/1	0.97	0.10	111,111,111,111	0
80	MG	1	3594	1/1	0.97	0.16	92,92,92,92	0
80	MG	1	3410	1/1	0.97	0.33	92,92,92,92	0
80	MG	1	3423	1/1	0.97	0.36	102,102,102,102	0
80	MG	8	201	1/1	0.97	0.25	94,94,94,94	0
80	MG	5	3515	1/1	0.97	0.23	106,106,106,106	0
80	MG	5	3571	1/1	0.97	0.14	94,94,94,94	0
80	MG	5	3509	1/1	0.97	0.40	91,91,91,91	0
80	MG	6	1971	1/1	0.97	0.26	133,133,133,133	0
80	MG	O6	201	1/1	0.97	0.36	132,132,132,132	0
80	MG	6	2026	1/1	0.97	0.19	142,142,142,142	0
80	MG	5	3413	1/1	0.97	0.28	98,98,98,98	0
80	MG	5	3525	1/1	0.97	0.40	91,91,91,91	0
80	MG	2	1923	1/1	0.97	0.12	140,140,140,140	0
80	MG	5	3508	1/1	0.98	0.26	96,96,96,96	0
80	MG	5	3416	1/1	0.98	0.21	86,86,86,86	0
80	MG	1	3679	1/1	0.98	0.17	82,82,82,82	0
80	MG	5	3767	1/1	0.98	0.33	89,89,89,89	0
80	MG	5	3653	1/1	0.98	0.36	91,91,91,91	0
80	MG	2	1949	1/1	0.98	0.25	137,137,137,137	0
80	MG	1	3680	1/1	0.98	0.25	79,79,79,79	0
80	MG	1	3535	1/1	0.98	0.34	82,82,82,82	0
80	MG	5	3511	1/1	0.98	0.14	96,96,96,96	0
80	MG	1	3823	1/1	0.98	0.33	79,79,79,79	0
80	MG	2	1957	1/1	0.98	0.14	139,139,139,139	0
80	MG	1	3771	1/1	0.98	0.23	89,89,89,89	1
80	MG	1	3593	1/1	0.98	0.15	93,93,93,93	0
80	MG	5	3521	1/1	0.98	0.34	133,133,133,133	0
80	MG	1	3665	1/1	0.98	0.18	82,82,82,82	0
80	MG	3	213	1/1	0.98	0.17	124,124,124,124	0
80	MG	5	3532	1/1	0.98	0.38	84,84,84,84	0
80	MG	1	3545	1/1	0.99	0.34	81,81,81,81	0
80	MG	1	3542	1/1	0.99	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	o4	502	1/1	0.99	0.34	136,136,136,136	1
80	MG	2	1939	1/1	0.99	0.24	109,109,109,109	0
80	MG	1	3407	1/1	0.99	0.40	86,86,86,86	0
80	MG	5	3752	1/1	0.99	0.20	91,91,91,91	0
80	MG	1	3481	1/1	0.99	0.29	78,78,78,78	0
80	MG	1	3772	1/1	0.99	0.19	90,90,90,90	0
80	MG	1	3534	1/1	0.99	0.41	77,77,77,77	0
80	MG	1	3586	1/1	0.99	0.17	86,86,86,86	0
80	MG	1	3695	1/1	0.99	0.48	74,74,74,74	0
80	MG	5	3657	1/1	0.99	0.24	93,93,93,93	0
80	MG	1	3465	1/1	1.00	0.18	114,114,114,114	0
80	MG	1	3717	1/1	1.00	0.29	83,83,83,83	0
82	ZN	q0	500	1/1	1.00	0.17	93,93,93,93	0
80	MG	4	219	1/1	-	-	97,97,97,97	1
80	MG	5	3667	1/1	-0.27	0.49	200,200,200,200	0
80	MG	c1	201	1/1	-0.01	0.98	126,126,126,126	0
80	MG	2	2018	1/1	0.00	0.28	138,138,138,138	0
80	MG	6	2060	1/1	0.02	0.51	139,139,139,139	0
80	MG	2	1926	1/1	0.06	0.33	151,151,151,151	0
80	MG	d3	201	1/1	0.12	0.63	122,122,122,122	0
80	MG	2	1997	1/1	0.18	0.34	128,128,128,128	0
80	MG	5	3463	1/1	0.22	2.00	94,94,94,94	0
80	MG	6	1996	1/1	0.24	1.33	119,119,119,119	0
80	MG	c1	202	1/1	0.25	0.54	113,113,113,113	0
80	MG	8	203	1/1	0.27	0.81	105,105,105,105	0
80	MG	1	3670	1/1	0.28	0.37	108,108,108,108	0
80	MG	6	1986	1/1	0.28	0.38	132,132,132,132	0
80	MG	S1	301	1/1	0.29	0.30	172,172,172,172	0
80	MG	1	3523	1/1	0.30	0.40	119,119,119,119	0
80	MG	6	1965	1/1	0.33	0.48	144,144,144,144	0
80	MG	5	3800	1/1	0.33	0.41	122,122,122,122	1
80	MG	5	3640	1/1	0.33	0.94	107,107,107,107	0
80	MG	5	3480	1/1	0.34	0.90	107,107,107,107	0
80	MG	5	3822	1/1	0.36	0.61	102,102,102,102	0
80	MG	1	3799	1/1	0.36	0.12	148,148,148,148	0
80	MG	6	1964	1/1	0.36	0.20	143,143,143,143	0
80	MG	2	2025	1/1	0.37	0.22	142,142,142,142	0
80	MG	5	3728	1/1	0.39	0.71	87,87,87,87	0
80	MG	6	1913	1/1	0.41	0.68	101,101,101,101	0
80	MG	n6	201	1/1	0.43	1.04	104,104,104,104	0
80	MG	3	203	1/1	0.44	0.20	122,122,122,122	0
80	MG	5	3705	1/1	0.44	1.23	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3510	1/1	0.44	0.26	142,142,142,142	0
80	MG	6	1957	1/1	0.45	0.36	102,102,102,102	0
80	MG	5	3426	1/1	0.45	0.82	90,90,90,90	0
80	MG	3	201	1/1	0.46	0.40	95,95,95,95	0
80	MG	1	3562	1/1	0.47	0.22	124,124,124,124	0
80	MG	1	3432	1/1	0.47	0.22	140,140,140,140	0
80	MG	1	3782	1/1	0.47	0.22	93,93,93,93	1
80	MG	1	3569	1/1	0.47	0.97	94,94,94,94	0
80	MG	6	1908	1/1	0.47	1.43	99,99,99,99	0
80	MG	3	205	1/1	0.48	0.22	126,126,126,126	0
80	MG	2	2019	1/1	0.48	0.18	125,125,125,125	1
80	MG	1	3564	1/1	0.49	0.52	92,92,92,92	0
80	MG	2	2024	1/1	0.51	0.34	123,123,123,123	0
80	MG	O4	502	1/1	0.52	0.79	104,104,104,104	0
80	MG	1	3517	1/1	0.52	0.76	89,89,89,89	0
80	MG	2	1908	1/1	0.53	0.77	118,118,118,118	0
80	MG	1	3687	1/1	0.54	0.72	79,79,79,79	0
80	MG	5	3701	1/1	0.54	0.63	101,101,101,101	0
80	MG	5	3740	1/1	0.55	0.71	100,100,100,100	0
80	MG	5	3698	1/1	0.55	0.44	105,105,105,105	0
80	MG	6	2029	1/1	0.55	0.33	148,148,148,148	0
80	MG	1	3868	1/1	0.55	0.94	111,111,111,111	0
80	MG	O3	202	1/1	0.56	0.65	93,93,93,93	0
80	MG	5	3643	1/1	0.56	0.36	108,108,108,108	0
80	MG	5	3635	1/1	0.57	0.54	109,109,109,109	0
80	MG	2	2026	1/1	0.57	1.07	103,103,103,103	0
80	MG	5	3811	1/1	0.57	0.34	97,97,97,97	1
80	MG	o3	201	1/1	0.58	0.79	76,76,76,76	0
80	MG	5	3619	1/1	0.58	0.73	99,99,99,99	0
80	MG	6	2038	1/1	0.58	0.47	118,118,118,118	1
80	MG	1	3832	1/1	0.59	0.16	115,115,115,115	1
80	MG	1	3813	1/1	0.59	0.23	123,123,123,123	0
80	MG	Q2	502	1/1	0.59	0.29	126,126,126,126	0
80	MG	1	3550	1/1	0.59	1.57	80,80,80,80	0
80	MG	M6	201	1/1	0.59	0.52	86,86,86,86	0
80	MG	5	3783	1/1	0.60	0.18	134,134,134,134	0
80	MG	1	3860	1/1	0.60	0.85	92,92,92,92	0
80	MG	5	3668	1/1	0.60	0.13	154,154,154,154	0
80	MG	5	3669	1/1	0.60	0.34	116,116,116,116	0
80	MG	5	3457	1/1	0.60	1.30	81,81,81,81	0
80	MG	1	3515	1/1	0.60	0.50	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3834	1/1	0.60	0.14	120,120,120,120	0
80	MG	1	3862	1/1	0.60	0.59	85,85,85,85	0
80	MG	L6	202	1/1	0.61	0.26	101,101,101,101	0
80	MG	8	206	1/1	0.61	0.48	112,112,112,112	0
80	MG	2	2012	1/1	0.61	0.14	173,173,173,173	0
80	MG	1	3763	1/1	0.61	0.53	90,90,90,90	0
80	MG	5	3672	1/1	0.61	0.27	106,106,106,106	0
80	MG	7	202	1/1	0.62	0.10	173,173,173,173	0
80	MG	1	3464	1/1	0.62	0.34	101,101,101,101	0
80	MG	6	2035	1/1	0.62	0.16	113,113,113,113	1
80	MG	5	3691	1/1	0.62	0.37	125,125,125,125	0
80	MG	1	3708	1/1	0.62	0.80	90,90,90,90	0
80	MG	1	3789	1/1	0.62	0.34	102,102,102,102	1
80	MG	5	3444	1/1	0.63	0.36	117,117,117,117	0
80	MG	3	207	1/1	0.63	0.34	129,129,129,129	0
80	MG	6	1995	1/1	0.64	0.51	117,117,117,117	0
80	MG	5	3762	1/1	0.64	0.36	116,116,116,116	1
80	MG	1	3674	1/1	0.64	0.49	101,101,101,101	0
80	MG	1	3608	1/1	0.64	0.40	107,107,107,107	1
80	MG	1	3505	1/1	0.64	0.62	101,101,101,101	0
80	MG	q2	504	1/1	0.64	0.53	94,94,94,94	0
80	MG	5	3803	1/1	0.65	0.19	159,159,159,159	0
80	MG	1	3567	1/1	0.65	0.52	97,97,97,97	0
82	ZN	D7	101	1/1	0.65	0.07	337,337,337,337	0
80	MG	5	3556	1/1	0.65	1.68	86,86,86,86	0
80	MG	2	1973	1/1	0.65	0.60	107,107,107,107	0
80	MG	5	3608	1/1	0.65	0.37	94,94,94,94	0
80	MG	5	3516	1/1	0.65	0.43	116,116,116,116	0
80	MG	5	3722	1/1	0.66	0.28	131,131,131,131	0
80	MG	1	3883	1/1	0.66	0.29	88,88,88,88	0
80	MG	5	3707	1/1	0.66	1.01	99,99,99,99	0
80	MG	6	2048	1/1	0.66	0.16	188,188,188,188	0
80	MG	5	3595	1/1	0.67	0.68	91,91,91,91	0
80	MG	1	3885	1/1	0.67	0.20	124,124,124,124	0
80	MG	5	3779	1/1	0.67	0.12	137,137,137,137	0
80	MG	1	3492	1/1	0.67	0.59	82,82,82,82	0
80	MG	5	3565	1/1	0.67	0.53	113,113,113,113	0
80	MG	8	207	1/1	0.68	0.17	129,129,129,129	0
80	MG	1	3598	1/1	0.68	0.42	95,95,95,95	0
80	MG	6	1981	1/1	0.68	0.54	125,125,125,125	0
80	MG	6	2034	1/1	0.69	0.28	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3464	1/1	0.69	0.70	95,95,95,95	0
80	MG	5	3430	1/1	0.69	0.52	88,88,88,88	0
80	MG	6	1927	1/1	0.69	0.26	114,114,114,114	0
80	MG	5	3471	1/1	0.69	0.45	125,125,125,125	0
80	MG	1	3457	1/1	0.69	0.27	107,107,107,107	0
80	MG	5	3771	1/1	0.69	0.14	127,127,127,127	0
80	MG	6	1939	1/1	0.69	0.82	102,102,102,102	0
80	MG	c7	201	1/1	0.69	0.16	138,138,138,138	0
80	MG	6	2050	1/1	0.70	1.38	104,104,104,104	0
80	MG	1	3580	1/1	0.70	0.48	96,96,96,96	0
80	MG	5	3493	1/1	0.70	0.76	83,83,83,83	0
80	MG	1	3418	1/1	0.70	0.45	74,74,74,74	0
80	MG	5	3834	1/1	0.70	0.47	79,79,79,79	0
80	MG	5	3713	1/1	0.70	0.68	88,88,88,88	0
80	MG	1	3706	1/1	0.71	0.99	88,88,88,88	0
80	MG	1	3712	1/1	0.71	0.46	87,87,87,87	0
80	MG	6	2031	1/1	0.71	0.24	137,137,137,137	1
80	MG	1	3865	1/1	0.71	0.30	185,185,185,185	0
80	MG	5	3766	1/1	0.72	0.17	106,106,106,106	0
80	MG	1	3548	1/1	0.72	0.56	87,87,87,87	0
80	MG	5	3764	1/1	0.72	0.66	101,101,101,101	1
80	MG	1	3829	1/1	0.72	0.65	101,101,101,101	1
80	MG	5	3735	1/1	0.72	0.50	102,102,102,102	0
80	MG	1	3727	1/1	0.72	0.40	79,79,79,79	0
80	MG	1	3659	1/1	0.73	1.39	86,86,86,86	0
80	MG	5	3731	1/1	0.73	0.62	89,89,89,89	0
80	MG	2	2000	1/1	0.73	0.21	130,130,130,130	0
80	MG	5	3483	1/1	0.73	0.33	104,104,104,104	0
80	MG	2	2006	1/1	0.73	0.21	138,138,138,138	0
80	MG	1	3442	1/1	0.73	0.37	132,132,132,132	0
80	MG	5	3491	1/1	0.73	1.00	97,97,97,97	0
80	MG	5	3661	1/1	0.73	0.30	141,141,141,141	0
80	MG	N0	201	1/1	0.73	0.49	88,88,88,88	0
80	MG	5	3774	1/1	0.73	0.12	104,104,104,104	1
80	MG	6	1901	1/1	0.73	1.07	106,106,106,106	0
80	MG	6	1940	1/1	0.73	0.59	112,112,112,112	0
80	MG	1	3815	1/1	0.73	0.27	133,133,133,133	0
80	MG	5	3738	1/1	0.74	0.81	96,96,96,96	0
80	MG	1	3709	1/1	0.74	0.54	77,77,77,77	0
80	MG	2	1947	1/1	0.74	0.91	91,91,91,91	0
80	MG	4	207	1/1	0.74	0.66	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	4	214	1/1	0.74	0.62	100,100,100,100	0
80	MG	1	3498	1/1	0.75	0.45	108,108,108,108	0
80	MG	5	3772	1/1	0.75	0.11	152,152,152,152	1
80	MG	2	2008	1/1	0.75	0.17	130,130,130,130	0
80	MG	1	3739	1/1	0.75	0.75	100,100,100,100	0
80	MG	1	3507	1/1	0.75	0.17	139,139,139,139	0
80	MG	5	3736	1/1	0.75	0.49	89,89,89,89	0
80	MG	1	3858	1/1	0.75	0.47	107,107,107,107	0
80	MG	5	3724	1/1	0.75	0.39	118,118,118,118	0
80	MG	6	2041	1/1	0.75	0.70	105,105,105,105	0
80	MG	5	3847	1/1	0.75	0.71	137,137,137,137	0
80	MG	1	3779	1/1	0.75	0.21	108,108,108,108	0
80	MG	6	1992	1/1	0.76	0.23	196,196,196,196	0
80	MG	5	3768	1/1	0.76	0.47	91,91,91,91	1
80	MG	5	3664	1/1	0.76	0.44	81,81,81,81	0
80	MG	o3	202	1/1	0.76	0.35	84,84,84,84	0
80	MG	M0	302	1/1	0.76	0.21	98,98,98,98	0
80	MG	1	3463	1/1	0.76	0.22	106,106,106,106	0
80	MG	l2	302	1/1	0.76	0.38	90,90,90,90	0
80	MG	1	3819	1/1	0.76	0.21	114,114,114,114	0
80	MG	5	3543	1/1	0.76	0.45	112,112,112,112	0
80	MG	5	3551	1/1	0.76	0.18	131,131,131,131	0
80	MG	1	3820	1/1	0.76	0.18	94,94,94,94	1
80	MG	5	3694	1/1	0.77	0.42	98,98,98,98	0
80	MG	5	3539	1/1	0.77	0.30	100,100,100,100	0
80	MG	1	3600	1/1	0.77	0.09	168,168,168,168	1
80	MG	o2	201	1/1	0.77	0.40	85,85,85,85	0
80	MG	5	3478	1/1	0.77	0.35	109,109,109,109	0
80	MG	5	3620	1/1	0.77	0.37	92,92,92,92	0
80	MG	5	3627	1/1	0.77	1.02	97,97,97,97	0
80	MG	1	3658	1/1	0.77	1.05	76,76,76,76	0
80	MG	6	2015	1/1	0.77	0.24	140,140,140,140	0
80	MG	l3	401	1/1	0.77	0.46	83,83,83,83	0
80	MG	1	3448	1/1	0.77	0.74	103,103,103,103	0
80	MG	1	3876	1/1	0.77	0.64	134,134,134,134	0
80	MG	1	3831	1/1	0.77	0.30	146,146,146,146	0
80	MG	1	3859	1/1	0.77	0.28	103,103,103,103	0
80	MG	2	1927	1/1	0.77	0.04	169,169,169,169	0
80	MG	5	3488	1/1	0.78	0.71	83,83,83,83	0
80	MG	1	3721	1/1	0.78	0.29	83,83,83,83	0
80	MG	5	3796	1/1	0.78	0.21	129,129,129,129	0
80	MG	5	3513	1/1	0.78	0.50	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	N8	201	1/1	0.78	0.28	116,116,116,116	0
80	MG	1	3576	1/1	0.78	1.29	88,88,88,88	0
80	MG	1	3671	1/1	0.78	0.23	108,108,108,108	0
80	MG	1	3741	1/1	0.78	1.13	101,101,101,101	0
80	MG	5	3733	1/1	0.78	0.21	106,106,106,106	0
80	MG	1	3480	1/1	0.78	0.60	84,84,84,84	0
80	MG	6	1983	1/1	0.79	0.19	146,146,146,146	0
80	MG	5	3506	1/1	0.79	0.56	95,95,95,95	0
80	MG	1	3842	1/1	0.79	0.57	104,104,104,104	0
80	MG	6	1954	1/1	0.79	0.38	119,119,119,119	0
80	MG	O1	201	1/1	0.79	1.10	102,102,102,102	0
80	MG	5	3607	1/1	0.79	0.40	99,99,99,99	0
80	MG	5	3750	1/1	0.79	0.60	92,92,92,92	0
80	MG	5	3604	1/1	0.79	0.15	127,127,127,127	1
80	MG	1	3715	1/1	0.79	0.35	76,76,76,76	0
80	MG	4	202	1/1	0.79	0.48	97,97,97,97	0
80	MG	1	3552	1/1	0.79	0.42	76,76,76,76	0
80	MG	5	3846	1/1	0.79	0.58	116,116,116,116	0
80	MG	1	3506	1/1	0.79	0.10	122,122,122,122	0
80	MG	5	3466	1/1	0.79	1.14	113,113,113,113	0
80	MG	6	1975	1/1	0.80	0.28	136,136,136,136	0
80	MG	6	1903	1/1	0.80	0.29	122,122,122,122	0
80	MG	6	1941	1/1	0.80	0.16	168,168,168,168	0
80	MG	5	3610	1/1	0.80	0.12	115,115,115,115	0
80	MG	5	3588	1/1	0.80	0.54	83,83,83,83	0
80	MG	1	3804	1/1	0.80	0.53	87,87,87,87	1
80	MG	5	3637	1/1	0.80	1.07	108,108,108,108	0
80	MG	1	3504	1/1	0.80	0.71	101,101,101,101	0
80	MG	5	3489	1/1	0.80	1.01	91,91,91,91	0
80	MG	1	3588	1/1	0.80	0.55	95,95,95,95	0
80	MG	1	3809	1/1	0.80	0.29	118,118,118,118	0
80	MG	1	3724	1/1	0.80	0.39	81,81,81,81	0
80	MG	5	3804	1/1	0.80	0.15	167,167,167,167	0
80	MG	1	3827	1/1	0.81	0.67	79,79,79,79	1
80	MG	1	3870	1/1	0.81	0.43	86,86,86,86	0
80	MG	1	3811	1/1	0.81	0.38	83,83,83,83	0
80	MG	1	3451	1/1	0.81	0.36	95,95,95,95	0
80	MG	1	3835	1/1	0.81	0.44	87,87,87,87	0
80	MG	6	2014	1/1	0.81	0.40	109,109,109,109	0
80	MG	1	3742	1/1	0.81	0.18	107,107,107,107	0
80	MG	1	3759	1/1	0.81	0.96	76,76,76,76	0
80	MG	1	3514	1/1	0.81	0.31	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3460	1/1	0.81	0.32	90,90,90,90	0
80	MG	1	3843	1/1	0.81	0.27	104,104,104,104	1
80	MG	5	3592	1/1	0.81	0.58	80,80,80,80	0
80	MG	1	3591	1/1	0.81	0.28	104,104,104,104	0
80	MG	1	3767	1/1	0.81	0.33	77,77,77,77	0
80	MG	2	1964	1/1	0.81	0.56	98,98,98,98	0
80	MG	4	209	1/1	0.81	0.64	87,87,87,87	0
80	MG	m7	202	1/1	0.81	0.33	86,86,86,86	0
80	MG	5	3788	1/1	0.81	0.37	116,116,116,116	1
80	MG	1	3570	1/1	0.82	0.61	96,96,96,96	0
80	MG	5	3522	1/1	0.82	1.02	94,94,94,94	0
80	MG	5	3782	1/1	0.82	0.31	93,93,93,93	1
80	MG	2	1930	1/1	0.82	1.44	89,89,89,89	0
80	MG	5	3723	1/1	0.82	0.28	127,127,127,127	0
80	MG	2	2013	1/1	0.82	0.33	96,96,96,96	0
80	MG	5	3801	1/1	0.82	0.58	109,109,109,109	0
80	MG	2	1951	1/1	0.82	0.34	121,121,121,121	0
80	MG	6	1923	1/1	0.82	0.30	122,122,122,122	0
80	MG	2	1958	1/1	0.82	0.33	112,112,112,112	0
80	MG	1	3614	1/1	0.82	0.30	101,101,101,101	0
80	MG	6	1928	1/1	0.82	0.14	121,121,121,121	1
80	MG	5	3432	1/1	0.82	0.24	86,86,86,86	1
80	MG	2	1978	1/1	0.82	0.07	138,138,138,138	0
80	MG	8	208	1/1	0.82	0.72	80,80,80,80	0
80	MG	2	1946	1/1	0.82	0.38	109,109,109,109	0
80	MG	5	3586	1/1	0.82	0.25	79,79,79,79	0
80	MG	5	3487	1/1	0.83	0.26	106,106,106,106	0
80	MG	6	1966	1/1	0.83	0.13	148,148,148,148	0
82	ZN	E1	501	1/1	0.83	0.04	245,245,245,245	0
80	MG	5	3775	1/1	0.83	0.18	133,133,133,133	1
80	MG	1	3844	1/1	0.83	0.37	98,98,98,98	0
80	MG	2	1905	1/1	0.83	0.25	144,144,144,144	0
80	MG	5	3831	1/1	0.83	0.67	89,89,89,89	0
80	MG	5	3514	1/1	0.83	0.29	93,93,93,93	0
80	MG	6	1956	1/1	0.83	0.51	113,113,113,113	0
80	MG	1	3796	1/1	0.83	0.35	104,104,104,104	1
80	MG	1	3730	1/1	0.83	0.37	70,70,70,70	0
80	MG	5	3599	1/1	0.83	0.27	97,97,97,97	0
80	MG	5	3517	1/1	0.83	0.17	116,116,116,116	0
80	MG	1	3640	1/1	0.83	0.31	84,84,84,84	1
80	MG	6	2018	1/1	0.83	0.09	167,167,167,167	0
81	8UZ	1	3890	33/33	0.83	0.34	108,108,108,108	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	d9	103	1/1	0.83	0.29	152,152,152,152	0
80	MG	M0	301	1/1	0.84	0.12	93,93,93,93	0
81	8UZ	2	2031	33/33	0.84	0.31	123,123,123,123	0
80	MG	5	3558	1/1	0.84	0.74	97,97,97,97	0
80	MG	1	3778	1/1	0.84	0.18	116,116,116,116	0
80	MG	2	1903	1/1	0.84	0.42	115,115,115,115	0
80	MG	7	206	1/1	0.84	0.17	142,142,142,142	0
80	MG	1	3704	1/1	0.84	0.23	94,94,94,94	0
80	MG	s8	301	1/1	0.84	0.25	110,110,110,110	0
80	MG	1	3807	1/1	0.84	0.12	139,139,139,139	0
80	MG	1	3553	1/1	0.84	0.57	90,90,90,90	0
80	MG	L7	302	1/1	0.84	0.47	89,89,89,89	0
80	MG	2	1972	1/1	0.84	0.23	132,132,132,132	0
80	MG	5	3742	1/1	0.85	0.31	92,92,92,92	0
80	MG	5	3553	1/1	0.85	0.13	145,145,145,145	0
80	MG	1	3731	1/1	0.85	0.26	71,71,71,71	0
80	MG	5	3818	1/1	0.85	1.71	91,91,91,91	0
80	MG	5	3693	1/1	0.85	0.10	108,108,108,108	0
80	MG	2	1992	1/1	0.85	0.54	145,145,145,145	0
80	MG	2	2002	1/1	0.85	0.32	120,120,120,120	0
80	MG	5	3624	1/1	0.85	0.57	84,84,84,84	0
80	MG	5	3830	1/1	0.85	0.26	130,130,130,130	0
80	MG	1	3584	1/1	0.85	0.32	88,88,88,88	0
80	MG	5	3835	1/1	0.85	0.48	101,101,101,101	0
80	MG	q2	502	1/1	0.85	0.41	109,109,109,109	0
80	MG	2	1933	1/1	0.85	0.12	137,137,137,137	0
80	MG	5	3547	1/1	0.85	0.29	130,130,130,130	0
80	MG	5	3692	1/1	0.85	0.30	137,137,137,137	0
80	MG	2	1932	1/1	0.85	0.28	120,120,120,120	0
80	MG	L9	201	1/1	0.85	0.29	111,111,111,111	0
80	MG	2	1967	1/1	0.85	0.49	103,103,103,103	0
80	MG	5	3776	1/1	0.85	0.18	107,107,107,107	1
80	MG	5	3501	1/1	0.85	0.51	100,100,100,100	0
80	MG	5	3647	1/1	0.85	0.47	71,71,71,71	0
80	MG	5	3527	1/1	0.86	0.48	93,93,93,93	0
81	8UZ	1	3888	33/33	0.86	0.18	127,127,127,127	0
80	MG	5	3823	1/1	0.86	0.24	113,113,113,113	0
80	MG	5	3406	1/1	0.86	0.51	79,79,79,79	0
80	MG	L6	203	1/1	0.86	1.03	101,101,101,101	0
80	MG	7	203	1/1	0.86	0.14	172,172,172,172	0
80	MG	5	3609	1/1	0.86	0.13	104,104,104,104	0
80	MG	1	3684	1/1	0.86	0.39	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3460	1/1	0.86	0.59	95,95,95,95	0
80	MG	1	3833	1/1	0.86	0.36	98,98,98,98	0
80	MG	1	3688	1/1	0.86	0.26	97,97,97,97	0
80	MG	5	3848	1/1	0.86	0.21	138,138,138,138	0
80	MG	2	1928	1/1	0.86	0.42	143,143,143,143	0
80	MG	6	1948	1/1	0.87	0.34	111,111,111,111	0
80	MG	6	1902	1/1	0.87	0.36	111,111,111,111	0
80	MG	6	1987	1/1	0.87	0.09	142,142,142,142	0
80	MG	8	204	1/1	0.87	0.29	109,109,109,109	0
80	MG	1	3443	1/1	0.87	0.44	86,86,86,86	0
80	MG	5	3492	1/1	0.87	0.65	100,100,100,100	0
81	8UZ	1	3894	33/33	0.87	0.34	126,126,126,126	0
80	MG	5	3727	1/1	0.87	0.76	72,72,72,72	0
80	MG	5	3791	1/1	0.88	0.20	111,111,111,111	0
80	MG	2	1980	1/1	0.88	0.15	136,136,136,136	0
81	8UZ	4	220	33/33	0.88	0.31	103,103,103,103	0
80	MG	6	2002	1/1	0.88	0.59	114,114,114,114	0
80	MG	5	3611	1/1	0.88	0.31	111,111,111,111	0
80	MG	5	3469	1/1	0.88	0.10	147,147,147,147	0
80	MG	M5	303	1/1	0.88	0.15	111,111,111,111	0
80	MG	1	3776	1/1	0.88	0.46	108,108,108,108	0
80	MG	1	3555	1/1	0.88	0.23	89,89,89,89	0
80	MG	2	1975	1/1	0.88	0.28	132,132,132,132	0
80	MG	1	3846	1/1	0.88	0.26	91,91,91,91	0
80	MG	5	3585	1/1	0.88	0.46	93,93,93,93	0
80	MG	2	2014	1/1	0.88	0.31	104,104,104,104	0
80	MG	6	1980	1/1	0.88	1.02	116,116,116,116	0
80	MG	1	3673	1/1	0.88	0.55	93,93,93,93	0
80	MG	1	3429	1/1	0.88	0.27	111,111,111,111	0
80	MG	6	1984	1/1	0.88	0.20	136,136,136,136	0
80	MG	5	3792	1/1	0.88	0.21	110,110,110,110	0
80	MG	1	3750	1/1	0.88	1.24	89,89,89,89	0
80	MG	1	3716	1/1	0.88	0.35	84,84,84,84	0
80	MG	1	3866	1/1	0.88	0.23	130,130,130,130	0
80	MG	1	3830	1/1	0.88	0.16	86,86,86,86	0
80	MG	1	3484	1/1	0.89	0.20	84,84,84,84	1
80	MG	5	3810	1/1	0.89	0.31	83,83,83,83	0
80	MG	2	1971	1/1	0.89	0.37	127,127,127,127	0
80	MG	5	3433	1/1	0.89	0.30	85,85,85,85	0
80	MG	1	3656	1/1	0.89	0.42	97,97,97,97	0
80	MG	1	3449	1/1	0.89	0.32	97,97,97,97	0
80	MG	1	3531	1/1	0.89	0.36	88,88,88,88	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	2	1935	1/1	0.89	0.13	144,144,144,144	0
80	MG	1	3628	1/1	0.89	1.11	77,77,77,77	0
80	MG	1	3797	1/1	0.89	0.17	148,148,148,148	0
80	MG	1	3707	1/1	0.89	0.27	83,83,83,83	1
80	MG	1	3884	1/1	0.89	1.09	90,90,90,90	0
80	MG	1	3705	1/1	0.89	0.31	82,82,82,82	0
80	MG	5	3402	1/1	0.89	0.50	73,73,73,73	0
80	MG	5	3465	1/1	0.89	0.22	110,110,110,110	1
80	MG	1	3538	1/1	0.89	0.36	83,83,83,83	0
80	MG	5	3808	1/1	0.89	0.20	99,99,99,99	0
80	MG	5	3689	1/1	0.89	0.27	120,120,120,120	0
80	MG	2	1911	1/1	0.89	0.42	113,113,113,113	0
80	MG	1	3516	1/1	0.89	0.12	97,97,97,97	1
80	MG	1	3852	1/1	0.89	0.72	100,100,100,100	0
80	MG	1	3478	1/1	0.89	0.24	84,84,84,84	0
80	MG	2	2007	1/1	0.89	0.15	140,140,140,140	0
80	MG	5	3597	1/1	0.89	0.25	86,86,86,86	0
80	MG	5	3458	1/1	0.89	0.99	97,97,97,97	0
80	MG	1	3857	1/1	0.89	0.23	123,123,123,123	0
80	MG	l3	403	1/1	0.90	0.17	87,87,87,87	1
80	MG	5	3468	1/1	0.90	0.12	135,135,135,135	0
80	MG	5	3685	1/1	0.90	0.26	95,95,95,95	0
80	MG	1	3554	1/1	0.90	0.29	87,87,87,87	0
80	MG	5	3838	1/1	0.90	0.13	154,154,154,154	0
80	MG	N6	201	1/1	0.90	1.42	103,103,103,103	1
80	MG	5	3629	1/1	0.90	0.19	109,109,109,109	0
80	MG	5	3663	1/1	0.90	0.23	85,85,85,85	1
80	MG	5	3554	1/1	0.90	0.06	151,151,151,151	0
80	MG	5	3770	1/1	0.90	0.59	102,102,102,102	0
80	MG	5	3448	1/1	0.90	0.39	83,83,83,83	0
80	MG	5	3816	1/1	0.90	0.43	66,66,66,66	0
80	MG	1	3646	1/1	0.90	0.25	85,85,85,85	0
80	MG	6	2022	1/1	0.90	0.09	137,137,137,137	0
80	MG	5	3729	1/1	0.90	0.89	81,81,81,81	0
80	MG	1	3503	1/1	0.90	0.18	103,103,103,103	0
80	MG	5	3842	1/1	0.90	0.36	137,137,137,137	0
80	MG	1	3875	1/1	0.90	0.27	89,89,89,89	0
80	MG	2	1979	1/1	0.90	0.22	144,144,144,144	0
80	MG	SM	302	1/1	0.90	0.28	114,114,114,114	0
80	MG	1	3615	1/1	0.90	0.10	93,93,93,93	1
80	MG	1	3768	1/1	0.90	0.36	69,69,69,69	0
80	MG	1	3621	1/1	0.90	0.09	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	O7	103	1/1	0.90	0.42	95,95,95,95	1
80	MG	6	1925	1/1	0.90	0.47	118,118,118,118	0
80	MG	5	3665	1/1	0.90	0.18	123,123,123,123	0
80	MG	1	3743	1/1	0.90	0.20	109,109,109,109	0
80	MG	5	3690	1/1	0.90	0.45	112,112,112,112	0
81	8UZ	2	2029	33/33	0.90	0.18	134,134,134,134	0
80	MG	6	1974	1/1	0.90	0.24	137,137,137,137	0
80	MG	3	209	1/1	0.90	0.09	138,138,138,138	0
80	MG	C9	201	1/1	0.91	0.10	152,152,152,152	0
80	MG	5	3844	1/1	0.91	0.36	93,93,93,93	0
80	MG	5	3684	1/1	0.91	0.49	93,93,93,93	0
80	MG	S6	301	1/1	0.91	0.06	172,172,172,172	0
80	MG	6	2028	1/1	0.91	0.43	113,113,113,113	0
80	MG	1	3592	1/1	0.91	0.19	90,90,90,90	0
80	MG	SM	301	1/1	0.91	0.28	123,123,123,123	0
80	MG	2	1974	1/1	0.91	0.17	137,137,137,137	0
80	MG	1	3765	1/1	0.91	0.21	92,92,92,92	0
80	MG	1	3445	1/1	0.91	0.40	79,79,79,79	0
80	MG	5	3704	1/1	0.91	0.70	73,73,73,73	0
80	MG	1	3412	1/1	0.91	0.28	92,92,92,92	0
80	MG	5	3656	1/1	0.91	0.20	88,88,88,88	0
81	8UZ	3	214	33/33	0.91	0.18	99,99,99,99	0
80	MG	6	1958	1/1	0.91	0.62	97,97,97,97	0
81	8UZ	1	3892	33/33	0.91	0.29	110,110,110,110	0
80	MG	1	3488	1/1	0.91	0.40	74,74,74,74	0
80	MG	5	3837	1/1	0.91	0.35	123,123,123,123	0
80	MG	5	3763	1/1	0.91	0.20	89,89,89,89	1
80	MG	1	3634	1/1	0.91	0.21	80,80,80,80	1
80	MG	5	3534	1/1	0.91	0.41	96,96,96,96	0
80	MG	6	2024	1/1	0.91	0.38	101,101,101,101	1
80	MG	1	3404	1/1	0.91	0.77	87,87,87,87	0
80	MG	1	3426	1/1	0.91	0.79	94,94,94,94	0
80	MG	1	3849	1/1	0.91	0.38	74,74,74,74	0
80	MG	1	3881	1/1	0.91	0.18	127,127,127,127	0
80	MG	2	1985	1/1	0.91	0.09	156,156,156,156	0
80	MG	6	1942	1/1	0.91	0.25	129,129,129,129	0
80	MG	5	3827	1/1	0.91	0.49	91,91,91,91	1
80	MG	1	3539	1/1	0.91	0.39	85,85,85,85	0
80	MG	5	3563	1/1	0.91	0.17	121,121,121,121	0
80	MG	5	3777	1/1	0.91	0.17	124,124,124,124	0
80	MG	6	2004	1/1	0.91	0.35	132,132,132,132	0
80	MG	2	1934	1/1	0.91	0.20	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3601	1/1	0.92	0.10	114,114,114,114	0
80	MG	1	3777	1/1	0.92	0.12	86,86,86,86	1
80	MG	5	3666	1/1	0.92	0.55	143,143,143,143	0
80	MG	C4	201	1/1	0.92	0.09	144,144,144,144	0
80	MG	6	1998	1/1	0.92	0.06	149,149,149,149	0
80	MG	5	3716	1/1	0.92	0.13	102,102,102,102	0
80	MG	4	212	1/1	0.92	0.36	72,72,72,72	0
80	MG	5	3673	1/1	0.92	0.58	84,84,84,84	0
80	MG	5	3414	1/1	0.92	0.27	94,94,94,94	0
80	MG	5	3428	1/1	0.92	0.45	80,80,80,80	0
80	MG	8	209	1/1	0.92	0.10	117,117,117,117	0
80	MG	5	3825	1/1	0.92	0.15	149,149,149,149	0
80	MG	6	2058	1/1	0.92	0.20	113,113,113,113	0
80	MG	5	3821	1/1	0.92	0.20	145,145,145,145	0
80	MG	1	3788	1/1	0.92	0.21	101,101,101,101	1
81	8UZ	5	3854	33/33	0.92	0.22	117,117,117,117	0
80	MG	2	1952	1/1	0.92	0.20	115,115,115,115	0
80	MG	1	3532	1/1	0.92	0.60	83,83,83,83	0
80	MG	5	3798	1/1	0.92	0.19	130,130,130,130	0
80	MG	5	3542	1/1	0.92	0.30	110,110,110,110	0
80	MG	5	3754	1/1	0.92	0.26	85,85,85,85	0
80	MG	2	1986	1/1	0.92	0.08	144,144,144,144	0
80	MG	6	2001	1/1	0.92	0.18	142,142,142,142	0
80	MG	2	1918	1/1	0.92	0.17	122,122,122,122	0
80	MG	5	3712	1/1	0.92	0.13	92,92,92,92	1
80	MG	3	211	1/1	0.92	0.09	140,140,140,140	0
80	MG	1	3557	1/1	0.92	0.45	88,88,88,88	0
80	MG	1	3702	1/1	0.92	0.32	81,81,81,81	0
80	MG	5	3467	1/1	0.92	0.09	143,143,143,143	0
80	MG	1	3764	1/1	0.92	0.39	92,92,92,92	0
80	MG	5	3417	1/1	0.92	0.18	91,91,91,91	0
80	MG	2	1921	1/1	0.92	0.15	120,120,120,120	0
80	MG	1	3726	1/1	0.92	0.47	72,72,72,72	0
80	MG	1	3689	1/1	0.92	0.18	85,85,85,85	1
80	MG	1	3748	1/1	0.92	0.67	83,83,83,83	0
80	MG	5	3505	1/1	0.92	0.24	86,86,86,86	0
80	MG	5	3809	1/1	0.92	0.29	87,87,87,87	0
80	MG	5	3674	1/1	0.92	0.15	133,133,133,133	0
80	MG	2	1987	1/1	0.92	0.07	164,164,164,164	0
80	MG	1	3662	1/1	0.93	0.27	94,94,94,94	0
80	MG	2	1938	1/1	0.93	0.27	116,116,116,116	0
80	MG	2	1910	1/1	0.93	0.11	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3753	1/1	0.93	0.24	81,81,81,81	0
80	MG	5	3474	1/1	0.93	0.16	148,148,148,148	0
80	MG	5	3717	1/1	0.93	0.11	100,100,100,100	0
80	MG	5	3578	1/1	0.93	0.32	87,87,87,87	0
80	MG	5	3450	1/1	0.93	0.24	88,88,88,88	0
80	MG	1	3758	1/1	0.93	0.37	76,76,76,76	0
80	MG	1	3762	1/1	0.93	0.27	90,90,90,90	0
81	8UZ	5	3853	33/33	0.93	0.21	91,91,91,91	33
80	MG	5	3633	1/1	0.93	0.06	112,112,112,112	0
80	MG	3	202	1/1	0.93	0.31	93,93,93,93	0
81	8UZ	1	3887	33/33	0.93	0.17	120,120,120,120	0
80	MG	5	3442	1/1	0.93	0.51	83,83,83,83	0
80	MG	5	3452	1/1	0.93	0.43	84,84,84,84	0
80	MG	17	301	1/1	0.93	0.34	79,79,79,79	0
80	MG	5	3626	1/1	0.93	0.36	89,89,89,89	0
80	MG	2	1970	1/1	0.93	0.09	133,133,133,133	0
80	MG	1	3787	1/1	0.93	0.44	85,85,85,85	1
80	MG	1	3405	1/1	0.93	0.40	84,84,84,84	0
80	MG	2	1931	1/1	0.93	0.22	116,116,116,116	0
81	8UZ	1	3895	33/33	0.93	0.15	119,119,119,119	0
80	MG	6	2006	1/1	0.93	0.21	136,136,136,136	0
80	MG	1	3501	1/1	0.93	0.12	109,109,109,109	0
80	MG	2	1982	1/1	0.93	0.18	139,139,139,139	0
80	MG	1	3401	1/1	0.93	0.55	84,84,84,84	0
80	MG	6	1937	1/1	0.93	0.18	111,111,111,111	0
80	MG	6	1962	1/1	0.93	0.11	131,131,131,131	0
80	MG	5	3749	1/1	0.93	0.21	108,108,108,108	0
80	MG	5	3659	1/1	0.93	0.15	128,128,128,128	0
80	MG	1	3824	1/1	0.93	0.10	117,117,117,117	0
80	MG	1	3678	1/1	0.93	0.37	79,79,79,79	0
81	8UZ	1	3891	33/33	0.93	0.23	89,89,89,89	0
80	MG	6	1977	1/1	0.93	0.13	142,142,142,142	0
80	MG	5	3490	1/1	0.93	1.22	85,85,85,85	0
80	MG	6	1936	1/1	0.93	0.36	106,106,106,106	0
80	MG	L3	402	1/1	0.93	0.24	86,86,86,86	0
80	MG	M7	203	1/1	0.93	0.24	78,78,78,78	0
80	MG	8	210	1/1	0.93	0.43	123,123,123,123	0
80	MG	1	3583	1/1	0.93	0.10	128,128,128,128	0
80	MG	6	1930	1/1	0.94	0.22	117,117,117,117	0
80	MG	5	3579	1/1	0.94	0.34	91,91,91,91	0
80	MG	6	1907	1/1	0.94	0.14	117,117,117,117	0
80	MG	1	3490	1/1	0.94	0.32	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3528	1/1	0.94	0.23	94,94,94,94	1
80	MG	1	3735	1/1	0.94	0.15	83,83,83,83	0
80	MG	5	3590	1/1	0.94	0.19	79,79,79,79	0
80	MG	1	3417	1/1	0.94	0.26	80,80,80,80	0
80	MG	2	1948	1/1	0.94	0.27	134,134,134,134	0
80	MG	1	3818	1/1	0.94	0.18	81,81,81,81	1
80	MG	1	3837	1/1	0.94	0.36	80,80,80,80	0
80	MG	1	3651	1/1	0.94	0.67	79,79,79,79	0
80	MG	5	3422	1/1	0.94	0.22	90,90,90,90	0
80	MG	6	2027	1/1	0.94	0.23	137,137,137,137	0
80	MG	1	3736	1/1	0.94	0.26	101,101,101,101	0
80	MG	1	3540	1/1	0.94	0.49	84,84,84,84	0
80	MG	c9	201	1/1	0.94	0.07	139,139,139,139	0
80	MG	1	3631	1/1	0.94	0.26	78,78,78,78	1
80	MG	5	3807	1/1	0.94	0.46	97,97,97,97	0
80	MG	2	1936	1/1	0.94	0.15	131,131,131,131	0
80	MG	4	201	1/1	0.94	0.28	100,100,100,100	0
80	MG	4	217	1/1	0.94	0.37	93,93,93,93	0
80	MG	1	3474	1/1	0.94	0.24	83,83,83,83	0
80	MG	2	1984	1/1	0.94	0.12	151,151,151,151	0
80	MG	1	3597	1/1	0.94	0.16	93,93,93,93	0
82	ZN	O4	501	1/1	0.94	0.08	181,181,181,181	0
80	MG	2	2015	1/1	0.94	0.35	126,126,126,126	0
80	MG	5	3741	1/1	0.94	0.34	115,115,115,115	0
80	MG	6	1912	1/1	0.94	0.16	116,116,116,116	0
80	MG	2	1998	1/1	0.94	0.71	118,118,118,118	0
80	MG	1	3649	1/1	0.94	0.22	84,84,84,84	1
80	MG	1	3414	1/1	0.94	0.25	85,85,85,85	0
80	MG	6	2007	1/1	0.94	0.11	144,144,144,144	0
80	MG	5	3479	1/1	0.94	0.32	119,119,119,119	0
80	MG	1	3565	1/1	0.94	0.32	94,94,94,94	0
80	MG	1	3612	1/1	0.94	0.30	94,94,94,94	0
80	MG	2	1912	1/1	0.94	0.11	125,125,125,125	0
80	MG	5	3730	1/1	0.94	0.20	95,95,95,95	1
80	MG	1	3625	1/1	0.94	1.33	96,96,96,96	0
80	MG	6	2055	1/1	0.94	0.34	97,97,97,97	1
80	MG	5	3434	1/1	0.94	0.10	93,93,93,93	0
80	MG	2	1925	1/1	0.94	0.05	158,158,158,158	0
80	MG	5	3408	1/1	0.94	0.30	81,81,81,81	0
80	MG	1	3681	1/1	0.94	0.26	78,78,78,78	0
80	MG	1	3878	1/1	0.94	0.23	97,97,97,97	0
80	MG	1	3850	1/1	0.94	0.61	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3540	1/1	0.94	0.15	110,110,110,110	0
80	MG	1	3521	1/1	0.94	0.36	114,114,114,114	0
80	MG	5	3718	1/1	0.94	0.35	97,97,97,97	0
80	MG	5	3655	1/1	0.95	0.28	95,95,95,95	0
80	MG	3	204	1/1	0.95	0.11	127,127,127,127	0
80	MG	1	3422	1/1	0.95	0.27	97,97,97,97	0
80	MG	1	3568	1/1	0.95	0.60	102,102,102,102	0
80	MG	2	1907	1/1	0.95	0.11	168,168,168,168	0
80	MG	1	3838	1/1	0.95	0.34	75,75,75,75	0
80	MG	5	3520	1/1	0.95	0.45	123,123,123,123	0
80	MG	1	3874	1/1	0.95	0.54	89,89,89,89	0
80	MG	2	1902	1/1	0.95	0.18	115,115,115,115	1
80	MG	6	1919	1/1	0.95	0.11	137,137,137,137	0
80	MG	5	3475	1/1	0.95	0.14	146,146,146,146	0
80	MG	L6	201	1/1	0.95	0.11	114,114,114,114	0
80	MG	5	3405	1/1	0.95	0.46	79,79,79,79	0
80	MG	d9	102	1/1	0.95	0.09	171,171,171,171	0
80	MG	5	3412	1/1	0.95	0.10	99,99,99,99	0
80	MG	1	3616	1/1	0.95	0.29	85,85,85,85	0
80	MG	6	1999	1/1	0.95	0.14	146,146,146,146	0
80	MG	6	2017	1/1	0.95	0.07	119,119,119,119	0
80	MG	2	2021	1/1	0.95	0.32	135,135,135,135	0
80	MG	1	3626	1/1	0.95	0.18	104,104,104,104	0
80	MG	1	3430	1/1	0.95	0.17	104,104,104,104	0
80	MG	6	1933	1/1	0.95	0.15	109,109,109,109	0
80	MG	c8	202	1/1	0.95	0.07	149,149,149,149	0
80	MG	5	3679	1/1	0.95	0.19	107,107,107,107	0
80	MG	1	3556	1/1	0.95	0.21	91,91,91,91	0
80	MG	5	3415	1/1	0.95	0.23	92,92,92,92	0
80	MG	5	3683	1/1	0.95	0.31	116,116,116,116	0
80	MG	1	3714	1/1	0.95	0.22	81,81,81,81	0
80	MG	5	3453	1/1	0.95	0.34	88,88,88,88	0
80	MG	1	3821	1/1	0.95	0.17	89,89,89,89	0
80	MG	1	3635	1/1	0.95	0.30	76,76,76,76	0
80	MG	5	3536	1/1	0.95	0.10	106,106,106,106	0
80	MG	2	2003	1/1	0.95	0.24	113,113,113,113	1
80	MG	5	3503	1/1	0.95	0.39	96,96,96,96	0
80	MG	5	3732	1/1	0.95	0.54	91,91,91,91	0
80	MG	1	3710	1/1	0.95	0.22	84,84,84,84	0
80	MG	1	3604	1/1	0.95	0.12	105,105,105,105	0
80	MG	l2	301	1/1	0.95	0.38	93,93,93,93	0
80	MG	1	3855	1/1	0.95	0.20	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	2	1959	1/1	0.95	0.20	129,129,129,129	0
80	MG	6	1931	1/1	0.95	0.44	107,107,107,107	0
80	MG	1	3543	1/1	0.95	0.54	72,72,72,72	0
80	MG	1	3546	1/1	0.95	0.71	77,77,77,77	0
80	MG	5	3799	1/1	0.95	0.12	110,110,110,110	1
80	MG	N7	201	1/1	0.95	0.34	138,138,138,138	0
80	MG	7	204	1/1	0.95	0.12	170,170,170,170	0
80	MG	5	3575	1/1	0.95	0.14	95,95,95,95	0
80	MG	1	3790	1/1	0.95	0.19	89,89,89,89	1
80	MG	2	1965	1/1	0.95	0.12	127,127,127,127	0
80	MG	2	1962	1/1	0.95	0.19	134,134,134,134	0
80	MG	1	3693	1/1	0.95	0.36	73,73,73,73	0
80	MG	1	3487	1/1	0.95	0.33	83,83,83,83	0
80	MG	1	3415	1/1	0.95	0.27	81,81,81,81	0
80	MG	2	1920	1/1	0.95	0.24	116,116,116,116	0
80	MG	1	3606	1/1	0.95	0.31	97,97,97,97	0
80	MG	5	3499	1/1	0.95	0.63	97,97,97,97	0
80	MG	5	3594	1/1	0.95	0.39	91,91,91,91	0
80	MG	5	3418	1/1	0.95	0.35	79,79,79,79	0
80	MG	1	3810	1/1	0.95	0.22	82,82,82,82	0
80	MG	1	3686	1/1	0.96	0.25	85,85,85,85	0
80	MG	5	3472	1/1	0.96	0.09	130,130,130,130	0
80	MG	1	3424	1/1	0.96	0.20	111,111,111,111	0
80	MG	1	3643	1/1	0.96	0.34	75,75,75,75	0
80	MG	C6	201	1/1	0.96	0.07	173,173,173,173	0
80	MG	1	3752	1/1	0.96	0.23	81,81,81,81	0
80	MG	D2	201	1/1	0.96	0.15	139,139,139,139	0
80	MG	1	3754	1/1	0.96	0.32	80,80,80,80	0
80	MG	1	3439	1/1	0.96	0.06	118,118,118,118	0
80	MG	6	1943	1/1	0.96	0.10	136,136,136,136	0
80	MG	1	3613	1/1	0.96	0.19	99,99,99,99	0
80	MG	5	3589	1/1	0.96	0.20	82,82,82,82	0
80	MG	5	3756	1/1	0.96	0.22	93,93,93,93	0
80	MG	1	3756	1/1	0.96	0.27	76,76,76,76	0
80	MG	1	3694	1/1	0.96	0.15	70,70,70,70	0
80	MG	2	1966	1/1	0.96	0.10	134,134,134,134	1
80	MG	1	3558	1/1	0.96	0.35	113,113,113,113	0
80	MG	5	3545	1/1	0.96	0.13	130,130,130,130	0
80	MG	1	3825	1/1	0.96	0.22	97,97,97,97	0
80	MG	1	3698	1/1	0.96	0.31	82,82,82,82	0
80	MG	1	3696	1/1	0.96	0.18	86,86,86,86	0
80	MG	5	3630	1/1	0.96	0.13	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3451	1/1	0.96	0.24	80,80,80,80	0
80	MG	5	3675	1/1	0.96	0.33	96,96,96,96	0
80	MG	1	3475	1/1	0.96	0.30	84,84,84,84	0
80	MG	1	3454	1/1	0.96	0.22	92,92,92,92	0
80	MG	5	3699	1/1	0.96	0.25	97,97,97,97	1
80	MG	5	3494	1/1	0.96	0.24	97,97,97,97	0
80	MG	1	3595	1/1	0.96	0.47	84,84,84,84	0
80	MG	1	3435	1/1	0.96	0.17	103,103,103,103	1
80	MG	1	3458	1/1	0.96	0.07	106,106,106,106	0
80	MG	5	3429	1/1	0.96	0.23	80,80,80,80	0
80	MG	5	3646	1/1	0.96	0.40	85,85,85,85	0
80	MG	1	3466	1/1	0.96	0.09	115,115,115,115	0
80	MG	1	3840	1/1	0.96	0.24	99,99,99,99	0
80	MG	5	3577	1/1	0.96	0.24	96,96,96,96	0
80	MG	2	1919	1/1	0.96	0.27	122,122,122,122	0
80	MG	6	2057	1/1	0.96	0.20	130,130,130,130	0
80	MG	5	3790	1/1	0.96	0.20	90,90,90,90	0
80	MG	1	3647	1/1	0.96	0.41	78,78,78,78	0
80	MG	5	3421	1/1	0.96	0.30	91,91,91,91	0
80	MG	5	3401	1/1	0.96	0.44	77,77,77,77	0
80	MG	6	1932	1/1	0.96	0.26	112,112,112,112	0
80	MG	5	3561	1/1	0.96	0.15	130,130,130,130	0
80	MG	5	3815	1/1	0.96	0.15	97,97,97,97	1
80	MG	6	1997	1/1	0.96	0.33	137,137,137,137	0
80	MG	2	1983	1/1	0.96	0.11	138,138,138,138	0
80	MG	1	3873	1/1	0.96	0.12	135,135,135,135	0
80	MG	7	207	1/1	0.96	0.38	102,102,102,102	0
80	MG	1	3672	1/1	0.96	0.25	103,103,103,103	0
80	MG	1	3803	1/1	0.96	0.57	89,89,89,89	1
80	MG	6	2012	1/1	0.96	0.06	131,131,131,131	0
80	MG	1	3692	1/1	0.96	0.33	79,79,79,79	0
80	MG	1	3479	1/1	0.96	0.31	83,83,83,83	0
80	MG	1	3493	1/1	0.96	0.21	90,90,90,90	1
80	MG	1	3419	1/1	0.96	0.31	81,81,81,81	0
80	MG	5	3719	1/1	0.96	0.84	77,77,77,77	1
80	MG	6	1914	1/1	0.96	0.30	109,109,109,109	0
80	MG	2	2020	1/1	0.97	0.32	155,155,155,155	0
80	MG	1	3653	1/1	0.97	0.21	87,87,87,87	0
80	MG	5	3755	1/1	0.97	0.10	90,90,90,90	1
80	MG	1	3723	1/1	0.97	0.28	79,79,79,79	0
80	MG	6	2011	1/1	0.97	0.27	132,132,132,132	0
80	MG	5	3739	1/1	0.97	0.22	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3676	1/1	0.97	0.31	80,80,80,80	0
80	MG	5	3746	1/1	0.97	0.34	82,82,82,82	0
80	MG	6	2052	1/1	0.97	0.25	179,179,179,179	0
80	MG	1	3518	1/1	0.97	0.25	96,96,96,96	0
80	MG	6	1949	1/1	0.97	0.16	114,114,114,114	0
80	MG	1	3622	1/1	0.97	0.20	110,110,110,110	0
80	MG	5	3531	1/1	0.97	0.38	84,84,84,84	0
80	MG	1	3836	1/1	0.97	0.31	98,98,98,98	0
80	MG	5	3537	1/1	0.97	0.23	105,105,105,105	0
80	MG	1	3511	1/1	0.97	0.19	102,102,102,102	0
80	MG	5	3560	1/1	0.97	0.20	130,130,130,130	0
80	MG	1	3471	1/1	0.97	0.39	89,89,89,89	0
80	MG	5	3523	1/1	0.97	0.30	93,93,93,93	0
80	MG	1	3826	1/1	0.97	0.75	105,105,105,105	0
80	MG	6	1951	1/1	0.97	0.28	102,102,102,102	0
80	MG	1	3632	1/1	0.97	0.08	88,88,88,88	0
80	MG	5	3582	1/1	0.97	0.44	89,89,89,89	0
80	MG	1	3637	1/1	0.97	0.40	70,70,70,70	0
80	MG	1	3657	1/1	0.97	0.30	94,94,94,94	0
82	ZN	q2	501	1/1	0.97	0.14	211,211,211,211	0
80	MG	5	3720	1/1	0.97	0.20	113,113,113,113	0
80	MG	1	3527	1/1	0.97	0.29	86,86,86,86	0
80	MG	5	3745	1/1	0.97	0.19	135,135,135,135	0
80	MG	6	1952	1/1	0.97	0.36	105,105,105,105	0
80	MG	6	1990	1/1	0.97	0.21	153,153,153,153	0
80	MG	1	3770	1/1	0.97	0.11	100,100,100,100	0
80	MG	5	3677	1/1	0.97	0.18	106,106,106,106	0
80	MG	1	3476	1/1	0.97	0.24	82,82,82,82	0
80	MG	6	1918	1/1	0.97	0.06	134,134,134,134	0
80	MG	5	3576	1/1	0.97	0.59	90,90,90,90	0
80	MG	5	3642	1/1	0.97	0.15	106,106,106,106	0
80	MG	5	3446	1/1	0.97	0.10	84,84,84,84	0
80	MG	1	3433	1/1	0.97	0.11	96,96,96,96	0
80	MG	1	3733	1/1	0.97	0.29	73,73,73,73	0
80	MG	5	3530	1/1	0.97	0.14	93,93,93,93	0
80	MG	5	3587	1/1	0.97	0.20	90,90,90,90	0
80	MG	1	3467	1/1	0.97	0.17	100,100,100,100	0
80	MG	1	3574	1/1	0.97	0.30	85,85,85,85	0
80	MG	2	2009	1/1	0.97	0.22	132,132,132,132	0
82	ZN	q3	501	1/1	0.97	0.12	138,138,138,138	0
80	MG	1	3494	1/1	0.97	0.45	83,83,83,83	0
80	MG	1	3839	1/1	0.97	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	1	3700	1/1	0.97	0.27	81,81,81,81	0
80	MG	1	3473	1/1	0.97	0.61	78,78,78,78	0
80	MG	6	1953	1/1	0.97	0.28	105,105,105,105	0
80	MG	S4	301	1/1	0.97	0.19	135,135,135,135	0
80	MG	1	3581	1/1	0.97	0.18	102,102,102,102	0
80	MG	1	3652	1/1	0.97	0.26	86,86,86,86	0
82	ZN	o4	501	1/1	0.97	0.06	182,182,182,182	0
80	MG	5	3634	1/1	0.97	0.09	150,150,150,150	0
80	MG	m7	201	1/1	0.97	0.22	93,93,93,93	0
80	MG	1	3497	1/1	0.97	0.21	98,98,98,98	0
80	MG	1	3607	1/1	0.97	0.16	102,102,102,102	1
80	MG	5	3709	1/1	0.97	0.19	110,110,110,110	0
80	MG	1	3882	1/1	0.97	0.28	146,146,146,146	0
80	MG	L7	301	1/1	0.97	0.27	83,83,83,83	0
80	MG	1	3725	1/1	0.97	0.18	75,75,75,75	0
80	MG	1	3781	1/1	0.97	0.21	84,84,84,84	1
80	MG	5	3581	1/1	0.97	0.23	100,100,100,100	1
80	MG	1	3486	1/1	0.97	0.40	83,83,83,83	0
80	MG	6	1924	1/1	0.97	0.51	116,116,116,116	0
80	MG	M5	302	1/1	0.97	0.33	97,97,97,97	0
80	MG	5	3648	1/1	0.97	0.30	80,80,80,80	0
80	MG	1	3438	1/1	0.97	0.11	106,106,106,106	0
80	MG	1	3627	1/1	0.97	0.26	80,80,80,80	0
80	MG	1	3791	1/1	0.97	0.22	88,88,88,88	0
80	MG	1	3701	1/1	0.97	0.35	87,87,87,87	0
80	MG	1	3869	1/1	0.97	0.27	165,165,165,165	0
80	MG	1	3871	1/1	0.97	0.23	97,97,97,97	1
80	MG	1	3453	1/1	0.97	0.14	94,94,94,94	0
80	MG	1	3533	1/1	0.97	0.40	82,82,82,82	0
80	MG	6	2005	1/1	0.97	1.06	93,93,93,93	0
80	MG	6	2019	1/1	0.97	0.16	116,116,116,116	0
80	MG	1	3437	1/1	0.98	0.14	103,103,103,103	0
80	MG	1	3585	1/1	0.98	0.26	84,84,84,84	0
80	MG	5	3700	1/1	0.98	0.23	101,101,101,101	0
80	MG	5	3495	1/1	0.98	0.45	92,92,92,92	0
80	MG	5	3441	1/1	0.98	0.19	86,86,86,86	0
80	MG	5	3849	1/1	0.98	0.07	150,150,150,150	0
80	MG	5	3631	1/1	0.98	0.20	125,125,125,125	0
80	MG	5	3600	1/1	0.98	0.27	100,100,100,100	0
80	MG	5	3403	1/1	0.98	0.35	82,82,82,82	0
80	MG	1	3522	1/1	0.98	0.06	115,115,115,115	0
80	MG	1	3629	1/1	0.98	0.67	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3786	1/1	0.98	0.19	104,104,104,104	0
80	MG	5	3622	1/1	0.98	0.25	84,84,84,84	0
80	MG	5	3615	1/1	0.98	0.21	128,128,128,128	0
80	MG	1	3402	1/1	0.98	0.34	91,91,91,91	0
80	MG	6	1929	1/1	0.98	0.12	121,121,121,121	0
80	MG	5	3574	1/1	0.98	0.24	99,99,99,99	0
80	MG	1	3648	1/1	0.98	0.23	77,77,77,77	0
80	MG	6	2020	1/1	0.98	0.11	174,174,174,174	0
80	MG	6	1906	1/1	0.98	0.23	112,112,112,112	0
80	MG	1	3529	1/1	0.98	0.29	85,85,85,85	0
80	MG	5	3681	1/1	0.98	0.07	103,103,103,103	0
80	MG	1	3513	1/1	0.98	0.11	103,103,103,103	1
80	MG	5	3710	1/1	0.98	0.25	105,105,105,105	0
80	MG	5	3793	1/1	0.98	0.29	97,97,97,97	1
80	MG	5	3625	1/1	0.98	0.34	85,85,85,85	0
80	MG	1	3691	1/1	0.98	0.16	81,81,81,81	0
80	MG	1	3816	1/1	0.98	0.43	99,99,99,99	1
80	MG	1	3602	1/1	0.98	0.16	115,115,115,115	0
80	MG	1	3489	1/1	0.98	0.19	78,78,78,78	0
80	MG	3	210	1/1	0.98	0.07	136,136,136,136	0
80	MG	5	3813	1/1	0.98	0.23	87,87,87,87	0
80	MG	6	2053	1/1	0.98	0.42	114,114,114,114	0
80	MG	6	1976	1/1	0.98	0.11	140,140,140,140	0
80	MG	5	3410	1/1	0.98	0.20	90,90,90,90	0
80	MG	6	1944	1/1	0.98	0.08	154,154,154,154	0
80	MG	2	1960	1/1	0.98	0.18	127,127,127,127	0
80	MG	5	3687	1/1	0.98	0.22	103,103,103,103	0
80	MG	5	3411	1/1	0.98	0.15	96,96,96,96	0
80	MG	L2	301	1/1	0.98	0.23	80,80,80,80	0
80	MG	1	3618	1/1	0.98	0.14	85,85,85,85	0
80	MG	O3	201	1/1	0.98	0.25	83,83,83,83	0
80	MG	5	3420	1/1	0.98	0.19	94,94,94,94	1
80	MG	1	3654	1/1	0.98	0.19	95,95,95,95	0
80	MG	5	3564	1/1	0.98	0.23	113,113,113,113	0
80	MG	5	3449	1/1	0.98	0.37	82,82,82,82	0
80	MG	1	3719	1/1	0.98	0.15	87,87,87,87	1
80	MG	5	3828	1/1	0.98	0.10	111,111,111,111	0
80	MG	1	3406	1/1	0.98	0.24	91,91,91,91	0
80	MG	1	3536	1/1	0.98	0.28	80,80,80,80	0
80	MG	5	3427	1/1	0.98	0.46	79,79,79,79	0
80	MG	1	3722	1/1	0.98	0.20	79,79,79,79	1
80	MG	1	3645	1/1	0.98	0.19	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3591	1/1	0.98	0.15	86,86,86,86	0
80	MG	1	3502	1/1	0.98	0.17	105,105,105,105	0
80	MG	1	3786	1/1	0.98	0.15	99,99,99,99	0
80	MG	1	3537	1/1	0.98	0.20	85,85,85,85	1
80	MG	5	3569	1/1	0.98	0.23	94,94,94,94	0
80	MG	5	3623	1/1	0.98	0.40	84,84,84,84	0
80	MG	1	3573	1/1	0.98	0.27	85,85,85,85	0
80	MG	1	3801	1/1	0.98	0.08	136,136,136,136	0
80	MG	1	3747	1/1	0.98	0.29	86,86,86,86	0
80	MG	5	3502	1/1	0.98	0.63	94,94,94,94	0
80	MG	1	3519	1/1	0.98	0.15	99,99,99,99	0
80	MG	5	3425	1/1	0.98	0.31	80,80,80,80	0
80	MG	5	3424	1/1	0.98	0.26	85,85,85,85	0
80	MG	m0	301	1/1	0.98	0.29	95,95,95,95	0
80	MG	5	3795	1/1	0.98	0.13	118,118,118,118	0
80	MG	5	3485	1/1	0.98	0.24	107,107,107,107	1
80	MG	1	3794	1/1	0.98	0.20	82,82,82,82	0
80	MG	6	2049	1/1	0.98	0.17	142,142,142,142	0
80	MG	5	3482	1/1	0.98	0.14	106,106,106,106	1
80	MG	1	3491	1/1	0.98	0.24	84,84,84,84	0
80	MG	5	3836	1/1	0.98	0.17	111,111,111,111	0
80	MG	5	3462	1/1	0.98	0.47	95,95,95,95	0
80	MG	3	208	1/1	0.98	0.19	138,138,138,138	0
82	ZN	d6	500	1/1	0.99	0.14	136,136,136,136	0
80	MG	n3	201	1/1	0.99	0.32	81,81,81,81	0
80	MG	6	1960	1/1	0.99	0.35	102,102,102,102	0
80	MG	5	3447	1/1	0.99	0.29	84,84,84,84	0
80	MG	1	3470	1/1	0.99	0.32	90,90,90,90	0
80	MG	1	3485	1/1	0.99	0.44	77,77,77,77	0
80	MG	5	3407	1/1	0.99	0.29	85,85,85,85	0
80	MG	5	3435	1/1	0.99	0.22	95,95,95,95	0
80	MG	1	3577	1/1	0.99	0.23	104,104,104,104	0
82	ZN	D6	500	1/1	0.99	0.14	131,131,131,131	0
80	MG	5	3440	1/1	0.99	0.26	86,86,86,86	0
80	MG	1	3660	1/1	0.99	0.27	103,103,103,103	0
80	MG	1	3572	1/1	0.99	0.38	79,79,79,79	0
80	MG	1	3697	1/1	0.99	0.24	85,85,85,85	0
80	MG	1	3403	1/1	0.99	0.27	89,89,89,89	0
80	MG	1	3472	1/1	0.99	0.30	90,90,90,90	0
80	MG	5	3645	1/1	0.99	0.39	82,82,82,82	0
80	MG	5	3455	1/1	0.99	0.24	96,96,96,96	0
80	MG	1	3408	1/1	0.99	0.40	86,86,86,86	0

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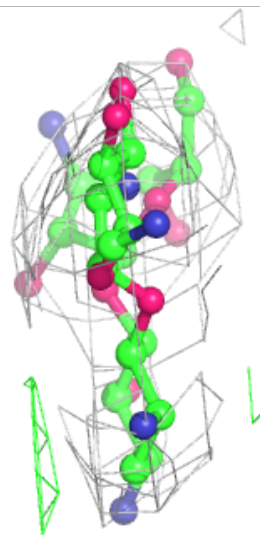
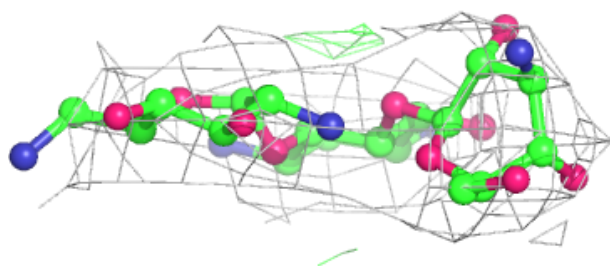
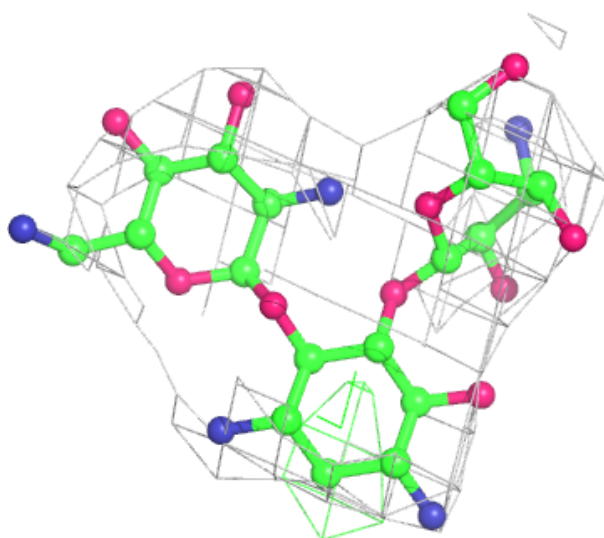
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	MG	5	3649	1/1	0.99	0.24	82,82,82,82	1
82	ZN	d9	101	1/1	0.99	0.11	151,151,151,151	0
80	MG	6	1970	1/1	0.99	0.37	134,134,134,134	0
82	ZN	Q2	501	1/1	0.99	0.07	173,173,173,173	0
80	MG	1	3541	1/1	0.99	0.23	82,82,82,82	0
80	MG	5	3686	1/1	0.99	0.20	104,104,104,104	0
80	MG	5	3584	1/1	0.99	0.37	91,91,91,91	0
80	MG	5	3814	1/1	0.99	0.40	78,78,78,78	0
80	MG	1	3520	1/1	0.99	0.14	105,105,105,105	0
80	MG	5	3618	1/1	0.99	0.12	136,136,136,136	0
82	ZN	D9	101	1/1	0.99	0.14	130,130,130,130	0
80	MG	5	3572	1/1	0.99	0.22	97,97,97,97	0
80	MG	5	3726	1/1	0.99	0.39	81,81,81,81	0
80	MG	1	3500	1/1	0.99	0.12	110,110,110,110	0
80	MG	5	3671	1/1	0.99	0.32	100,100,100,100	0
80	MG	5	3580	1/1	0.99	0.36	89,89,89,89	0
80	MG	M7	202	1/1	0.99	0.22	88,88,88,88	1
80	MG	5	3500	1/1	0.99	0.50	100,100,100,100	1
80	MG	5	3454	1/1	0.99	0.36	87,87,87,87	0
80	MG	5	3652	1/1	0.99	0.46	89,89,89,89	0
80	MG	6	1911	1/1	0.99	0.23	105,105,105,105	0
80	MG	1	3845	1/1	1.00	0.10	107,107,107,107	0
82	ZN	o7	501	1/1	1.00	0.23	109,109,109,109	0
82	ZN	Q0	500	1/1	1.00	0.14	105,105,105,105	0
82	ZN	O7	101	1/1	1.00	0.20	99,99,99,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

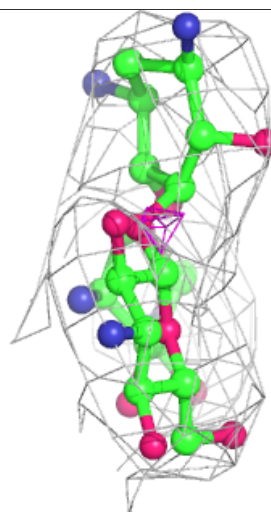
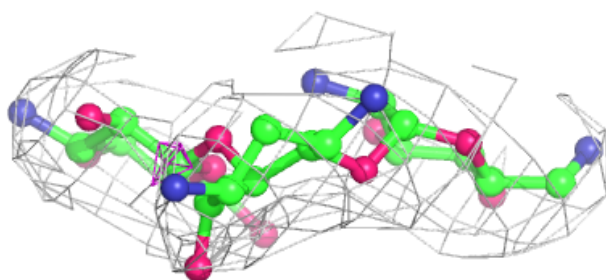
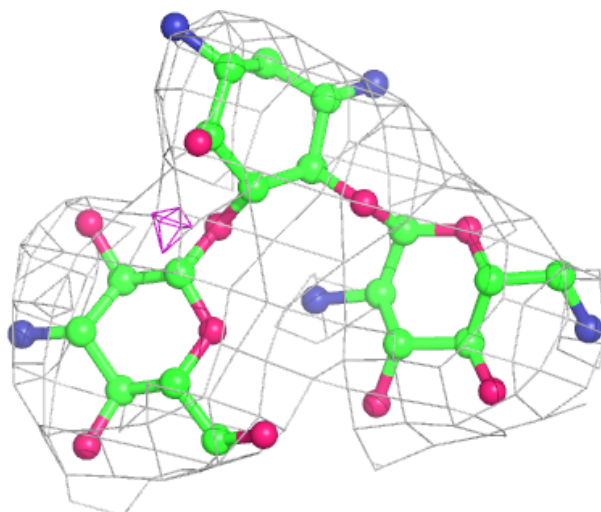
Electron density around 8UZ 7 209:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



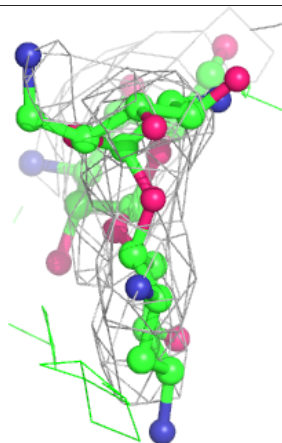
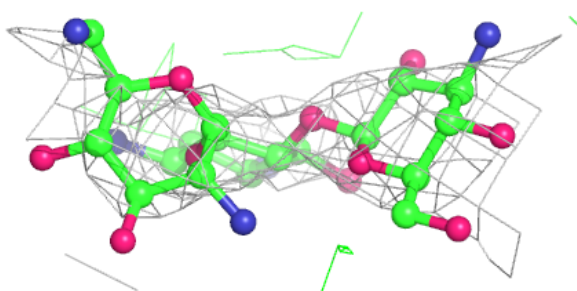
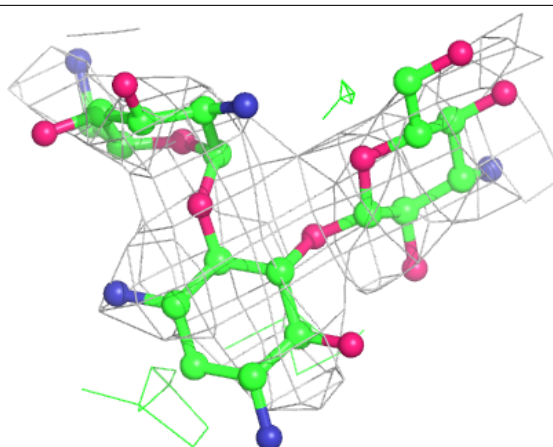
Electron density around 8UZ 5 3856:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



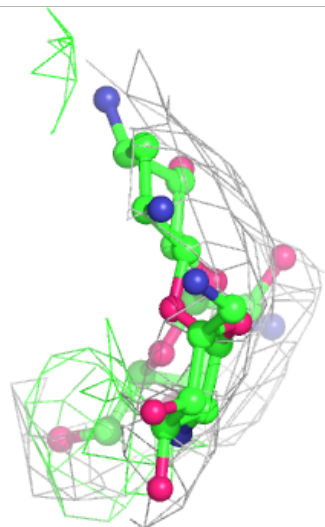
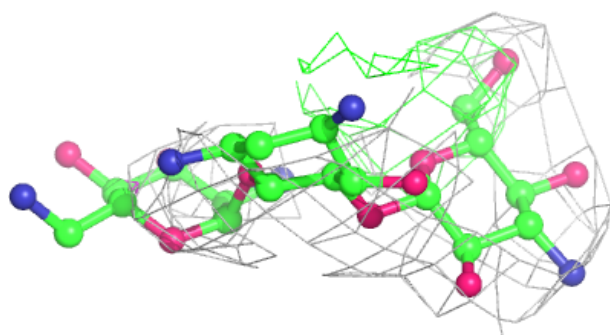
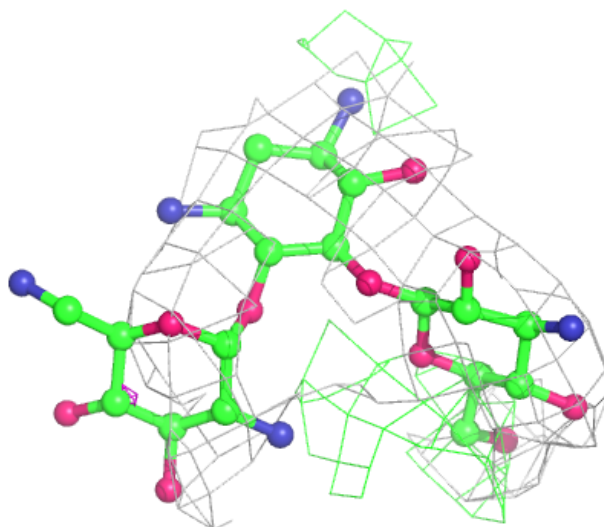
Electron density around 8UZ 5 3852:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



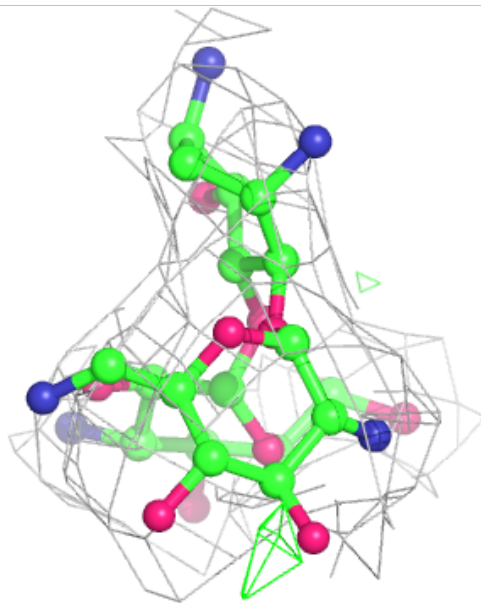
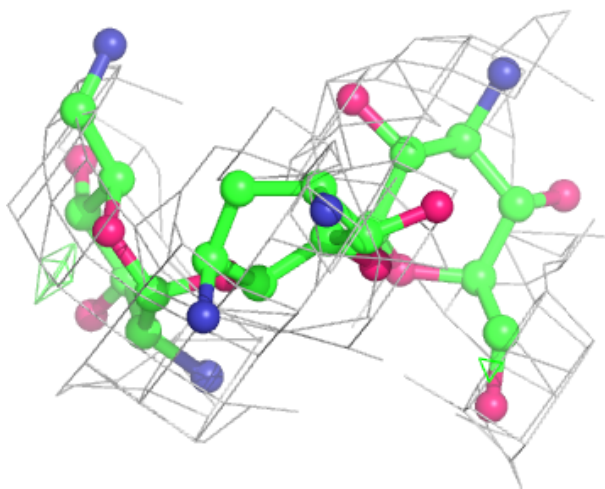
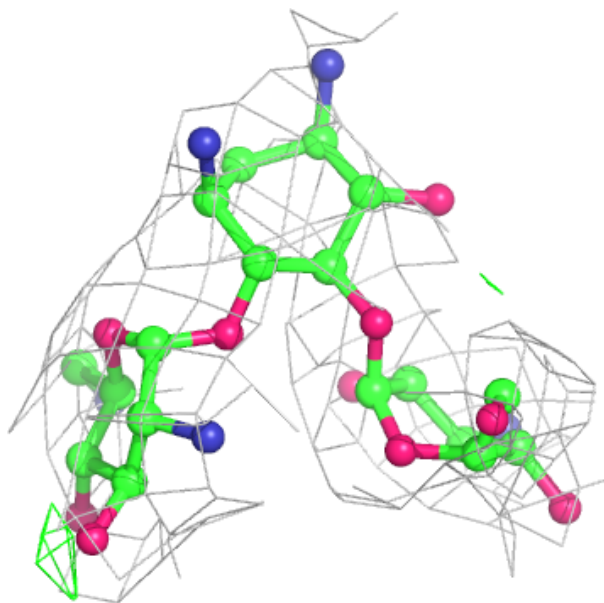
Electron density around 8UZ 5 3855:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



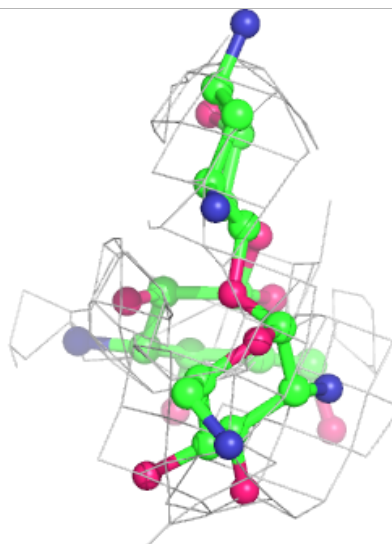
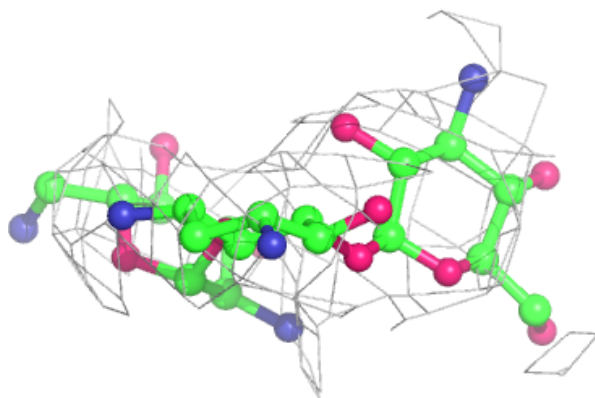
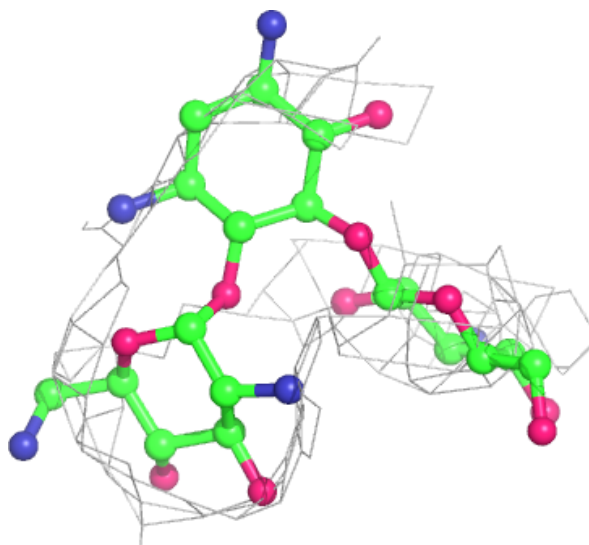
Electron density around 8UZ 5 3857:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



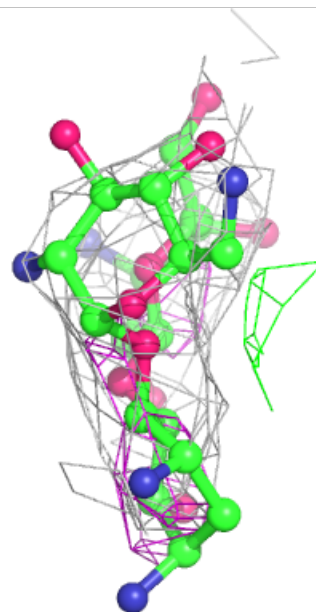
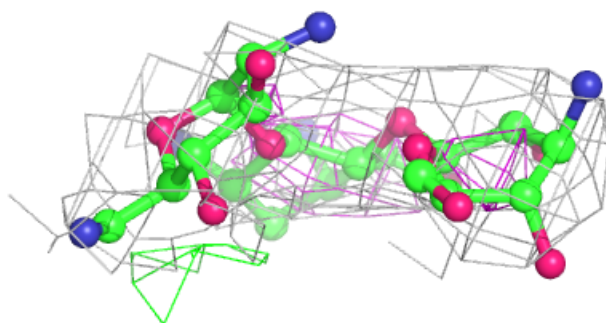
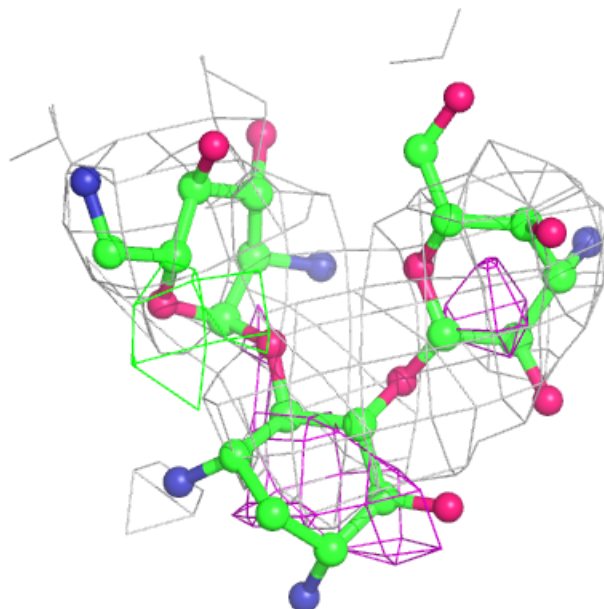
Electron density around 8UZ 2 2030:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



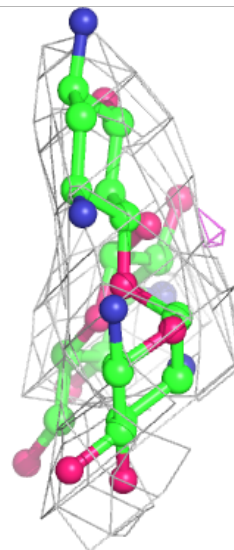
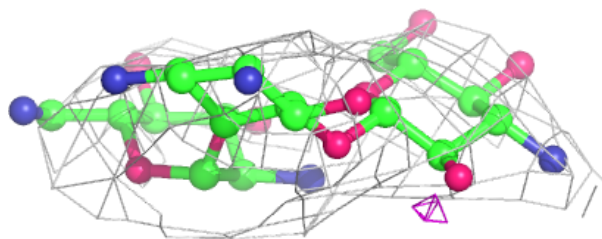
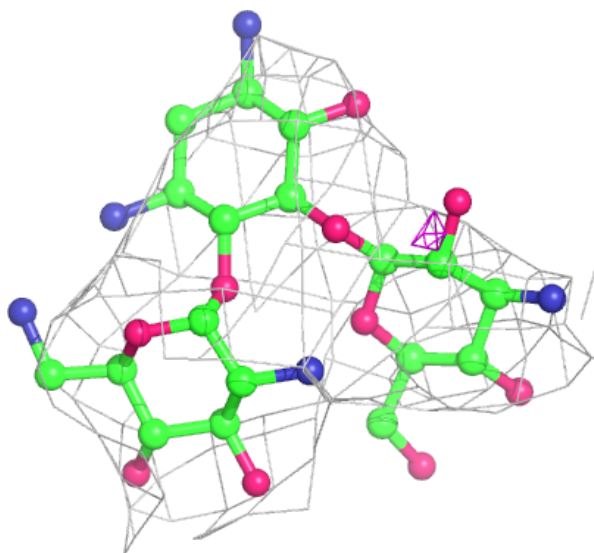
Electron density around 8UZ 1 3893:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



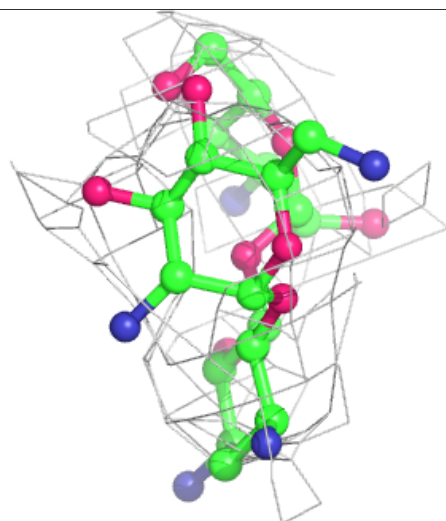
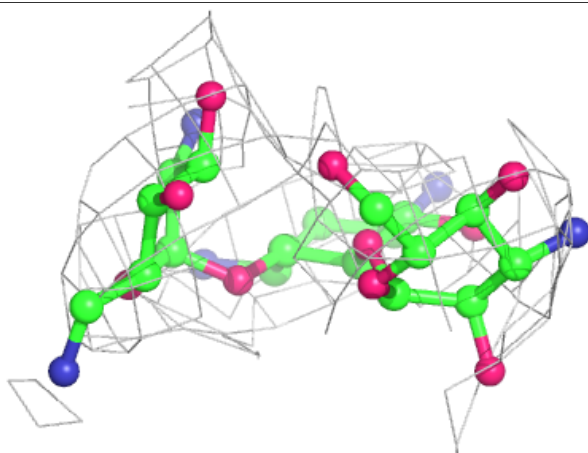
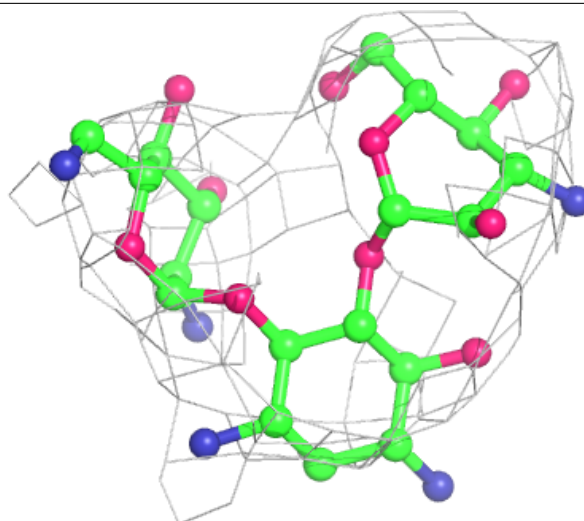
Electron density around 8UZ 1 3889:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



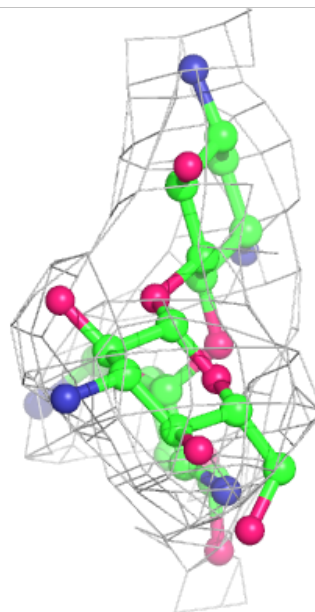
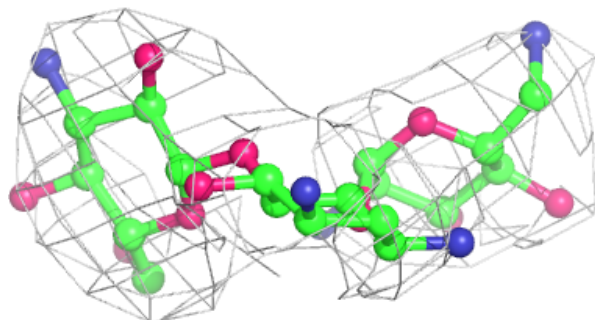
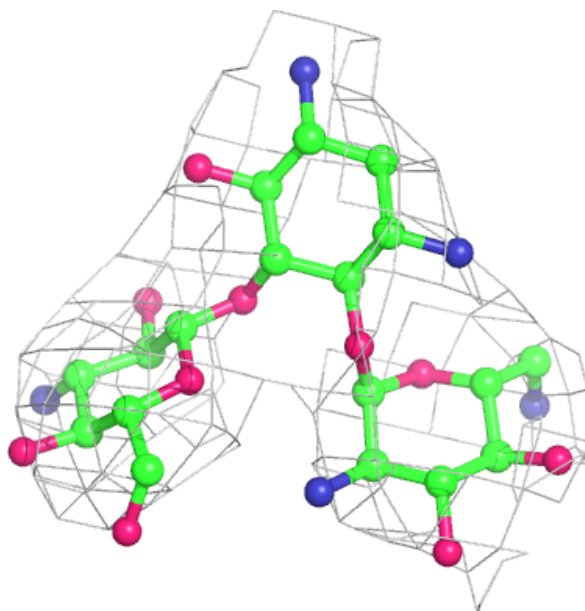
Electron density around 8UZ 6 2061:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



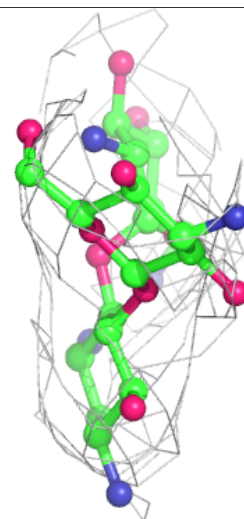
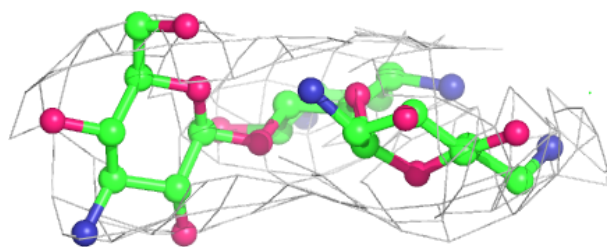
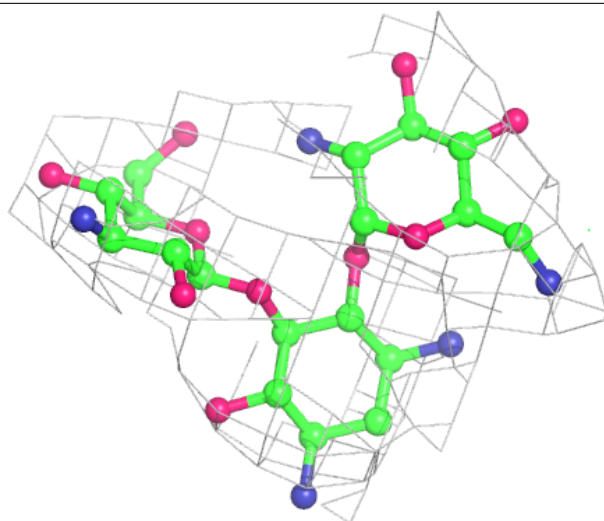
Electron density around 8UZ 5 3850:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



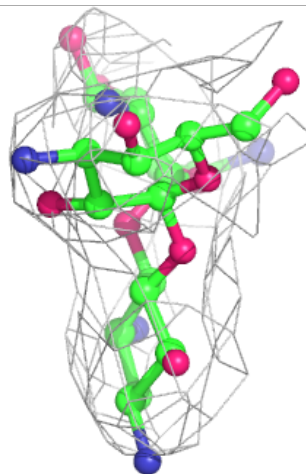
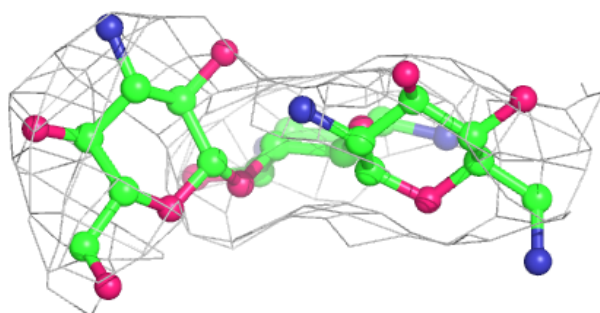
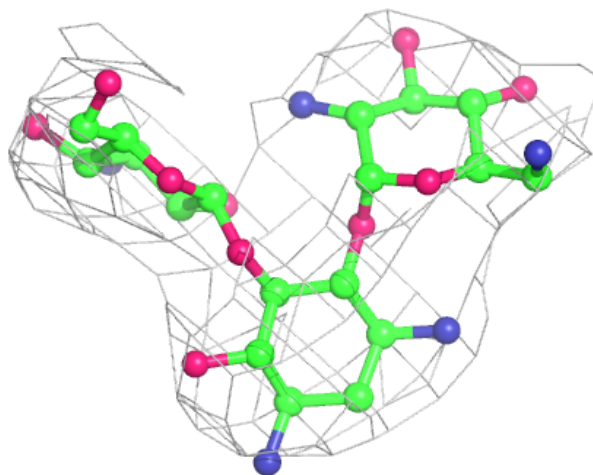
Electron density around 8UZ 5 3851:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



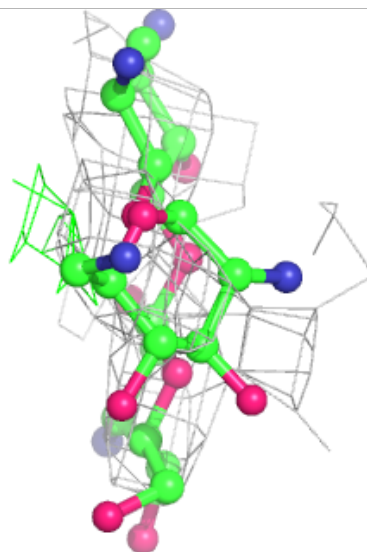
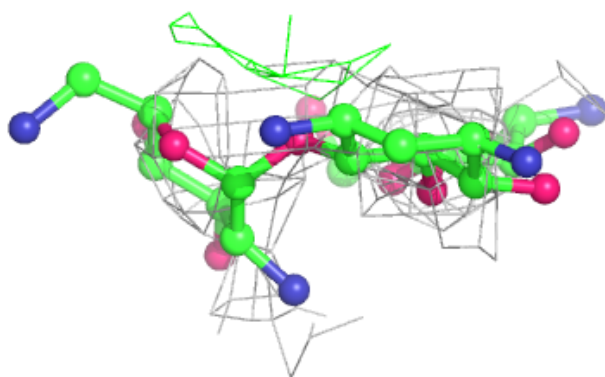
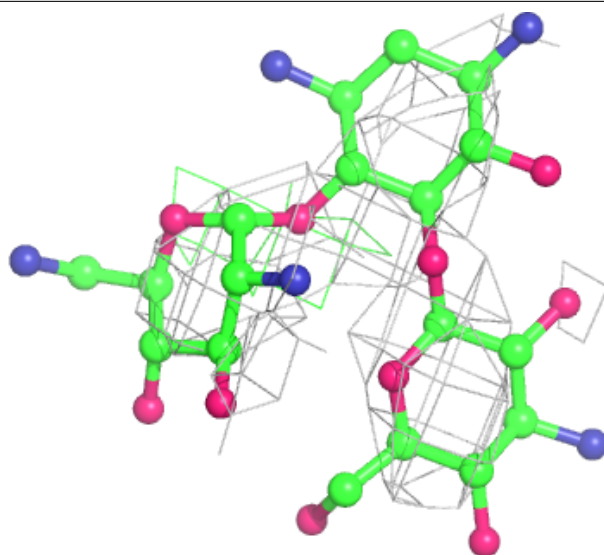
Electron density around 8UZ 1 3886:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



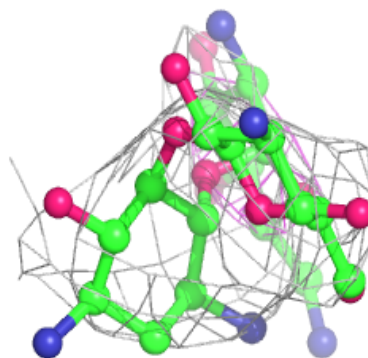
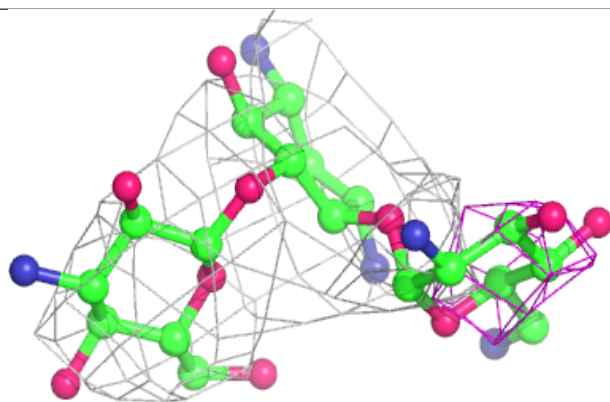
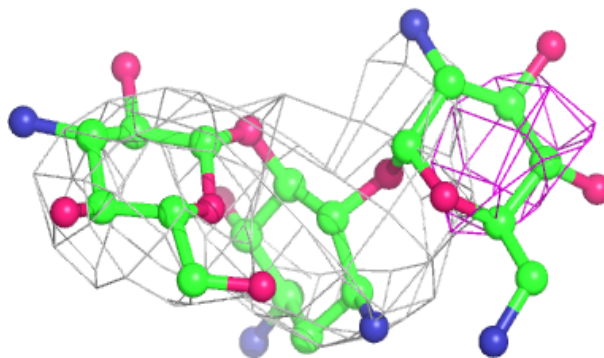
Electron density around 8UZ 1 3890:

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and green (positive)



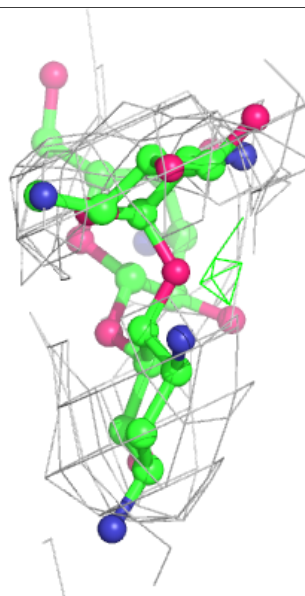
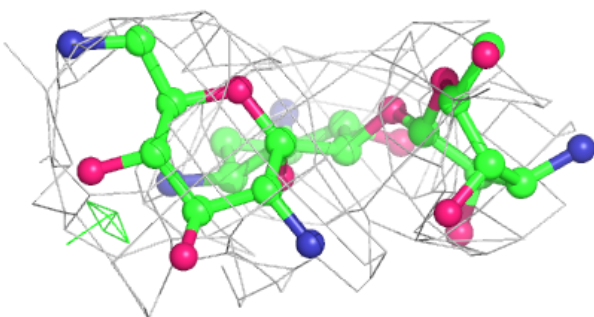
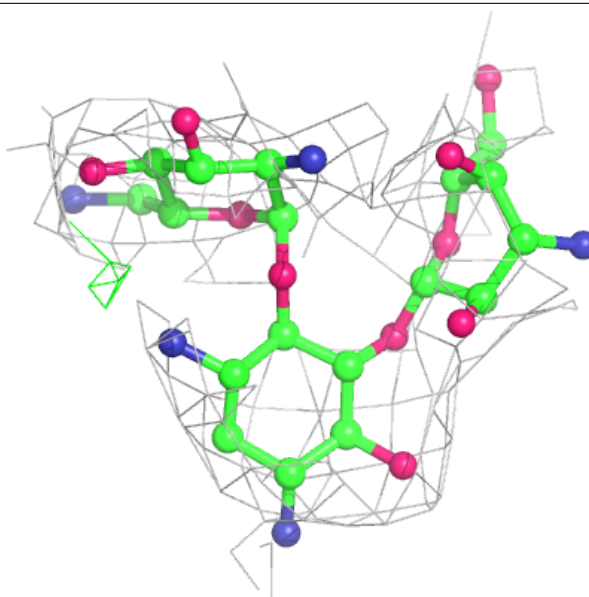
Electron density around 8UZ 2 2031:

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and green (positive)



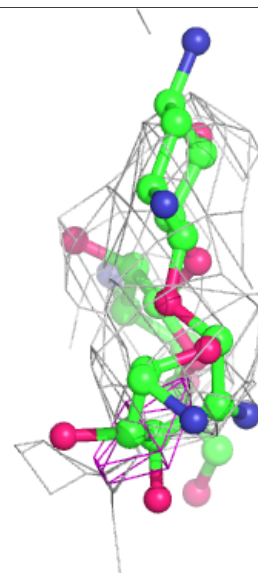
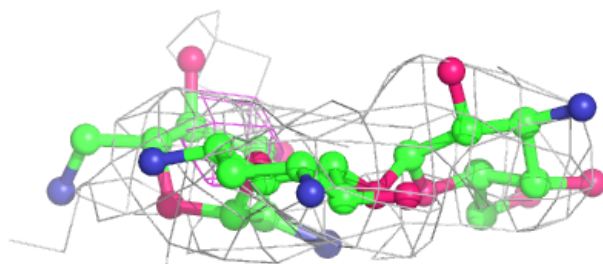
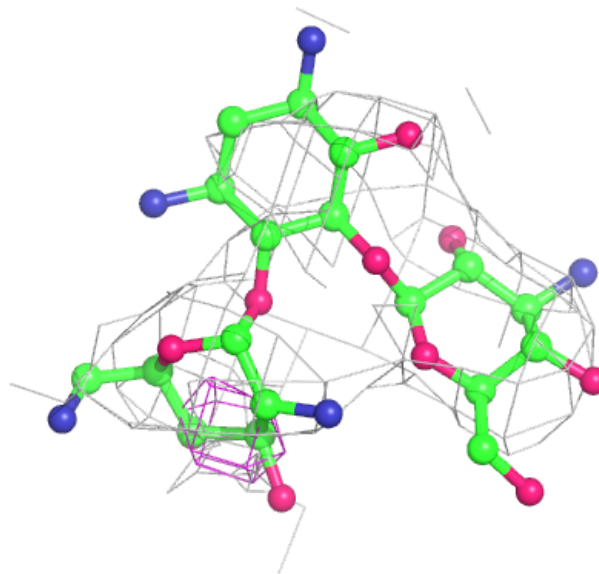
Electron density around 8UZ 1 3888:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



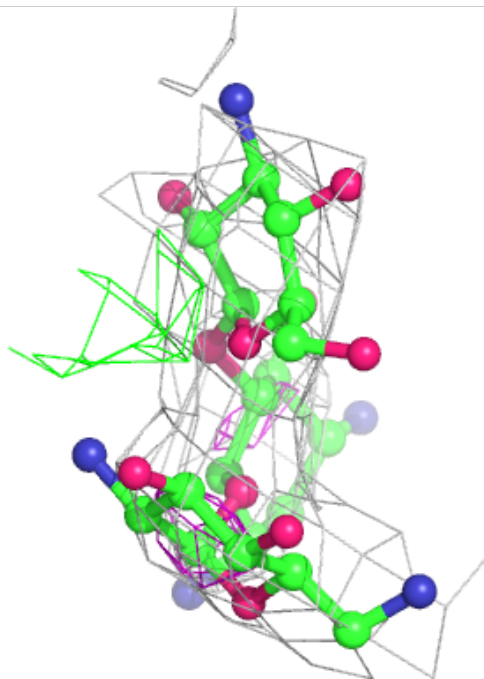
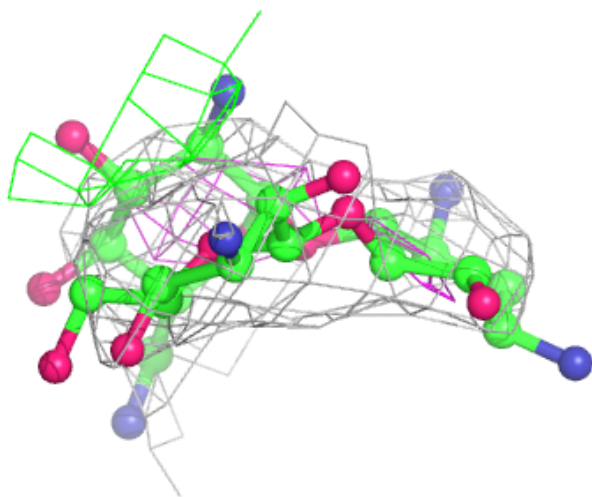
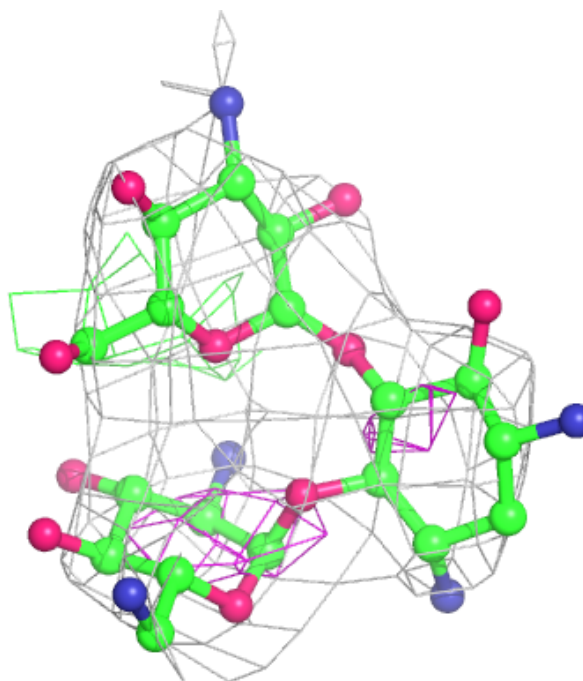
Electron density around 8UZ 1 3894:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



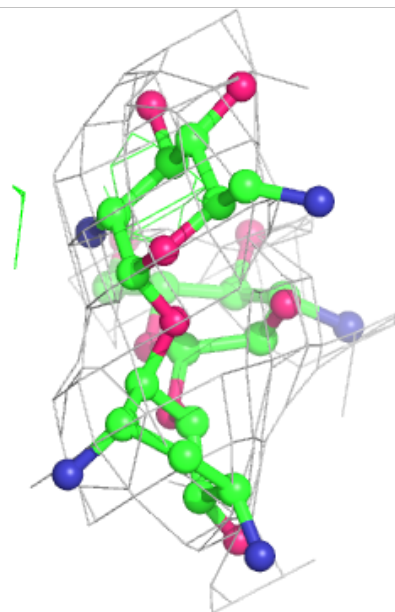
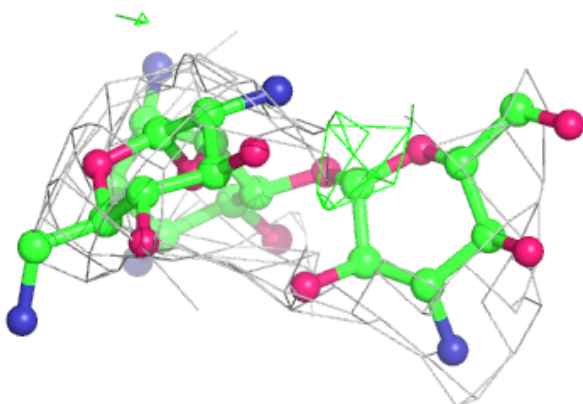
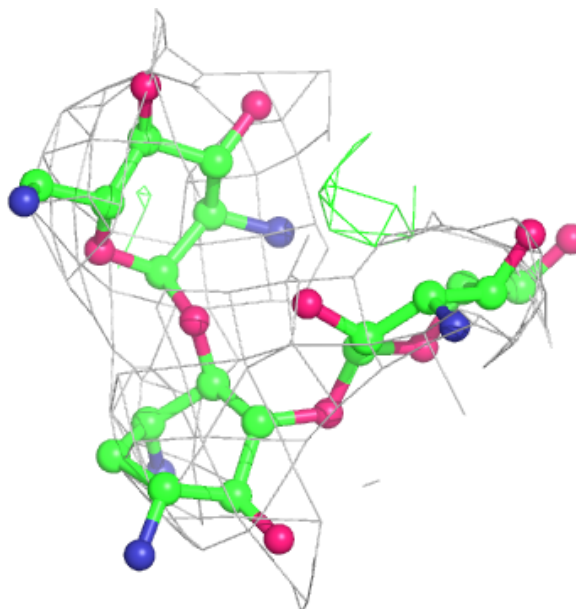
Electron density around 8UZ 4 220:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



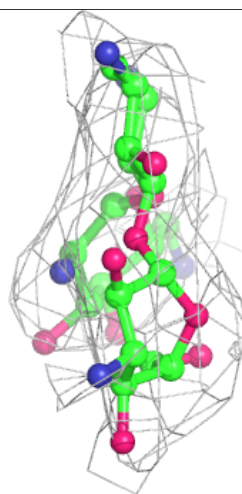
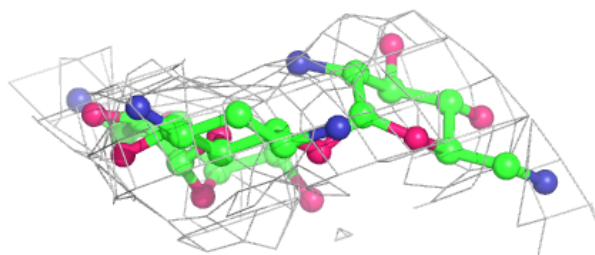
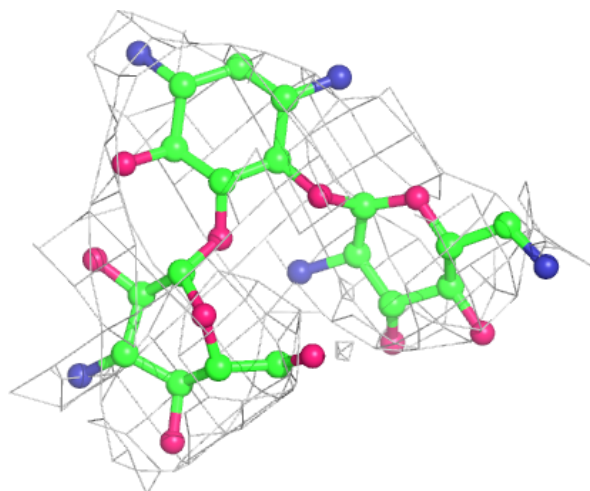
Electron density around 8UZ 2 2029:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



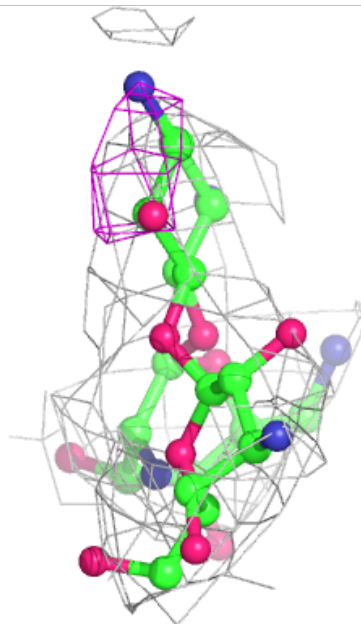
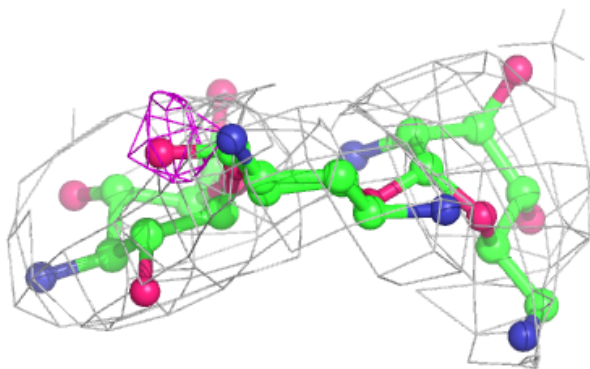
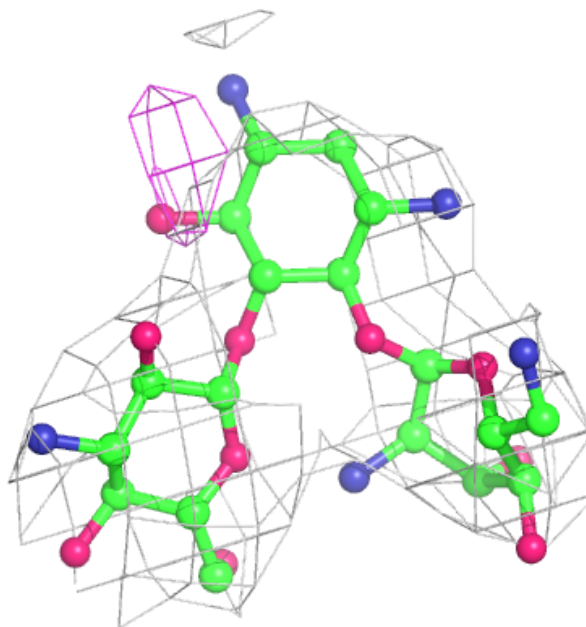
Electron density around 8UZ 3 214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



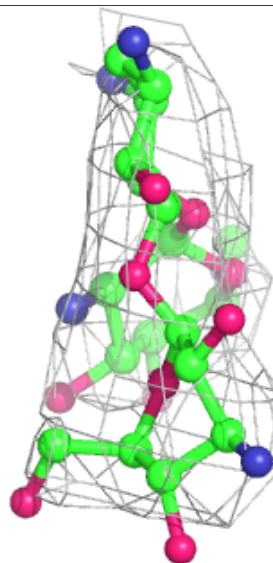
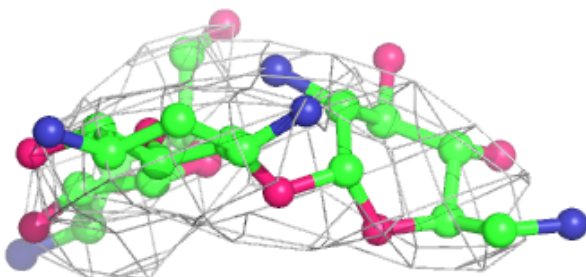
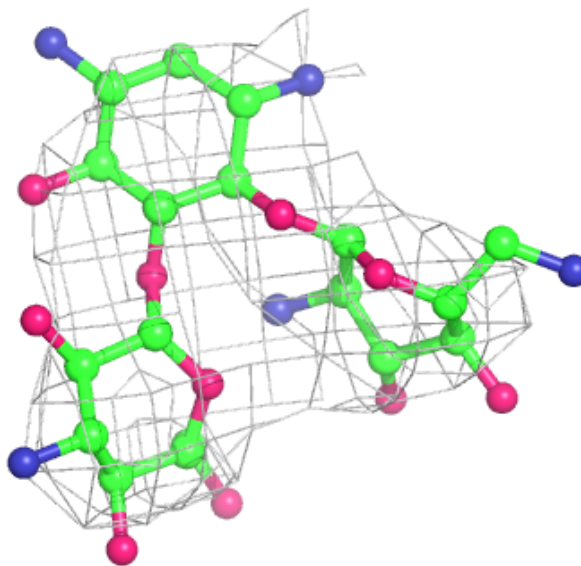
Electron density around 8UZ 1 3892:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



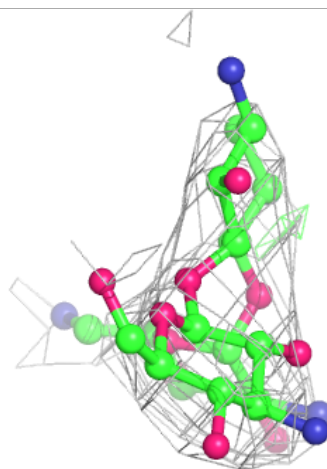
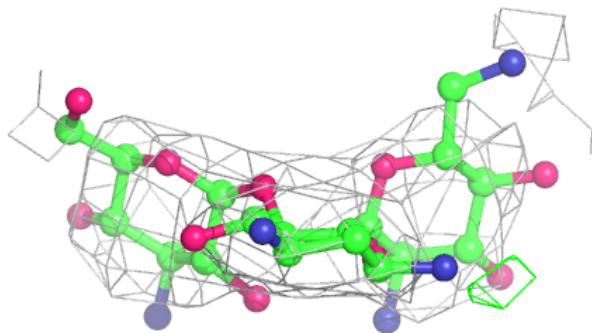
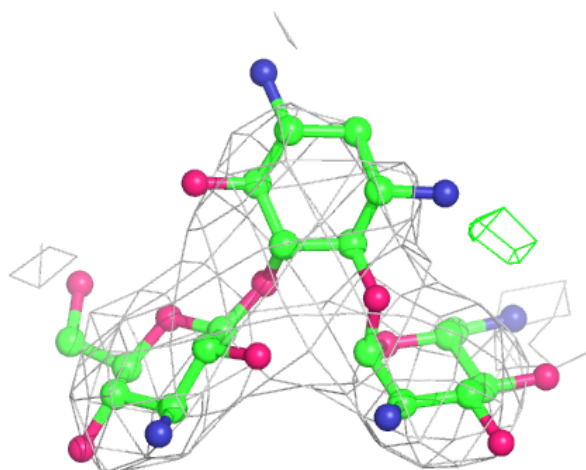
Electron density around 8UZ 5 3854:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



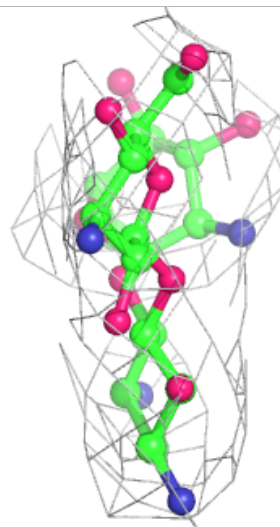
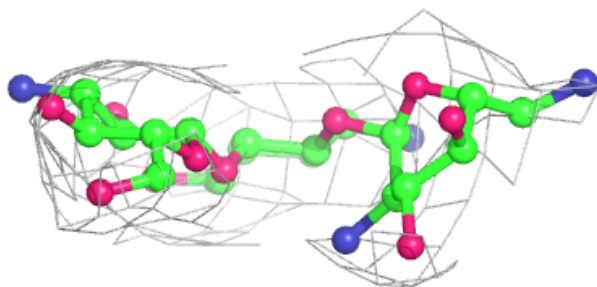
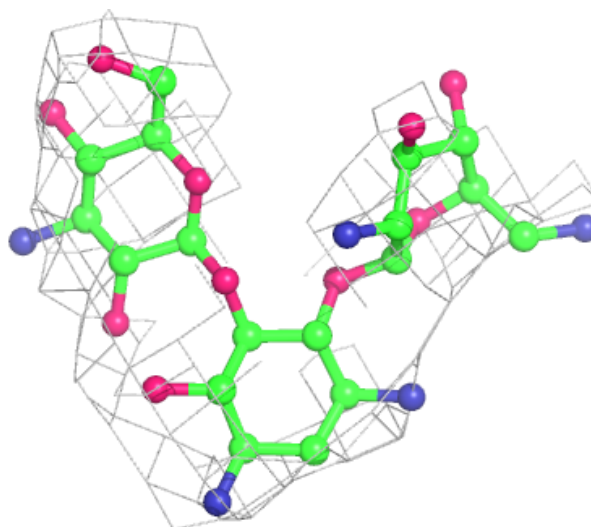
Electron density around 8UZ 5 3853:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



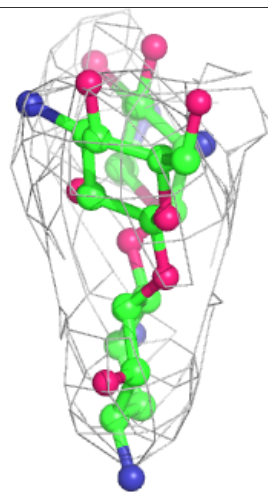
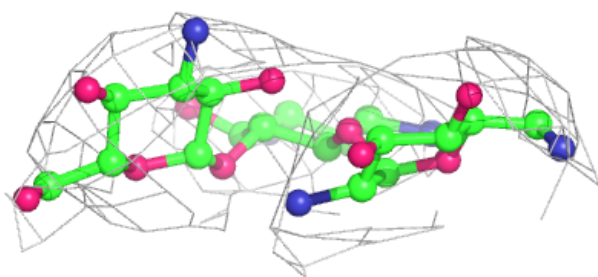
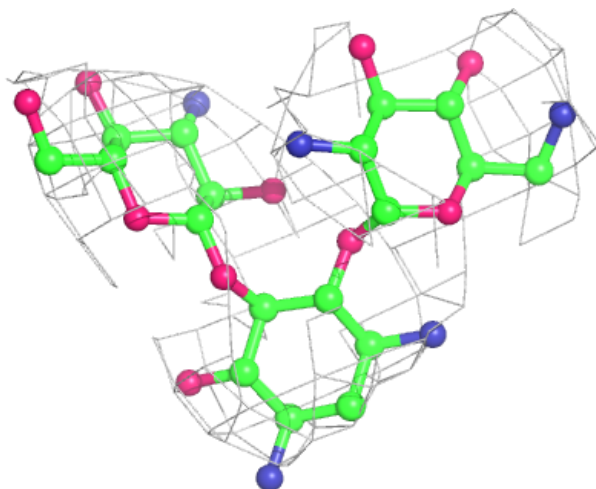
Electron density around 8UZ 1 3887:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



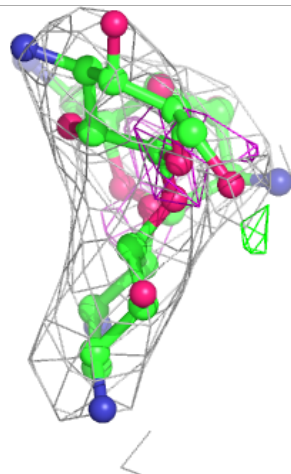
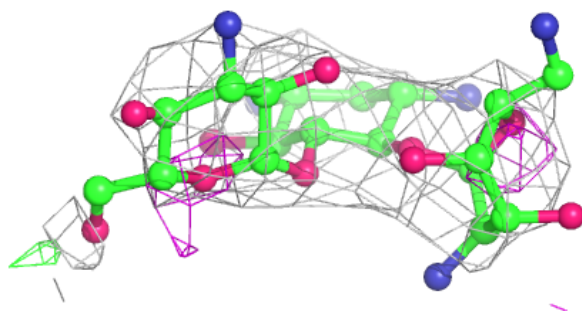
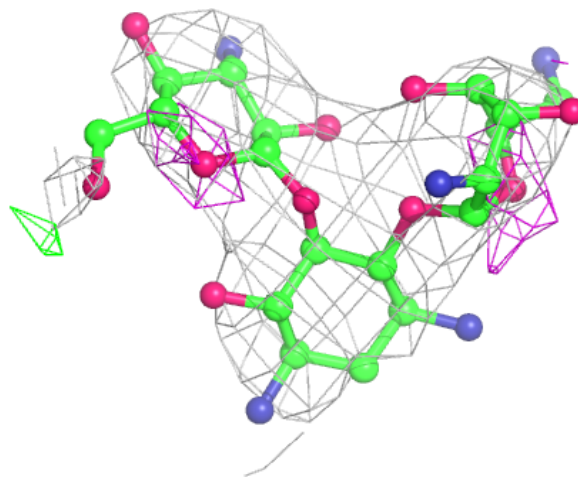
Electron density around 8UZ 1 3895:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 8UZ 1 3891:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.