



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:23 PM UTC

PDB ID : 5NDG / pdb_00005ndg
Title : Crystal structure of geneticin (G418) bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-03-08
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

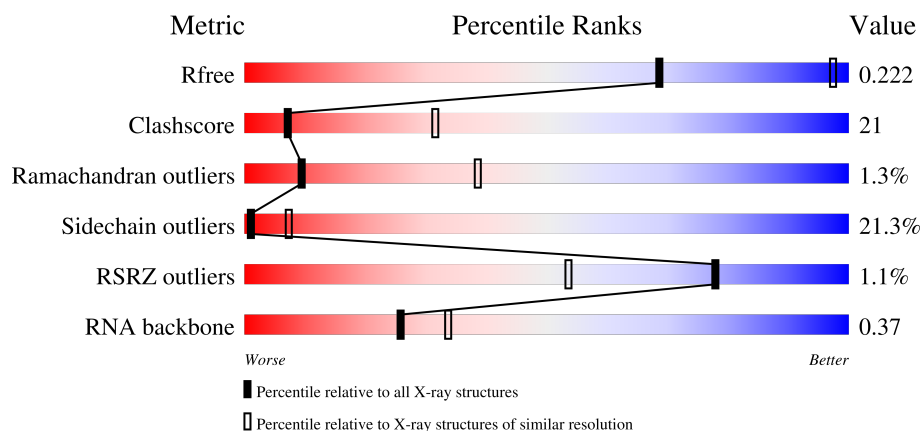
1 Overall quality at a glance

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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	206	
2	s0	206	

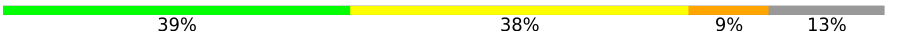
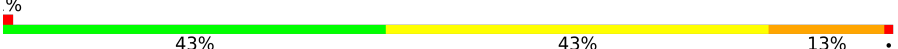
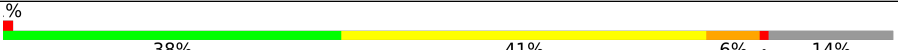
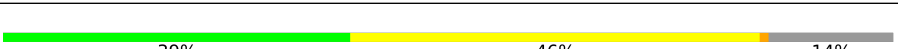
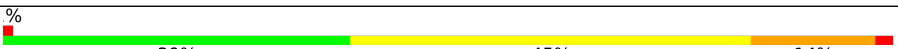
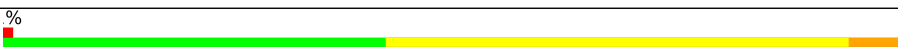
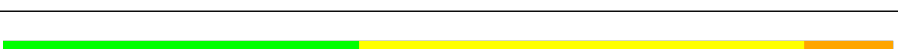
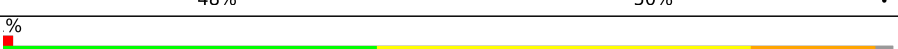
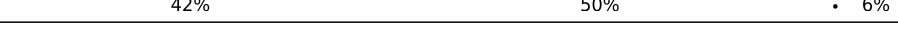
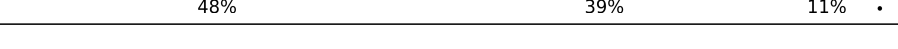
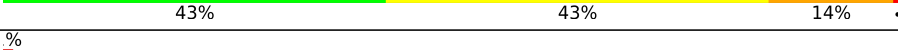
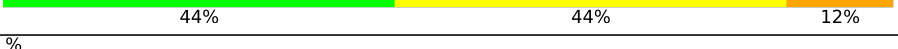
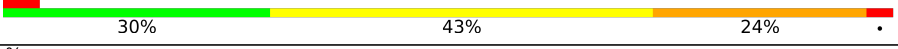
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	S1	216	
3	s1	216	
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	236	
8	s6	236	
9	S7	185	
9	s7	185	
10	S8	200	
10	s8	200	
11	S9	185	
11	s9	185	
12	C0	105	
12	c0	105	
13	C1	156	
13	c1	156	
14	C2	143	
14	c2	143	
15	C3	150	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	c3	150	
16	C4	128	
16	c4	128	
17	C5	141	
17	c5	141	
18	C6	141	
18	c6	141	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	107	
22	d0	107	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	70	
27	d5	70	

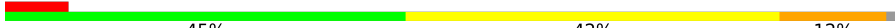
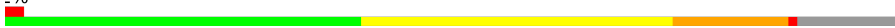
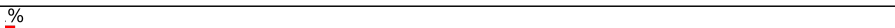
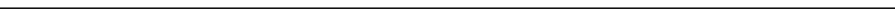
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	60	
32	e0	60	
33	E1	152	
33	e1	152	
34	SR	318	
34	sR	318	
35	SM	272	
35	sM	272	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	

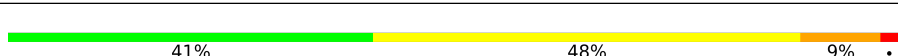
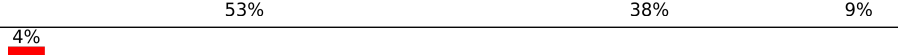
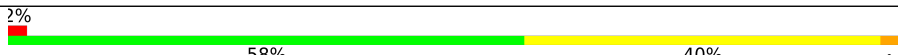
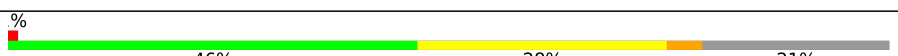
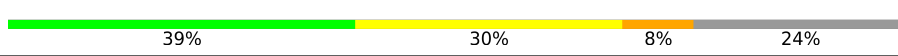
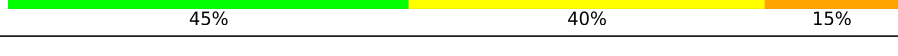
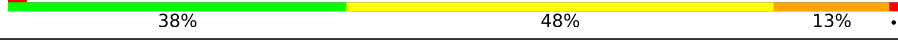
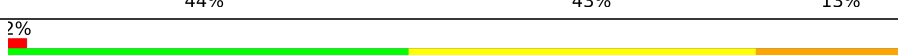
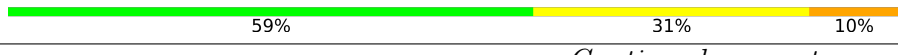
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	176	
43	l6	176	
44	L7	223	
44	l7	223	
45	L8	233	
45	l8	233	
46	L9	191	
46	l9	191	
47	M0	221	
47	m0	221	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	M7	184	
53	m7	184	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	98	
58	n2	98	
59	N3	135	
59	n3	135	
60	N4	155	
60	n4	155	
61	N5	121	
61	n5	121	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	

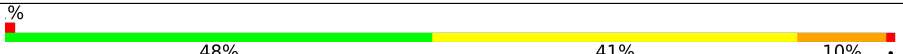
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
65	n9	58	
66	O0	100	
66	o0	100	
67	O1	109	
67	o1	109	
68	O2	127	
68	o2	127	
69	O3	106	
69	o3	106	
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	84	
73	o7	84	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	p0	312	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3720	-	-	-	X
81	MG	1	3771	-	-	-	X
81	MG	2	1921	-	-	-	X
81	MG	2	1993	-	-	-	X
81	MG	2	2000	-	-	-	X
81	MG	5	3693	-	-	-	X
81	MG	s8	302	-	-	-	X

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 397710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1688	Total	C	N	O	P	0	0	0
			35985	16089	6386	11822	1688			
1	6	1700	Total	C	N	O	P	0	0	0
			36234	16201	6426	11907	1700			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	185	Total	C	N	O	0	0	0
			1486	954	266	266			

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	92	Total	C	N	O	S	0	0	0
			752	487	122	141	2			
12	c0	92	Total	C	N	O	S	0	0	0
			741	478	121	140	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	142	Total	C	N	O	S	0	0	0
			1146	735	217	191	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	120	Total	C	N	O	S	0	0	0
			870	548	152	168	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	117	Total	C	N	O	S	0	0	0
			911	568	174	167	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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

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

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	105	Total	C	N	O	S	0	0	0
			837	529	152	155	1			
22	d0	101	Total	C	N	O	S	0	0	0
			805	512	145	147	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	313	Total	C	N	O	S	0	0	0
			2403	1521	411	463	8			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	157	Total	C	N	O	P	0	0	0
			3333	1491	584	1101	157			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	294	Total	C	N	O	S	0	0	0
			2357	1491	410	454	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	190	Total	C	N	O	S	0	0	0
			1510	957	273	276	4			

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

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

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

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

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

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

Continued on next page...

Continued from previous page...

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

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O	S	0	0	0
			1420	882	281	257				
53	m7	175	Total	C	N	O	S	0	0	0
			1378	856	273	249				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	170	Total	C	N	O	S	0	0	0
			1432	922	265	242	3			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	135	Total	C	N	O	S	0	0	0
			997	625	188	177	7			
59	n3	134	Total	C	N	O	S	0	0	0
			993	623	187	176	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	124	Total	C	N	O	0	0	0
			976	614	190	172			

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	84	Total	C	N	O	S	0	0	0
			665	405	145	110	5			
73	o7	82	Total	C	N	O	S	0	0	0
			650	396	142	107	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	49	Total	C	N	O	S	0	0	0
			431	269	96	64	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

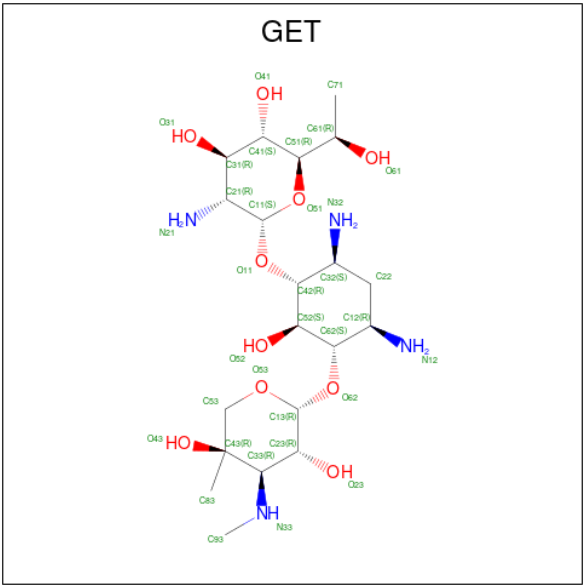
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	d3	2	Total 2	Mg 2	0	0
81	sM	1	Total 1	Mg 1	0	0
81	5	443	Total 443	Mg 443	1	0
81	7	8	Total 8	Mg 8	0	0
81	8	14	Total 14	Mg 14	0	0
81	l2	4	Total 4	Mg 4	0	0
81	l3	4	Total 4	Mg 4	0	0
81	l4	1	Total 1	Mg 1	0	0
81	l7	2	Total 2	Mg 2	0	0
81	l9	1	Total 1	Mg 1	0	0
81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

Continued on next page...

Continued from previous page...

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

- Molecule 82 is GENETICIN (CCD ID: GET) (formula: C₂₀H₄₀N₄O₁₀).



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

Continued on next page...

Continued from previous page...

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

- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

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

- Molecule 84 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

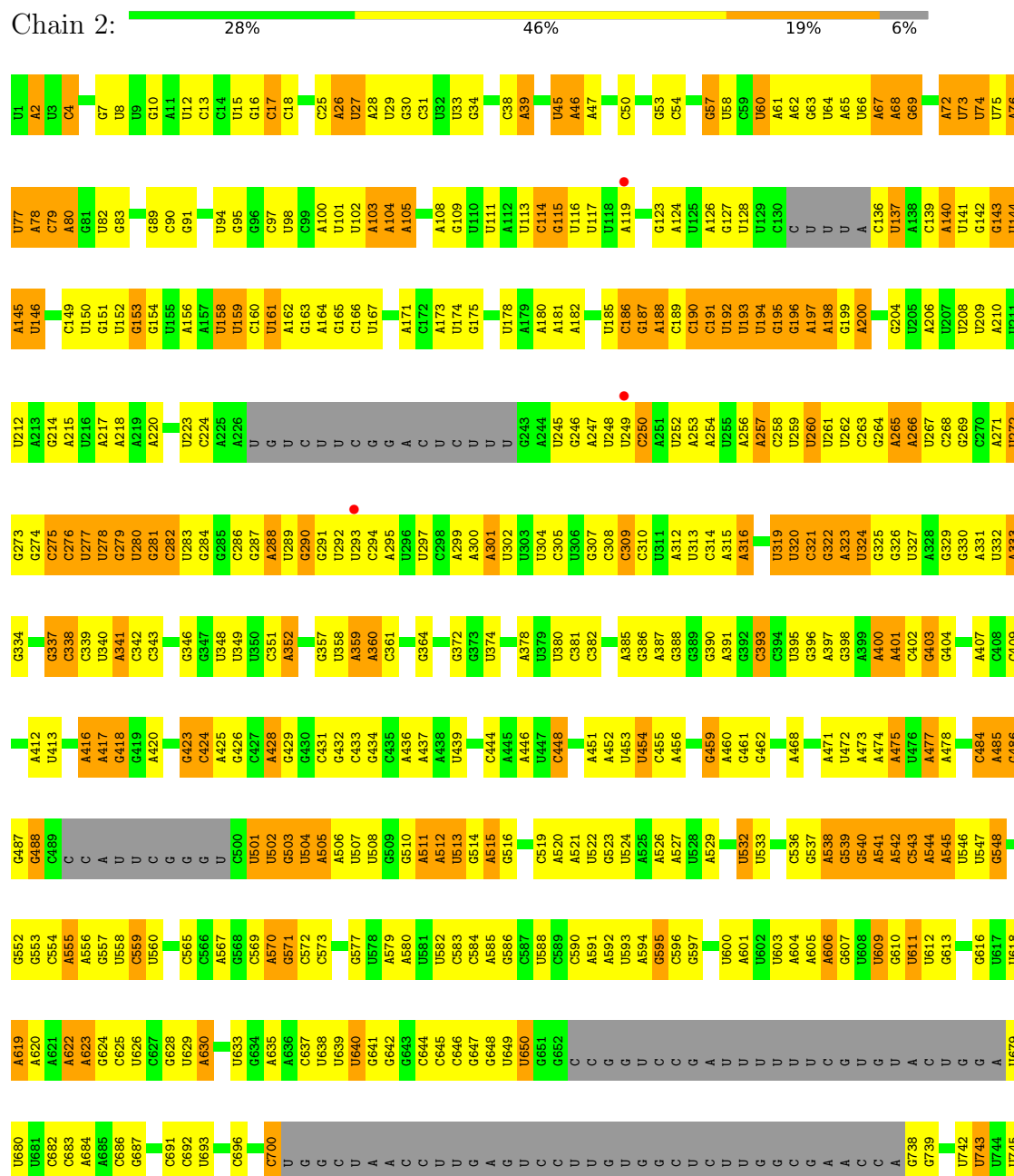
Continued from previous page...

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

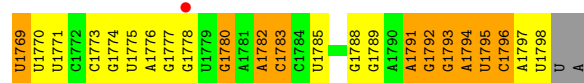
3 Residue-property plots

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

• Molecule 1: 18S ribosomal RNA

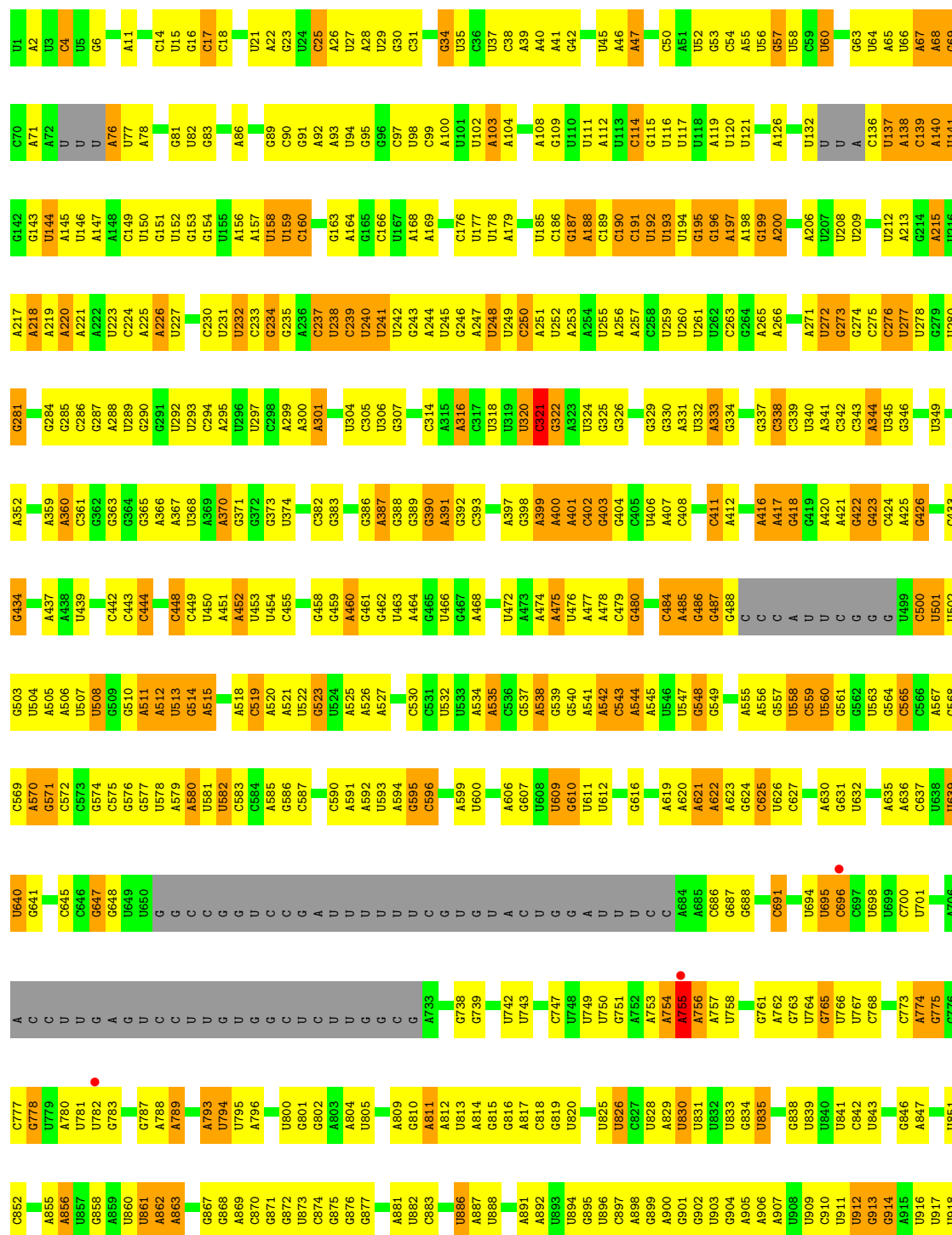


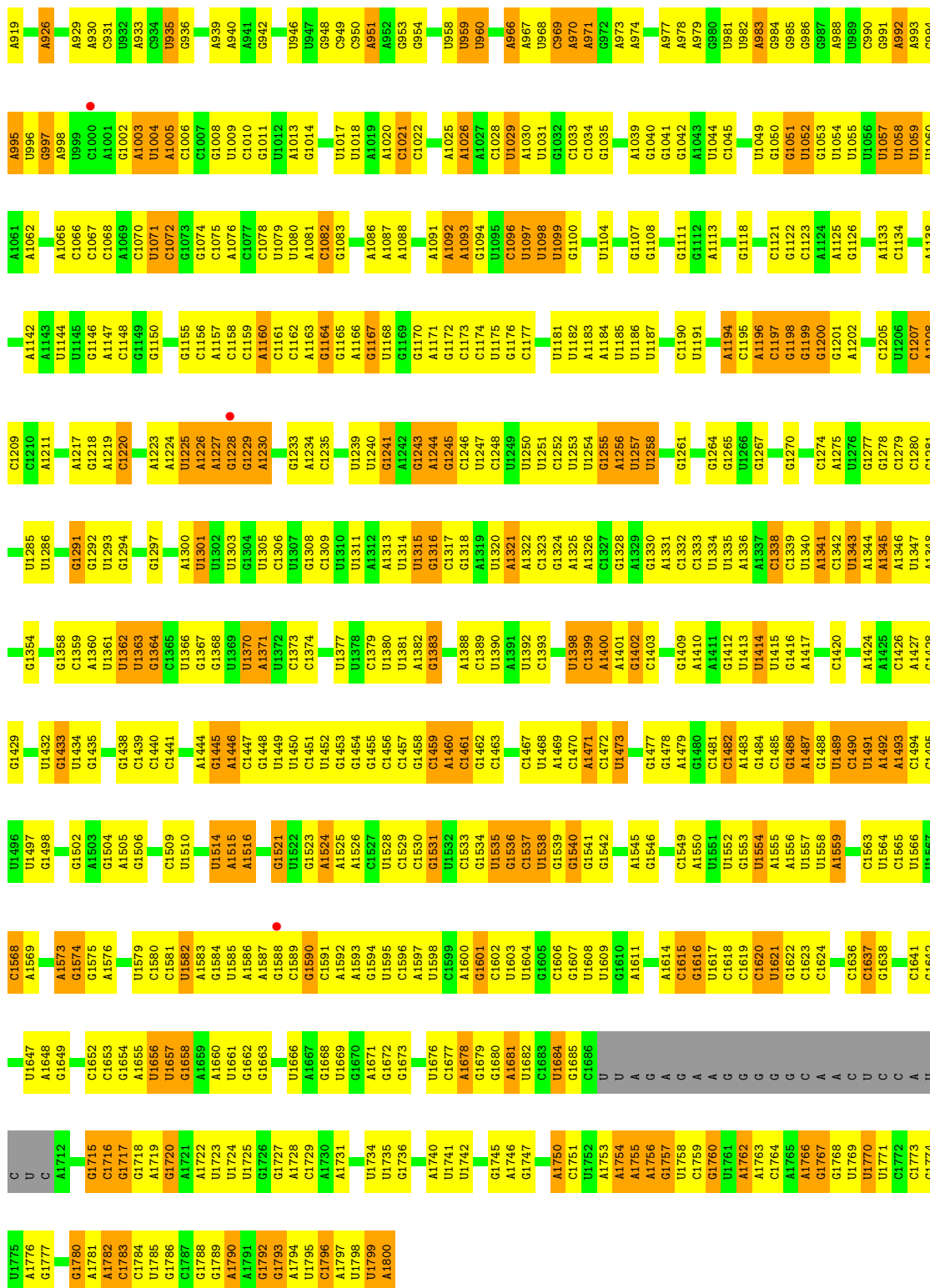
A	A1625	U1564	C1500	U1482	G1364	G1292	G1213	G1149	G1085	C1021	A951	U886	A812	A746
A	U1626	C1565	C1501	U1432	C1365	U1293		G1150	A1086	C1022	A952	A887	U813	C747
C	U1627	U1566	G1502	G1433	G1366	G1294	A1217	A1151	A1087	U1023	G953	U888	A814	U748
U	U1628	C1567	G1503	U1434	G1367		G1218	A1152	A1088	A1024	G954	U889	G815	U749
C	G1629	C1568	G1504	G1435	G1368	U1297	A1219	G1154		U1025	A955	G816	G816	
C	U1630	A1569	A1505	A1436	U1369	U1298	C1220	G1155	A1091	A1026	C956	A891	A817	A753
A	A1631	A1570	G1506	U1437	U1370	G1299	A1221	G1156	A1092	A1027	G957	A892	G818	A754
U		C1571	U1508	U1438	U1372	A1300	C1222	A1157	A1093	C1028	U958		G819	A755
C	C1634	G1572	U1509	C1439	U1373	U1301	A1223	A1158	A1094	U1029	U959		U820	A756
U1710	A1635	G1573	U1510	U1442	A1375	U1305	A1224	C1159	A1095	U1030	U960	U896	U757	
C1711	C1636	A1574	U1511	U1443		C1306	U1225	C1159	A1096	U1031		U897	U758	
A1712	C1637	G1575	U1512	A1444	A1376		A1226	A1160	A1097	G1032	U964	G898	U759	A760
A1713		A1576	G1513	G1445	U1378	C1306	A1227	C1161	U1098	C1033	U965	G899	A760	
A1714			G1514	G1446	U1379	A1312	A1228	C1162	U1099	C1034	A866	A900	G761	
C1715	C1641	U1579	U1515	A1446	C1379	A1313	G1229	A1163	G1100	G1035		U828		
C1716	C1642	C1580	A1515	C1447	U1380	A1314	A1230	G1164	G1101		C969	U902	G765	
U1643	U1643	C1581	A1516	G1448	U1381	U1313	A1231	G1165	U1102	A1039	A970	U903	U831	U766
G1718	G1644	U1582	U1517	U1449	G1383	G1316	U1232	A1166	G1103	G1040	A971	G904	U832	U767
A1719	G1645	A1583	C1518	U1450	G1384	G1317	G1233	U1167	U1104	G1041	G972	A905	U833	C768
G1720	C1646	U1584		C1451	G1385	U1318	A1234	U1168	C1105	G1042	A973		G834	A769
		U1585	G1521	U1452	G1386			G1169	U1106	A1043	A974	U908	U835	A770
G1726	G1649	A1586	U1522	G1453	A1387	A1321	C1235	G1170	U1107	U1044	C975	U909	U836	A771
G1727	U1650	A1587	G1523	G1454	A1388	A1322	A1236	A1171	G1108	U1045		C910	U837	G772
A1728	A1651	G1588	A1524	G1455	C1389	G1323	G1237	G1172	G1109	G1046	A978	U911	G838	C773
C1729		C1589	A1525	C1456	U1390	G1324	G1241	C1173	G1110	G1047	A979	U912	A774	
A1730	G1654	G1590	A1526	C1457	A1391	A1325		C1174	G1111	G1048	G980		G846	C775
A1731	A1655	C1591	C1527	G1458	U1392	A1326	A1244	U1175		U1049		G914		G776
A1732	U1656	A1592	U1528	C1459	C1393	C1327	G1245	U1176	U1115	A1050	A983	U916	C849	C777
C1733	U1657	C1593	G1529	A1460	G1394	A1328			A1116	U1051	G984	U917	A850	G778
U1734	G1658	G1594	C1530	C1461	G1395	A1329	U1249	G1179	U1117	U1052	G985	U918	U851	U779
U1735	A1659	U1595	G1531	G1462	U1396	G1330	U1250	C1180	G1118	G1053	G986	U918	G852	A780
G1736	A1660	C1596	U1532		U1397		U1251	U1181	G1119	U1054	G987	A919	G853	U781
	U1661	A1597	C1533	A1469	U1398	U1335	U1252	U1182	U1120	U1055	A988	U920	U854	U782
C1739	G1662	U1598	G1534	C1470	C1399	A1336	G1253	A1183	G1121	U1056	U989	U921	A855	U783
A1740	U1663	C1599	U1535	A1471	A1400	A1337	U1254	A1184	C1122	U1057	C990		A856	C784
U1741	C1664	A1600	G1536	C1472	A1401	C1338	G1255	U1185		U1058	G991	A924	U857	U785
U1742		G1601	C1537	U1473	G1402	U1339	A1256	U1186	A1125	U1059	A992	G925	U858	C786
	A1671	C1602	U1538	G1474	C1403	U1340	U1257	G1188	G1126	U1060	A993	A926	G859	G787
G1745	G1672	U1603	G1539	A1475	C1404	A1341	U1258		G1127	A1061	G994	U928	U860	A788
A1746	G1673	G1540	C1342			C1342	U1259	U1191	C1128	A1062	A995	U928	A789	
G1747	C1674	G1605	U1541	G1478	U1407	U1343	U1260	C1192	U1129	U1063	A996	A929	A863	U790
	C1675	G1606	G1542	A1479	G1408	A1344	G1261	A1193	G1130	G1064	G997	A930	U864	A791
A1750	U1676	G1607	A1543	G1480	G1409	A1345	U1262	A1194	A1131	A1065	A998	C931	U865	U792
C1751	G1677	U1608	U1544	A1410	A1411	A1346		C1195	A1132	C1066	U999	U932	G866	A793
U1752		U1609		C1481		U1347	G1268	A1196	A1133	C1067	C1000	U932	G867	U794
A1753	A1681	G1610	C1549	C1482	G1412	A1348		C1197	C1134	C1068	A1001	A933	G868	U795
A1754	U1682	A1550	A1550	G1486	U1413	G1349	C1274	G1198	U1135	C1068	G1002	C934	A869	A796
A1755	U1683	U1612	U1551	A1487	U1414	U1350	A1275	G1199	U1136	A1069	G1003	U935	A870	
C1683	G1683	U1552	G1351	G1488	U1415	G1351	G1200	G1201	A1137	C1070	U1004	G936	C870	
G1757	U1684	A1614	G1553	U1489	G1416	G1352	G1278	G1202	A1138	U1071		A940	G871	U800
U1758	G1685	C1615	U1554	C1490	A1417	U1353	C1279	A1203	A1139	G1074		A941	G872	G801
C1759		G1616	A1555	U1491		G1354	G1280	A1202	G1140		C1006	A942	U873	G802
G1760	U1617	U1617	A1556	A1492	C1420		G1281	A1204	G1141	C1077		G942	C874	A803
U1761	U1761	C1618	U1557	A1493	A1424	G1358	U1286	C1205	A1142	C1078	G1011	C943	A804	U805
A1762	G	C	U1558	C1494	A1425	G1359	U1287	U1206	A1143	U1079	U1012	A944	G875	
	G	C	A1559	C1495	A1426	C1359	G1288	C1207	U1144	U1080		U945	A806	
	G	U1621	U1560	U1486	C1426	A1360	G1288	A1208	U1145	A1081	U1015	U946	A807	
A1765	U1661	U1497	U1561	U1497	A1427	A1361	U1289	A1082	G1146	C1082		U947	U882	U808
G1766	G1622	G1498	C1562	U1497	A1428	U1362	U1290	A1147	A1019	A1084		G948	C883	A809
G1767	G	C	U1562	U1497	A1428	U1362	U1290	A1147	A1019	A1084		G948	A884	
G1768	C	C1624	C1563	G1499	G1429	U1363	G1291	A1211	C1148		A1020	C950	G885	A811



• Molecule 1: 18S ribosomal RNA

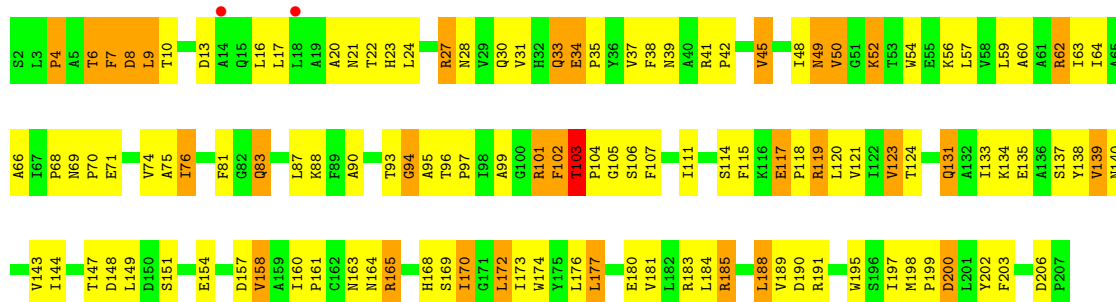
Chain 6: 32% 46% 16% 6%



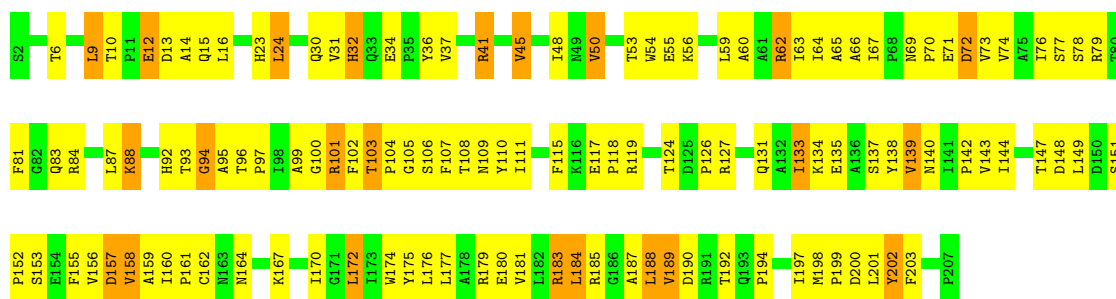


- Molecule 2: 40S ribosomal protein S0-A

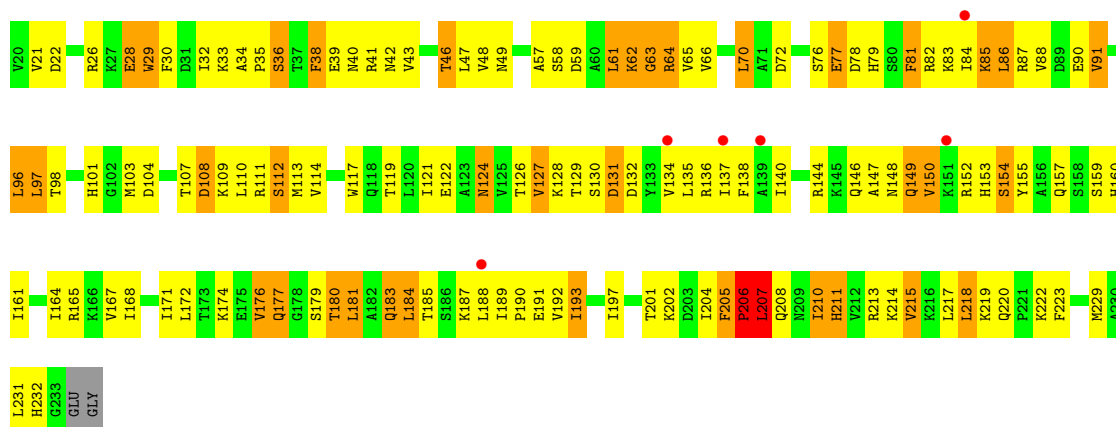




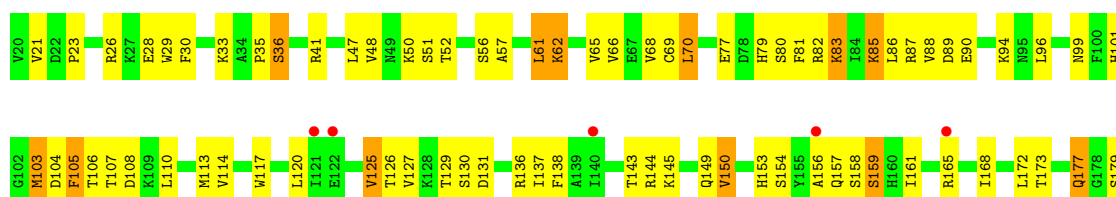
• Molecule 2: 40S ribosomal protein S0-A



• Molecule 3: 40S ribosomal protein S1-A

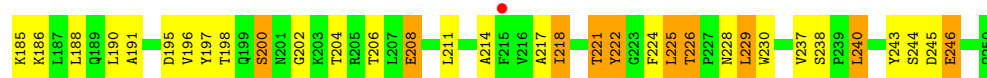
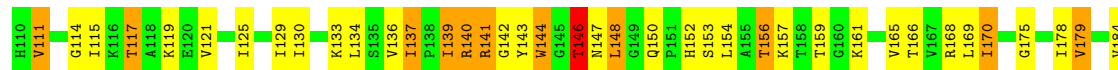


• Molecule 3: 40S ribosomal protein S1-A

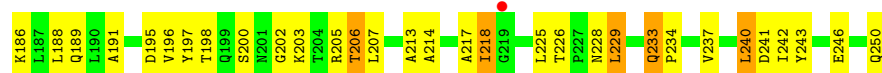
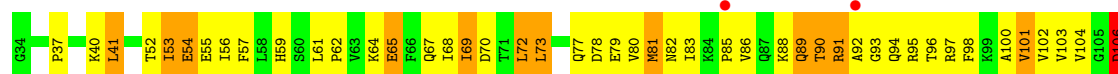




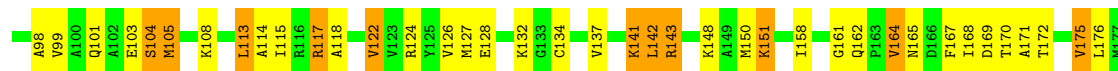
• Molecule 4: 40S ribosomal protein S2



• Molecule 4: 40S ribosomal protein S2

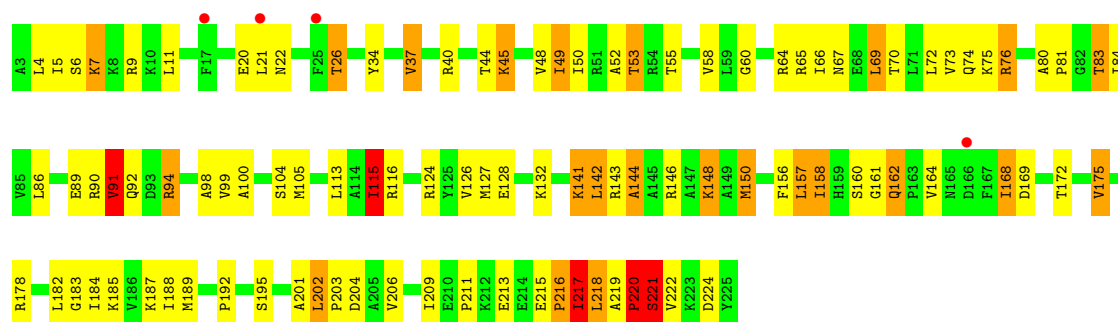


• Molecule 5: 40S ribosomal protein S3

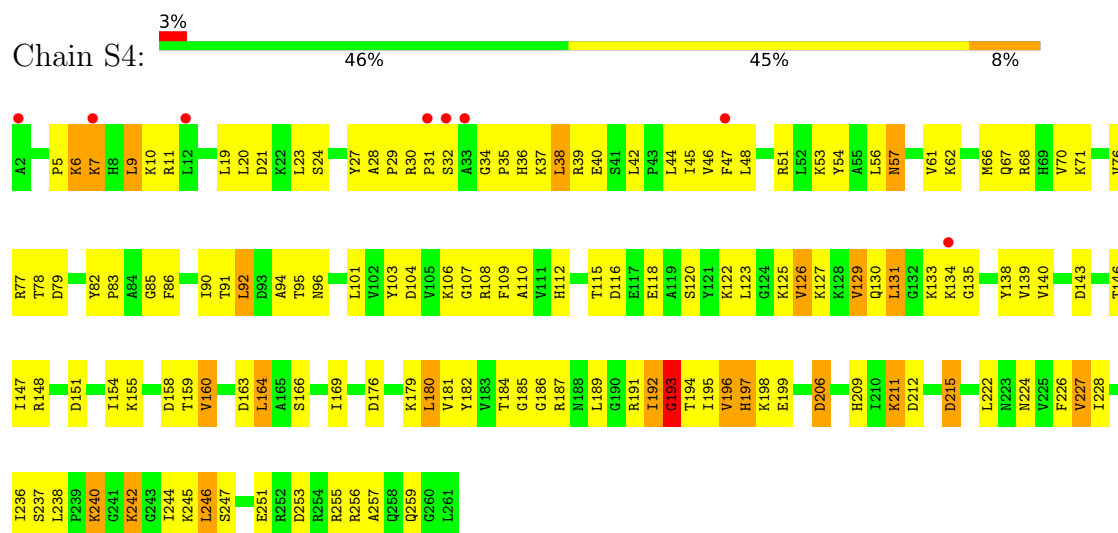


• Molecule 5: 40S ribosomal protein S3

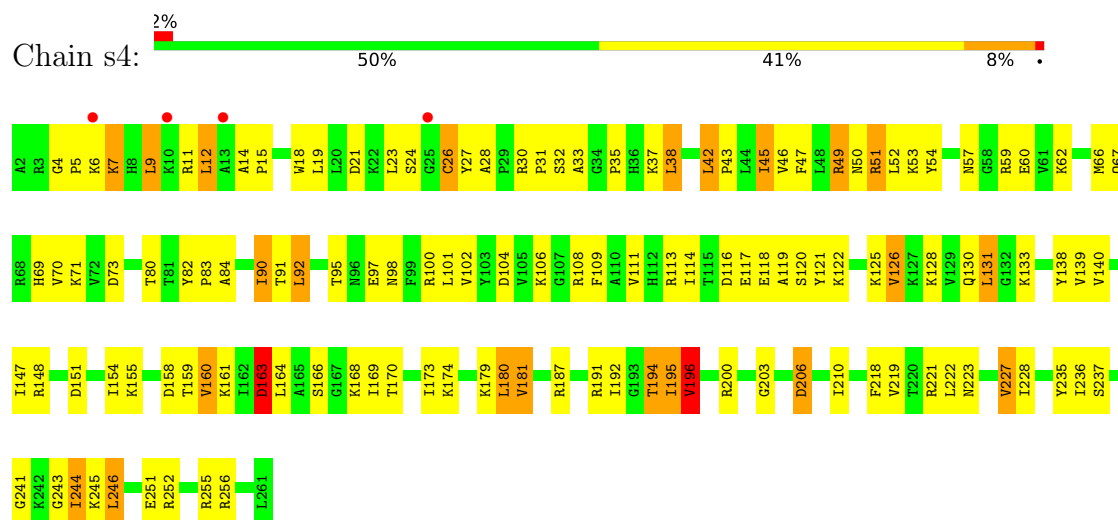




• Molecule 6: 40S ribosomal protein S4-A

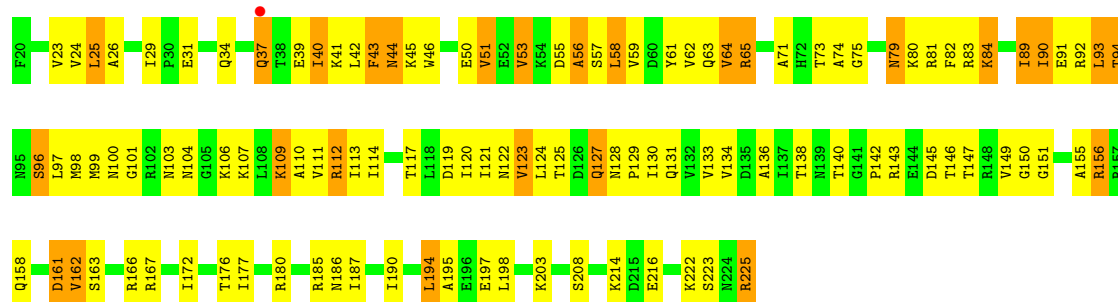


• Molecule 6: 40S ribosomal protein S4-A

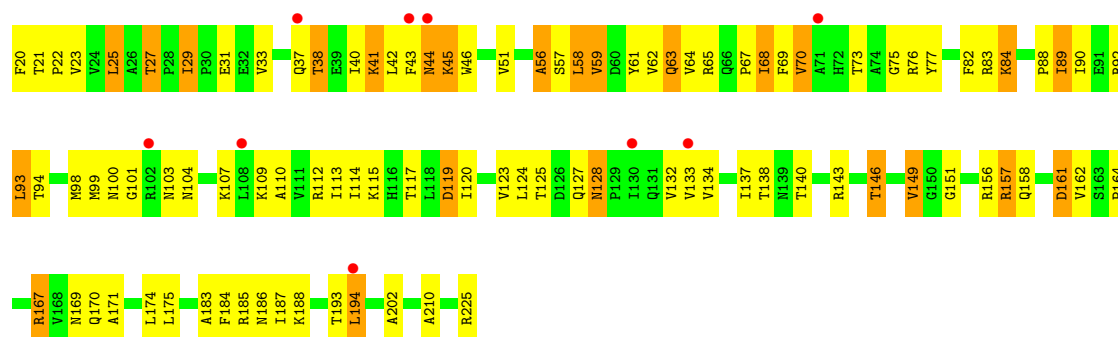


• Molecule 7: 40S ribosomal protein S5

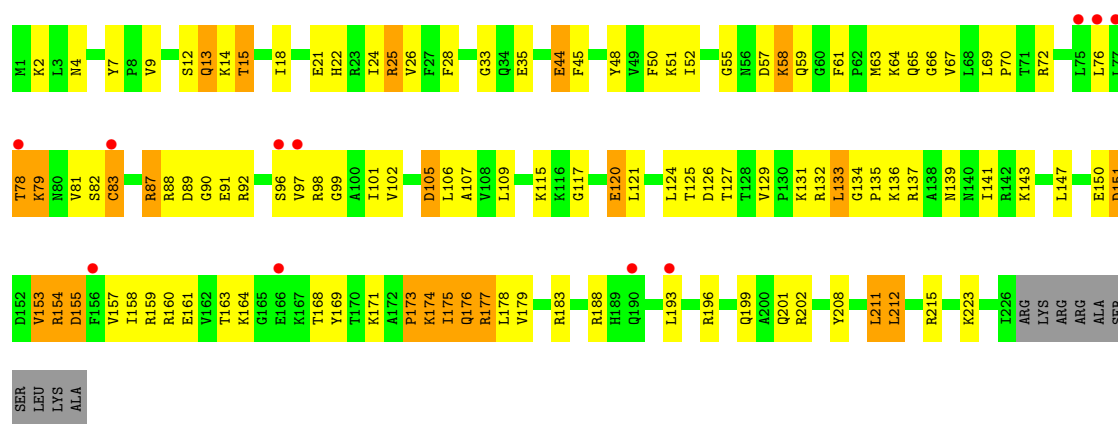




• Molecule 7: 40S ribosomal protein S5

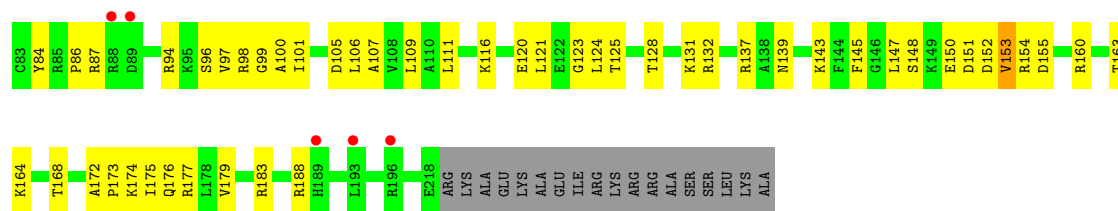


• Molecule 8: 40S ribosomal protein S6-A

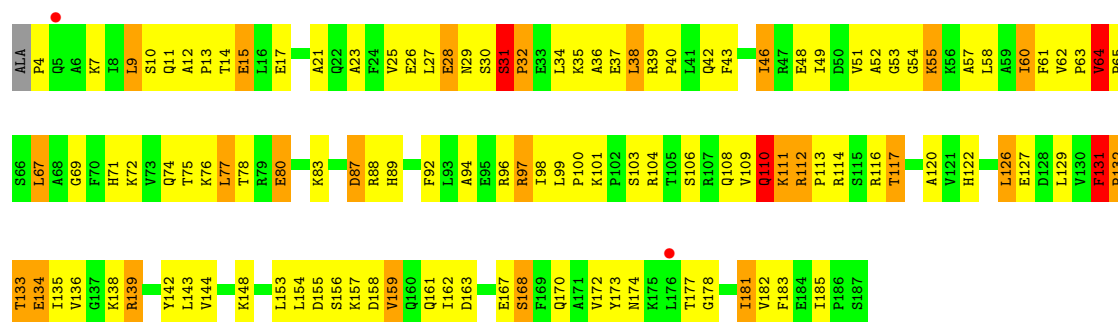


• Molecule 8: 40S ribosomal protein S6-A

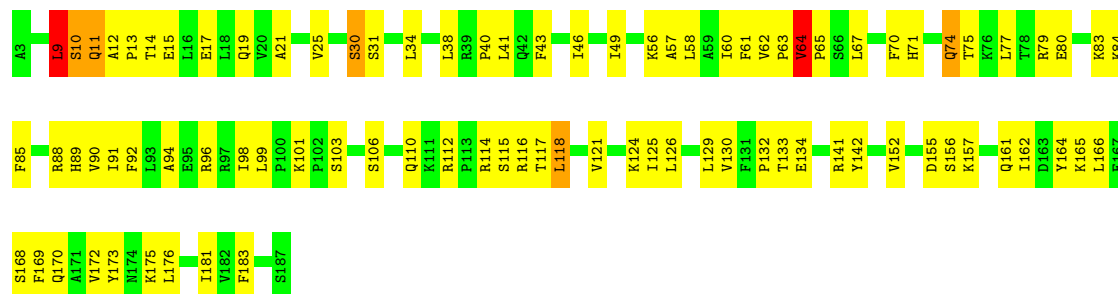




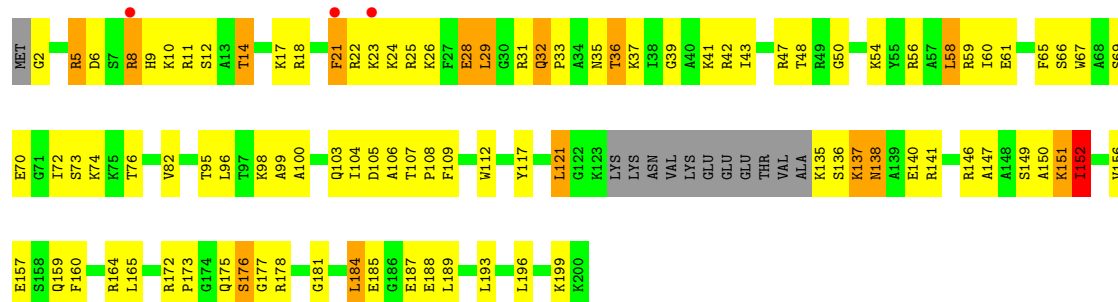
• Molecule 9: 40S ribosomal protein S7-A



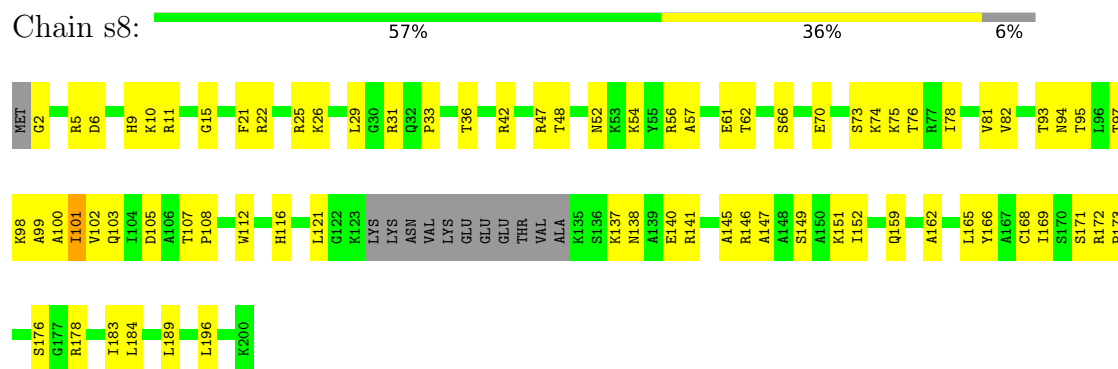
• Molecule 9: 40S ribosomal protein S7-A



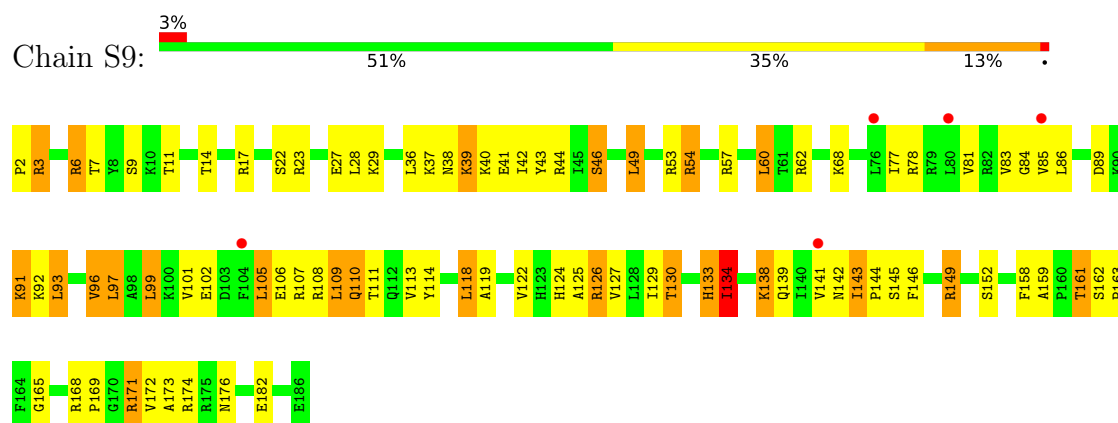
• Molecule 10: 40S ribosomal protein S8-A



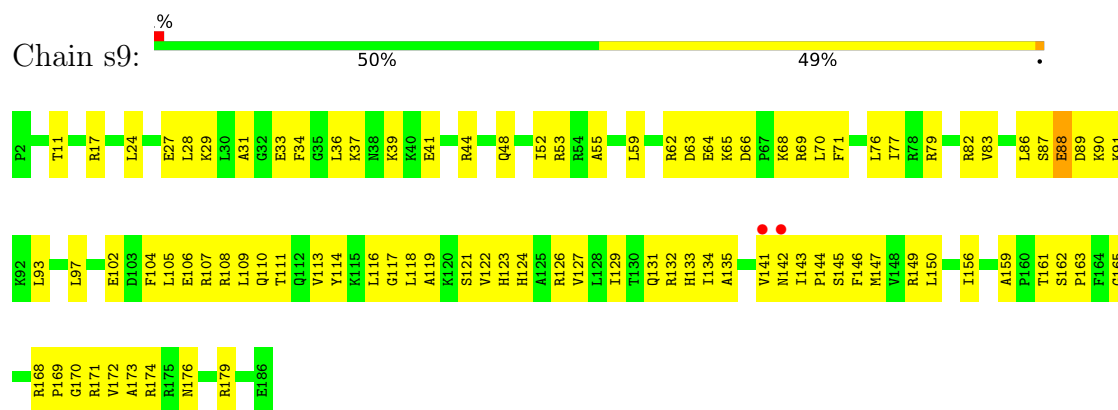
• Molecule 10: 40S ribosomal protein S8-A



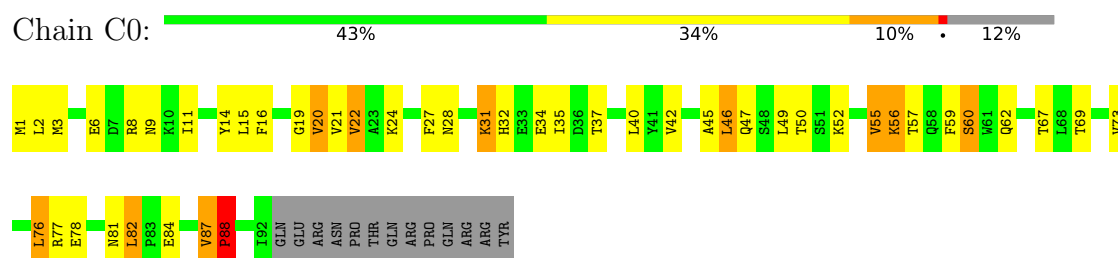
• Molecule 11: 40S ribosomal protein S9-A



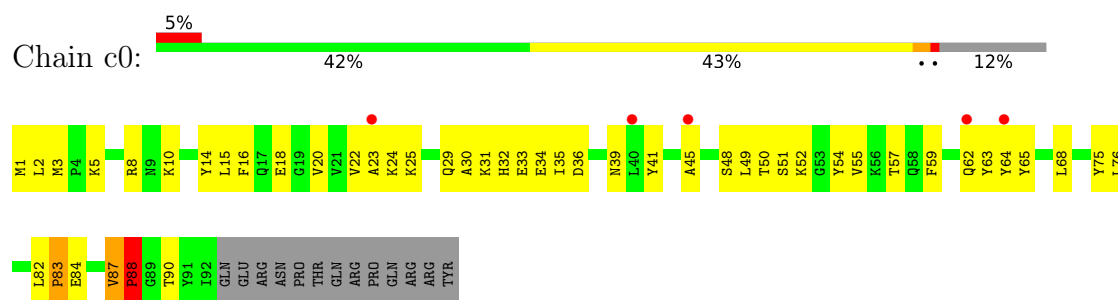
• Molecule 11: 40S ribosomal protein S9-A



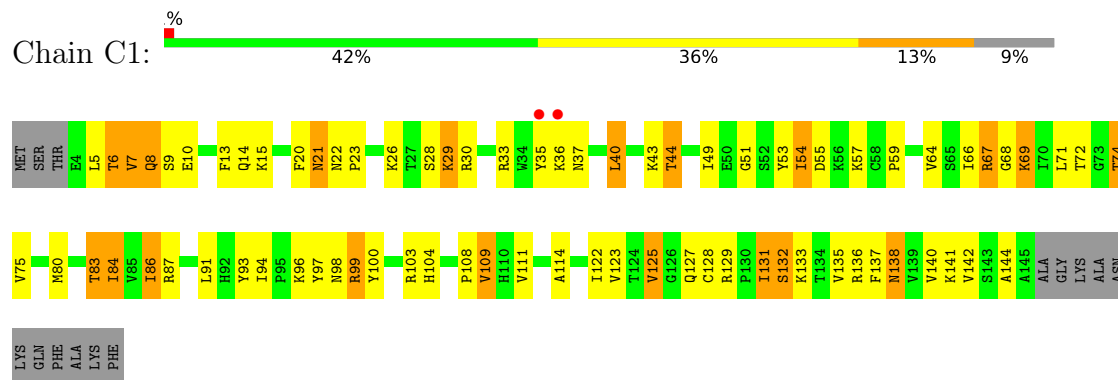
• Molecule 12: 40S ribosomal protein S10-A



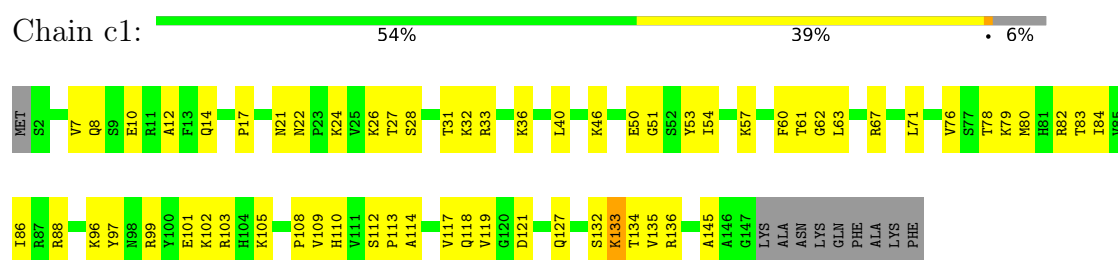
• Molecule 12: 40S ribosomal protein S10-A



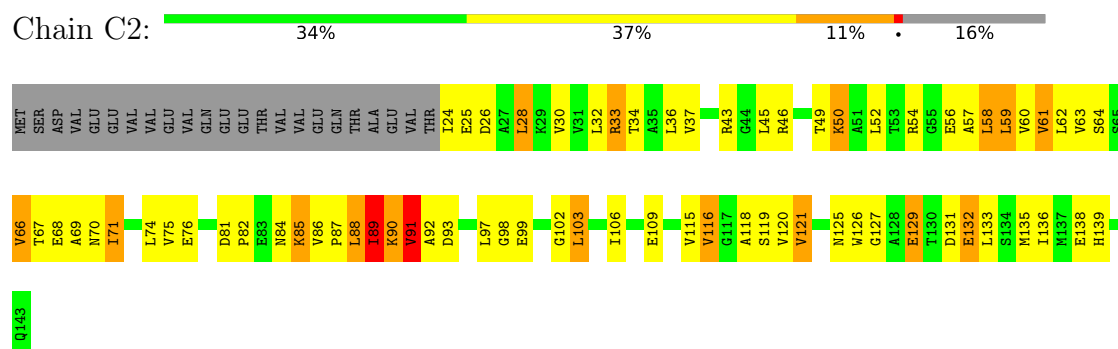
- Molecule 13: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S11-A

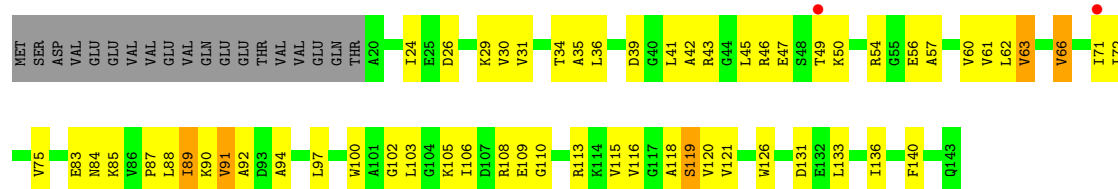


- Molecule 14: 40S ribosomal protein S12

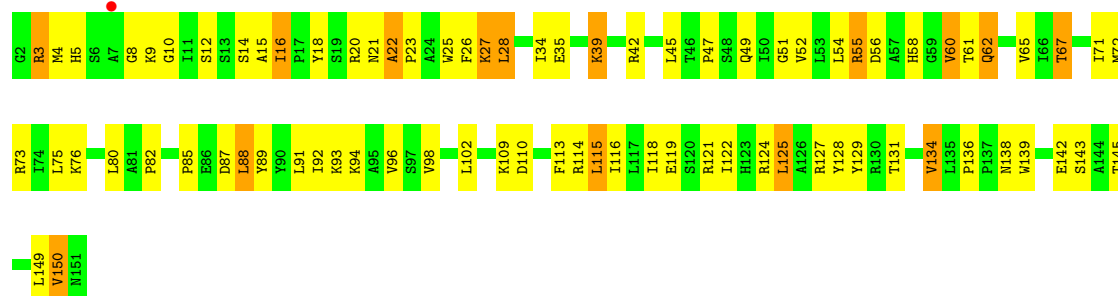


- Molecule 14: 40S ribosomal protein S12

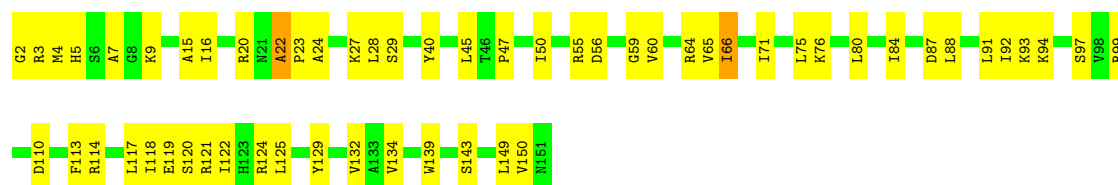




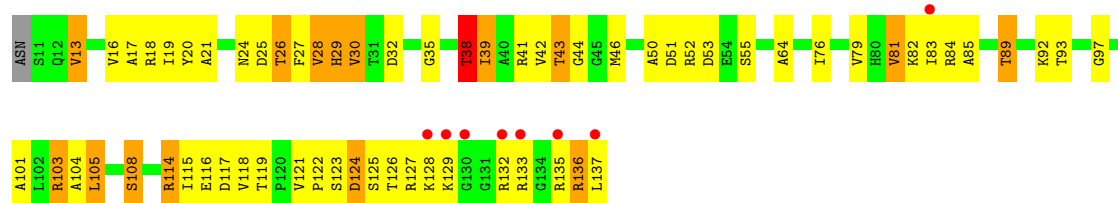
• Molecule 15: 40S ribosomal protein S13



• Molecule 15: 40S ribosomal protein S13



• Molecule 16: 40S ribosomal protein S14-A

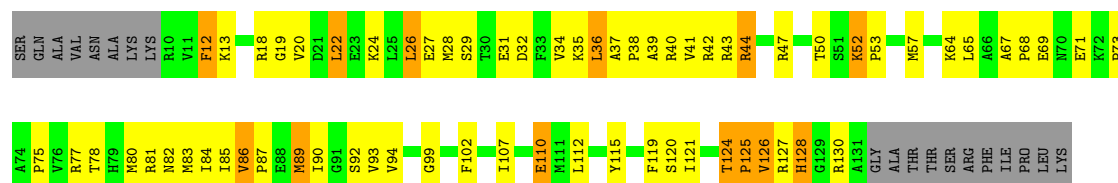


• Molecule 16: 40S ribosomal protein S14-A

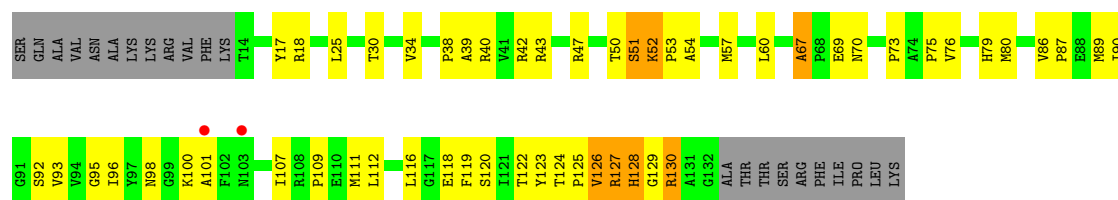




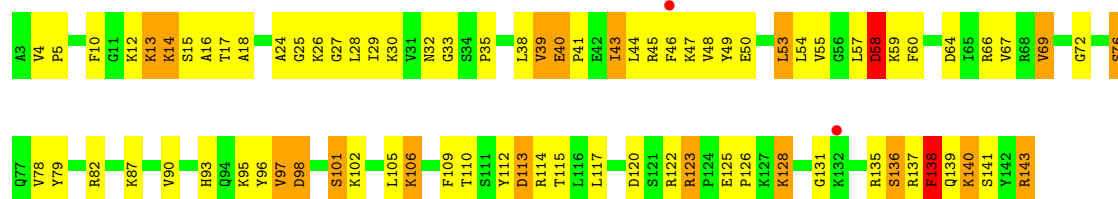
- Molecule 17: 40S ribosomal protein S15



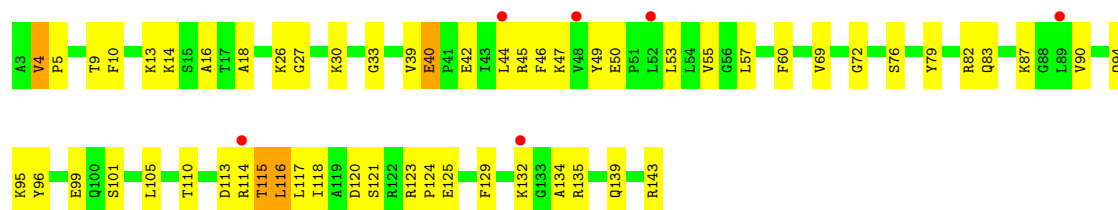
- Molecule 17: 40S ribosomal protein S15



- Molecule 18: 40S ribosomal protein S16-A

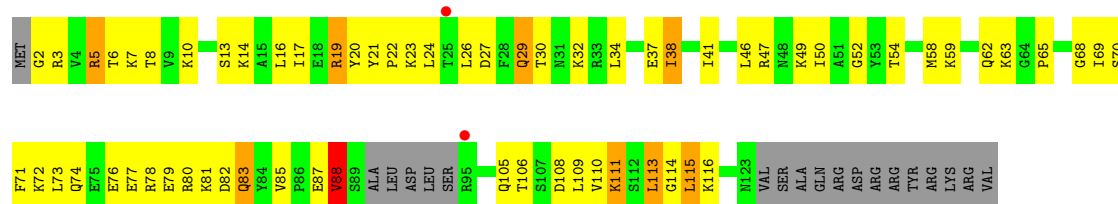


- Molecule 18: 40S ribosomal protein S16-A

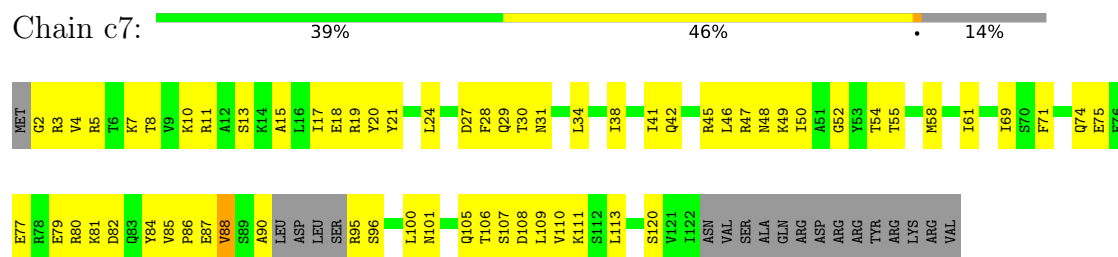


- Molecule 19: 40S ribosomal protein S17-A

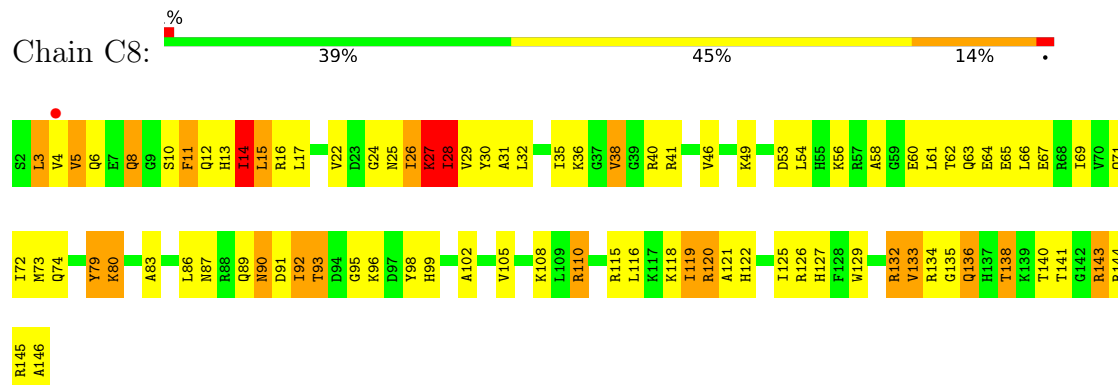




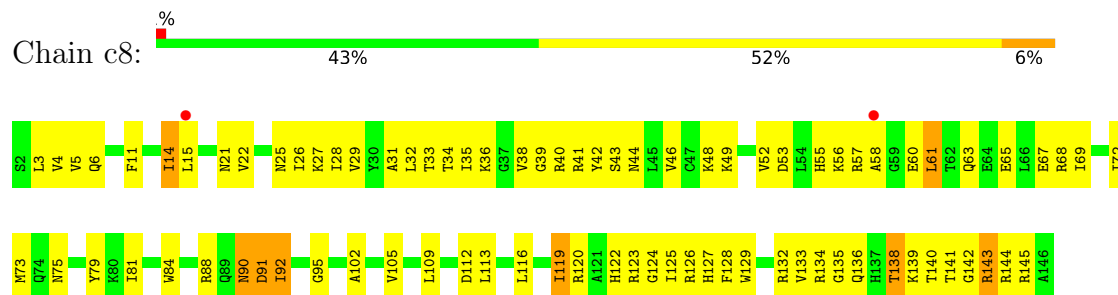
• Molecule 19: 40S ribosomal protein S17-A



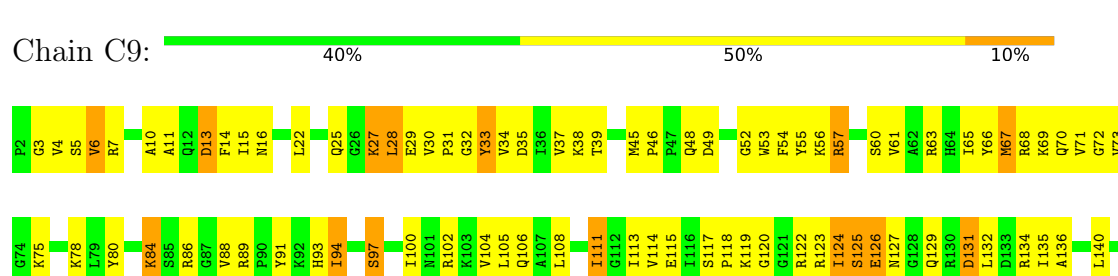
• Molecule 20: 40S ribosomal protein S18-A



• Molecule 20: 40S ribosomal protein S18-A



• Molecule 21: 40S ribosomal protein S19-A



E144

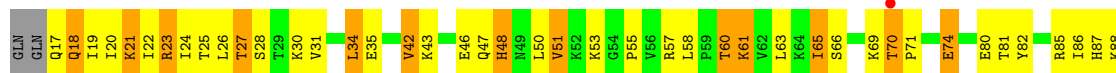
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  3% 48% 50%



- Molecule 22: 40S ribosomal protein S20

Chain D0:  % 42% 42% 14%



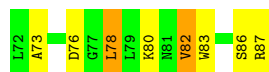
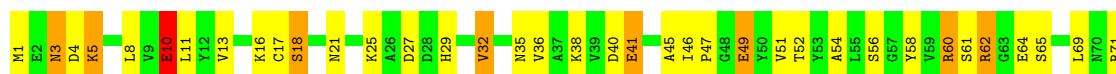
- Molecule 22: 40S ribosomal protein S20

Chain d0:  4% 42% 50% 6%



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  48% 39% 11%

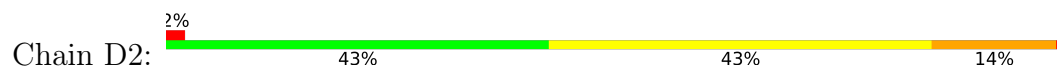


- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  62% 38%



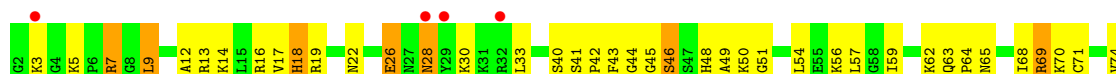
• Molecule 24: 40S ribosomal protein S22-A



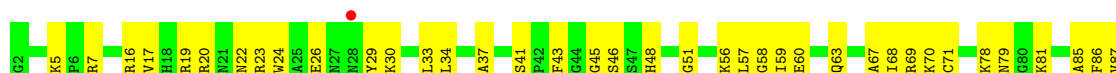
• Molecule 24: 40S ribosomal protein S22-A



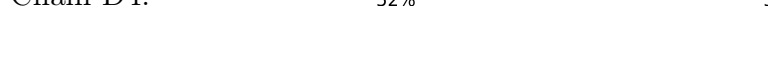
• Molecule 25: 40S ribosomal protein S23-A



• Molecule 25: 40S ribosomal protein S23-A

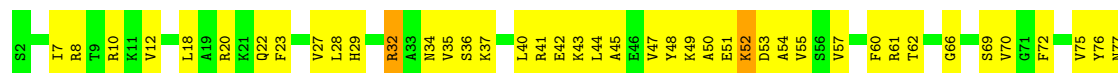


• Molecule 26: 40S ribosomal protein S24-A





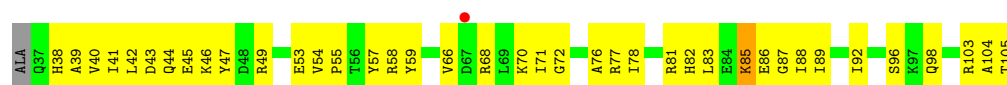
• Molecule 26: 40S ribosomal protein S24-A



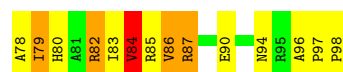
• Molecule 27: 40S ribosomal protein S25-A



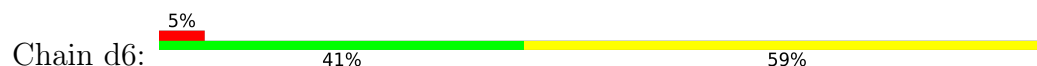
• Molecule 27: 40S ribosomal protein S25-A

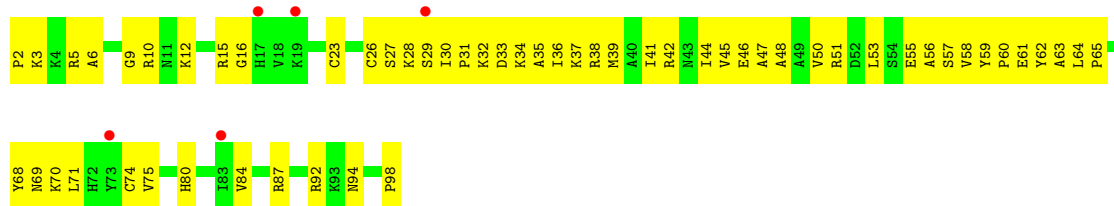


• Molecule 28: 40S ribosomal protein S26-B



• Molecule 28: 40S ribosomal protein S26-B





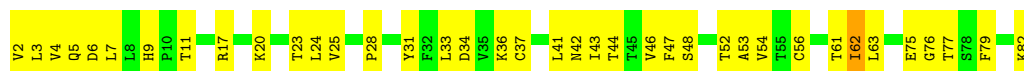
- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 60% 31% 9%



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 53% 46% .



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 38% 46% 14% .



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 63% 37%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 51% 40% 9%

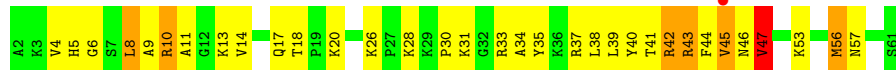


- Molecule 31: 40S ribosomal protein S29-A

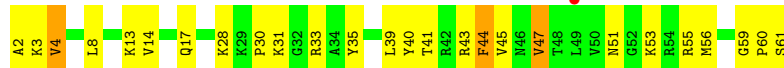
Chain d9: 68% 30% .



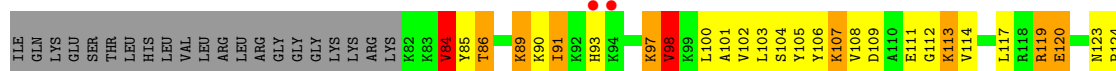
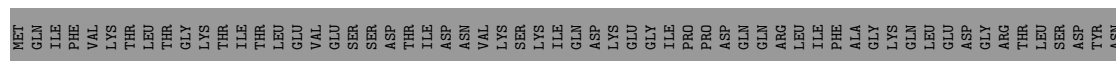
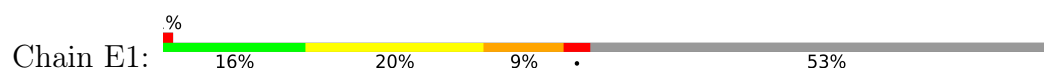
- Molecule 32: 40S ribosomal protein S30-A



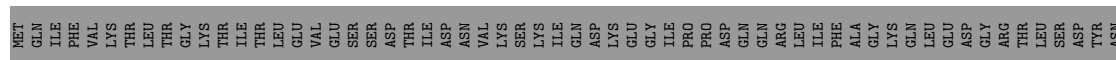
- Molecule 32: 40S ribosomal protein S30-A



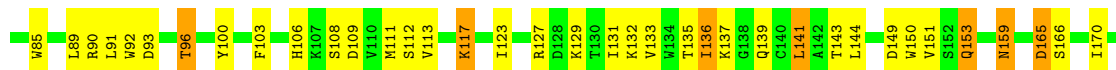
- Molecule 33: Ubiquitin-40S ribosomal protein S31

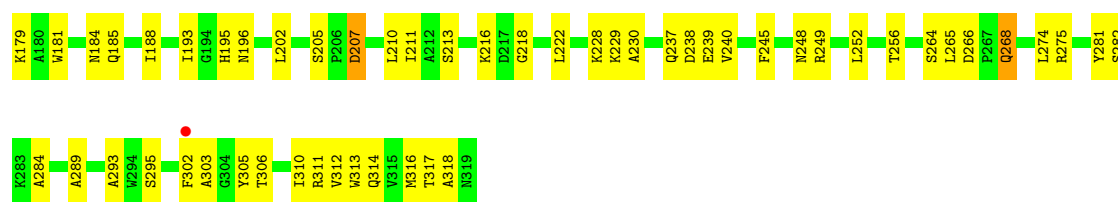


- Molecule 33: Ubiquitin-40S ribosomal protein S31



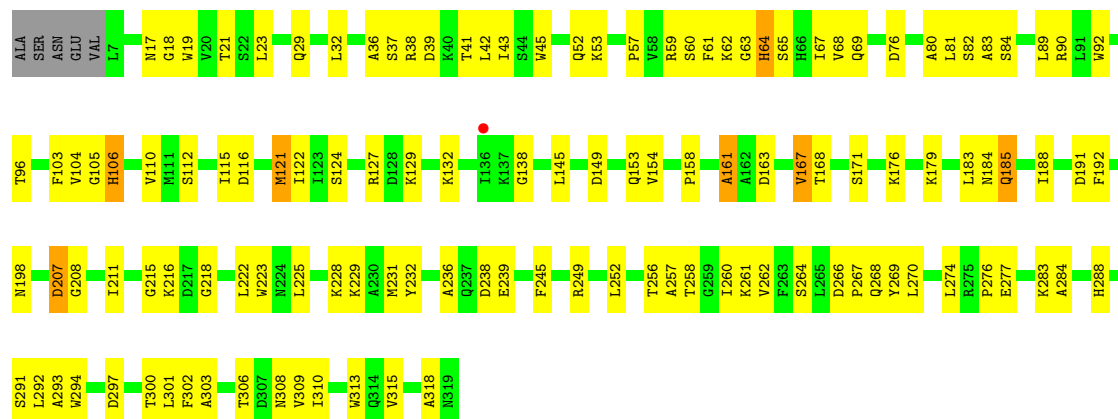
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein





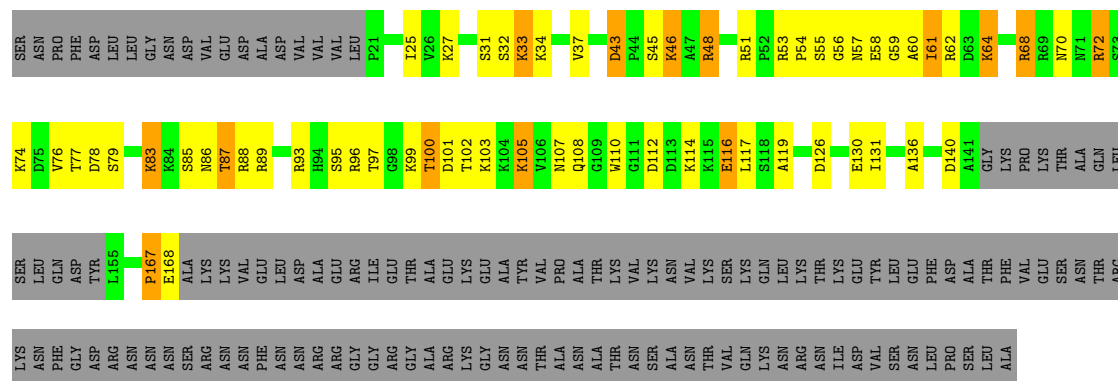
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 59% 37%



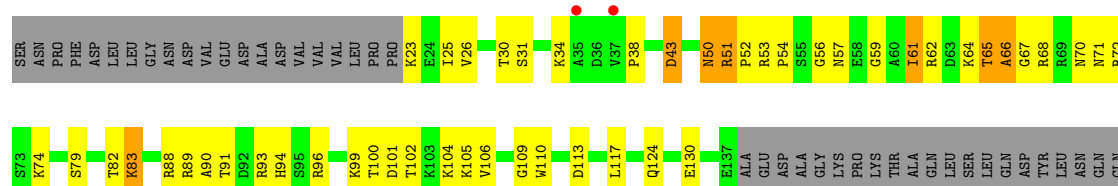
• Molecule 35: Suppressor protein STM1

Chain SM: 27% 18% 5% 50%



• Molecule 35: Suppressor protein STM1

Chain sM: 24% 16% 58%



ALA	ASN	ASN	GLN	PHE	ASN	LYS	VAL	PRO	GLU	ASN	GLU	LYS	LYS	VAL	GLU	GLY	THR	ALA	GLY	LYS	LYS	GLY	ALA	ALA	PRO	ALA	ALA	THR	VAL	ASN	LYS	VAL	VAL	THR	SER	LYS	GLN	LYS	LEU	ASN	ARG	LYS	THR	LYS	THR	LYS	ASP	GLU	VAL	THR	ALA		
ARG	LYS	ASN	PHE	GLY	ASP	ARG	ASN	ASN	ASN	SER	ALA	ARG	LYS	ASN	ASN	PHE	ASN	ASP	ARG	GLY	GLY	ILE	GLY	ARG	GLY	ALA	ALA	GLY	LYS	GLY	ASN	ALA	THR	THR	VAL	GLN	LYS	GLN	LEU	ASN	ARG	LYS	THR	ASN	ILE	ASP	VAL	VAL	SER	SER	LEU	THR	ALA

• Molecule 36: 25S ribosomal RNA

Chain 1: 28% 46% 15% 9%

U829	G763	C695	A559	C	U429	G360	C288	A221	G145	G75	G
A830	U764	C696	G560	U	U430	A361	A289		U146	G76	U
C831	C765	A697	C561	G		U362	G290	C225	U147	A77	
G832	U698	C636	C562	C494	U434	G363	C291	C226	G148		
G833	U766	C637	U563	C495	C435	G364	C292	G227	U149	U83	
	U767	C638	C564	C496	A436		C293	U228	A150	U84	
A836	G770	G701	U565	C497	G437	A367	U294	G229		U85	
A837	A771	C702	U640	A498	A438	U370	A295	U230	U154	G86	
C838	G703	G704	C641	G567	C439	G371	A296	G231	G155	U87	
C839	A775	U704	U642	A501	A440	A372	G297	G232	A157	A88	
C840	U776	A705	U643	U502		A373	U298	C233		U14	
A841	U777	A706	G644	C503	U				C90	A15	
		U707	A645	C503	G		G301	G236	G161	G91	
A843	G781	G708	A646	U507	U	G376	U302	G237		G92	
	U782	A709	A647	U508	G		G303	A238	U19	G93	
A846	A783	A710	C648	U509	U	G379	G304	G239	C166	G94	
A847	G785	G712	A649	G510	U	U380	U305	U240	U168	A95	
A848			A585	G511	U		A306	G241	U169	G21	
							A307	C242	G170	G98	
C849	A796	U713	G588	C515	G	G383	A308	G243	G171	A99	
U850	G787	U714	C590	A516	U	A385		G244	G172	A100	
C851	C788	A715	G591	G517	G	A386		U245	G173		
	A789	A716	A592	G518	U	A387		C246	G174	G104	
G854	U790	C717	C593	A519	C			U247	C175		
U855	A791	U718	U594	U520	C	G390	A317	U248			
G856	G792	U719	U594	A521	C	A391	A318	U249		A109	
C857	C793	A720	G595	A521	C	G392	A319	U250	U182	G110	
C858	U794	G721	C596	A521	C	U393	G320	G251	C111	C111	
C859	G795	G722	C597	U524	U	G394	U393	U252	U112	G36	
C860	U796	U723	A598	C525	G	C394	C321	U252	C113	U37	
C861	U797	U724	C599	C526	C	A395	U322		A114	U38	
U862	G798	G725	U664	C527	C	A396	A323	U255	A115	A39	
C863	C799	G726	G601	U528	C	A397	A324	G256	A116	A40	
C864	G800	G727	A602	A529	C	A398	A325	U257	U117	G41	
	A801		A603	G530	U	A399		G258	U118	C42	
G869	C802	C730	G604	G531	U	U400	U329		U119	A43	
C870	C803	U731	U665	A532	G	U401	G330	U261	U190	U44	
U871	C804	C732	C606	A533	U	A402		U262	C192		
	G805		A607	U534	G	C403	G335		A122	A49	
C873	A806	A738	U673	G535	G	C404	A336	A265	A123		
U874	A807	G739	C674	U536	G	U405	G337	A266	G196	A52	
G875	U808	G740	C675	U536	U	G406	A338	G267	U124	G53	
A876	C809	U741	C676	C539	A	A407	C339	A268	A198	C54	
	A810		A677	C539	G	A408	C339	G269	A199	G55	
G878	U811	C745	U678	C542	G	A409	G341	U270	C200	G55	
U879	G812	A746	U679	C543	G				G128		
C881	U814	U748	U681	U545	G		A342	C271	U129	G59	
A882	G815	C749	U682	C546	A	G412	U343	G271	A130	A60	
A883	A816	G750	U683	C547	A		A344	G274	C131	G61	
U884	A817	A751	C684	U547	U	G415	G345	U275	C132	A62	
U885	C818	C752	U685	U548	C	A418	G347	U276	U133	G62	
C886	U819	C753	C686	A621	U	G419	A348	G277	C134	G64	
			A622	A550	C	G420		U278	U135	A65	
			U687	A551	C	A421	C349	U279	G136	A66	
			C688	G552	G	G422	A350	U280	A213	A67	
G891	G822		U689	C552	C	A423	A351	G281	U138	C68	
U892	C823	C757	C690	U553	A	A424	A352	G282	G139	C69	
C893	C824	C758	A690	A554	U	G425	G353	A284	C140	A70	
G894	U825	U759	A691	U555	U	G426		U285	C141	A71	
A895	G826	G760	A692	U556	U	U427	A357	A285	G217	C72	
A896	A927	A761	A693	U557	U	C427	G358	U286	C142	C73	
	A928	U762	U694	A557	C	A428	U359	C287	G143	G74	

U1873	A1804	C1660	U1533	G1464	G1392	G1319	A	A1182	U1108	U1041	C969	U899
A1874	C1805	G1661	A1534	A1467	A1393	U1322	A	G1186	U1109	U1042	A970	G900
G1875	A1806	C1662	A1535	A1468	C1396	U1325	C	C1187	U1110	U1043	G971	G901
U1876	G1807	C1663	G1536	U1471	U1397	A1326	G	U1188	G1112	A1047	A973	U905
G1877	G1808	U1600	A1537	U1472	U1398	U1327	C	C1189	G1113	A1048	G975	A906
A1878	G1809	G1664	G1538	G1473	A1399	C1327	U	A1190	U1114	C1049	G976	G907
A1879	A1810	C1665	A1539	U1477	G1400	U1328	C	U1191	G1115	U1050	C977	G908
U1880	U1873	G1666	U1540	A1478	A1401	U1329	A	C1192	G1116	U1051	G978	G909
A1881	A1667	A1667	G1541	A1479	C1402	A1330	G	A1193	G1117	U1052	G979	G910
A1886	G1668	C1669	G1542	U1477	C1403	U1334	G	G1194	C1118	A1053	A980	C911
U1887	U1740	U1606	G1543	U1478	G1404	U1335	A	A1195	U1122	A1054	U981	G912
U1888	G1744	U1607	G1547	U1480	A1407	U1336	G	C1198	U1123	A1055	C982	A913
U1889	C1745	C1609	C1548	A1481	G1408	U1337	U	C1199	U1124	U1056	A992	A914
A1891	G1677	G1610	U1549	A1482	U1409	C1338	G	A1200	U1125	A1057	G993	A915
G1892	G1678	G1611	C1550	G1483	C1411	C1339	G	C1201	G1126	U1058	G994	G916
U1821	A1679	A1612	U1553	U1484	G1412	G1340	G	A1202	G1127	G1059	G995	A917
A1893	G1680	A1613	U1554	G1485	G1413	U1341	U	A1203	U1128	U1060	U995	A920
U1894	U1681	C1614	U1555	G1486	G1414	U1342	A	A1204	U1129	A1061	A996	A921
A1895	U1682	C1615	U1556	G1487	C1416	A1343	A	A1205	A1130	A1062	A997	G922
A1901	A1683	U1616	C1556	U1488	G1417	G1344	C	G1206	G1131	G1063	C1000	C923
C1904	U1686	G1617	A1557	A1489	A1418	G1345	A	G1207	G1132	A1064	G1001	G924
G1905	U1687	A1619	A1558	A1490	A1419	G1346	A	U1208	G1133	A1065	A1002	A925
G1906	U1688	U1620	A1559	A1491	C1420	U1347	C	G1209	G1134	G1066	A1003	A926
C1907	U1688	A1621	G1561	U1495	G1421	U1348	U	U1210	U1138	U1070	U1004	C927
A1908	C1690	U1622	C1562	C1496	G1422	G	C	G1213	G1139	U1071	G1005	C928
A1909	C1691	A1625	C1563	C1497	U1427	A	C	G1219	G1140	G1072	A1006	A929
A1910	U1691	U1629	U1564	A1498	A1428	U1353	C	C1219	A1143	U1073	U1007	U930
A1913	U1696	U1629	G1565	A1499	G1429	U1354	C	A1221	U1144	U1078	A1008	C931
U1914	C1767	U1629	U1566	A1501	U1430	G1354	C	G1222	U1145	A1079	A1009	G932
G1914	U1697	U1629	U1567	C1502	G1431	U1355	C	A1223	G1146	A1080	G1010	A933
A1915	G1700	A1632	U1568	A1503	C1432	U1356	C	G1226	G1147	U1081	U1014	U935
C1842	C1701	C1634	U1569	A1504	A1433	G1357	C	G1227	G1152	U1082	C1016	A936
C1844	A1704	G1635	C1505	C1506	G1434	U1357	C	G1228	A1153	G1083	G1017	G937
G1845	C1779	U1636	A1506	A1507	U1435	U1361	C	C1229	C1155	A1084	C1018	U943
C1846	G1780	A1637	U1572	C1507	U1436	G1362	C	G	C1156	A1085	G1019	C944
A1847	C1781	A1638	G1573	C1508	C1437	A1363	C	A	G1157	A1086	G1020	U945
G1848	U1782	A1639	A1575	A1509	U1438	C1364	C	C	A1158	G1087	U1021	U946
C1849	U1783	G1640	G1576	G1510	U1439	G1365	C	G	A1159	G1090	C1023	G947
G1850	G1784	U1641	U1511	U1512	G1440	G1366	C	G	C1160	C1092	G1024	G950
G1851	U1785	A1642	U1513	U1514	G1441	U1367	C	G	G1161	A1093	A1025	A951
G1852	G1786	A1643	G1515	G1516	U1442	U1368	C	G	U1162	A1094	A1026	A952
U1853	A1714	C1644	A1515	C1516	G1443	A1369	C	G	A1163	U1095	A1027	G953
C1854	U1716	U1645	C1581	C1517	U1444	G1374	C	G	G1164	U1096	U1028	U956
U1855	U1717	G1646	C1582	G1518	U1445	G1375	C	A	A1165	G1097	G1029	C957
C1856	G1718	A1647	A1583	U1519	A1446	C1376	C	U	A1169	A1098	A1030	C958
G1857	G1719	A1648	U1584	G1520	G1447	G1380	C	G	A1170	A1099	U1033	C959
A1858	U1720	U1649	C1585	G1521	U1448	A1381	C	G	G1175	U1100	U1034	U960
A1859	U1721	G1650	G1586	U1522	A1449	G1386	C	A	C1176	G1101	G1035	U961
G1860	U1722	U1651	U1587	U1523	G1450	U1387	C	A	G1177	A1102	C1037	G963
U1944	A1723	G1652	A1588	A1524	U1455	U1388	C	U	G1178	A1103	C1038	U966
A1945	U1724	G1653	A1589	G1525	A1456	G1389	C	C	G1179	A1104	A1105	A967
A1946	C1725	A1654	G1590	U1526	U1456	A1460	C	G	A1180	C1107	U1039	G968
G1947	A1798	G1655	G1591	U1527	A1461	A1461	C	G	A1181			
G1948	U1726	A1656	G1592	U1528	A1462	A1462	C	G				
C1869	G1727	A1657	A1593	G1529	A1463	C1391	C	G				
C1870	A1728	G1658	A1594	G1528			C	G				
U1871	A1729	A1594	A1462	G1528			C	G				
U1950	C1872						C	G				
C1951							C	G				



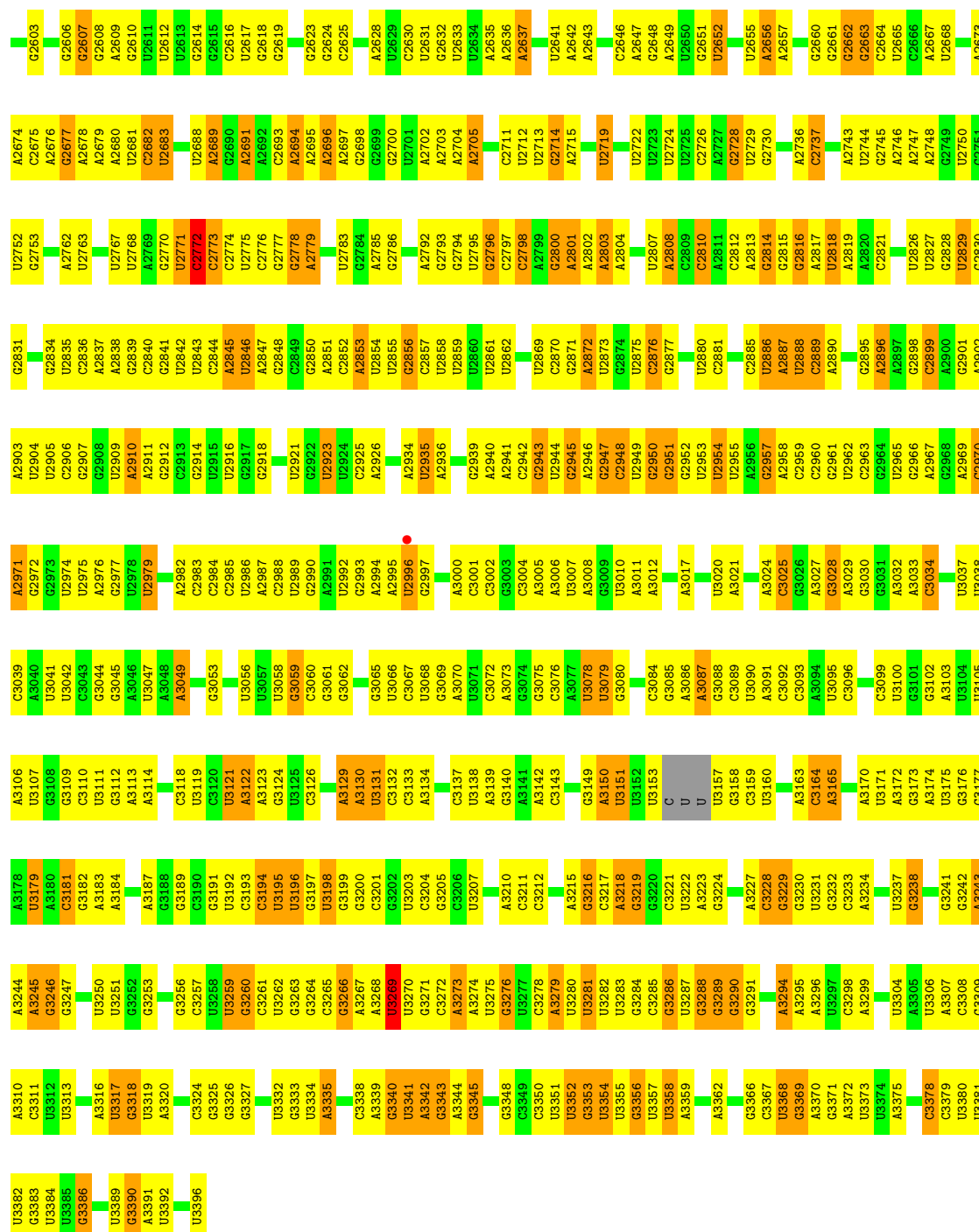
G2937	G3003	A3073	C3145	G3216	G3288	U3357	G	A213	G281	U370	G
A2940	C3004	G3074	G3146	C3217	G3289	U3358	U	G214	G282	G371	U
A3005	A3005	G3075	U3151	A3218	G3290	U3359	U3	G215	G283	A372	G
A2941	A3006	C3076	U3152	G3219	G3291	C3360	C	G216	A284	A373	C
C2942	U3007	A3077	U3153	G3220	A3294	G3361	C7	G217	U285	U376	C
G2943	A3008	U3078	C	G3221	A3295	U3362	C8	G218	U286	A377	C
U2944	U3079	G3080	U	G3222	C3298	U3363	U9	G219	U287	A378	U
G2945	A3012	U3081	U	A3227	A3299	U3364	C10	G220	C291	A379	C
A2946	U3013	C3082	U	C3228	G3303	U3365	A11	G221	U292	U380	U
G2947	U3014	G3083	U	G3229	G3304	G3366	A12	G222	G293	U381	G
C2948	C3018	C3084	G3159	G3230	U3305	C3367	A13	G223	A295	U382	C
U2949	U3019	G3085	U3160	G3231	A3306	U3368	U14	G224	A296	U383	U
G2950	U3020	A3086		G3232	A3307	G3369	G15	G225	U297	A386	U
G2951	A3021	A3087	C3163	G3233	U3308	A3372	G18	G226	U298	A387	C
U2952	G3022	C3088	A3164	U3237	U3309	U3373	U19	G227	G299	G388	C
U2953	U3023	A3089	A3165	G3238	C3308	U3374	A20	G228	G303	A389	U
U2954	A3024			G3239	G3309	A3375	G21	G229	G304	U	U
U2955	C3025			G3240	A3310	U3376	U84	G230	C312	G392	G
A2956	G3026	C3092	U3168	G3241		G3377	G22	G231	U313	G393	G
G2957	A3027	C3093	U3169	A3242	U3313	C3378	A23	G232	G315	G394	G
	C2960	U3037	U3170	A3243	A3314	U3379	G24	G233	U316	A398	G
U2962	G3028	A3039	U3171	A3244	G3315	C3380	U25	G234	A317	A399	U
	A3029	A3040	A3172	A3245	G3316	U3381	A26	G235	A318	G400	A
	G3030	C3096	G3173	G3246	U3317	U3382	G27	G236	A319	U401	G
		G3097	A3174	G3247	U3318	U3383	G28	G237	U314	A402	G
		G3098	U3175		G3319	U3384	G29	G238	G316	G403	G
		C3099	U3176		A3320	U3385	G30	G239	U317	G404	G
		U3100	G3177		C3321	U3386	G33	G240	U318	U405	A
			A3106			C3322	G34	G241	G172	G406	U
		U3107	U3179			U3323	A35	G242	G173	A407	A
		G3108	A3180			U3324	C36	G243	C174	U408	C
		U3111	C3181			G3325	G37	G244	C175	A409	U
		G3112	G3182			U3326	U37	G245	U181	U410	C
		C3115	A3183			G3327	U38	G246	U182	G420	G
			A3184			U3328	A39	G247	U183	G421	C
			U3185			U3329	A40	G248	U184	G422	U
			A3186			U3330	G41	G249	U185	A423	U
			A3187			U3331	C42	G250	U186	G424	U
						U3332	A43	G251	U187	U425	C
						U3333	U44	G252	U188	G426	U
						U3334	A45	G253	U189	C427	C
						U3335	U46	G254	U190	U428	U
						U3336	C47	G255	U191	U429	G
						U3337	A48	G256	C192	U430	U
						U3338	U49	G257	U193	U431	C
						U3339	A50		U194	U432	U
						U3340	A51		U195	U433	U
						U3341	A52		G196	C435	U
						U3342	G53		G197	A439	U
						U3343	C54		U120	A351	U
						U3344	A57		A122	A352	U
						U3345	G58		U126	G353	U
						U3346	U58		G127	U359	U
						U3347	G59			G360	G
						U3348	A60		C132	A361	U
						U3349	U60		U133	U362	G
						U3350	A61		U134	G363	U
						U3351	A62		C136	G364	U
						U3352	G63			U411	U
						U3353	A63			G510	U
						U3354	G64			G511	U
						U3355	A65				
						G3356					

• Molecule 36: 25S ribosomal RNA

Chain 5:  31% 46% 15% 8%

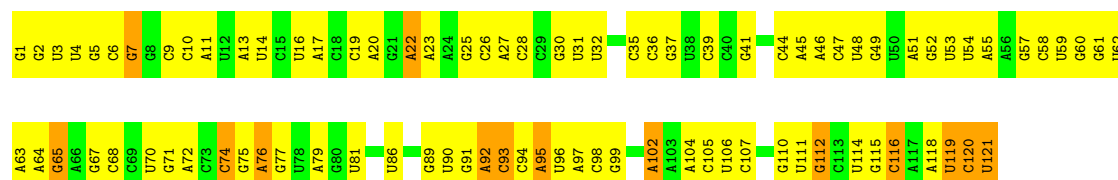
A1509	A1435	C1358	C1284	G1206	G1140	C1000	C937	C861	U797	G728	G658	C593	U512
G1510	U1436	C1359	G1285	G1207	C1141	G1001	C928	C862	G798	C729	G659	U594	G513
U1511	U1437	C1360	A1286	U1208	A1142	A1002	A929	U885	G799	C730	A660	G595	G514
U1512	U1438	C1361	A1287	G1209	A1143	A1003	U930	A866	G800	U731	G661	C596	C515
A1515	U1439	C1362	C1297	U1210	G1144	A1006	C931	C867	A801	C732	U662	G597	A516
C1516	U1440	C1363	C1298	U1211	G1145	U1007	U932	C868	C802		C663	A598	G517
G1517	G1443	C1364	U1299	A1212	C1146	U1008	A933	C869	C803		U664	C599	G518
U1520	U1444	G1367	A1301	G1213	G1147	A1009	A936	C870	C804		A665	G600	A519
G1521	U1445	U1368	A1302	U1214	G1148	U1010	G937	U874	A806		A672	U601	U520
U1522	U1446	A1369	A1303	U1215	U1149	A1011	C938	C875	U673		G674	A602	A521
A1524	G1447	U1378	U1305	C1219	U1151	G1012		A876	A808			G604	U528
U1525		G1379	G1306	U1220	G1152	G1013	U942	C877			A677	G609	A529
G1526	G1450	U1380	C1307	A1221	A1153	U1014	U943	C878			G678	G610	A532
C1527	C1451	A1381	U1309	G1223	A1154	C1015	U944	U879	U814		U679	A611	A533
U1528	A1459	C1385	C1312	G1229	C1155	U1016	U955	G880	G680		U680	U612	U534
A1529	A1460	G1386	G1313	G1230	C1156	C1017	U946	C881	G681		U681	G613	G535
	A1461	U1387	C1314	A1231	G1157	G1018	U947	A882	A816		U682	C614	
	A1462	U1388	U1315	G1232	U1158	U1019		A883	A817		U683	U615	U540
	A1468	G1391	C1316	U1235	A1165	G1020	A952	U884	C818		U684	U616	U541
A1534	C1469	C1392	A1317	G1236	U1166	G1021	G953	U885	U819		U685	G617	G542
A1535	U1470	G1393	G1318	G1237	U1167	A1026	U954	C886	A820		U686	C618	C543
G1536	U1471	A1394	G1319	U1241	A1170	A1027	U956	C887	U821		U687	A619	
	U1472	A1395	C1320	G1242	G1175	A1028	C957	U888	C822		U688	U620	C546
A1538	U1473	C1397	U1321	G1243	C1176	U1029	C958	C889	C824		U689	A621	
U1540	G1474	U1398	G1322	A1244	G1177	G1030	U966	C890	U825		A690	A622	
A1541	A1475	G1399	U1323	A1245	U1178	A1031	U967	U891	G826		A691	G625	U549
G1543	U1476	G1400	G1324	A1246	A1179	C1032	U968	U892	U827		A692	A693	A550
	A1477	A1401	C1325	A1247	U1180	C1033	C969	C893	A828		C694	U626	A551
		A1402	U1326	U1248	A1181	U1034	A962	C894	U829		C695	U627	G552
		C1403	A1327	G1249	U1182	U1035	C963	A895	A830		C696	A628	U553
		U1405	C1328	G1250	A1183	A1040		A896	A831		U629	U630	A554
		A1406	U1329	A1251	C1184	G1036	U966	U897	U834		A630	U631	U555
		A1407	C1330	A1252	U1185	C1037	C968	U898	C835		U632	G633	U556
		G1408	A1331	U1253	C1186	U1038	C969	U900	A836		G634	C634	U557
			U1332		G1187	C1039		G901	A837		U704	A559	U558
			C1333		U1110	A1040	A973	A906	C838		A705	G635	G560
			U1334		U1111	C1043	G974	G907	C839		U706	C561	C562
			C1335		U1112	U1044	C975	G908	C840		G708	C637	
			U1336		U1121	A1045		G909	A841			C638	
			C1337		U1122	A1046		G910	A842			G639	G566
			U1338		U1123	A1047	U979	C911	A843			U640	G567
			G1340		U1124	A1048		G912	G844			C641	
			U1341		U1125	U1049	U986	G913	G845			U642	C576
			C1342		U1126	U1050	U987	A914	A846			U643	C577
			A1343		G1127	U1054	U988	A915	A847			A578	G644
			G1344		U1128	A1055	U989	G916	A786			A645	A579
			U1345		U1129	A1056	U990	A917	G787			C580	C580
			G1346		A1130	A1057	U991	C918	C788			U648	U551
			U1347		U1131	A1062	U992	U919	A789			G649	G582
			C1348		U1132	G1063	U993	U920	U790			C650	C586
			A		U1133	A1064	U994	A921	A791			G651	C587
			U		G1134	A1065	U995	U922	G792			U652	U587
			U		U1135	G1066	U996	C923	G793			C654	G588
			G1352		U1138	U1070	U997	G924	U794			C655	A589
			C1281		A1203	U1071	U998	A925	G795			G590	G590
			G1283		A1205		U999	A926	U796			A656	A592

C	U	C	U	U	A	G1928	C1857	G1790	U1721	U1645	G1576
U	U	C	U	G	C	G1929	A1858	C1791	U1722	G1646	G1577
C	G	C	U	G	C	A1930	A1859	C1792	U1723	A1647	C1578
C	C	C	U	G	C			G1793	U1724	A1648	C1579
G	C	C	U	A	C	A1933	G1863	G1794	G1727	G1653	A1580
C	G	C	U	G	U	G1935	A1864	U1795	G1728	A1654	C1581
C	C	G	G	G	G		C1866	A1796	G1729	G1655	C1582
C	C	G	G	G	G	G1940	A1867	A1798	G1730	A1656	A1583
C	U	U	U	C	U	C1941	A1799	A1799	A1731	C1657	U1584
C	U	U	U	C	U	U1942	G1868	A1800	U1732	G1658	
A	U	C	G	U	C	U1943	U1871	U1801	U1733	U1659	A1587
G	C	C	G	C	C		C1872	C1802	G1734	U1588	A1588
G	U	G	G	U	G		A1873	C1803	G1735	C1660	A1589
G	U	C	C	U	C	G1947	U1874	C1803	G1736	G1590	U1590
C	U	C	C	U	C	G1948	A1875		U1737	G1661	G1591
A	U	U	U	A	U	G1949	G1876	G1807	U1737	C1663	G1592
U	G	G	U	A	U		U1877	G1808	U1738	G1664	A1593
U	C	C	G	G	G	G1952	U1877	A1809	U1739	C1665	A1594
C	U	C	U	C	C	G1953	G1878	A1810	U1740	G1666	U1595
C	U	C	C	A	C		A1879	G1811	U1741	A1657	C1596
C	U	C	C	U	C	G	U1880	G1812	G1742	G1668	C1597
C	U	U	C	G	U	U	A	A1813	U1743		G1598
C	U	U	C	G	U	G	A	A1814	G1744	C1671	G1599
U	C	C	C	U	C	U	U1884	U1815	C1745	U1672	U1600
A	U	U	U	G	U	G	U1885	A1816	U1746	G1673	U1601
C	U	C	A	C	A	A	A1886	G1817	G1747	A1602	A1602
C	U	C	G	U	C	G	U1887	U1818		G1675	A1603
C	U	C	G	U	C	G	A1888			A1674	G1604
C	U	C	C	U	C	C	G1889		A1750	A1676	A1605
C	C	C	C	G	C			U1821	G1751	G1677	U1606
C	C	C	C	C	C		U1894	C1822			U1607
C	U	C	C	A	C		A1895	A1923	C1756	G1680	C1608
C	U	C	C	U	C		A1896	U1824		U1681	
C	U	C	C	C	U		G1897	G1825	C1759	U1682	
C	U	C	C	C	U	U		C1826	U1760	A1683	
C	A	C	C	A	C	G	A1901	C1827	C1761	C1683	A1613
C	U	C	C	A	C	U	G1902	A1828	C1762	U1686	A1614
C	U	C	U	U	C		U1903		U1763	U1687	C1615
C	U	C	U	U	C		C1904	C1832	U1764	U1688	C1616
C	U	C	U	G	G	A	G1905	G1833	U1765	G1617	C1617
C	C	C	C	C	C	A	C1906	U1834	G1766	G1618	G1618
C	C	C	C	C	C	C	C1907		C1767	A1619	A1619
U	U	U	U	G	G		A1908	U1837	U1768	U1620	U1620
C	C	C	C	C	C		A1909	G1838	A1696	C1628	U1629
C	C	C	C	C	C		A1910	A1839	G1770	C1701	U1630
C	C	C	C	C	C		U1911	U1840	C1771	U1631	C1631
C	C	C	C	C	C		A1912	A1841	U1772	G1700	U1629
C	U	U	U	G	G		A1913	A1842		C1701	U1630
C	U	U	U	G	G		G1914	C1843		U1702	C1632
C	U	U	U	G	G		A1915	C1844	G1775	U1703	A1632
C	U	C	C	C	C						C1633
C	U	C	C	C	C		C1918	C1846	G1778	C1709	
C	U	U	U	U	U		G1919	A1847	C1779	C1710	U1636
C	U	U	U	A	U		U1920	G1848	G1780	C1711	A1637
C	C	C	C	A	C		A1921	C1849	U1782	C1711	A1638
C	C	C	C	G	C						
C	C	C	C	U	C		A1922	A1850	U1783	A1715	C1639
C	U	C	U	A	C		C1923	G1851	G1784	U1716	G1640
C	U	C	U	G	C		U1924	G1852	U1785	U1717	A1641
C	U	C	U	G	U		U1925	U1853		G1718	A1642
C	C	C	C	G	C		C1926	C1854	C1788	G1719	A1643
C	C	C	C	C	C		C1927	C1789	C1789	U1720	C1644

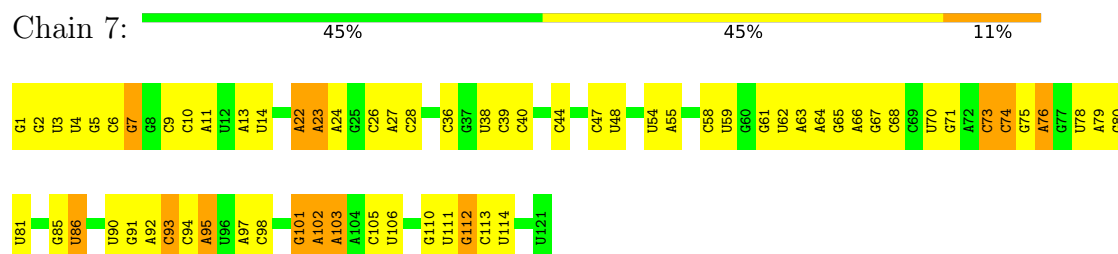


● Molecule 37: 5S ribosomal RNA

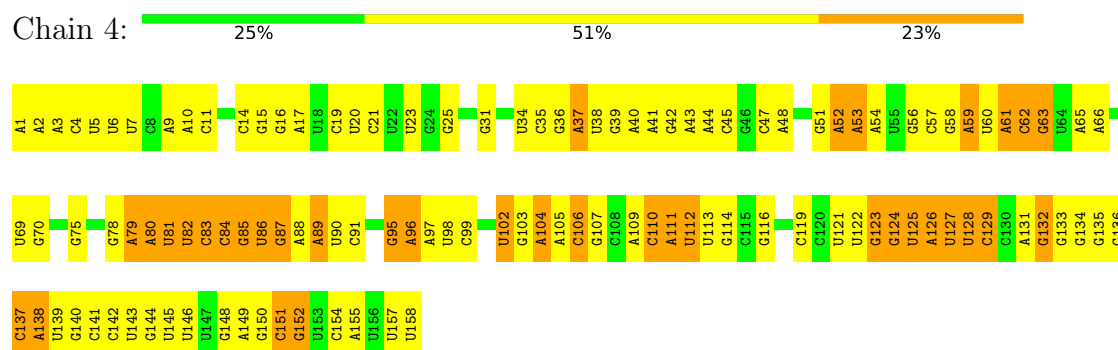
Chain 3:



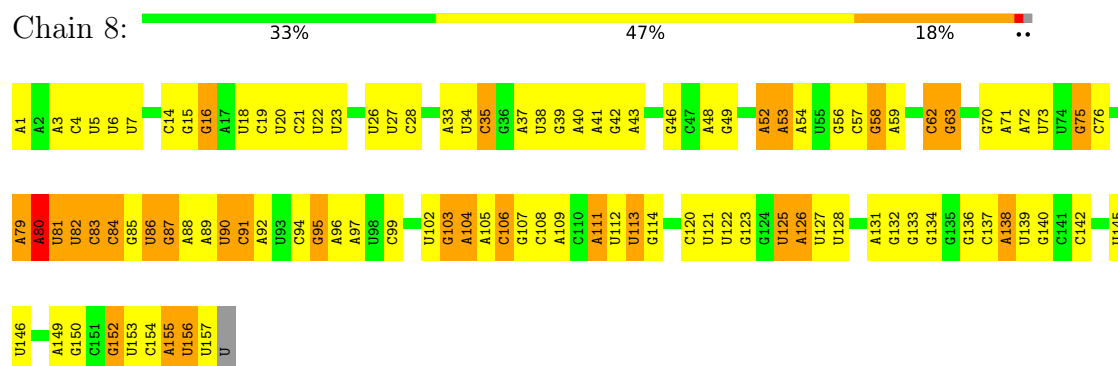
- Molecule 37: 5S ribosomal RNA



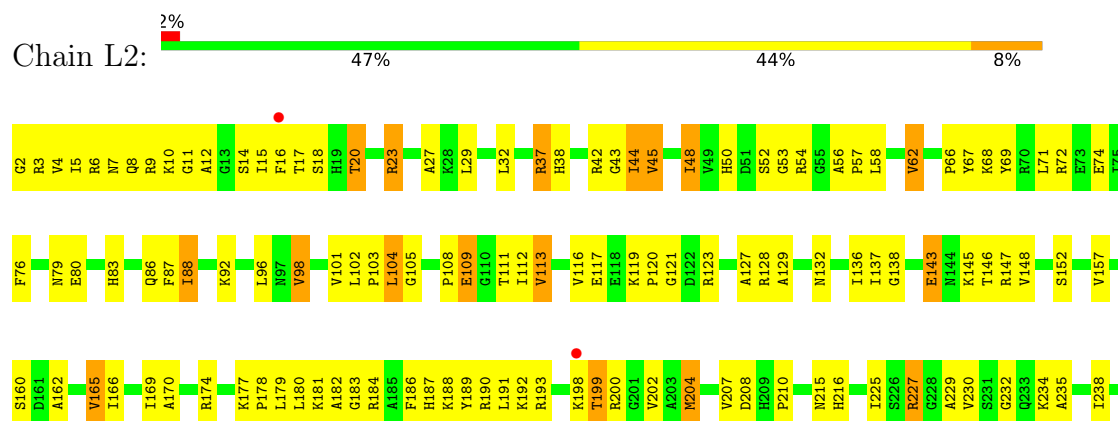
- Molecule 38: 5.8S ribosomal RNA

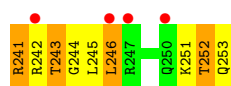


- Molecule 38: 5.8S ribosomal RNA

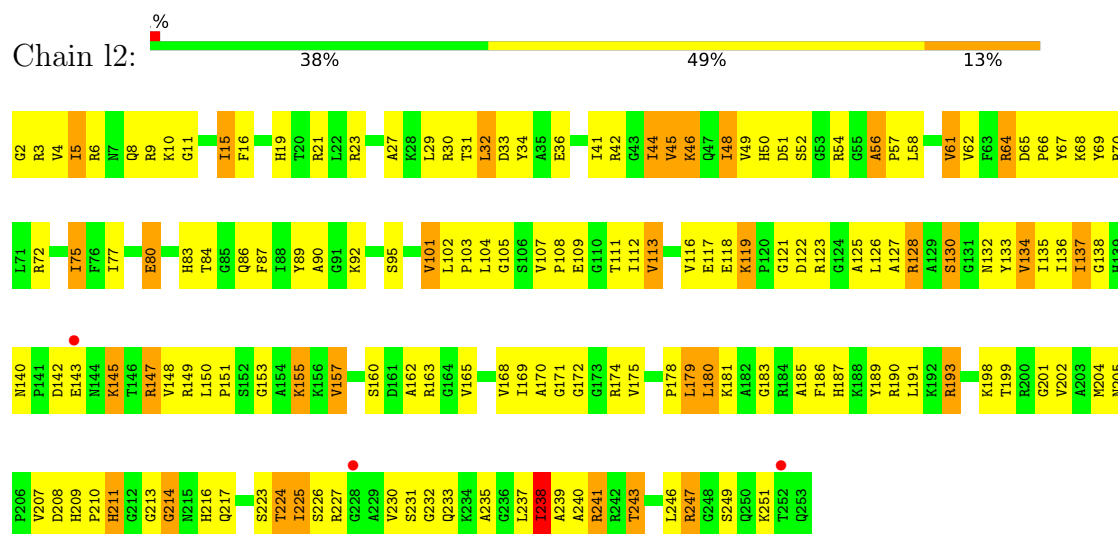


- Molecule 39: 60S ribosomal protein L2-A

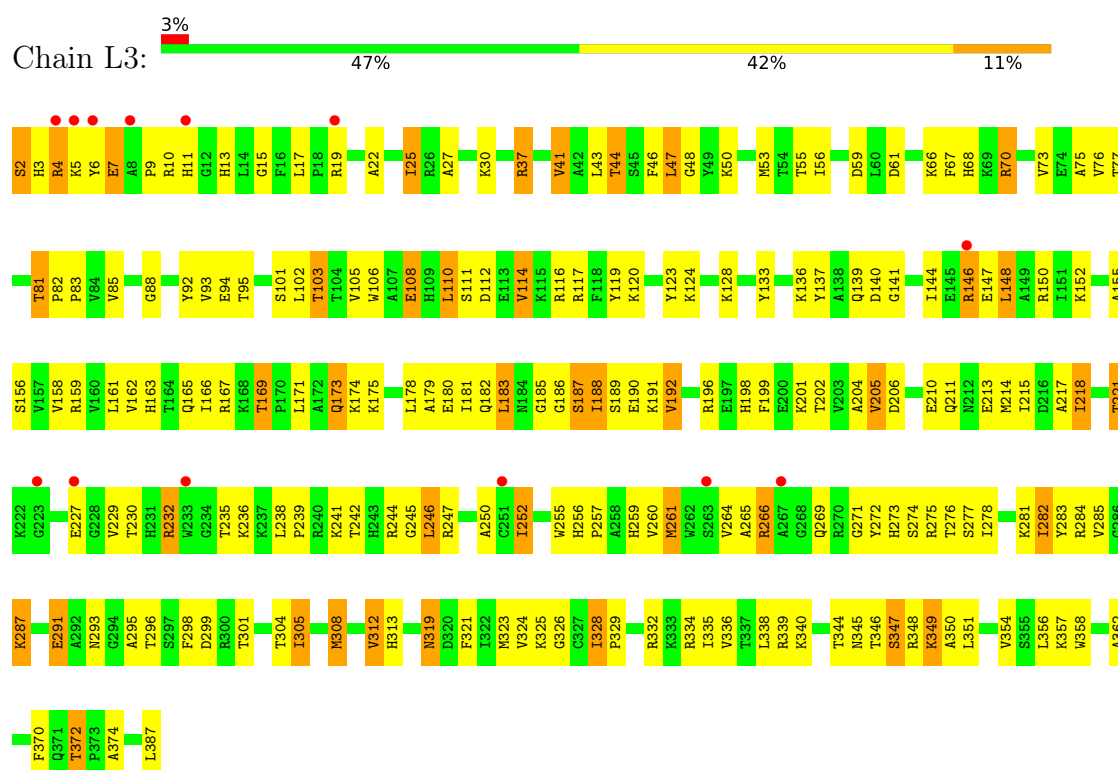




• Molecule 39: 60S ribosomal protein L2-A

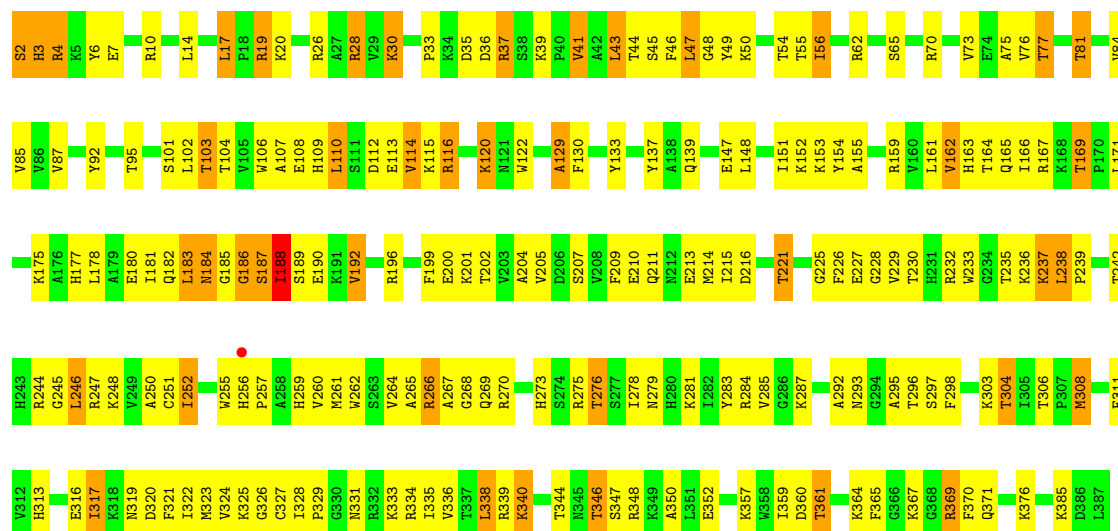


• Molecule 40: 60S ribosomal protein L3

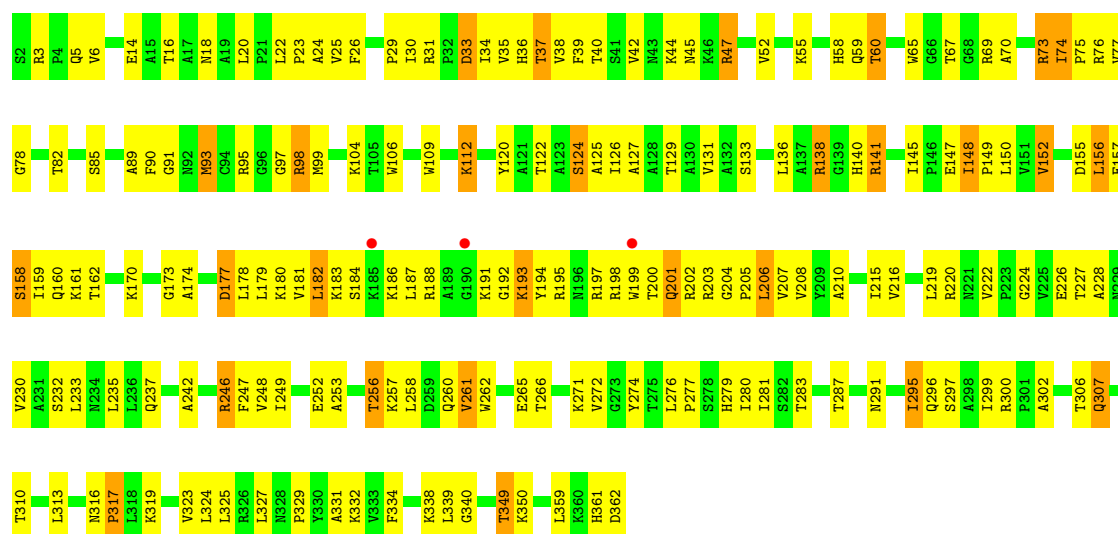


• Molecule 40: 60S ribosomal protein L3

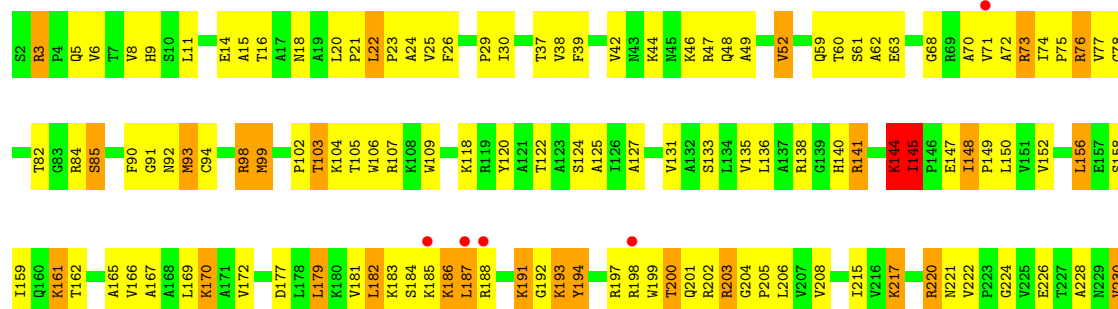


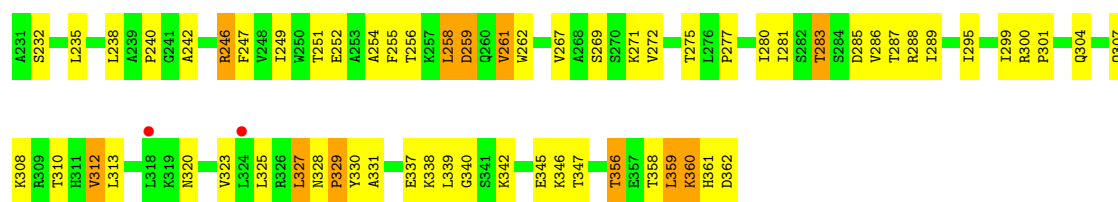


• Molecule 41: 60S ribosomal protein L4-A

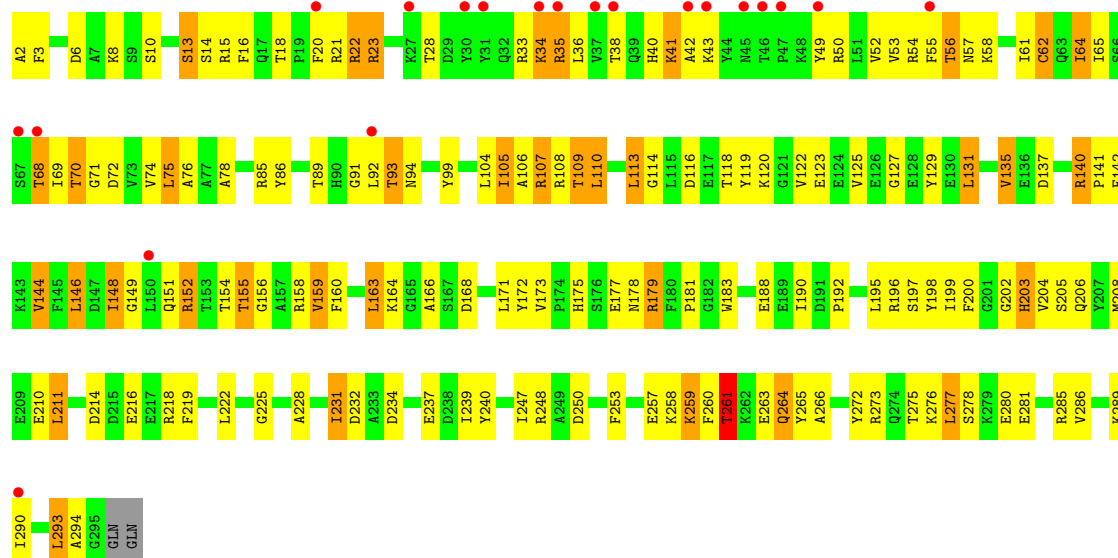


• Molecule 41: 60S ribosomal protein L4-A





• Molecule 42: 60S ribosomal protein L5



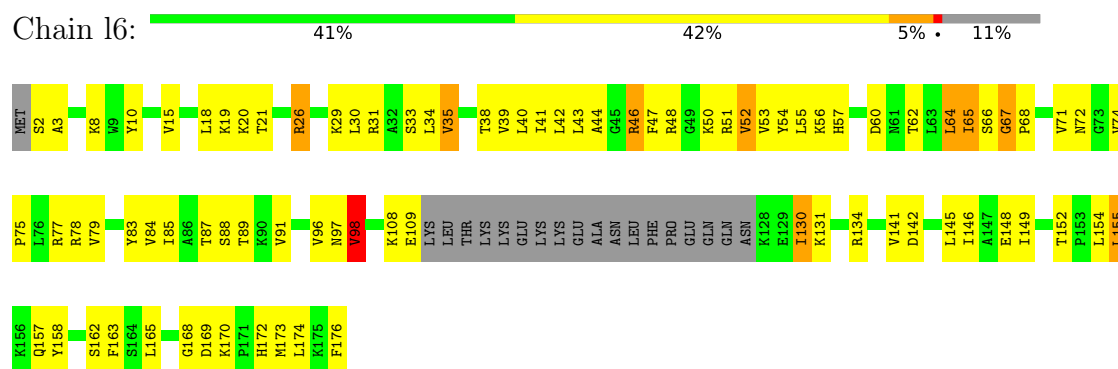
• Molecule 42: 60S ribosomal protein L5



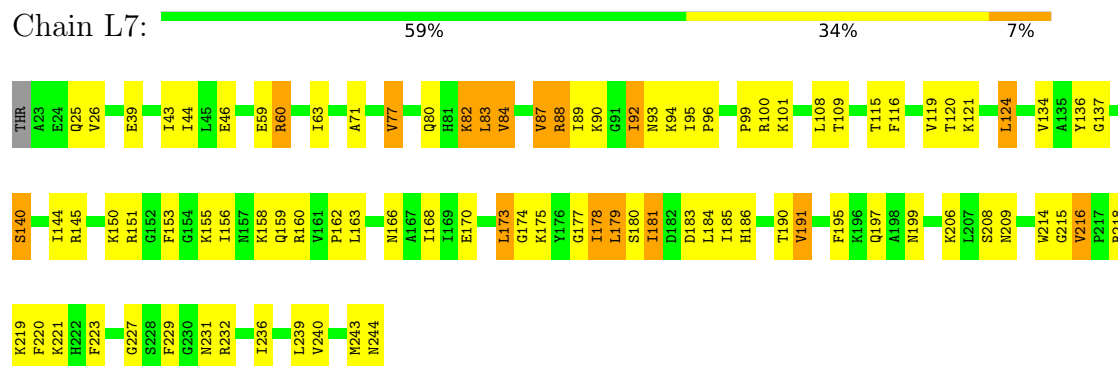
• Molecule 43: 60S ribosomal protein L6-A



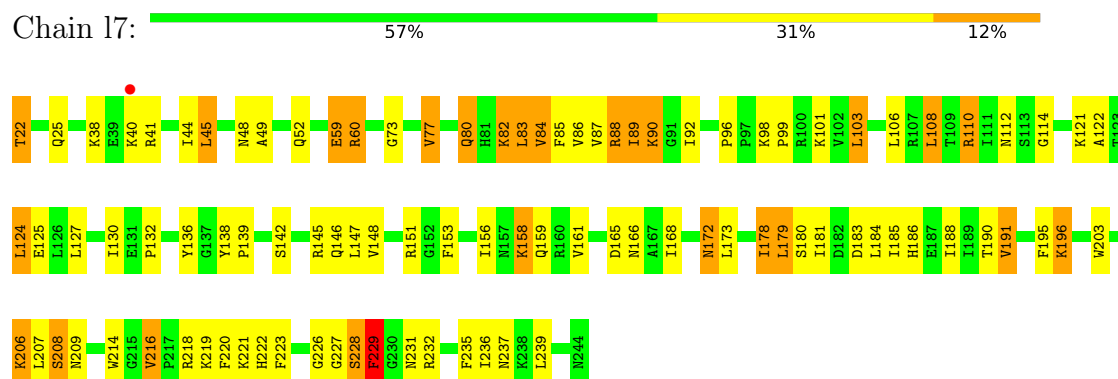
- Molecule 43: 60S ribosomal protein L6-A



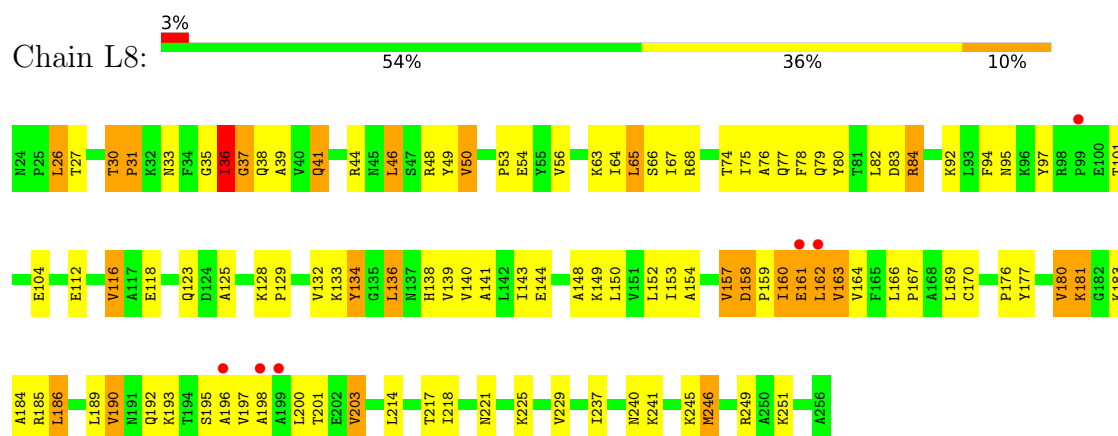
- Molecule 44: 60S ribosomal protein L7-A



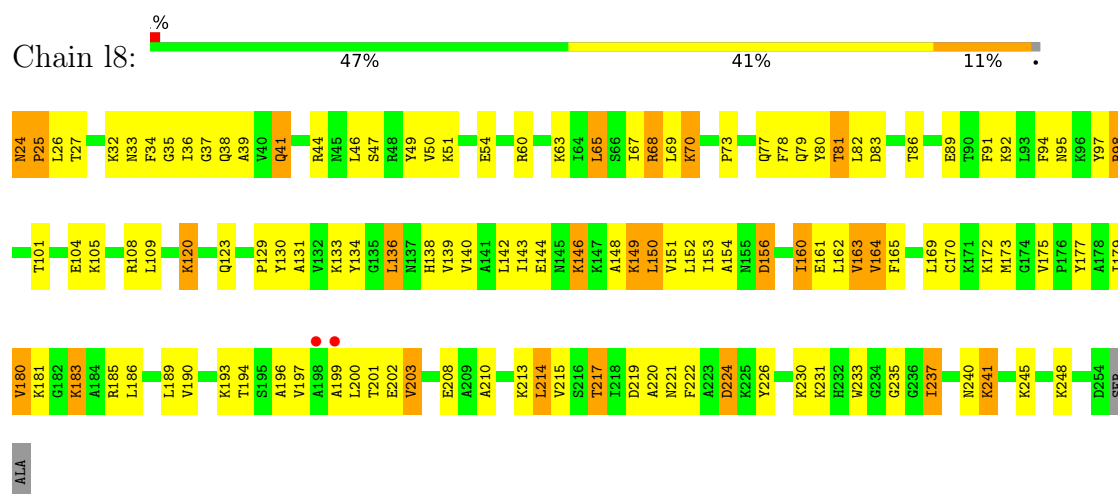
- Molecule 44: 60S ribosomal protein L7-A



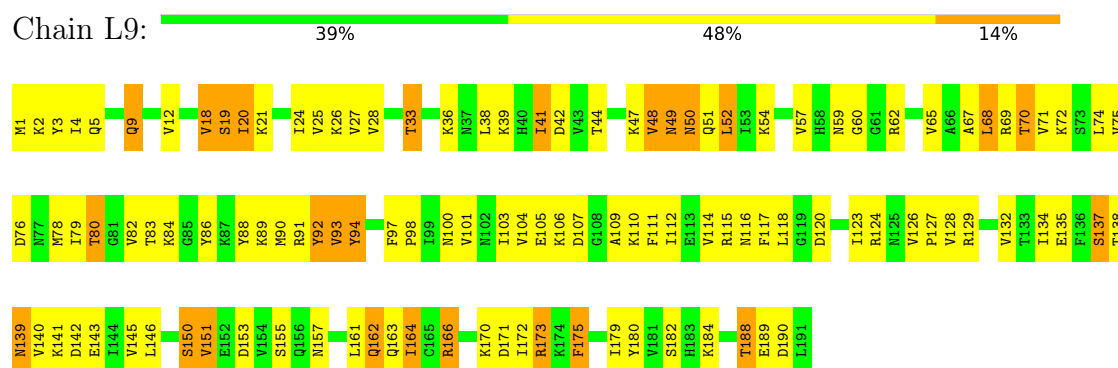
- Molecule 45: 60S ribosomal protein L8-A



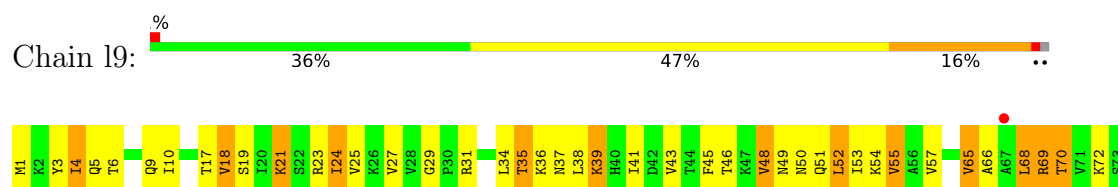
- Molecule 45: 60S ribosomal protein L8-A

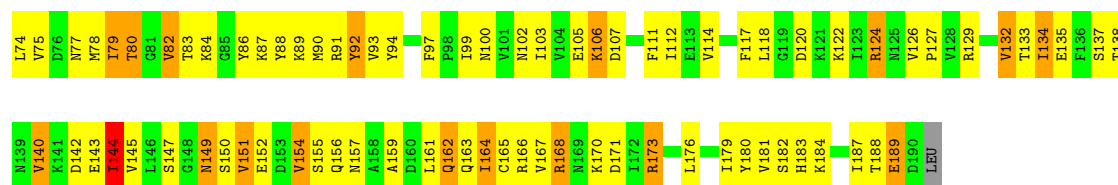


- Molecule 46: 60S ribosomal protein L9-A



- Molecule 46: 60S ribosomal protein L9-A

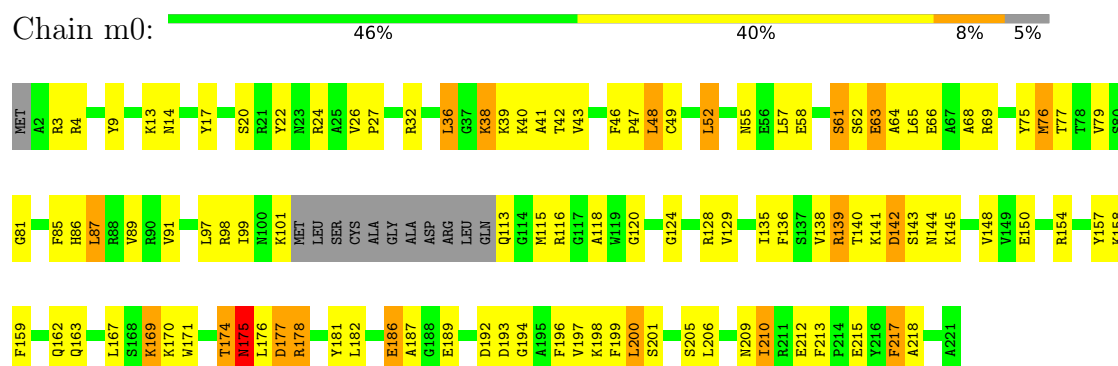




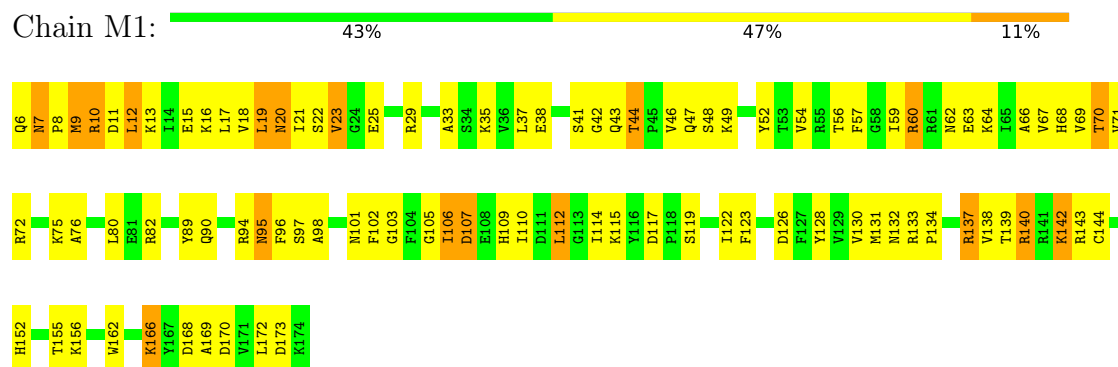
• Molecule 47: 60S ribosomal protein L10



• Molecule 47: 60S ribosomal protein L10

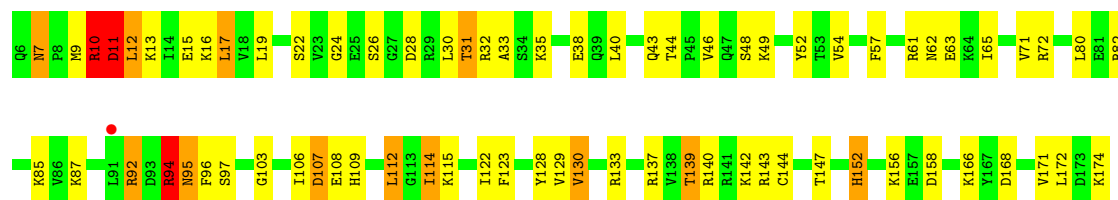


• Molecule 48: 60S ribosomal protein L11-A

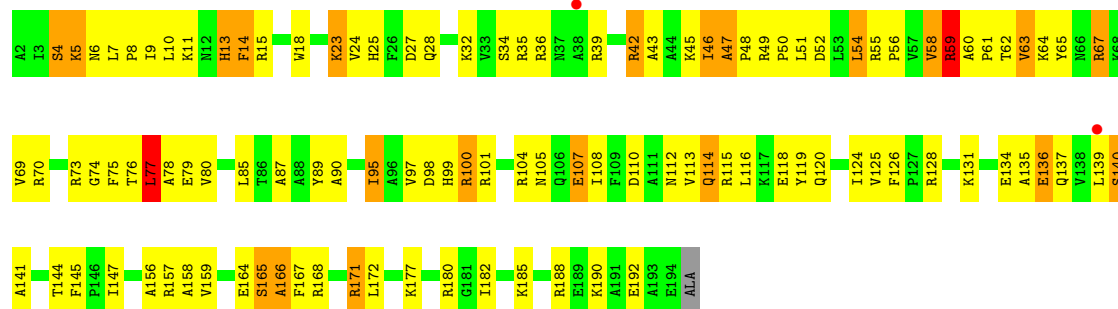
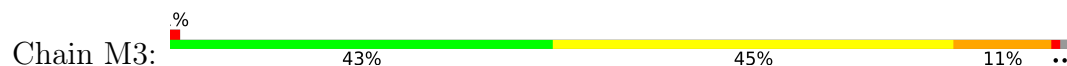


• Molecule 48: 60S ribosomal protein L11-A

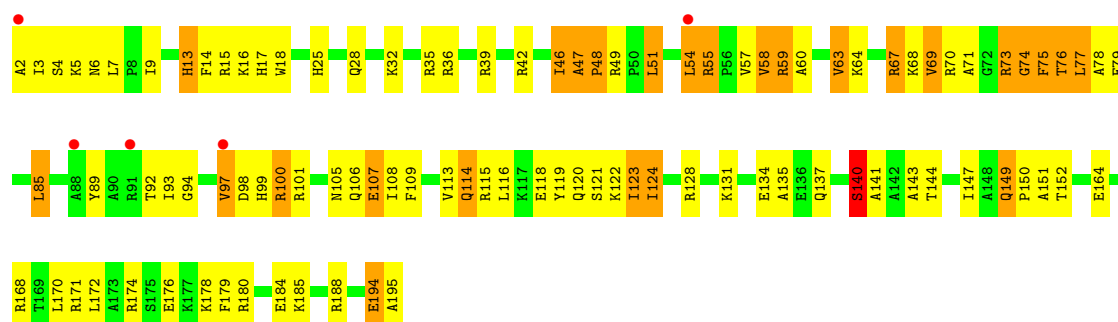




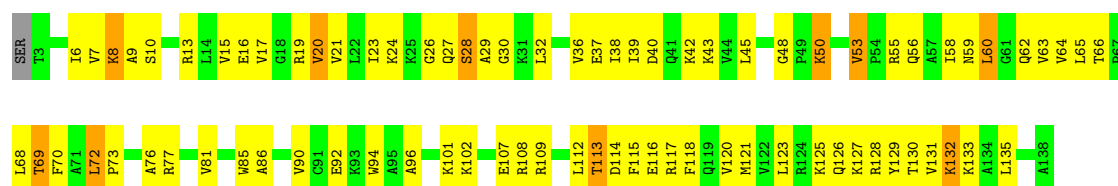
• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A

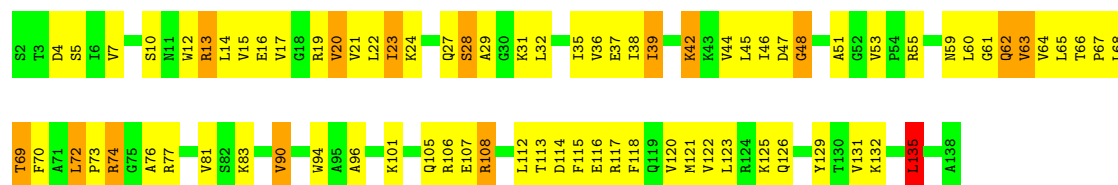


• Molecule 50: 60S ribosomal protein L14-A

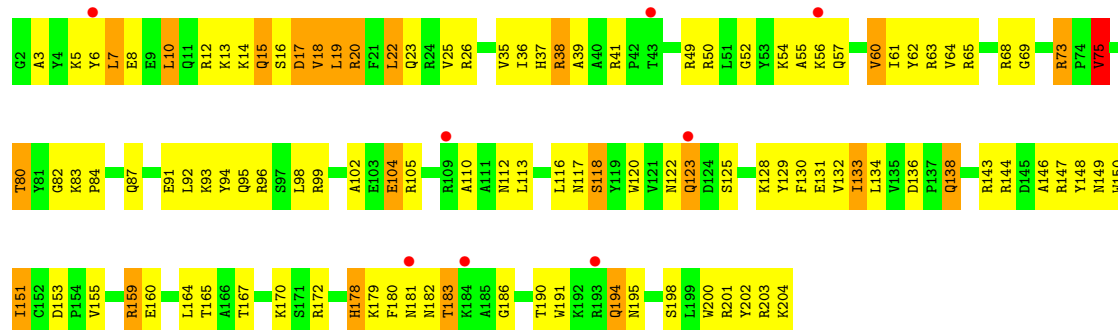


• Molecule 50: 60S ribosomal protein L14-A

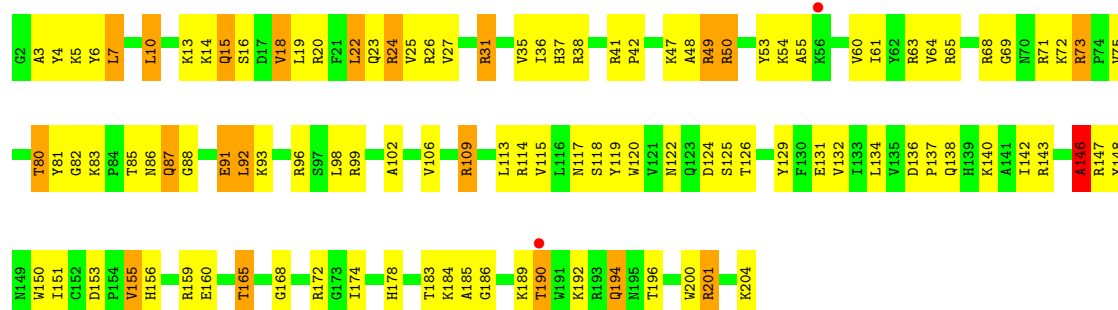




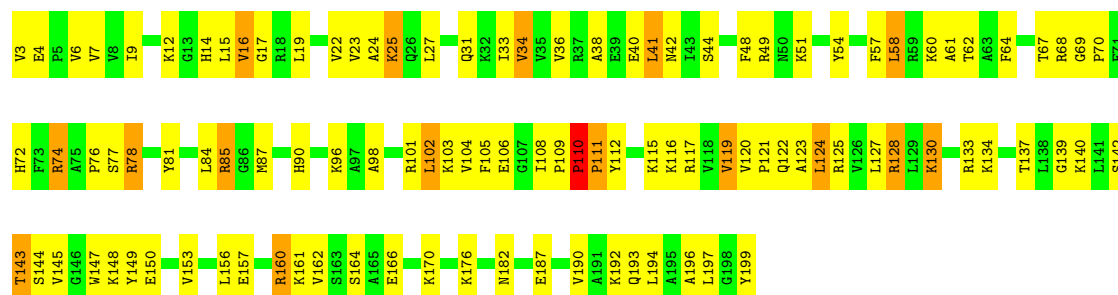
• Molecule 51: 60S ribosomal protein L15-A



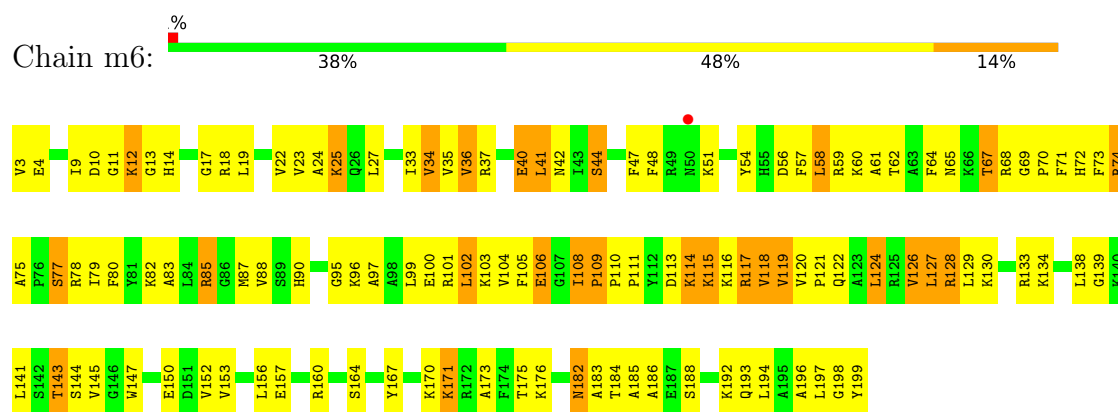
• Molecule 51: 60S ribosomal protein L15-A



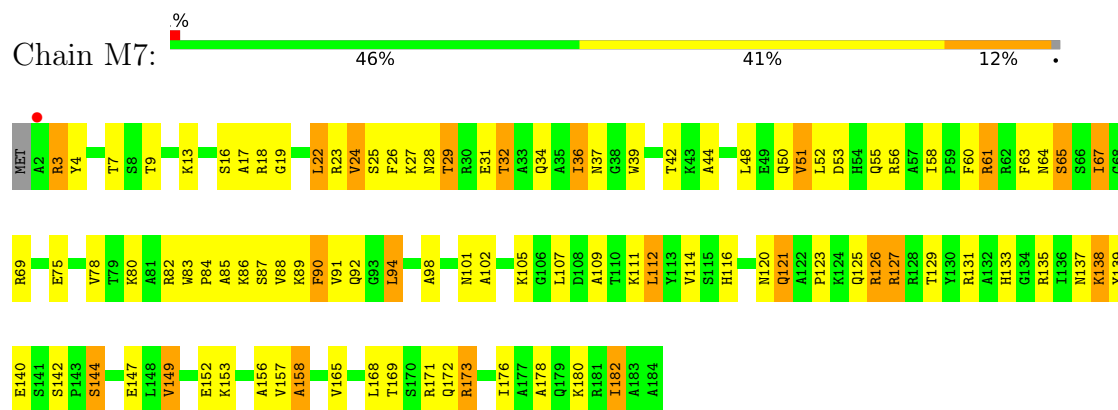
• Molecule 52: 60S ribosomal protein L16-A



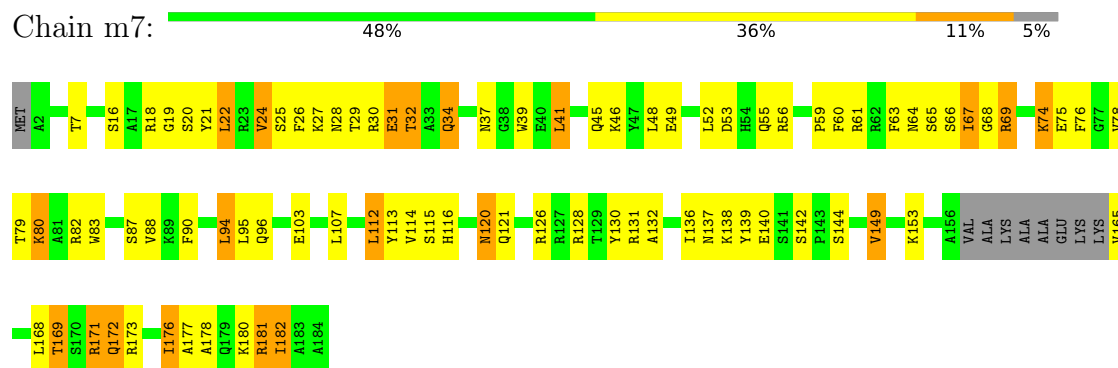
• Molecule 52: 60S ribosomal protein L16-A



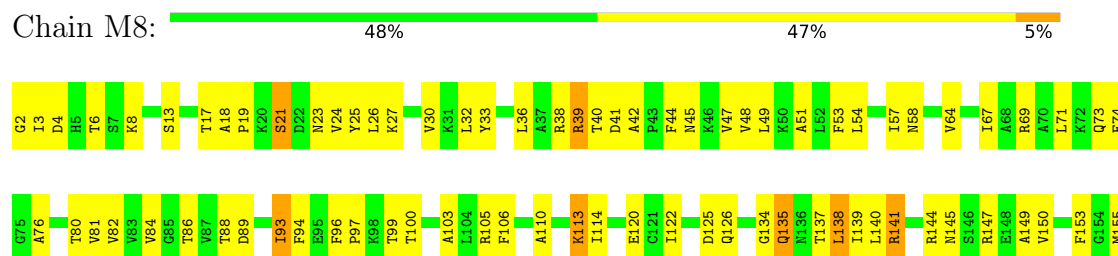
• Molecule 53: 60S ribosomal protein L17-A



• Molecule 53: 60S ribosomal protein L17-A

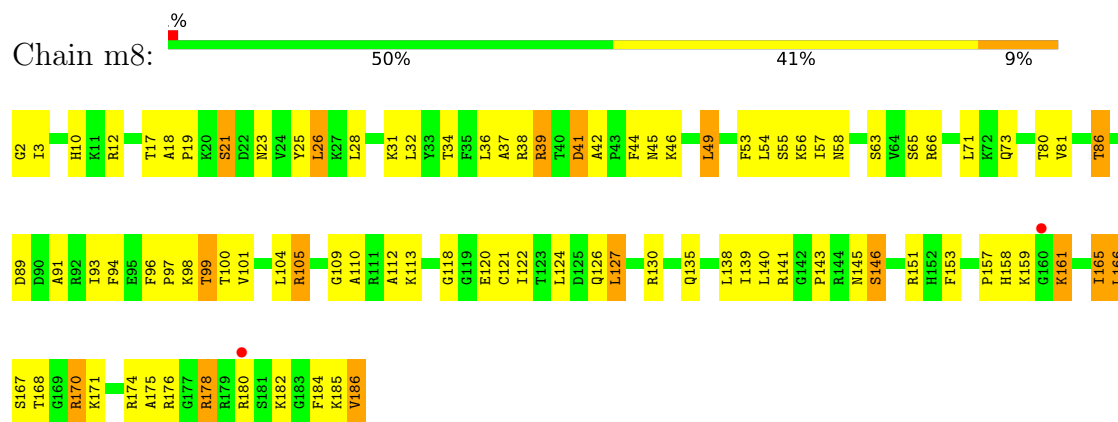


• Molecule 54: 60S ribosomal protein L18-A

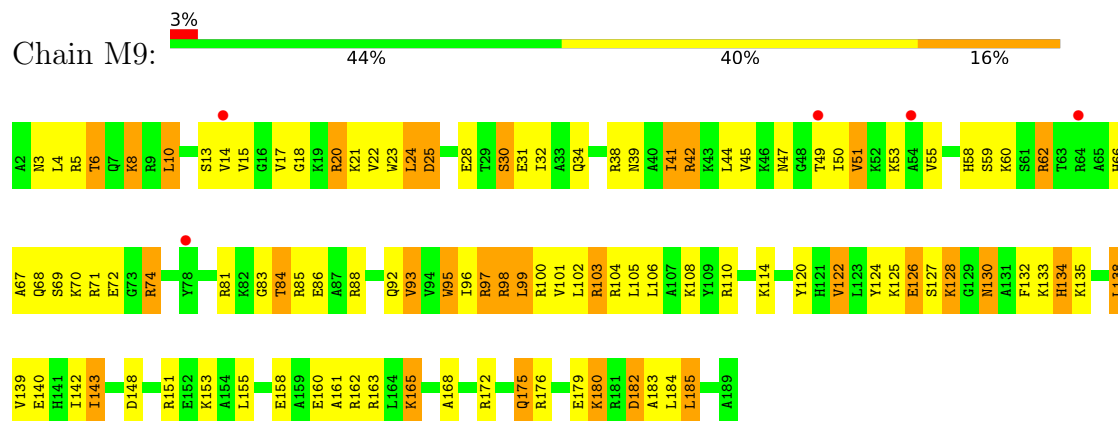




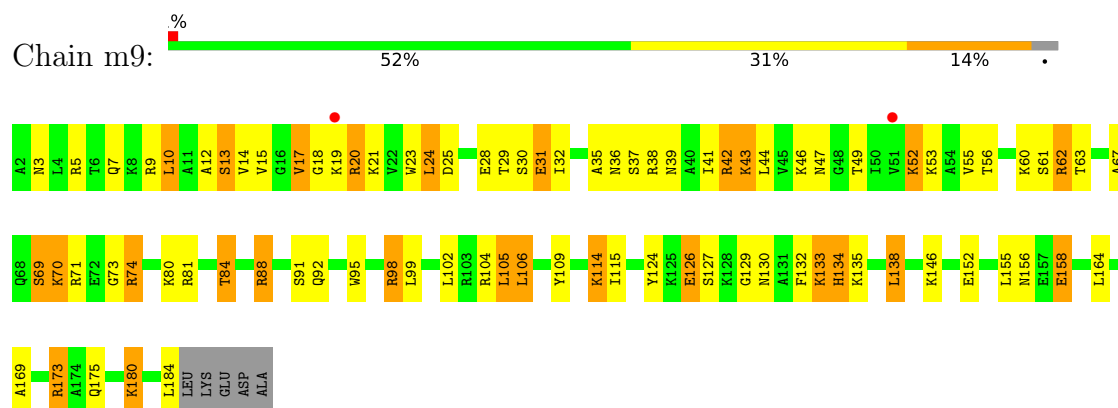
• Molecule 54: 60S ribosomal protein L18-A



• Molecule 55: 60S ribosomal protein L19-A

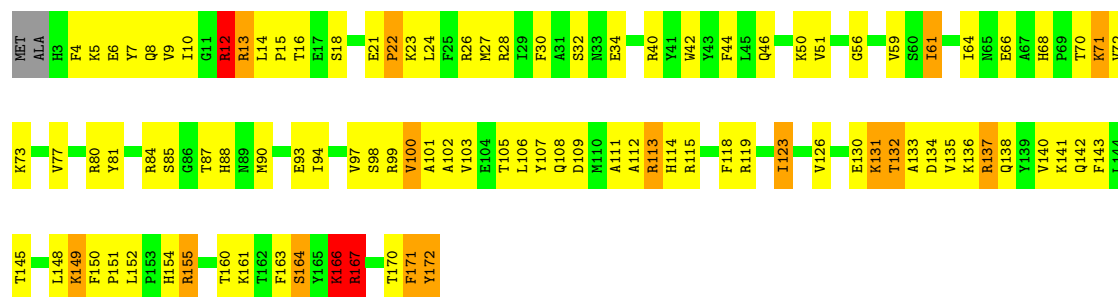


• Molecule 55: 60S ribosomal protein L19-A

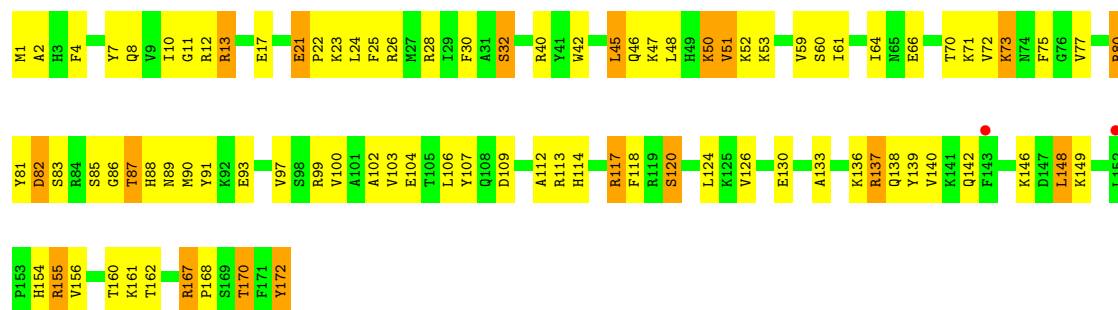


• Molecule 56: 60S ribosomal protein L20-A

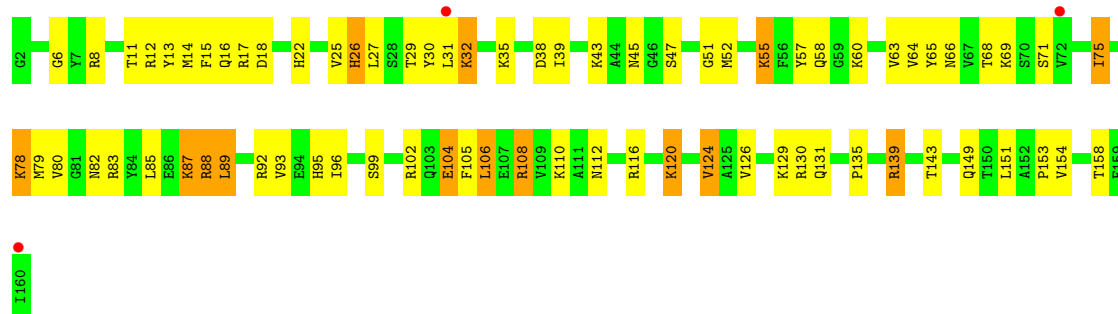




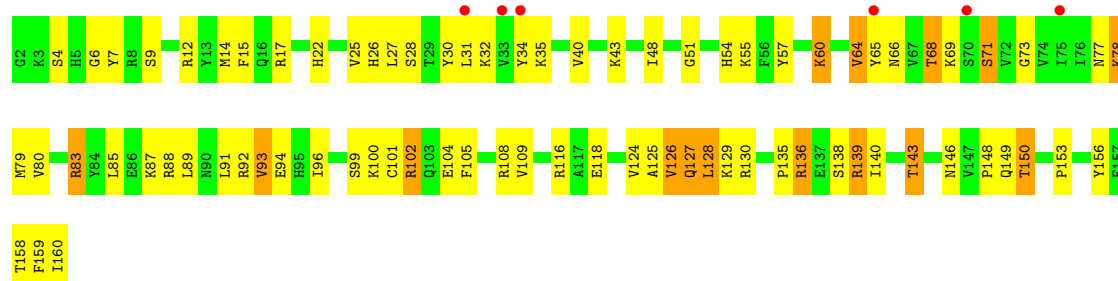
- Molecule 56: 60S ribosomal protein L20-A



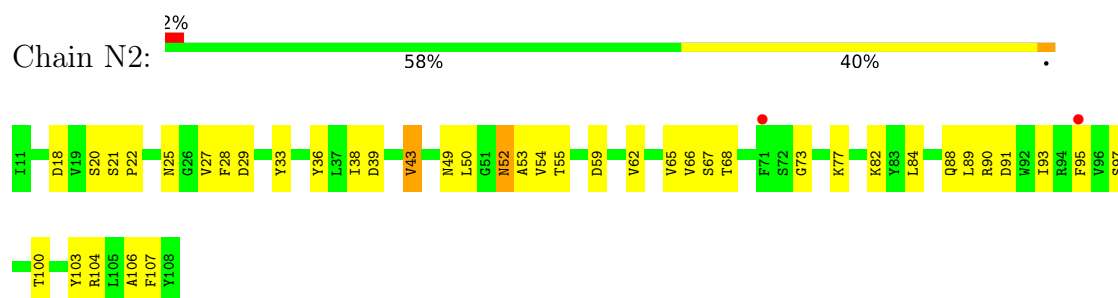
- Molecule 57: 60S ribosomal protein L21-A



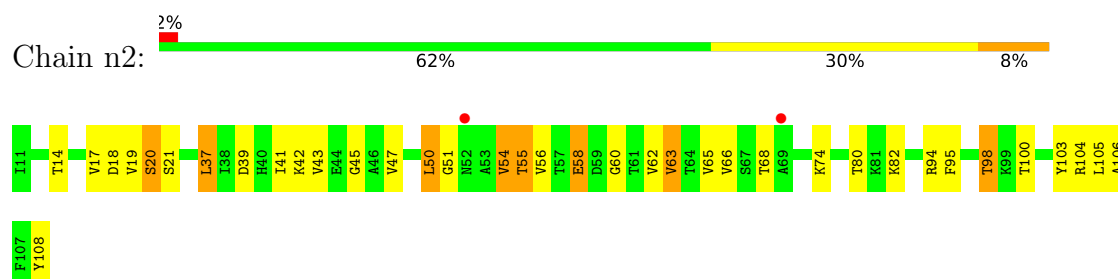
- Molecule 57: 60S ribosomal protein L21-A



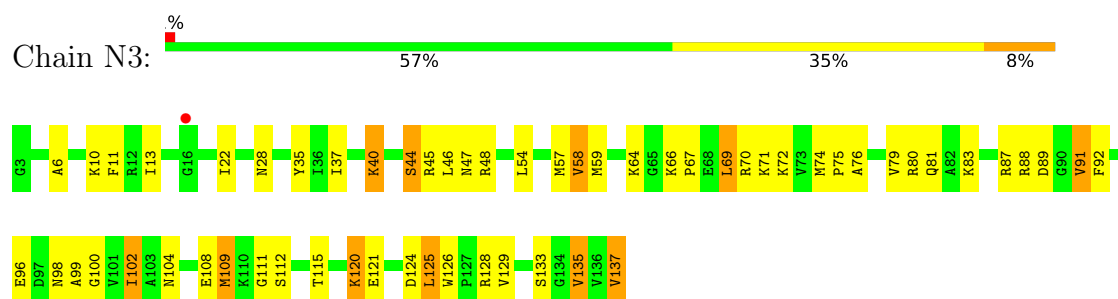
- Molecule 58: 60S ribosomal protein L22-A



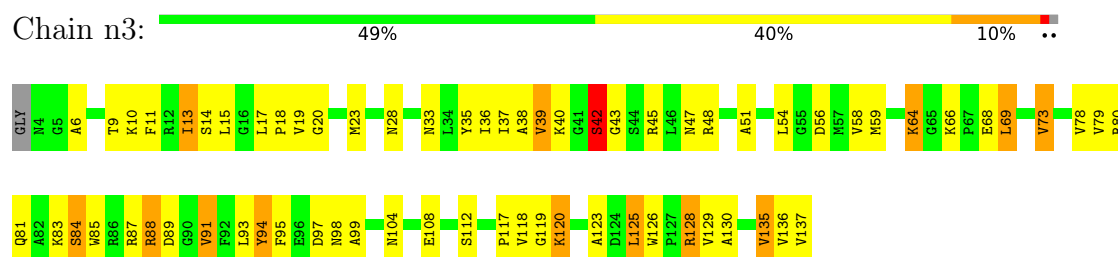
- Molecule 58: 60S ribosomal protein L22-A



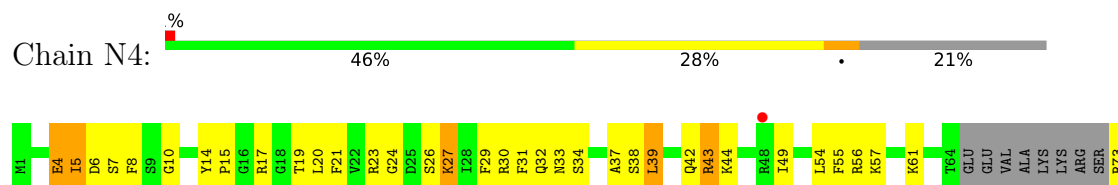
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A

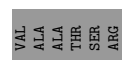
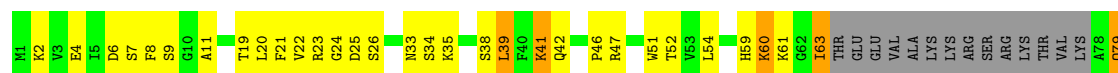


- Molecule 60: 60S ribosomal protein L24-A

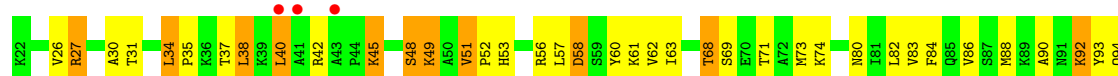




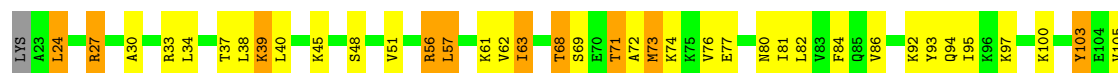
• Molecule 60: 60S ribosomal protein L24-A



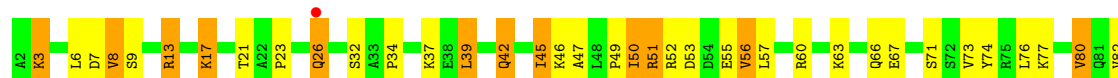
• Molecule 61: 60S ribosomal protein L25



• Molecule 61: 60S ribosomal protein L25

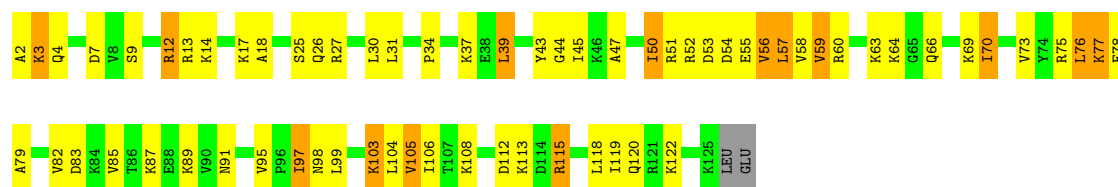


• Molecule 62: 60S ribosomal protein L26-A



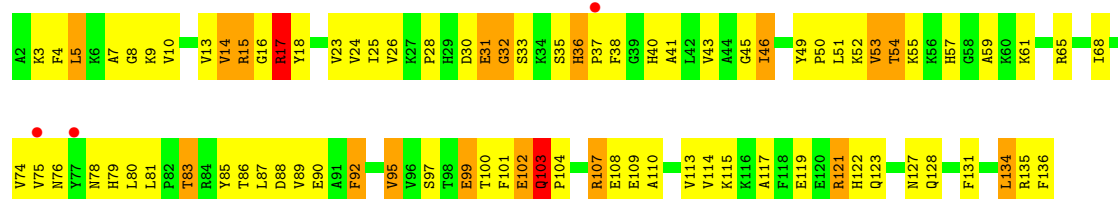
• Molecule 62: 60S ribosomal protein L26-A

Chain n6: 46% 41% 11%



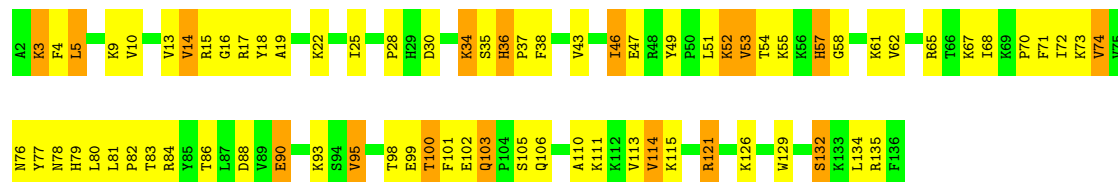
• Molecule 63: 60S ribosomal protein L27-A

Chain N7: 2% 38% 48% 13%



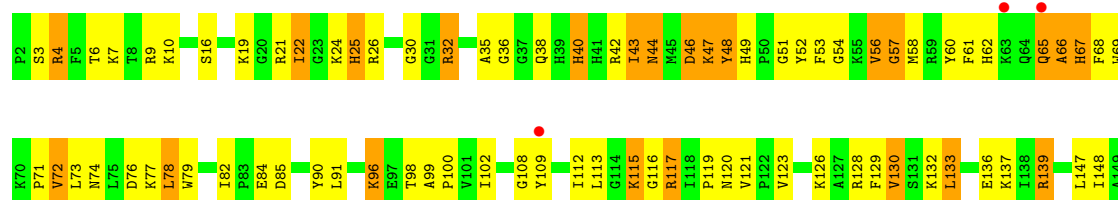
• Molecule 63: 60S ribosomal protein L27-A

Chain n7: 44% 43% 13%



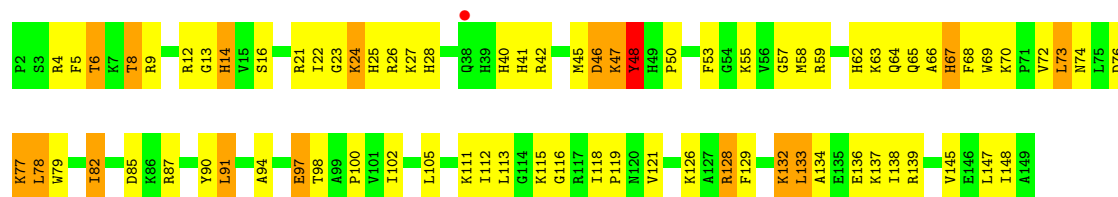
• Molecule 64: 60S ribosomal protein L28

Chain N8: 2% 45% 39% 16%



• Molecule 64: 60S ribosomal protein L28

Chain n8: 47% 41% 11%



- Molecule 65: 60S ribosomal protein L29

Chain N9:  59% 31% 10%

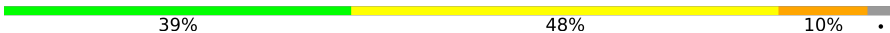


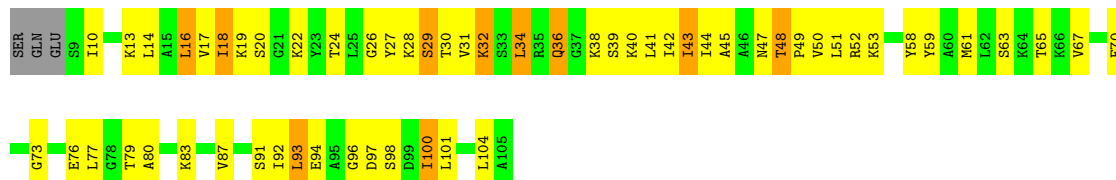
- Molecule 65: 60S ribosomal protein L29

Chain n9:  5% 47% 45% 9%



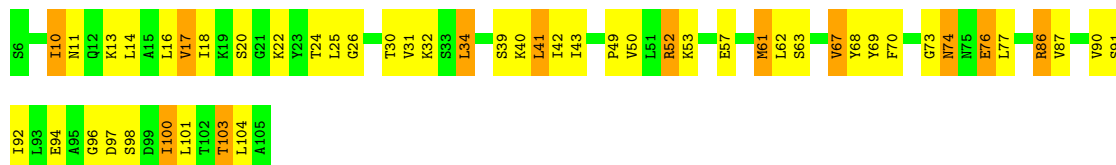
- Molecule 66: 60S ribosomal protein L30

Chain O0:  39% 48% 10%



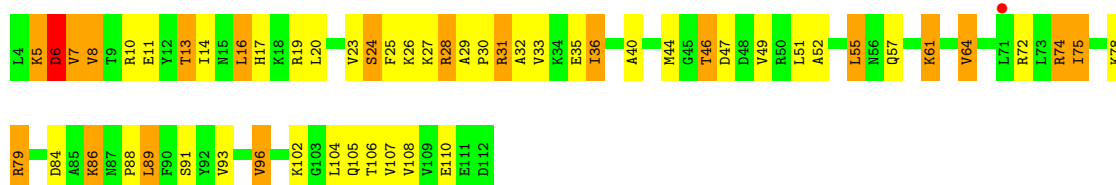
- Molecule 66: 60S ribosomal protein L30

Chain o0:  50% 38% 12%

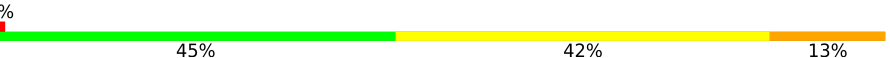


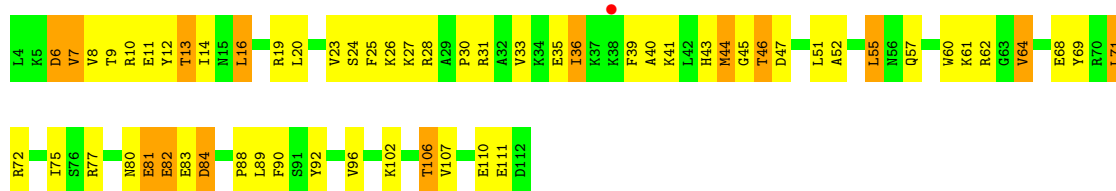
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  50% 32% 17%

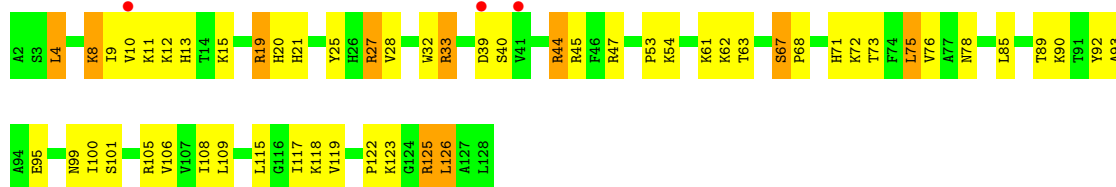


- Molecule 67: 60S ribosomal protein L31-A

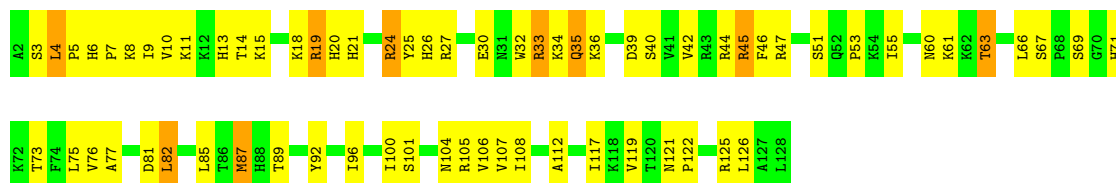
Chain o1:  45% 42% 13%



• Molecule 68: 60S ribosomal protein L32



• Molecule 68: 60S ribosomal protein L32



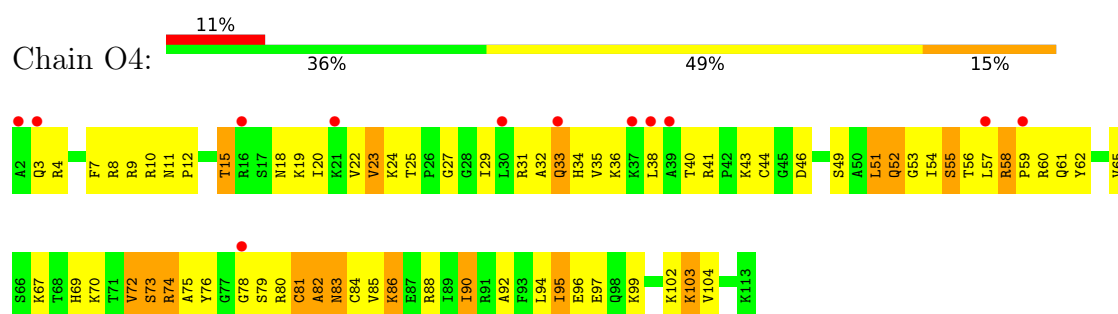
• Molecule 69: 60S ribosomal protein L33-A



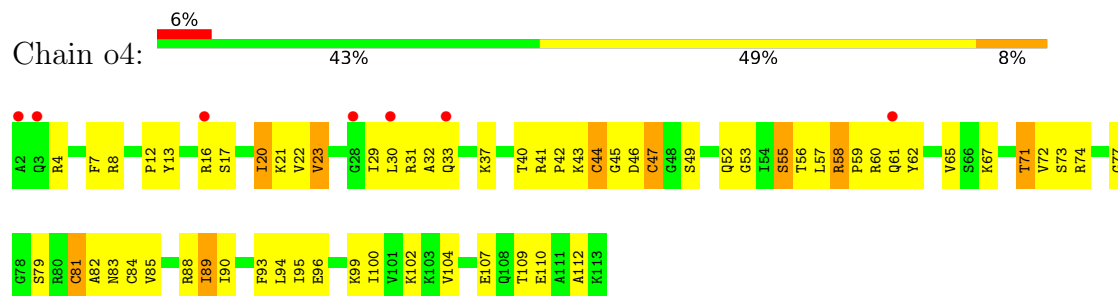
• Molecule 69: 60S ribosomal protein L33-A



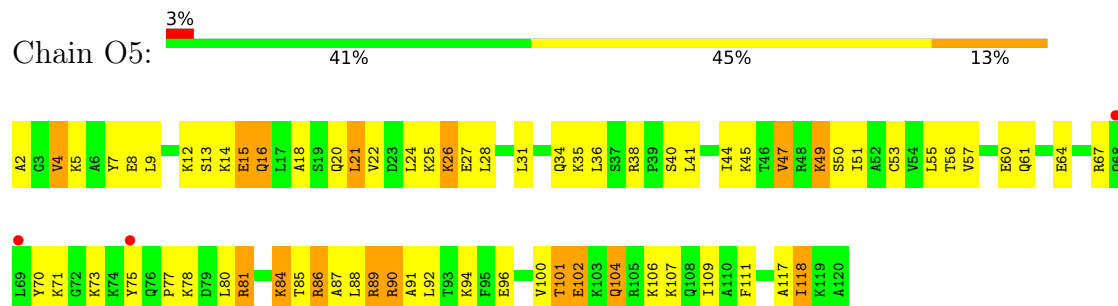
• Molecule 70: 60S ribosomal protein L34-A



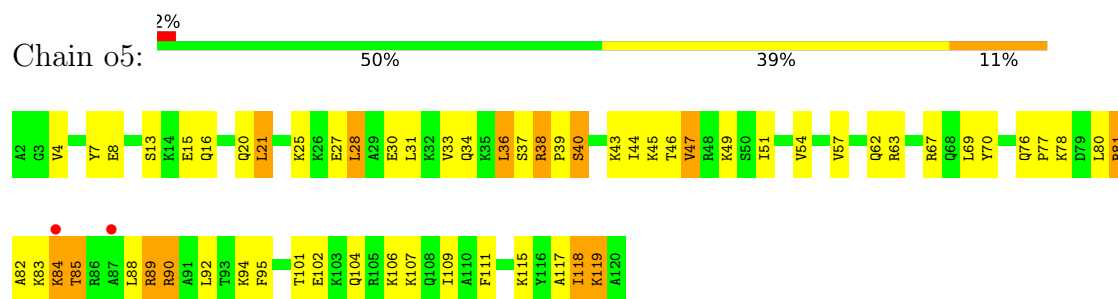
- Molecule 70: 60S ribosomal protein L34-A



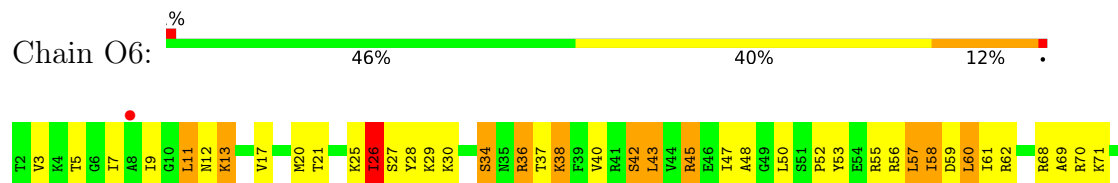
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A



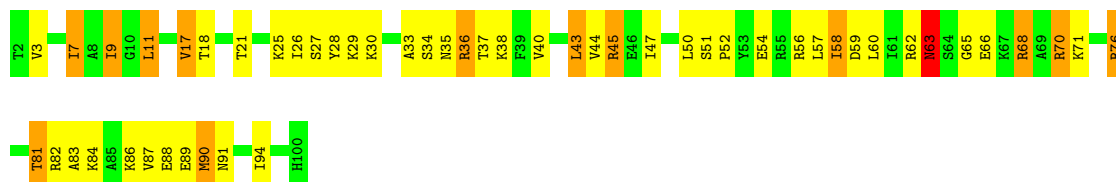
- Molecule 72: 60S ribosomal protein L36-A





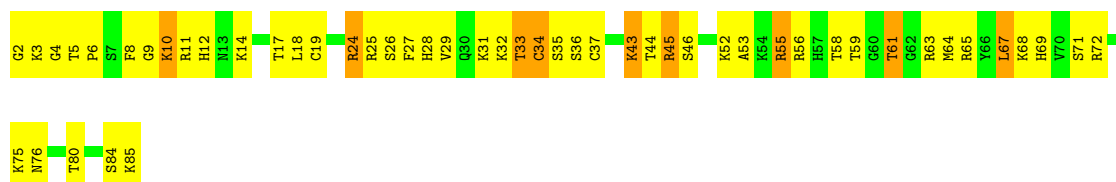
- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 47% 38% 13% .



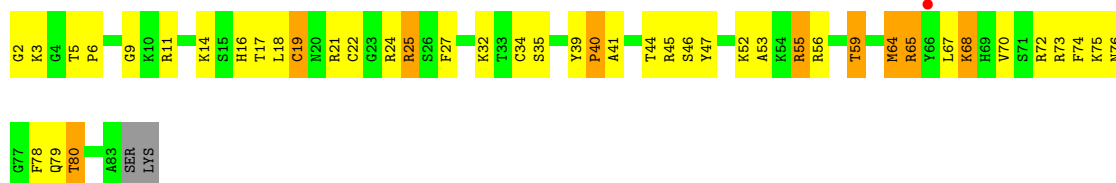
- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 39% 50% 11%



- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 45% 42% 11% .



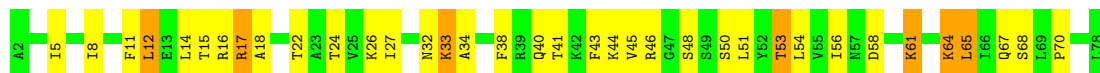
- Molecule 74: 60S ribosomal protein L38

Chain O8: 53% 35% 12%

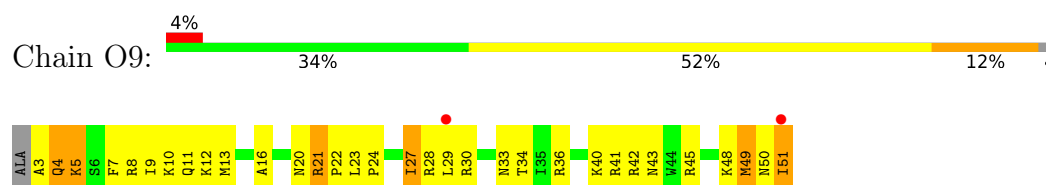


- Molecule 74: 60S ribosomal protein L38

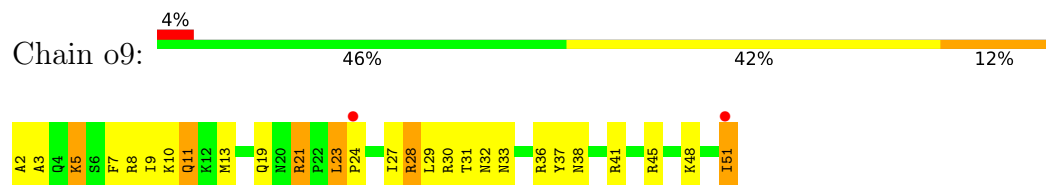
Chain o8: 53% 38% 9%



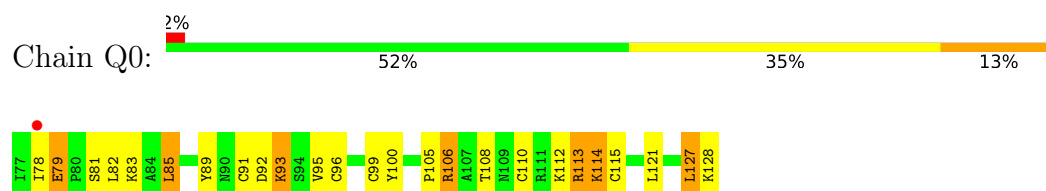
- Molecule 75: 60S ribosomal protein L39



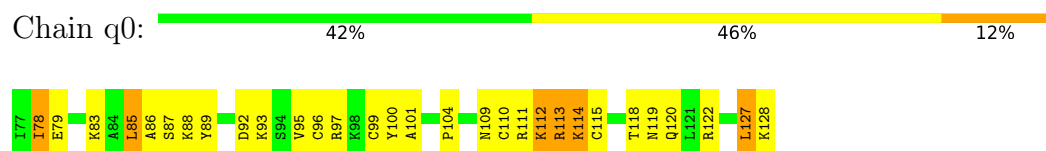
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



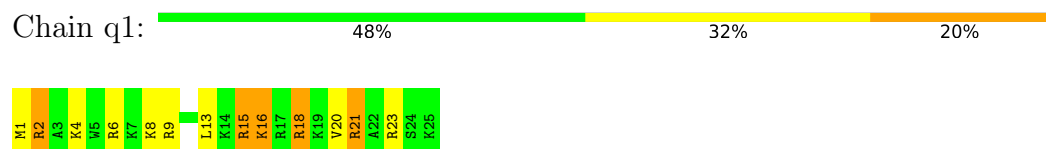
- Molecule 76: Ubiquitin-60S ribosomal protein L40



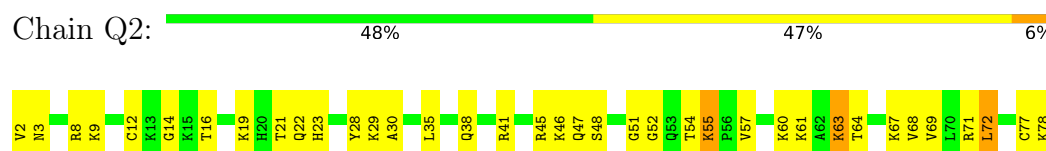
- Molecule 77: 60S ribosomal protein L41-A

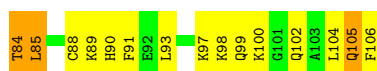


- Molecule 77: 60S ribosomal protein L41-A

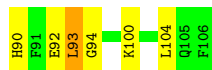


- Molecule 78: 60S ribosomal protein L42-A

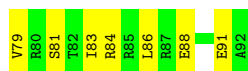




- Molecule 78: 60S ribosomal protein L42-A



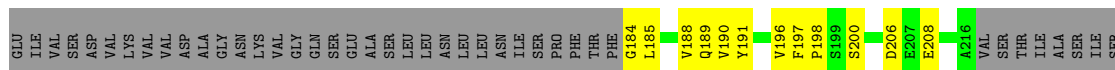
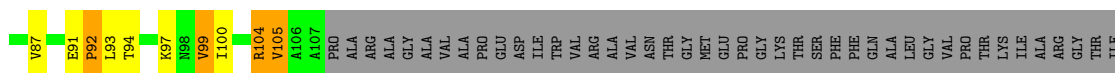
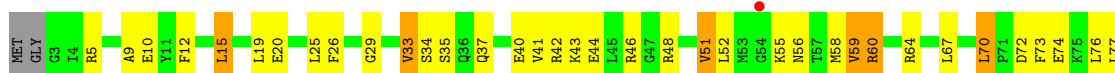
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 60S acidic ribosomal protein P0



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	443.59Å 297.32Å 300.15Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	91.75 – 3.70 91.75 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (91.75-3.70) 89.5 (91.75-3.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.253 (Not available) , 0.222	Depositor DCC
R_{free} test set	16296 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 118.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	397710	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

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

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: MG, GET, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.34	0/40250	0.61	1/62707 (0.0%)
1	6	0.34	0/40528	0.59	5/63141 (0.0%)
2	S0	0.30	0/1617	0.69	4/2215 (0.2%)
2	s0	0.31	0/1623	0.66	0/2222
3	S1	0.31	0/1735	0.72	0/2335
3	s1	0.28	0/1748	0.61	0/2352
4	S2	0.31	0/1665	0.68	1/2263 (0.0%)
4	s2	0.36	0/1665	0.65	0/2263
5	S3	0.36	0/1759	0.62	0/2368
5	s3	0.30	0/1759	0.67	2/2368 (0.1%)
6	S4	0.30	0/2109	0.65	1/2839 (0.0%)
6	s4	0.36	1/2109 (0.0%)	0.67	0/2839
7	S5	0.30	0/1629	0.63	0/2202
7	s5	0.28	0/1629	0.63	0/2202
8	S6	0.27	0/1823	0.57	0/2439
8	s6	0.34	0/1779	0.61	0/2379
9	S7	0.35	0/1506	0.78	4/2028 (0.2%)
9	s7	0.41	1/1511 (0.1%)	0.77	3/2036 (0.1%)
10	S8	0.34	0/1514	0.69	0/2021
10	s8	0.41	0/1514	0.68	1/2021 (0.0%)
11	S9	0.31	0/1519	0.64	0/2035
11	s9	0.32	0/1519	0.63	0/2035
12	C0	0.32	0/769	0.89	3/1039 (0.3%)
12	c0	0.34	0/757	0.84	1/1022 (0.1%)
13	C1	0.35	0/1172	0.74	1/1580 (0.1%)
13	c1	0.41	0/1194	0.71	0/1610
14	C2	0.32	0/878	0.75	0/1192
14	c2	0.30	0/898	0.78	2/1220 (0.2%)
15	C3	0.35	0/1215	0.70	2/1638 (0.1%)
15	c3	0.36	0/1215	0.72	2/1638 (0.1%)
16	C4	0.34	0/901	0.71	0/1217
16	c4	0.29	0/960	0.71	2/1290 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.43	1/988 (0.1%)	0.77	0/1327
17	c5	0.38	0/959	0.79	2/1288 (0.2%)
18	C6	0.37	0/1125	0.81	3/1510 (0.2%)
18	c6	0.60	2/1125 (0.2%)	0.66	2/1510 (0.1%)
19	C7	0.30	0/920	0.68	0/1233
19	c7	0.33	0/915	0.70	0/1227
20	C8	0.33	0/1211	0.77	4/1628 (0.2%)
20	c8	0.30	0/1211	0.68	0/1628
21	C9	0.38	0/1130	0.70	0/1517
21	c9	0.31	0/1130	0.67	0/1517
22	D0	0.33	0/847	0.66	0/1145
22	d0	0.35	0/815	0.62	0/1102
23	D1	0.33	0/693	0.61	0/935
23	d1	0.29	0/693	0.62	0/935
24	D2	0.34	0/1038	0.78	4/1395 (0.3%)
24	d2	0.37	0/1038	0.65	0/1395
25	D3	0.40	0/1139	0.81	0/1518
25	d3	0.42	0/1139	0.72	0/1518
26	D4	0.26	0/1087	0.69	3/1449 (0.2%)
26	d4	0.34	0/1087	0.71	0/1449
27	D5	0.37	0/571	0.82	0/768
27	d5	0.31	0/566	0.59	0/761
28	D6	0.61	1/782 (0.1%)	0.81	2/1047 (0.2%)
28	d6	0.33	0/782	0.67	0/1047
29	D7	0.30	0/620	0.66	0/838
29	d7	0.32	0/620	0.75	0/838
30	D8	0.97	1/499 (0.2%)	0.61	0/670
30	d8	0.69	1/499 (0.2%)	0.63	0/670
31	D9	0.41	0/452	0.85	2/600 (0.3%)
31	d9	0.36	0/452	0.68	0/600
32	E0	0.39	0/483	0.70	0/643
32	e0	0.42	0/483	0.80	0/643
33	E1	0.44	0/577	1.13	5/770 (0.6%)
33	e1	0.41	0/358	0.83	0/477
34	SR	0.24	0/2490	0.53	1/3389 (0.0%)
34	sR	0.25	0/2456	0.53	0/3343
35	SM	0.37	0/994	0.80	1/1335 (0.1%)
35	sM	0.41	0/882	0.78	0/1180
36	1	0.43	0/73692	0.70	18/114882 (0.0%)
36	5	0.45	0/74873	0.70	13/116727 (0.0%)
37	3	0.37	0/2883	0.59	0/4491
37	7	0.34	0/2883	0.53	0/4491
38	4	0.43	0/3746	0.71	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.47	0/3724	0.75	1/5798 (0.0%)
39	L2	0.41	0/1948	0.79	0/2617
39	l2	0.47	0/1946	0.84	3/2614 (0.1%)
40	L3	0.44	0/3146	0.73	0/4228
40	l3	0.49	0/3146	0.79	1/4228 (0.0%)
41	L4	0.41	0/2800	0.79	1/3790 (0.0%)
41	l4	0.46	0/2800	0.80	3/3790 (0.1%)
42	L5	0.35	0/2407	0.66	0/3247
42	l5	0.31	0/2408	0.58	0/3248
43	L6	0.45	0/1260	0.76	0/1694
43	l6	0.49	0/1269	0.80	0/1705
44	L7	0.43	0/1821	0.69	0/2451
44	l7	0.46	0/1828	0.70	0/2461
45	L8	0.37	1/1836 (0.1%)	0.66	3/2481 (0.1%)
45	l8	0.39	0/1795	0.70	0/2429
46	L9	0.41	0/1539	0.72	0/2073
46	l9	0.43	0/1531	0.77	0/2062
47	M0	0.46	0/1726	0.73	0/2314
47	m0	0.41	0/1732	0.79	3/2323 (0.1%)
48	M1	0.37	0/1374	0.73	0/1842
48	m1	0.31	0/1374	0.67	2/1842 (0.1%)
49	M3	0.44	2/1568 (0.1%)	0.80	0/2106
49	m3	0.42	0/1573	0.80	2/2113 (0.1%)
50	M4	0.42	0/1068	0.74	0/1438
50	m4	0.49	0/1074	0.76	1/1446 (0.1%)
51	M5	0.41	0/1757	0.74	0/2354
51	m5	0.46	0/1757	0.84	2/2354 (0.1%)
52	M6	0.54	0/1585	0.78	0/2128
52	m6	0.54	0/1585	0.80	0/2128
53	M7	0.47	0/1443	0.79	0/1944
53	m7	0.50	0/1400	0.82	0/1882
54	M8	0.35	0/1465	0.68	0/1965
54	m8	0.39	0/1465	0.70	0/1965
55	M9	0.35	0/1538	0.62	0/2050
55	m9	0.38	0/1499	0.64	0/1998
56	N0	0.43	0/1468	0.72	1/1973 (0.1%)
56	n0	0.51	1/1481 (0.1%)	0.75	0/1990
57	N1	0.42	0/1300	0.72	0/1743
57	n1	0.36	0/1300	0.65	1/1743 (0.1%)
58	N2	0.30	0/794	0.61	0/1076
58	n2	0.30	0/794	0.58	0/1076
59	N3	0.44	0/1012	0.74	0/1361
59	n3	0.52	0/1008	0.82	0/1356

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.38	0/937	0.62	0/1243
60	n4	0.38	0/959	0.67	0/1267
61	N5	0.41	0/979	0.75	0/1321
61	n5	0.48	0/974	0.81	1/1314 (0.1%)
62	N6	0.40	0/1004	0.81	0/1341
62	n6	0.43	0/987	0.85	0/1318
63	N7	0.39	0/1118	0.69	2/1497 (0.1%)
63	n7	0.41	0/1118	0.67	0/1497
64	N8	0.40	0/1204	0.85	2/1612 (0.1%)
64	n8	0.40	0/1204	0.77	3/1612 (0.2%)
65	N9	0.39	0/473	0.69	0/629
65	n9	0.43	0/473	0.89	2/629 (0.3%)
66	O0	0.32	0/751	0.61	0/1008
66	o0	0.38	0/775	0.63	0/1040
67	O1	0.42	0/890	0.77	0/1196
67	o1	0.45	0/897	0.84	2/1205 (0.2%)
68	O2	0.45	0/1041	0.77	0/1394
68	o2	0.50	0/1041	0.78	0/1394
69	O3	0.49	0/868	0.79	0/1168
69	o3	0.56	0/868	0.84	0/1168
70	O4	0.39	0/890	0.75	0/1189
70	o4	0.43	0/890	0.77	0/1189
71	O5	0.39	0/978	0.75	2/1301 (0.2%)
71	o5	0.42	0/974	0.75	0/1297
72	O6	0.40	1/778 (0.1%)	0.68	0/1034
72	o6	0.37	0/777	0.79	3/1033 (0.3%)
73	O7	0.49	0/680	0.88	0/901
73	o7	0.54	0/665	0.89	0/882
74	O8	0.34	0/618	0.67	0/826
74	o8	0.37	0/614	0.68	0/822
75	O9	0.42	0/438	0.78	0/581
75	o9	0.51	0/443	0.74	0/588
76	Q0	0.49	0/423	0.89	0/562
76	q0	0.60	0/423	0.92	0/562
77	Q1	0.37	0/234	0.71	0/300
77	q1	0.45	0/234	0.70	0/300
78	Q2	0.40	0/860	0.70	0/1136
78	q2	0.39	0/860	0.72	0/1136
79	Q3	0.38	0/701	0.68	0/934
79	q3	0.37	0/701	0.72	0/934
80	p0	0.26	0/1067	0.58	0/1439
All	All	0.40	13/423555 (0.0%)	0.69	136/621249 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D8	5	THR	C-N	20.70	1.82	1.33
18	c6	4	VAL	C-N	15.22	1.69	1.33
30	d8	5	THR	C-N	14.20	1.67	1.33
28	D6	59	TYR	C-N	13.44	1.65	1.33
17	C5	67	ALA	C-N	8.15	1.52	1.33

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C6	40	GLU	CA-C-N	-10.78	106.36	119.84
18	C6	40	GLU	C-N-CA	-10.78	106.36	119.84
12	C0	87	VAL	CA-C-N	10.74	133.26	119.84
12	C0	87	VAL	C-N-CA	10.74	133.26	119.84
41	L4	340	GLY	N-CA-C	-8.63	101.73	112.77

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	35985	0	18101	1210	0
1	6	36234	0	18227	1059	0
2	S0	1577	0	1567	98	0
2	s0	1583	0	1578	98	0
3	S1	1709	0	1784	124	0
3	s1	1722	0	1793	75	0
4	S2	1635	0	1723	89	0
4	s2	1635	0	1723	85	0
5	S3	1734	0	1817	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	81	0
6	S4	2068	0	2154	96	0
6	s4	2068	0	2154	95	0
7	S5	1609	0	1675	107	0
7	s5	1609	0	1675	76	0
8	S6	1799	0	1879	92	0
8	s6	1755	0	1846	80	0
9	S7	1481	0	1572	90	0
9	s7	1486	0	1576	72	0
10	S8	1489	0	1525	87	0
10	s8	1489	0	1525	67	0
11	S9	1494	0	1572	77	0
11	s9	1494	0	1573	100	0
12	C0	752	0	719	33	0
12	c0	741	0	691	46	0
13	C1	1146	0	1213	73	0
13	c1	1168	0	1233	54	0
14	C2	870	0	876	54	0
14	c2	890	0	887	47	0
15	C3	1192	0	1255	69	0
15	c3	1192	0	1255	49	0
16	C4	891	0	883	74	0
16	c4	949	0	985	59	0
17	C5	967	0	998	47	0
17	c5	939	0	968	60	0
18	C6	1105	0	1166	64	0
18	c6	1105	0	1166	60	0
19	C7	911	0	921	52	0
19	c7	906	0	910	63	0
20	C8	1192	0	1222	86	0
20	c8	1192	0	1222	92	0
21	C9	1112	0	1124	75	0
21	c9	1112	0	1124	69	0
22	D0	837	0	901	49	0
22	d0	805	0	874	48	0
23	D1	684	0	672	40	0
23	d1	684	0	672	45	0
24	D2	1021	0	1060	72	0
24	d2	1021	0	1060	57	0
25	D3	1121	0	1196	59	0
25	d3	1121	0	1196	59	0
26	D4	1073	0	1132	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	65	0
27	D5	563	0	603	60	0
27	d5	558	0	598	34	0
28	D6	769	0	814	59	0
28	d6	769	0	815	62	0
29	D7	610	0	633	25	0
29	d7	610	0	633	42	0
30	D8	497	0	535	32	0
30	d8	497	0	535	19	0
31	D9	442	0	428	20	0
31	d9	442	0	428	14	0
32	E0	475	0	525	30	0
32	e0	475	0	525	39	0
33	E1	566	0	603	32	0
33	e1	352	0	364	23	0
34	SR	2437	0	2389	75	0
34	sR	2403	0	2353	80	0
35	SM	985	0	939	55	0
35	sM	874	0	875	66	0
36	1	65838	0	33085	2147	0
36	5	66891	0	33617	2006	0
37	3	2579	0	1303	94	0
37	7	2579	0	1304	71	0
38	4	3353	0	1695	161	0
38	8	3333	0	1684	121	0
39	L2	1914	0	1981	119	0
39	l2	1912	0	1976	144	0
40	L3	3075	0	3142	171	0
40	l3	3075	0	3142	156	0
41	L4	2748	0	2859	153	0
41	l4	2748	0	2859	150	0
42	L5	2357	0	2309	134	0
42	l5	2359	0	2311	116	0
43	L6	1239	0	1326	64	0
43	l6	1248	0	1339	71	0
44	L7	1784	0	1862	68	0
44	l7	1791	0	1869	91	0
45	L8	1804	0	1877	89	0
45	l8	1763	0	1819	98	0
46	L9	1518	0	1587	96	0
46	l9	1510	0	1576	100	0
47	M0	1690	0	1727	83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	m0	1696	0	1731	86	0
48	M1	1353	0	1383	72	0
48	m1	1353	0	1383	52	0
49	M3	1543	0	1608	92	0
49	m3	1548	0	1613	98	0
50	M4	1053	0	1149	69	0
50	m4	1059	0	1154	72	0
51	M5	1720	0	1779	109	0
51	m5	1720	0	1779	100	0
52	M6	1555	0	1659	85	0
52	m6	1555	0	1659	121	0
53	M7	1420	0	1437	76	0
53	m7	1378	0	1404	69	0
54	M8	1441	0	1543	63	0
54	m8	1441	0	1543	68	0
55	M9	1521	0	1617	99	0
55	m9	1482	0	1578	69	0
56	N0	1432	0	1470	77	0
56	n0	1445	0	1487	79	0
57	N1	1276	0	1323	58	0
57	n1	1276	0	1323	76	0
58	N2	778	0	791	29	0
58	n2	778	0	791	21	0
59	N3	997	0	1043	54	0
59	n3	993	0	1040	61	0
60	N4	925	0	933	35	0
60	n4	946	0	1019	49	0
61	N5	964	0	1025	63	0
61	n5	959	0	1023	53	0
62	N6	993	0	1081	40	0
62	n6	976	0	1064	52	0
63	N7	1092	0	1155	73	0
63	n7	1092	0	1155	57	0
64	N8	1173	0	1215	87	0
64	n8	1173	0	1215	71	0
65	N9	462	0	491	20	0
65	n9	462	0	491	24	0
66	O0	743	0	797	43	0
66	o0	767	0	816	41	0
67	O1	876	0	912	54	0
67	o1	883	0	918	39	0
68	O2	1020	0	1090	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	o2	1020	0	1090	48	0
69	O3	850	0	880	34	0
69	o3	850	0	880	42	0
70	O4	880	0	944	82	0
70	o4	880	0	943	61	0
71	O5	969	0	1078	66	0
71	o5	965	0	1067	53	0
72	O6	771	0	849	39	0
72	o6	770	0	846	36	0
73	O7	665	0	669	46	0
73	o7	650	0	650	42	0
74	O8	612	0	682	26	0
74	o8	608	0	671	28	0
75	O9	431	0	470	25	0
75	o9	436	0	475	28	0
76	Q0	417	0	455	23	0
76	q0	417	0	455	23	0
77	Q1	233	0	284	14	0
77	q1	233	0	284	11	0
78	Q2	847	0	916	33	0
78	q2	847	0	915	26	0
79	Q3	694	0	736	47	0
79	q3	694	0	736	49	0
80	p0	1052	0	1028	35	0
81	1	407	0	0	0	0
81	2	111	0	0	0	0
81	3	9	0	0	0	0
81	4	25	0	0	0	0
81	5	443	0	0	0	0
81	6	112	0	0	0	0
81	7	8	0	0	0	0
81	8	14	0	0	0	0
81	C0	1	0	0	0	0
81	C4	2	0	0	0	0
81	C8	1	0	0	0	0
81	D2	2	0	0	0	0
81	D9	1	0	0	0	0
81	L2	3	0	0	0	0
81	L3	2	0	0	0	0
81	L5	1	0	0	0	0
81	L6	1	0	0	0	0
81	L8	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	M0	2	0	0	0	0
81	M4	1	0	0	0	0
81	M5	1	0	0	0	0
81	M6	1	0	0	0	0
81	M7	6	0	0	0	0
81	N2	1	0	0	0	0
81	N7	1	0	0	0	0
81	N8	2	0	0	0	0
81	O2	3	0	0	0	0
81	O3	2	0	0	0	0
81	O5	1	0	0	0	0
81	O6	2	0	0	0	0
81	O7	1	0	0	0	0
81	O8	1	0	0	0	0
81	O9	1	0	0	0	0
81	Q2	1	0	0	0	0
81	S1	1	0	0	0	0
81	S8	1	0	0	0	0
81	SM	1	0	0	0	0
81	c3	1	0	0	0	0
81	d3	2	0	0	0	0
81	l2	4	0	0	0	0
81	l3	4	0	0	0	0
81	l4	1	0	0	0	0
81	l7	2	0	0	0	0
81	l9	1	0	0	0	0
81	m0	1	0	0	0	0
81	m6	1	0	0	0	0
81	m7	5	0	0	0	0
81	n0	2	0	0	0	0
81	n3	2	0	0	0	0
81	n4	1	0	0	0	0
81	n5	1	0	0	0	0
81	n7	1	0	0	0	0
81	o2	2	0	0	0	0
81	o3	3	0	0	0	0
81	o5	1	0	0	0	0
81	o7	5	0	0	0	0
81	q2	4	0	0	0	0
81	s8	2	0	0	0	0
81	sM	1	0	0	0	0
82	1	204	0	240	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	2	102	0	120	20	0
82	5	272	0	320	37	0
82	6	102	0	120	15	0
82	n6	34	0	40	3	0
83	D6	1	0	0	0	0
83	D7	1	0	0	0	0
83	D9	1	0	0	0	0
83	E1	1	0	0	0	0
83	O4	1	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	Q3	1	0	0	0	0
83	d6	1	0	0	0	0
83	d7	1	0	0	0	0
83	d9	1	0	0	0	0
83	e1	1	0	0	0	0
83	o4	1	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	q3	1	0	0	0	0
84	1	367	0	0	47	0
84	2	99	0	0	18	0
84	3	18	0	0	0	0
84	4	7	0	0	0	0
84	5	365	0	0	41	0
84	6	111	0	0	11	0
84	7	11	0	0	1	0
84	8	7	0	0	0	0
84	C1	1	0	0	0	0
84	C3	1	0	0	1	0
84	C6	1	0	0	0	0
84	C9	2	0	0	0	0
84	D3	1	0	0	0	0
84	D9	1	0	0	0	0
84	L2	1	0	0	1	0
84	L3	1	0	0	0	0
84	L4	1	0	0	1	0
84	M0	2	0	0	0	0
84	M5	1	0	0	0	0
84	M6	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	M7	4	0	0	0	0
84	N1	3	0	0	0	0
84	N3	3	0	0	1	0
84	N5	1	0	0	1	0
84	N8	1	0	0	0	0
84	O1	2	0	0	0	0
84	O2	2	0	0	1	0
84	S4	1	0	0	0	0
84	SM	1	0	0	0	0
84	c3	1	0	0	0	0
84	c8	1	0	0	1	0
84	c9	2	0	0	0	0
84	d3	2	0	0	0	0
84	l2	1	0	0	0	0
84	l3	4	0	0	1	0
84	l4	2	0	0	0	0
84	l9	1	0	0	0	0
84	m0	1	0	0	0	0
84	m5	3	0	0	0	0
84	m6	1	0	0	1	0
84	m7	2	0	0	1	0
84	m9	2	0	0	1	0
84	n1	3	0	0	0	0
84	n3	3	0	0	1	0
84	o2	3	0	0	1	0
84	o4	2	0	0	1	0
84	o7	1	0	0	0	0
84	q2	1	0	0	0	0
All	All	397710	0	294943	14049	0

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 21.

The worst 5 of 14049 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)
18:c6:4:VAL:C	18:c6:5:PRO:N	1.69	1.45
30:D8:5:THR:C	30:D8:6:PRO:N	1.82	1.36
1:2:1761:U:H3'	82:2:2013:GET:H611	1.34	1.10
40:l3:41:VAL:HA	40:l3:185:GLY:HA3	1.30	1.08
40:l3:296:THR:HG22	40:l3:298:PHE:H	1.13	1.07

There are no symmetry-related clashes.

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	
2	S0	204/206 (99%)	174 (85%)	26 (13%)	4 (2%)	6	32
2	s0	204/206 (99%)	176 (86%)	23 (11%)	5 (2%)	4	29
3	S1	212/216 (98%)	162 (76%)	45 (21%)	5 (2%)	4	29
3	s1	214/216 (99%)	195 (91%)	15 (7%)	4 (2%)	6	33
4	S2	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	14	45
4	s2	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	56
5	S3	221/223 (99%)	202 (91%)	15 (7%)	4 (2%)	6	34
5	s3	221/223 (99%)	195 (88%)	18 (8%)	8 (4%)	2	23
6	S4	258/260 (99%)	226 (88%)	30 (12%)	2 (1%)	16	48
6	s4	258/260 (99%)	234 (91%)	21 (8%)	3 (1%)	10	40
7	S5	204/206 (99%)	178 (87%)	21 (10%)	5 (2%)	4	29
7	s5	204/206 (99%)	183 (90%)	18 (9%)	3 (2%)	8	36
8	S6	224/236 (95%)	209 (93%)	9 (4%)	6 (3%)	4	27
8	s6	216/236 (92%)	196 (91%)	17 (8%)	3 (1%)	9	37
9	S7	182/185 (98%)	154 (85%)	20 (11%)	8 (4%)	2	19
9	s7	183/185 (99%)	157 (86%)	23 (13%)	3 (2%)	7	35
10	S8	184/200 (92%)	160 (87%)	23 (12%)	1 (0%)	24	56
10	s8	184/200 (92%)	171 (93%)	11 (6%)	2 (1%)	11	42
11	S9	183/185 (99%)	162 (88%)	20 (11%)	1 (0%)	24	56
11	s9	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
12	C0	90/105 (86%)	77 (86%)	10 (11%)	3 (3%)	3	25
12	c0	90/105 (86%)	65 (72%)	19 (21%)	6 (7%)	1	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C1	140/156 (90%)	128 (91%)	10 (7%)	2 (1%)	9	37
13	c1	144/156 (92%)	130 (90%)	11 (8%)	3 (2%)	5	31
14	C2	118/143 (82%)	87 (74%)	27 (23%)	4 (3%)	3	25
14	c2	122/143 (85%)	89 (73%)	25 (20%)	8 (7%)	1	13
15	C3	148/150 (99%)	134 (90%)	12 (8%)	2 (1%)	9	37
15	c3	148/150 (99%)	129 (87%)	16 (11%)	3 (2%)	6	32
16	C4	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	48
16	c4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
17	C5	120/141 (85%)	100 (83%)	18 (15%)	2 (2%)	7	34
17	c5	117/141 (83%)	99 (85%)	14 (12%)	4 (3%)	3	25
18	C6	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	3	26
18	c6	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	50
19	C7	113/136 (83%)	100 (88%)	12 (11%)	1 (1%)	14	45
19	c7	115/136 (85%)	104 (90%)	10 (9%)	1 (1%)	14	45
20	C8	143/145 (99%)	123 (86%)	17 (12%)	3 (2%)	5	31
20	c8	143/145 (99%)	122 (85%)	18 (13%)	3 (2%)	5	31
21	C9	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
21	c9	141/143 (99%)	128 (91%)	12 (8%)	1 (1%)	18	50
22	D0	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
22	d0	99/107 (92%)	88 (89%)	9 (9%)	2 (2%)	6	32
23	D1	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	4	29
23	d1	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	16	48
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	48
25	D3	142/144 (99%)	119 (84%)	19 (13%)	4 (3%)	4	27
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
26	D4	132/134 (98%)	121 (92%)	8 (6%)	3 (2%)	5	30
26	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	8	36
27	D5	68/70 (97%)	52 (76%)	14 (21%)	2 (3%)	3	26
27	d5	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
28	D6	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	d6	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	11	42
29	D7	79/81 (98%)	69 (87%)	9 (11%)	1 (1%)	9	38
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	9	38
30	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
30	d8	61/63 (97%)	52 (85%)	9 (15%)	0	100	100
31	D9	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
31	d9	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	2	21
32	E0	58/60 (97%)	51 (88%)	4 (7%)	3 (5%)	1	17
32	e0	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	1	17
33	E1	69/152 (45%)	44 (64%)	19 (28%)	6 (9%)	0	8
33	e1	41/152 (27%)	31 (76%)	8 (20%)	2 (5%)	1	17
34	SR	316/318 (99%)	298 (94%)	18 (6%)	0	100	100
34	sR	311/318 (98%)	291 (94%)	19 (6%)	1 (0%)	36	65
35	SM	131/272 (48%)	116 (88%)	12 (9%)	3 (2%)	5	30
35	sM	113/272 (42%)	94 (83%)	13 (12%)	6 (5%)	1	16
39	L2	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
39	l2	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	30	60
40	L3	384/386 (100%)	352 (92%)	30 (8%)	2 (0%)	24	56
40	l3	384/386 (100%)	361 (94%)	19 (5%)	4 (1%)	12	43
41	L4	359/361 (99%)	321 (89%)	35 (10%)	3 (1%)	16	48
41	l4	359/361 (99%)	322 (90%)	31 (9%)	6 (2%)	7	34
42	L5	292/296 (99%)	264 (90%)	23 (8%)	5 (2%)	7	34
42	l5	292/296 (99%)	276 (94%)	16 (6%)	0	100	100
43	L6	152/176 (86%)	142 (93%)	6 (4%)	4 (3%)	4	28
43	l6	153/176 (87%)	139 (91%)	11 (7%)	3 (2%)	6	32
44	L7	220/223 (99%)	205 (93%)	15 (7%)	0	100	100
44	l7	221/223 (99%)	210 (95%)	9 (4%)	2 (1%)	14	45
45	L8	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	7	34
45	l8	229/233 (98%)	201 (88%)	23 (10%)	5 (2%)	5	31
46	L9	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	24	56
46	l9	188/191 (98%)	176 (94%)	9 (5%)	3 (2%)	7	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	M0	204/221 (92%)	193 (95%)	11 (5%)	0	100	100
47	m0	205/221 (93%)	186 (91%)	18 (9%)	1 (0%)	24	56
48	M1	167/169 (99%)	136 (81%)	29 (17%)	2 (1%)	10	40
48	m1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	2	23
49	M3	191/194 (98%)	172 (90%)	14 (7%)	5 (3%)	4	28
49	m3	192/194 (99%)	162 (84%)	25 (13%)	5 (3%)	4	28
50	M4	134/137 (98%)	123 (92%)	9 (7%)	2 (2%)	8	36
50	m4	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
51	M5	201/203 (99%)	181 (90%)	18 (9%)	2 (1%)	12	43
51	m5	201/203 (99%)	185 (92%)	13 (6%)	3 (2%)	8	36
52	M6	195/197 (99%)	182 (93%)	11 (6%)	2 (1%)	12	43
52	m6	195/197 (99%)	185 (95%)	10 (5%)	0	100	100
53	M7	181/184 (98%)	168 (93%)	11 (6%)	2 (1%)	11	42
53	m7	171/184 (93%)	159 (93%)	12 (7%)	0	100	100
54	M8	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	24	56
54	m8	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
55	M9	186/188 (99%)	174 (94%)	10 (5%)	2 (1%)	11	42
55	m9	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	21	52
56	N0	168/172 (98%)	154 (92%)	12 (7%)	2 (1%)	10	40
56	n0	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
57	N1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	21	52
57	n1	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	21	52
58	N2	96/98 (98%)	86 (90%)	10 (10%)	0	100	100
58	n2	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	12	43
59	N3	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
59	n3	132/135 (98%)	128 (97%)	3 (2%)	1 (1%)	16	48
60	N4	118/155 (76%)	110 (93%)	8 (7%)	0	100	100
60	n4	114/155 (74%)	106 (93%)	8 (7%)	0	100	100
61	N5	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
61	n5	118/121 (98%)	102 (86%)	15 (13%)	1 (1%)	16	48
62	N6	124/126 (98%)	116 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	n6	122/126 (97%)	116 (95%)	4 (3%)	2 (2%)	7	35
63	N7	133/135 (98%)	120 (90%)	11 (8%)	2 (2%)	8	36
63	n7	133/135 (98%)	117 (88%)	14 (10%)	2 (2%)	8	36
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	3	25
64	n8	146/148 (99%)	128 (88%)	16 (11%)	2 (1%)	9	37
65	N9	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
65	n9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	2	23
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
66	o0	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
67	O1	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	4	27
67	o1	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	33
68	O2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
68	o2	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
69	O3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
69	o3	104/106 (98%)	93 (89%)	11 (11%)	0	100	100
70	O4	110/112 (98%)	102 (93%)	6 (6%)	2 (2%)	6	34
70	o4	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	45
71	O5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	7	34
71	o5	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	14	45
72	O6	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	12	43
72	o6	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	12	43
73	O7	82/84 (98%)	76 (93%)	5 (6%)	1 (1%)	10	40
73	o7	80/84 (95%)	74 (92%)	5 (6%)	1 (1%)	9	38
74	O8	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
74	o8	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	9	38
75	O9	47/50 (94%)	43 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	5	31
76	Q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	6	32
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	32
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Q2	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
78	q2	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
79	Q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
79	q3	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
80	p0	134/312 (43%)	121 (90%)	12 (9%)	1 (1%)	18	50
All	All	22212/23608 (94%)	19993 (90%)	1922 (9%)	297 (1%)	9	38

5 of 297 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	207	LEU
8	S6	153	VAL
9	S7	111	LYS
12	C0	87	VAL
12	C0	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	127 (77%)	37 (23%)	1	6
2	s0	165/173 (95%)	133 (81%)	32 (19%)	1	9
3	S1	191/192 (100%)	144 (75%)	47 (25%)	1	5
3	s1	192/192 (100%)	158 (82%)	34 (18%)	2	12
4	S2	176/176 (100%)	131 (74%)	45 (26%)	0	4
4	s2	176/176 (100%)	132 (75%)	44 (25%)	0	4
5	S3	182/182 (100%)	142 (78%)	40 (22%)	1	7
5	s3	182/182 (100%)	141 (78%)	41 (22%)	1	6
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	9
6	s4	221/221 (100%)	176 (80%)	45 (20%)	1	8
7	S5	173/173 (100%)	140 (81%)	33 (19%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	s5	153/173 (88%)	123 (80%)	30 (20%)	1	9
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	8
9	S7	165/165 (100%)	127 (77%)	38 (23%)	1	6
10	S8	150/161 (93%)	126 (84%)	24 (16%)	2	15
11	S9	158/158 (100%)	123 (78%)	35 (22%)	1	7
12	C0	77/98 (79%)	63 (82%)	14 (18%)	2	11
13	C1	127/137 (93%)	104 (82%)	23 (18%)	2	12
14	C2	88/119 (74%)	64 (73%)	24 (27%)	0	3
15	C3	127/127 (100%)	104 (82%)	23 (18%)	2	12
16	C4	81/97 (84%)	59 (73%)	22 (27%)	0	3
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	8
18	C6	117/117 (100%)	89 (76%)	28 (24%)	1	5
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	8
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	4
20	c8	65/128 (51%)	55 (85%)	10 (15%)	2	16
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	6
21	c9	17/115 (15%)	14 (82%)	3 (18%)	2	12
22	D0	98/100 (98%)	73 (74%)	25 (26%)	0	4
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	7
24	D2	110/110 (100%)	86 (78%)	24 (22%)	1	7
25	D3	119/119 (100%)	93 (78%)	26 (22%)	1	7
26	D4	112/112 (100%)	85 (76%)	27 (24%)	1	5
27	D5	61/61 (100%)	39 (64%)	22 (36%)	0	1
28	D6	83/83 (100%)	59 (71%)	24 (29%)	0	2
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	15
30	D8	56/56 (100%)	38 (68%)	18 (32%)	0	2
31	D9	47/47 (100%)	35 (74%)	12 (26%)	0	4
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	9
33	E1	62/135 (46%)	41 (66%)	21 (34%)	0	1
34	SR	259/260 (100%)	223 (86%)	36 (14%)	3	19
34	sR	202/260 (78%)	182 (90%)	20 (10%)	7	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SM	97/227 (43%)	72 (74%)	25 (26%)	0	4
35	sM	36/227 (16%)	28 (78%)	8 (22%)	1	7
39	L2	193/194 (100%)	155 (80%)	38 (20%)	1	9
39	l2	192/194 (99%)	145 (76%)	47 (24%)	1	5
40	L3	320/322 (99%)	254 (79%)	66 (21%)	1	8
40	l3	318/322 (99%)	240 (76%)	78 (24%)	1	5
41	L4	288/288 (100%)	236 (82%)	52 (18%)	2	12
41	l4	288/288 (100%)	219 (76%)	69 (24%)	1	5
42	L5	242/244 (99%)	186 (77%)	56 (23%)	1	6
42	l5	243/244 (100%)	195 (80%)	48 (20%)	1	9
43	L6	134/153 (88%)	101 (75%)	33 (25%)	1	5
43	l6	135/153 (88%)	112 (83%)	23 (17%)	2	13
44	L7	186/187 (100%)	159 (86%)	27 (14%)	3	17
44	l7	187/187 (100%)	155 (83%)	32 (17%)	2	13
45	L8	187/191 (98%)	149 (80%)	38 (20%)	1	8
45	l8	177/191 (93%)	138 (78%)	39 (22%)	1	7
46	L9	171/171 (100%)	127 (74%)	44 (26%)	0	4
46	l9	170/171 (99%)	126 (74%)	44 (26%)	0	4
47	M0	177/187 (95%)	145 (82%)	32 (18%)	2	12
47	m0	177/187 (95%)	138 (78%)	39 (22%)	1	7
48	M1	147/147 (100%)	117 (80%)	30 (20%)	1	8
48	m1	147/147 (100%)	117 (80%)	30 (20%)	1	8
49	M3	154/154 (100%)	118 (77%)	36 (23%)	1	6
49	m3	154/154 (100%)	125 (81%)	29 (19%)	1	10
50	M4	107/108 (99%)	85 (79%)	22 (21%)	1	8
50	m4	108/108 (100%)	86 (80%)	22 (20%)	1	8
51	M5	175/175 (100%)	144 (82%)	31 (18%)	2	12
51	m5	175/175 (100%)	145 (83%)	30 (17%)	2	13
52	M6	160/160 (100%)	126 (79%)	34 (21%)	1	7
52	m6	160/160 (100%)	123 (77%)	37 (23%)	1	6
53	M7	140/146 (96%)	102 (73%)	38 (27%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	m7	139/146 (95%)	98 (70%)	41 (30%)	0	2
54	M8	150/150 (100%)	120 (80%)	30 (20%)	1	9
54	m8	150/150 (100%)	121 (81%)	29 (19%)	1	9
55	M9	153/153 (100%)	108 (71%)	45 (29%)	0	2
55	m9	149/153 (97%)	107 (72%)	42 (28%)	0	3
56	N0	155/156 (99%)	121 (78%)	34 (22%)	1	7
56	n0	156/156 (100%)	125 (80%)	31 (20%)	1	9
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	6
57	n1	136/136 (100%)	110 (81%)	26 (19%)	1	10
58	N2	85/85 (100%)	76 (89%)	9 (11%)	6	27
58	n2	85/85 (100%)	70 (82%)	15 (18%)	2	12
59	N3	103/103 (100%)	87 (84%)	16 (16%)	2	15
59	n3	103/103 (100%)	84 (82%)	19 (18%)	1	11
60	N4	85/129 (66%)	72 (85%)	13 (15%)	3	16
60	n4	97/129 (75%)	82 (84%)	15 (16%)	2	15
61	N5	104/105 (99%)	76 (73%)	28 (27%)	0	4
61	n5	104/105 (99%)	81 (78%)	23 (22%)	1	7
62	N6	109/109 (100%)	83 (76%)	26 (24%)	1	5
62	n6	107/109 (98%)	83 (78%)	24 (22%)	1	7
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	9
63	n7	115/115 (100%)	87 (76%)	28 (24%)	1	5
64	N8	118/118 (100%)	93 (79%)	25 (21%)	1	7
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	7
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	12
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	9
66	O0	81/84 (96%)	62 (76%)	19 (24%)	1	6
66	o0	84/84 (100%)	67 (80%)	17 (20%)	1	8
67	O1	92/96 (96%)	69 (75%)	23 (25%)	0	4
67	o1	94/96 (98%)	72 (77%)	22 (23%)	1	6
68	O2	109/109 (100%)	88 (81%)	21 (19%)	1	9
68	o2	109/109 (100%)	85 (78%)	24 (22%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	15
69	o3	90/90 (100%)	72 (80%)	18 (20%)	1	9
70	O4	95/95 (100%)	71 (75%)	24 (25%)	0	4
70	o4	95/95 (100%)	79 (83%)	16 (17%)	2	13
71	O5	104/104 (100%)	83 (80%)	21 (20%)	1	8
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	6
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	3
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	2
73	O7	69/69 (100%)	51 (74%)	18 (26%)	0	4
73	o7	67/69 (97%)	53 (79%)	14 (21%)	1	7
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	7
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	9
75	O9	45/45 (100%)	33 (73%)	12 (27%)	0	4
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2	15
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1	10
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	13
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4	20
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1	5
78	q2	90/90 (100%)	78 (87%)	12 (13%)	4	20
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	13
79	q3	71/71 (100%)	54 (76%)	17 (24%)	1	5
80	p0	105/254 (41%)	86 (82%)	19 (18%)	2	12
All	All	16042/17195 (93%)	12630 (79%)	3412 (21%)	1	7

5 of 3412 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	8	ARG
39	l2	107	VAL
67	o1	61	LYS
72	O6	45	ARG
69	O3	107	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
40	l3	293	ASN
54	m8	5	HIS
41	l4	213	ASN
47	m0	73	ASN
58	n2	49	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1680/1800 (93%)	464 (27%)	67 (3%)
1	6	1695/1800 (94%)	427 (25%)	51 (3%)
36	1	3071/3396 (90%)	768 (25%)	101 (3%)
36	5	3120/3396 (91%)	745 (23%)	109 (3%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	49 (31%)	6 (3%)
38	8	156/158 (98%)	42 (26%)	8 (5%)
All	All	10119/10950 (92%)	2530 (25%)	344 (3%)

5 of 2530 RNA backbone outliers are listed below:

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

5 of 344 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1260 ligands modelled in this entry, 1239 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	GET	1	3809	-	35,36,36	0.36	0	43,55,55	1.09	5 (11%)
82	GET	1	3813	-	35,36,36	0.44	0	43,55,55	1.91	9 (20%)
82	GET	6	2015	-	35,36,36	2.10	11 (31%)	43,55,55	2.97	20 (46%)
82	GET	5	3850	-	35,36,36	0.35	0	43,55,55	1.23	5 (11%)
82	GET	5	3844	-	35,36,36	0.35	0	43,55,55	1.55	8 (18%)
82	GET	2	2012	-	35,36,36	0.37	0	43,55,55	1.02	3 (6%)
82	GET	5	3848	-	35,36,36	0.35	0	43,55,55	1.79	7 (16%)
82	GET	2	2014	-	35,36,36	0.44	0	43,55,55	1.33	5 (11%)
82	GET	5	3846	-	35,36,36	0.40	0	43,55,55	1.15	2 (4%)
82	GET	5	3851	-	35,36,36	0.30	0	43,55,55	0.70	1 (2%)
82	GET	1	3812	-	35,36,36	0.45	0	43,55,55	1.23	3 (6%)
82	GET	6	2014	-	35,36,36	0.24	0	43,55,55	1.10	4 (9%)
82	GET	1	3811	-	35,36,36	0.34	0	43,55,55	0.65	1 (2%)
82	GET	5	3847	-	35,36,36	0.46	0	43,55,55	1.55	7 (16%)
82	GET	n6	201	-	35,36,36	0.27	0	43,55,55	1.17	4 (9%)
82	GET	2	2013	-	35,36,36	0.37	0	43,55,55	0.96	3 (6%)
82	GET	6	2013	-	35,36,36	0.25	0	43,55,55	0.70	1 (2%)
82	GET	5	3849	-	35,36,36	0.51	0	43,55,55	1.32	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	GET	5	3845	-	35,36,36	0.40	0	43,55,55	0.95	2 (4%)
82	GET	1	3810	-	35,36,36	0.41	0	43,55,55	1.67	7 (16%)
82	GET	1	3808	-	35,36,36	0.35	0	43,55,55	1.65	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GET	1	3809	-	-	10/13/74/74	0/3/3/3
82	GET	1	3813	-	-	6/13/74/74	0/3/3/3
82	GET	6	2015	-	-	5/13/74/74	0/3/3/3
82	GET	5	3850	-	-	6/13/74/74	0/3/3/3
82	GET	5	3844	-	-	5/13/74/74	0/3/3/3
82	GET	2	2012	-	-	3/13/74/74	1/3/3/3
82	GET	5	3848	-	-	3/13/74/74	0/3/3/3
82	GET	2	2014	-	-	5/13/74/74	1/3/3/3
82	GET	5	3846	-	-	5/13/74/74	0/3/3/3
82	GET	5	3851	-	-	6/13/74/74	0/3/3/3
82	GET	1	3812	-	-	6/13/74/74	0/3/3/3
82	GET	6	2014	-	-	6/13/74/74	0/3/3/3
82	GET	1	3811	-	-	1/13/74/74	0/3/3/3
82	GET	5	3847	-	-	8/13/74/74	0/3/3/3
82	GET	n6	201	-	-	6/13/74/74	0/3/3/3
82	GET	2	2013	-	-	6/13/74/74	0/3/3/3
82	GET	6	2013	-	-	2/13/74/74	0/3/3/3
82	GET	5	3849	-	-	4/13/74/74	0/3/3/3
82	GET	5	3845	-	-	1/13/74/74	0/3/3/3
82	GET	1	3810	-	-	2/13/74/74	0/3/3/3
82	GET	1	3808	-	-	9/13/74/74	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	6	2015	GET	C23-C33	5.33	1.64	1.53
82	6	2015	GET	C53-C43	3.95	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	6	2015	GET	C22-C12	3.80	1.61	1.53
82	6	2015	GET	C41-C31	3.47	1.61	1.52
82	6	2015	GET	C33-N33	3.21	1.49	1.45

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	5	3848	GET	C23-C33-N33	-7.62	90.62	110.84
82	6	2015	GET	C11-C21-N21	7.35	123.45	110.20
82	6	2015	GET	O31-C31-C21	-7.02	97.61	110.22
82	1	3810	GET	O11-C11-C21	6.91	119.38	108.08
82	5	3847	GET	O11-C11-C21	5.93	117.79	108.08

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	2	2013	GET	C41-C51-C61-O61
82	2	2013	GET	C41-C51-C61-C71
82	2	2013	GET	O51-C51-C61-O61
82	2	2014	GET	C21-C11-O11-C42
82	2	2014	GET	C23-C33-N33-C93

All (2) ring outliers are listed below:

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

21 monomers are involved in 113 short contacts:

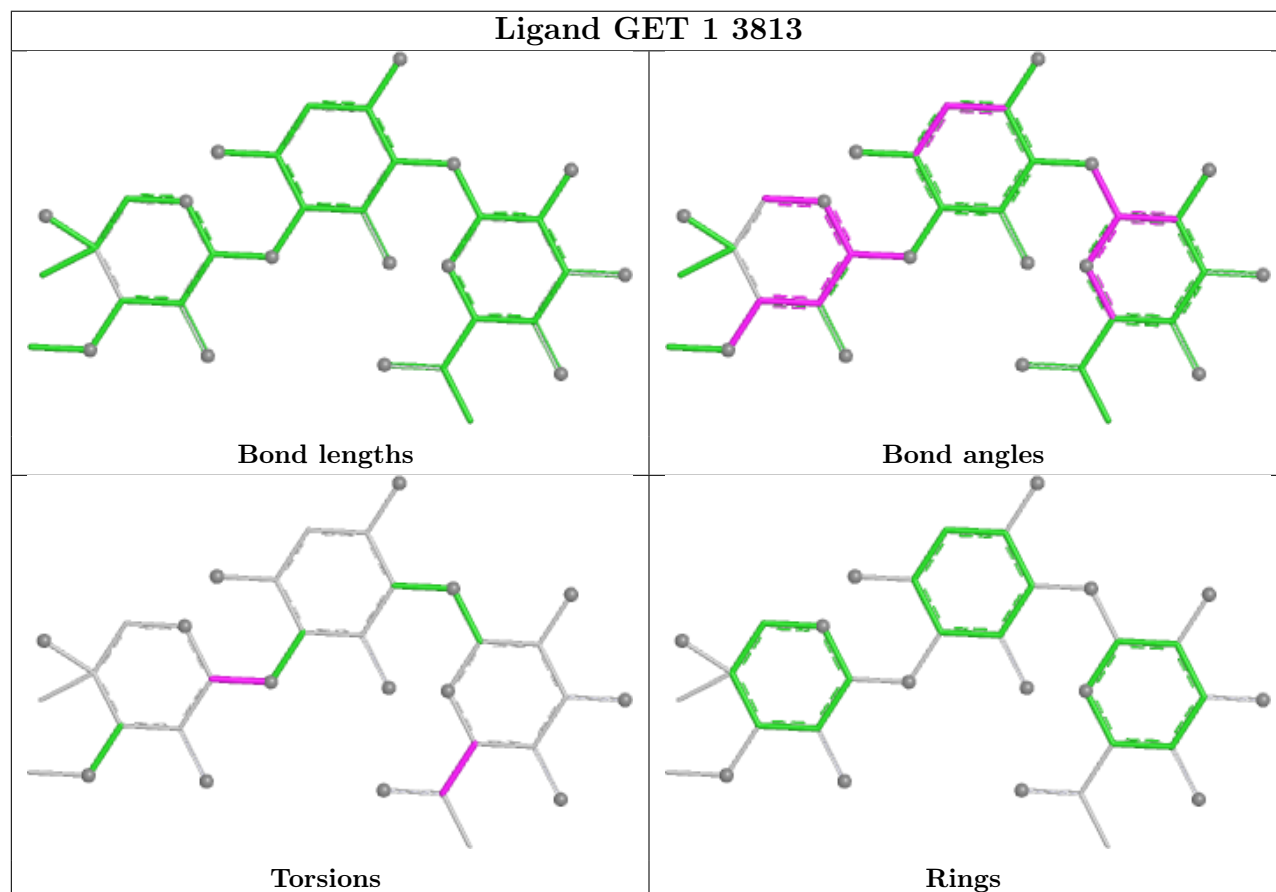
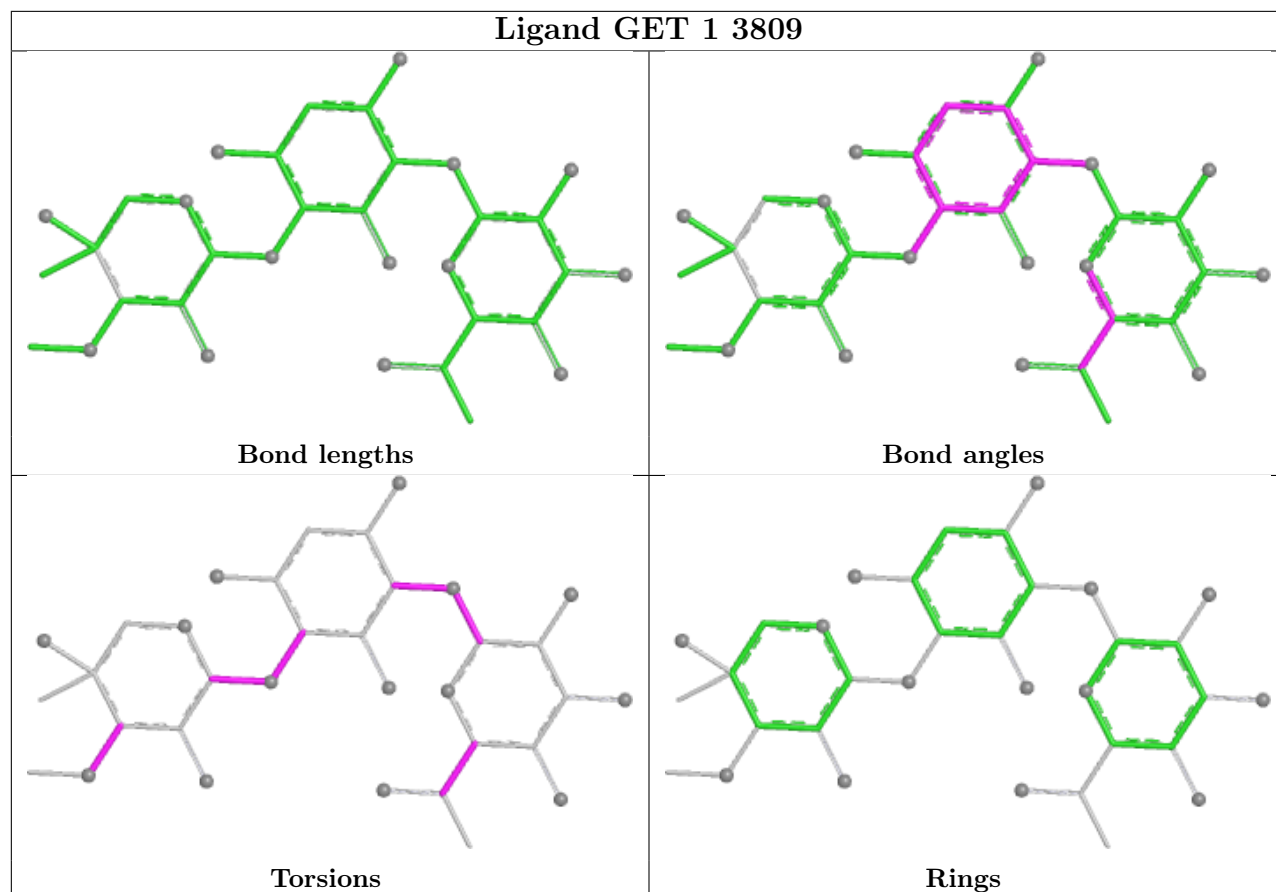
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	1	3809	GET	1	0
82	1	3813	GET	3	0
82	6	2015	GET	2	0
82	5	3850	GET	7	0
82	5	3844	GET	10	0
82	2	2012	GET	9	0
82	5	3848	GET	4	0
82	2	2014	GET	3	0
82	5	3846	GET	4	0

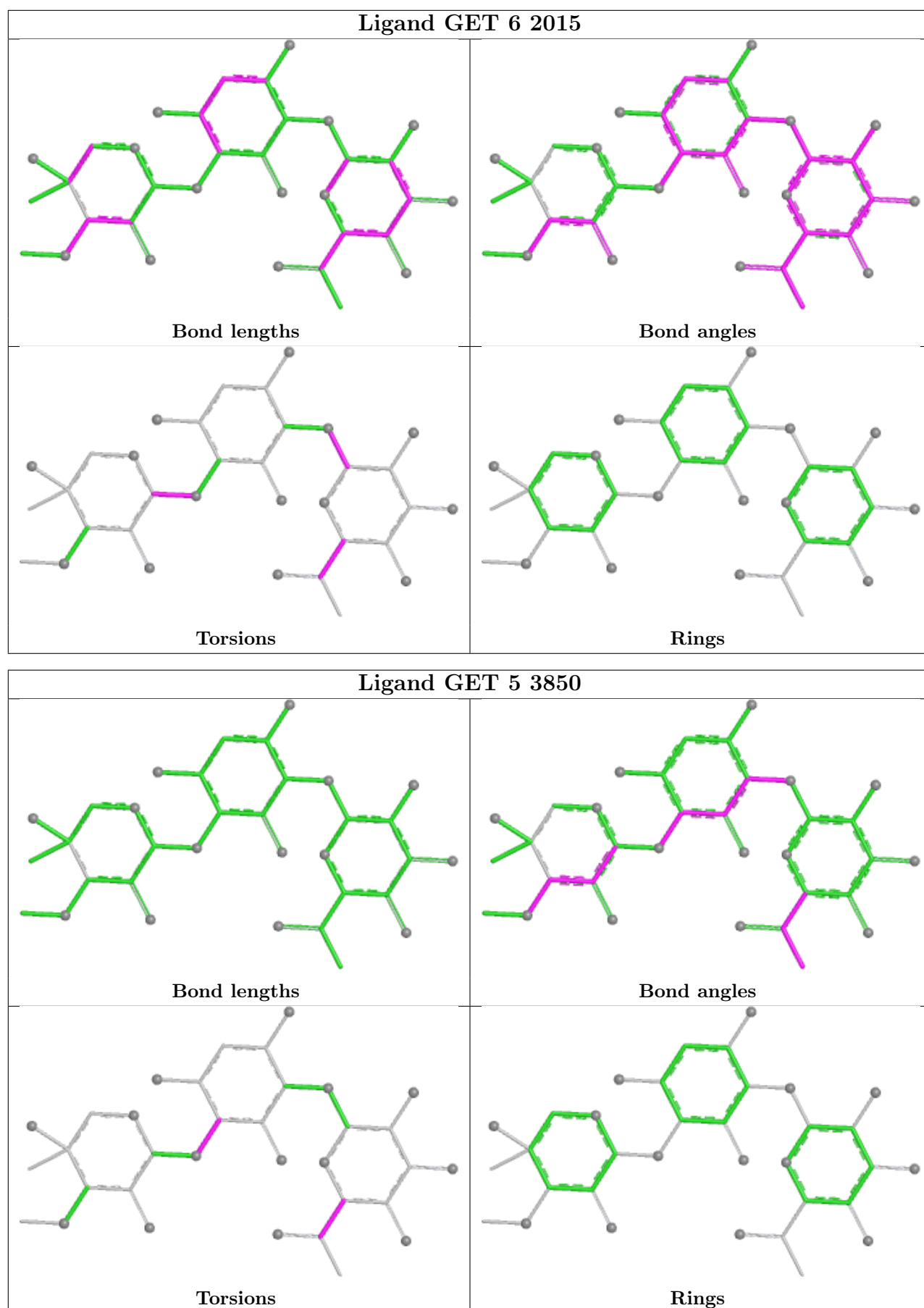
Continued on next page...

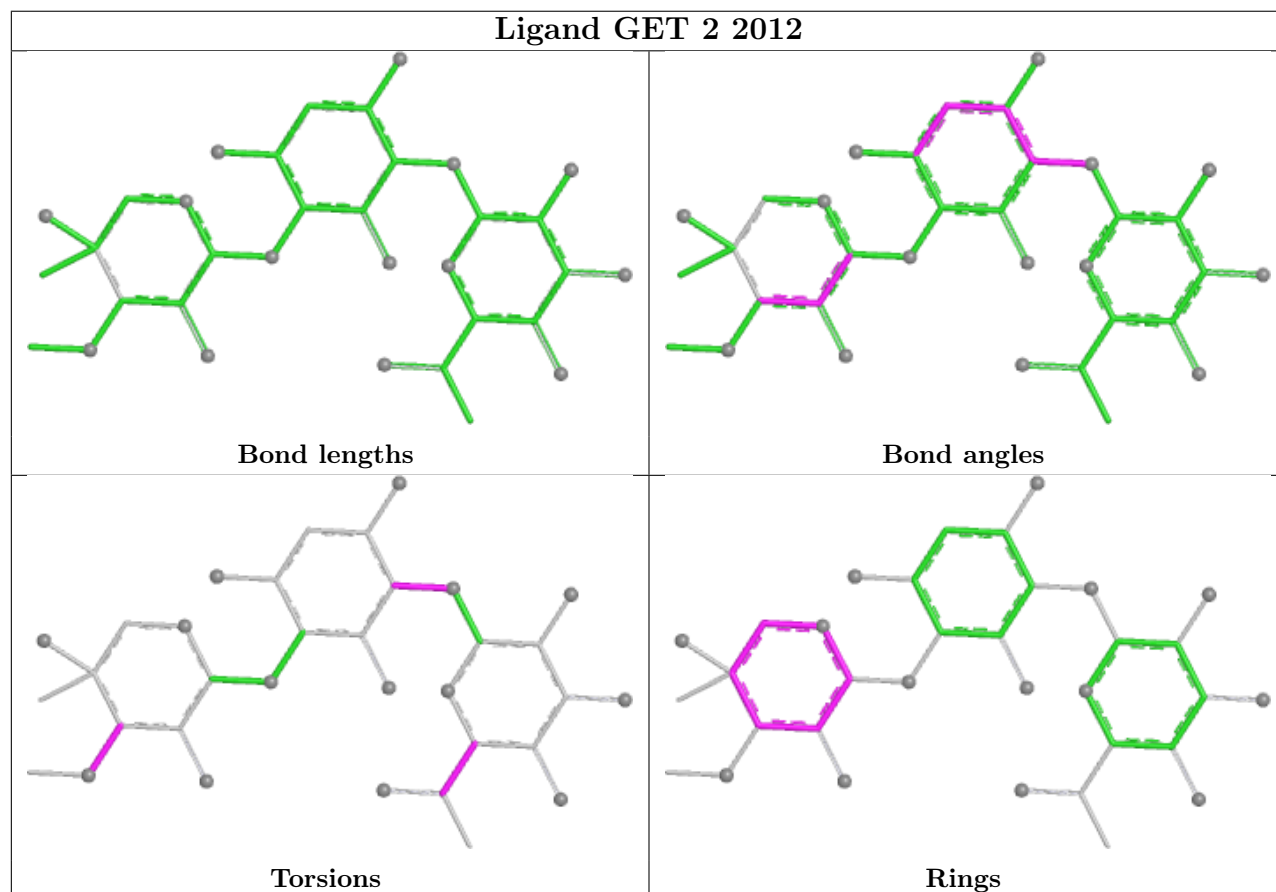
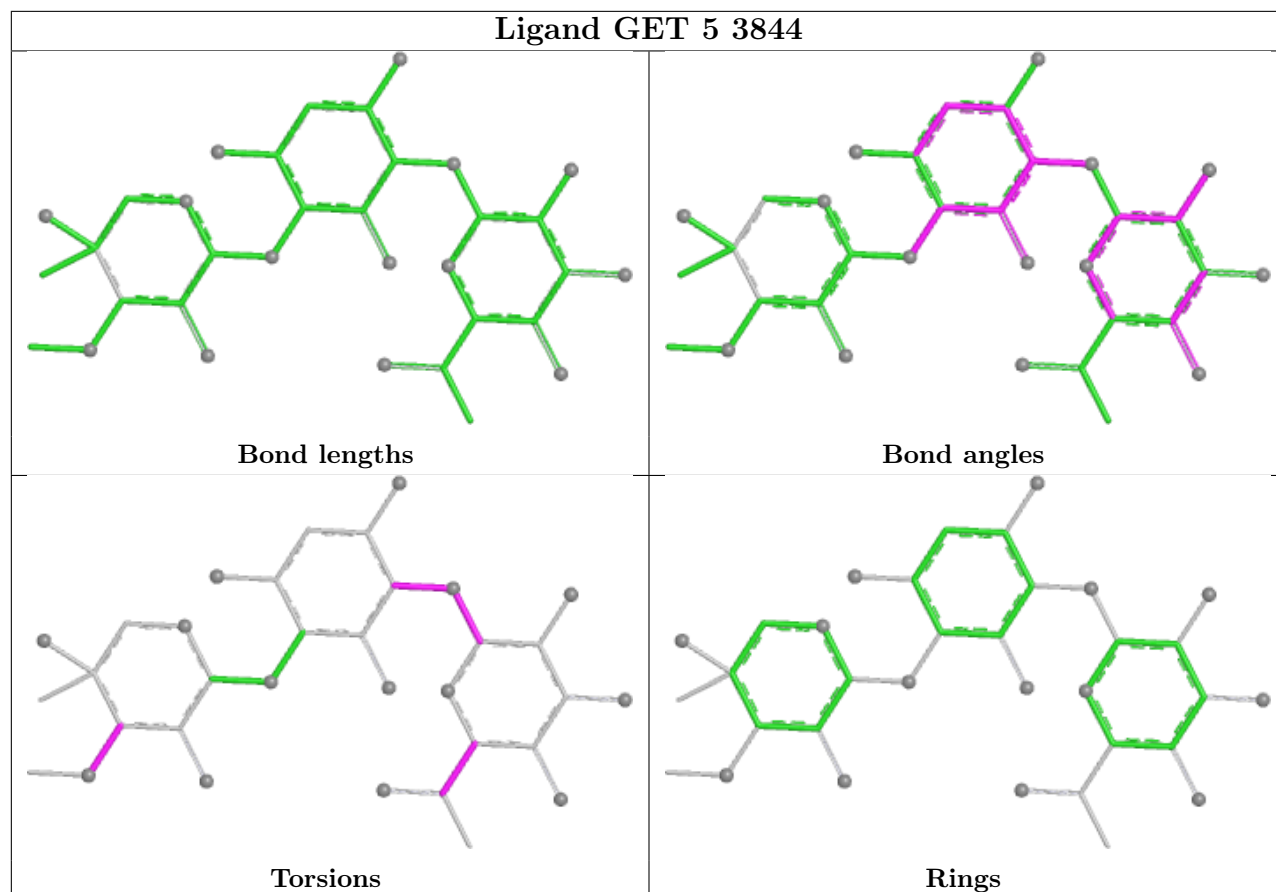
Continued from previous page...

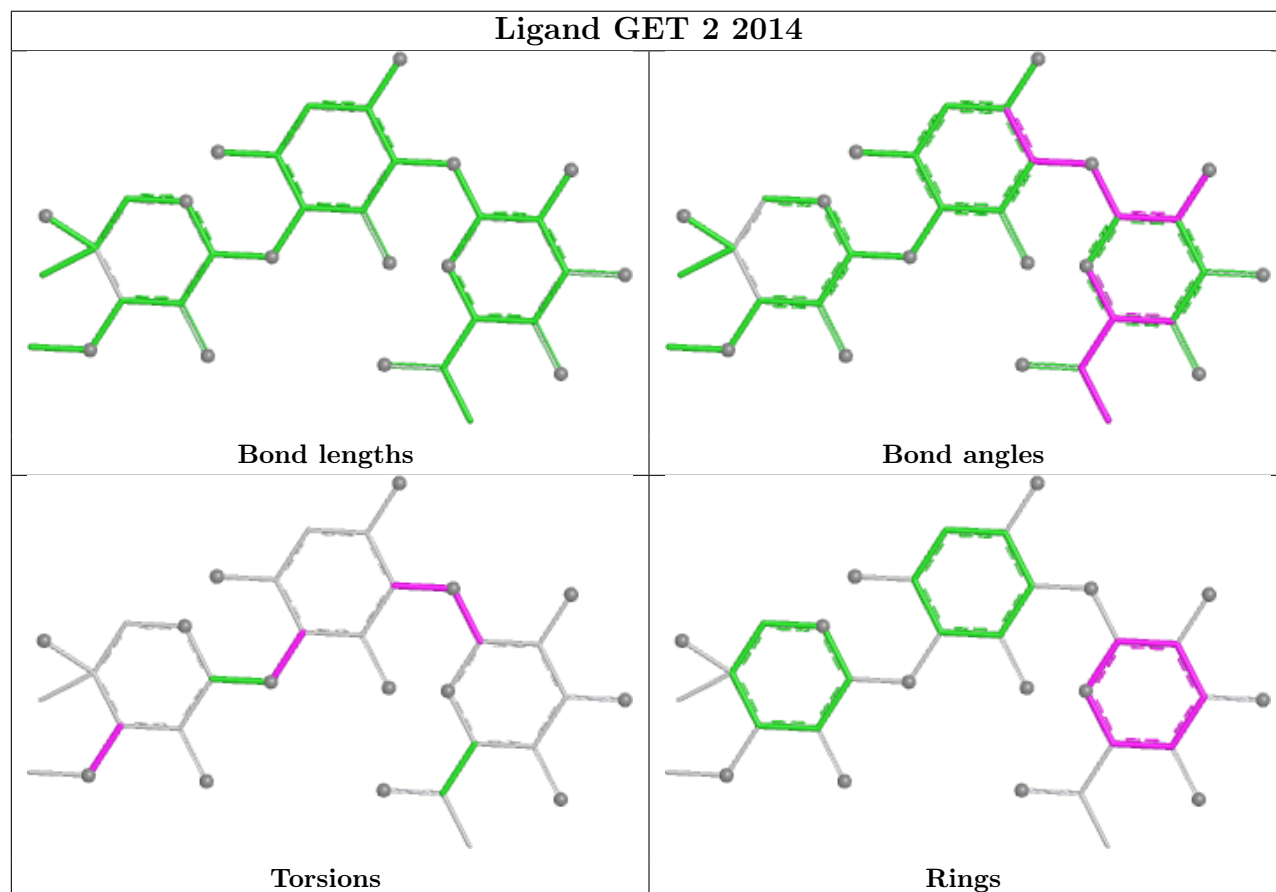
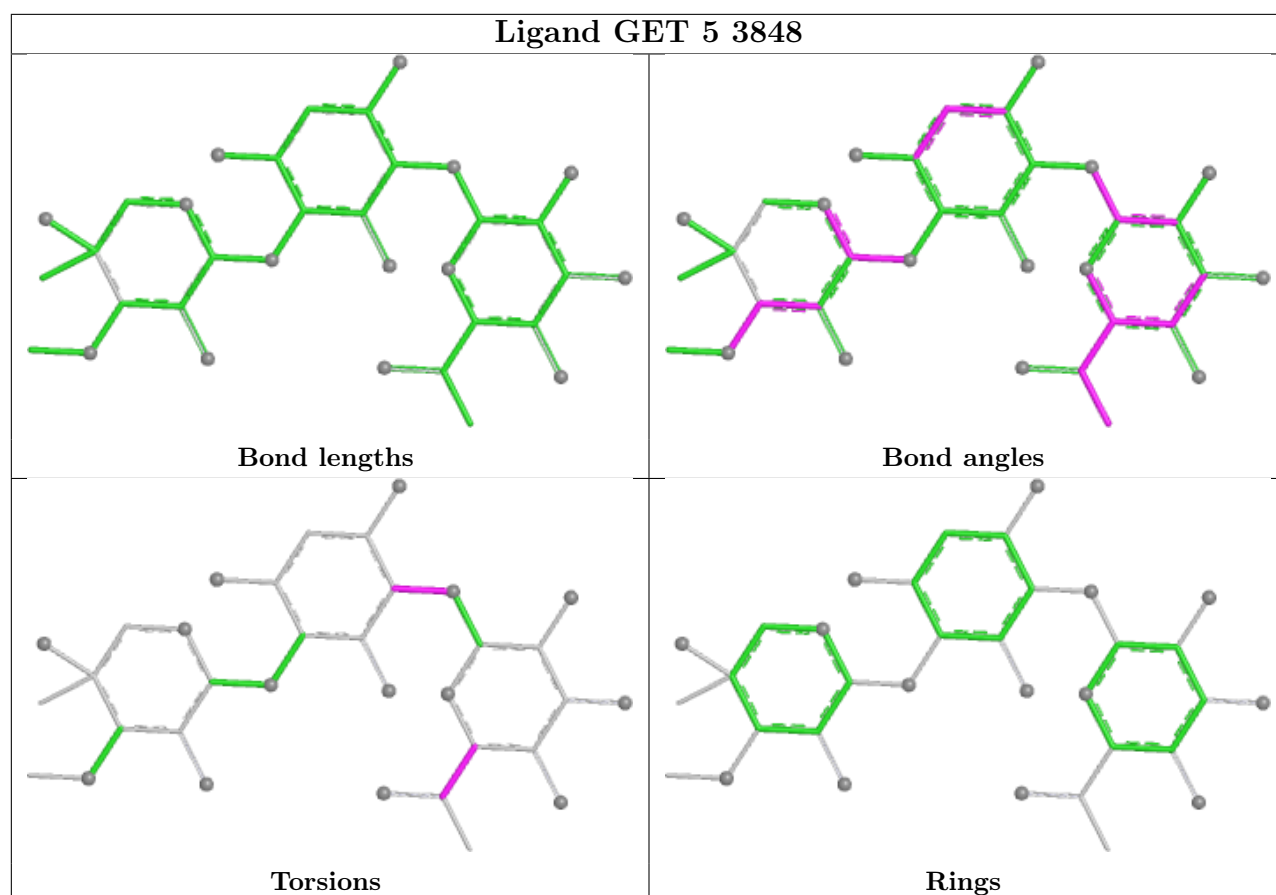
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	5	3851	GET	4	0
82	1	3812	GET	5	0
82	6	2014	GET	2	0
82	1	3811	GET	5	0
82	5	3847	GET	3	0
82	n6	201	GET	3	0
82	2	2013	GET	8	0
82	6	2013	GET	11	0
82	5	3849	GET	4	0
82	5	3845	GET	3	0
82	1	3810	GET	13	0
82	1	3808	GET	11	0

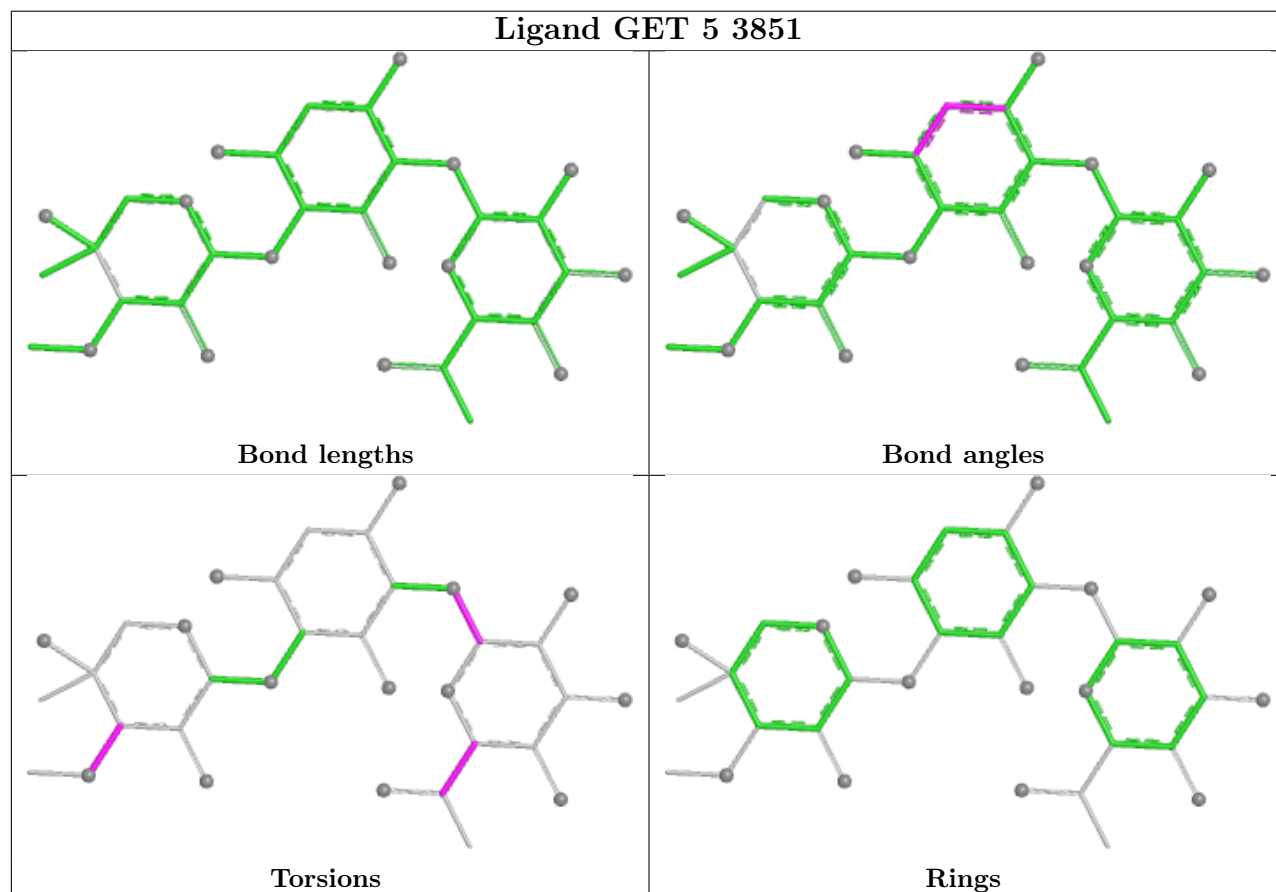
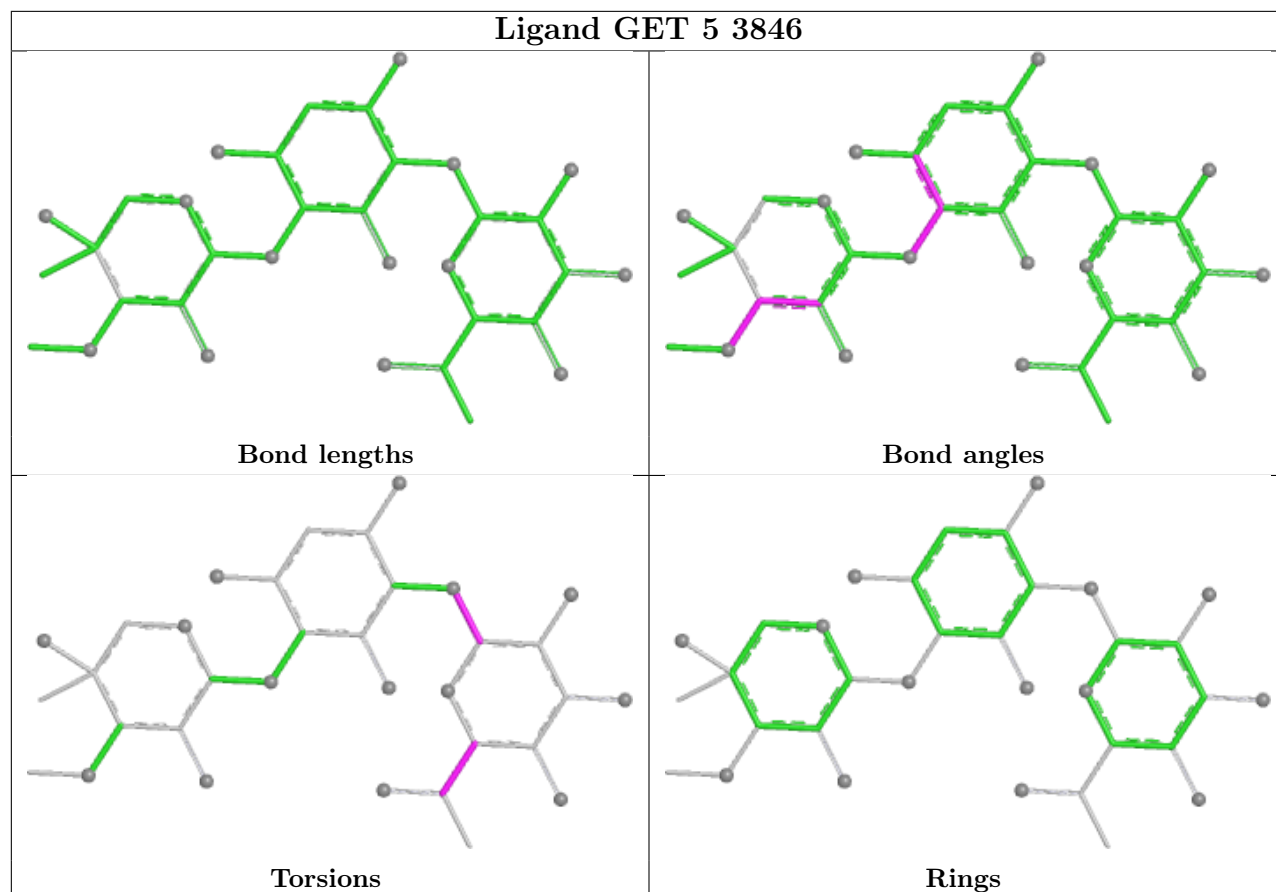
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

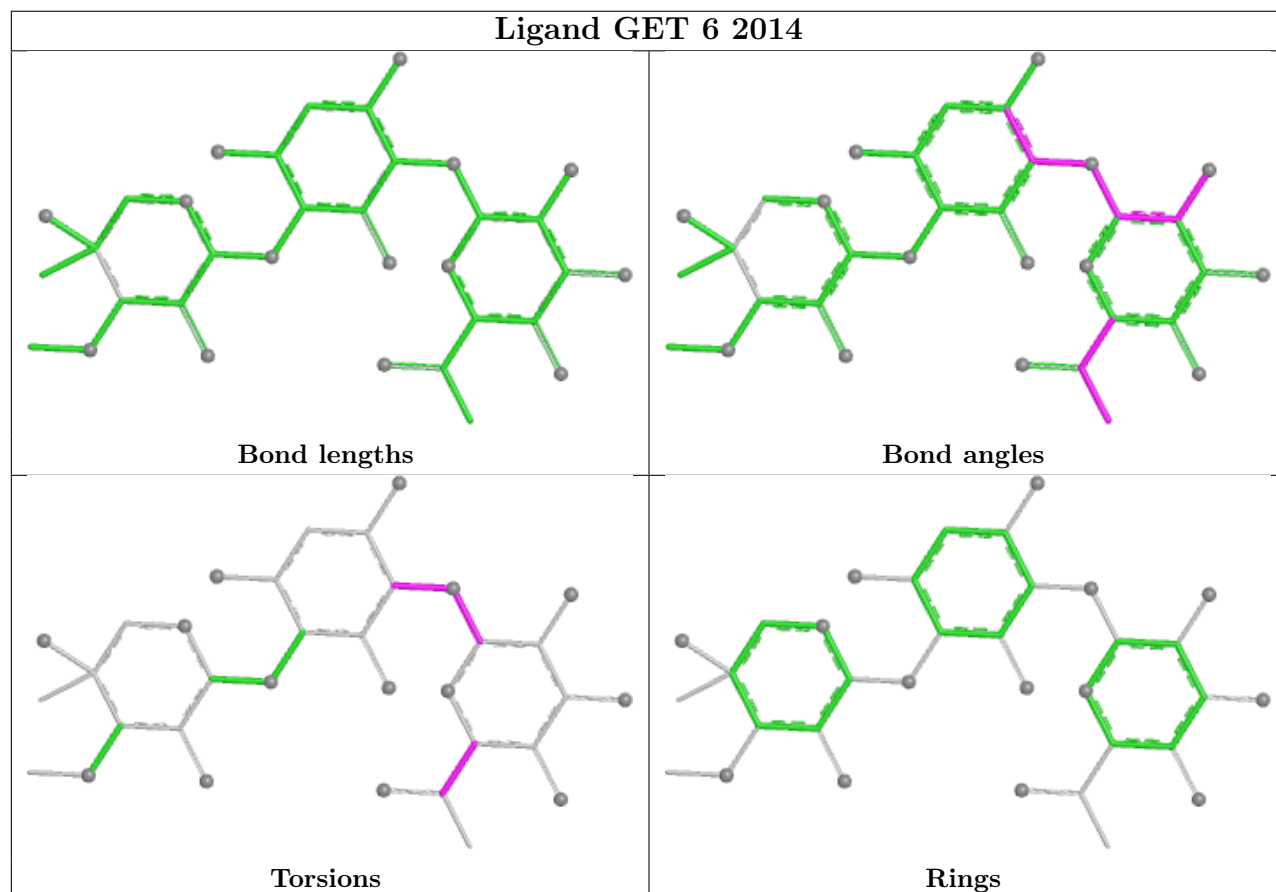
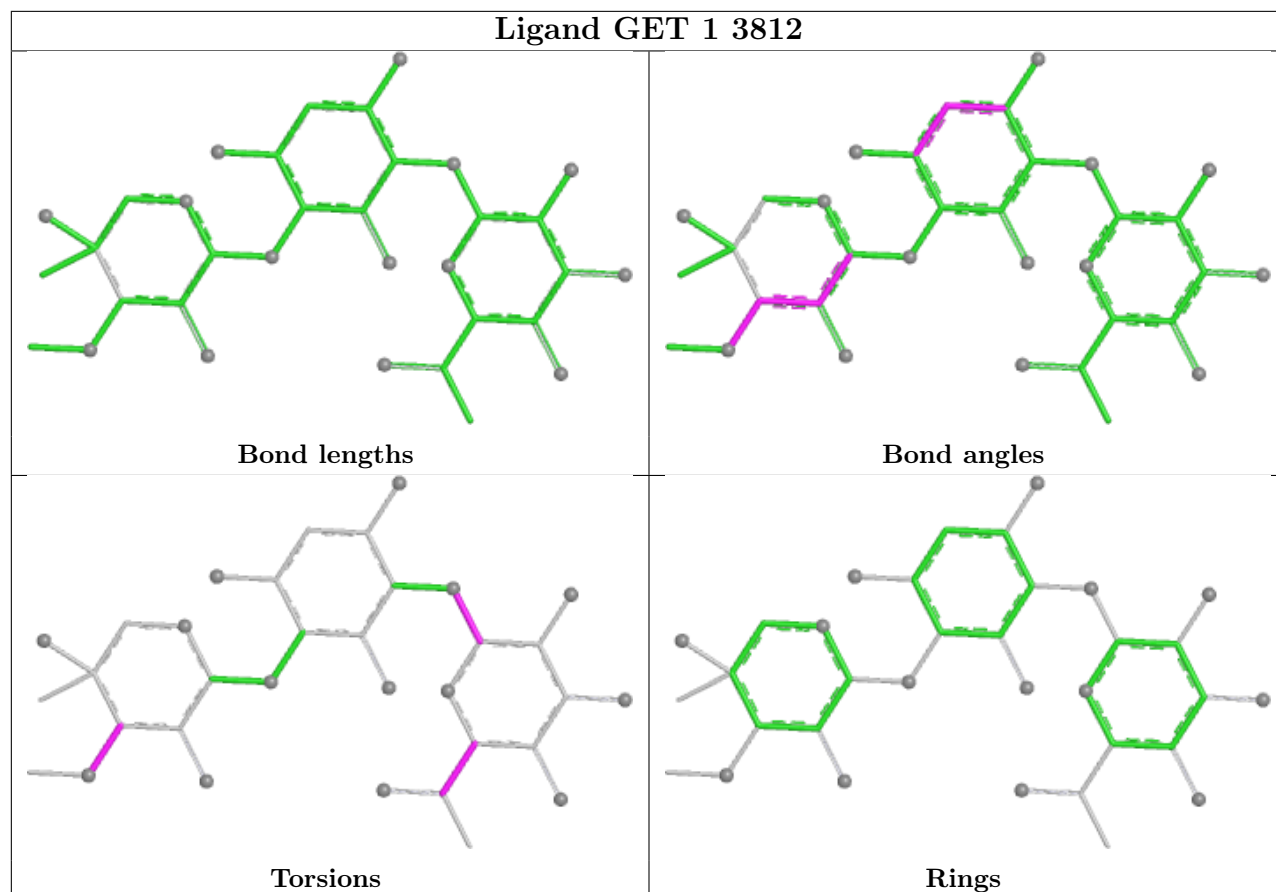


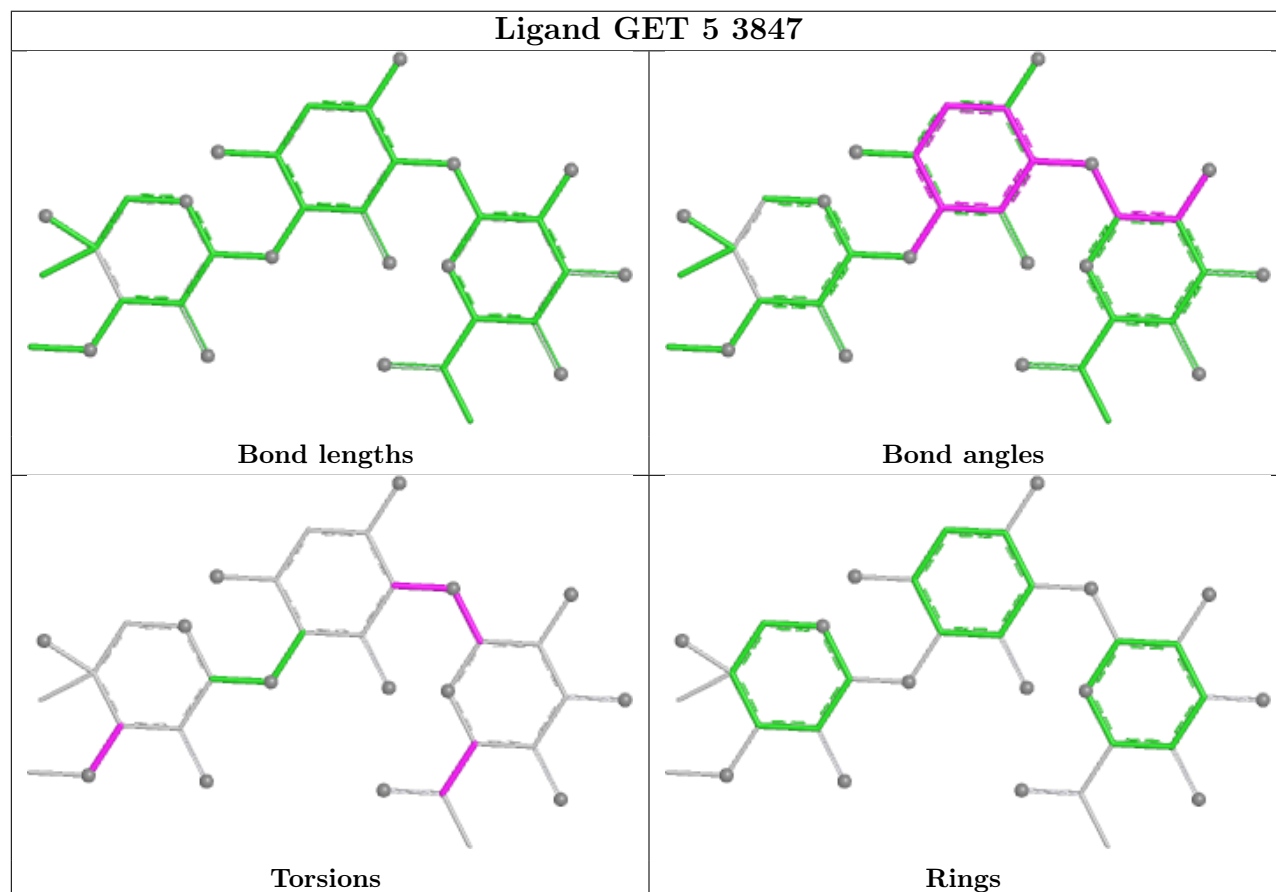
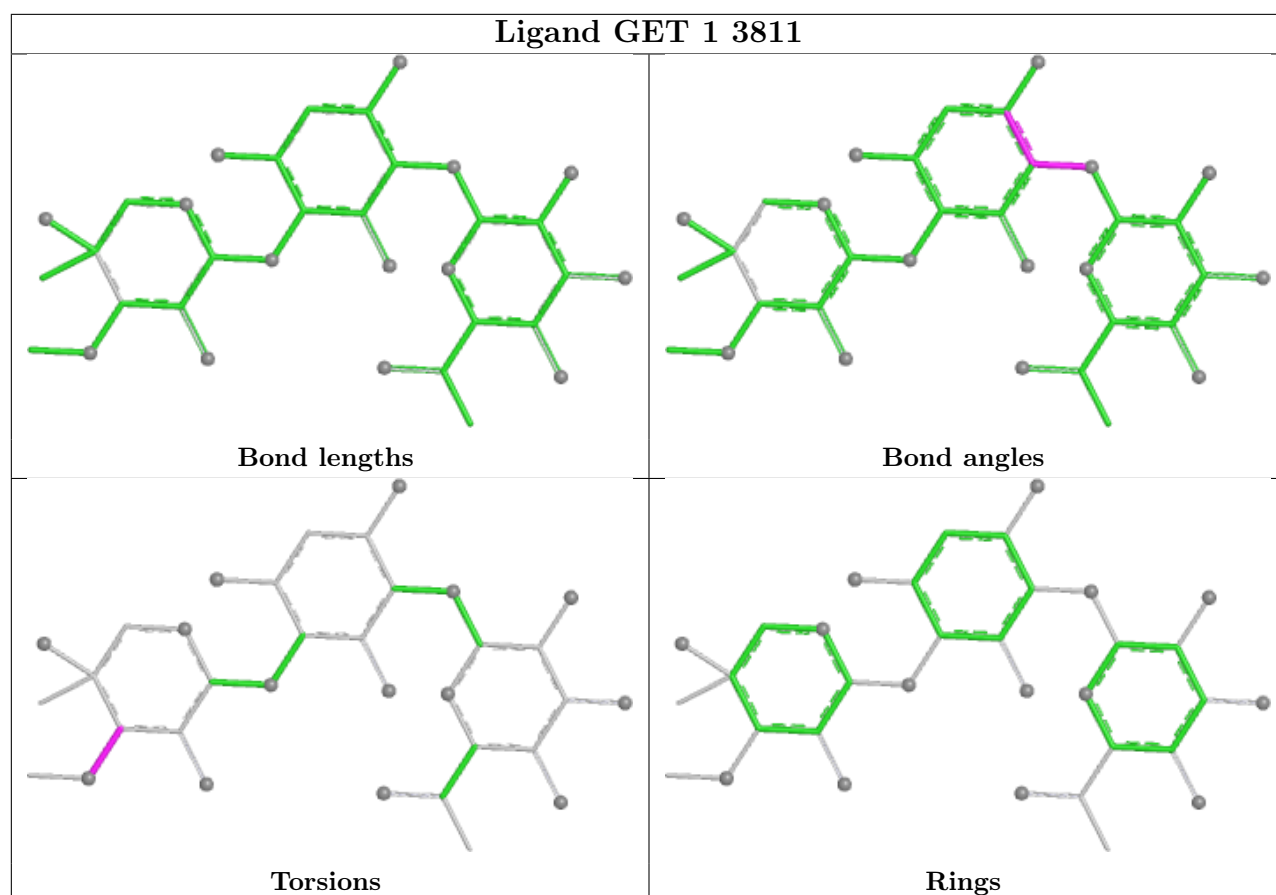


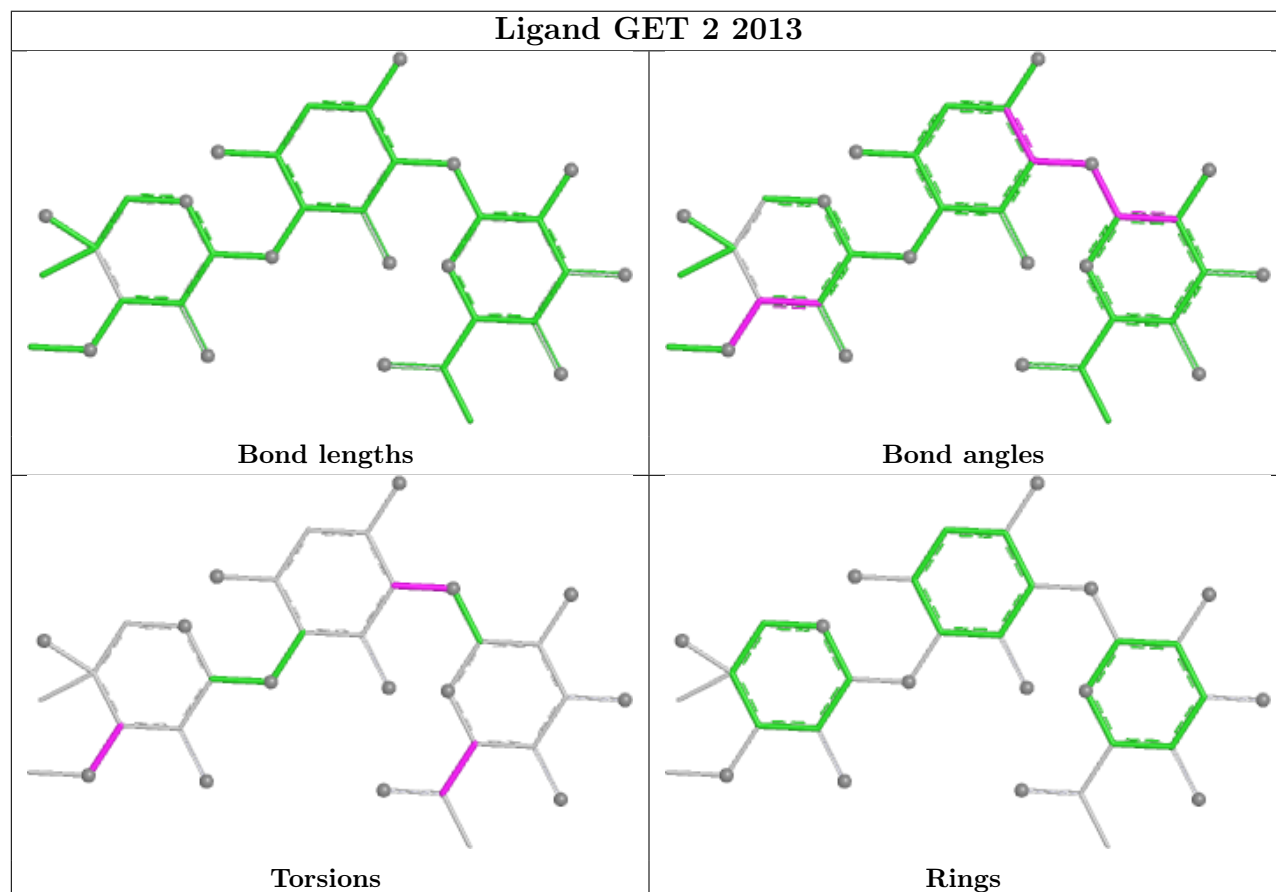
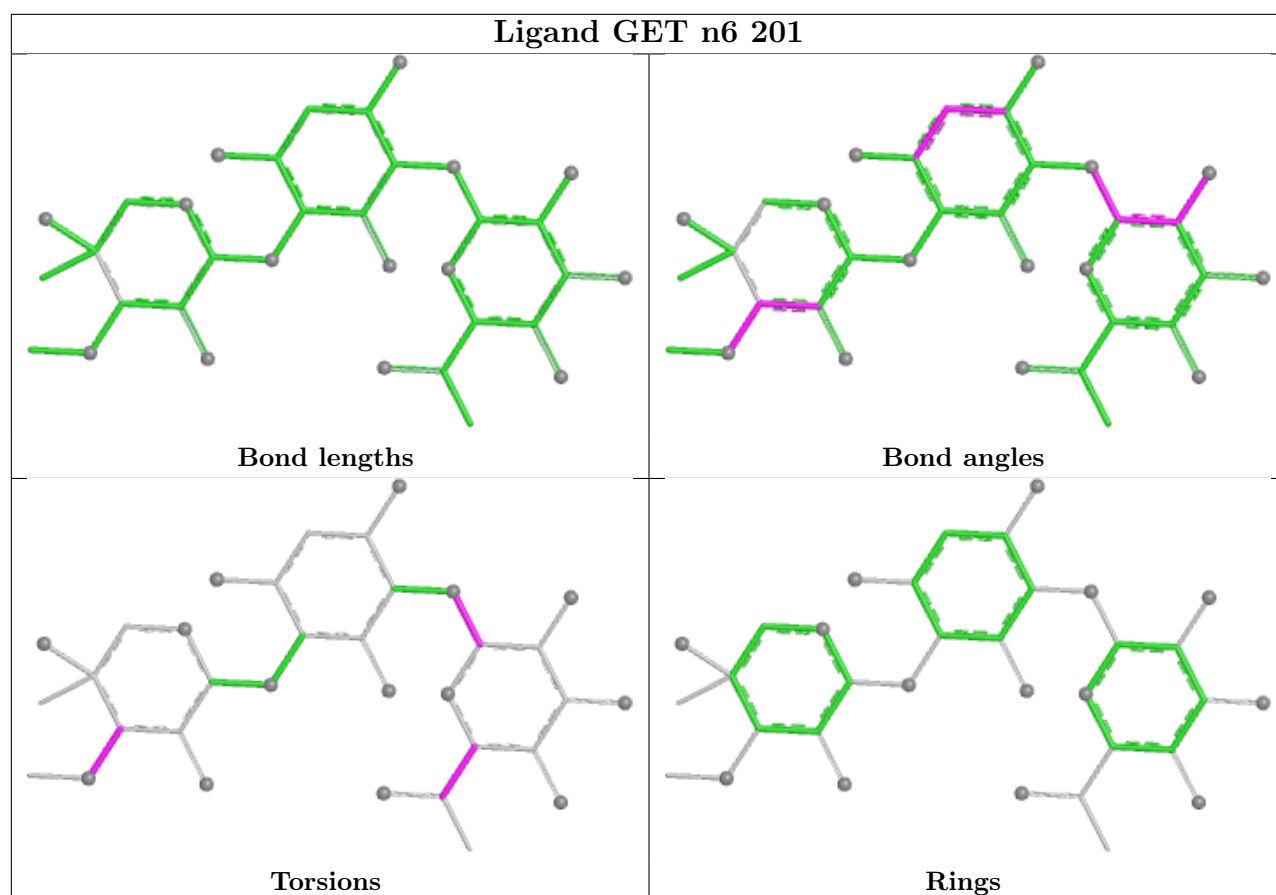


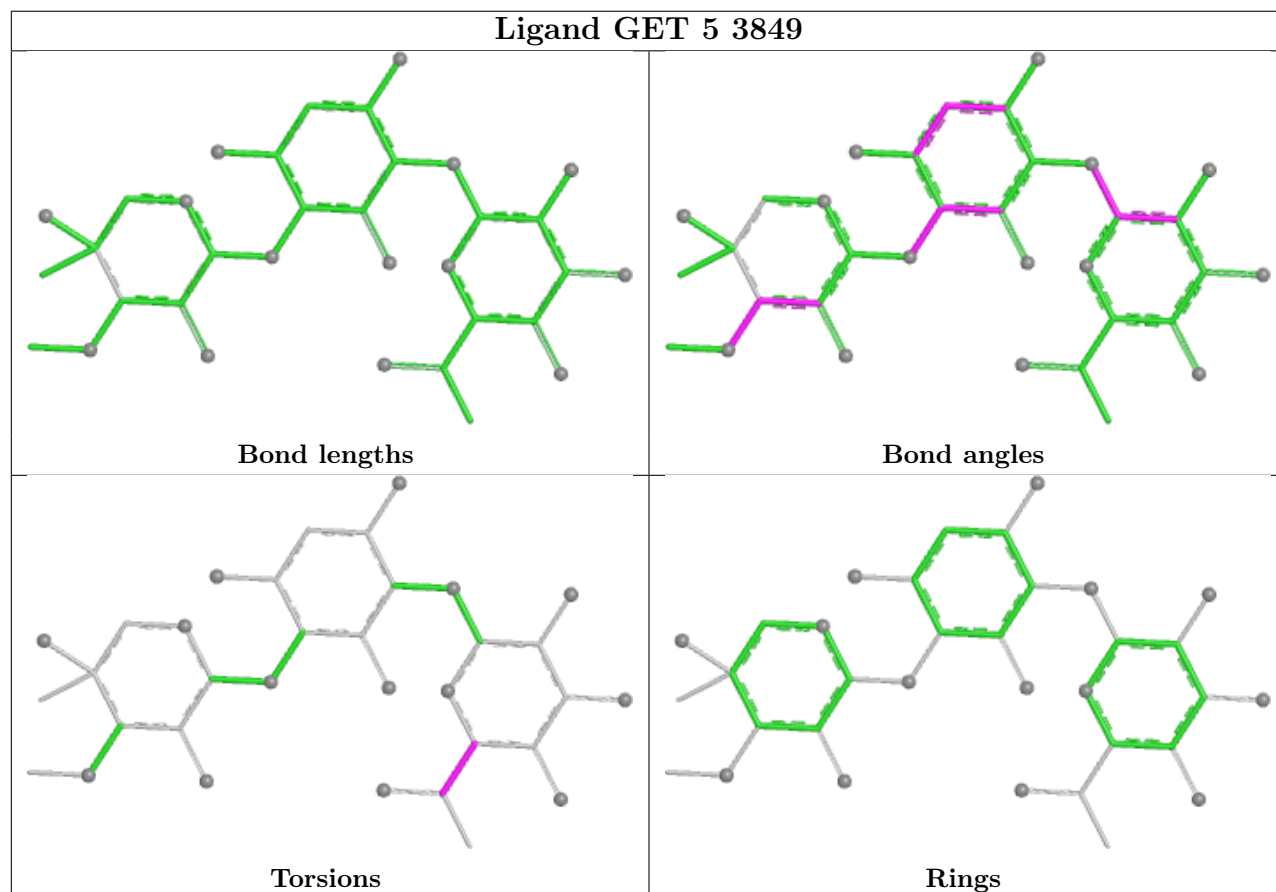
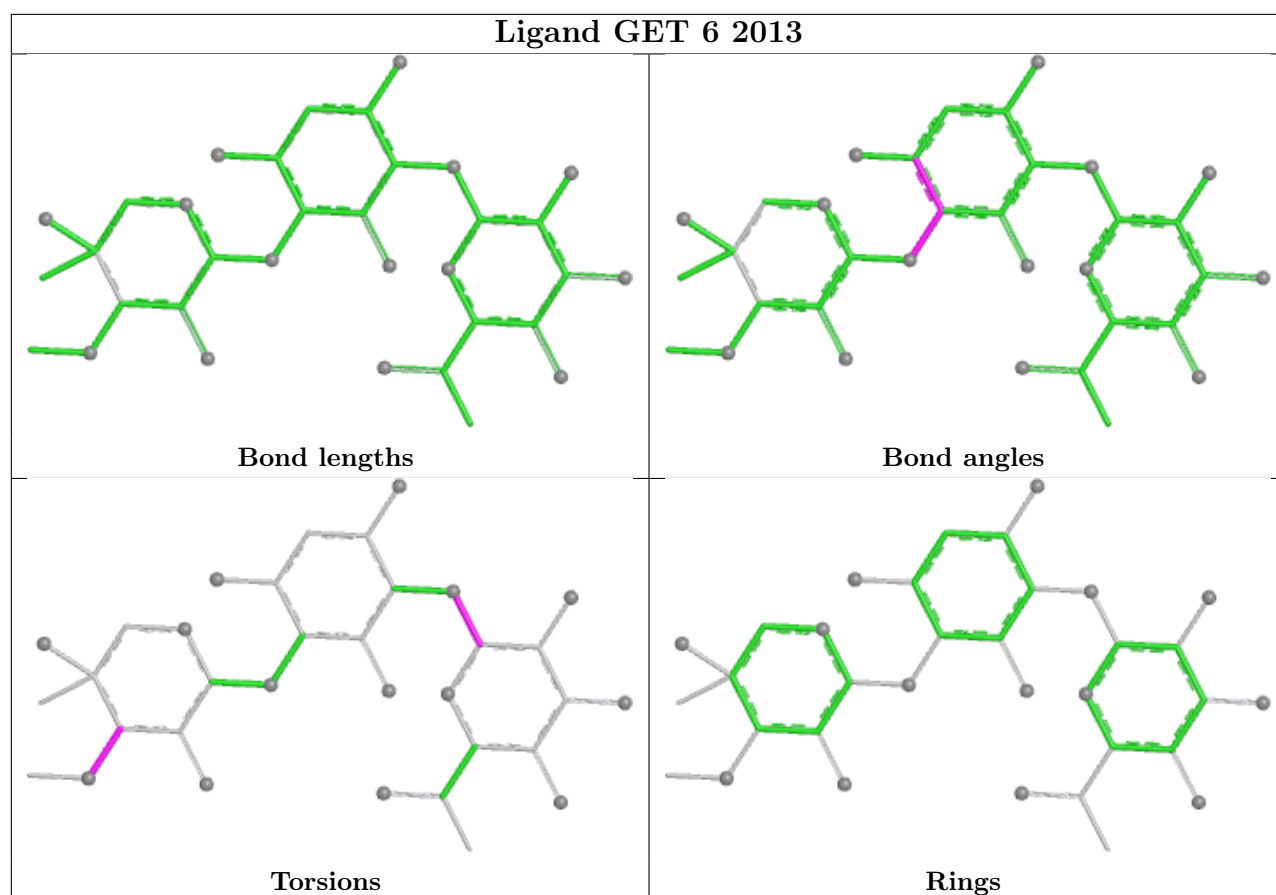


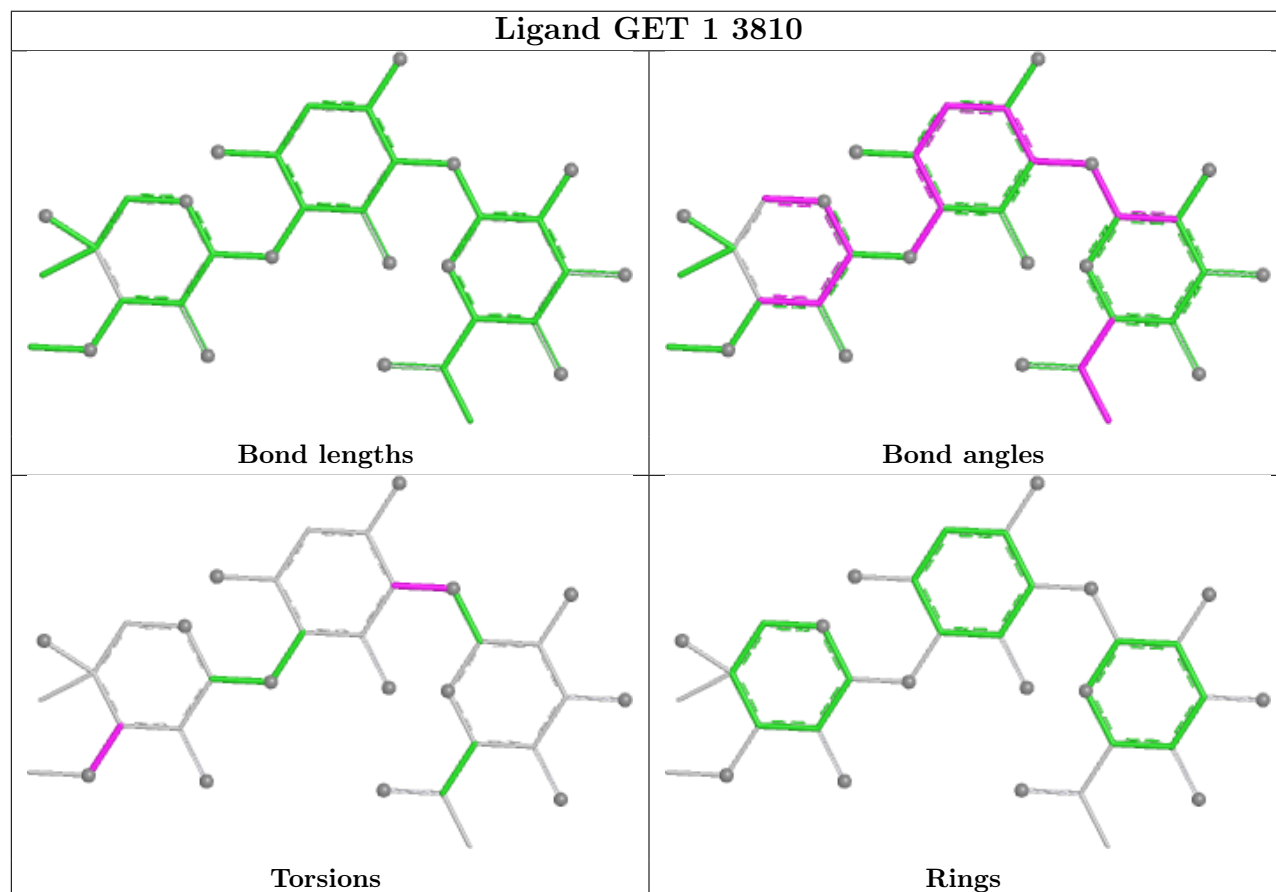
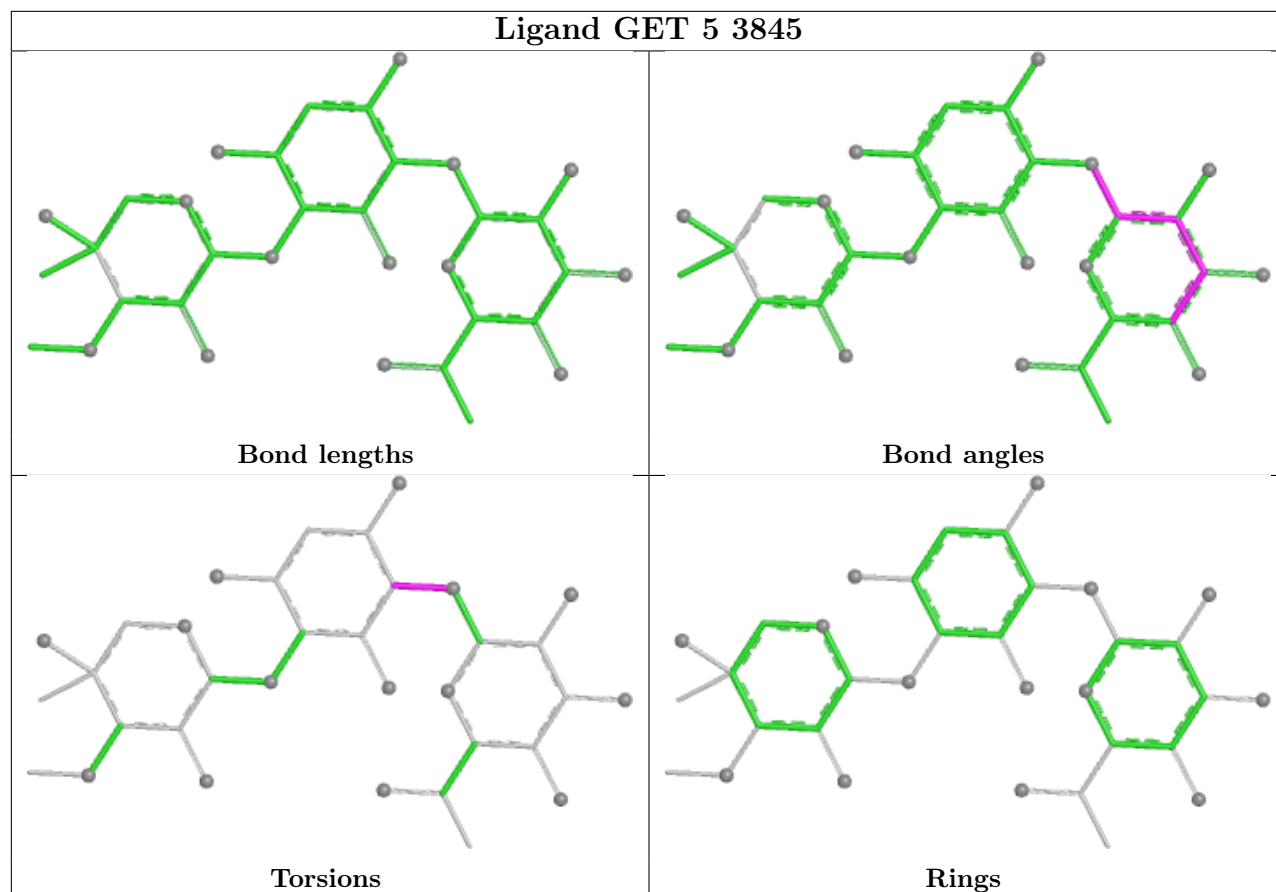


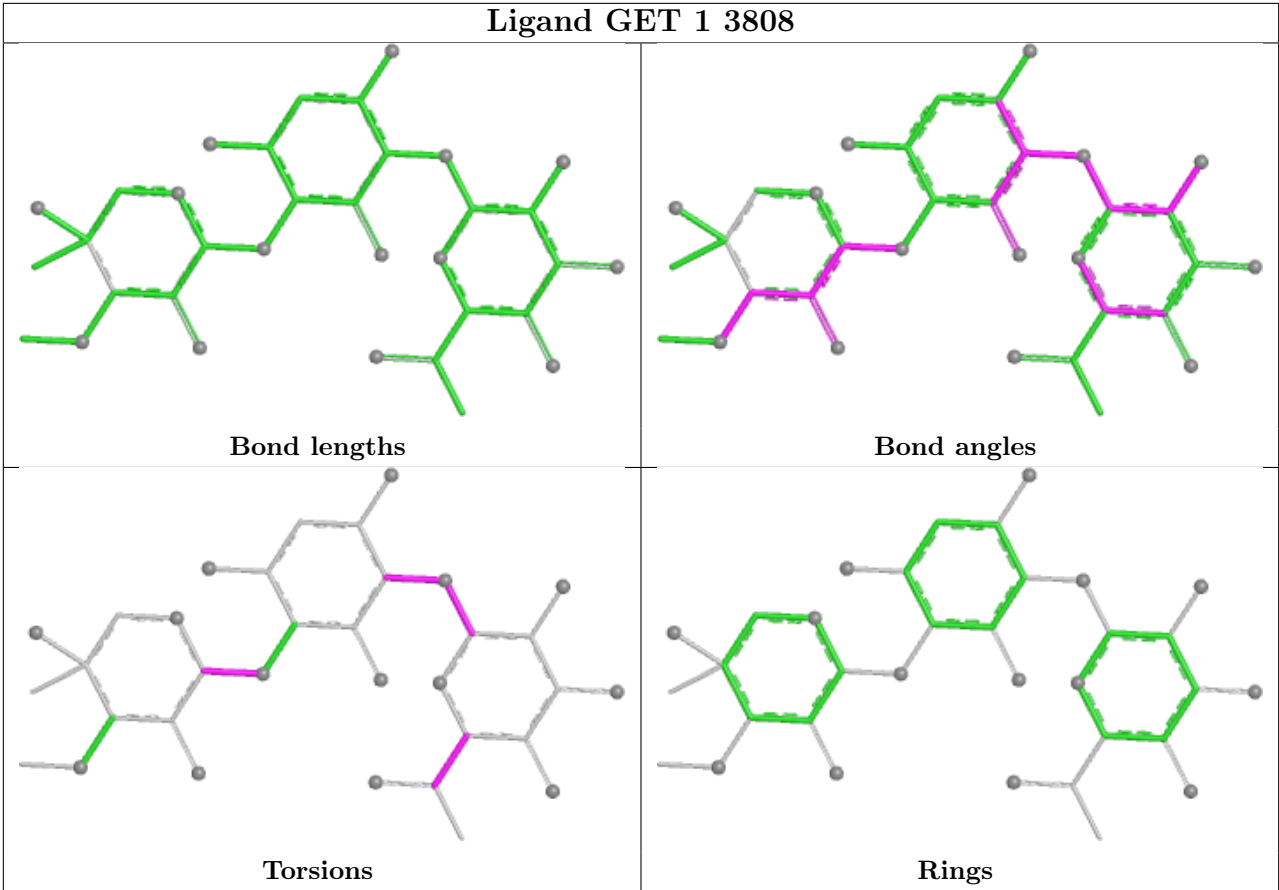












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	3.84

Continued on next page...

Continued from previous page...

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1688/1800 (93%)	-0.17	7 (0%) 88 72	109, 170, 289, 329	0
1	6	1700/1800 (94%)	-0.23	6 (0%) 88 72	101, 171, 254, 295	0
2	S0	206/206 (100%)	0.05	2 (0%) 79 55	173, 208, 229, 240	0
2	s0	206/206 (100%)	-0.10	0 100 100	171, 192, 212, 220	0
3	S1	214/216 (99%)	0.23	6 (2%) 55 34	194, 239, 265, 270	0
3	s1	216/216 (100%)	0.02	5 (2%) 61 38	171, 207, 229, 241	0
4	S2	217/217 (100%)	-0.02	4 (1%) 67 42	147, 178, 199, 213	0
4	s2	217/217 (100%)	-0.13	4 (1%) 67 42	144, 169, 192, 211	0
5	S3	223/223 (100%)	-0.13	1 (0%) 88 72	133, 156, 222, 235	0
5	s3	223/223 (100%)	0.06	4 (1%) 67 42	168, 198, 240, 247	0
6	S4	260/260 (100%)	0.17	8 (3%) 51 32	175, 227, 242, 258	0
6	s4	260/260 (100%)	0.10	4 (1%) 72 46	126, 174, 193, 231	0
7	S5	206/206 (100%)	-0.07	1 (0%) 87 69	153, 185, 199, 206	0
7	s5	206/206 (100%)	0.30	9 (4%) 39 25	199, 217, 245, 248	0
8	S6	226/236 (95%)	0.22	11 (4%) 35 23	166, 211, 269, 303	0
8	s6	218/236 (92%)	-0.11	7 (3%) 50 31	128, 177, 205, 214	0
9	S7	184/185 (99%)	0.26	2 (1%) 78 53	209, 268, 310, 313	0
9	s7	185/185 (100%)	-0.09	0 100 100	166, 204, 230, 235	0
10	S8	188/200 (94%)	0.17	3 (1%) 70 45	160, 200, 261, 281	0
10	s8	188/200 (94%)	0.03	0 100 100	124, 153, 209, 238	0
11	S9	185/185 (100%)	0.14	5 (2%) 56 35	162, 210, 238, 253	0
11	s9	185/185 (100%)	-0.00	2 (1%) 78 53	151, 188, 220, 261	0
12	C0	92/105 (87%)	-0.07	0 100 100	141, 170, 190, 194	0
12	c0	92/105 (87%)	0.36	5 (5%) 31 21	197, 228, 244, 246	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	142/156 (91%)	0.35	2 (1%) 73 48	161, 194, 232, 265	0
13	c1	146/156 (93%)	-0.10	0 100 100	128, 142, 181, 197	0
14	C2	120/143 (83%)	-0.08	0 100 100	212, 235, 252, 258	0
14	c2	124/143 (86%)	-0.03	2 (1%) 70 45	275, 290, 306, 315	0
15	C3	150/150 (100%)	0.06	1 (0%) 84 63	167, 208, 244, 247	0
15	c3	150/150 (100%)	-0.14	0 100 100	138, 161, 184, 191	0
16	C4	127/128 (99%)	0.34	8 (6%) 26 18	147, 201, 230, 236	0
16	c4	128/128 (100%)	0.14	9 (7%) 22 16	136, 198, 216, 223	0
17	C5	122/141 (86%)	-0.07	0 100 100	134, 163, 182, 196	0
17	c5	119/141 (84%)	0.11	2 (1%) 69 43	179, 214, 233, 237	0
18	C6	141/141 (100%)	0.07	2 (1%) 73 48	133, 170, 188, 197	0
18	c6	141/141 (100%)	0.47	6 (4%) 40 25	177, 226, 241, 246	0
19	C7	117/136 (86%)	0.10	2 (1%) 69 43	162, 195, 242, 247	0
19	c7	117/136 (86%)	0.06	0 100 100	190, 206, 225, 229	0
20	C8	145/145 (100%)	-0.15	1 (0%) 84 63	133, 172, 206, 215	0
20	c8	145/145 (100%)	0.01	2 (1%) 73 48	175, 221, 248, 254	0
21	C9	143/143 (100%)	-0.08	0 100 100	138, 163, 181, 198	0
21	c9	143/143 (100%)	0.26	5 (3%) 47 30	197, 234, 253, 259	0
22	D0	105/107 (98%)	-0.06	1 (0%) 79 55	125, 164, 196, 202	0
22	d0	101/107 (94%)	0.30	4 (3%) 42 27	171, 227, 255, 261	0
23	D1	87/87 (100%)	-0.25	0 100 100	182, 200, 226, 237	0
23	d1	87/87 (100%)	-0.29	0 100 100	170, 179, 208, 215	0
24	D2	129/129 (100%)	0.11	2 (1%) 70 45	176, 195, 212, 224	0
24	d2	129/129 (100%)	-0.07	1 (0%) 82 60	142, 159, 172, 186	0
25	D3	144/144 (100%)	0.10	4 (2%) 55 34	130, 139, 163, 169	0
25	d3	144/144 (100%)	0.09	1 (0%) 84 63	122, 131, 147, 164	0
26	D4	134/134 (100%)	0.14	2 (1%) 72 46	186, 230, 242, 250	0
26	d4	134/134 (100%)	0.04	2 (1%) 72 46	146, 190, 211, 227	0
27	D5	70/70 (100%)	0.03	3 (4%) 40 25	175, 202, 214, 217	0
27	d5	69/70 (98%)	0.09	1 (1%) 73 48	223, 244, 254, 258	0
28	D6	97/97 (100%)	0.45	5 (5%) 33 22	145, 167, 227, 233	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.23	5 (5%) 33 22	140, 154, 218, 222	0
29	D7	81/81 (100%)	-0.13	0 100 100	196, 233, 277, 288	0
29	d7	81/81 (100%)	-0.16	0 100 100	161, 181, 221, 225	0
30	D8	63/63 (100%)	-0.25	0 100 100	169, 197, 216, 226	0
30	d8	63/63 (100%)	-0.21	0 100 100	187, 211, 225, 229	0
31	D9	53/53 (100%)	0.24	0 100 100	125, 132, 160, 170	0
31	d9	53/53 (100%)	0.37	0 100 100	180, 191, 224, 249	0
32	E0	60/60 (100%)	-0.07	1 (1%) 69 43	137, 178, 205, 210	0
32	e0	60/60 (100%)	-0.02	1 (1%) 69 43	141, 182, 208, 215	0
33	E1	71/152 (46%)	0.15	2 (2%) 55 34	157, 207, 238, 244	0
33	e1	45/152 (29%)	0.24	0 100 100	198, 263, 280, 283	0
34	SR	318/318 (100%)	-0.36	1 (0%) 90 76	189, 218, 242, 262	0
34	sR	313/318 (98%)	-0.13	1 (0%) 90 76	221, 240, 258, 318	0
35	SM	135/272 (49%)	-0.01	0 100 100	133, 155, 230, 255	0
35	sM	115/272 (42%)	0.23	2 (1%) 69 43	154, 179, 231, 293	0
36	1	3078/3396 (90%)	-0.30	9 (0%) 90 76	82, 131, 236, 350	0
36	5	3127/3396 (92%)	-0.39	5 (0%) 91 80	83, 121, 213, 304	0
37	3	121/121 (100%)	-0.41	0 100 100	92, 159, 191, 204	0
37	7	121/121 (100%)	-0.28	0 100 100	95, 170, 205, 211	0
38	4	158/158 (100%)	-0.26	0 100 100	100, 159, 221, 285	0
38	8	157/158 (99%)	-0.40	0 100 100	96, 132, 183, 217	0
39	L2	252/252 (100%)	0.17	6 (2%) 59 37	104, 154, 189, 209	0
39	l2	252/252 (100%)	-0.01	3 (1%) 76 51	97, 127, 152, 170	0
40	L3	386/386 (100%)	-0.04	13 (3%) 48 30	84, 121, 147, 180	0
40	l3	386/386 (100%)	-0.21	1 (0%) 90 76	83, 111, 131, 164	0
41	L4	361/361 (100%)	-0.02	3 (0%) 82 60	94, 144, 170, 183	0
41	l4	361/361 (100%)	-0.06	7 (1%) 66 42	91, 125, 147, 160	0
42	L5	294/296 (99%)	0.29	20 (6%) 23 17	127, 188, 205, 210	0
42	l5	294/296 (99%)	0.20	12 (4%) 41 26	141, 197, 221, 235	0
43	L6	156/176 (88%)	-0.20	3 (1%) 66 42	109, 127, 147, 163	0
43	l6	157/176 (89%)	-0.23	0 100 100	105, 118, 143, 164	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/223 (99%)	-0.19	0 100 100	95, 123, 164, 193	0
44	l7	223/223 (100%)	-0.21	1 (0%) 88 72	96, 114, 149, 189	0
45	L8	233/233 (100%)	0.18	6 (2%) 57 35	188, 228, 265, 283	0
45	l8	231/233 (99%)	0.00	2 (0%) 81 58	152, 178, 213, 223	0
46	L9	191/191 (100%)	-0.22	0 100 100	113, 131, 146, 172	0
46	l9	190/191 (99%)	-0.22	1 (0%) 87 69	110, 125, 145, 154	0
47	M0	208/221 (94%)	-0.19	0 100 100	97, 115, 162, 181	0
47	m0	209/221 (94%)	-0.12	0 100 100	102, 125, 180, 194	0
48	M1	169/169 (100%)	-0.18	0 100 100	151, 165, 173, 175	0
48	m1	169/169 (100%)	-0.01	1 (0%) 85 66	171, 191, 201, 204	0
49	M3	193/194 (99%)	0.01	2 (1%) 79 55	109, 185, 219, 232	0
49	m3	194/194 (100%)	0.17	5 (2%) 57 35	102, 156, 197, 209	0
50	M4	136/137 (99%)	-0.23	0 100 100	118, 129, 144, 153	0
50	m4	137/137 (100%)	-0.20	0 100 100	113, 121, 146, 176	0
51	M5	203/203 (100%)	0.49	8 (3%) 43 28	117, 163, 193, 205	0
51	m5	203/203 (100%)	0.18	2 (0%) 79 55	106, 133, 154, 163	0
52	M6	197/197 (100%)	-0.18	0 100 100	83, 97, 140, 150	0
52	m6	197/197 (100%)	-0.14	1 (0%) 87 69	85, 97, 139, 147	0
53	M7	183/184 (99%)	-0.21	1 (0%) 87 69	92, 108, 159, 196	0
53	m7	175/184 (95%)	-0.12	0 100 100	91, 104, 140, 157	0
54	M8	185/185 (100%)	-0.01	0 100 100	103, 149, 173, 180	0
54	m8	185/185 (100%)	-0.04	2 (1%) 78 53	102, 131, 147, 155	0
55	M9	188/188 (100%)	0.19	5 (2%) 56 35	137, 167, 298, 318	0
55	m9	183/188 (97%)	-0.00	2 (1%) 78 53	114, 135, 212, 223	0
56	N0	170/172 (98%)	-0.15	0 100 100	104, 121, 143, 156	0
56	n0	172/172 (100%)	-0.19	2 (1%) 76 51	100, 116, 137, 154	0
57	N1	159/159 (100%)	0.17	3 (1%) 66 42	100, 136, 196, 205	0
57	n1	159/159 (100%)	0.15	6 (3%) 44 28	110, 134, 182, 186	0
58	N2	98/98 (100%)	-0.02	2 (2%) 65 41	186, 205, 216, 219	0
58	n2	98/98 (100%)	0.06	2 (2%) 65 41	159, 174, 187, 190	0
59	N3	135/135 (100%)	-0.09	1 (0%) 84 63	95, 117, 129, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	134/135 (99%)	-0.30	0 100 100	89, 104, 116, 128	0
60	N4	122/155 (78%)	0.16	2 (1%) 70 45	123, 163, 280, 283	0
60	n4	118/155 (76%)	-0.10	0 100 100	103, 136, 235, 242	0
61	N5	121/121 (100%)	0.13	3 (2%) 58 36	143, 176, 210, 245	0
61	n5	120/121 (99%)	0.06	0 100 100	119, 143, 165, 189	0
62	N6	126/126 (100%)	-0.09	2 (1%) 70 45	130, 150, 177, 192	0
62	n6	124/126 (98%)	-0.29	0 100 100	113, 138, 166, 177	0
63	N7	135/135 (100%)	0.37	3 (2%) 62 39	209, 238, 257, 269	0
63	n7	135/135 (100%)	-0.08	0 100 100	155, 177, 193, 203	0
64	N8	148/148 (100%)	0.19	3 (2%) 65 41	92, 165, 197, 210	0
64	n8	148/148 (100%)	0.11	1 (0%) 84 63	92, 144, 169, 173	0
65	N9	58/58 (100%)	0.05	0 100 100	93, 154, 197, 203	0
65	n9	58/58 (100%)	0.63	3 (5%) 33 22	96, 150, 197, 206	0
66	O0	97/100 (97%)	-0.08	0 100 100	197, 217, 237, 241	0
66	o0	100/100 (100%)	-0.29	0 100 100	151, 166, 186, 197	0
67	O1	109/109 (100%)	0.07	1 (0%) 81 58	116, 141, 173, 183	0
67	o1	109/109 (100%)	-0.07	1 (0%) 81 58	105, 132, 166, 186	0
68	O2	127/127 (100%)	0.09	3 (2%) 59 37	89, 118, 134, 153	0
68	o2	127/127 (100%)	-0.05	0 100 100	88, 111, 124, 154	0
69	O3	106/106 (100%)	-0.05	1 (0%) 81 58	88, 103, 119, 122	0
69	o3	106/106 (100%)	-0.07	0 100 100	89, 101, 116, 123	0
70	O4	112/112 (100%)	0.62	12 (10%) 11 12	138, 186, 249, 258	0
70	o4	112/112 (100%)	0.31	7 (6%) 26 18	113, 144, 201, 211	0
71	O5	119/119 (100%)	0.12	3 (2%) 58 36	162, 182, 210, 218	0
71	o5	119/119 (100%)	-0.00	2 (1%) 69 43	129, 152, 174, 182	0
72	O6	99/99 (100%)	0.28	1 (1%) 79 55	170, 194, 221, 241	0
72	o6	99/99 (100%)	-0.05	0 100 100	150, 162, 186, 207	0
73	O7	84/84 (100%)	0.02	0 100 100	103, 129, 178, 189	0
73	o7	82/84 (97%)	0.18	1 (1%) 76 51	94, 111, 140, 153	0
74	O8	77/77 (100%)	0.01	1 (1%) 75 50	194, 216, 228, 229	0
74	o8	77/77 (100%)	-0.08	0 100 100	154, 174, 185, 187	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	49/50 (98%)	0.60	2 (4%) 41 26	122, 135, 142, 146	0
75	o9	50/50 (100%)	0.32	2 (4%) 42 27	106, 117, 127, 129	0
76	Q0	52/52 (100%)	-0.24	1 (1%) 66 42	100, 107, 147, 156	0
76	q0	52/52 (100%)	-0.10	0 100 100	101, 111, 138, 145	0
77	Q1	25/25 (100%)	0.38	0 100 100	113, 125, 130, 132	0
77	q1	25/25 (100%)	0.43	0 100 100	113, 121, 125, 126	0
78	Q2	105/105 (100%)	-0.13	0 100 100	113, 143, 167, 178	0
78	q2	105/105 (100%)	-0.18	2 (1%) 66 42	109, 144, 170, 189	0
79	Q3	91/91 (100%)	0.10	0 100 100	118, 158, 189, 203	0
79	q3	91/91 (100%)	-0.15	1 (1%) 78 53	102, 129, 153, 167	0
80	p0	138/312 (44%)	-0.01	1 (0%) 84 63	202, 229, 270, 271	0
All	All	32690/34558 (94%)	-0.08	373 (1%) 78 53	82, 159, 244, 350	0

The worst 5 of 373 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	C4	133	ARG	6.7
42	L5	38	THR	6.6
42	l5	69	ILE	5.9
42	L5	31	TYR	5.8
63	N7	37	PRO	5.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	2	1967	1/1	0.03	0.19	175,175,175,175	0
81	MG	1	3704	1/1	0.03	0.16	195,195,195,195	0
81	MG	4	211	1/1	0.09	0.27	142,142,142,142	0
81	MG	6	2000	1/1	0.17	0.29	123,123,123,123	0
81	MG	2	1965	1/1	0.18	0.18	162,162,162,162	0
81	MG	2	1970	1/1	0.19	0.18	145,145,145,145	0
81	MG	2	1988	1/1	0.20	0.18	202,202,202,202	0
81	MG	S1	301	1/1	0.27	0.19	193,193,193,193	0
81	MG	2	1985	1/1	0.27	0.29	133,133,133,133	0
81	MG	1	3781	1/1	0.28	0.30	137,137,137,137	0
81	MG	6	1918	1/1	0.30	0.39	123,123,123,123	0
81	MG	4	213	1/1	0.31	0.14	178,178,178,178	0
81	MG	1	3807	1/1	0.32	0.24	173,173,173,173	0
81	MG	2	1984	1/1	0.34	0.14	192,192,192,192	0
81	MG	5	3835	1/1	0.36	0.20	157,157,157,157	0
81	MG	1	3802	1/1	0.37	0.25	133,133,133,133	0
81	MG	5	3648	1/1	0.40	0.15	147,147,147,147	0
81	MG	1	3777	1/1	0.46	0.15	117,117,117,117	0
81	MG	2	1915	1/1	0.47	0.27	125,125,125,125	0
81	MG	5	3842	1/1	0.47	0.28	105,105,105,105	0
81	MG	5	3810	1/1	0.48	0.24	115,115,115,115	0
81	MG	4	216	1/1	0.48	0.12	143,143,143,143	0
81	MG	1	3681	1/1	0.48	0.26	128,128,128,128	0
81	MG	8	212	1/1	0.48	0.14	110,110,110,110	0
81	MG	5	3820	1/1	0.49	0.35	123,123,123,123	0
81	MG	6	1978	1/1	0.49	0.26	158,158,158,158	0
81	MG	5	3673	1/1	0.50	0.18	132,132,132,132	0
81	MG	2	1931	1/1	0.50	0.23	140,140,140,140	0
81	MG	5	3812	1/1	0.50	0.33	90,90,90,90	0
81	MG	5	3818	1/1	0.50	0.21	129,129,129,129	0
81	MG	1	3543	1/1	0.51	0.22	134,134,134,134	0
81	MG	5	3603	1/1	0.51	0.25	143,143,143,143	0
81	MG	2	1986	1/1	0.51	0.22	139,139,139,139	0
81	MG	6	1959	1/1	0.51	0.23	165,165,165,165	0
81	MG	5	3805	1/1	0.51	0.16	161,161,161,161	0
81	MG	1	3423	1/1	0.51	0.21	159,159,159,159	0
81	MG	5	3794	1/1	0.52	0.16	122,122,122,122	0
81	MG	5	3804	1/1	0.52	0.15	168,168,168,168	0
81	MG	S8	301	1/1	0.52	0.21	161,161,161,161	0
81	MG	1	3783	1/1	0.52	0.17	140,140,140,140	0
81	MG	7	204	1/1	0.52	0.21	171,171,171,171	0
81	MG	6	1939	1/1	0.52	0.16	156,156,156,156	0
81	MG	O9	101	1/1	0.53	0.14	124,124,124,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	2	1911	1/1	0.53	0.36	150,150,150,150	0
81	MG	1	3784	1/1	0.53	0.20	146,146,146,146	0
81	MG	3	205	1/1	0.53	0.23	149,149,149,149	0
81	MG	6	1999	1/1	0.54	0.12	206,206,206,206	0
81	MG	1	3540	1/1	0.54	0.23	115,115,115,115	0
81	MG	5	3811	1/1	0.54	0.28	115,115,115,115	0
81	MG	5	3559	1/1	0.54	0.16	139,139,139,139	0
81	MG	7	208	1/1	0.54	0.16	132,132,132,132	0
81	MG	4	215	1/1	0.54	0.19	133,133,133,133	0
81	MG	5	3777	1/1	0.55	0.26	91,91,91,91	0
81	MG	6	2006	1/1	0.55	0.37	126,126,126,126	0
81	MG	2	1966	1/1	0.56	0.18	152,152,152,152	0
81	MG	1	3795	1/1	0.56	0.21	133,133,133,133	0
81	MG	6	1995	1/1	0.56	0.25	157,157,157,157	0
81	MG	2	1979	1/1	0.57	0.18	147,147,147,147	0
81	MG	2	1916	1/1	0.57	0.18	158,158,158,158	0
81	MG	6	1903	1/1	0.57	0.28	128,128,128,128	0
81	MG	1	3485	1/1	0.57	0.11	143,143,143,143	0
81	MG	6	1931	1/1	0.57	0.12	169,169,169,169	0
81	MG	1	3789	1/1	0.58	0.34	128,128,128,128	0
81	MG	1	3691	1/1	0.58	0.17	152,152,152,152	0
81	MG	4	208	1/1	0.58	0.32	130,130,130,130	0
81	MG	1	3799	1/1	0.58	0.25	112,112,112,112	0
81	MG	1	3530	1/1	0.58	0.23	111,111,111,111	0
81	MG	1	3806	1/1	0.58	0.16	141,141,141,141	0
81	MG	1	3689	1/1	0.59	0.14	141,141,141,141	0
81	MG	6	1952	1/1	0.59	0.15	175,175,175,175	0
81	MG	5	3551	1/1	0.59	0.17	105,105,105,105	0
81	MG	1	3804	1/1	0.59	0.13	128,128,128,128	0
81	MG	5	3829	1/1	0.59	0.17	124,124,124,124	0
81	MG	o3	203	1/1	0.59	0.32	99,99,99,99	0
81	MG	6	1998	1/1	0.60	0.21	124,124,124,124	0
81	MG	4	202	1/1	0.60	0.25	131,131,131,131	0
81	MG	2	2008	1/1	0.60	0.29	117,117,117,117	0
81	MG	2	1950	1/1	0.60	0.21	126,126,126,126	0
81	MG	6	2008	1/1	0.60	0.17	111,111,111,111	0
81	MG	5	3830	1/1	0.60	0.21	131,131,131,131	0
81	MG	1	3763	1/1	0.61	0.23	118,118,118,118	0
81	MG	5	3647	1/1	0.61	0.16	143,143,143,143	0
81	MG	d3	202	1/1	0.61	0.31	125,125,125,125	0
81	MG	1	3769	1/1	0.61	0.20	115,115,115,115	0
81	MG	5	3717	1/1	0.61	0.29	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3728	1/1	0.61	0.19	98,98,98,98	0
81	MG	5	3750	1/1	0.61	0.29	99,99,99,99	0
81	MG	SM	301	1/1	0.61	0.22	126,126,126,126	0
81	MG	2	1980	1/1	0.62	0.11	202,202,202,202	1
81	MG	1	3425	1/1	0.62	0.30	122,122,122,122	0
81	MG	1	3788	1/1	0.62	0.23	140,140,140,140	0
81	MG	5	3752	1/1	0.62	0.12	164,164,164,164	0
81	MG	6	1958	1/1	0.62	0.20	120,120,120,120	0
81	MG	5	3793	1/1	0.62	0.22	128,128,128,128	0
81	MG	5	3611	1/1	0.62	0.29	99,99,99,99	0
81	MG	6	2004	1/1	0.62	0.23	124,124,124,124	0
81	MG	1	3724	1/1	0.62	0.29	125,125,125,125	0
81	MG	1	3745	1/1	0.62	0.26	133,133,133,133	0
81	MG	5	3677	1/1	0.62	0.36	112,112,112,112	0
81	MG	6	2003	1/1	0.63	0.17	119,119,119,119	0
81	MG	1	3780	1/1	0.63	0.20	104,104,104,104	0
81	MG	4	212	1/1	0.63	0.20	142,142,142,142	0
81	MG	6	1980	1/1	0.63	0.19	106,106,106,106	0
81	MG	C8	201	1/1	0.63	0.15	161,161,161,161	0
81	MG	2	1921	1/1	0.63	0.49	125,125,125,125	0
81	MG	5	3807	1/1	0.63	0.22	145,145,145,145	0
81	MG	5	3727	1/1	0.63	0.36	103,103,103,103	0
81	MG	8	205	1/1	0.63	0.19	102,102,102,102	0
81	MG	1	3429	1/1	0.63	0.23	136,136,136,136	0
81	MG	1	3744	1/1	0.63	0.27	111,111,111,111	0
81	MG	5	3722	1/1	0.64	0.23	84,84,84,84	0
81	MG	2	1953	1/1	0.64	0.20	151,151,151,151	0
81	MG	5	3597	1/1	0.64	0.12	151,151,151,151	0
81	MG	5	3667	1/1	0.64	0.21	119,119,119,119	0
81	MG	5	3598	1/1	0.64	0.20	137,137,137,137	0
81	MG	1	3720	1/1	0.64	0.40	122,122,122,122	0
81	MG	5	3706	1/1	0.64	0.29	93,93,93,93	0
81	MG	2	1907	1/1	0.64	0.21	145,145,145,145	0
81	MG	5	3823	1/1	0.64	0.28	103,103,103,103	0
81	MG	5	3789	1/1	0.65	0.14	102,102,102,102	0
81	MG	6	1954	1/1	0.65	0.19	176,176,176,176	0
81	MG	2	1935	1/1	0.65	0.19	147,147,147,147	0
81	MG	6	1985	1/1	0.65	0.20	127,127,127,127	0
81	MG	5	3693	1/1	0.65	0.46	95,95,95,95	0
81	MG	1	3486	1/1	0.65	0.11	151,151,151,151	0
81	MG	5	3666	1/1	0.65	0.30	102,102,102,102	0
81	MG	1	3542	1/1	0.66	0.26	127,127,127,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	2	1952	1/1	0.66	0.31	145,145,145,145	0
81	MG	5	3669	1/1	0.66	0.21	103,103,103,103	0
81	MG	2	1996	1/1	0.66	0.22	103,103,103,103	0
81	MG	5	3514	1/1	0.66	0.32	109,109,109,109	0
81	MG	5	3720	1/1	0.67	0.23	119,119,119,119	0
81	MG	1	3662	1/1	0.67	0.22	114,114,114,114	0
81	MG	5	3636	1/1	0.67	0.15	109,109,109,109	0
81	MG	1	3693	1/1	0.67	0.22	116,116,116,116	0
81	MG	1	3674	1/1	0.67	0.16	115,115,115,115	0
81	MG	5	3467	1/1	0.67	0.29	106,106,106,106	0
81	MG	1	3782	1/1	0.67	0.16	123,123,123,123	0
81	MG	1	3733	1/1	0.68	0.09	110,110,110,110	0
81	MG	5	3519	1/1	0.68	0.18	122,122,122,122	0
81	MG	1	3673	1/1	0.68	0.35	110,110,110,110	0
81	MG	1	3452	1/1	0.68	0.30	93,93,93,93	0
81	MG	5	3774	1/1	0.68	0.17	98,98,98,98	0
81	MG	5	3712	1/1	0.68	0.12	104,104,104,104	0
81	MG	6	2010	1/1	0.68	0.21	109,109,109,109	0
81	MG	1	3761	1/1	0.68	0.31	96,96,96,96	0
81	MG	2	1983	1/1	0.68	0.21	144,144,144,144	0
81	MG	1	3712	1/1	0.69	0.25	125,125,125,125	0
81	MG	5	3438	1/1	0.69	0.27	117,117,117,117	0
81	MG	5	3637	1/1	0.69	0.09	122,122,122,122	0
81	MG	5	3561	1/1	0.69	0.19	137,137,137,137	0
81	MG	1	3653	1/1	0.69	0.30	98,98,98,98	0
81	MG	2	2007	1/1	0.69	0.35	126,126,126,126	0
81	MG	5	3825	1/1	0.69	0.23	107,107,107,107	0
81	MG	1	3513	1/1	0.69	0.14	139,139,139,139	0
81	MG	5	3495	1/1	0.70	0.17	133,133,133,133	0
81	MG	2	1959	1/1	0.70	0.17	151,151,151,151	0
81	MG	1	3426	1/1	0.70	0.20	126,126,126,126	0
81	MG	1	3716	1/1	0.70	0.15	104,104,104,104	0
81	MG	4	223	1/1	0.70	0.12	99,99,99,99	0
81	MG	2	1995	1/1	0.70	0.21	123,123,123,123	0
81	MG	5	3564	1/1	0.70	0.21	109,109,109,109	0
81	MG	1	3671	1/1	0.70	0.20	118,118,118,118	0
81	MG	1	3487	1/1	0.70	0.32	105,105,105,105	0
81	MG	6	1966	1/1	0.71	0.16	140,140,140,140	0
81	MG	1	3565	1/1	0.71	0.35	86,86,86,86	0
81	MG	1	3579	1/1	0.71	0.16	120,120,120,120	0
81	MG	1	3743	1/1	0.71	0.17	147,147,147,147	0
81	MG	1	3505	1/1	0.71	0.30	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3549	1/1	0.72	0.18	83,83,83,83	0
81	MG	6	1946	1/1	0.72	0.18	163,163,163,163	0
81	MG	6	1947	1/1	0.72	0.11	165,165,165,165	0
81	MG	5	3814	1/1	0.72	0.33	109,109,109,109	0
81	MG	6	1901	1/1	0.72	0.24	122,122,122,122	0
81	MG	1	3732	1/1	0.72	0.29	91,91,91,91	0
81	MG	5	3758	1/1	0.72	0.25	100,100,100,100	0
81	MG	5	3762	1/1	0.72	0.19	100,100,100,100	0
81	MG	5	3769	1/1	0.72	0.32	106,106,106,106	0
81	MG	5	3426	1/1	0.72	0.15	81,81,81,81	0
81	MG	2	1940	1/1	0.72	0.34	119,119,119,119	0
81	MG	5	3684	1/1	0.72	0.11	125,125,125,125	0
81	MG	6	1929	1/1	0.72	0.23	139,139,139,139	0
81	MG	6	2002	1/1	0.72	0.22	121,121,121,121	0
81	MG	1	3723	1/1	0.72	0.10	119,119,119,119	0
81	MG	2	1927	1/1	0.72	0.20	140,140,140,140	0
81	MG	5	3643	1/1	0.72	0.17	104,104,104,104	0
81	MG	q2	503	1/1	0.72	0.31	106,106,106,106	0
81	MG	6	2005	1/1	0.73	0.26	101,101,101,101	0
81	MG	2	1951	1/1	0.73	0.24	127,127,127,127	0
81	MG	5	3792	1/1	0.73	0.13	108,108,108,108	0
81	MG	1	3711	1/1	0.73	0.23	116,116,116,116	0
81	MG	2	1993	1/1	0.73	0.44	121,121,121,121	0
81	MG	c3	200	1/1	0.73	0.27	127,127,127,127	0
81	MG	5	3836	1/1	0.73	0.17	128,128,128,128	0
81	MG	1	3798	1/1	0.73	0.25	85,85,85,85	0
81	MG	1	3762	1/1	0.73	0.23	90,90,90,90	0
81	MG	7	205	1/1	0.73	0.14	154,154,154,154	0
81	MG	6	1915	1/1	0.73	0.12	133,133,133,133	0
81	MG	1	3584	1/1	0.73	0.27	109,109,109,109	0
81	MG	1	3553	1/1	0.73	0.24	97,97,97,97	0
81	MG	5	3623	1/1	0.73	0.19	104,104,104,104	0
81	MG	1	3786	1/1	0.73	0.19	123,123,123,123	0
81	MG	1	3771	1/1	0.74	0.41	82,82,82,82	0
81	MG	1	3439	1/1	0.74	0.22	117,117,117,117	0
81	MG	1	3517	1/1	0.74	0.32	124,124,124,124	0
81	MG	2	2009	1/1	0.74	0.17	110,110,110,110	0
81	MG	1	3680	1/1	0.74	0.07	148,148,148,148	0
81	MG	4	219	1/1	0.74	0.13	117,117,117,117	0
81	MG	s8	302	1/1	0.74	0.45	112,112,112,112	0
81	MG	5	3700	1/1	0.74	0.14	90,90,90,90	0
81	MG	5	3702	1/1	0.74	0.25	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3518	1/1	0.74	0.15	128,128,128,128	0
81	MG	1	3668	1/1	0.75	0.21	131,131,131,131	0
81	MG	4	206	1/1	0.75	0.16	97,97,97,97	0
81	MG	5	3799	1/1	0.75	0.29	91,91,91,91	0
81	MG	5	3744	1/1	0.75	0.27	94,94,94,94	0
81	MG	1	3746	1/1	0.75	0.16	118,118,118,118	0
81	MG	2	1937	1/1	0.75	0.20	120,120,120,120	0
81	MG	2	2003	1/1	0.75	0.15	141,141,141,141	0
81	MG	5	3658	1/1	0.75	0.07	117,117,117,117	0
81	MG	1	3441	1/1	0.75	0.18	108,108,108,108	0
81	MG	3	202	1/1	0.75	0.15	133,133,133,133	0
81	MG	2	1957	1/1	0.75	0.21	126,126,126,126	0
81	MG	l3	403	1/1	0.75	0.25	106,106,106,106	0
81	MG	l7	302	1/1	0.75	0.14	93,93,93,93	0
81	MG	n4	201	1/1	0.75	0.27	114,114,114,114	0
81	MG	6	2001	1/1	0.75	0.18	168,168,168,168	0
81	MG	5	3725	1/1	0.75	0.20	100,100,100,100	0
81	MG	2	1962	1/1	0.76	0.12	164,164,164,164	0
81	MG	1	3474	1/1	0.76	0.15	136,136,136,136	0
81	MG	L2	301	1/1	0.76	0.17	97,97,97,97	0
81	MG	O6	201	1/1	0.76	0.14	167,167,167,167	0
81	MG	1	3587	1/1	0.76	0.30	123,123,123,123	0
81	MG	5	3463	1/1	0.76	0.30	99,99,99,99	0
81	MG	5	3838	1/1	0.76	0.23	101,101,101,101	0
81	MG	1	3767	1/1	0.76	0.29	88,88,88,88	0
81	MG	6	1993	1/1	0.76	0.12	142,142,142,142	0
81	MG	5	3736	1/1	0.76	0.13	157,157,157,157	0
81	MG	5	3501	1/1	0.76	0.19	96,96,96,96	0
81	MG	5	3682	1/1	0.76	0.23	95,95,95,95	0
81	MG	1	3639	1/1	0.76	0.10	134,134,134,134	0
81	MG	5	3634	1/1	0.76	0.18	102,102,102,102	0
81	MG	6	1997	1/1	0.76	0.22	111,111,111,111	0
81	MG	5	3764	1/1	0.76	0.14	114,114,114,114	0
81	MG	1	3805	1/1	0.76	0.09	154,154,154,154	0
81	MG	5	3821	1/1	0.76	0.17	92,92,92,92	0
81	MG	2	1934	1/1	0.77	0.21	128,128,128,128	0
81	MG	1	3659	1/1	0.77	0.10	87,87,87,87	0
81	MG	5	3708	1/1	0.77	0.18	134,134,134,134	0
81	MG	6	1919	1/1	0.77	0.15	123,123,123,123	0
81	MG	1	3582	1/1	0.77	0.18	100,100,100,100	0
81	MG	1	3525	1/1	0.77	0.12	161,161,161,161	0
81	MG	4	225	1/1	0.77	0.11	156,156,156,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3819	1/1	0.77	0.24	90,90,90,90	0
81	MG	2	1969	1/1	0.77	0.20	140,140,140,140	0
81	MG	5	3516	1/1	0.77	0.14	99,99,99,99	0
81	MG	1	3731	1/1	0.77	0.25	105,105,105,105	0
81	MG	1	3635	1/1	0.77	0.18	93,93,93,93	0
81	MG	1	3764	1/1	0.77	0.24	110,110,110,110	0
81	MG	o5	201	1/1	0.77	0.20	120,120,120,120	0
81	MG	1	3473	1/1	0.77	0.17	131,131,131,131	0
81	MG	4	218	1/1	0.78	0.25	134,134,134,134	0
81	MG	5	3493	1/1	0.78	0.20	102,102,102,102	0
81	MG	5	3579	1/1	0.78	0.17	102,102,102,102	0
81	MG	6	1910	1/1	0.78	0.25	94,94,94,94	0
81	MG	1	3609	1/1	0.78	0.32	98,98,98,98	0
81	MG	5	3672	1/1	0.78	0.13	119,119,119,119	0
81	MG	5	3796	1/1	0.78	0.23	124,124,124,124	0
81	MG	5	3506	1/1	0.78	0.31	84,84,84,84	0
81	MG	1	3670	1/1	0.78	0.06	127,127,127,127	0
81	MG	5	3618	1/1	0.78	0.15	123,123,123,123	0
81	MG	5	3745	1/1	0.78	0.19	80,80,80,80	0
81	MG	2	1904	1/1	0.78	0.19	158,158,158,158	0
81	MG	6	1961	1/1	0.78	0.07	197,197,197,197	0
81	MG	5	3753	1/1	0.78	0.27	117,117,117,117	0
81	MG	5	3757	1/1	0.78	0.15	115,115,115,115	0
81	MG	1	3773	1/1	0.78	0.28	89,89,89,89	0
81	MG	1	3776	1/1	0.78	0.22	101,101,101,101	0
81	MG	1	3801	1/1	0.78	0.20	114,114,114,114	0
81	MG	2	1941	1/1	0.78	0.21	126,126,126,126	0
83	ZN	d7	101	1/1	0.78	0.08	247,247,247,247	0
81	MG	L2	303	1/1	0.79	0.23	115,115,115,115	0
81	MG	5	3689	1/1	0.79	0.33	89,89,89,89	0
81	MG	5	3490	1/1	0.79	0.24	102,102,102,102	0
81	MG	O2	202	1/1	0.79	0.27	84,84,84,84	0
81	MG	2	1954	1/1	0.79	0.12	128,128,128,128	0
81	MG	5	3703	1/1	0.79	0.14	110,110,110,110	0
81	MG	1	3757	1/1	0.79	0.16	123,123,123,123	0
81	MG	6	1957	1/1	0.79	0.12	175,175,175,175	0
81	MG	5	3710	1/1	0.79	0.14	114,114,114,114	0
81	MG	1	3518	1/1	0.79	0.16	126,126,126,126	0
81	MG	1	3634	1/1	0.79	0.19	74,74,74,74	0
81	MG	6	1909	1/1	0.79	0.28	120,120,120,120	0
81	MG	1	3727	1/1	0.79	0.12	123,123,123,123	0
81	MG	5	3529	1/1	0.79	0.21	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	8	211	1/1	0.79	0.37	110,110,110,110	0
81	MG	5	3545	1/1	0.79	0.24	89,89,89,89	0
81	MG	2	1999	1/1	0.79	0.23	104,104,104,104	0
81	MG	1	3697	1/1	0.79	0.16	127,127,127,127	0
81	MG	19	201	1/1	0.79	0.39	113,113,113,113	0
81	MG	n0	201	1/1	0.79	0.20	109,109,109,109	0
81	MG	1	3467	1/1	0.79	0.23	101,101,101,101	0
81	MG	2	2000	1/1	0.79	0.49	118,118,118,118	0
81	MG	1	3675	1/1	0.79	0.29	112,112,112,112	0
81	MG	2	1990	1/1	0.79	0.25	93,93,93,93	0
81	MG	6	1940	1/1	0.79	0.22	115,115,115,115	0
81	MG	5	3740	1/1	0.80	0.20	98,98,98,98	0
81	MG	5	3430	1/1	0.80	0.19	100,100,100,100	0
81	MG	2	1945	1/1	0.80	0.23	131,131,131,131	0
81	MG	5	3747	1/1	0.80	0.14	112,112,112,112	0
81	MG	2	1920	1/1	0.80	0.14	162,162,162,162	0
81	MG	1	3699	1/1	0.80	0.11	126,126,126,126	0
81	MG	1	3736	1/1	0.80	0.22	103,103,103,103	0
81	MG	5	3492	1/1	0.80	0.13	111,111,111,111	0
81	MG	6	1955	1/1	0.80	0.17	171,171,171,171	0
81	MG	5	3606	1/1	0.80	0.17	107,107,107,107	0
81	MG	5	3833	1/1	0.80	0.45	103,103,103,103	0
81	MG	1	3408	1/1	0.80	0.29	109,109,109,109	0
81	MG	5	3766	1/1	0.80	0.12	103,103,103,103	0
81	MG	5	3613	1/1	0.80	0.21	105,105,105,105	0
81	MG	5	3617	1/1	0.80	0.08	127,127,127,127	0
81	MG	2	1975	1/1	0.80	0.17	133,133,133,133	0
81	MG	5	3786	1/1	0.80	0.11	110,110,110,110	0
81	MG	1	3499	1/1	0.80	0.11	91,91,91,91	0
81	MG	5	3633	1/1	0.80	0.14	98,98,98,98	0
81	MG	1	3454	1/1	0.80	0.20	93,93,93,93	0
81	MG	5	3635	1/1	0.80	0.15	115,115,115,115	0
81	MG	6	1965	1/1	0.80	0.14	154,154,154,154	0
81	MG	5	3797	1/1	0.80	0.15	139,139,139,139	0
81	MG	1	3717	1/1	0.80	0.13	116,116,116,116	0
81	MG	5	3801	1/1	0.80	0.09	86,86,86,86	0
81	MG	4	222	1/1	0.80	0.10	123,123,123,123	0
81	MG	1	3458	1/1	0.80	0.28	91,91,91,91	0
81	MG	2	1930	1/1	0.80	0.12	149,149,149,149	0
81	MG	1	3660	1/1	0.80	0.34	108,108,108,108	0
81	MG	2	1994	1/1	0.80	0.18	136,136,136,136	0
81	MG	L3	402	1/1	0.81	0.17	128,128,128,128	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	6	1986	1/1	0.81	0.18	91,91,91,91	0
81	MG	M7	205	1/1	0.81	0.28	101,101,101,101	0
81	MG	2	1913	1/1	0.81	0.19	142,142,142,142	0
81	MG	8	206	1/1	0.81	0.12	97,97,97,97	0
81	MG	1	3794	1/1	0.81	0.21	117,117,117,117	0
81	MG	1	3524	1/1	0.81	0.32	130,130,130,130	0
81	MG	1	3460	1/1	0.81	0.33	99,99,99,99	0
81	MG	6	1902	1/1	0.81	0.12	136,136,136,136	0
81	MG	1	3592	1/1	0.81	0.33	87,87,87,87	0
81	MG	6	1974	1/1	0.81	0.18	169,169,169,169	0
81	MG	5	3455	1/1	0.81	0.14	133,133,133,133	0
81	MG	5	3460	1/1	0.81	0.12	140,140,140,140	0
81	MG	1	3463	1/1	0.81	0.20	94,94,94,94	0
81	MG	1	3489	1/1	0.81	0.24	114,114,114,114	0
81	MG	q2	504	1/1	0.81	0.33	107,107,107,107	0
81	MG	5	3558	1/1	0.81	0.26	115,115,115,115	0
81	MG	5	3678	1/1	0.82	0.16	105,105,105,105	0
81	MG	5	3737	1/1	0.82	0.16	112,112,112,112	0
81	MG	1	3791	1/1	0.82	0.17	107,107,107,107	0
81	MG	1	3404	1/1	0.82	0.31	91,91,91,91	0
81	MG	5	3491	1/1	0.82	0.14	108,108,108,108	0
81	MG	6	2011	1/1	0.82	0.23	111,111,111,111	0
81	MG	3	201	1/1	0.82	0.21	102,102,102,102	0
81	MG	5	3562	1/1	0.82	0.12	134,134,134,134	0
81	MG	2	1972	1/1	0.82	0.19	134,134,134,134	0
81	MG	5	3755	1/1	0.82	0.19	97,97,97,97	0
81	MG	5	3756	1/1	0.82	0.38	90,90,90,90	0
81	MG	1	3475	1/1	0.82	0.15	139,139,139,139	0
81	MG	5	3423	1/1	0.82	0.24	89,89,89,89	0
81	MG	1	3490	1/1	0.82	0.33	103,103,103,103	0
81	MG	4	203	1/1	0.82	0.09	160,160,160,160	0
81	MG	1	3785	1/1	0.82	0.14	120,120,120,120	0
81	MG	1	3721	1/1	0.82	0.15	86,86,86,86	0
81	MG	5	3526	1/1	0.82	0.16	119,119,119,119	0
81	MG	1	3413	1/1	0.82	0.21	112,112,112,112	0
81	MG	5	3676	1/1	0.82	0.34	106,106,106,106	0
81	MG	1	3548	1/1	0.82	0.08	144,144,144,144	0
81	MG	5	3790	1/1	0.82	0.11	105,105,105,105	0
81	MG	1	3545	1/1	0.83	0.12	114,114,114,114	0
81	MG	5	3624	1/1	0.83	0.09	92,92,92,92	0
81	MG	1	3401	1/1	0.83	0.19	97,97,97,97	0
81	MG	1	3538	1/1	0.83	0.10	153,153,153,153	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3749	1/1	0.83	0.21	83,83,83,83	0
81	MG	1	3790	1/1	0.83	0.22	98,98,98,98	0
81	MG	2	1982	1/1	0.83	0.17	152,152,152,152	0
81	MG	5	3802	1/1	0.83	0.22	113,113,113,113	0
81	MG	7	206	1/1	0.83	0.30	100,100,100,100	0
81	MG	6	1925	1/1	0.83	0.37	115,115,115,115	0
81	MG	1	3612	1/1	0.83	0.10	91,91,91,91	0
81	MG	5	3806	1/1	0.83	0.12	118,118,118,118	0
81	MG	8	210	1/1	0.83	0.27	103,103,103,103	0
81	MG	1	3507	1/1	0.83	0.18	91,91,91,91	0
81	MG	2	2001	1/1	0.83	0.27	109,109,109,109	0
81	MG	5	3590	1/1	0.83	0.22	90,90,90,90	0
81	MG	s8	301	1/1	0.83	0.13	124,124,124,124	0
81	MG	1	3748	1/1	0.83	0.21	102,102,102,102	0
81	MG	1	3751	1/1	0.83	0.07	181,181,181,181	0
81	MG	1	3583	1/1	0.83	0.08	100,100,100,100	0
81	MG	1	3725	1/1	0.83	0.11	111,111,111,111	0
81	MG	1	3703	1/1	0.83	0.29	106,106,106,106	0
81	MG	5	3729	1/1	0.83	0.15	111,111,111,111	0
81	MG	1	3645	1/1	0.83	0.22	92,92,92,92	0
81	MG	6	1908	1/1	0.83	0.25	103,103,103,103	0
81	MG	1	3713	1/1	0.84	0.13	133,133,133,133	0
81	MG	2	1902	1/1	0.84	0.08	145,145,145,145	0
81	MG	5	3824	1/1	0.84	0.33	98,98,98,98	0
81	MG	6	1956	1/1	0.84	0.13	168,168,168,168	0
81	MG	6	1904	1/1	0.84	0.24	123,123,123,123	0
81	MG	5	3782	1/1	0.84	0.37	85,85,85,85	0
81	MG	5	3464	1/1	0.84	0.22	99,99,99,99	0
81	MG	5	3724	1/1	0.84	0.30	98,98,98,98	0
81	MG	1	3688	1/1	0.84	0.15	114,114,114,114	0
81	MG	5	3660	1/1	0.84	0.40	89,89,89,89	0
81	MG	5	3477	1/1	0.84	0.20	95,95,95,95	0
81	MG	1	3419	1/1	0.84	0.13	161,161,161,161	0
81	MG	1	3568	1/1	0.84	0.43	79,79,79,79	0
81	MG	1	3793	1/1	0.84	0.14	111,111,111,111	1
81	MG	1	3516	1/1	0.84	0.14	118,118,118,118	0
81	MG	5	3601	1/1	0.84	0.16	95,95,95,95	0
81	MG	2	1926	1/1	0.84	0.09	117,117,117,117	0
81	MG	5	3499	1/1	0.84	0.20	92,92,92,92	0
81	MG	2	1901	1/1	0.84	0.15	140,140,140,140	0
81	MG	6	2012	1/1	0.84	0.28	116,116,116,116	0
81	MG	4	207	1/1	0.84	0.11	132,132,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3809	1/1	0.84	0.23	119,119,119,119	0
81	MG	5	3691	1/1	0.84	0.33	91,91,91,91	0
81	MG	M0	301	1/1	0.84	0.30	101,101,101,101	0
81	MG	2	1998	1/1	0.84	0.14	224,224,224,224	0
81	MG	5	3813	1/1	0.84	0.16	104,104,104,104	0
81	MG	2	2004	1/1	0.84	0.11	136,136,136,136	0
81	MG	1	3676	1/1	0.84	0.22	97,97,97,97	0
81	MG	1	3588	1/1	0.84	0.20	115,115,115,115	0
81	MG	4	214	1/1	0.84	0.14	147,147,147,147	0
81	MG	M7	203	1/1	0.85	0.24	85,85,85,85	0
81	MG	5	3671	1/1	0.85	0.11	125,125,125,125	0
81	MG	2	1968	1/1	0.85	0.09	132,132,132,132	0
81	MG	5	3817	1/1	0.85	0.09	105,105,105,105	0
81	MG	5	3596	1/1	0.85	0.15	128,128,128,128	0
81	MG	2	2002	1/1	0.85	0.09	214,214,214,214	0
81	MG	1	3663	1/1	0.85	0.20	101,101,101,101	0
81	MG	6	1953	1/1	0.85	0.08	171,171,171,171	0
81	MG	5	3602	1/1	0.85	0.16	138,138,138,138	0
81	MG	1	3506	1/1	0.85	0.14	96,96,96,96	0
81	MG	5	3687	1/1	0.85	0.14	89,89,89,89	0
81	MG	1	3617	1/1	0.85	0.21	88,88,88,88	0
81	MG	1	3737	1/1	0.85	0.12	143,143,143,143	0
81	MG	1	3620	1/1	0.85	0.12	108,108,108,108	0
81	MG	5	3834	1/1	0.85	0.25	98,98,98,98	0
81	MG	1	3412	1/1	0.85	0.27	104,104,104,104	0
81	MG	5	3775	1/1	0.85	0.15	115,115,115,115	0
81	MG	6	1905	1/1	0.85	0.21	128,128,128,128	0
81	MG	5	3619	1/1	0.85	0.32	89,89,89,89	0
81	MG	1	3509	1/1	0.85	0.35	97,97,97,97	0
81	MG	2	1938	1/1	0.85	0.15	128,128,128,128	0
81	MG	5	3628	1/1	0.85	0.19	107,107,107,107	0
81	MG	5	3791	1/1	0.85	0.09	125,125,125,125	0
81	MG	1	3644	1/1	0.85	0.32	92,92,92,92	0
81	MG	6	1972	1/1	0.85	0.15	136,136,136,136	0
81	MG	6	1911	1/1	0.85	0.29	108,108,108,108	0
81	MG	1	3434	1/1	0.85	0.26	99,99,99,99	0
81	MG	5	3411	1/1	0.85	0.23	89,89,89,89	0
81	MG	2	1944	1/1	0.85	0.18	127,127,127,127	0
81	MG	1	3656	1/1	0.85	0.17	96,96,96,96	0
81	MG	1	3658	1/1	0.85	0.12	204,204,204,204	0
81	MG	5	3652	1/1	0.85	0.24	88,88,88,88	0
81	MG	5	3657	1/1	0.85	0.20	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3420	1/1	0.85	0.16	137,137,137,137	0
81	MG	5	3739	1/1	0.85	0.43	83,83,83,83	0
81	MG	6	1994	1/1	0.85	0.12	175,175,175,175	0
81	MG	1	3726	1/1	0.85	0.20	115,115,115,115	0
82	GET	2	2014	34/34	0.85	0.13	145,145,145,145	0
81	MG	M4	201	1/1	0.85	0.11	135,135,135,135	0
81	MG	5	3822	1/1	0.86	0.15	105,105,105,105	0
81	MG	5	3444	1/1	0.86	0.41	87,87,87,87	0
81	MG	2	1989	1/1	0.86	0.14	125,125,125,125	0
81	MG	1	3643	1/1	0.86	0.10	89,89,89,89	0
81	MG	5	3828	1/1	0.86	0.15	103,103,103,103	0
81	MG	2	1939	1/1	0.86	0.22	125,125,125,125	0
81	MG	5	3568	1/1	0.86	0.12	89,89,89,89	0
81	MG	1	3448	1/1	0.86	0.44	90,90,90,90	0
81	MG	5	3589	1/1	0.86	0.12	88,88,88,88	0
81	MG	2	1910	1/1	0.86	0.09	160,160,160,160	0
81	MG	1	3523	1/1	0.86	0.31	114,114,114,114	0
81	MG	5	3731	1/1	0.86	0.12	97,97,97,97	0
81	MG	5	3482	1/1	0.86	0.18	72,72,72,72	0
81	MG	1	3686	1/1	0.86	0.22	94,94,94,94	0
81	MG	1	3752	1/1	0.86	0.10	145,145,145,145	0
81	MG	1	3595	1/1	0.86	0.20	86,86,86,86	0
81	MG	7	207	1/1	0.86	0.29	99,99,99,99	0
81	MG	2	1974	1/1	0.86	0.15	137,137,137,137	0
81	MG	6	1913	1/1	0.86	0.16	149,149,149,149	0
81	MG	6	1970	1/1	0.86	0.16	123,123,123,123	0
81	MG	1	3690	1/1	0.86	0.21	107,107,107,107	0
81	MG	L3	401	1/1	0.86	0.23	81,81,81,81	0
81	MG	1	3476	1/1	0.86	0.06	194,194,194,194	0
81	MG	8	214	1/1	0.86	0.14	113,113,113,113	0
81	MG	L6	201	1/1	0.86	0.12	111,111,111,111	0
81	MG	1	3417	1/1	0.86	0.15	129,129,129,129	0
81	MG	1	3618	1/1	0.86	0.18	90,90,90,90	0
81	MG	1	3571	1/1	0.86	0.16	80,80,80,80	0
81	MG	n3	202	1/1	0.86	0.28	93,93,93,93	0
81	MG	4	210	1/1	0.86	0.13	114,114,114,114	0
81	MG	2	2011	1/1	0.86	0.13	93,93,93,93	0
81	MG	5	3433	1/1	0.86	0.20	83,83,83,83	0
81	MG	5	3436	1/1	0.86	0.09	83,83,83,83	0
81	MG	5	3767	1/1	0.86	0.18	91,91,91,91	0
81	MG	1	3539	1/1	0.86	0.10	139,139,139,139	0
81	MG	5	3772	1/1	0.86	0.39	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	O3	202	1/1	0.87	0.19	97,97,97,97	0
81	MG	5	3680	1/1	0.87	0.25	83,83,83,83	0
81	MG	1	3415	1/1	0.87	0.25	103,103,103,103	0
81	MG	6	1982	1/1	0.87	0.09	181,181,181,181	0
81	MG	2	1987	1/1	0.87	0.17	144,144,144,144	0
81	MG	d3	201	1/1	0.87	0.28	107,107,107,107	0
81	MG	5	3505	1/1	0.87	0.31	85,85,85,85	0
81	MG	2	1992	1/1	0.87	0.07	130,130,130,130	0
81	MG	5	3826	1/1	0.87	0.36	101,101,101,101	0
81	MG	5	3768	1/1	0.87	0.16	115,115,115,115	0
81	MG	1	3740	1/1	0.87	0.12	80,80,80,80	0
81	MG	5	3701	1/1	0.87	0.21	121,121,121,121	0
81	MG	5	3832	1/1	0.87	0.28	102,102,102,102	0
81	MG	5	3773	1/1	0.87	0.20	94,94,94,94	0
81	MG	1	3742	1/1	0.87	0.15	90,90,90,90	0
81	MG	2	1960	1/1	0.87	0.13	154,154,154,154	0
81	MG	L2	302	1/1	0.87	0.36	99,99,99,99	0
81	MG	1	3504	1/1	0.87	0.23	87,87,87,87	0
81	MG	5	3785	1/1	0.87	0.10	144,144,144,144	0
81	MG	1	3446	1/1	0.87	0.15	102,102,102,102	0
81	MG	5	3532	1/1	0.87	0.44	93,93,93,93	0
81	MG	5	3536	1/1	0.87	0.14	89,89,89,89	0
81	MG	5	3538	1/1	0.87	0.11	99,99,99,99	0
81	MG	1	3422	1/1	0.87	0.10	129,129,129,129	0
81	MG	5	3546	1/1	0.87	0.38	87,87,87,87	0
81	MG	5	3441	1/1	0.87	0.22	82,82,82,82	0
81	MG	5	3726	1/1	0.87	0.26	107,107,107,107	0
81	MG	1	3611	1/1	0.87	0.11	109,109,109,109	0
81	MG	5	3649	1/1	0.87	0.09	151,151,151,151	0
81	MG	C0	201	1/1	0.87	0.16	126,126,126,126	0
81	MG	5	3458	1/1	0.87	0.20	117,117,117,117	0
81	MG	C4	202	1/1	0.87	0.12	116,116,116,116	0
81	MG	1	3677	1/1	0.87	0.37	97,97,97,97	0
81	MG	1	3706	1/1	0.87	0.19	107,107,107,107	0
81	MG	6	1967	1/1	0.87	0.09	152,152,152,152	0
81	MG	5	3475	1/1	0.87	0.24	107,107,107,107	0
81	MG	o3	201	1/1	0.87	0.19	97,97,97,97	0
81	MG	2	1964	1/1	0.87	0.13	130,130,130,130	0
81	MG	5	3480	1/1	0.87	0.23	90,90,90,90	0
81	MG	o7	505	1/1	0.87	0.11	111,111,111,111	0
81	MG	6	2009	1/1	0.87	0.10	98,98,98,98	0
81	MG	5	3675	1/1	0.87	0.30	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	O3	201	1/1	0.87	0.18	88,88,88,88	0
82	GET	6	2015	34/34	0.87	0.14	145,145,145,145	0
81	MG	6	1930	1/1	0.87	0.12	155,155,155,155	0
81	MG	5	3778	1/1	0.88	0.11	96,96,96,96	0
81	MG	5	3781	1/1	0.88	0.10	115,115,115,115	0
81	MG	6	1936	1/1	0.88	0.13	113,113,113,113	0
81	MG	4	217	1/1	-	-	113,113,113,113	1
81	MG	1	3778	1/1	0.88	0.14	91,91,91,91	0
81	MG	1	3440	1/1	0.88	0.11	114,114,114,114	0
81	MG	6	1945	1/1	0.88	0.15	153,153,153,153	0
81	MG	1	3574	1/1	0.88	0.15	87,87,87,87	0
81	MG	1	3575	1/1	0.88	0.16	92,92,92,92	0
81	MG	1	3427	1/1	0.88	0.17	122,122,122,122	0
81	MG	5	3837	1/1	0.88	0.33	96,96,96,96	0
81	MG	D2	201	1/1	0.88	0.13	184,184,184,184	0
81	MG	5	3839	1/1	0.88	0.24	105,105,105,105	0
81	MG	5	3840	1/1	0.88	0.25	98,98,98,98	0
81	MG	5	3841	1/1	0.88	0.31	102,102,102,102	0
81	MG	5	3743	1/1	0.88	0.22	99,99,99,99	0
81	MG	2	1961	1/1	0.88	0.13	139,139,139,139	0
81	MG	1	3622	1/1	0.88	0.18	80,80,80,80	0
81	MG	1	3633	1/1	0.88	0.18	74,74,74,74	0
81	MG	3	206	1/1	0.88	0.06	161,161,161,161	0
81	MG	1	3500	1/1	0.88	0.29	102,102,102,102	0
81	MG	1	3585	1/1	0.88	0.20	102,102,102,102	0
81	MG	5	3557	1/1	0.88	0.16	111,111,111,111	0
81	MG	5	3754	1/1	0.88	0.08	98,98,98,98	0
81	MG	1	3556	1/1	0.88	0.19	88,88,88,88	0
81	MG	5	3808	1/1	0.88	0.09	84,84,84,84	0
81	MG	2	1933	1/1	0.88	0.12	135,135,135,135	0
81	MG	l2	304	1/1	0.88	0.08	116,116,116,116	0
81	MG	6	1914	1/1	0.88	0.10	159,159,159,159	0
81	MG	5	3645	1/1	0.88	0.12	93,93,93,93	0
81	MG	1	3472	1/1	0.88	0.19	137,137,137,137	0
81	MG	m0	301	1/1	0.88	0.13	107,107,107,107	0
81	MG	5	3763	1/1	0.88	0.14	105,105,105,105	0
81	MG	6	1916	1/1	0.88	0.18	121,121,121,121	0
81	MG	5	3815	1/1	0.88	0.18	85,85,85,85	0
81	MG	1	3569	1/1	0.88	0.32	88,88,88,88	0
81	MG	M5	301	1/1	0.88	0.13	130,130,130,130	0
81	MG	5	3713	1/1	0.88	0.20	89,89,89,89	0
81	MG	M6	201	1/1	0.88	0.38	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3797	1/1	0.88	0.13	90,90,90,90	0
81	MG	5	3659	1/1	0.88	0.13	107,107,107,107	0
81	MG	1	3651	1/1	0.88	0.16	86,86,86,86	0
81	MG	1	3604	1/1	0.88	0.14	94,94,94,94	0
82	GET	5	3850	34/34	0.88	0.14	110,110,110,110	0
81	MG	5	3412	1/1	0.88	0.12	97,97,97,97	0
81	MG	5	3474	1/1	0.89	0.30	104,104,104,104	0
81	MG	2	1928	1/1	0.89	0.12	95,95,95,95	0
81	MG	2	1922	1/1	0.89	0.17	124,124,124,124	0
81	MG	5	3594	1/1	0.89	0.23	84,84,84,84	0
81	MG	1	3715	1/1	0.89	0.19	108,108,108,108	0
81	MG	1	3750	1/1	0.89	0.07	169,169,169,169	0
81	MG	5	3489	1/1	0.89	0.12	91,91,91,91	0
81	MG	5	3599	1/1	0.89	0.19	95,95,95,95	0
81	MG	2	1923	1/1	0.89	0.15	134,134,134,134	0
81	MG	1	3586	1/1	0.89	0.08	145,145,145,145	0
81	MG	1	3792	1/1	0.89	0.15	96,96,96,96	0
81	MG	5	3604	1/1	0.89	0.20	96,96,96,96	0
81	MG	5	3696	1/1	0.89	0.21	81,81,81,81	0
81	MG	2	1947	1/1	0.89	0.11	157,157,157,157	0
81	MG	1	3758	1/1	0.89	0.24	92,92,92,92	0
81	MG	5	3612	1/1	0.89	0.19	105,105,105,105	0
81	MG	1	3471	1/1	0.89	0.16	147,147,147,147	0
81	MG	5	3616	1/1	0.89	0.14	104,104,104,104	0
81	MG	1	3590	1/1	0.89	0.30	95,95,95,95	0
81	MG	7	203	1/1	0.89	0.06	180,180,180,180	0
81	MG	1	3566	1/1	0.89	0.36	80,80,80,80	0
81	MG	1	3648	1/1	0.89	0.25	92,92,92,92	0
81	MG	5	3620	1/1	0.89	0.12	108,108,108,108	0
81	MG	5	3513	1/1	0.89	0.18	85,85,85,85	0
81	MG	1	3594	1/1	0.89	0.26	89,89,89,89	0
81	MG	8	204	1/1	0.89	0.20	108,108,108,108	0
81	MG	1	3444	1/1	0.89	0.15	104,104,104,104	0
81	MG	1	3770	1/1	0.89	0.26	135,135,135,135	0
81	MG	1	3655	1/1	0.89	0.07	106,106,106,106	0
81	MG	1	3416	1/1	0.89	0.10	121,121,121,121	0
81	MG	5	3416	1/1	0.89	0.23	90,90,90,90	1
81	MG	1	3447	1/1	0.89	0.33	90,90,90,90	0
81	MG	5	3638	1/1	0.89	0.11	94,94,94,94	0
81	MG	5	3730	1/1	0.89	0.11	98,98,98,98	1
81	MG	1	3572	1/1	0.89	0.13	87,87,87,87	0
81	MG	6	1924	1/1	0.89	0.24	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3542	1/1	0.89	0.22	82,82,82,82	0
81	MG	m7	204	1/1	0.89	0.16	86,86,86,86	0
81	MG	5	3738	1/1	0.89	0.16	76,76,76,76	0
81	MG	2	1909	1/1	0.89	0.14	160,160,160,160	0
81	MG	1	3615	1/1	0.89	0.07	93,93,93,93	0
81	MG	n5	201	1/1	0.89	0.31	98,98,98,98	0
81	MG	6	1992	1/1	0.89	0.10	164,164,164,164	0
81	MG	1	3741	1/1	0.89	0.08	92,92,92,92	0
81	MG	2	1903	1/1	0.89	0.08	201,201,201,201	0
81	MG	6	1933	1/1	0.89	0.20	106,106,106,106	0
81	MG	6	1996	1/1	0.89	0.13	125,125,125,125	0
81	MG	1	3481	1/1	0.89	0.09	130,130,130,130	0
81	MG	6	1938	1/1	0.89	0.17	115,115,115,115	0
81	MG	1	3431	1/1	0.89	0.15	75,75,75,75	0
81	MG	5	3565	1/1	0.89	0.22	100,100,100,100	0
82	GET	5	3851	34/34	0.89	0.08	154,154,154,154	0
81	MG	N2	201	1/1	0.89	0.11	193,193,193,193	0
81	MG	5	3699	1/1	0.90	0.13	107,107,107,107	1
81	MG	5	3454	1/1	0.90	0.07	148,148,148,148	0
81	MG	1	3803	1/1	0.90	0.36	115,115,115,115	0
81	MG	5	3843	1/1	0.90	0.19	116,116,116,116	0
81	MG	5	3803	1/1	0.90	0.08	81,81,81,81	0
81	MG	1	3695	1/1	0.90	0.09	122,122,122,122	0
81	MG	1	3641	1/1	0.90	0.33	93,93,93,93	0
81	MG	5	3461	1/1	0.90	0.22	108,108,108,108	0
81	MG	1	3768	1/1	0.90	0.32	93,93,93,93	0
81	MG	5	3522	1/1	0.90	0.08	132,132,132,132	0
81	MG	5	3760	1/1	0.90	0.12	81,81,81,81	0
81	MG	2	1912	1/1	0.90	0.13	147,147,147,147	0
81	MG	sM	301	1/1	0.90	0.08	147,147,147,147	0
81	MG	5	3714	1/1	0.90	0.23	134,134,134,134	0
81	MG	5	3469	1/1	0.90	0.19	98,98,98,98	0
81	MG	5	3472	1/1	0.90	0.17	103,103,103,103	0
81	MG	8	213	1/1	0.90	0.11	118,118,118,118	0
81	MG	5	3605	1/1	0.90	0.10	98,98,98,98	0
81	MG	l2	301	1/1	0.90	0.17	91,91,91,91	0
81	MG	1	3591	1/1	0.90	0.18	97,97,97,97	0
81	MG	2	1971	1/1	0.90	0.08	123,123,123,123	0
81	MG	1	3685	1/1	0.90	0.17	113,113,113,113	0
81	MG	1	3710	1/1	0.90	0.10	118,118,118,118	0
81	MG	5	3424	1/1	0.90	0.13	84,84,84,84	0
81	MG	m6	201	1/1	0.90	0.36	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3488	1/1	0.90	0.15	82,82,82,82	0
81	MG	2	1963	1/1	0.90	0.10	141,141,141,141	0
81	MG	5	3779	1/1	0.90	0.12	106,106,106,106	0
81	MG	5	3428	1/1	0.90	0.20	93,93,93,93	0
81	MG	5	3732	1/1	0.90	0.13	114,114,114,114	0
81	MG	2	2006	1/1	0.90	0.12	105,105,105,105	0
81	MG	5	3432	1/1	0.90	0.19	92,92,92,92	0
81	MG	5	3787	1/1	0.90	0.19	109,109,109,109	0
81	MG	o7	502	1/1	0.90	0.15	100,100,100,100	0
81	MG	5	3681	1/1	0.90	0.23	96,96,96,96	0
81	MG	o7	506	1/1	0.90	0.13	104,104,104,104	0
81	MG	1	3491	1/1	0.90	0.18	108,108,108,108	0
81	MG	1	3714	1/1	0.90	0.14	145,145,145,145	0
81	MG	2	1929	1/1	0.90	0.08	144,144,144,144	0
82	GET	1	3812	34/34	0.90	0.10	158,158,158,158	0
81	MG	1	3531	1/1	0.90	0.09	113,113,113,113	0
81	MG	5	3569	1/1	0.90	0.14	85,85,85,85	0
81	MG	2	1925	1/1	0.90	0.09	141,141,141,141	0
81	MG	5	3580	1/1	0.90	0.08	111,111,111,111	0
81	MG	1	3528	1/1	0.91	0.12	105,105,105,105	0
81	MG	6	1937	1/1	0.91	0.11	120,120,120,120	0
81	MG	1	3529	1/1	0.91	0.16	85,85,85,85	0
81	MG	1	3624	1/1	0.91	0.13	86,86,86,86	0
81	MG	1	3765	1/1	0.91	0.22	103,103,103,103	0
81	MG	5	3574	1/1	0.91	0.21	107,107,107,107	0
81	MG	5	3577	1/1	0.91	0.06	129,129,129,129	0
81	MG	1	3694	1/1	0.91	0.08	103,103,103,103	0
81	MG	1	3465	1/1	0.91	0.23	99,99,99,99	0
81	MG	5	3584	1/1	0.91	0.11	88,88,88,88	0
81	MG	2	1958	1/1	0.91	0.08	132,132,132,132	0
81	MG	1	3665	1/1	0.91	0.09	109,109,109,109	0
81	MG	5	3504	1/1	0.91	0.23	88,88,88,88	0
81	MG	1	3534	1/1	0.91	0.14	101,101,101,101	0
81	MG	5	3800	1/1	0.91	0.21	97,97,97,97	0
81	MG	1	3772	1/1	0.91	0.15	122,122,122,122	0
81	MG	5	3510	1/1	0.91	0.14	109,109,109,109	0
81	MG	5	3511	1/1	0.91	0.14	125,125,125,125	0
81	MG	1	3638	1/1	0.91	0.07	138,138,138,138	0
81	MG	1	3495	1/1	0.91	0.16	97,97,97,97	0
81	MG	5	3746	1/1	0.91	0.22	71,71,71,71	0
81	MG	1	3515	1/1	0.91	0.05	147,147,147,147	0
81	MG	1	3496	1/1	0.91	0.14	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3779	1/1	0.91	0.06	144,144,144,144	0
81	MG	5	3751	1/1	0.91	0.24	87,87,87,87	0
81	MG	1	3468	1/1	0.91	0.24	108,108,108,108	0
81	MG	1	3578	1/1	0.91	0.16	109,109,109,109	0
81	MG	1	3647	1/1	0.91	0.18	92,92,92,92	0
81	MG	2	1976	1/1	0.91	0.12	152,152,152,152	0
81	MG	5	3534	1/1	0.91	0.12	98,98,98,98	0
81	MG	5	3816	1/1	0.91	0.19	111,111,111,111	0
81	MG	5	3692	1/1	0.91	0.17	88,88,88,88	0
81	MG	5	3465	1/1	0.91	0.22	83,83,83,83	0
81	MG	5	3695	1/1	0.91	0.21	86,86,86,86	0
81	MG	1	3409	1/1	0.91	0.12	103,103,103,103	0
81	MG	1	3682	1/1	0.91	0.11	130,130,130,130	0
81	MG	5	3471	1/1	0.91	0.15	99,99,99,99	0
81	MG	6	1973	1/1	0.91	0.15	107,107,107,107	0
81	MG	1	3652	1/1	0.91	0.12	102,102,102,102	0
81	MG	2	2010	1/1	0.91	0.12	139,139,139,139	0
81	MG	5	3631	1/1	0.91	0.15	99,99,99,99	0
81	MG	5	3707	1/1	0.91	0.13	132,132,132,132	0
82	GET	2	2013	34/34	0.91	0.11	140,140,140,140	0
81	MG	5	3552	1/1	0.91	0.14	95,95,95,95	0
82	GET	1	3808	34/34	0.91	0.12	106,106,106,106	0
81	MG	5	3554	1/1	0.91	0.10	103,103,103,103	0
81	MG	1	3552	1/1	0.91	0.19	86,86,86,86	0
81	MG	5	3478	1/1	0.91	0.15	95,95,95,95	0
81	MG	6	1932	1/1	0.91	0.11	120,120,120,120	0
81	MG	2	1948	1/1	0.91	0.07	172,172,172,172	0
81	MG	1	3559	1/1	0.92	0.11	90,90,90,90	0
81	MG	5	3456	1/1	0.92	0.21	130,130,130,130	0
81	MG	6	1944	1/1	0.92	0.07	190,190,190,190	0
81	MG	1	3560	1/1	0.92	0.19	82,82,82,82	0
81	MG	1	3747	1/1	0.92	0.11	101,101,101,101	0
81	MG	2	1949	1/1	0.92	0.05	176,176,176,176	0
81	MG	5	3655	1/1	0.92	0.09	89,89,89,89	0
81	MG	6	1950	1/1	0.92	0.10	193,193,193,193	0
81	MG	6	1951	1/1	0.92	0.07	224,224,224,224	0
81	MG	5	3555	1/1	0.92	0.11	108,108,108,108	0
81	MG	5	3556	1/1	0.92	0.06	106,106,106,106	1
81	MG	5	3661	1/1	0.92	0.15	97,97,97,97	0
81	MG	5	3662	1/1	0.92	0.09	114,114,114,114	0
81	MG	5	3665	1/1	0.92	0.17	92,92,92,92	0
81	MG	5	3466	1/1	0.92	0.11	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	2	1919	1/1	0.92	0.07	184,184,184,184	0
81	MG	5	3468	1/1	0.92	0.24	96,96,96,96	0
81	MG	2	1905	1/1	0.92	0.14	154,154,154,154	0
81	MG	1	3649	1/1	0.92	0.20	92,92,92,92	0
81	MG	4	220	1/1	0.92	0.15	117,117,117,117	0
81	MG	1	3754	1/1	0.92	0.17	110,110,110,110	0
81	MG	1	3698	1/1	0.92	0.09	113,113,113,113	0
81	MG	5	3476	1/1	0.92	0.08	108,108,108,108	1
81	MG	1	3414	1/1	0.92	0.12	119,119,119,119	0
81	MG	5	3575	1/1	0.92	0.18	97,97,97,97	0
81	MG	1	3760	1/1	0.92	0.08	147,147,147,147	0
81	MG	6	1960	1/1	0.92	0.07	169,169,169,169	0
81	MG	2	1917	1/1	0.92	0.05	160,160,160,160	0
81	MG	5	3582	1/1	0.92	0.21	88,88,88,88	0
81	MG	5	3485	1/1	0.92	0.17	89,89,89,89	0
81	MG	6	1964	1/1	0.92	0.10	164,164,164,164	0
81	MG	3	204	1/1	0.92	0.07	147,147,147,147	0
81	MG	5	3591	1/1	0.92	0.24	98,98,98,98	0
81	MG	5	3784	1/1	0.92	0.10	98,98,98,98	0
81	MG	1	3493	1/1	0.92	0.13	106,106,106,106	0
81	MG	1	3627	1/1	0.92	0.15	78,78,78,78	0
81	MG	5	3407	1/1	0.92	0.21	87,87,87,87	0
81	MG	5	3410	1/1	0.92	0.21	84,84,84,84	0
81	MG	6	1969	1/1	0.92	0.12	181,181,181,181	0
81	MG	5	3600	1/1	0.92	0.14	89,89,89,89	0
81	MG	3	208	1/1	0.92	0.08	162,162,162,162	0
81	MG	5	3500	1/1	0.92	0.26	87,87,87,87	0
81	MG	3	209	1/1	0.92	0.10	141,141,141,141	0
81	MG	5	3419	1/1	0.92	0.18	86,86,86,86	0
81	MG	6	1922	1/1	0.92	0.14	113,113,113,113	0
81	MG	5	3711	1/1	0.92	0.20	86,86,86,86	0
81	MG	1	3547	1/1	0.92	0.07	92,92,92,92	0
81	MG	5	3508	1/1	0.92	0.19	107,107,107,107	0
81	MG	1	3511	1/1	0.92	0.16	113,113,113,113	0
81	MG	o2	202	1/1	0.92	0.25	92,92,92,92	0
81	MG	1	3684	1/1	0.92	0.08	101,101,101,101	0
81	MG	5	3429	1/1	0.92	0.17	92,92,92,92	0
81	MG	M7	201	1/1	0.92	0.26	105,105,105,105	0
81	MG	5	3515	1/1	0.92	0.15	109,109,109,109	0
81	MG	1	3470	1/1	0.92	0.11	132,132,132,132	0
81	MG	M7	204	1/1	0.92	0.06	94,94,94,94	0
81	MG	5	3435	1/1	0.92	0.11	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3521	1/1	0.92	0.14	151,151,151,151	0
81	MG	q2	505	1/1	0.92	0.11	126,126,126,126	0
81	MG	1	3597	1/1	0.92	0.10	105,105,105,105	0
81	MG	4	209	1/1	0.92	0.19	111,111,111,111	0
81	MG	5	3527	1/1	0.92	0.17	116,116,116,116	0
82	GET	1	3809	34/34	0.92	0.16	101,101,101,101	0
82	GET	1	3810	34/34	0.92	0.12	108,108,108,108	0
81	MG	5	3528	1/1	0.92	0.14	105,105,105,105	0
82	GET	1	3813	34/34	0.92	0.19	103,103,103,103	0
81	MG	N8	202	1/1	0.92	0.27	108,108,108,108	0
81	MG	1	3484	1/1	0.92	0.09	157,157,157,157	0
81	MG	5	3448	1/1	0.92	0.24	97,97,97,97	0
82	GET	n6	201	34/34	0.92	0.09	128,128,128,128	0
81	MG	1	3430	1/1	0.92	0.23	92,92,92,92	0
81	MG	5	3827	1/1	0.93	0.26	81,81,81,81	0
81	MG	6	1963	1/1	0.93	0.06	197,197,197,197	0
81	MG	5	3401	1/1	0.93	0.10	76,76,76,76	0
81	MG	5	3570	1/1	0.93	0.09	91,91,91,91	0
81	MG	5	3831	1/1	0.93	0.12	76,76,76,76	0
81	MG	1	3522	1/1	0.93	0.06	104,104,104,104	1
81	MG	6	1912	1/1	0.93	0.13	127,127,127,127	0
81	MG	1	3729	1/1	0.93	0.06	171,171,171,171	0
81	MG	D2	202	1/1	0.93	0.06	180,180,180,180	0
81	MG	1	3581	1/1	0.93	0.14	113,113,113,113	0
81	MG	5	3494	1/1	0.93	0.05	129,129,129,129	0
81	MG	5	3418	1/1	0.93	0.28	77,77,77,77	0
81	MG	5	3585	1/1	0.93	0.55	69,69,69,69	0
81	MG	5	3497	1/1	0.93	0.19	93,93,93,93	0
81	MG	1	3421	1/1	0.93	0.10	144,144,144,144	0
81	MG	1	3550	1/1	0.93	0.29	94,94,94,94	0
81	MG	1	3696	1/1	0.93	0.13	92,92,92,92	0
81	MG	1	3402	1/1	0.93	0.16	102,102,102,102	0
81	MG	1	3488	1/1	0.93	0.19	108,108,108,108	0
81	MG	1	3625	1/1	0.93	0.07	89,89,89,89	1
81	MG	1	3701	1/1	0.93	0.16	96,96,96,96	0
81	MG	5	3431	1/1	0.93	0.09	101,101,101,101	0
81	MG	5	3780	1/1	0.93	0.07	85,85,85,85	0
81	MG	8	203	1/1	0.93	0.04	112,112,112,112	0
81	MG	6	1984	1/1	0.93	0.11	135,135,135,135	0
81	MG	5	3512	1/1	0.93	0.06	121,121,121,121	0
81	MG	D9	102	1/1	0.93	0.24	126,126,126,126	0
81	MG	5	3434	1/1	0.93	0.14	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3461	1/1	0.93	0.11	104,104,104,104	0
81	MG	5	3704	1/1	0.93	0.21	84,84,84,84	0
81	MG	6	1988	1/1	0.93	0.15	120,120,120,120	0
81	MG	6	1990	1/1	0.93	0.08	139,139,139,139	0
81	MG	5	3440	1/1	0.93	0.19	83,83,83,83	0
81	MG	12	302	1/1	0.93	0.08	95,95,95,95	0
81	MG	12	303	1/1	0.93	0.20	91,91,91,91	0
81	MG	4	201	1/1	0.93	0.15	130,130,130,130	0
81	MG	13	402	1/1	0.93	0.09	91,91,91,91	0
81	MG	M7	202	1/1	0.93	0.15	100,100,100,100	0
81	MG	14	401	1/1	0.93	0.16	95,95,95,95	0
81	MG	5	3524	1/1	0.93	0.13	132,132,132,132	0
81	MG	1	3705	1/1	0.93	0.14	114,114,114,114	0
81	MG	1	3510	1/1	0.93	0.17	105,105,105,105	0
81	MG	4	204	1/1	0.93	0.07	160,160,160,160	0
81	MG	1	3589	1/1	0.93	0.06	139,139,139,139	1
81	MG	m7	205	1/1	0.93	0.26	77,77,77,77	0
81	MG	1	3562	1/1	0.93	0.19	92,92,92,92	0
81	MG	5	3627	1/1	0.93	0.15	103,103,103,103	0
81	MG	6	1941	1/1	0.93	0.08	145,145,145,145	0
81	MG	1	3533	1/1	0.93	0.20	110,110,110,110	0
81	MG	5	3462	1/1	0.93	0.13	104,104,104,104	0
81	MG	5	3540	1/1	0.93	0.12	89,89,89,89	0
81	MG	1	3445	1/1	0.93	0.12	105,105,105,105	0
81	MG	5	3543	1/1	0.93	0.23	97,97,97,97	0
81	MG	1	3537	1/1	0.93	0.08	143,143,143,143	0
81	MG	o7	504	1/1	0.93	0.12	80,80,80,80	0
81	MG	O5	201	1/1	0.93	0.06	165,165,165,165	0
81	MG	5	3547	1/1	0.93	0.18	87,87,87,87	0
81	MG	6	1949	1/1	0.93	0.06	172,172,172,172	0
81	MG	1	3492	1/1	0.93	0.14	109,109,109,109	0
81	MG	O6	202	1/1	0.93	0.10	150,150,150,150	0
81	MG	1	3424	1/1	0.93	0.11	114,114,114,114	0
81	MG	5	3742	1/1	0.93	0.09	107,107,107,107	0
81	MG	1	3599	1/1	0.93	0.34	87,87,87,87	0
81	MG	1	3683	1/1	0.93	0.10	98,98,98,98	0
81	MG	1	3477	1/1	0.93	0.11	138,138,138,138	0
82	GET	1	3811	34/34	0.93	0.10	147,147,147,147	0
81	MG	1	3607	1/1	0.93	0.15	90,90,90,90	0
81	MG	2	1906	1/1	0.93	0.12	155,155,155,155	0
82	GET	6	2014	34/34	0.93	0.09	132,132,132,132	0
81	MG	6	1907	1/1	0.93	0.11	122,122,122,122	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	GET	5	3844	34/34	0.93	0.13	100,100,100,100	0
82	GET	5	3846	34/34	0.93	0.09	138,138,138,138	0
82	GET	5	3848	34/34	0.93	0.10	127,127,127,127	0
81	MG	1	3610	1/1	0.93	0.12	100,100,100,100	0
81	MG	1	3435	1/1	0.93	0.17	102,102,102,102	0
81	MG	4	221	1/1	0.93	0.09	137,137,137,137	0
83	ZN	D7	101	1/1	0.93	0.06	287,287,287,287	0
81	MG	5	3566	1/1	0.93	0.08	93,93,93,93	0
81	MG	1	3457	1/1	0.94	0.34	81,81,81,81	0
81	MG	5	3578	1/1	-	-	120,120,120,120	1
81	MG	5	3553	1/1	0.94	0.12	98,98,98,98	0
81	MG	2	1997	1/1	0.94	0.07	200,200,200,200	0
81	MG	5	3470	1/1	0.94	0.16	96,96,96,96	0
81	MG	1	3700	1/1	0.94	0.07	97,97,97,97	0
81	MG	1	3512	1/1	0.94	0.07	110,110,110,110	0
81	MG	5	3663	1/1	0.94	0.20	95,95,95,95	0
81	MG	2	1955	1/1	0.94	0.09	134,134,134,134	0
81	MG	Q2	502	1/1	0.94	0.12	122,122,122,122	0
81	MG	2	1914	1/1	0.94	0.07	195,195,195,195	0
81	MG	1	3632	1/1	0.94	0.09	62,62,62,62	0
81	MG	5	3765	1/1	0.94	0.25	91,91,91,91	0
81	MG	1	3462	1/1	0.94	0.15	98,98,98,98	0
81	MG	1	3707	1/1	0.94	0.18	86,86,86,86	0
81	MG	1	3708	1/1	0.94	0.33	83,83,83,83	0
81	MG	C4	201	1/1	0.94	0.10	176,176,176,176	0
81	MG	1	3483	1/1	0.94	0.12	150,150,150,150	0
81	MG	1	3521	1/1	0.94	0.14	101,101,101,101	0
81	MG	5	3573	1/1	0.94	0.14	113,113,113,113	0
81	MG	2	1946	1/1	0.94	0.10	115,115,115,115	0
81	MG	1	3640	1/1	0.94	0.06	105,105,105,105	0
81	MG	8	207	1/1	0.94	0.10	115,115,115,115	0
81	MG	5	3576	1/1	0.94	0.06	125,125,125,125	0
81	MG	1	3503	1/1	0.94	0.09	97,97,97,97	0
81	MG	1	3642	1/1	0.94	0.07	103,103,103,103	0
81	MG	1	3602	1/1	0.94	0.24	87,87,87,87	0
81	MG	1	3577	1/1	0.94	0.09	109,109,109,109	0
81	MG	6	1968	1/1	0.94	0.17	130,130,130,130	0
81	MG	1	3605	1/1	0.94	0.11	85,85,85,85	0
81	MG	6	1917	1/1	0.94	0.15	122,122,122,122	0
81	MG	6	1971	1/1	0.94	0.04	192,192,192,192	0
81	MG	l3	401	1/1	0.94	0.18	84,84,84,84	0
81	MG	5	3503	1/1	0.94	0.13	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3418	1/1	0.94	0.11	152,152,152,152	0
81	MG	1	3407	1/1	0.94	0.06	109,109,109,109	1
81	MG	6	1920	1/1	0.94	0.09	134,134,134,134	0
81	MG	5	3507	1/1	0.94	0.18	103,103,103,103	0
81	MG	6	1975	1/1	0.94	0.09	161,161,161,161	0
81	MG	5	3509	1/1	0.94	0.19	111,111,111,111	0
81	MG	6	1977	1/1	0.94	0.05	197,197,197,197	0
81	MG	6	1921	1/1	0.94	0.09	115,115,115,115	0
81	MG	6	1979	1/1	0.94	0.19	113,113,113,113	0
81	MG	n0	202	1/1	0.94	0.20	103,103,103,103	0
81	MG	n3	201	1/1	0.94	0.07	89,89,89,89	0
81	MG	1	3687	1/1	0.94	0.24	79,79,79,79	0
81	MG	1	3580	1/1	0.94	0.07	121,121,121,121	0
81	MG	6	1983	1/1	0.94	0.08	152,152,152,152	0
81	MG	M0	302	1/1	0.94	0.19	96,96,96,96	0
81	MG	5	3437	1/1	0.94	0.09	91,91,91,91	0
81	MG	o3	202	1/1	0.94	0.08	102,102,102,102	0
81	MG	6	1928	1/1	0.94	0.14	114,114,114,114	0
81	MG	5	3520	1/1	0.94	0.08	144,144,144,144	0
81	MG	3	203	1/1	0.94	0.04	142,142,142,142	0
81	MG	6	1987	1/1	0.94	0.11	169,169,169,169	0
81	MG	5	3523	1/1	0.94	0.09	113,113,113,113	0
81	MG	2	1908	1/1	0.94	0.09	163,163,163,163	0
81	MG	q2	502	1/1	0.94	0.29	107,107,107,107	0
81	MG	6	1989	1/1	0.94	0.06	125,125,125,125	0
81	MG	5	3451	1/1	0.94	0.12	97,97,97,97	0
81	MG	5	3452	1/1	0.94	0.24	96,96,96,96	0
82	GET	2	2012	34/34	0.94	0.09	131,131,131,131	0
81	MG	1	3728	1/1	0.94	0.11	93,93,93,93	0
81	MG	2	1943	1/1	0.94	0.17	97,97,97,97	0
81	MG	5	3733	1/1	0.94	0.46	88,88,88,88	0
81	MG	5	3734	1/1	0.94	0.31	88,88,88,88	0
81	MG	1	3554	1/1	0.94	0.15	96,96,96,96	0
81	MG	5	3457	1/1	0.94	0.06	141,141,141,141	0
81	MG	5	3537	1/1	0.94	0.10	100,100,100,100	0
81	MG	6	1935	1/1	0.94	0.10	124,124,124,124	0
82	GET	6	2013	34/34	0.94	0.09	132,132,132,132	0
81	MG	1	3616	1/1	0.94	0.19	88,88,88,88	0
81	MG	1	3555	1/1	0.94	0.15	96,96,96,96	0
81	MG	1	3657	1/1	0.94	0.10	97,97,97,97	0
82	GET	5	3845	34/34	0.94	0.10	119,119,119,119	0
81	MG	2	1918	1/1	0.94	0.11	181,181,181,181	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	N7	201	1/1	0.94	0.09	204,204,204,204	0
81	MG	1	3738	1/1	0.94	0.22	87,87,87,87	0
81	MG	4	205	1/1	0.94	0.11	118,118,118,118	0
81	MG	5	3651	1/1	0.94	0.16	91,91,91,91	0
81	MG	5	3550	1/1	0.94	0.08	99,99,99,99	0
81	MG	1	3619	1/1	0.94	0.09	92,92,92,92	0
83	ZN	e1	501	1/1	0.94	0.05	282,282,282,282	0
81	MG	1	3464	1/1	0.95	0.24	102,102,102,102	0
81	MG	5	3450	1/1	0.95	0.36	94,94,94,94	0
81	MG	5	3719	1/1	0.95	0.23	88,88,88,88	0
81	MG	1	3411	1/1	0.95	0.12	106,106,106,106	0
81	MG	1	3561	1/1	0.95	0.15	87,87,87,87	0
81	MG	1	3478	1/1	0.95	0.10	133,133,133,133	0
81	MG	5	3567	1/1	0.95	0.07	88,88,88,88	0
81	MG	5	3644	1/1	0.95	0.05	103,103,103,103	0
81	MG	1	3739	1/1	0.95	0.09	114,114,114,114	0
81	MG	5	3798	1/1	0.95	0.35	88,88,88,88	0
81	MG	O7	102	1/1	0.95	0.08	121,121,121,121	0
81	MG	1	3614	1/1	0.95	0.21	91,91,91,91	0
81	MG	1	3563	1/1	0.95	0.20	82,82,82,82	0
81	MG	5	3650	1/1	0.95	0.10	79,79,79,79	0
81	MG	6	1976	1/1	0.95	0.05	149,149,149,149	0
81	MG	1	3564	1/1	0.95	0.26	88,88,88,88	0
81	MG	4	224	1/1	0.95	0.08	144,144,144,144	0
81	MG	1	3456	1/1	0.95	0.43	78,78,78,78	0
81	MG	1	3437	1/1	0.95	0.19	104,104,104,104	0
81	MG	5	3403	1/1	0.95	0.12	94,94,94,94	0
81	MG	m7	201	1/1	0.95	0.06	84,84,84,84	0
81	MG	5	3581	1/1	0.95	0.12	112,112,112,112	0
81	MG	5	3406	1/1	0.95	0.17	86,86,86,86	0
81	MG	1	3567	1/1	0.95	0.21	81,81,81,81	0
81	MG	1	3526	1/1	0.95	0.07	133,133,133,133	0
81	MG	2	1942	1/1	0.95	0.15	123,123,123,123	0
81	MG	6	1948	1/1	0.95	0.09	167,167,167,167	0
81	MG	5	3525	1/1	0.95	0.05	128,128,128,128	0
81	MG	5	3593	1/1	0.95	0.13	102,102,102,102	0
81	MG	o2	201	1/1	0.95	0.15	92,92,92,92	0
81	MG	5	3748	1/1	0.95	0.17	97,97,97,97	0
81	MG	1	3459	1/1	0.95	0.17	100,100,100,100	0
81	MG	5	3595	1/1	0.95	0.18	94,94,94,94	0
81	MG	1	3514	1/1	0.95	0.07	144,144,144,144	0
81	MG	1	3626	1/1	0.95	0.20	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3421	1/1	0.95	0.13	90,90,90,90	0
81	MG	1	3433	1/1	0.95	0.11	111,111,111,111	0
81	MG	1	3722	1/1	0.95	0.11	92,92,92,92	0
81	MG	6	1991	1/1	0.95	0.10	198,198,198,198	0
81	MG	1	3755	1/1	0.95	0.10	111,111,111,111	0
81	MG	5	3481	1/1	0.95	0.10	90,90,90,90	0
81	MG	5	3759	1/1	0.95	0.09	82,82,82,82	0
81	MG	1	3630	1/1	0.95	0.38	78,78,78,78	0
81	MG	2	2005	1/1	0.95	0.10	169,169,169,169	0
81	MG	5	3487	1/1	0.95	0.17	84,84,84,84	0
81	MG	5	3607	1/1	0.95	0.17	101,101,101,101	0
81	MG	1	3576	1/1	0.95	0.17	101,101,101,101	0
81	MG	1	3600	1/1	0.95	0.08	87,87,87,87	0
81	MG	5	3694	1/1	0.95	0.11	89,89,89,89	0
81	MG	1	3450	1/1	0.95	0.22	90,90,90,90	0
81	MG	5	3614	1/1	0.95	0.13	95,95,95,95	0
81	MG	1	3536	1/1	0.95	0.07	163,163,163,163	0
81	MG	M7	206	1/1	0.95	0.21	93,93,93,93	0
81	MG	6	1962	1/1	0.95	0.09	191,191,191,191	0
81	MG	1	3443	1/1	0.95	0.06	117,117,117,117	0
81	MG	1	3672	1/1	0.95	0.15	107,107,107,107	0
81	MG	5	3439	1/1	0.95	0.09	87,87,87,87	0
81	MG	1	3557	1/1	0.95	0.13	108,108,108,108	0
82	GET	5	3847	34/34	0.95	0.14	101,101,101,101	0
81	MG	1	3800	1/1	0.95	0.19	111,111,111,111	0
82	GET	5	3849	34/34	0.95	0.14	101,101,101,101	0
81	MG	5	3442	1/1	0.95	0.06	88,88,88,88	0
81	MG	5	3629	1/1	0.95	0.14	93,93,93,93	0
81	MG	5	3783	1/1	0.95	0.06	105,105,105,105	0
81	MG	5	3502	1/1	0.95	0.12	83,83,83,83	0
81	MG	5	3632	1/1	0.95	0.08	118,118,118,118	0
81	MG	O2	203	1/1	0.95	0.12	92,92,92,92	0
81	MG	1	3613	1/1	0.96	0.10	88,88,88,88	0
81	MG	5	3646	1/1	0.96	0.08	131,131,131,131	0
81	MG	1	3527	1/1	0.96	0.15	103,103,103,103	0
81	MG	l7	301	1/1	0.96	0.08	92,92,92,92	0
81	MG	1	3598	1/1	0.96	0.14	101,101,101,101	0
81	MG	5	3761	1/1	0.96	0.23	88,88,88,88	0
81	MG	1	3549	1/1	0.96	0.16	145,145,145,145	0
81	MG	1	3520	1/1	0.96	0.10	103,103,103,103	0
81	MG	1	3469	1/1	0.96	0.12	120,120,120,120	0
81	MG	m7	202	1/1	0.96	0.13	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	3	207	1/1	0.96	0.07	159,159,159,159	0
81	MG	1	3692	1/1	0.96	0.08	127,127,127,127	0
81	MG	1	3775	1/1	0.96	0.08	98,98,98,98	0
81	MG	1	3796	1/1	0.96	0.11	100,100,100,100	0
81	MG	5	3716	1/1	0.96	0.23	66,66,66,66	0
81	MG	N8	201	1/1	0.96	0.06	119,119,119,119	0
81	MG	5	3718	1/1	0.96	0.07	103,103,103,103	0
81	MG	5	3479	1/1	0.96	0.09	93,93,93,93	0
81	MG	5	3517	1/1	0.96	0.14	123,123,123,123	0
81	MG	5	3721	1/1	0.96	0.06	93,93,93,93	0
81	MG	6	1942	1/1	0.96	0.05	146,146,146,146	0
81	MG	5	3404	1/1	0.96	0.13	89,89,89,89	0
81	MG	1	3654	1/1	0.96	0.09	95,95,95,95	0
81	MG	5	3484	1/1	0.96	0.10	85,85,85,85	0
81	MG	5	3446	1/1	0.96	0.16	87,87,87,87	0
81	MG	o7	503	1/1	0.96	0.05	126,126,126,126	0
81	MG	5	3668	1/1	0.96	0.12	86,86,86,86	0
81	MG	5	3615	1/1	0.96	0.07	108,108,108,108	0
81	MG	5	3670	1/1	0.96	0.10	112,112,112,112	0
81	MG	1	3508	1/1	0.96	0.05	98,98,98,98	0
81	MG	5	3409	1/1	0.96	0.21	88,88,88,88	0
81	MG	5	3788	1/1	0.96	0.13	98,98,98,98	0
81	MG	1	3734	1/1	0.96	0.07	120,120,120,120	0
81	MG	5	3572	1/1	0.96	0.12	87,87,87,87	1
81	MG	5	3735	1/1	0.96	0.07	102,102,102,102	0
81	MG	1	3410	1/1	0.96	0.17	94,94,94,94	0
81	MG	2	1936	1/1	0.96	0.05	140,140,140,140	0
81	MG	5	3415	1/1	0.96	0.10	89,89,89,89	0
81	MG	5	3625	1/1	0.96	0.07	99,99,99,99	0
81	MG	5	3626	1/1	0.96	0.11	106,106,106,106	0
81	MG	8	201	1/1	0.96	0.11	99,99,99,99	0
81	MG	1	3428	1/1	0.96	0.09	140,140,140,140	0
81	MG	5	3683	1/1	0.96	0.12	116,116,116,116	0
81	MG	1	3546	1/1	0.96	0.07	98,98,98,98	0
81	MG	5	3533	1/1	0.96	0.13	91,91,91,91	0
81	MG	1	3558	1/1	0.96	0.19	90,90,90,90	0
81	MG	8	208	1/1	0.96	0.06	123,123,123,123	0
81	MG	L8	301	1/1	0.96	0.15	182,182,182,182	0
81	MG	5	3498	1/1	0.96	0.10	94,94,94,94	0
81	MG	O8	101	1/1	0.96	0.09	168,168,168,168	0
81	MG	1	3432	1/1	0.96	0.10	94,94,94,94	0
81	MG	1	3646	1/1	0.96	0.08	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	5	3427	1/1	0.96	0.07	85,85,85,85	0
81	MG	5	3698	1/1	0.96	0.08	80,80,80,80	0
81	MG	6	2007	1/1	0.96	0.04	148,148,148,148	0
81	MG	5	3592	1/1	0.96	0.18	97,97,97,97	0
81	MG	1	3664	1/1	0.96	0.10	99,99,99,99	0
81	MG	1	3735	1/1	0.97	0.10	98,98,98,98	0
81	MG	5	3413	1/1	0.97	0.09	97,97,97,97	0
81	MG	2	1956	1/1	0.97	0.05	130,130,130,130	0
81	MG	5	3586	1/1	0.97	0.10	80,80,80,80	0
81	MG	5	3587	1/1	0.97	0.05	95,95,95,95	0
81	MG	5	3654	1/1	0.97	0.05	96,96,96,96	0
81	MG	5	3795	1/1	0.97	0.05	104,104,104,104	1
81	MG	1	3551	1/1	0.97	0.07	138,138,138,138	0
81	MG	5	3656	1/1	0.97	0.11	96,96,96,96	0
81	MG	1	3570	1/1	0.97	0.09	92,92,92,92	0
81	MG	1	3679	1/1	0.97	0.07	102,102,102,102	0
81	MG	6	1906	1/1	0.97	0.06	119,119,119,119	0
81	MG	5	3422	1/1	0.97	0.12	91,91,91,91	0
81	MG	2	1991	1/1	0.97	0.12	182,182,182,182	0
81	MG	L5	301	1/1	0.97	0.07	135,135,135,135	0
81	MG	1	3449	1/1	0.97	0.16	100,100,100,100	0
81	MG	1	3593	1/1	0.97	0.10	91,91,91,91	0
81	MG	1	3573	1/1	0.97	0.08	92,92,92,92	0
81	MG	1	3535	1/1	0.97	0.07	153,153,153,153	0
81	MG	1	3519	1/1	0.97	0.11	94,94,94,94	0
81	MG	5	3541	1/1	0.97	0.09	91,91,91,91	0
81	MG	5	3741	1/1	0.97	0.08	92,92,92,92	0
81	MG	2	1981	1/1	0.97	0.10	135,135,135,135	0
81	MG	2	1932	1/1	0.97	0.08	137,137,137,137	0
81	MG	5	3544	1/1	0.97	0.15	81,81,81,81	0
81	MG	1	3453	1/1	0.97	0.07	98,98,98,98	0
81	MG	5	3674	1/1	0.97	0.05	98,98,98,98	0
81	MG	1	3749	1/1	0.97	0.09	80,80,80,80	0
81	MG	1	3718	1/1	0.97	0.08	83,83,83,83	0
81	MG	5	3608	1/1	0.97	0.06	108,108,108,108	1
81	MG	1	3719	1/1	0.97	0.13	86,86,86,86	0
81	MG	5	3679	1/1	0.97	0.14	98,98,98,98	0
81	MG	1	3628	1/1	0.97	0.12	83,83,83,83	0
81	MG	1	3753	1/1	0.97	0.06	129,129,129,129	0
81	MG	1	3601	1/1	0.97	0.08	95,95,95,95	0
81	MG	6	1923	1/1	0.97	0.09	119,119,119,119	0
81	MG	1	3631	1/1	0.97	0.07	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3756	1/1	0.97	0.24	94,94,94,94	0
81	MG	5	3688	1/1	0.97	0.06	140,140,140,140	0
81	MG	5	3443	1/1	0.97	0.07	89,89,89,89	0
81	MG	6	1926	1/1	0.97	0.07	121,121,121,121	0
81	MG	5	3445	1/1	0.97	0.06	86,86,86,86	0
81	MG	5	3621	1/1	0.97	0.05	98,98,98,98	0
81	MG	6	1927	1/1	0.97	0.05	123,123,123,123	0
81	MG	2	1977	1/1	0.97	0.04	134,134,134,134	0
81	MG	O2	201	1/1	0.97	0.07	101,101,101,101	0
81	MG	5	3563	1/1	0.97	0.05	140,140,140,140	0
81	MG	1	3603	1/1	0.97	0.09	84,84,84,84	0
81	MG	1	3541	1/1	0.97	0.10	119,119,119,119	0
81	MG	1	3466	1/1	0.97	0.07	111,111,111,111	0
81	MG	5	3771	1/1	0.97	0.35	93,93,93,93	0
81	MG	5	3630	1/1	0.97	0.13	86,86,86,86	0
81	MG	1	3637	1/1	0.97	0.11	89,89,89,89	0
81	MG	6	1934	1/1	0.97	0.07	124,124,124,124	0
81	MG	1	3405	1/1	0.97	0.08	108,108,108,108	0
81	MG	5	3402	1/1	0.97	0.07	88,88,88,88	0
81	MG	1	3479	1/1	0.97	0.08	122,122,122,122	0
81	MG	1	3480	1/1	0.97	0.11	127,127,127,127	1
81	MG	5	3405	1/1	0.97	0.09	88,88,88,88	0
81	MG	1	3766	1/1	0.97	0.10	104,104,104,104	0
81	MG	5	3642	1/1	0.97	0.07	116,116,116,116	0
81	MG	6	1981	1/1	0.97	0.08	133,133,133,133	0
81	MG	8	202	1/1	0.97	0.07	114,114,114,114	0
81	MG	5	3715	1/1	0.97	0.08	86,86,86,86	0
81	MG	5	3408	1/1	0.97	0.06	86,86,86,86	0
81	MG	2	1924	1/1	0.97	0.08	141,141,141,141	0
81	MG	1	3497	1/1	0.97	0.07	106,106,106,106	0
81	MG	1	3436	1/1	0.97	0.11	104,104,104,104	0
81	MG	1	3544	1/1	0.98	0.07	116,116,116,116	0
81	MG	1	3606	1/1	0.98	0.12	92,92,92,92	0
81	MG	1	3636	1/1	0.98	0.07	85,85,85,85	0
81	MG	m7	203	1/1	0.98	0.09	88,88,88,88	0
81	MG	5	3535	1/1	0.98	0.05	103,103,103,103	0
81	MG	5	3609	1/1	0.98	0.03	103,103,103,103	0
81	MG	5	3571	1/1	0.98	0.06	87,87,87,87	0
81	MG	5	3697	1/1	0.98	0.08	98,98,98,98	0
81	MG	5	3653	1/1	0.98	0.09	94,94,94,94	0
81	MG	1	3501	1/1	0.98	0.09	95,95,95,95	0
81	MG	1	3621	1/1	0.98	0.04	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3608	1/1	0.98	0.09	100,100,100,100	0
81	MG	n7	201	1/1	0.98	0.19	148,148,148,148	1
81	MG	5	3539	1/1	0.98	0.07	93,93,93,93	0
81	MG	1	3678	1/1	0.98	0.08	89,89,89,89	0
81	MG	5	3473	1/1	0.98	0.06	109,109,109,109	0
81	MG	5	3705	1/1	0.98	0.04	116,116,116,116	0
81	MG	7	201	1/1	0.98	0.09	92,92,92,92	0
81	MG	7	202	1/1	0.98	0.07	152,152,152,152	0
81	MG	1	3774	1/1	0.98	0.12	148,148,148,148	0
81	MG	1	3623	1/1	0.98	0.11	93,93,93,93	0
81	MG	1	3596	1/1	0.98	0.12	107,107,107,107	0
81	MG	5	3709	1/1	0.98	0.07	112,112,112,112	0
81	MG	5	3414	1/1	0.98	0.06	94,94,94,94	0
81	MG	5	3622	1/1	0.98	0.06	106,106,106,106	0
81	MG	5	3583	1/1	0.98	0.04	90,90,90,90	0
81	MG	2	1973	1/1	0.98	0.09	135,135,135,135	1
81	MG	1	3406	1/1	0.98	0.05	110,110,110,110	0
81	MG	5	3417	1/1	0.98	0.12	87,87,87,87	0
81	MG	5	3449	1/1	0.98	0.10	95,95,95,95	0
81	MG	1	3661	1/1	0.98	0.04	106,106,106,106	0
81	MG	5	3483	1/1	0.98	0.06	94,94,94,94	0
81	MG	1	3730	1/1	0.98	0.06	123,123,123,123	0
81	MG	8	209	1/1	0.98	0.11	111,111,111,111	0
81	MG	1	3451	1/1	0.98	0.08	89,89,89,89	0
81	MG	2	1978	1/1	0.98	0.07	138,138,138,138	0
81	MG	1	3709	1/1	0.98	0.10	114,114,114,114	0
81	MG	5	3723	1/1	0.98	0.10	92,92,92,92	0
81	MG	1	3442	1/1	0.98	0.07	133,133,133,133	0
81	MG	1	3532	1/1	0.98	0.04	113,113,113,113	0
81	MG	1	3666	1/1	0.98	0.15	107,107,107,107	0
81	MG	5	3560	1/1	0.98	0.09	133,133,133,133	0
81	MG	1	3667	1/1	0.98	0.04	110,110,110,110	0
81	MG	5	3640	1/1	0.98	0.07	84,84,84,84	0
81	MG	5	3776	1/1	0.98	0.08	93,93,93,93	0
81	MG	1	3438	1/1	0.98	0.07	109,109,109,109	0
81	MG	l3	404	1/1	0.98	0.10	85,85,85,85	0
81	MG	1	3669	1/1	0.98	0.06	98,98,98,98	0
81	MG	5	3685	1/1	0.98	0.05	126,126,126,126	0
81	MG	1	3455	1/1	0.98	0.08	89,89,89,89	0
83	ZN	E1	501	1/1	0.98	0.04	209,209,209,209	0
81	MG	1	3650	1/1	0.98	0.03	110,110,110,110	0
83	ZN	d9	101	1/1	0.98	0.04	184,184,184,184	0

Continued on next page...

Continued from previous page...

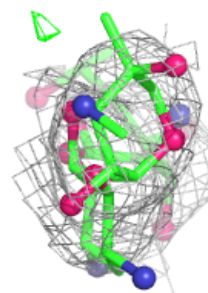
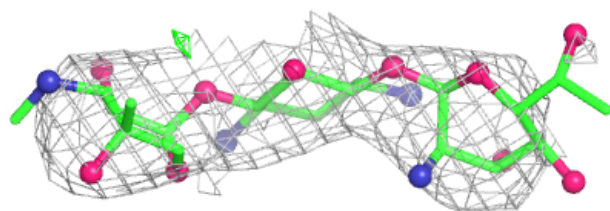
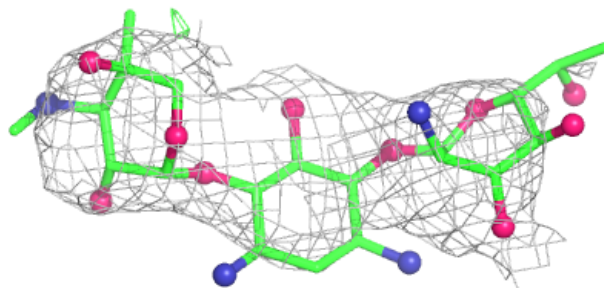
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	6	1943	1/1	0.98	0.10	157,157,157,157	0
83	ZN	q2	501	1/1	0.98	0.04	167,167,167,167	0
81	MG	5	3420	1/1	0.99	0.10	88,88,88,88	0
81	MG	1	3502	1/1	0.99	0.05	92,92,92,92	0
81	MG	1	3498	1/1	0.99	0.05	97,97,97,97	0
81	MG	5	3486	1/1	0.99	0.08	92,92,92,92	0
81	MG	1	3629	1/1	0.99	0.06	86,86,86,86	0
81	MG	5	3459	1/1	0.99	0.05	124,124,124,124	0
81	MG	1	3702	1/1	0.99	0.09	101,101,101,101	0
81	MG	5	3639	1/1	0.99	0.10	85,85,85,85	0
81	MG	5	3447	1/1	0.99	0.11	92,92,92,92	0
81	MG	5	3686	1/1	0.99	0.08	108,108,108,108	0
81	MG	5	3641	1/1	0.99	0.06	90,90,90,90	0
81	MG	5	3664	1/1	0.99	0.09	111,111,111,111	0
81	MG	5	3425	1/1	0.99	0.07	81,81,81,81	0
81	MG	5	3690	1/1	0.99	0.07	100,100,100,100	0
81	MG	1	3759	1/1	0.99	0.04	112,112,112,112	0
81	MG	1	3482	1/1	0.99	0.05	136,136,136,136	0
81	MG	1	3403	1/1	0.99	0.10	99,99,99,99	0
81	MG	1	3494	1/1	0.99	0.05	102,102,102,102	0
81	MG	5	3770	1/1	0.99	0.03	106,106,106,106	0
81	MG	5	3496	1/1	0.99	0.07	102,102,102,102	0
81	MG	5	3453	1/1	0.99	0.06	112,112,112,112	0
81	MG	5	3548	1/1	0.99	0.05	90,90,90,90	0
83	ZN	O4	500	1/1	0.99	0.03	192,192,192,192	0
83	ZN	Q2	501	1/1	0.99	0.03	170,170,170,170	0
83	ZN	Q3	501	1/1	0.99	0.03	177,177,177,177	0
83	ZN	d6	500	1/1	0.99	0.02	147,147,147,147	0
81	MG	5	3530	1/1	0.99	0.04	104,104,104,104	0
81	MG	5	3531	1/1	0.99	0.03	99,99,99,99	0
81	MG	5	3610	1/1	0.99	0.04	106,106,106,106	0
83	ZN	o4	500	1/1	0.99	0.04	143,143,143,143	0
81	MG	1	3787	1/1	0.99	0.09	157,157,157,157	0
83	ZN	q3	501	1/1	0.99	0.03	138,138,138,138	0
83	ZN	Q0	500	1/1	1.00	0.02	98,98,98,98	0
83	ZN	D9	101	1/1	1.00	0.02	124,124,124,124	0
83	ZN	D6	500	1/1	1.00	0.02	149,149,149,149	0
83	ZN	o7	501	1/1	1.00	0.07	115,115,115,115	0
83	ZN	q0	500	1/1	1.00	0.01	100,100,100,100	0
81	MG	5	3588	1/1	1.00	0.03	88,88,88,88	0
83	ZN	O7	101	1/1	1.00	0.02	130,130,130,130	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.

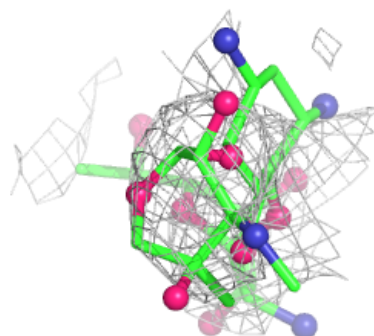
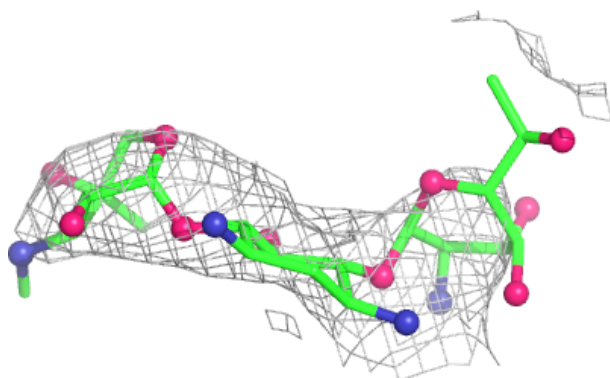
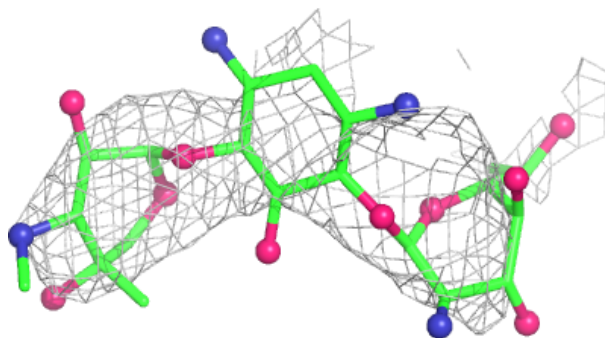
Electron density around GET 2 2014:

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

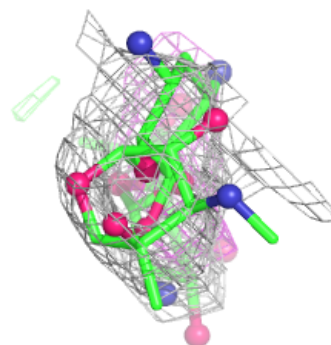
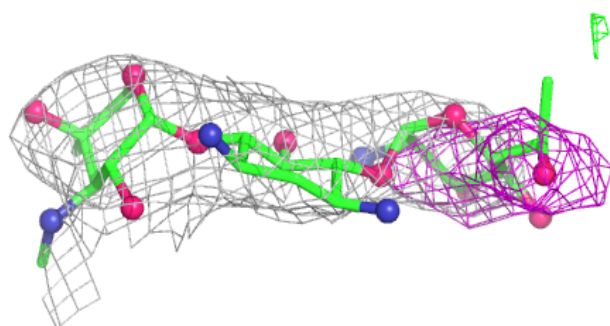
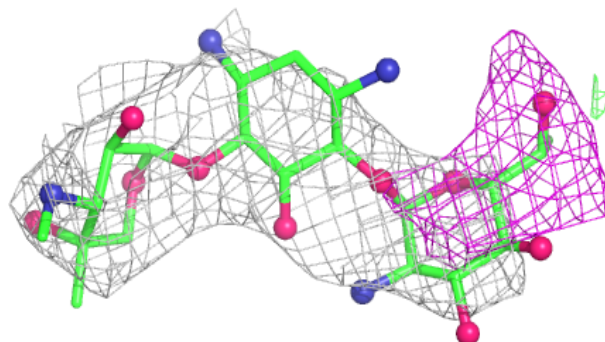


Electron density around GET 6 2015:

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

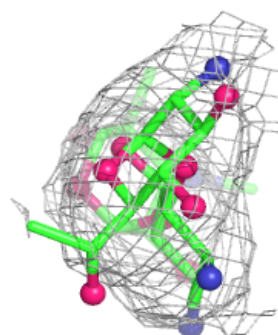
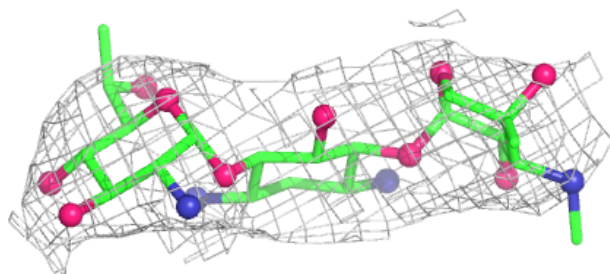
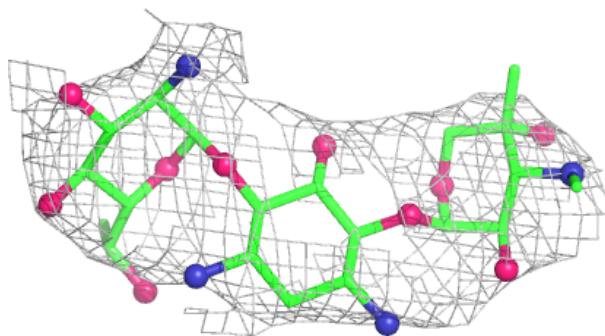
**Electron density around GET 5 3850:**

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

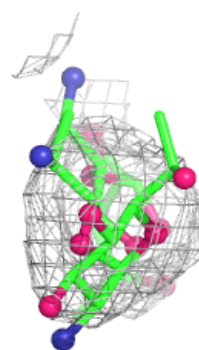
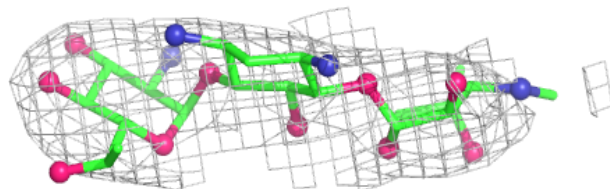
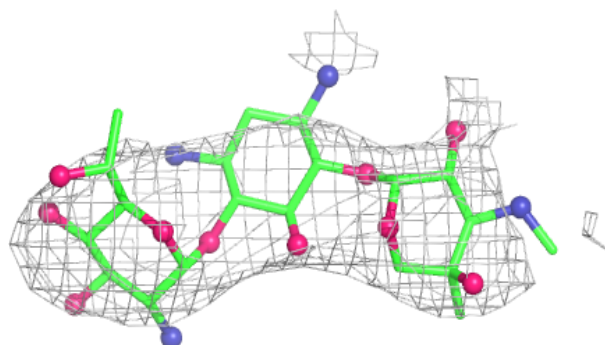


Electron density around GET 5 3851:

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

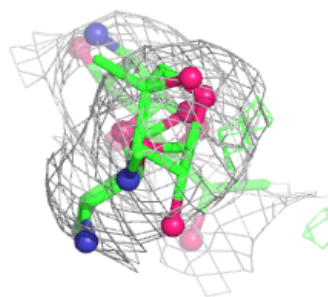
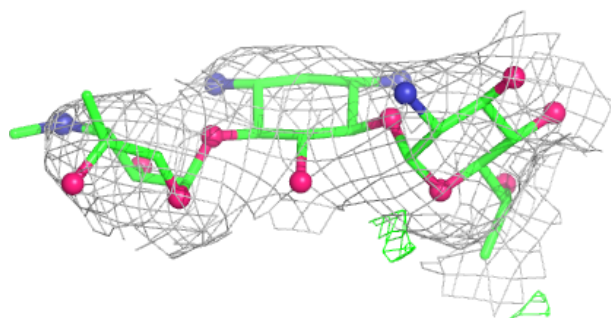
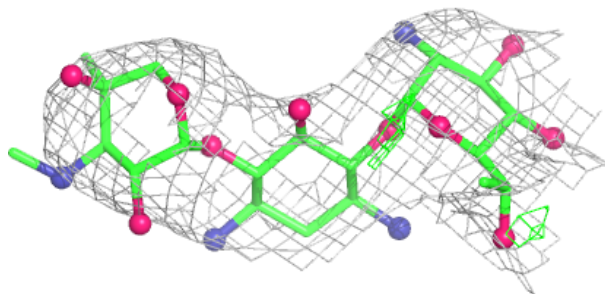
**Electron density around GET 1 3812:**

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

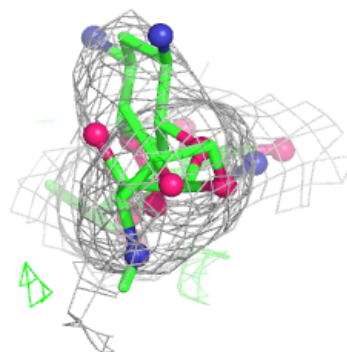
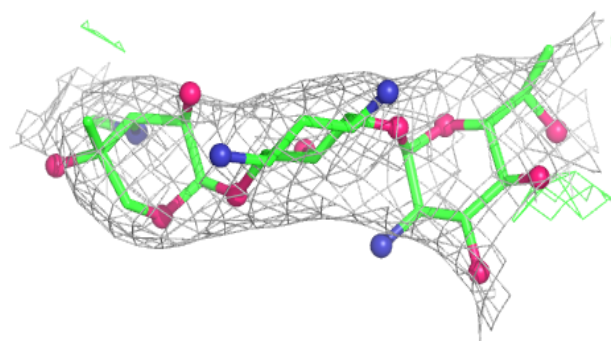
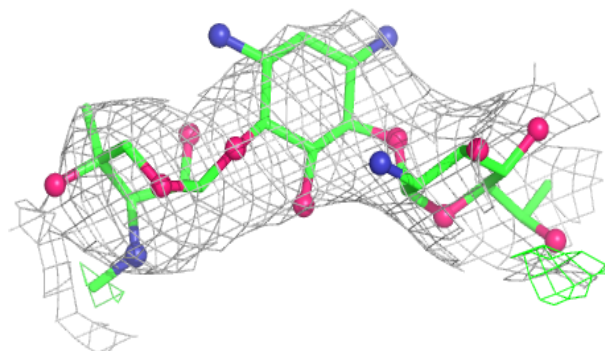


Electron density around GET 2 2013:

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

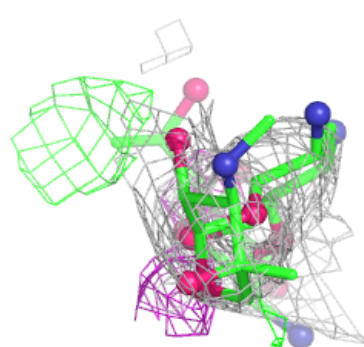
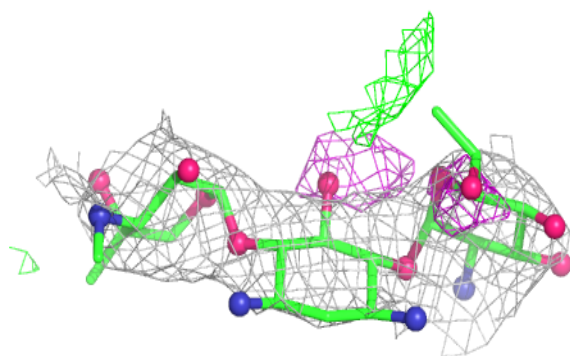
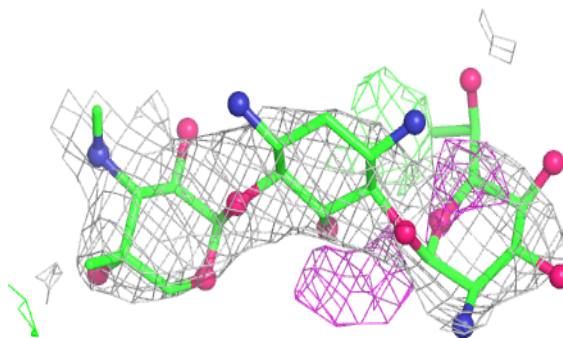
**Electron density around GET 1 3808:**

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

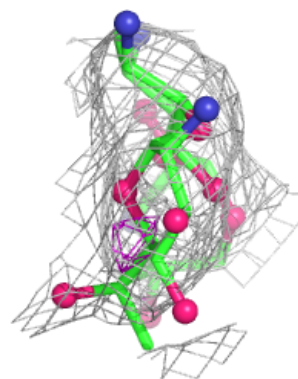
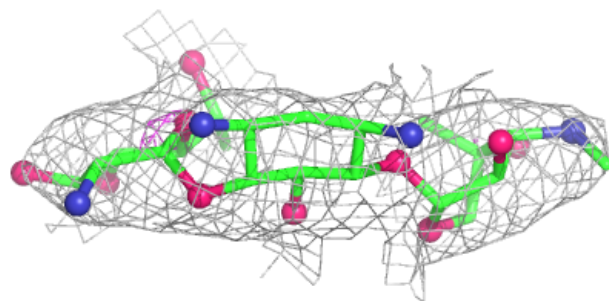
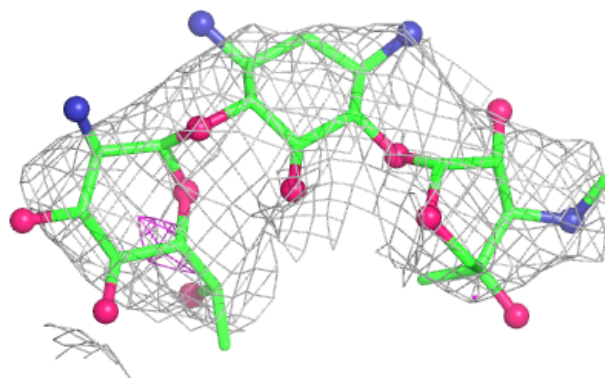


Electron density around GET 1 3809:

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

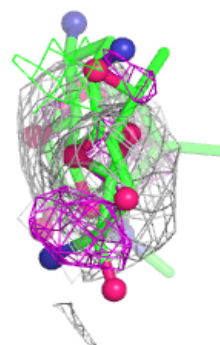
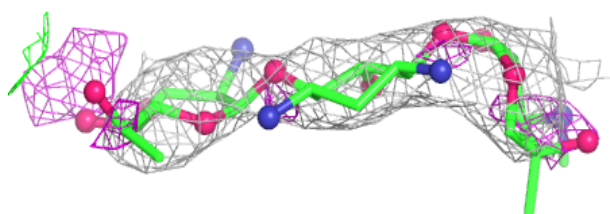
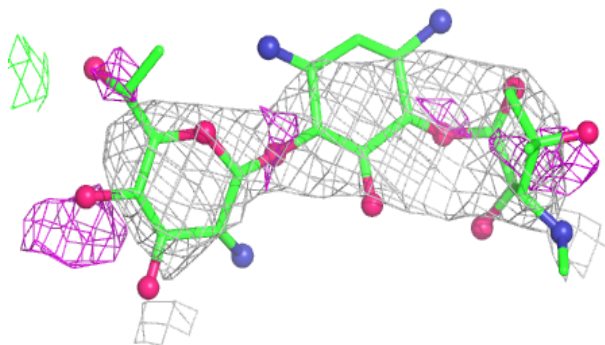
**Electron density around GET 1 3810:**

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

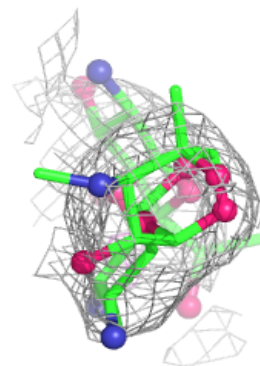
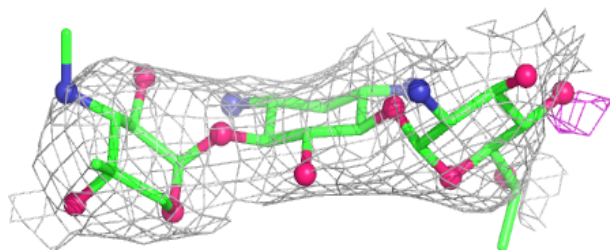
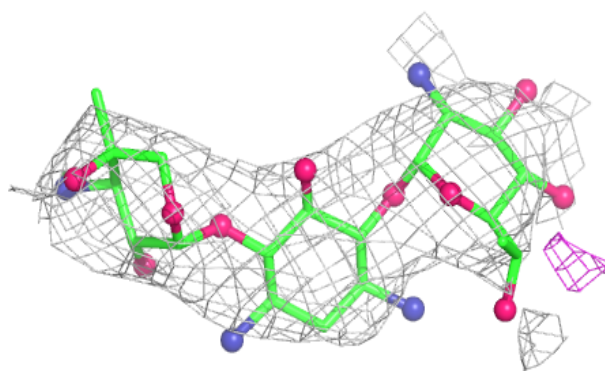


Electron density around GET 1 3813:

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

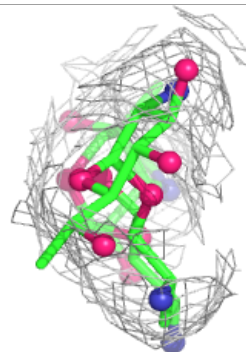
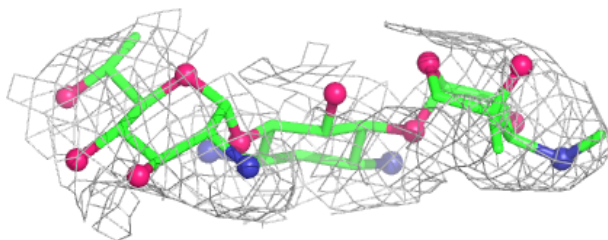
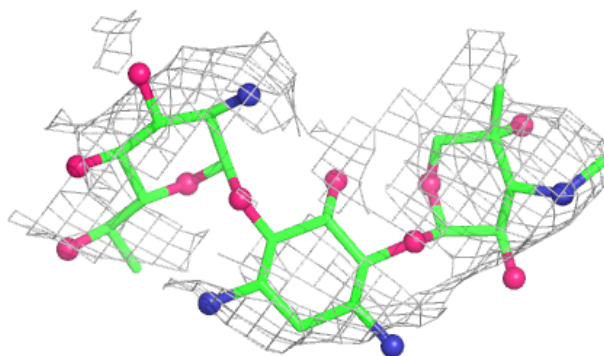
**Electron density around GET n6 201:**

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

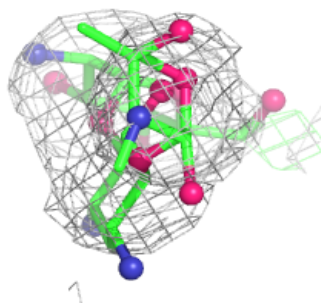
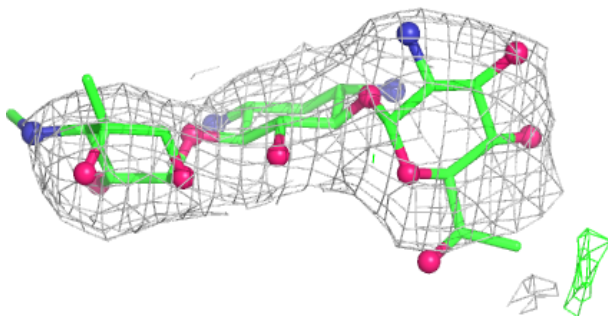
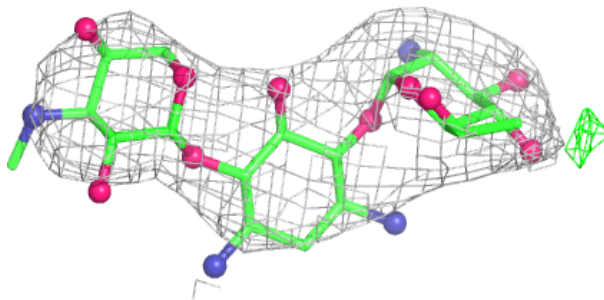


Electron density around GET 1 3811:

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

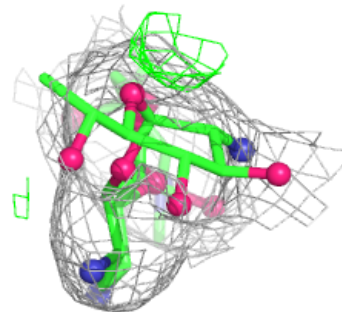
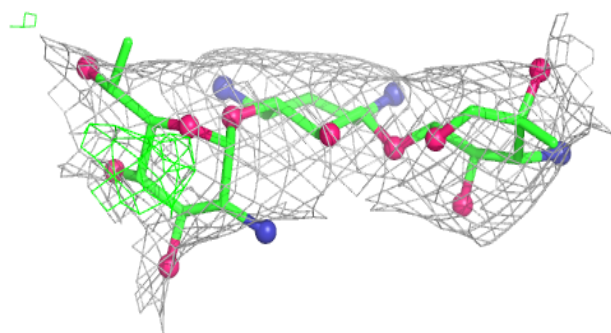
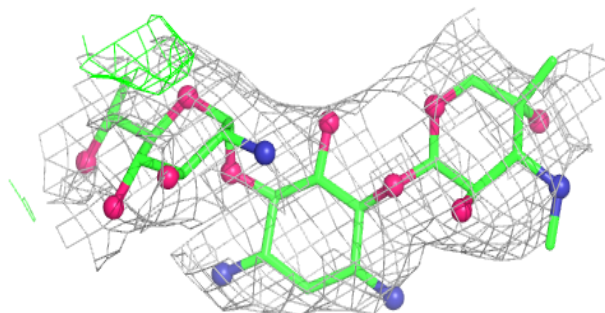
**Electron density around GET 6 2014:**

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

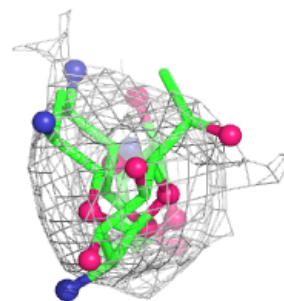
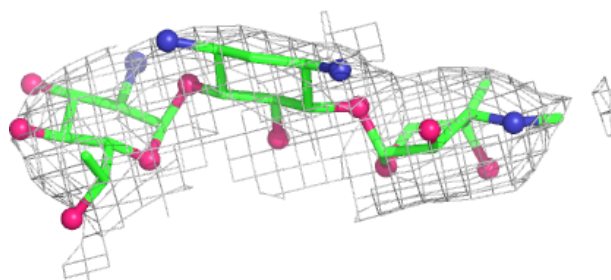
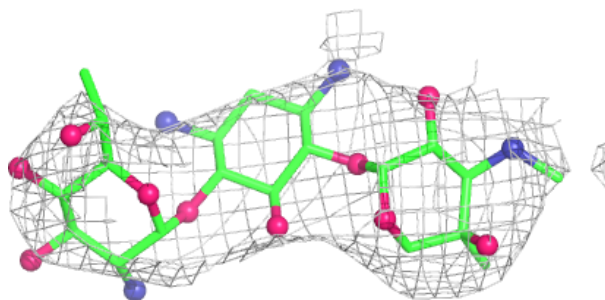


Electron density around GET 5 3844:

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

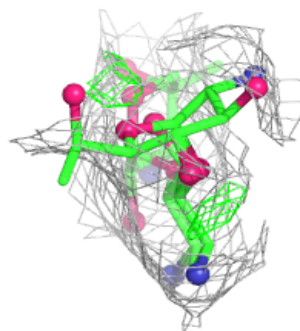
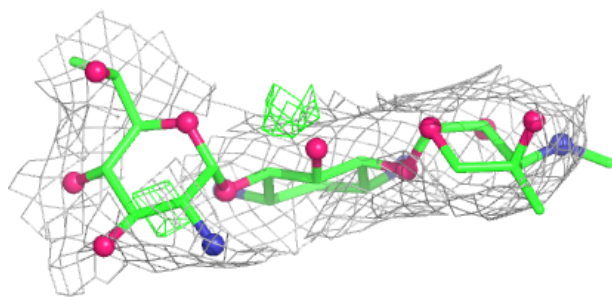
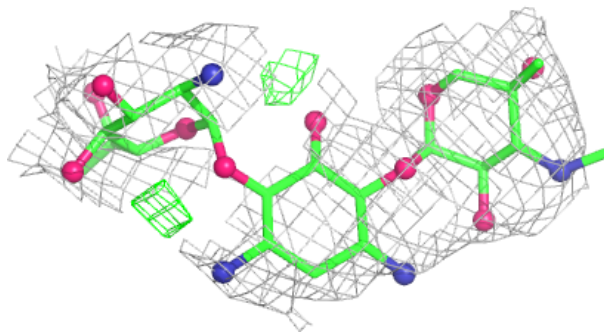
**Electron density around GET 5 3846:**

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

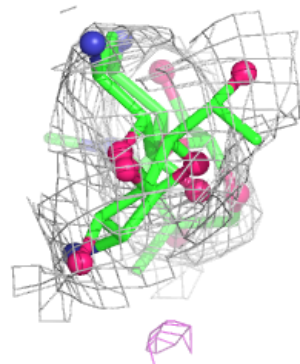
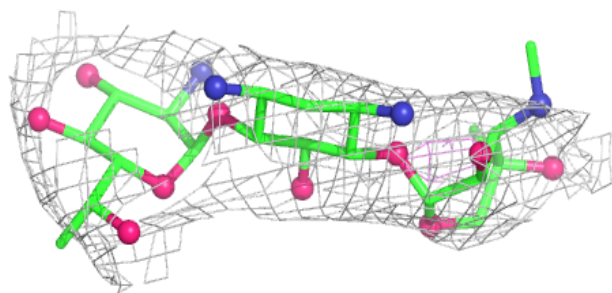
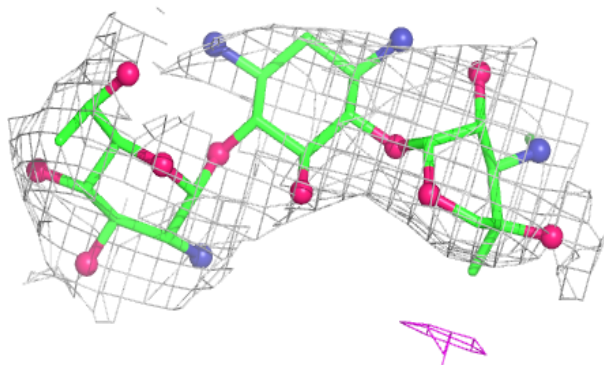


Electron density around GET 5 3848:

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

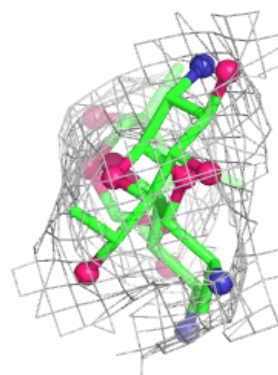
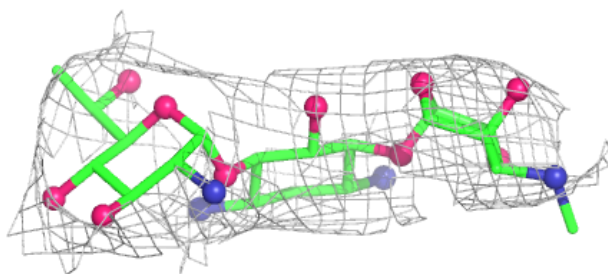
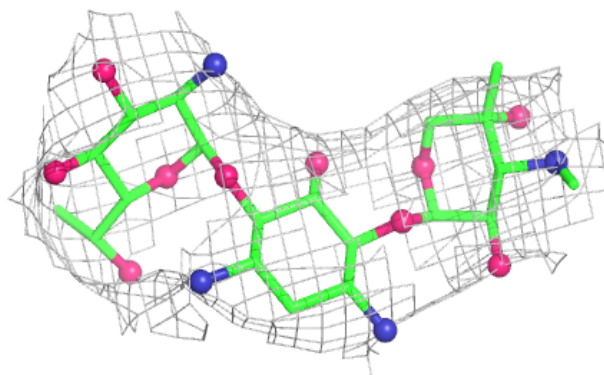
**Electron density around GET 2 2012:**

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

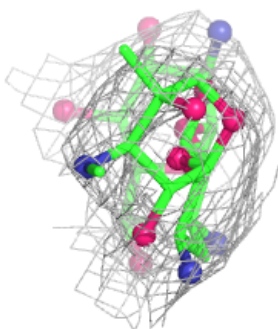
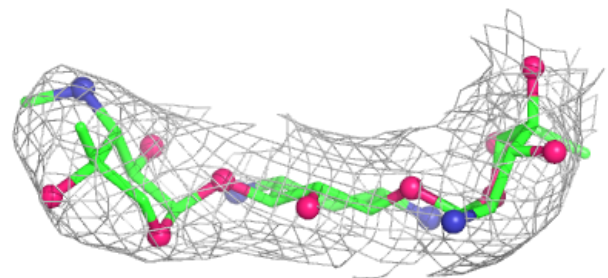
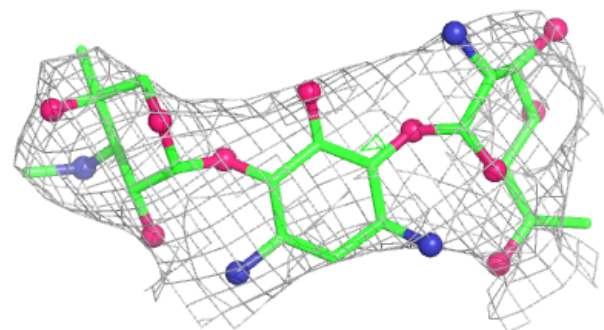


Electron density around GET 6 2013:

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

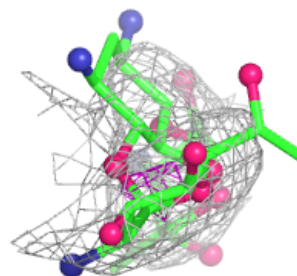
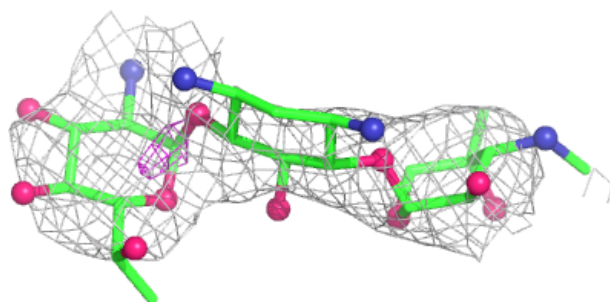
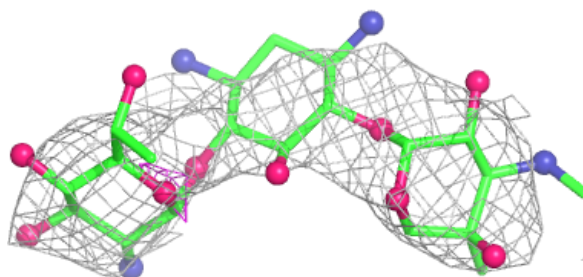
**Electron density around GET 5 3845:**

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

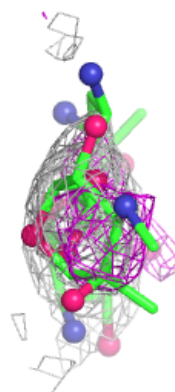
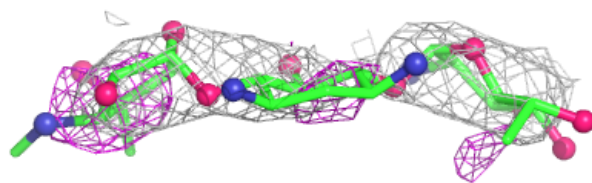
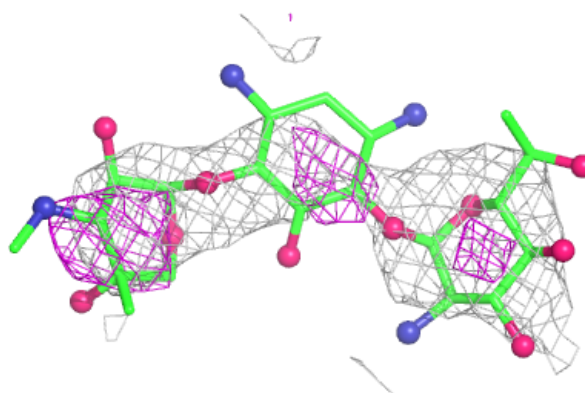


Electron density around GET 5 3847:

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

**Electron density around GET 5 3849:**

$2mF_o-DF_c$ (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.