



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 11:09 pm BST

PDB ID : 5NDV  
Title : Crystal structure of Paromomycin bound to the yeast 80S ribosome  
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2017-03-09  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

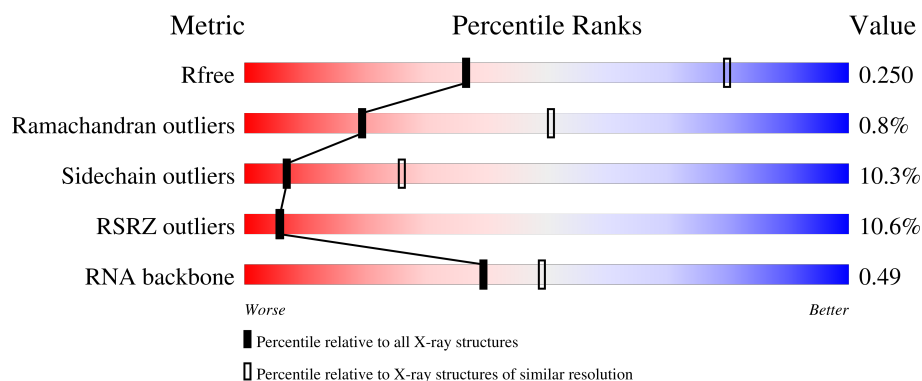
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



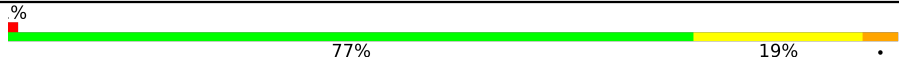
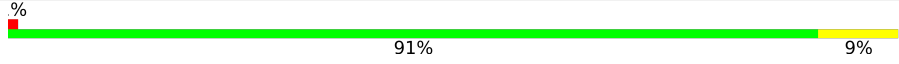
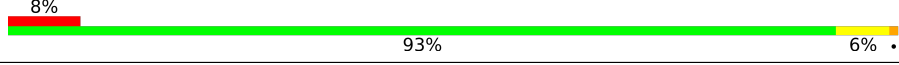
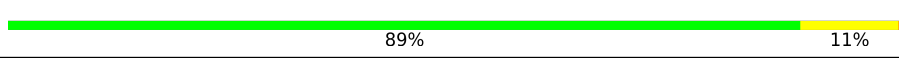
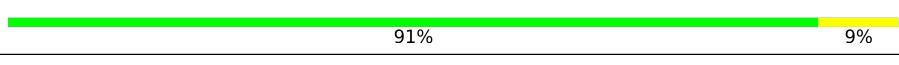
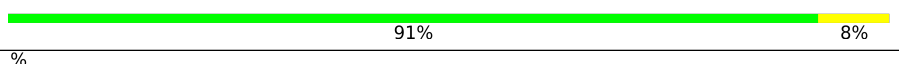
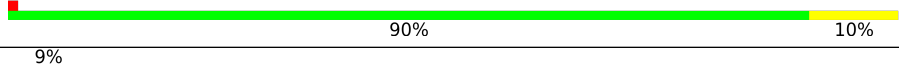
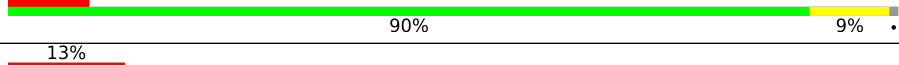
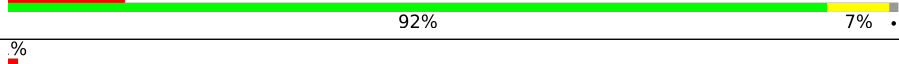



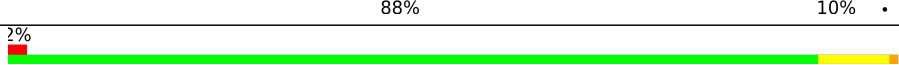
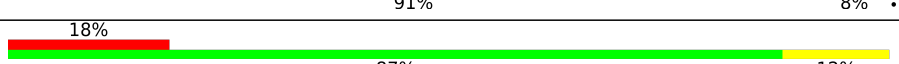

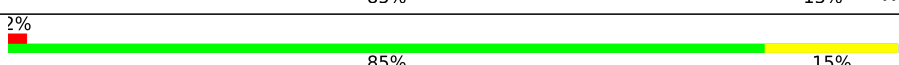
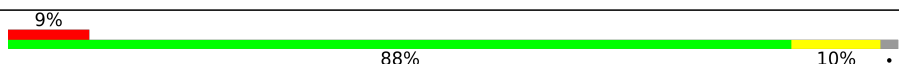

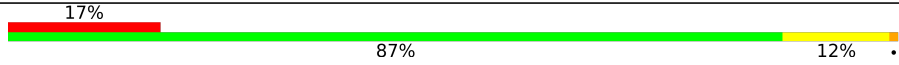

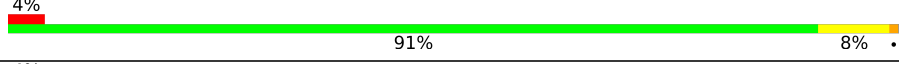
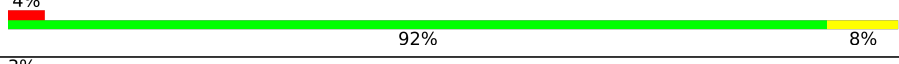
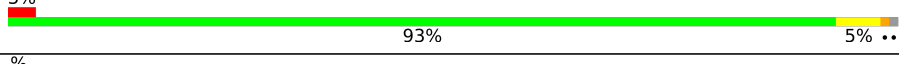
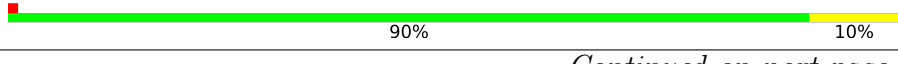

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	
1	5	3396	
2	3	121	
2	7	121	
3	4	158	

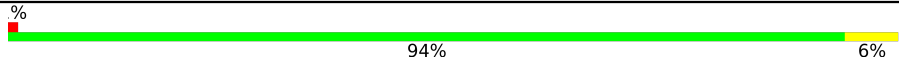
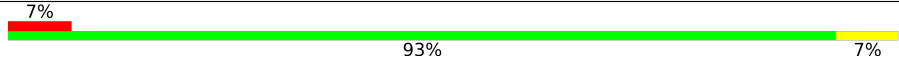
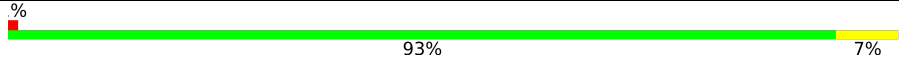
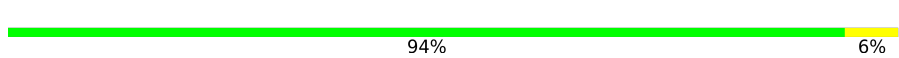


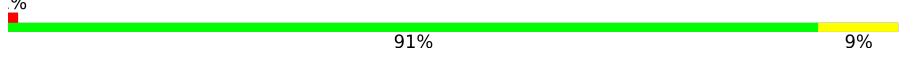
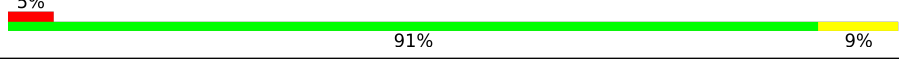

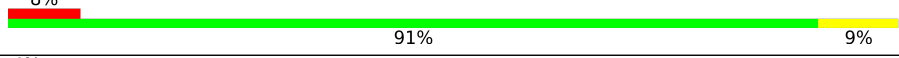

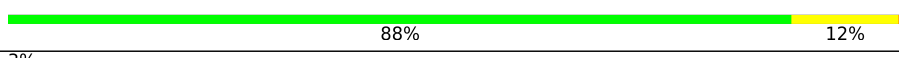
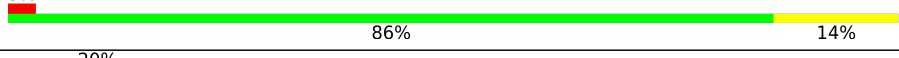
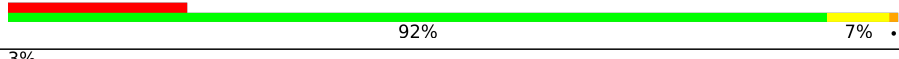
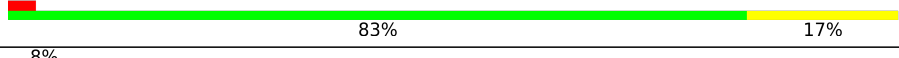
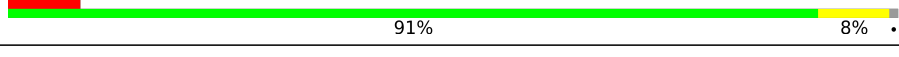
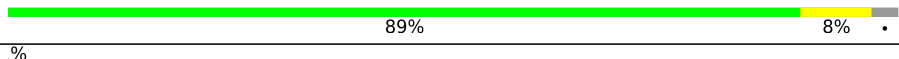
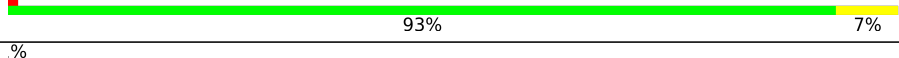




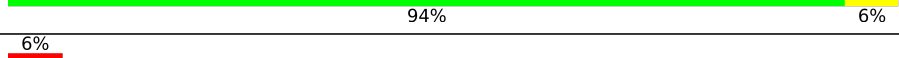
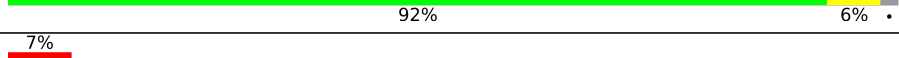
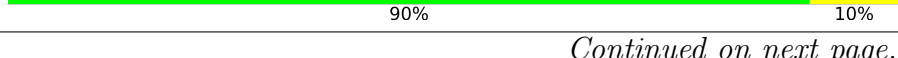
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Mol	Chain	Length	Quality of chain
3	8	158	
4	L2	248	
4	l2	248	
5	L3	386	
5	l3	386	
6	L4	361	
6	l4	361	
7	L5	296	
7	l5	296	
8	L6	176	
8	l6	176	
9	L7	226	
9	l7	226	
10	L8	231	
10	l8	231	
11	L9	191	
11	l9	191	
12	M0	221	
12	m0	221	
13	M1	169	
13	m1	169	
14	M3	194	
14	m3	194	
15	M4	137	
15	m4	137	

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Mol	Chain	Length	Quality of chain
16	M5	203	
16	m5	203	
17	M6	197	
17	m6	197	
18	M7	184	
18	m7	184	
19	M8	185	
19	m8	185	
20	M9	188	
20	m9	188	
21	N0	172	
21	n0	172	
22	N1	159	
22	n1	159	
23	N2	99	
23	n2	99	
24	N3	136	
24	n3	136	
25	N4	155	
25	n4	155	
26	N5	120	
26	n5	120	
27	N6	125	
27	n6	125	
28	N7	135	

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Mol	Chain	Length	Quality of chain
28	n7	135	
29	N8	148	
29	n8	148	
30	N9	58	
30	n9	58	
31	O0	100	
31	o0	100	
32	O1	112	
32	o1	112	
33	O2	127	
33	o2	127	
34	O3	106	
34	o3	106	
35	O4	112	
35	o4	112	
36	O5	119	
36	o5	119	
37	O6	99	
37	o6	99	
38	O7	87	
38	o7	87	
39	O8	77	
39	o8	77	
40	O9	50	
40	o9	50	

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Mol	Chain	Length	Quality of chain
41	Q0	52	
41	q0	52	
42	Q1	25	
42	q1	25	
43	Q2	105	
43	q2	105	
44	Q3	91	
44	q3	91	
45	2	1800	
45	6	1800	
46	S0	206	
46	s0	206	
47	S1	216	
47	s1	216	
48	S2	217	
48	s2	217	
49	S3	223	
49	s3	223	
50	S4	260	
50	s4	260	
51	S5	206	
51	s5	206	
52	S6	236	
53	S7	186	
53	s7	186	

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Mol	Chain	Length	Quality of chain
54	S8	200	
54	s8	200	
55	S9	185	
55	s9	185	
56	C0	105	
56	c0	105	
57	C1	146	
57	c1	146	
58	C2	143	
58	c2	143	
59	C3	150	
59	c3	150	
60	C4	128	
60	c4	128	
61	C5	141	
61	c5	141	
62	C6	142	
62	c6	142	
63	C7	136	
63	c7	136	
64	C8	145	
64	c8	145	
65	C9	143	
65	c9	143	
66	D0	109	

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Mol	Chain	Length	Quality of chain
66	d0	109	
67	D1	87	
67	d1	87	
68	D2	129	
68	d2	129	
69	D3	144	
69	d3	144	
70	D4	134	
70	d4	134	
71	D5	70	
71	d5	70	
72	D6	97	
72	d6	97	
73	D7	81	
73	d7	81	
74	D8	63	
74	d8	63	
75	D9	53	
75	d9	53	
76	E0	62	
76	e0	62	
77	SR	318	
77	sR	318	
78	SM	272	
78	sM	272	

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Mol	Chain	Length	Quality of chain
79	s6	218	<div> <div>39%</div> <div>90%</div> <div>9%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
80	PAR	5	3423	-	-	-	X
81	MG	1	3491	-	-	-	X
81	MG	1	3521	-	-	-	X
81	MG	1	3548	-	-	-	X
81	MG	1	3577	-	-	-	X
81	MG	1	3591	-	-	-	X
81	MG	1	3593	-	-	-	X
81	MG	1	3632	-	-	-	X
81	MG	1	3634	-	-	-	X
81	MG	1	3682	-	-	-	X
81	MG	1	3711	-	-	-	X
81	MG	1	3795	-	-	-	X
81	MG	1	3830	-	-	-	X
81	MG	1	3847	-	-	-	X
81	MG	1	3860	-	-	-	X
81	MG	1	3871	-	-	-	X
81	MG	1	3884	-	-	-	X
81	MG	1	3903	-	-	-	X
81	MG	1	3904	-	-	-	X
81	MG	1	3905	-	-	-	X
81	MG	1	3924	-	-	-	X
81	MG	1	3946	-	-	-	X
81	MG	1	3957	-	-	-	X
81	MG	1	3963	-	-	-	X
81	MG	1	3975	-	-	-	X
81	MG	1	3979	-	-	-	X
81	MG	1	3982	-	-	-	X
81	MG	1	3993	-	-	-	X
81	MG	1	3998	-	-	-	X
81	MG	1	4015	-	-	-	X
81	MG	1	4018	-	-	-	X
81	MG	1	4020	-	-	-	X
81	MG	1	4026	-	-	-	X
81	MG	1	4033	-	-	-	X
81	MG	1	4062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	4084	-	-	-	X
81	MG	1	4089	-	-	-	X
81	MG	1	4095	-	-	-	X
81	MG	1	4098	-	-	-	X
81	MG	1	4099	-	-	-	X
81	MG	1	4100	-	-	-	X
81	MG	1	4102	-	-	-	X
81	MG	1	4107	-	-	-	X
81	MG	1	4108	-	-	-	X
81	MG	1	4109	-	-	-	X
81	MG	1	4118	-	-	-	X
81	MG	1	4121	-	-	-	X
81	MG	1	4136	-	-	-	X
81	MG	1	4139	-	-	-	X
81	MG	1	4155	-	-	-	X
81	MG	1	4173	-	-	-	X
81	MG	1	4175	-	-	-	X
81	MG	1	4180	-	-	-	X
81	MG	1	4184	-	-	-	X
81	MG	1	4186	-	-	-	X
81	MG	1	4198	-	-	-	X
81	MG	2	1923	-	-	-	X
81	MG	2	1932	-	-	-	X
81	MG	2	1937	-	-	-	X
81	MG	2	1940	-	-	-	X
81	MG	2	1982	-	-	-	X
81	MG	2	2003	-	-	-	X
81	MG	2	2010	-	-	-	X
81	MG	2	2011	-	-	-	X
81	MG	2	2019	-	-	-	X
81	MG	2	2025	-	-	-	X
81	MG	2	2026	-	-	-	X
81	MG	2	2044	-	-	-	X
81	MG	2	2048	-	-	-	X
81	MG	2	2059	-	-	-	X
81	MG	2	2061	-	-	-	X
81	MG	2	2094	-	-	-	X
81	MG	2	2103	-	-	-	X
81	MG	2	2111	-	-	-	X
81	MG	2	2113	-	-	-	X
81	MG	5	3529	-	-	-	X
81	MG	5	3535	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3536	-	-	-	X
81	MG	5	3537	-	-	-	X
81	MG	5	3561	-	-	-	X
81	MG	5	3658	-	-	-	X
81	MG	5	3677	-	-	-	X
81	MG	5	3679	-	-	-	X
81	MG	5	3681	-	-	-	X
81	MG	5	3685	-	-	-	X
81	MG	5	3690	-	-	-	X
81	MG	5	3700	-	-	-	X
81	MG	5	3701	-	-	-	X
81	MG	5	3708	-	-	-	X
81	MG	5	3729	-	-	-	X
81	MG	5	3769	-	-	-	X
81	MG	5	3793	-	-	-	X
81	MG	5	3794	-	-	-	X
81	MG	5	3826	-	-	-	X
81	MG	5	3827	-	-	-	X
81	MG	5	3828	-	-	-	X
81	MG	5	3839	-	-	-	X
81	MG	5	3840	-	-	-	X
81	MG	5	3841	-	-	-	X
81	MG	5	3842	-	-	-	X
81	MG	5	3844	-	-	-	X
81	MG	5	3845	-	-	-	X
81	MG	5	3846	-	-	-	X
81	MG	5	3853	-	-	-	X
81	MG	5	3878	-	-	-	X
81	MG	5	3910	-	-	-	X
81	MG	5	3915	-	-	-	X
81	MG	5	3927	-	-	-	X
81	MG	5	3928	-	-	-	X
81	MG	5	3951	-	-	-	X
81	MG	5	3952	-	-	-	X
81	MG	5	3953	-	-	-	X
81	MG	5	3959	-	-	-	X
81	MG	5	3966	-	-	-	X
81	MG	5	3983	-	-	-	X
81	MG	5	3985	-	-	-	X
81	MG	5	3987	-	-	-	X
81	MG	5	3989	-	-	-	X
81	MG	5	3994	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3998	-	-	-	X
81	MG	5	3999	-	-	-	X
81	MG	5	4000	-	-	-	X
81	MG	5	4003	-	-	-	X
81	MG	5	4012	-	-	-	X
81	MG	5	4013	-	-	-	X
81	MG	5	4019	-	-	-	X
81	MG	5	4025	-	-	-	X
81	MG	5	4038	-	-	-	X
81	MG	5	4057	-	-	-	X
81	MG	5	4058	-	-	-	X
81	MG	5	4059	-	-	-	X
81	MG	5	4062	-	-	-	X
81	MG	5	4066	-	-	-	X
81	MG	5	4067	-	-	-	X
81	MG	5	4068	-	-	-	X
81	MG	5	4079	-	-	-	X
81	MG	5	4082	-	-	-	X
81	MG	5	4085	-	-	-	X
81	MG	5	4090	-	-	-	X
81	MG	5	4091	-	-	-	X
81	MG	5	4098	-	-	-	X
81	MG	5	4099	-	-	-	X
81	MG	5	4100	-	-	-	X
81	MG	5	4105	-	-	-	X
81	MG	5	4111	-	-	-	X
81	MG	5	4115	-	-	-	X
81	MG	5	4116	-	-	-	X
81	MG	6	1921	-	-	-	X
81	MG	6	1922	-	-	-	X
81	MG	6	1937	-	-	-	X
81	MG	6	1966	-	-	-	X
81	MG	6	1986	-	-	-	X
81	MG	6	2011	-	-	-	X
81	MG	6	2013	-	-	-	X
81	MG	6	2020	-	-	-	X
81	MG	6	2058	-	-	-	X
81	MG	6	2060	-	-	-	X
81	MG	6	2064	-	-	-	X
81	MG	6	2065	-	-	-	X
81	MG	6	2067	-	-	-	X
81	MG	6	2070	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	6	2071	-	-	-	X
81	MG	7	204	-	-	-	X
81	MG	7	211	-	-	-	X
81	MG	8	209	-	-	-	X
81	MG	8	212	-	-	-	X
81	MG	8	219	-	-	-	X
81	MG	8	220	-	-	-	X
81	MG	8	222	-	-	-	X
81	MG	8	223	-	-	-	X
81	MG	D3	202	-	-	-	X
81	MG	L3	402	-	-	-	X
81	MG	L7	302	-	-	-	X
81	MG	N8	203	-	-	-	X
81	MG	O2	202	-	-	-	X
81	MG	d3	204	-	-	-	X
81	MG	m9	204	-	-	-	X
81	MG	o2	204	-	-	-	X
81	MG	q3	502	-	-	-	X

## 2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 397978 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3078	Total	C	N	O	P	0	0	0
			65834	29406	11864	21486	3078			
1	5	3087	Total	C	N	O	P	0	0	0
			66030	29494	11905	21544	3087			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	157	Total	C	N	O	P	0	0	0
			3333	1491	584	1101	157			
3	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L2	248	Total	C	N	O	S	0	0	0
			1884	1173	382	328	1			
4	l2	248	Total	C	N	O	S	0	0	0
			1884	1173	382	328	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			
5	l3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			
6	l4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L5	293	Total	C	N	O	S	0	0	0
			2353	1489	409	453	2			
7	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L7	226	Total	C	N	O	S	0	0	0
			1818	1171	331	315	1			
9	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L8	231	Total	C	N	O	S	0	0	0
			1793	1145	321	324	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L9	189	Total	C	N	O	S	0	0	0
			1502	953	272	273	4			
11	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M0	217	Total	C	N	O	S	0	0	0
			1759	1114	333	305	7			
12	m0	219	Total	C	N	O	S	0	0	0
			1773	1122	336	308	7			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	M7	175	Total	C	N	O	0	0	0
			1378	856	273	249			
18	m7	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	M9	185	Total	C	N	O	0	0	0
			1499	923	323	253			
20	m9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	N2	99	Total	C	N	O		0	0	0
			787	511	129	147				
23	n2	98	Total	C	N	O		0	0	0
			778	505	127	146				

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	N3	132	Total	C	N	O	S	0	0	0
			981	617	184	173	7			
24	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	N4	63	Total	C	N	O	S	0	0	0
			521	336	102	82	1			
25	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	N5	118	Total	C	N	O	S	0	0	0
			946	608	166	170	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	N6	125	Total	C	N	O		0	0	0
			984	620	191	173				
27	n6	123	Total	C	N	O		0	0	0
			967	608	188	171				

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	O1	106	Total	C	N	O	S	0	0	0
			849	541	164	143	1			
32	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	O2	125	Total	C	N	O	S	0	0	0
			1007	638	203	165	1			
33	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	O4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			
35	o4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	O6	97	Total	C	N	O	S	0	0	0
			750	469	149	130	2			
37	o6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	O7	84	Total	C	N	O	S	0	0	0
			665	405	145	110	5			
38	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-B.

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

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	2	1712	Total	C	N	O	P	0	0	0
			36485	16312	6462	11999	1712			
45	6	1683	Total	C	N	O	P	0	0	0
			35865	16035	6355	11792	1683			

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	S0	206	Total	C	N	O	S	0	0	0
			1581	1017	278	284	2			
46	s0	206	Total	C	N	O	S	0	0	0
			1581	1017	278	284	2			

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	S1	211	Total	C	N	O	S	0	0	0
			1688	1071	305	308	4			
47	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 48 is a protein called 40S ribosomal protein S2.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	S3	209	Total	C	N	O	S	0	0	0
			1621	1028	297	290	6			
49	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	S4	256	Total	C	N	O	S	0	0	0
			2044	1300	385	356	3			
50	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	S6	200	Total	C	N	O	S	0	0	0
			1593	997	313	280	3			

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	S7	179	Total	C	N	O	0	0	0
			1442	926	259	257			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	s7	186	Total	C	N	O	0	0	0
			1492	957	267	268			

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	S9	174	Total	C	N	O	S	0	0	0
			1418	900	273	244	1			
55	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	C0	90	Total	C	N	O	S	0	0	0
			742	481	120	139	2			
56	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	C1	139	Total	C	N	O	S	0	0	0
			1127	724	214	186	3			
57	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	C2	102	Total	C	N	O	S	0	0	0
			764	485	132	145	2			
58	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 59 is a protein called 40S ribosomal protein S13.

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

- Molecule 60 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	C5	116	Total	C	N	O	S	0	0	0
			918	583	171	157	7			
61	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	C6	136	Total	C	N	O	0	0	0
			1064	682	195	187			
62	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	C7	115	Total	C	N	O	S	0	0	0
			901	562	172	165	2			
63	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	C8	143	Total	C	N	O	S	0	0	0
			1178	734	235	207	2			
64	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	C9	137	Total	C	N	O	S	0	0	0
			1072	669	202	199	2			
65	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 66 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	D0	102	Total	C	N	O	S	0	0	0
			818	519	148	150	1			
66	d0	109	Total	C	N	O	S	0	0	0
			873	549	159	164	1			

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

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

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

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	D9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			
75	d9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
76	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 77 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	SR	317	Total	C	N	O	S	0	0	0
			2432	1537	416	471	8			
77	sR	318	Total	C	N	O	S	0	0	0
			2437	1540	417	472	8			

- Molecule 78 is a protein called Suppressor protein STM1.

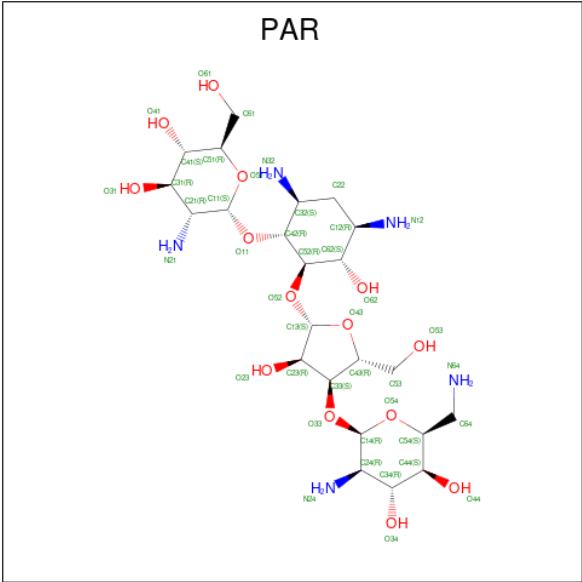
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	SM	147	Total	C	N	O		0	0	0
			1044	616	209	219				
78	sM	95	Total	C	N	O		0	0	0
			635	376	131	128				

- Molecule 79 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 80 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	1	1	Total 42	C 23	N 5	O 14	0	0
80	1	1	Total 42	C 23	N 5	O 14	0	0
80	3	1	Total 42	C 23	N 5	O 14	0	0
80	3	1	Total 42	C 23	N 5	O 14	0	0
80	3	1	Total 42	C 23	N 5	O 14	0	0
80	4	1	Total 42	C 23	N 5	O 14	0	0
80	4	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	2	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0
80	5	1	Total 42	C 23	N 5	O 14	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	7	1	Total	C	N	O	0	0
			42	23	5	14		
80	7	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	8	1	Total	C	N	O	0	0
			42	23	5	14		
80	8	1	Total	C	N	O	0	0
			42	23	5	14		
80	n3	1	Total	C	N	O	0	0
			42	23	5	14		
80	o2	1	Total	C	N	O	0	0
			42	23	5	14		
80	6	1	Total	C	N	O	0	0
			42	23	5	14		
80	6	1	Total	C	N	O	0	0
			42	23	5	14		
80	6	1	Total	C	N	O	0	0
			42	23	5	14		
80	6	1	Total	C	N	O	0	0
			42	23	5	14		
80	6	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	1	762	Total	Mg	0	0
			762	762		
81	3	15	Total	Mg	0	0
			15	15		
81	4	35	Total	Mg	0	0
			35	35		
81	L2	6	Total	Mg	0	0
			6	6		
81	L3	5	Total	Mg	0	0
			5	5		
81	L4	3	Total	Mg	0	0
			3	3		
81	L5	3	Total	Mg	0	0
			3	3		
81	L7	2	Total	Mg	0	0
			2	2		
81	L8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	L9	4	Total 4	Mg 4	0	0
81	M0	1	Total 1	Mg 1	0	0
81	M3	1	Total 1	Mg 1	0	0
81	M4	3	Total 3	Mg 3	0	0
81	M5	9	Total 9	Mg 9	0	0
81	M6	5	Total 5	Mg 5	0	0
81	M7	6	Total 6	Mg 6	0	0
81	M8	2	Total 2	Mg 2	0	0
81	M9	2	Total 2	Mg 2	0	0
81	N0	1	Total 1	Mg 1	0	0
81	N1	3	Total 3	Mg 3	0	0
81	N3	4	Total 4	Mg 4	0	0
81	N5	1	Total 1	Mg 1	0	0
81	N6	5	Total 5	Mg 5	0	0
81	N7	2	Total 2	Mg 2	0	0
81	N8	3	Total 3	Mg 3	0	0
81	O0	1	Total 1	Mg 1	0	0
81	O1	3	Total 3	Mg 3	0	0
81	O2	3	Total 3	Mg 3	0	0
81	O3	2	Total 2	Mg 2	0	0
81	O4	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	O6	1	Total 1	Mg 1	0	0
81	O7	4	Total 4	Mg 4	0	0
81	O9	1	Total 1	Mg 1	0	0
81	Q1	1	Total 1	Mg 1	0	0
81	Q2	5	Total 5	Mg 5	0	0
81	Q3	2	Total 2	Mg 2	0	0
81	2	212	Total 212	Mg 212	0	0
81	S2	2	Total 2	Mg 2	0	0
81	S6	1	Total 1	Mg 1	0	0
81	S7	1	Total 1	Mg 1	0	0
81	S9	1	Total 1	Mg 1	0	0
81	C8	1	Total 1	Mg 1	0	0
81	C9	2	Total 2	Mg 2	0	0
81	D3	2	Total 2	Mg 2	0	0
81	D6	1	Total 1	Mg 1	0	0
81	5	698	Total 698	Mg 698	0	0
81	7	12	Total 12	Mg 12	0	0
81	8	23	Total 23	Mg 23	0	0
81	l2	3	Total 3	Mg 3	0	0
81	l3	9	Total 9	Mg 9	0	0
81	l4	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	l7	6	Total 6	Mg 6	0	0
81	l8	1	Total 1	Mg 1	0	0
81	l9	1	Total 1	Mg 1	0	0
81	m0	3	Total 3	Mg 3	0	0
81	m5	2	Total 2	Mg 2	0	0
81	m6	4	Total 4	Mg 4	0	0
81	m7	9	Total 9	Mg 9	0	0
81	m8	1	Total 1	Mg 1	0	0
81	m9	5	Total 5	Mg 5	0	0
81	n0	6	Total 6	Mg 6	0	0
81	n1	2	Total 2	Mg 2	0	0
81	n2	1	Total 1	Mg 1	0	0
81	n3	3	Total 3	Mg 3	0	0
81	n5	1	Total 1	Mg 1	0	0
81	n6	4	Total 4	Mg 4	0	0
81	n8	4	Total 4	Mg 4	0	0
81	n9	1	Total 1	Mg 1	0	0
81	o0	3	Total 3	Mg 3	0	0
81	o1	3	Total 3	Mg 3	0	0
81	o2	3	Total 3	Mg 3	0	0
81	o3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	o4	1	Total 1	Mg 1	0	0
81	o7	2	Total 2	Mg 2	0	0
81	q0	1	Total 1	Mg 1	0	0
81	q2	1	Total 1	Mg 1	0	0
81	q3	1	Total 1	Mg 1	0	0
81	6	169	Total 169	Mg 169	0	0
81	s2	1	Total 1	Mg 1	0	0
81	s4	1	Total 1	Mg 1	0	0
81	s6	2	Total 2	Mg 2	0	0
81	s8	1	Total 1	Mg 1	0	0
81	c1	1	Total 1	Mg 1	0	0
81	c4	3	Total 3	Mg 3	0	0
81	c9	2	Total 2	Mg 2	0	0
81	d2	1	Total 1	Mg 1	0	0
81	d3	5	Total 5	Mg 5	0	0
81	d4	1	Total 1	Mg 1	0	0
81	d6	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	O4	1	Total 1	Zn 1	0	0
82	O7	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	Q0	1	Total 1	Zn 1	0	0
82	Q2	1	Total 1	Zn 1	0	0
82	Q3	1	Total 1	Zn 1	0	0
82	D6	1	Total 1	Zn 1	0	0
82	D7	1	Total 1	Zn 1	0	0
82	D9	1	Total 1	Zn 1	0	0
82	o4	1	Total 1	Zn 1	0	0
82	o7	1	Total 1	Zn 1	0	0
82	q0	1	Total 1	Zn 1	0	0
82	q2	1	Total 1	Zn 1	0	0
82	q3	1	Total 1	Zn 1	0	0
82	d6	1	Total 1	Zn 1	0	0
82	d7	1	Total 1	Zn 1	0	0
82	d9	1	Total 1	Zn 1	0	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	500	Total 500	O 500	0	0
83	3	7	Total 7	O 7	0	0
83	4	15	Total 15	O 15	0	0
83	L2	5	Total 5	O 5	0	0
83	L3	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	L4	2	Total 2	O 2	0	0
83	L5	1	Total 1	O 1	0	0
83	L7	1	Total 1	O 1	0	0
83	M5	2	Total 2	O 2	0	0
83	M6	2	Total 2	O 2	0	0
83	M7	4	Total 4	O 4	0	0
83	N0	2	Total 2	O 2	0	0
83	N1	1	Total 1	O 1	0	0
83	N3	3	Total 3	O 3	0	0
83	N6	2	Total 2	O 2	0	0
83	N7	2	Total 2	O 2	0	0
83	N8	2	Total 2	O 2	0	0
83	N9	2	Total 2	O 2	0	0
83	O0	1	Total 1	O 1	0	0
83	O2	2	Total 2	O 2	0	0
83	O3	2	Total 2	O 2	0	0
83	O4	1	Total 1	O 1	0	0
83	O7	1	Total 1	O 1	0	0
83	Q2	4	Total 4	O 4	0	0
83	2	122	Total 122	O 122	0	0
83	S1	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	S9	1	Total 1	O 1	0	0
83	C3	1	Total 1	O 1	0	0
83	C6	1	Total 1	O 1	0	0
83	C7	1	Total 1	O 1	0	0
83	C9	1	Total 1	O 1	0	0
83	D3	4	Total 4	O 4	0	0
83	5	477	Total 477	O 477	0	0
83	7	12	Total 12	O 12	0	0
83	8	7	Total 7	O 7	0	0
83	l2	5	Total 5	O 5	0	0
83	l3	2	Total 2	O 2	0	0
83	l5	1	Total 1	O 1	0	0
83	l7	1	Total 1	O 1	0	0
83	l9	1	Total 1	O 1	0	0
83	m0	1	Total 1	O 1	0	0
83	m6	1	Total 1	O 1	0	0
83	m7	2	Total 2	O 2	0	0
83	m9	1	Total 1	O 1	0	0
83	n0	2	Total 2	O 2	0	0
83	n1	2	Total 2	O 2	0	0
83	n3	3	Total 3	O 3	0	0

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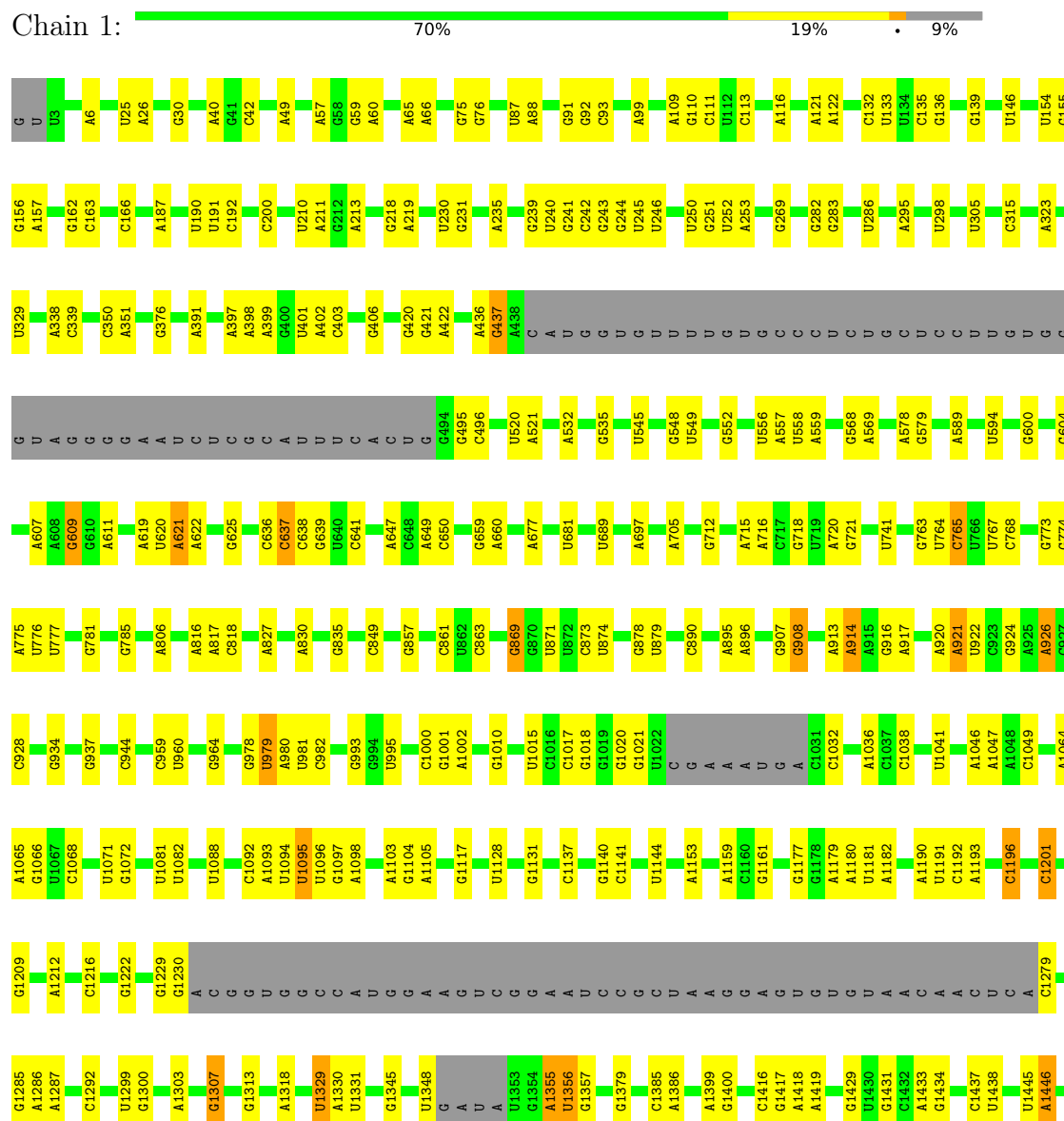
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	n6	1	Total 1	O 1	0	0
83	n7	1	Total 1	O 1	0	0
83	n8	3	Total 3	O 3	0	0
83	o2	3	Total 3	O 3	0	0
83	6	113	Total 113	O 113	0	0
83	c3	4	Total 4	O 4	0	0
83	c4	1	Total 1	O 1	0	0
83	c6	1	Total 1	O 1	0	0
83	c9	1	Total 1	O 1	0	0
83	d3	1	Total 1	O 1	0	0
83	d6	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.

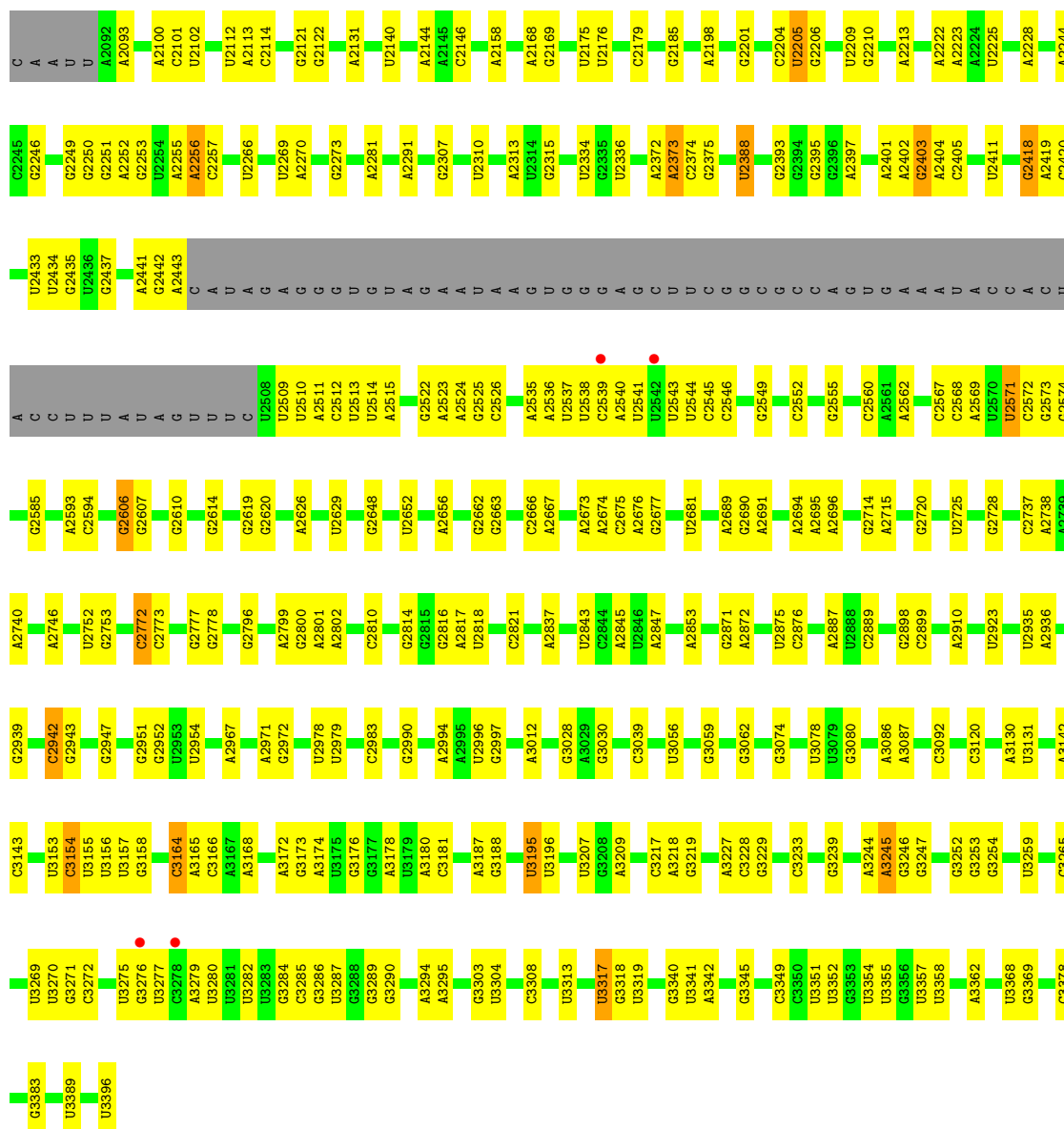
#### • Molecule 1: 25S ribosomal RNA



G3383	G3386	G3390	G3393	G3394	G3395	G3396	U3270	G3271	A3272	G3273	U3274	G3275	G3276	G3277	G3278	A3279	U3280	U3281	G3286	G3287	G3288	G3289	A3295	U3304	A3305	U3306	G3309	A3316	U3317	G3318	U3319	A3320	A3335	U3341	A3342	G3343	A3344	G3345	A3347	G3350	U3351	U3352	G3353	U3354	U3355	A3362	G3367	U3368	G3369	A3375	G3378	U3382	U3151	U3152	U3153	C	U	U	U	G3158	A3163	A3164	A3165	G3166	A3167	U3168	U3169	A3170	U3171	A3172	G3173	A3174	U3175	A3176	U3179	A3180	C3181	A3187	G3194	U3195	U3196	G3202	U3207	A3210	C3217	A3218	G3219	C3228	G3229	A3244	A3245	G3246	G3247	G3253	U3254	U3255	U3256	U3257	U3258	U3259	U3260	U3261	U3262	U3263	U3264	U3265	U3266	U3267	U3268	U3269	U3270	U3271	U3272	U3273	U3274	U3275	U3276	U3277	U3278	U3279	U3280	U3281	U3282	U3283	U3284	U3285	U3286	U3287	U3288	U3289	U3290	U3291	U3292	U3293	U3294	U3295	U3296	U3297	U3298	U3299	U3300	U3301	U3302	U3303	U3304	U3305	U3306	U3307	U3308	U3309	U3310	U3311	U3312	U3313	U3314	U3315	U3316	U3317	U3318	U3319	U3320	U3321	U3322	U3323	U3324	U3325	U3326	U3327	U3328	U3329	U3330	U3331	U3332	U3333	U3334	U3335	U3336	U3337	U3338	U3339	U3340	U3341	U3342	U3343	U3344	U3345	U3346	U3347	U3348	U3349	U3350	U3351	U3352	U3353	U3354	U3355	U3356	U3357	U3358	U3359	U3360	U3361	U3362	U3363	U3364	U3365	U3366	U3367	U3368	U3369	U3370	U3371	U3372	U3373	U3374	U3375	U3376	U3377	U3378	U3379	U3380	U3381	U3382	U3383	U3384	U3385	U3386	U3387	U3388	U3389	U3390	U3391	U3392	U3393	U3394	U3395	U3396	U3397	U3398	U3399	U3400	U3401	U3402	U3403	U3404	U3405	U3406	U3407	U3408	U3409	U3410	U3411	U3412	U3413	U3414	U3415	U3416	U3417	U3418	U3419	U3420	U3421	U3422	U3423	U3424	U3425	U3426	U3427	U3428	U3429	U3430	U3431	U3432	U3433	U3434	U3435	U3436	U3437	U3438	U3439	U3440	U3441	U3442	U3443	U3444	U3445	U3446	U3447	U3448	U3449	U3450	U3451	U3452	U3453	U3454	U3455	U3456	U3457	U3458	U3459	U3460	U3461	U3462	U3463	U3464	U3465	U3466	U3467	U3468	U3469	U3470	U3471	U3472	U3473	U3474	U3475	U3476	U3477	U3478	U3479	U3480	U3481	U3482	U3483	U3484	U3485	U3486	U3487	U3488	U3489	U3490	U3491	U3492	U3493	U3494	U3495	U3496	U3497	U3498	U3499	U3500	U3501	U3502	U3503	U3504	U3505	U3506	U3507	U3508	U3509	U3510	U3511	U3512	U3513	U3514	U3515	U3516	U3517	U3518	U3519	U3520	U3521	U3522	U3523	U3524	U3525	U3526	U3527	U3528	U3529	U3530	U3531	U3532	U3533	U3534	U3535	U3536	U3537	U3538	U3539	U3540	U3541	U3542	U3543	U3544	U3545	U3546	U3547	U3548	U3549	U3550	U3551	U3552	U3553	U3554	U3555	U3556	U3557	U3558	U3559	U3560	U3561	U3562	U3563	U3564	U3565	U3566	U3567	U3568	U3569	U3570	U3571	U3572	U3573	U3574	U3575	U3576	U3577	U3578	U3579	U3580	U3581	U3582	U3583	U3584	U3585	U3586	U3587	U3588	U3589	U3590	U3591	U3592	U3593	U3594	U3595	U3596	U3597	U3598	U3599	U3600	U3601	U3602	U3603	U3604	U3605	U3606	U3607	U3608	U3609	U3610	U3611	U3612	U3613	U3614	U3615	U3616	U3617	U3618	U3619	U3620	U3621	U3622	U3623	U3624	U3625	U3626	U3627	U3628	U3629	U3630	U3631	U3632	U3633	U3634	U3635	U3636	U3637	U3638	U3639	U3640	U3641	U3642	U3643	U3644	U3645	U3646	U3647	U3648	U3649	U3650	U3651	U3652	U3653	U3654	U3655	U3656	U3657	U3658	U3659	U3660	U3661	U3662	U3663	U3664	U3665	U3666	U3667	U3668	U3669	U3670	U3671	U3672	U3673	U3674	U3675	U3676	U3677	U3678	U3679	U3680	U3681	U3682	U3683	U3684	U3685	U3686	U3687	U3688	U3689	U3690	U3691	U3692	U3693	U3694	U3695	U3696	U3697	U3698	U3699	U3700	U3701	U3702	U3703	U3704	U3705	U3706	U3707	U3708	U3709	U3710	U3711	U3712	U3713	U3714	U3715	U3716	U3717	U3718	U3719	U3720	U3721	U3722	U3723	U3724	U3725	U3726	U3727	U3728	U3729	U3730	U3731	U3732	U3733	U3734	U3735	U3736	U3737	U3738	U3739	U3740	U3741	U3742	U3743	U3744	U3745	U3746	U3747	U3748	U3749	U3750	U3751	U3752	U3753	U3754	U3755	U3756	U3757	U3758	U3759	U3760	U3761	U3762	U3763	U3764	U3765	U3766	U3767	U3768	U3769	U3770	U3771	U3772	U3773	U3774	U3775	U3776	U3777	U3778	U3779	U3780	U3781	U3782	U3783	U3784	U3785	U3786	U3787	U3788	U3789	U3790	U3791	U3792	U3793	U3794	U3795	U3796	U3797	U3798	U3799	U3800	U3801	U3802	U3803	U3804	U3805	U3806	U3807	U3808	U3809	U3810	U3811	U3812	U3813	U3814	U3815	U3816	U3817	U3818	U3819	U3820	U3821	U3822	U3823	U3824	U3825	U3826	U3827	U3828	U3829	U3830	U3831	U3832	U3833	U3834	U3835	U3836	U3837	U3838	U3839	U3840	U3841	U3842	U3843	U3844	U3845	U3846	U3847	U3848	U3849	U3850	U3851	U3852	U3853	U3854	U3855	U3856	U3857	U3858	U3859	U3860	U3861	U3862	U3863	U3864	U3865	U3866	U3867	U3868	U3869	U3870	U3871	U3872	U3873	U3874	U3875	U3876	U3877	U3878	U3879	U3880	U3881	U3882	U3883	U3884	U3885	U3886	U3887	U3888	U3889	U3890	U3891	U3892	U3893	U3894	U3895	U3896	U3897	U3898	U3899	U3900	U3901	U3902	U3903	U3904	U3905	U3906	U3907	U3908	U3909	U3910	U3911	U3912	U3913	U3914	U3915	U3916	U3917	U3918	U3919	U3920	U3921	U3922	U3923	U3924	U3925	U3926	U3927	U3928	U3929	U3930	U3931	U3932	U3933	U3934	U3935	U3936	U3937	U3938	U3939	U3940	U3941	U3942	U3943	U3944	U3945	U3946	U3947	U3948	U3949	U3950	U3951	U3952	U3953	U3954	U3955	U3956	U3957	U3958	U3959	U3960	U3961	U3962	U3963	U3964	U3965	U3966	U3967	U3968	U3969	U3970	U3971	U3972	U3973	U3974	U3975	U3976	U3977	U3978	U3979	U3980	U3981	U3982	U3983	U3984	U3985	U3986	U3987	U3988	U3989	U3990	U3991	U3992	U3993	U3994	U3995	U3996	U3997	U3998	U3999	U4000	U4001	U4002	U4003	U4004	U4005	U4006	U4007	U4008	U4009	U4010	U4011	U4012	U4013	U4014	U4015	U4016	U4017	U4018	U4019	U4020	U4021	U4022	U4023	U4024	U4025	U4026	U4027	U4028	U4029	U4030	U4031	U4032	U4033	U4034	U4035	U4036	U4037	U4038	U4039	U4040	U4041	U4042	U4043	U4044	U4045	U4046	U4047	U4048	U4049	U4050	U4051	U4052	U4053	U4054	U4055	U4056	U4057	U4058	U4059	U4060	U4061	U4062	U4063	U4064	U4065	U4066	U4067	U4068	U4069	U4070	U4071	U4072	U4073	U4074	U4075	U4076	U4077	U4078	U4079	U4080	U4081	U4082	U4083	U4084	U4085	U4086	U4087	U4088	U4089	U4090	U4091	U4092	U4093	U4094	U4095	U4096	U4097	U4098	U4099	U4100	U4101	U4102	U4103	U4104	U4105	U4106	U4107	U4108	U4109	U4110	U4111	U4112	U4113	U4114	U4115	U4116	U4117	U4118	U4119	U4120	U4121	U4122	U4123	U4124	U4125	U4126	U4127	U4128	U4129	U4130	U4131	U4132	U4133	U4134	U4135	U4136	U4137	U4138	U4139	U4140	U4141	U4142	U4143	U4144	U4145	U4146	U4147	U4148	U4149	U4150	U4151	U4152	U4153	U4154	U4155	U4156	U4157	U4158	U4159	U4160	U4161	U4162	U4163	U4164	U4165	U4166	U4167	U4168	U4169	U4170	U4171	U4172	U4173	U4174	U4175	U4176	U4177	U4178	U4179	U4180	U4181	U4182	U4183	U4184	U4185	U4186	U4187	U4188	U4189	U4190	U4191	U4192	U4193	U4194	U4195	U4196	U4197	U4198	U4199	U4200	U4201	U4202	U4203	U4204	U4205	U4206	U4207	U4208	U4209	U4210	U4211	U4212	U4213	U4214	U4215	U4216	U4217	U4218	U4219	U4220	U4221	U4222	U4223	U4224	U4225	U4226	U4227	U4228	U4229	U4230	U4231	U4232	U4233	U4234	U4235	U4236	U4237	U4238	U4239	U4240	U4241	U4242	U4243	U4244	U4245	U4246	U4247	U4248	U4249	U4250	U4251	U4252	U4253	U4254	U4255	U4256	U4257	U4258	U4259	U4260	U4261	U4262	U4263	U4264	U4265	U4266	U4267	U4268	U4269	U4270	U4271	U4272	U4273	U4274	U4275	U4276	U4277	U4278	U4279	U4280	U4281	U4282	U4283	U4284	U4285	U4286	U4287	U4288	U4289	U4290	U4291	U4292	U4293	U4294	U4295	U4296	U4297	U4298	U4299	U4300	U4301	U4302	U4303	U4304	U4305	U4306	U4307	U4308	U4309	U4310	U4311	U4312	U4313	U4314	U4315	U4316	U4317	U4318	U4319	U4320	U4321	U4322	U4323	U4324	U4325	U4326	U4327	U4328	U4329	U4330	U4331	U4332	U4333	U4334	U4335	U4336	U4337	U4338	U4339	U4340	U4341	U4342	U4343	U4344	U4345	U4346	U4347	U4348	U4349	U4350	U4351	U4352	U4353	U4354	U4355	U4356	U4357	U4358	U4359	U4360	U4361	U4362	U4363	U4364	U4365	U4366	U4367	U4368	U4369	U4370	U4371	U4372	U4373	U4374	U4375	U4376	U4377	U4378	U4379	U4380	U4381	U4382	U4383	U4384	U4385	U4386	U4387	U4388	U4389	U4390	U4391
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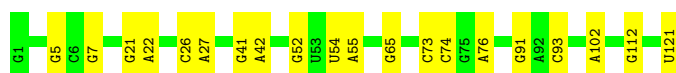


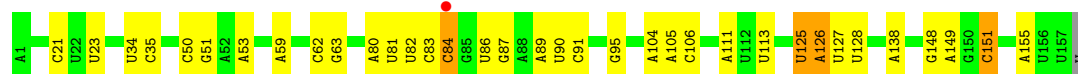
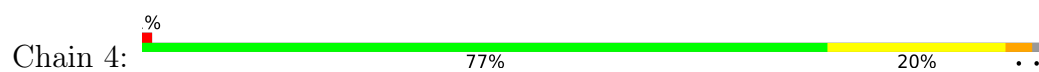




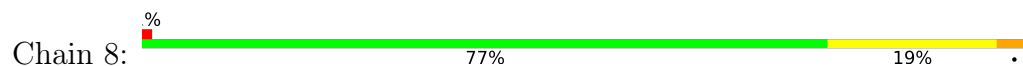
• Molecule 2: 5S ribosomal RNA

Chain 7: 83% 17%

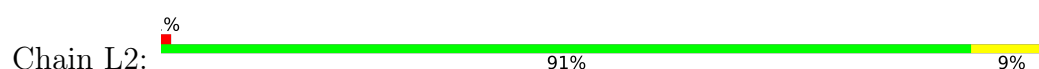




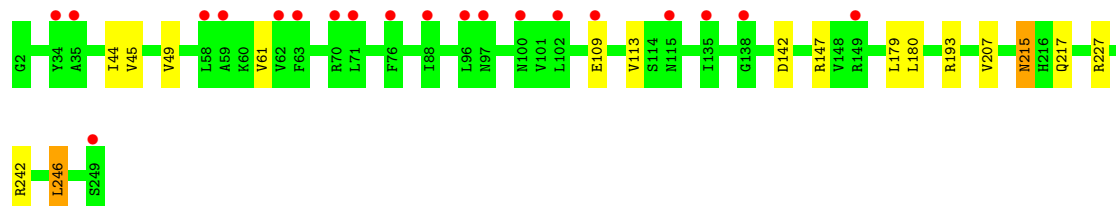
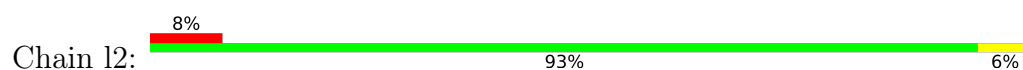
- Molecule 3: 5.8S ribosomal RNA



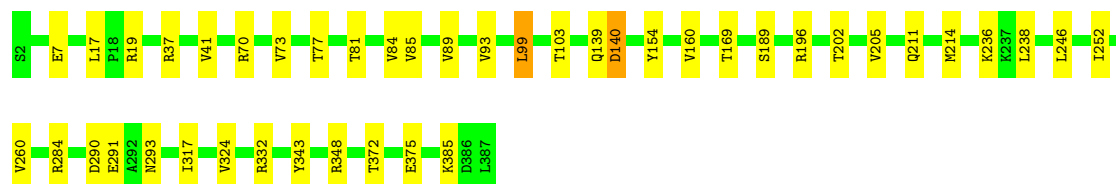
- Molecule 4: 60S ribosomal protein L2-A



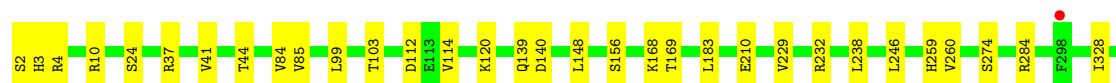
- Molecule 4: 60S ribosomal protein L2-A



- Molecule 5: 60S ribosomal protein L3



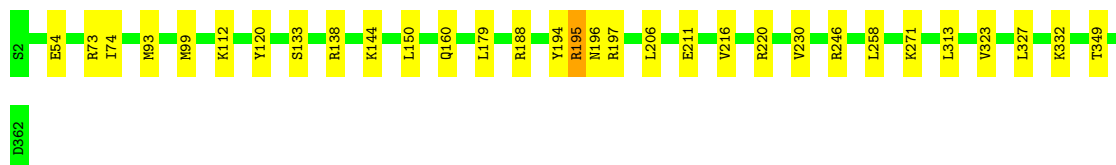
- Molecule 5: 60S ribosomal protein L3





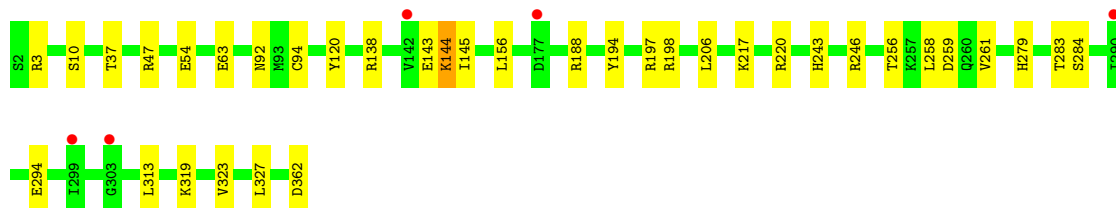
- Molecule 6: 60S ribosomal protein L4-A

Chain L4: 91% 8%



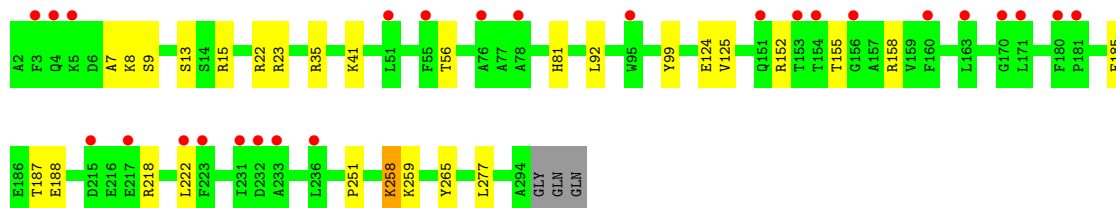
- Molecule 6: 60S ribosomal protein L4-A

Chain l4: 90% 10%



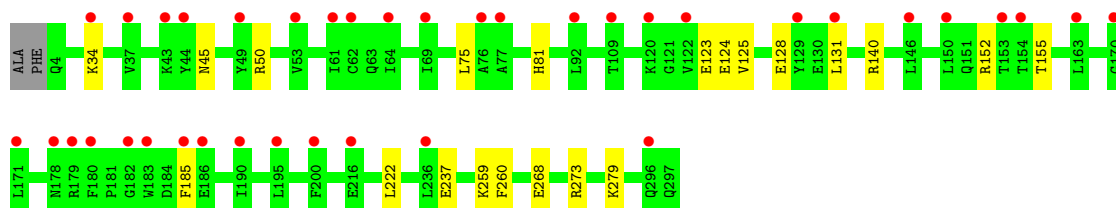
- Molecule 7: 60S ribosomal protein L5

Chain L5: 9% 90% 9%



- Molecule 7: 60S ribosomal protein L5

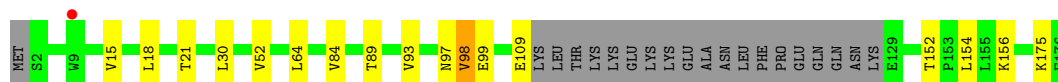
Chain l5: 13% 92% 7%



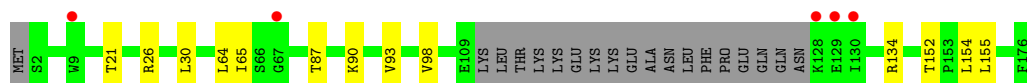
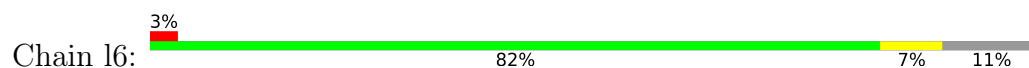
- Molecule 8: 60S ribosomal protein L6-A

Chain L6: 79% 9% 11%





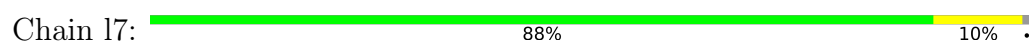
- Molecule 8: 60S ribosomal protein L6-A



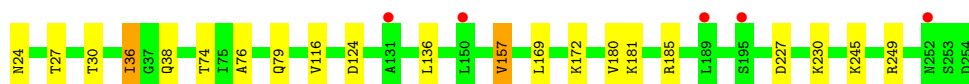
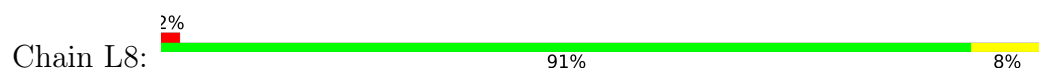
- Molecule 9: 60S ribosomal protein L7-A



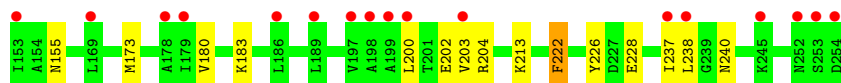
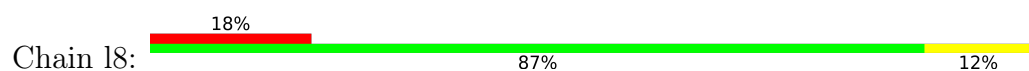
- Molecule 9: 60S ribosomal protein L7-A



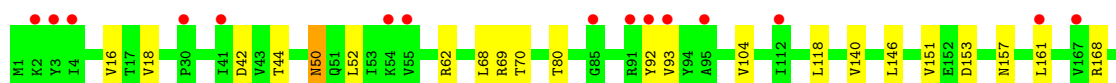
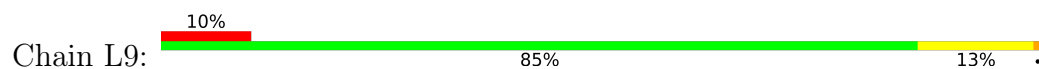
- Molecule 10: 60S ribosomal protein L8-A

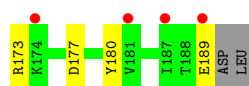


- Molecule 10: 60S ribosomal protein L8-A

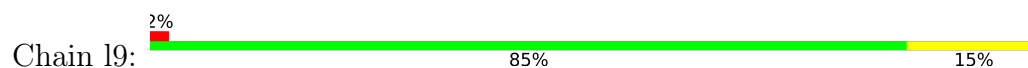


- Molecule 11: 60S ribosomal protein L9-A

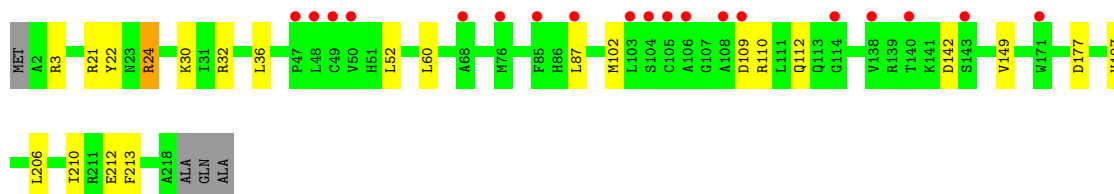




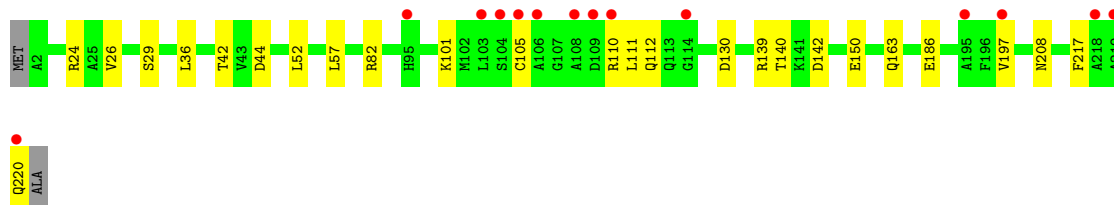
- Molecule 11: 60S ribosomal protein L9-A



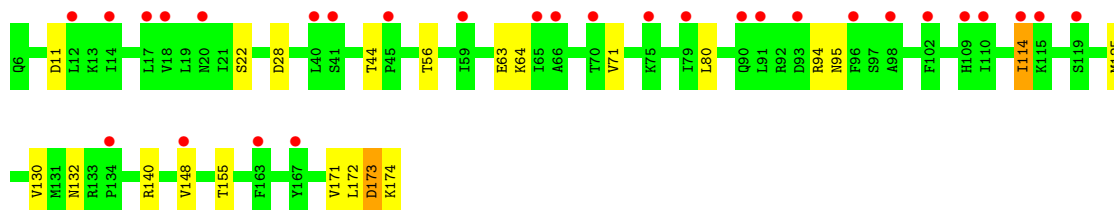
- Molecule 12: 60S ribosomal protein L10



- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-B



- Molecule 13: 60S ribosomal protein L11-B





- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



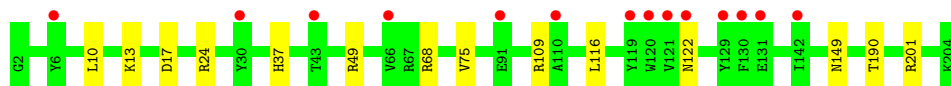
- Molecule 15: 60S ribosomal protein L14-A



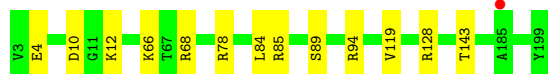
- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A



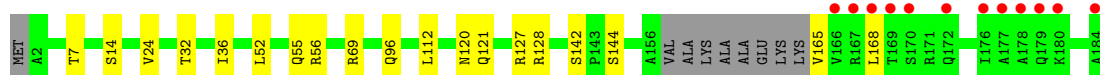
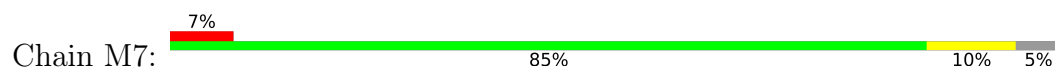
- Molecule 17: 60S ribosomal protein L16-A



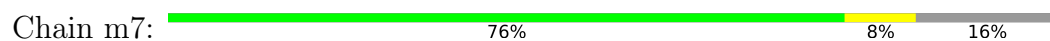
- Molecule 17: 60S ribosomal protein L16-A



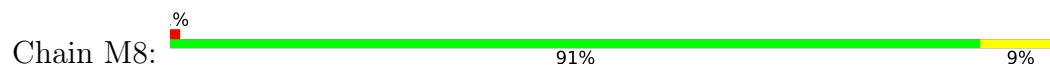
- Molecule 18: 60S ribosomal protein L17-A



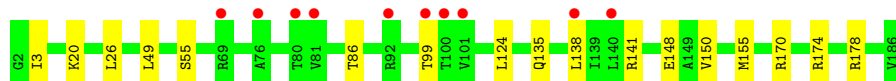
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 19: 60S ribosomal protein L18-A



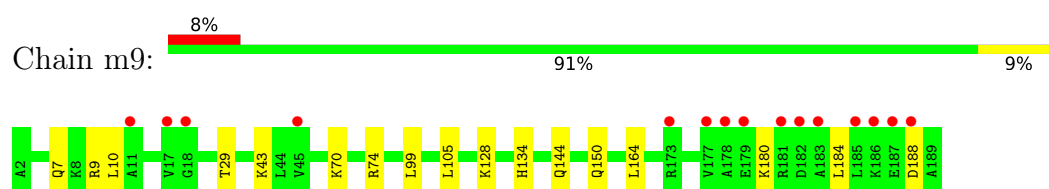
- Molecule 19: 60S ribosomal protein L18-A



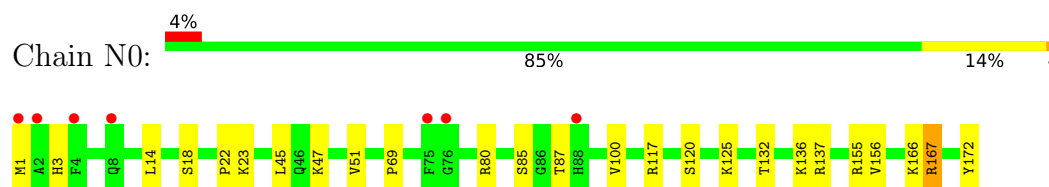
- Molecule 20: 60S ribosomal protein L19-A



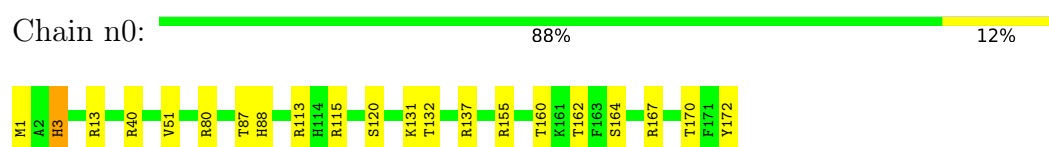
- Molecule 20: 60S ribosomal protein L19-A



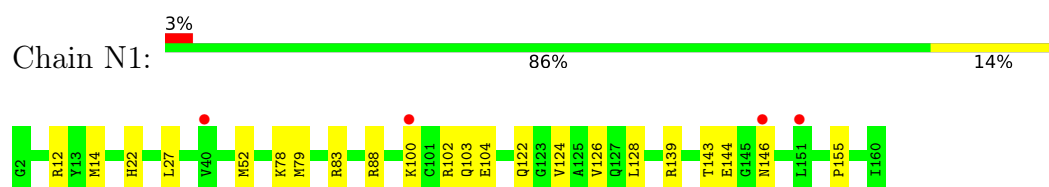
- Molecule 21: 60S ribosomal protein L20-A



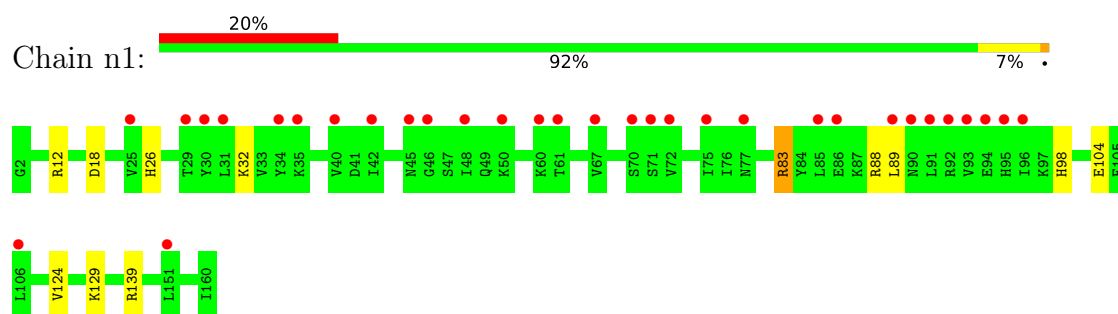
- Molecule 21: 60S ribosomal protein L20-A



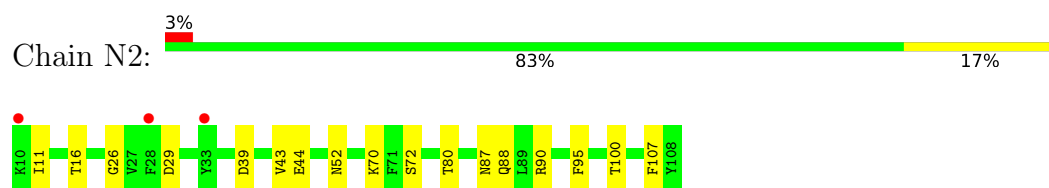
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 22: 60S ribosomal protein L21-A



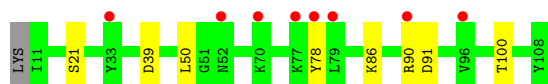
- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A

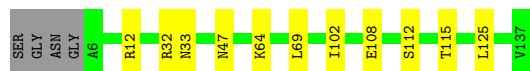






- Molecule 24: 60S ribosomal protein L23-A

Chain N3: 89% 8% .



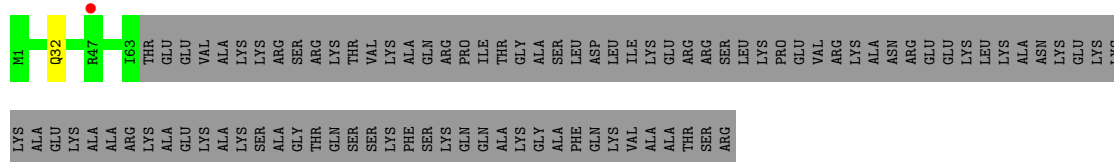
- Molecule 24: 60S ribosomal protein L23-A

Chain n3: 93% 7% .



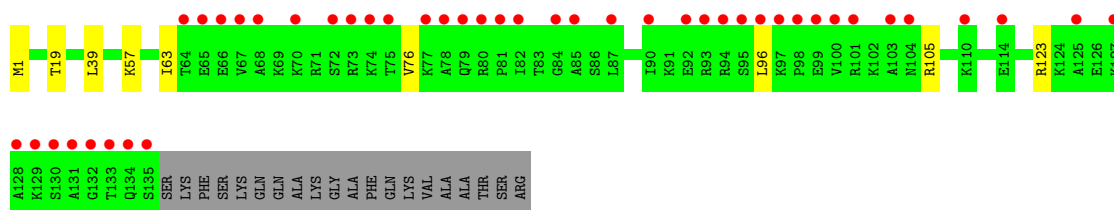
- Molecule 25: 60S ribosomal protein L24-A

Chain N4: 40% 59% .



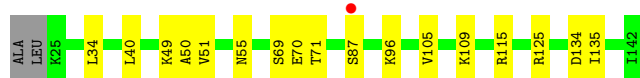
- Molecule 25: 60S ribosomal protein L24-A

Chain n4: 28% 81% 6% 13% .



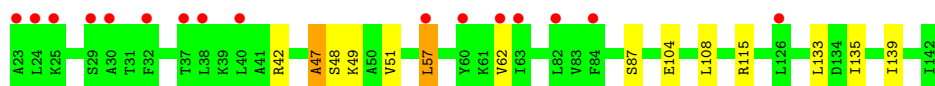
- Molecule 26: 60S ribosomal protein L25

Chain N5: 84% 14% .

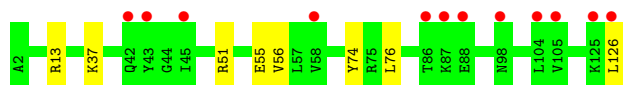


- Molecule 26: 60S ribosomal protein L25

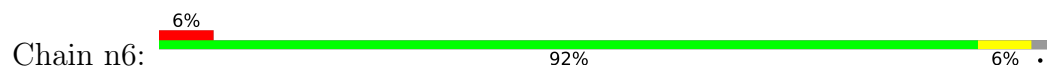
Chain n5: 13% 88% 10% .



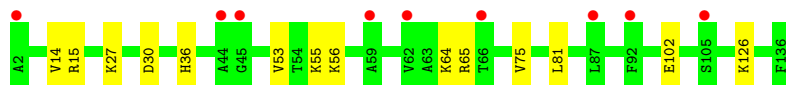
- Molecule 27: 60S ribosomal protein L26-A



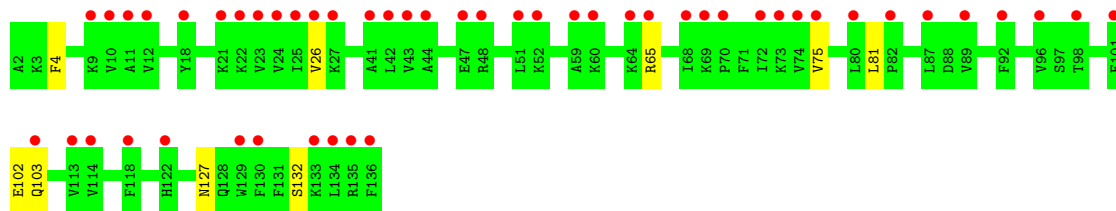
- Molecule 27: 60S ribosomal protein L26-A



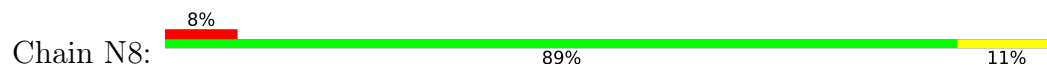
- Molecule 28: 60S ribosomal protein L27-A



- Molecule 28: 60S ribosomal protein L27-A

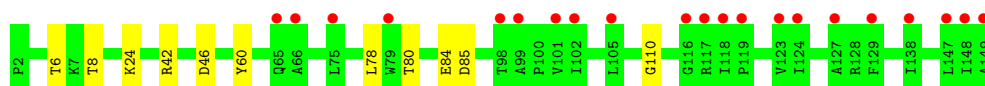


- Molecule 29: 60S ribosomal protein L28

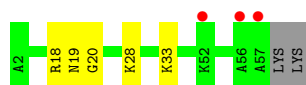
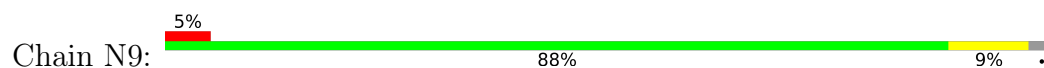


- Molecule 29: 60S ribosomal protein L28

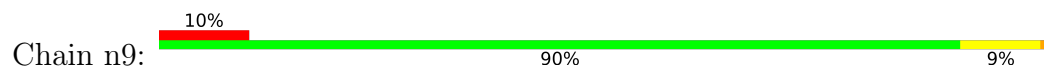




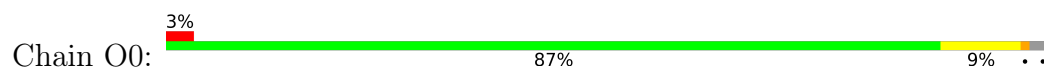
- Molecule 30: 60S ribosomal protein L29



- Molecule 30: 60S ribosomal protein L29



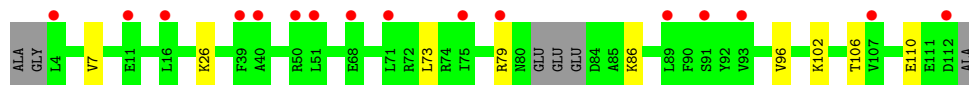
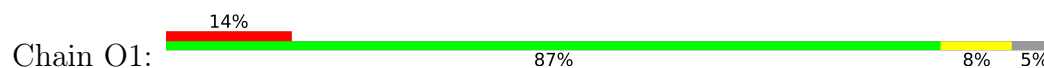
- Molecule 31: 60S ribosomal protein L30



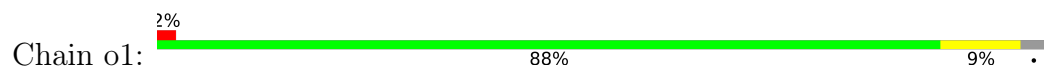
- Molecule 31: 60S ribosomal protein L30



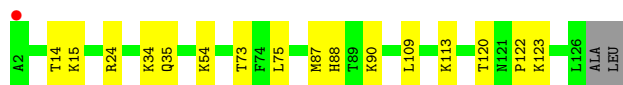
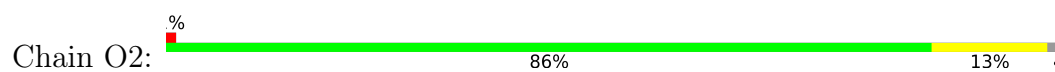
- Molecule 32: 60S ribosomal protein L31-A



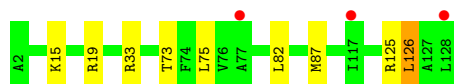
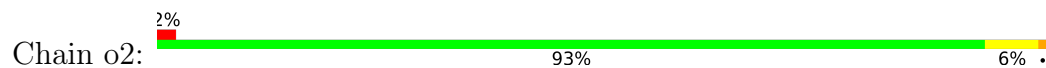
- Molecule 32: 60S ribosomal protein L31-A



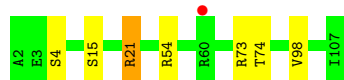
- Molecule 33: 60S ribosomal protein L32



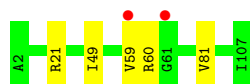
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L33-A



- Molecule 34: 60S ribosomal protein L33-A



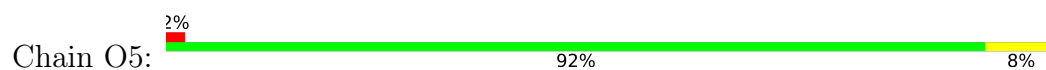
- Molecule 35: 60S ribosomal protein L34-A



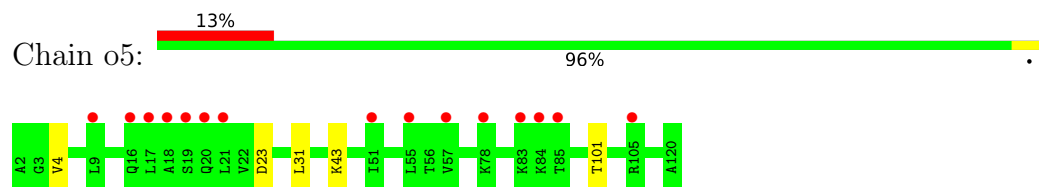
- Molecule 35: 60S ribosomal protein L34-A



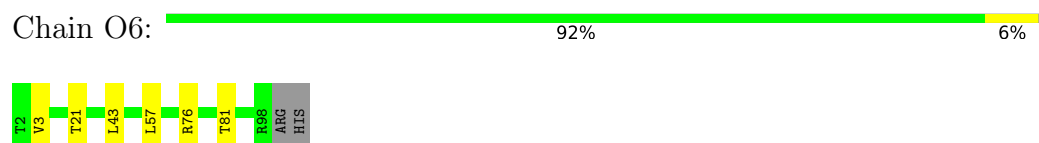
- Molecule 36: 60S ribosomal protein L35-A



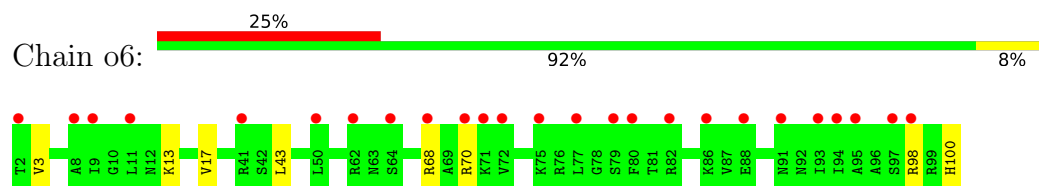
- Molecule 36: 60S ribosomal protein L35-A



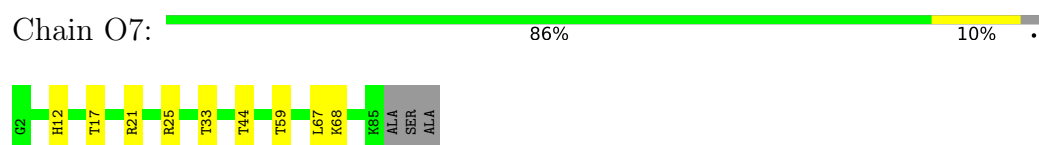
- Molecule 37: 60S ribosomal protein L36-A



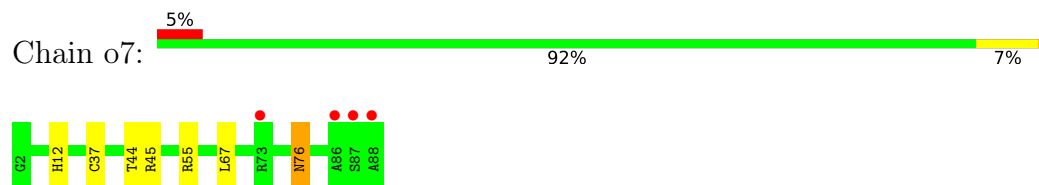
- Molecule 37: 60S ribosomal protein L36-A



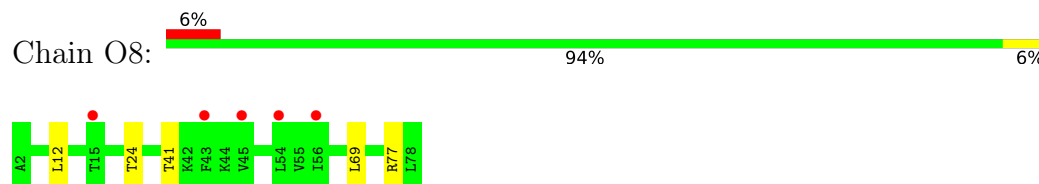
- Molecule 38: 60S ribosomal protein L37-A



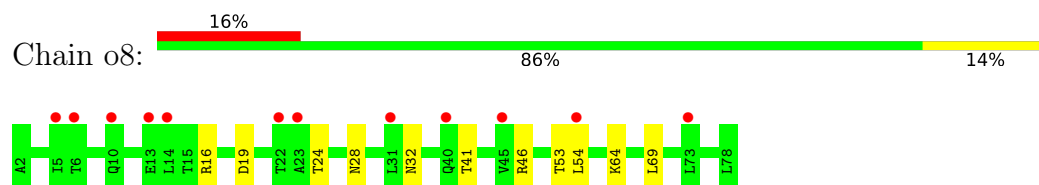
- Molecule 38: 60S ribosomal protein L37-A



- Molecule 39: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39

Chain O9:  88% 12%



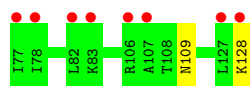
- Molecule 40: 60S ribosomal protein L39

Chain o9:  4% 96% .




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Q0:  15% 96% .




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain q0:  4% 87% 13%




- Molecule 42: 60S ribosomal protein L41-B

Chain Q1:  84% 16%




- Molecule 42: 60S ribosomal protein L41-B

Chain q1:  76% 24%

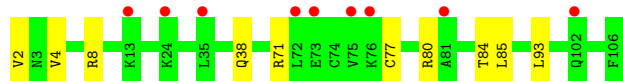
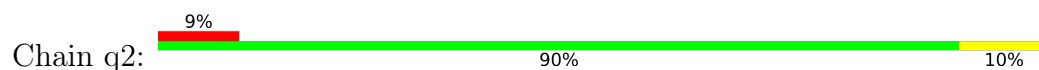


- Molecule 43: 60S ribosomal protein L42-A

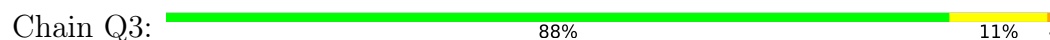
Chain Q2:  16% 89% 11%



- Molecule 43: 60S ribosomal protein L42-A



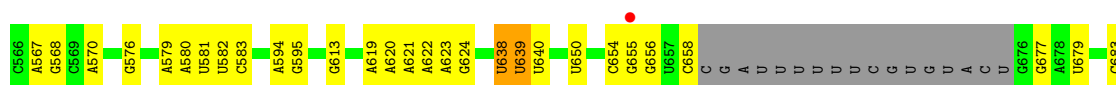
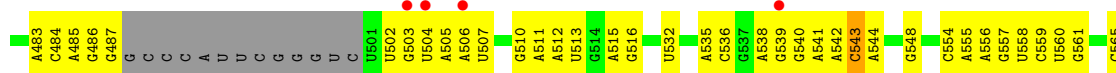
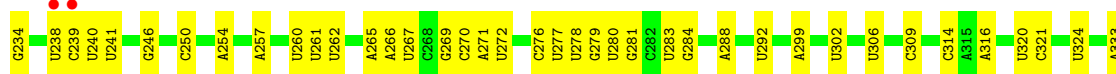
- Molecule 44: 60S ribosomal protein L43-A

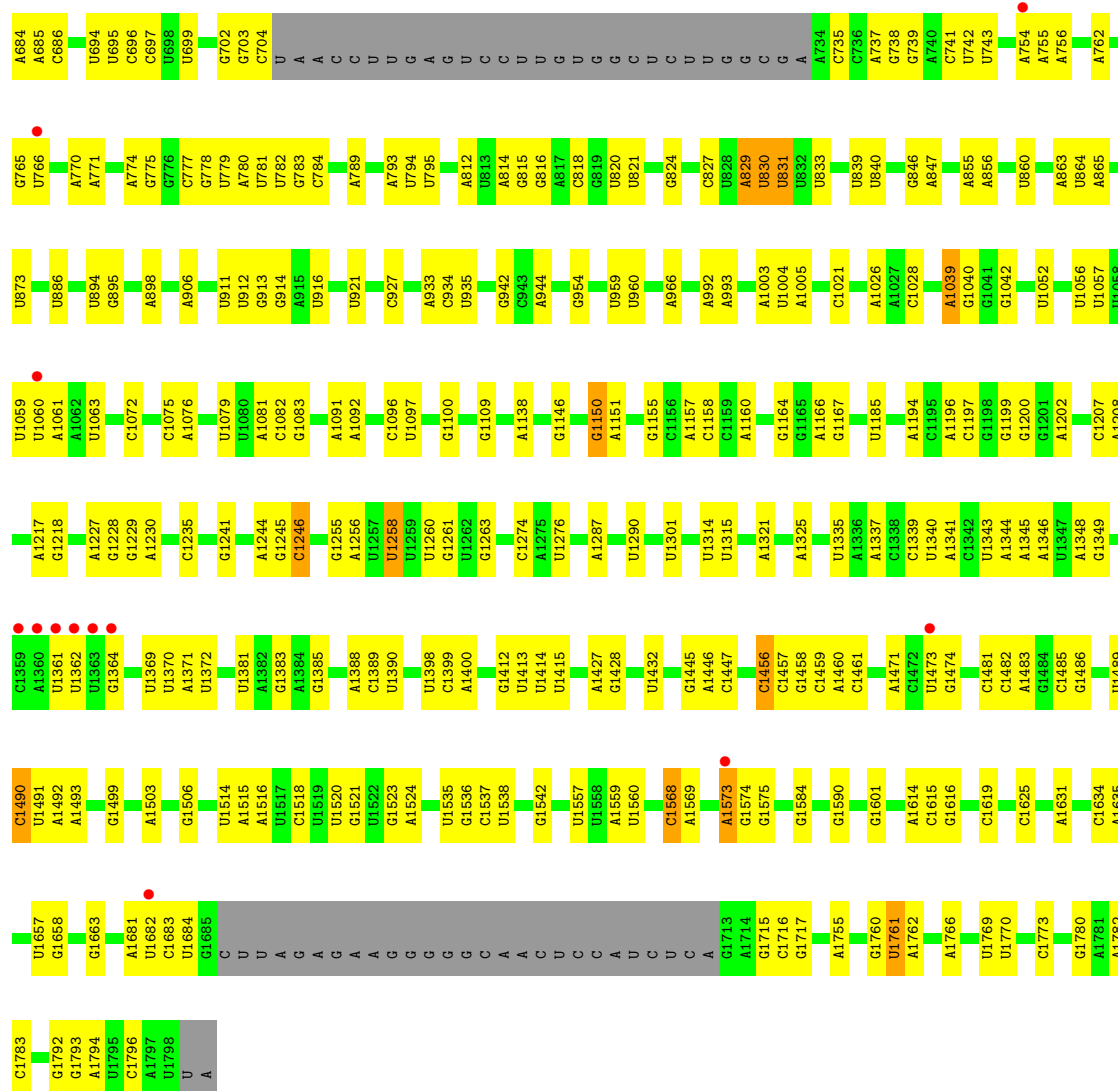


- Molecule 44: 60S ribosomal protein L43-A

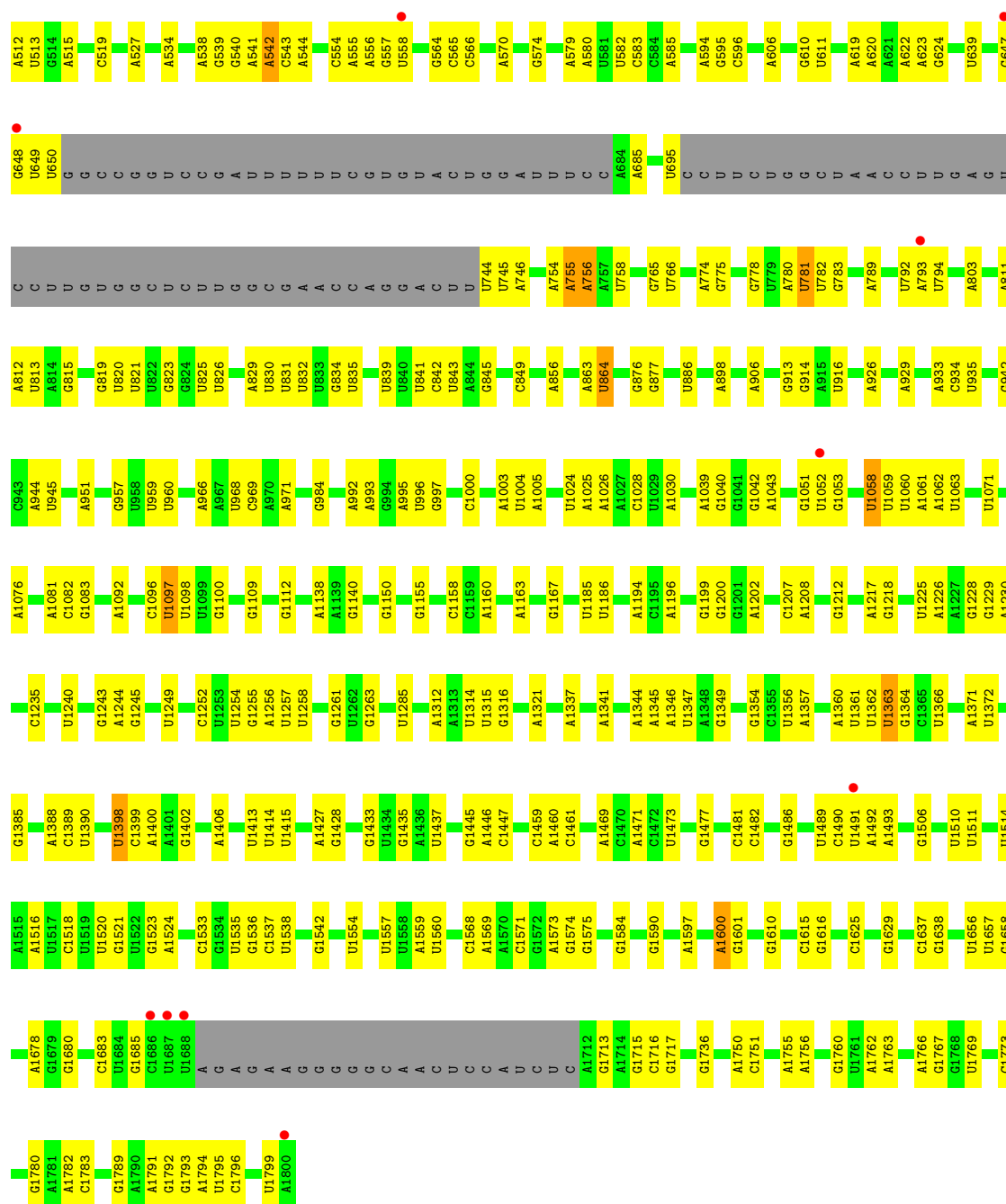


- Molecule 45: 18S ribosomal RNA



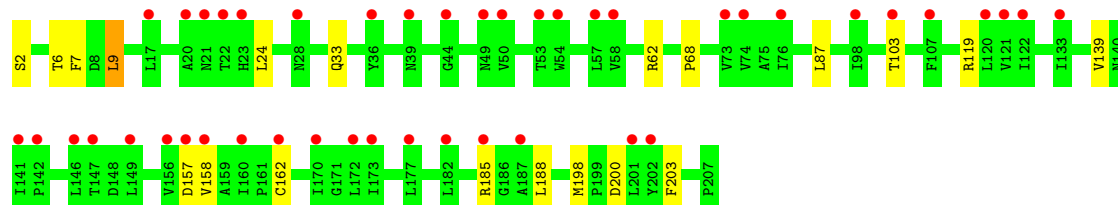




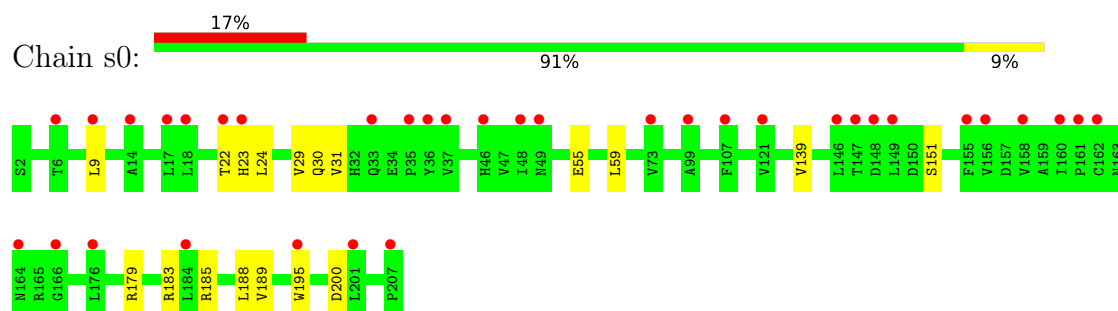


• Molecule 46: 40S ribosomal protein S0-A

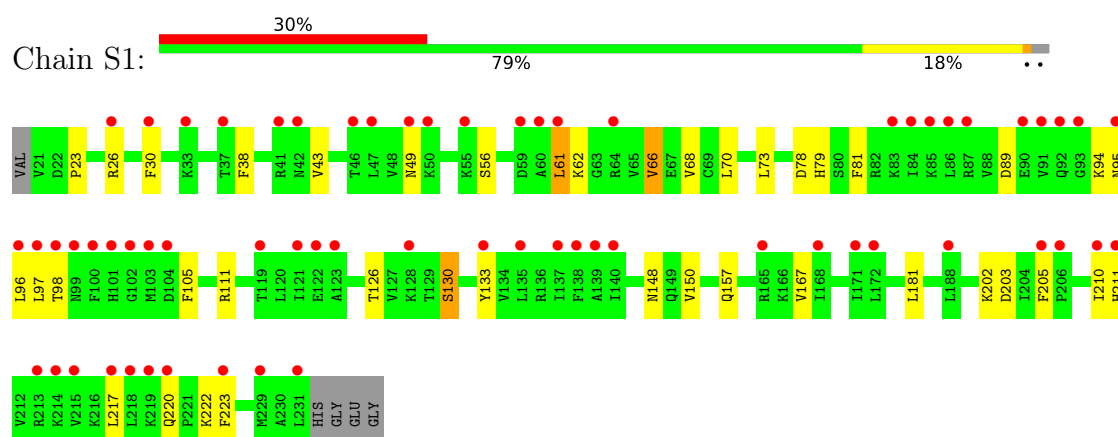
Chain S0: 21% 90% 9%



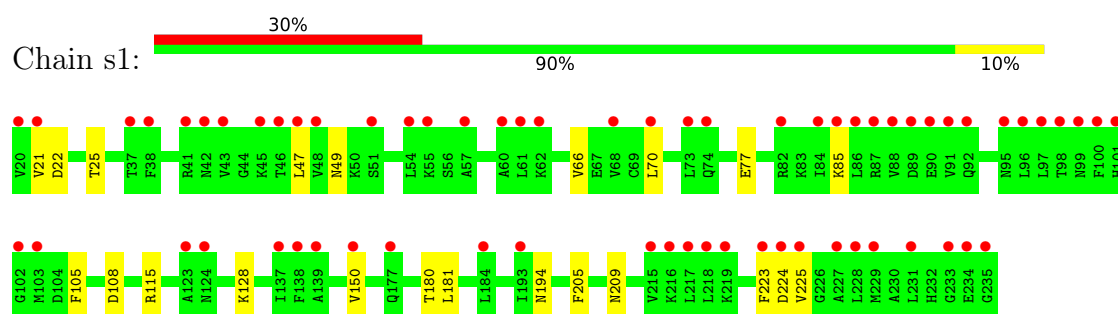
- Molecule 46: 40S ribosomal protein S0-A



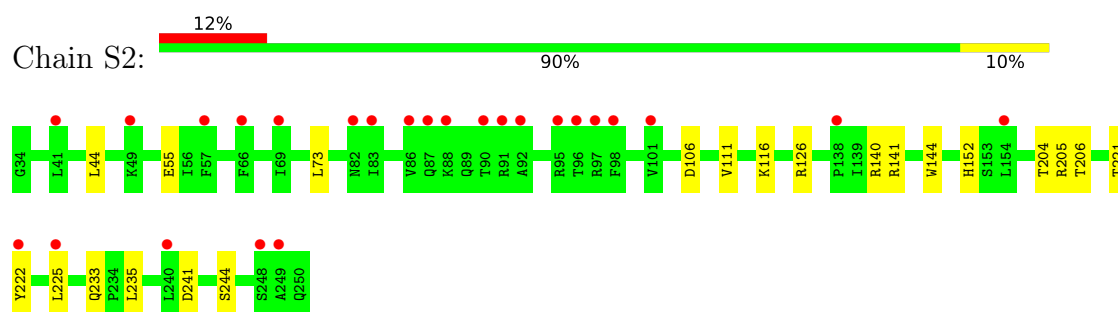
- Molecule 47: 40S ribosomal protein S1-A



- Molecule 47: 40S ribosomal protein S1-A

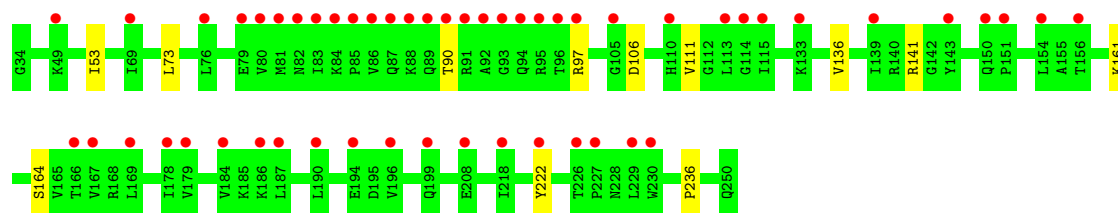


- Molecule 48: 40S ribosomal protein S2

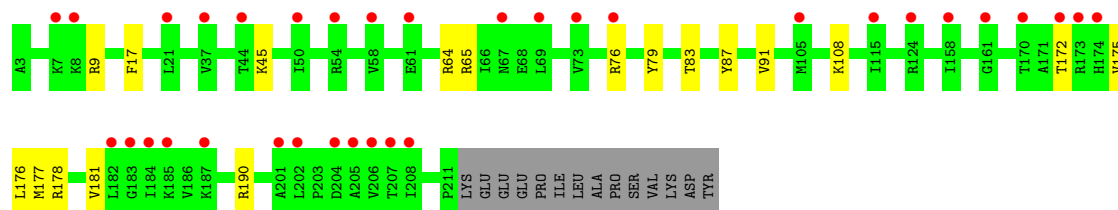
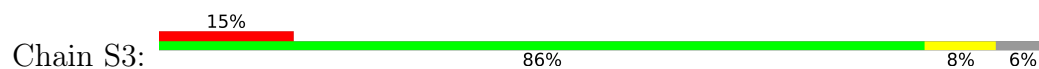


- Molecule 48: 40S ribosomal protein S2

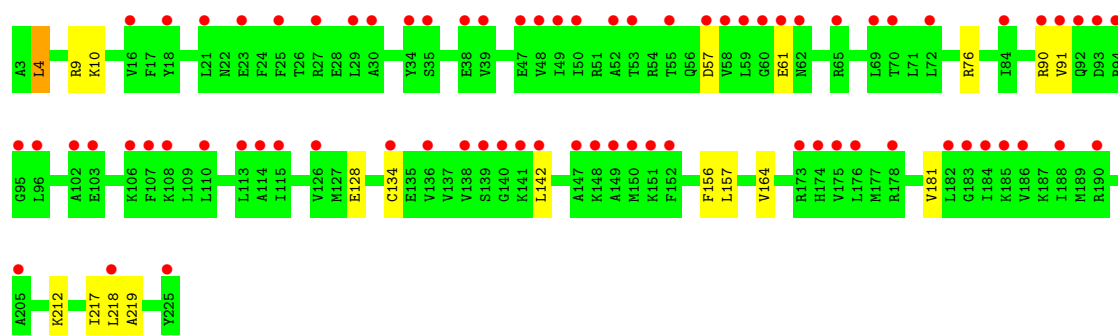




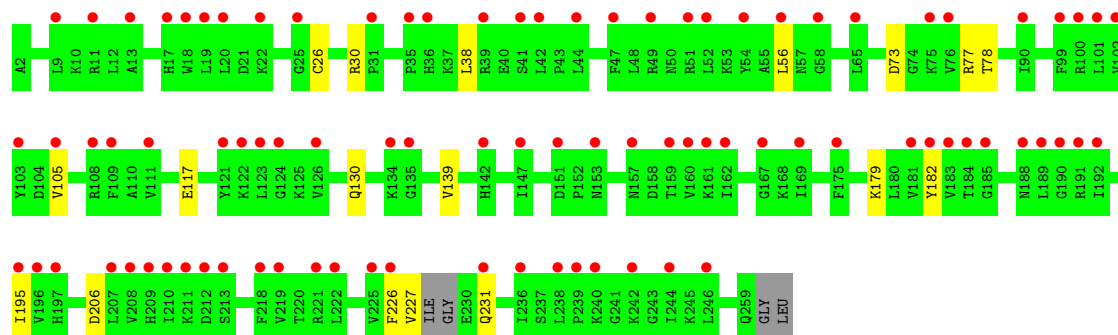
• Molecule 49: 40S ribosomal protein S3



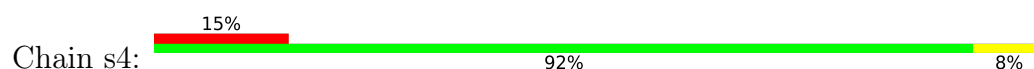
• Molecule 49: 40S ribosomal protein S3

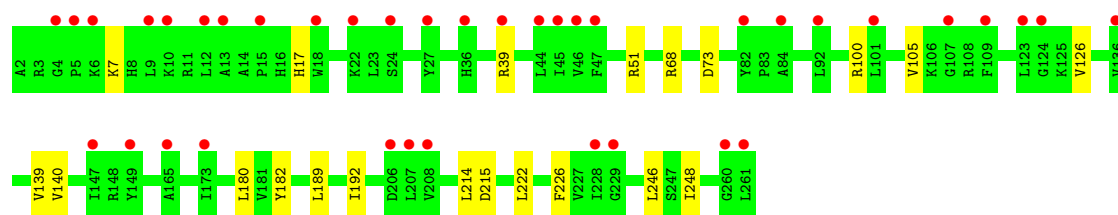


• Molecule 50: 40S ribosomal protein S4-A

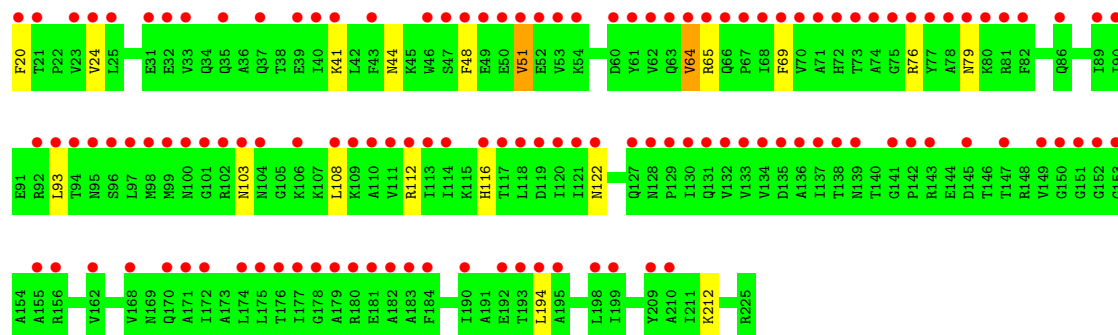
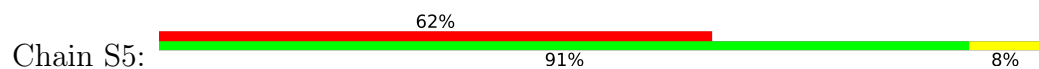


• Molecule 50: 40S ribosomal protein S4-A

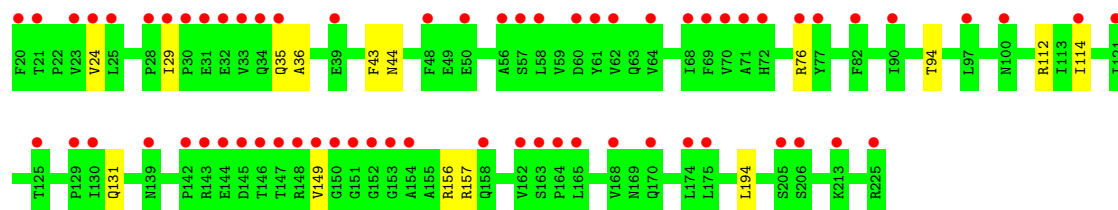




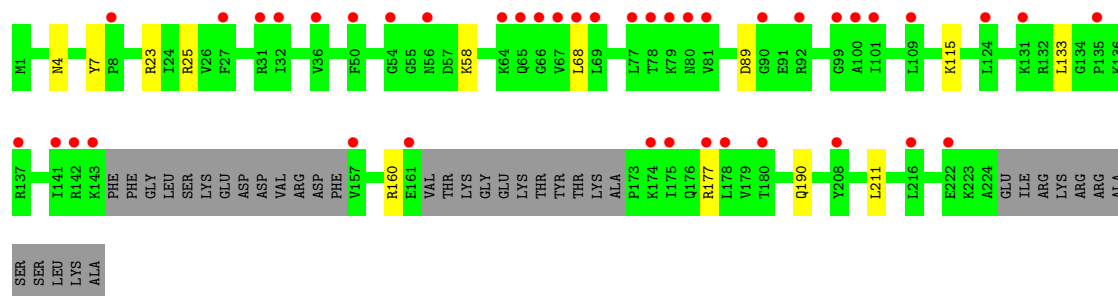
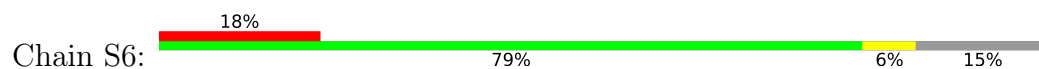
• Molecule 51: 40S ribosomal protein S5



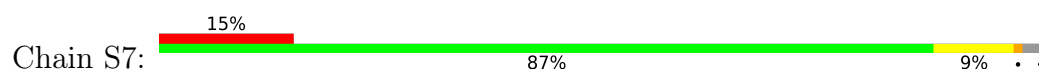
• Molecule 51: 40S ribosomal protein S5

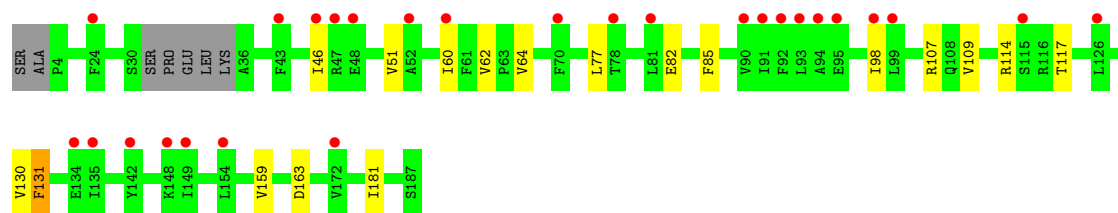


• Molecule 52: 40S ribosomal protein S6-A

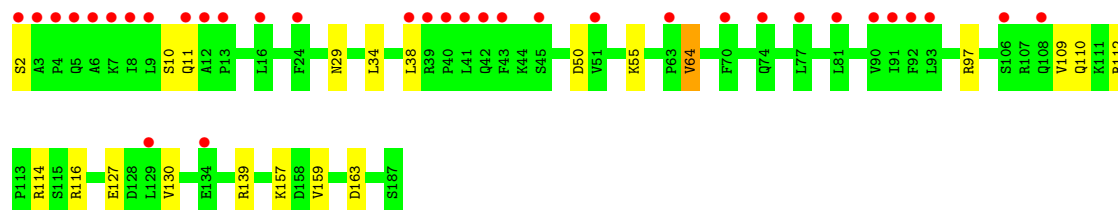
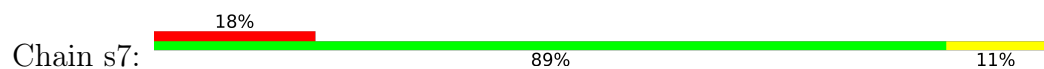


• Molecule 53: 40S ribosomal protein S7-A

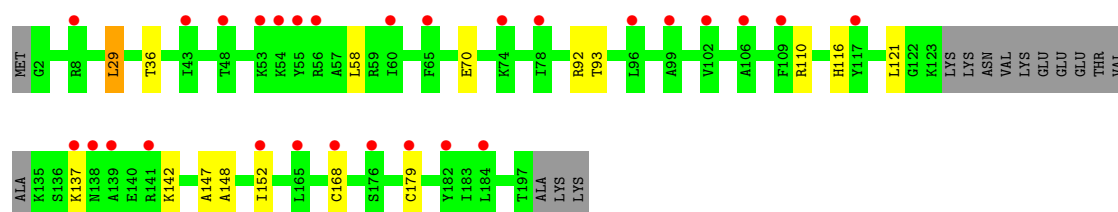
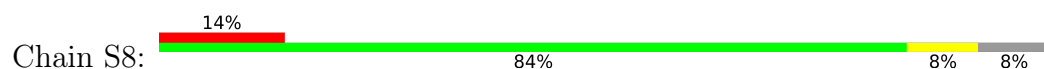




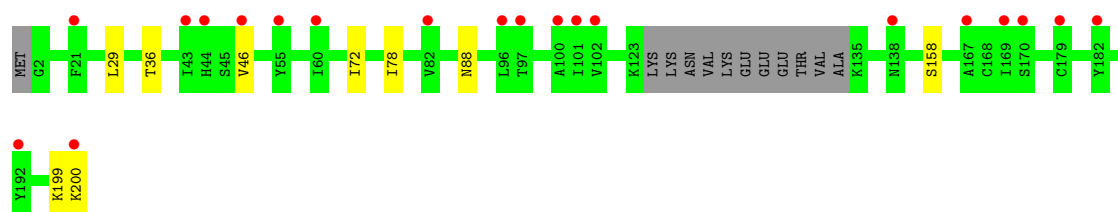
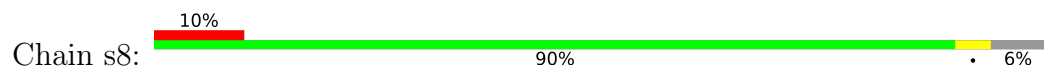
• Molecule 53: 40S ribosomal protein S7-A



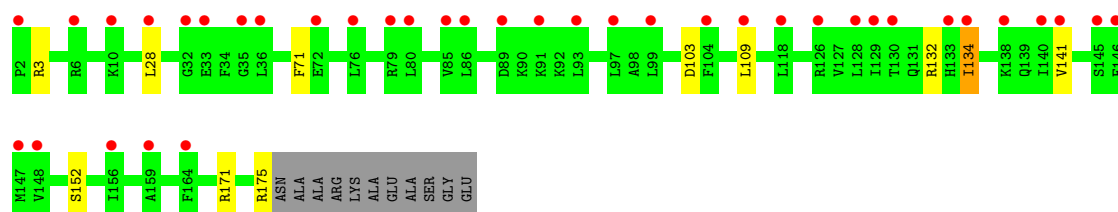
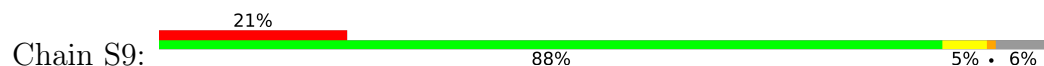
• Molecule 54: 40S ribosomal protein S8-A



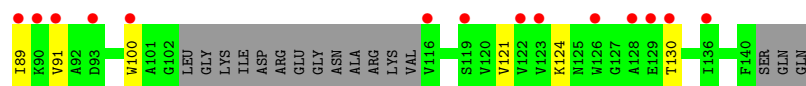
• Molecule 54: 40S ribosomal protein S8-A



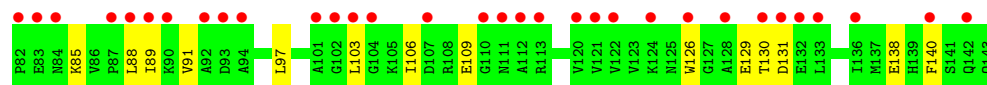
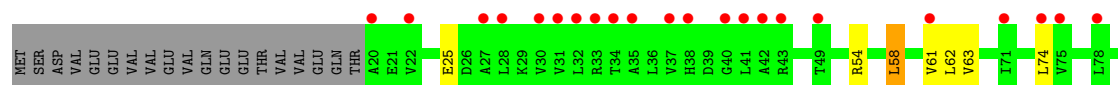
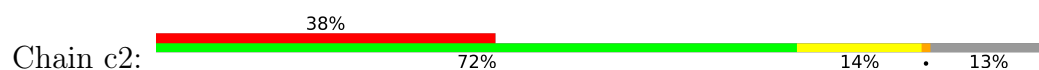
• Molecule 55: 40S ribosomal protein S9-A



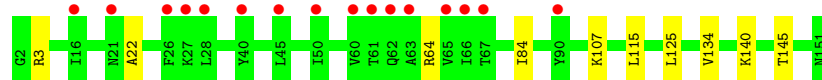
- Chain C2:
- 
- | Residue Type | Count | Percentage |
|--------------|-------|------------|
| Red          | 23    | 23%        |
| Green        | 59    | 59%        |
| Yellow       | 12    | 12%        |
| Grey         | 29    | 29%        |
- Sequence: MET SER ASP VAL GLU VAL VAL VAL VAL GLN GLU GLU THR THR THR VAL VAL GLN GLU D26 L28 K29 D39 G40 L41 A42 R43 L52 G55 E56 A57 L58 L59 V60 V61 L62 V63 V66 A69 V75 F82 E83 N84 K85 L86



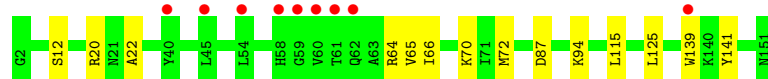
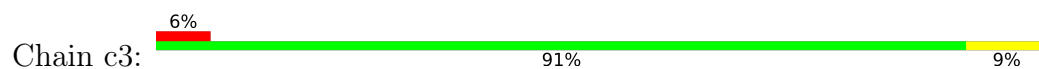
- Molecule 58: 40S ribosomal protein S12



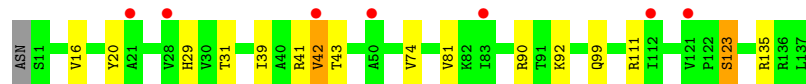
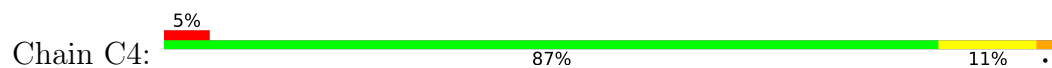
- Molecule 59: 40S ribosomal protein S13



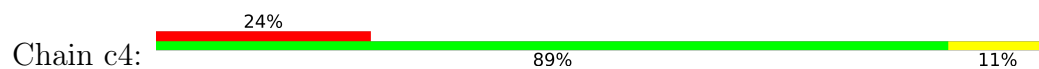
- Molecule 59: 40S ribosomal protein S13



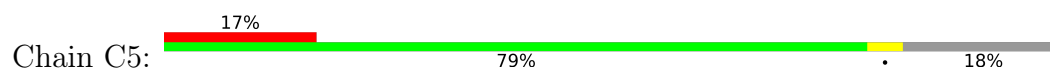
- Molecule 60: 40S ribosomal protein S14-B

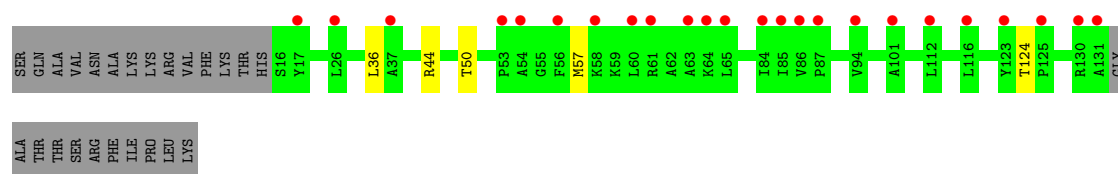


- Molecule 60: 40S ribosomal protein S14-B

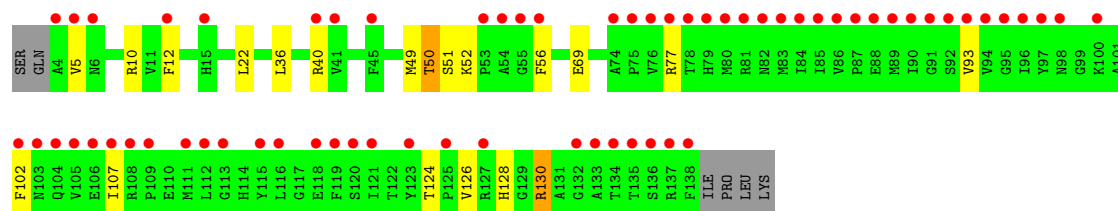
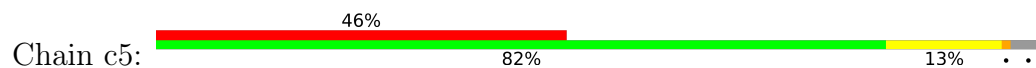


- Molecule 61: 40S ribosomal protein S15

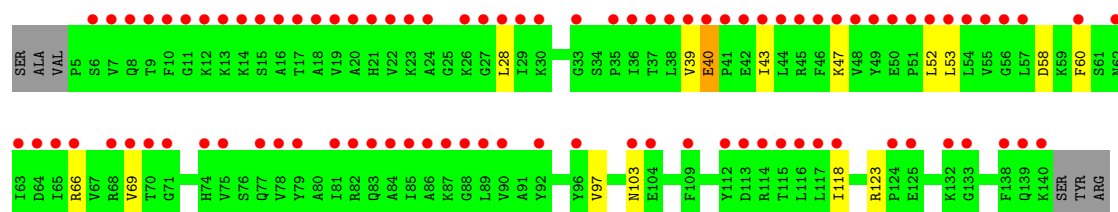
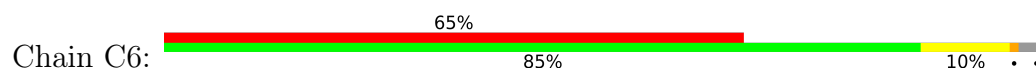




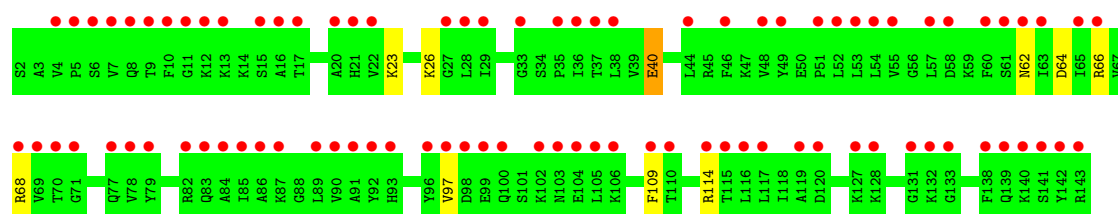
- Molecule 61: 40S ribosomal protein S15



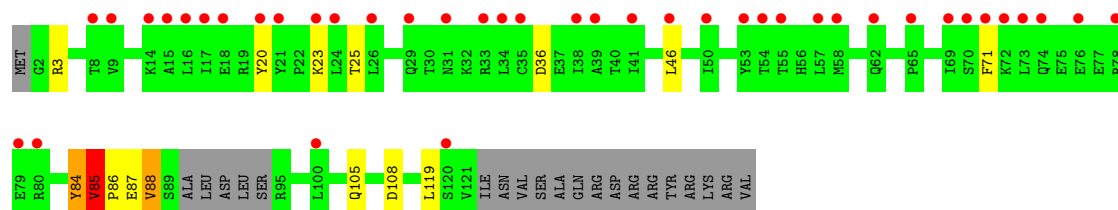
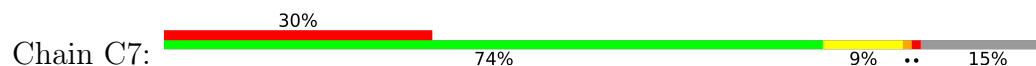
- Molecule 62: 40S ribosomal protein S16-A



- Molecule 62: 40S ribosomal protein S16-A

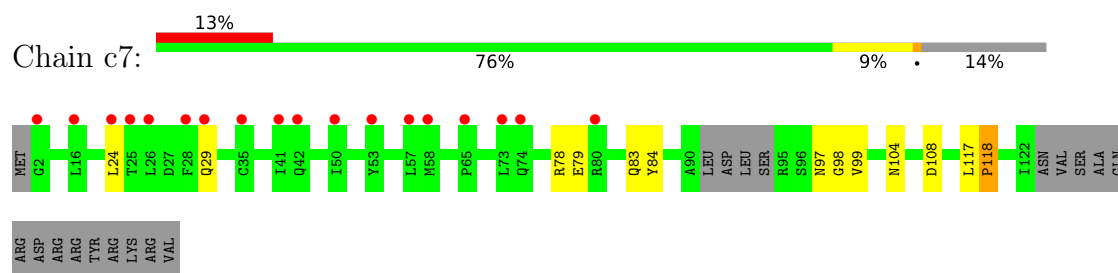


- Molecule 63: 40S ribosomal protein S17-A

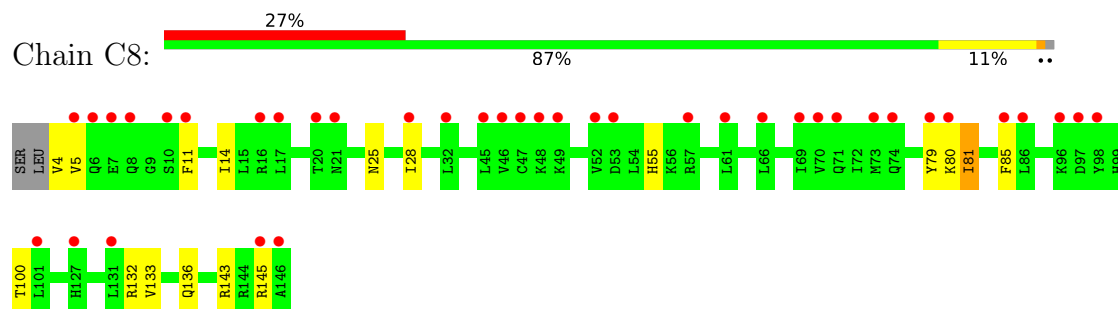




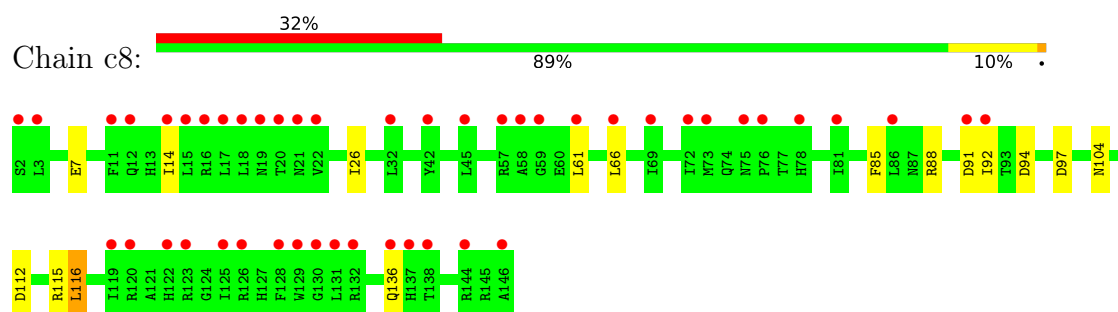
- Molecule 63: 40S ribosomal protein S17-A



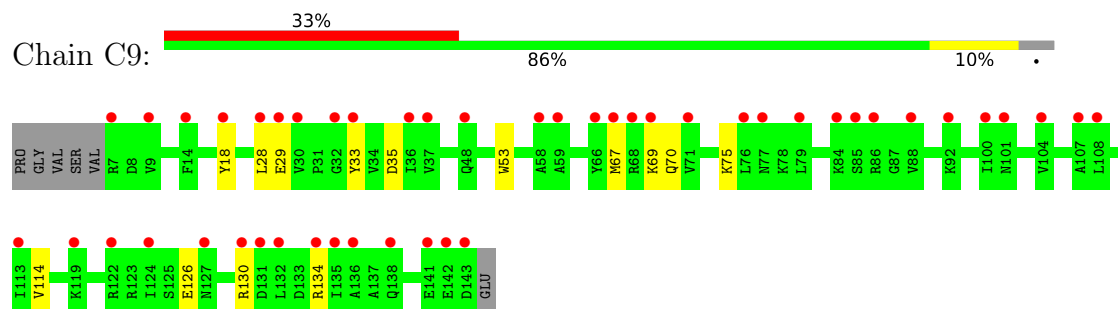
- Molecule 64: 40S ribosomal protein S18-A



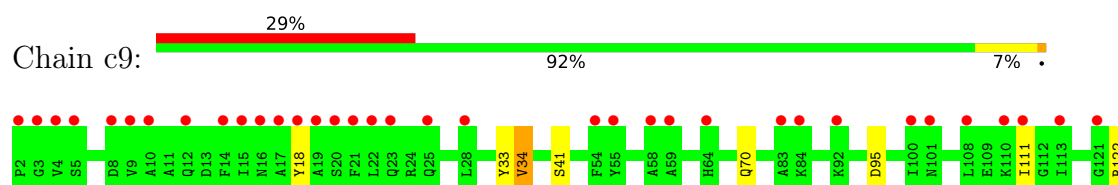
- Molecule 64: 40S ribosomal protein S18-A



- Molecule 65: 40S ribosomal protein S19-A

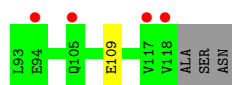
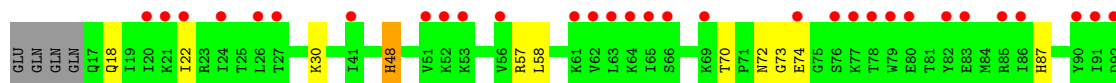
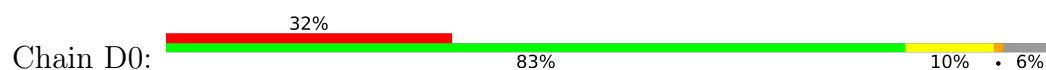


- Molecule 65: 40S ribosomal protein S19-A

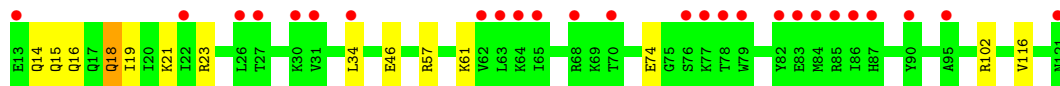
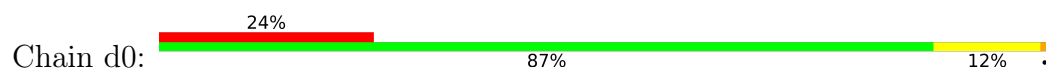




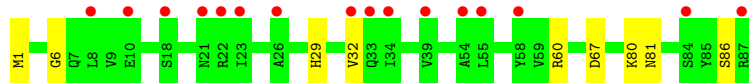
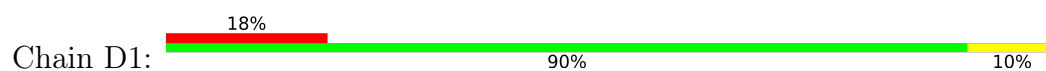
- Molecule 66: 40S ribosomal protein S20



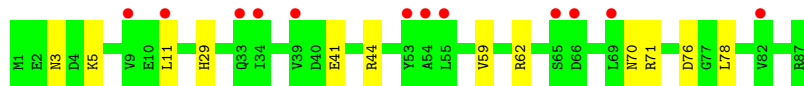
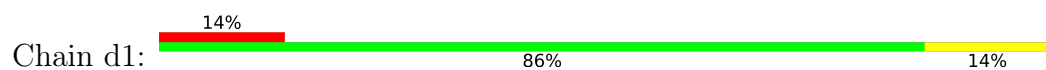
- Molecule 66: 40S ribosomal protein S20



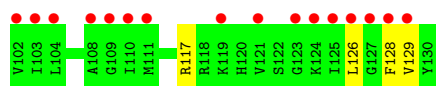
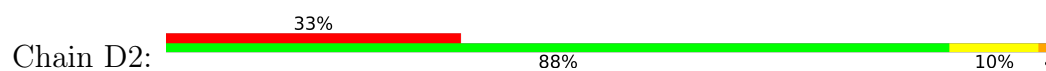
- Molecule 67: 40S ribosomal protein S21-A



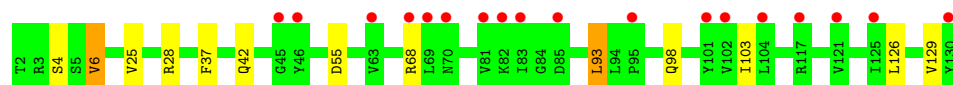
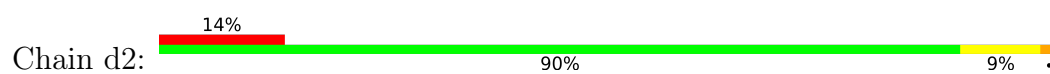
- Molecule 67: 40S ribosomal protein S21-A



- Molecule 68: 40S ribosomal protein S22-A



- Molecule 68: 40S ribosomal protein S22-A



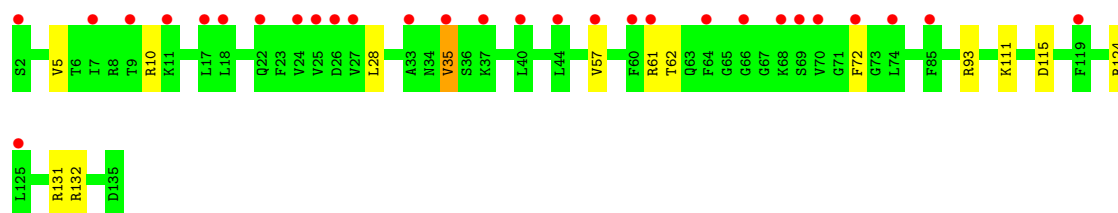
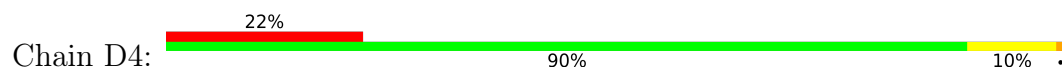
- Molecule 69: 40S ribosomal protein S23-A



- Molecule 69: 40S ribosomal protein S23-A



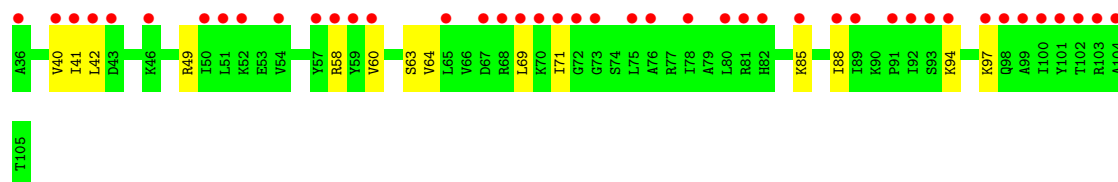
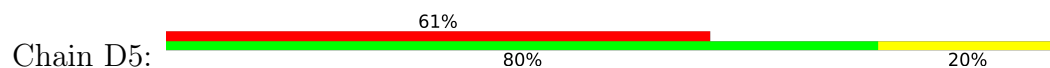
- Molecule 70: 40S ribosomal protein S24-A



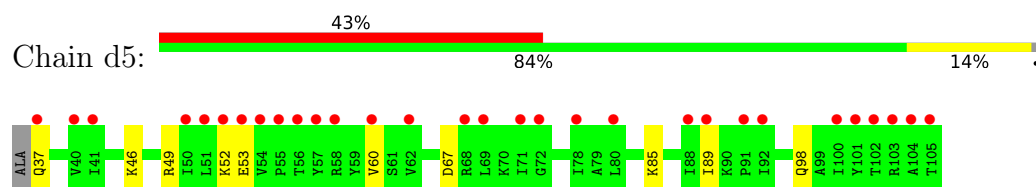
- Molecule 70: 40S ribosomal protein S24-A



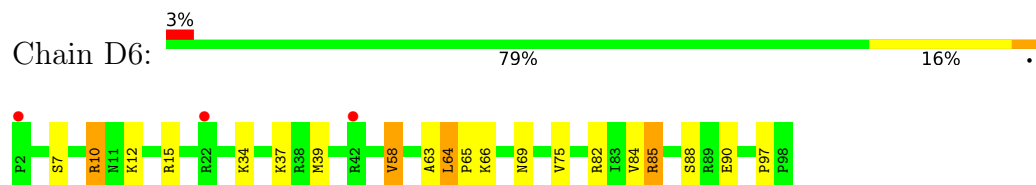
- Molecule 71: 40S ribosomal protein S25-A



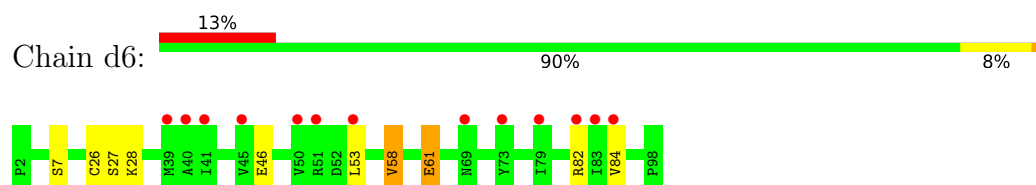
- Molecule 71: 40S ribosomal protein S25-A



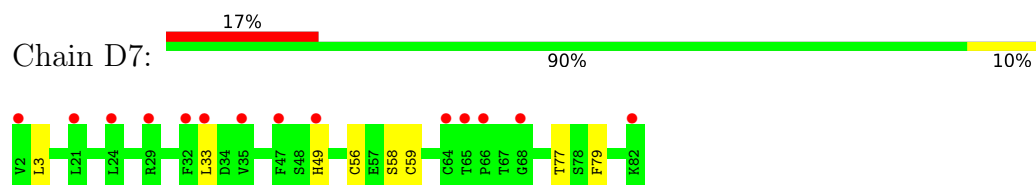
- Molecule 72: 40S ribosomal protein S26-B



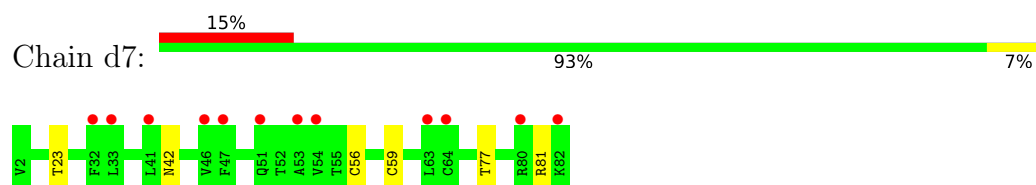
- Molecule 72: 40S ribosomal protein S26-B



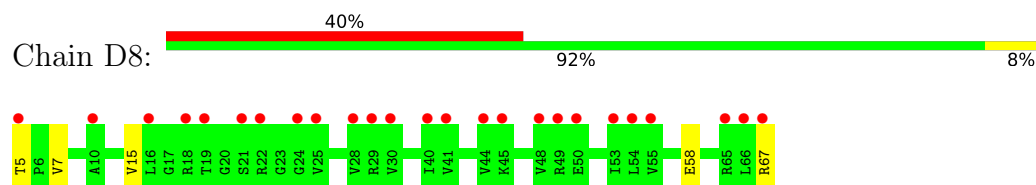
- Molecule 73: 40S ribosomal protein S27-A



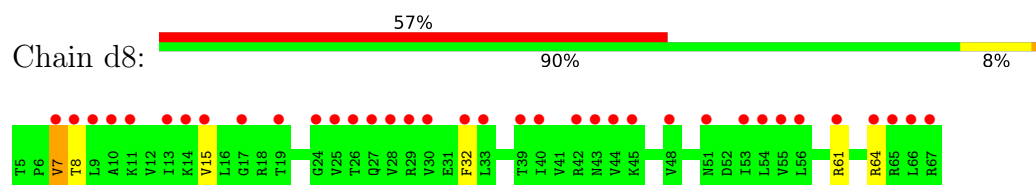
- Molecule 73: 40S ribosomal protein S27-A



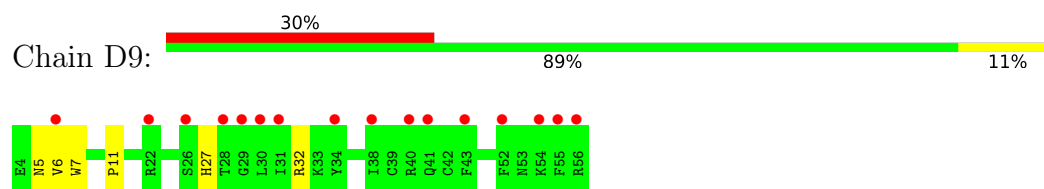
- Molecule 74: 40S ribosomal protein S28-A



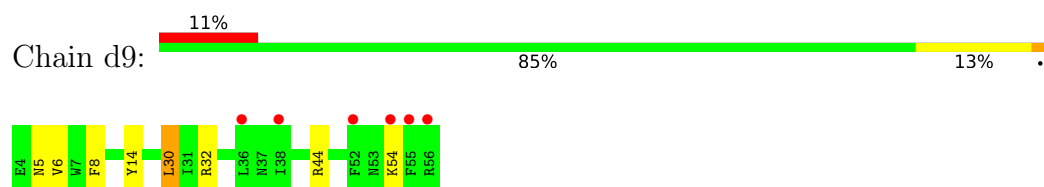
- Molecule 74: 40S ribosomal protein S28-A



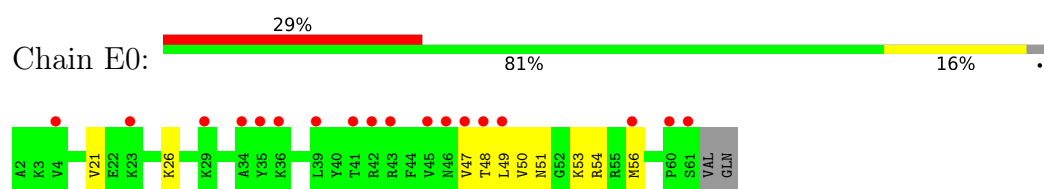
- Molecule 75: 40S ribosomal protein S29-A



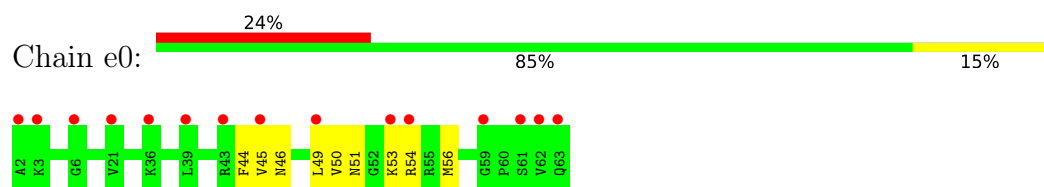
- Molecule 75: 40S ribosomal protein S29-A



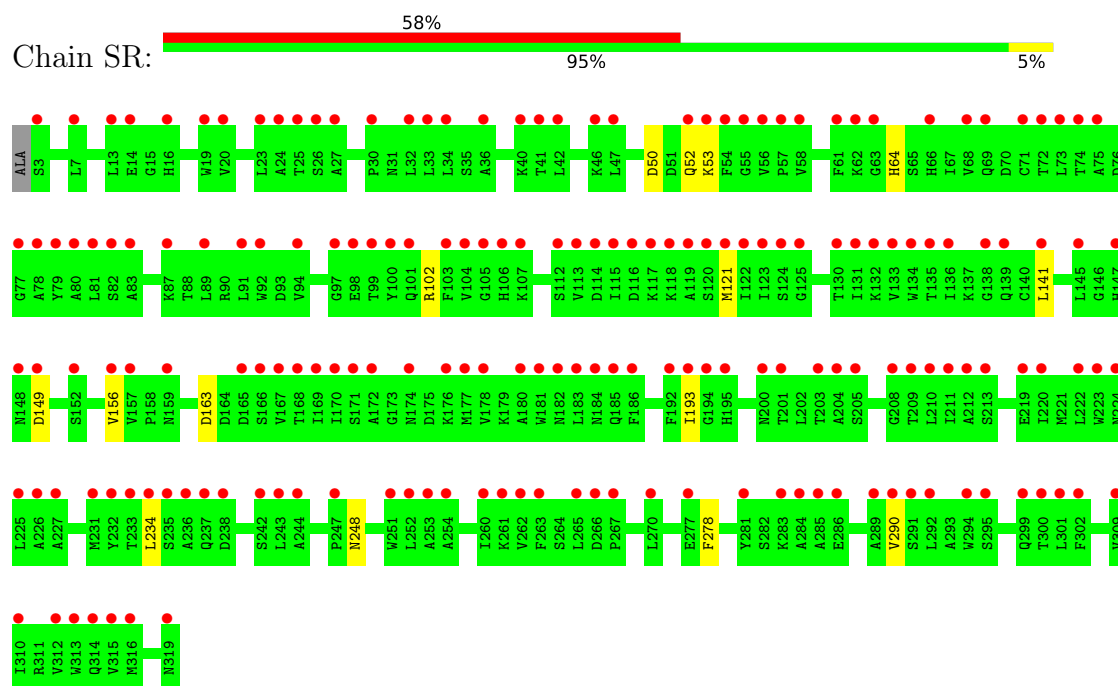
- Molecule 76: 40S ribosomal protein S30-A



- Molecule 76: 40S ribosomal protein S30-A

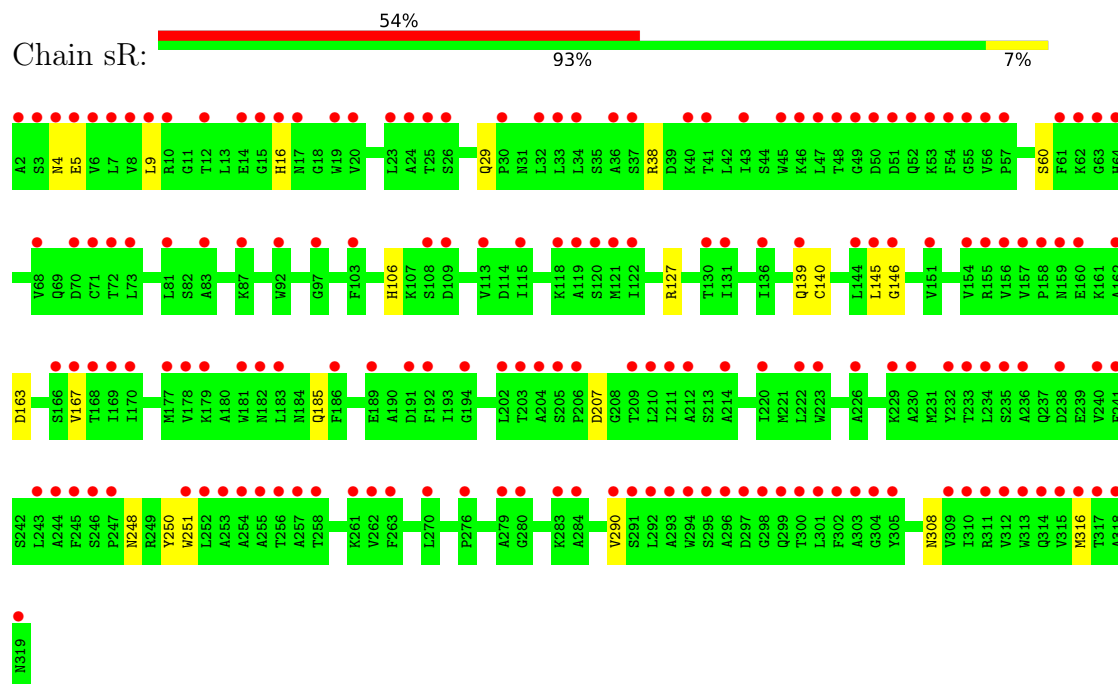


- Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein



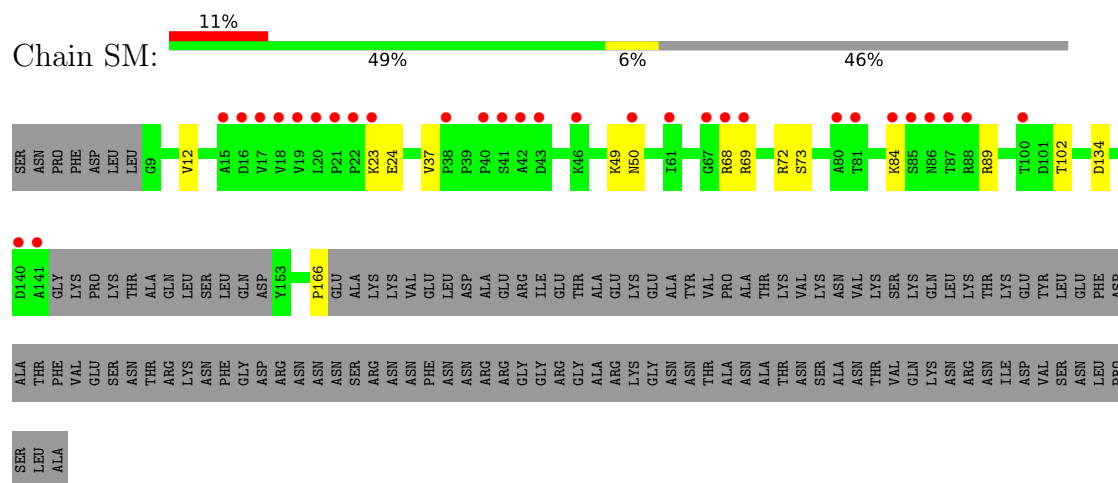
- Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



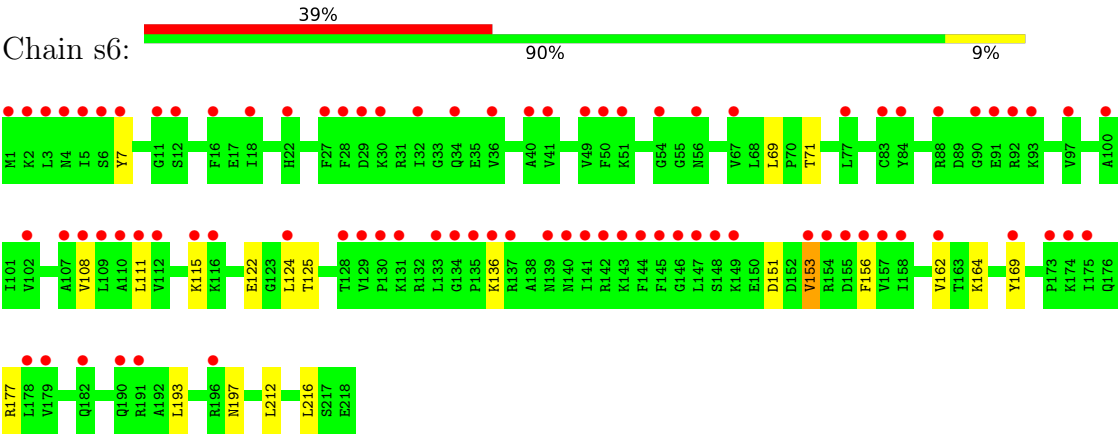
- Molecule 78: Suppressor protein STM1

Chain SM:



ARG	ARG	GLY	GLY	ARG	GLY	ALA	ARG	LYS	GLY	ASN	ASN	THR	ALA	ALA	ALA	THR	ASN	SER	ALA	ASN	THR	THR	VAL	GLN	LYS	ASN	ARG	ASN	ASP	VAL	SER	ASN	LEU	PRO	SER	SER	LEU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 79: 40S ribosomal protein S6-A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.53Å 293.33Å 295.79Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	146.66 – 3.30 146.66 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (146.66-3.30) 91.8 (146.66-3.30)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.203 , 0.250 0.203 , 0.250	Depositor DCC
$R_{free}$ test set	21969 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 92.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	397978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.67	4/73685 (0.0%)	1.11	189/114868 (0.2%)
1	5	0.55	2/73908 (0.0%)	1.02	101/115221 (0.1%)
2	3	0.51	0/2883	0.98	2/4491 (0.0%)
2	7	0.43	0/2883	0.89	0/4491
3	4	0.69	0/3724	1.14	14/5798 (0.2%)
3	8	0.51	0/3746	1.07	21/5832 (0.4%)
4	L2	0.46	0/1918	0.67	2/2577 (0.1%)
4	l2	0.35	0/1918	0.60	1/2577 (0.0%)
5	L3	0.42	0/3152	0.61	1/4239 (0.0%)
5	l3	0.43	1/3152 (0.0%)	0.59	0/4239
6	L4	0.45	0/2801	0.62	0/3792
6	l4	0.38	0/2801	0.59	0/3792
7	L5	0.35	0/2403	0.54	0/3242
7	l5	0.32	0/2408	0.50	0/3248
8	L6	0.38	0/1260	0.55	0/1694
8	l6	0.38	0/1269	0.56	0/1705
9	L7	0.40	0/1855	0.56	0/2496
9	l7	0.36	0/1828	0.57	0/2461
10	L8	0.40	0/1825	0.56	0/2466
10	l8	0.32	0/1795	0.55	1/2429 (0.0%)
11	L9	0.40	0/1523	0.60	0/2051
11	l9	0.38	0/1539	0.56	0/2073
12	M0	0.43	0/1796	0.61	0/2409
12	m0	0.40	0/1810	0.59	1/2428 (0.0%)
13	M1	0.34	0/1374	0.61	0/1842
13	m1	0.30	0/1374	0.53	1/1842 (0.1%)
14	M3	0.41	0/1568	0.59	1/2106 (0.0%)
14	m3	0.37	0/1573	0.58	0/2113
15	M4	0.36	0/1068	0.55	0/1438
15	m4	0.35	0/1074	0.55	0/1446
16	M5	0.45	0/1757	0.60	0/2354
16	m5	0.33	0/1757	0.53	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	M6	0.45	0/1585	0.56	0/2128
17	m6	0.46	0/1585	0.60	0/2128
18	M7	0.44	0/1400	0.62	0/1882
18	m7	0.42	0/1250	0.60	0/1683
19	M8	0.43	0/1465	0.61	0/1965
19	m8	0.34	0/1465	0.57	0/1965
20	M9	0.38	0/1516	0.56	2/2020 (0.1%)
20	m9	0.34	0/1538	0.49	0/2050
21	N0	0.41	0/1481	0.59	0/1990
21	n0	0.38	0/1481	0.53	0/1990
22	N1	0.41	0/1300	0.58	0/1743
22	n1	0.35	0/1300	0.54	0/1743
23	N2	0.35	0/803	0.61	0/1087
23	n2	0.32	0/794	0.55	0/1076
24	N3	0.45	0/996	0.62	0/1340
24	n3	0.43	0/1018	0.59	0/1369
25	N4	0.40	0/533	0.53	0/707
25	n4	0.33	0/1052	0.53	0/1398
26	N5	0.44	0/961	0.61	1/1296 (0.1%)
26	n5	0.34	0/974	0.59	1/1314 (0.1%)
27	N6	0.43	0/995	0.62	0/1329
27	n6	0.38	0/978	0.58	0/1307
28	N7	0.51	2/1118 (0.2%)	0.58	0/1497
28	n7	0.33	0/1118	0.52	0/1497
29	N8	0.40	0/1204	0.66	0/1612
29	n8	0.33	0/1204	0.59	0/1612
30	N9	0.40	0/455	0.54	0/607
30	n9	0.34	0/473	0.55	0/629
31	O0	0.38	0/751	0.54	0/1008
31	o0	0.31	0/775	0.54	0/1040
32	O1	0.39	0/862	0.56	0/1157
32	o1	0.42	0/897	0.57	0/1205
33	O2	0.45	0/1028	0.59	0/1376
33	o2	0.41	0/1041	0.66	1/1394 (0.1%)
34	O3	0.46	0/868	0.65	1/1168 (0.1%)
34	o3	0.41	0/868	0.56	0/1168
35	O4	0.41	0/891	0.63	1/1191 (0.1%)
35	o4	0.34	0/891	0.55	0/1191
36	O5	0.45	0/978	0.62	1/1301 (0.1%)
36	o5	0.32	0/974	0.51	0/1297
37	O6	0.41	0/756	0.58	0/1005
37	o6	0.31	0/778	0.51	0/1034
38	O7	0.51	0/680	0.70	0/901

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	o7	0.40	0/696	0.64	0/923
39	O8	0.36	0/618	0.54	0/826
39	o8	0.32	0/614	0.62	0/822
40	O9	0.49	0/443	0.67	0/588
40	o9	0.40	0/443	0.54	0/588
41	Q0	0.44	0/423	0.62	0/562
41	q0	0.46	0/423	0.63	0/562
42	Q1	0.36	0/234	0.45	0/300
42	q1	0.35	0/234	0.52	0/300
43	Q2	0.43	0/860	0.62	0/1136
43	q2	0.35	0/860	0.55	0/1136
44	Q3	0.48	0/701	0.70	2/934 (0.2%)
44	q3	0.35	0/701	0.58	0/934
45	2	0.42	0/40808	0.94	54/63582 (0.1%)
45	6	0.39	0/40116	0.91	42/62502 (0.1%)
46	S0	0.30	0/1621	0.54	1/2220 (0.0%)
46	s0	0.31	0/1621	0.54	1/2220 (0.0%)
47	S1	0.33	0/1713	0.64	1/2305 (0.0%)
47	s1	0.29	0/1748	0.54	0/2352
48	S2	0.32	0/1665	0.53	0/2263
48	s2	0.32	0/1665	0.58	0/2263
49	S3	0.31	0/1643	0.50	0/2210
49	s3	0.29	0/1759	0.55	1/2368 (0.0%)
50	S4	0.32	0/2084	0.57	0/2804
50	s4	0.32	0/2109	0.56	0/2839
51	S5	0.27	0/1629	0.56	0/2202
51	s5	0.29	0/1629	0.53	0/2202
52	S6	0.31	0/1611	0.52	0/2151
53	S7	0.30	0/1465	0.56	0/1971
53	s7	0.31	0/1517	0.58	0/2044
54	S8	0.34	0/1491	0.57	1/1992 (0.1%)
54	s8	0.32	0/1514	0.50	0/2021
55	S9	0.30	0/1443	0.54	0/1934
55	s9	0.30	0/1519	0.53	0/2035
56	C0	0.29	0/759	0.56	1/1025 (0.1%)
56	c0	0.29	0/776	0.73	4/1047 (0.4%)
57	C1	0.37	0/1153	0.57	0/1554
57	c1	0.34	0/1194	0.57	0/1610
58	C2	0.33	0/771	0.64	0/1044
58	c2	0.30	0/898	0.66	1/1220 (0.1%)
59	C3	0.32	0/1215	0.51	0/1638
59	c3	0.29	0/1215	0.50	0/1638
60	C4	0.31	0/901	0.60	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	c4	0.30	0/960	0.58	0/1290
61	C5	0.30	0/937	0.52	0/1258
61	c5	0.35	0/1060	0.64	0/1426
62	C6	0.29	0/1083	0.55	1/1452 (0.1%)
62	c6	0.29	0/1131	0.52	0/1518
63	C7	0.31	0/910	0.70	3/1219 (0.2%)
63	c7	0.30	0/914	0.64	1/1224 (0.1%)
64	C8	0.38	1/1197 (0.1%)	0.51	0/1609
64	c8	0.29	0/1211	0.58	1/1628 (0.1%)
65	C9	0.29	0/1089	0.50	0/1461
65	c9	0.29	0/1130	0.47	0/1517
66	D0	0.29	0/828	0.51	0/1119
66	d0	0.31	0/883	0.58	0/1193
67	D1	0.29	0/693	0.54	0/935
67	d1	0.30	0/693	0.59	0/935
68	D2	0.32	0/1038	0.56	0/1395
68	d2	0.31	0/1038	0.55	1/1395 (0.1%)
69	D3	0.40	0/1139	0.56	0/1518
69	d3	0.36	0/1139	0.54	0/1518
70	D4	0.31	0/1087	0.54	0/1449
70	d4	0.34	0/1087	0.57	1/1449 (0.1%)
71	D5	0.28	0/571	0.60	0/768
71	d5	0.26	0/566	0.45	0/761
72	D6	0.43	0/782	0.73	3/1047 (0.3%)
72	d6	0.32	0/782	0.59	0/1047
73	D7	0.30	0/620	0.58	0/838
73	d7	0.29	0/620	0.55	0/838
74	D8	0.29	0/499	0.57	0/670
74	d8	0.29	0/499	0.58	0/670
75	D9	0.40	0/453	0.62	0/602
75	d9	0.39	0/453	0.63	1/602 (0.2%)
76	E0	0.33	0/483	0.56	0/643
76	e0	0.34	0/499	0.61	0/665
77	SR	0.26	0/2485	0.51	0/3383
77	sR	0.27	0/2490	0.53	0/3390
78	SM	0.32	0/1053	0.57	1/1418 (0.1%)
78	sM	0.67	1/638 (0.2%)	0.51	0/860
79	s6	0.31	0/1779	0.51	0/2379
All	All	0.48	11/419528 (0.0%)	0.87	465/615687 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	l2	0	1
6	L4	0	1
7	L5	0	5
10	L8	0	3
10	l8	0	3
13	M1	0	1
13	m1	0	1
14	M3	0	1
15	m4	0	1
16	M5	0	1
20	M9	0	1
21	N0	0	3
21	n0	0	2
23	N2	0	2
26	n5	0	1
28	n7	0	1
29	n8	0	1
30	N9	0	1
30	n9	0	1
31	O0	0	1
33	O2	0	1
33	o2	0	1
35	o4	0	1
38	o7	0	1
43	Q2	0	1
47	S1	0	2
48	S2	0	1
48	s2	0	2
49	s3	0	1
51	S5	0	1
51	s5	0	1
53	S7	0	2
53	s7	0	5
54	S8	0	1
55	s9	0	4
57	c1	0	1
58	C2	0	1
58	c2	0	2
60	C4	0	3
61	c5	0	1
62	C6	0	1
62	c6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	C7	0	2
63	c7	0	1
65	C9	0	1
66	D0	0	2
68	D2	0	3
70	d4	0	3
71	D5	0	1
72	D6	0	3
73	D7	0	1
75	D9	0	2
75	d9	0	1
77	SR	0	2
77	sR	0	1
78	SM	0	1
78	sM	0	1
All	All	0	92

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	sM	51	ARG	C-N	14.96	1.62	1.34
28	N7	36	HIS	C-N	9.18	1.51	1.34
64	C8	81	ILE	C-N	-9.18	1.16	1.34
1	5	1152	G	N9-C4	-8.15	1.31	1.38
1	1	2606	G	N9-C4	-7.56	1.31	1.38

The worst 5 of 465 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-N9	-14.66	117.20	126.00
1	5	1152	G	N3-C4-C5	12.74	134.97	128.60
3	8	84	C	N1-C2-O2	12.54	126.42	118.90
1	1	2606	G	C5-N7-C8	-12.29	98.15	104.30
1	1	2606	G	N3-C4-C5	12.25	134.72	128.60

There are no chirality outliers.

5 of 92 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	L4	196	ASN	Peptide
7	L5	124	GLU	Peptide

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Mol	Chain	Res	Type	Group
7	L5	251	PRO	Peptide
7	L5	7	ALA	Peptide
7	L5	8	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L2	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
4	l2	246/248 (99%)	229 (93%)	16 (6%)	1 (0%)	34	66
5	L3	384/386 (100%)	355 (92%)	27 (7%)	2 (0%)	29	61
5	l3	384/386 (100%)	359 (94%)	25 (6%)	0	100	100
6	L4	359/361 (99%)	334 (93%)	24 (7%)	1 (0%)	41	71
6	l4	359/361 (99%)	318 (89%)	39 (11%)	2 (1%)	25	57
7	L5	291/296 (98%)	260 (89%)	29 (10%)	2 (1%)	22	54
7	l5	292/296 (99%)	261 (89%)	30 (10%)	1 (0%)	41	71
8	L6	152/176 (86%)	142 (93%)	8 (5%)	2 (1%)	12	40
8	l6	153/176 (87%)	136 (89%)	16 (10%)	1 (1%)	22	54
9	L7	224/226 (99%)	206 (92%)	17 (8%)	1 (0%)	34	66
9	l7	221/226 (98%)	202 (91%)	18 (8%)	1 (0%)	29	61
10	L8	229/231 (99%)	199 (87%)	27 (12%)	3 (1%)	12	40
10	l8	229/231 (99%)	190 (83%)	35 (15%)	4 (2%)	9	35
11	L9	187/191 (98%)	167 (89%)	19 (10%)	1 (0%)	29	61
11	l9	189/191 (99%)	176 (93%)	11 (6%)	2 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M0	215/221 (97%)	196 (91%)	18 (8%)	1 (0%)	29	61
12	m0	217/221 (98%)	200 (92%)	17 (8%)	0	100	100
13	M1	167/169 (99%)	146 (87%)	18 (11%)	3 (2%)	8	35
13	m1	167/169 (99%)	140 (84%)	25 (15%)	2 (1%)	13	42
14	M3	191/194 (98%)	171 (90%)	19 (10%)	1 (0%)	29	61
14	m3	192/194 (99%)	157 (82%)	34 (18%)	1 (0%)	29	61
15	M4	134/137 (98%)	121 (90%)	12 (9%)	1 (1%)	22	54
15	m4	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
16	M5	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
16	m5	201/203 (99%)	184 (92%)	16 (8%)	1 (0%)	29	61
17	M6	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
17	m6	195/197 (99%)	183 (94%)	11 (6%)	1 (0%)	29	61
18	M7	171/184 (93%)	164 (96%)	7 (4%)	0	100	100
18	m7	153/184 (83%)	142 (93%)	11 (7%)	0	100	100
19	M8	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	29	61
19	m8	183/185 (99%)	166 (91%)	15 (8%)	2 (1%)	14	45
20	M9	183/188 (97%)	162 (88%)	21 (12%)	0	100	100
20	m9	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
21	N0	170/172 (99%)	151 (89%)	18 (11%)	1 (1%)	25	57
21	n0	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	N1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	12	40
22	n1	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	57
23	N2	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7	31
23	n2	96/99 (97%)	86 (90%)	10 (10%)	0	100	100
24	N3	130/136 (96%)	124 (95%)	6 (5%)	0	100	100
24	n3	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
25	N4	61/155 (39%)	56 (92%)	5 (8%)	0	100	100
25	n4	133/155 (86%)	121 (91%)	10 (8%)	2 (2%)	10	38
26	N5	116/120 (97%)	104 (90%)	11 (10%)	1 (1%)	17	48
26	n5	118/120 (98%)	105 (89%)	11 (9%)	2 (2%)	9	35
27	N6	123/125 (98%)	119 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	n6	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
28	N7	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
28	n7	133/135 (98%)	117 (88%)	15 (11%)	1 (1%)	19	51
29	N8	146/148 (99%)	133 (91%)	12 (8%)	1 (1%)	22	54
29	n8	146/148 (99%)	128 (88%)	18 (12%)	0	100	100
30	N9	54/58 (93%)	46 (85%)	8 (15%)	0	100	100
30	n9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	8	35
31	O0	95/100 (95%)	91 (96%)	3 (3%)	1 (1%)	14	45
31	o0	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	15	46
32	O1	102/112 (91%)	98 (96%)	3 (3%)	1 (1%)	15	46
32	o1	107/112 (96%)	96 (90%)	11 (10%)	0	100	100
33	O2	123/127 (97%)	114 (93%)	8 (6%)	1 (1%)	19	51
33	o2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
34	O3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
34	o3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
35	O4	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
35	o4	110/112 (98%)	99 (90%)	10 (9%)	1 (1%)	17	48
36	O5	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	48
36	o5	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
37	O6	95/99 (96%)	83 (87%)	11 (12%)	1 (1%)	14	45
37	o6	97/99 (98%)	83 (86%)	14 (14%)	0	100	100
38	O7	82/87 (94%)	78 (95%)	4 (5%)	0	100	100
38	o7	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
39	O8	75/77 (97%)	66 (88%)	9 (12%)	0	100	100
39	o8	75/77 (97%)	63 (84%)	12 (16%)	0	100	100
40	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
40	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
41	Q0	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
41	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	32
42	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
42	q1	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	Q2	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
43	q2	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
44	Q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
44	q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
46	S0	204/206 (99%)	179 (88%)	22 (11%)	3 (2%)	10	38
46	s0	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	61
47	S1	209/216 (97%)	161 (77%)	40 (19%)	8 (4%)	3	19
47	s1	214/216 (99%)	186 (87%)	26 (12%)	2 (1%)	17	48
48	S2	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	17	48
48	s2	215/217 (99%)	187 (87%)	28 (13%)	0	100	100
49	S3	207/223 (93%)	188 (91%)	19 (9%)	0	100	100
49	s3	221/223 (99%)	187 (85%)	33 (15%)	1 (0%)	29	61
50	S4	252/260 (97%)	219 (87%)	31 (12%)	2 (1%)	19	51
50	s4	258/260 (99%)	224 (87%)	34 (13%)	0	100	100
51	S5	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	15	46
51	s5	204/206 (99%)	177 (87%)	25 (12%)	2 (1%)	15	46
52	S6	194/236 (82%)	174 (90%)	20 (10%)	0	100	100
53	S7	175/186 (94%)	138 (79%)	35 (20%)	2 (1%)	14	45
53	s7	184/186 (99%)	155 (84%)	28 (15%)	1 (0%)	29	61
54	S8	181/200 (90%)	157 (87%)	22 (12%)	2 (1%)	14	45
54	s8	184/200 (92%)	162 (88%)	21 (11%)	1 (0%)	29	61
55	S9	172/185 (93%)	140 (81%)	31 (18%)	1 (1%)	25	57
55	s9	183/185 (99%)	165 (90%)	18 (10%)	0	100	100
56	C0	88/105 (84%)	73 (83%)	14 (16%)	1 (1%)	14	45
56	c0	92/105 (88%)	65 (71%)	19 (21%)	8 (9%)	1	5
57	C1	137/146 (94%)	126 (92%)	10 (7%)	1 (1%)	22	54
57	c1	144/146 (99%)	130 (90%)	12 (8%)	2 (1%)	11	38
58	C2	98/143 (68%)	70 (71%)	25 (26%)	3 (3%)	4	23
58	c2	122/143 (85%)	91 (75%)	28 (23%)	3 (2%)	5	27
59	C3	148/150 (99%)	129 (87%)	18 (12%)	1 (1%)	22	54
59	c3	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	C4	125/128 (98%)	98 (78%)	25 (20%)	2 (2%)	9	36
60	c4	126/128 (98%)	108 (86%)	17 (14%)	1 (1%)	19	51
61	C5	114/141 (81%)	101 (89%)	13 (11%)	0	100	100
61	c5	133/141 (94%)	100 (75%)	29 (22%)	4 (3%)	4	24
62	C6	134/142 (94%)	114 (85%)	19 (14%)	1 (1%)	22	54
62	c6	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
63	C7	111/136 (82%)	94 (85%)	14 (13%)	3 (3%)	5	26
63	c7	113/136 (83%)	95 (84%)	12 (11%)	6 (5%)	2	12
64	C8	141/145 (97%)	111 (79%)	28 (20%)	2 (1%)	11	38
64	c8	143/145 (99%)	126 (88%)	15 (10%)	2 (1%)	11	38
65	C9	135/143 (94%)	120 (89%)	14 (10%)	1 (1%)	22	54
65	c9	141/143 (99%)	125 (89%)	15 (11%)	1 (1%)	22	54
66	D0	100/109 (92%)	90 (90%)	10 (10%)	0	100	100
66	d0	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	17	48
67	D1	85/87 (98%)	67 (79%)	15 (18%)	3 (4%)	3	21
67	d1	85/87 (98%)	74 (87%)	10 (12%)	1 (1%)	13	42
68	D2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	9	36
68	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	51
69	D3	142/144 (99%)	120 (84%)	21 (15%)	1 (1%)	22	54
69	d3	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
70	D4	132/134 (98%)	117 (89%)	13 (10%)	2 (2%)	10	38
70	d4	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
71	D5	68/70 (97%)	54 (79%)	11 (16%)	3 (4%)	2	16
71	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
72	D6	95/97 (98%)	69 (73%)	22 (23%)	4 (4%)	3	17
72	d6	95/97 (98%)	75 (79%)	18 (19%)	2 (2%)	7	31
73	D7	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
73	d7	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
74	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
74	d8	61/63 (97%)	48 (79%)	12 (20%)	1 (2%)	9	36
75	D9	51/53 (96%)	43 (84%)	7 (14%)	1 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	d9	51/53 (96%)	43 (84%)	8 (16%)	0	100	100
76	E0	58/62 (94%)	50 (86%)	7 (12%)	1 (2%)	9	35
76	e0	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4	22
77	SR	315/318 (99%)	274 (87%)	41 (13%)	0	100	100
77	sR	316/318 (99%)	278 (88%)	37 (12%)	1 (0%)	41	71
78	SM	143/272 (53%)	117 (82%)	25 (18%)	1 (1%)	22	54
78	sM	89/272 (33%)	73 (82%)	15 (17%)	1 (1%)	14	45
79	s6	216/218 (99%)	183 (85%)	30 (14%)	3 (1%)	11	38
All	All	21808/22972 (95%)	19331 (89%)	2311 (11%)	166 (1%)	19	51

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L6	98	VAL
10	L8	36	ILE
10	L8	116	VAL
11	L9	50	ASN
33	O2	123	LYS

### 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	
4	L2	190/190 (100%)	169 (89%)	21 (11%)	6	23
4	l2	190/190 (100%)	174 (92%)	16 (8%)	11	35
5	L3	322/322 (100%)	280 (87%)	42 (13%)	4	17
5	l3	322/322 (100%)	287 (89%)	35 (11%)	6	24
6	L4	288/288 (100%)	258 (90%)	30 (10%)	7	25
6	l4	288/288 (100%)	253 (88%)	35 (12%)	5	20
7	L5	242/244 (99%)	220 (91%)	22 (9%)	9	31
7	l5	243/244 (100%)	223 (92%)	20 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L6	134/153 (88%)	118 (88%)	16 (12%)	5	21
8	l6	135/153 (88%)	123 (91%)	12 (9%)	9	32
9	L7	190/190 (100%)	169 (89%)	21 (11%)	6	23
9	l7	187/190 (98%)	164 (88%)	23 (12%)	4	20
10	L8	186/190 (98%)	169 (91%)	17 (9%)	9	31
10	l8	177/190 (93%)	155 (88%)	22 (12%)	4	19
11	L9	169/171 (99%)	143 (85%)	26 (15%)	2	12
11	l9	171/171 (100%)	144 (84%)	27 (16%)	2	11
12	M0	185/187 (99%)	163 (88%)	22 (12%)	5	21
12	m0	186/187 (100%)	162 (87%)	24 (13%)	4	18
13	M1	147/147 (100%)	127 (86%)	20 (14%)	3	16
13	m1	147/147 (100%)	125 (85%)	22 (15%)	3	13
14	M3	154/154 (100%)	139 (90%)	15 (10%)	8	29
14	m3	154/154 (100%)	140 (91%)	14 (9%)	9	31
15	M4	107/108 (99%)	99 (92%)	8 (8%)	13	39
15	m4	108/108 (100%)	95 (88%)	13 (12%)	5	20
16	M5	175/175 (100%)	164 (94%)	11 (6%)	18	47
16	m5	175/175 (100%)	162 (93%)	13 (7%)	13	40
17	M6	160/160 (100%)	147 (92%)	13 (8%)	11	36
17	m6	160/160 (100%)	150 (94%)	10 (6%)	18	47
18	M7	139/146 (95%)	120 (86%)	19 (14%)	3	16
18	m7	125/146 (86%)	110 (88%)	15 (12%)	5	20
19	M8	150/150 (100%)	134 (89%)	16 (11%)	6	25
19	m8	150/150 (100%)	135 (90%)	15 (10%)	7	27
20	M9	151/153 (99%)	135 (89%)	16 (11%)	6	25
20	m9	153/153 (100%)	136 (89%)	17 (11%)	6	23
21	N0	156/156 (100%)	134 (86%)	22 (14%)	3	16
21	n0	156/156 (100%)	136 (87%)	20 (13%)	4	18
22	N1	136/136 (100%)	116 (85%)	20 (15%)	3	14
22	n1	136/136 (100%)	124 (91%)	12 (9%)	10	33
23	N2	86/86 (100%)	73 (85%)	13 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	n2	85/86 (99%)	77 (91%)	8 (9%)	8	30
24	N3	102/104 (98%)	91 (89%)	11 (11%)	6	24
24	n3	104/104 (100%)	94 (90%)	10 (10%)	8	29
25	N4	55/129 (43%)	54 (98%)	1 (2%)	59	78
25	n4	100/129 (78%)	93 (93%)	7 (7%)	15	43
26	N5	103/104 (99%)	88 (85%)	15 (15%)	3	14
26	n5	104/104 (100%)	92 (88%)	12 (12%)	5	22
27	N6	108/108 (100%)	100 (93%)	8 (7%)	13	40
27	n6	106/108 (98%)	98 (92%)	8 (8%)	13	39
28	N7	115/115 (100%)	103 (90%)	12 (10%)	7	25
28	n7	115/115 (100%)	108 (94%)	7 (6%)	18	48
29	N8	118/118 (100%)	102 (86%)	16 (14%)	3	16
29	n8	118/118 (100%)	108 (92%)	10 (8%)	10	35
30	N9	44/46 (96%)	40 (91%)	4 (9%)	9	31
30	n9	46/46 (100%)	41 (89%)	5 (11%)	6	24
31	O0	81/84 (96%)	72 (89%)	9 (11%)	6	23
31	o0	84/84 (100%)	75 (89%)	9 (11%)	6	25
32	O1	89/96 (93%)	81 (91%)	8 (9%)	9	32
32	o1	94/96 (98%)	84 (89%)	10 (11%)	6	25
33	O2	108/109 (99%)	94 (87%)	14 (13%)	4	17
33	o2	109/109 (100%)	101 (93%)	8 (7%)	14	41
34	O3	90/90 (100%)	83 (92%)	7 (8%)	12	38
34	o3	90/90 (100%)	85 (94%)	5 (6%)	21	52
35	O4	95/95 (100%)	88 (93%)	7 (7%)	13	40
35	o4	95/95 (100%)	88 (93%)	7 (7%)	13	40
36	O5	104/104 (100%)	96 (92%)	8 (8%)	13	38
36	o5	103/104 (99%)	98 (95%)	5 (5%)	25	56
37	O6	79/81 (98%)	74 (94%)	5 (6%)	18	47
37	o6	81/81 (100%)	73 (90%)	8 (10%)	8	28
38	O7	69/70 (99%)	60 (87%)	9 (13%)	4	17
38	o7	70/70 (100%)	63 (90%)	7 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	O8	68/68 (100%)	63 (93%)	5 (7%)	13	40
39	o8	67/68 (98%)	56 (84%)	11 (16%)	2	10
40	O9	45/45 (100%)	39 (87%)	6 (13%)	4	17
40	o9	45/45 (100%)	43 (96%)	2 (4%)	28	59
41	Q0	47/47 (100%)	45 (96%)	2 (4%)	29	59
41	q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
42	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	8
42	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
43	Q2	90/90 (100%)	79 (88%)	11 (12%)	5	20
43	q2	90/90 (100%)	80 (89%)	10 (11%)	6	23
44	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	16
44	q3	71/71 (100%)	64 (90%)	7 (10%)	8	28
46	S0	166/173 (96%)	149 (90%)	17 (10%)	7	27
46	s0	166/173 (96%)	150 (90%)	16 (10%)	8	29
47	S1	189/192 (98%)	156 (82%)	33 (18%)	2	8
47	s1	192/192 (100%)	172 (90%)	20 (10%)	7	25
48	S2	176/176 (100%)	158 (90%)	18 (10%)	7	27
48	s2	176/176 (100%)	166 (94%)	10 (6%)	20	51
49	S3	169/182 (93%)	151 (89%)	18 (11%)	6	25
49	s3	182/182 (100%)	165 (91%)	17 (9%)	9	30
50	S4	219/221 (99%)	203 (93%)	16 (7%)	14	41
50	s4	221/221 (100%)	200 (90%)	21 (10%)	8	29
51	S5	173/173 (100%)	155 (90%)	18 (10%)	7	25
51	s5	173/173 (100%)	161 (93%)	12 (7%)	15	44
52	S6	167/201 (83%)	154 (92%)	13 (8%)	12	38
53	S7	160/166 (96%)	145 (91%)	15 (9%)	8	30
53	s7	166/166 (100%)	150 (90%)	16 (10%)	8	29
54	S8	148/161 (92%)	135 (91%)	13 (9%)	10	33
54	s8	150/161 (93%)	142 (95%)	8 (5%)	22	53
55	S9	152/158 (96%)	141 (93%)	11 (7%)	14	41
55	s9	158/158 (100%)	146 (92%)	12 (8%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	C0	77/98 (79%)	71 (92%)	6 (8%)	12	38
56	c0	73/98 (74%)	68 (93%)	5 (7%)	16	44
57	C1	126/129 (98%)	110 (87%)	16 (13%)	4	19
57	c1	129/129 (100%)	117 (91%)	12 (9%)	9	30
58	C2	82/119 (69%)	69 (84%)	13 (16%)	2	11
58	c2	88/119 (74%)	72 (82%)	16 (18%)	1	7
59	C3	127/127 (100%)	118 (93%)	9 (7%)	14	42
59	c3	127/127 (100%)	116 (91%)	11 (9%)	10	34
60	C4	81/97 (84%)	68 (84%)	13 (16%)	2	11
60	c4	97/97 (100%)	84 (87%)	13 (13%)	4	16
61	C5	96/117 (82%)	91 (95%)	5 (5%)	23	54
61	c5	103/117 (88%)	86 (84%)	17 (16%)	2	10
62	C6	113/118 (96%)	100 (88%)	13 (12%)	5	22
62	c6	118/118 (100%)	108 (92%)	10 (8%)	10	35
63	C7	94/124 (76%)	81 (86%)	13 (14%)	3	16
63	c7	92/124 (74%)	86 (94%)	6 (6%)	17	46
64	C8	126/128 (98%)	111 (88%)	15 (12%)	5	21
64	c8	128/128 (100%)	114 (89%)	14 (11%)	6	24
65	C9	110/115 (96%)	98 (89%)	12 (11%)	6	24
65	c9	115/115 (100%)	104 (90%)	11 (10%)	8	29
66	D0	96/102 (94%)	85 (88%)	11 (12%)	5	22
66	d0	102/102 (100%)	88 (86%)	14 (14%)	3	16
67	D1	74/74 (100%)	68 (92%)	6 (8%)	11	36
67	d1	74/74 (100%)	63 (85%)	11 (15%)	3	13
68	D2	110/110 (100%)	98 (89%)	12 (11%)	6	24
68	d2	110/110 (100%)	97 (88%)	13 (12%)	5	21
69	D3	119/119 (100%)	111 (93%)	8 (7%)	16	45
69	d3	119/119 (100%)	112 (94%)	7 (6%)	19	49
70	D4	112/112 (100%)	99 (88%)	13 (12%)	5	22
70	d4	112/112 (100%)	104 (93%)	8 (7%)	14	42
71	D5	61/61 (100%)	51 (84%)	10 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	d5	61/61 (100%)	51 (84%)	10 (16%)	2	10
72	D6	83/83 (100%)	69 (83%)	14 (17%)	2	9
72	d6	83/83 (100%)	73 (88%)	10 (12%)	5	20
73	D7	70/70 (100%)	63 (90%)	7 (10%)	7	27
73	d7	70/70 (100%)	64 (91%)	6 (9%)	10	35
74	D8	56/56 (100%)	51 (91%)	5 (9%)	9	32
74	d8	56/56 (100%)	50 (89%)	6 (11%)	6	25
75	D9	47/47 (100%)	44 (94%)	3 (6%)	17	46
75	d9	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	E0	51/53 (96%)	42 (82%)	9 (18%)	2	8
76	e0	53/53 (100%)	46 (87%)	7 (13%)	4	17
77	SR	259/261 (99%)	246 (95%)	13 (5%)	24	55
77	sR	259/261 (99%)	238 (92%)	21 (8%)	11	36
78	SM	97/227 (43%)	85 (88%)	12 (12%)	4	19
78	sM	54/227 (24%)	50 (93%)	4 (7%)	13	40
79	s6	187/187 (100%)	168 (90%)	19 (10%)	7	27
All	All	18408/19292 (95%)	16513 (90%)	1895 (10%)	7	26

5 of 1895 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
73	D7	56	CYS
66	d0	16	GLN
11	l9	93	VAL
64	c8	97	ASP
78	sM	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
6	l4	316	ASN
28	n7	78	ASN
77	sR	182	ASN
12	m0	112	GLN
24	n3	47	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3069/3396 (90%)	618 (20%)	56 (1%)
1	5	3080/3396 (90%)	657 (21%)	53 (1%)
2	3	120/121 (99%)	22 (18%)	1 (0%)
2	7	120/121 (99%)	20 (16%)	0
3	4	156/158 (98%)	35 (22%)	4 (2%)
3	8	157/158 (99%)	35 (22%)	7 (4%)
45	2	1708/1800 (94%)	485 (28%)	33 (1%)
45	6	1678/1800 (93%)	453 (26%)	39 (2%)
All	All	10088/10950 (92%)	2325 (23%)	193 (1%)

5 of 2325 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	25	U
1	1	26	A
1	1	30	G
1	1	40	A

5 of 193 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1573	G
1	5	3303	G
1	5	1815	U
1	5	2372	A
3	8	82	U

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 2242 ligands modelled in this entry, 2155 are monoatomic - leaving 87 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	$\# Z  > 2$
80	PAR	1	3414	-	45,45,45	0.21	0	64,67,67	1.05	4 (6%)
80	PAR	1	3428	81	45,45,45	0.22	0	64,67,67	0.99	2 (3%)
80	PAR	5	3428	81	45,45,45	0.39	0	64,67,67	1.21	5 (7%)
80	PAR	1	3406	-	45,45,45	0.21	0	64,67,67	0.89	4 (6%)
80	PAR	6	1903	-	45,45,45	0.18	0	64,67,67	0.88	1 (1%)
80	PAR	5	3420	-	45,45,45	0.23	0	64,67,67	1.30	7 (10%)
80	PAR	6	1901	-	45,45,45	0.25	0	64,67,67	0.92	2 (3%)
80	PAR	5	3425	-	45,45,45	0.22	0	64,67,67	0.98	4 (6%)
80	PAR	5	3424	-	45,45,45	0.23	0	64,67,67	1.02	3 (4%)
80	PAR	7	202	-	45,45,45	0.18	0	64,67,67	0.87	3 (4%)
80	PAR	1	3429	-	45,45,45	0.23	0	64,67,67	1.26	4 (6%)
80	PAR	2	1902	-	45,45,45	0.24	0	64,67,67	1.34	5 (7%)
80	PAR	5	3415	-	45,45,45	0.26	0	64,67,67	1.01	2 (3%)
80	PAR	5	3414	-	45,45,45	0.19	0	64,67,67	0.80	4 (6%)
80	PAR	1	3412	-	45,45,45	0.21	0	64,67,67	1.23	8 (12%)
80	PAR	5	3401	-	45,45,45	0.27	0	64,67,67	1.01	2 (3%)
80	PAR	3	203	-	45,45,45	0.21	0	64,67,67	0.99	3 (4%)
80	PAR	5	3427	-	45,45,45	0.22	0	64,67,67	1.05	3 (4%)
80	PAR	1	3426	-	45,45,45	0.25	0	64,67,67	1.02	3 (4%)
80	PAR	1	3420	-	45,45,45	0.20	0	64,67,67	0.99	3 (4%)
80	PAR	5	3422	-	45,45,45	0.20	0	64,67,67	0.91	4 (6%)
80	PAR	1	3403	81	45,45,45	0.22	0	64,67,67	0.92	1 (1%)
80	PAR	6	1906	-	45,45,45	0.20	0	64,67,67	0.75	2 (3%)
80	PAR	7	201	-	45,45,45	0.17	0	64,67,67	0.75	2 (3%)
80	PAR	8	201	-	45,45,45	0.24	0	64,67,67	1.01	5 (7%)
80	PAR	1	3417	-	45,45,45	0.17	0	64,67,67	0.88	2 (3%)
80	PAR	1	3427	-	45,45,45	0.21	0	64,67,67	0.83	3 (4%)
80	PAR	1	3404	-	45,45,45	0.22	0	64,67,67	0.92	2 (3%)
80	PAR	1	3411	-	45,45,45	0.32	0	64,67,67	1.68	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
80	PAR	1	3430	-	45,45,45	0.24	0	64,67,67	0.95	3 (4%)
80	PAR	5	3410	-	45,45,45	0.17	0	64,67,67	0.87	2 (3%)
80	PAR	1	3405	-	45,45,45	0.24	0	64,67,67	0.89	2 (3%)
80	PAR	1	3415	-	45,45,45	0.25	0	64,67,67	0.88	3 (4%)
80	PAR	4	201	-	45,45,45	0.29	0	64,67,67	1.21	5 (7%)
80	PAR	5	3426	-	45,45,45	0.23	0	64,67,67	0.89	1 (1%)
80	PAR	1	3435	-	45,45,45	0.38	0	64,67,67	1.31	4 (6%)
80	PAR	5	3419	-	45,45,45	0.33	0	64,67,67	1.27	8 (12%)
80	PAR	1	3419	-	45,45,45	0.22	0	64,67,67	1.15	5 (7%)
80	PAR	5	3407	-	45,45,45	0.20	0	64,67,67	0.81	3 (4%)
80	PAR	1	3434	-	45,45,45	0.20	0	64,67,67	0.89	5 (7%)
80	PAR	4	202	-	45,45,45	0.26	0	64,67,67	1.06	4 (6%)
80	PAR	6	1904	-	45,45,45	0.21	0	64,67,67	0.90	3 (4%)
80	PAR	1	3408	-	45,45,45	0.22	0	64,67,67	1.07	5 (7%)
80	PAR	8	202	-	45,45,45	0.22	0	64,67,67	0.88	1 (1%)
80	PAR	5	3416	-	45,45,45	0.22	0	64,67,67	0.91	3 (4%)
80	PAR	1	3401	-	45,45,45	0.18	0	64,67,67	1.22	2 (3%)
80	PAR	2	1903	-	45,45,45	0.22	0	64,67,67	0.84	3 (4%)
80	PAR	5	3406	81	45,45,45	0.27	0	64,67,67	0.95	5 (7%)
80	PAR	1	3416	-	45,45,45	0.28	0	64,67,67	1.13	5 (7%)
80	PAR	5	3423	-	45,45,45	0.21	0	64,67,67	0.96	4 (6%)
80	PAR	n3	201	-	45,45,45	0.24	0	64,67,67	1.07	4 (6%)
80	PAR	5	3403	-	45,45,45	0.25	0	64,67,67	1.02	3 (4%)
80	PAR	1	3425	-	45,45,45	0.28	0	64,67,67	1.17	5 (7%)
80	PAR	5	3405	-	45,45,45	0.22	0	64,67,67	0.80	2 (3%)
80	PAR	2	1905	-	45,45,45	0.20	0	64,67,67	0.79	4 (6%)
80	PAR	1	3413	-	45,45,45	0.20	0	64,67,67	0.66	1 (1%)
80	PAR	5	3418	-	45,45,45	0.24	0	64,67,67	1.08	3 (4%)
80	PAR	5	3417	-	45,45,45	0.16	0	64,67,67	0.78	2 (3%)
80	PAR	1	3432	-	45,45,45	0.25	0	64,67,67	1.11	2 (3%)
80	PAR	5	3421	-	45,45,45	0.20	0	64,67,67	1.25	2 (3%)
80	PAR	5	3412	-	45,45,45	0.21	0	64,67,67	0.89	2 (3%)
80	PAR	1	3423	-	45,45,45	0.20	0	64,67,67	0.75	1 (1%)
80	PAR	5	3409	-	45,45,45	0.22	0	64,67,67	0.98	4 (6%)
80	PAR	2	1901	-	45,45,45	0.19	0	64,67,67	0.74	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
80	PAR	5	3408	-	45,45,45	0.22	0	64,67,67	0.91	3 (4%)
80	PAR	1	3437	1	45,45,45	0.19	0	64,67,67	0.73	2 (3%)
80	PAR	6	1905	-	45,45,45	0.20	0	64,67,67	1.05	4 (6%)
80	PAR	1	3410	-	45,45,45	0.36	0	64,67,67	1.38	8 (12%)
80	PAR	3	201	-	45,45,45	0.26	0	64,67,67	1.46	5 (7%)
80	PAR	1	3409	-	45,45,45	0.29	0	64,67,67	1.45	4 (6%)
80	PAR	3	202	81	45,45,45	0.21	0	64,67,67	1.06	3 (4%)
80	PAR	1	3402	-	45,45,45	0.21	0	64,67,67	0.78	2 (3%)
80	PAR	1	3407	-	45,45,45	0.21	0	64,67,67	0.95	3 (4%)
80	PAR	1	3436	-	45,45,45	0.23	0	64,67,67	1.01	3 (4%)
80	PAR	5	3404	-	45,45,45	0.24	0	64,67,67	1.22	4 (6%)
80	PAR	1	3418	-	45,45,45	0.26	0	64,67,67	0.87	2 (3%)
80	PAR	6	1902	-	45,45,45	0.24	0	64,67,67	0.98	3 (4%)
80	PAR	o2	201	-	45,45,45	0.28	0	64,67,67	1.17	4 (6%)
80	PAR	1	3433	-	45,45,45	0.27	0	64,67,67	1.24	6 (9%)
80	PAR	1	3421	-	45,45,45	0.21	0	64,67,67	0.93	2 (3%)
80	PAR	5	3402	-	45,45,45	0.20	0	64,67,67	1.05	2 (3%)
80	PAR	2	1904	-	45,45,45	0.21	0	64,67,67	1.42	4 (6%)
80	PAR	5	3411	-	45,45,45	0.24	0	64,67,67	1.13	5 (7%)
80	PAR	5	3413	-	45,45,45	0.21	0	64,67,67	1.40	6 (9%)
80	PAR	1	3424	-	45,45,45	0.16	0	64,67,67	0.71	2 (3%)
80	PAR	1	3422	-	45,45,45	0.22	0	64,67,67	1.05	3 (4%)
80	PAR	1	3431	-	45,45,45	0.19	0	64,67,67	1.13	3 (4%)

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
80	PAR	1	3414	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3428	81	-	3/18/94/94	0/4/4/4
80	PAR	5	3428	81	-	7/18/94/94	0/4/4/4
80	PAR	1	3406	-	-	2/18/94/94	0/4/4/4
80	PAR	6	1903	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3420	-	-	3/18/94/94	1/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	6	1901	-	-	2/18/94/94	0/4/4/4
80	PAR	5	3425	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3424	-	-	4/18/94/94	0/4/4/4
80	PAR	7	202	-	-	8/18/94/94	0/4/4/4
80	PAR	1	3429	-	-	3/18/94/94	0/4/4/4
80	PAR	2	1902	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3415	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3414	-	-	1/18/94/94	1/4/4/4
80	PAR	1	3412	-	-	4/18/94/94	0/4/4/4
80	PAR	5	3401	-	-	6/18/94/94	0/4/4/4
80	PAR	3	203	-	-	4/18/94/94	1/4/4/4
80	PAR	5	3427	-	-	3/18/94/94	1/4/4/4
80	PAR	1	3426	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3420	-	-	1/18/94/94	0/4/4/4
80	PAR	5	3422	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3403	81	-	5/18/94/94	0/4/4/4
80	PAR	6	1906	-	-	5/18/94/94	0/4/4/4
80	PAR	7	201	-	-	3/18/94/94	0/4/4/4
80	PAR	8	201	-	-	1/18/94/94	0/4/4/4
80	PAR	1	3417	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3427	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3404	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3411	-	-	8/18/94/94	0/4/4/4
80	PAR	1	3430	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3410	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3405	-	-	11/18/94/94	0/4/4/4
80	PAR	1	3415	-	-	4/18/94/94	0/4/4/4
80	PAR	4	201	-	-	6/18/94/94	1/4/4/4
80	PAR	5	3426	-	-	4/18/94/94	1/4/4/4
80	PAR	1	3435	-	-	11/18/94/94	0/4/4/4
80	PAR	5	3419	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3419	-	-	7/18/94/94	1/4/4/4
80	PAR	5	3407	-	-	9/18/94/94	0/4/4/4
80	PAR	1	3434	-	-	6/18/94/94	0/4/4/4
80	PAR	4	202	-	-	3/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	6	1904	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3408	-	-	3/18/94/94	0/4/4/4
80	PAR	8	202	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3416	-	-	2/18/94/94	0/4/4/4
80	PAR	1	3401	-	-	5/18/94/94	0/4/4/4
80	PAR	2	1903	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3406	81	-	5/18/94/94	0/4/4/4
80	PAR	1	3416	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3423	-	-	5/18/94/94	0/4/4/4
80	PAR	n3	201	-	-	8/18/94/94	0/4/4/4
80	PAR	5	3403	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3425	-	-	10/18/94/94	0/4/4/4
80	PAR	5	3405	-	-	7/18/94/94	0/4/4/4
80	PAR	2	1905	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3413	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3418	-	-	6/18/94/94	0/4/4/4
80	PAR	5	3417	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3432	-	-	3/18/94/94	1/4/4/4
80	PAR	5	3421	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3412	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3423	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3409	-	-	9/18/94/94	0/4/4/4
80	PAR	2	1901	-	-	1/18/94/94	0/4/4/4
80	PAR	5	3408	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3437	1	-	5/18/94/94	0/4/4/4
80	PAR	6	1905	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3410	-	-	6/18/94/94	0/4/4/4
80	PAR	3	201	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3409	-	-	9/18/94/94	1/4/4/4
80	PAR	3	202	81	-	8/18/94/94	0/4/4/4
80	PAR	1	3402	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3407	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3436	-	-	9/18/94/94	0/4/4/4
80	PAR	5	3404	-	-	8/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	1	3418	-	-	7/18/94/94	1/4/4/4
80	PAR	6	1902	-	-	9/18/94/94	0/4/4/4
80	PAR	o2	201	-	-	10/18/94/94	0/4/4/4
80	PAR	1	3433	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3421	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3402	-	-	8/18/94/94	0/4/4/4
80	PAR	2	1904	-	-	4/18/94/94	0/4/4/4
80	PAR	5	3411	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3413	-	-	2/18/94/94	0/4/4/4
80	PAR	1	3424	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3422	-	-	8/18/94/94	0/4/4/4
80	PAR	1	3431	-	-	5/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3409	PAR	O11-C11-C21	8.93	123.60	108.22
80	5	3421	PAR	O52-C13-O43	-8.23	102.52	111.43
80	2	1904	PAR	O52-C13-O43	-7.82	102.97	111.43
80	1	3431	PAR	O52-C13-O43	-7.17	103.67	111.43
80	5	3413	PAR	O11-C11-C21	6.84	120.00	108.22

There are no chirality outliers.

5 of 474 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	1	3401	PAR	C23-C13-O52-C52
80	1	3401	PAR	C24-C14-O33-C33
80	1	3402	PAR	C23-C13-O52-C52
80	1	3403	PAR	C21-C11-O11-C42
80	1	3403	PAR	C23-C13-O52-C52

5 of 10 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	1	3409	PAR	C12-C22-C32-C42-C52-C62
80	5	3414	PAR	C12-C22-C32-C42-C52-C62

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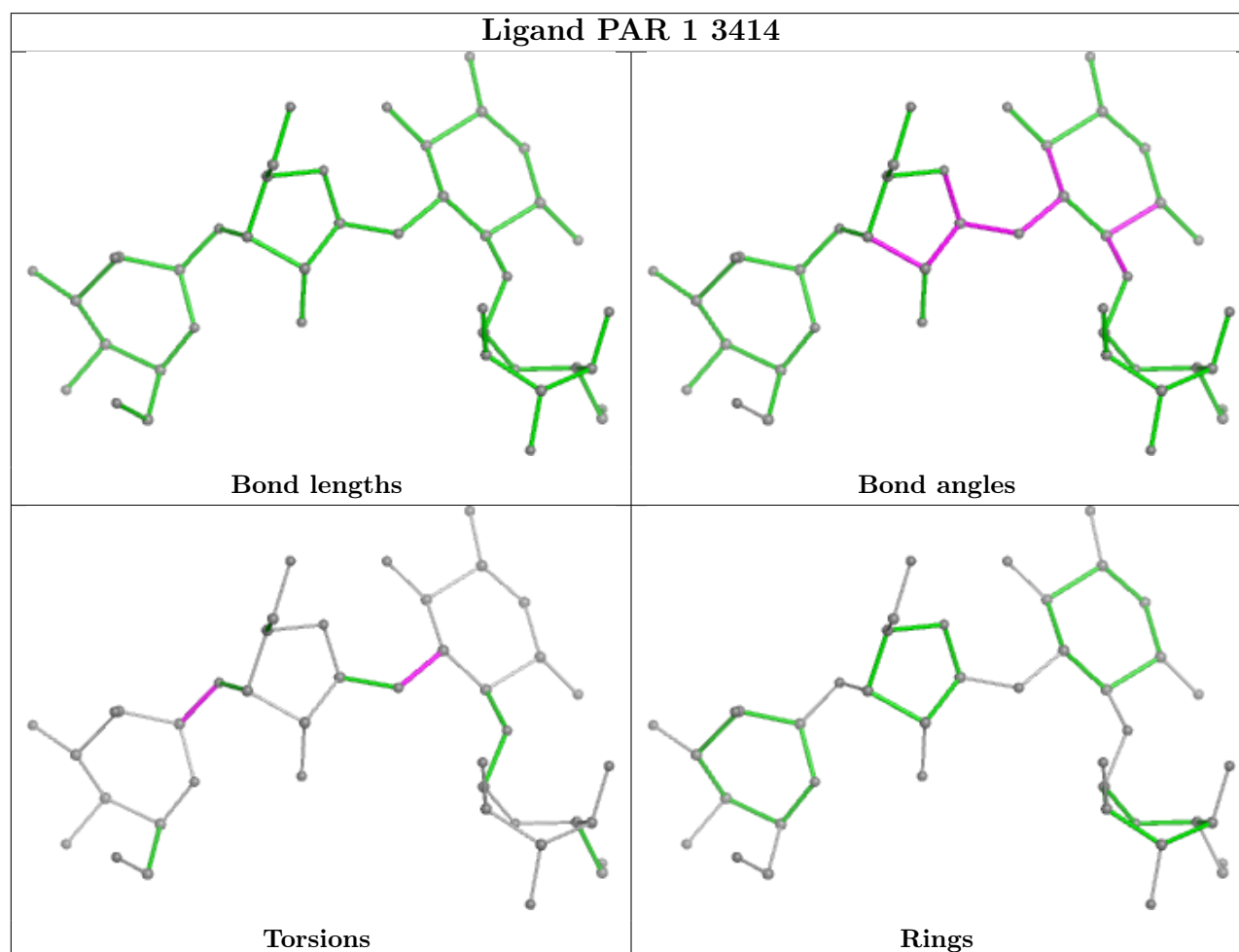


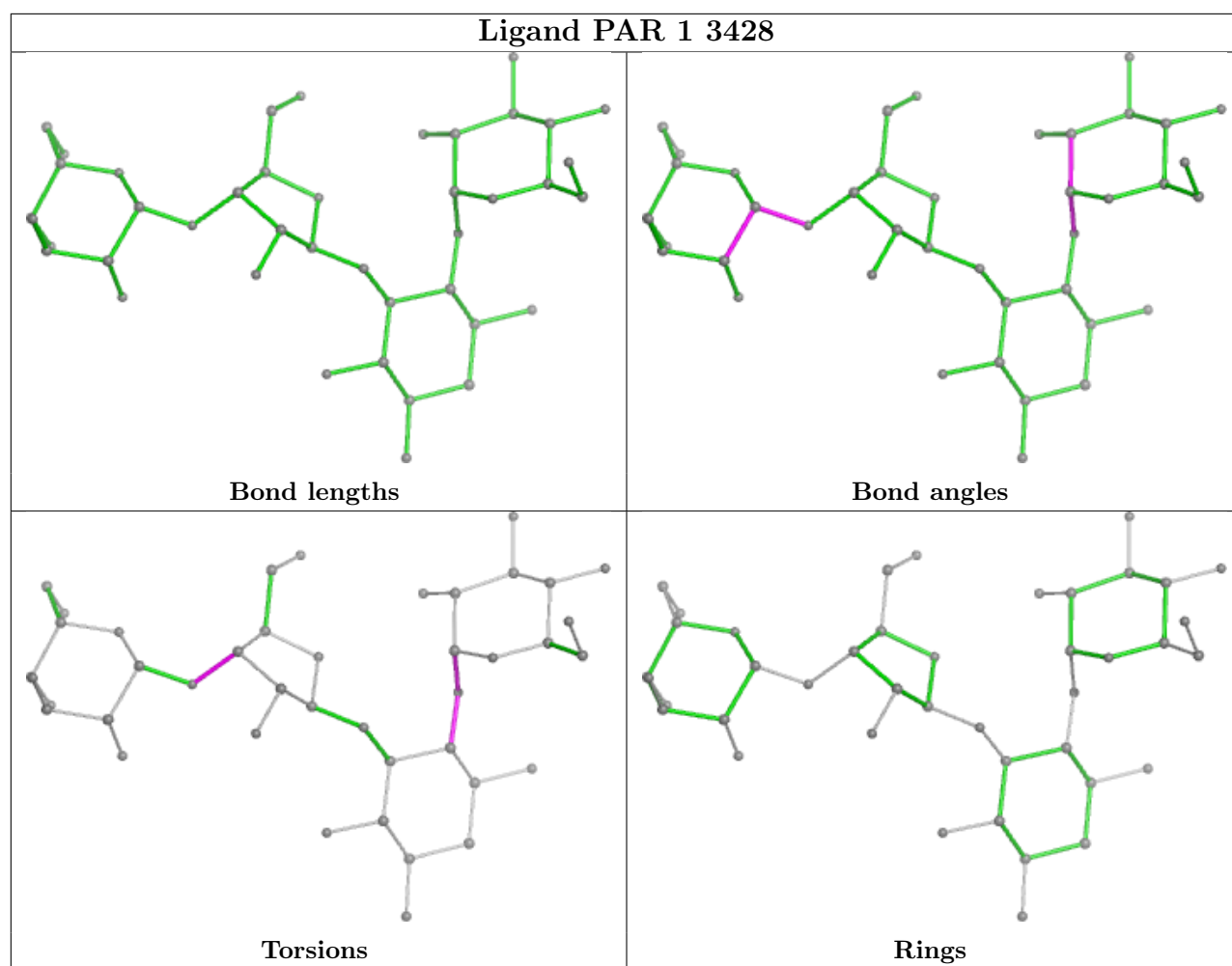
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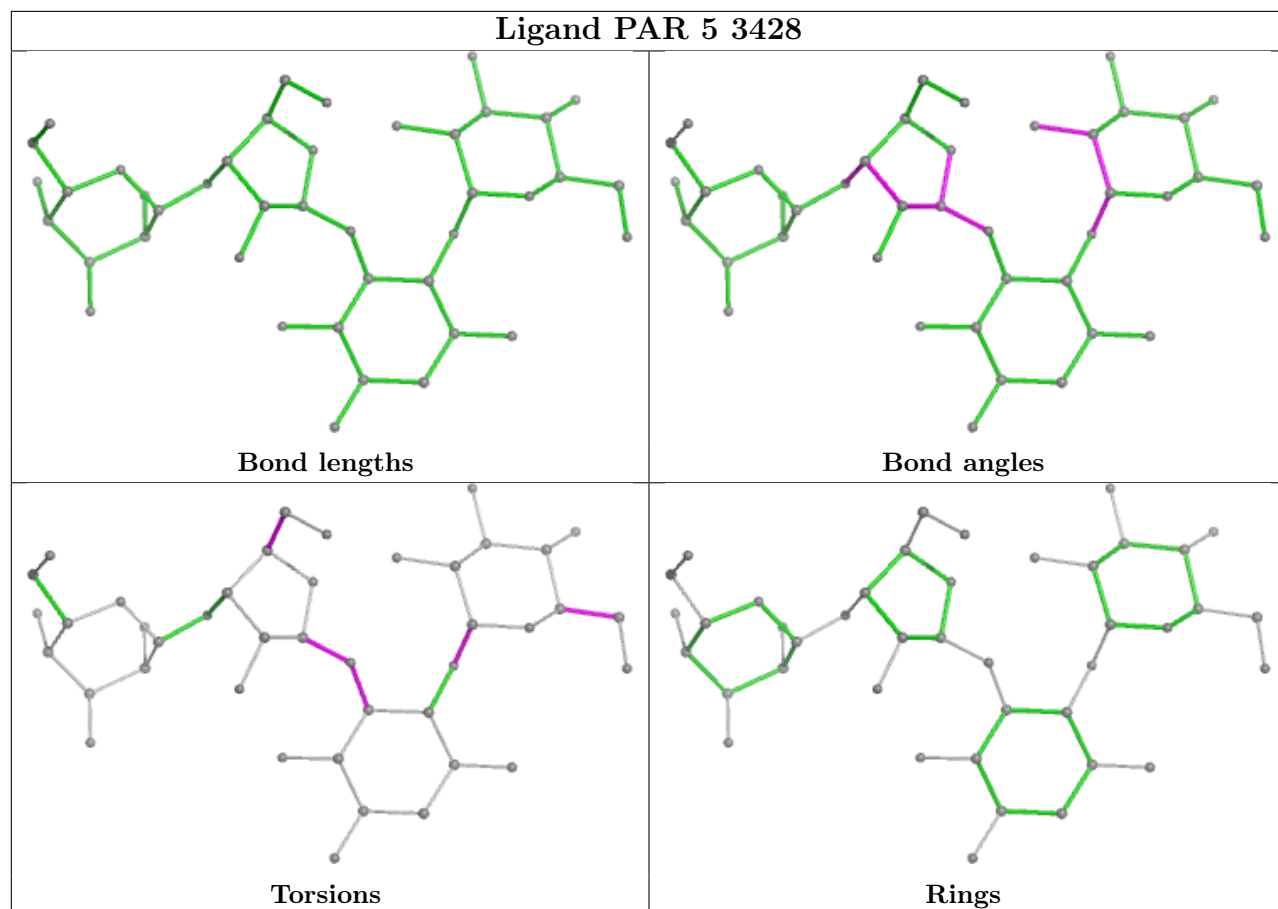
Mol	Chain	Res	Type	Atoms
80	4	201	PAR	C12-C22-C32-C42-C52-C62
80	3	203	PAR	C12-C22-C32-C42-C52-C62
80	1	3418	PAR	C14-C24-C34-C44-C54-O54

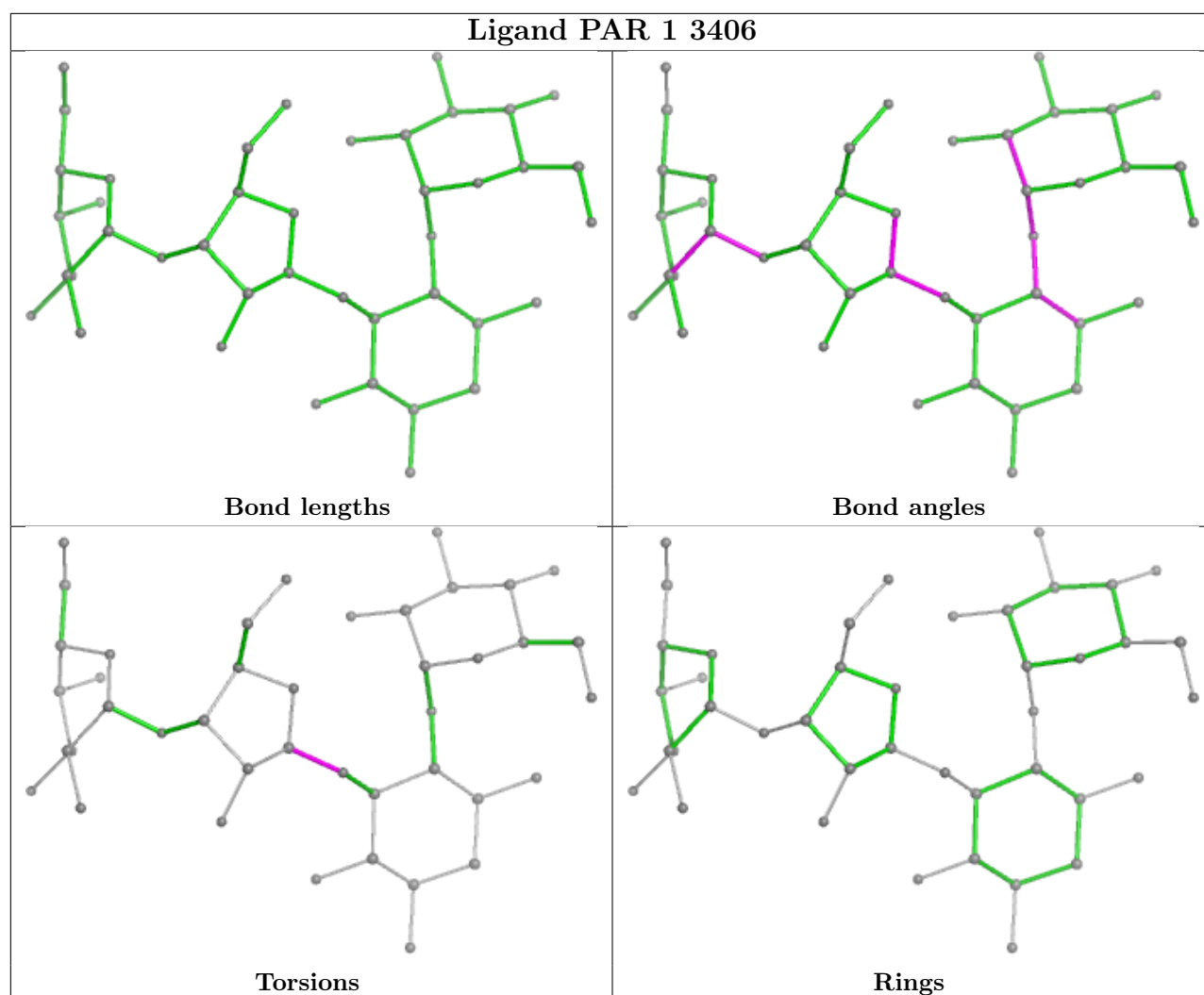
No monomer is involved in short contacts.

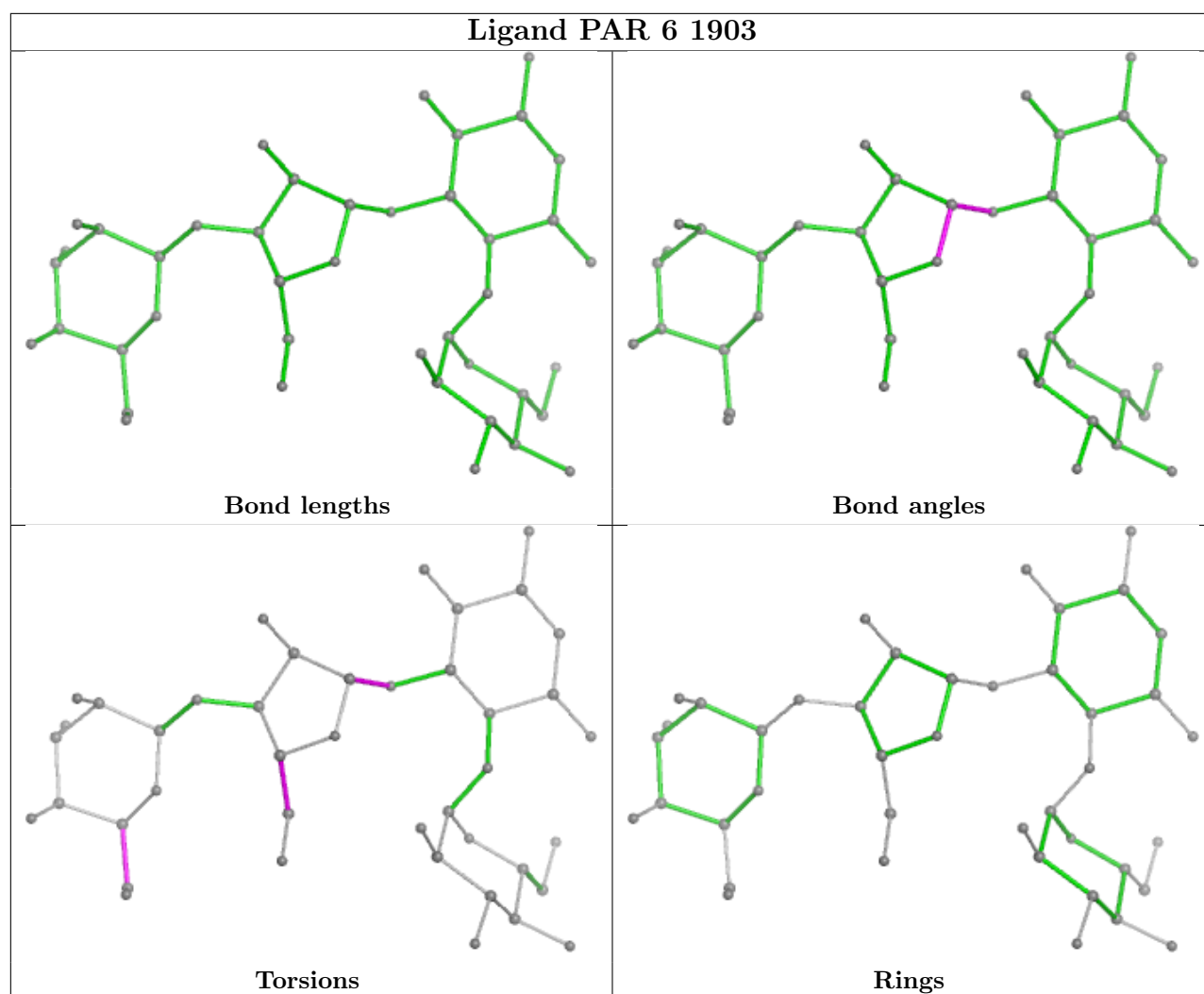
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

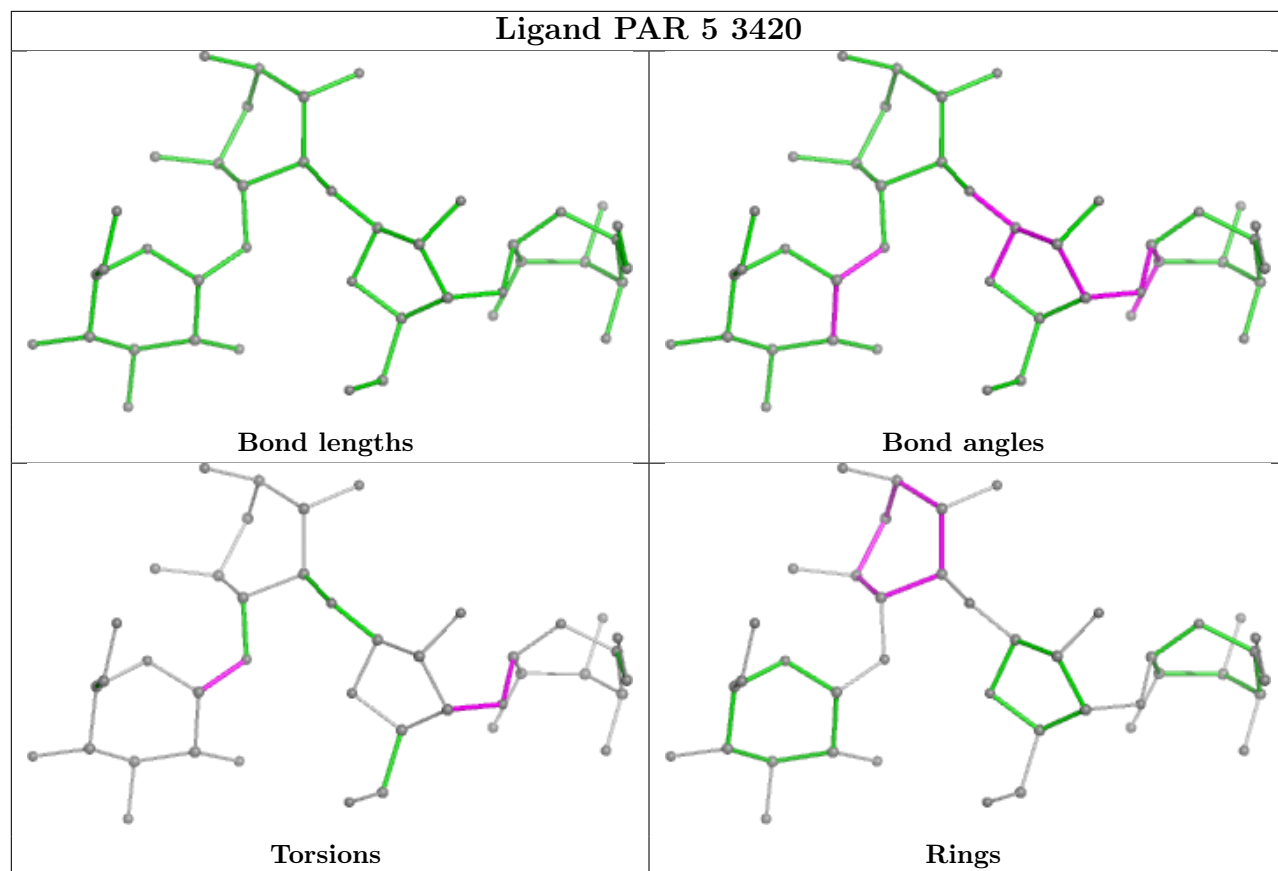




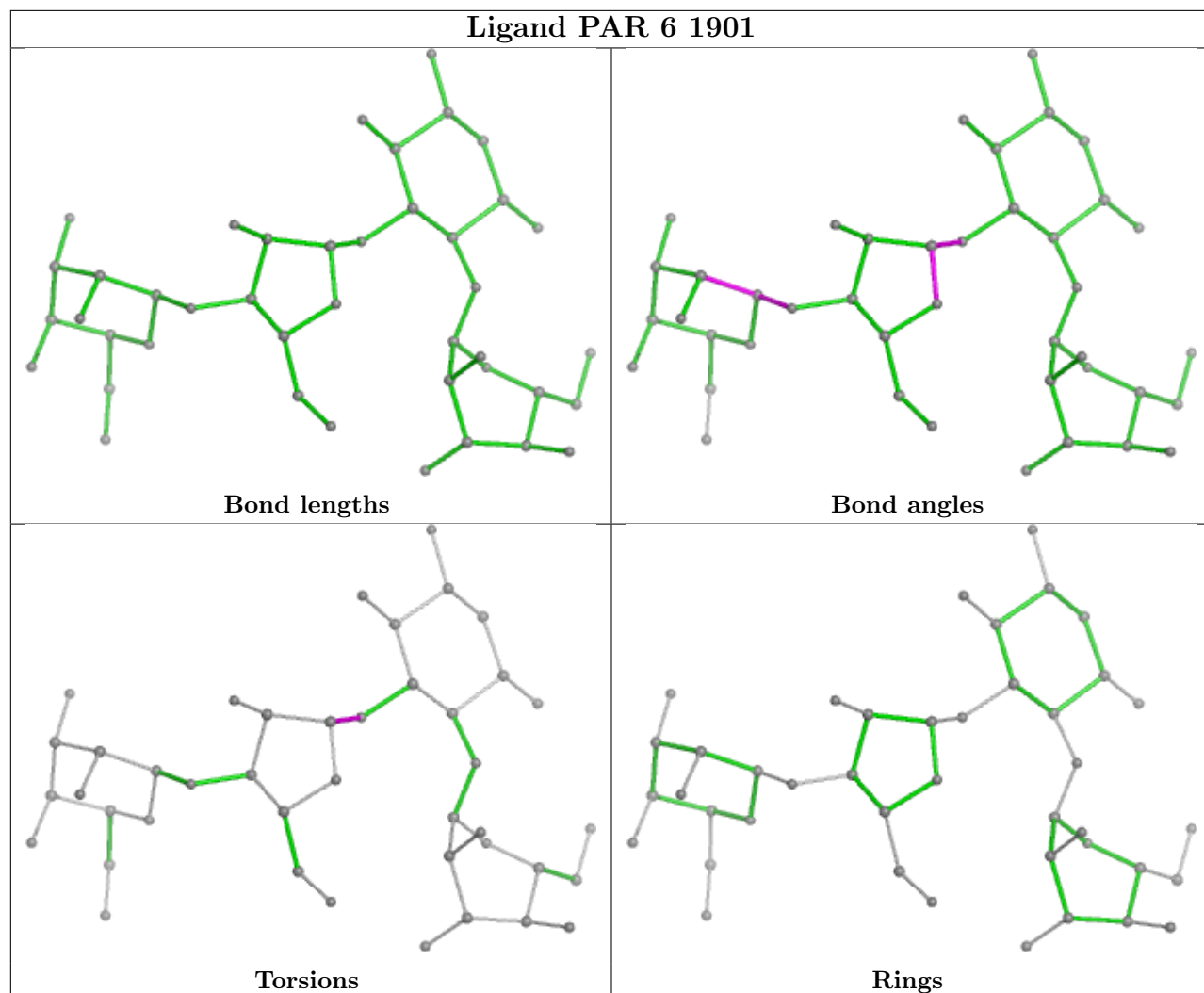




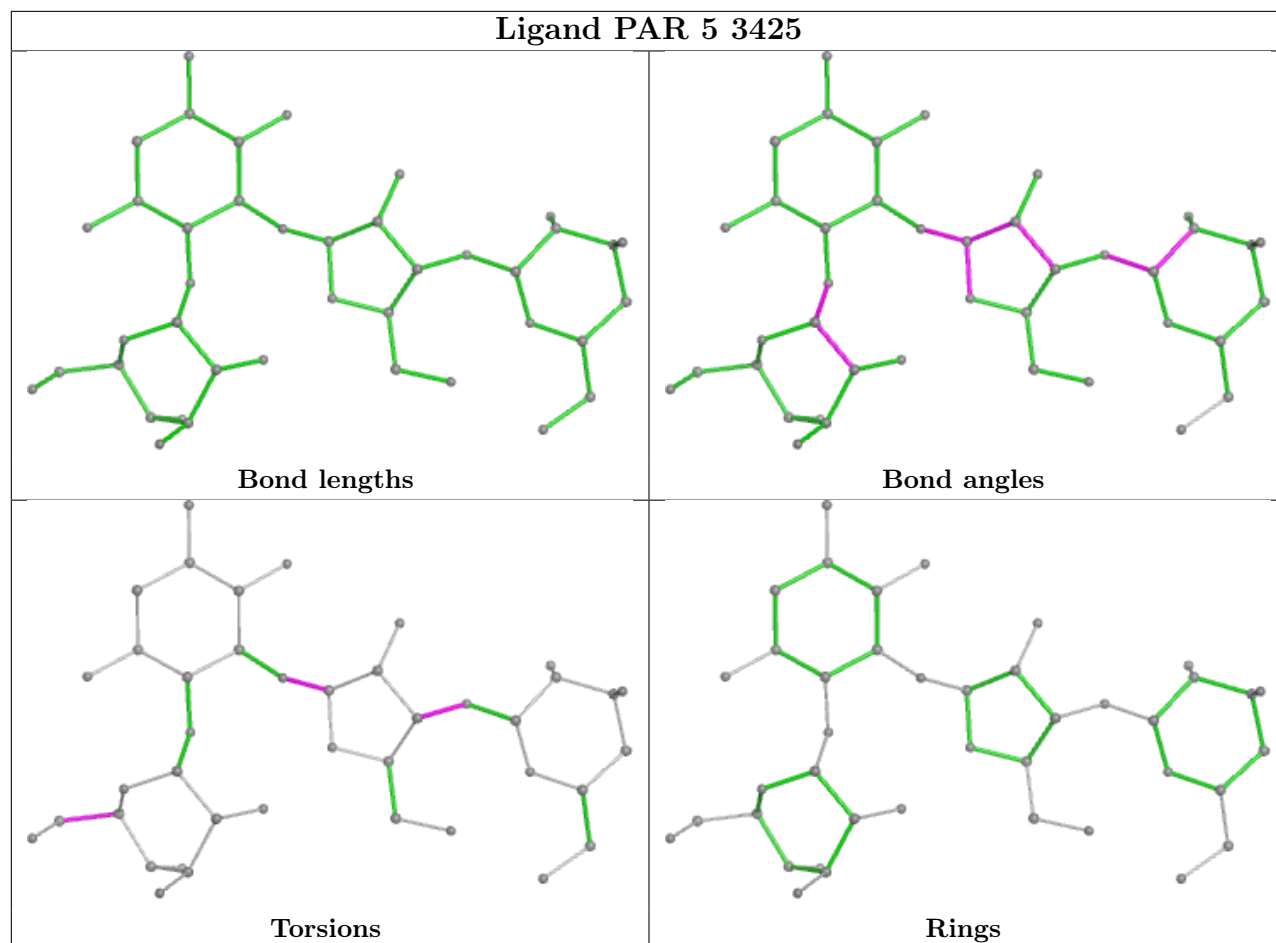




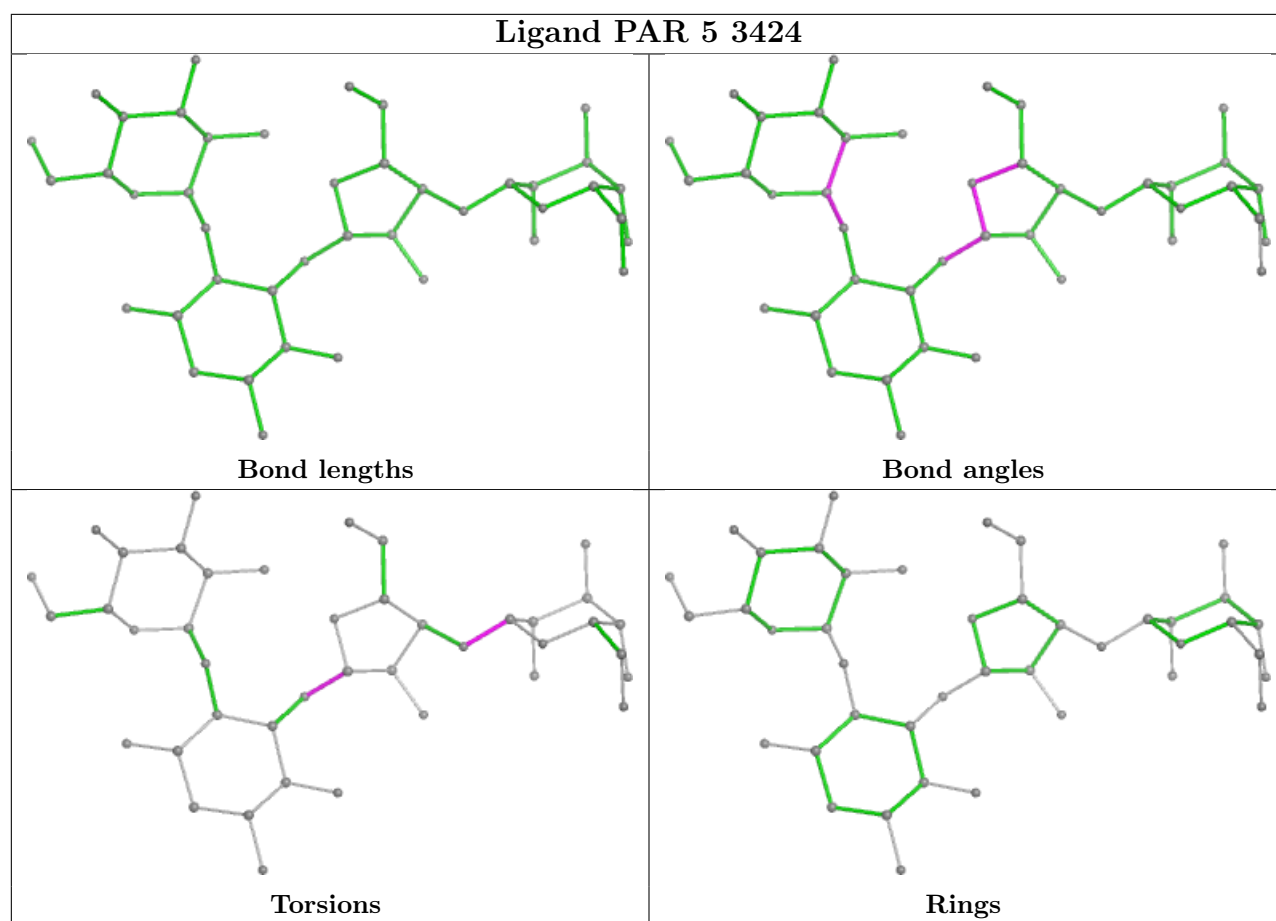
## Ligand PAR 6 1901



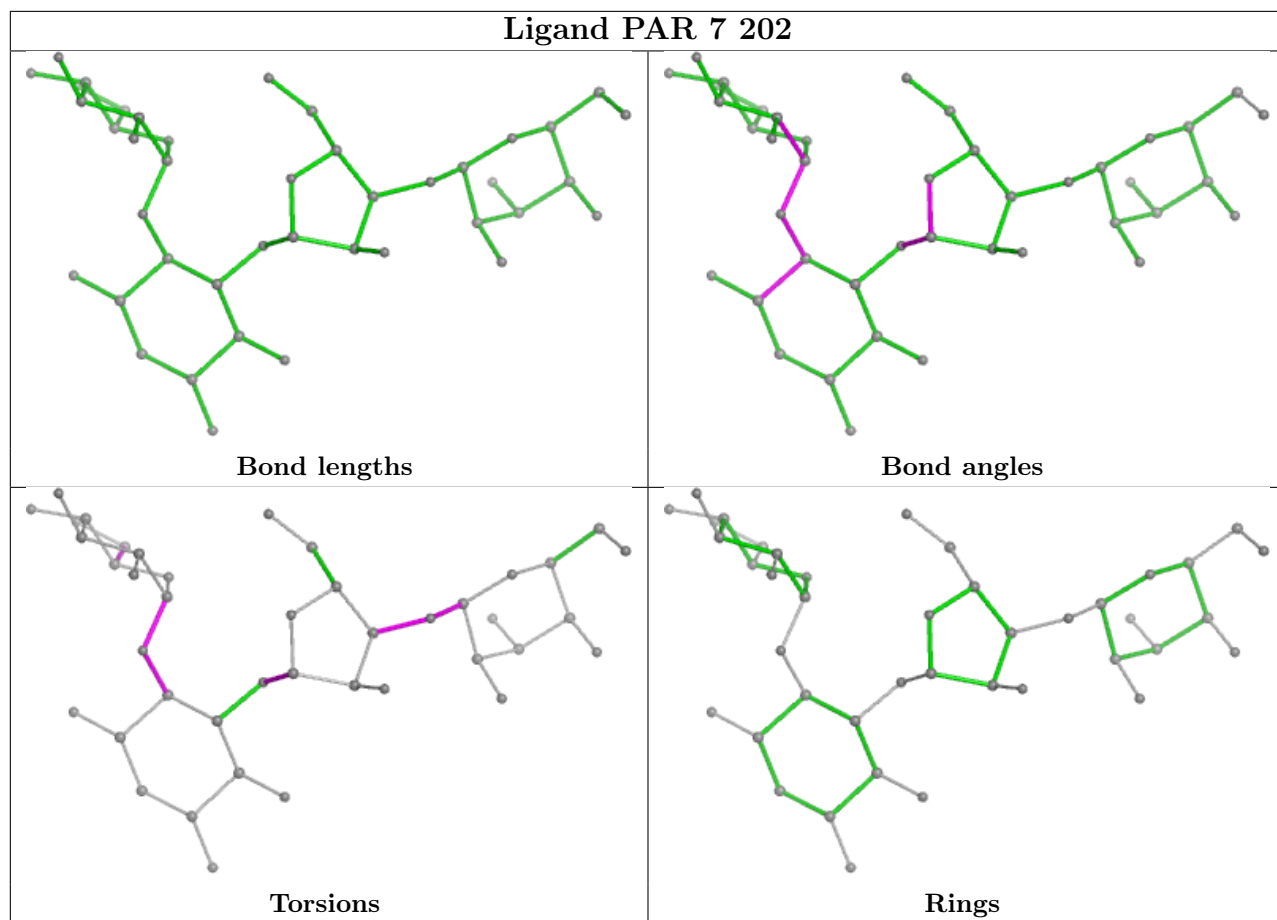
## Ligand PAR 5 3425

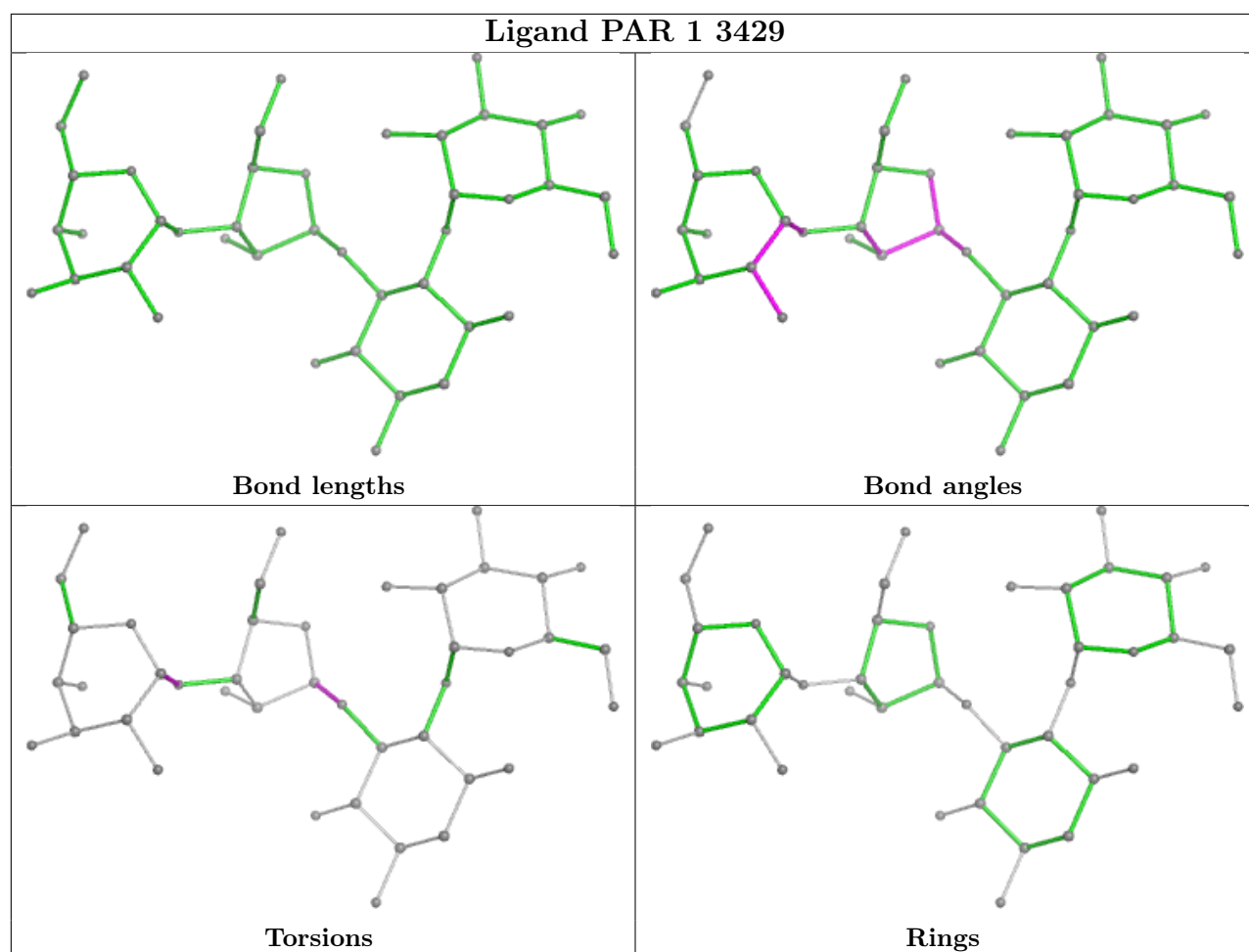






## Ligand PAR 7 202

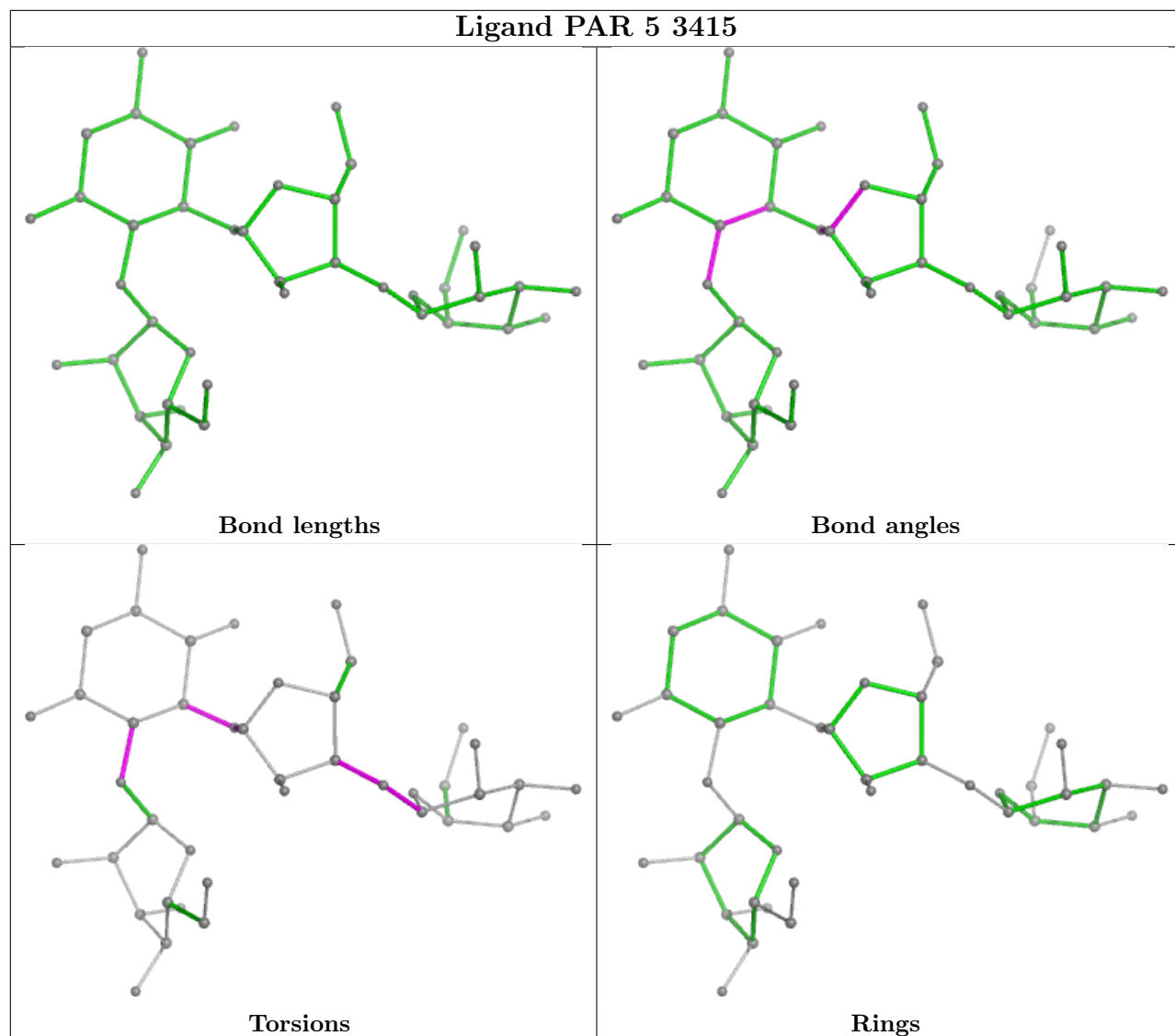


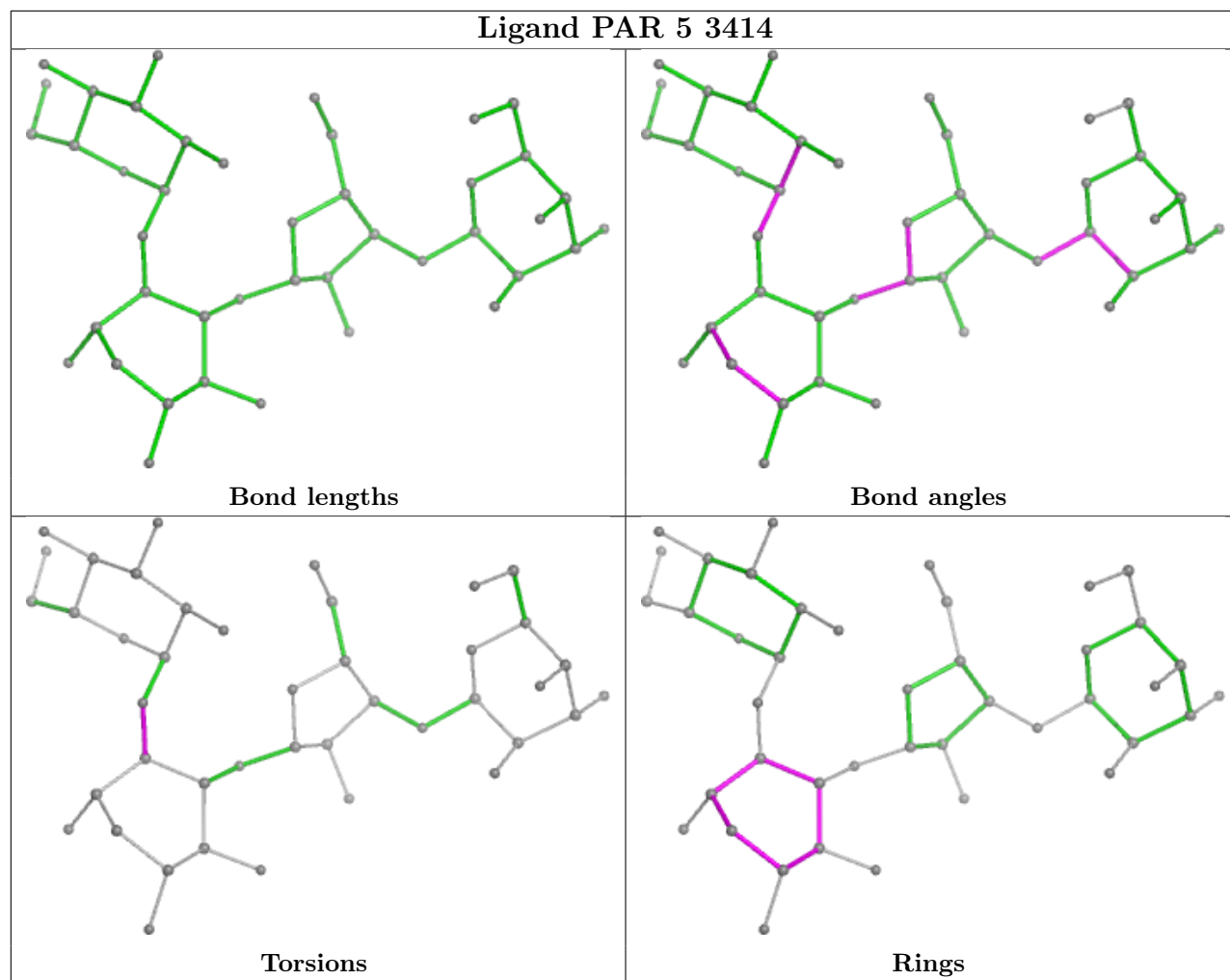


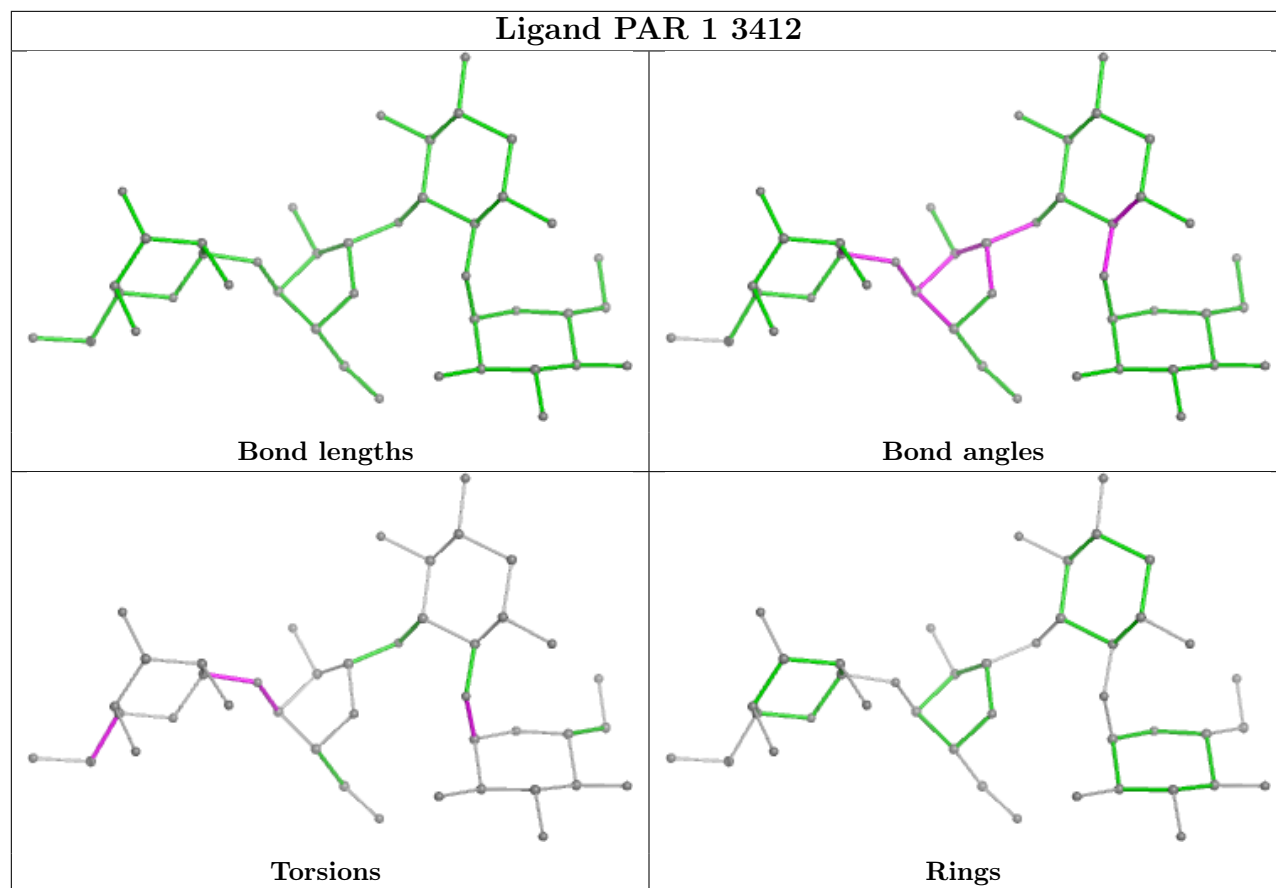
Ligand PAR 2 1902

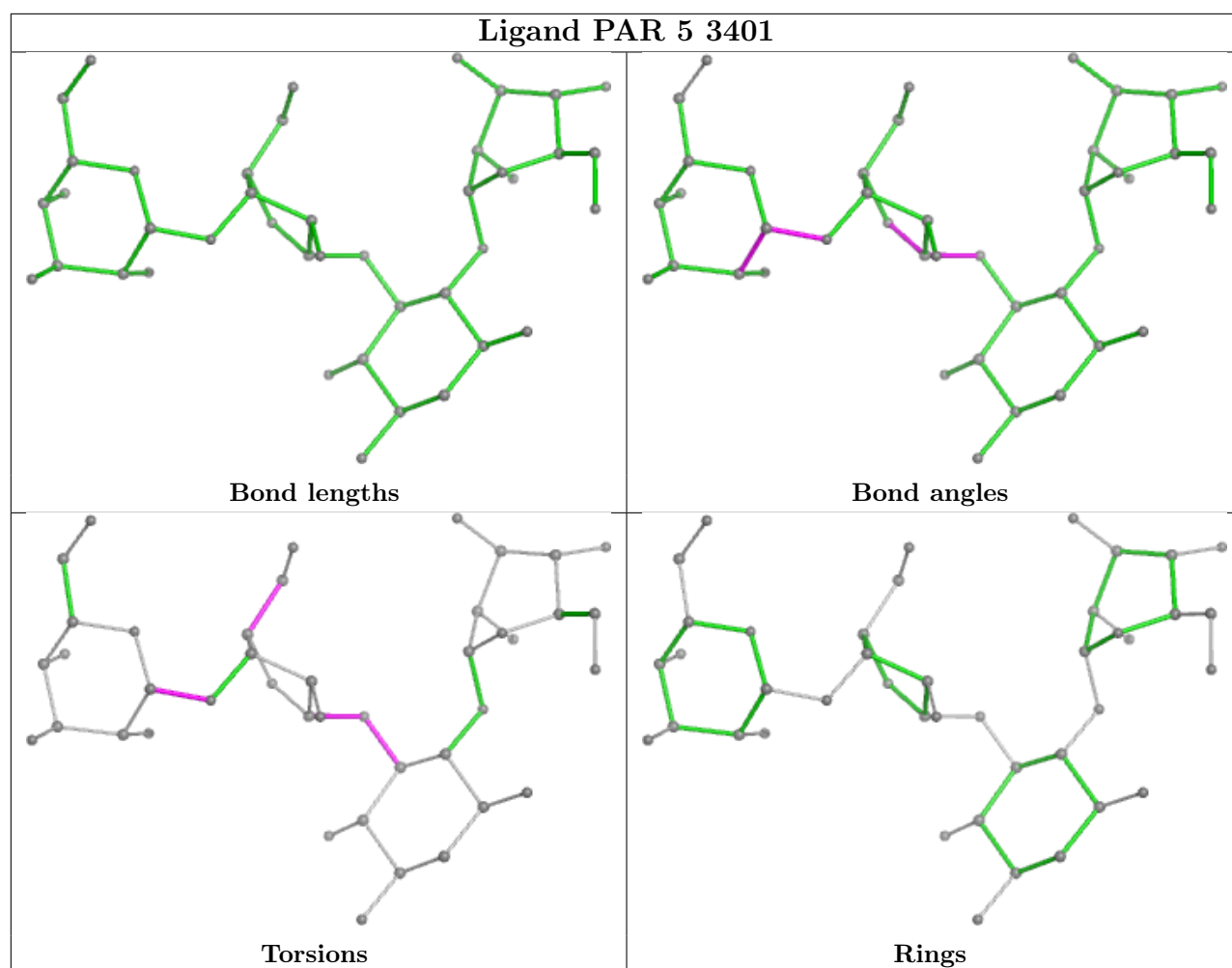
The figure displays four panels of structural analysis for Ligand PAR 2 1902. Each panel shows a 3D ball-and-stick model of the molecule, which consists of a central pyrazole ring connected to a benzene ring and a pyridine ring. The panels are labeled as follows:

- Bond lengths:** Shows the bond lengths for the molecule. The bonds are color-coded: green for standard bonds, magenta for bonds of interest, and grey for other bonds.
- Bond angles:** Shows the bond angles for the molecule. The bonds are color-coded: green for standard bonds, magenta for bonds of interest, and grey for other bonds.
- Torsions:** Shows the torsion angles for the molecule. The bonds are color-coded: green for standard bonds, magenta for bonds of interest, and grey for other bonds.
- Rings:** Shows the ring angles for the molecule. The bonds are color-coded: green for standard bonds, magenta for bonds of interest, and grey for other bonds.



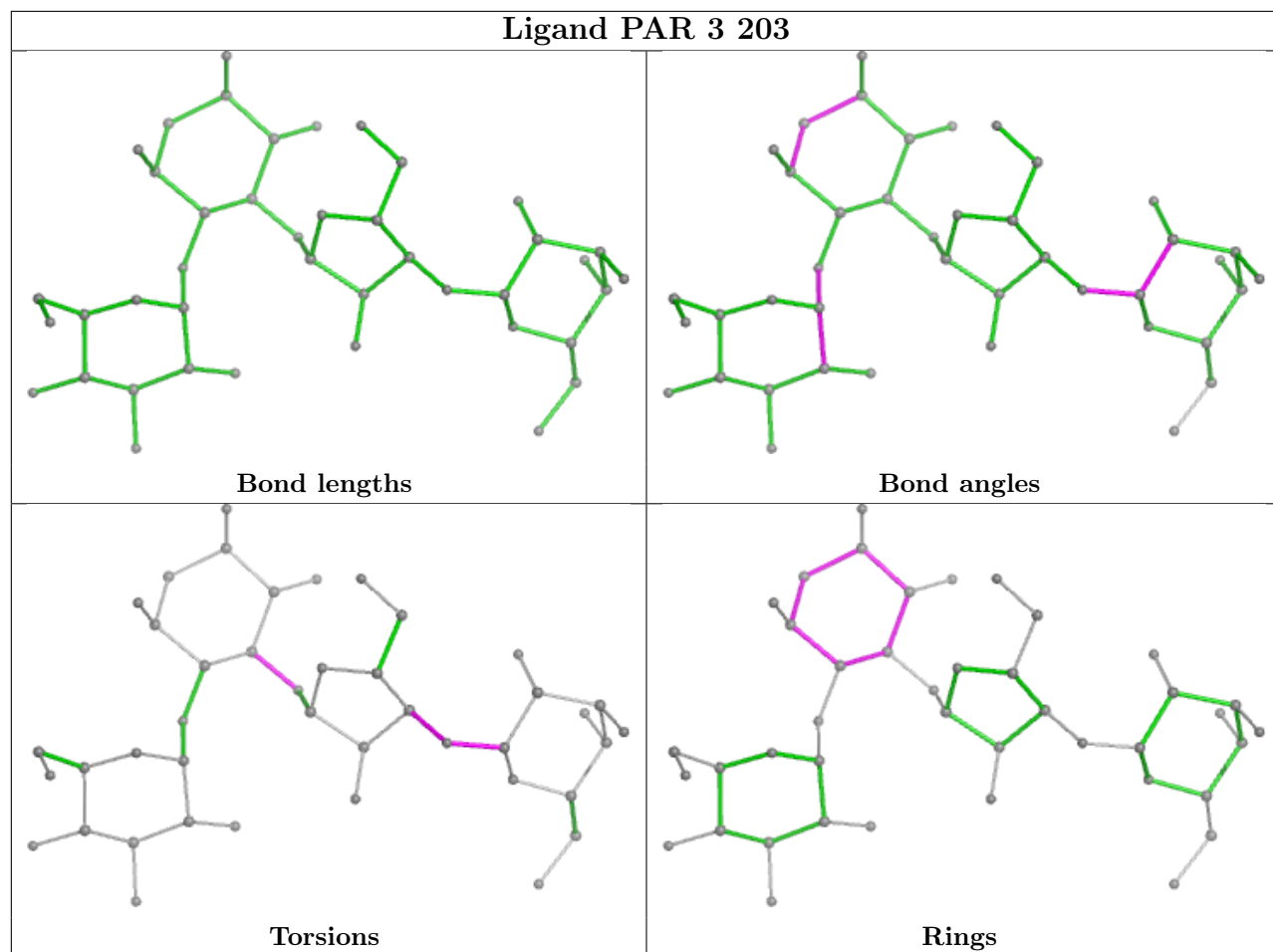


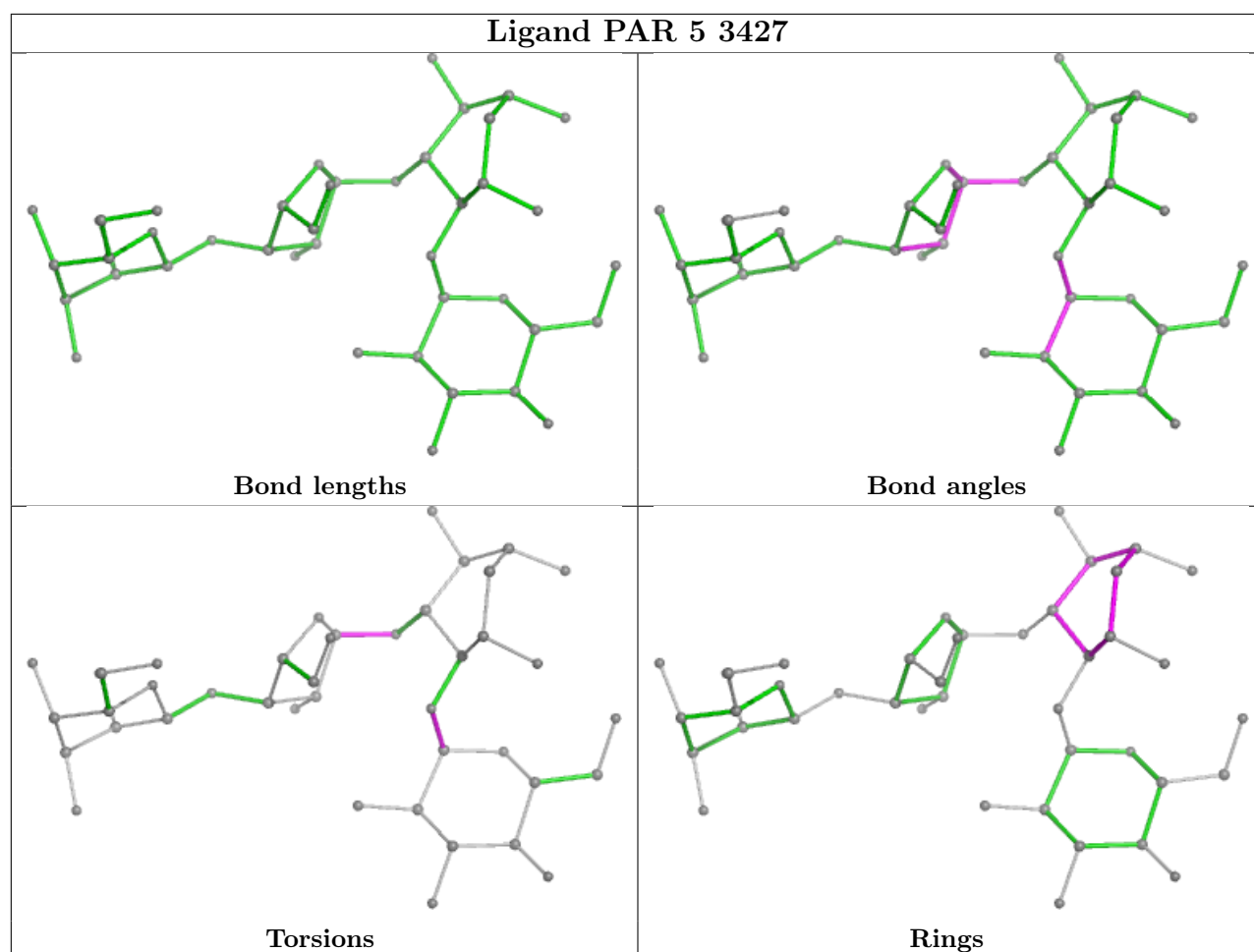


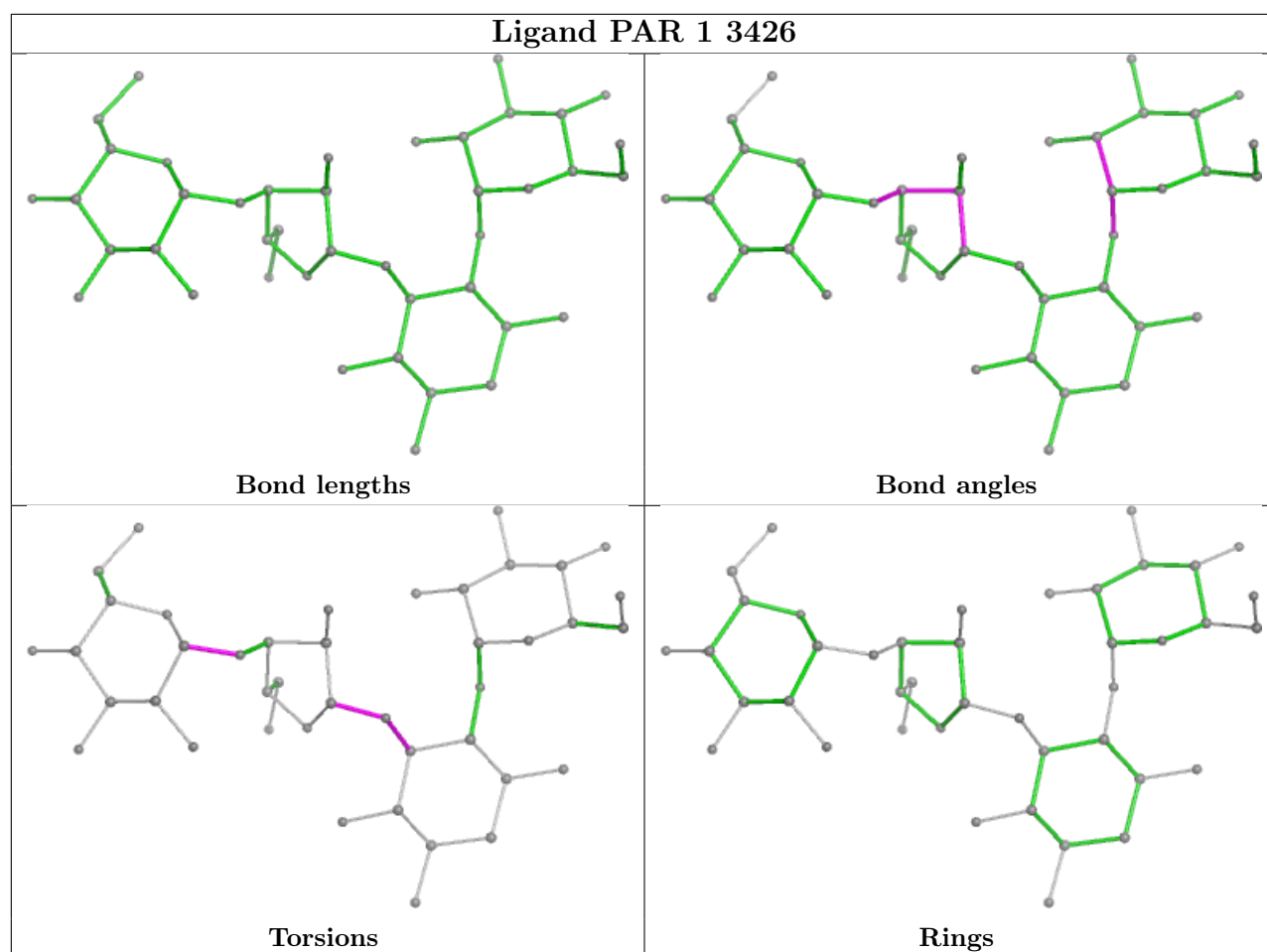


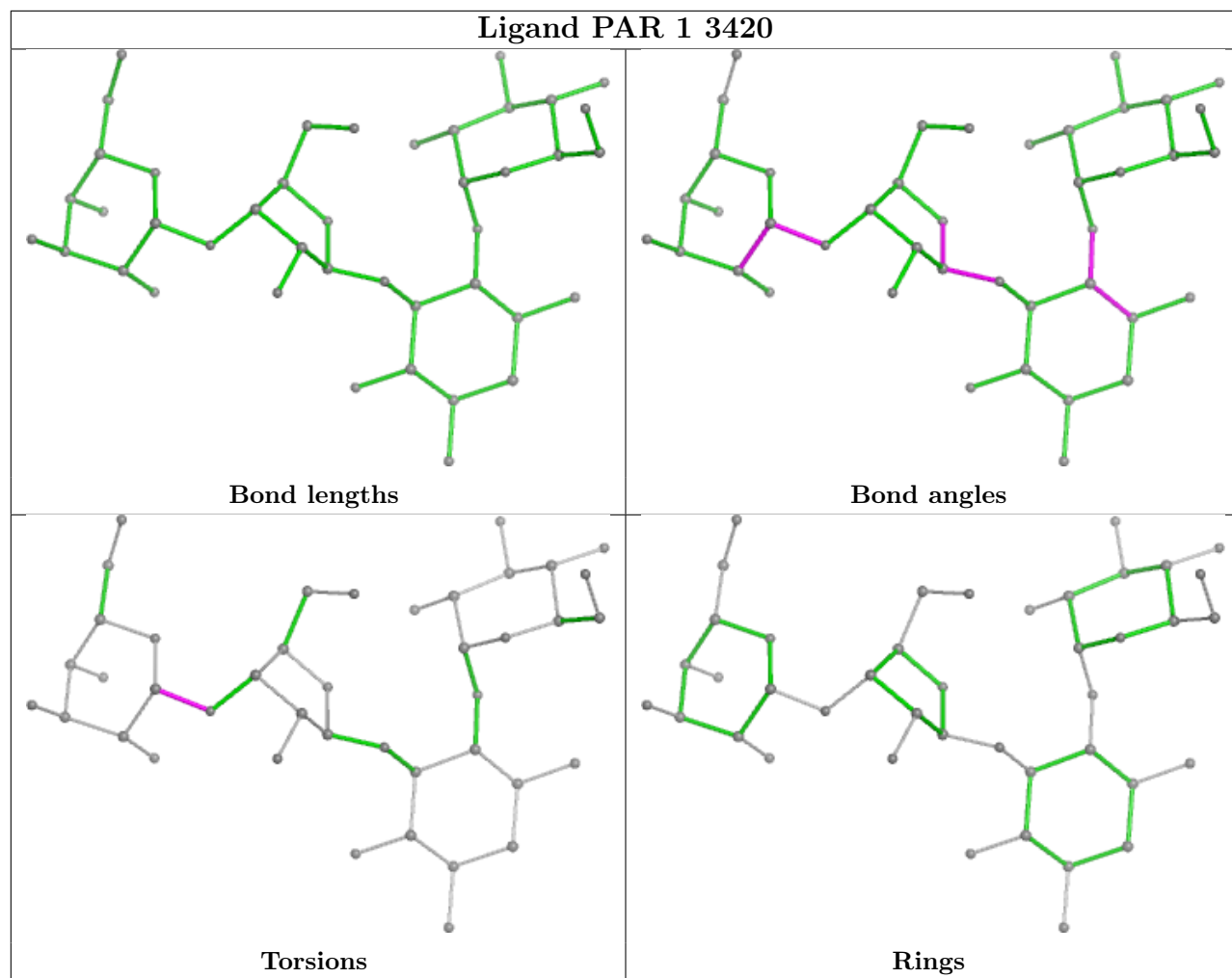


## Ligand PAR 3 203

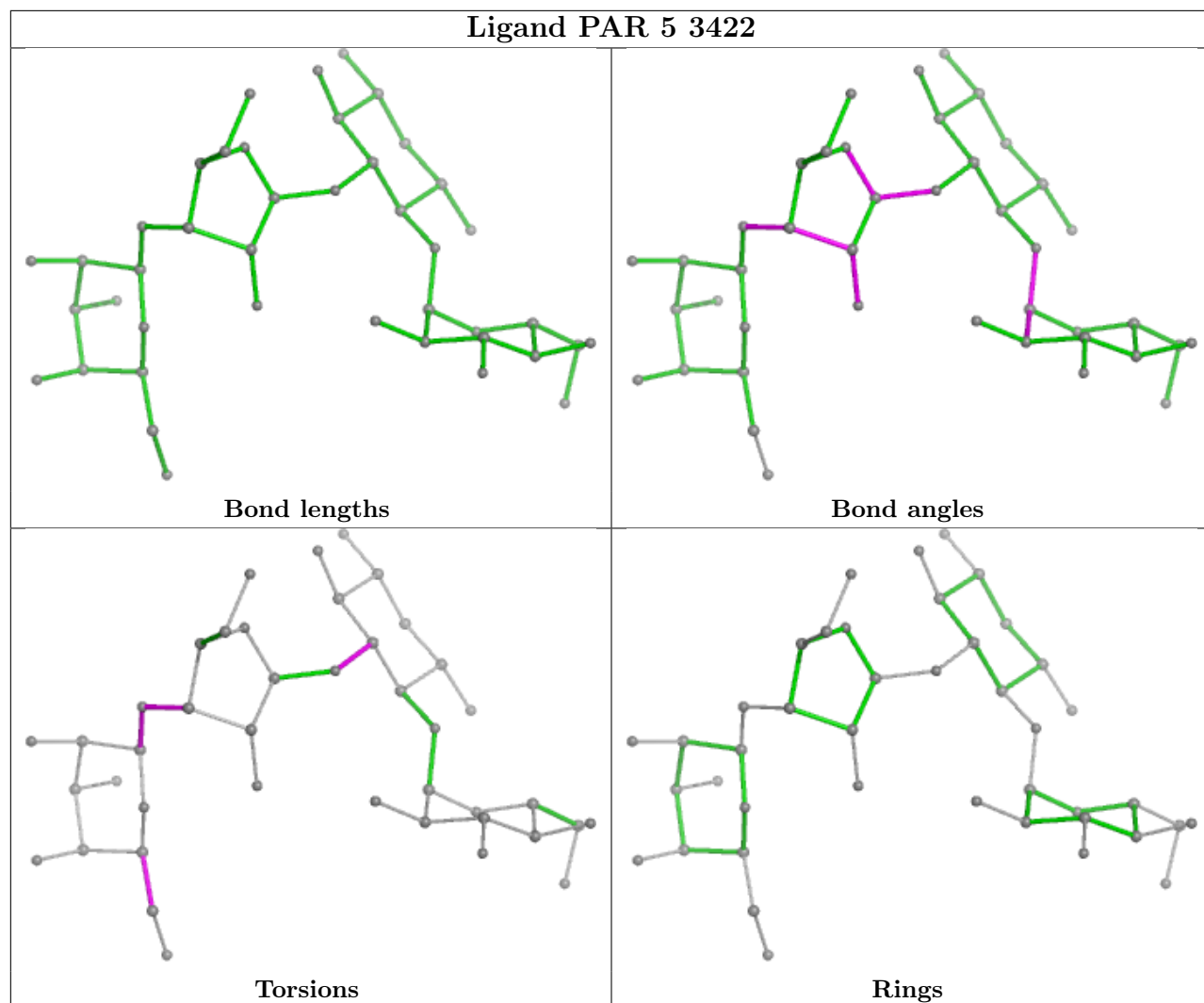


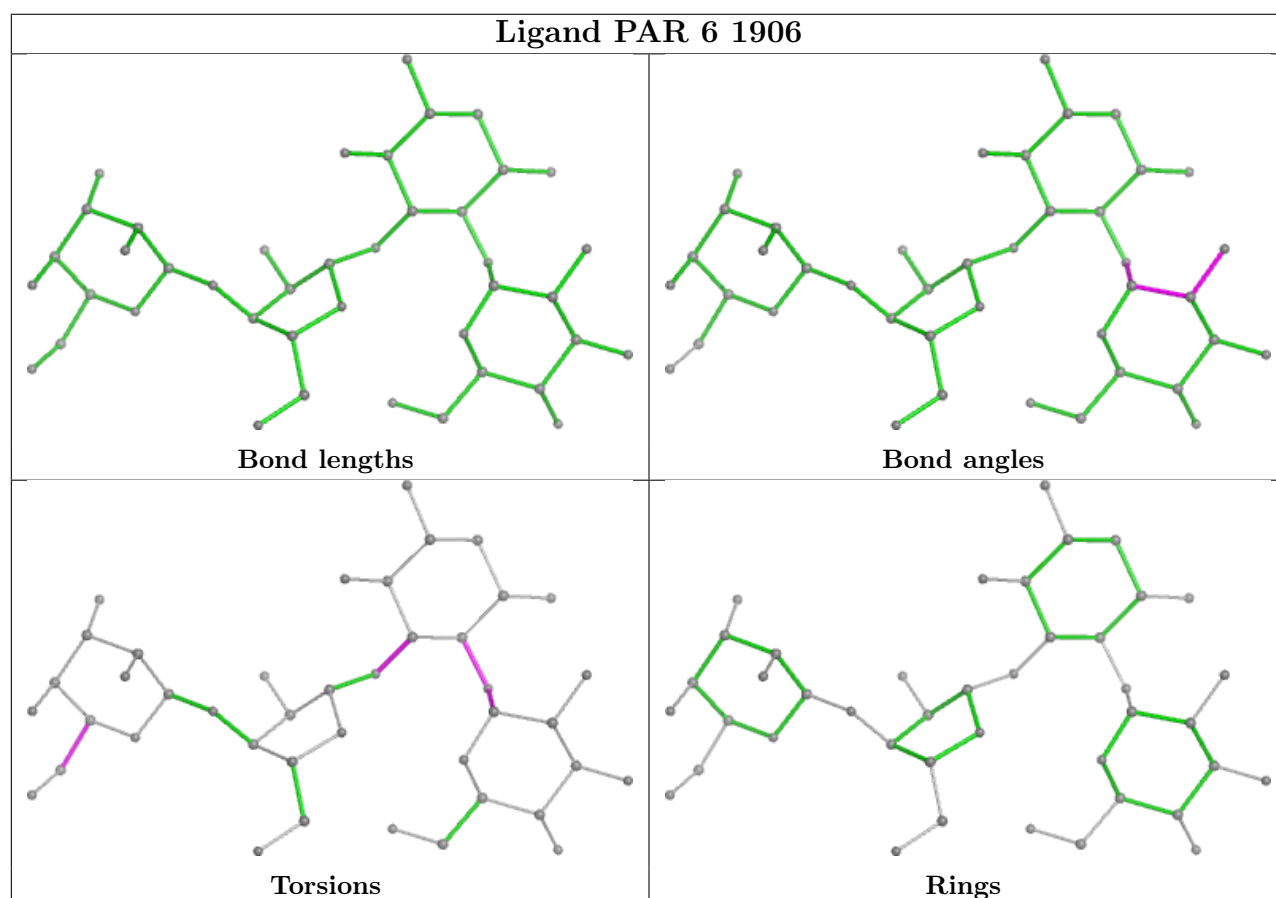
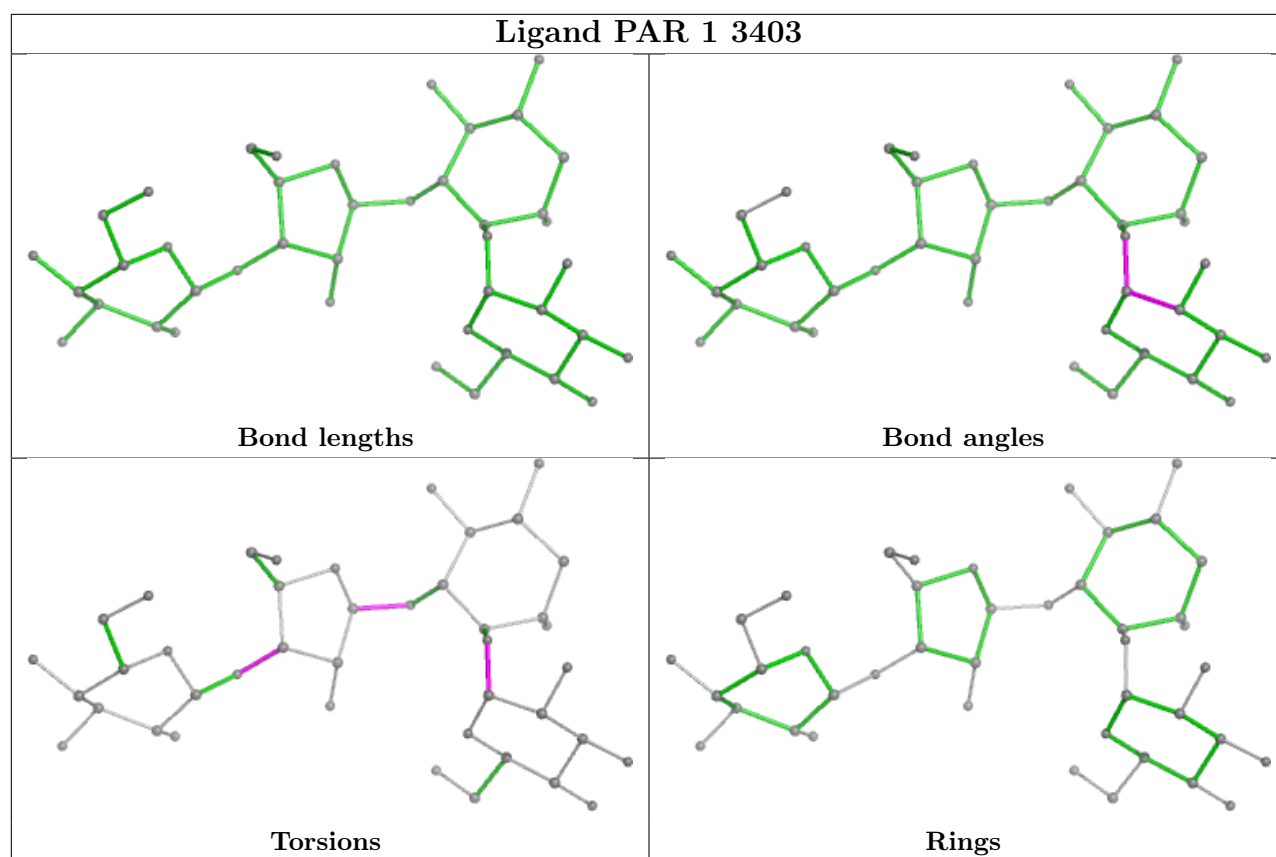




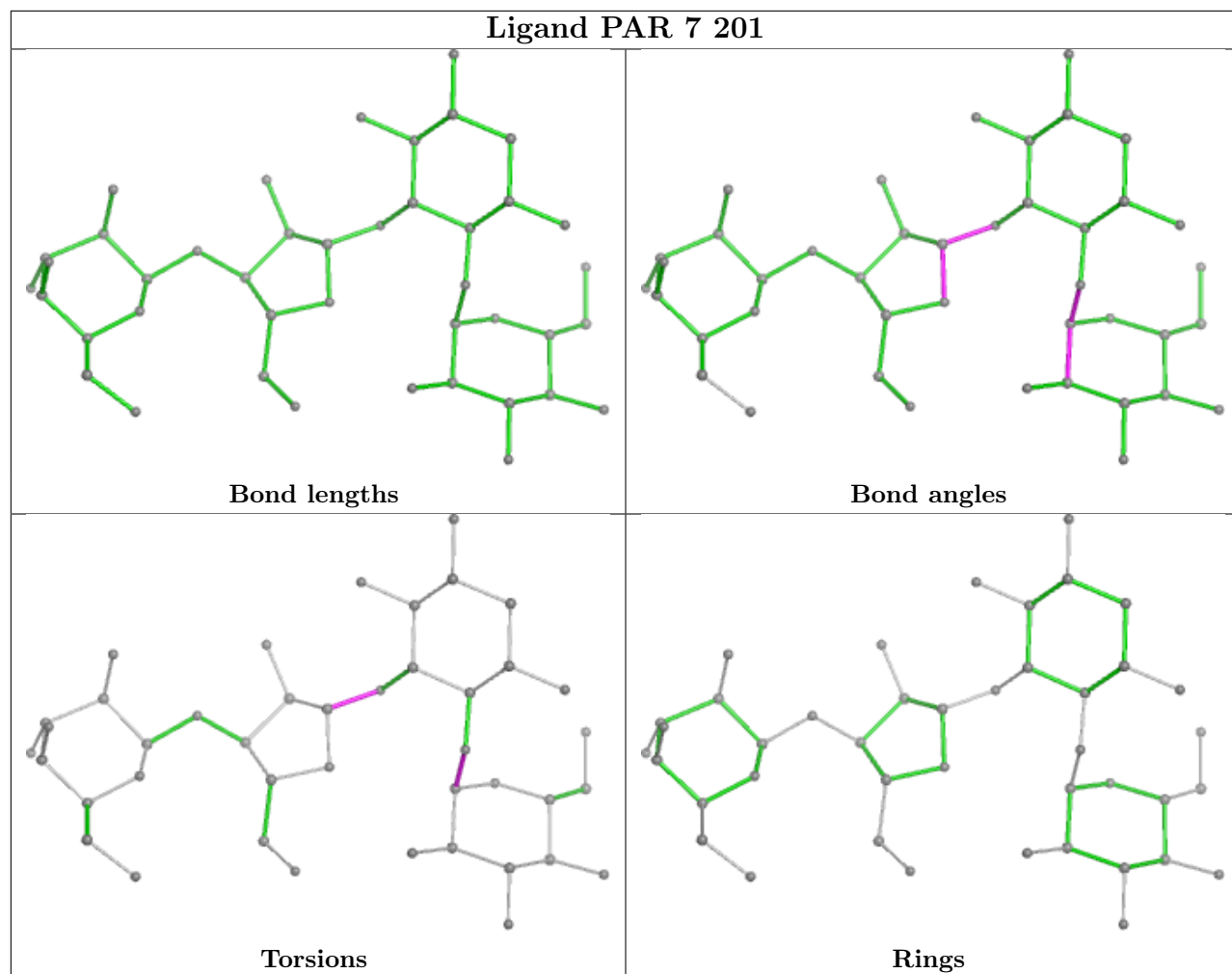


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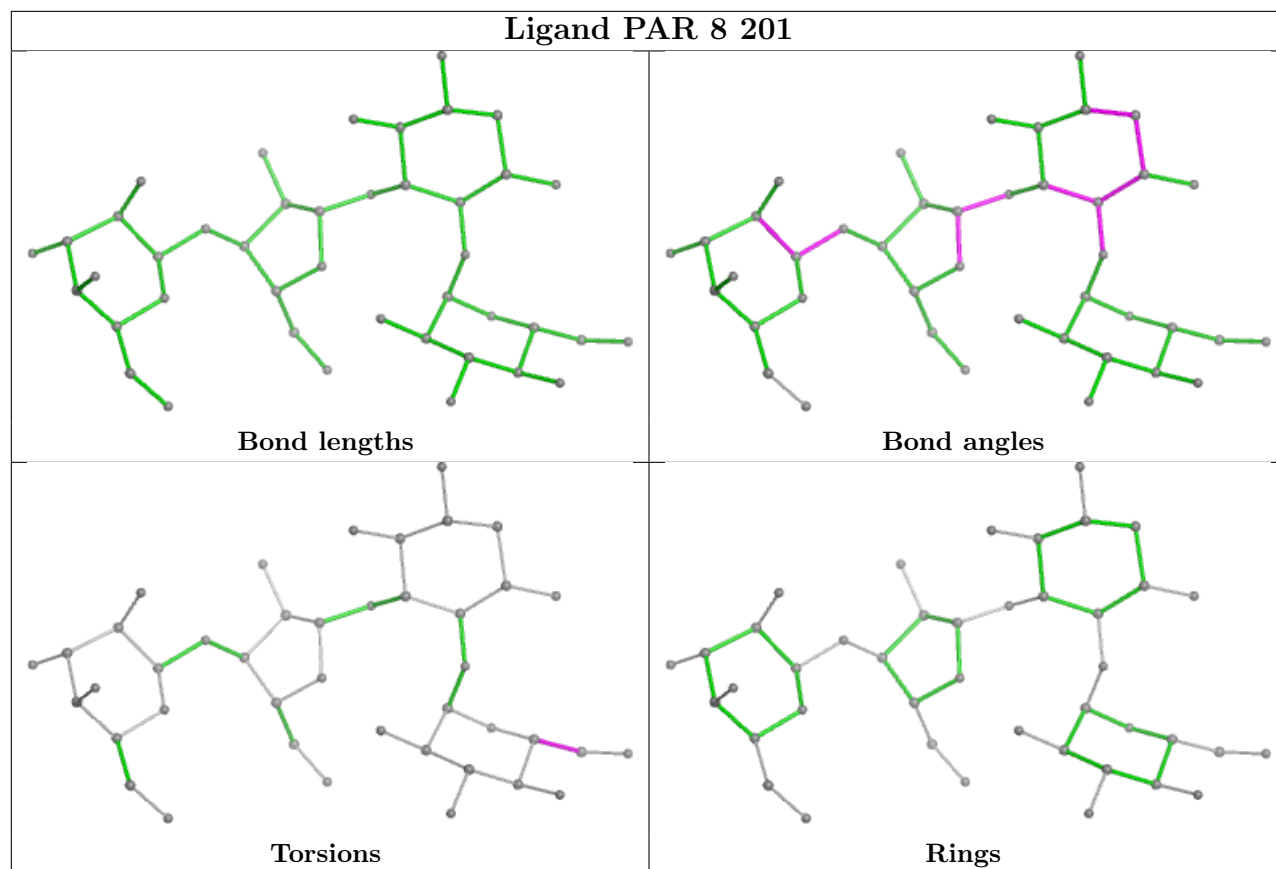




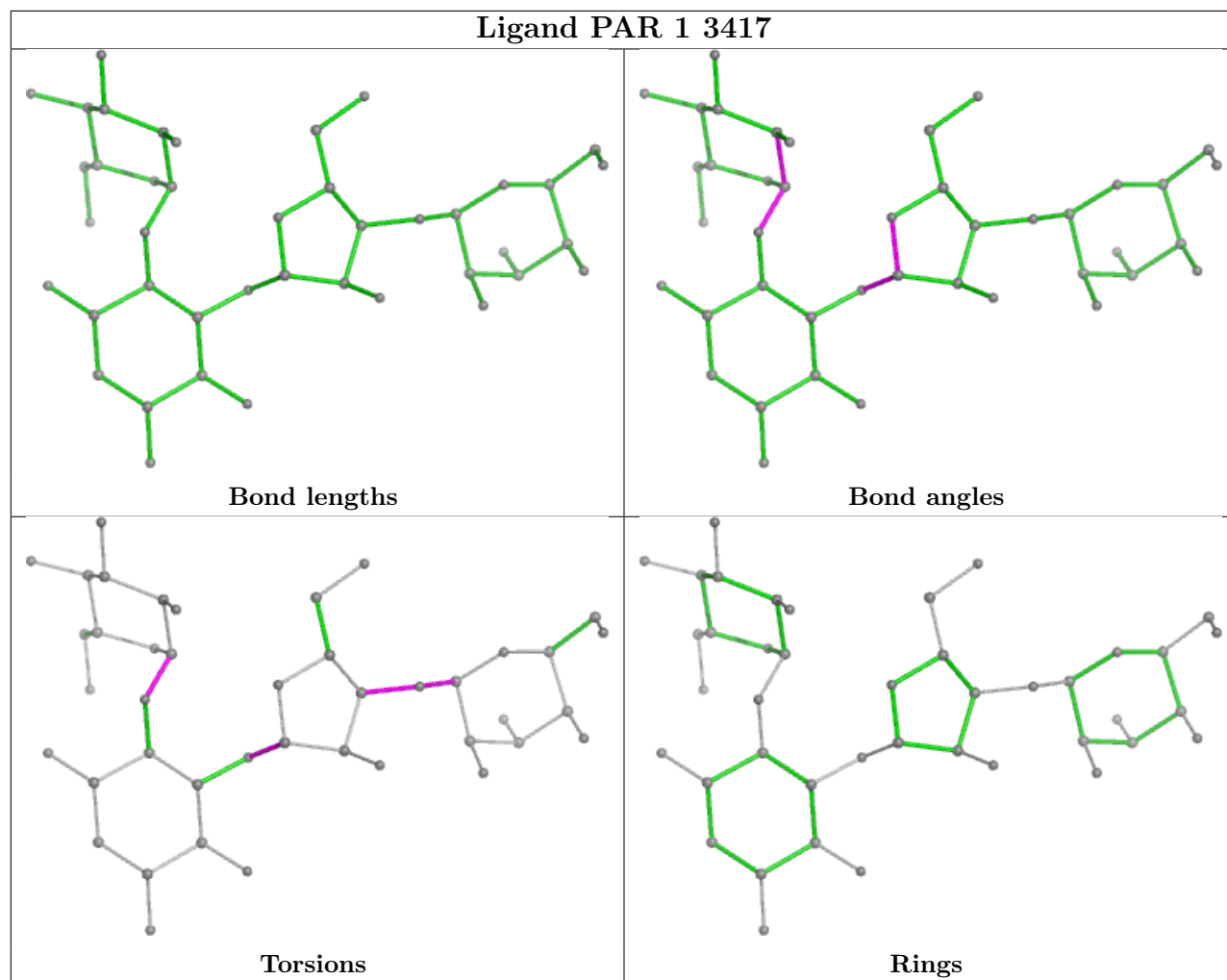
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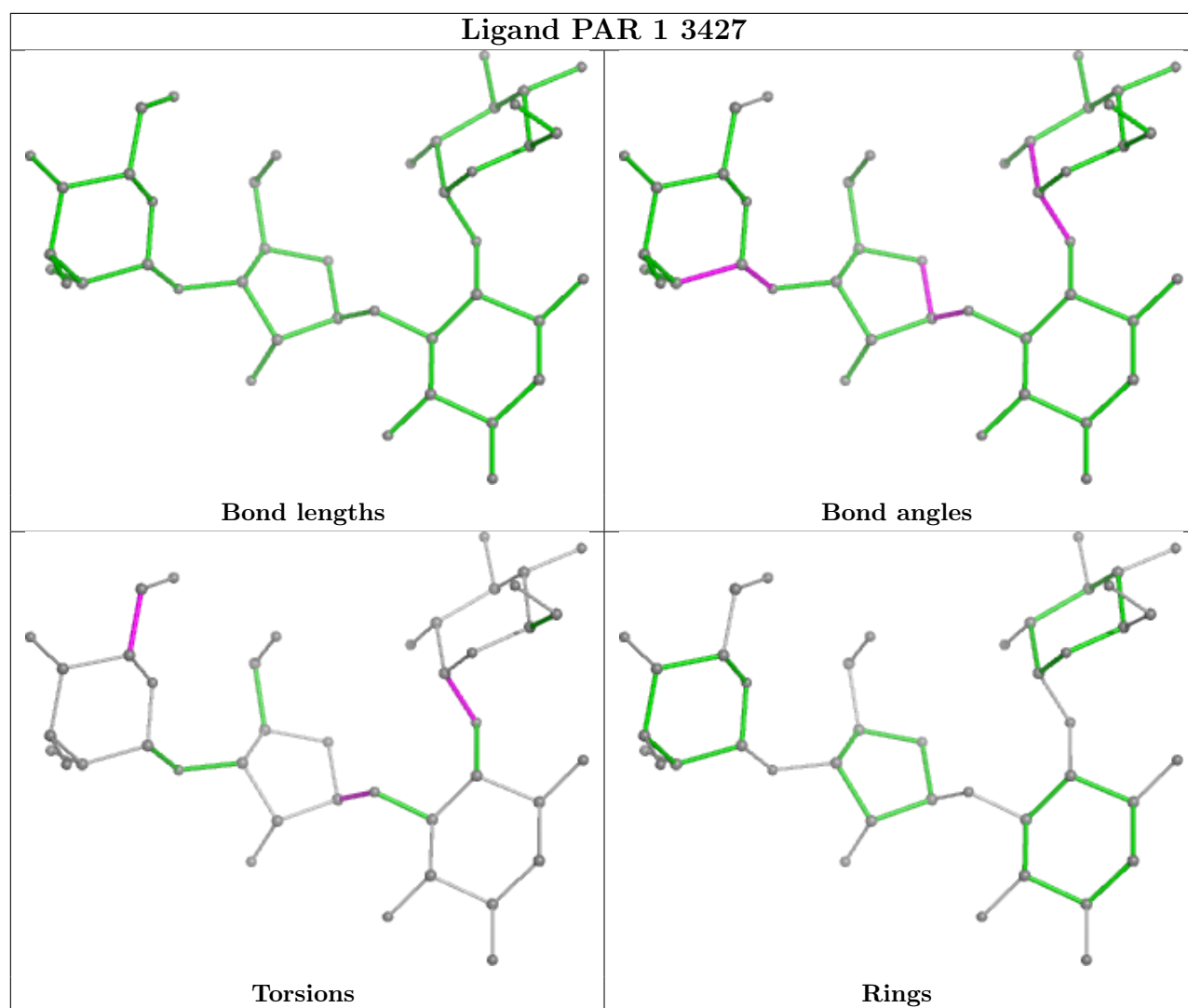


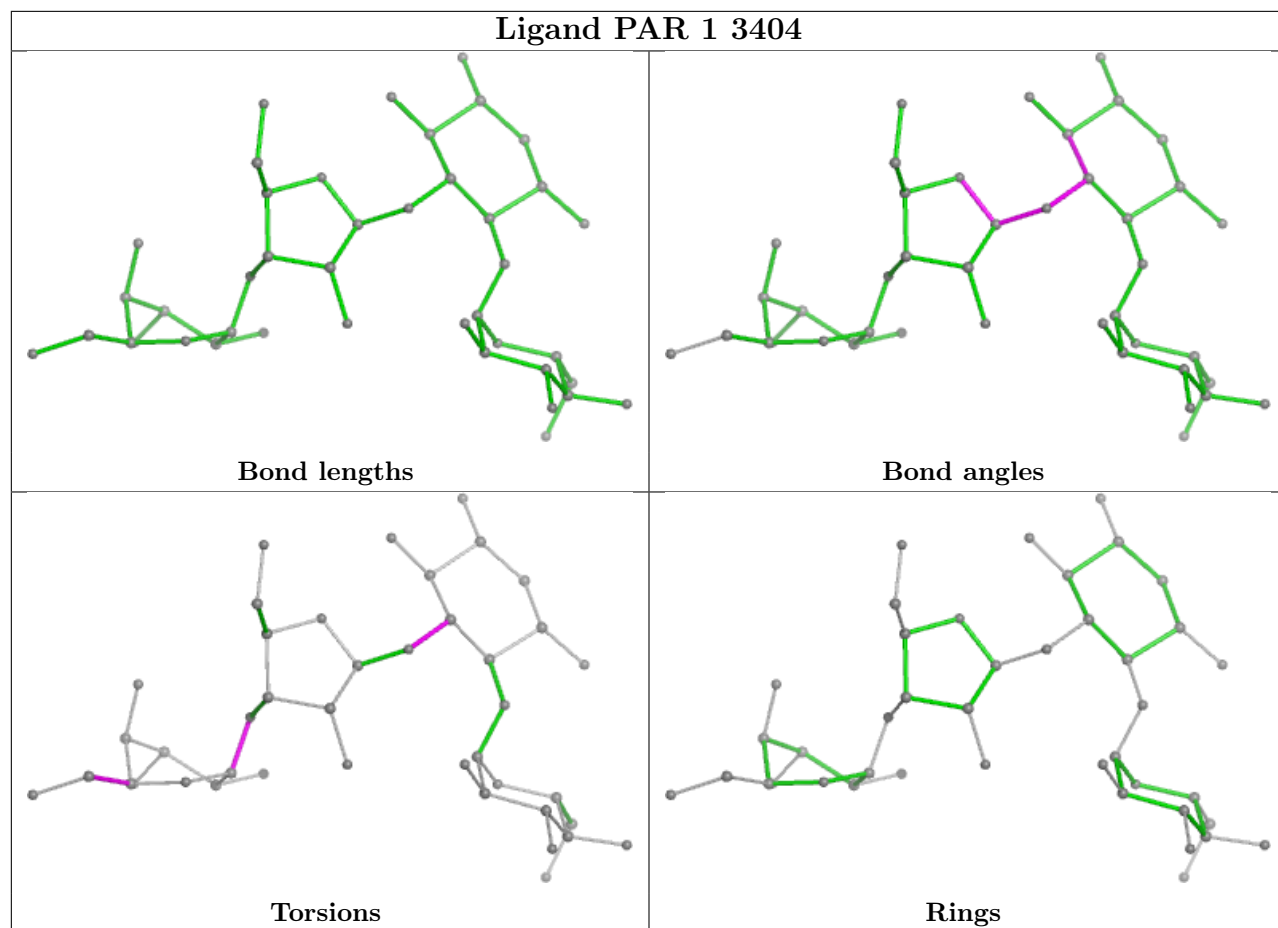
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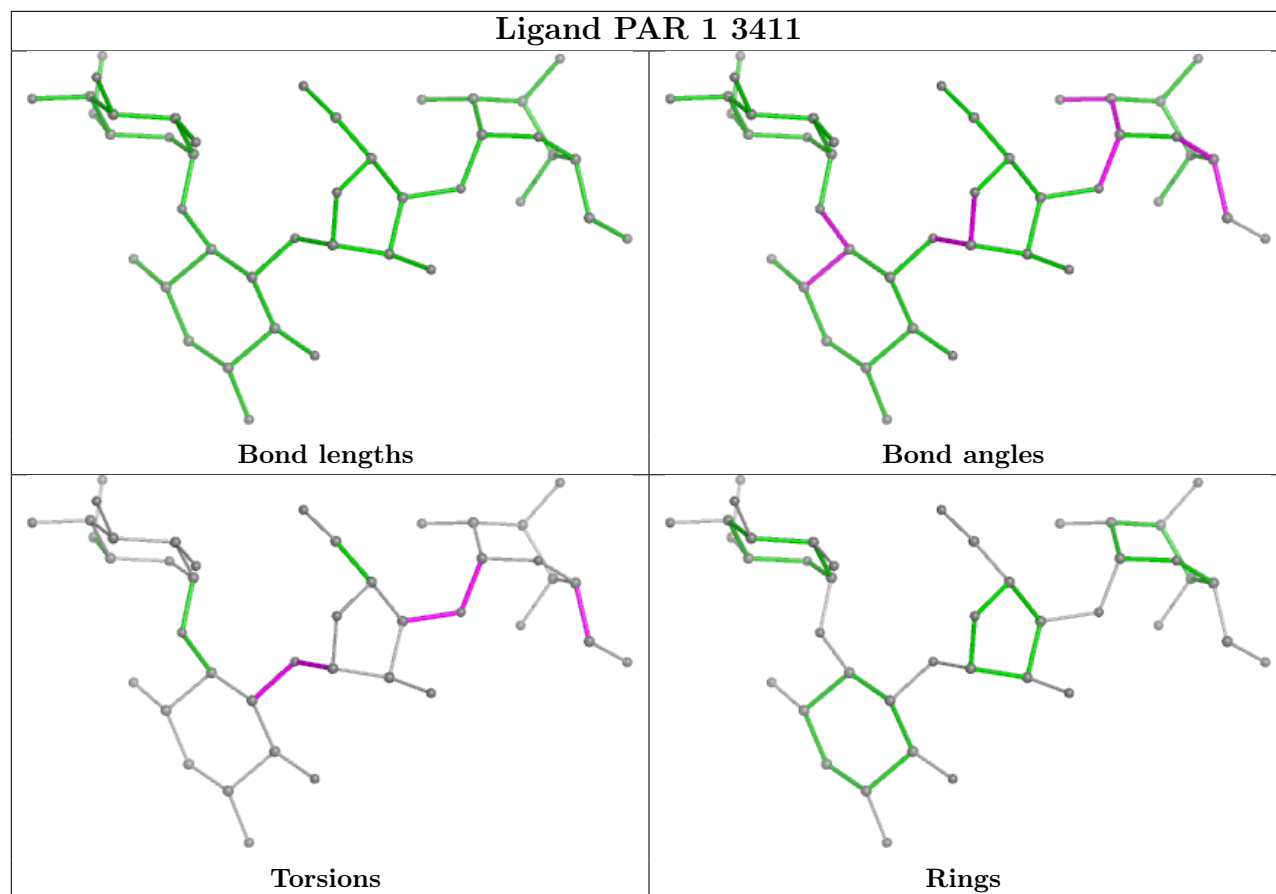


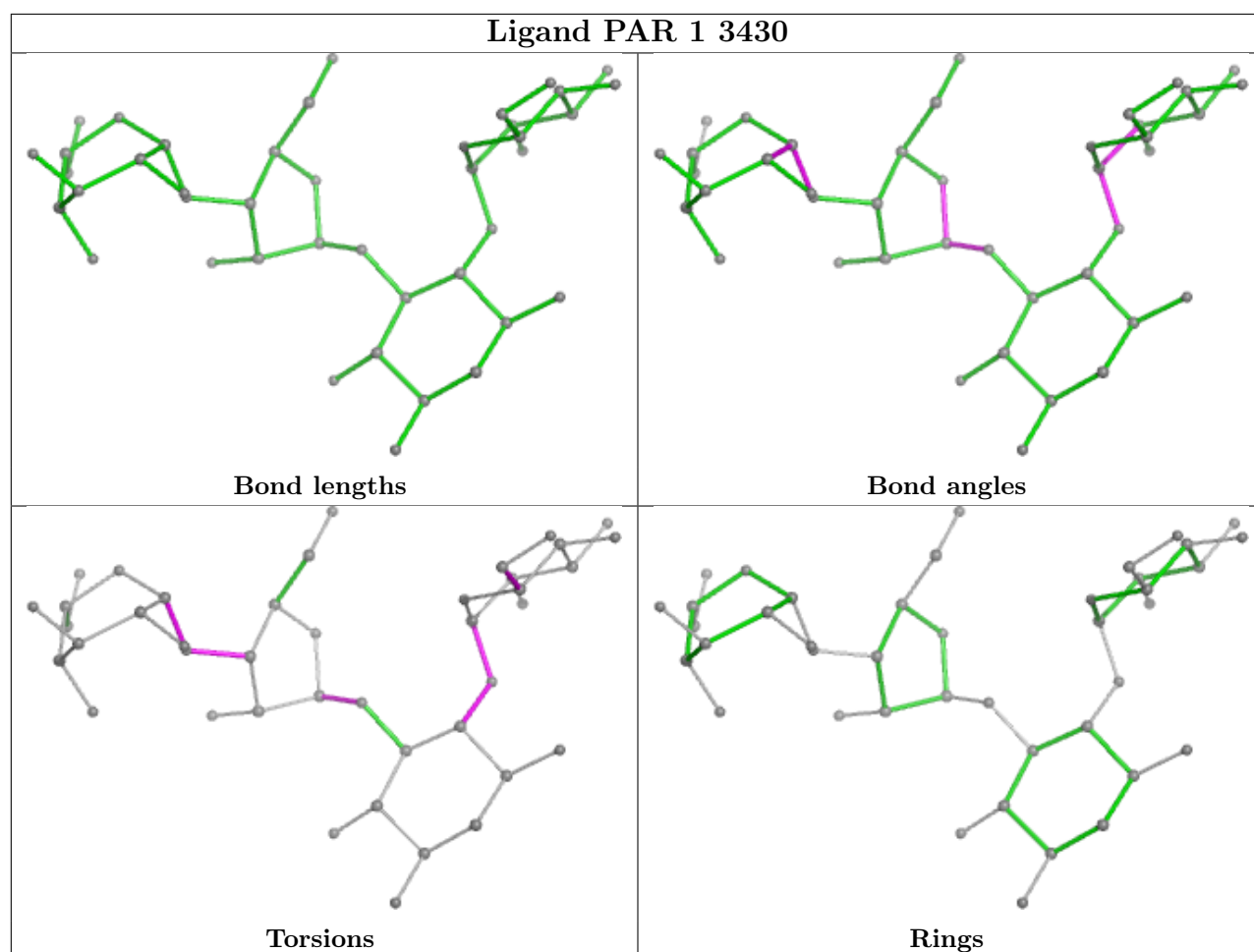


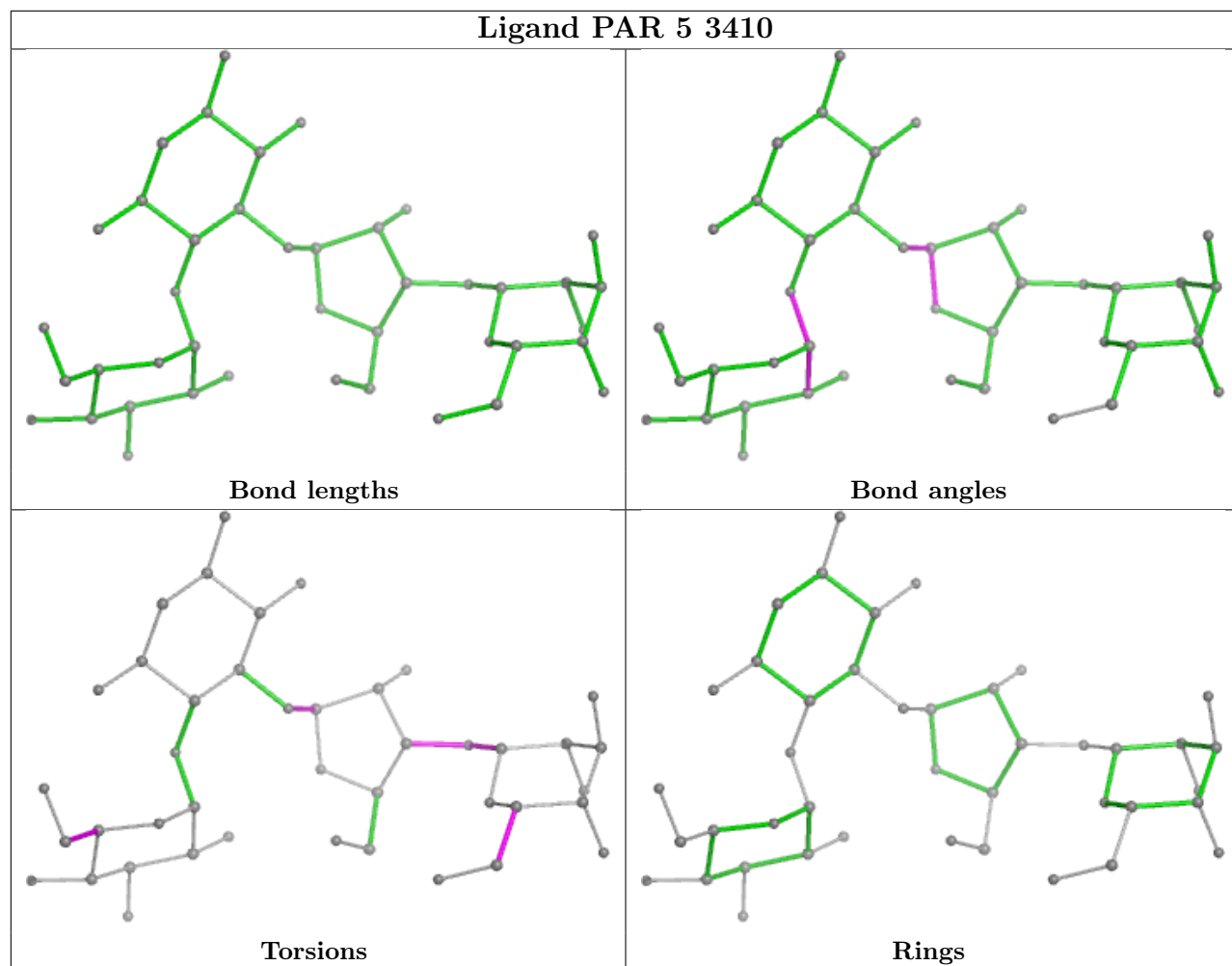


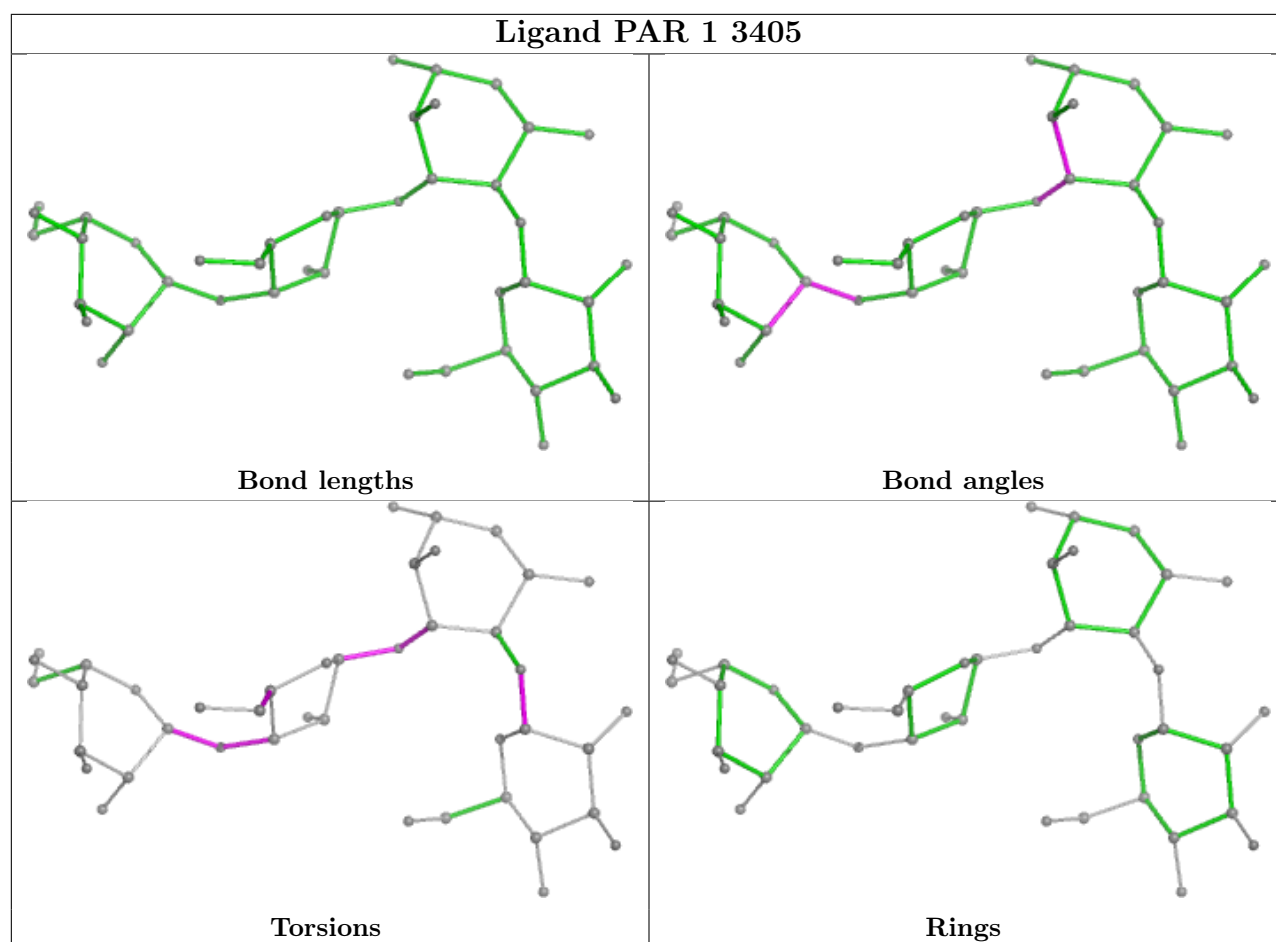


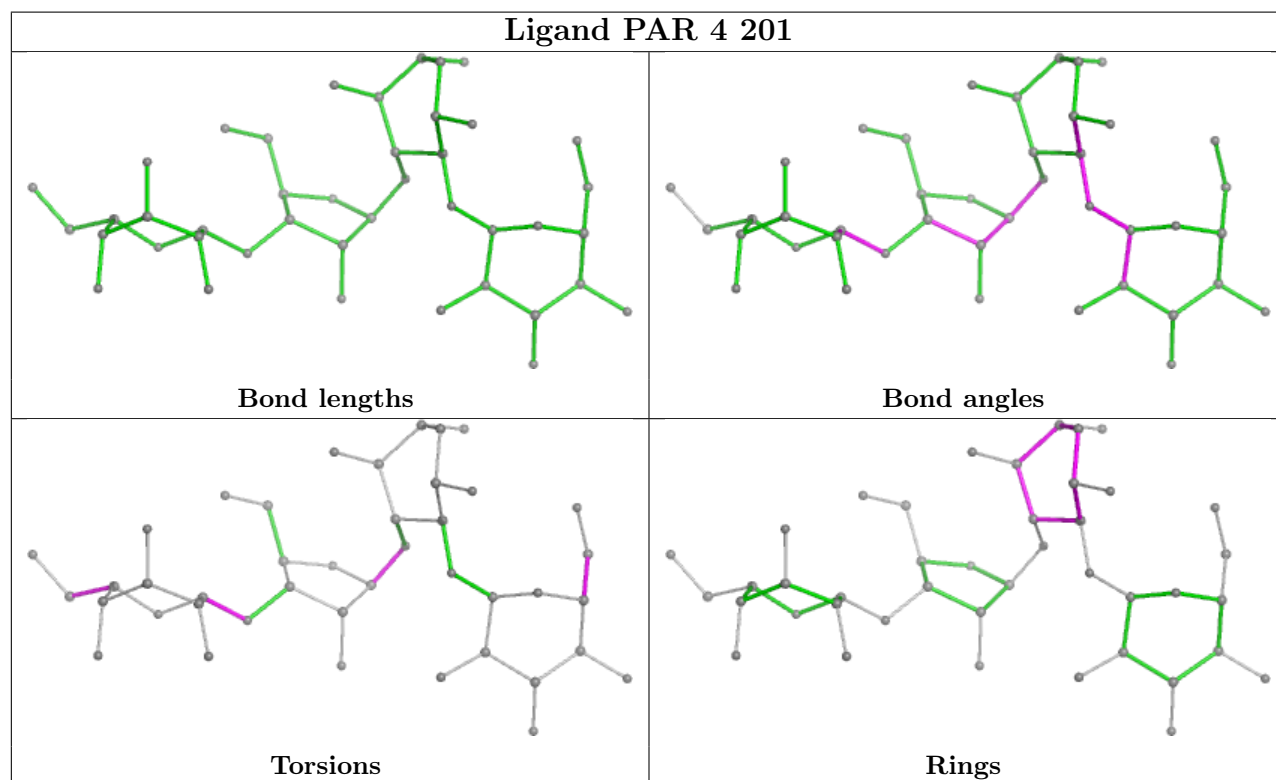
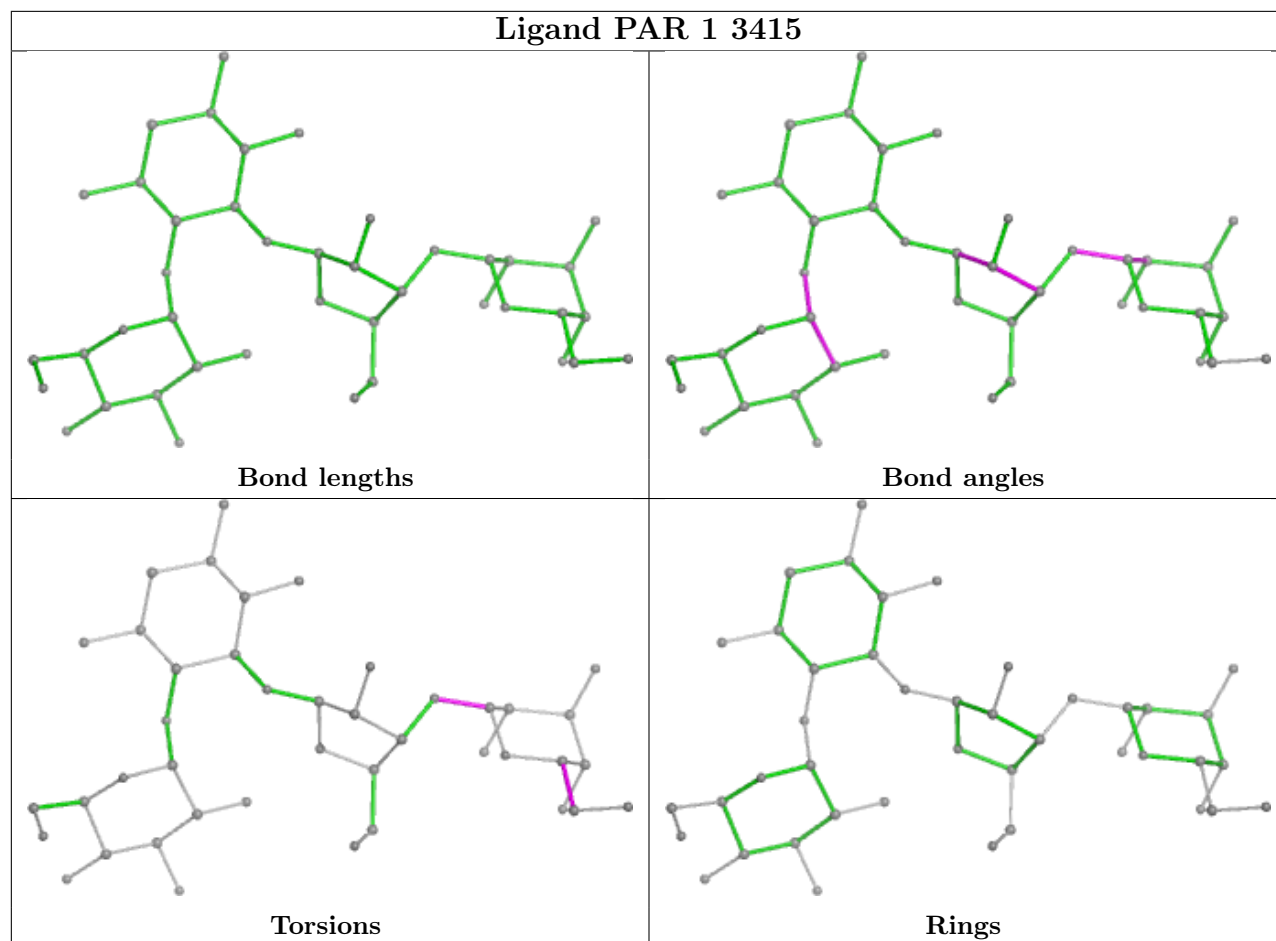




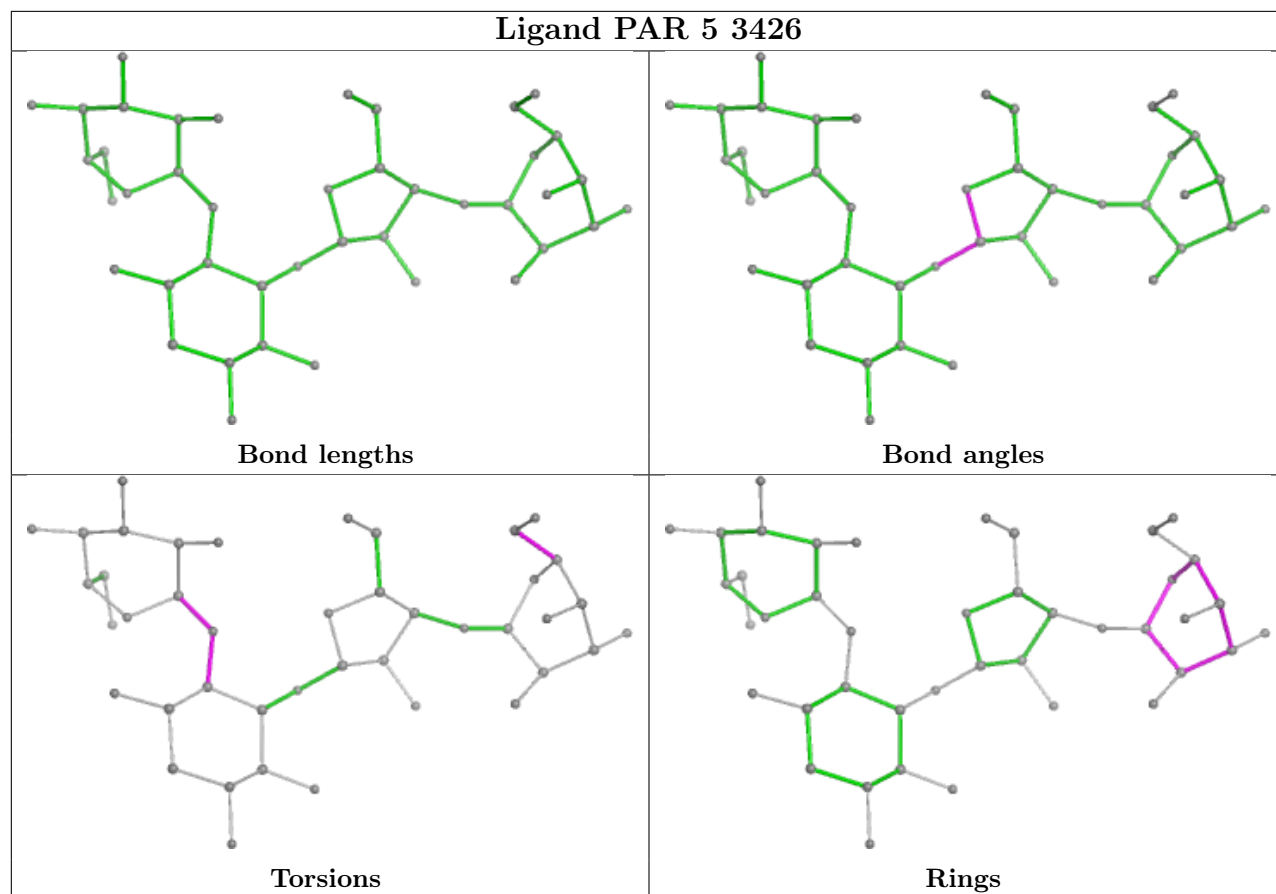


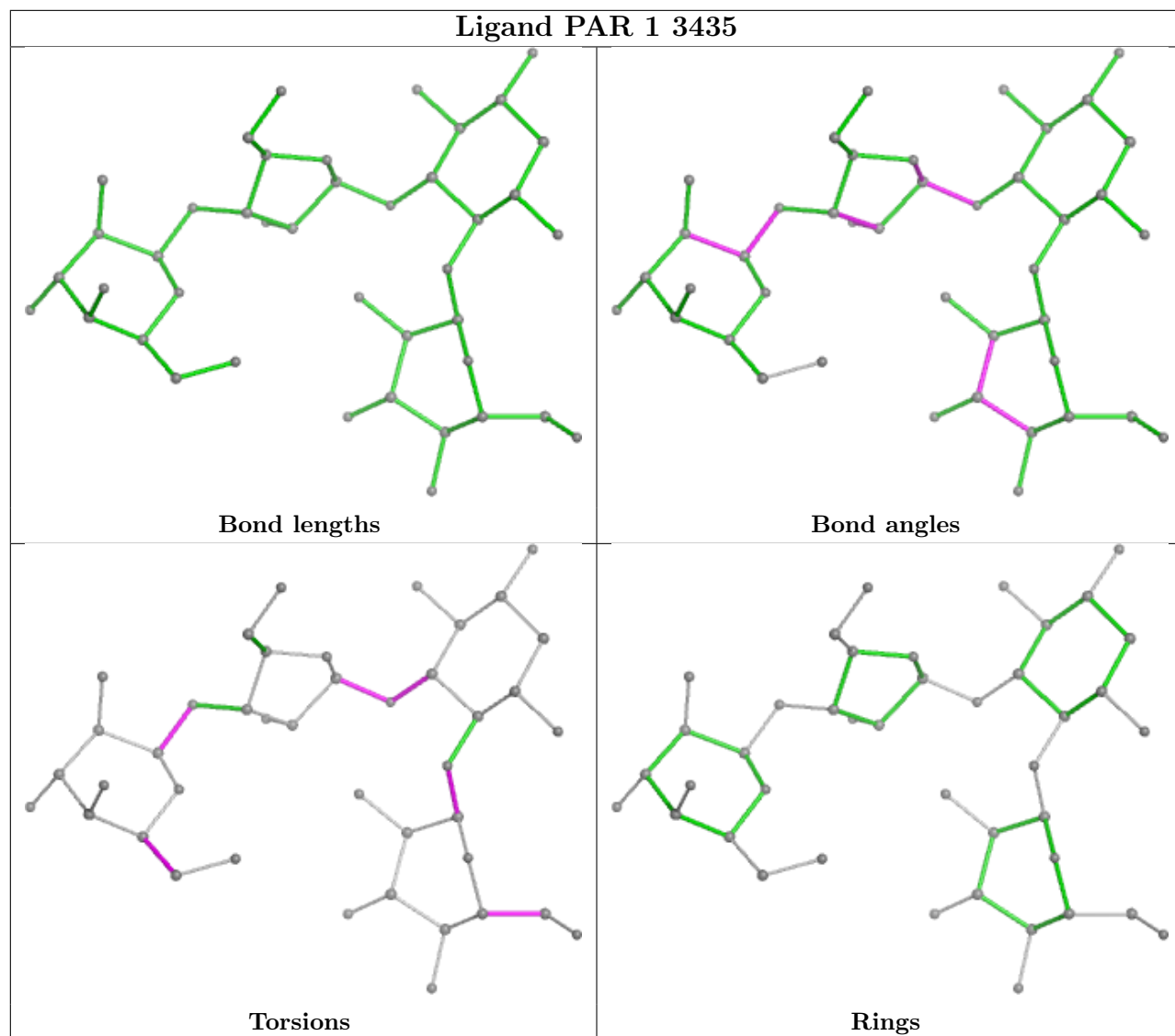


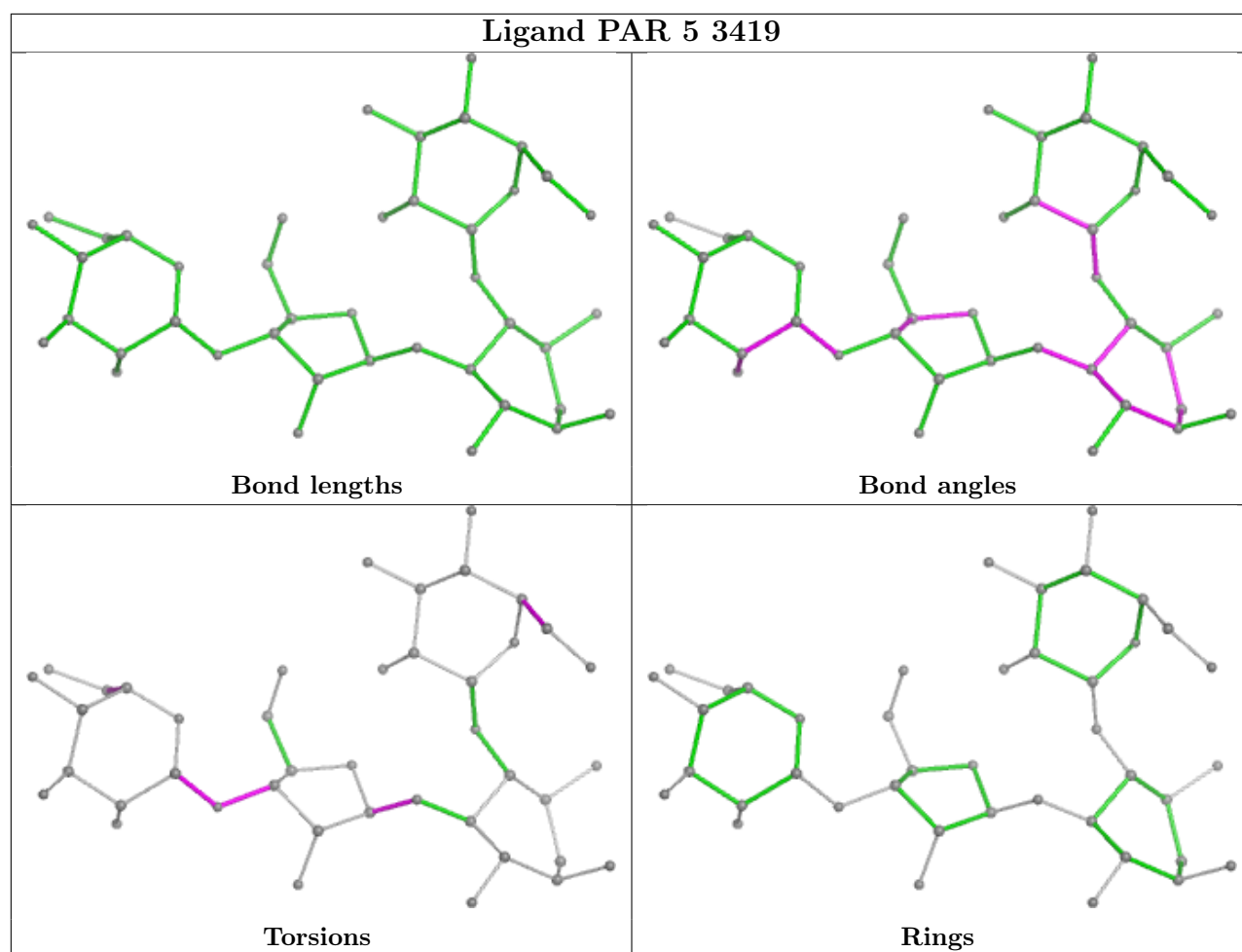




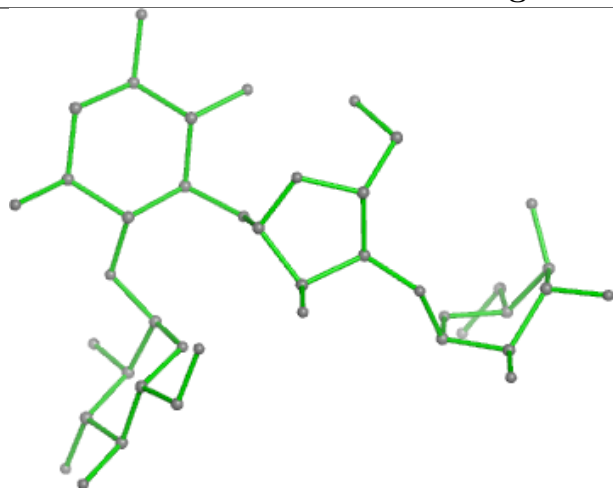




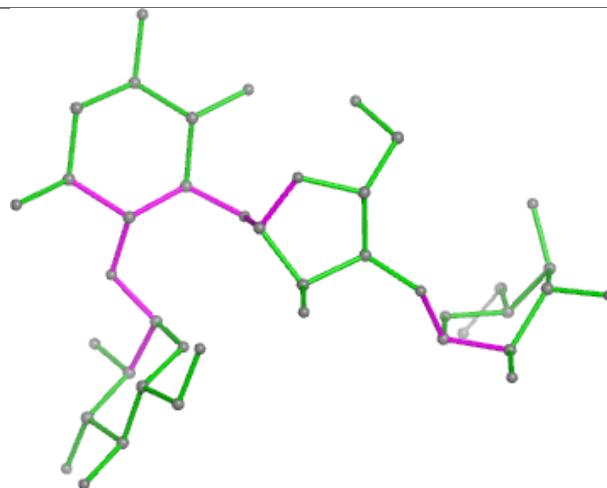




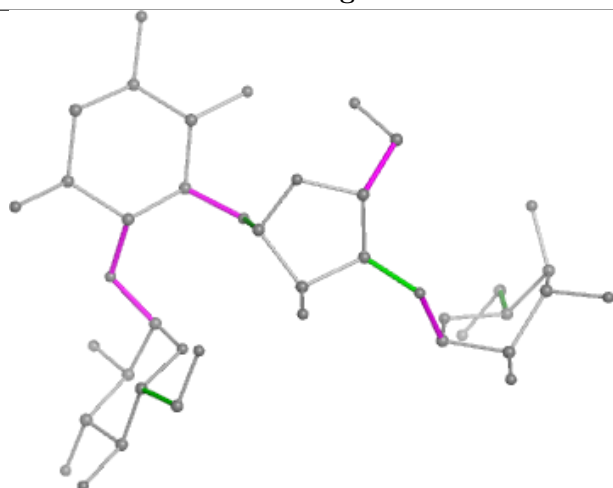
## Ligand PAR 1 3419



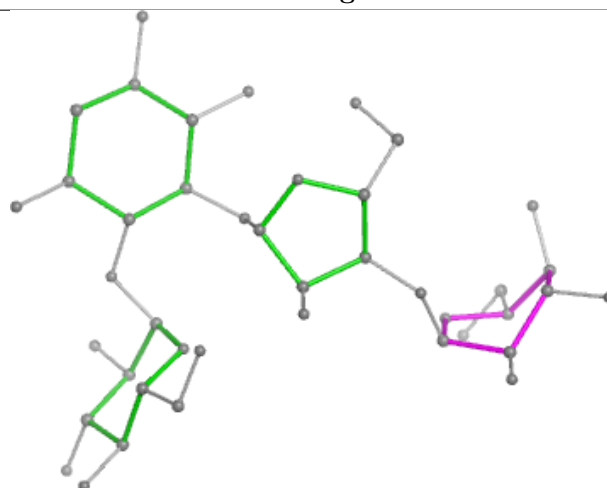
Bond lengths



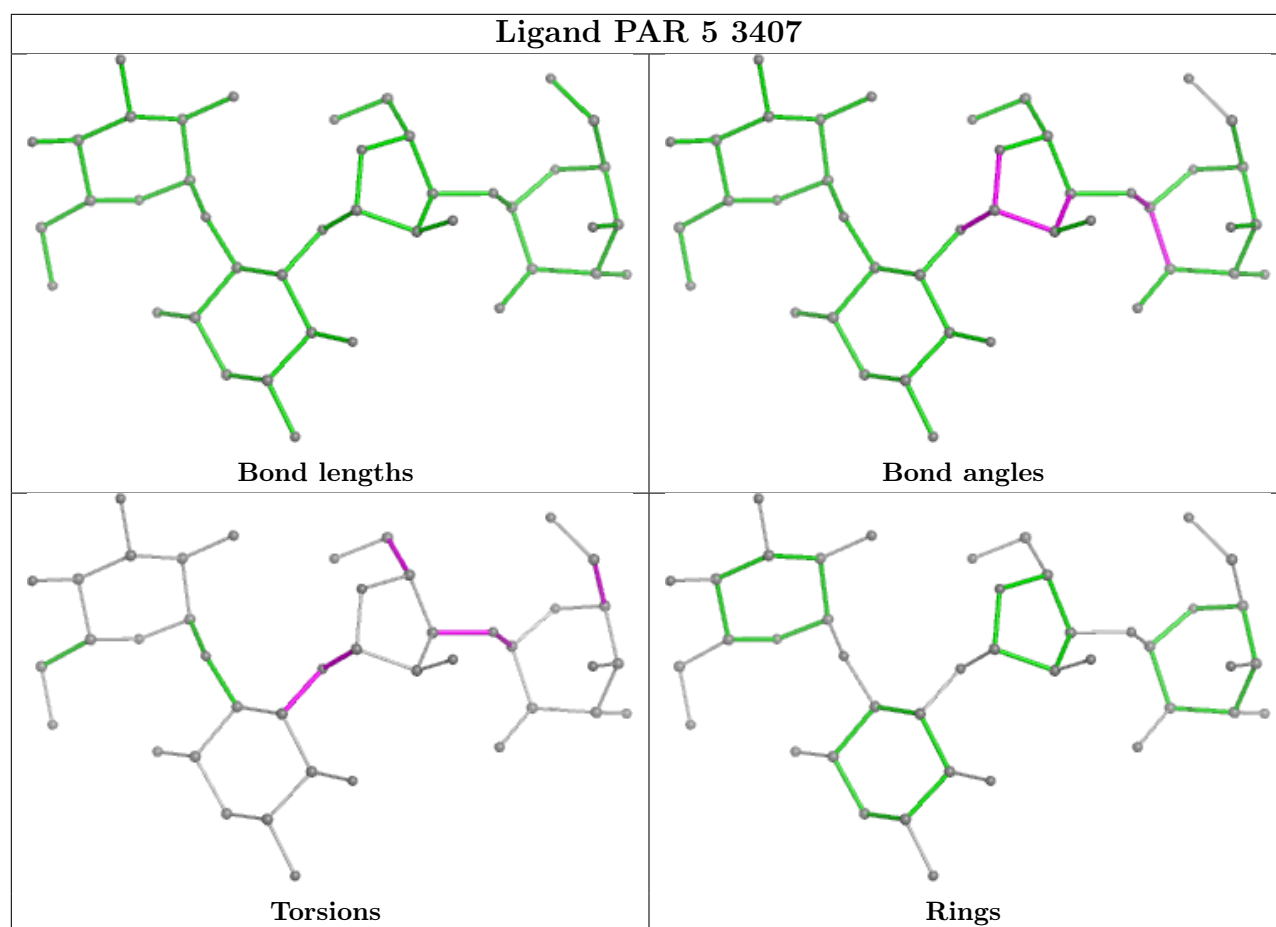
Bond angles

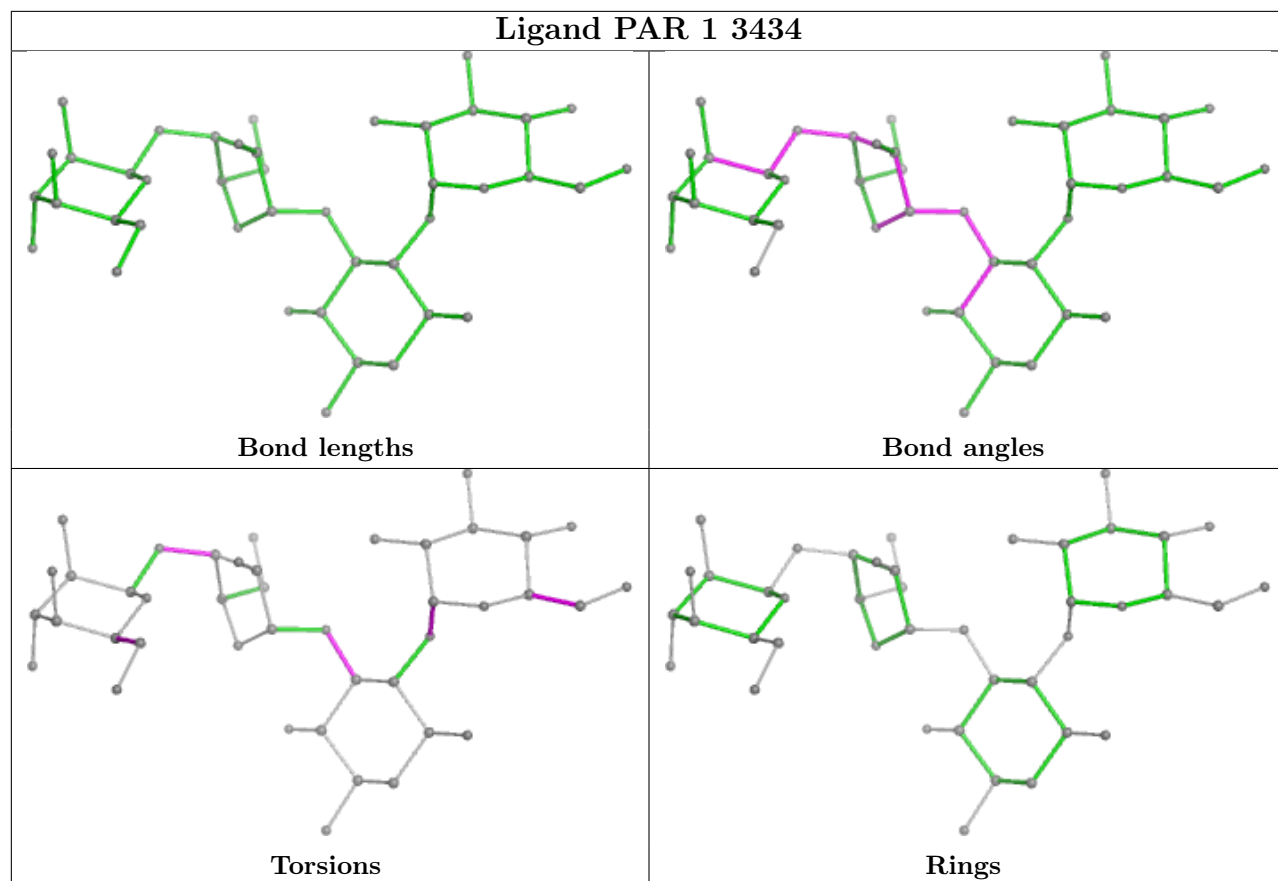


Torsions

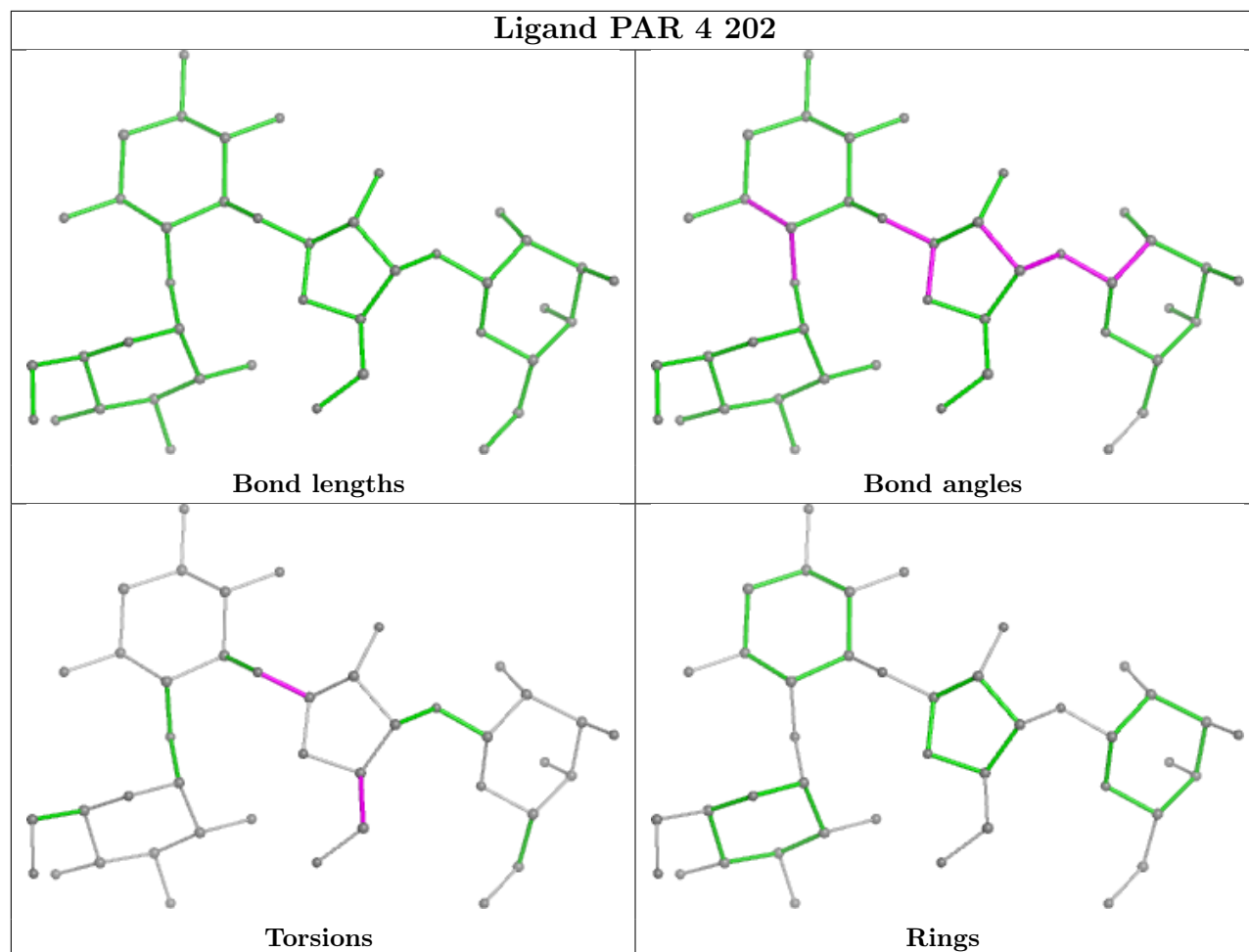


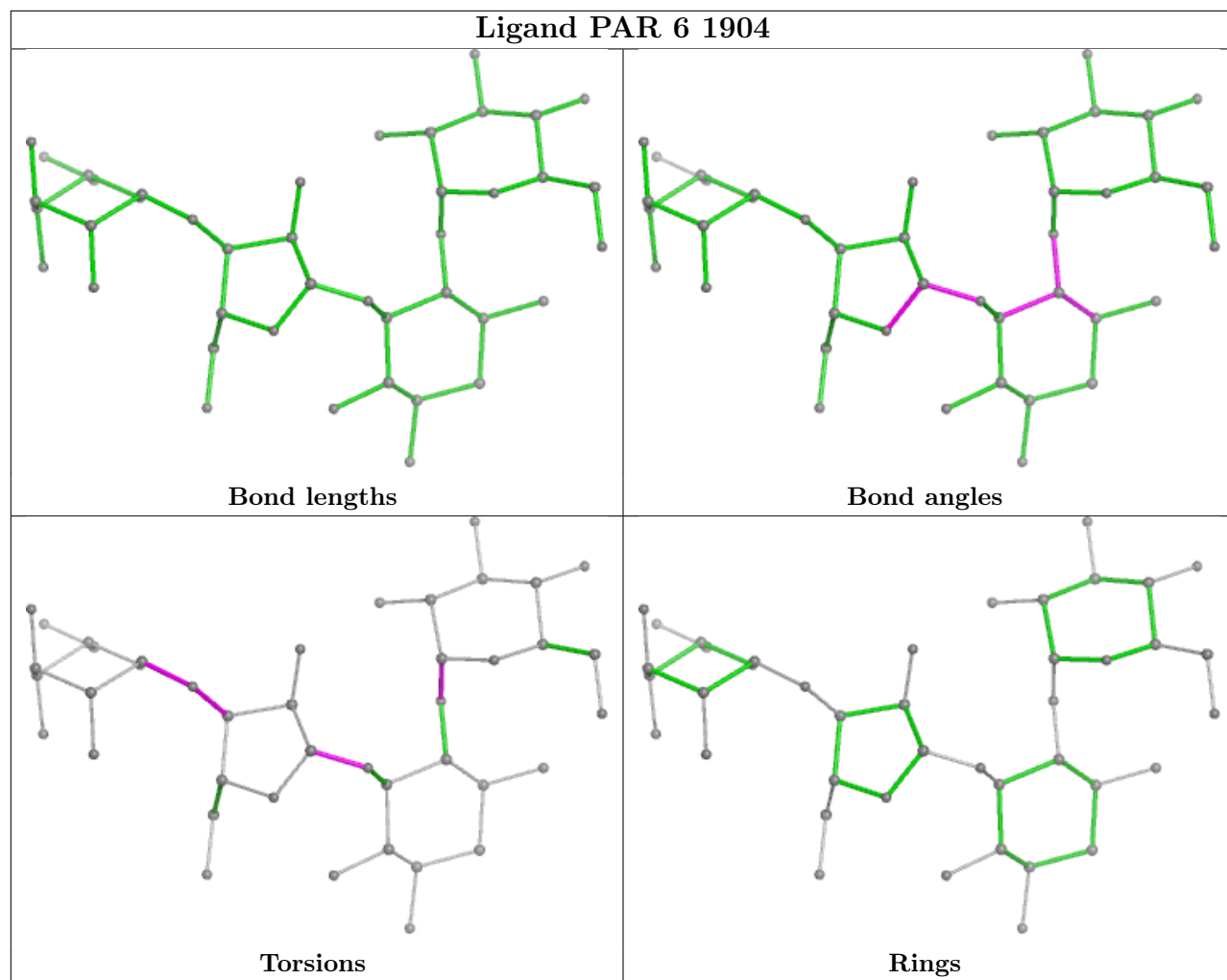
Rings



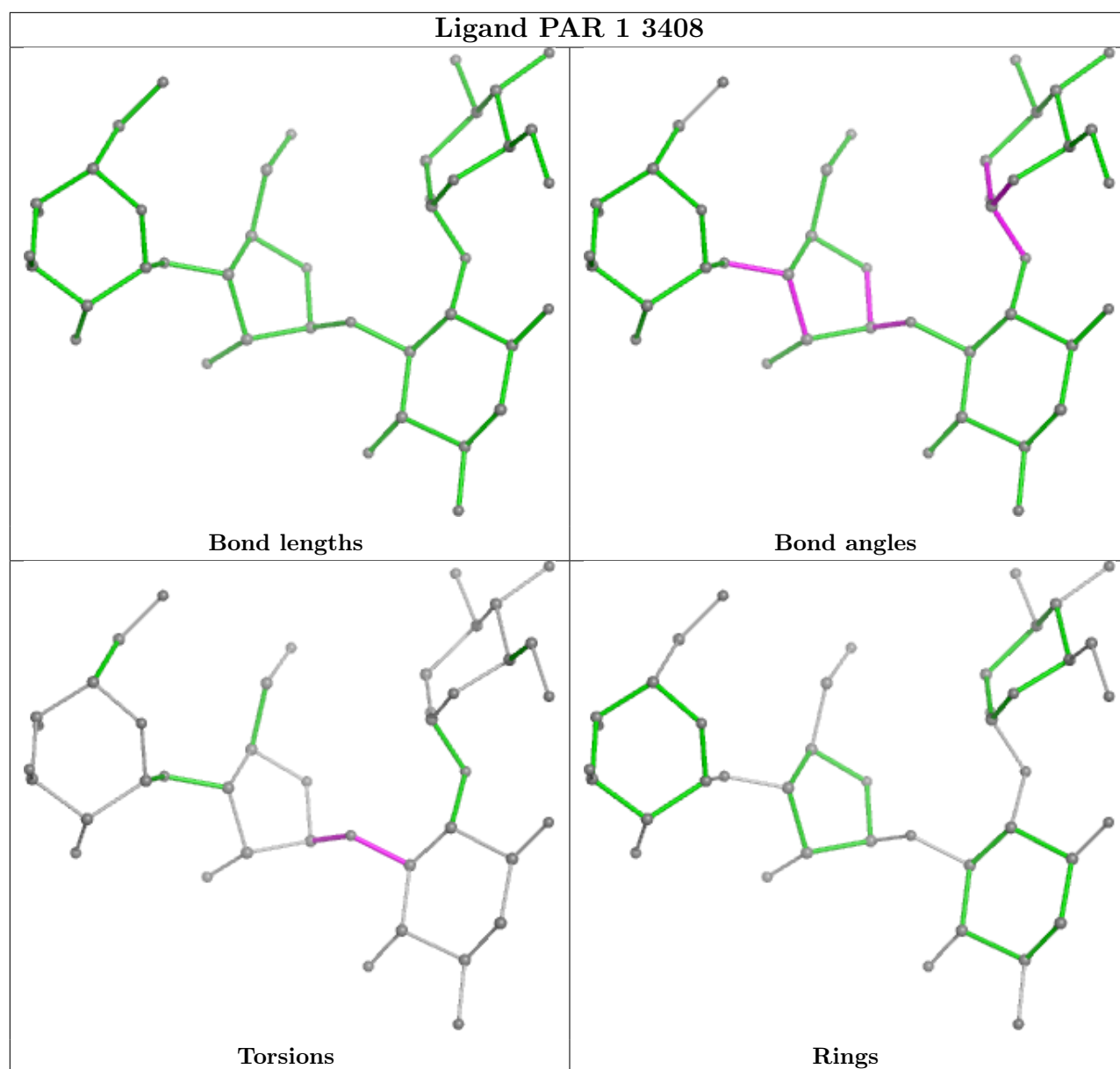


## Ligand PAR 4 202

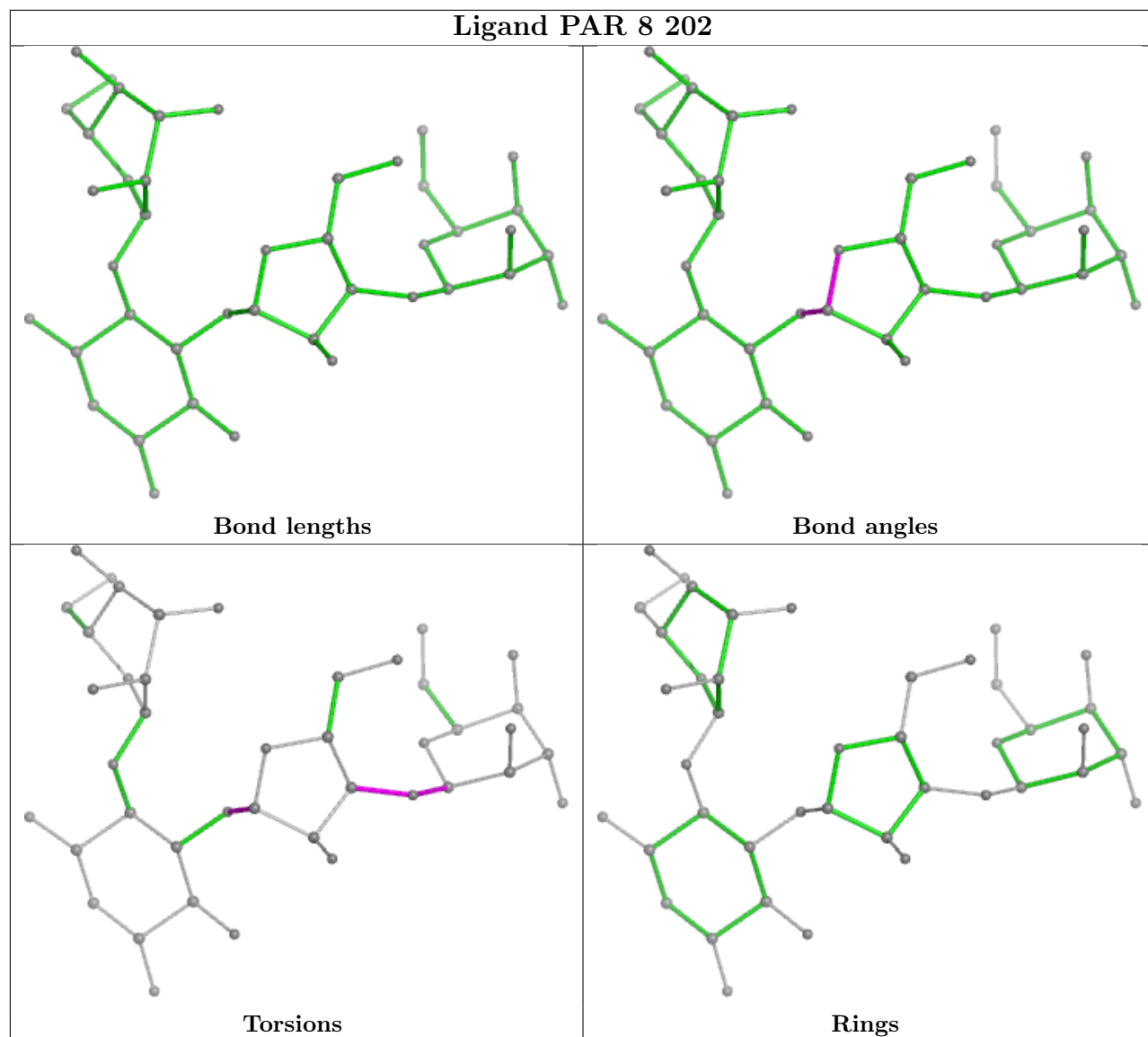


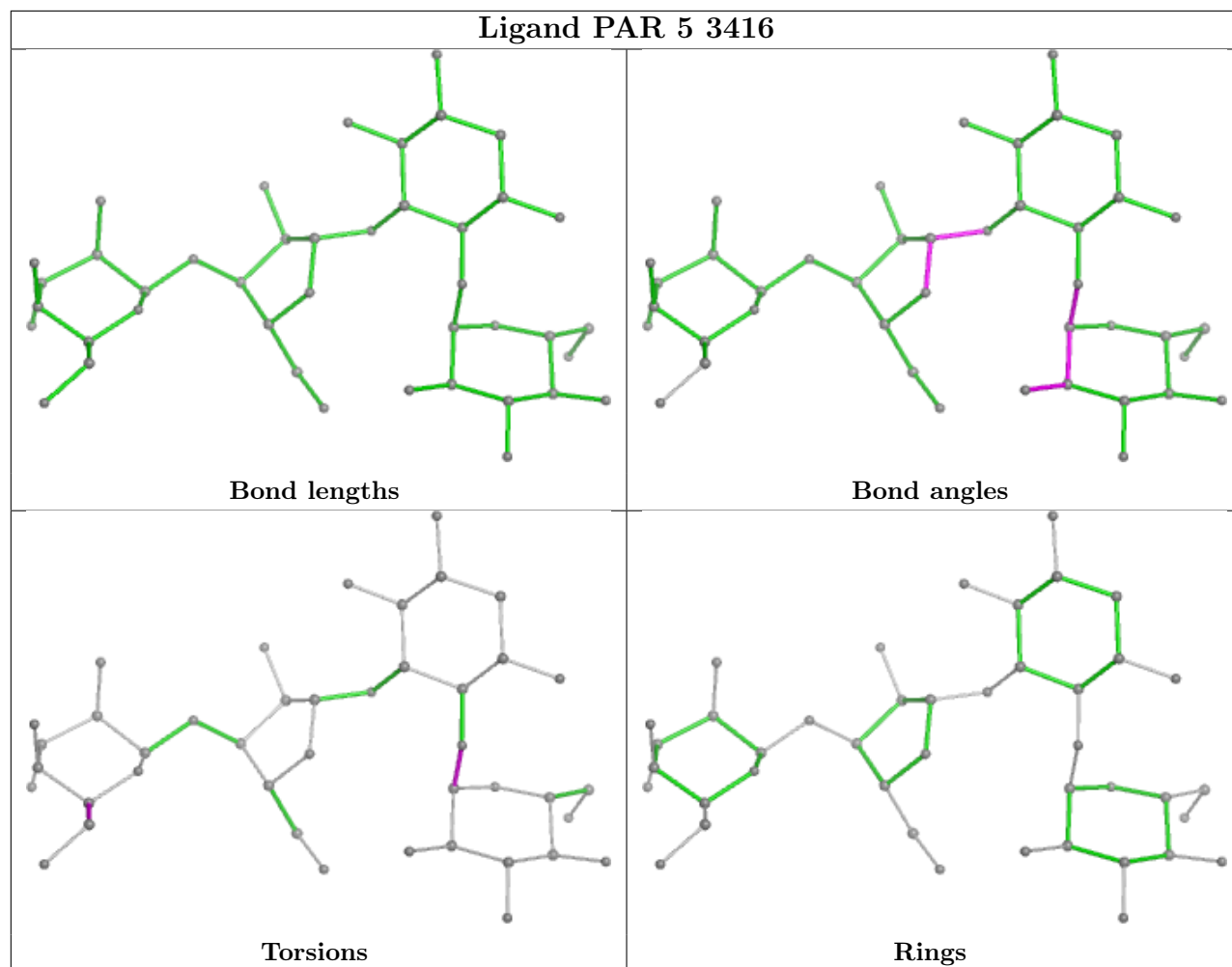


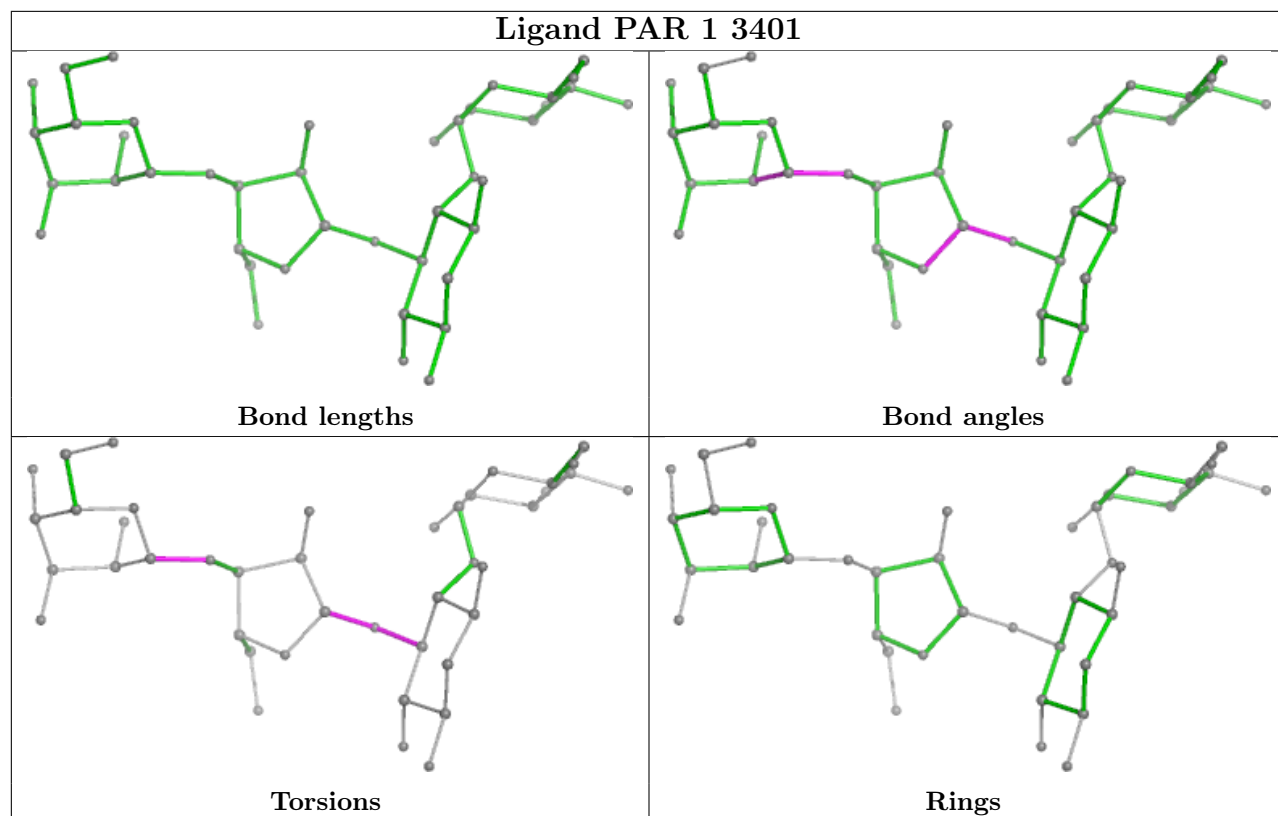


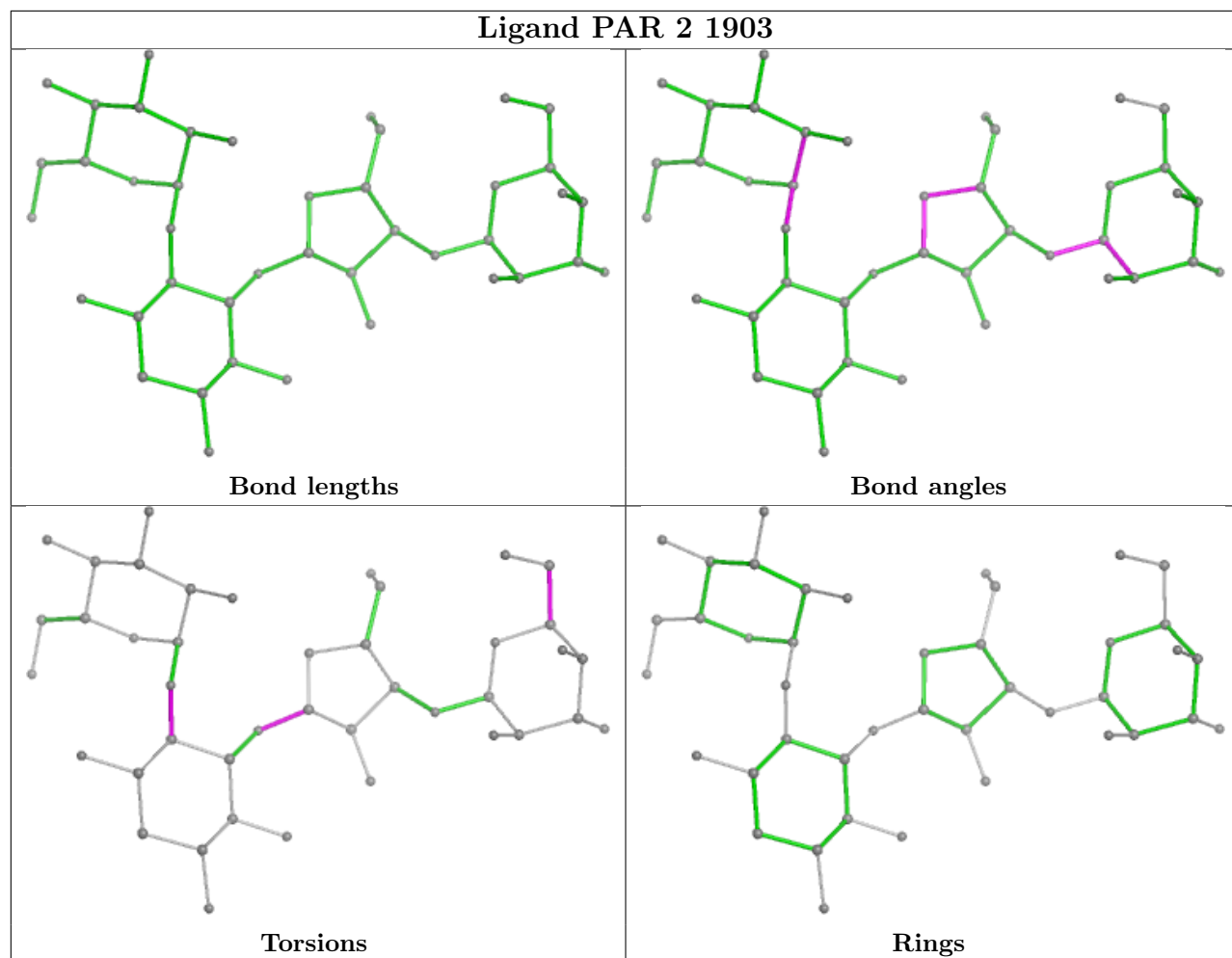


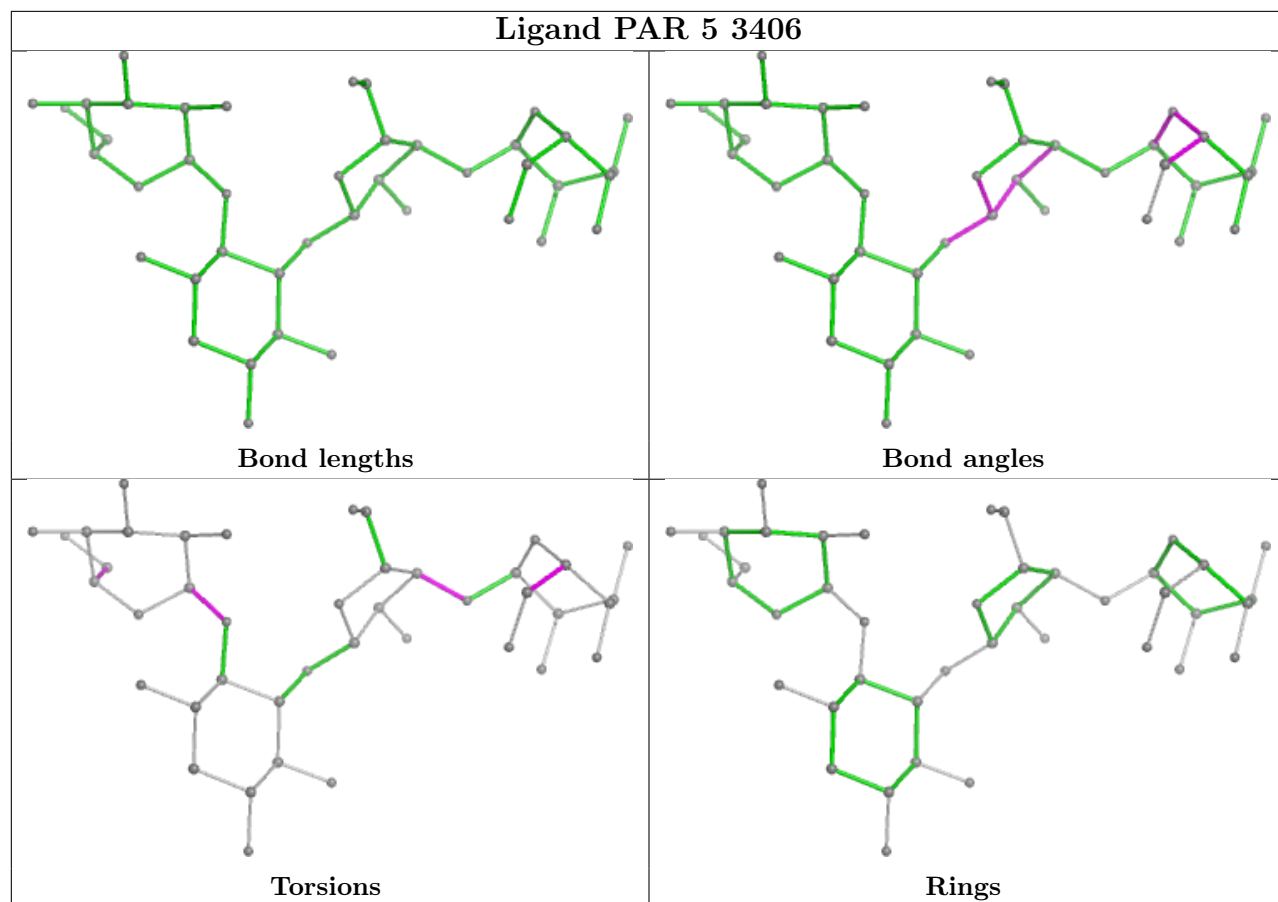
## Ligand PAR 8 202

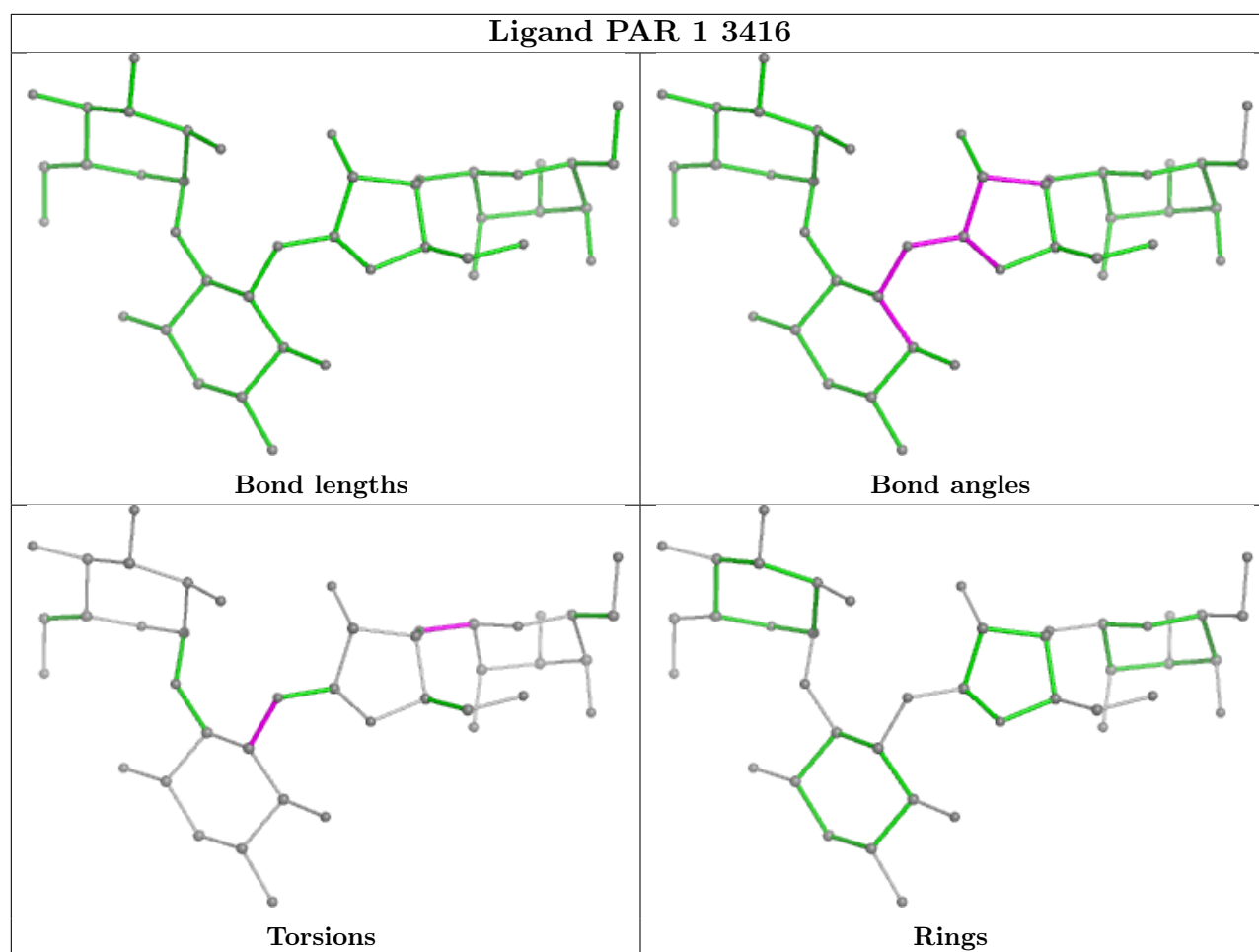


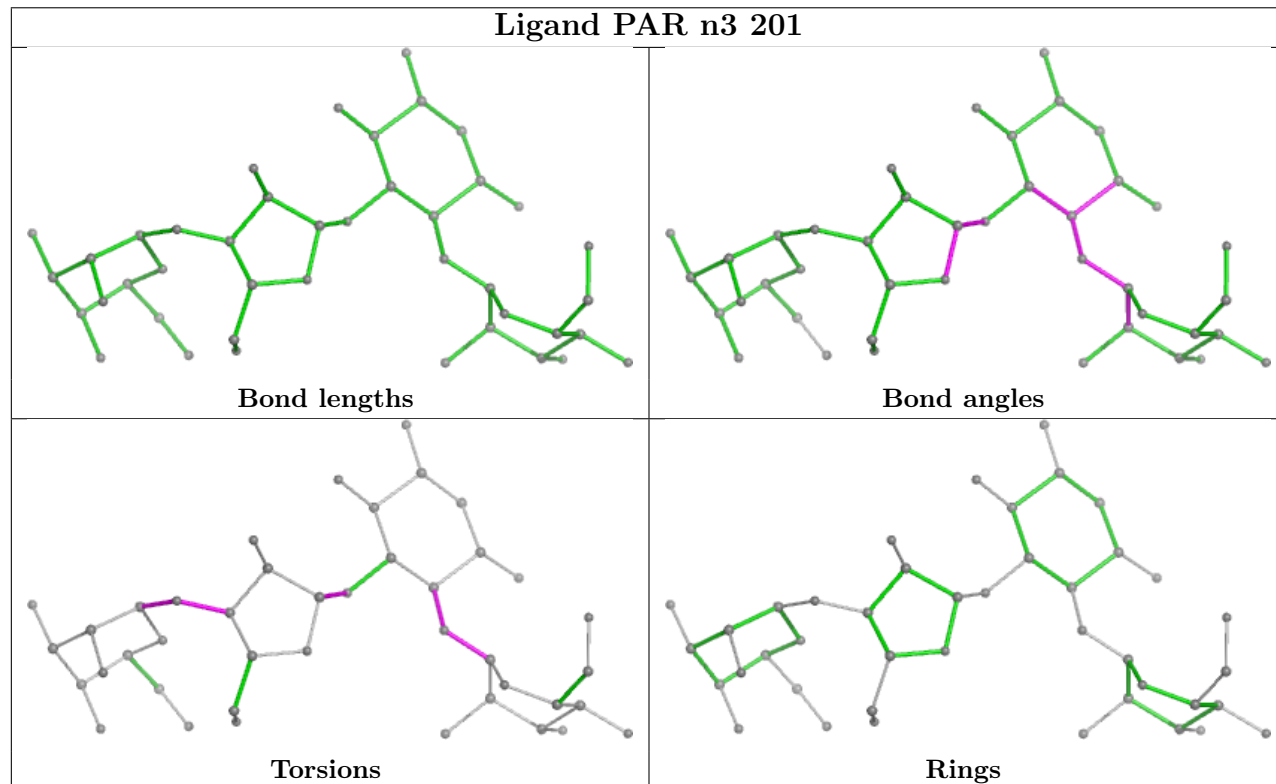
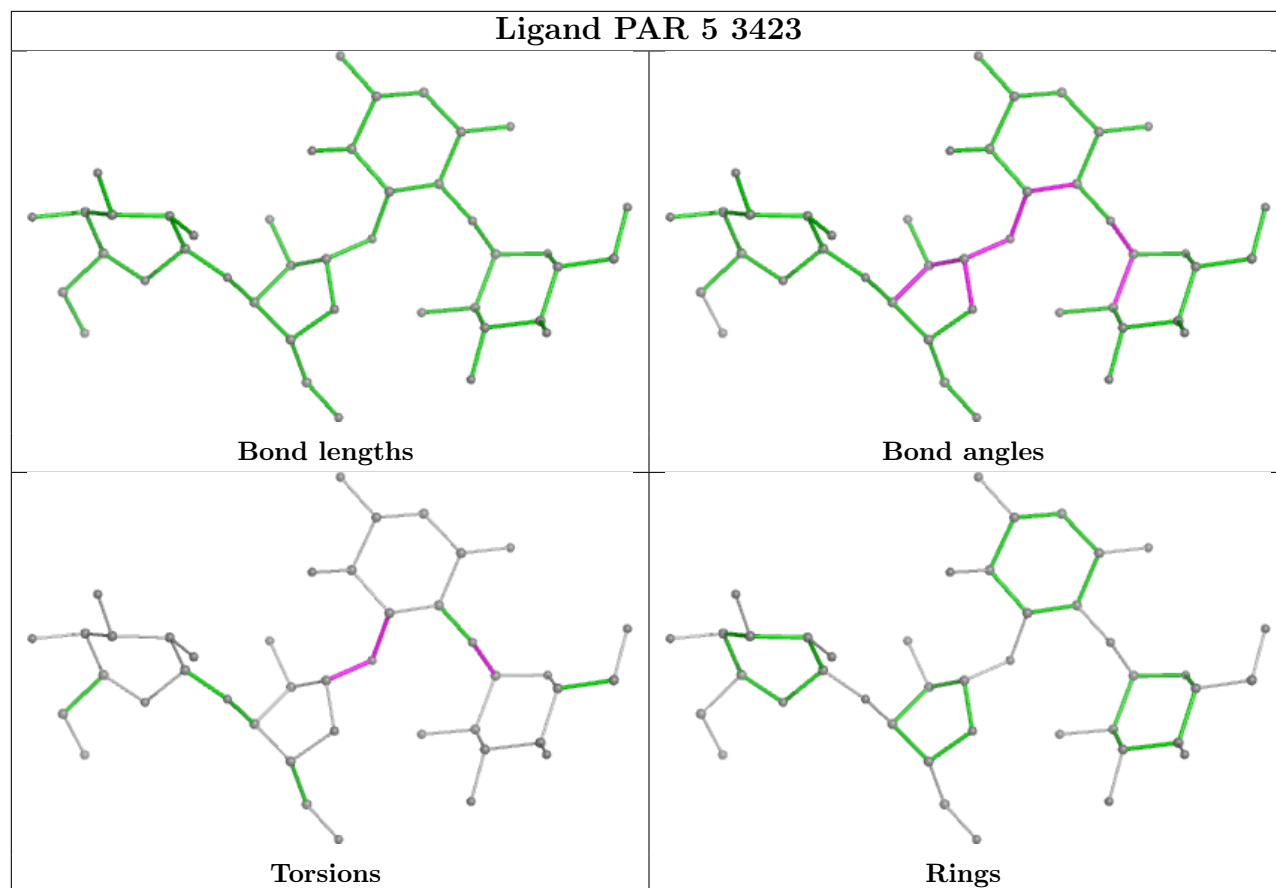




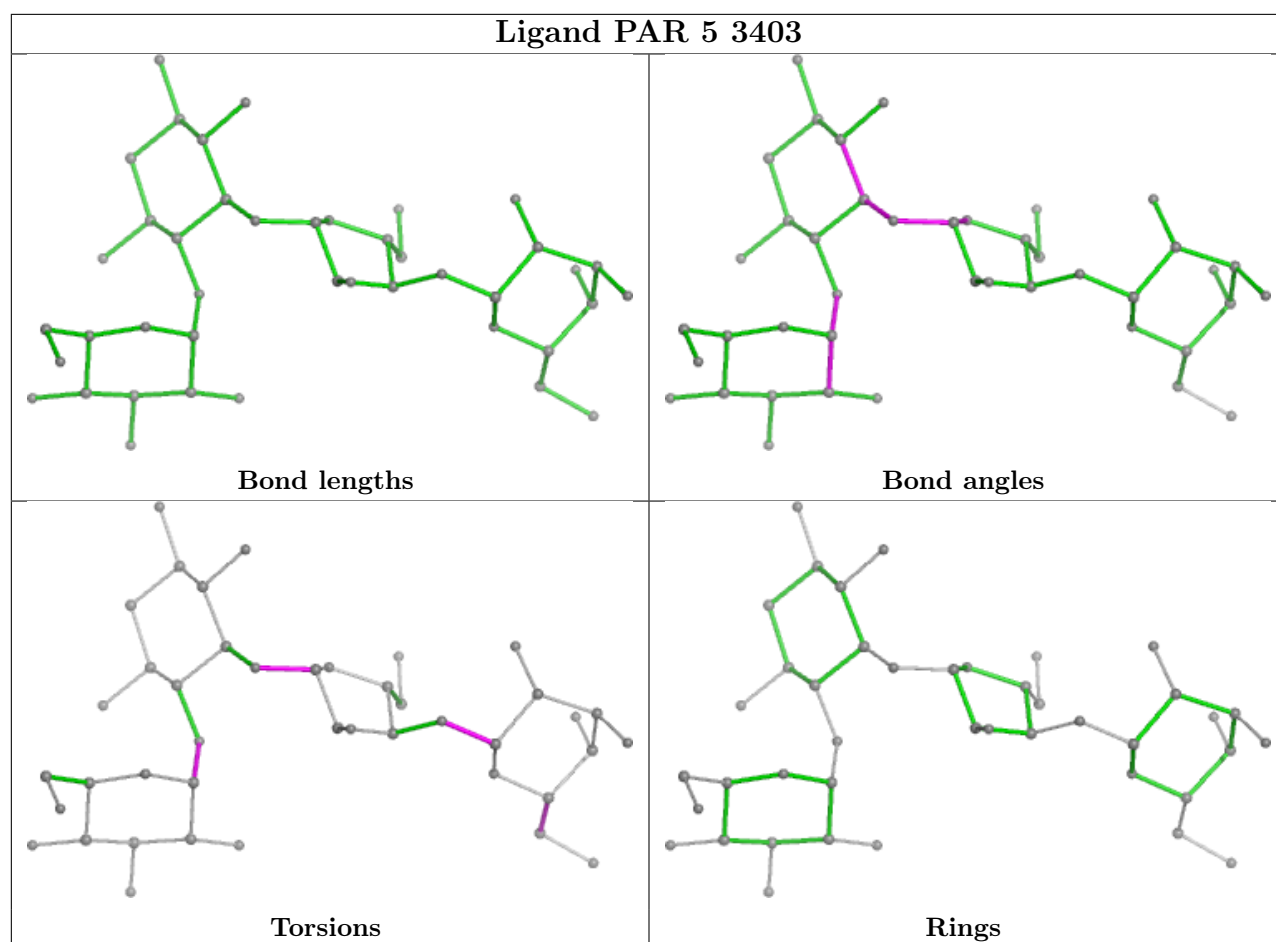


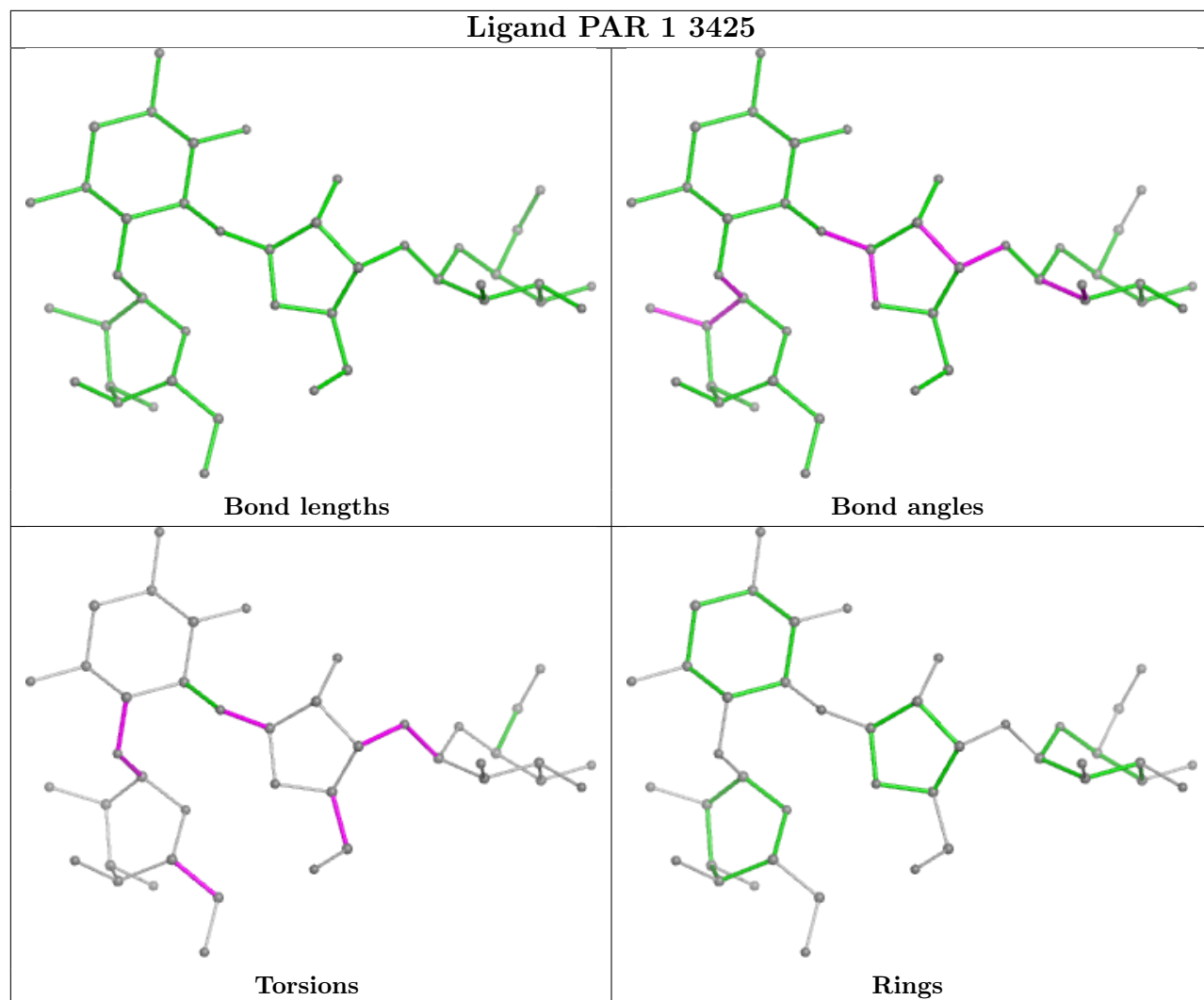


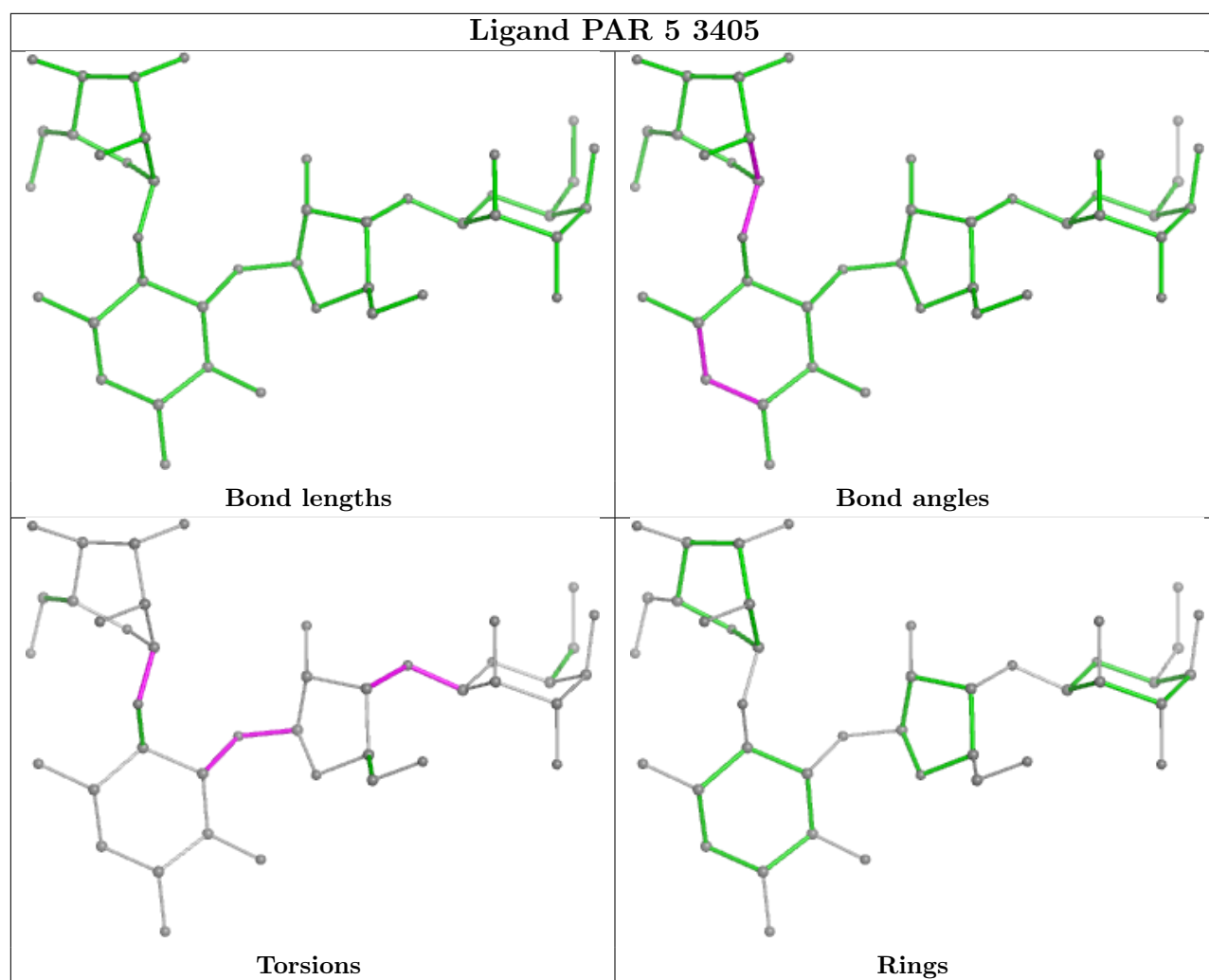


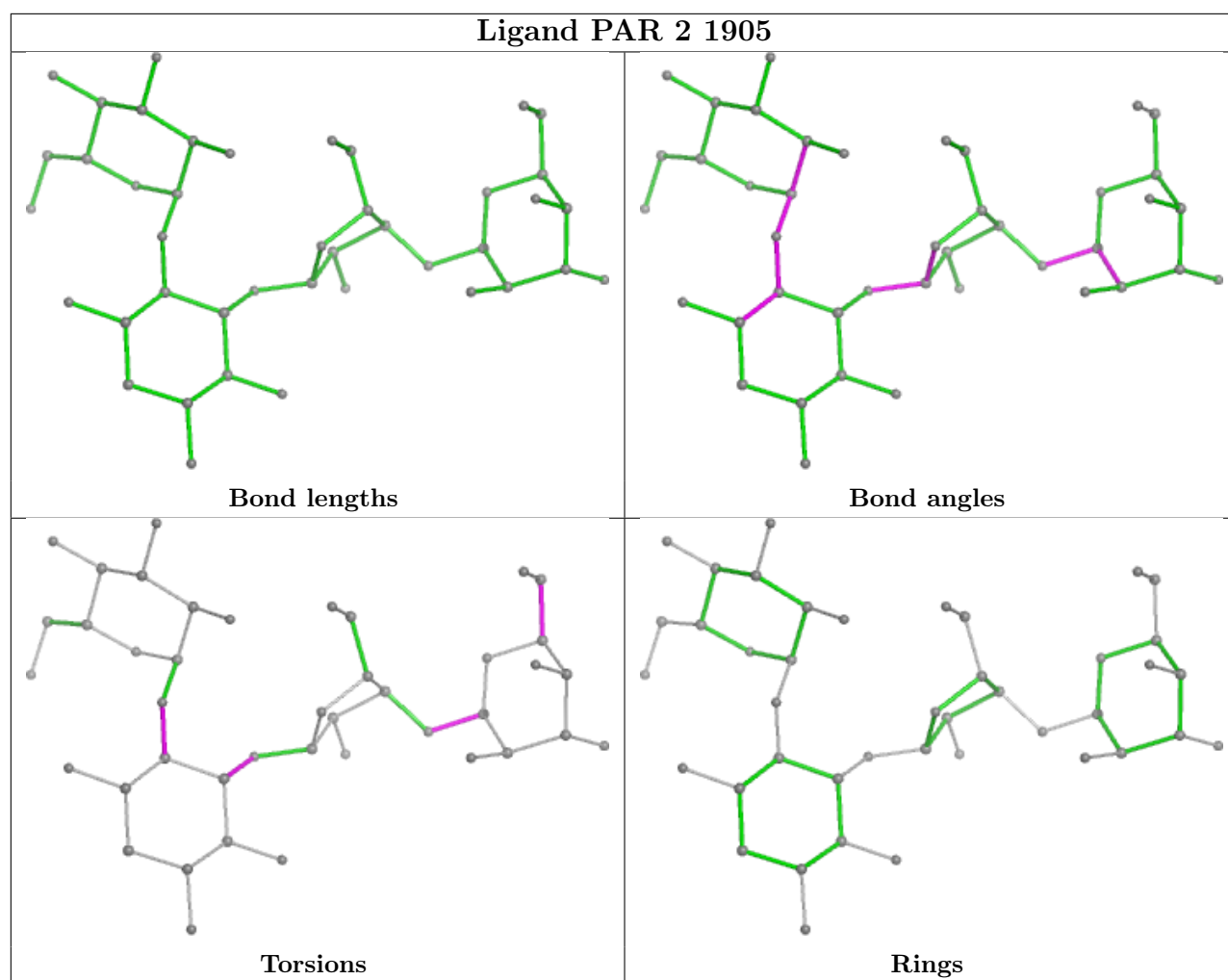


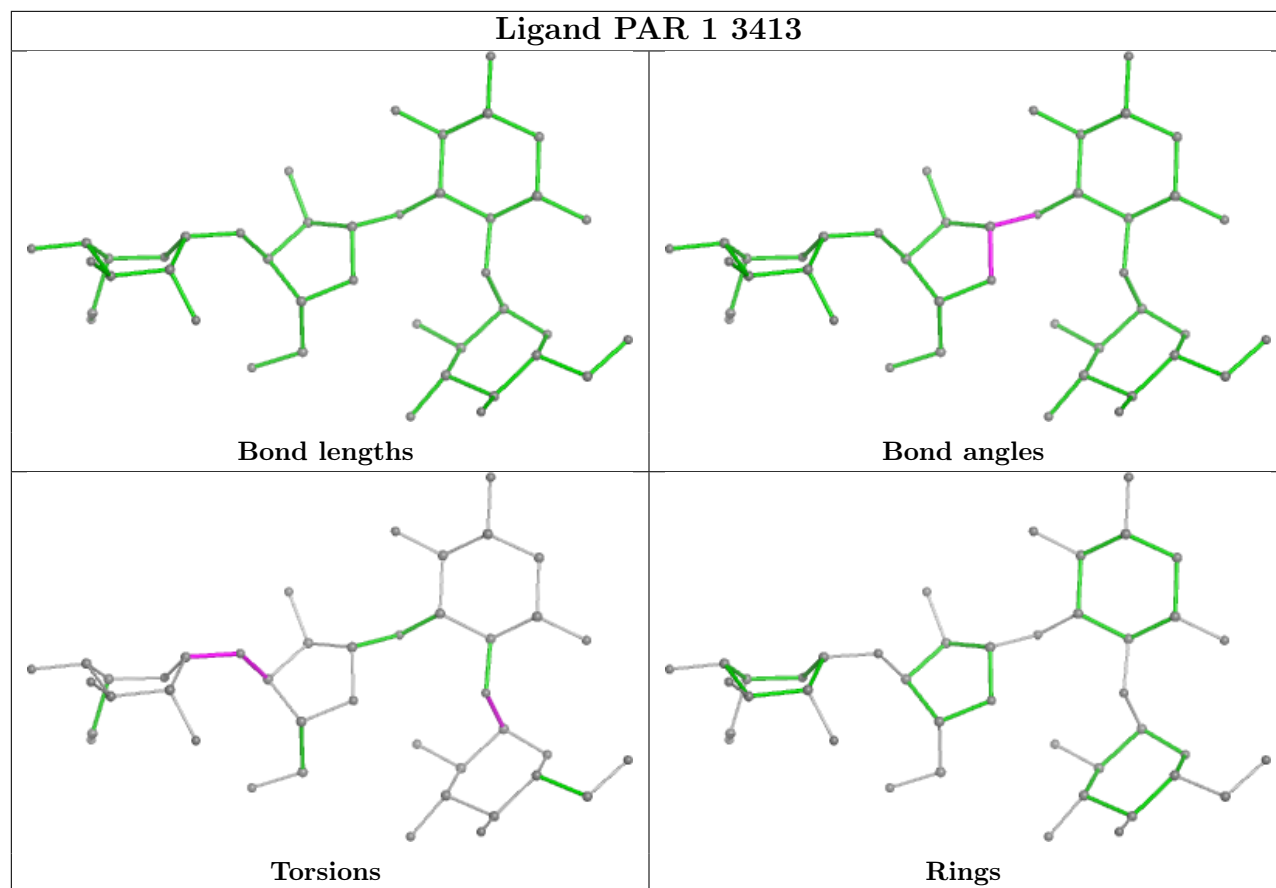




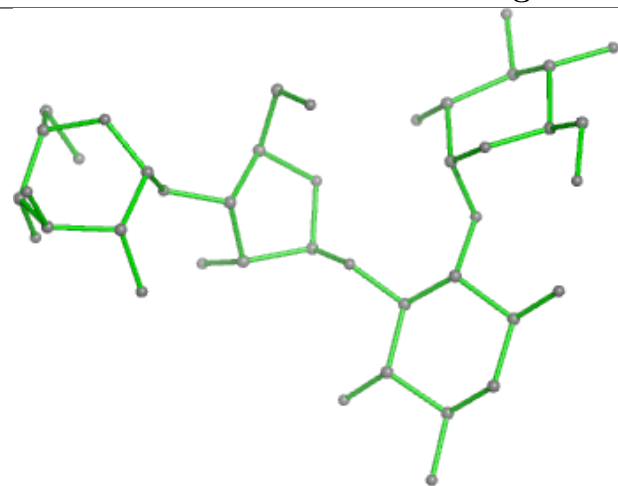




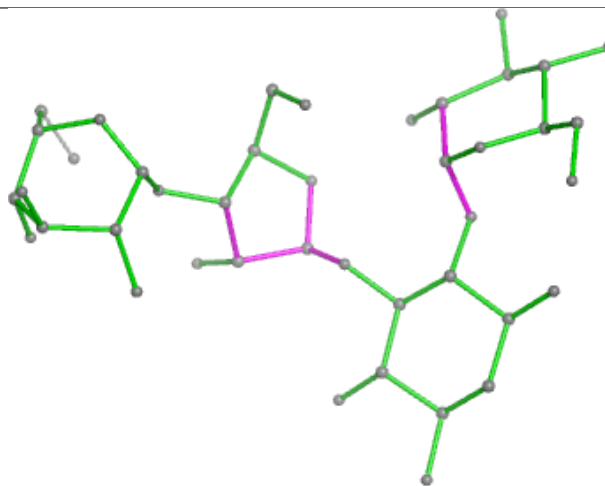




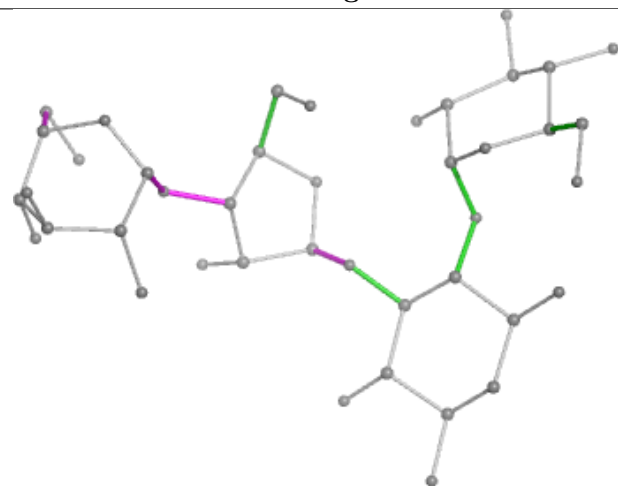
## Ligand PAR 5 3418



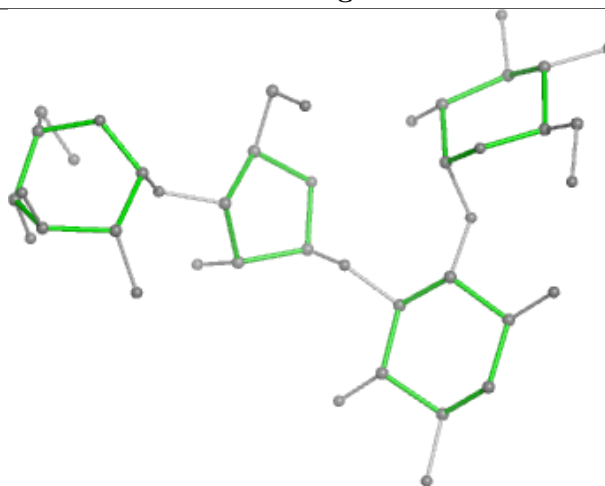
Bond lengths



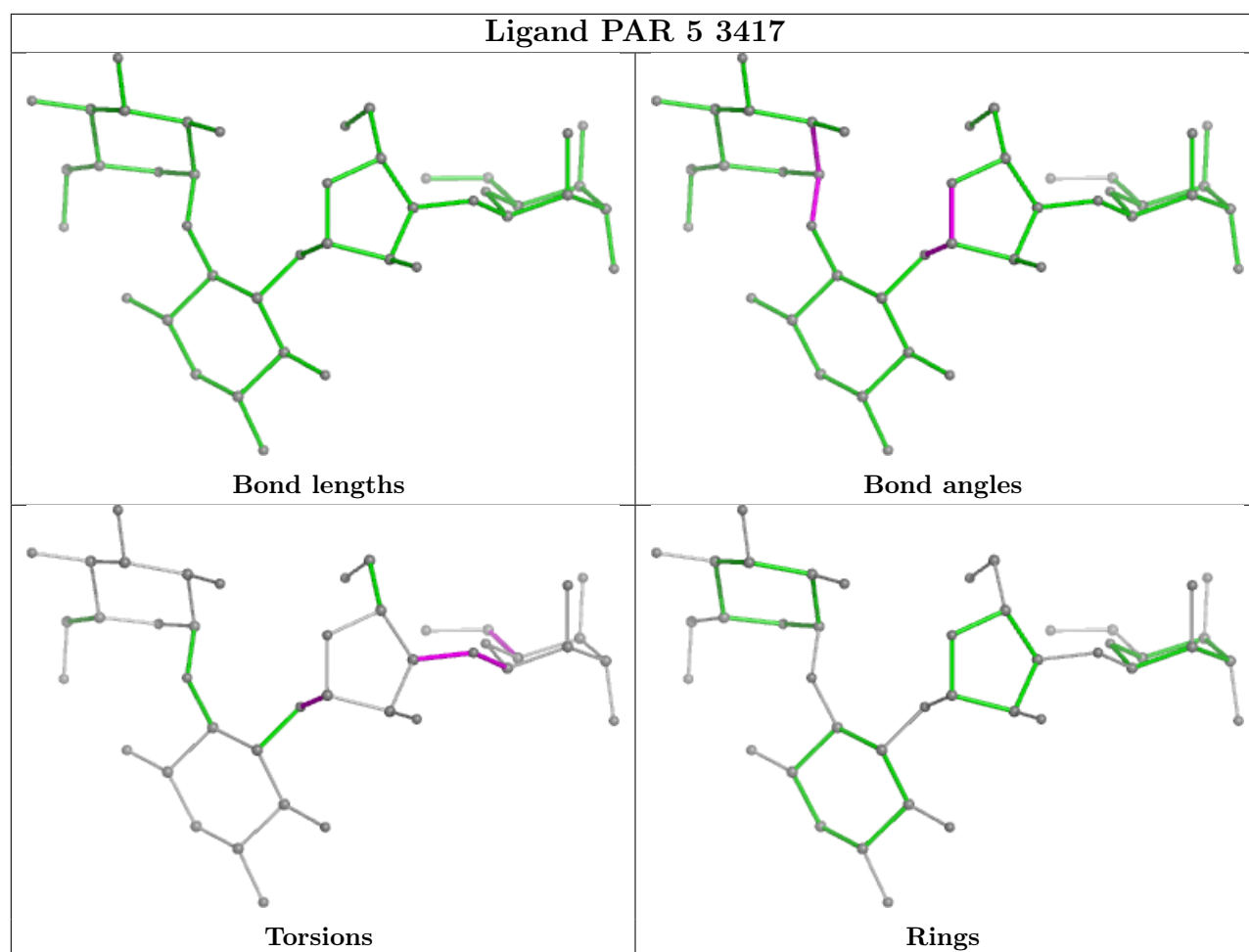
Bond angles

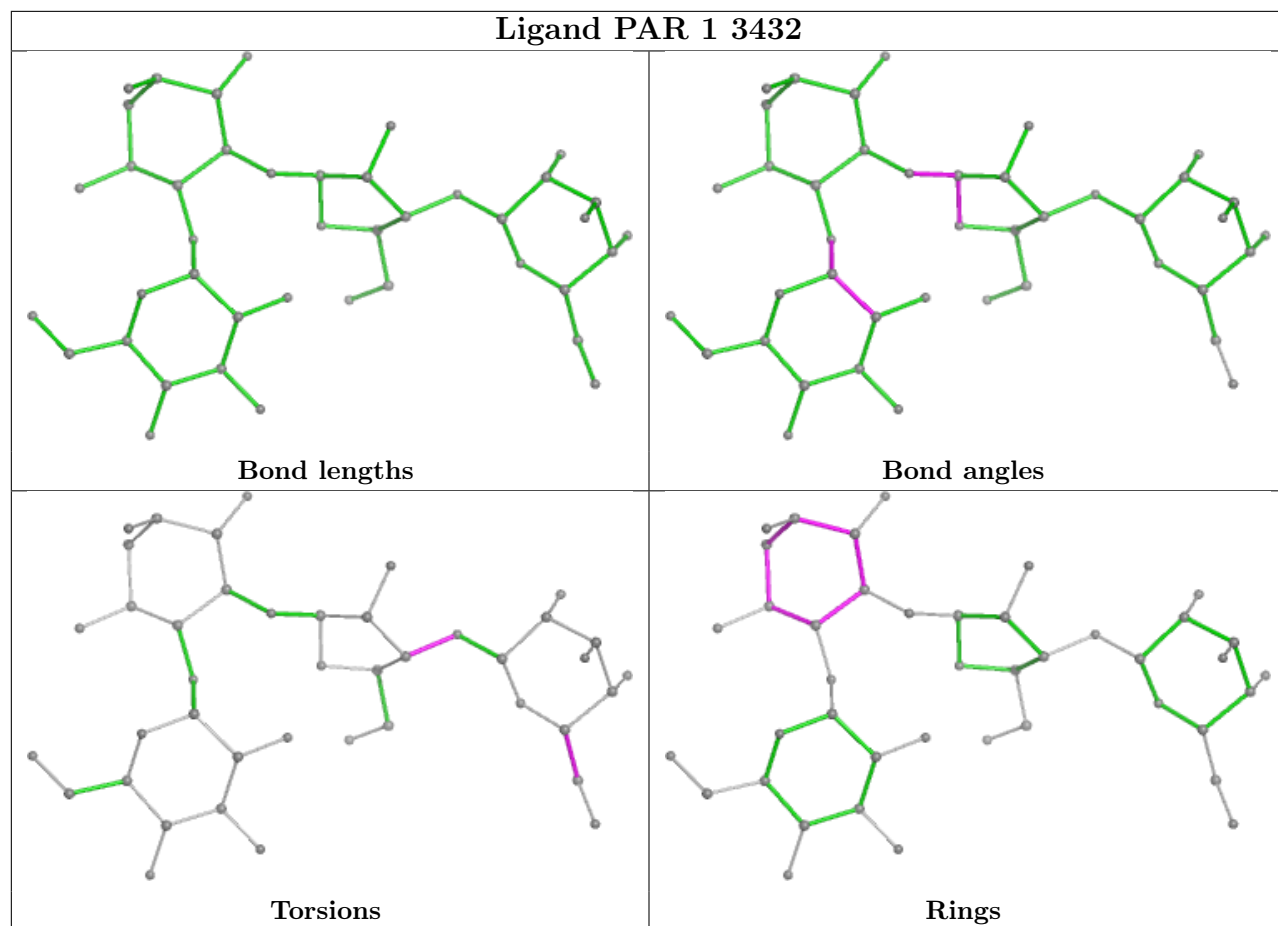


Torsions

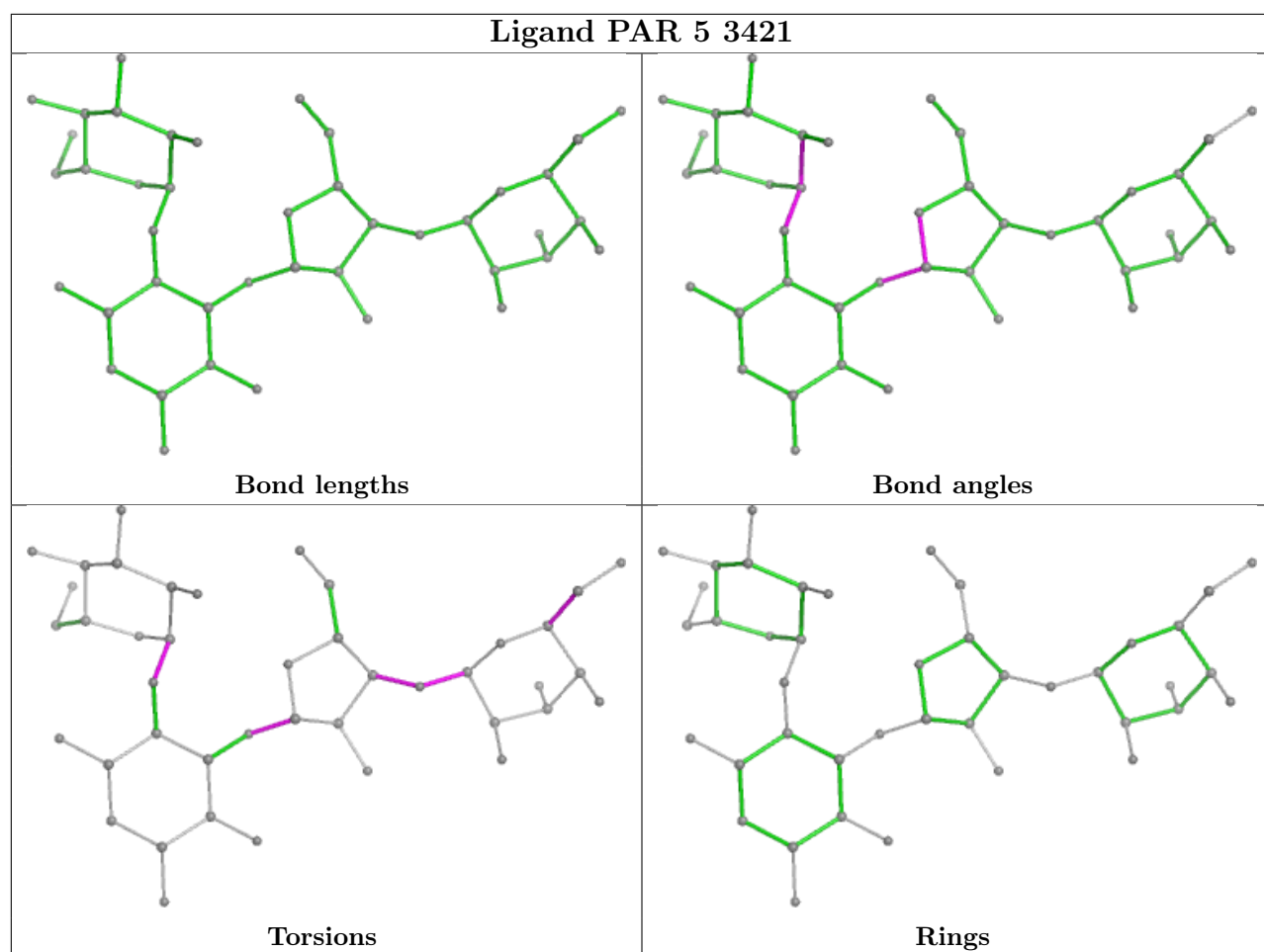


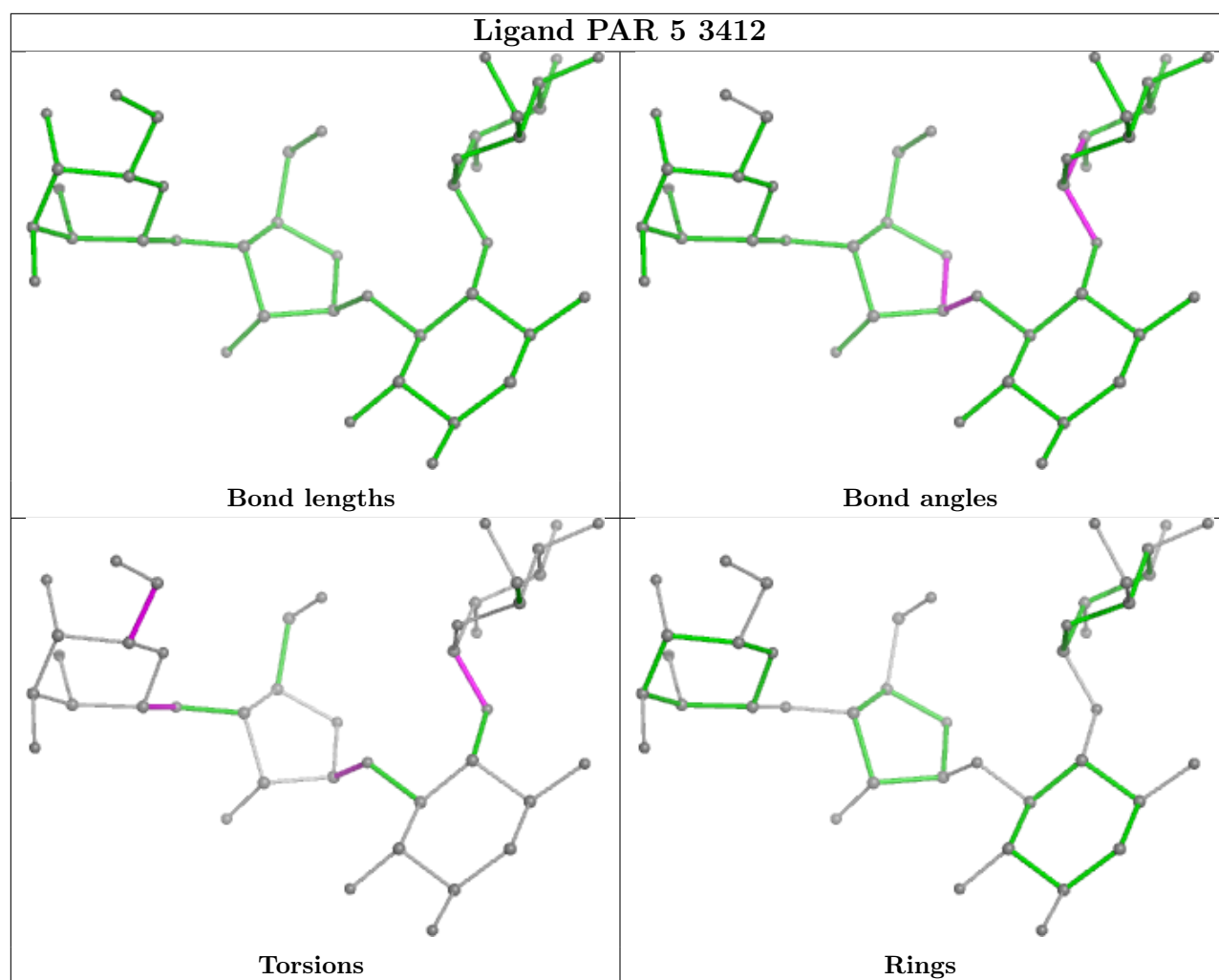
Rings

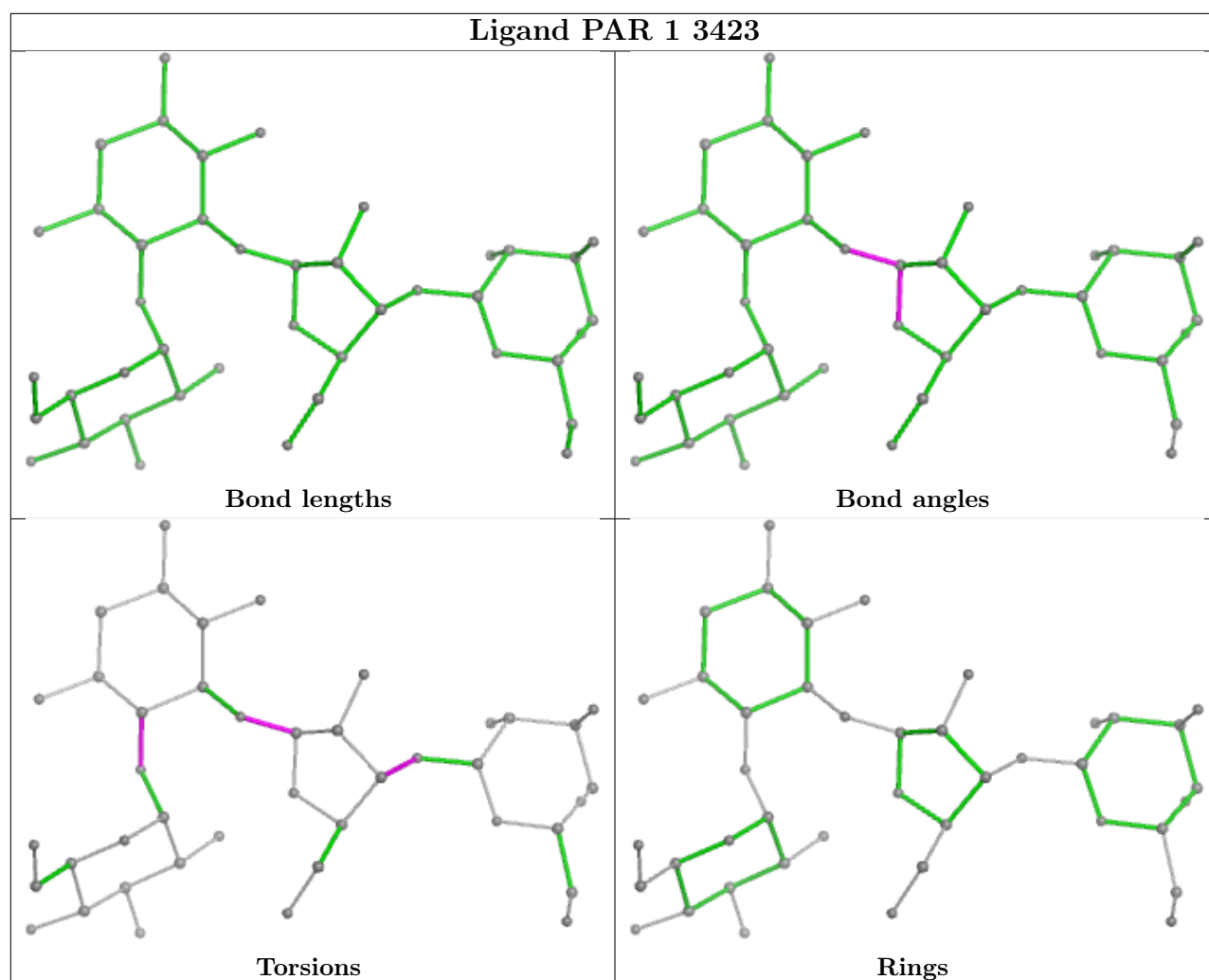


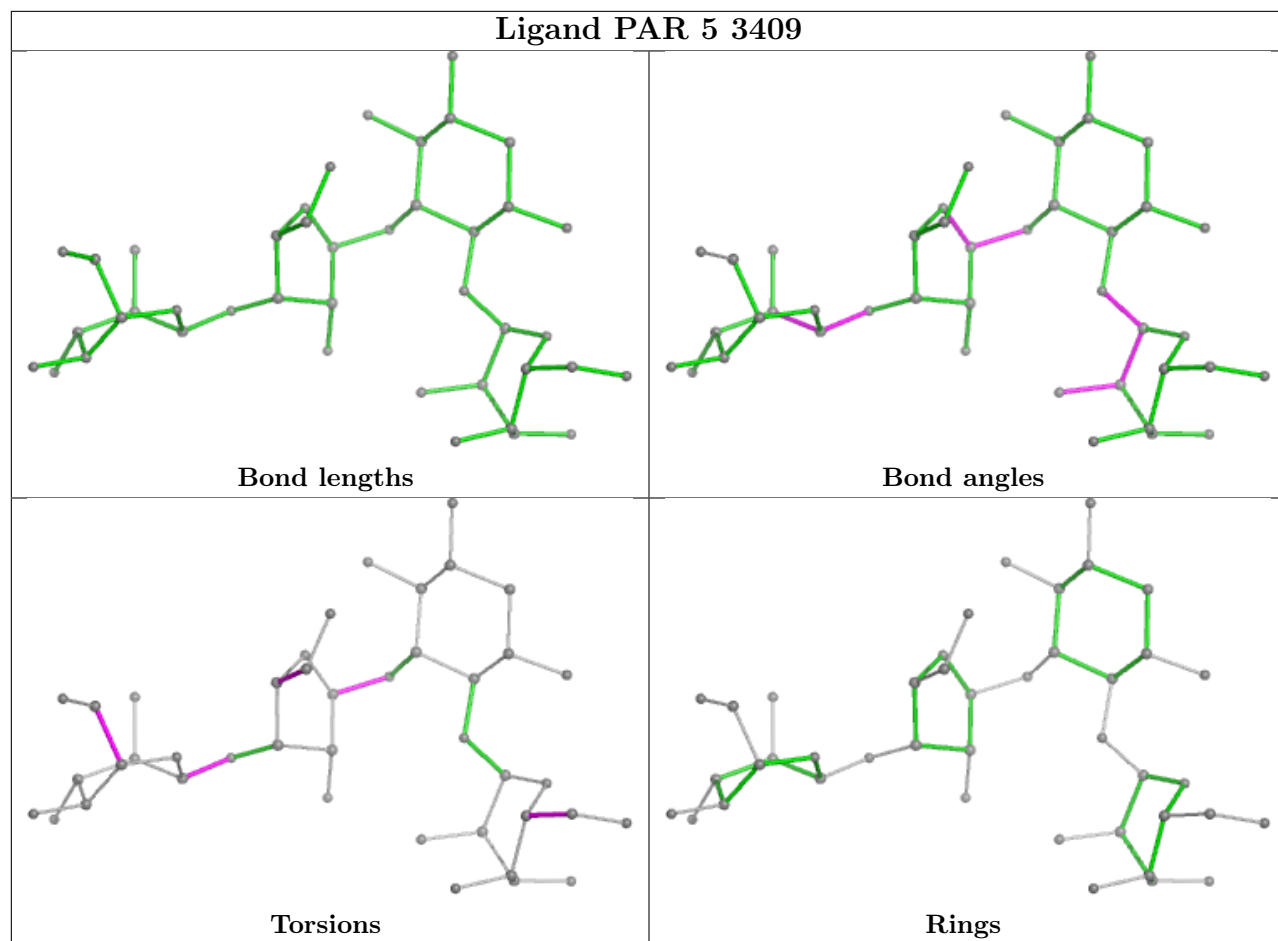


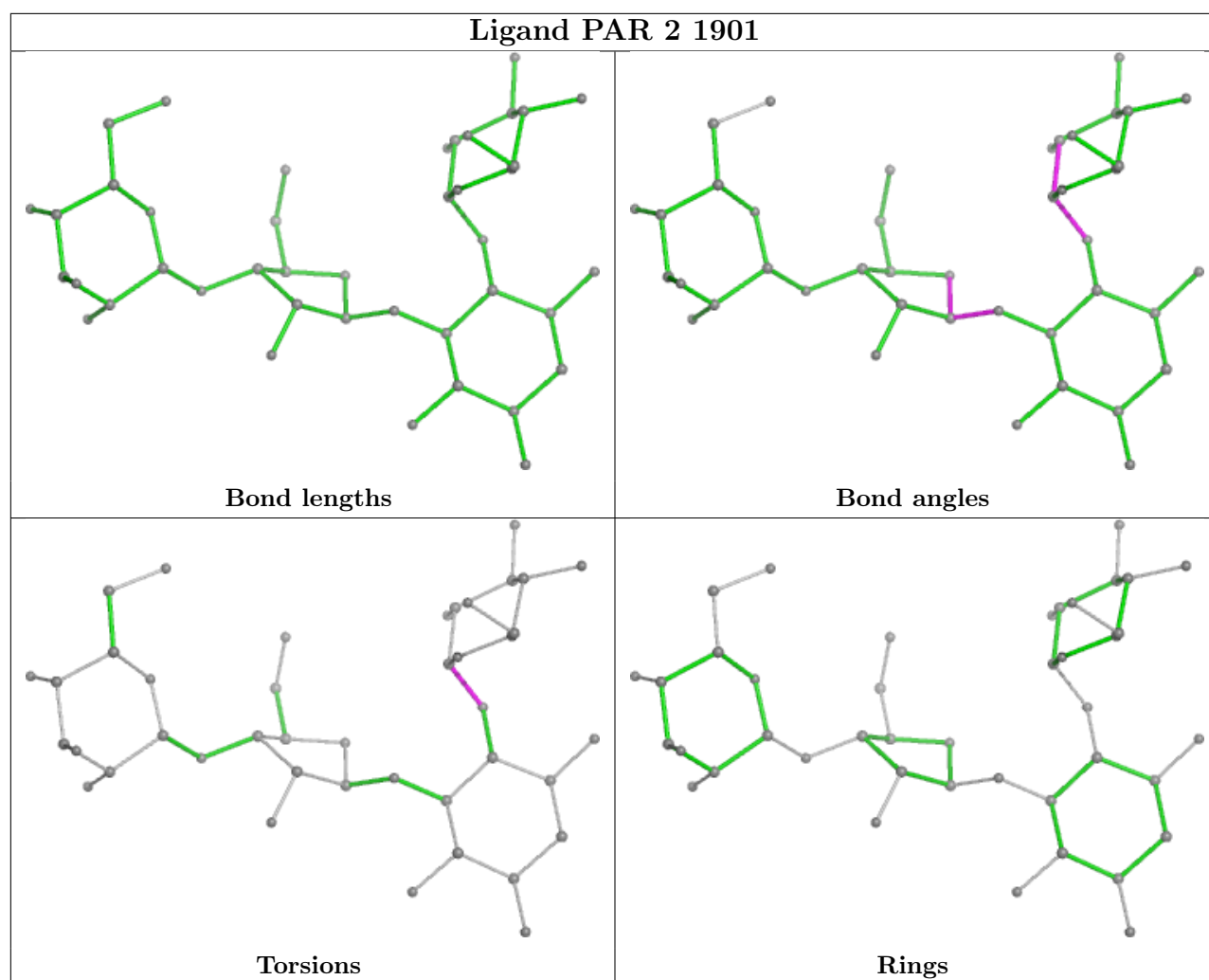


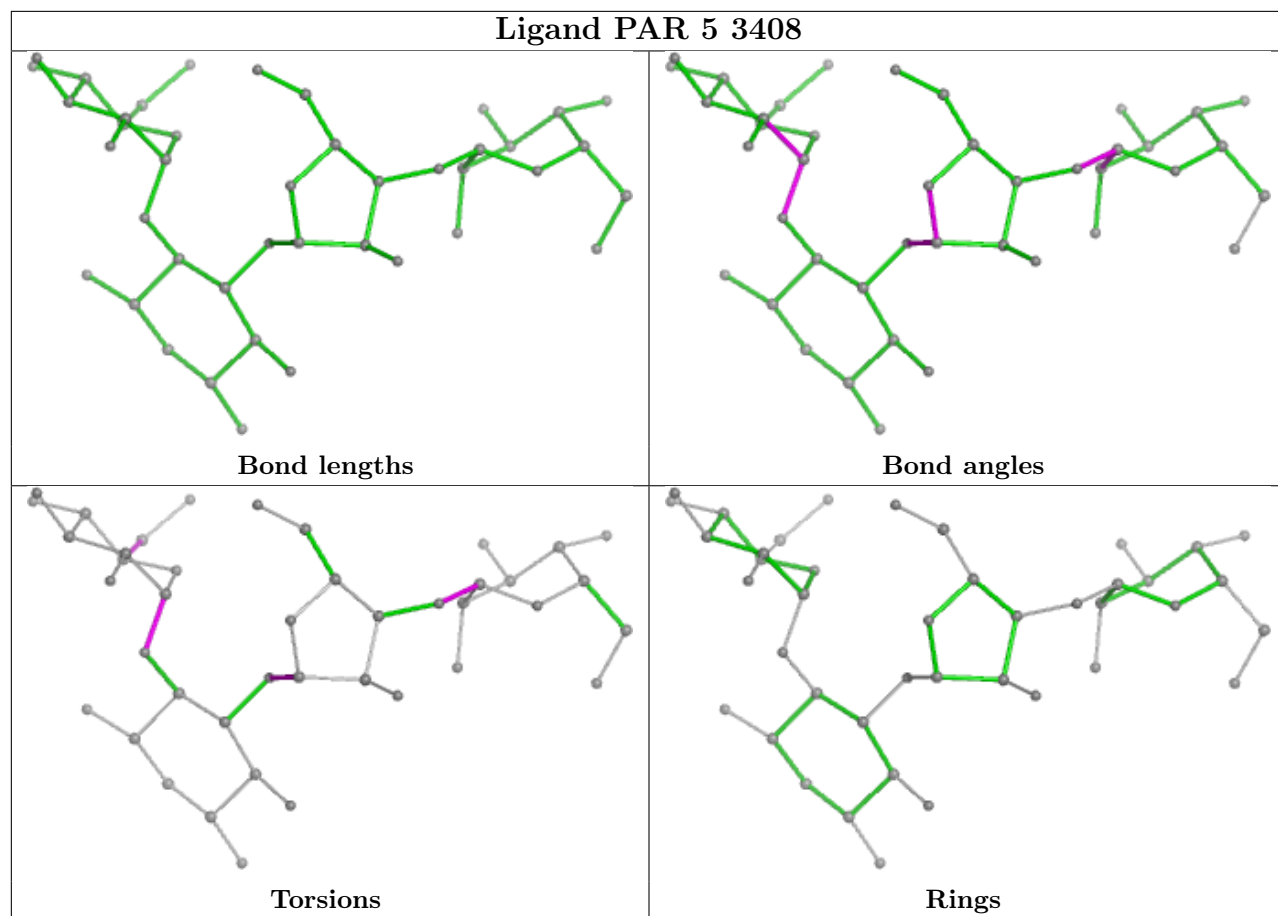


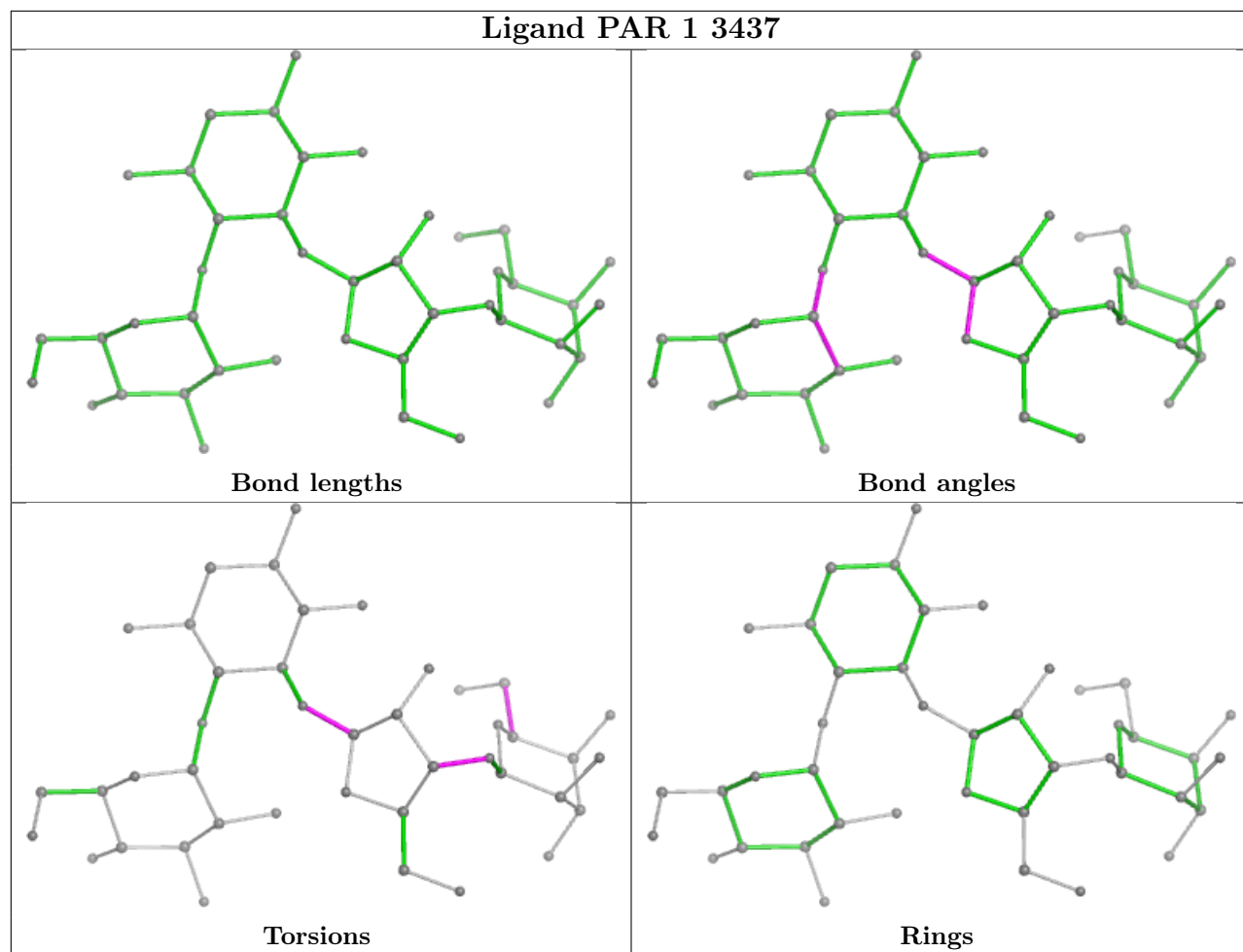


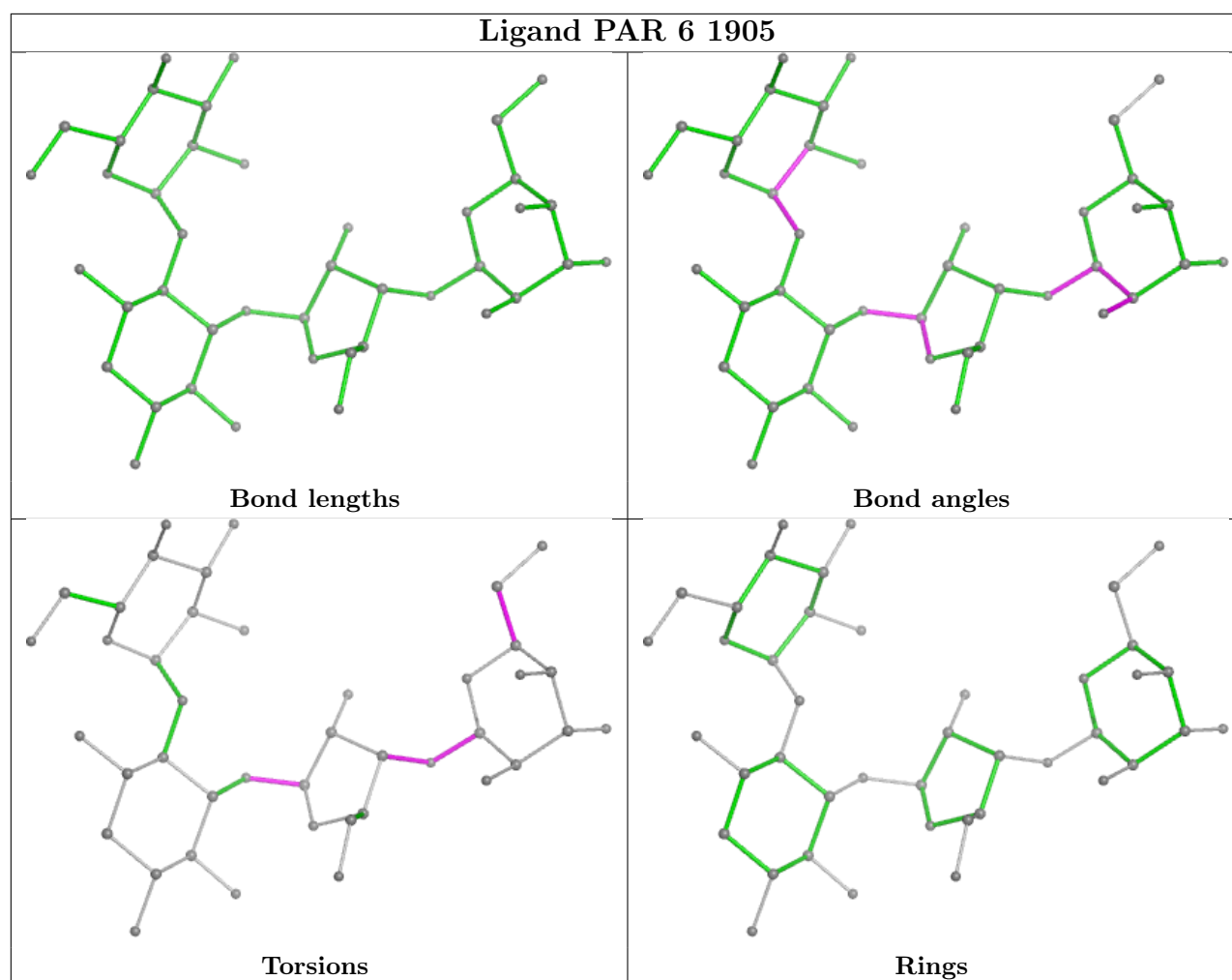




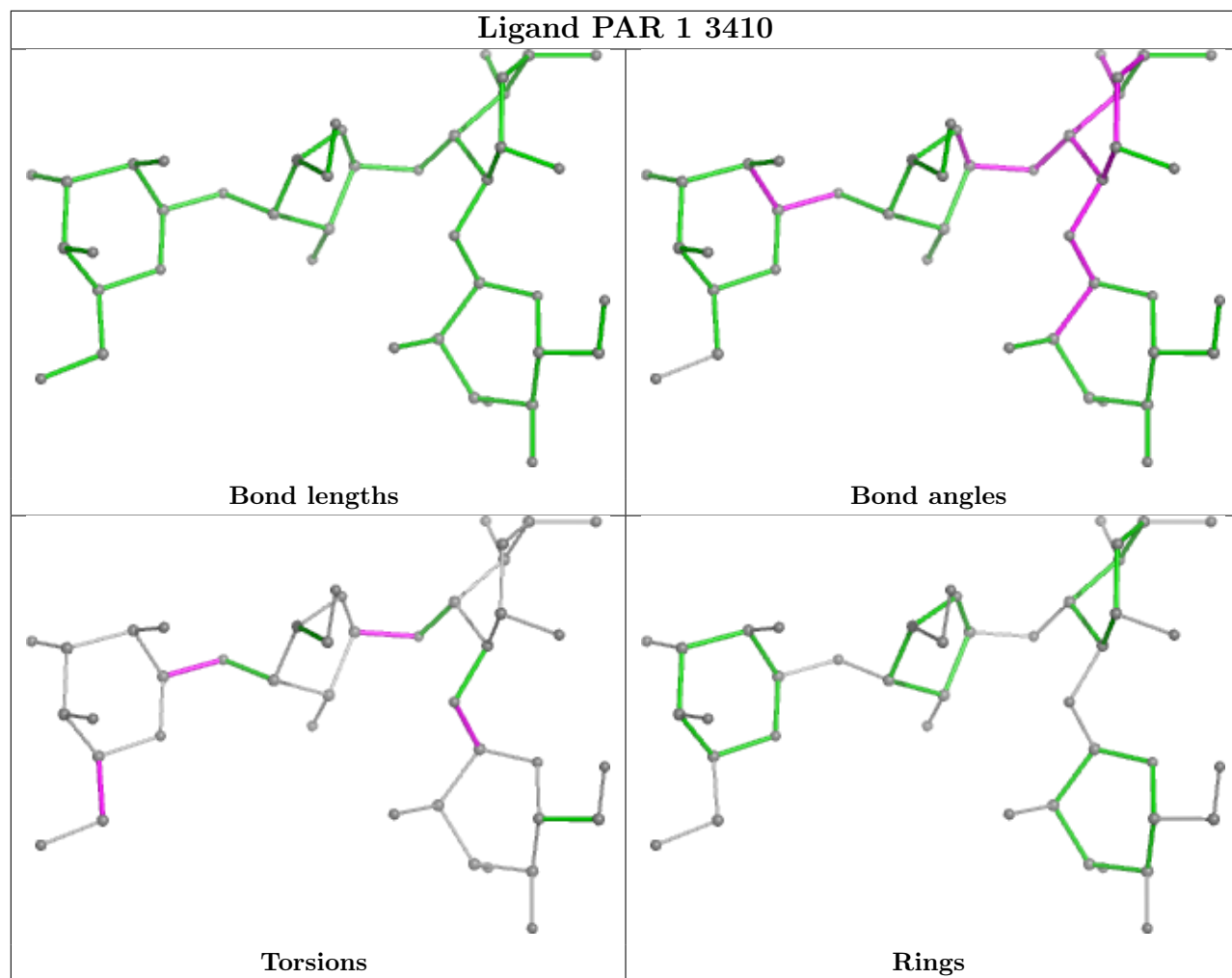




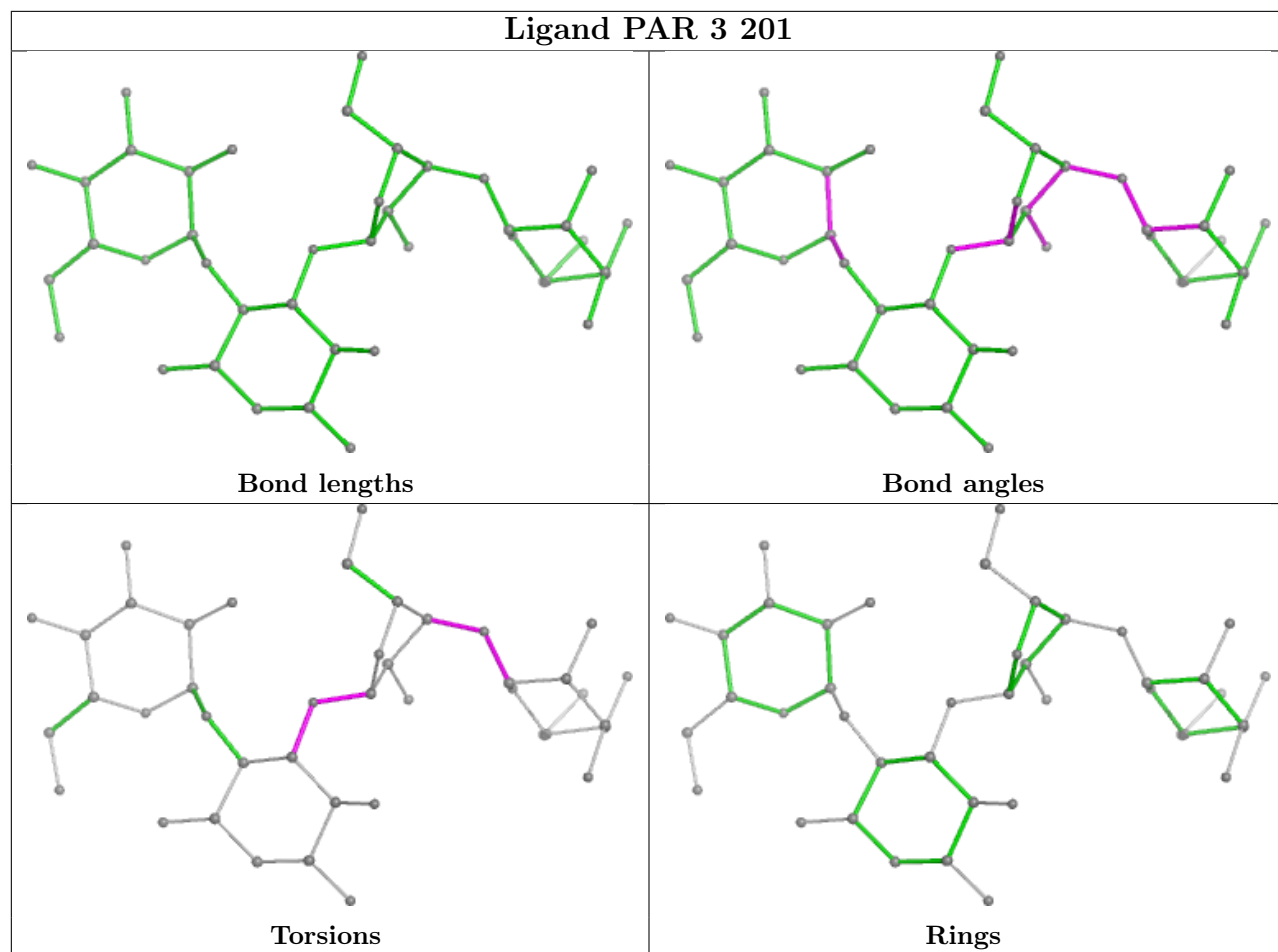


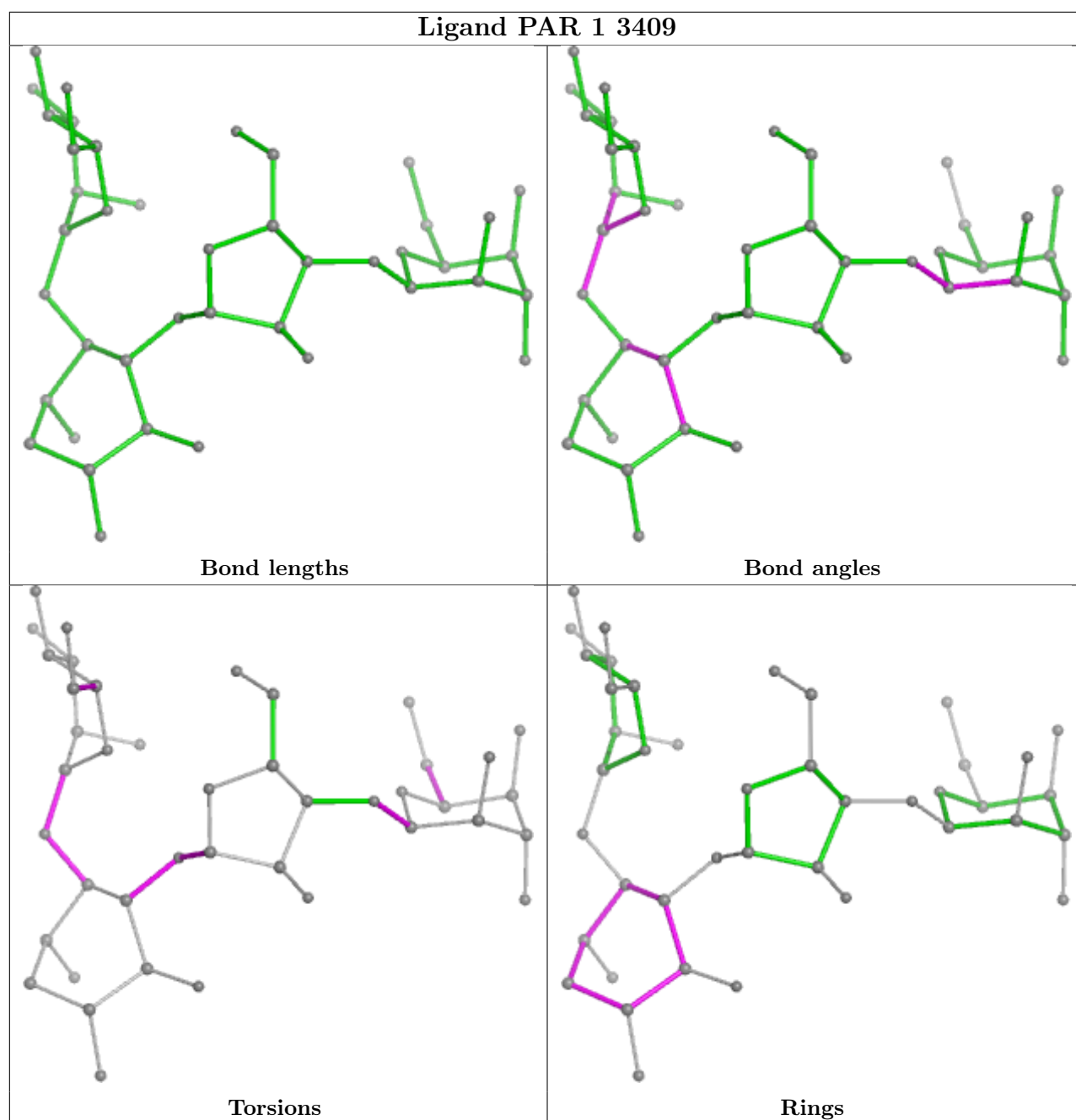


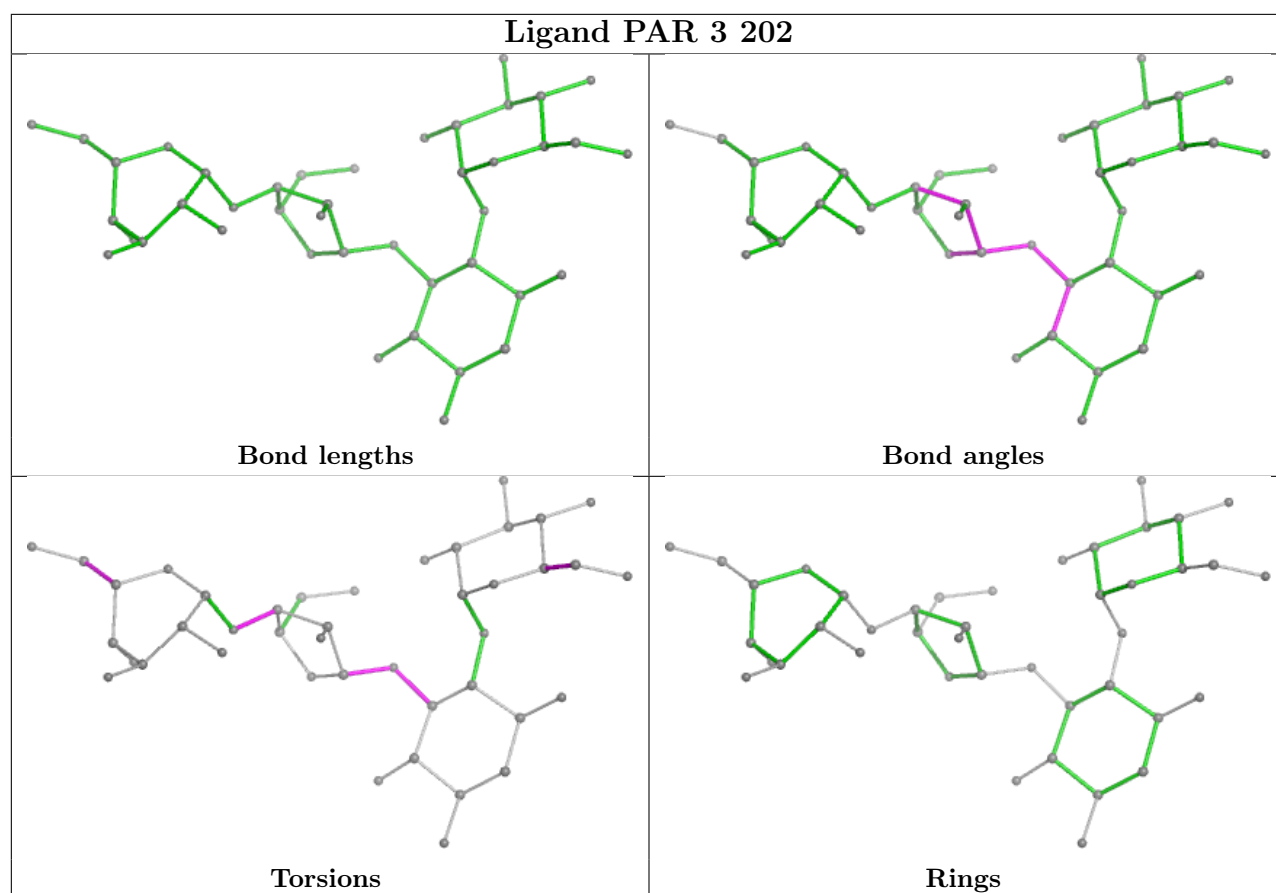




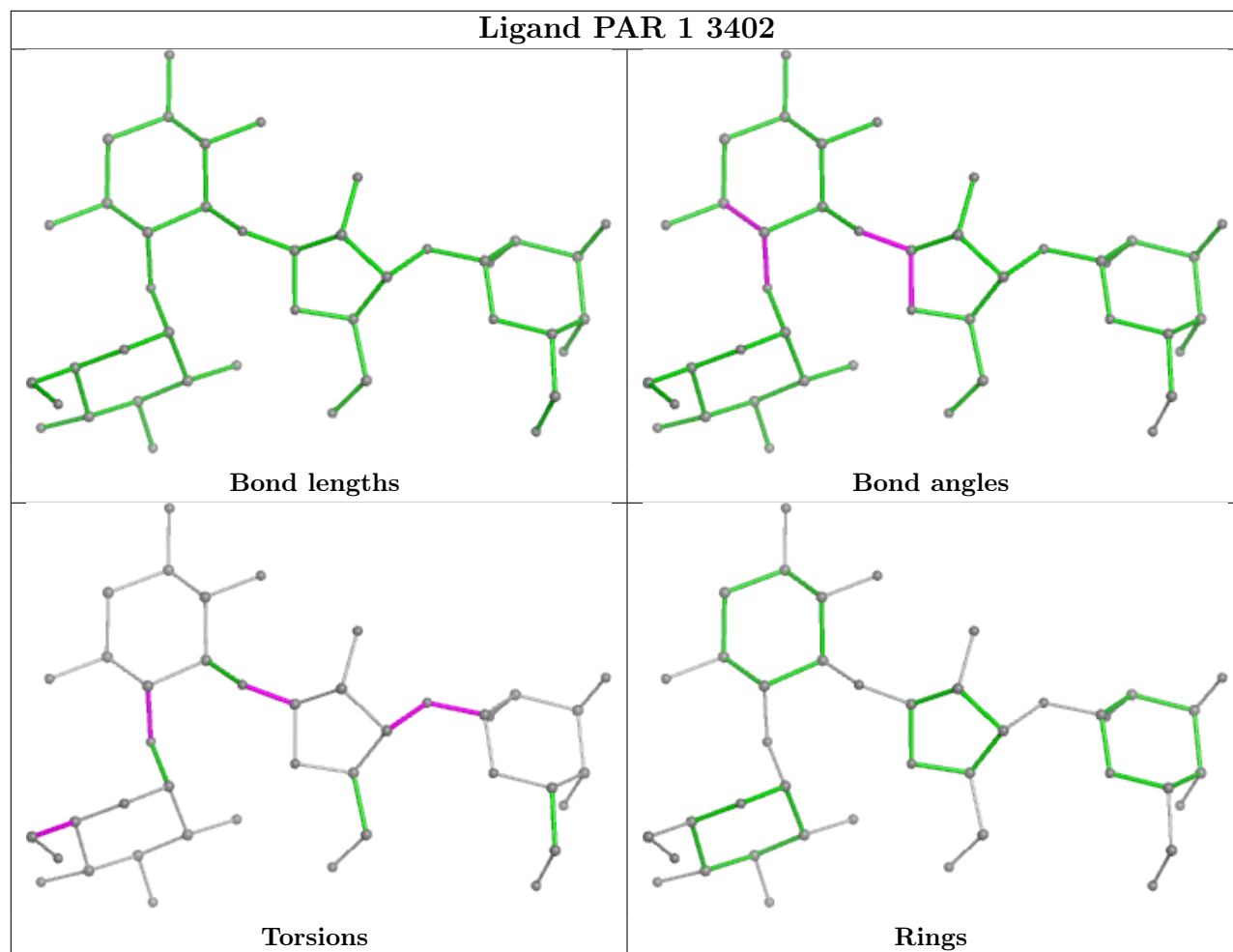
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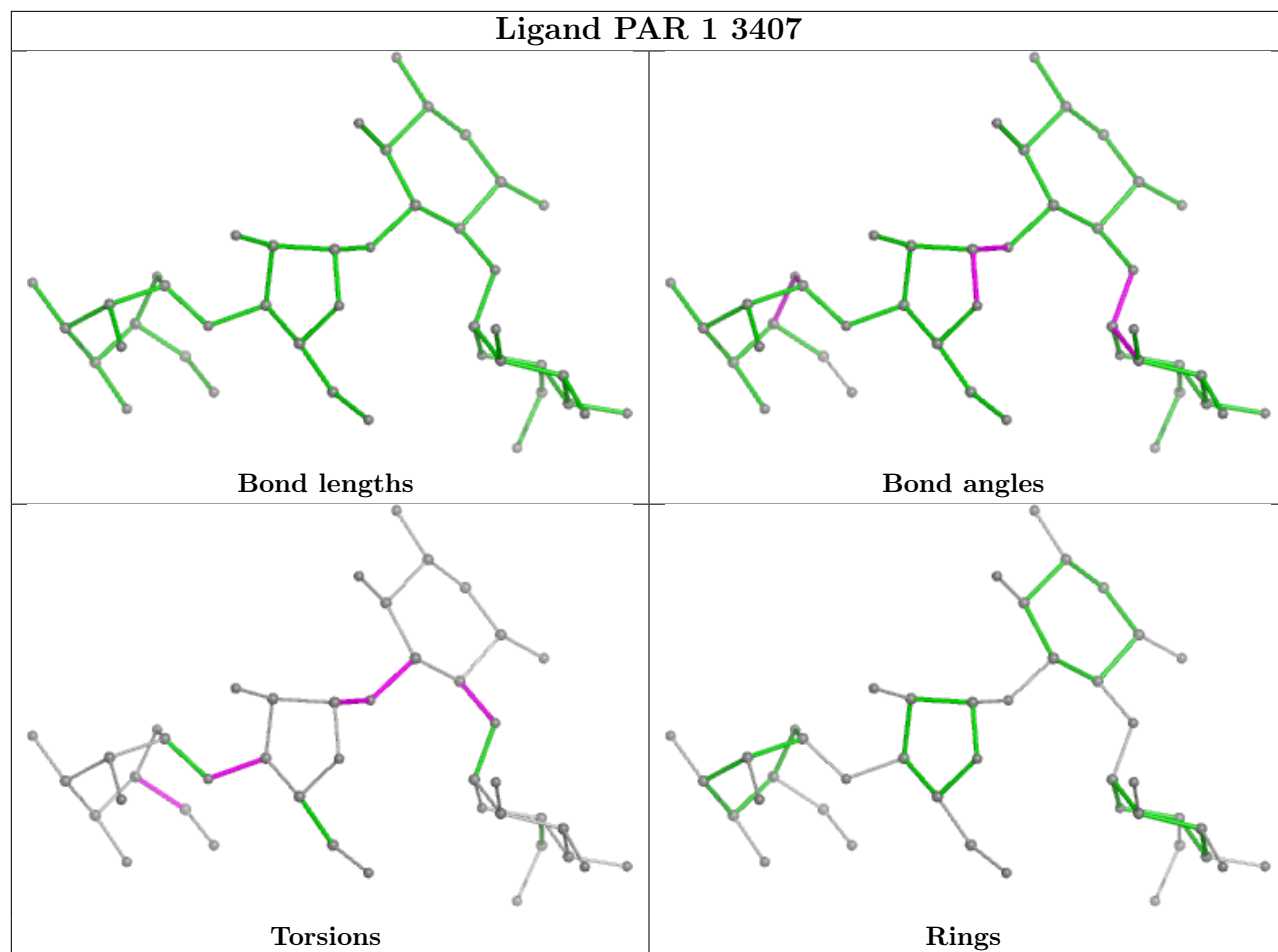




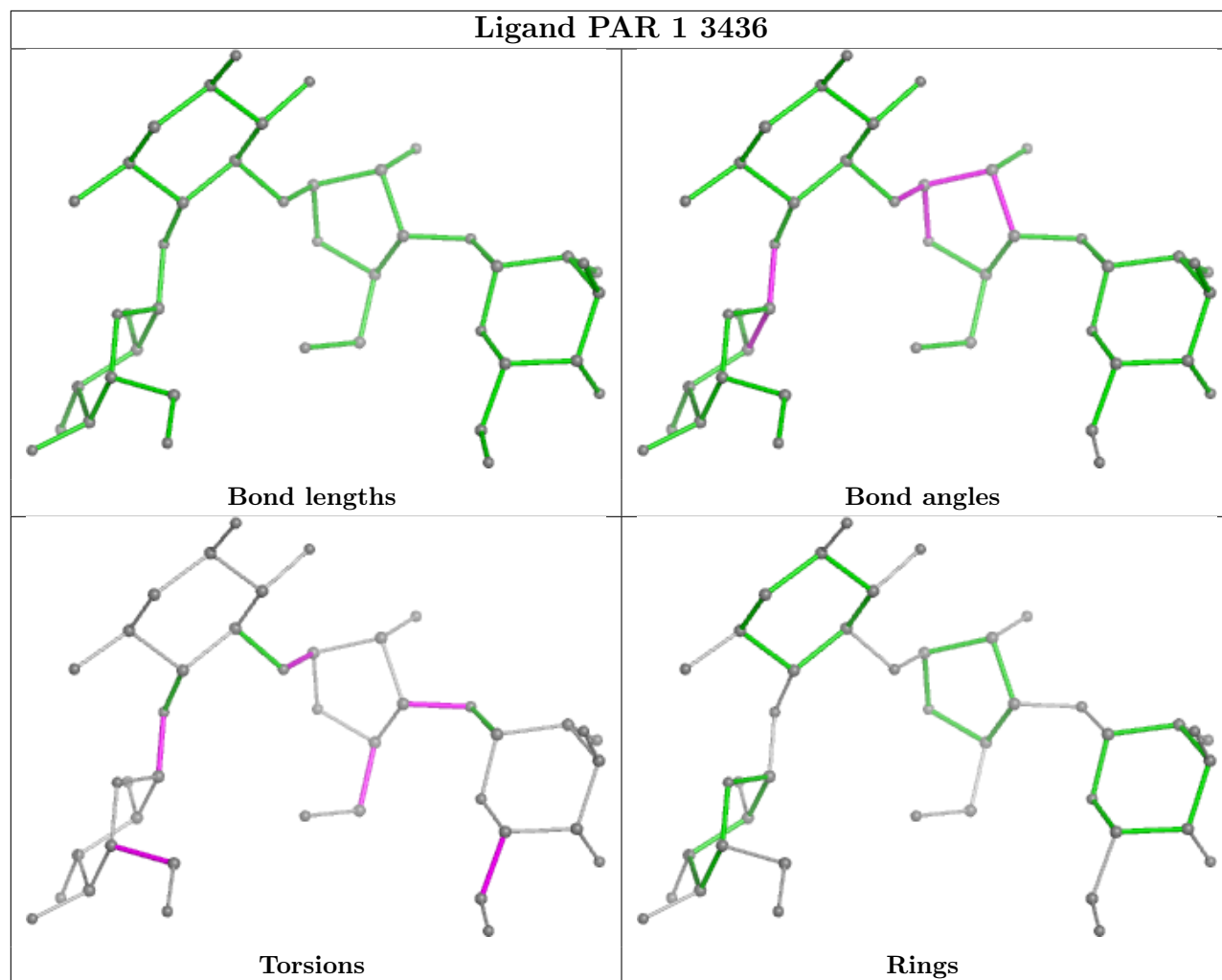


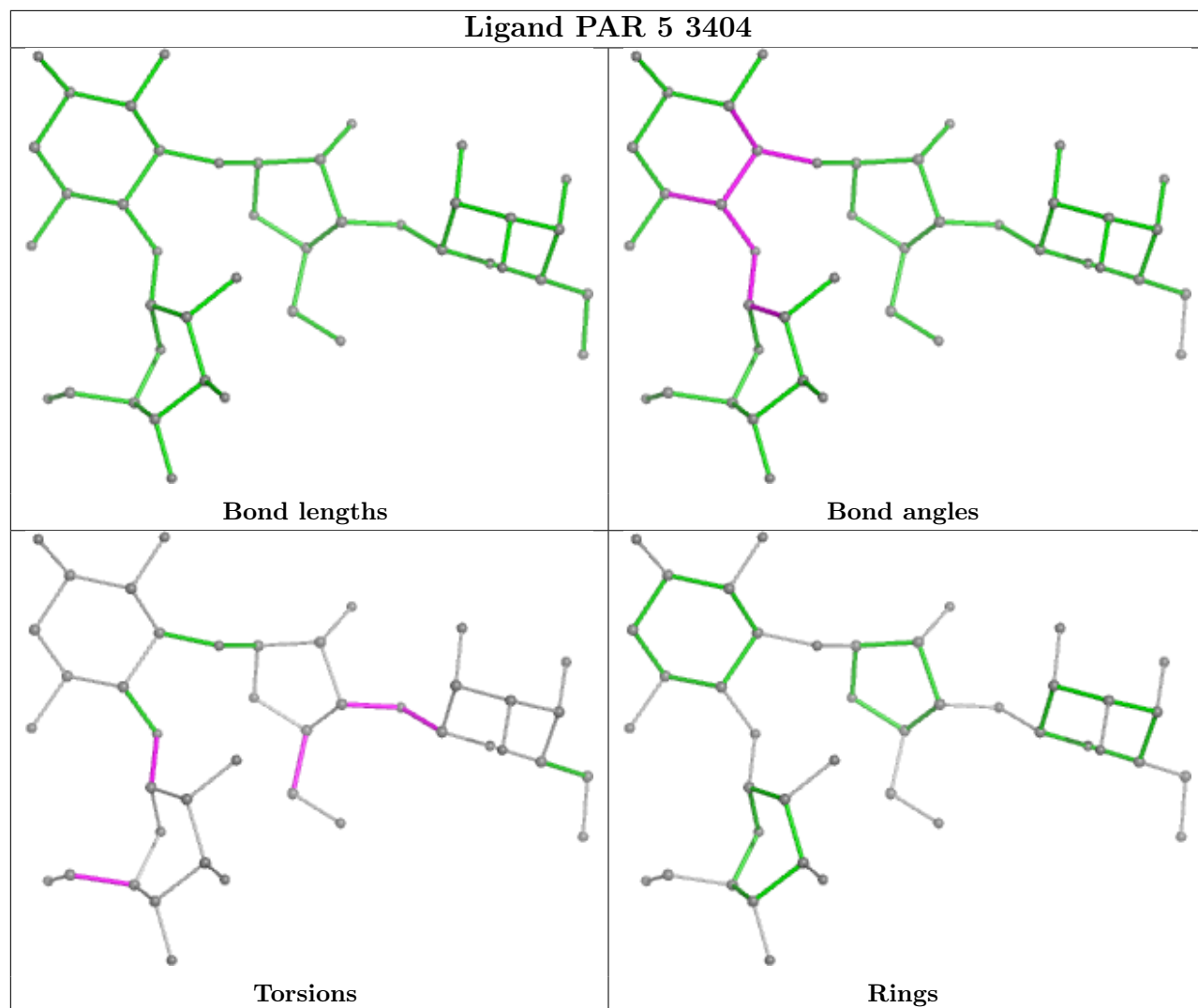
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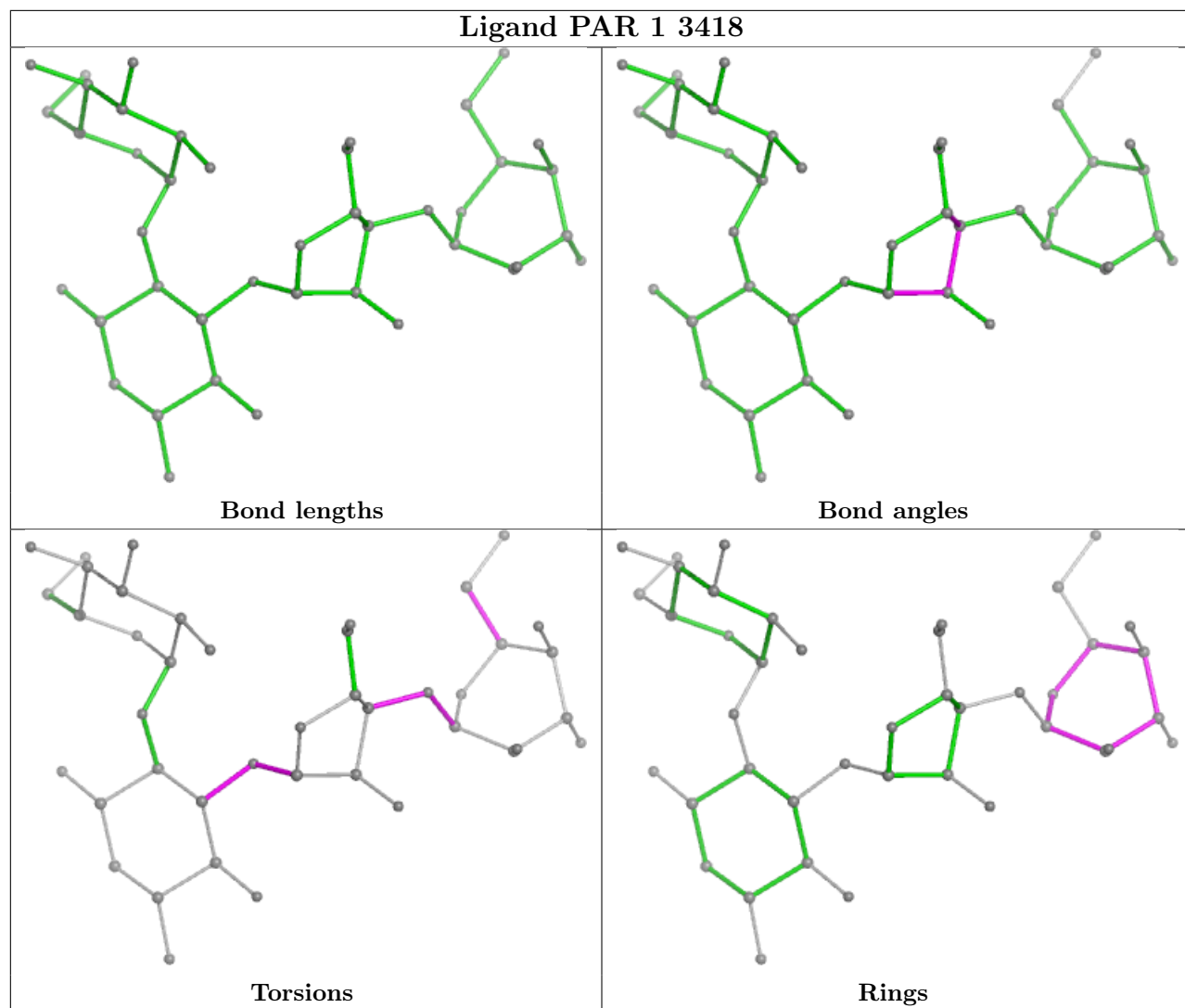


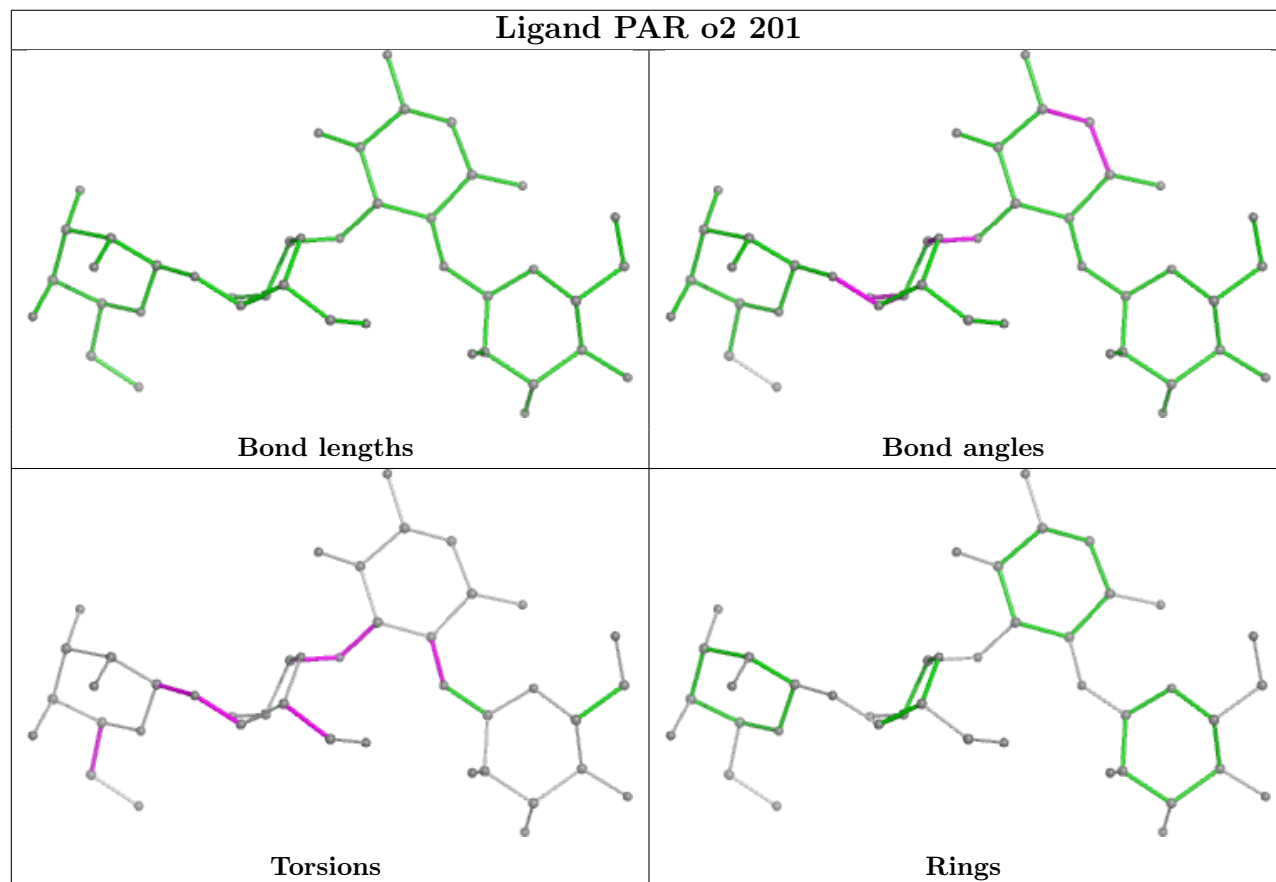
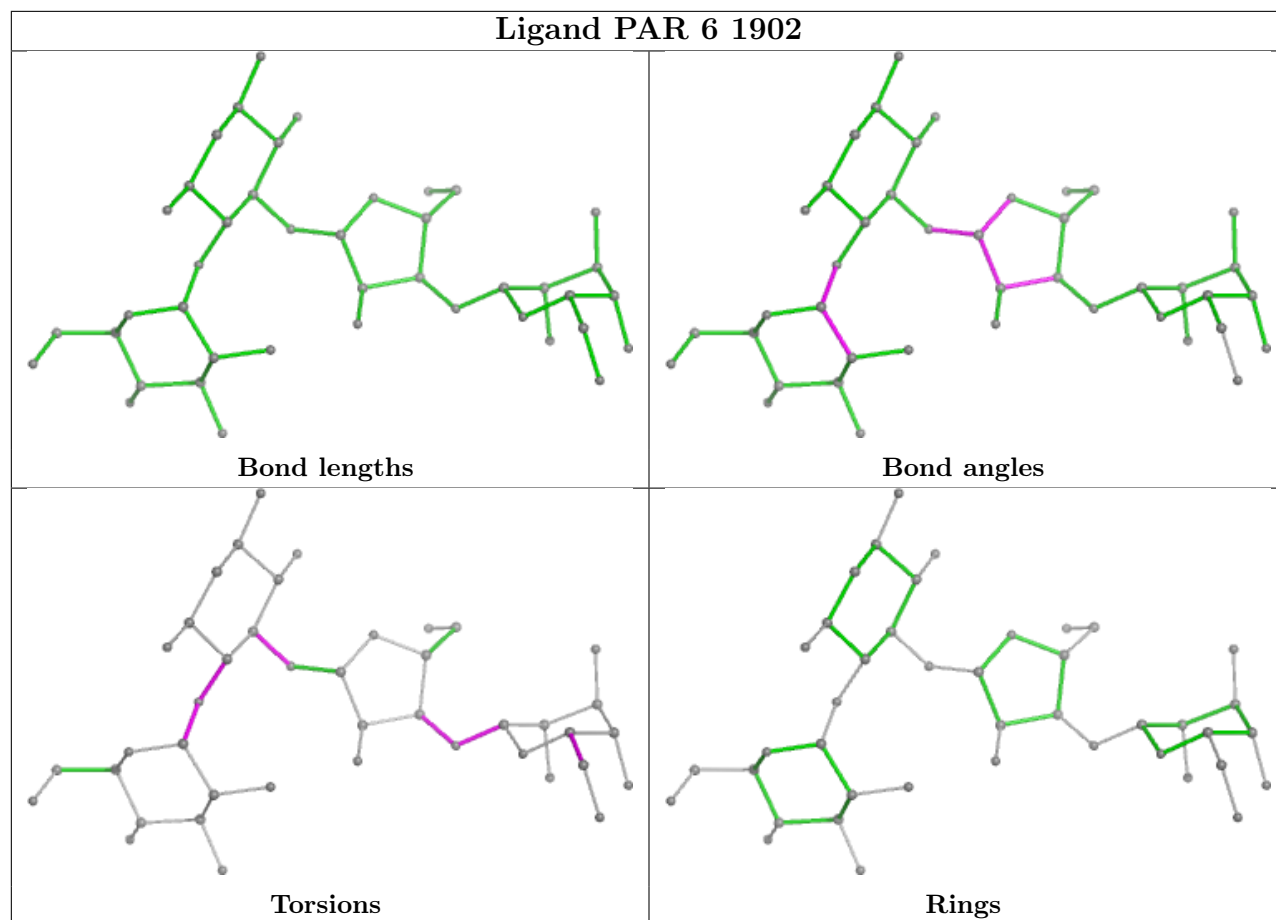
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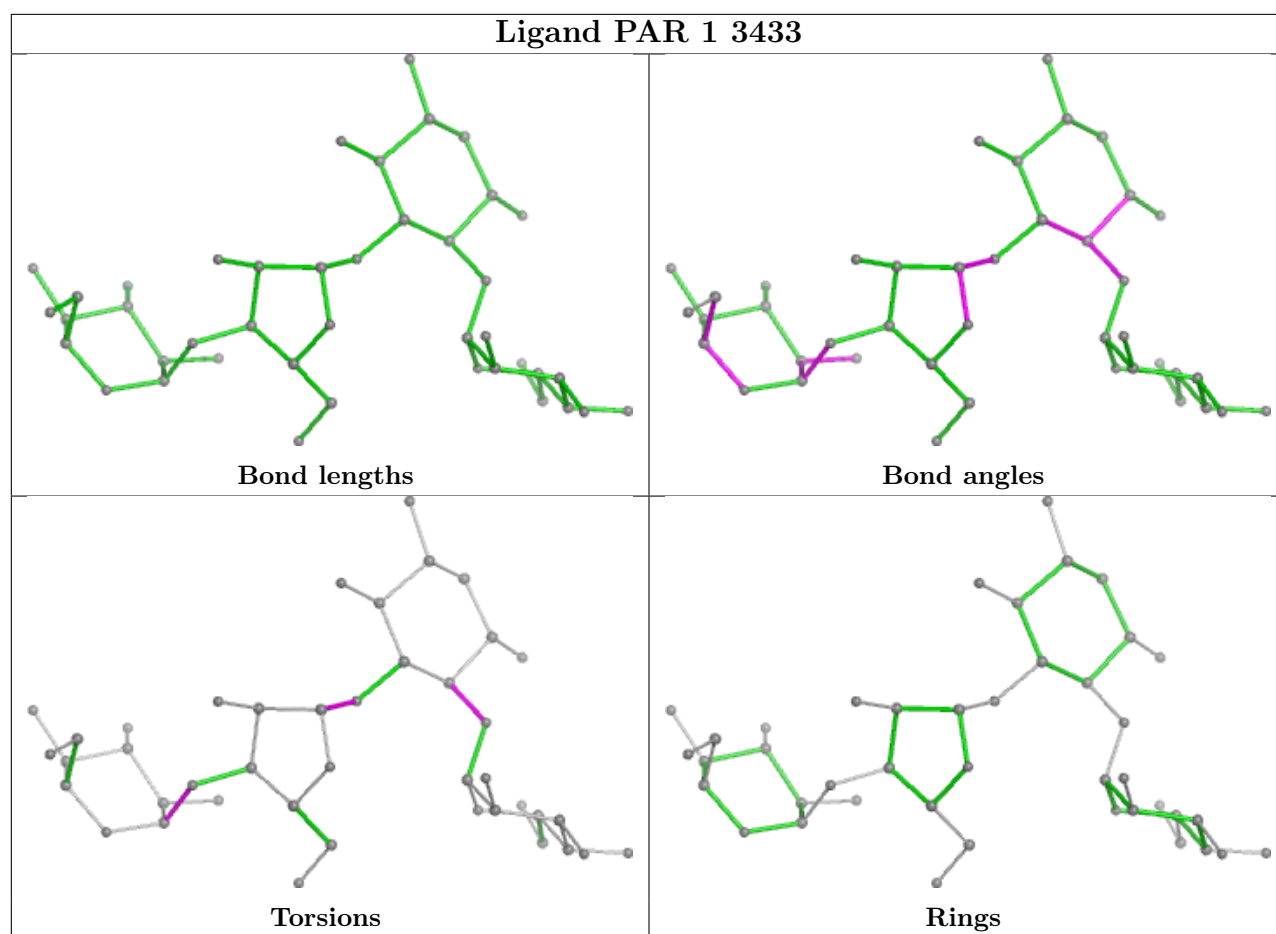


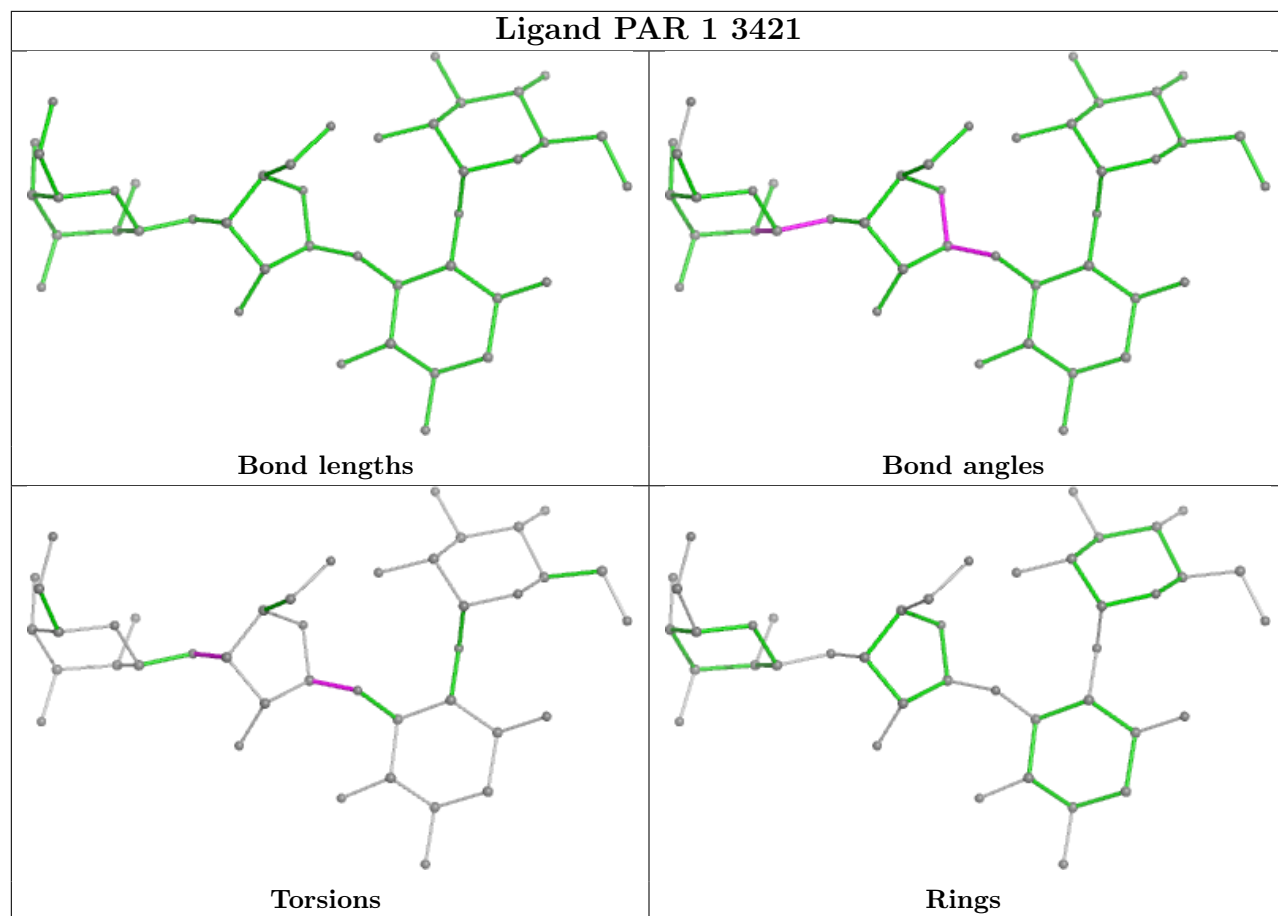


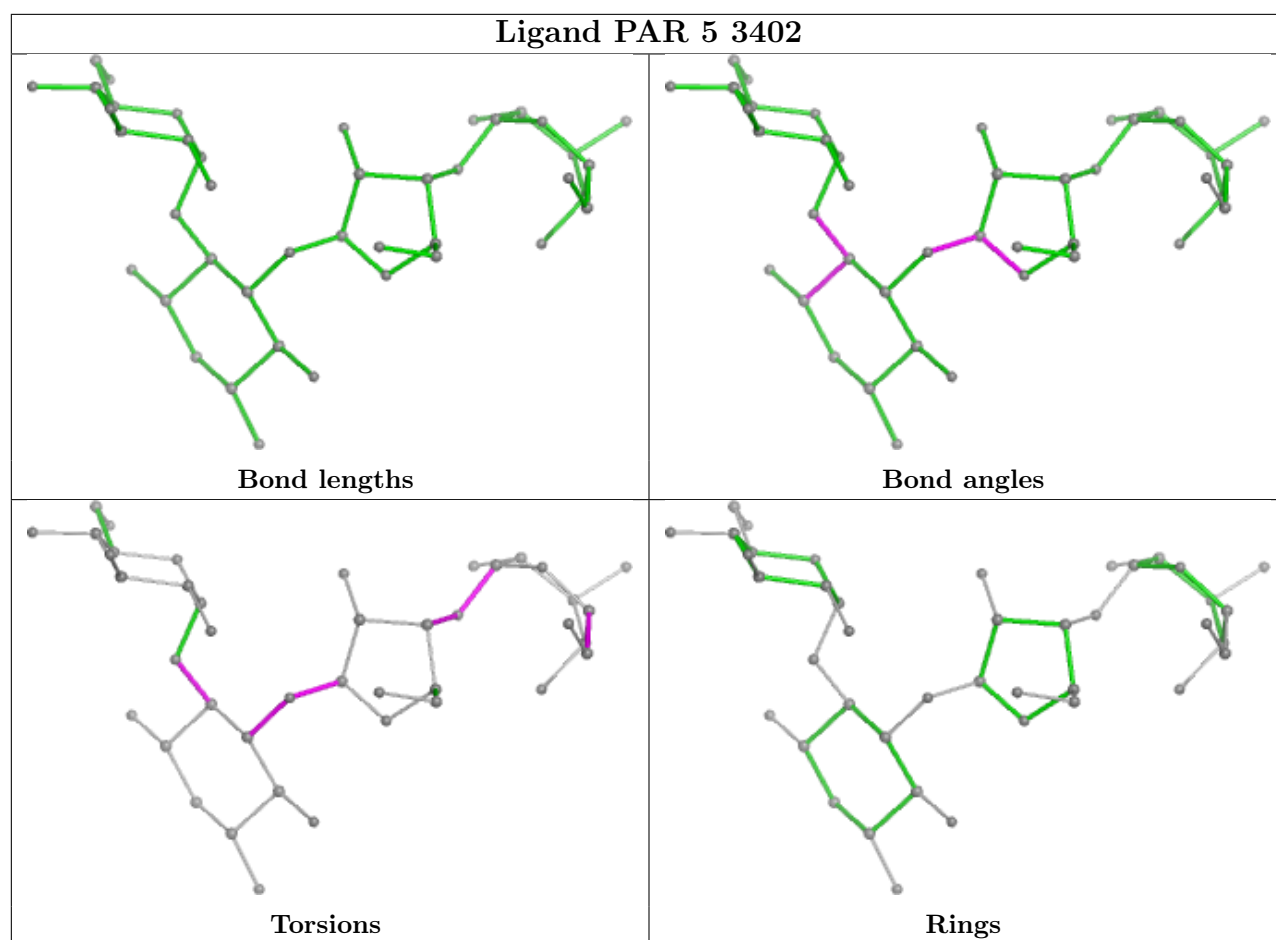


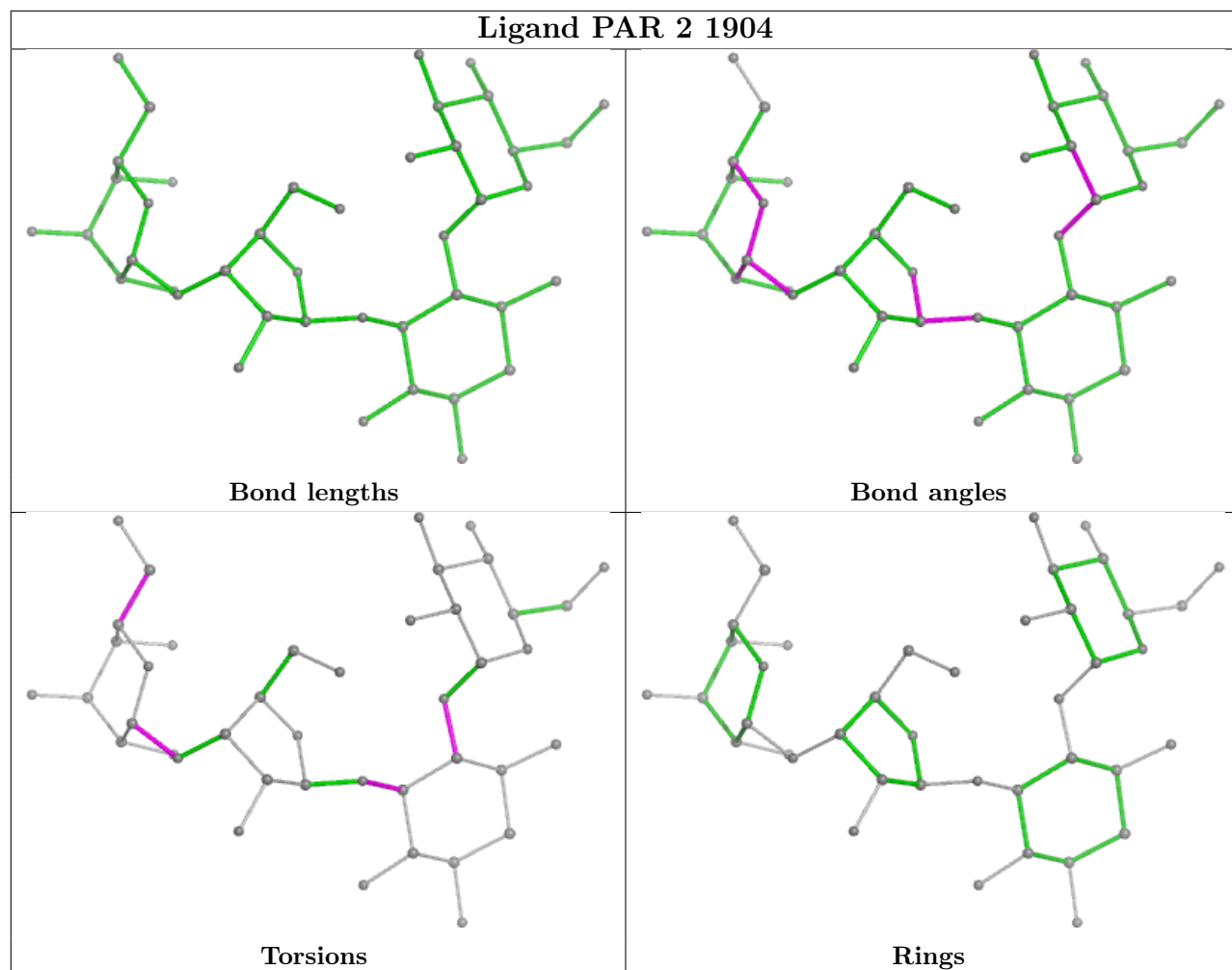


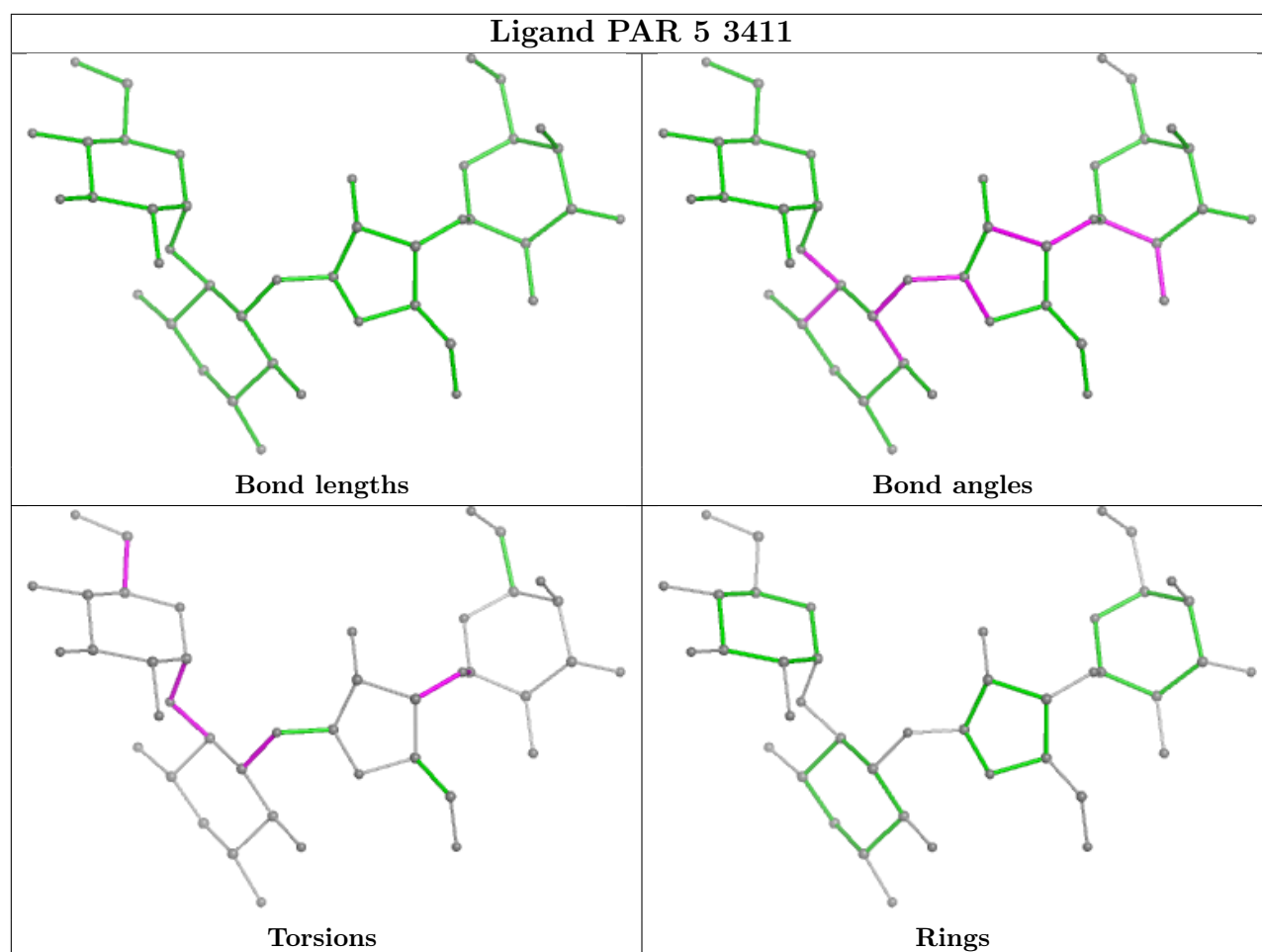


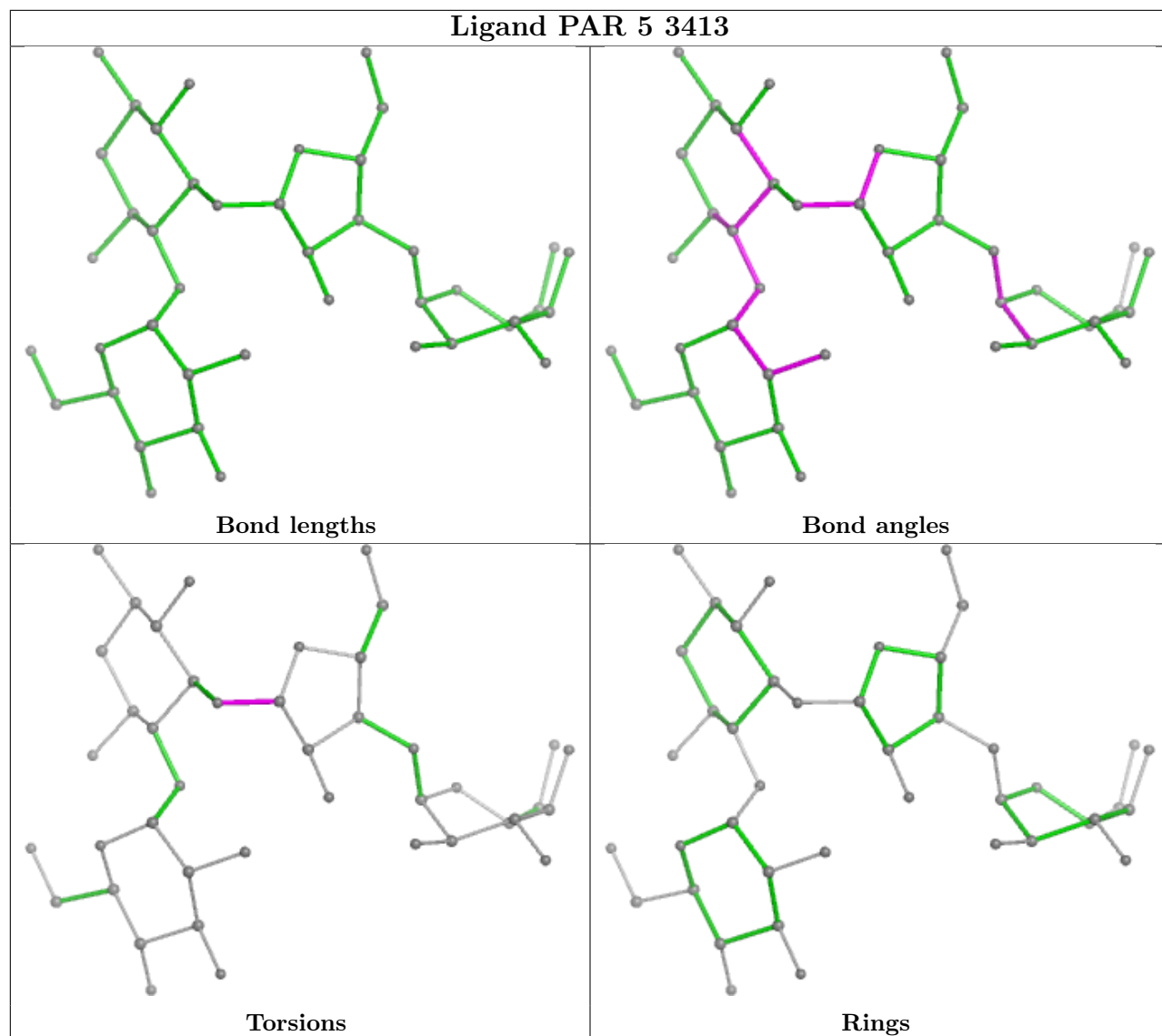




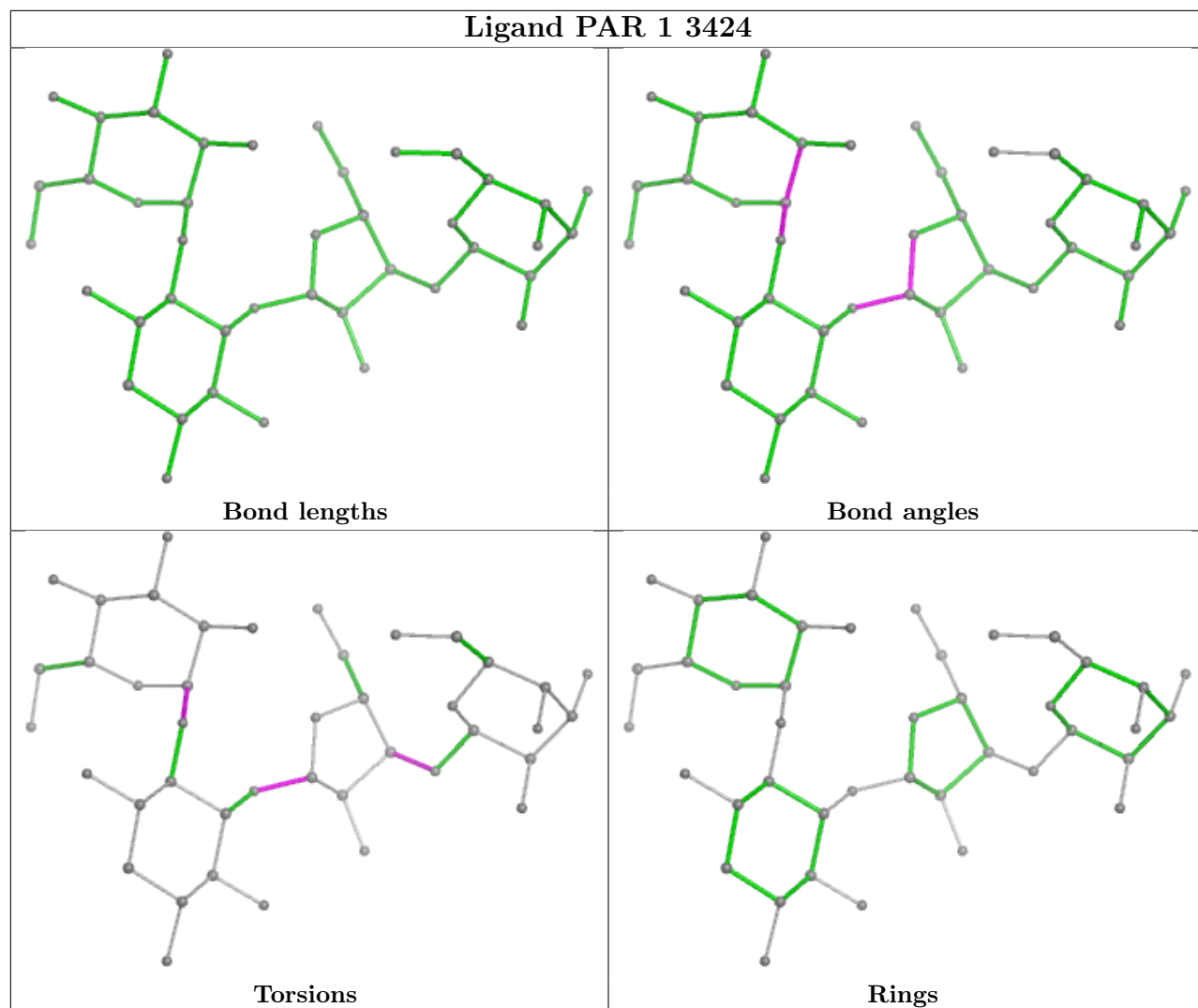


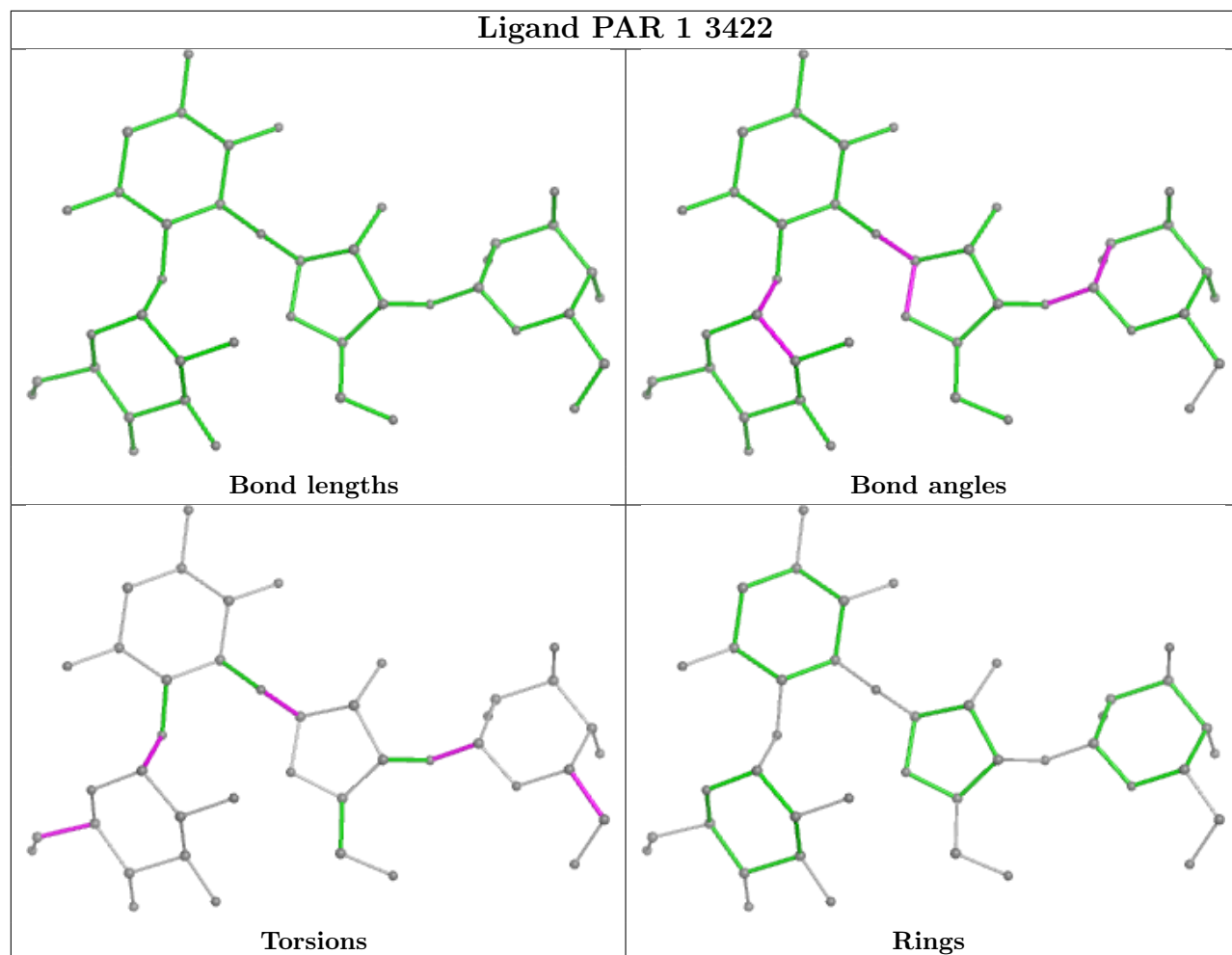


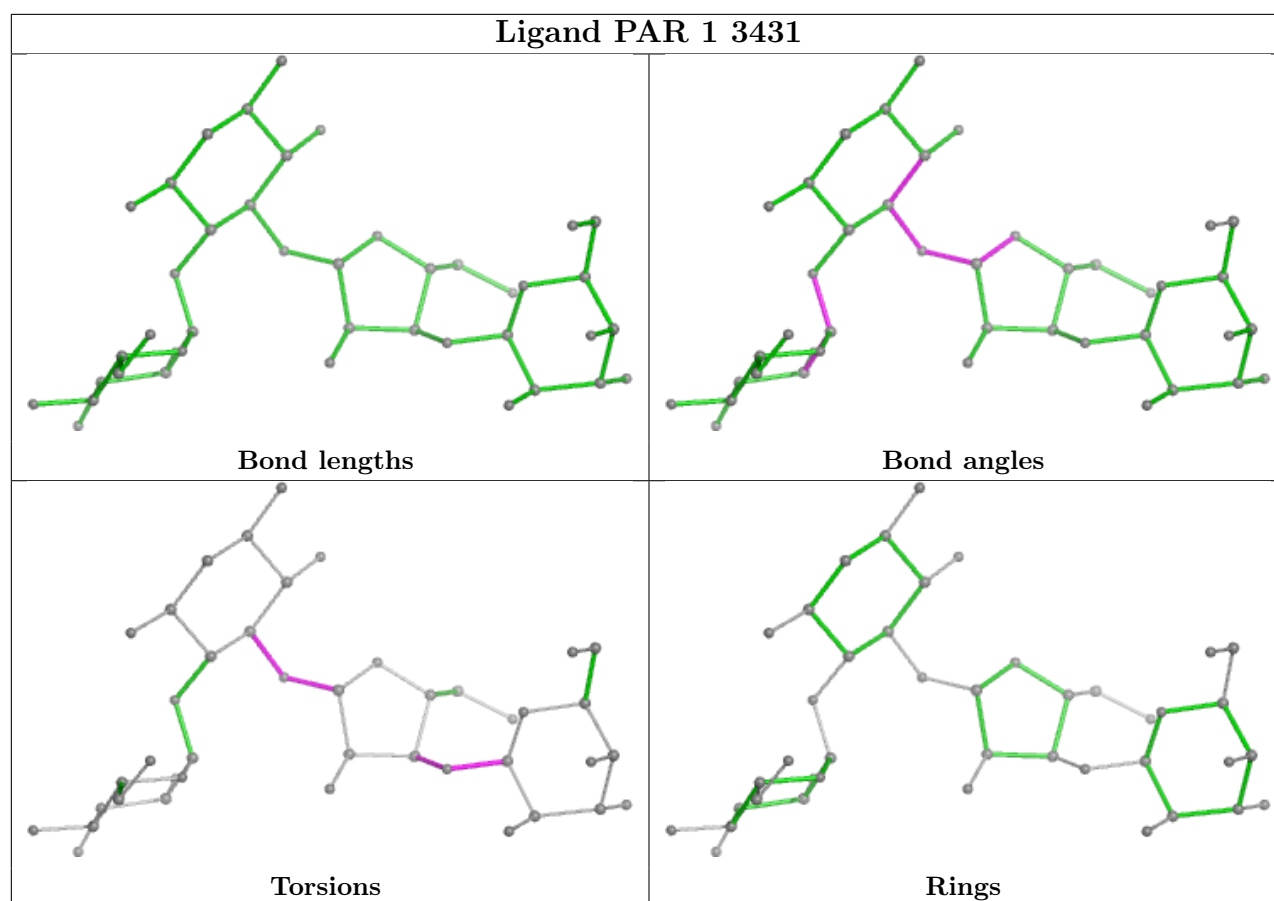












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
78	sM	1
64	C8	1
5	l3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	51:ARG	C	52:PRO	N	1.62
1	C8	81:ILE	C	82:PRO	N	1.16
1	l3	168:LYS	C	169:THR	N	1.16

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	3078/3396 (90%)	0.18	9 (0%) 94 94	29, 61, 151, 275	0
1	5	3087/3396 (90%)	0.20	17 (0%) 89 90	36, 77, 179, 287	0
2	3	121/121 (100%)	0.00	0 100 100	49, 98, 117, 142	0
2	7	121/121 (100%)	-0.12	0 100 100	50, 115, 151, 169	0
3	4	157/158 (99%)	0.19	1 (0%) 89 90	36, 58, 138, 255	0
3	8	158/158 (100%)	0.17	2 (1%) 77 77	48, 90, 161, 264	0
4	L2	248/248 (100%)	0.33	2 (0%) 86 86	22, 47, 66, 101	0
4	l2	248/248 (100%)	0.76	20 (8%) 12 11	49, 86, 120, 160	0
5	L3	386/386 (100%)	0.18	0 100 100	28, 69, 100, 156	0
5	l3	386/386 (100%)	0.02	1 (0%) 94 94	26, 64, 92, 160	0
6	L4	361/361 (100%)	0.12	0 100 100	23, 65, 101, 156	0
6	l4	361/361 (100%)	0.21	5 (1%) 75 75	32, 84, 121, 155	0
7	L5	293/296 (98%)	0.75	26 (8%) 9 10	72, 111, 149, 179	0
7	l5	294/296 (99%)	0.89	38 (12%) 3 3	81, 139, 182, 214	0
8	L6	156/176 (88%)	0.05	1 (0%) 89 90	47, 76, 109, 146	0
8	l6	157/176 (89%)	0.35	5 (3%) 47 46	55, 81, 127, 162	0
9	L7	226/226 (100%)	0.07	0 100 100	37, 63, 117, 200	0
9	l7	223/226 (98%)	0.11	0 100 100	43, 70, 123, 195	0
10	L8	231/231 (100%)	0.60	5 (2%) 62 60	48, 83, 139, 171	0
10	l8	231/231 (100%)	0.92	41 (17%) 1 1	93, 143, 197, 244	0
11	L9	189/191 (98%)	0.80	19 (10%) 7 6	56, 87, 120, 156	0
11	l9	191/191 (100%)	0.38	3 (1%) 72 70	52, 77, 100, 189	0
12	M0	217/221 (98%)	0.67	19 (8%) 10 10	47, 83, 141, 196	0
12	m0	219/221 (99%)	0.67	14 (6%) 19 19	49, 76, 148, 220	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M1	169/169 (100%)	1.02	29 (17%) 1 1	86, 113, 147, 170	0
13	m1	169/169 (100%)	1.01	28 (16%) 1 2	101, 142, 176, 196	0
14	M3	193/194 (99%)	0.38	7 (3%) 42 40	33, 75, 134, 214	0
14	m3	194/194 (100%)	0.44	8 (4%) 37 35	60, 120, 172, 211	0
15	M4	136/137 (99%)	0.33	4 (2%) 51 50	52, 78, 107, 152	0
15	m4	137/137 (100%)	0.14	1 (0%) 87 88	51, 77, 124, 152	0
16	M5	203/203 (100%)	0.37	3 (1%) 73 72	26, 50, 67, 80	0
16	m5	203/203 (100%)	0.85	14 (6%) 16 16	62, 96, 123, 139	0
17	M6	197/197 (100%)	0.33	1 (0%) 91 91	36, 57, 97, 118	0
17	m6	197/197 (100%)	-0.01	0 100 100	35, 54, 107, 138	0
18	M7	175/184 (95%)	0.43	12 (6%) 16 16	30, 52, 139, 184	0
18	m7	155/184 (84%)	0.12	0 100 100	39, 55, 86, 143	0
19	M8	185/185 (100%)	0.26	2 (1%) 80 81	43, 65, 91, 111	0
19	m8	185/185 (100%)	0.48	10 (5%) 25 24	53, 93, 121, 143	0
20	M9	185/188 (98%)	0.26	0 100 100	45, 72, 158, 198	0
20	m9	188/188 (100%)	0.54	15 (7%) 12 11	50, 83, 212, 255	0
21	N0	172/172 (100%)	0.68	7 (4%) 37 35	51, 72, 105, 144	0
21	n0	172/172 (100%)	0.40	0 100 100	45, 71, 101, 139	0
22	N1	159/159 (100%)	0.54	4 (2%) 57 54	45, 74, 130, 198	0
22	n1	159/159 (100%)	1.10	32 (20%) 1 1	62, 90, 155, 204	0
23	N2	99/99 (100%)	0.32	3 (3%) 50 49	77, 110, 147, 168	0
23	n2	98/99 (98%)	0.76	8 (8%) 11 11	85, 120, 146, 169	0
24	N3	132/136 (97%)	0.20	0 100 100	38, 66, 93, 155	0
24	n3	136/136 (100%)	0.28	2 (1%) 73 72	33, 58, 98, 150	0
25	N4	63/155 (40%)	0.55	1 (1%) 72 70	52, 74, 98, 121	0
25	n4	135/155 (87%)	1.53	44 (32%) 0 0	44, 140, 224, 256	0
26	N5	118/120 (98%)	0.40	1 (0%) 86 86	42, 62, 91, 116	0
26	n5	120/120 (100%)	1.01	16 (13%) 3 3	59, 95, 135, 176	0
27	N6	125/125 (100%)	0.73	12 (9%) 8 8	34, 71, 101, 131	0
27	n6	123/125 (98%)	0.50	7 (5%) 23 23	55, 85, 123, 139	0
28	N7	135/135 (100%)	0.82	9 (6%) 17 17	57, 84, 115, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	n7	135/135 (100%)	1.80	50 (37%) 0 0	99, 132, 175, 194	0
29	N8	148/148 (100%)	0.64	12 (8%) 12 11	27, 63, 117, 156	0
29	n8	148/148 (100%)	0.83	21 (14%) 2 2	34, 104, 145, 167	0
30	N9	56/58 (96%)	0.57	3 (5%) 25 24	34, 80, 137, 171	0
30	n9	58/58 (100%)	0.75	6 (10%) 6 6	53, 112, 157, 189	0
31	O0	97/100 (97%)	0.70	3 (3%) 49 48	51, 76, 110, 145	0
31	o0	100/100 (100%)	0.16	3 (3%) 50 49	82, 117, 167, 201	0
32	O1	106/112 (94%)	1.14	16 (15%) 2 2	50, 77, 130, 149	0
32	o1	109/112 (97%)	0.53	2 (1%) 68 67	43, 75, 137, 178	0
33	O2	125/127 (98%)	0.23	1 (0%) 86 86	29, 55, 78, 114	0
33	o2	127/127 (100%)	0.32	3 (2%) 59 56	35, 65, 92, 147	0
34	O3	106/106 (100%)	0.18	1 (0%) 84 84	37, 55, 95, 133	0
34	o3	106/106 (100%)	0.31	2 (1%) 66 65	37, 59, 106, 127	0
35	O4	112/112 (100%)	0.66	5 (4%) 33 32	41, 61, 123, 175	0
35	o4	112/112 (100%)	0.97	16 (14%) 2 2	60, 96, 167, 193	0
36	O5	119/119 (100%)	0.41	2 (1%) 70 68	42, 75, 107, 130	0
36	o5	119/119 (100%)	0.81	15 (12%) 3 3	78, 108, 138, 167	0
37	O6	97/99 (97%)	0.26	0 100 100	51, 75, 108, 125	0
37	o6	99/99 (100%)	1.37	25 (25%) 0 0	95, 131, 170, 205	0
38	O7	84/87 (96%)	0.10	0 100 100	29, 43, 76, 102	0
38	o7	87/87 (100%)	0.54	4 (4%) 32 30	37, 71, 122, 180	0
39	O8	77/77 (100%)	0.55	5 (6%) 18 18	63, 94, 148, 185	0
39	o8	77/77 (100%)	1.09	12 (15%) 2 2	87, 121, 154, 182	0
40	O9	50/50 (100%)	0.41	0 100 100	37, 54, 77, 83	0
40	o9	50/50 (100%)	0.40	2 (4%) 38 36	57, 72, 95, 108	0
41	Q0	52/52 (100%)	1.14	8 (15%) 2 2	57, 76, 122, 133	0
41	q0	52/52 (100%)	0.46	2 (3%) 40 37	48, 62, 91, 122	0
42	Q1	25/25 (100%)	0.30	0 100 100	52, 66, 82, 94	0
42	q1	25/25 (100%)	0.19	0 100 100	61, 74, 90, 92	0
43	Q2	105/105 (100%)	0.90	17 (16%) 1 2	31, 66, 119, 192	0
43	q2	105/105 (100%)	0.73	9 (8%) 10 10	59, 102, 140, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
44	Q3	91/91 (100%)	0.09	0	100	100	33, 53, 85, 98	0
44	q3	91/91 (100%)	0.14	0	100	100	44, 83, 118, 135	0
45	2	1712/1800 (95%)	0.24	27 (1%)	72	70	55, 120, 223, 318	0
45	6	1683/1800 (93%)	0.20	23 (1%)	75	75	57, 119, 222, 300	0
46	S0	206/206 (100%)	1.14	44 (21%)	0	1	92, 133, 170, 223	0
46	s0	206/206 (100%)	1.00	35 (16%)	1	1	98, 140, 187, 229	0
47	S1	211/216 (97%)	1.47	64 (30%)	0	0	89, 142, 196, 244	0
47	s1	216/216 (100%)	1.55	65 (30%)	0	0	94, 145, 190, 236	0
48	S2	217/217 (100%)	0.72	25 (11%)	4	4	76, 119, 159, 170	0
48	s2	217/217 (100%)	1.31	53 (24%)	0	0	74, 120, 156, 179	0
49	S3	209/223 (93%)	1.00	34 (16%)	1	2	87, 131, 176, 214	0
49	s3	223/223 (100%)	1.67	75 (33%)	0	0	97, 140, 196, 224	0
50	S4	256/260 (98%)	1.67	89 (34%)	0	0	92, 137, 169, 240	0
50	s4	260/260 (100%)	0.99	38 (14%)	2	2	80, 125, 157, 209	0
51	S5	206/206 (100%)	2.79	127 (61%)	0	0	107, 158, 207, 239	0
51	s5	206/206 (100%)	1.56	66 (32%)	0	0	108, 156, 202, 234	0
52	S6	200/236 (84%)	1.03	42 (21%)	1	1	77, 138, 206, 301	0
53	S7	179/186 (96%)	0.86	27 (15%)	2	2	97, 147, 192, 216	0
53	s7	186/186 (100%)	1.00	34 (18%)	1	1	101, 162, 213, 267	0
54	S8	185/200 (92%)	1.03	28 (15%)	2	2	63, 106, 162, 218	0
54	s8	188/200 (94%)	0.85	20 (10%)	6	6	65, 104, 156, 206	0
55	S9	174/185 (94%)	1.31	38 (21%)	0	1	98, 145, 187, 217	0
55	s9	185/185 (100%)	1.23	45 (24%)	0	0	93, 130, 177, 209	0
56	C0	90/105 (85%)	0.64	10 (11%)	5	5	120, 153, 193, 210	0
56	c0	96/105 (91%)	1.33	31 (32%)	0	0	119, 171, 207, 261	0
57	C1	139/146 (95%)	1.01	14 (10%)	7	6	68, 98, 146, 171	0
57	c1	146/146 (100%)	0.88	17 (11%)	4	4	70, 96, 165, 231	0
58	C2	102/143 (71%)	1.90	33 (32%)	0	0	147, 210, 256, 296	0
58	c2	124/143 (86%)	1.85	54 (43%)	0	0	170, 230, 275, 291	0
59	C3	150/150 (100%)	0.77	16 (10%)	6	5	65, 107, 140, 180	0
59	c3	150/150 (100%)	0.32	9 (6%)	21	21	78, 127, 170, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
60	C4	127/128 (99%)	0.34	7 (5%)	25	23	71, 133, 184, 207	0
60	c4	128/128 (100%)	1.19	31 (24%)	0	0	77, 138, 177, 239	0
61	C5	116/141 (82%)	1.15	24 (20%)	1	1	97, 149, 199, 225	0
61	c5	135/141 (95%)	2.29	65 (48%)	0	0	111, 152, 206, 244	0
62	C6	136/142 (95%)	2.90	92 (67%)	0	0	88, 160, 201, 253	0
62	c6	142/142 (100%)	2.64	88 (61%)	0	0	98, 160, 210, 264	0
63	C7	115/136 (84%)	1.68	41 (35%)	0	0	109, 149, 191, 223	0
63	c7	117/136 (86%)	1.02	18 (15%)	2	2	104, 152, 200, 226	0
64	C8	143/145 (98%)	1.40	39 (27%)	0	0	104, 163, 211, 244	0
64	c8	145/145 (100%)	1.48	47 (32%)	0	0	103, 149, 196, 217	0
65	C9	137/143 (95%)	1.76	47 (34%)	0	0	104, 168, 206, 231	0
65	c9	143/143 (100%)	1.48	41 (28%)	0	0	117, 170, 215, 240	0
66	D0	102/109 (93%)	1.57	35 (34%)	0	0	92, 163, 218, 276	0
66	d0	109/109 (100%)	1.20	26 (23%)	0	0	91, 159, 218, 265	0
67	D1	87/87 (100%)	0.99	16 (18%)	1	1	101, 130, 167, 213	0
67	d1	87/87 (100%)	0.88	12 (13%)	2	2	101, 131, 176, 206	0
68	D2	129/129 (100%)	1.47	42 (32%)	0	0	73, 110, 134, 165	0
68	d2	129/129 (100%)	0.92	18 (13%)	2	2	85, 111, 133, 175	0
69	D3	144/144 (100%)	0.52	1 (0%)	87	88	63, 86, 109, 154	0
69	d3	144/144 (100%)	0.53	7 (4%)	29	27	61, 86, 107, 141	0
70	D4	134/134 (100%)	1.06	29 (21%)	0	1	106, 155, 191, 221	0
70	d4	134/134 (100%)	1.05	23 (17%)	1	1	100, 140, 175, 195	0
71	D5	70/70 (100%)	2.78	43 (61%)	0	0	137, 193, 229, 237	0
71	d5	69/70 (98%)	1.95	30 (43%)	0	0	131, 174, 211, 238	0
72	D6	97/97 (100%)	0.48	3 (3%)	49	48	67, 105, 176, 218	0
72	d6	97/97 (100%)	1.05	13 (13%)	3	3	79, 111, 173, 203	0
73	D7	81/81 (100%)	1.08	14 (17%)	1	1	84, 127, 181, 205	0
73	d7	81/81 (100%)	0.69	12 (14%)	2	2	96, 147, 202, 227	0
74	D8	63/63 (100%)	1.76	25 (39%)	0	0	114, 146, 173, 198	0
74	d8	63/63 (100%)	2.64	36 (57%)	0	0	110, 163, 192, 218	0
75	D9	53/53 (100%)	1.41	16 (30%)	0	0	101, 121, 151, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	d9	53/53 (100%)	0.68	6 (11%) 5 5	106, 127, 150, 180	0
76	E0	60/62 (96%)	1.47	18 (30%) 0 0	76, 140, 183, 197	0
76	e0	62/62 (100%)	1.52	15 (24%) 0 0	74, 133, 181, 208	0
77	SR	317/318 (99%)	2.50	184 (58%) 0 0	137, 198, 248, 295	0
77	sR	318/318 (100%)	2.42	171 (53%) 0 0	136, 194, 243, 296	0
78	SM	147/272 (54%)	1.18	30 (20%) 1 1	74, 137, 205, 240	0
78	sM	95/272 (34%)	1.29	24 (25%) 0 0	99, 146, 191, 217	0
79	s6	218/218 (100%)	1.82	84 (38%) 0 0	75, 136, 176, 211	0
All	All	32255/33922 (95%)	0.67	3409 (10%) 6 6	22, 100, 194, 318	0

The worst 5 of 3409 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
76	e0	63	GLN	14.3
51	S5	152	GLY	13.9
51	S5	71	ALA	13.9
51	S5	151	GLY	12.3
51	S5	70	VAL	11.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
81	MG	5	3796	1/1	-0.24	0.33	165,165,165,165	0
81	MG	8	220	1/1	0.09	0.42	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	2059	1/1	0.13	0.58	114,114,114,114	0
81	MG	5	3878	1/1	0.18	0.62	118,118,118,118	0
81	MG	2	1947	1/1	0.18	0.27	110,110,110,110	0
81	MG	5	4057	1/1	0.19	0.62	117,117,117,117	0
81	MG	1	4093	1/1	0.23	0.32	86,86,86,86	0
81	MG	1	4118	1/1	0.26	0.45	88,88,88,88	0
81	MG	2	2084	1/1	0.26	0.35	105,105,105,105	0
81	MG	1	3968	1/1	0.27	0.18	81,81,81,81	0
81	MG	1	3853	1/1	0.27	0.28	62,62,62,62	0
81	MG	5	3944	1/1	0.31	0.26	118,118,118,118	0
81	MG	5	3839	1/1	0.36	1.23	88,88,88,88	0
81	MG	2	2048	1/1	0.38	0.83	84,84,84,84	0
81	MG	5	3983	1/1	0.39	0.46	92,92,92,92	0
81	MG	6	2009	1/1	0.39	0.17	126,126,126,126	0
81	MG	5	3942	1/1	0.40	0.29	108,108,108,108	0
81	MG	1	4155	1/1	0.40	0.76	40,40,40,40	1
81	MG	m5	302	1/1	0.40	0.39	82,82,82,82	0
81	MG	1	4043	1/1	0.40	0.17	91,91,91,91	0
81	MG	5	4090	1/1	0.42	0.76	85,85,85,85	0
81	MG	8	213	1/1	0.43	0.38	67,67,67,67	0
81	MG	1	4036	1/1	0.43	0.34	80,80,80,80	0
81	MG	18	301	1/1	0.44	0.39	109,109,109,109	0
81	MG	5	3893	1/1	0.44	0.30	68,68,68,68	0
81	MG	5	3536	1/1	0.44	0.57	51,51,51,51	1
81	MG	1	3998	1/1	0.45	0.50	86,86,86,86	0
81	MG	6	1944	1/1	0.45	0.34	95,95,95,95	0
81	MG	5	3966	1/1	0.45	0.62	92,92,92,92	0
81	MG	5	4079	1/1	0.46	0.55	105,105,105,105	0
81	MG	2	2007	1/1	0.46	0.33	67,67,67,67	0
81	MG	1	3903	1/1	0.47	0.50	68,68,68,68	0
81	MG	5	3967	1/1	0.47	0.31	100,100,100,100	0
81	MG	1	3851	1/1	0.47	0.28	86,86,86,86	0
81	MG	3	206	1/1	0.47	0.27	87,87,87,87	0
81	MG	1	4100	1/1	0.48	0.63	94,94,94,94	0
81	MG	6	1943	1/1	0.48	0.29	89,89,89,89	0
81	MG	1	4117	1/1	0.50	0.16	114,114,114,114	0
81	MG	D3	202	1/1	0.51	0.45	79,79,79,79	0
81	MG	1	3507	1/1	0.52	0.23	65,65,65,65	0
81	MG	5	3789	1/1	0.52	0.37	70,70,70,70	0
81	MG	1	4035	1/1	0.52	0.18	98,98,98,98	0
81	MG	1	4114	1/1	0.53	0.38	76,76,76,76	0
81	MG	1	4099	1/1	0.53	0.58	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	4059	1/1	0.53	0.43	98,98,98,98	0
81	MG	1	3857	1/1	0.53	0.30	57,57,57,57	0
81	MG	6	2028	1/1	0.53	0.24	126,126,126,126	0
81	MG	c9	201	1/1	0.53	0.09	115,115,115,115	0
81	MG	1	3502	1/1	0.54	0.22	66,66,66,66	0
81	MG	6	1946	1/1	0.54	0.23	84,84,84,84	0
81	MG	6	1952	1/1	0.54	0.17	103,103,103,103	0
81	MG	5	4091	1/1	0.55	0.55	75,75,75,75	0
81	MG	2	2069	1/1	0.55	0.28	96,96,96,96	0
81	MG	1	3849	1/1	0.55	0.20	56,56,56,56	0
81	MG	6	2063	1/1	0.55	0.37	88,88,88,88	0
81	MG	1	3521	1/1	0.55	0.41	49,49,49,49	1
81	MG	5	4033	1/1	0.56	0.18	88,88,88,88	0
81	MG	5	3685	1/1	0.56	0.64	59,59,59,59	0
81	MG	c1	201	1/1	0.56	0.35	78,78,78,78	0
81	MG	5	4025	1/1	0.56	0.50	71,71,71,71	0
81	MG	1	3924	1/1	0.57	0.56	58,58,58,58	0
81	MG	2	2061	1/1	0.57	0.50	105,105,105,105	0
81	MG	5	3999	1/1	0.57	0.47	71,71,71,71	0
81	MG	8	223	1/1	0.57	0.53	99,99,99,99	0
81	MG	5	4019	1/1	0.57	0.80	86,86,86,86	0
81	MG	5	4085	1/1	0.57	0.42	88,88,88,88	0
81	MG	6	2064	1/1	0.57	0.95	65,65,65,65	0
81	MG	6	1937	1/1	0.57	0.76	72,72,72,72	0
81	MG	5	3914	1/1	0.57	0.34	97,97,97,97	0
81	MG	d3	202	1/1	0.57	0.27	87,87,87,87	0
81	MG	5	3647	1/1	0.58	0.29	56,56,56,56	0
81	MG	5	3896	1/1	0.58	0.19	68,68,68,68	0
81	MG	5	3646	1/1	0.58	0.15	66,66,66,66	0
81	MG	5	4105	1/1	0.58	0.59	54,54,54,54	0
81	MG	6	2045	1/1	0.58	0.24	117,117,117,117	0
81	MG	1	4133	1/1	0.59	0.31	69,69,69,69	0
81	MG	5	3874	1/1	0.59	0.35	75,75,75,75	0
81	MG	3	209	1/1	0.59	0.26	80,80,80,80	0
81	MG	L7	302	1/1	0.59	0.56	62,62,62,62	0
81	MG	1	3752	1/1	0.59	0.36	46,46,46,46	0
81	MG	5	3619	1/1	0.59	0.36	70,70,70,70	0
81	MG	n0	206	1/1	0.59	0.27	72,72,72,72	0
81	MG	o1	201	1/1	0.59	0.21	72,72,72,72	0
81	MG	q3	502	1/1	0.59	0.41	81,81,81,81	0
81	MG	5	4009	1/1	0.59	0.20	97,97,97,97	0
81	MG	5	3927	1/1	0.59	0.67	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3632	1/1	0.60	0.55	45,45,45,45	0
81	MG	5	3855	1/1	0.60	0.40	74,74,74,74	0
81	MG	8	216	1/1	0.60	0.28	82,82,82,82	0
81	MG	2	2043	1/1	0.60	0.20	85,85,85,85	0
81	MG	1	3963	1/1	0.60	0.45	52,52,52,52	0
81	MG	6	2075	1/1	0.60	0.23	98,98,98,98	0
81	MG	17	305	1/1	0.60	0.30	62,62,62,62	0
81	MG	1	4033	1/1	0.60	0.41	55,55,55,55	0
81	MG	2	1954	1/1	0.60	0.11	133,133,133,133	0
81	MG	5	3906	1/1	0.61	0.32	92,92,92,92	0
81	MG	5	3794	1/1	0.61	0.95	124,124,124,124	0
81	MG	1	3605	1/1	0.61	0.25	61,61,61,61	0
81	MG	2	2044	1/1	0.61	0.55	67,67,67,67	0
81	MG	5	3840	1/1	0.61	0.91	89,89,89,89	0
81	MG	5	4068	1/1	0.61	0.47	75,75,75,75	0
81	MG	6	2054	1/1	0.61	0.18	110,110,110,110	0
81	MG	N8	203	1/1	0.61	0.43	61,61,61,61	1
81	MG	2	1929	1/1	0.61	0.23	78,78,78,78	0
81	MG	1	4107	1/1	0.61	0.45	64,64,64,64	0
81	MG	1	3640	1/1	0.61	0.27	57,57,57,57	0
81	MG	5	4099	1/1	0.61	0.59	58,58,58,58	0
81	MG	L5	301	1/1	0.61	0.34	84,84,84,84	0
81	MG	2	2025	1/1	0.62	0.41	75,75,75,75	0
81	MG	1	3593	1/1	0.62	0.63	50,50,50,50	0
81	MG	5	4044	1/1	0.62	0.33	64,64,64,64	0
81	MG	5	3945	1/1	0.62	0.18	103,103,103,103	0
81	MG	5	3890	1/1	0.62	0.36	78,78,78,78	0
81	MG	8	225	1/1	0.62	0.22	77,77,77,77	0
81	MG	l3	408	1/1	0.62	0.25	71,71,71,71	0
81	MG	5	4066	1/1	0.62	0.68	88,88,88,88	0
81	MG	1	3654	1/1	0.62	0.35	47,47,47,47	0
81	MG	1	4020	1/1	0.62	0.49	49,49,49,49	1
81	MG	5	3994	1/1	0.62	0.51	59,59,59,59	0
81	MG	2	2054	1/1	0.62	0.28	86,86,86,86	0
81	MG	O1	202	1/1	0.62	0.33	63,63,63,63	0
81	MG	2	2020	1/1	0.62	0.37	83,83,83,83	0
81	MG	m8	201	1/1	0.63	0.36	72,72,72,72	0
81	MG	m9	204	1/1	0.63	0.52	79,79,79,79	0
81	MG	5	4070	1/1	0.63	0.30	113,113,113,113	0
81	MG	1	4184	1/1	0.63	0.87	67,67,67,67	0
81	MG	1	3982	1/1	0.63	0.48	62,62,62,62	0
81	MG	1	3526	1/1	0.63	0.36	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	2070	1/1	0.63	0.31	119,119,119,119	0
81	MG	1	4091	1/1	0.63	0.36	82,82,82,82	0
81	MG	1	4004	1/1	0.63	0.21	89,89,89,89	0
81	MG	L9	201	1/1	0.63	0.14	80,80,80,80	0
81	MG	n6	204	1/1	0.64	0.21	83,83,83,83	0
81	MG	5	3660	1/1	0.64	0.18	86,86,86,86	0
81	MG	1	4180	1/1	0.64	0.49	55,55,55,55	1
81	MG	1	4121	1/1	0.64	0.56	88,88,88,88	0
81	MG	5	3877	1/1	0.64	0.39	66,66,66,66	0
81	MG	1	3840	1/1	0.64	0.39	58,58,58,58	0
81	MG	5	3887	1/1	0.64	0.37	79,79,79,79	0
81	MG	2	2074	1/1	0.64	0.22	89,89,89,89	0
81	MG	1	3957	1/1	0.64	0.41	55,55,55,55	0
81	MG	5	3841	1/1	0.65	1.24	82,82,82,82	0
81	MG	2	2083	1/1	0.65	0.38	101,101,101,101	0
81	MG	2	1932	1/1	0.65	0.47	83,83,83,83	0
81	MG	1	3711	1/1	0.65	0.41	44,44,44,44	0
81	MG	5	4067	1/1	0.65	0.80	94,94,94,94	0
81	MG	6	2037	1/1	0.65	0.33	102,102,102,102	0
81	MG	5	4125	1/1	0.65	0.21	78,78,78,78	0
81	MG	8	212	1/1	0.65	0.54	74,74,74,74	0
81	MG	1	4113	1/1	0.65	0.39	79,79,79,79	0
81	MG	8	215	1/1	0.65	0.32	72,72,72,72	0
81	MG	5	3581	1/1	0.65	0.40	55,55,55,55	0
81	MG	5	4073	1/1	0.65	0.25	77,77,77,77	0
81	MG	8	222	1/1	0.65	0.42	78,78,78,78	0
81	MG	5	4037	1/1	0.65	0.23	65,65,65,65	0
81	MG	1	4065	1/1	0.66	0.37	69,69,69,69	0
81	MG	7	204	1/1	0.66	0.44	65,65,65,65	0
81	MG	6	1981	1/1	0.66	0.33	77,77,77,77	0
81	MG	6	1998	1/1	0.66	0.39	74,74,74,74	0
81	MG	7	213	1/1	0.66	0.34	76,76,76,76	0
81	MG	5	3827	1/1	0.66	0.90	70,70,70,70	0
81	MG	1	4186	1/1	0.66	0.74	43,43,43,43	0
81	MG	2	1931	1/1	0.66	0.25	98,98,98,98	0
81	MG	1	4160	1/1	0.66	0.34	65,65,65,65	0
81	MG	N1	202	1/1	0.66	0.33	61,61,61,61	0
81	MG	5	3901	1/1	0.66	0.29	94,94,94,94	0
81	MG	6	2067	1/1	0.66	0.78	75,75,75,75	0
81	MG	6	1915	1/1	0.66	0.25	73,73,73,73	0
81	MG	5	3903	1/1	0.66	0.35	87,87,87,87	0
81	MG	5	3989	1/1	0.66	0.60	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3559	1/1	0.66	0.39	47,47,47,47	0
81	MG	5	4034	1/1	0.67	0.09	102,102,102,102	0
81	MG	2	2103	1/1	0.67	0.49	73,73,73,73	0
81	MG	6	2060	1/1	0.67	0.60	88,88,88,88	0
81	MG	2	2081	1/1	0.67	0.31	79,79,79,79	0
81	MG	6	1972	1/1	0.67	0.15	107,107,107,107	0
81	MG	5	4000	1/1	0.67	0.44	78,78,78,78	0
81	MG	L4	402	1/1	0.67	0.33	54,54,54,54	0
81	MG	5	3842	1/1	0.67	1.44	78,78,78,78	0
81	MG	4	230	1/1	0.67	0.24	61,61,61,61	0
81	MG	5	3677	1/1	0.67	0.70	55,55,55,55	0
81	MG	2	2111	1/1	0.68	0.58	72,72,72,72	0
81	MG	2	2113	1/1	0.68	0.40	95,95,95,95	0
81	MG	8	219	1/1	0.68	0.45	60,60,60,60	0
81	MG	5	4108	1/1	0.68	0.31	70,70,70,70	0
81	MG	4	223	1/1	0.68	0.33	65,65,65,65	0
81	MG	6	1966	1/1	0.68	0.41	88,88,88,88	0
81	MG	6	2065	1/1	0.68	0.59	66,66,66,66	0
81	MG	1	3795	1/1	0.68	0.79	68,68,68,68	1
81	MG	5	3911	1/1	0.68	0.33	63,63,63,63	0
81	MG	1	4038	1/1	0.68	0.32	83,83,83,83	0
81	MG	5	3871	1/1	0.68	0.32	75,75,75,75	0
81	MG	6	1921	1/1	0.68	0.42	70,70,70,70	0
81	MG	5	4119	1/1	0.69	0.18	89,89,89,89	0
81	MG	1	3847	1/1	0.69	0.43	77,77,77,77	0
81	MG	O1	201	1/1	0.69	0.30	64,64,64,64	0
81	MG	o0	203	1/1	0.69	0.23	102,102,102,102	0
81	MG	1	3884	1/1	0.69	0.42	62,62,62,62	0
81	MG	2	2094	1/1	0.69	0.43	95,95,95,95	0
81	MG	1	3591	1/1	0.69	1.09	77,77,77,77	0
81	MG	6	2071	1/1	0.69	0.91	78,78,78,78	0
81	MG	5	3910	1/1	0.69	0.57	74,74,74,74	0
81	MG	6	2020	1/1	0.69	0.40	101,101,101,101	0
81	MG	1	4166	1/1	0.69	0.36	77,77,77,77	0
81	MG	5	3853	1/1	0.69	0.63	68,68,68,68	0
81	MG	d3	204	1/1	0.69	0.47	69,69,69,69	0
81	MG	2	2115	1/1	0.70	0.38	118,118,118,118	0
81	MG	3	215	1/1	0.70	0.31	72,72,72,72	0
81	MG	5	3529	1/1	0.70	0.58	55,55,55,55	0
81	MG	1	4018	1/1	0.70	0.46	50,50,50,50	0
81	MG	5	4098	1/1	0.70	0.46	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4057	1/1	0.70	0.11	89,89,89,89	0
81	MG	5	3701	1/1	0.70	0.72	70,70,70,70	0
81	MG	5	3729	1/1	0.70	0.42	63,63,63,63	0
81	MG	2	1950	1/1	0.70	0.14	133,133,133,133	0
81	MG	5	4076	1/1	0.70	0.14	99,99,99,99	0
81	MG	1	3876	1/1	0.71	0.19	66,66,66,66	1
81	MG	1	3975	1/1	0.71	0.49	71,71,71,71	0
81	MG	2	2024	1/1	0.71	0.23	78,78,78,78	0
81	MG	2	1937	1/1	0.71	0.42	69,69,69,69	0
81	MG	5	3700	1/1	0.71	0.90	62,62,62,62	0
81	MG	5	4013	1/1	0.71	0.42	87,87,87,87	0
81	MG	2	1940	1/1	0.71	0.96	78,78,78,78	0
81	MG	3	210	1/1	0.71	0.13	91,91,91,91	0
81	MG	5	3559	1/1	0.71	0.22	75,75,75,75	0
81	MG	1	4089	1/1	0.71	0.43	89,89,89,89	0
81	MG	1	3860	1/1	0.71	0.43	54,54,54,54	0
81	MG	5	3955	1/1	0.71	0.29	54,54,54,54	0
81	MG	6	1953	1/1	0.71	0.23	96,96,96,96	0
81	MG	5	3625	1/1	0.71	0.34	68,68,68,68	0
81	MG	5	3828	1/1	0.71	0.62	64,64,64,64	0
81	MG	5	4061	1/1	0.71	0.32	64,64,64,64	0
81	MG	2	1976	1/1	0.71	0.17	113,113,113,113	0
81	MG	6	1965	1/1	0.72	0.24	104,104,104,104	0
81	MG	5	3561	1/1	0.72	0.68	81,81,81,81	0
81	MG	1	3548	1/1	0.72	0.46	67,67,67,67	0
81	MG	5	4045	1/1	0.72	0.24	67,67,67,67	0
81	MG	5	3960	1/1	0.72	0.39	44,44,44,44	0
81	MG	5	3615	1/1	0.72	0.31	82,82,82,82	0
81	MG	6	2011	1/1	0.72	0.52	69,69,69,69	0
81	MG	2	2091	1/1	0.72	0.20	81,81,81,81	0
81	MG	1	3965	1/1	0.72	0.27	53,53,53,53	1
81	MG	6	2029	1/1	0.72	0.31	77,77,77,77	0
81	MG	2	1986	1/1	0.72	0.32	82,82,82,82	0
81	MG	6	2041	1/1	0.72	0.18	101,101,101,101	0
81	MG	1	4095	1/1	0.72	0.41	86,86,86,86	0
81	MG	o1	203	1/1	0.72	0.14	74,74,74,74	0
81	MG	o2	204	1/1	0.72	0.41	62,62,62,62	0
81	MG	2	2016	1/1	0.72	0.32	84,84,84,84	0
81	MG	2	2019	1/1	0.72	0.50	81,81,81,81	0
81	MG	5	3846	1/1	0.72	1.03	89,89,89,89	0
81	MG	1	4123	1/1	0.72	0.25	70,70,70,70	1
81	MG	6	2070	1/1	0.72	0.79	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4183	1/1	0.72	0.16	96,96,96,96	0
81	MG	1	4131	1/1	0.72	0.20	71,71,71,71	0
81	MG	1	3967	1/1	0.72	0.18	77,77,77,77	0
81	MG	6	1947	1/1	0.72	0.20	113,113,113,113	0
81	MG	5	3875	1/1	0.72	0.34	75,75,75,75	0
81	MG	17	304	1/1	0.72	0.24	66,66,66,66	0
81	MG	5	3980	1/1	0.73	0.28	97,97,97,97	0
81	MG	6	1992	1/1	0.73	0.32	86,86,86,86	0
81	MG	n6	201	1/1	0.73	0.31	71,71,71,71	0
81	MG	2	2026	1/1	0.73	0.46	69,69,69,69	0
81	MG	n8	201	1/1	0.73	0.18	55,55,55,55	0
81	MG	6	2014	1/1	0.73	0.37	89,89,89,89	0
81	MG	2	2078	1/1	0.73	0.11	100,100,100,100	0
81	MG	6	2024	1/1	0.73	0.11	119,119,119,119	0
81	MG	1	3955	1/1	0.73	0.25	59,59,59,59	0
81	MG	5	3998	1/1	0.73	0.56	63,63,63,63	0
81	MG	2	1991	1/1	0.73	0.33	91,91,91,91	0
81	MG	1	4187	1/1	0.73	0.29	50,50,50,50	0
81	MG	5	3572	1/1	0.73	0.29	72,72,72,72	0
81	MG	6	2053	1/1	0.73	0.26	123,123,123,123	0
81	MG	5	3769	1/1	0.73	0.58	53,53,53,53	0
81	MG	6	1924	1/1	0.73	0.33	83,83,83,83	0
81	MG	1	3806	1/1	0.73	0.35	50,50,50,50	0
81	MG	6	1941	1/1	0.73	0.30	80,80,80,80	0
81	MG	1	3785	1/1	0.73	0.32	69,69,69,69	0
81	MG	O2	202	1/1	0.73	0.64	44,44,44,44	0
81	MG	5	3622	1/1	0.73	0.31	69,69,69,69	0
81	MG	5	3959	1/1	0.73	0.43	59,59,59,59	0
81	MG	5	4038	1/1	0.73	0.51	68,68,68,68	0
81	MG	1	4070	1/1	0.73	0.17	84,84,84,84	0
81	MG	1	3634	1/1	0.73	0.72	48,48,48,48	0
81	MG	m9	203	1/1	0.73	0.14	78,78,78,78	0
81	MG	2	2071	1/1	0.73	0.25	67,67,67,67	0
81	MG	1	3904	1/1	0.74	0.40	63,63,63,63	0
81	MG	5	4087	1/1	0.74	0.26	85,85,85,85	0
81	MG	1	4098	1/1	0.74	0.83	89,89,89,89	0
81	MG	6	2034	1/1	0.74	0.36	70,70,70,70	0
81	MG	5	3951	1/1	0.74	0.48	55,55,55,55	0
81	MG	5	3952	1/1	0.74	0.60	57,57,57,57	0
81	MG	5	3586	1/1	0.74	0.30	64,64,64,64	0
81	MG	1	4173	1/1	0.74	0.41	58,58,58,58	0
81	MG	1	4174	1/1	0.74	0.34	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	4116	1/1	0.74	0.49	61,61,61,61	0
81	MG	5	3812	1/1	0.74	0.34	55,55,55,55	0
81	MG	1	4079	1/1	0.74	0.28	59,59,59,59	0
81	MG	2	1912	1/1	0.74	0.23	92,92,92,92	0
81	MG	2	1923	1/1	0.74	0.41	55,55,55,55	0
81	MG	2	2010	1/1	0.74	0.48	64,64,64,64	0
81	MG	1	4085	1/1	0.74	0.36	62,62,62,62	0
80	PAR	5	3423	42/42	0.74	0.41	86,86,86,86	42
81	MG	5	3679	1/1	0.74	0.50	52,52,52,52	0
81	MG	1	3974	1/1	0.74	0.39	58,58,58,58	0
81	MG	1	3715	1/1	0.74	0.37	46,46,46,46	0
81	MG	1	4198	1/1	0.74	0.49	68,68,68,68	0
81	MG	3	216	1/1	0.75	0.13	72,72,72,72	0
81	MG	5	3987	1/1	0.75	0.69	77,77,77,77	0
81	MG	5	3708	1/1	0.75	0.59	59,59,59,59	0
81	MG	5	4126	1/1	0.75	0.30	78,78,78,78	0
81	MG	2	2108	1/1	0.75	0.22	110,110,110,110	0
81	MG	5	3924	1/1	0.75	0.31	75,75,75,75	0
81	MG	1	4062	1/1	0.75	0.44	48,48,48,48	0
81	MG	1	4111	1/1	0.75	0.35	65,65,65,65	0
81	MG	4	236	1/1	0.75	0.35	50,50,50,50	0
81	MG	5	3631	1/1	0.75	0.32	62,62,62,62	0
81	MG	6	1919	1/1	0.75	0.35	85,85,85,85	1
81	MG	Q2	505	1/1	0.75	0.28	42,42,42,42	0
81	MG	5	4082	1/1	0.75	0.51	79,79,79,79	0
81	MG	1	3964	1/1	0.75	0.27	58,58,58,58	0
81	MG	1	3993	1/1	0.75	0.41	46,46,46,46	0
81	MG	1	4115	1/1	0.75	0.22	98,98,98,98	0
81	MG	l3	405	1/1	0.75	0.37	66,66,66,66	0
81	MG	1	4139	1/1	0.75	0.46	50,50,50,50	0
81	MG	5	4092	1/1	0.75	0.29	67,67,67,67	0
81	MG	6	1949	1/1	0.75	0.21	83,83,83,83	0
81	MG	1	3979	1/1	0.75	0.40	63,63,63,63	0
81	MG	2	2011	1/1	0.75	0.48	101,101,101,101	0
81	MG	6	1956	1/1	0.75	0.14	105,105,105,105	0
81	MG	5	3844	1/1	0.75	0.89	81,81,81,81	0
81	MG	5	4050	1/1	0.75	0.26	57,57,57,57	1
81	MG	5	4111	1/1	0.75	1.12	75,75,75,75	0
81	MG	5	4115	1/1	0.75	0.70	74,74,74,74	0
81	MG	d3	205	1/1	0.75	0.34	78,78,78,78	0
81	MG	5	3633	1/1	0.76	0.38	56,56,56,56	0
81	MG	1	3513	1/1	0.76	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4112	1/1	0.76	0.32	73,73,73,73	0
81	MG	2	1992	1/1	0.76	0.38	75,75,75,75	0
80	PAR	6	1902	42/42	0.76	0.38	87,87,87,87	42
81	MG	5	4031	1/1	0.76	0.16	91,91,91,91	0
81	MG	1	3873	1/1	0.76	0.32	69,69,69,69	0
81	MG	5	3915	1/1	0.76	0.41	97,97,97,97	0
81	MG	l3	404	1/1	0.76	0.21	65,65,65,65	0
81	MG	1	3728	1/1	0.76	0.39	49,49,49,49	0
81	MG	5	4123	1/1	0.76	0.21	84,84,84,84	0
81	MG	S2	302	1/1	0.76	0.15	84,84,84,84	0
81	MG	3	214	1/1	0.76	0.14	73,73,73,73	0
81	MG	6	1922	1/1	0.76	0.49	73,73,73,73	0
81	MG	1	4031	1/1	0.76	0.32	44,44,44,44	1
81	MG	m0	303	1/1	0.76	0.32	69,69,69,69	0
81	MG	1	3660	1/1	0.76	0.25	55,55,55,55	0
81	MG	8	209	1/1	0.76	0.40	66,66,66,66	0
81	MG	5	3756	1/1	0.76	0.32	55,55,55,55	0
82	ZN	d7	101	1/1	0.76	0.14	261,261,261,261	0
81	MG	1	4026	1/1	0.77	0.43	37,37,37,37	1
81	MG	6	1986	1/1	0.77	0.41	81,81,81,81	0
81	MG	5	3928	1/1	0.77	0.47	76,76,76,76	0
81	MG	2	2085	1/1	0.77	0.39	76,76,76,76	0
81	MG	1	3989	1/1	0.77	0.32	60,60,60,60	0
81	MG	2	2093	1/1	0.77	0.34	69,69,69,69	0
81	MG	5	3614	1/1	0.77	0.24	94,94,94,94	0
81	MG	n9	101	1/1	0.77	0.37	65,65,65,65	0
81	MG	1	3969	1/1	0.77	0.31	77,77,77,77	0
81	MG	6	2026	1/1	0.77	0.25	76,76,76,76	0
81	MG	5	3953	1/1	0.77	0.51	49,49,49,49	0
81	MG	1	4034	1/1	0.77	0.31	66,66,66,66	0
81	MG	1	3590	1/1	0.77	0.40	49,49,49,49	0
81	MG	5	3793	1/1	0.77	0.67	89,89,89,89	0
81	MG	5	3962	1/1	0.77	0.18	81,81,81,81	0
81	MG	5	4062	1/1	0.77	0.55	85,85,85,85	0
81	MG	2	2062	1/1	0.77	0.27	124,124,124,124	0
80	PAR	5	3403	42/42	0.77	0.34	84,84,84,84	42
81	MG	6	2058	1/1	0.77	0.40	121,121,121,121	0
81	MG	1	4108	1/1	0.77	0.70	83,83,83,83	0
81	MG	5	3982	1/1	0.77	0.19	75,75,75,75	0
81	MG	1	4109	1/1	0.77	0.50	78,78,78,78	0
81	MG	1	3830	1/1	0.77	0.51	45,45,45,45	0
81	MG	5	3988	1/1	0.77	0.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3658	1/1	0.77	0.55	61,61,61,61	0
81	MG	5	3909	1/1	0.77	0.38	62,62,62,62	0
81	MG	1	3905	1/1	0.77	0.62	44,44,44,44	1
81	MG	2	1982	1/1	0.77	0.46	63,63,63,63	0
81	MG	5	3913	1/1	0.77	0.32	74,74,74,74	0
81	MG	L3	402	1/1	0.77	0.52	55,55,55,55	0
81	MG	5	4012	1/1	0.77	0.42	80,80,80,80	0
81	MG	5	3681	1/1	0.77	0.91	56,56,56,56	0
81	MG	5	3845	1/1	0.77	0.91	68,68,68,68	0
81	MG	1	3900	1/1	0.78	0.12	70,70,70,70	0
80	PAR	5	3428	42/42	0.78	0.23	120,120,120,120	0
81	MG	1	3669	1/1	0.78	0.35	55,55,55,55	0
81	MG	6	1939	1/1	0.78	0.14	104,104,104,104	0
81	MG	5	4058	1/1	0.78	0.41	75,75,75,75	0
81	MG	1	3621	1/1	0.78	0.37	49,49,49,49	0
81	MG	1	4119	1/1	0.78	0.23	80,80,80,80	0
81	MG	3	213	1/1	0.78	0.14	89,89,89,89	0
81	MG	5	3937	1/1	0.78	0.24	76,76,76,76	0
81	MG	M6	202	1/1	0.78	0.31	52,52,52,52	0
81	MG	1	4056	1/1	0.78	0.21	69,69,69,69	0
81	MG	N6	204	1/1	0.78	0.23	56,56,56,56	0
81	MG	6	2062	1/1	0.78	0.14	108,108,108,108	0
81	MG	7	214	1/1	0.78	0.21	89,89,89,89	0
81	MG	N7	202	1/1	0.78	0.14	72,72,72,72	0
81	MG	2	1961	1/1	0.78	0.31	76,76,76,76	0
81	MG	2	1963	1/1	0.78	0.26	112,112,112,112	0
81	MG	1	3914	1/1	0.78	0.40	75,75,75,75	0
81	MG	5	4030	1/1	0.78	0.14	88,88,88,88	0
80	PAR	3	201	42/42	0.78	0.20	95,95,95,95	42
81	MG	1	3890	1/1	0.78	0.11	52,52,52,52	0
81	MG	4	226	1/1	0.78	0.38	60,60,60,60	0
81	MG	1	4136	1/1	0.78	0.44	47,47,47,47	1
81	MG	6	2013	1/1	0.78	0.43	83,83,83,83	0
81	MG	Q2	506	1/1	0.78	0.29	51,51,51,51	0
81	MG	5	3537	1/1	0.78	0.41	49,49,49,49	0
81	MG	M6	203	1/1	0.79	0.34	56,56,56,56	0
80	PAR	2	1905	42/42	0.79	0.32	80,80,80,80	42
81	MG	5	3872	1/1	0.79	0.34	72,72,72,72	0
81	MG	5	3510	1/1	0.79	0.32	68,68,68,68	0
81	MG	N6	203	1/1	0.79	0.27	55,55,55,55	0
81	MG	5	3964	1/1	0.79	0.20	67,67,67,67	1
81	MG	5	3535	1/1	0.79	0.53	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	4	203	1/1	0.79	0.30	44,44,44,44	0
81	MG	5	3879	1/1	0.79	0.18	137,137,137,137	0
81	MG	5	3981	1/1	0.79	0.30	79,79,79,79	0
81	MG	5	3883	1/1	0.79	0.37	73,73,73,73	0
81	MG	2	1968	1/1	0.79	0.15	129,129,129,129	0
81	MG	5	3985	1/1	0.79	0.61	79,79,79,79	0
81	MG	5	3741	1/1	0.79	0.29	58,58,58,58	0
81	MG	4	205	1/1	0.79	0.39	46,46,46,46	0
81	MG	4	216	1/1	0.79	0.31	41,41,41,41	0
81	MG	5	3774	1/1	0.79	0.38	59,59,59,59	1
81	MG	5	3902	1/1	0.79	0.36	80,80,80,80	0
81	MG	5	4100	1/1	0.79	0.42	60,60,60,60	0
80	PAR	6	1906	42/42	0.79	0.27	120,120,120,120	0
81	MG	5	3792	1/1	0.79	0.40	50,50,50,50	0
81	MG	1	3682	1/1	0.79	0.46	61,61,61,61	0
81	MG	1	3615	1/1	0.79	0.33	72,72,72,72	0
81	MG	2	2003	1/1	0.79	0.51	66,66,66,66	0
81	MG	6	2055	1/1	0.79	0.20	106,106,106,106	0
81	MG	4	232	1/1	0.79	0.25	51,51,51,51	0
81	MG	5	4122	1/1	0.79	0.34	68,68,68,68	0
81	MG	5	3826	1/1	0.79	0.77	78,78,78,78	0
81	MG	6	1920	1/1	0.79	0.26	70,70,70,70	1
81	MG	1	3875	1/1	0.79	0.21	64,64,64,64	1
81	MG	2	1910	1/1	0.79	0.32	80,80,80,80	0
81	MG	1	4164	1/1	0.79	0.27	69,69,69,69	0
81	MG	7	211	1/1	0.79	0.50	72,72,72,72	0
81	MG	1	3491	1/1	0.79	0.45	58,58,58,58	0
81	MG	1	3852	1/1	0.79	0.17	63,63,63,63	0
81	MG	1	3935	1/1	0.79	0.27	56,56,56,56	0
81	MG	L8	301	1/1	0.79	0.25	73,73,73,73	0
81	MG	1	4175	1/1	0.79	0.62	69,69,69,69	0
81	MG	5	3946	1/1	0.79	0.29	72,72,72,72	0
81	MG	M4	201	1/1	0.79	0.24	59,59,59,59	0
81	MG	1	3946	1/1	0.79	0.50	56,56,56,56	0
81	MG	2	1973	1/1	0.80	0.44	82,82,82,82	0
81	MG	1	4084	1/1	0.80	0.42	62,62,62,62	0
81	MG	1	3786	1/1	0.80	0.34	67,67,67,67	0
81	MG	1	3791	1/1	0.80	0.28	62,62,62,62	0
81	MG	1	3564	1/1	0.80	0.29	48,48,48,48	0
81	MG	1	3577	1/1	0.80	0.44	48,48,48,48	0
81	MG	1	3871	1/1	0.80	0.65	59,59,59,59	0
81	MG	1	3586	1/1	0.80	0.35	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3508	1/1	0.80	0.11	72,72,72,72	0
80	PAR	5	3427	42/42	0.80	0.35	94,94,94,94	42
81	MG	2	2109	1/1	0.80	0.32	103,103,103,103	0
81	MG	5	3690	1/1	0.80	0.81	59,59,59,59	0
81	MG	2	2014	1/1	0.80	0.35	67,67,67,67	0
81	MG	5	3886	1/1	0.80	0.14	75,75,75,75	0
81	MG	1	4102	1/1	0.80	0.47	66,66,66,66	0
81	MG	n0	203	1/1	0.80	0.22	60,60,60,60	0
81	MG	1	4104	1/1	0.80	0.34	55,55,55,55	0
81	MG	S2	301	1/1	0.80	0.32	91,91,91,91	0
81	MG	2	1917	1/1	0.80	0.49	88,88,88,88	0
81	MG	1	4039	1/1	0.80	0.26	72,72,72,72	0
81	MG	2	1924	1/1	0.80	0.23	63,63,63,63	0
81	MG	6	2042	1/1	0.80	0.34	98,98,98,98	0
81	MG	1	4042	1/1	0.80	0.18	63,63,63,63	0
81	MG	1	3948	1/1	0.80	0.43	42,42,42,42	0
81	MG	5	4003	1/1	0.80	0.41	64,64,64,64	0
81	MG	1	3990	1/1	0.80	0.32	56,56,56,56	0
81	MG	5	4011	1/1	0.80	0.72	63,63,63,63	0
81	MG	1	3883	1/1	0.80	0.35	67,67,67,67	0
81	MG	1	3768	1/1	0.80	0.26	77,77,77,77	0
81	MG	2	2058	1/1	0.80	0.54	58,58,58,58	0
81	MG	5	3805	1/1	0.80	0.33	68,68,68,68	0
81	MG	1	3680	1/1	0.80	0.36	62,62,62,62	0
81	MG	5	3922	1/1	0.80	0.16	87,87,87,87	0
81	MG	5	3814	1/1	0.80	0.36	63,63,63,63	0
81	MG	1	4015	1/1	0.80	0.78	65,65,65,65	0
81	MG	5	3585	1/1	0.80	0.27	73,73,73,73	0
81	MG	1	4076	1/1	0.80	0.38	61,61,61,61	0
81	MG	c4	201	1/1	0.80	0.14	118,118,118,118	0
81	MG	5	4043	1/1	0.80	0.31	66,66,66,66	0
81	MG	2	1957	1/1	0.80	0.23	81,81,81,81	0
81	MG	1	3894	1/1	0.80	0.27	60,60,60,60	0
81	MG	M6	204	1/1	0.80	0.25	65,65,65,65	0
81	MG	1	4080	1/1	0.80	0.31	64,64,64,64	0
81	MG	2	1919	1/1	0.81	0.24	73,73,73,73	0
81	MG	5	3935	1/1	0.81	0.71	59,59,59,59	0
81	MG	8	210	1/1	0.81	0.28	62,62,62,62	0
81	MG	1	3525	1/1	0.81	0.45	54,54,54,54	0
81	MG	5	3941	1/1	0.81	0.26	113,113,113,113	0
81	MG	1	3639	1/1	0.81	0.20	78,78,78,78	0
81	MG	1	4007	1/1	0.81	0.46	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	2089	1/1	0.81	0.22	93,93,93,93	0
81	MG	M9	201	1/1	0.81	0.43	65,65,65,65	0
81	MG	6	1977	1/1	0.81	0.12	107,107,107,107	0
81	MG	2	2092	1/1	0.81	0.23	71,71,71,71	0
81	MG	1	4105	1/1	0.81	0.23	63,63,63,63	0
81	MG	2	2018	1/1	0.81	0.10	99,99,99,99	0
81	MG	N3	201	1/1	0.81	0.29	82,82,82,82	0
81	MG	1	4125	1/1	0.81	0.41	58,58,58,58	0
81	MG	5	3669	1/1	0.81	0.25	48,48,48,48	0
81	MG	1	4013	1/1	0.81	0.70	70,70,70,70	0
81	MG	N7	201	1/1	0.81	0.22	64,64,64,64	0
81	MG	5	4069	1/1	0.81	0.28	69,69,69,69	1
81	MG	1	3861	1/1	0.81	0.24	44,44,44,44	0
81	MG	2	2028	1/1	0.81	0.37	73,73,73,73	0
81	MG	5	3972	1/1	0.81	0.28	68,68,68,68	0
81	MG	1	3683	1/1	0.81	0.56	49,49,49,49	0
81	MG	1	3985	1/1	0.81	0.46	61,61,61,61	0
81	MG	6	2035	1/1	0.81	0.24	87,87,87,87	0
81	MG	C9	202	1/1	0.81	0.11	133,133,133,133	0
81	MG	L3	405	1/1	0.81	0.18	73,73,73,73	0
81	MG	D6	102	1/1	0.81	0.36	79,79,79,79	0
81	MG	2	1964	1/1	0.81	0.15	102,102,102,102	0
81	MG	6	2049	1/1	0.81	0.25	74,74,74,74	0
81	MG	1	4048	1/1	0.81	0.22	50,50,50,50	0
81	MG	n8	202	1/1	0.81	0.42	52,52,52,52	1
81	MG	1	3698	1/1	0.81	0.52	62,62,62,62	0
81	MG	5	3990	1/1	0.81	0.14	91,91,91,91	0
81	MG	6	2059	1/1	0.81	0.20	118,118,118,118	0
81	MG	1	4161	1/1	0.81	0.18	61,61,61,61	1
81	MG	5	3785	1/1	0.81	0.38	53,53,53,53	0
81	MG	5	3904	1/1	0.81	0.42	89,89,89,89	0
81	MG	q0	202	1/1	0.81	0.40	67,67,67,67	0
81	MG	2	1980	1/1	0.81	0.39	66,66,66,66	0
81	MG	5	4112	1/1	0.81	0.82	69,69,69,69	0
81	MG	2	1907	1/1	0.81	0.14	81,81,81,81	0
81	MG	5	3560	1/1	0.81	0.09	92,92,92,92	0
81	MG	1	4029	1/1	0.81	0.42	40,40,40,40	0
81	MG	1	3809	1/1	0.81	0.27	59,59,59,59	0
81	MG	5	3580	1/1	0.81	0.29	60,60,60,60	0
81	MG	c4	203	1/1	0.81	0.19	118,118,118,118	0
81	MG	2	2072	1/1	0.81	0.16	83,83,83,83	0
81	MG	5	4024	1/1	0.81	0.37	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
80	PAR	5	3405	42/42	0.81	0.23	131,131,131,131	0
81	MG	2	2001	1/1	0.81	0.17	80,80,80,80	0
81	MG	5	3611	1/1	0.81	0.33	67,67,67,67	0
81	MG	5	3734	1/1	0.82	0.73	65,65,65,65	0
81	MG	5	3738	1/1	0.82	0.41	54,54,54,54	0
81	MG	6	1975	1/1	0.82	0.07	104,104,104,104	1
81	MG	l3	406	1/1	0.82	0.25	62,62,62,62	0
81	MG	1	3954	1/1	0.82	0.24	65,65,65,65	0
81	MG	1	3638	1/1	0.82	0.30	68,68,68,68	0
81	MG	5	3573	1/1	0.82	0.22	76,76,76,76	0
81	MG	6	1995	1/1	0.82	0.36	71,71,71,71	0
81	MG	6	1997	1/1	0.82	0.38	80,80,80,80	0
81	MG	5	3899	1/1	0.82	0.21	73,73,73,73	0
81	MG	6	2001	1/1	0.82	0.24	105,105,105,105	0
81	MG	5	3772	1/1	0.82	0.35	73,73,73,73	0
81	MG	1	3981	1/1	0.82	0.34	57,57,57,57	0
81	MG	m6	201	1/1	0.82	0.35	52,52,52,52	0
81	MG	O9	101	1/1	0.82	0.45	48,48,48,48	1
81	MG	6	2016	1/1	0.82	0.34	95,95,95,95	0
81	MG	1	3821	1/1	0.82	0.26	52,52,52,52	0
81	MG	L9	203	1/1	0.82	0.19	71,71,71,71	0
81	MG	5	4097	1/1	0.82	0.43	52,52,52,52	0
81	MG	Q3	502	1/1	0.82	0.34	51,51,51,51	0
81	MG	2	2098	1/1	0.82	0.29	79,79,79,79	0
81	MG	2	2100	1/1	0.82	0.60	58,58,58,58	0
81	MG	2	2037	1/1	0.82	0.10	123,123,123,123	0
81	MG	5	4010	1/1	0.82	0.32	74,74,74,74	0
81	MG	6	2039	1/1	0.82	0.33	69,69,69,69	0
81	MG	5	3620	1/1	0.82	0.54	79,79,79,79	0
81	MG	2	2104	1/1	0.82	0.77	82,82,82,82	0
81	MG	1	3962	1/1	0.82	0.41	44,44,44,44	0
81	MG	1	3862	1/1	0.82	0.25	62,62,62,62	0
81	MG	1	3864	1/1	0.82	0.24	47,47,47,47	0
81	MG	5	4120	1/1	0.82	0.21	58,58,58,58	0
81	MG	5	3837	1/1	0.82	0.30	53,53,53,53	0
81	MG	5	3639	1/1	0.82	0.39	54,54,54,54	0
81	MG	1	4073	1/1	0.82	0.13	80,80,80,80	0
81	MG	M7	205	1/1	0.82	0.26	45,45,45,45	0
81	MG	2	1922	1/1	0.82	0.27	60,60,60,60	1
80	PAR	1	3413	42/42	0.82	0.27	64,64,64,64	42
81	MG	2	2000	1/1	0.82	0.13	78,78,78,78	0
81	MG	2	2063	1/1	0.82	0.44	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
80	PAR	5	3422	42/42	0.82	0.20	105,105,105,105	0
81	MG	1	4002	1/1	0.82	0.56	75,75,75,75	0
81	MG	2	2004	1/1	0.82	0.34	69,69,69,69	0
81	MG	1	3947	1/1	0.82	0.33	54,54,54,54	0
81	MG	5	3693	1/1	0.82	0.38	51,51,51,51	0
81	MG	1	4192	1/1	0.82	0.71	62,62,62,62	0
81	MG	1	3592	1/1	0.82	0.71	63,63,63,63	0
81	MG	1	4140	1/1	0.82	0.27	56,56,56,56	1
81	MG	5	3724	1/1	0.82	0.51	78,78,78,78	0
81	MG	5	3880	1/1	0.82	0.58	77,77,77,77	0
81	MG	6	1962	1/1	0.82	0.37	110,110,110,110	0
81	MG	1	3949	1/1	0.82	0.45	38,38,38,38	1
81	MG	5	3861	1/1	0.83	0.38	64,64,64,64	0
81	MG	1	3695	1/1	0.83	0.38	50,50,50,50	1
81	MG	5	3697	1/1	0.83	0.69	60,60,60,60	0
81	MG	5	3873	1/1	0.83	0.39	66,66,66,66	0
81	MG	1	4027	1/1	0.83	0.41	42,42,42,42	0
81	MG	1	3818	1/1	0.83	0.27	54,54,54,54	0
81	MG	M4	203	1/1	0.83	0.15	64,64,64,64	0
81	MG	M5	303	1/1	0.83	0.32	44,44,44,44	1
81	MG	l3	407	1/1	0.83	0.40	51,51,51,51	0
80	PAR	o2	201	42/42	0.83	0.32	51,51,51,51	42
81	MG	1	4000	1/1	0.83	0.24	54,54,54,54	0
81	MG	5	3974	1/1	0.83	0.42	59,59,59,59	0
81	MG	1	4078	1/1	0.83	0.25	71,71,71,71	0
81	MG	M7	202	1/1	0.83	0.47	40,40,40,40	0
81	MG	1	3882	1/1	0.83	0.17	74,74,74,74	0
81	MG	5	3767	1/1	0.83	0.37	66,66,66,66	0
81	MG	5	4084	1/1	0.83	0.20	69,69,69,69	0
81	MG	5	3892	1/1	0.83	0.25	66,66,66,66	0
81	MG	5	3986	1/1	0.83	0.61	78,78,78,78	0
81	MG	M8	201	1/1	0.83	0.32	63,63,63,63	0
81	MG	1	3530	1/1	0.83	0.34	37,37,37,37	0
81	MG	1	4171	1/1	0.83	0.36	52,52,52,52	0
81	MG	n6	202	1/1	0.83	0.10	69,69,69,69	0
81	MG	5	3598	1/1	0.83	0.38	82,82,82,82	0
81	MG	6	2036	1/1	0.83	0.43	80,80,80,80	0
81	MG	1	4005	1/1	0.83	0.33	64,64,64,64	0
81	MG	1	3789	1/1	0.83	0.44	54,54,54,54	0
81	MG	2	2095	1/1	0.83	0.42	78,78,78,78	0
81	MG	1	4010	1/1	0.83	0.50	53,53,53,53	0
81	MG	6	2044	1/1	0.83	0.22	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	4	231	1/1	0.83	0.28	49,49,49,49	0
80	PAR	1	3433	42/42	0.83	0.27	64,64,64,64	42
81	MG	6	2051	1/1	0.83	0.26	110,110,110,110	0
81	MG	2	2031	1/1	0.83	0.13	98,98,98,98	0
81	MG	1	4014	1/1	0.83	0.90	70,70,70,70	0
81	MG	5	3822	1/1	0.83	0.11	65,65,65,65	0
81	MG	5	4118	1/1	0.83	0.27	66,66,66,66	0
81	MG	1	3503	1/1	0.83	0.26	56,56,56,56	0
81	MG	5	4016	1/1	0.83	0.37	77,77,77,77	0
81	MG	1	4096	1/1	0.83	0.30	62,62,62,62	0
81	MG	5	4021	1/1	0.83	0.61	64,64,64,64	0
81	MG	1	4097	1/1	0.83	0.25	63,63,63,63	0
81	MG	2	2049	1/1	0.83	0.56	88,88,88,88	0
81	MG	6	2066	1/1	0.83	0.37	55,55,55,55	0
81	MG	6	1938	1/1	0.83	0.09	99,99,99,99	0
81	MG	1	4053	1/1	0.83	0.35	55,55,55,55	0
81	MG	2	1978	1/1	0.83	0.21	79,79,79,79	0
81	MG	6	2072	1/1	0.83	0.42	74,74,74,74	0
81	MG	7	212	1/1	0.83	0.22	60,60,60,60	0
81	MG	2	1979	1/1	0.83	0.30	77,77,77,77	0
81	MG	5	3673	1/1	0.83	0.33	51,51,51,51	0
81	MG	5	4035	1/1	0.83	0.17	85,85,85,85	0
81	MG	L5	303	1/1	0.83	0.20	86,86,86,86	0
81	MG	1	3987	1/1	0.83	0.33	54,54,54,54	0
81	MG	5	3483	1/1	0.83	0.33	53,53,53,53	0
80	PAR	n3	201	42/42	0.83	0.30	63,63,63,63	42
81	MG	5	3513	1/1	0.83	0.57	76,76,76,76	0
81	MG	1	3972	1/1	0.84	0.39	84,84,84,84	0
81	MG	1	4116	1/1	0.84	0.31	107,107,107,107	0
81	MG	1	3874	1/1	0.84	0.20	67,67,67,67	1
81	MG	5	3847	1/1	0.84	0.33	96,96,96,96	0
81	MG	5	3852	1/1	0.84	0.41	55,55,55,55	0
81	MG	1	3930	1/1	0.84	0.40	45,45,45,45	0
81	MG	1	3500	1/1	0.84	0.76	71,71,71,71	0
81	MG	17	303	1/1	0.84	0.25	69,69,69,69	0
81	MG	1	3501	1/1	0.84	0.57	78,78,78,78	0
81	MG	6	2004	1/1	0.84	0.74	77,77,77,77	0
81	MG	5	3867	1/1	0.84	0.26	66,66,66,66	0
81	MG	5	3469	1/1	0.84	0.36	46,46,46,46	0
81	MG	1	3614	1/1	0.84	0.26	71,71,71,71	0
81	MG	1	4030	1/1	0.84	0.37	48,48,48,48	0
81	MG	3	218	1/1	0.84	0.40	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3984	1/1	0.84	0.36	52,52,52,52	0
81	MG	5	3707	1/1	0.84	0.60	58,58,58,58	0
81	MG	1	3855	1/1	0.84	0.23	51,51,51,51	0
81	MG	5	3713	1/1	0.84	0.48	56,56,56,56	0
81	MG	2	2066	1/1	0.84	0.35	82,82,82,82	0
81	MG	1	4092	1/1	0.84	0.20	62,62,62,62	0
80	PAR	1	3403	42/42	0.84	0.31	58,58,58,58	42
81	MG	1	3889	1/1	0.84	0.32	54,54,54,54	0
81	MG	1	4145	1/1	0.84	0.28	52,52,52,52	0
81	MG	2	1987	1/1	0.84	0.59	81,81,81,81	0
81	MG	5	3991	1/1	0.84	0.17	66,66,66,66	0
81	MG	5	3764	1/1	0.84	0.34	56,56,56,56	0
81	MG	5	3995	1/1	0.84	0.26	49,49,49,49	0
81	MG	o1	202	1/1	0.84	0.50	69,69,69,69	0
81	MG	1	4146	1/1	0.84	0.46	55,55,55,55	0
81	MG	2	2080	1/1	0.84	0.17	81,81,81,81	0
80	PAR	5	3404	42/42	0.84	0.23	90,90,90,90	0
81	MG	1	3956	1/1	0.84	0.23	67,67,67,67	0
81	MG	1	3630	1/1	0.84	0.29	51,51,51,51	0
81	MG	1	4041	1/1	0.84	0.15	69,69,69,69	0
81	MG	5	3603	1/1	0.84	0.24	65,65,65,65	0
81	MG	L4	401	1/1	0.84	0.23	49,49,49,49	0
81	MG	1	3896	1/1	0.84	0.28	76,76,76,76	0
81	MG	5	4014	1/1	0.84	0.39	71,71,71,71	0
81	MG	1	4001	1/1	0.84	0.22	62,62,62,62	0
81	MG	1	3899	1/1	0.84	0.22	76,76,76,76	0
80	PAR	1	3401	42/42	0.84	0.22	87,87,87,87	42
81	MG	1	4054	1/1	0.84	0.29	75,75,75,75	0
81	MG	1	4055	1/1	0.84	0.20	60,60,60,60	0
81	MG	5	4027	1/1	0.84	0.52	69,69,69,69	0
80	PAR	1	3426	42/42	0.84	0.28	82,82,82,82	0
81	MG	1	3868	1/1	0.84	0.32	39,39,39,39	0
81	MG	s8	301	1/1	0.84	0.32	70,70,70,70	0
81	MG	M4	202	1/1	0.84	0.30	60,60,60,60	0
81	MG	5	3835	1/1	0.84	0.37	57,57,57,57	0
81	MG	5	3936	1/1	0.84	0.54	60,60,60,60	1
81	MG	1	3788	1/1	0.84	0.27	68,68,68,68	0
81	MG	2	1936	1/1	0.84	0.54	59,59,59,59	0
81	MG	1	3549	1/1	0.84	0.34	49,49,49,49	0
81	MG	1	3971	1/1	0.84	0.19	69,69,69,69	0
82	ZN	D7	101	1/1	0.84	0.16	173,173,173,173	0
81	MG	5	3667	1/1	0.84	0.37	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3643	1/1	0.85	0.24	60,60,60,60	0
81	MG	6	1940	1/1	0.85	0.11	100,100,100,100	0
81	MG	5	4109	1/1	0.85	0.87	79,79,79,79	0
81	MG	2	1911	1/1	0.85	0.14	79,79,79,79	0
81	MG	1	3538	1/1	0.85	0.38	35,35,35,35	0
81	MG	2	1915	1/1	0.85	0.33	82,82,82,82	0
81	MG	2	2106	1/1	0.85	0.17	84,84,84,84	0
81	MG	1	3546	1/1	0.85	0.18	43,43,43,43	0
80	PAR	1	3405	42/42	0.85	0.35	44,44,44,44	42
81	MG	1	4195	1/1	0.85	0.31	60,60,60,60	0
81	MG	6	1954	1/1	0.85	0.16	98,98,98,98	0
81	MG	L9	204	1/1	0.85	0.29	60,60,60,60	0
81	MG	6	1959	1/1	0.85	0.29	119,119,119,119	0
81	MG	1	3923	1/1	0.85	0.42	45,45,45,45	0
81	MG	5	3876	1/1	0.85	0.28	74,74,74,74	0
81	MG	2	2116	1/1	0.85	0.38	93,93,93,93	0
81	MG	1	4199	1/1	0.85	0.19	47,47,47,47	0
80	PAR	1	3435	42/42	0.85	0.31	40,40,40,40	42
81	MG	1	3839	1/1	0.85	0.29	47,47,47,47	0
81	MG	M5	309	1/1	0.85	0.37	43,43,43,43	0
81	MG	5	4004	1/1	0.85	0.27	72,72,72,72	0
81	MG	2	2041	1/1	0.85	0.11	126,126,126,126	0
81	MG	1	3973	1/1	0.85	0.36	71,71,71,71	0
81	MG	1	3932	1/1	0.85	0.28	44,44,44,44	0
81	MG	2	1941	1/1	0.85	0.28	75,75,75,75	0
81	MG	2	1943	1/1	0.85	0.64	82,82,82,82	0
81	MG	5	3521	1/1	0.85	0.28	55,55,55,55	0
81	MG	8	217	1/1	0.85	0.24	69,69,69,69	0
81	MG	5	3898	1/1	0.85	0.24	66,66,66,66	0
80	PAR	8	201	42/42	0.85	0.28	79,79,79,79	42
81	MG	5	3530	1/1	0.85	0.29	43,43,43,43	0
81	MG	1	4103	1/1	0.85	0.49	57,57,57,57	0
81	MG	6	2017	1/1	0.85	0.20	93,93,93,93	0
81	MG	1	4061	1/1	0.85	0.32	41,41,41,41	1
81	MG	5	3743	1/1	0.85	0.29	54,54,54,54	1
81	MG	5	3747	1/1	0.85	0.60	60,60,60,60	0
81	MG	2	1956	1/1	0.85	0.23	119,119,119,119	0
81	MG	5	3541	1/1	0.85	0.47	41,41,41,41	0
81	MG	5	3546	1/1	0.85	0.30	59,59,59,59	0
81	MG	17	302	1/1	0.85	0.41	57,57,57,57	0
81	MG	5	3553	1/1	0.85	0.32	64,64,64,64	0
81	MG	5	3771	1/1	0.85	0.37	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4147	1/1	0.85	0.32	51,51,51,51	0
81	MG	5	3916	1/1	0.85	0.29	96,96,96,96	0
81	MG	1	3941	1/1	0.85	0.36	72,72,72,72	0
81	MG	5	3777	1/1	0.85	0.42	45,45,45,45	0
81	MG	M9	202	1/1	0.85	0.34	61,61,61,61	0
80	PAR	8	202	42/42	0.85	0.30	62,62,62,62	42
81	MG	1	3848	1/1	0.85	0.58	62,62,62,62	0
80	PAR	1	3436	42/42	0.85	0.22	85,85,85,85	0
81	MG	n0	202	1/1	0.85	0.23	59,59,59,59	0
80	PAR	1	3431	42/42	0.85	0.25	67,67,67,67	42
81	MG	5	3938	1/1	0.85	0.25	74,74,74,74	0
81	MG	n1	202	1/1	0.85	0.50	63,63,63,63	0
81	MG	1	3511	1/1	0.85	0.11	73,73,73,73	0
80	PAR	5	3411	42/42	0.85	0.29	83,83,83,83	0
81	MG	5	3597	1/1	0.85	0.32	65,65,65,65	0
80	PAR	4	201	42/42	0.85	0.31	43,43,43,43	42
80	PAR	2	1901	42/42	0.85	0.32	82,82,82,82	42
81	MG	5	3947	1/1	0.85	0.28	57,57,57,57	0
81	MG	5	3950	1/1	0.85	0.34	61,61,61,61	0
81	MG	6	2068	1/1	0.85	0.63	71,71,71,71	0
81	MG	L2	306	1/1	0.85	0.37	51,51,51,51	0
81	MG	1	4176	1/1	0.85	0.71	78,78,78,78	0
81	MG	O7	104	1/1	0.85	0.31	43,43,43,43	0
81	MG	6	2074	1/1	0.85	0.32	81,81,81,81	0
81	MG	5	3616	1/1	0.85	0.14	81,81,81,81	0
81	MG	1	4177	1/1	0.85	0.39	57,57,57,57	0
81	MG	Q1	1301	1/1	0.85	0.44	58,58,58,58	0
81	MG	5	3621	1/1	0.85	0.49	65,65,65,65	0
81	MG	1	3496	1/1	0.85	0.50	52,52,52,52	0
81	MG	1	4181	1/1	0.85	0.26	49,49,49,49	0
81	MG	5	3626	1/1	0.85	0.32	60,60,60,60	0
81	MG	L4	403	1/1	0.85	0.36	39,39,39,39	0
81	MG	1	3797	1/1	0.85	0.19	53,53,53,53	0
81	MG	5	4101	1/1	0.85	0.81	67,67,67,67	0
81	MG	1	3499	1/1	0.85	0.51	52,52,52,52	0
81	MG	1	3603	1/1	0.86	0.33	52,52,52,52	0
80	PAR	1	3406	42/42	0.86	0.38	68,68,68,68	42
81	MG	1	4154	1/1	0.86	0.35	38,38,38,38	0
81	MG	2	1938	1/1	0.86	0.27	85,85,85,85	0
81	MG	1	3612	1/1	0.86	0.17	74,74,74,74	0
81	MG	5	3851	1/1	0.86	0.68	61,61,61,61	0
81	MG	M8	202	1/1	0.86	0.67	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	7	208	1/1	0.86	0.11	117,117,117,117	0
81	MG	4	212	1/1	0.86	0.19	57,57,57,57	0
81	MG	2	2052	1/1	0.86	0.25	95,95,95,95	0
81	MG	2	1999	1/1	0.86	0.17	74,74,74,74	0
80	PAR	1	3410	42/42	0.86	0.33	52,52,52,52	42
81	MG	6	2030	1/1	0.86	0.39	71,71,71,71	0
81	MG	8	204	1/1	0.86	0.69	69,69,69,69	0
81	MG	1	3996	1/1	0.86	0.49	78,78,78,78	0
81	MG	5	3993	1/1	0.86	0.28	64,64,64,64	0
81	MG	2	2060	1/1	0.86	0.41	103,103,103,103	0
81	MG	1	3953	1/1	0.86	0.18	54,54,54,54	0
80	PAR	6	1905	42/42	0.86	0.20	112,112,112,112	0
81	MG	5	4072	1/1	0.86	0.19	65,65,65,65	0
81	MG	1	3532	1/1	0.86	0.28	48,48,48,48	0
81	MG	2	2112	1/1	0.86	0.51	72,72,72,72	0
81	MG	2	2065	1/1	0.86	0.36	76,76,76,76	0
81	MG	5	3683	1/1	0.86	0.55	53,53,53,53	0
81	MG	6	2052	1/1	0.86	0.22	72,72,72,72	0
81	MG	5	4007	1/1	0.86	0.61	76,76,76,76	0
81	MG	2	1958	1/1	0.86	0.18	114,114,114,114	0
81	MG	1	3623	1/1	0.86	0.19	63,63,63,63	1
81	MG	5	3807	1/1	0.86	0.23	60,60,60,60	0
81	MG	1	3781	1/1	0.86	0.33	51,51,51,51	1
81	MG	1	3784	1/1	0.86	0.39	56,56,56,56	0
81	MG	6	1951	1/1	0.86	0.20	78,78,78,78	0
81	MG	5	4095	1/1	0.86	0.29	56,56,56,56	1
81	MG	1	3628	1/1	0.86	0.65	54,54,54,54	0
81	MG	5	4015	1/1	0.86	0.30	78,78,78,78	0
81	MG	5	3824	1/1	0.86	0.34	59,59,59,59	0
81	MG	5	3954	1/1	0.86	0.45	55,55,55,55	0
81	MG	2	1969	1/1	0.86	0.16	114,114,114,114	0
81	MG	5	4104	1/1	0.86	0.42	52,52,52,52	0
81	MG	2	1970	1/1	0.86	0.09	118,118,118,118	0
81	MG	2	1972	1/1	0.86	0.55	92,92,92,92	0
81	MG	m7	205	1/1	0.86	0.26	60,60,60,60	0
81	MG	5	3961	1/1	0.86	0.22	60,60,60,60	0
81	MG	6	1979	1/1	0.86	0.13	90,90,90,90	0
81	MG	6	1980	1/1	0.86	0.14	105,105,105,105	0
81	MG	m9	201	1/1	0.86	0.22	63,63,63,63	0
81	MG	1	3560	1/1	0.86	0.17	42,42,42,42	0
81	MG	5	3720	1/1	0.86	0.33	65,65,65,65	0
81	MG	c9	202	1/1	0.86	0.15	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	6	1993	1/1	0.86	0.35	76,76,76,76	0
81	MG	5	4113	1/1	0.86	0.88	74,74,74,74	0
81	MG	5	3723	1/1	0.86	0.32	69,69,69,69	0
80	PAR	1	3437	42/42	0.86	0.31	64,64,64,64	42
81	MG	O4	202	1/1	0.86	0.24	59,59,59,59	0
81	MG	1	3451	1/1	0.87	0.33	36,36,36,36	0
81	MG	6	1983	1/1	0.87	0.32	88,88,88,88	0
81	MG	1	3676	1/1	0.87	0.21	64,64,64,64	0
81	MG	6	1988	1/1	0.87	0.64	62,62,62,62	0
81	MG	L3	403	1/1	0.87	0.29	57,57,57,57	0
81	MG	1	3678	1/1	0.87	0.25	58,58,58,58	1
81	MG	5	3644	1/1	0.87	0.48	59,59,59,59	0
81	MG	5	3645	1/1	0.87	0.30	62,62,62,62	0
80	PAR	5	3413	42/42	0.87	0.29	72,72,72,72	42
80	PAR	5	3421	42/42	0.87	0.19	102,102,102,102	0
81	MG	1	4008	1/1	0.87	0.47	50,50,50,50	0
81	MG	5	3799	1/1	0.87	0.23	47,47,47,47	0
80	PAR	1	3404	42/42	0.87	0.27	53,53,53,53	42
81	MG	1	3631	1/1	0.87	0.34	47,47,47,47	0
81	MG	m9	205	1/1	0.87	0.39	75,75,75,75	0
81	MG	n0	201	1/1	0.87	0.14	59,59,59,59	0
81	MG	O1	203	1/1	0.87	0.27	74,74,74,74	0
80	PAR	5	3402	42/42	0.87	0.23	81,81,81,81	42
81	MG	5	3818	1/1	0.87	0.33	60,60,60,60	0
81	MG	5	3821	1/1	0.87	0.26	62,62,62,62	0
81	MG	2	2086	1/1	0.87	0.33	95,95,95,95	0
81	MG	5	3823	1/1	0.87	0.33	78,78,78,78	0
81	MG	1	4148	1/1	0.87	0.35	47,47,47,47	0
81	MG	5	3825	1/1	0.87	0.93	67,67,67,67	0
81	MG	5	3680	1/1	0.87	0.24	60,60,60,60	0
81	MG	5	3550	1/1	0.87	0.28	55,55,55,55	0
81	MG	1	3701	1/1	0.87	0.30	46,46,46,46	0
81	MG	2	1959	1/1	0.87	0.31	92,92,92,92	0
81	MG	6	2040	1/1	0.87	0.42	66,66,66,66	0
81	MG	5	3925	1/1	0.87	0.34	73,73,73,73	0
81	MG	1	3702	1/1	0.87	0.42	42,42,42,42	0
81	MG	5	3838	1/1	0.87	0.25	57,57,57,57	0
81	MG	1	3600	1/1	0.87	0.42	52,52,52,52	0
81	MG	Q2	504	1/1	0.87	0.22	42,42,42,42	0
81	MG	6	2050	1/1	0.87	0.42	80,80,80,80	0
81	MG	2	2097	1/1	0.87	0.49	62,62,62,62	0
81	MG	M3	201	1/1	0.87	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3714	1/1	0.87	0.22	44,44,44,44	0
81	MG	2	2101	1/1	0.87	0.52	61,61,61,61	0
81	MG	3	217	1/1	0.87	0.18	60,60,60,60	0
81	MG	1	3558	1/1	0.87	0.53	36,36,36,36	0
81	MG	1	3523	1/1	0.87	0.31	50,50,50,50	0
80	PAR	5	3425	42/42	0.87	0.29	75,75,75,75	42
81	MG	5	3726	1/1	0.87	0.62	69,69,69,69	0
81	MG	1	3642	1/1	0.87	0.17	63,63,63,63	0
81	MG	5	3856	1/1	0.87	0.24	51,51,51,51	0
81	MG	5	3857	1/1	0.87	0.23	60,60,60,60	0
81	MG	4	214	1/1	0.87	0.35	63,63,63,63	0
80	PAR	5	3409	42/42	0.87	0.32	56,56,56,56	42
81	MG	5	4046	1/1	0.87	0.34	68,68,68,68	0
81	MG	5	3958	1/1	0.87	0.24	61,61,61,61	1
81	MG	5	4055	1/1	0.87	0.21	56,56,56,56	0
81	MG	1	3895	1/1	0.87	0.24	65,65,65,65	0
81	MG	1	3782	1/1	0.87	0.21	82,82,82,82	0
81	MG	1	3961	1/1	0.87	0.20	40,40,40,40	0
81	MG	5	3751	1/1	0.87	0.42	50,50,50,50	0
81	MG	6	1958	1/1	0.87	0.33	81,81,81,81	0
81	MG	2	1988	1/1	0.87	0.14	86,86,86,86	0
81	MG	5	4065	1/1	0.87	0.17	100,100,100,100	0
81	MG	1	4037	1/1	0.87	0.21	97,97,97,97	0
81	MG	5	3624	1/1	0.87	0.39	76,76,76,76	0
80	PAR	3	203	42/42	0.87	0.26	78,78,78,78	0
81	MG	1	3665	1/1	0.87	0.32	54,54,54,54	0
81	MG	5	3979	1/1	0.87	0.31	73,73,73,73	0
81	MG	14	401	1/1	0.87	0.18	62,62,62,62	0
81	MG	5	4071	1/1	0.87	0.14	56,56,56,56	0
81	MG	2	1981	1/1	0.88	0.29	61,61,61,61	0
81	MG	5	3640	1/1	0.88	0.26	49,49,49,49	0
80	PAR	3	202	42/42	0.88	0.31	55,55,55,55	42
81	MG	2	1984	1/1	0.88	0.74	59,59,59,59	0
81	MG	5	4114	1/1	0.88	0.29	52,52,52,52	0
81	MG	5	3984	1/1	0.88	0.56	85,85,85,85	0
81	MG	1	3909	1/1	0.88	0.86	65,65,65,65	0
81	MG	O6	201	1/1	0.88	0.37	56,56,56,56	0
81	MG	O7	102	1/1	0.88	0.25	43,43,43,43	0
81	MG	4	233	1/1	0.88	0.36	57,57,57,57	0
81	MG	5	4121	1/1	0.88	0.17	65,65,65,65	0
81	MG	1	3913	1/1	0.88	0.39	66,66,66,66	0
81	MG	2	1996	1/1	0.88	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
80	PAR	1	3417	42/42	0.88	0.31	66,66,66,66	42
81	MG	1	4094	1/1	0.88	0.24	84,84,84,84	0
81	MG	1	4162	1/1	0.88	0.24	63,63,63,63	0
81	MG	6	1974	1/1	0.88	0.12	110,110,110,110	0
81	MG	1	3915	1/1	0.88	0.40	69,69,69,69	0
81	MG	1	3917	1/1	0.88	0.31	69,69,69,69	0
81	MG	1	3635	1/1	0.88	0.31	49,49,49,49	0
81	MG	1	3527	1/1	0.88	0.25	32,32,32,32	0
81	MG	1	3610	1/1	0.88	0.20	58,58,58,58	0
80	PAR	7	202	42/42	0.88	0.27	59,59,59,59	42
81	MG	6	1984	1/1	0.88	0.17	89,89,89,89	0
81	MG	5	4006	1/1	0.88	0.61	68,68,68,68	0
80	PAR	1	3434	42/42	0.88	0.20	85,85,85,85	42
81	MG	2	2117	1/1	0.88	0.30	90,90,90,90	0
81	MG	1	3713	1/1	0.88	0.28	53,53,53,53	0
81	MG	8	214	1/1	0.88	0.17	61,61,61,61	0
81	MG	1	3945	1/1	0.88	0.18	49,49,49,49	0
81	MG	5	3881	1/1	0.88	0.23	58,58,58,58	0
81	MG	1	3653	1/1	0.88	0.32	51,51,51,51	0
81	MG	6	2002	1/1	0.88	0.60	64,64,64,64	0
81	MG	1	3519	1/1	0.88	0.31	43,43,43,43	0
81	MG	5	3709	1/1	0.88	0.36	54,54,54,54	0
81	MG	1	4044	1/1	0.88	0.25	48,48,48,48	0
81	MG	5	4017	1/1	0.88	0.88	67,67,67,67	0
81	MG	5	3467	1/1	0.88	0.49	49,49,49,49	0
81	MG	13	402	1/1	0.88	0.13	59,59,59,59	0
81	MG	1	4046	1/1	0.88	0.23	49,49,49,49	0
81	MG	1	4047	1/1	0.88	0.20	50,50,50,50	0
81	MG	1	3881	1/1	0.88	0.22	72,72,72,72	0
81	MG	2	2034	1/1	0.88	0.09	113,113,113,113	0
81	MG	5	3517	1/1	0.88	0.30	57,57,57,57	0
81	MG	2	2036	1/1	0.88	0.12	127,127,127,127	0
81	MG	2	1935	1/1	0.88	0.35	78,78,78,78	0
81	MG	1	3617	1/1	0.88	0.20	75,75,75,75	0
81	MG	5	3531	1/1	0.88	0.48	49,49,49,49	0
81	MG	2	2042	1/1	0.88	0.12	126,126,126,126	0
81	MG	M5	304	1/1	0.88	0.28	61,61,61,61	0
81	MG	1	3731	1/1	0.88	0.52	52,52,52,52	0
81	MG	2	2046	1/1	0.88	0.29	60,60,60,60	0
81	MG	1	3663	1/1	0.88	0.34	48,48,48,48	0
81	MG	5	3770	1/1	0.88	0.48	59,59,59,59	0
81	MG	5	3547	1/1	0.88	0.25	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3921	1/1	0.88	0.26	91,91,91,91	0
81	MG	6	2046	1/1	0.88	0.33	118,118,118,118	0
81	MG	1	3841	1/1	0.88	0.31	60,60,60,60	0
81	MG	5	3773	1/1	0.88	0.32	80,80,80,80	0
81	MG	1	3756	1/1	0.88	0.21	47,47,47,47	0
81	MG	M6	205	1/1	0.88	0.37	53,53,53,53	0
81	MG	2	2056	1/1	0.88	0.42	80,80,80,80	0
81	MG	5	3788	1/1	0.88	0.24	68,68,68,68	0
81	MG	2	1948	1/1	0.88	0.21	85,85,85,85	0
81	MG	5	3565	1/1	0.88	0.22	80,80,80,80	0
81	MG	1	4060	1/1	0.88	0.24	58,58,58,58	0
81	MG	2	1951	1/1	0.88	0.09	134,134,134,134	0
81	MG	3	211	1/1	0.88	0.24	86,86,86,86	0
81	MG	1	3539	1/1	0.88	0.21	30,30,30,30	0
81	MG	1	3958	1/1	0.88	0.26	59,59,59,59	0
81	MG	1	3769	1/1	0.88	0.25	54,54,54,54	0
81	MG	1	4069	1/1	0.88	0.21	74,74,74,74	0
81	MG	5	3813	1/1	0.88	1.07	70,70,70,70	0
81	MG	1	4126	1/1	0.88	0.34	35,35,35,35	0
81	MG	1	3520	1/1	0.88	0.40	51,51,51,51	0
81	MG	o2	203	1/1	0.88	0.26	49,49,49,49	0
81	MG	N3	204	1/1	0.88	0.34	53,53,53,53	0
81	MG	5	3613	1/1	0.88	0.23	80,80,80,80	0
81	MG	2	1967	1/1	0.88	0.32	100,100,100,100	0
81	MG	1	3897	1/1	0.88	0.19	56,56,56,56	0
81	MG	2	2075	1/1	0.88	0.14	95,95,95,95	0
80	PAR	1	3432	42/42	0.88	0.30	51,51,51,51	42
81	MG	N6	205	1/1	0.88	0.36	67,67,67,67	0
81	MG	1	3783	1/1	0.88	0.22	57,57,57,57	0
81	MG	2	2082	1/1	0.88	0.26	119,119,119,119	0
80	PAR	5	3426	42/42	0.88	0.26	56,56,56,56	42
81	MG	1	4142	1/1	0.88	0.20	83,83,83,83	0
81	MG	1	3596	1/1	0.88	0.18	44,44,44,44	0
81	MG	1	4022	1/1	0.88	0.26	47,47,47,47	1
81	MG	1	4024	1/1	0.88	0.66	61,61,61,61	0
81	MG	5	3754	1/1	0.89	0.18	53,53,53,53	0
81	MG	1	3537	1/1	0.89	0.37	31,31,31,31	0
81	MG	4	206	1/1	0.89	0.31	48,48,48,48	0
81	MG	5	3888	1/1	0.89	0.30	61,61,61,61	0
81	MG	5	3610	1/1	0.89	0.20	81,81,81,81	0
81	MG	1	3670	1/1	0.89	0.27	57,57,57,57	1
81	MG	N1	203	1/1	0.89	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3493	1/1	0.89	0.18	50,50,50,50	0
81	MG	1	3991	1/1	0.89	0.30	41,41,41,41	1
81	MG	5	4008	1/1	0.89	0.70	59,59,59,59	0
80	PAR	6	1901	42/42	0.89	0.27	90,90,90,90	0
81	MG	2	2105	1/1	0.89	0.27	62,62,62,62	0
81	MG	1	4157	1/1	0.89	0.35	44,44,44,44	0
81	MG	1	4158	1/1	0.89	0.20	55,55,55,55	0
81	MG	6	1971	1/1	0.89	0.16	89,89,89,89	0
81	MG	2	2039	1/1	0.89	0.23	113,113,113,113	0
81	MG	1	4159	1/1	0.89	0.16	55,55,55,55	1
81	MG	1	3994	1/1	0.89	0.49	61,61,61,61	0
81	MG	6	1976	1/1	0.89	0.37	89,89,89,89	0
81	MG	1	3952	1/1	0.89	0.19	63,63,63,63	0
81	MG	1	3997	1/1	0.89	0.38	80,80,80,80	0
81	MG	5	4018	1/1	0.89	0.56	95,95,95,95	0
81	MG	L2	305	1/1	0.89	0.35	47,47,47,47	0
81	MG	1	3893	1/1	0.89	0.24	71,71,71,71	0
81	MG	1	3498	1/1	0.89	0.49	66,66,66,66	0
81	MG	5	3806	1/1	0.89	0.24	65,65,65,65	0
81	MG	6	1987	1/1	0.89	0.21	68,68,68,68	0
80	PAR	2	1904	42/42	0.89	0.18	107,107,107,107	0
81	MG	5	3809	1/1	0.89	0.34	49,49,49,49	0
81	MG	S9	201	1/1	0.89	0.24	126,126,126,126	0
81	MG	2	2053	1/1	0.89	0.20	100,100,100,100	0
81	MG	8	224	1/1	0.89	0.60	59,59,59,59	0
81	MG	1	4106	1/1	0.89	0.57	68,68,68,68	0
81	MG	5	3815	1/1	0.89	0.34	55,55,55,55	0
81	MG	2	1971	1/1	0.89	0.43	73,73,73,73	0
81	MG	5	3648	1/1	0.89	0.24	59,59,59,59	0
81	MG	6	2006	1/1	0.89	0.48	76,76,76,76	0
81	MG	5	3656	1/1	0.89	0.35	40,40,40,40	0
80	PAR	1	3414	42/42	0.89	0.24	63,63,63,63	42
81	MG	5	3939	1/1	0.89	0.29	74,74,74,74	0
81	MG	1	3550	1/1	0.89	0.24	64,64,64,64	0
81	MG	5	4049	1/1	0.89	0.18	73,73,73,73	0
81	MG	O7	105	1/1	0.89	0.28	41,41,41,41	0
81	MG	5	3506	1/1	0.89	0.25	55,55,55,55	0
81	MG	6	2023	1/1	0.89	0.29	90,90,90,90	0
81	MG	1	3854	1/1	0.89	0.27	52,52,52,52	0
81	MG	6	2025	1/1	0.89	0.23	85,85,85,85	0
80	PAR	5	3415	42/42	0.89	0.23	83,83,83,83	0
80	PAR	5	3401	42/42	0.89	0.20	78,78,78,78	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3858	1/1	0.89	0.17	106,106,106,106	0
81	MG	1	3641	1/1	0.89	0.20	57,57,57,57	0
81	MG	m6	203	1/1	0.89	0.27	55,55,55,55	1
81	MG	5	4063	1/1	0.89	0.36	80,80,80,80	0
81	MG	m7	206	1/1	0.89	0.28	50,50,50,50	0
81	MG	2	2067	1/1	0.89	0.25	75,75,75,75	0
81	MG	6	2038	1/1	0.89	0.25	105,105,105,105	0
81	MG	1	3465	1/1	0.89	0.26	34,34,34,34	0
81	MG	5	3689	1/1	0.89	0.31	59,59,59,59	0
81	MG	1	3504	1/1	0.89	0.36	58,58,58,58	0
81	MG	1	4067	1/1	0.89	0.16	54,54,54,54	0
81	MG	1	3568	1/1	0.89	0.26	55,55,55,55	0
81	MG	1	3481	1/1	0.89	0.24	48,48,48,48	0
81	MG	1	4120	1/1	0.89	0.28	81,81,81,81	0
81	MG	n0	205	1/1	0.89	0.12	62,62,62,62	0
81	MG	2	2076	1/1	0.89	0.46	92,92,92,92	0
81	MG	1	3870	1/1	0.89	0.23	36,36,36,36	1
81	MG	n3	204	1/1	0.89	0.35	50,50,50,50	0
81	MG	1	4122	1/1	0.89	0.24	68,68,68,68	0
81	MG	5	4080	1/1	0.89	0.16	64,64,64,64	0
81	MG	5	3558	1/1	0.89	0.31	70,70,70,70	0
81	MG	5	4083	1/1	0.89	0.29	78,78,78,78	0
81	MG	5	3969	1/1	0.89	0.28	55,55,55,55	0
81	MG	5	3970	1/1	0.89	0.28	59,59,59,59	0
81	MG	1	3727	1/1	0.89	0.51	39,39,39,39	1
81	MG	M5	307	1/1	0.89	0.37	43,43,43,43	0
81	MG	5	3975	1/1	0.89	0.33	57,57,57,57	0
81	MG	5	3978	1/1	0.89	0.27	72,72,72,72	0
80	PAR	1	3427	42/42	0.89	0.26	65,65,65,65	42
81	MG	1	3927	1/1	0.89	0.18	53,53,53,53	0
81	MG	o4	202	1/1	0.89	0.16	89,89,89,89	0
81	MG	o7	503	1/1	0.89	0.28	58,58,58,58	0
81	MG	5	3868	1/1	0.89	0.16	57,57,57,57	0
81	MG	1	3729	1/1	0.89	0.47	44,44,44,44	0
81	MG	1	3730	1/1	0.89	0.70	47,47,47,47	0
81	MG	1	3587	1/1	0.89	0.50	53,53,53,53	0
81	MG	5	4102	1/1	0.89	0.24	48,48,48,48	1
81	MG	5	3740	1/1	0.89	0.44	68,68,68,68	0
81	MG	1	4032	1/1	0.89	0.34	41,41,41,41	0
81	MG	1	3940	1/1	0.89	0.41	37,37,37,37	0
81	MG	6	1927	1/1	0.89	0.43	73,73,73,73	0
81	MG	5	3745	1/1	0.89	0.69	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3837	1/1	0.89	0.35	63,63,63,63	0
81	MG	5	3748	1/1	0.89	0.24	50,50,50,50	0
81	MG	1	3744	1/1	0.89	0.31	39,39,39,39	0
81	MG	5	3992	1/1	0.89	0.37	59,59,59,59	0
81	MG	5	3752	1/1	0.89	0.12	60,60,60,60	0
81	MG	5	3742	1/1	0.90	0.25	53,53,53,53	0
81	MG	2	2012	1/1	0.90	0.10	104,104,104,104	0
81	MG	5	3595	1/1	0.90	0.15	83,83,83,83	0
80	PAR	5	3419	42/42	0.90	0.27	57,57,57,57	0
81	MG	6	1950	1/1	0.90	0.23	83,83,83,83	0
81	MG	4	204	1/1	0.90	0.53	51,51,51,51	0
81	MG	5	3750	1/1	0.90	0.37	46,46,46,46	0
81	MG	5	3602	1/1	0.90	0.14	87,87,87,87	0
81	MG	5	3884	1/1	0.90	0.15	67,67,67,67	0
81	MG	1	3535	1/1	0.90	0.42	36,36,36,36	1
81	MG	5	4002	1/1	0.90	0.32	66,66,66,66	0
81	MG	1	3739	1/1	0.90	0.27	43,43,43,43	0
81	MG	1	3740	1/1	0.90	0.36	42,42,42,42	0
81	MG	5	4005	1/1	0.90	0.25	85,85,85,85	0
81	MG	5	3763	1/1	0.90	0.36	42,42,42,42	0
81	MG	6	1969	1/1	0.90	0.31	101,101,101,101	0
81	MG	1	3820	1/1	0.90	0.21	54,54,54,54	0
81	MG	1	3563	1/1	0.90	0.10	55,55,55,55	0
81	MG	2	1945	1/1	0.90	0.17	88,88,88,88	0
81	MG	4	220	1/1	0.90	0.30	45,45,45,45	0
81	MG	1	3825	1/1	0.90	0.21	65,65,65,65	0
81	MG	8	206	1/1	0.90	0.20	56,56,56,56	0
81	MG	4	224	1/1	0.90	0.34	55,55,55,55	0
81	MG	1	3681	1/1	0.90	0.37	53,53,53,53	0
81	MG	1	3919	1/1	0.90	0.32	48,48,48,48	0
81	MG	1	3921	1/1	0.90	0.28	40,40,40,40	0
81	MG	5	3781	1/1	0.90	0.40	49,49,49,49	0
81	MG	2	2040	1/1	0.90	0.30	123,123,123,123	0
81	MG	1	4011	1/1	0.90	0.77	54,54,54,54	0
80	PAR	1	3418	42/42	0.90	0.21	69,69,69,69	42
81	MG	1	4059	1/1	0.90	0.33	53,53,53,53	0
81	MG	1	3970	1/1	0.90	0.20	55,55,55,55	0
81	MG	1	3607	1/1	0.90	0.71	57,57,57,57	1
81	MG	5	3795	1/1	0.90	0.12	106,106,106,106	0
81	MG	5	4029	1/1	0.90	0.35	57,57,57,57	0
81	MG	1	4017	1/1	0.90	0.35	57,57,57,57	0
80	PAR	1	3420	42/42	0.90	0.21	65,65,65,65	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3804	1/1	0.90	0.26	48,48,48,48	0
81	MG	O2	203	1/1	0.90	0.16	38,38,38,38	0
81	MG	1	3773	1/1	0.90	0.38	47,47,47,47	0
81	MG	1	4068	1/1	0.90	0.33	51,51,51,51	0
81	MG	5	3930	1/1	0.90	0.34	50,50,50,50	0
81	MG	5	3931	1/1	0.90	0.46	54,54,54,54	0
81	MG	5	3933	1/1	0.90	0.60	42,42,42,42	0
81	MG	1	3775	1/1	0.90	0.35	47,47,47,47	0
81	MG	5	3651	1/1	0.90	0.17	63,63,63,63	1
81	MG	6	2021	1/1	0.90	0.46	85,85,85,85	0
81	MG	5	4048	1/1	0.90	0.27	66,66,66,66	0
81	MG	5	3653	1/1	0.90	0.57	45,45,45,45	0
81	MG	1	3569	1/1	0.90	0.17	61,61,61,61	0
81	MG	5	4052	1/1	0.90	0.21	53,53,53,53	0
80	PAR	1	3422	42/42	0.90	0.27	51,51,51,51	42
81	MG	5	3490	1/1	0.90	0.35	50,50,50,50	0
81	MG	5	3662	1/1	0.90	0.41	56,56,56,56	0
81	MG	6	2032	1/1	0.90	0.23	78,78,78,78	0
81	MG	5	3504	1/1	0.90	0.23	53,53,53,53	0
81	MG	2	1975	1/1	0.90	0.31	94,94,94,94	0
81	MG	1	3649	1/1	0.90	0.51	37,37,37,37	0
81	MG	5	3674	1/1	0.90	0.31	49,49,49,49	0
81	MG	5	3949	1/1	0.90	0.15	58,58,58,58	1
81	MG	1	3944	1/1	0.90	0.44	48,48,48,48	0
81	MG	Q2	502	1/1	0.90	0.28	38,38,38,38	0
81	MG	1	3983	1/1	0.90	0.30	51,51,51,51	1
81	MG	5	3834	1/1	0.90	0.12	77,77,77,77	0
81	MG	1	4190	1/1	0.90	0.21	73,73,73,73	0
81	MG	5	3836	1/1	0.90	0.28	51,51,51,51	0
81	MG	1	3891	1/1	0.90	0.23	59,59,59,59	0
81	MG	5	3684	1/1	0.90	0.57	55,55,55,55	0
81	MG	5	4074	1/1	0.90	0.13	71,71,71,71	0
81	MG	2	1983	1/1	0.90	0.74	68,68,68,68	0
81	MG	5	3533	1/1	0.90	0.24	50,50,50,50	0
81	MG	1	4124	1/1	0.90	0.40	69,69,69,69	0
81	MG	5	4081	1/1	0.90	0.28	102,102,102,102	0
81	MG	Q3	503	1/1	0.90	0.28	54,54,54,54	0
81	MG	M0	301	1/1	0.90	0.21	54,54,54,54	0
81	MG	2	2073	1/1	0.90	0.16	99,99,99,99	0
81	MG	1	3892	1/1	0.90	0.14	72,72,72,72	0
81	MG	1	3583	1/1	0.90	0.25	49,49,49,49	0
81	MG	o2	202	1/1	0.90	0.47	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4128	1/1	0.90	0.33	47,47,47,47	0
81	MG	1	4130	1/1	0.90	0.26	38,38,38,38	1
81	MG	2	2079	1/1	0.90	0.29	75,75,75,75	0
81	MG	5	3976	1/1	0.90	0.34	58,58,58,58	0
81	MG	5	4096	1/1	0.90	0.25	52,52,52,52	0
81	MG	5	3714	1/1	0.90	0.28	58,58,58,58	0
81	MG	1	4088	1/1	0.90	0.69	79,79,79,79	0
81	MG	6	1916	1/1	0.90	0.21	79,79,79,79	0
81	MG	1	3542	1/1	0.90	0.24	38,38,38,38	0
81	MG	5	3859	1/1	0.90	0.41	51,51,51,51	0
81	MG	1	4134	1/1	0.90	0.36	69,69,69,69	0
81	MG	2	2002	1/1	0.90	0.16	79,79,79,79	0
81	MG	5	4103	1/1	0.90	0.47	52,52,52,52	0
80	PAR	5	3424	42/42	0.90	0.28	65,65,65,65	42
81	MG	6	1934	1/1	0.90	0.41	83,83,83,83	0
80	PAR	5	3414	42/42	0.90	0.22	67,67,67,67	42
81	MG	d2	201	1/1	0.90	0.43	84,84,84,84	0
81	MG	5	3736	1/1	0.90	0.37	46,46,46,46	0
80	PAR	1	3407	42/42	0.90	0.33	69,69,69,69	42
81	MG	5	4110	1/1	0.90	0.77	82,82,82,82	0
80	PAR	5	3418	42/42	0.90	0.24	98,98,98,98	0
80	PAR	6	1904	42/42	0.90	0.28	72,72,72,72	0
81	MG	1	3522	1/1	0.91	0.31	52,52,52,52	0
81	MG	5	3468	1/1	0.91	0.32	44,44,44,44	0
81	MG	1	3910	1/1	0.91	0.54	48,48,48,48	0
81	MG	5	3666	1/1	0.91	0.18	44,44,44,44	0
81	MG	5	4094	1/1	0.91	0.28	48,48,48,48	0
81	MG	6	1933	1/1	0.91	0.70	92,92,92,92	0
81	MG	5	3481	1/1	0.91	0.24	47,47,47,47	0
81	MG	1	3911	1/1	0.91	0.35	43,43,43,43	0
81	MG	5	3671	1/1	0.91	0.45	56,56,56,56	0
81	MG	5	3965	1/1	0.91	0.36	58,58,58,58	0
81	MG	N8	202	1/1	0.91	0.15	59,59,59,59	0
81	MG	5	3500	1/1	0.91	0.52	56,56,56,56	0
81	MG	4	228	1/1	0.91	0.17	47,47,47,47	0
81	MG	2	2055	1/1	0.91	0.35	56,56,56,56	0
81	MG	1	4049	1/1	0.91	0.26	51,51,51,51	0
81	MG	5	3973	1/1	0.91	0.32	47,47,47,47	1
81	MG	1	4051	1/1	0.91	0.33	51,51,51,51	0
81	MG	1	3719	1/1	0.91	0.16	42,42,42,42	0
81	MG	1	3540	1/1	0.91	0.34	33,33,33,33	0
81	MG	1	4170	1/1	0.91	0.43	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3688	1/1	0.91	0.31	59,59,59,59	0
80	PAR	7	201	42/42	0.91	0.21	85,85,85,85	0
81	MG	1	3570	1/1	0.91	0.34	60,60,60,60	0
81	MG	2	1977	1/1	0.91	0.10	96,96,96,96	0
81	MG	5	3854	1/1	0.91	0.21	65,65,65,65	0
81	MG	1	4009	1/1	0.91	0.42	46,46,46,46	0
81	MG	1	3918	1/1	0.91	0.20	70,70,70,70	0
81	MG	1	3492	1/1	0.91	0.36	47,47,47,47	0
81	MG	6	1968	1/1	0.91	0.23	77,77,77,77	0
81	MG	5	3858	1/1	0.91	0.28	62,62,62,62	0
80	PAR	6	1903	42/42	0.91	0.26	74,74,74,74	0
81	MG	5	3542	1/1	0.91	0.62	50,50,50,50	0
81	MG	5	3544	1/1	0.91	0.41	55,55,55,55	0
80	PAR	1	3402	42/42	0.91	0.19	62,62,62,62	42
81	MG	1	4063	1/1	0.91	0.38	47,47,47,47	0
81	MG	5	3548	1/1	0.91	0.38	52,52,52,52	0
81	MG	1	3850	1/1	0.91	0.14	57,57,57,57	0
81	MG	1	3926	1/1	0.91	0.31	53,53,53,53	0
81	MG	5	3555	1/1	0.91	0.46	54,54,54,54	0
81	MG	L7	301	1/1	0.91	0.24	52,52,52,52	0
81	MG	1	3885	1/1	0.91	0.17	67,67,67,67	0
81	MG	1	3929	1/1	0.91	0.32	47,47,47,47	1
81	MG	5	3737	1/1	0.91	0.36	43,43,43,43	0
81	MG	8	207	1/1	0.91	0.12	79,79,79,79	0
81	MG	8	208	1/1	0.91	0.21	71,71,71,71	0
81	MG	1	4188	1/1	0.91	0.20	57,57,57,57	0
81	MG	2	1993	1/1	0.91	0.26	83,83,83,83	0
81	MG	2	1909	1/1	0.91	0.20	88,88,88,88	0
81	MG	2	1997	1/1	0.91	0.16	81,81,81,81	0
81	MG	6	2000	1/1	0.91	0.09	107,107,107,107	0
81	MG	5	3885	1/1	0.91	0.19	65,65,65,65	0
81	MG	1	3888	1/1	0.91	0.21	42,42,42,42	0
81	MG	1	3790	1/1	0.91	0.15	62,62,62,62	0
81	MG	1	4194	1/1	0.91	0.25	50,50,50,50	0
81	MG	5	3889	1/1	0.91	0.36	66,66,66,66	0
81	MG	1	4074	1/1	0.91	0.49	57,57,57,57	0
81	MG	5	3891	1/1	0.91	0.17	68,68,68,68	0
81	MG	5	3588	1/1	0.91	0.20	69,69,69,69	0
81	MG	1	4196	1/1	0.91	0.24	46,46,46,46	1
81	MG	5	3895	1/1	0.91	0.19	56,56,56,56	0
81	MG	12	303	1/1	0.91	0.43	66,66,66,66	0
81	MG	1	3976	1/1	0.91	0.22	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3753	1/1	0.91	0.31	57,57,57,57	0
81	MG	5	4020	1/1	0.91	0.41	100,100,100,100	0
81	MG	2	2006	1/1	0.91	0.14	66,66,66,66	0
81	MG	1	3978	1/1	0.91	0.20	68,68,68,68	0
81	MG	1	3933	1/1	0.91	0.15	65,65,65,65	1
81	MG	5	3604	1/1	0.91	0.23	62,62,62,62	0
81	MG	5	3607	1/1	0.91	0.24	49,49,49,49	0
81	MG	5	3905	1/1	0.91	0.21	121,121,121,121	0
81	MG	5	3768	1/1	0.91	0.26	55,55,55,55	0
81	MG	5	3907	1/1	0.91	0.28	81,81,81,81	0
80	PAR	2	1902	42/42	0.91	0.27	74,74,74,74	0
81	MG	m0	302	1/1	0.91	0.20	66,66,66,66	0
81	MG	M5	305	1/1	0.91	0.28	52,52,52,52	0
81	MG	1	4081	1/1	0.91	0.23	63,63,63,63	0
81	MG	2	2099	1/1	0.91	0.35	57,57,57,57	0
81	MG	1	3551	1/1	0.91	0.36	46,46,46,46	0
80	PAR	1	3412	42/42	0.91	0.25	67,67,67,67	0
81	MG	6	2043	1/1	0.91	0.18	97,97,97,97	0
81	MG	1	4087	1/1	0.91	0.49	67,67,67,67	0
81	MG	5	3917	1/1	0.91	0.47	72,72,72,72	0
81	MG	5	3918	1/1	0.91	0.44	60,60,60,60	0
81	MG	m9	202	1/1	0.91	0.21	80,80,80,80	0
81	MG	5	3920	1/1	0.91	0.40	65,65,65,65	0
81	MG	5	3779	1/1	0.91	0.38	52,52,52,52	0
81	MG	5	4051	1/1	0.91	0.31	61,61,61,61	0
81	MG	1	3943	1/1	0.91	0.32	40,40,40,40	0
81	MG	1	3803	1/1	0.91	0.27	55,55,55,55	0
81	MG	1	3622	1/1	0.91	0.43	54,54,54,54	0
81	MG	1	3760	1/1	0.91	0.13	43,43,43,43	0
81	MG	2	1942	1/1	0.91	0.20	77,77,77,77	0
81	MG	1	4143	1/1	0.91	0.47	62,62,62,62	0
81	MG	n2	201	1/1	0.91	0.15	97,97,97,97	0
81	MG	5	3627	1/1	0.91	0.27	59,59,59,59	0
81	MG	2	2033	1/1	0.91	0.23	75,75,75,75	0
81	MG	5	3934	1/1	0.91	0.46	58,58,58,58	0
81	MG	1	3810	1/1	0.91	0.36	96,96,96,96	0
81	MG	5	3635	1/1	0.91	0.16	59,59,59,59	0
81	MG	5	3638	1/1	0.91	0.25	58,58,58,58	0
81	MG	1	3811	1/1	0.91	0.07	64,64,64,64	0
80	PAR	1	3419	42/42	0.91	0.24	59,59,59,59	0
81	MG	1	3625	1/1	0.91	0.23	36,36,36,36	1
81	MG	4	213	1/1	0.91	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3867	1/1	0.91	0.53	47,47,47,47	0
81	MG	s2	301	1/1	0.91	0.12	95,95,95,95	0
81	MG	S6	301	1/1	0.91	0.33	118,118,118,118	0
80	PAR	1	3430	42/42	0.91	0.20	65,65,65,65	42
81	MG	N6	202	1/1	0.91	0.30	50,50,50,50	0
81	MG	5	3649	1/1	0.91	0.35	50,50,50,50	0
81	MG	5	3820	1/1	0.91	0.19	59,59,59,59	0
81	MG	5	3650	1/1	0.91	0.40	46,46,46,46	0
81	MG	4	217	1/1	0.91	0.32	72,72,72,72	0
81	MG	6	1908	1/1	0.91	0.23	76,76,76,76	0
81	MG	6	1910	1/1	0.91	0.19	78,78,78,78	0
80	PAR	1	3415	42/42	0.91	0.27	46,46,46,46	42
81	MG	d4	201	1/1	0.91	0.22	91,91,91,91	0
81	MG	5	3447	1/1	0.91	0.21	45,45,45,45	0
81	MG	5	4086	1/1	0.91	0.16	79,79,79,79	0
81	MG	1	4101	1/1	0.92	0.23	113,113,113,113	0
81	MG	5	3848	1/1	0.92	0.27	95,95,95,95	0
81	MG	5	3696	1/1	0.92	0.29	59,59,59,59	0
81	MG	1	4169	1/1	0.92	0.28	48,48,48,48	0
81	MG	5	3698	1/1	0.92	0.28	49,49,49,49	0
81	MG	1	3939	1/1	0.92	0.30	49,49,49,49	1
81	MG	2	2077	1/1	0.92	0.06	121,121,121,121	0
81	MG	5	3706	1/1	0.92	0.39	64,64,64,64	0
81	MG	1	3886	1/1	0.92	0.34	38,38,38,38	0
81	MG	1	3838	1/1	0.92	0.27	53,53,53,53	0
81	MG	1	3762	1/1	0.92	0.17	54,54,54,54	0
81	MG	1	3494	1/1	0.92	0.41	44,44,44,44	0
81	MG	5	3563	1/1	0.92	0.26	85,85,85,85	0
81	MG	1	3556	1/1	0.92	0.28	36,36,36,36	0
81	MG	5	3869	1/1	0.92	0.14	64,64,64,64	0
81	MG	5	3567	1/1	0.92	0.18	73,73,73,73	0
81	MG	5	3570	1/1	0.92	0.21	110,110,110,110	0
81	MG	L5	302	1/1	0.92	0.23	68,68,68,68	0
81	MG	5	4124	1/1	0.92	0.40	81,81,81,81	0
81	MG	1	4052	1/1	0.92	0.22	50,50,50,50	0
81	MG	5	3730	1/1	0.92	0.47	55,55,55,55	0
81	MG	5	3732	1/1	0.92	0.50	50,50,50,50	0
81	MG	1	3509	1/1	0.92	0.10	74,74,74,74	0
81	MG	1	3633	1/1	0.92	0.41	49,49,49,49	0
81	MG	2	2088	1/1	0.92	0.35	64,64,64,64	0
81	MG	1	3776	1/1	0.92	0.46	52,52,52,52	0
80	PAR	5	3416	42/42	0.92	0.23	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	L9	202	1/1	0.92	0.29	58,58,58,58	0
81	MG	1	3693	1/1	0.92	0.31	46,46,46,46	0
80	PAR	5	3412	42/42	0.92	0.21	47,47,47,47	42
81	MG	5	3744	1/1	0.92	0.79	58,58,58,58	0
81	MG	1	3898	1/1	0.92	0.09	70,70,70,70	0
81	MG	5	3746	1/1	0.92	0.30	50,50,50,50	0
81	MG	1	3467	1/1	0.92	0.28	31,31,31,31	0
81	MG	1	3470	1/1	0.92	0.26	42,42,42,42	0
81	MG	5	3605	1/1	0.92	0.12	71,71,71,71	0
81	MG	2	1928	1/1	0.92	0.22	75,75,75,75	0
81	MG	1	4193	1/1	0.92	0.34	66,66,66,66	0
81	MG	5	3894	1/1	0.92	0.15	57,57,57,57	0
80	PAR	4	202	42/42	0.92	0.24	49,49,49,49	42
81	MG	5	3612	1/1	0.92	0.14	70,70,70,70	0
81	MG	5	3897	1/1	0.92	0.31	55,55,55,55	0
81	MG	1	3486	1/1	0.92	0.20	38,38,38,38	0
81	MG	6	1999	1/1	0.92	0.30	82,82,82,82	0
81	MG	5	3757	1/1	0.92	0.22	57,57,57,57	0
81	MG	1	3959	1/1	0.92	0.29	52,52,52,52	0
81	MG	2	2022	1/1	0.92	0.22	79,79,79,79	0
81	MG	5	4023	1/1	0.92	0.43	60,60,60,60	0
81	MG	1	3544	1/1	0.92	0.28	32,32,32,32	0
81	MG	6	2008	1/1	0.92	0.59	98,98,98,98	0
81	MG	5	3617	1/1	0.92	0.20	69,69,69,69	0
81	MG	1	3908	1/1	0.92	0.65	49,49,49,49	0
81	MG	1	3643	1/1	0.92	0.32	55,55,55,55	0
81	MG	M6	201	1/1	0.92	0.30	53,53,53,53	0
81	MG	2	2029	1/1	0.92	0.34	81,81,81,81	0
81	MG	14	403	1/1	0.92	0.31	80,80,80,80	0
81	MG	17	301	1/1	0.92	0.19	58,58,58,58	0
81	MG	1	4072	1/1	0.92	0.23	80,80,80,80	0
81	MG	1	3646	1/1	0.92	0.19	42,42,42,42	0
81	MG	5	3912	1/1	0.92	0.20	63,63,63,63	0
81	MG	1	3545	1/1	0.92	0.28	37,37,37,37	0
81	MG	1	4075	1/1	0.92	0.34	55,55,55,55	0
81	MG	5	4039	1/1	0.92	0.64	56,56,56,56	0
81	MG	1	3863	1/1	0.92	0.17	46,46,46,46	0
81	MG	5	3782	1/1	0.92	0.26	46,46,46,46	0
81	MG	2	2038	1/1	0.92	0.13	109,109,109,109	0
81	MG	1	3722	1/1	0.92	0.29	50,50,50,50	0
81	MG	1	3652	1/1	0.92	0.35	41,41,41,41	0
81	MG	1	3916	1/1	0.92	0.28	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	1952	1/1	0.92	0.20	132,132,132,132	0
81	MG	1	4138	1/1	0.92	0.27	55,55,55,55	0
81	MG	5	3431	1/1	0.92	0.25	42,42,42,42	0
81	MG	5	3437	1/1	0.92	0.22	43,43,43,43	0
81	MG	1	3578	1/1	0.92	0.24	41,41,41,41	0
81	MG	1	4028	1/1	0.92	0.28	45,45,45,45	0
81	MG	1	3869	1/1	0.92	0.28	44,44,44,44	0
81	MG	5	3932	1/1	0.92	0.35	54,54,54,54	1
81	MG	1	3616	1/1	0.92	0.24	53,53,53,53	0
81	MG	2	2050	1/1	0.92	0.44	67,67,67,67	0
81	MG	2	2051	1/1	0.92	0.21	96,96,96,96	0
81	MG	5	3810	1/1	0.92	0.21	50,50,50,50	0
81	MG	5	3652	1/1	0.92	0.41	49,49,49,49	0
81	MG	1	3659	1/1	0.92	0.16	53,53,53,53	0
81	MG	N6	201	1/1	0.92	0.11	57,57,57,57	1
81	MG	5	3940	1/1	0.92	0.16	73,73,73,73	0
81	MG	1	3581	1/1	0.92	0.34	42,42,42,42	0
81	MG	6	2056	1/1	0.92	0.08	126,126,126,126	0
81	MG	5	3659	1/1	0.92	0.34	43,43,43,43	0
81	MG	5	3819	1/1	0.92	0.21	60,60,60,60	0
81	MG	1	4090	1/1	0.92	0.38	66,66,66,66	0
81	MG	1	3812	1/1	0.92	0.21	52,52,52,52	0
81	MG	2	2057	1/1	0.92	0.29	75,75,75,75	0
81	MG	5	3948	1/1	0.92	0.27	53,53,53,53	0
81	MG	1	4151	1/1	0.92	0.24	40,40,40,40	0
81	MG	4	219	1/1	0.92	0.27	54,54,54,54	0
81	MG	1	4152	1/1	0.92	0.17	47,47,47,47	1
81	MG	1	4153	1/1	0.92	0.81	50,50,50,50	0
81	MG	o3	201	1/1	0.92	0.36	59,59,59,59	0
80	PAR	5	3420	42/42	0.92	0.29	77,77,77,77	0
80	PAR	1	3425	42/42	0.92	0.23	48,48,48,48	42
81	MG	5	3678	1/1	0.92	0.23	50,50,50,50	0
81	MG	1	3928	1/1	0.92	0.21	46,46,46,46	0
81	MG	6	1907	1/1	0.92	0.28	93,93,93,93	0
81	MG	s6	302	1/1	0.92	0.33	68,68,68,68	0
81	MG	1	3505	1/1	0.92	0.22	64,64,64,64	0
81	MG	1	3588	1/1	0.92	0.35	47,47,47,47	0
81	MG	5	3540	1/1	0.92	0.24	48,48,48,48	0
81	MG	c4	202	1/1	0.92	0.22	119,119,119,119	0
81	MG	1	3826	1/1	0.92	0.23	37,37,37,37	1
81	MG	6	1917	1/1	0.92	0.35	71,71,71,71	0
81	MG	1	3672	1/1	0.92	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3687	1/1	0.92	0.24	58,58,58,58	0
81	MG	1	3986	1/1	0.92	0.30	51,51,51,51	0
81	MG	5	3843	1/1	0.92	0.64	86,86,86,86	0
81	MG	6	1923	1/1	0.92	0.41	65,65,65,65	0
81	MG	L2	304	1/1	0.92	0.29	44,44,44,44	0
81	MG	d6	102	1/1	0.92	0.26	85,85,85,85	0
80	PAR	1	3429	42/42	0.92	0.24	58,58,58,58	42
81	MG	5	3692	1/1	0.92	0.38	56,56,56,56	0
81	MG	5	4093	1/1	0.93	0.31	60,60,60,60	0
81	MG	1	3704	1/1	0.93	0.19	42,42,42,42	0
81	MG	5	3956	1/1	0.93	0.51	56,56,56,56	0
81	MG	5	3833	1/1	0.93	0.30	56,56,56,56	0
81	MG	1	4172	1/1	0.93	0.27	41,41,41,41	0
81	MG	1	4012	1/1	0.93	0.40	56,56,56,56	0
81	MG	1	3624	1/1	0.93	0.22	34,34,34,34	0
81	MG	1	3780	1/1	0.93	0.32	42,42,42,42	0
81	MG	6	1936	1/1	0.93	0.23	84,84,84,84	0
81	MG	O7	103	1/1	0.93	0.31	37,37,37,37	0
81	MG	1	4064	1/1	0.93	0.17	44,44,44,44	0
80	PAR	1	3428	42/42	0.93	0.21	58,58,58,58	0
80	PAR	5	3410	42/42	0.93	0.23	75,75,75,75	0
81	MG	1	3573	1/1	0.93	0.30	45,45,45,45	0
81	MG	5	4107	1/1	0.93	0.28	52,52,52,52	0
81	MG	1	4019	1/1	0.93	0.38	52,52,52,52	0
81	MG	5	3971	1/1	0.93	0.17	58,58,58,58	0
81	MG	1	3602	1/1	0.93	0.22	55,55,55,55	0
81	MG	1	3576	1/1	0.93	0.20	39,39,39,39	0
81	MG	2	1990	1/1	0.93	0.28	88,88,88,88	0
81	MG	1	4023	1/1	0.93	0.30	49,49,49,49	0
81	MG	1	3724	1/1	0.93	0.37	31,31,31,31	0
81	MG	5	3702	1/1	0.93	0.56	61,61,61,61	0
81	MG	5	3703	1/1	0.93	0.55	58,58,58,58	0
81	MG	6	1955	1/1	0.93	0.30	91,91,91,91	0
81	MG	5	4117	1/1	0.93	0.24	62,62,62,62	0
81	MG	1	4189	1/1	0.93	0.30	77,77,77,77	0
81	MG	5	3562	1/1	0.93	0.12	94,94,94,94	0
81	MG	6	1960	1/1	0.93	0.24	110,110,110,110	0
81	MG	2	1906	1/1	0.93	0.25	80,80,80,80	0
81	MG	1	4025	1/1	0.93	0.20	41,41,41,41	0
81	MG	5	3566	1/1	0.93	0.42	81,81,81,81	0
81	MG	1	4191	1/1	0.93	0.32	48,48,48,48	0
81	MG	5	3568	1/1	0.93	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3722	1/1	0.93	0.16	74,74,74,74	0
81	MG	1	3787	1/1	0.93	0.11	97,97,97,97	0
81	MG	1	3936	1/1	0.93	0.14	65,65,65,65	0
81	MG	7	205	1/1	0.93	0.12	93,93,93,93	0
81	MG	7	206	1/1	0.93	0.20	116,116,116,116	0
81	MG	5	3725	1/1	0.93	0.31	63,63,63,63	0
81	MG	2	2087	1/1	0.93	0.27	70,70,70,70	0
81	MG	5	3728	1/1	0.93	0.29	61,61,61,61	1
81	MG	5	3578	1/1	0.93	0.26	48,48,48,48	0
81	MG	1	3980	1/1	0.93	0.21	54,54,54,54	0
81	MG	8	203	1/1	0.93	0.18	56,56,56,56	0
80	PAR	1	3416	42/42	0.93	0.23	52,52,52,52	0
81	MG	8	205	1/1	0.93	0.27	55,55,55,55	0
81	MG	2	1916	1/1	0.93	0.26	86,86,86,86	0
81	MG	6	1989	1/1	0.93	0.22	75,75,75,75	0
81	MG	6	1991	1/1	0.93	0.40	62,62,62,62	0
80	PAR	1	3408	42/42	0.93	0.24	44,44,44,44	42
81	MG	1	3536	1/1	0.93	0.31	37,37,37,37	0
81	MG	2	2009	1/1	0.93	0.29	70,70,70,70	0
81	MG	2	1921	1/1	0.93	0.27	72,72,72,72	0
81	MG	8	211	1/1	0.93	0.24	66,66,66,66	0
81	MG	1	3856	1/1	0.93	0.18	49,49,49,49	0
81	MG	5	3600	1/1	0.93	0.15	93,93,93,93	0
81	MG	1	3675	1/1	0.93	0.32	64,64,64,64	0
81	MG	1	3637	1/1	0.93	0.49	45,45,45,45	0
81	MG	2	1925	1/1	0.93	0.33	58,58,58,58	0
81	MG	6	2005	1/1	0.93	0.67	62,62,62,62	0
81	MG	2	2017	1/1	0.93	0.23	93,93,93,93	0
81	MG	1	3736	1/1	0.93	0.24	58,58,58,58	0
81	MG	1	3988	1/1	0.93	0.22	56,56,56,56	0
81	MG	1	3582	1/1	0.93	0.57	40,40,40,40	0
81	MG	2	2021	1/1	0.93	0.28	73,73,73,73	0
81	MG	1	4144	1/1	0.93	0.34	40,40,40,40	1
81	MG	1	3804	1/1	0.93	0.28	45,45,45,45	0
81	MG	1	3613	1/1	0.93	0.19	63,63,63,63	0
81	MG	1	4040	1/1	0.93	0.22	59,59,59,59	0
81	MG	1	3906	1/1	0.93	0.31	38,38,38,38	0
81	MG	1	4150	1/1	0.93	0.25	62,62,62,62	0
81	MG	1	3807	1/1	0.93	0.20	49,49,49,49	0
80	PAR	1	3424	42/42	0.93	0.28	76,76,76,76	0
80	PAR	5	3406	42/42	0.93	0.22	51,51,51,51	42
81	MG	4	209	1/1	0.93	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3755	1/1	0.93	0.18	51,51,51,51	0
81	MG	1	3912	1/1	0.93	0.39	44,44,44,44	0
81	MG	6	2031	1/1	0.93	0.75	64,64,64,64	0
81	MG	C8	201	1/1	0.93	0.18	137,137,137,137	0
81	MG	5	3628	1/1	0.93	0.20	59,59,59,59	0
81	MG	N0	201	1/1	0.93	0.46	60,60,60,60	0
81	MG	5	3908	1/1	0.93	0.12	86,86,86,86	0
81	MG	5	3775	1/1	0.93	0.59	60,60,60,60	0
80	PAR	5	3407	42/42	0.93	0.23	51,51,51,51	42
81	MG	1	3441	1/1	0.93	0.28	30,30,30,30	0
81	MG	5	3780	1/1	0.93	0.32	51,51,51,51	0
81	MG	2	1953	1/1	0.93	0.15	131,131,131,131	0
81	MG	5	4040	1/1	0.93	0.24	49,49,49,49	0
81	MG	m6	204	1/1	0.93	0.38	49,49,49,49	0
81	MG	5	4041	1/1	0.93	0.18	70,70,70,70	0
81	MG	5	3434	1/1	0.93	0.34	46,46,46,46	0
81	MG	1	4003	1/1	0.93	0.27	40,40,40,40	0
81	MG	5	3787	1/1	0.93	0.30	59,59,59,59	0
81	MG	2	1955	1/1	0.93	0.09	133,133,133,133	0
81	MG	5	3456	1/1	0.93	0.28	43,43,43,43	0
81	MG	5	3790	1/1	0.93	0.11	76,76,76,76	0
81	MG	5	3791	1/1	0.93	0.16	70,70,70,70	0
81	MG	5	3466	1/1	0.93	0.31	45,45,45,45	0
81	MG	5	3923	1/1	0.93	0.11	112,112,112,112	0
81	MG	4	218	1/1	0.93	0.15	39,39,39,39	0
81	MG	n0	204	1/1	0.93	0.20	63,63,63,63	0
81	MG	2	2047	1/1	0.93	0.38	94,94,94,94	0
81	MG	N5	201	1/1	0.93	0.19	61,61,61,61	0
81	MG	6	2061	1/1	0.93	0.29	110,110,110,110	0
81	MG	n1	201	1/1	0.93	0.24	70,70,70,70	0
81	MG	5	3480	1/1	0.93	0.28	45,45,45,45	0
81	MG	5	3929	1/1	0.93	0.52	55,55,55,55	0
81	MG	5	3797	1/1	0.93	0.36	51,51,51,51	0
81	MG	1	3524	1/1	0.93	0.07	52,52,52,52	0
81	MG	5	3800	1/1	0.93	0.39	62,62,62,62	0
80	PAR	5	3408	42/42	0.93	0.22	58,58,58,58	42
81	MG	6	2069	1/1	0.93	0.28	54,54,54,54	0
81	MG	4	221	1/1	0.93	0.15	46,46,46,46	1
81	MG	5	3492	1/1	0.93	0.33	47,47,47,47	0
81	MG	1	4006	1/1	0.93	0.25	64,64,64,64	0
81	MG	5	3657	1/1	0.93	0.26	47,47,47,47	0
81	MG	5	3501	1/1	0.93	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3811	1/1	0.93	0.49	54,54,54,54	0
81	MG	1	4163	1/1	0.93	0.33	39,39,39,39	1
81	MG	2	1965	1/1	0.93	0.19	95,95,95,95	0
81	MG	1	3650	1/1	0.93	0.50	31,31,31,31	0
81	MG	5	3943	1/1	0.93	0.25	75,75,75,75	0
81	MG	4	227	1/1	0.93	0.08	76,76,76,76	0
81	MG	1	4165	1/1	0.93	0.33	42,42,42,42	0
81	MG	5	3518	1/1	0.93	0.22	52,52,52,52	0
81	MG	5	3519	1/1	0.93	0.30	48,48,48,48	0
81	MG	5	3672	1/1	0.93	0.23	40,40,40,40	0
81	MG	d3	201	1/1	0.93	0.33	68,68,68,68	0
81	MG	1	3770	1/1	0.93	0.38	45,45,45,45	1
81	MG	1	4167	1/1	0.93	0.20	65,65,65,65	0
81	MG	5	3676	1/1	0.93	0.28	42,42,42,42	0
81	MG	5	4088	1/1	0.93	0.17	70,70,70,70	0
81	MG	1	3772	1/1	0.93	0.37	49,49,49,49	0
81	MG	1	3462	1/1	0.93	0.40	30,30,30,30	0
81	MG	2	1974	1/1	0.93	0.19	101,101,101,101	0
81	MG	5	3453	1/1	0.94	0.24	45,45,45,45	0
81	MG	5	3808	1/1	0.94	0.18	54,54,54,54	1
81	MG	6	1913	1/1	0.94	0.14	72,72,72,72	0
81	MG	6	1914	1/1	0.94	0.17	81,81,81,81	0
81	MG	1	3746	1/1	0.94	0.40	36,36,36,36	0
81	MG	5	3463	1/1	0.94	0.43	44,44,44,44	0
81	MG	1	3747	1/1	0.94	0.28	36,36,36,36	0
81	MG	6	1918	1/1	0.94	0.31	71,71,71,71	0
81	MG	5	4089	1/1	0.94	0.30	69,69,69,69	0
81	MG	1	3827	1/1	0.94	0.30	35,35,35,35	0
80	PAR	1	3423	42/42	0.94	0.23	54,54,54,54	0
81	MG	1	3831	1/1	0.94	0.24	37,37,37,37	0
81	MG	5	3470	1/1	0.94	0.26	45,45,45,45	0
81	MG	5	3816	1/1	0.94	0.18	58,58,58,58	0
81	MG	2	1926	1/1	0.94	0.36	62,62,62,62	0
81	MG	6	1929	1/1	0.94	0.25	80,80,80,80	0
81	MG	6	1930	1/1	0.94	0.25	86,86,86,86	0
81	MG	6	1931	1/1	0.94	0.20	94,94,94,94	0
81	MG	1	3835	1/1	0.94	0.36	45,45,45,45	0
81	MG	5	3661	1/1	0.94	0.35	47,47,47,47	0
81	MG	1	3589	1/1	0.94	0.63	49,49,49,49	0
81	MG	5	3484	1/1	0.94	0.27	58,58,58,58	0
81	MG	5	3489	1/1	0.94	0.26	46,46,46,46	0
81	MG	5	3668	1/1	0.94	0.31	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3510	1/1	0.94	0.11	68,68,68,68	0
81	MG	1	4178	1/1	0.94	0.32	54,54,54,54	0
81	MG	6	1942	1/1	0.94	0.19	105,105,105,105	0
81	MG	5	3494	1/1	0.94	0.17	64,64,64,64	0
81	MG	1	3757	1/1	0.94	0.31	45,45,45,45	0
81	MG	6	1945	1/1	0.94	0.31	71,71,71,71	0
81	MG	5	4106	1/1	0.94	0.37	73,73,73,73	0
81	MG	5	3830	1/1	0.94	0.27	56,56,56,56	0
81	MG	5	3832	1/1	0.94	0.55	52,52,52,52	0
81	MG	1	3618	1/1	0.94	0.19	68,68,68,68	0
81	MG	1	3566	1/1	0.94	0.23	43,43,43,43	0
81	MG	1	3765	1/1	0.94	0.18	68,68,68,68	0
81	MG	5	3509	1/1	0.94	0.13	72,72,72,72	0
81	MG	1	3684	1/1	0.94	0.35	43,43,43,43	0
81	MG	1	3688	1/1	0.94	0.29	39,39,39,39	0
81	MG	5	3515	1/1	0.94	0.17	61,61,61,61	0
81	MG	1	3691	1/1	0.94	0.28	42,42,42,42	0
81	MG	M5	301	1/1	0.94	0.22	39,39,39,39	0
81	MG	1	3480	1/1	0.94	0.22	39,39,39,39	0
81	MG	6	1961	1/1	0.94	0.20	98,98,98,98	0
81	MG	1	4045	1/1	0.94	0.30	44,44,44,44	0
81	MG	1	3547	1/1	0.94	0.17	65,65,65,65	0
81	MG	1	3697	1/1	0.94	0.69	58,58,58,58	0
81	MG	M5	308	1/1	0.94	0.39	58,58,58,58	0
80	PAR	5	3417	42/42	0.94	0.19	76,76,76,76	0
81	MG	5	3534	1/1	0.94	0.30	46,46,46,46	0
81	MG	1	3779	1/1	0.94	0.30	41,41,41,41	0
81	MG	1	3450	1/1	0.94	0.28	29,29,29,29	0
81	MG	1	3626	1/1	0.94	0.39	36,36,36,36	0
81	MG	1	4197	1/1	0.94	0.33	44,44,44,44	0
81	MG	1	3920	1/1	0.94	0.34	50,50,50,50	0
81	MG	7	207	1/1	0.94	0.18	118,118,118,118	0
81	MG	1	3488	1/1	0.94	0.23	43,43,43,43	0
81	MG	M7	204	1/1	0.94	0.22	42,42,42,42	0
81	MG	1	3707	1/1	0.94	0.36	40,40,40,40	0
81	MG	2	1962	1/1	0.94	0.12	106,106,106,106	0
81	MG	1	3655	1/1	0.94	0.29	52,52,52,52	0
81	MG	5	3865	1/1	0.94	0.13	58,58,58,58	0
81	MG	5	3866	1/1	0.94	0.19	68,68,68,68	0
81	MG	5	3996	1/1	0.94	0.33	54,54,54,54	0
81	MG	5	3549	1/1	0.94	0.49	50,50,50,50	0
81	MG	1	3925	1/1	0.94	0.20	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	2068	1/1	0.94	0.21	78,78,78,78	0
81	MG	6	1994	1/1	0.94	0.29	79,79,79,79	0
81	MG	1	3712	1/1	0.94	0.33	43,43,43,43	0
81	MG	6	1996	1/1	0.94	0.09	96,96,96,96	0
81	MG	5	3721	1/1	0.94	0.28	67,67,67,67	0
81	MG	2	1966	1/1	0.94	0.18	99,99,99,99	0
81	MG	1	3658	1/1	0.94	0.23	41,41,41,41	0
81	MG	1	3629	1/1	0.94	0.58	53,53,53,53	0
81	MG	N1	201	1/1	0.94	0.16	59,59,59,59	0
81	MG	1	3865	1/1	0.94	0.21	46,46,46,46	1
80	PAR	1	3409	42/42	0.94	0.22	38,38,38,38	42
81	MG	1	3661	1/1	0.94	0.26	46,46,46,46	0
81	MG	1	4135	1/1	0.94	0.31	37,37,37,37	1
81	MG	1	3721	1/1	0.94	0.26	47,47,47,47	1
81	MG	5	3882	1/1	0.94	0.38	55,55,55,55	0
81	MG	1	4137	1/1	0.94	0.21	61,61,61,61	0
81	MG	5	3569	1/1	0.94	0.26	78,78,78,78	0
81	MG	1	3934	1/1	0.94	0.19	57,57,57,57	0
81	MG	5	3571	1/1	0.94	0.15	92,92,92,92	0
81	MG	1	3662	1/1	0.94	0.34	45,45,45,45	0
81	MG	6	2018	1/1	0.94	0.23	89,89,89,89	0
81	MG	6	2019	1/1	0.94	0.19	107,107,107,107	0
81	MG	4	207	1/1	0.94	0.16	58,58,58,58	0
81	MG	4	208	1/1	0.94	0.27	55,55,55,55	0
81	MG	1	3792	1/1	0.94	0.22	45,45,45,45	0
81	MG	4	211	1/1	0.94	0.18	47,47,47,47	0
81	MG	1	3938	1/1	0.94	0.38	49,49,49,49	0
81	MG	1	4071	1/1	0.94	0.18	78,78,78,78	0
81	MG	5	4026	1/1	0.94	0.50	69,69,69,69	0
81	MG	5	3587	1/1	0.94	0.20	66,66,66,66	0
81	MG	1	3793	1/1	0.94	0.27	43,43,43,43	0
81	MG	5	3592	1/1	0.94	0.26	61,61,61,61	1
81	MG	4	215	1/1	0.94	0.24	42,42,42,42	0
81	MG	1	3794	1/1	0.94	0.23	55,55,55,55	0
81	MG	1	3552	1/1	0.94	0.36	61,61,61,61	0
81	MG	m0	301	1/1	0.94	0.09	58,58,58,58	0
81	MG	1	3796	1/1	0.94	0.29	52,52,52,52	0
81	MG	5	4036	1/1	0.94	0.51	68,68,68,68	0
81	MG	O3	202	1/1	0.94	0.20	56,56,56,56	0
81	MG	1	3877	1/1	0.94	0.42	46,46,46,46	0
81	MG	O4	203	1/1	0.94	0.10	59,59,59,59	0
81	MG	1	4077	1/1	0.94	0.28	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3878	1/1	0.94	0.38	54,54,54,54	1
81	MG	5	4042	1/1	0.94	0.27	69,69,69,69	0
81	MG	m7	208	1/1	0.94	0.30	43,43,43,43	0
81	MG	m7	209	1/1	0.94	0.29	47,47,47,47	0
81	MG	6	2048	1/1	0.94	0.29	88,88,88,88	0
81	MG	5	3609	1/1	0.94	0.29	59,59,59,59	0
81	MG	1	3606	1/1	0.94	0.24	74,74,74,74	0
81	MG	1	3801	1/1	0.94	0.30	47,47,47,47	0
81	MG	1	3666	1/1	0.94	0.30	49,49,49,49	0
81	MG	1	3668	1/1	0.94	0.25	53,53,53,53	0
81	MG	1	4156	1/1	0.94	0.21	44,44,44,44	1
81	MG	1	3452	1/1	0.94	0.35	30,30,30,30	0
81	MG	2	2005	1/1	0.94	0.22	58,58,58,58	0
81	MG	5	3776	1/1	0.94	0.49	48,48,48,48	0
81	MG	1	4086	1/1	0.94	0.47	55,55,55,55	0
81	MG	5	4056	1/1	0.94	0.22	48,48,48,48	0
81	MG	2	2110	1/1	0.94	0.46	78,78,78,78	0
80	PAR	2	1903	42/42	0.94	0.24	69,69,69,69	0
81	MG	1	3887	1/1	0.94	0.13	40,40,40,40	0
81	MG	1	3733	1/1	0.94	0.29	41,41,41,41	0
81	MG	n3	202	1/1	0.94	0.31	59,59,59,59	0
81	MG	n3	203	1/1	0.94	0.27	76,76,76,76	0
81	MG	2	2114	1/1	0.94	0.22	104,104,104,104	0
81	MG	n5	201	1/1	0.94	0.35	60,60,60,60	0
81	MG	L2	301	1/1	0.94	0.31	31,31,31,31	0
81	MG	L2	303	1/1	0.94	0.24	38,38,38,38	0
81	MG	n6	203	1/1	0.94	0.23	76,76,76,76	0
81	MG	1	3735	1/1	0.94	0.55	62,62,62,62	0
81	MG	6	2073	1/1	0.94	0.46	94,94,94,94	0
81	MG	2	2015	1/1	0.94	0.09	140,140,140,140	0
81	MG	2	1908	1/1	0.94	0.24	104,104,104,104	0
81	MG	n8	203	1/1	0.94	0.84	51,51,51,51	1
81	MG	s4	301	1/1	0.94	0.10	96,96,96,96	0
81	MG	n8	204	1/1	0.94	0.22	48,48,48,48	0
80	PAR	1	3421	42/42	0.94	0.24	43,43,43,43	42
81	MG	o0	201	1/1	0.94	0.25	89,89,89,89	0
81	MG	1	3673	1/1	0.94	0.28	52,52,52,52	0
80	PAR	1	3411	42/42	0.94	0.24	44,44,44,44	0
81	MG	1	3960	1/1	0.94	0.25	43,43,43,43	0
81	MG	2	1913	1/1	0.94	0.23	87,87,87,87	0
81	MG	L3	404	1/1	0.94	0.29	43,43,43,43	0
81	MG	1	3741	1/1	0.94	0.28	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	4077	1/1	0.94	0.28	74,74,74,74	0
81	MG	5	4078	1/1	0.94	0.28	63,63,63,63	0
81	MG	1	4168	1/1	0.94	0.13	64,64,64,64	0
81	MG	o7	502	1/1	0.94	0.34	48,48,48,48	0
81	MG	5	3803	1/1	0.94	0.18	47,47,47,47	0
81	MG	5	3435	1/1	0.94	0.25	44,44,44,44	0
81	MG	1	3562	1/1	0.94	0.40	44,44,44,44	0
81	MG	2	2027	1/1	0.94	0.20	69,69,69,69	0
81	MG	5	3545	1/1	0.95	0.24	55,55,55,55	0
81	MG	5	4028	1/1	0.95	0.20	78,78,78,78	0
81	MG	5	3663	1/1	0.95	0.24	57,57,57,57	0
81	MG	5	3665	1/1	0.95	0.24	46,46,46,46	0
81	MG	2	2035	1/1	0.95	0.11	116,116,116,116	0
81	MG	5	4032	1/1	0.95	0.16	75,75,75,75	0
81	MG	8	218	1/1	0.95	0.22	73,73,73,73	0
81	MG	1	3872	1/1	0.95	0.27	63,63,63,63	0
81	MG	1	3824	1/1	0.95	0.32	58,58,58,58	0
81	MG	8	221	1/1	0.95	0.11	86,86,86,86	0
81	MG	1	3732	1/1	0.95	0.37	50,50,50,50	0
81	MG	5	3802	1/1	0.95	0.23	48,48,48,48	1
81	MG	6	1963	1/1	0.95	0.39	97,97,97,97	0
81	MG	6	1964	1/1	0.95	0.18	108,108,108,108	0
81	MG	1	3609	1/1	0.95	0.15	56,56,56,56	0
81	MG	5	3551	1/1	0.95	0.43	54,54,54,54	1
81	MG	6	1967	1/1	0.95	0.31	80,80,80,80	0
81	MG	1	3734	1/1	0.95	0.35	43,43,43,43	0
81	MG	Q2	503	1/1	0.95	0.28	42,42,42,42	0
81	MG	l3	403	1/1	0.95	0.28	43,43,43,43	1
81	MG	1	4016	1/1	0.95	0.47	57,57,57,57	0
81	MG	1	3696	1/1	0.95	0.47	51,51,51,51	0
81	MG	1	3478	1/1	0.95	0.31	37,37,37,37	0
81	MG	1	3879	1/1	0.95	0.33	61,61,61,61	0
81	MG	1	3834	1/1	0.95	0.29	31,31,31,31	0
81	MG	1	4021	1/1	0.95	0.38	45,45,45,45	0
81	MG	5	3564	1/1	0.95	0.16	85,85,85,85	0
81	MG	1	3737	1/1	0.95	0.33	61,61,61,61	0
81	MG	1	3644	1/1	0.95	0.35	46,46,46,46	0
81	MG	1	3645	1/1	0.95	0.20	44,44,44,44	0
81	MG	5	3817	1/1	0.95	0.32	57,57,57,57	0
81	MG	5	4053	1/1	0.95	0.18	59,59,59,59	0
81	MG	S7	201	1/1	0.95	0.13	89,89,89,89	0
81	MG	1	3611	1/1	0.95	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	6	1990	1/1	0.95	0.27	69,69,69,69	0
81	MG	1	3671	1/1	0.95	0.43	52,52,52,52	0
81	MG	5	3691	1/1	0.95	0.55	58,58,58,58	0
81	MG	C9	201	1/1	0.95	0.16	121,121,121,121	0
81	MG	1	3705	1/1	0.95	0.38	44,44,44,44	0
81	MG	m6	202	1/1	0.95	0.22	53,53,53,53	0
81	MG	1	3842	1/1	0.95	0.22	43,43,43,43	1
81	MG	5	3575	1/1	0.95	0.24	58,58,58,58	0
81	MG	m7	202	1/1	0.95	0.23	48,48,48,48	0
81	MG	m7	203	1/1	0.95	0.20	49,49,49,49	0
81	MG	1	3843	1/1	0.95	0.14	48,48,48,48	0
81	MG	5	3699	1/1	0.95	0.24	48,48,48,48	0
81	MG	5	3430	1/1	0.95	0.22	45,45,45,45	0
81	MG	1	3506	1/1	0.95	0.12	65,65,65,65	0
81	MG	5	3831	1/1	0.95	0.32	66,66,66,66	0
81	MG	5	3582	1/1	0.95	0.31	54,54,54,54	0
81	MG	6	2007	1/1	0.95	0.48	90,90,90,90	0
81	MG	5	3584	1/1	0.95	0.31	67,67,67,67	0
81	MG	5	3432	1/1	0.95	0.37	43,43,43,43	0
81	MG	2	1985	1/1	0.95	0.36	46,46,46,46	0
81	MG	M7	203	1/1	0.95	0.28	45,45,45,45	0
81	MG	4	222	1/1	0.95	0.18	49,49,49,49	0
81	MG	5	3712	1/1	0.95	0.39	57,57,57,57	0
81	MG	5	3589	1/1	0.95	0.22	63,63,63,63	0
81	MG	5	3591	1/1	0.95	0.28	58,58,58,58	0
81	MG	5	3718	1/1	0.95	0.29	63,63,63,63	0
81	MG	5	3443	1/1	0.95	0.24	42,42,42,42	0
81	MG	5	3593	1/1	0.95	0.32	64,64,64,64	0
81	MG	6	2022	1/1	0.95	0.41	64,64,64,64	0
81	MG	5	3444	1/1	0.95	0.18	52,52,52,52	0
81	MG	2	1920	1/1	0.95	0.35	68,68,68,68	0
81	MG	1	3709	1/1	0.95	0.24	32,32,32,32	0
81	MG	5	3454	1/1	0.95	0.24	40,40,40,40	0
81	MG	1	4179	1/1	0.95	0.24	42,42,42,42	0
81	MG	5	3849	1/1	0.95	0.57	88,88,88,88	0
81	MG	2	2064	1/1	0.95	0.12	111,111,111,111	0
81	MG	4	225	1/1	0.95	0.10	62,62,62,62	1
81	MG	1	3754	1/1	0.95	0.14	52,52,52,52	0
81	MG	6	2033	1/1	0.95	0.34	70,70,70,70	0
81	MG	1	3594	1/1	0.95	0.38	45,45,45,45	0
81	MG	1	4132	1/1	0.95	0.25	37,37,37,37	0
81	MG	5	3735	1/1	0.95	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	2	1927	1/1	0.95	0.14	75,75,75,75	0
81	MG	5	3473	1/1	0.95	0.32	51,51,51,51	0
81	MG	5	3477	1/1	0.95	0.23	49,49,49,49	0
81	MG	1	4082	1/1	0.95	0.24	54,54,54,54	0
81	MG	o0	202	1/1	0.95	0.46	88,88,88,88	0
81	MG	5	3863	1/1	0.95	0.31	55,55,55,55	0
81	MG	1	4185	1/1	0.95	0.09	56,56,56,56	0
81	MG	5	3482	1/1	0.95	0.45	44,44,44,44	0
81	MG	1	3674	1/1	0.95	0.37	46,46,46,46	0
81	MG	1	3942	1/1	0.95	0.16	52,52,52,52	0
81	MG	6	2047	1/1	0.95	0.19	109,109,109,109	0
81	MG	5	3487	1/1	0.95	0.32	43,43,43,43	0
81	MG	5	3488	1/1	0.95	0.21	44,44,44,44	0
81	MG	N3	202	1/1	0.95	0.43	68,68,68,68	0
81	MG	1	3479	1/1	0.95	0.35	37,37,37,37	0
81	MG	4	237	1/1	0.95	0.39	68,68,68,68	0
81	MG	1	3598	1/1	0.95	0.29	41,41,41,41	0
81	MG	2	2008	1/1	0.95	0.30	76,76,76,76	0
81	MG	q2	502	1/1	0.95	0.23	70,70,70,70	0
81	MG	1	3571	1/1	0.95	0.27	40,40,40,40	0
81	MG	6	2057	1/1	0.95	0.09	126,126,126,126	0
81	MG	1	3992	1/1	0.95	0.24	47,47,47,47	1
81	MG	5	3629	1/1	0.95	0.10	66,66,66,66	0
81	MG	1	3802	1/1	0.95	0.14	42,42,42,42	0
81	MG	6	1911	1/1	0.95	0.26	73,73,73,73	0
81	MG	5	3758	1/1	0.95	0.33	48,48,48,48	0
81	MG	5	3760	1/1	0.95	0.23	50,50,50,50	0
81	MG	5	3761	1/1	0.95	0.33	45,45,45,45	0
81	MG	1	3763	1/1	0.95	0.10	56,56,56,56	0
81	MG	5	4001	1/1	0.95	0.24	63,63,63,63	0
81	MG	5	3634	1/1	0.95	0.14	55,55,55,55	0
81	MG	5	3765	1/1	0.95	0.17	52,52,52,52	1
81	MG	2	1944	1/1	0.95	0.23	84,84,84,84	0
81	MG	1	3572	1/1	0.95	0.31	41,41,41,41	0
81	MG	5	3514	1/1	0.95	0.26	57,57,57,57	0
81	MG	2	1946	1/1	0.95	0.24	74,74,74,74	0
81	MG	5	3641	1/1	0.95	0.18	45,45,45,45	0
81	MG	6	1926	1/1	0.95	0.31	70,70,70,70	0
81	MG	1	3438	1/1	0.95	0.33	36,36,36,36	0
81	MG	1	3620	1/1	0.95	0.22	68,68,68,68	0
81	MG	1	3808	1/1	0.95	0.23	51,51,51,51	0
81	MG	s6	301	1/1	0.95	0.09	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3516	1/1	0.95	0.18	47,47,47,47	0
81	MG	6	1932	1/1	0.95	0.41	87,87,87,87	0
81	MG	5	3525	1/1	0.95	0.32	52,52,52,52	0
81	MG	7	210	1/1	0.95	0.24	53,53,53,53	0
81	MG	1	3555	1/1	0.95	0.26	38,38,38,38	0
81	MG	3	204	1/1	0.95	0.16	84,84,84,84	0
81	MG	1	3686	1/1	0.95	0.20	45,45,45,45	0
81	MG	1	3531	1/1	0.95	0.31	41,41,41,41	0
81	MG	1	3866	1/1	0.95	0.31	38,38,38,38	0
81	MG	2	2096	1/1	0.95	0.18	76,76,76,76	0
81	MG	1	3814	1/1	0.95	0.27	47,47,47,47	0
81	MG	1	3608	1/1	0.95	0.25	50,50,50,50	0
81	MG	5	4022	1/1	0.95	0.87	64,64,64,64	0
81	MG	O4	204	1/1	0.95	0.24	63,63,63,63	0
81	MG	1	3778	1/1	0.95	0.29	50,50,50,50	1
81	MG	1	3664	1/1	0.95	0.37	50,50,50,50	0
81	MG	1	3823	1/1	0.95	0.25	42,42,42,42	0
81	MG	1	3832	1/1	0.96	0.27	45,45,45,45	0
81	MG	3	212	1/1	0.96	0.19	85,85,85,85	0
81	MG	6	1957	1/1	0.96	0.22	102,102,102,102	0
81	MG	1	3694	1/1	0.96	0.15	41,41,41,41	0
81	MG	5	3801	1/1	0.96	0.21	52,52,52,52	0
81	MG	l2	301	1/1	0.96	0.13	53,53,53,53	0
81	MG	l2	302	1/1	0.96	0.23	56,56,56,56	0
81	MG	1	4149	1/1	0.96	0.22	44,44,44,44	0
81	MG	l3	401	1/1	0.96	0.22	44,44,44,44	0
81	MG	1	3574	1/1	0.96	0.21	42,42,42,42	0
81	MG	1	3836	1/1	0.96	0.22	63,63,63,63	0
81	MG	5	3554	1/1	0.96	0.21	55,55,55,55	0
81	MG	1	3931	1/1	0.96	0.16	40,40,40,40	0
81	MG	5	3556	1/1	0.96	0.30	71,71,71,71	0
81	MG	D3	201	1/1	0.96	0.14	75,75,75,75	0
81	MG	6	1970	1/1	0.96	0.23	86,86,86,86	0
81	MG	1	3541	1/1	0.96	0.47	29,29,29,29	0
81	MG	1	3597	1/1	0.96	0.50	43,43,43,43	0
81	MG	l4	402	1/1	0.96	0.45	57,57,57,57	0
81	MG	1	3482	1/1	0.96	0.20	40,40,40,40	0
81	MG	5	3682	1/1	0.96	0.32	52,52,52,52	0
81	MG	1	3699	1/1	0.96	0.61	51,51,51,51	0
81	MG	6	1978	1/1	0.96	0.10	111,111,111,111	0
81	MG	M5	306	1/1	0.96	0.23	40,40,40,40	0
81	MG	5	3433	1/1	0.96	0.36	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3686	1/1	0.96	0.21	55,55,55,55	0
81	MG	6	1982	1/1	0.96	0.19	86,86,86,86	0
81	MG	1	3599	1/1	0.96	0.20	52,52,52,52	0
81	MG	1	3937	1/1	0.96	0.10	59,59,59,59	0
81	MG	2	1914	1/1	0.96	0.11	92,92,92,92	0
81	MG	5	3438	1/1	0.96	0.25	47,47,47,47	0
81	MG	m5	301	1/1	0.96	0.26	72,72,72,72	0
81	MG	5	4060	1/1	0.96	0.22	72,72,72,72	0
81	MG	5	3442	1/1	0.96	0.21	40,40,40,40	0
81	MG	1	3529	1/1	0.96	0.44	38,38,38,38	0
81	MG	1	3745	1/1	0.96	0.43	33,33,33,33	0
81	MG	5	4064	1/1	0.96	0.47	99,99,99,99	0
81	MG	5	3695	1/1	0.96	0.31	56,56,56,56	0
81	MG	5	3446	1/1	0.96	0.27	43,43,43,43	0
81	MG	1	3601	1/1	0.96	0.31	49,49,49,49	0
81	MG	5	3449	1/1	0.96	0.18	56,56,56,56	0
81	MG	m7	207	1/1	0.96	0.26	50,50,50,50	0
81	MG	5	3450	1/1	0.96	0.36	49,49,49,49	0
81	MG	5	3829	1/1	0.96	0.30	76,76,76,76	0
81	MG	5	3579	1/1	0.96	0.28	49,49,49,49	0
81	MG	1	3580	1/1	0.96	0.20	38,38,38,38	0
81	MG	1	3749	1/1	0.96	0.26	36,36,36,36	0
81	MG	2	1995	1/1	0.96	0.14	81,81,81,81	0
81	MG	5	4075	1/1	0.96	0.16	66,66,66,66	0
81	MG	5	3583	1/1	0.96	0.26	54,54,54,54	0
81	MG	5	3458	1/1	0.96	0.30	40,40,40,40	0
81	MG	1	3995	1/1	0.96	0.22	47,47,47,47	0
81	MG	1	3750	1/1	0.96	0.23	38,38,38,38	0
81	MG	6	2012	1/1	0.96	0.42	65,65,65,65	0
81	MG	5	3957	1/1	0.96	0.21	54,54,54,54	0
81	MG	1	3561	1/1	0.96	0.18	43,43,43,43	0
81	MG	6	2015	1/1	0.96	0.30	91,91,91,91	0
81	MG	1	3708	1/1	0.96	0.28	39,39,39,39	0
81	MG	1	3999	1/1	0.96	0.31	58,58,58,58	0
81	MG	5	3717	1/1	0.96	0.24	55,55,55,55	1
81	MG	M7	206	1/1	0.96	0.17	39,39,39,39	0
81	MG	5	3963	1/1	0.96	0.14	58,58,58,58	0
81	MG	1	3798	1/1	0.96	0.18	56,56,56,56	0
81	MG	5	3475	1/1	0.96	0.29	39,39,39,39	0
81	MG	1	3799	1/1	0.96	0.30	35,35,35,35	0
81	MG	5	3479	1/1	0.96	0.15	48,48,48,48	0
81	MG	1	3517	1/1	0.96	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3710	1/1	0.96	0.23	33,33,33,33	0
81	MG	6	2027	1/1	0.96	0.08	131,131,131,131	0
81	MG	1	3951	1/1	0.96	0.17	60,60,60,60	0
81	MG	1	3901	1/1	0.96	0.20	32,32,32,32	0
81	MG	1	3902	1/1	0.96	0.21	61,61,61,61	0
81	MG	5	3485	1/1	0.96	0.26	47,47,47,47	0
81	MG	5	3486	1/1	0.96	0.55	45,45,45,45	0
81	MG	1	3651	1/1	0.96	0.31	35,35,35,35	0
81	MG	1	3758	1/1	0.96	0.23	45,45,45,45	0
81	MG	1	3859	1/1	0.96	0.16	53,53,53,53	0
81	MG	1	3457	1/1	0.96	0.30	36,36,36,36	0
81	MG	5	3491	1/1	0.96	0.28	49,49,49,49	0
81	MG	5	3860	1/1	0.96	0.14	68,68,68,68	0
81	MG	1	3907	1/1	0.96	0.27	39,39,39,39	0
81	MG	1	3677	1/1	0.96	0.36	48,48,48,48	0
81	MG	5	3496	1/1	0.96	0.21	44,44,44,44	0
81	MG	5	3499	1/1	0.96	0.14	56,56,56,56	0
81	MG	1	4182	1/1	0.96	0.12	51,51,51,51	0
81	MG	4	235	1/1	0.96	0.37	43,43,43,43	0
81	MG	1	3584	1/1	0.96	0.37	43,43,43,43	0
81	MG	5	3870	1/1	0.96	0.19	63,63,63,63	0
81	MG	1	3679	1/1	0.96	0.25	70,70,70,70	0
81	MG	5	3623	1/1	0.96	0.25	59,59,59,59	0
81	MG	5	3749	1/1	0.96	0.26	45,45,45,45	0
81	MG	1	3766	1/1	0.96	0.15	55,55,55,55	0
81	MG	L2	302	1/1	0.96	0.28	46,46,46,46	0
81	MG	5	3511	1/1	0.96	0.17	45,45,45,45	0
81	MG	5	3997	1/1	0.96	0.55	51,51,51,51	0
81	MG	5	3512	1/1	0.96	0.42	61,61,61,61	0
81	MG	1	3487	1/1	0.96	0.38	37,37,37,37	0
81	MG	1	4129	1/1	0.96	0.28	56,56,56,56	0
81	MG	5	3630	1/1	0.96	0.12	59,59,59,59	0
81	MG	1	3534	1/1	0.96	0.28	46,46,46,46	0
81	MG	5	3516	1/1	0.96	0.21	55,55,55,55	0
81	MG	1	3656	1/1	0.96	0.29	48,48,48,48	0
81	MG	5	3762	1/1	0.96	0.41	45,45,45,45	0
81	MG	1	3966	1/1	0.96	0.62	50,50,50,50	0
81	MG	5	3636	1/1	0.96	0.21	53,53,53,53	0
81	MG	O2	201	1/1	0.96	0.22	43,43,43,43	0
81	MG	5	3520	1/1	0.96	0.42	47,47,47,47	0
81	MG	6	1925	1/1	0.96	0.29	76,76,76,76	0
81	MG	2	2030	1/1	0.96	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	7	209	1/1	0.96	0.11	96,96,96,96	0
81	MG	6	1928	1/1	0.96	0.36	72,72,72,72	0
81	MG	5	3522	1/1	0.96	0.21	54,54,54,54	0
81	MG	5	3523	1/1	0.96	0.28	44,44,44,44	0
81	MG	5	3524	1/1	0.96	0.12	54,54,54,54	1
81	MG	1	3771	1/1	0.96	0.32	40,40,40,40	0
81	MG	5	3526	1/1	0.96	0.41	52,52,52,52	0
81	MG	5	3528	1/1	0.96	0.33	52,52,52,52	0
81	MG	6	1935	1/1	0.96	0.32	78,78,78,78	0
81	MG	1	3458	1/1	0.96	0.24	40,40,40,40	0
81	MG	O3	201	1/1	0.96	0.39	56,56,56,56	0
81	MG	1	3725	1/1	0.96	0.27	40,40,40,40	1
81	MG	5	3532	1/1	0.96	0.40	46,46,46,46	0
81	MG	1	3461	1/1	0.96	0.26	37,37,37,37	0
81	MG	1	3685	1/1	0.96	0.31	41,41,41,41	0
81	MG	5	3655	1/1	0.96	0.25	43,43,43,43	0
81	MG	1	3453	1/1	0.96	0.28	40,40,40,40	0
81	MG	1	3463	1/1	0.96	0.39	39,39,39,39	0
81	MG	1	4083	1/1	0.96	0.34	44,44,44,44	0
81	MG	1	3690	1/1	0.96	0.21	44,44,44,44	0
81	MG	1	3828	1/1	0.96	0.42	43,43,43,43	0
81	MG	6	1948	1/1	0.96	0.21	111,111,111,111	0
81	MG	d3	203	1/1	0.96	0.15	80,80,80,80	0
81	MG	3	205	1/1	0.96	0.17	73,73,73,73	0
81	MG	5	3543	1/1	0.96	0.20	56,56,56,56	0
81	MG	1	3456	1/1	0.96	0.28	36,36,36,36	0
81	MG	5	3664	1/1	0.96	0.26	50,50,50,50	0
81	MG	1	3977	1/1	0.96	0.30	49,49,49,49	0
82	ZN	D9	101	1/1	0.96	0.12	112,112,112,112	0
82	ZN	o4	201	1/1	0.96	0.10	102,102,102,102	0
81	MG	1	3515	1/1	0.96	0.26	44,44,44,44	0
81	MG	1	3459	1/1	0.97	0.36	34,34,34,34	0
81	MG	4	229	1/1	0.97	0.11	57,57,57,57	0
81	MG	1	3533	1/1	0.97	0.29	33,33,33,33	0
81	MG	2	1998	1/1	0.97	0.24	79,79,79,79	0
81	MG	1	3777	1/1	0.97	0.20	44,44,44,44	0
81	MG	1	3449	1/1	0.97	0.29	35,35,35,35	0
81	MG	1	3743	1/1	0.97	0.37	35,35,35,35	0
81	MG	2	1949	1/1	0.97	0.15	102,102,102,102	0
81	MG	1	3667	1/1	0.97	0.21	52,52,52,52	0
81	MG	6	2003	1/1	0.97	0.60	71,71,71,71	0
81	MG	M7	201	1/1	0.97	0.34	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	3	207	1/1	0.97	0.19	83,83,83,83	0
81	MG	5	3755	1/1	0.97	0.29	59,59,59,59	0
81	MG	3	208	1/1	0.97	0.32	43,43,43,43	0
81	MG	5	3493	1/1	0.97	0.25	66,66,66,66	0
81	MG	1	3817	1/1	0.97	0.31	39,39,39,39	0
81	MG	6	2010	1/1	0.97	0.09	124,124,124,124	0
81	MG	5	3577	1/1	0.97	0.21	54,54,54,54	0
81	MG	5	4047	1/1	0.97	0.40	68,68,68,68	0
81	MG	1	3689	1/1	0.97	0.35	48,48,48,48	1
81	MG	5	3497	1/1	0.97	0.30	50,50,50,50	0
81	MG	1	3819	1/1	0.97	0.11	53,53,53,53	0
81	MG	1	3604	1/1	0.97	0.18	54,54,54,54	0
81	MG	6	1912	1/1	0.97	0.21	76,76,76,76	0
81	MG	1	3716	1/1	0.97	0.19	44,44,44,44	0
81	MG	1	3748	1/1	0.97	0.33	31,31,31,31	0
81	MG	5	4054	1/1	0.97	0.40	49,49,49,49	0
81	MG	1	3454	1/1	0.97	0.21	40,40,40,40	0
81	MG	5	3508	1/1	0.97	0.25	59,59,59,59	0
81	MG	1	3720	1/1	0.97	0.28	40,40,40,40	0
81	MG	1	3455	1/1	0.97	0.32	45,45,45,45	0
81	MG	1	4050	1/1	0.97	0.18	48,48,48,48	0
81	MG	1	3753	1/1	0.97	0.23	47,47,47,47	0
81	MG	1	3439	1/1	0.97	0.29	37,37,37,37	0
81	MG	1	3829	1/1	0.97	0.29	40,40,40,40	0
81	MG	1	3497	1/1	0.97	0.24	51,51,51,51	0
81	MG	5	3594	1/1	0.97	0.23	75,75,75,75	0
81	MG	5	3778	1/1	0.97	0.34	44,44,44,44	0
81	MG	1	3554	1/1	0.97	0.29	34,34,34,34	0
81	MG	5	3596	1/1	0.97	0.25	71,71,71,71	0
81	MG	2	2023	1/1	0.97	0.21	81,81,81,81	0
81	MG	1	3726	1/1	0.97	0.18	39,39,39,39	1
81	MG	5	3783	1/1	0.97	0.14	55,55,55,55	0
81	MG	5	3784	1/1	0.97	0.16	50,50,50,50	0
81	MG	2	1918	1/1	0.97	0.28	69,69,69,69	0
81	MG	5	3601	1/1	0.97	0.25	93,93,93,93	0
81	MG	5	3436	1/1	0.97	0.32	43,43,43,43	0
81	MG	1	3833	1/1	0.97	0.29	39,39,39,39	0
81	MG	13	409	1/1	0.97	0.21	55,55,55,55	1
81	MG	1	3485	1/1	0.97	0.26	32,32,32,32	0
81	MG	5	3439	1/1	0.97	0.26	45,45,45,45	0
81	MG	5	3606	1/1	0.97	0.16	67,67,67,67	0
81	MG	5	3440	1/1	0.97	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3694	1/1	0.97	0.40	52,52,52,52	0
81	MG	5	3608	1/1	0.97	0.34	52,52,52,52	0
81	MG	1	3443	1/1	0.97	0.26	32,32,32,32	0
81	MG	1	3575	1/1	0.97	0.33	38,38,38,38	0
81	MG	17	306	1/1	0.97	0.33	65,65,65,65	0
81	MG	5	3798	1/1	0.97	0.31	50,50,50,50	1
81	MG	19	201	1/1	0.97	0.26	56,56,56,56	0
81	MG	1	3700	1/1	0.97	0.29	38,38,38,38	0
81	MG	1	3445	1/1	0.97	0.42	28,28,28,28	0
81	MG	2	2032	1/1	0.97	0.22	90,90,90,90	0
81	MG	1	3595	1/1	0.97	0.27	46,46,46,46	0
81	MG	1	3767	1/1	0.97	0.07	62,62,62,62	0
81	MG	5	3451	1/1	0.97	0.24	42,42,42,42	0
81	MG	5	3704	1/1	0.97	0.24	51,51,51,51	0
81	MG	5	3900	1/1	0.97	0.41	75,75,75,75	0
81	MG	O0	201	1/1	0.97	0.12	63,63,63,63	0
81	MG	1	4066	1/1	0.97	0.26	47,47,47,47	0
81	MG	5	3455	1/1	0.97	0.23	47,47,47,47	0
81	MG	1	3475	1/1	0.97	0.30	32,32,32,32	0
81	MG	5	3538	1/1	0.97	0.38	46,46,46,46	0
81	MG	5	3539	1/1	0.97	0.42	44,44,44,44	0
81	MG	1	3880	1/1	0.97	0.32	43,43,43,43	0
81	MG	5	3715	1/1	0.97	0.38	57,57,57,57	0
81	MG	5	3459	1/1	0.97	0.32	45,45,45,45	0
81	MG	5	3460	1/1	0.97	0.23	42,42,42,42	0
81	MG	1	3543	1/1	0.97	0.40	34,34,34,34	0
81	MG	2	1933	1/1	0.97	0.21	78,78,78,78	0
81	MG	1	3579	1/1	0.97	0.16	51,51,51,51	0
81	MG	M5	302	1/1	0.97	0.25	35,35,35,35	0
81	MG	1	4110	1/1	0.97	0.33	63,63,63,63	0
81	MG	5	3632	1/1	0.97	0.27	59,59,59,59	0
81	MG	6	1973	1/1	0.97	0.10	113,113,113,113	0
81	MG	1	3489	1/1	0.97	0.30	37,37,37,37	0
81	MG	5	3727	1/1	0.97	0.43	55,55,55,55	0
81	MG	5	3919	1/1	0.97	0.59	58,58,58,58	0
81	MG	5	3471	1/1	0.97	0.32	47,47,47,47	0
81	MG	5	3472	1/1	0.97	0.32	52,52,52,52	0
81	MG	2	2045	1/1	0.97	0.26	74,74,74,74	0
81	MG	5	3731	1/1	0.97	0.44	54,54,54,54	0
81	MG	5	3637	1/1	0.97	0.39	53,53,53,53	0
81	MG	5	3552	1/1	0.97	0.15	56,56,56,56	1
81	MG	5	3926	1/1	0.97	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	5	3474	1/1	0.97	0.29	55,55,55,55	0
81	MG	6	1985	1/1	0.97	0.28	85,85,85,85	0
81	MG	1	3490	1/1	0.97	0.29	49,49,49,49	0
81	MG	5	3476	1/1	0.97	0.23	44,44,44,44	0
81	MG	1	3738	1/1	0.97	0.22	43,43,43,43	0
81	MG	5	3557	1/1	0.97	0.22	67,67,67,67	0
81	MG	5	3478	1/1	0.97	0.28	49,49,49,49	0
81	MG	2	2102	1/1	0.97	0.19	78,78,78,78	0
81	MG	1	3922	1/1	0.97	0.25	43,43,43,43	0
82	ZN	q3	501	1/1	0.97	0.19	96,96,96,96	0
81	MG	7	203	1/1	0.97	0.27	47,47,47,47	0
81	MG	5	3574	1/1	0.98	0.28	65,65,65,65	0
81	MG	1	3815	1/1	0.98	0.25	44,44,44,44	0
81	MG	5	3507	1/1	0.98	0.25	64,64,64,64	0
81	MG	4	210	1/1	0.98	0.17	47,47,47,47	0
81	MG	1	3816	1/1	0.98	0.33	43,43,43,43	0
81	MG	1	3460	1/1	0.98	0.41	33,33,33,33	0
81	MG	5	3654	1/1	0.98	0.33	48,48,48,48	0
81	MG	1	3717	1/1	0.98	0.25	35,35,35,35	0
81	MG	1	3718	1/1	0.98	0.28	34,34,34,34	0
81	MG	5	3739	1/1	0.98	0.18	50,50,50,50	0
81	MG	1	3477	1/1	0.98	0.22	35,35,35,35	0
81	MG	1	4141	1/1	0.98	0.15	51,51,51,51	0
81	MG	5	3445	1/1	0.98	0.28	48,48,48,48	0
81	MG	1	4058	1/1	0.98	0.42	73,73,73,73	0
81	MG	1	3448	1/1	0.98	0.23	35,35,35,35	0
81	MG	5	3448	1/1	0.98	0.23	49,49,49,49	0
81	MG	2	1930	1/1	0.98	0.35	70,70,70,70	0
81	MG	5	3590	1/1	0.98	0.33	62,62,62,62	0
81	MG	1	3822	1/1	0.98	0.21	50,50,50,50	0
81	MG	1	3751	1/1	0.98	0.26	42,42,42,42	0
81	MG	5	3452	1/1	0.98	0.27	47,47,47,47	0
81	MG	1	3440	1/1	0.98	0.11	39,39,39,39	0
81	MG	2	1934	1/1	0.98	0.12	75,75,75,75	0
81	MG	5	3670	1/1	0.98	0.19	46,46,46,46	0
81	MG	1	3444	1/1	0.98	0.30	32,32,32,32	0
81	MG	1	3495	1/1	0.98	0.27	41,41,41,41	0
81	MG	5	3527	1/1	0.98	0.44	54,54,54,54	0
81	MG	5	3599	1/1	0.98	0.21	84,84,84,84	0
81	MG	m7	204	1/1	0.98	0.41	53,53,53,53	0
81	MG	5	3675	1/1	0.98	0.19	50,50,50,50	0
81	MG	5	3759	1/1	0.98	0.28	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	3585	1/1	0.98	0.15	46,46,46,46	0
81	MG	2	1989	1/1	0.98	0.18	88,88,88,88	0
81	MG	1	3567	1/1	0.98	0.29	48,48,48,48	0
81	MG	5	3461	1/1	0.98	0.38	39,39,39,39	0
81	MG	5	3462	1/1	0.98	0.36	39,39,39,39	0
81	MG	2	1939	1/1	0.98	0.40	84,84,84,84	0
81	MG	5	3850	1/1	0.98	0.19	51,51,51,51	0
81	MG	5	3766	1/1	0.98	0.33	50,50,50,50	0
81	MG	5	3464	1/1	0.98	0.51	44,44,44,44	0
81	MG	5	3465	1/1	0.98	0.31	46,46,46,46	0
81	MG	1	3647	1/1	0.98	0.21	39,39,39,39	0
81	MG	1	3648	1/1	0.98	0.42	40,40,40,40	0
81	MG	2	1994	1/1	0.98	0.19	79,79,79,79	0
81	MG	1	3759	1/1	0.98	0.30	38,38,38,38	0
81	MG	1	3464	1/1	0.98	0.39	34,34,34,34	0
81	MG	1	3950	1/1	0.98	0.17	53,53,53,53	1
81	MG	2	2107	1/1	0.98	0.12	120,120,120,120	0
81	MG	1	3761	1/1	0.98	0.24	51,51,51,51	0
81	MG	5	3862	1/1	0.98	0.10	65,65,65,65	0
81	MG	1	3627	1/1	0.98	0.19	34,34,34,34	0
81	MG	5	3864	1/1	0.98	0.34	42,42,42,42	0
81	MG	1	3442	1/1	0.98	0.30	35,35,35,35	0
81	MG	5	3618	1/1	0.98	0.16	87,87,87,87	0
81	MG	4	234	1/1	0.98	0.26	46,46,46,46	0
81	MG	1	3514	1/1	0.98	0.16	63,63,63,63	1
81	MG	1	3703	1/1	0.98	0.26	40,40,40,40	0
81	MG	1	3483	1/1	0.98	0.17	41,41,41,41	0
81	MG	1	3484	1/1	0.98	0.30	35,35,35,35	0
81	MG	1	3446	1/1	0.98	0.21	35,35,35,35	0
81	MG	5	3786	1/1	0.98	0.32	53,53,53,53	0
81	MG	1	3518	1/1	0.98	0.22	46,46,46,46	0
81	MG	1	3657	1/1	0.98	0.18	49,49,49,49	0
81	MG	1	3468	1/1	0.98	0.40	33,33,33,33	0
81	MG	1	3844	1/1	0.98	0.20	44,44,44,44	1
81	MG	L3	401	1/1	0.98	0.26	46,46,46,46	0
81	MG	1	3845	1/1	0.98	0.28	38,38,38,38	0
81	MG	2	2013	1/1	0.98	0.11	86,86,86,86	0
81	MG	5	3968	1/1	0.98	0.38	48,48,48,48	0
81	MG	2	1960	1/1	0.98	0.17	90,90,90,90	0
81	MG	5	3710	1/1	0.98	0.28	50,50,50,50	0
81	MG	5	3711	1/1	0.98	0.34	54,54,54,54	0
81	MG	1	3846	1/1	0.98	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
81	MG	1	4127	1/1	0.98	0.16	39,39,39,39	0
81	MG	1	3447	1/1	0.98	0.25	39,39,39,39	0
81	MG	1	3636	1/1	0.98	0.43	48,48,48,48	0
81	MG	5	3716	1/1	0.98	0.23	58,58,58,58	0
81	MG	5	3977	1/1	0.98	0.18	71,71,71,71	0
81	MG	5	3429	1/1	0.98	0.29	42,42,42,42	0
81	MG	1	3742	1/1	0.98	0.38	32,32,32,32	0
81	MG	5	3719	1/1	0.98	0.43	63,63,63,63	0
81	MG	N3	203	1/1	0.98	0.33	45,45,45,45	0
81	MG	1	3471	1/1	0.98	0.46	37,37,37,37	0
81	MG	1	3472	1/1	0.98	0.28	39,39,39,39	0
81	MG	5	3642	1/1	0.98	0.15	56,56,56,56	0
82	ZN	Q3	501	1/1	0.98	0.17	64,64,64,64	0
82	ZN	D6	101	1/1	0.98	0.17	84,84,84,84	0
81	MG	1	3813	1/1	0.98	0.23	50,50,50,50	0
81	MG	5	3502	1/1	0.98	0.33	52,52,52,52	0
81	MG	5	3503	1/1	0.98	0.53	51,51,51,51	0
82	ZN	o7	501	1/1	0.98	0.16	71,71,71,71	0
82	ZN	q2	501	1/1	0.98	0.08	113,113,113,113	0
81	MG	1	3687	1/1	0.98	0.25	45,45,45,45	0
81	MG	5	3505	1/1	0.98	0.27	59,59,59,59	0
81	MG	5	3457	1/1	0.99	0.26	44,44,44,44	0
81	MG	5	3576	1/1	0.99	0.14	56,56,56,56	0
81	MG	1	3805	1/1	0.99	0.12	51,51,51,51	0
81	MG	1	3466	1/1	0.99	0.21	39,39,39,39	0
81	MG	1	3473	1/1	0.99	0.42	38,38,38,38	0
81	MG	5	3705	1/1	0.99	0.29	54,54,54,54	0
81	MG	1	3774	1/1	0.99	0.29	41,41,41,41	0
81	MG	5	3733	1/1	0.99	0.33	55,55,55,55	0
81	MG	6	1909	1/1	0.99	0.22	71,71,71,71	0
81	MG	1	3692	1/1	0.99	0.35	33,33,33,33	0
81	MG	m7	201	1/1	0.99	0.32	44,44,44,44	0
81	MG	5	3441	1/1	0.99	0.21	44,44,44,44	0
81	MG	1	3565	1/1	0.99	0.21	46,46,46,46	0
81	MG	1	3706	1/1	0.99	0.27	44,44,44,44	0
81	MG	1	3474	1/1	0.99	0.27	43,43,43,43	0
81	MG	1	3557	1/1	0.99	0.26	34,34,34,34	0
81	MG	1	3764	1/1	0.99	0.18	55,55,55,55	0
81	MG	N8	201	1/1	0.99	0.17	41,41,41,41	0
81	MG	1	3528	1/1	0.99	0.38	33,33,33,33	0
81	MG	1	3723	1/1	0.99	0.38	34,34,34,34	0
82	ZN	O4	201	1/1	0.99	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
82	ZN	O7	101	1/1	0.99	0.19	50,50,50,50	0
82	ZN	Q2	501	1/1	0.99	0.10	90,90,90,90	0
81	MG	1	3619	1/1	0.99	0.30	58,58,58,58	0
81	MG	5	3495	1/1	0.99	0.29	46,46,46,46	0
81	MG	2	2090	1/1	0.99	0.07	102,102,102,102	0
81	MG	1	3800	1/1	0.99	0.32	35,35,35,35	0
81	MG	5	3498	1/1	0.99	0.10	53,53,53,53	0
81	MG	1	3469	1/1	0.99	0.25	30,30,30,30	0
82	ZN	q0	201	1/1	0.99	0.16	58,58,58,58	0
81	MG	1	3476	1/1	0.99	0.27	34,34,34,34	0
81	MG	1	3512	1/1	0.99	0.15	59,59,59,59	0
82	ZN	d6	101	1/1	0.99	0.14	91,91,91,91	0
81	MG	1	3553	1/1	0.99	0.21	37,37,37,37	0
82	ZN	d9	101	1/1	0.99	0.11	123,123,123,123	0
82	ZN	Q0	500	1/1	1.00	0.15	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.