



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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

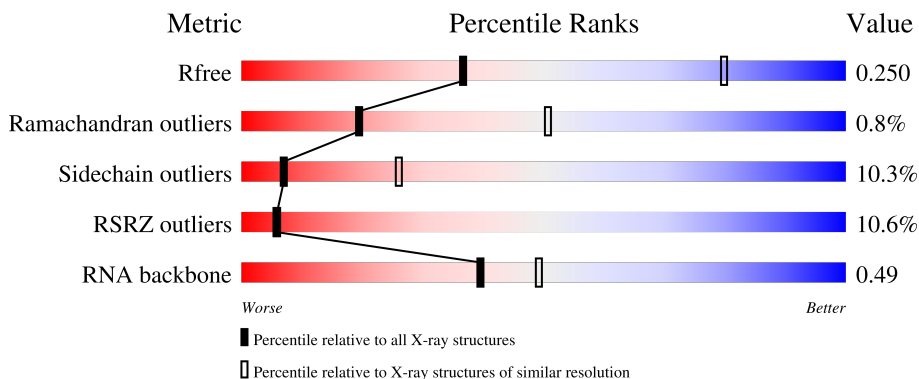
1 Overall quality at a glance

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 ≥ 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	

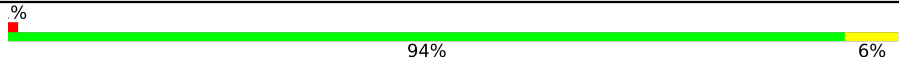
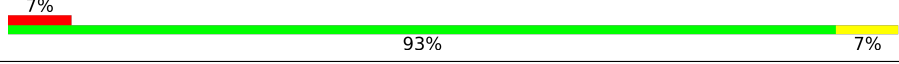
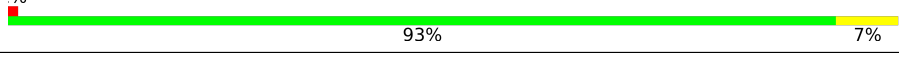
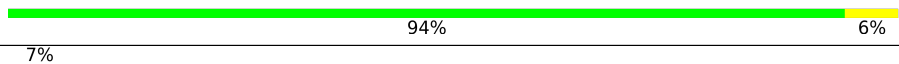

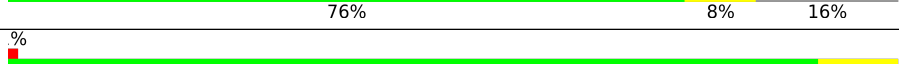
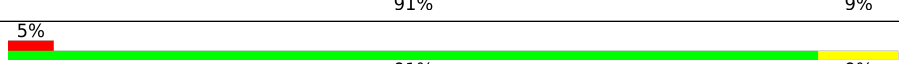
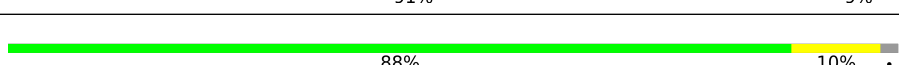
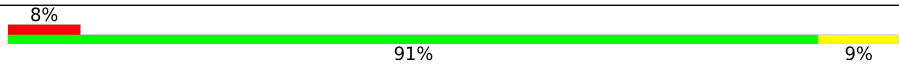

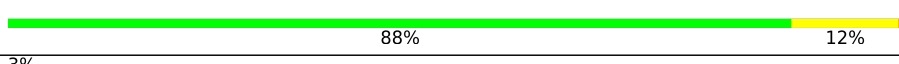
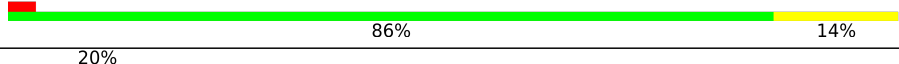
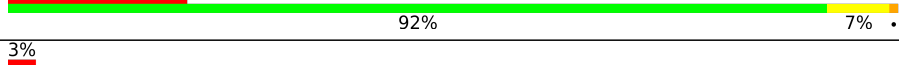

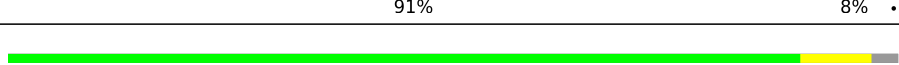
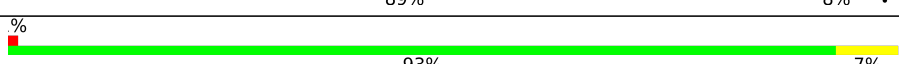
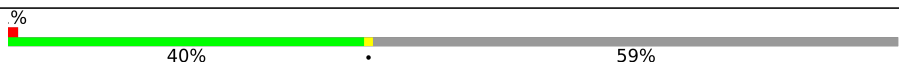


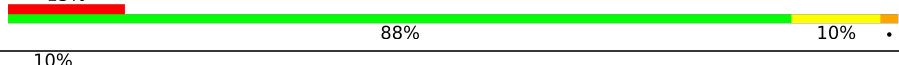
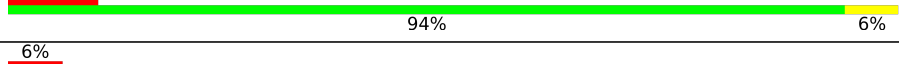
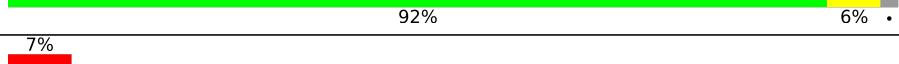
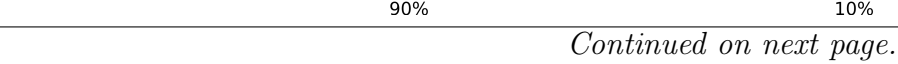


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	8	158	% 77% 19%
4	L2	248	% 91% 9%
4	l2	248	8% 93% 6%
5	L3	386	89% 11%
5	l3	386	91% 9%
6	L4	361	91% 8%
6	l4	361	% 90% 10%
7	L5	296	9% 90% 9%
7	l5	296	13% 92% 7%
8	L6	176	% 79% 9% 11%
8	l6	176	3% 82% 7% 11%
9	L7	226	90% 10%
9	l7	226	88% 10%
10	L8	231	2% 91% 8%
10	l8	231	18% 87% 12%
11	L9	191	10% 85% 13%
11	l9	191	2% 85% 15%
12	M0	221	9% 88% 10%
12	m0	221	6% 88% 11%
13	M1	169	17% 87% 12%
13	m1	169	17% 86% 13%
14	M3	194	4% 91% 8%
14	m3	194	4% 92% 8%
15	M4	137	3% 93% 5%
15	m4	137	% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	M5	203	 % 94% 6%
16	m5	203	 7% 93% 7%
17	M6	197	 % 93% 7%
17	m6	197	 94% 6%
18	M7	184	 7% 85% 10% 5%
18	m7	184	 76% 8% 16%
19	M8	185	 % 91% 9%
19	m8	185	 5% 91% 9%
20	M9	188	 88% 10%
20	m9	188	 8% 91% 9%
21	N0	172	 4% 85% 14%
21	n0	172	 88% 12%
22	N1	159	 3% 86% 14%
22	n1	159	 20% 92% 7%
23	N2	99	 3% 83% 17%
23	n2	99	 8% 91% 8%
24	N3	136	 89% 8%
24	n3	136	 % 93% 7%
25	N4	155	 % 40% 59%
25	n4	155	 28% 81% 6% 13%
26	N5	120	 % 84% 14%
26	n5	120	 13% 88% 10%
27	N6	125	 10% 94% 6%
27	n6	125	 6% 92% 6%
28	N7	135	 7% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	n7	135	37% 93% 7%
29	N8	148	8% 89% 11%
29	n8	148	14% 93% 7%
30	N9	58	5% 88% 9%
30	n9	58	10% 90% 9%
31	O0	100	3% 87% 9%
31	o0	100	3% 91% 8%
32	O1	112	14% 87% 8% 5%
32	o1	112	2% 88% 9%
33	O2	127	% 86% 13%
33	o2	127	2% 93% 6%
34	O3	106	% 93% 6%
34	o3	106	2% 95% 5%
35	O4	112	4% 94% 5%
35	o4	112	14% 92% 8%
36	O5	119	2% 92% 8%
36	o5	119	13% 96% .
37	O6	99	92% 6%
37	o6	99	25% 92% 8%
38	O7	87	86% 10%
38	o7	87	5% 92% 7%
39	O8	77	6% 94% 6%
39	o8	77	16% 86% 14%
40	O9	50	88% 12%
40	o9	50	4% 96% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	Q0	52	15% 96%
41	q0	52	4% 87% 13%
42	Q1	25	84% 16%
42	q1	25	76% 24%
43	Q2	105	16% 89% 11%
43	q2	105	9% 90% 10%
44	Q3	91	88% 11%
44	q3	91	92% 8%
45	2	1800	2% 67% 27% 5%
45	6	1800	% 67% 26% 6%
46	S0	206	21% 90% 9%
46	s0	206	17% 91% 9%
47	S1	216	30% 79% 18%
47	s1	216	30% 90% 10%
48	S2	217	12% 90% 10%
48	s2	217	24% 94% 6%
49	S3	223	15% 86% 8% 6%
49	s3	223	34% 91% 8%
50	S4	260	34% 92% 7%
50	s4	260	15% 92% 8%
51	S5	206	62% 91% 8%
51	s5	206	32% 93% 7%
52	S6	236	18% 79% 6% 15%
53	S7	186	15% 87% 9%
53	s7	186	18% 89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	S8	200	14% 84% 8% 8%
54	s8	200	10% 90% 6%
55	S9	185	21% 88% 5% 6%
55	s9	185	24% 91% 9%
56	C0	105	10% 79% 6% 14%
56	c0	105	30% 79% 9% 9%
57	C1	146	10% 84% 10% 5%
57	c1	146	12% 90% 9%
58	C2	143	23% 59% 12% 29%
58	c2	143	38% 72% 14% 13%
59	C3	150	11% 93% 7%
59	c3	150	6% 91% 9%
60	C4	128	5% 87% 11% ..
60	c4	128	24% 89% 11%
61	C5	141	17% 79% 18%
61	c5	141	46% 82% 13% ..
62	C6	142	65% 85% 10% ..
62	c6	142	62% 93% 6%
63	C7	136	30% 74% 9% .. 15%
63	c7	136	13% 76% 9% 14%
64	C8	145	27% 87% 11% ..
64	c8	145	32% 89% 10%
65	C9	143	33% 86% 10%
65	c9	143	29% 92% 7%
66	D0	109	32% 83% 10% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
66	d0	109	24% 87% 12%
67	D1	87	18% 90% 10%
67	d1	87	14% 86% 14%
68	D2	129	33% 88% 10%
68	d2	129	14% 90% 9%
69	D3	144	% 94% 6%
69	d3	144	5% 95% 5%
70	D4	134	22% 90% 10%
70	d4	134	17% 92% 7%
71	D5	70	61% 80% 20%
71	d5	70	43% 84% 14%
72	D6	97	3% 79% 16%
72	d6	97	13% 90% 8%
73	D7	81	17% 90% 10%
73	d7	81	15% 93% 7%
74	D8	63	40% 92% 8%
74	d8	63	57% 90% 8%
75	D9	53	30% 89% 11%
75	d9	53	11% 85% 13%
76	E0	62	29% 81% 16%
76	e0	62	24% 85% 15%
77	SR	318	58% 95% 5%
77	sR	318	54% 93% 7%
78	SM	272	11% 49% 6% 46%
78	sM	272	9% 33% 65%

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
			Total	C	N	O	P			
1	1	3078	Total 65834	C 29406	N 11864	O 21486	P 3078	0	0	0
1	5	3087	Total 66030	C 29494	N 11905	O 21544	P 3087	0	0	0

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

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

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

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

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

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

- 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			

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
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
			Total	C	N	O	S			
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
			Total	C	N	O			
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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

- 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			

Continued on next page...

Continued from previous page...

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			

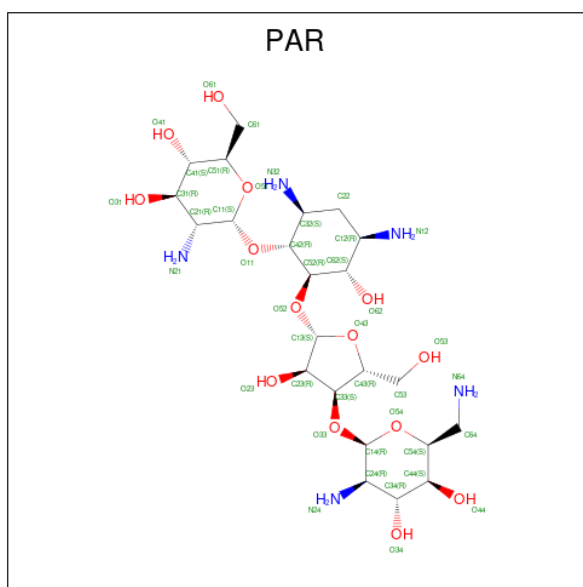
- Molecule 78 is a protein called Suppressor protein STM1.

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: C₂₃H₄₅N₅O₁₄).



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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
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	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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	O6	1	Total Mg 1 1	0	0
81	O7	4	Total Mg 4 4	0	0
81	O9	1	Total Mg 1 1	0	0
81	Q1	1	Total Mg 1 1	0	0
81	Q2	5	Total Mg 5 5	0	0
81	Q3	2	Total Mg 2 2	0	0
81	2	212	Total Mg 212 212	0	0
81	S2	2	Total Mg 2 2	0	0
81	S6	1	Total Mg 1 1	0	0
81	S7	1	Total Mg 1 1	0	0
81	S9	1	Total Mg 1 1	0	0
81	C8	1	Total Mg 1 1	0	0
81	C9	2	Total Mg 2 2	0	0
81	D3	2	Total Mg 2 2	0	0
81	D6	1	Total Mg 1 1	0	0
81	5	698	Total Mg 698 698	0	0
81	7	12	Total Mg 12 12	0	0
81	8	23	Total Mg 23 23	0	0
81	12	3	Total Mg 3 3	0	0
81	13	9	Total Mg 9 9	0	0
81	14	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

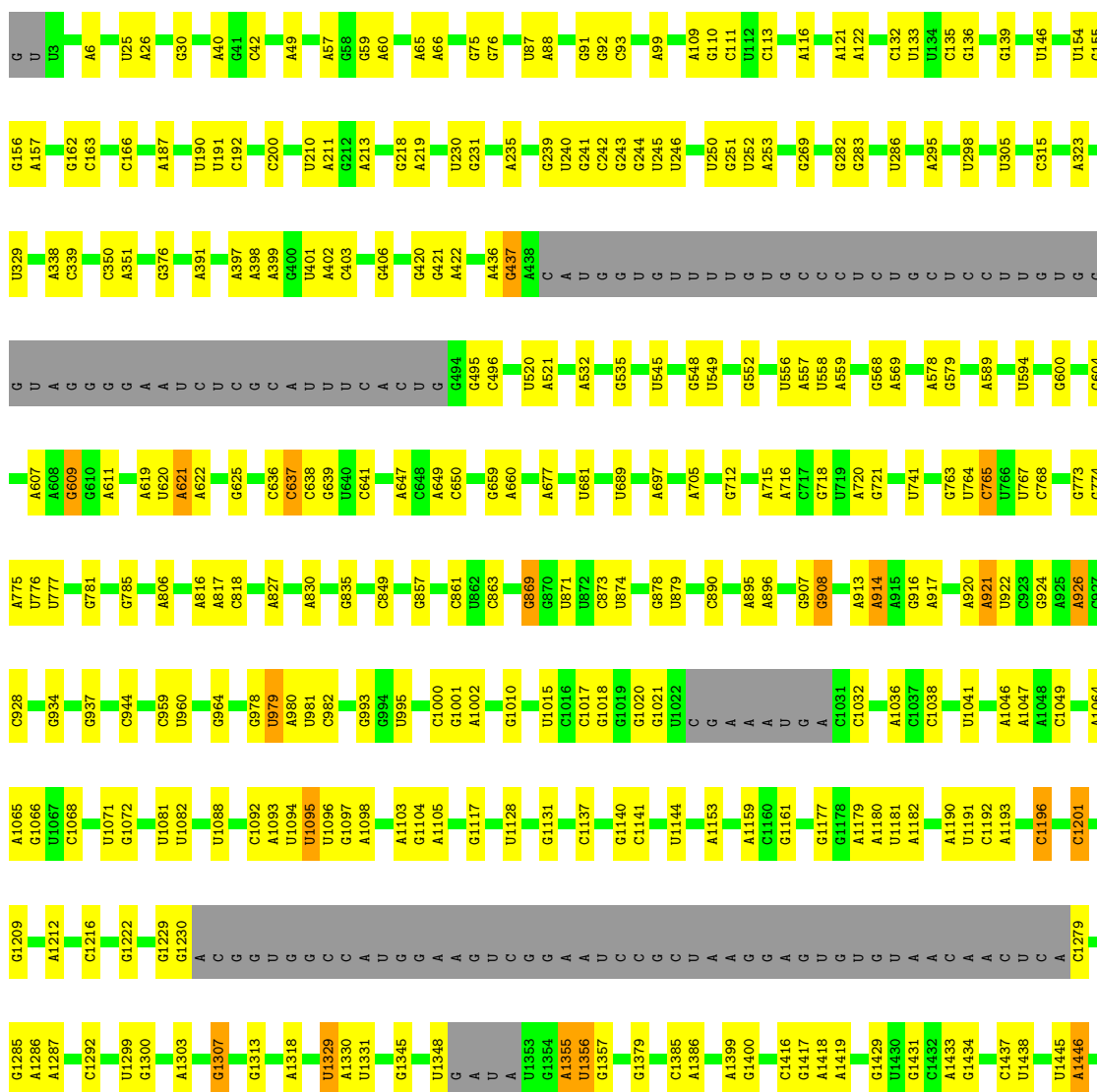
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	n6	1	Total O 1 1	0	0
83	n7	1	Total O 1 1	0	0
83	n8	3	Total O 3 3	0	0
83	o2	3	Total O 3 3	0	0
83	6	113	Total O 113 113	0	0
83	c3	4	Total O 4 4	0	0
83	c4	1	Total O 1 1	0	0
83	c6	1	Total O 1 1	0	0
83	c9	1	Total O 1 1	0	0
83	d3	1	Total O 1 1	0	0
83	d6	1	Total O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

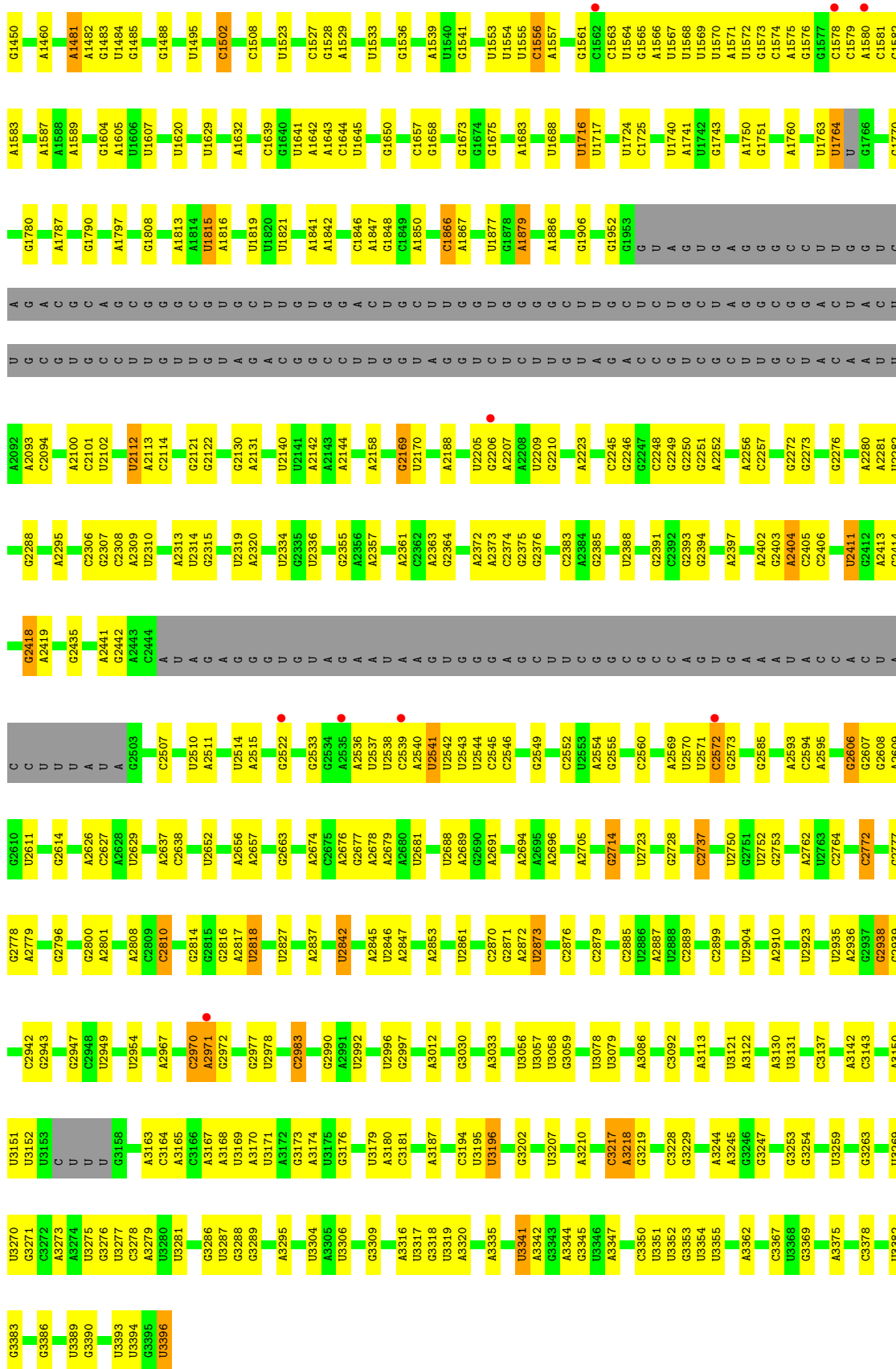
3 Residue-property plots [i](#)

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

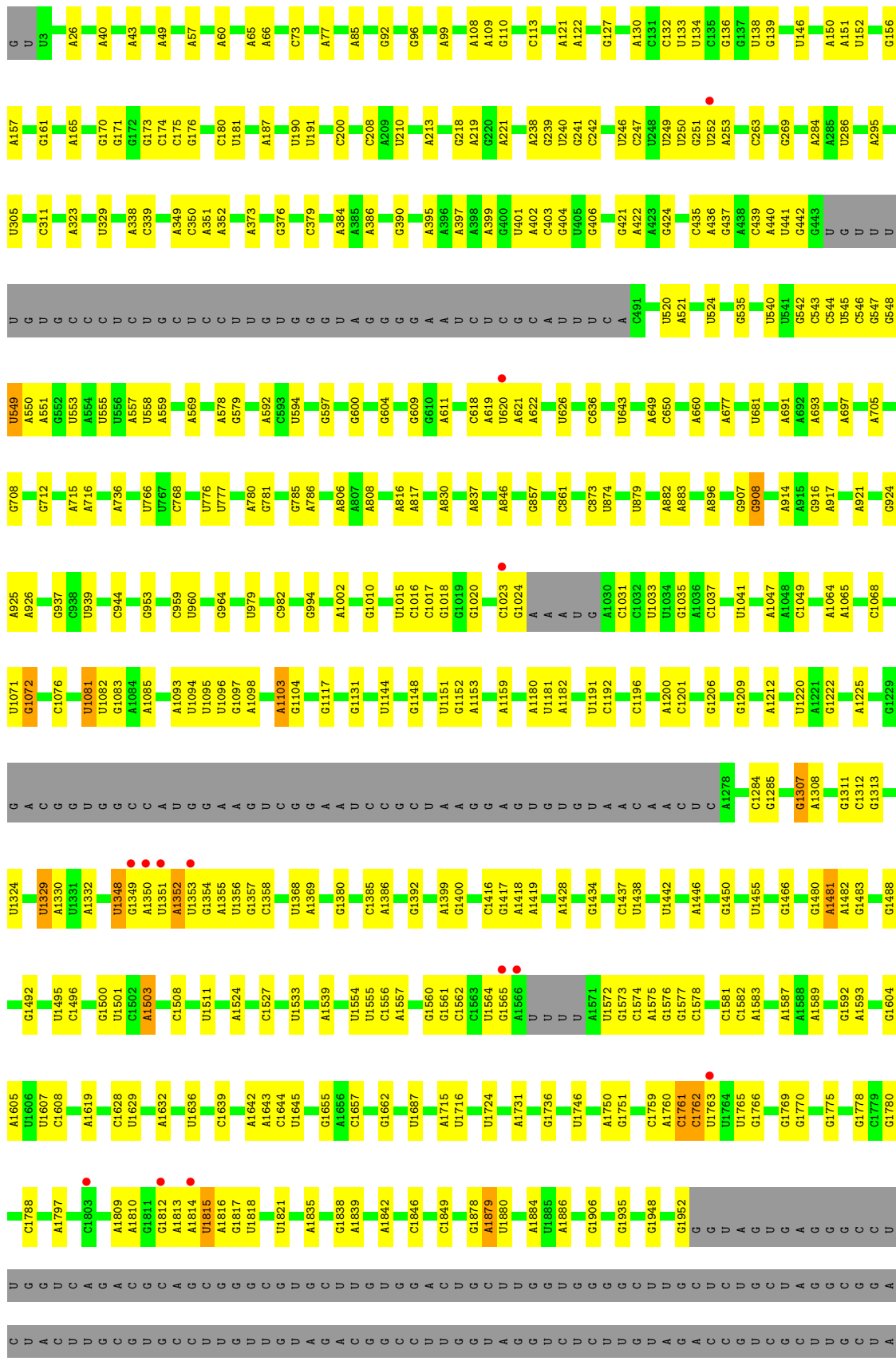
- Molecule 1: 25S ribosomal RNA

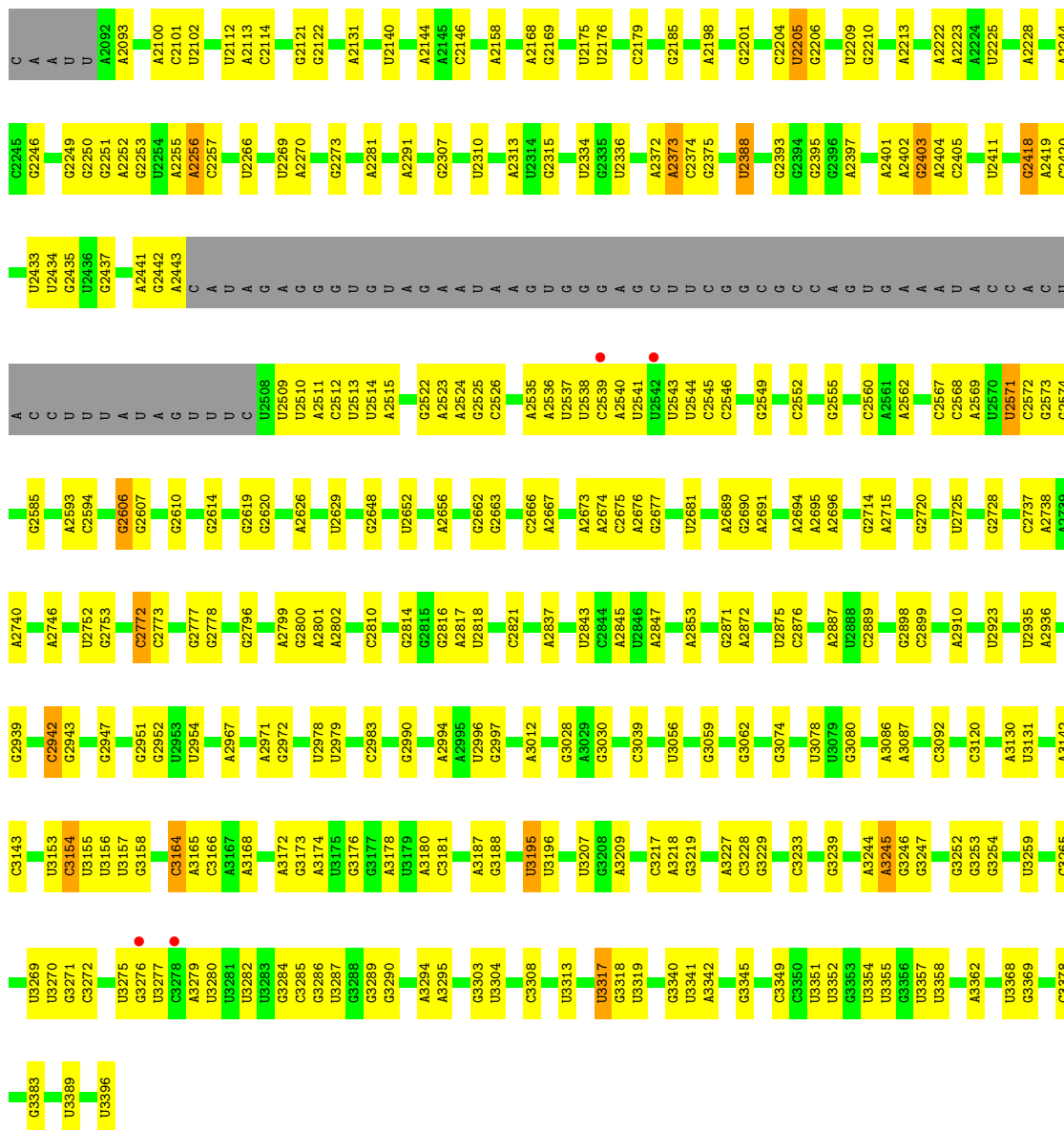
Chain 1:  70% 19% 9%



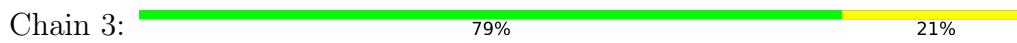


• Molecule 1: 25S ribosomal RNA

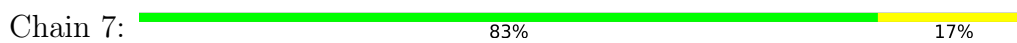




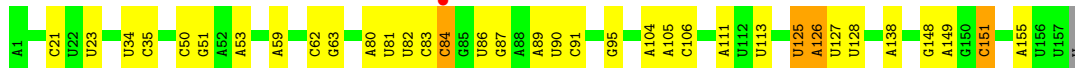
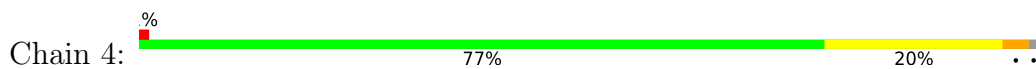
• Molecule 2: 5S ribosomal RNA



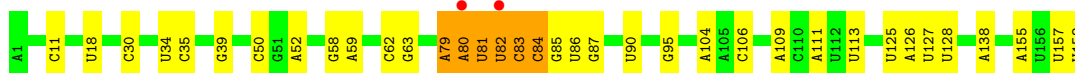
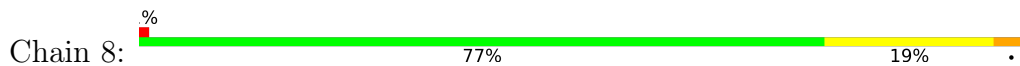
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



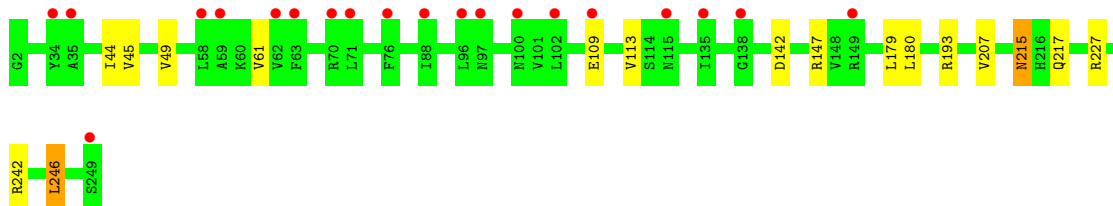
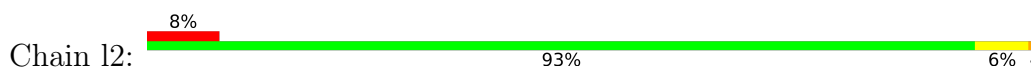
- Molecule 3: 5.8S ribosomal RNA



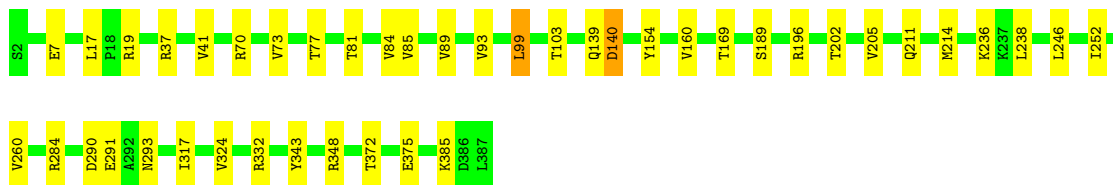
- Molecule 4: 60S ribosomal protein L2-A



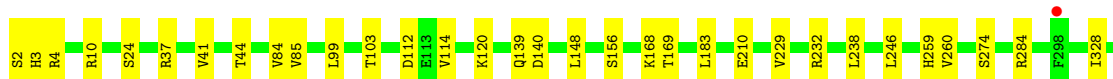
- Molecule 4: 60S ribosomal protein L2-A



- Molecule 5: 60S ribosomal protein L3



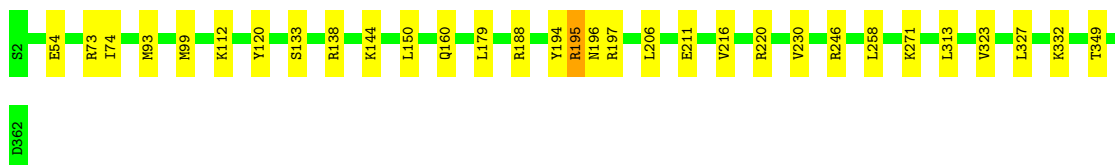
- Molecule 5: 60S ribosomal protein L3





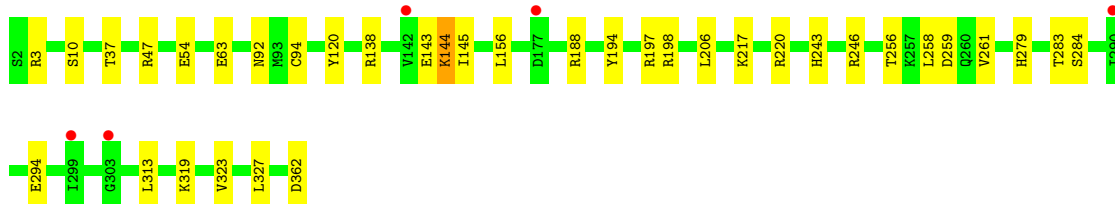
- Molecule 6: 60S ribosomal protein L4-A

Chain L4: 91% 8%



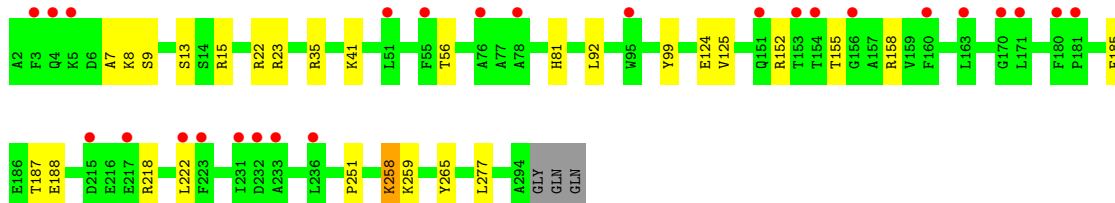
- Molecule 6: 60S ribosomal protein L4-A

Chain l4: 90% 10%



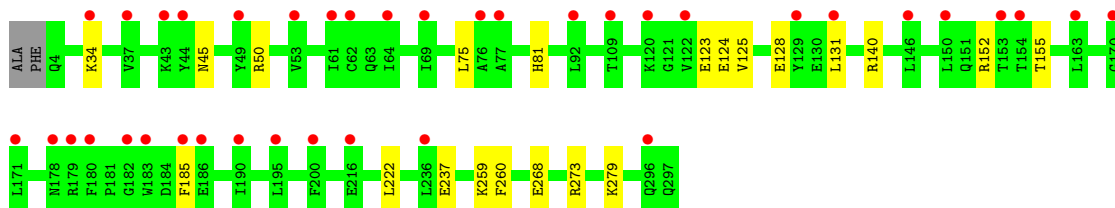
- Molecule 7: 60S ribosomal protein L5

Chain L5: 9% 90% 9%



- Molecule 7: 60S ribosomal protein L5

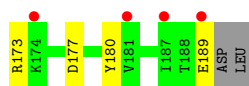
Chain l5: 13% 92% 7%



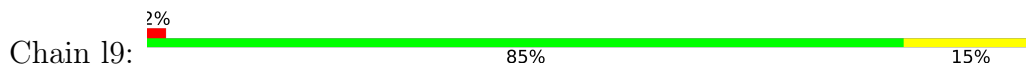
- Molecule 8: 60S ribosomal protein L6-A

Chain L6: 79% 9% 11%

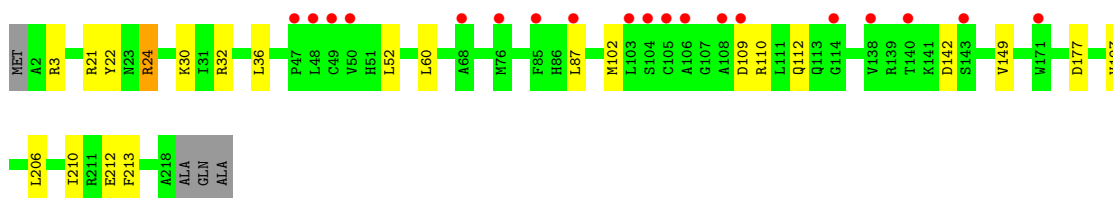
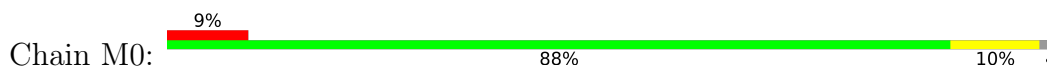




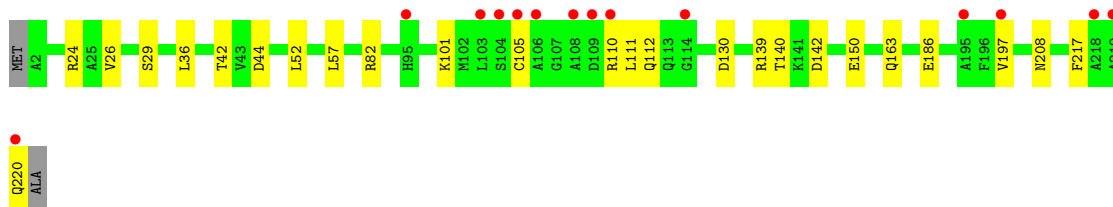
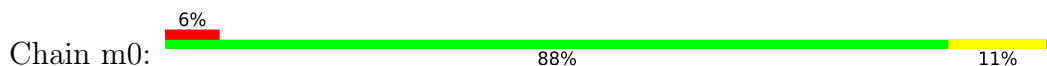
- Molecule 11: 60S ribosomal protein L9-A



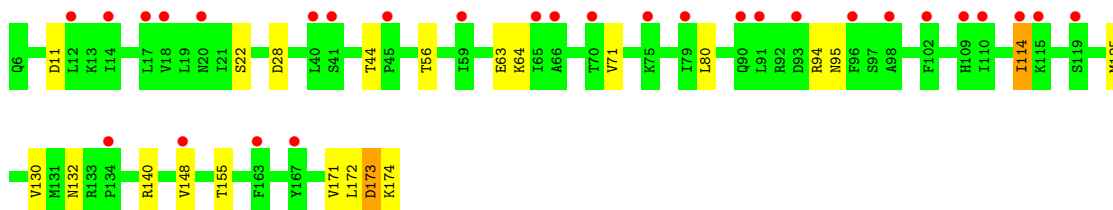
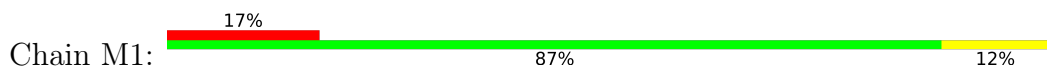
- Molecule 12: 60S ribosomal protein L10



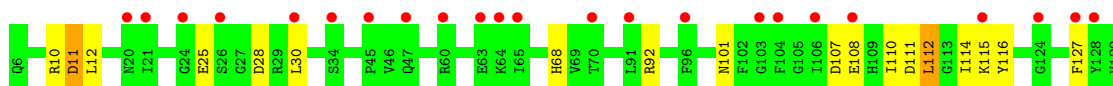
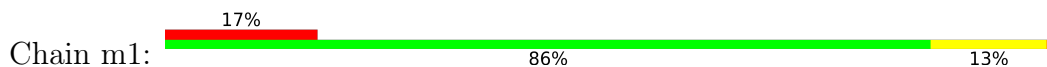
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-B

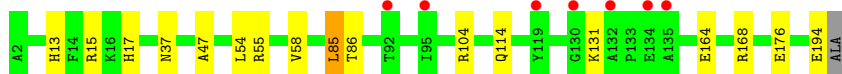
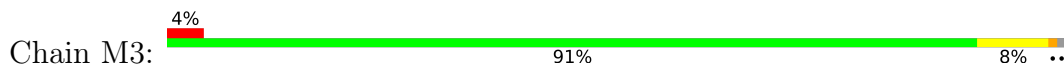


- Molecule 13: 60S ribosomal protein L11-B





- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



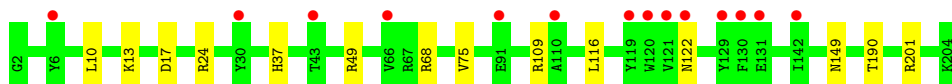
- Molecule 15: 60S ribosomal protein L14-A



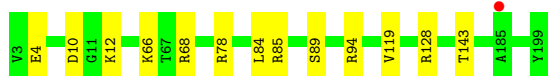
- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A



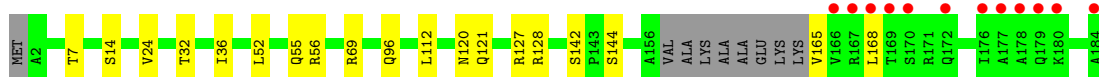
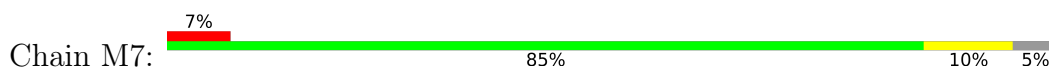
- Molecule 17: 60S ribosomal protein L16-A



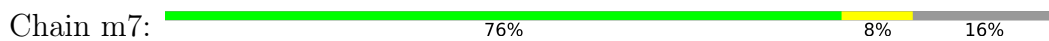
• Molecule 17: 60S ribosomal protein L16-A



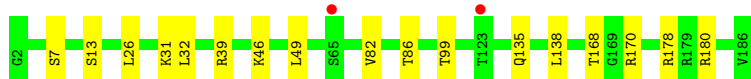
• Molecule 18: 60S ribosomal protein L17-A



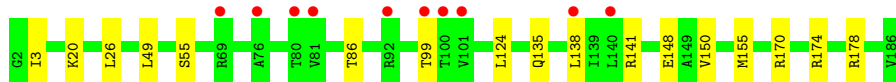
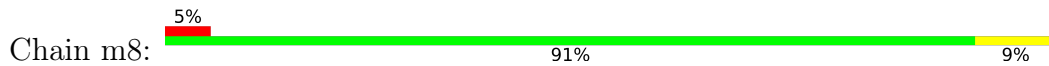
• Molecule 18: 60S ribosomal protein L17-A



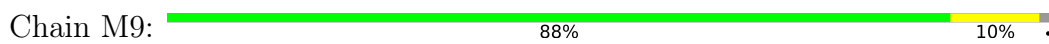
• Molecule 19: 60S ribosomal protein L18-A



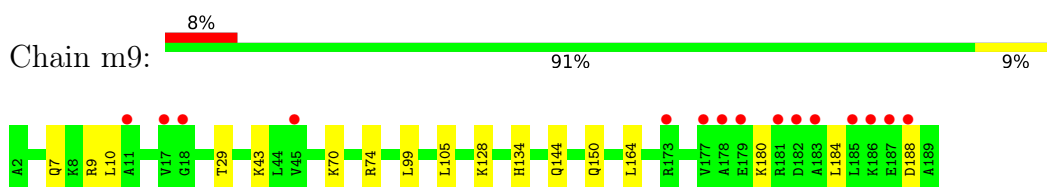
• Molecule 19: 60S ribosomal protein L18-A



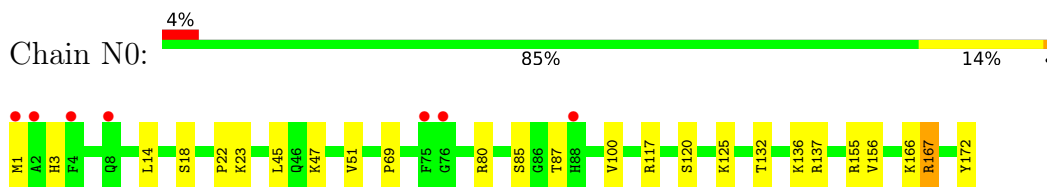
• Molecule 20: 60S ribosomal protein L19-A



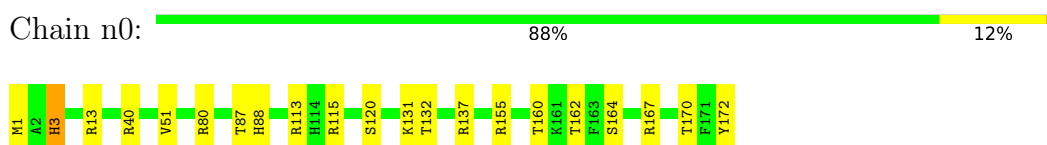
• Molecule 20: 60S ribosomal protein L19-A



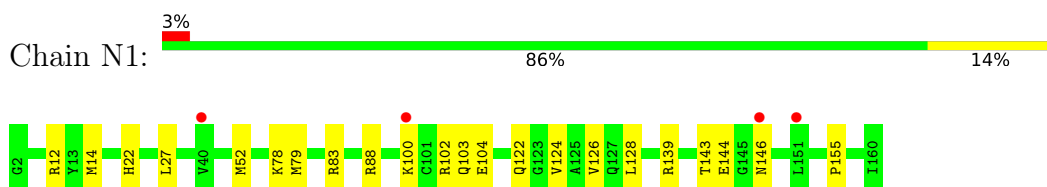
- Molecule 21: 60S ribosomal protein L20-A



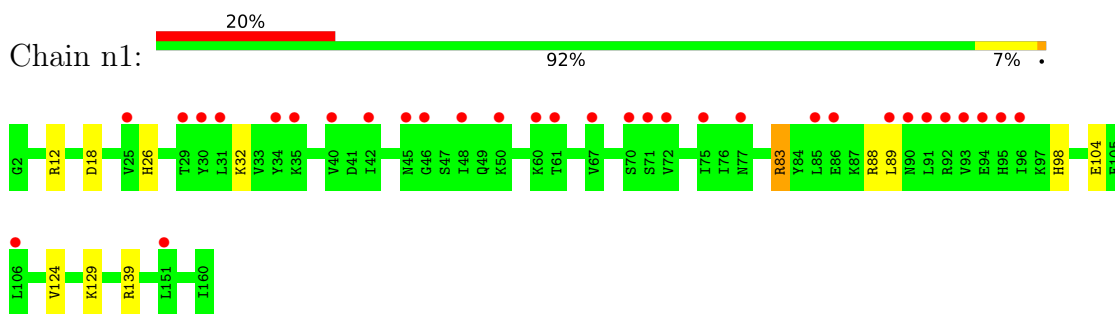
- Molecule 21: 60S ribosomal protein L20-A



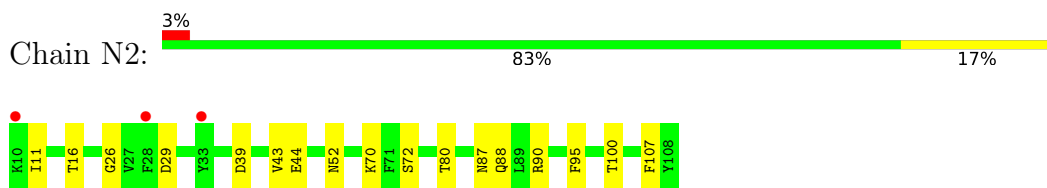
- Molecule 22: 60S ribosomal protein L21-A



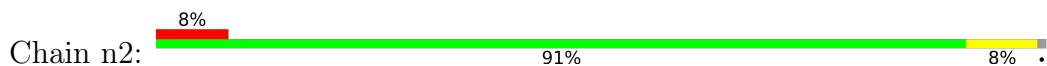
- Molecule 22: 60S ribosomal protein L21-A

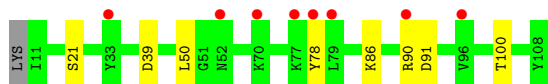


- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A

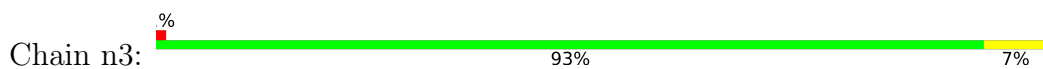




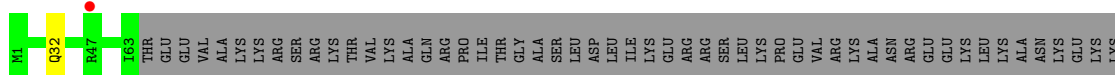
- Molecule 24: 60S ribosomal protein L23-A



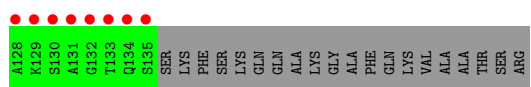
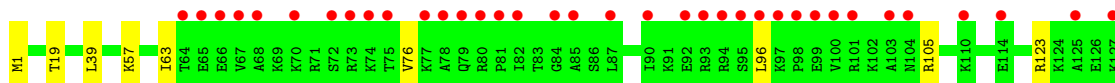
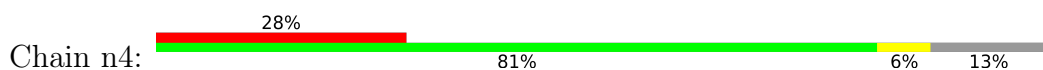
- Molecule 24: 60S ribosomal protein L23-A



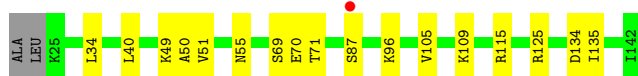
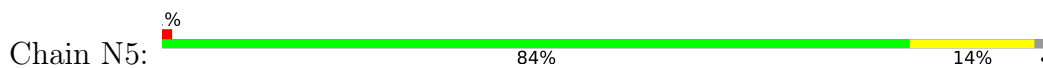
- Molecule 25: 60S ribosomal protein L24-A



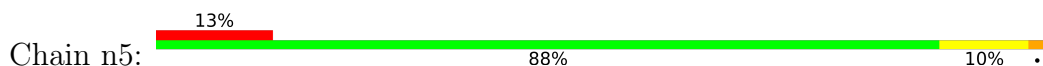
- Molecule 25: 60S ribosomal protein L24-A

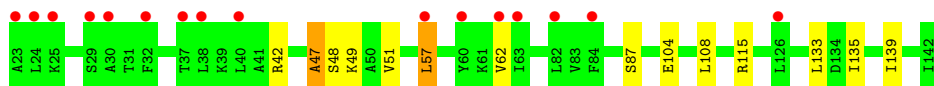


- Molecule 26: 60S ribosomal protein L25

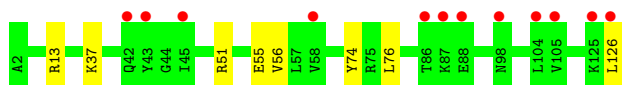


- Molecule 26: 60S ribosomal protein L25

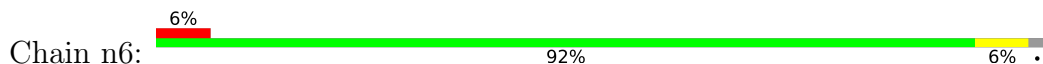




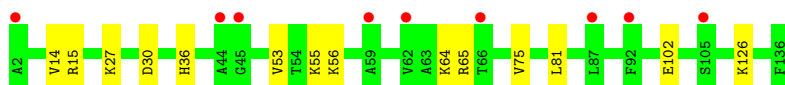
- Molecule 27: 60S ribosomal protein L26-A



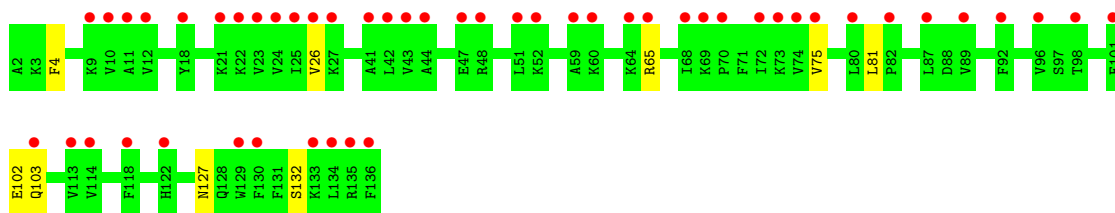
- Molecule 27: 60S ribosomal protein L26-A



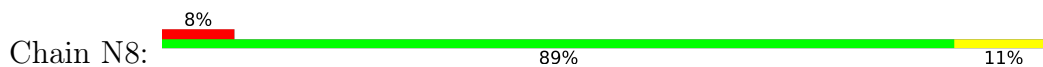
- Molecule 28: 60S ribosomal protein L27-A



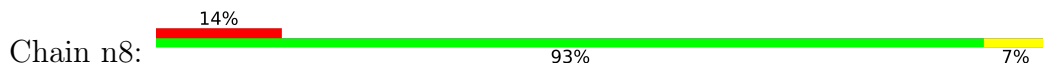
- Molecule 28: 60S ribosomal protein L27-A

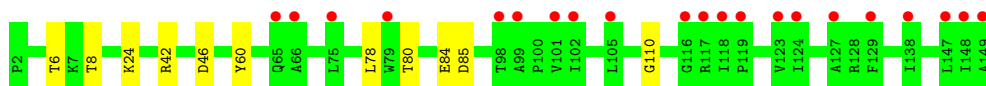


- Molecule 29: 60S ribosomal protein L28

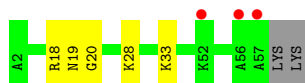
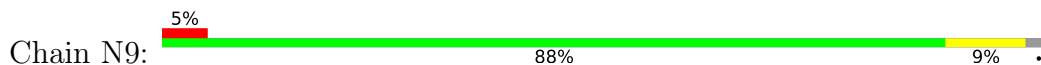


- Molecule 29: 60S ribosomal protein L28

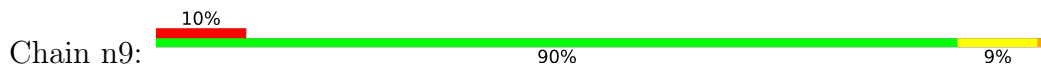




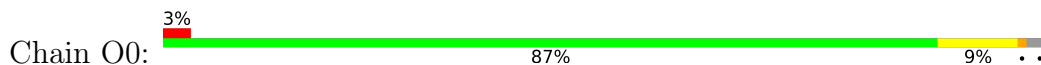
- Molecule 30: 60S ribosomal protein L29



- Molecule 30: 60S ribosomal protein L29



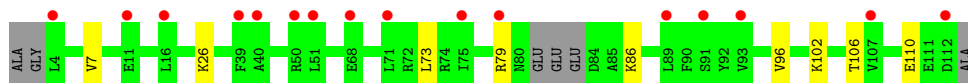
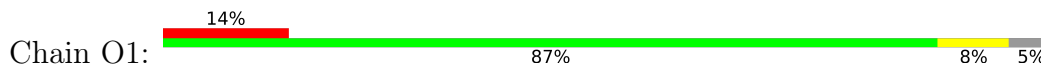
- Molecule 31: 60S ribosomal protein L30



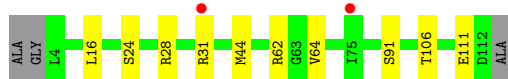
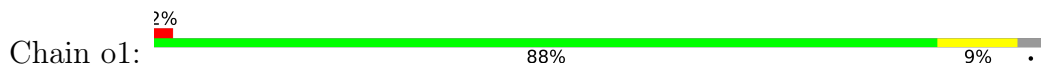
- Molecule 31: 60S ribosomal protein L30



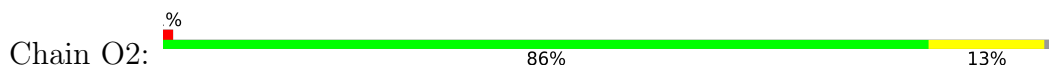
- Molecule 32: 60S ribosomal protein L31-A



- Molecule 32: 60S ribosomal protein L31-A



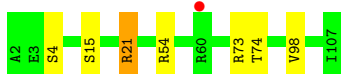
- Molecule 33: 60S ribosomal protein L32



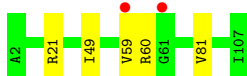
- Molecule 33: 60S ribosomal protein L32



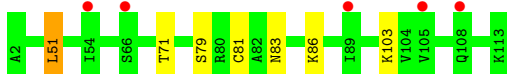
- Molecule 34: 60S ribosomal protein L33-A



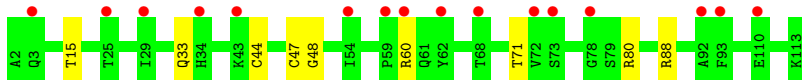
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A



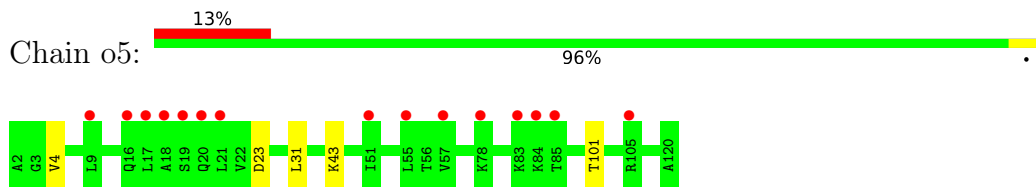
- Molecule 35: 60S ribosomal protein L34-A



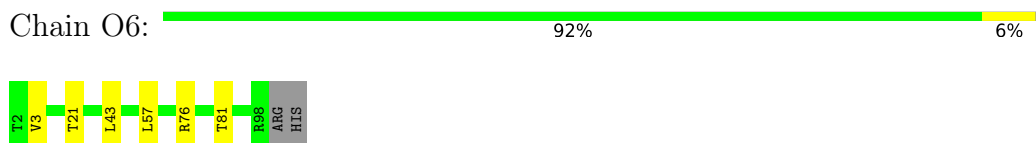
- Molecule 36: 60S ribosomal protein L35-A



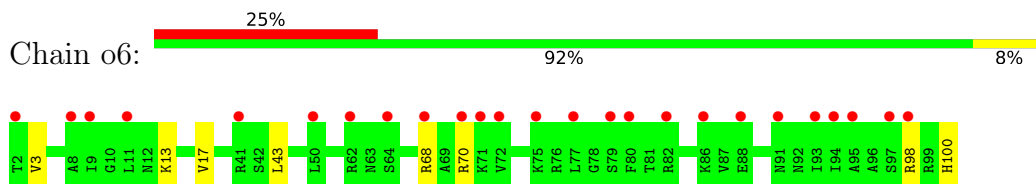
- Molecule 36: 60S ribosomal protein L35-A



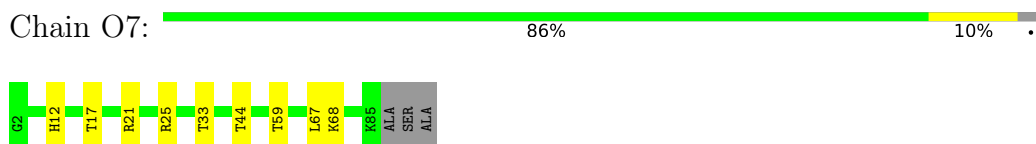
- Molecule 37: 60S ribosomal protein L36-A



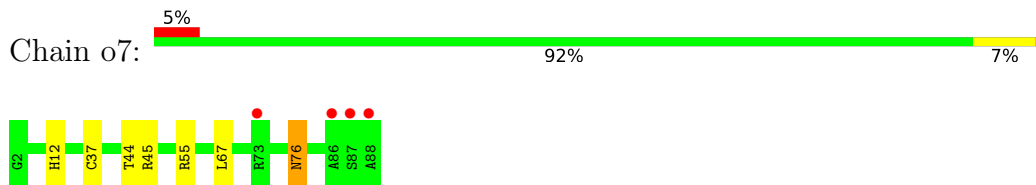
- Molecule 37: 60S ribosomal protein L36-A



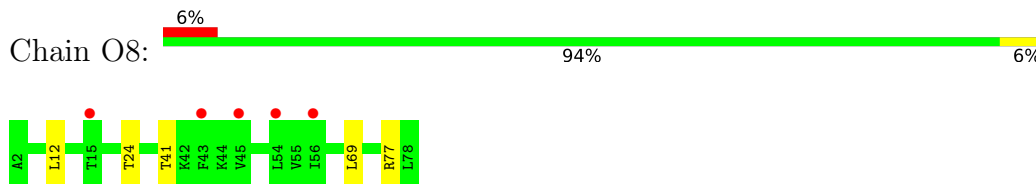
- Molecule 38: 60S ribosomal protein L37-A



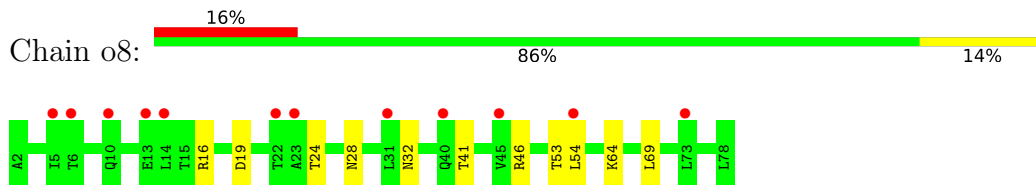
- Molecule 38: 60S ribosomal protein L37-A




- Molecule 39: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39

Chain O9:  88% 12%



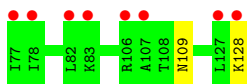
- Molecule 40: 60S ribosomal protein L39

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%

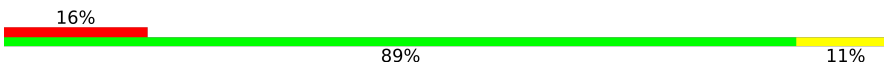


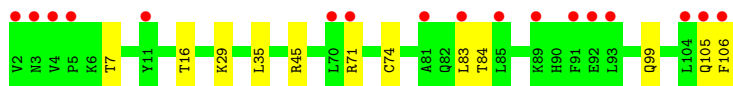
- Molecule 42: 60S ribosomal protein L41-B

Chain q1:  76% 24%

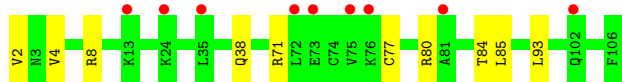
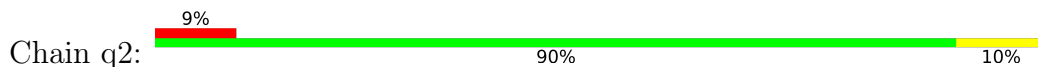


- Molecule 43: 60S ribosomal protein L42-A

Chain Q2:  16% 89% 11%



• Molecule 43: 60S ribosomal protein L42-A



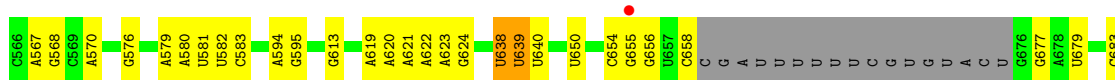
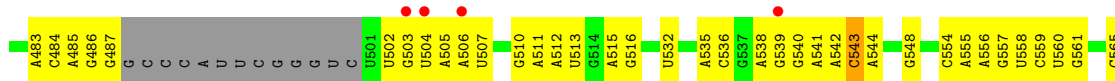
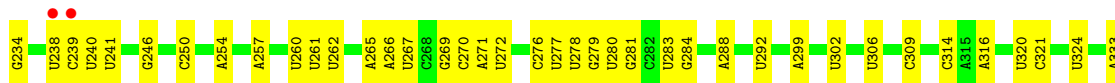
• Molecule 44: 60S ribosomal protein L43-A

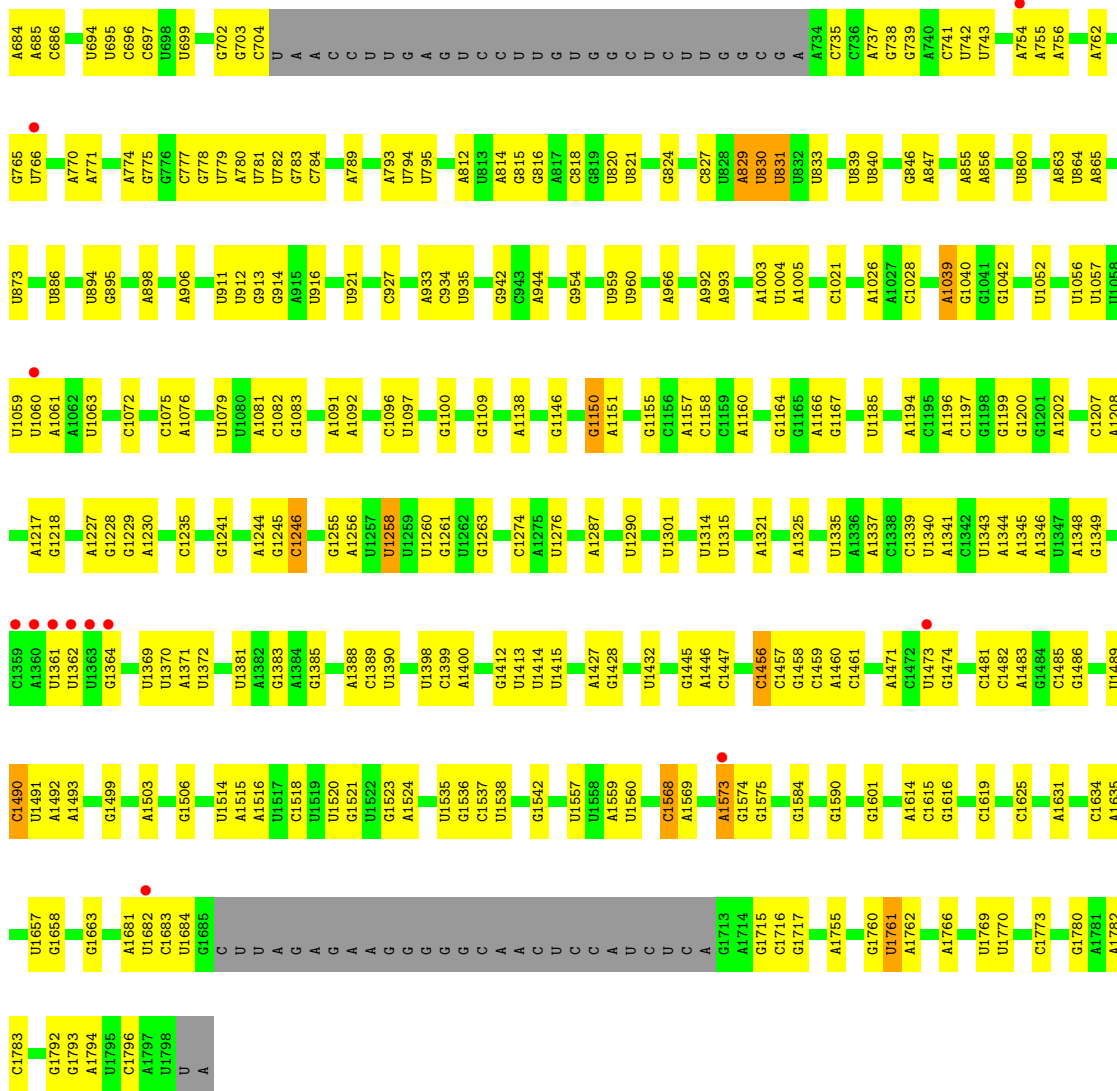


• Molecule 44: 60S ribosomal protein L43-A

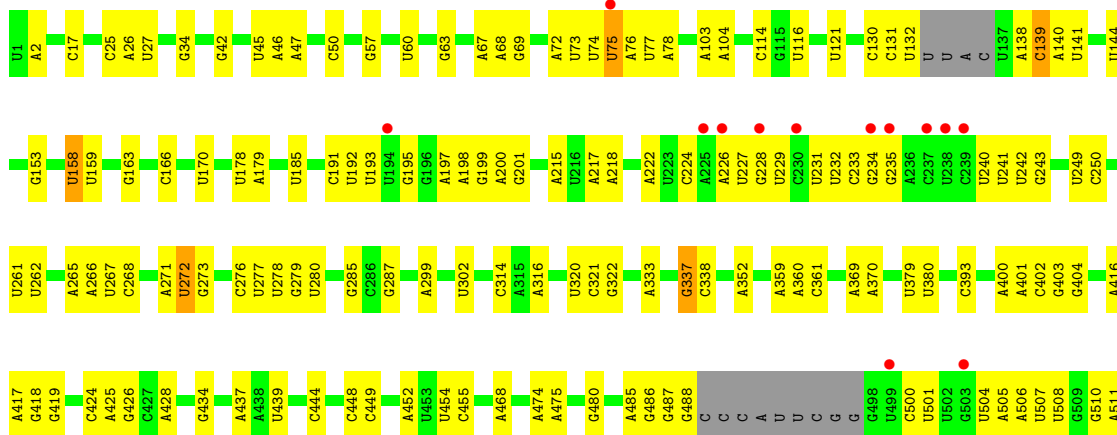


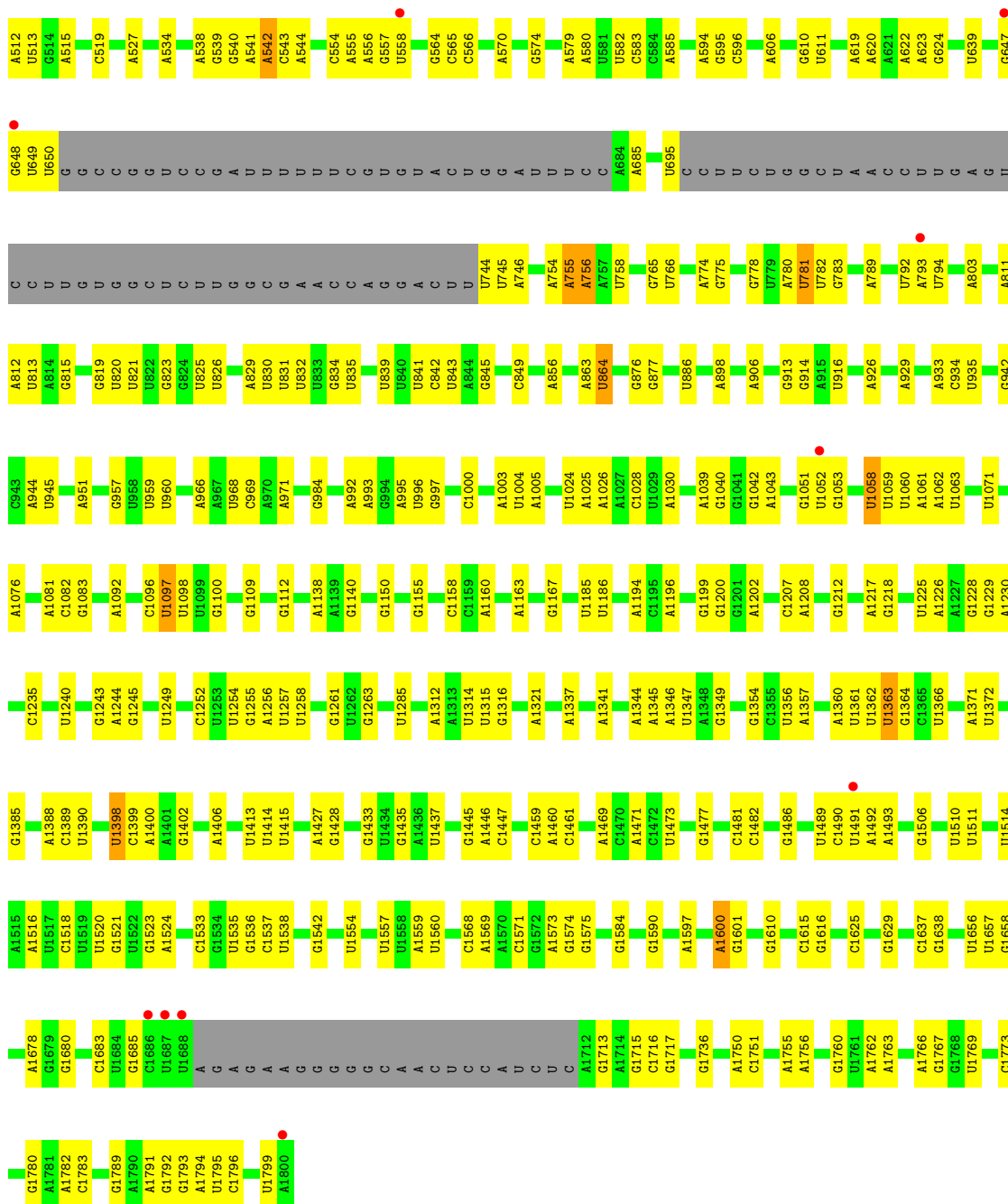
• Molecule 45: 18S ribosomal RNA



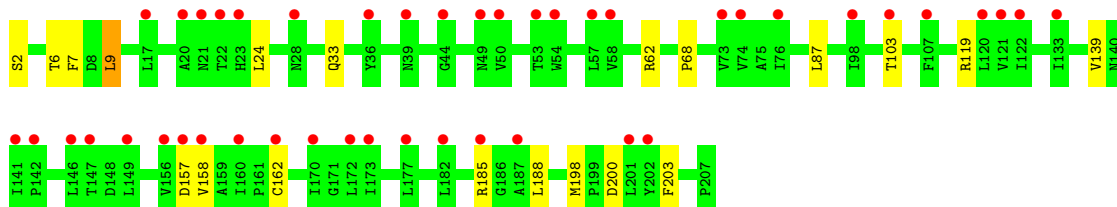


● Molecule 45: 18S ribosomal RNA

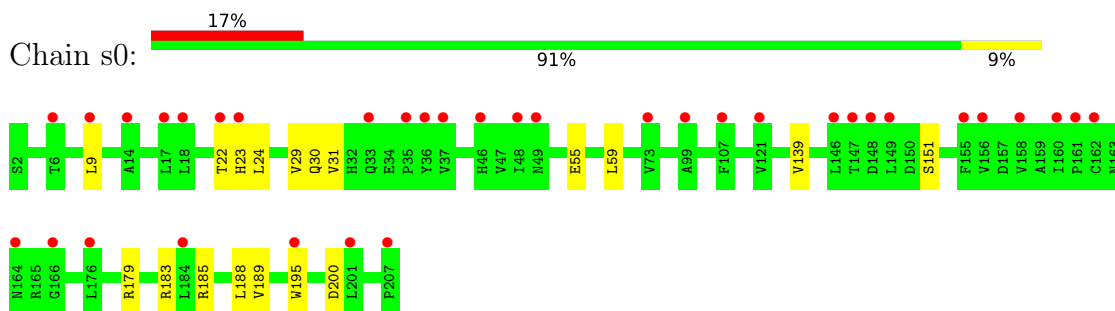




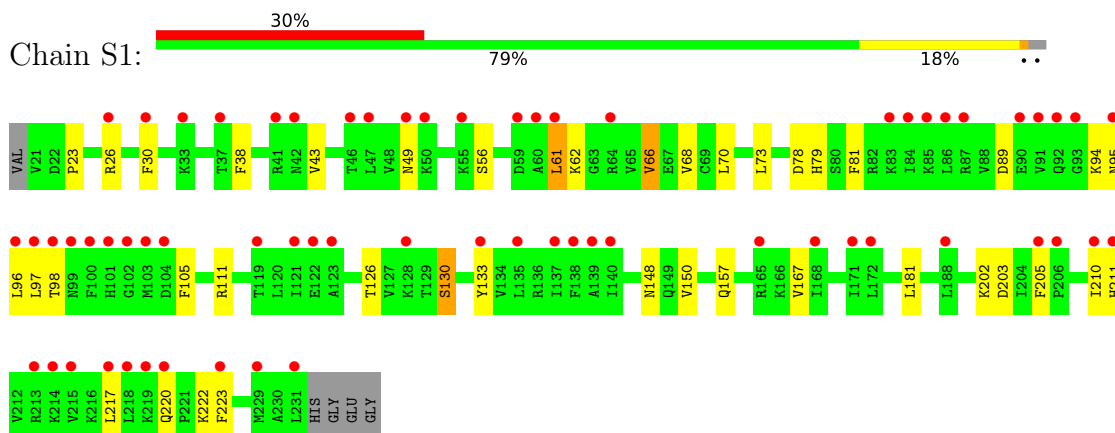
• Molecule 46: 40S ribosomal protein S0-A



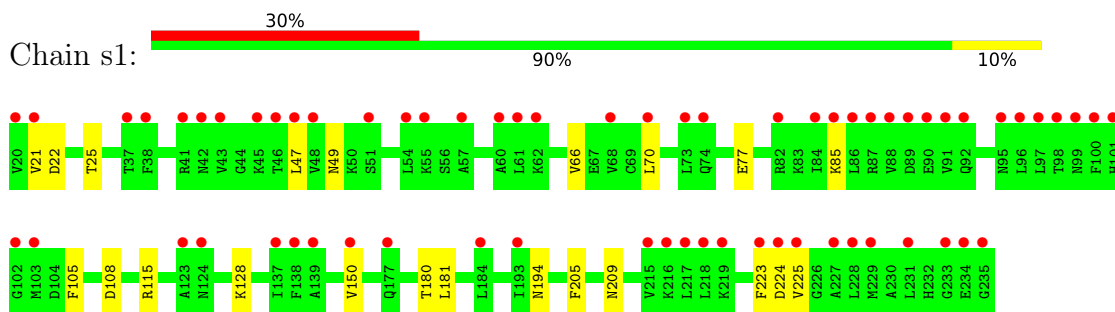
- Molecule 46: 40S ribosomal protein S0-A



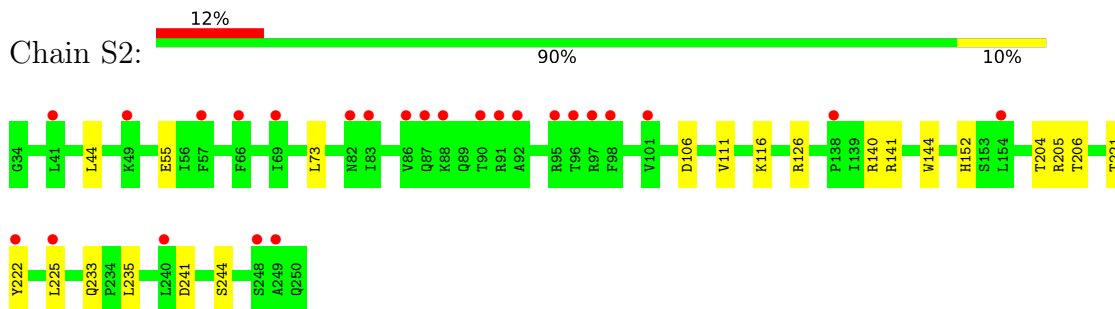
- Molecule 47: 40S ribosomal protein S1-A



- Molecule 47: 40S ribosomal protein S1-A

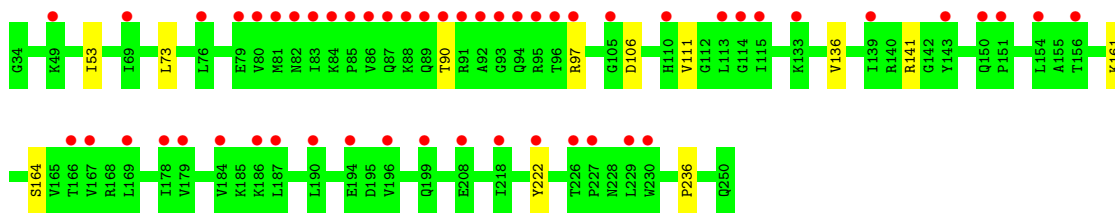


- Molecule 48: 40S ribosomal protein S2

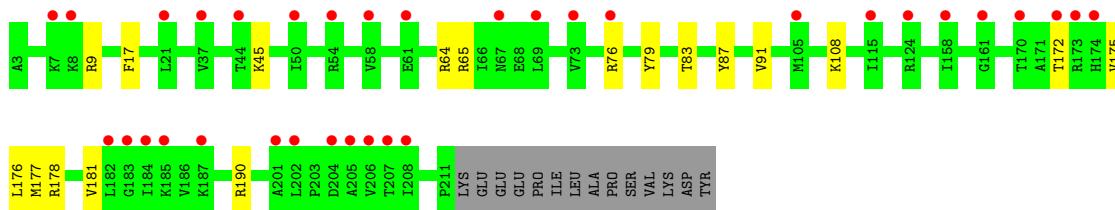
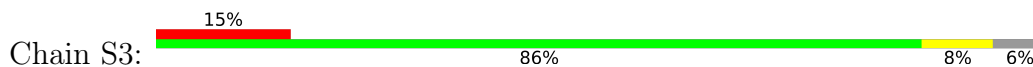


- Molecule 48: 40S ribosomal protein S2

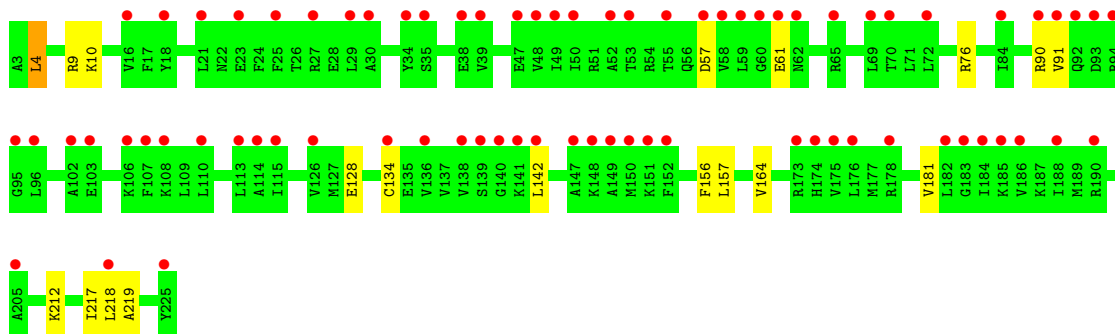
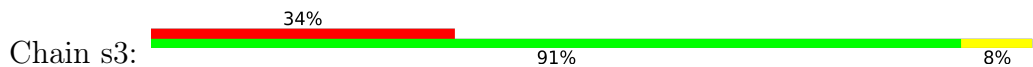




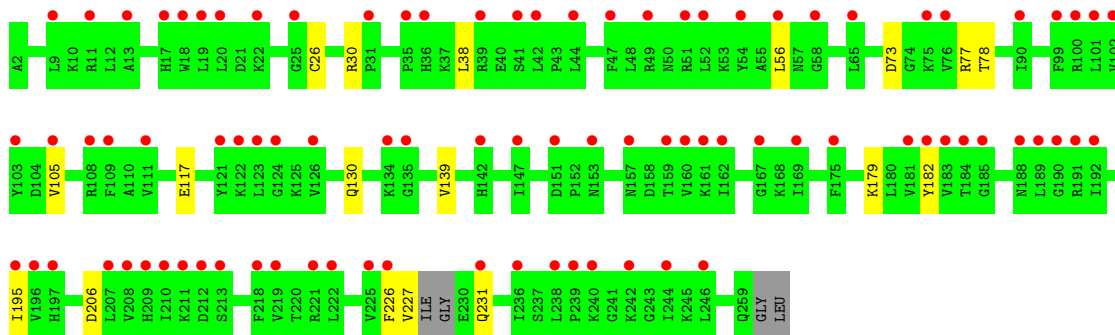
• Molecule 49: 40S ribosomal protein S3



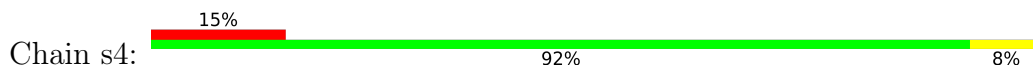
• Molecule 49: 40S ribosomal protein S3

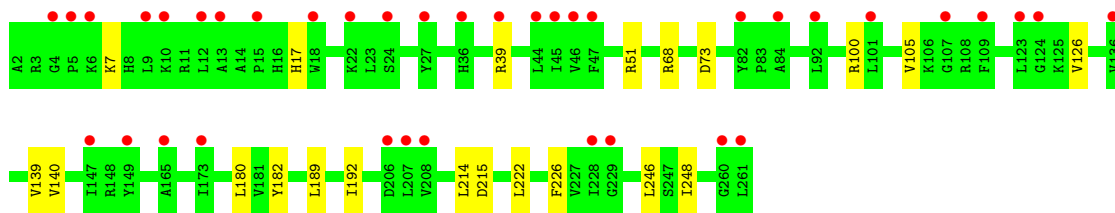


• Molecule 50: 40S ribosomal protein S4-A

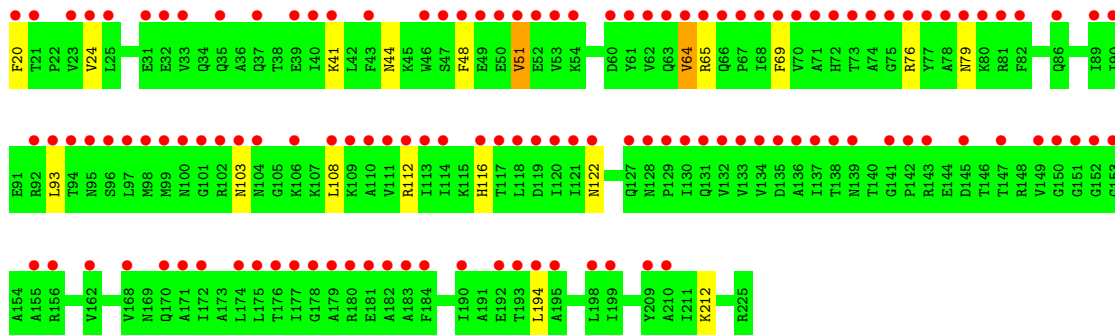
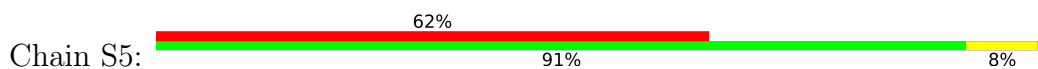


• Molecule 50: 40S ribosomal protein S4-A

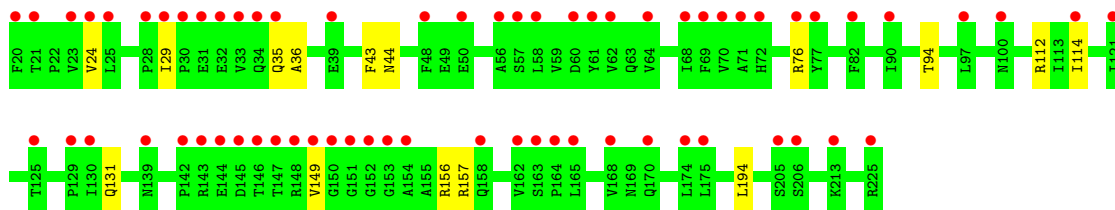
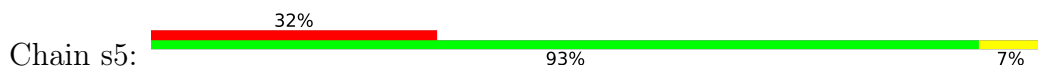




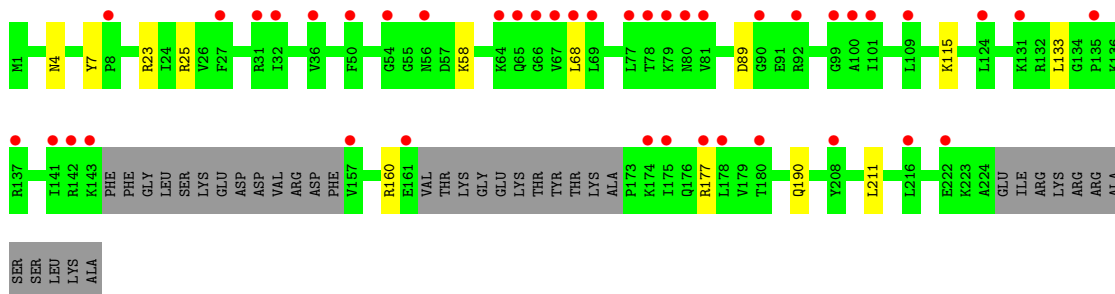
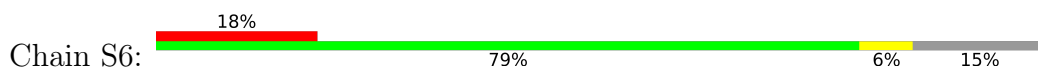
• Molecule 51: 40S ribosomal protein S5



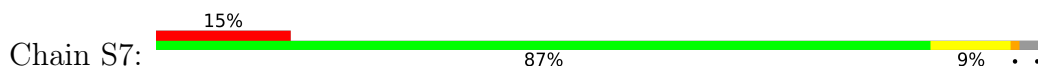
• Molecule 51: 40S ribosomal protein S5

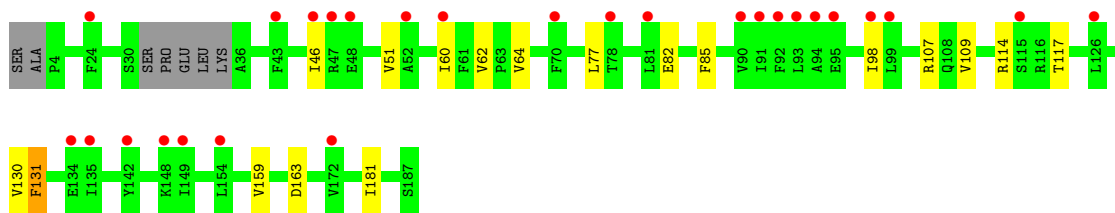


• Molecule 52: 40S ribosomal protein S6-A

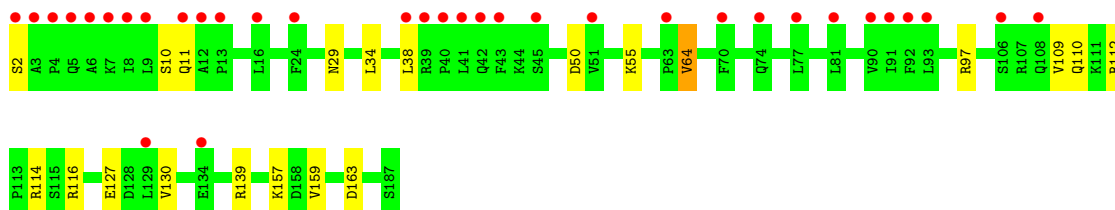
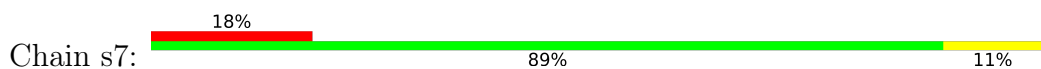


• Molecule 53: 40S ribosomal protein S7-A

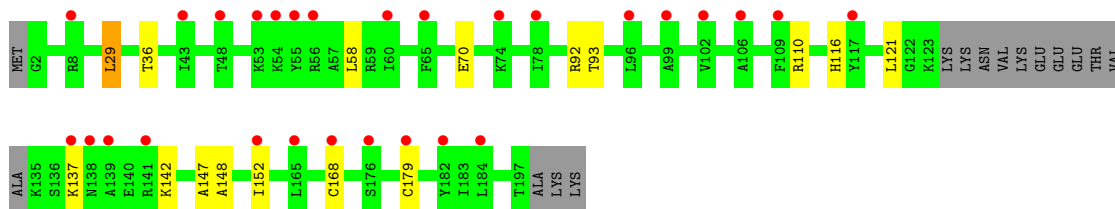
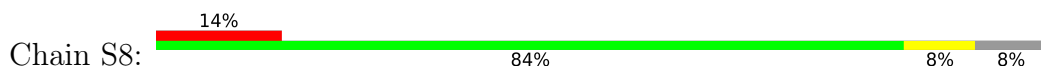




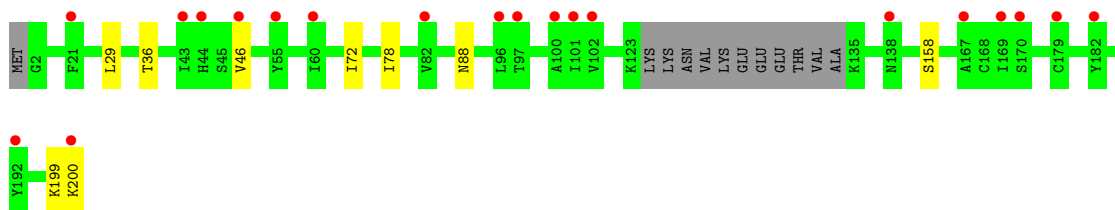
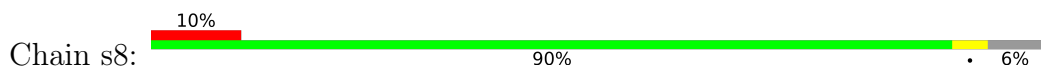
- Molecule 53: 40S ribosomal protein S7-A



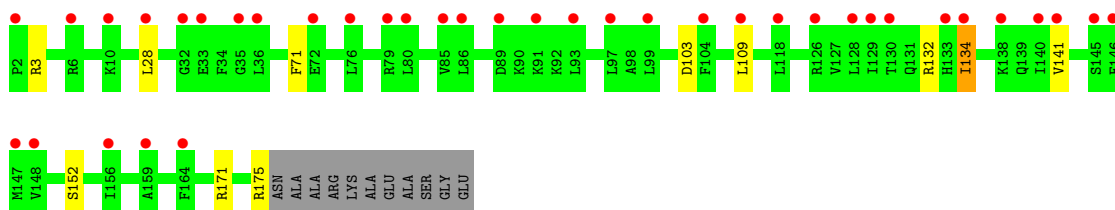
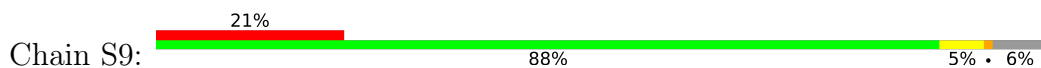
- Molecule 54: 40S ribosomal protein S8-A

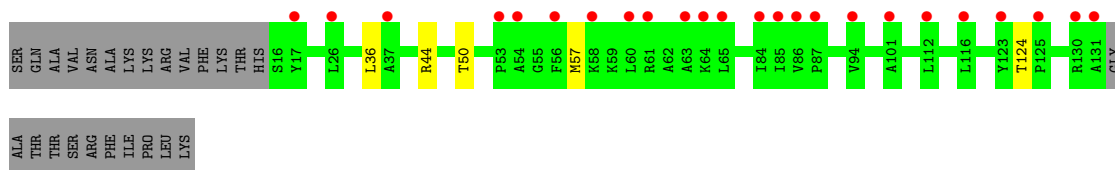


- Molecule 54: 40S ribosomal protein S8-A

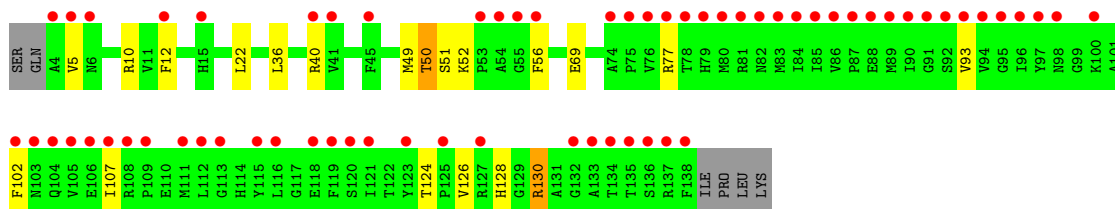
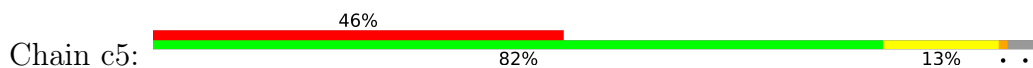


- Molecule 55: 40S ribosomal protein S9-A

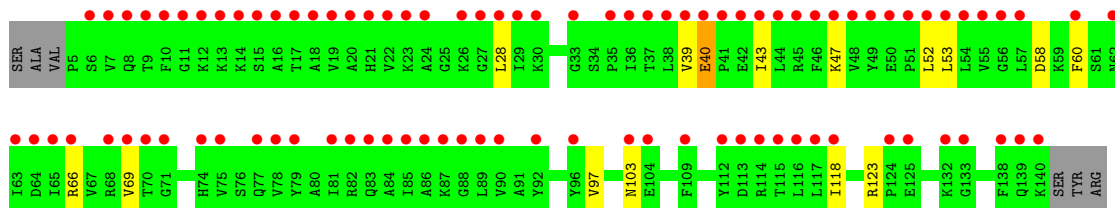
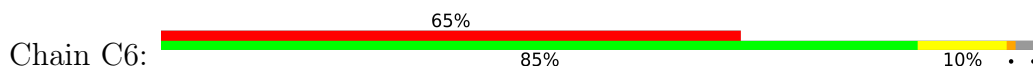




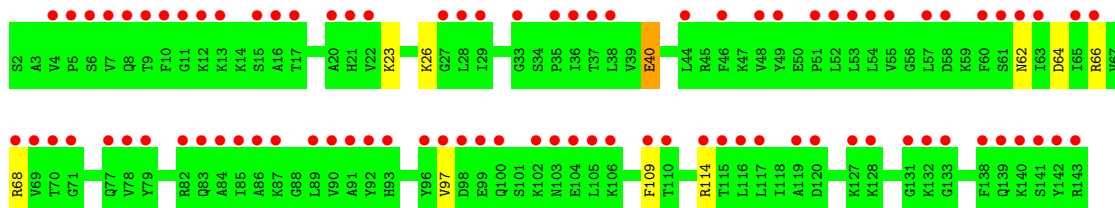
• Molecule 61: 40S ribosomal protein S15



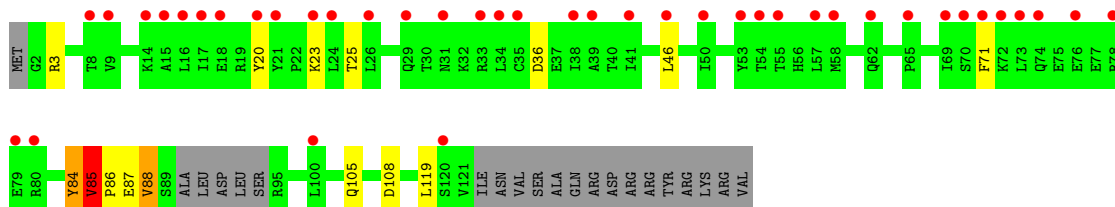
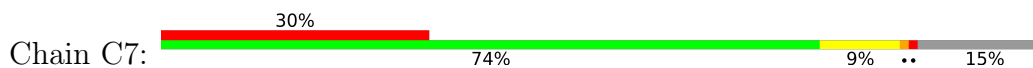
• Molecule 62: 40S ribosomal protein S16-A



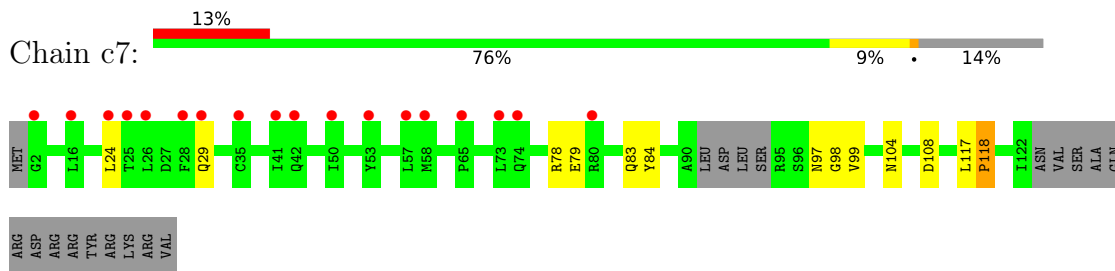
• Molecule 62: 40S ribosomal protein S16-A



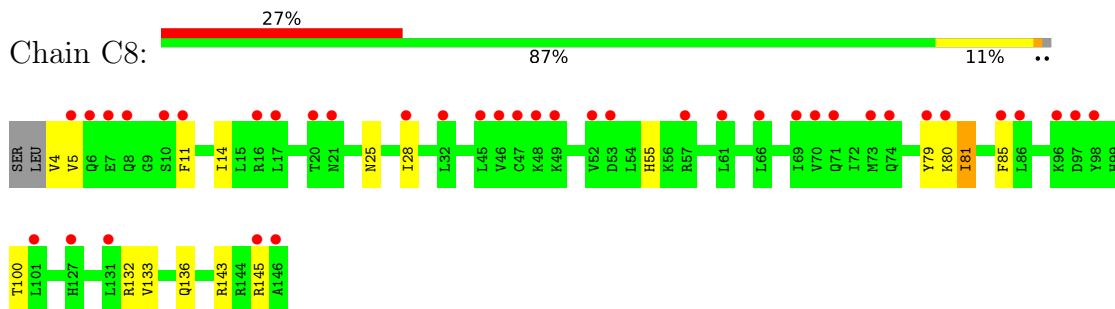
• Molecule 63: 40S ribosomal protein S17-A



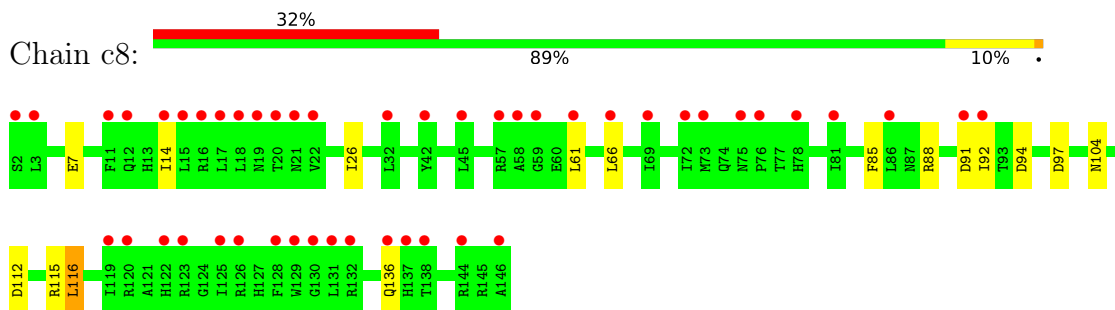
- Molecule 63: 40S ribosomal protein S17-A



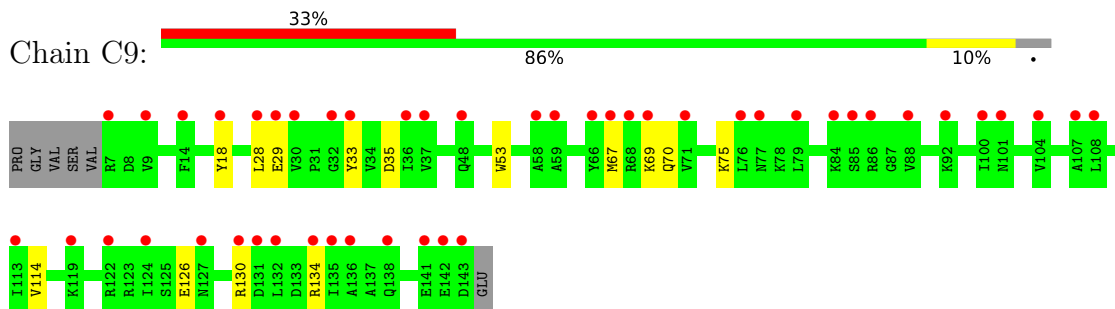
- Molecule 64: 40S ribosomal protein S18-A



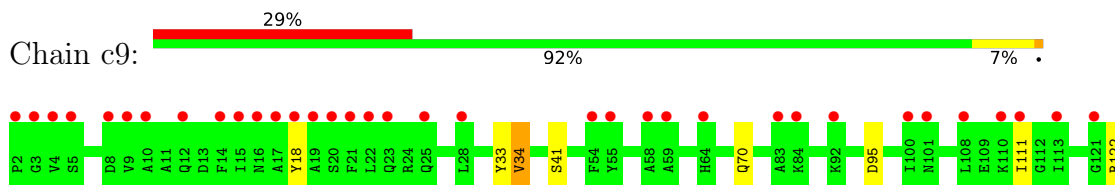
- Molecule 64: 40S ribosomal protein S18-A



- Molecule 65: 40S ribosomal protein S19-A

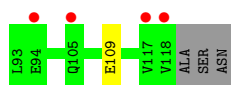
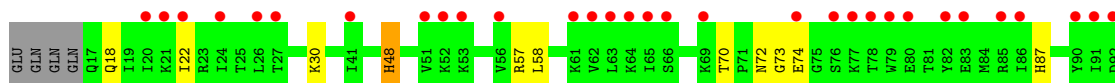
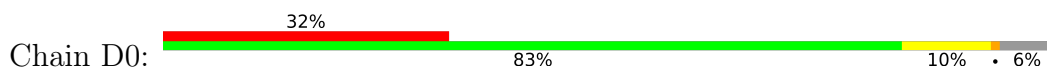


- Molecule 65: 40S ribosomal protein S19-A

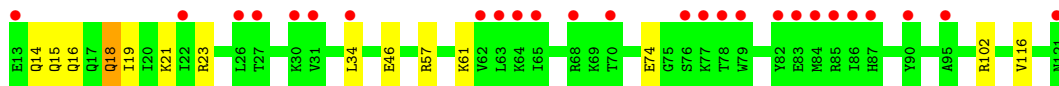
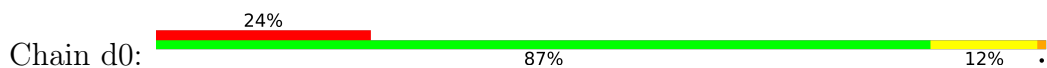




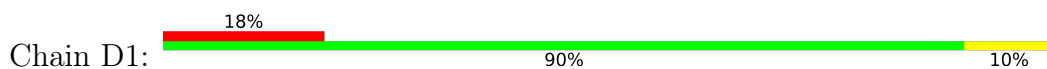
- Molecule 66: 40S ribosomal protein S20



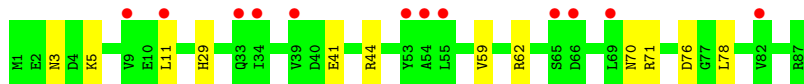
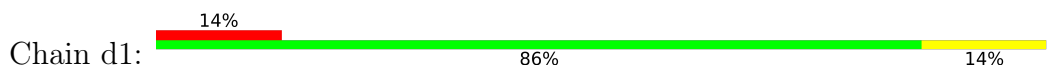
- Molecule 66: 40S ribosomal protein S20



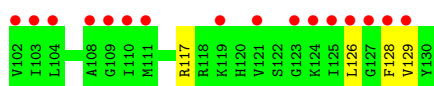
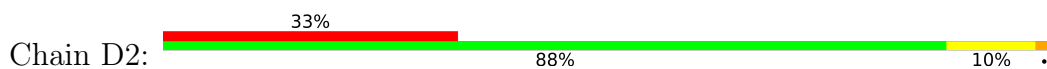
- Molecule 67: 40S ribosomal protein S21-A



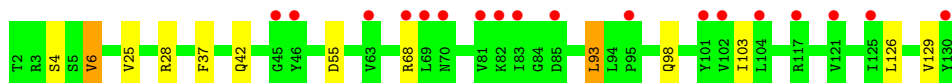
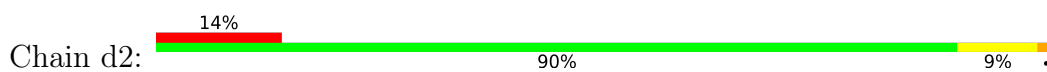
- Molecule 67: 40S ribosomal protein S21-A



- Molecule 68: 40S ribosomal protein S22-A



- Molecule 68: 40S ribosomal protein S22-A



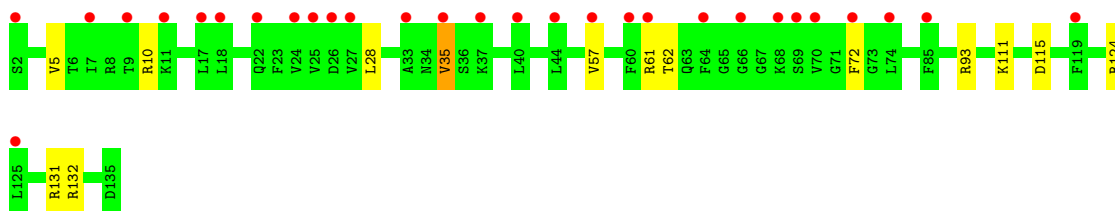
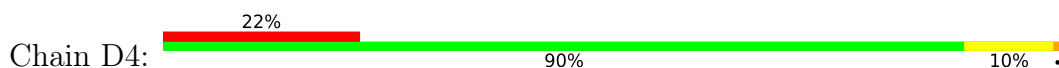
- Molecule 69: 40S ribosomal protein S23-A



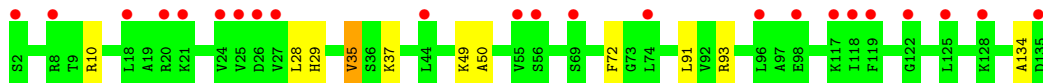
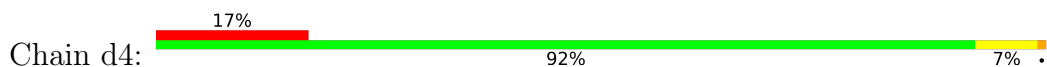
- Molecule 69: 40S ribosomal protein S23-A



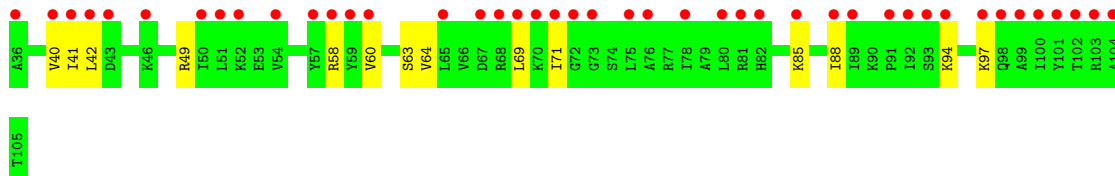
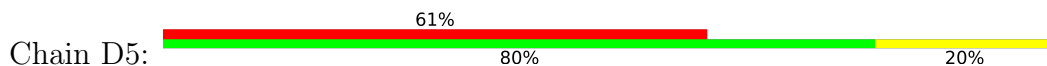
- Molecule 70: 40S ribosomal protein S24-A



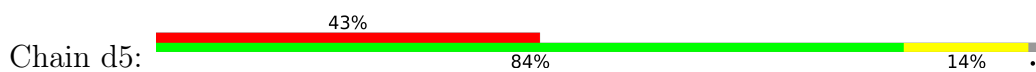
- Molecule 70: 40S ribosomal protein S24-A



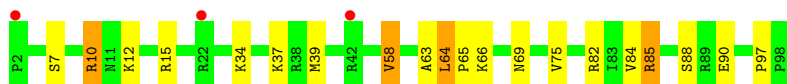
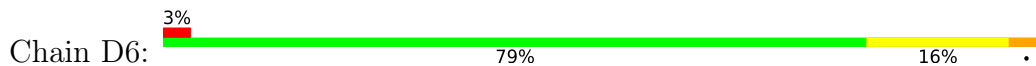
- Molecule 71: 40S ribosomal protein S25-A



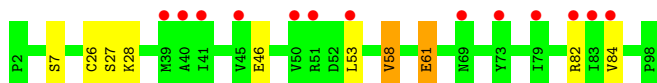
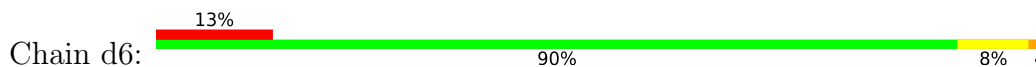
- Molecule 71: 40S ribosomal protein S25-A



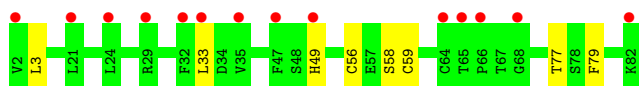
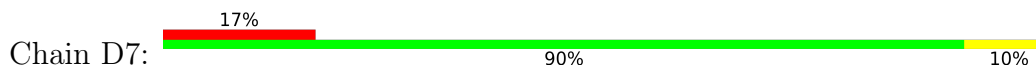
- Molecule 72: 40S ribosomal protein S26-B



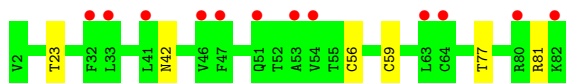
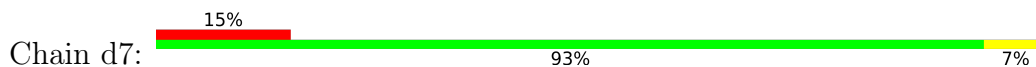
- Molecule 72: 40S ribosomal protein S26-B



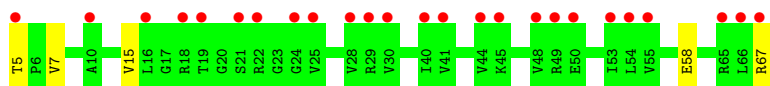
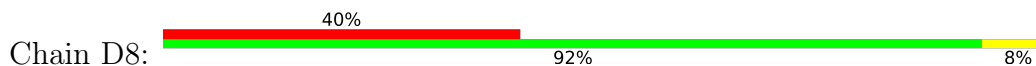
- Molecule 73: 40S ribosomal protein S27-A



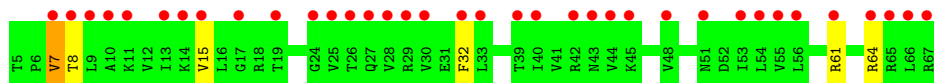
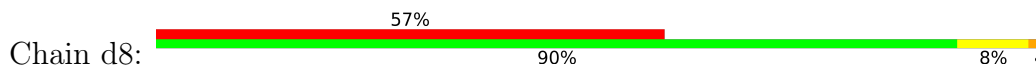
- Molecule 73: 40S ribosomal protein S27-A



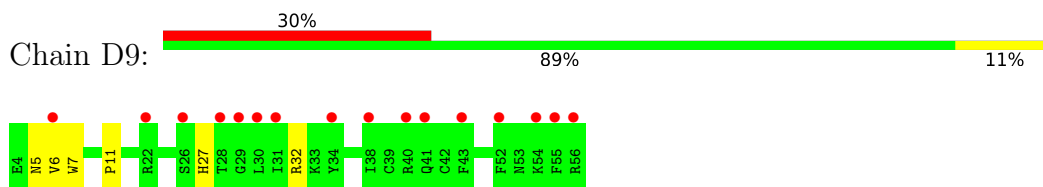
- Molecule 74: 40S ribosomal protein S28-A



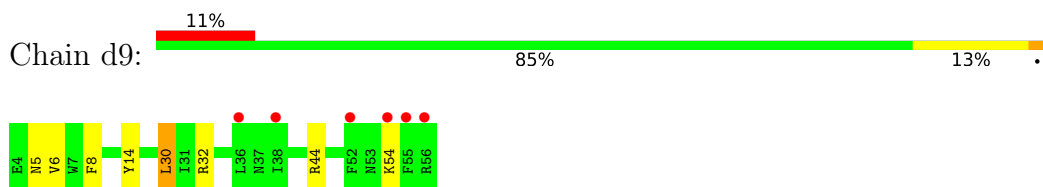
- Molecule 74: 40S ribosomal protein S28-A



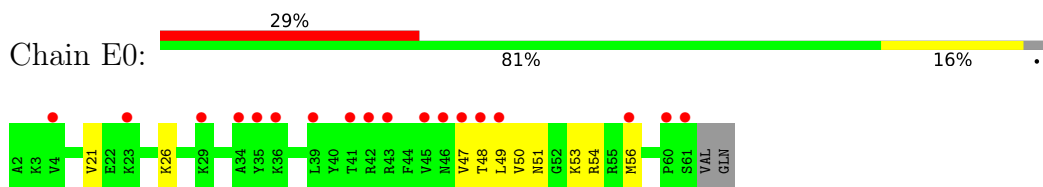
- Molecule 75: 40S ribosomal protein S29-A



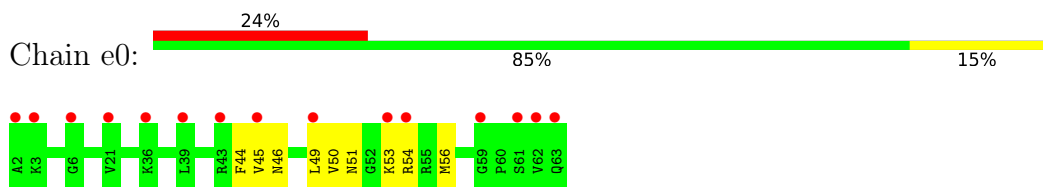
- Molecule 75: 40S ribosomal protein S29-A



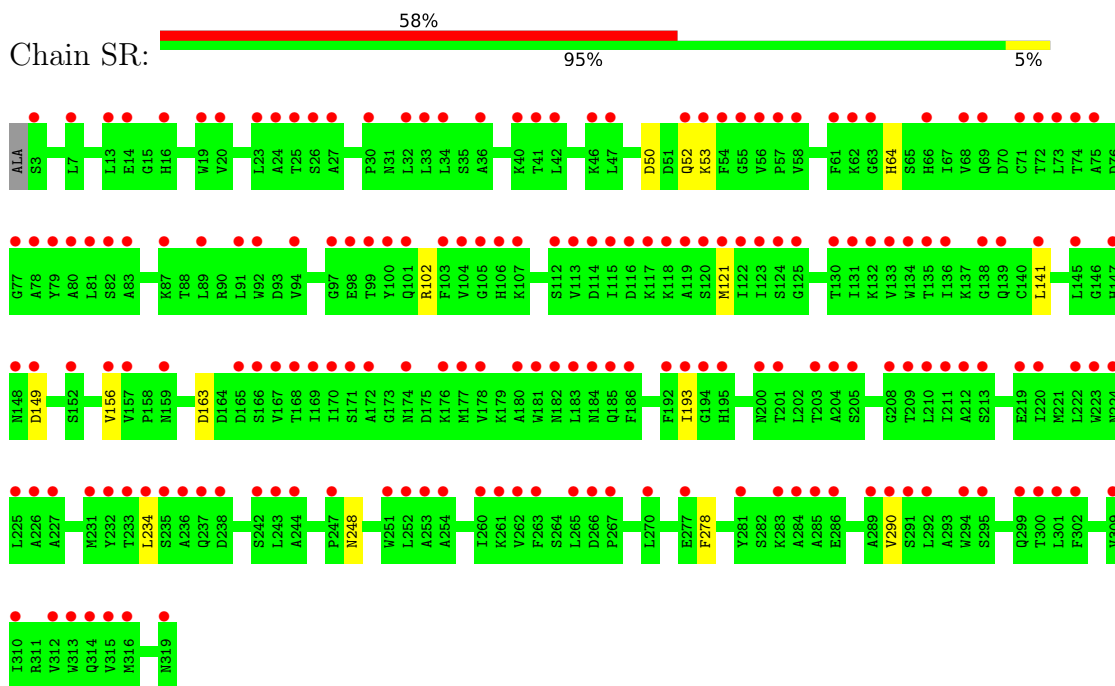
- Molecule 76: 40S ribosomal protein S30-A



- Molecule 76: 40S ribosomal protein S30-A

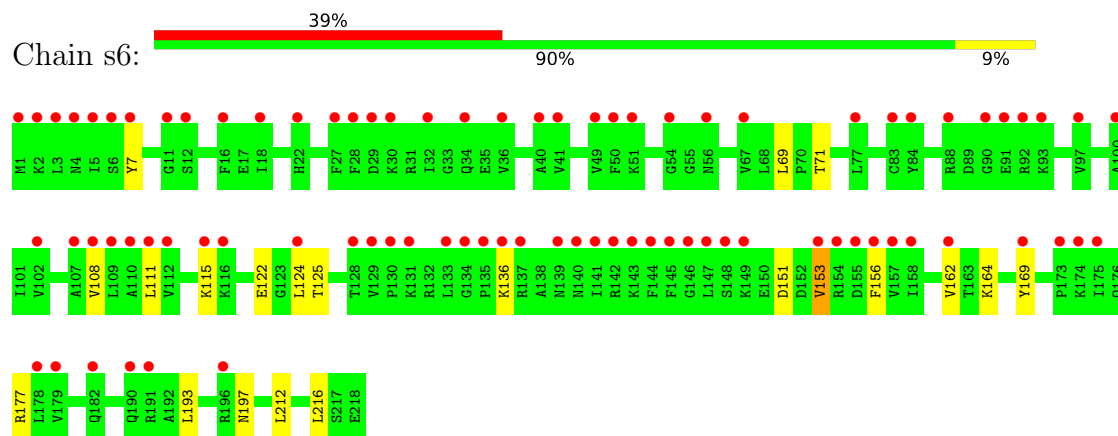


- Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein



ARG ARG ARG GLY GLY ARG GLY ALA ARG LYS GLY ASN ASN THR THR ALA ASN THR ALA ALA THR ASN SER ALA ASN VAL THR THR VAL GLN LYS ASN ARG ASN ILE ASP VAL SER ASN LEU PRO 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 3.33Å)	Xtrriage
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 ²)	77.3	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	397978	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

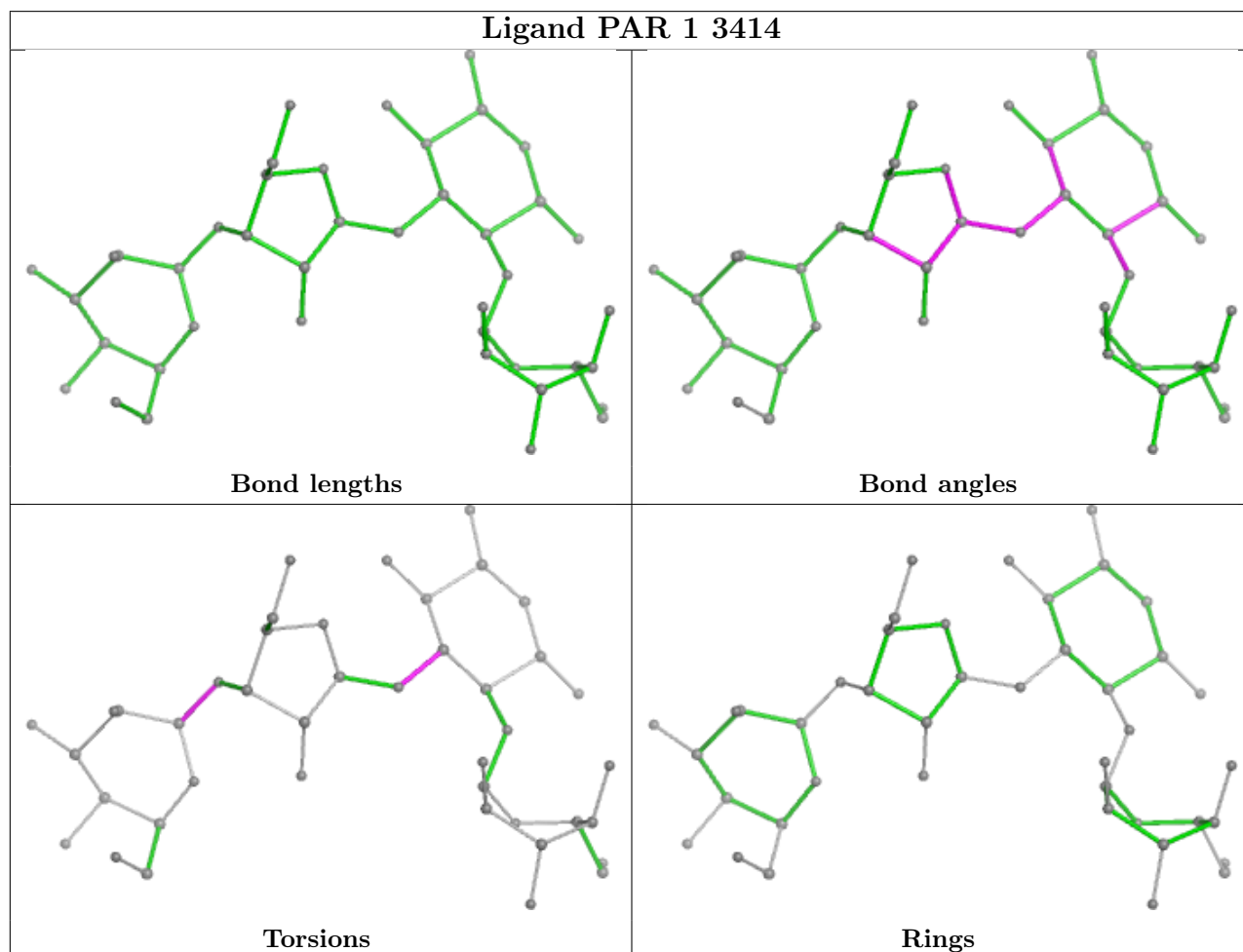
Continued on next page...

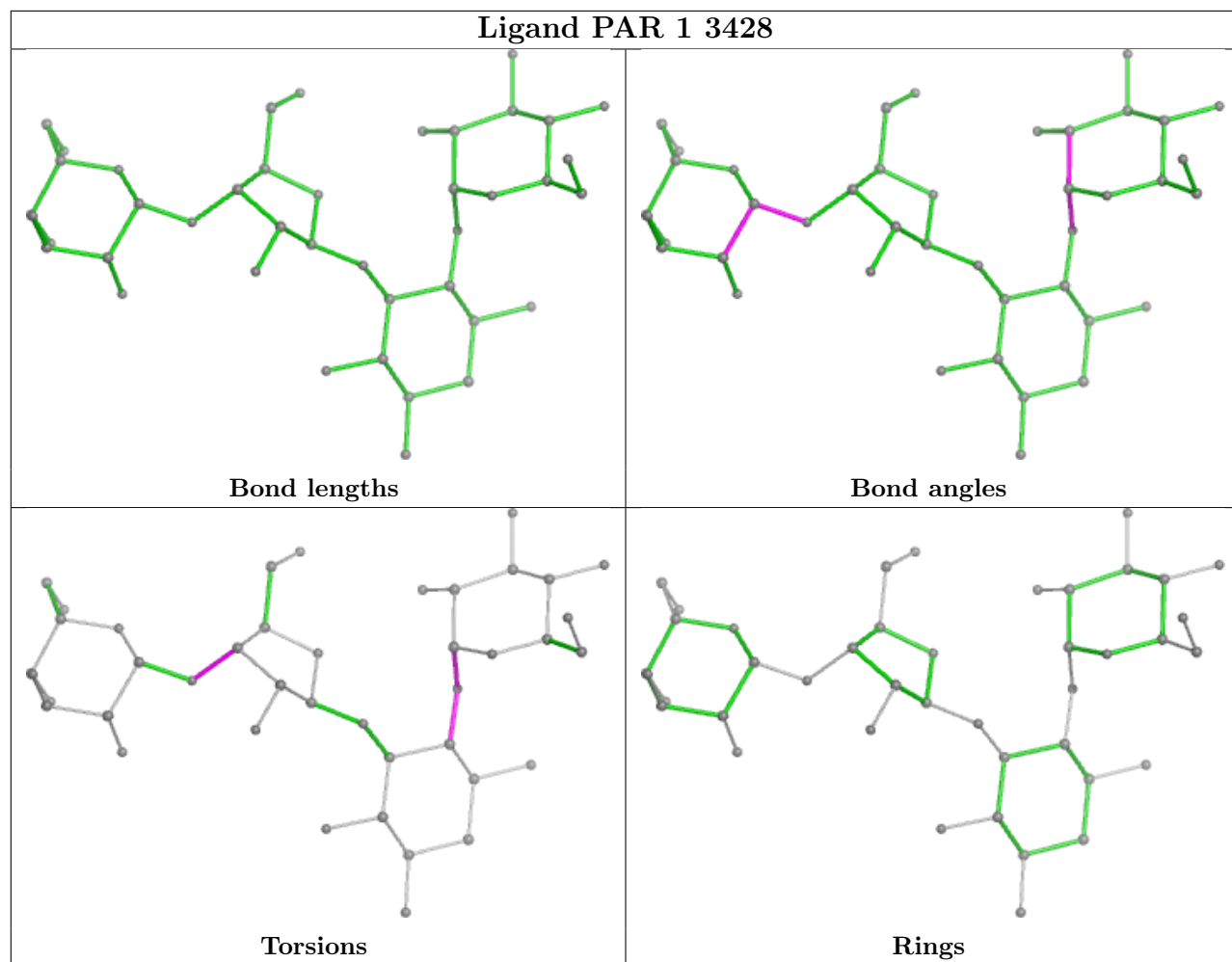
Continued from previous page...

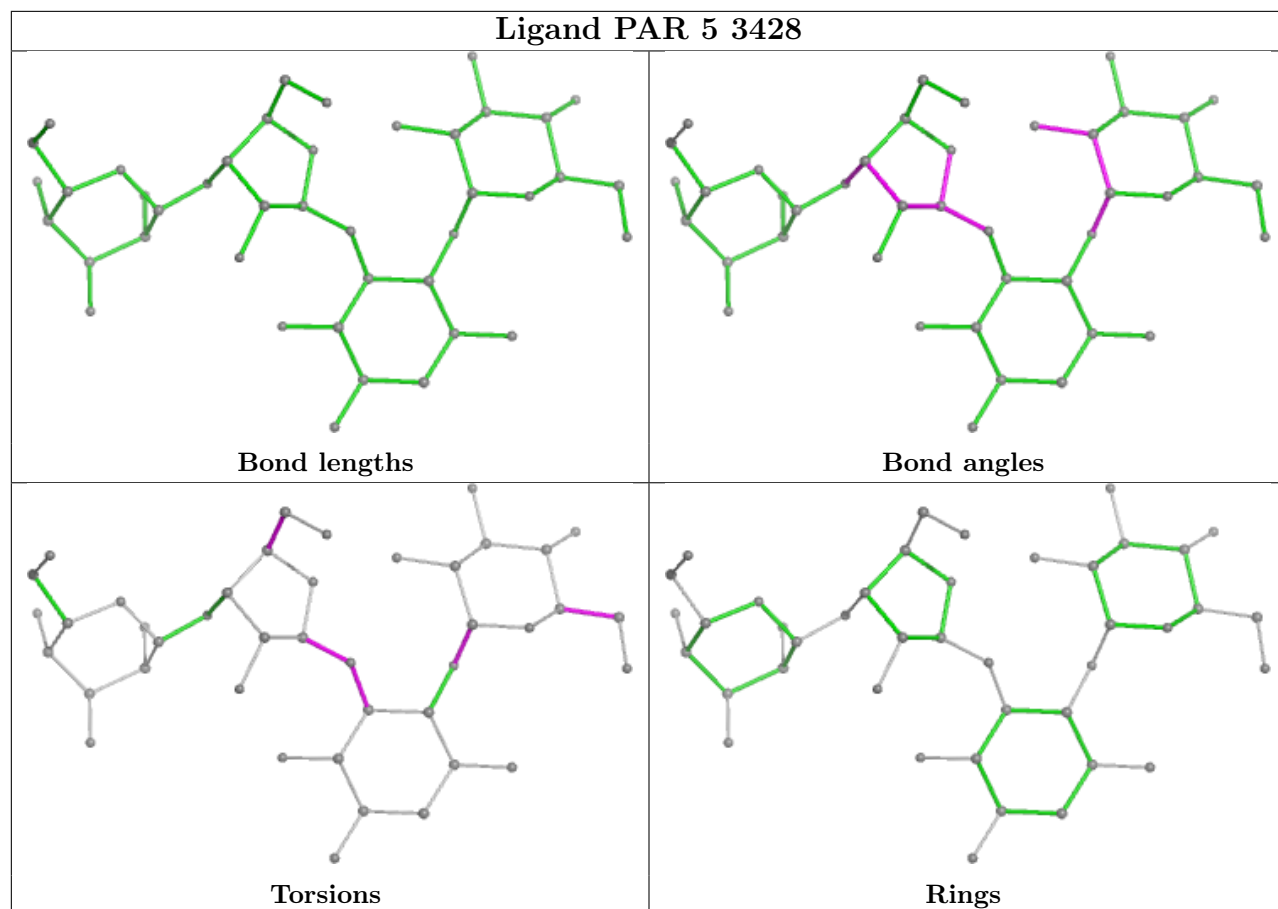
Mol	Chain	Res	Type	Atoms
80	4	201	PAR	C12-C22-C32-C42-C52-C62
80	3	203	PAR	C12-C22-C32-C42-C52-C62
80	1	3418	PAR	C14-C24-C34-C44-C54-O54

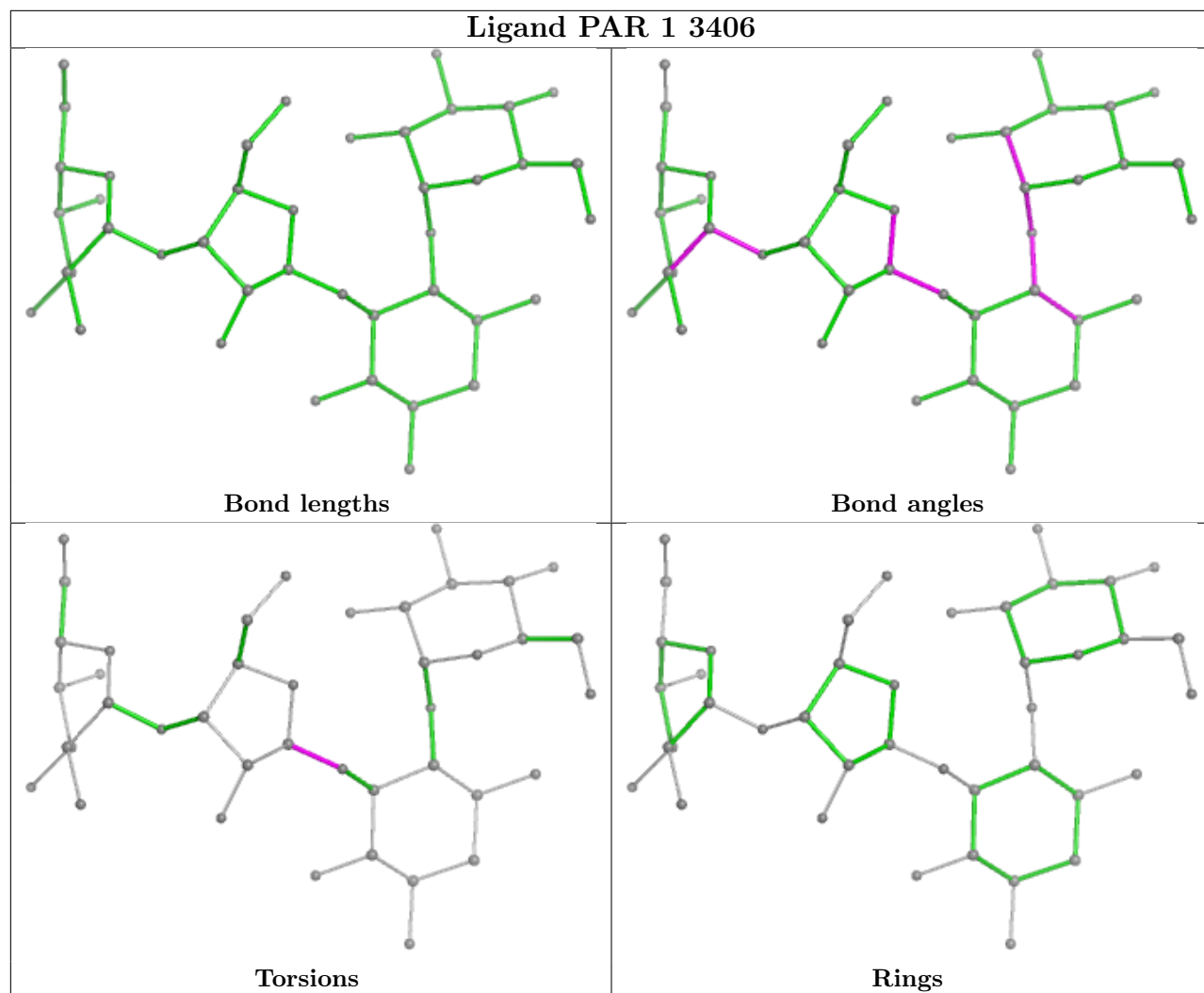
No monomer is involved in short contacts.

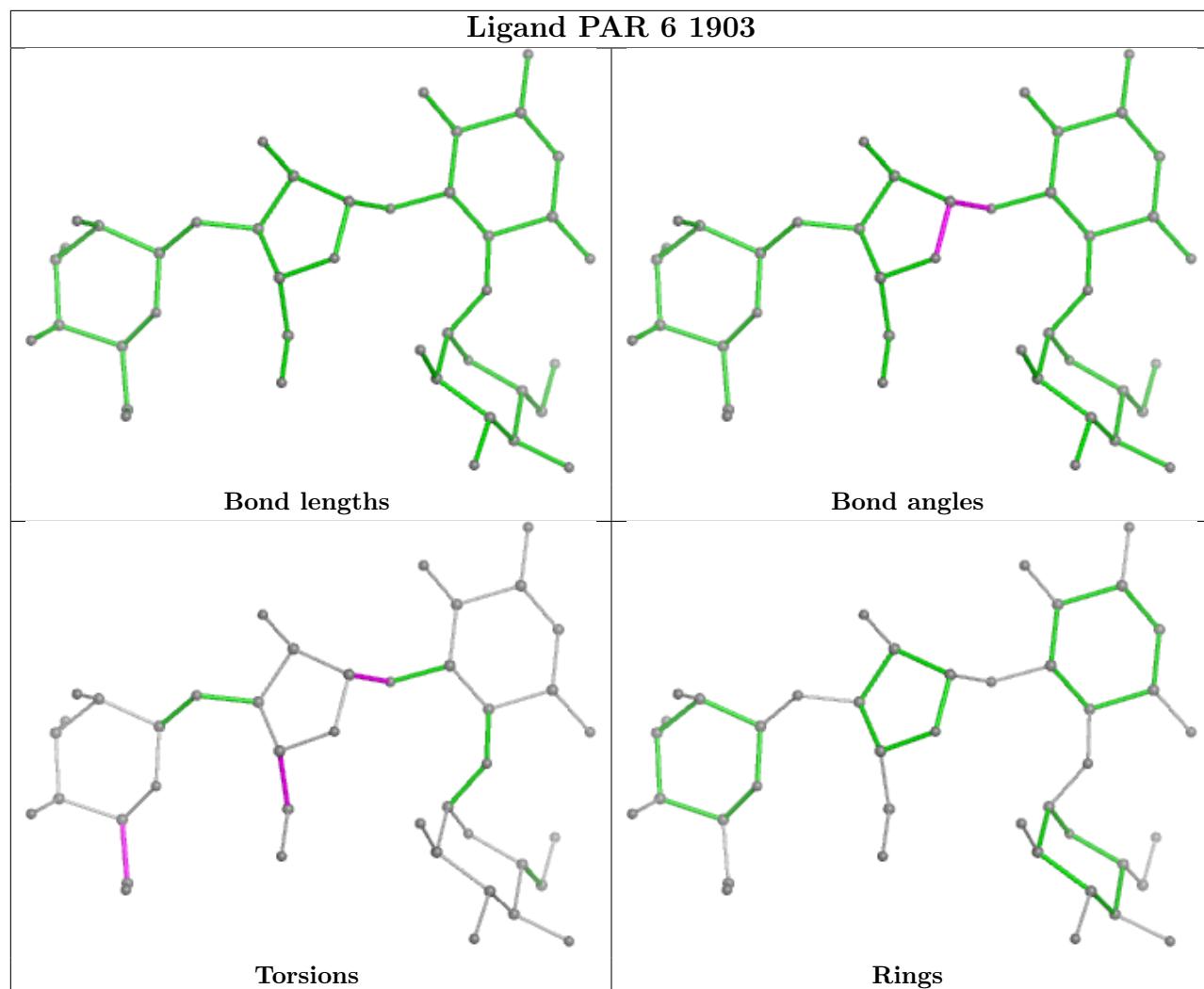
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

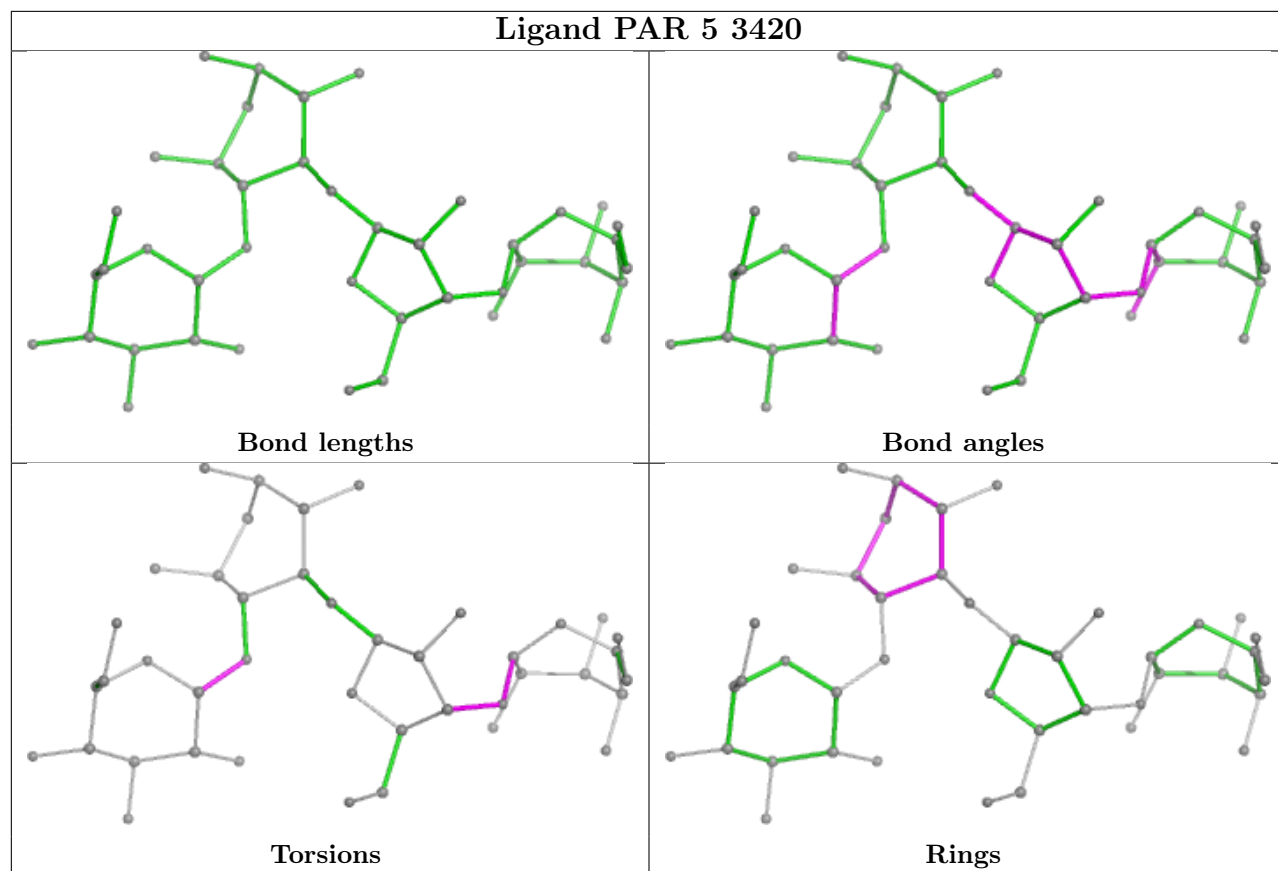


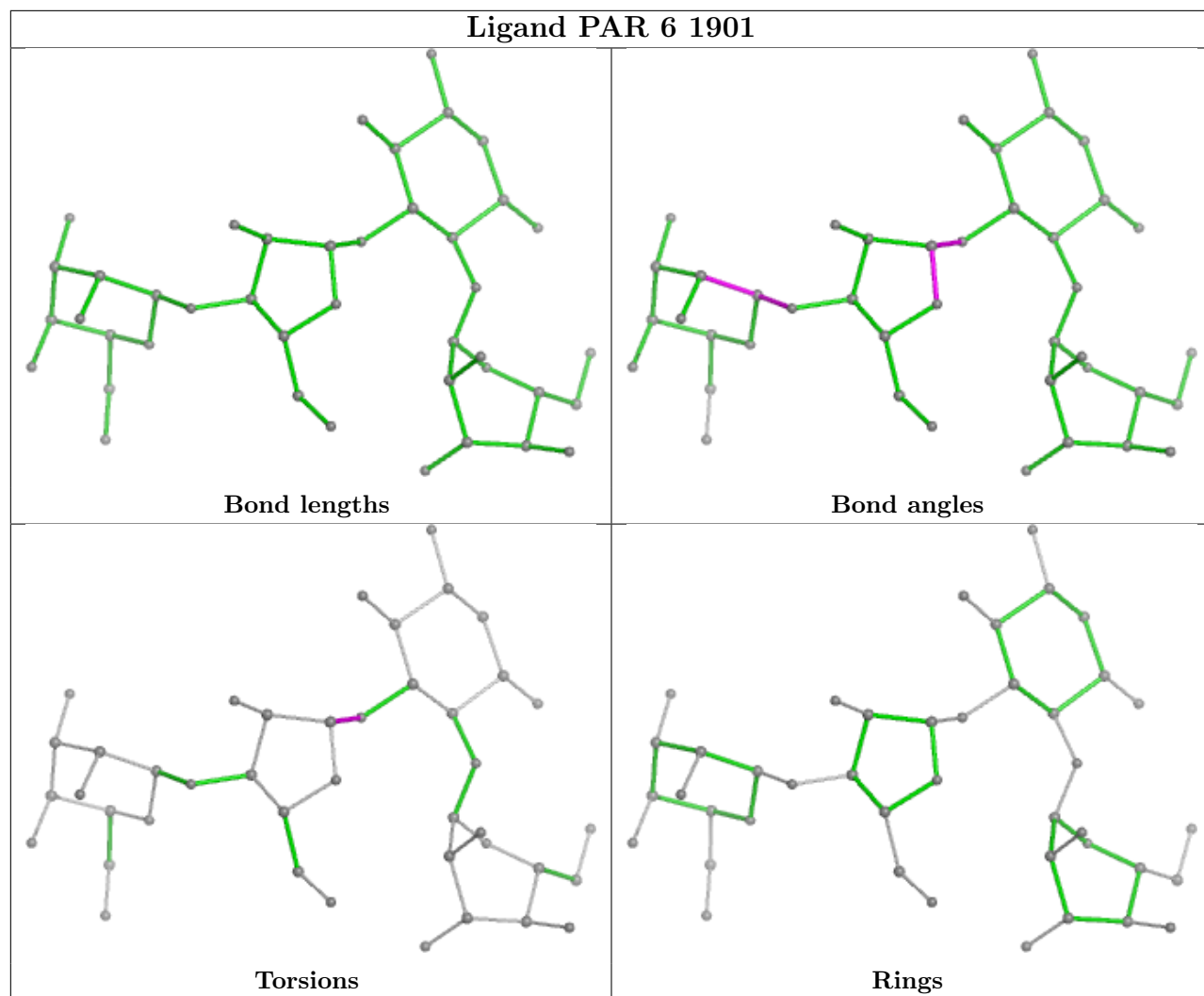


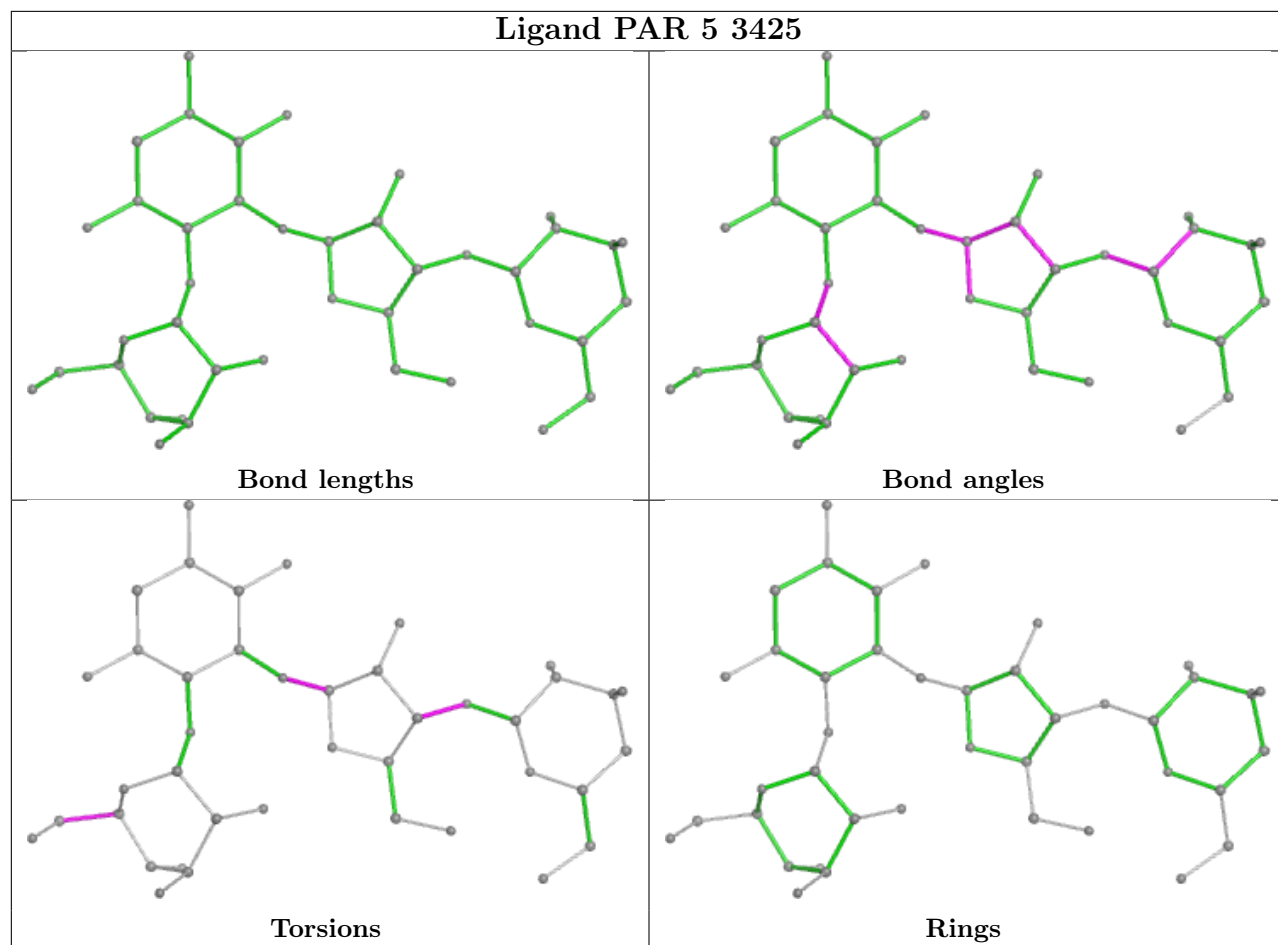


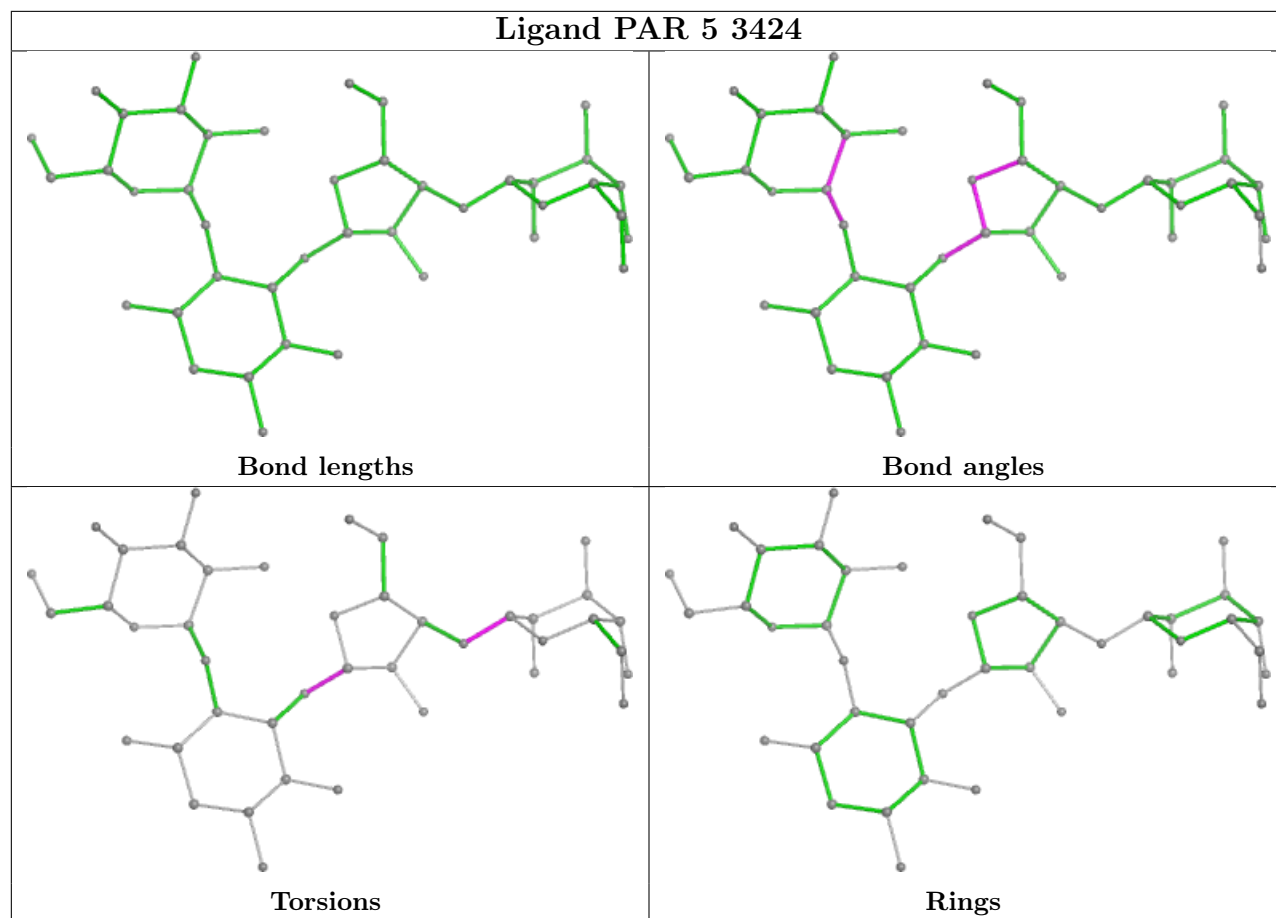


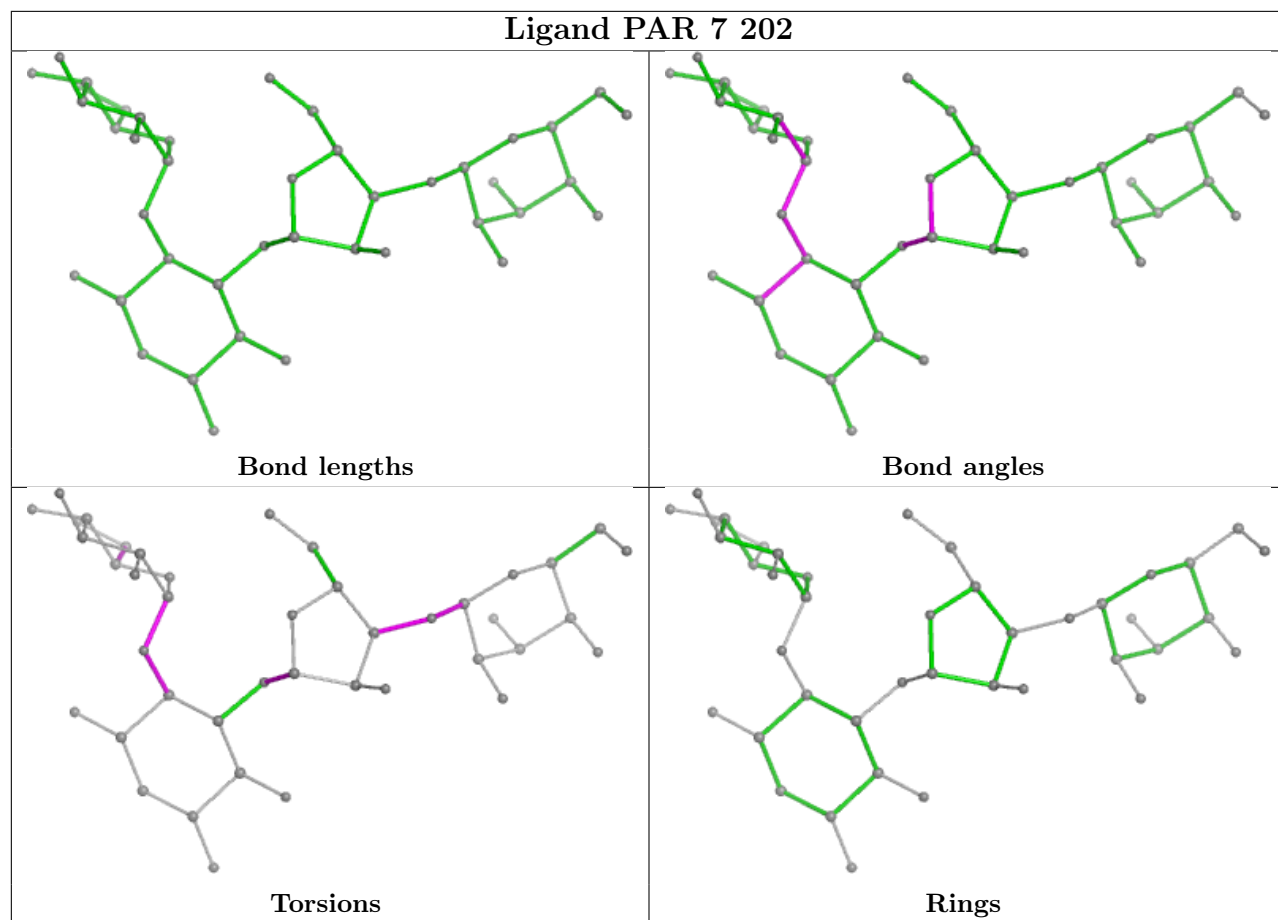


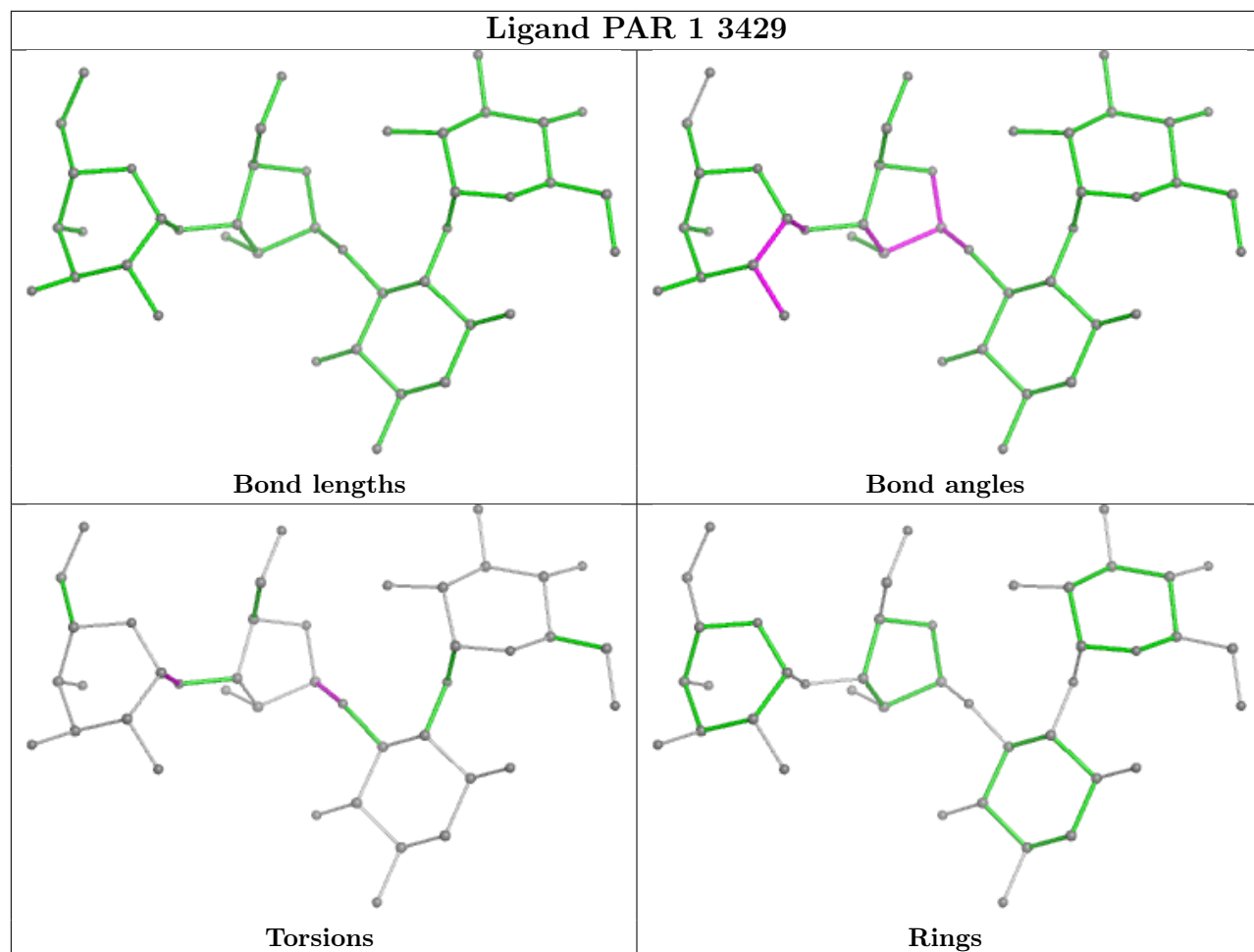


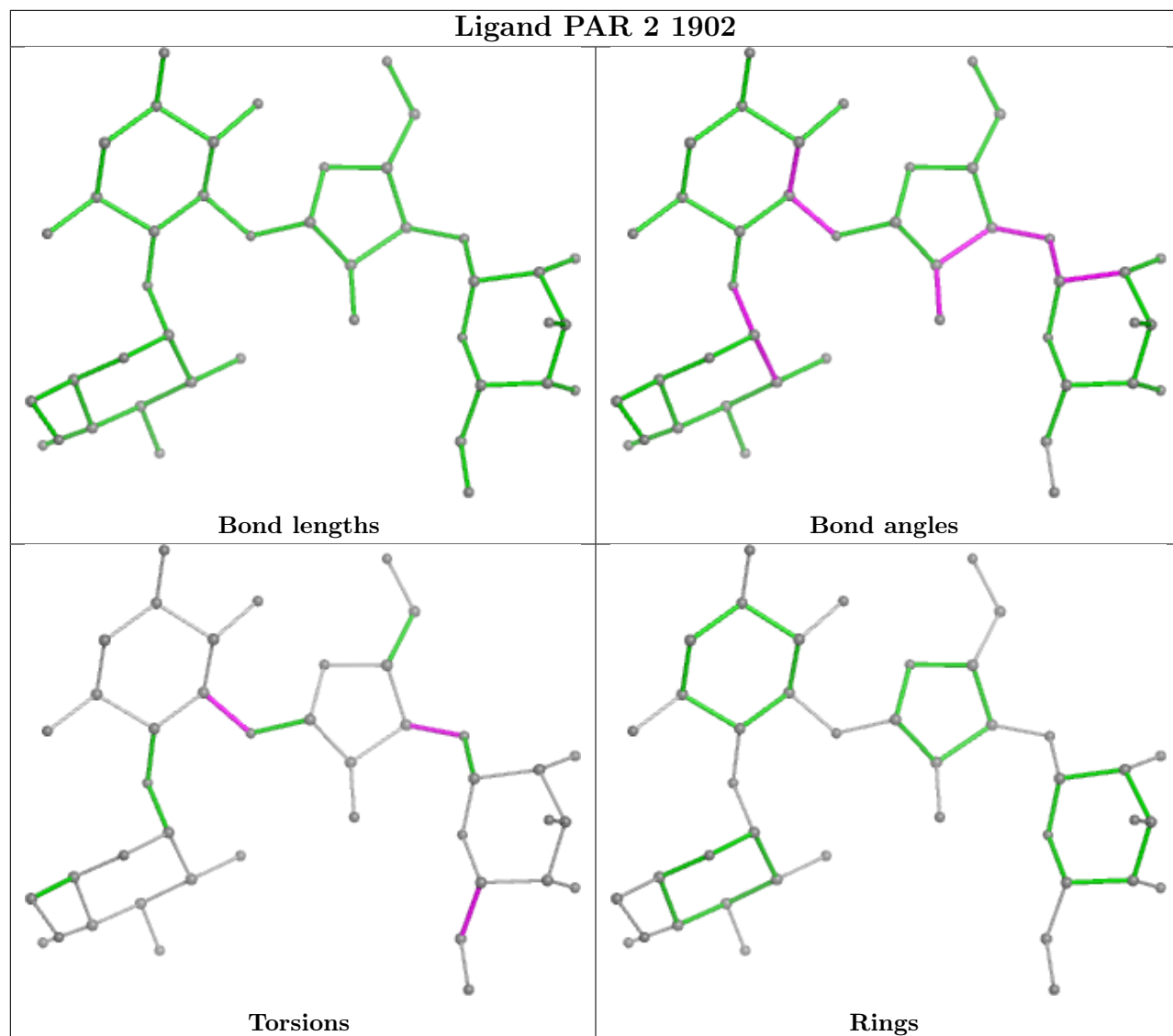


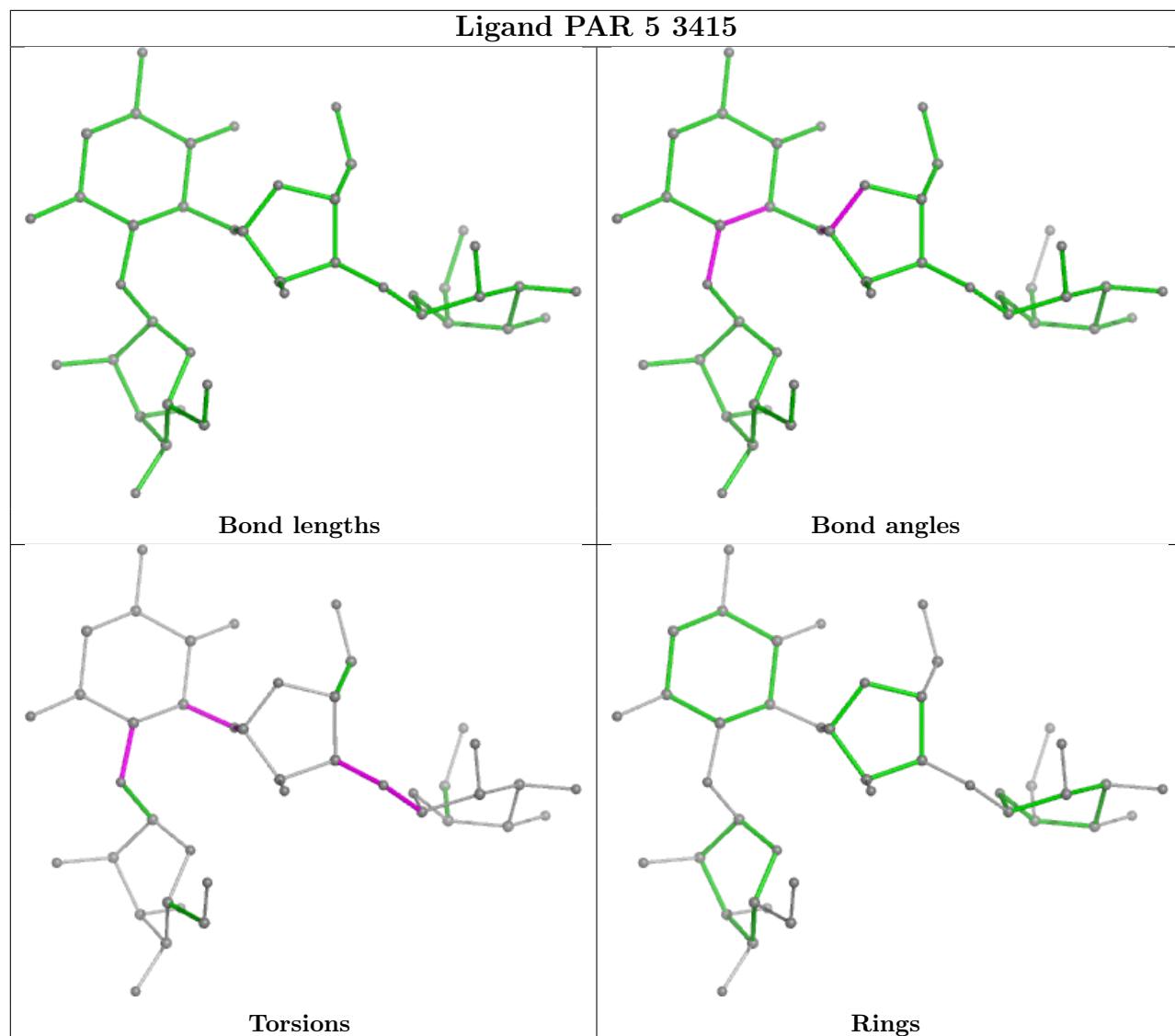


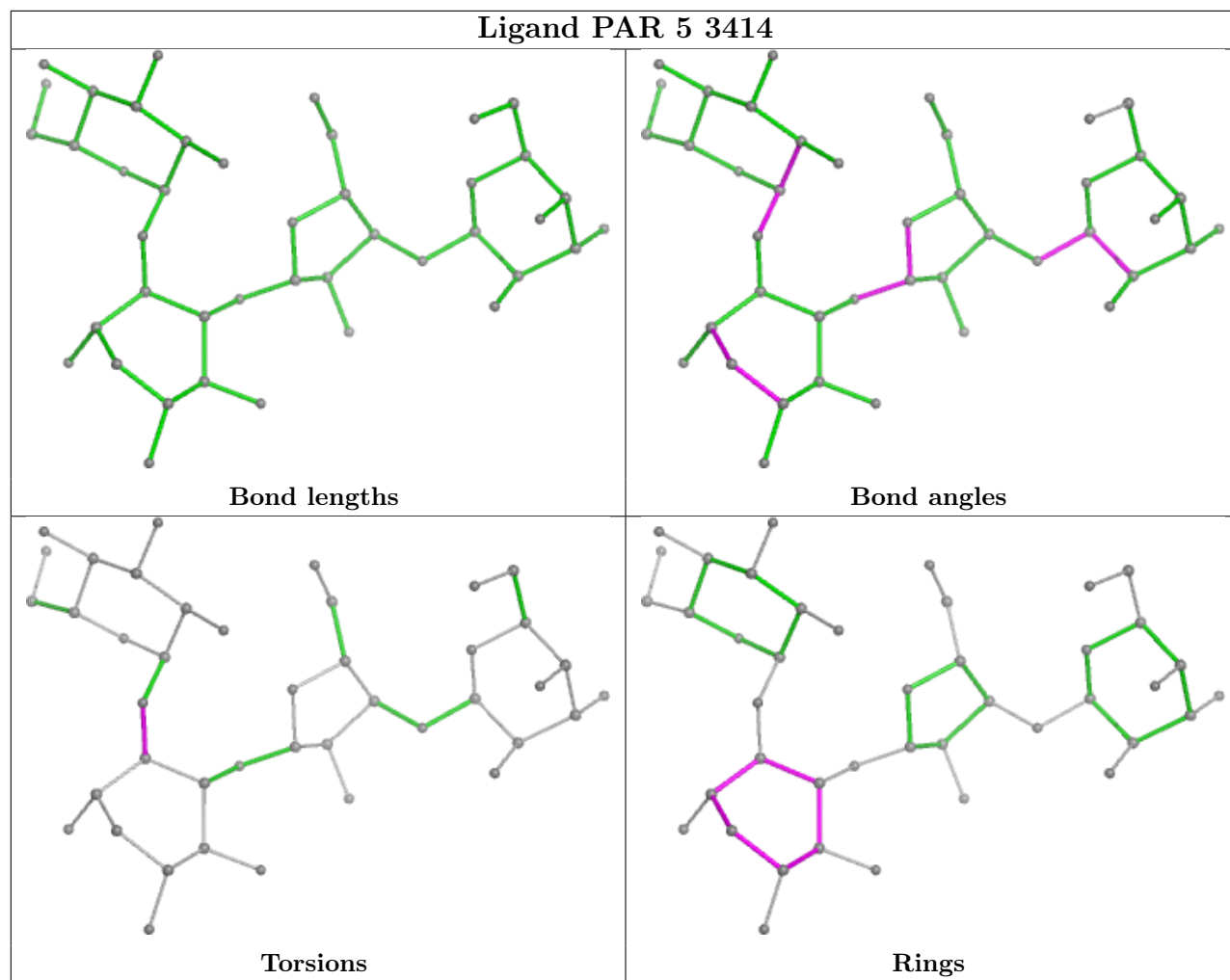


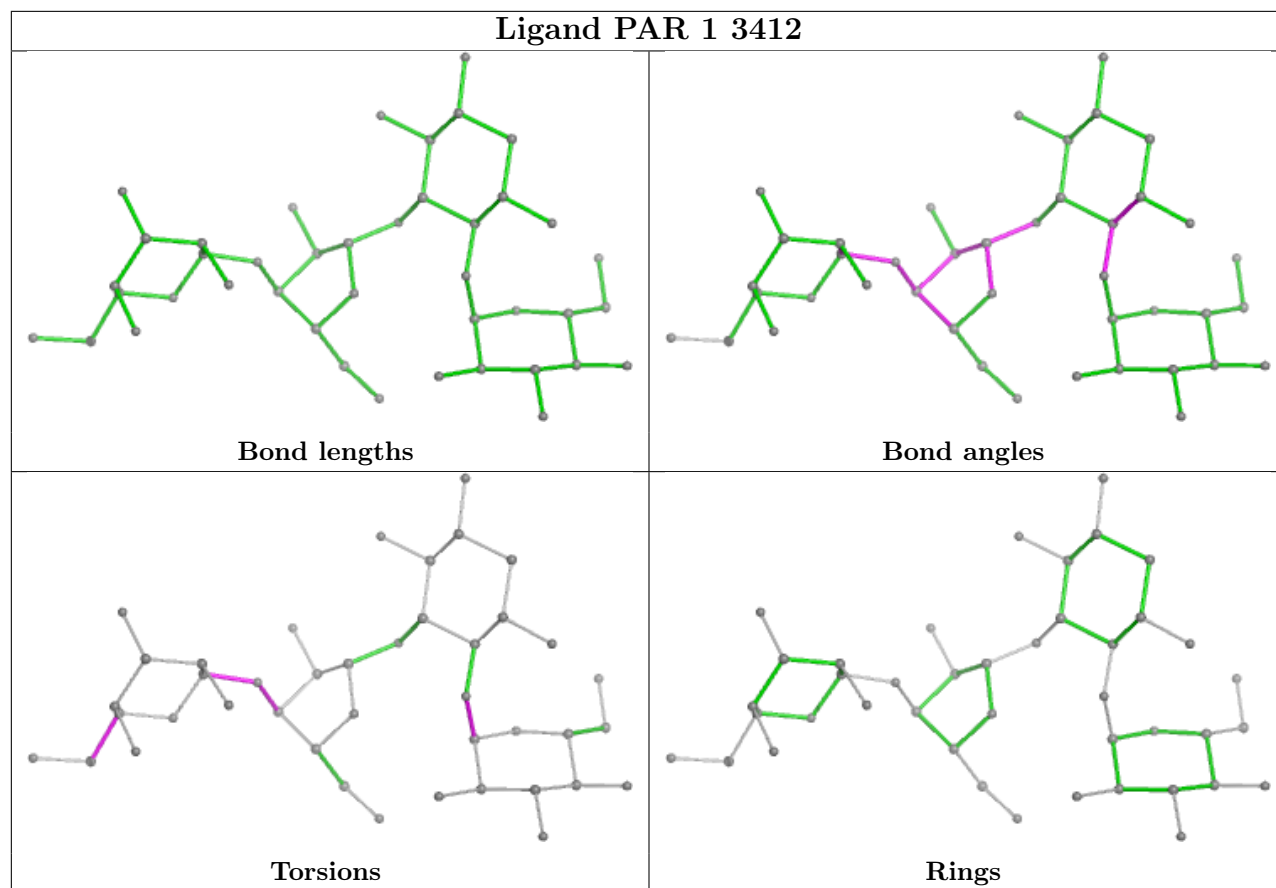


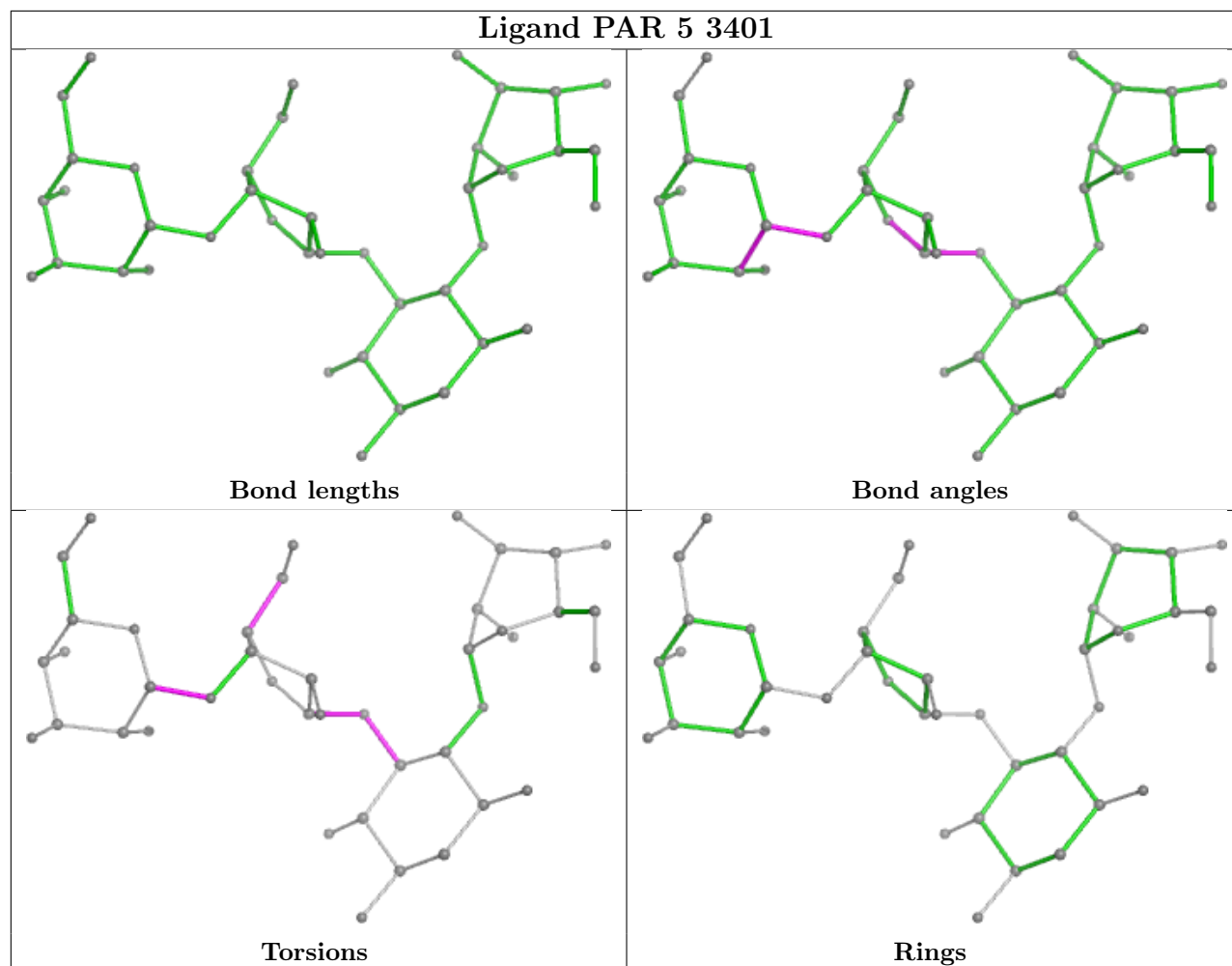


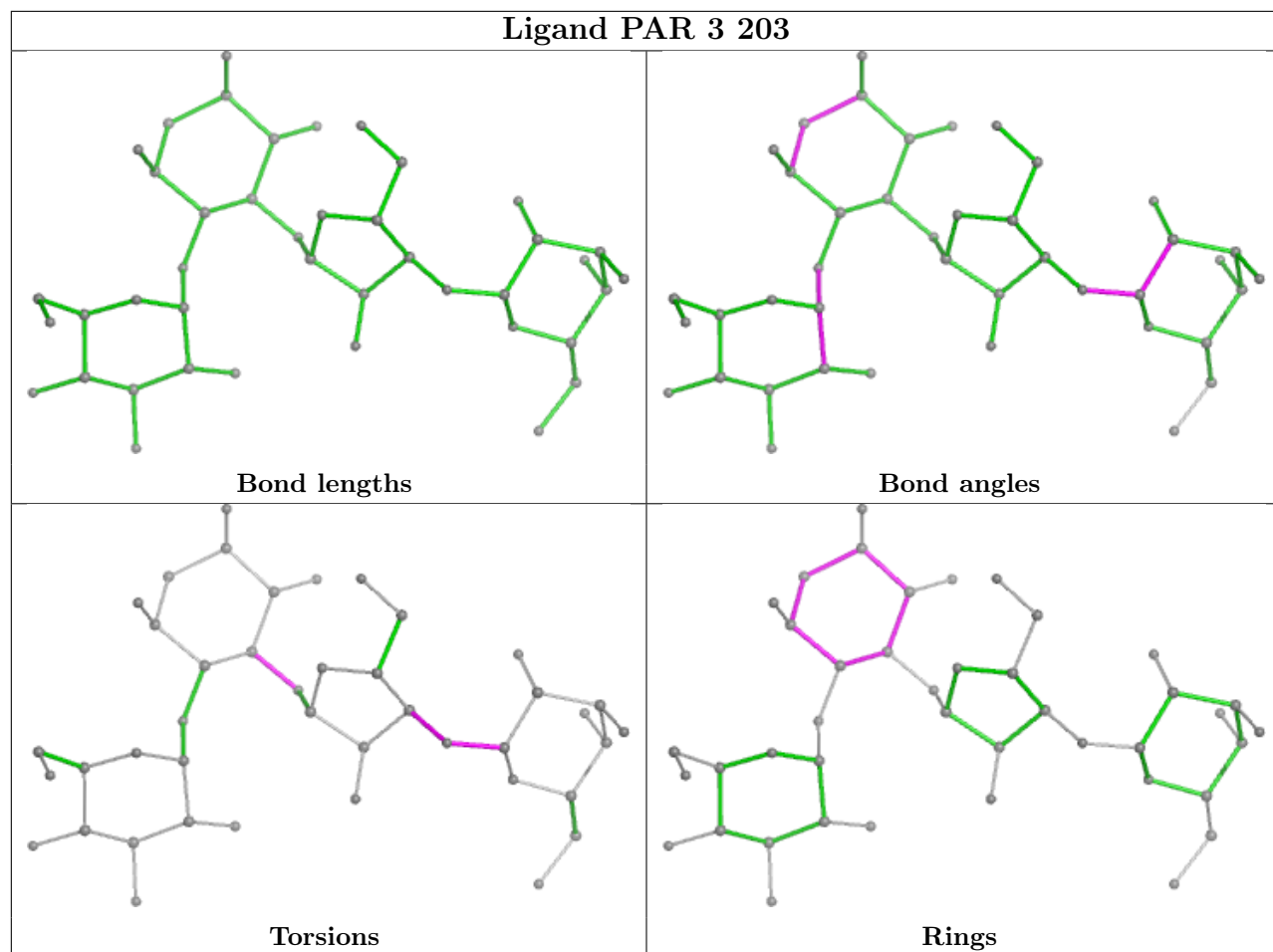


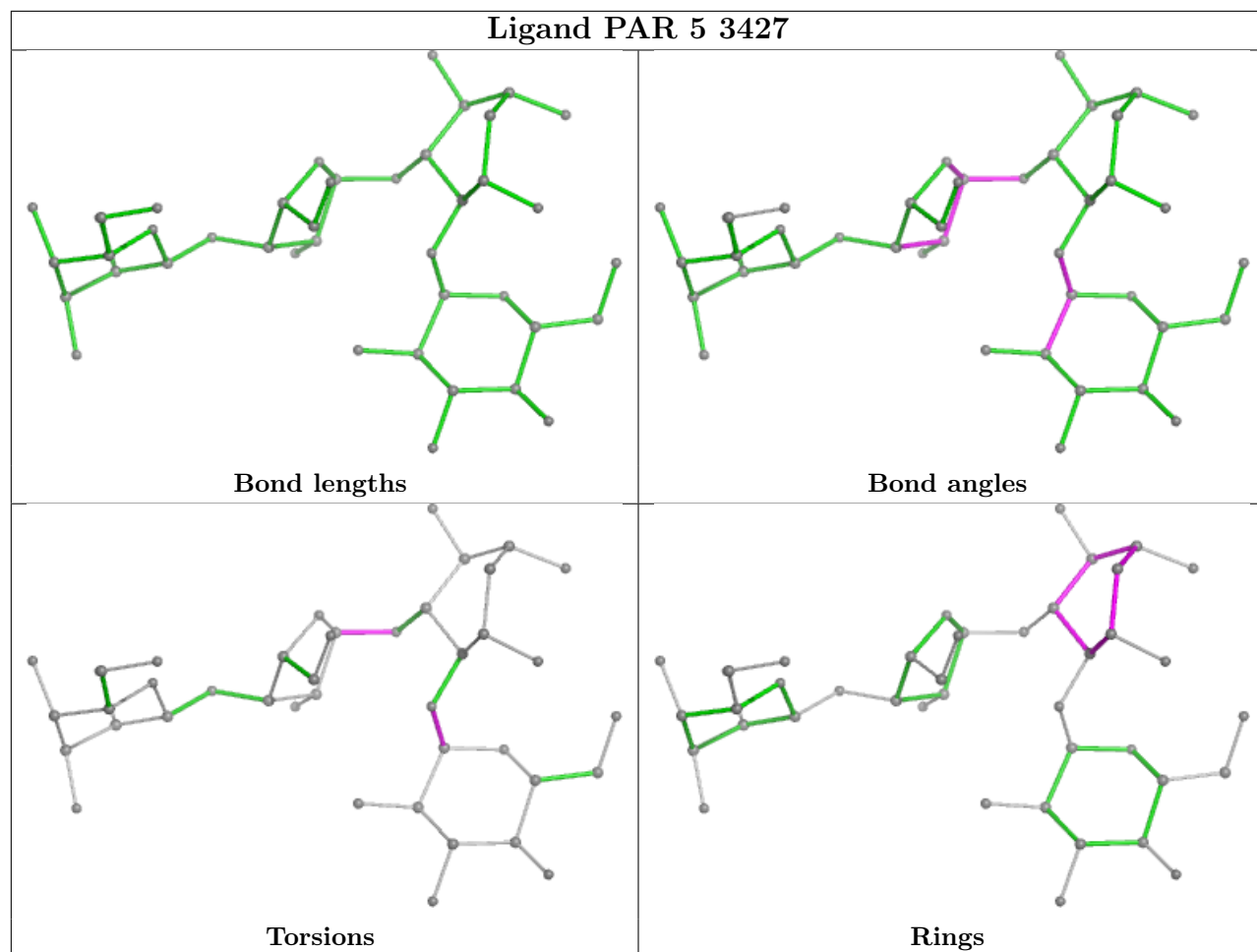


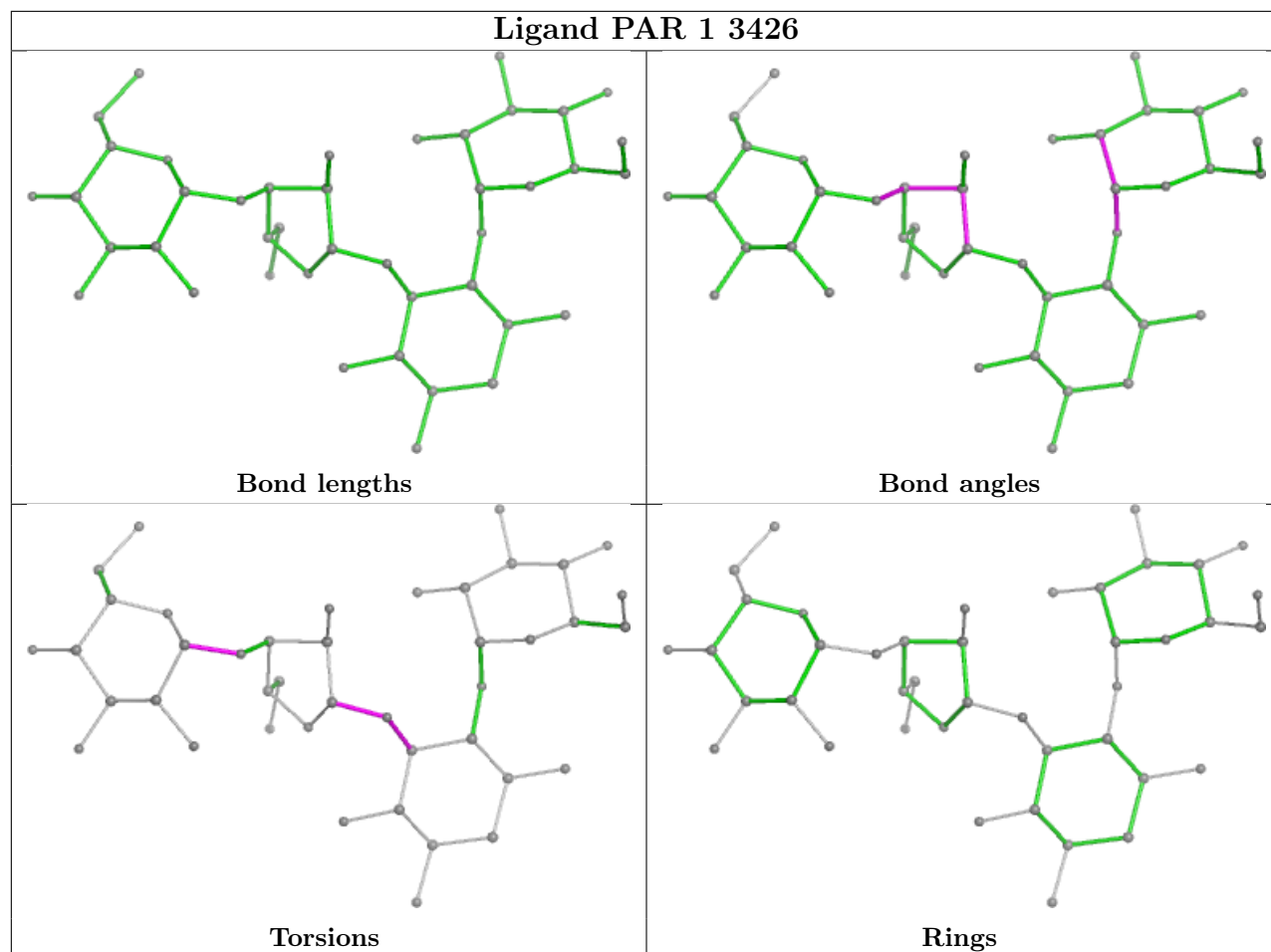


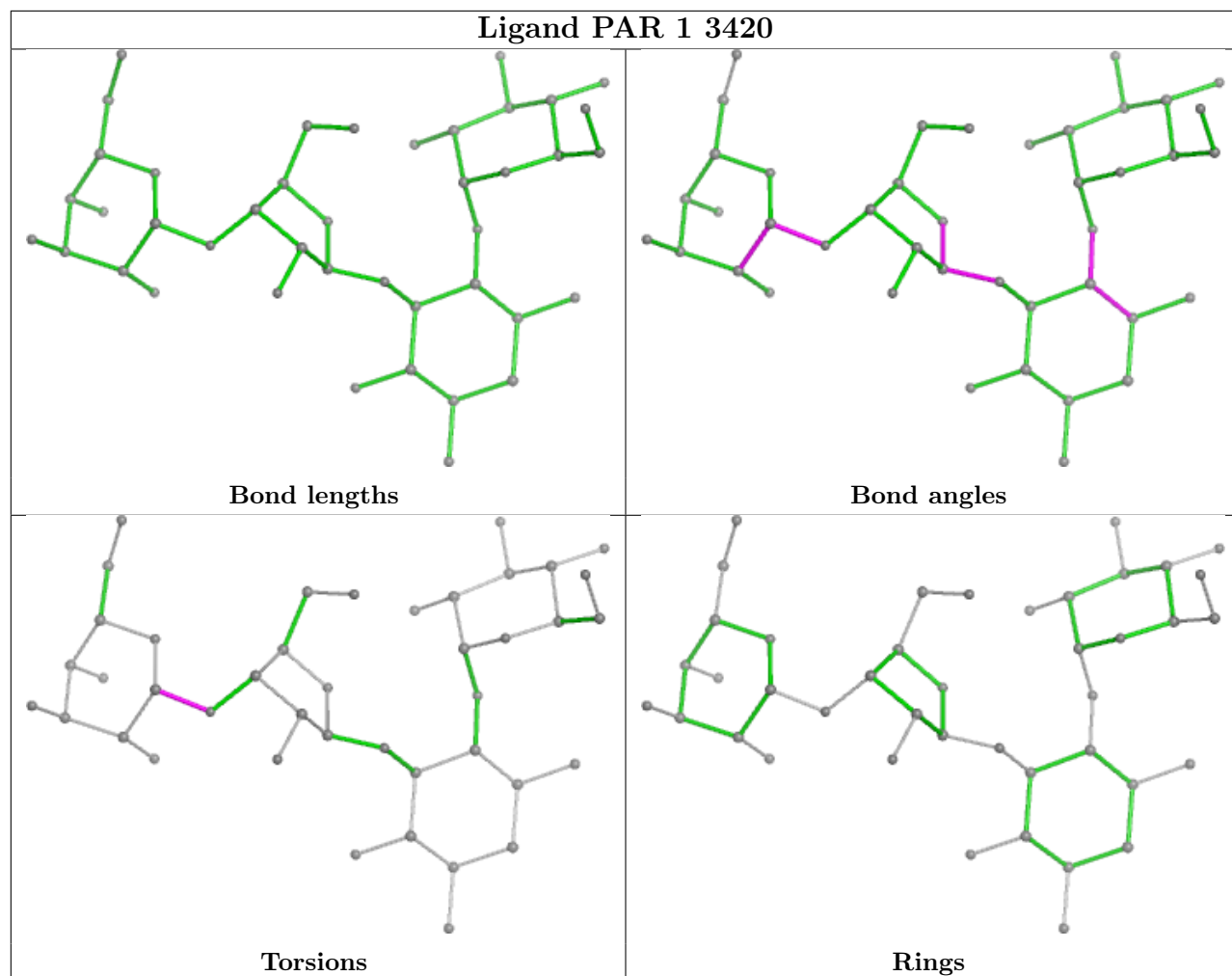


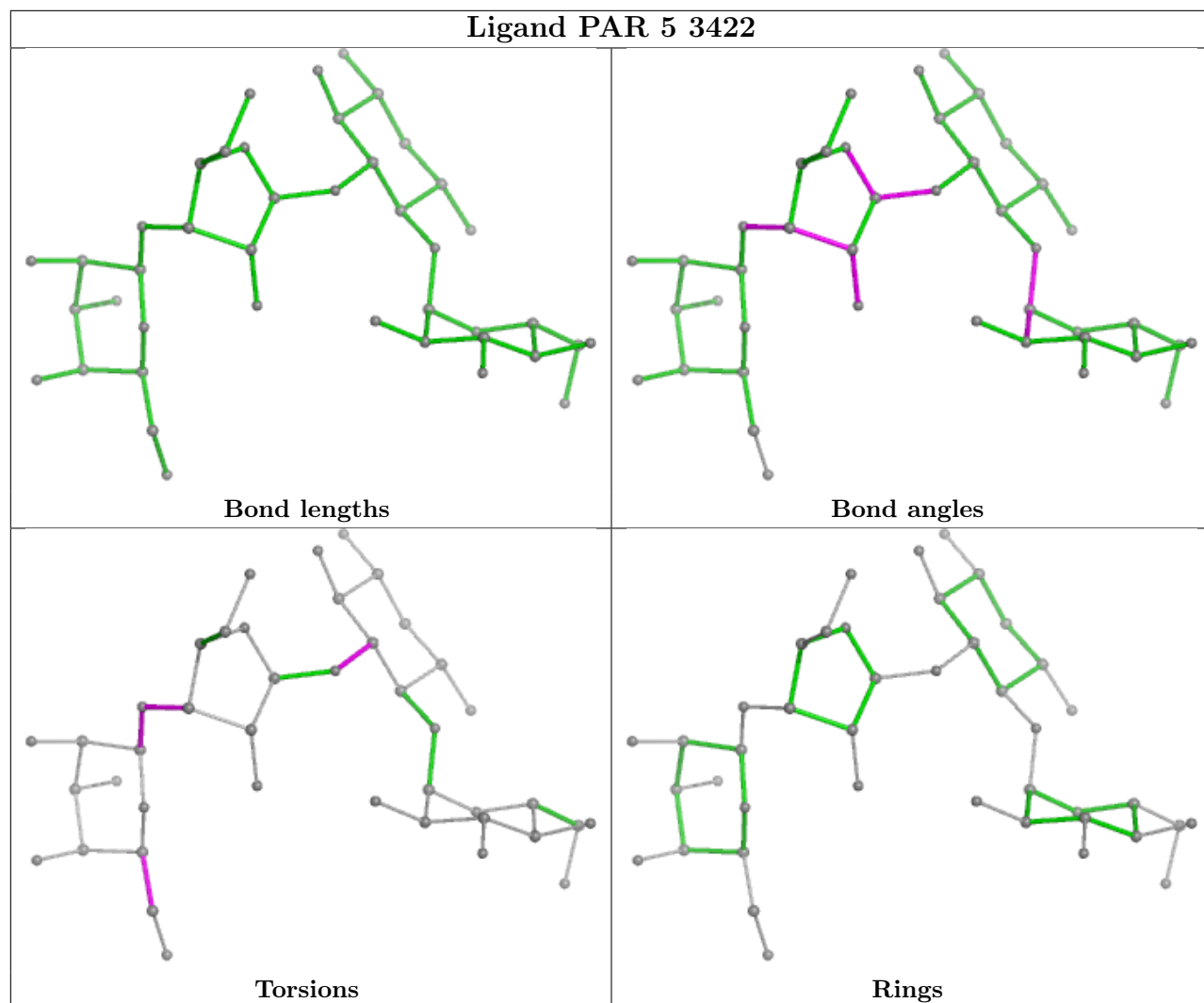


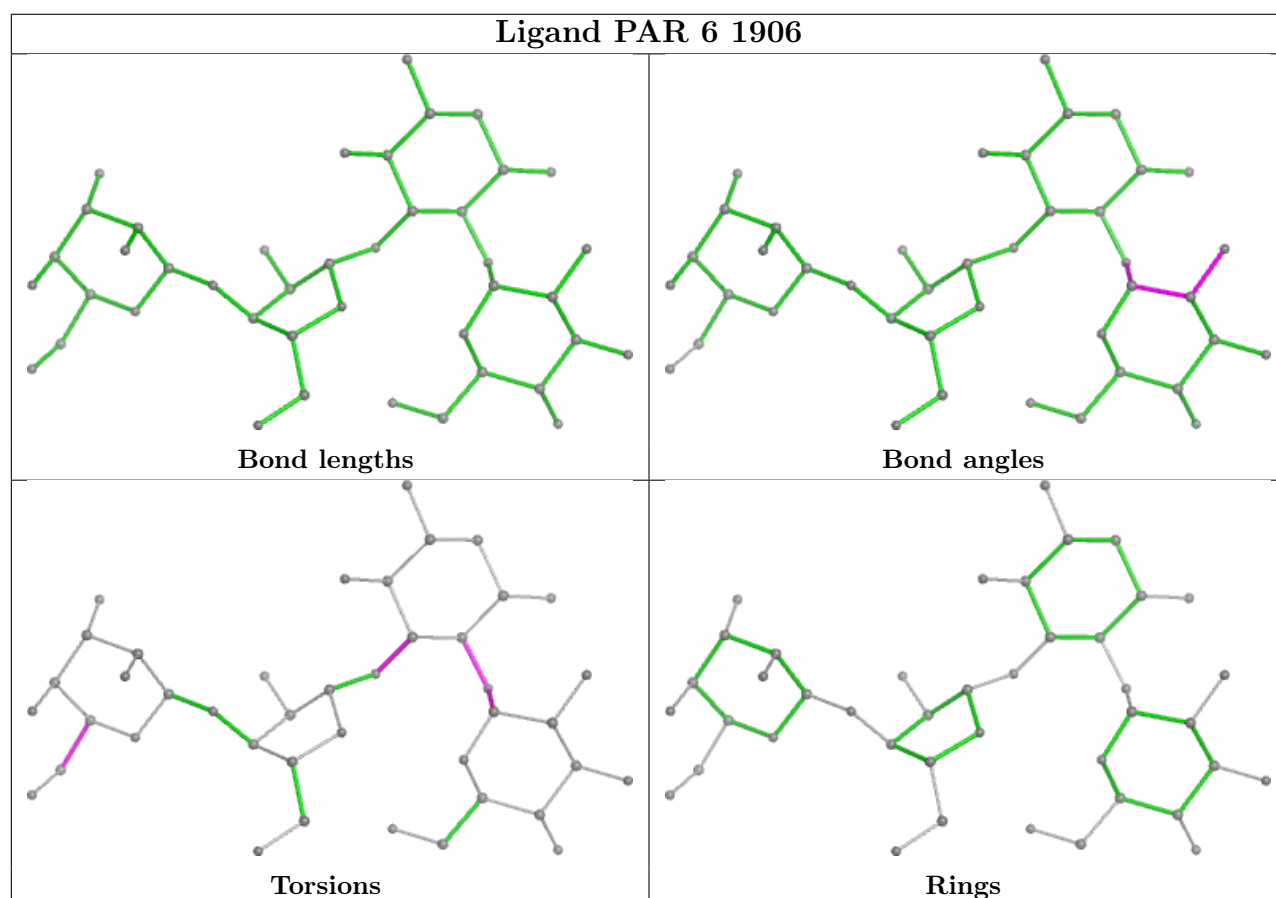
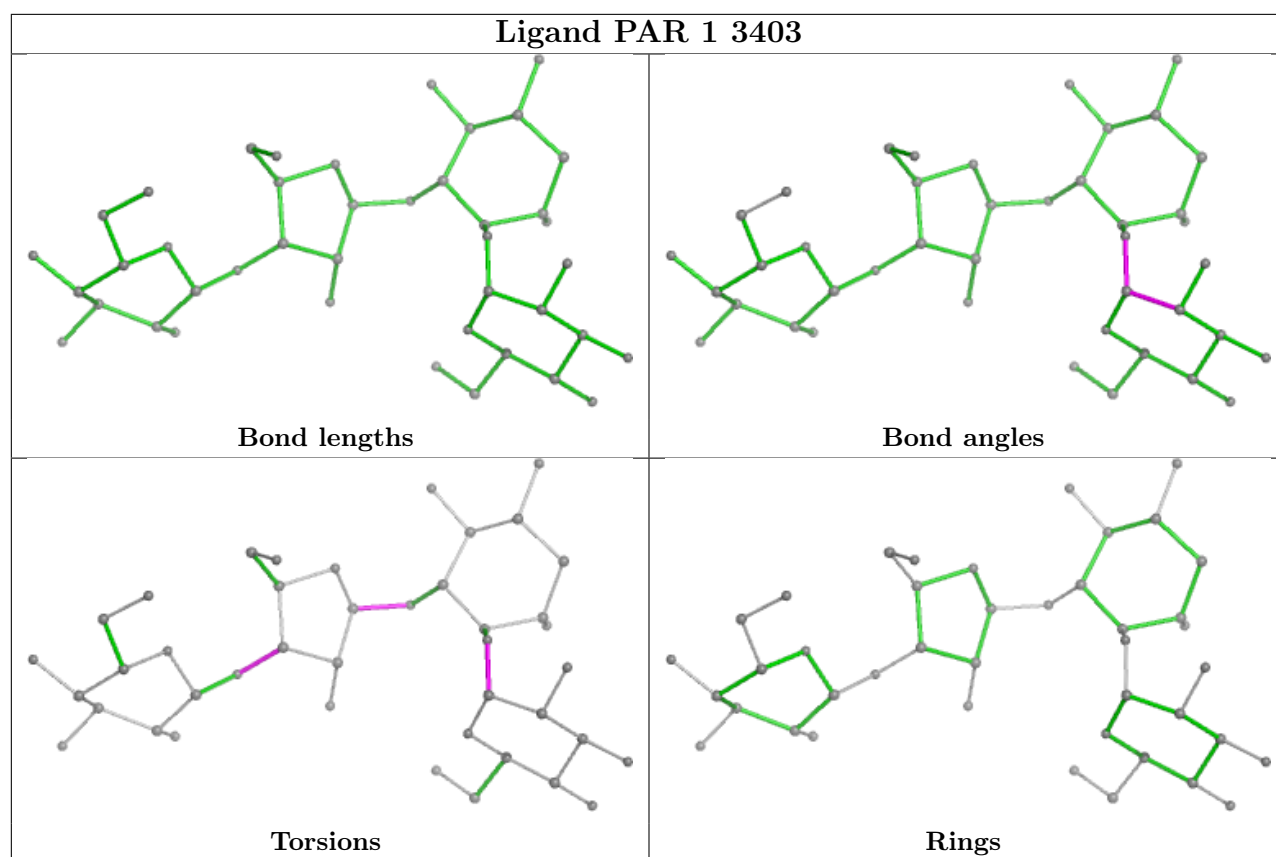


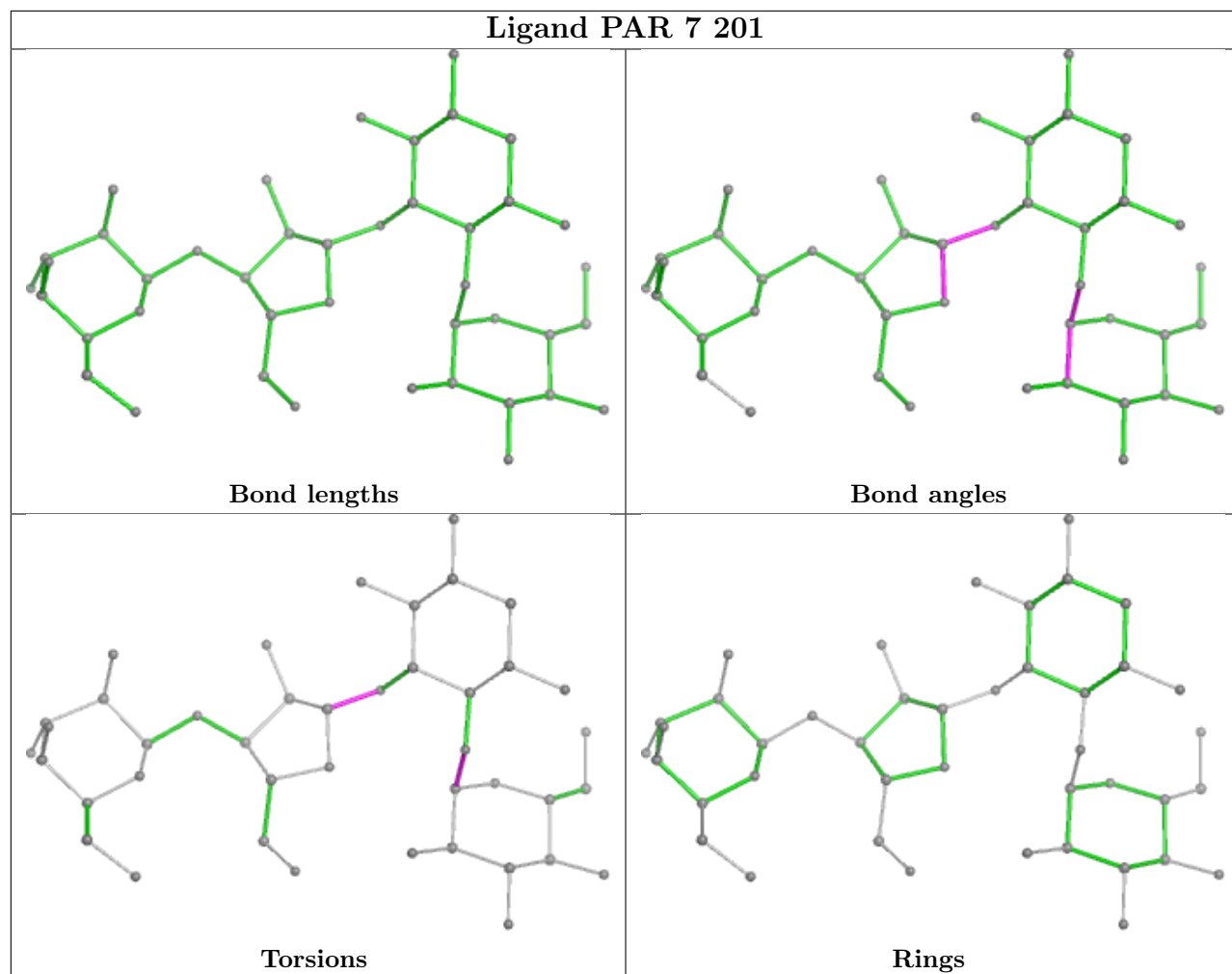


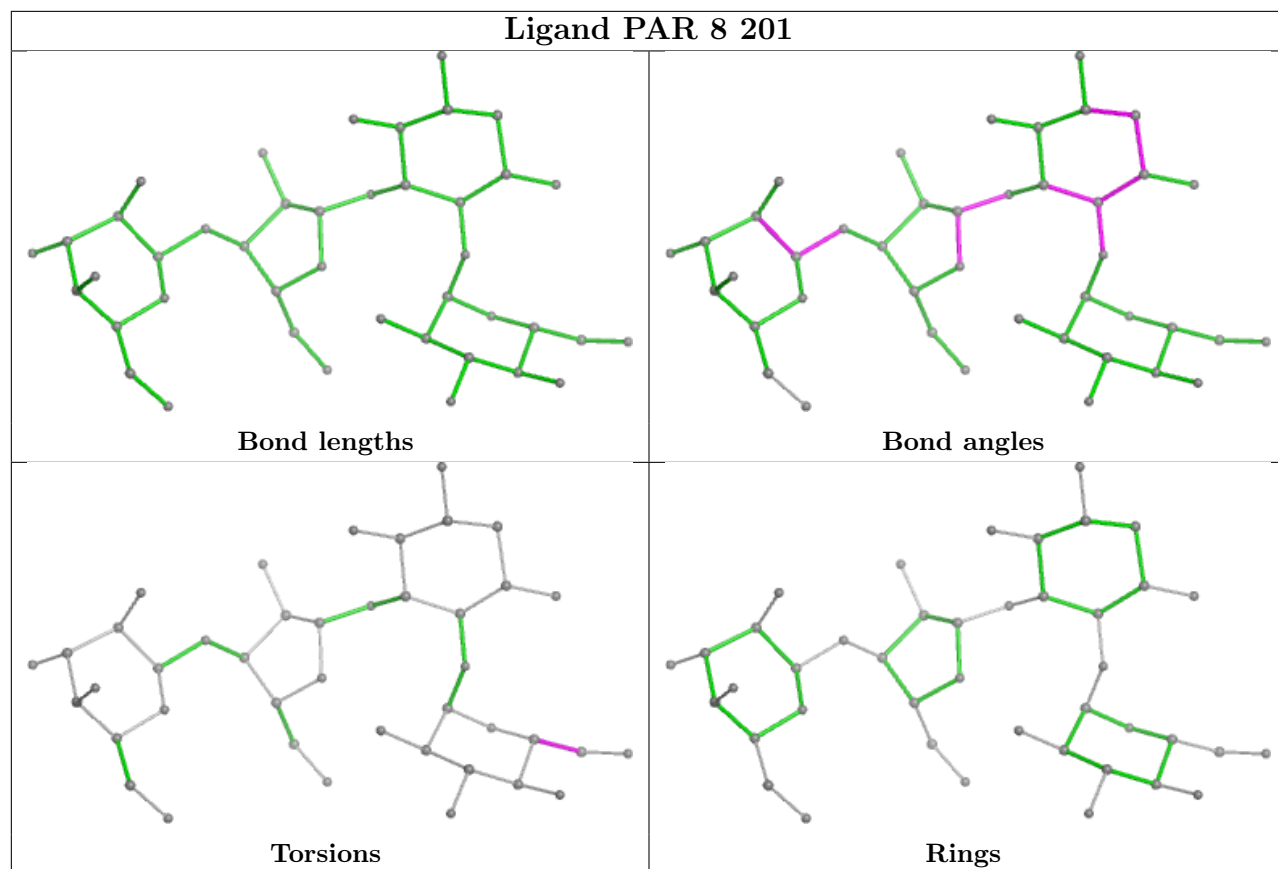


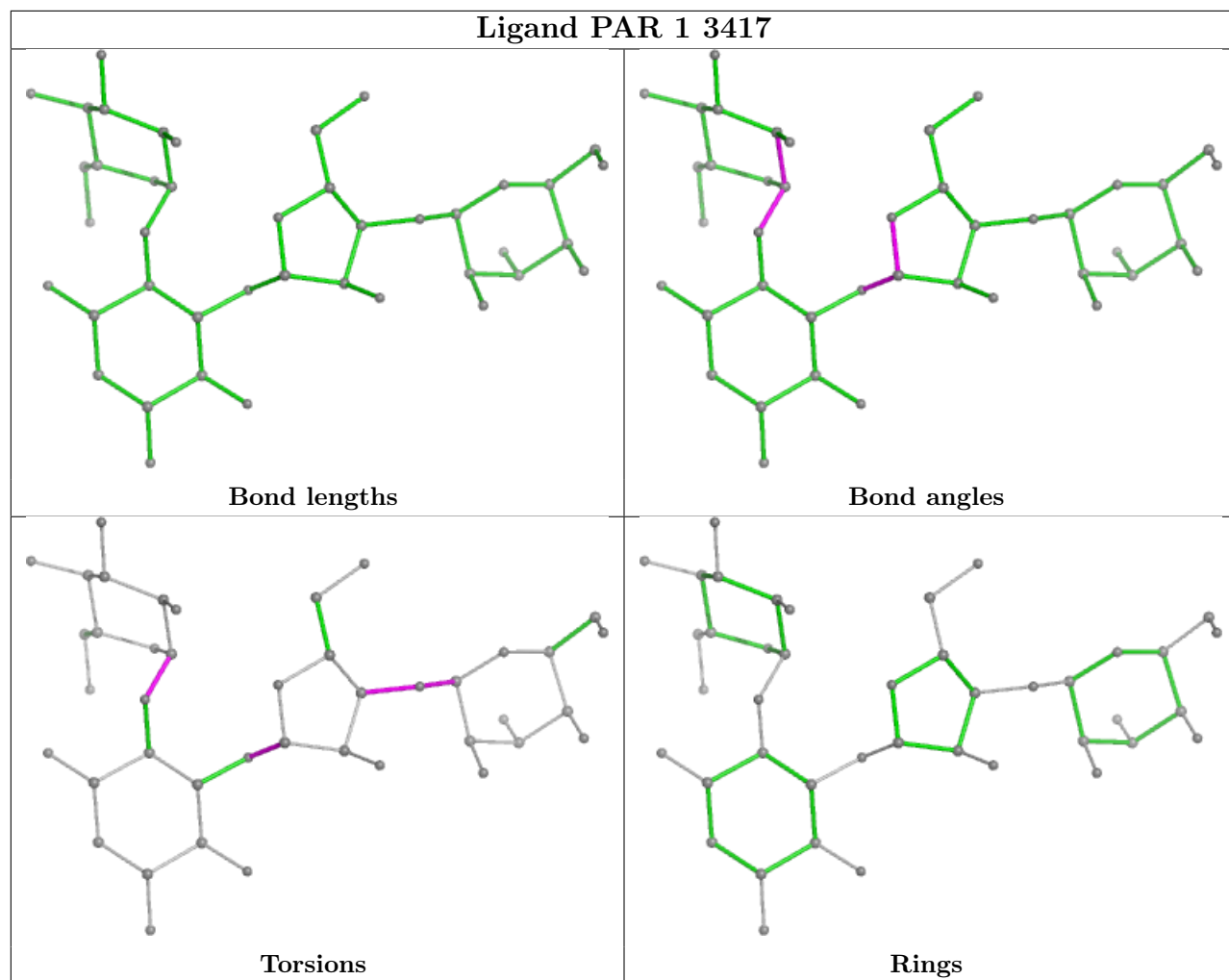


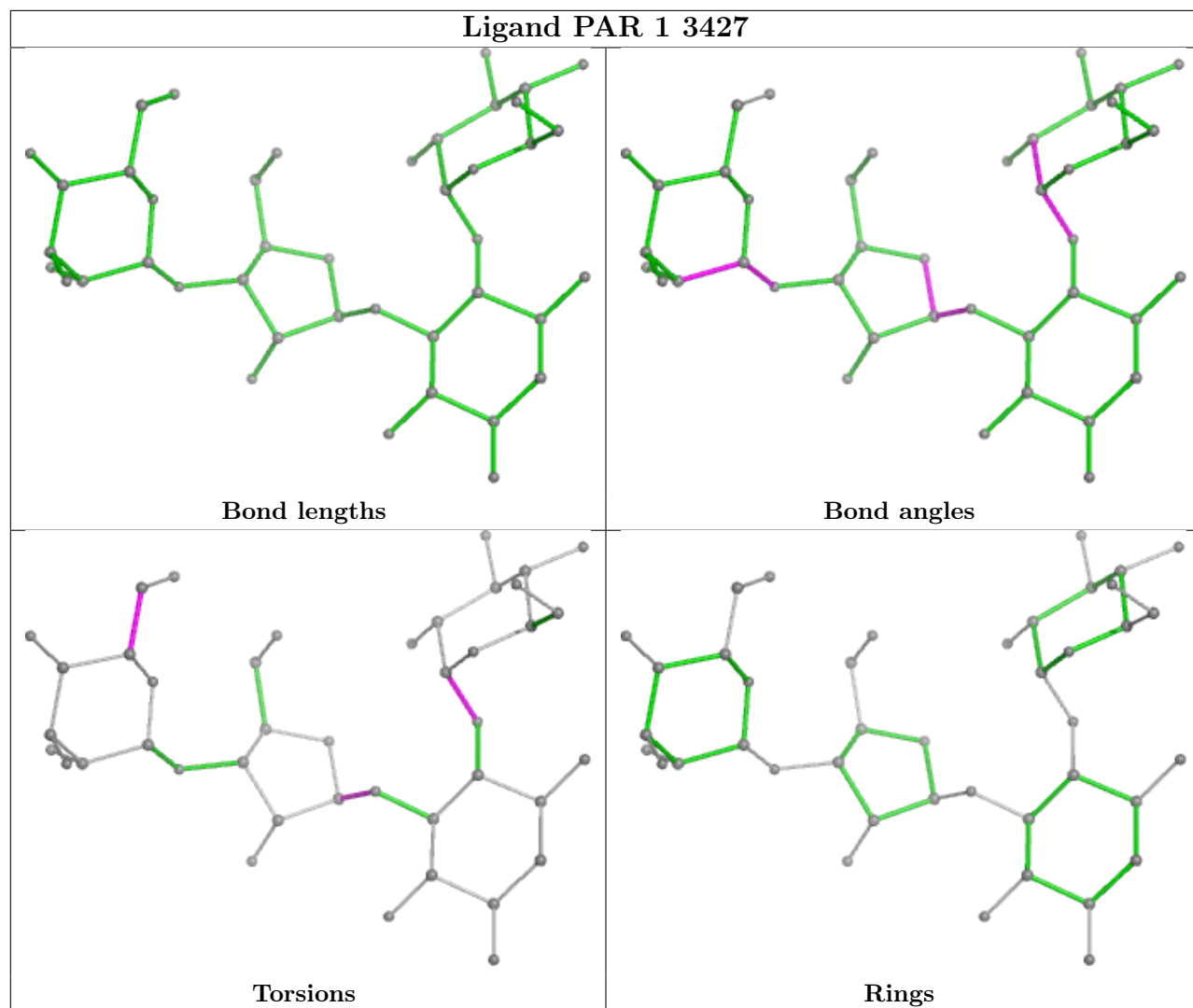


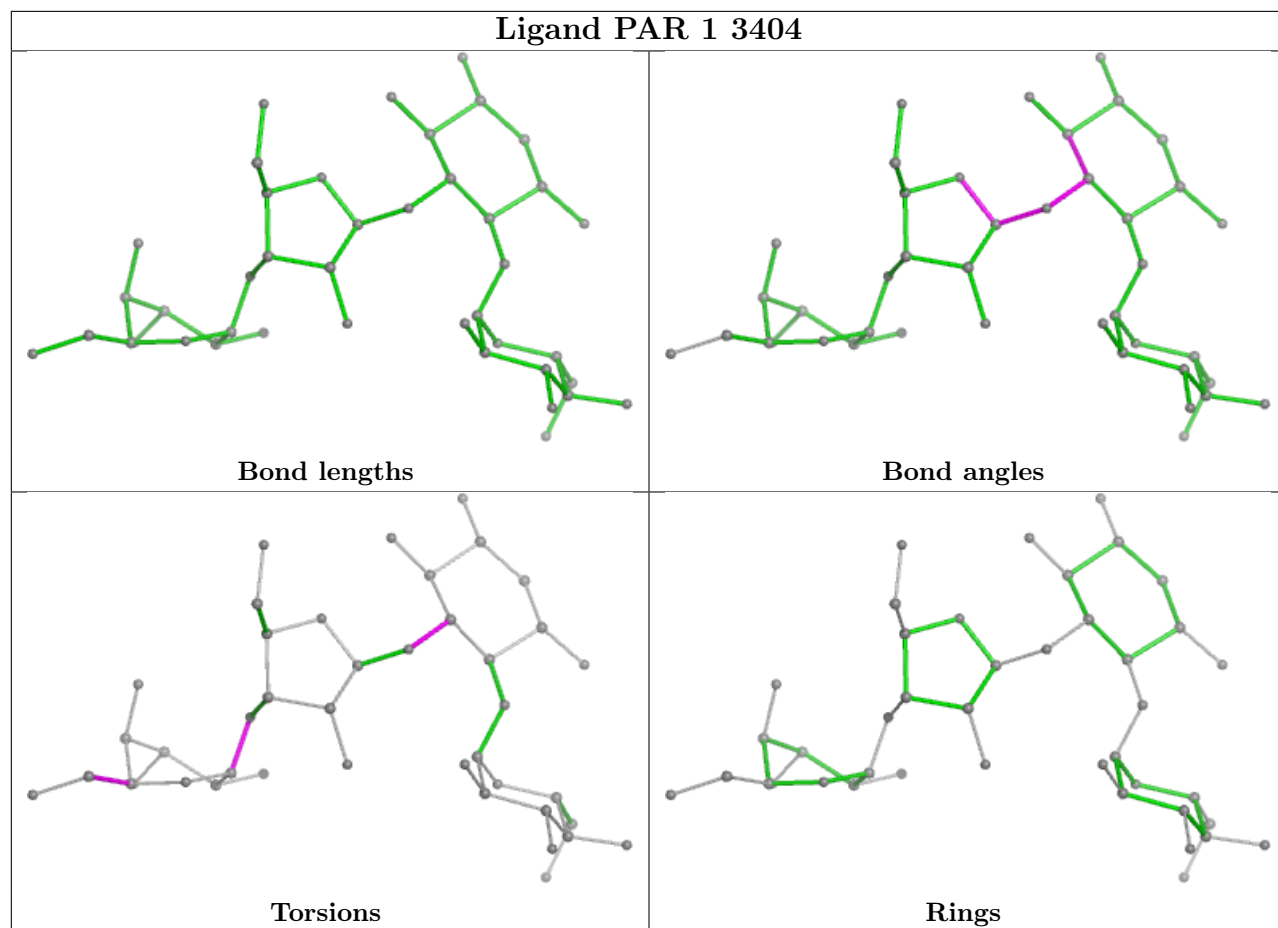


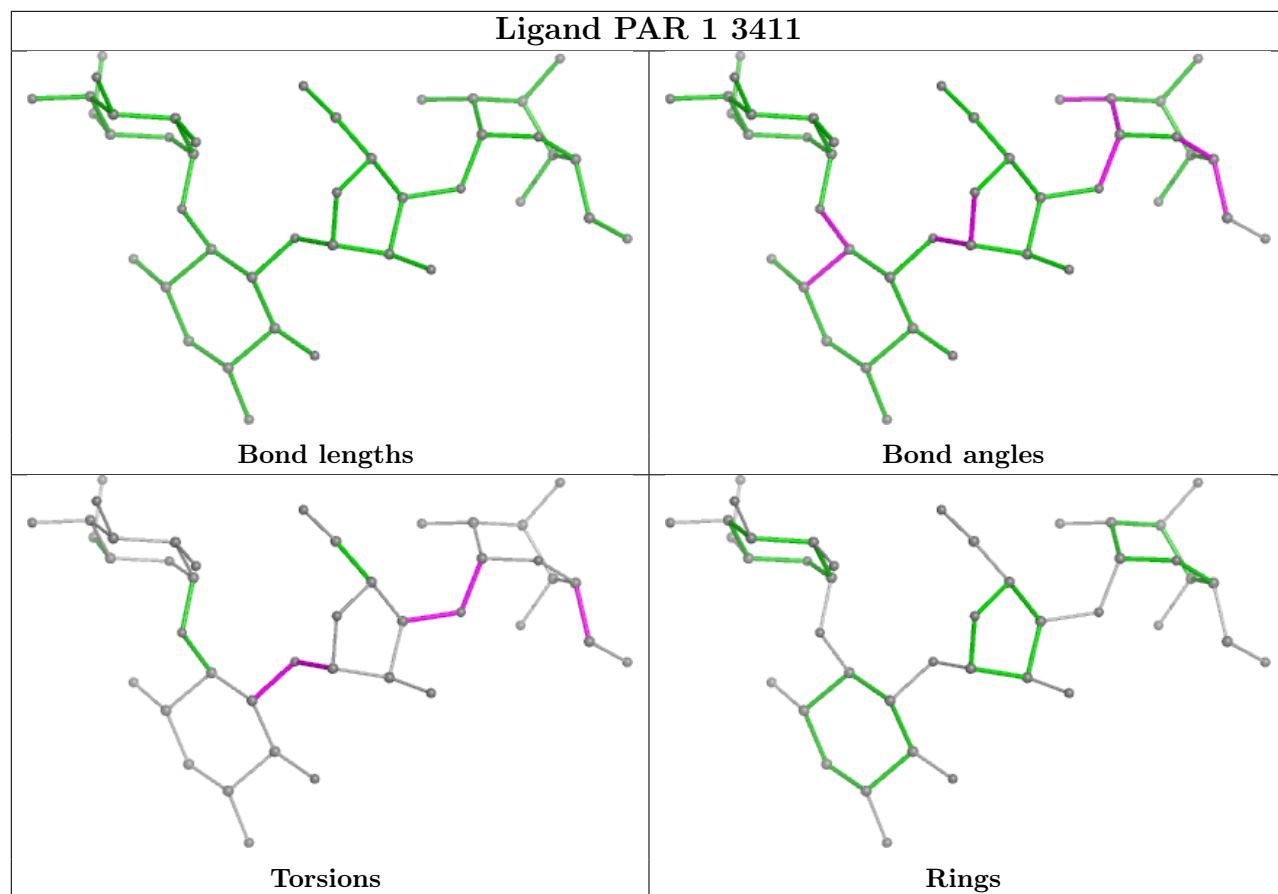


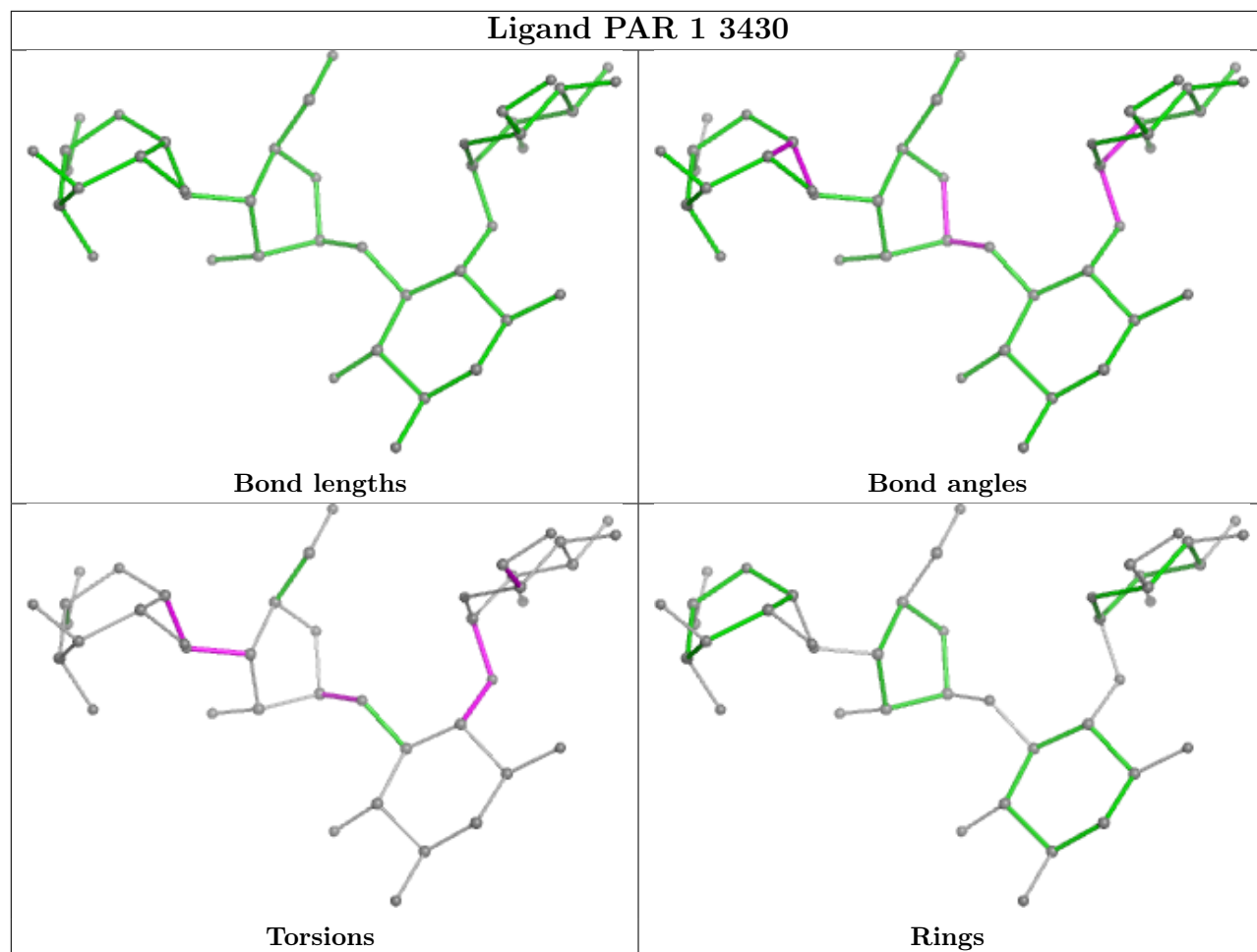


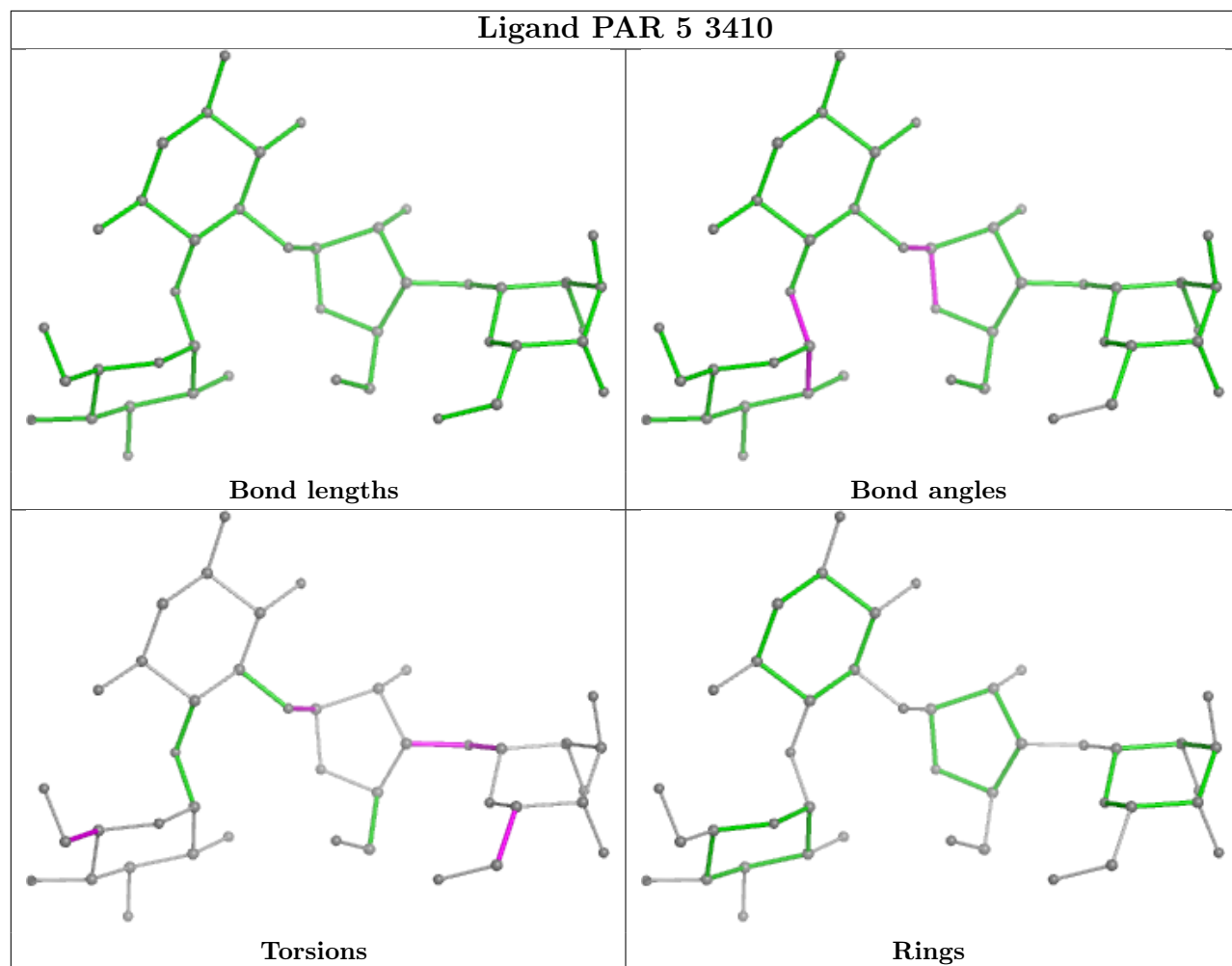


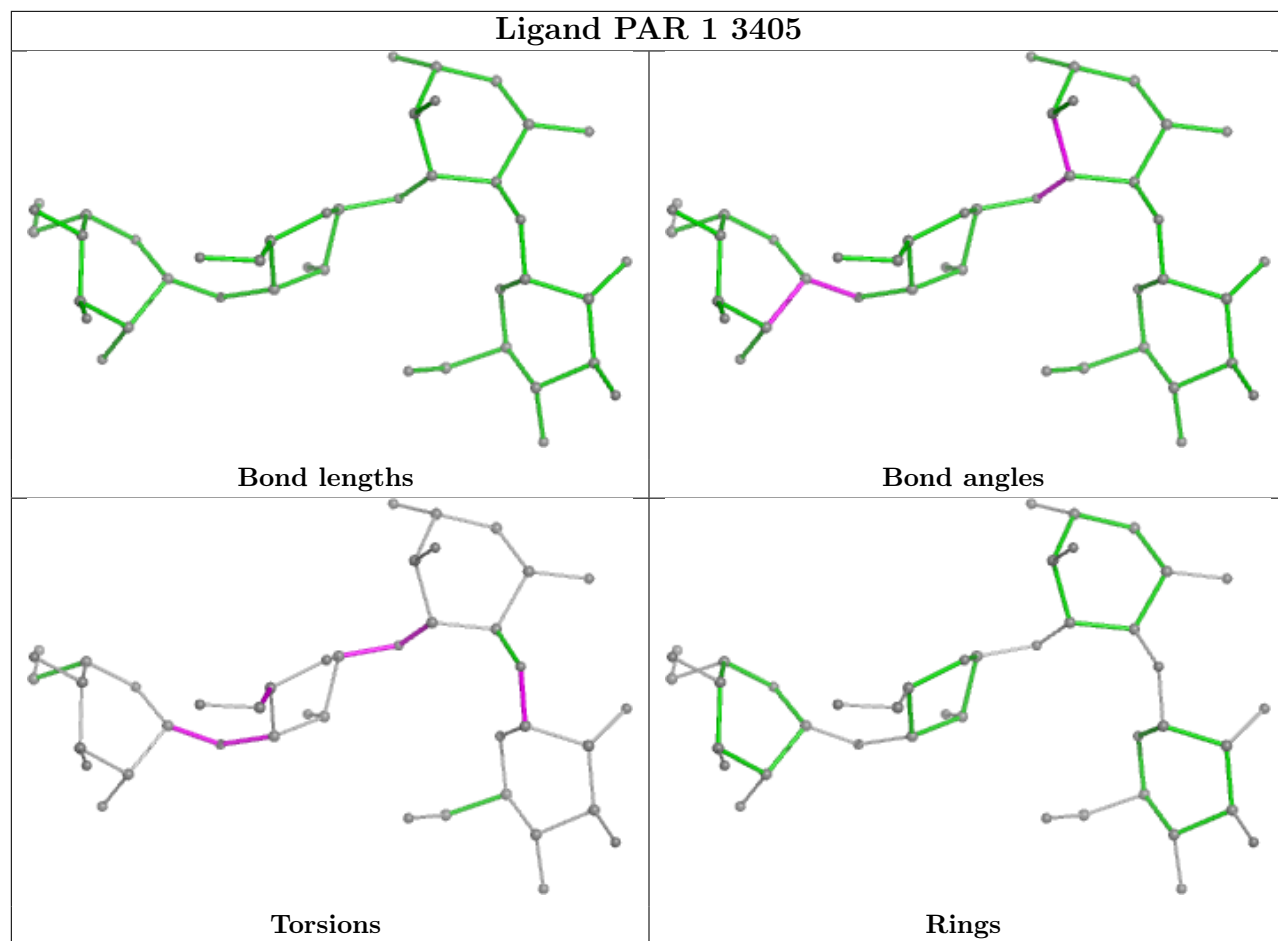


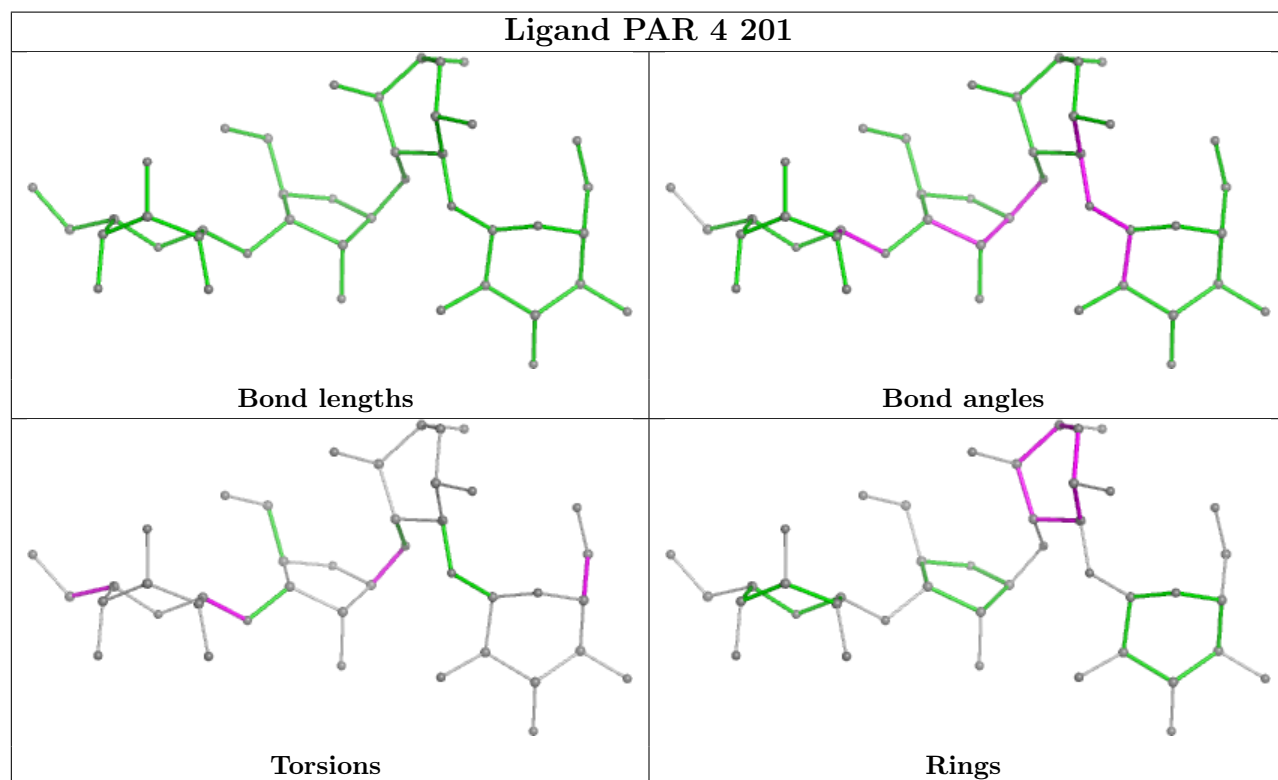
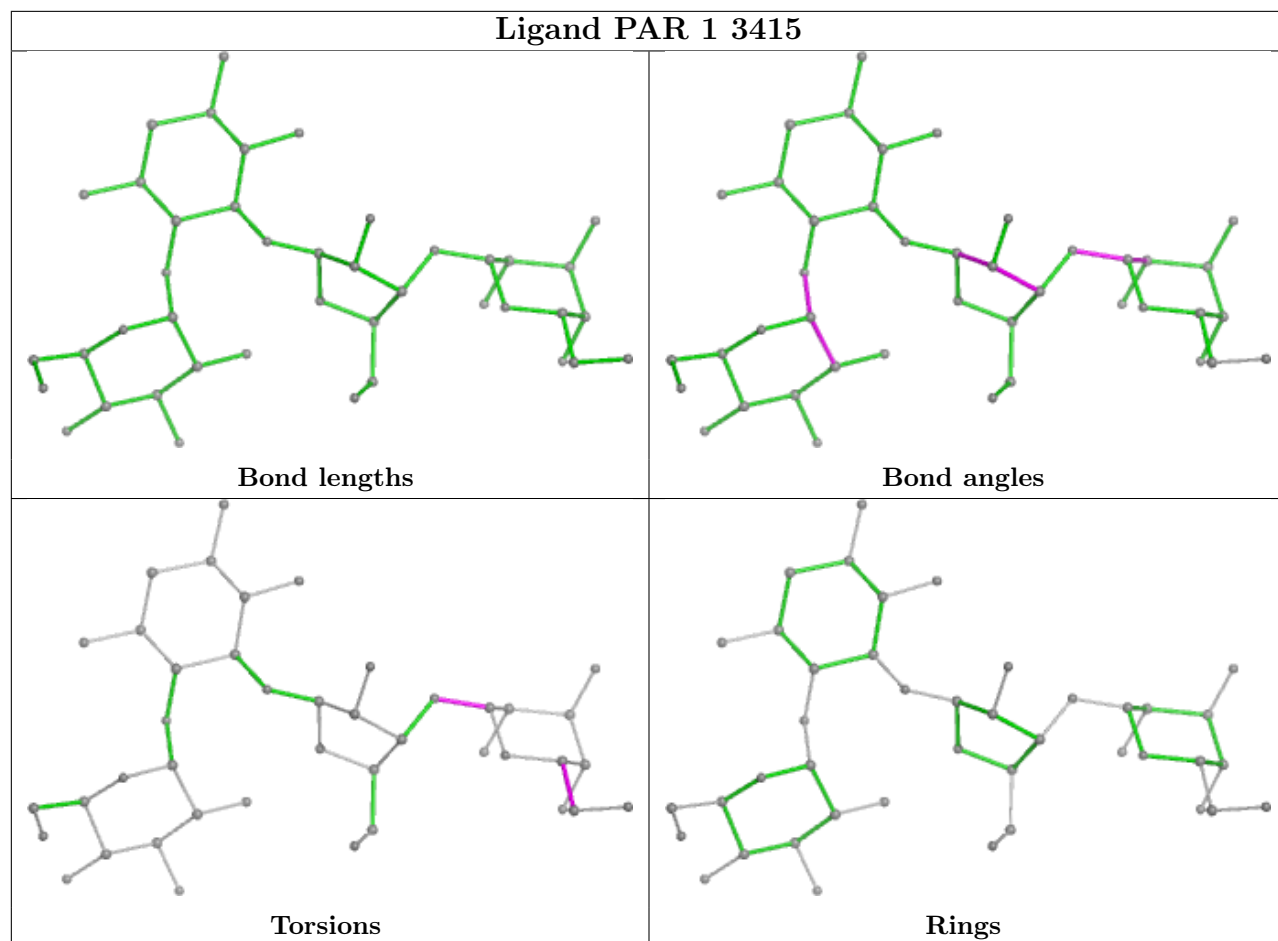


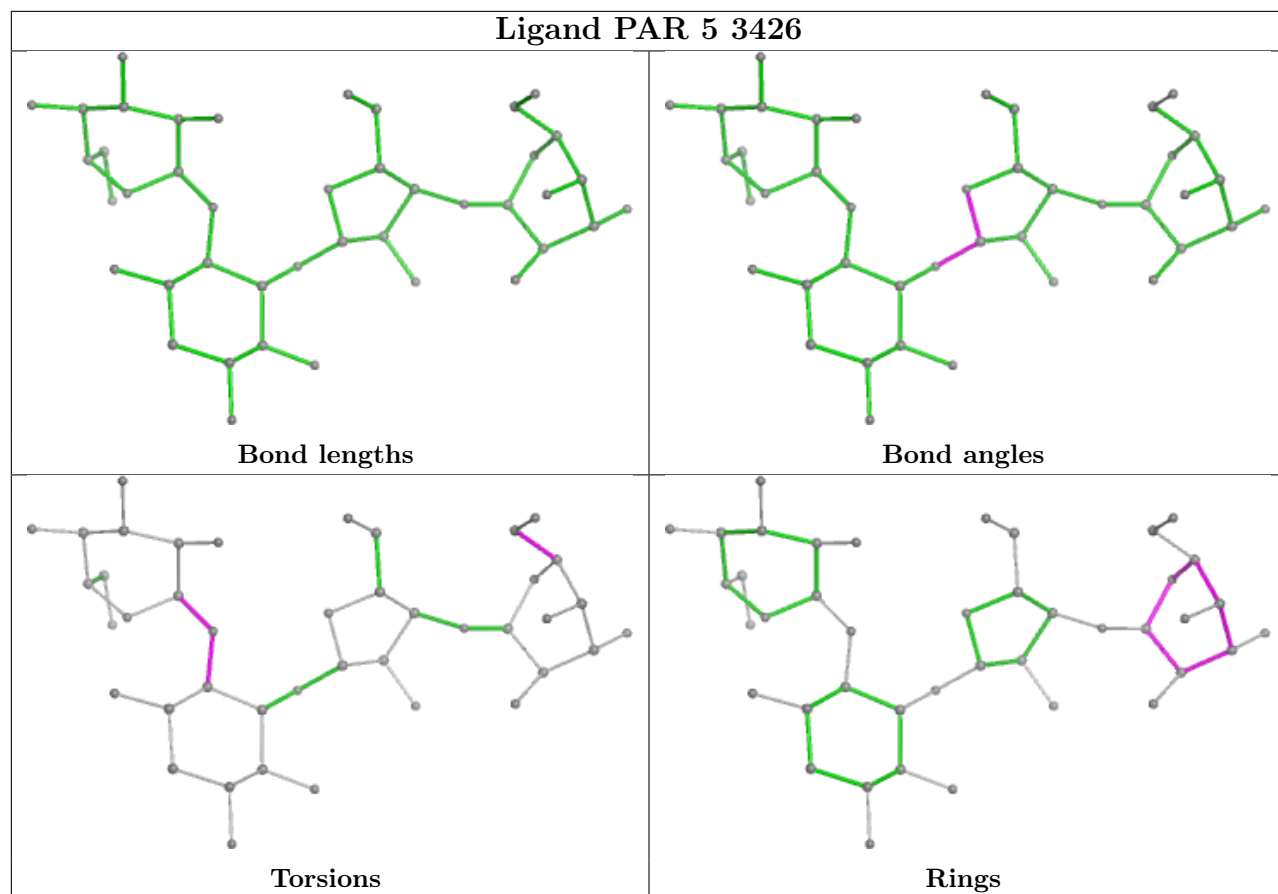


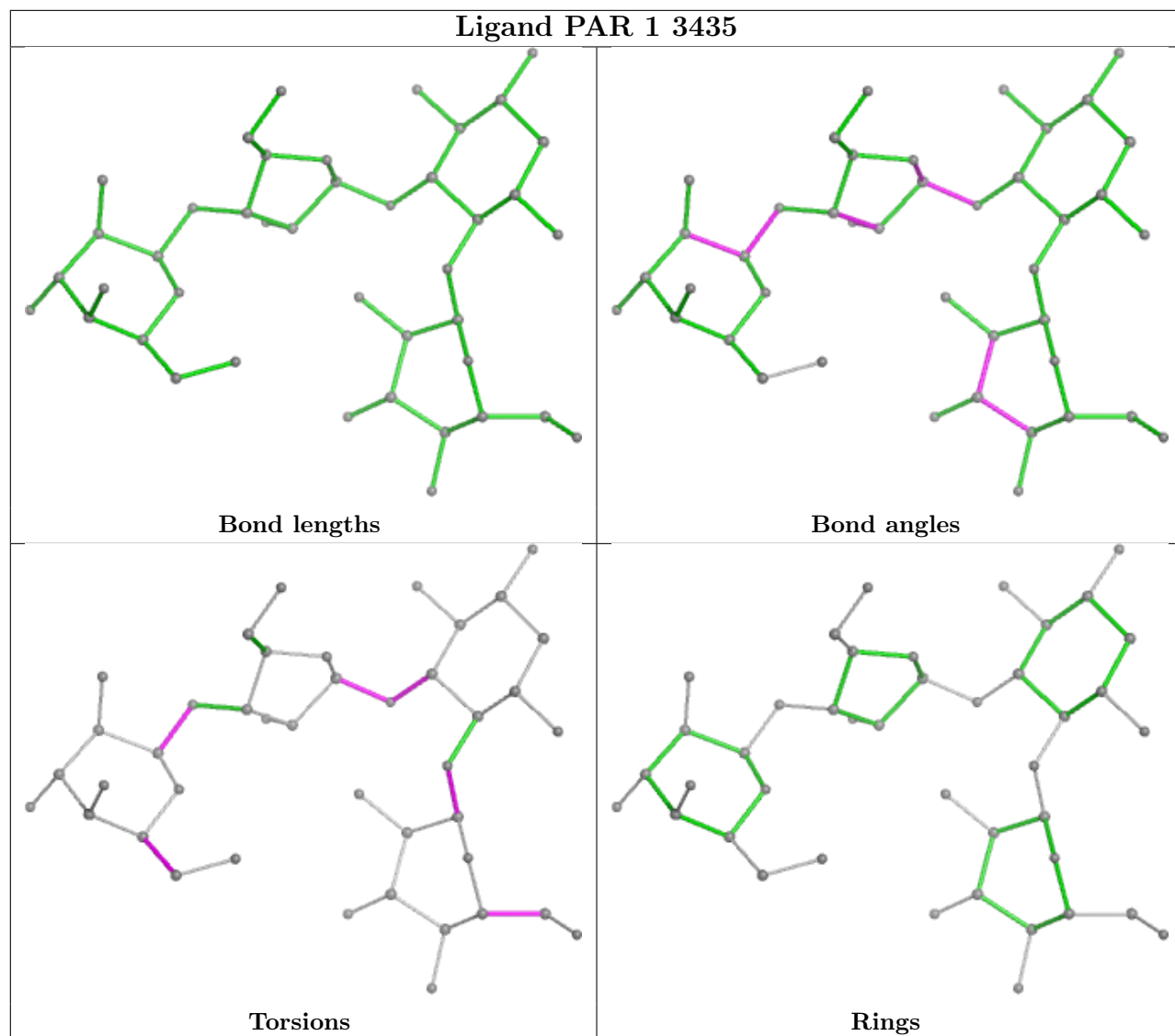


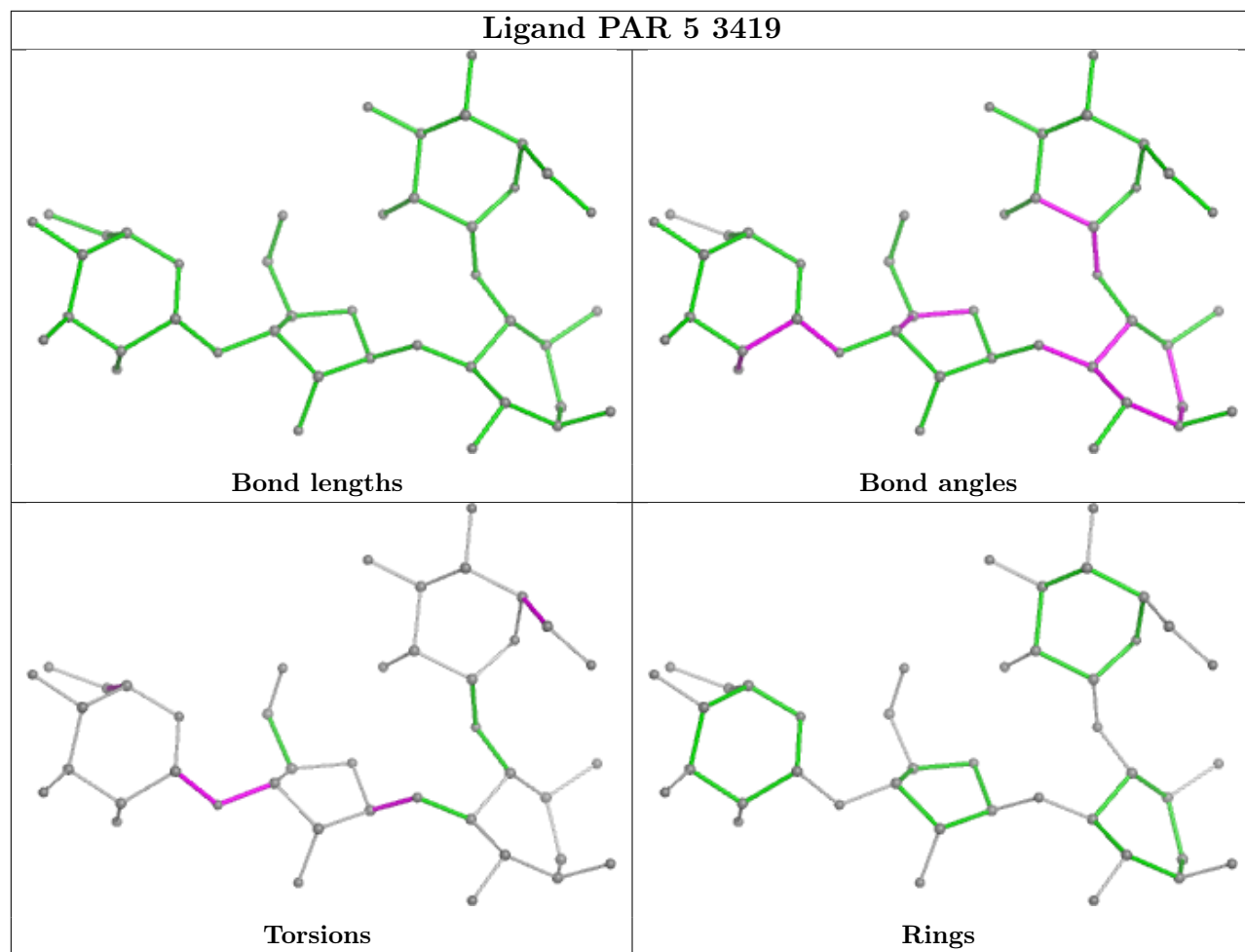


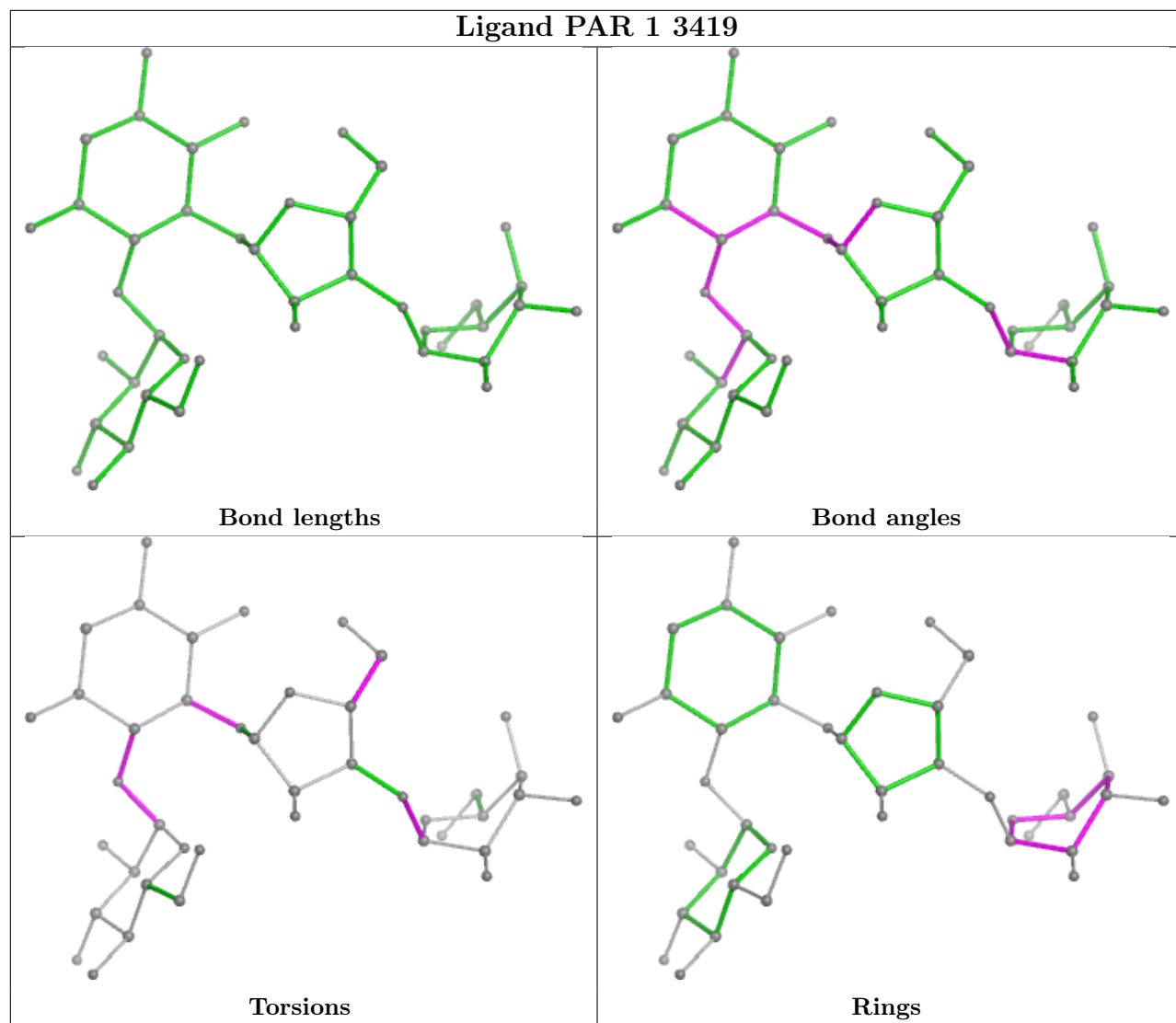


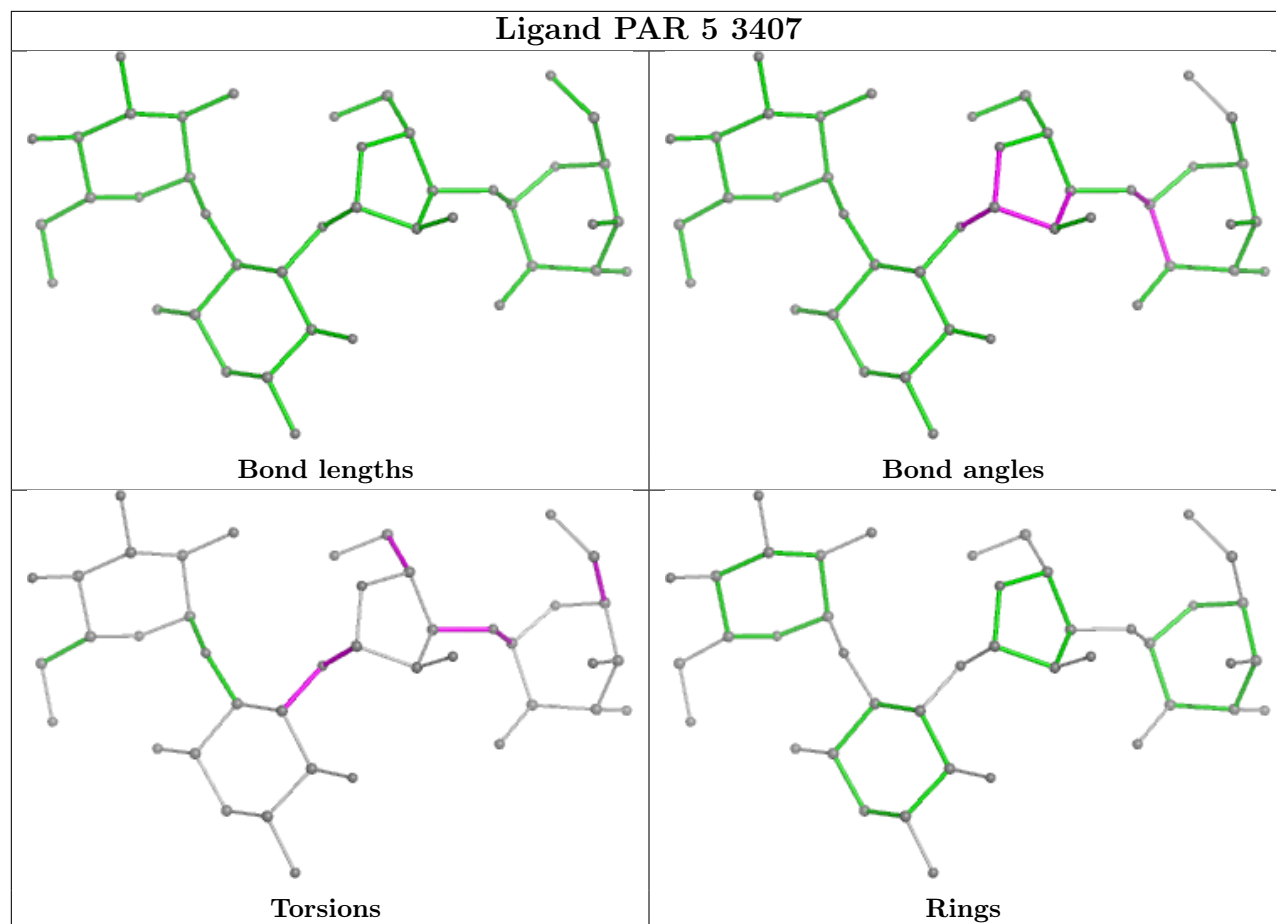


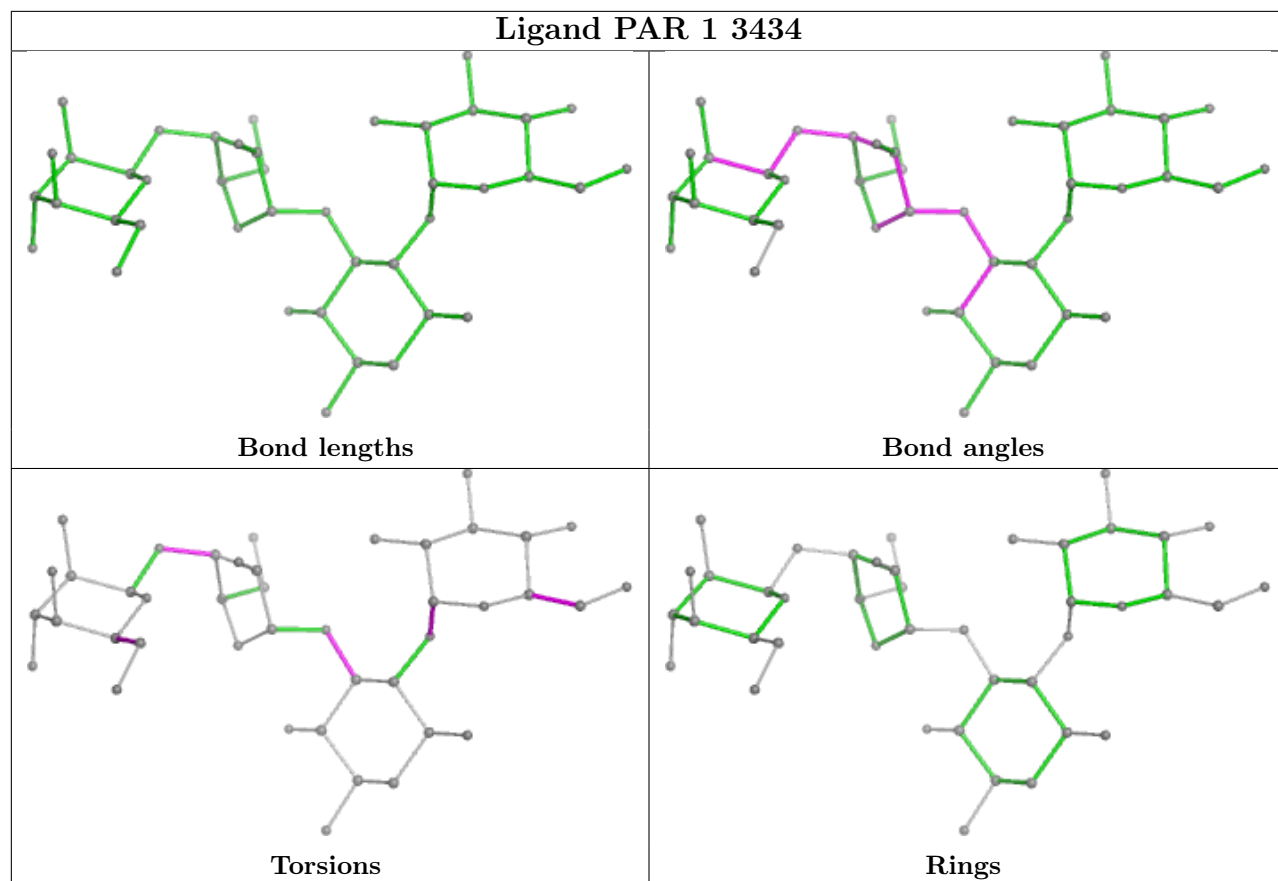


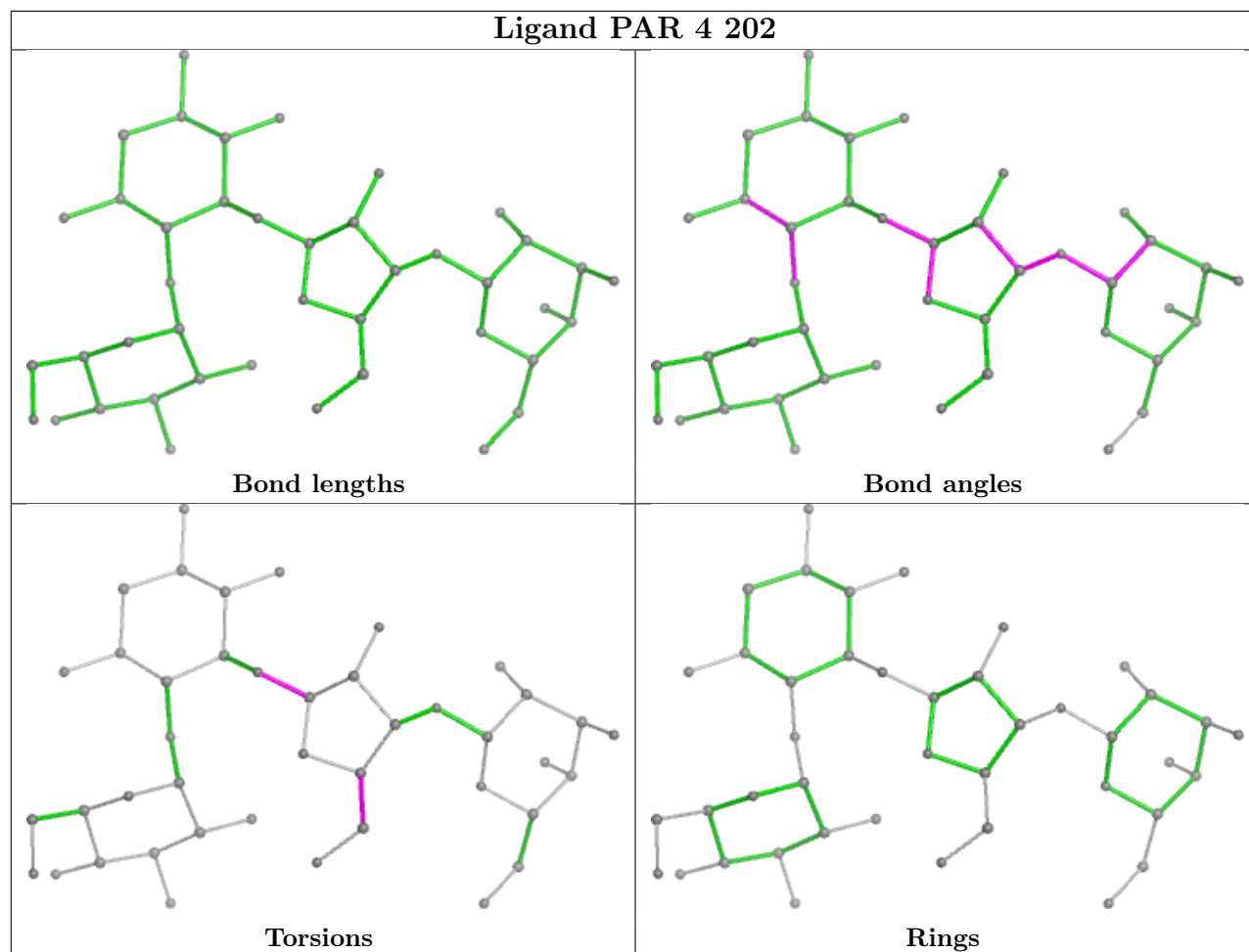


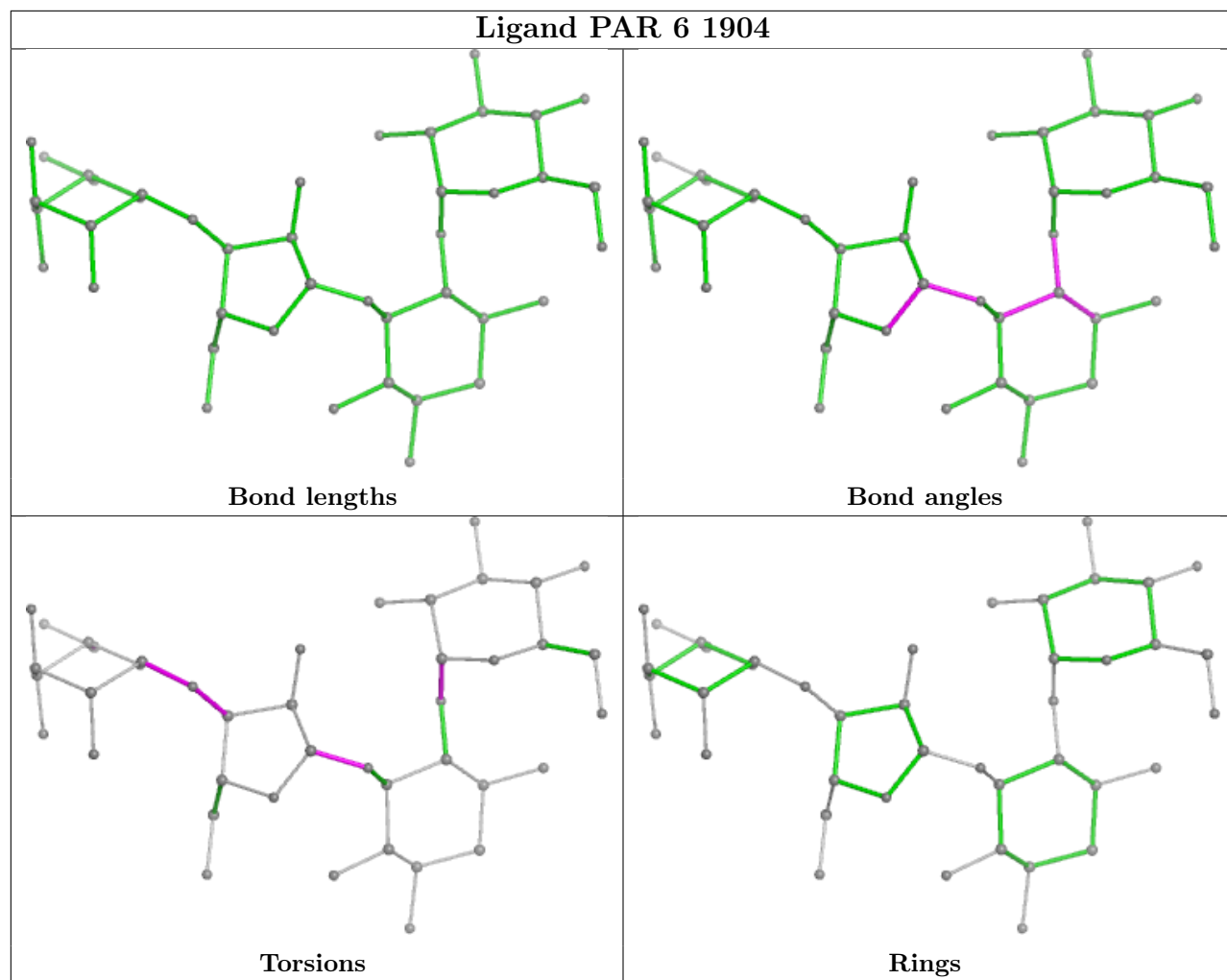


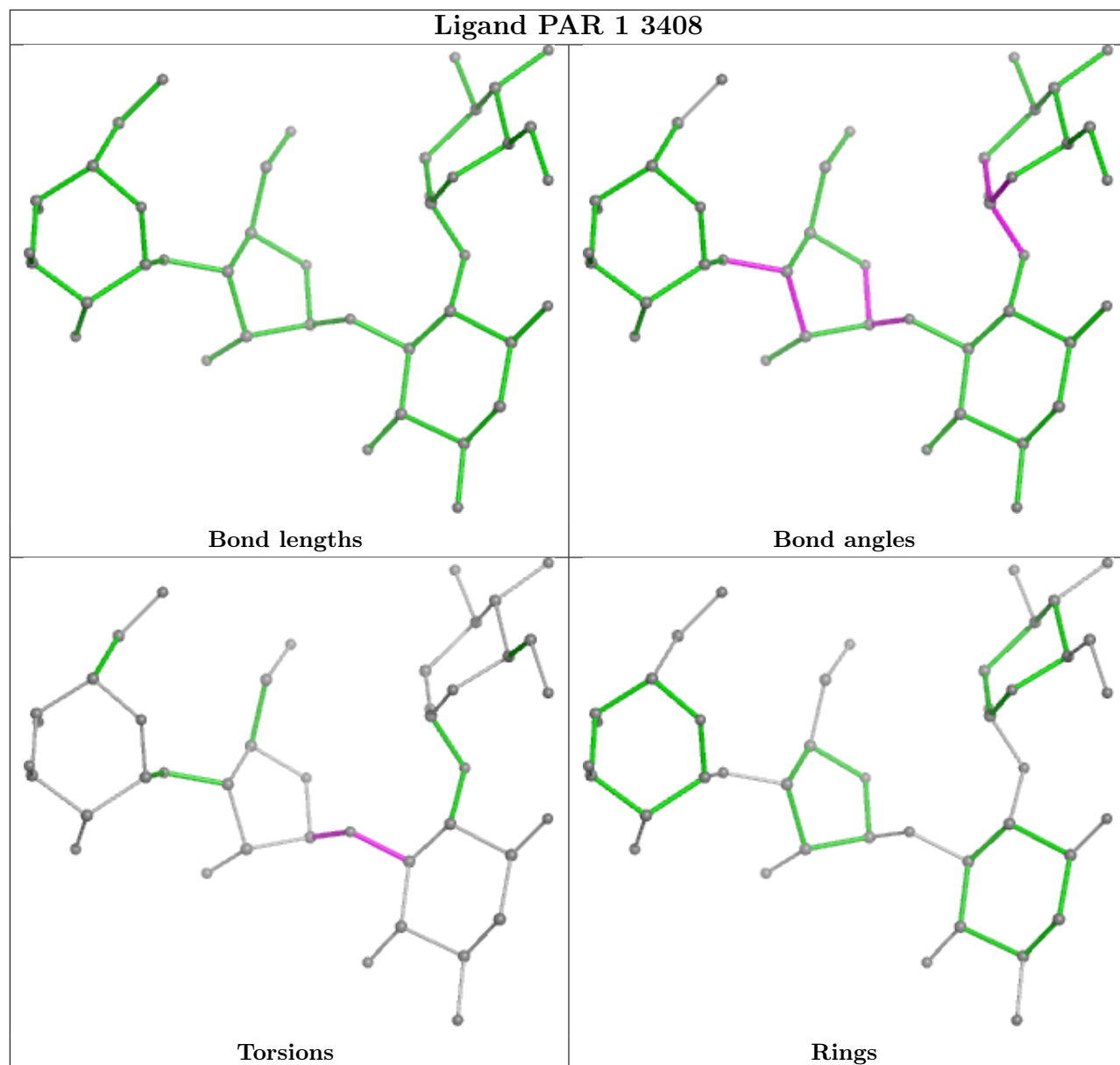


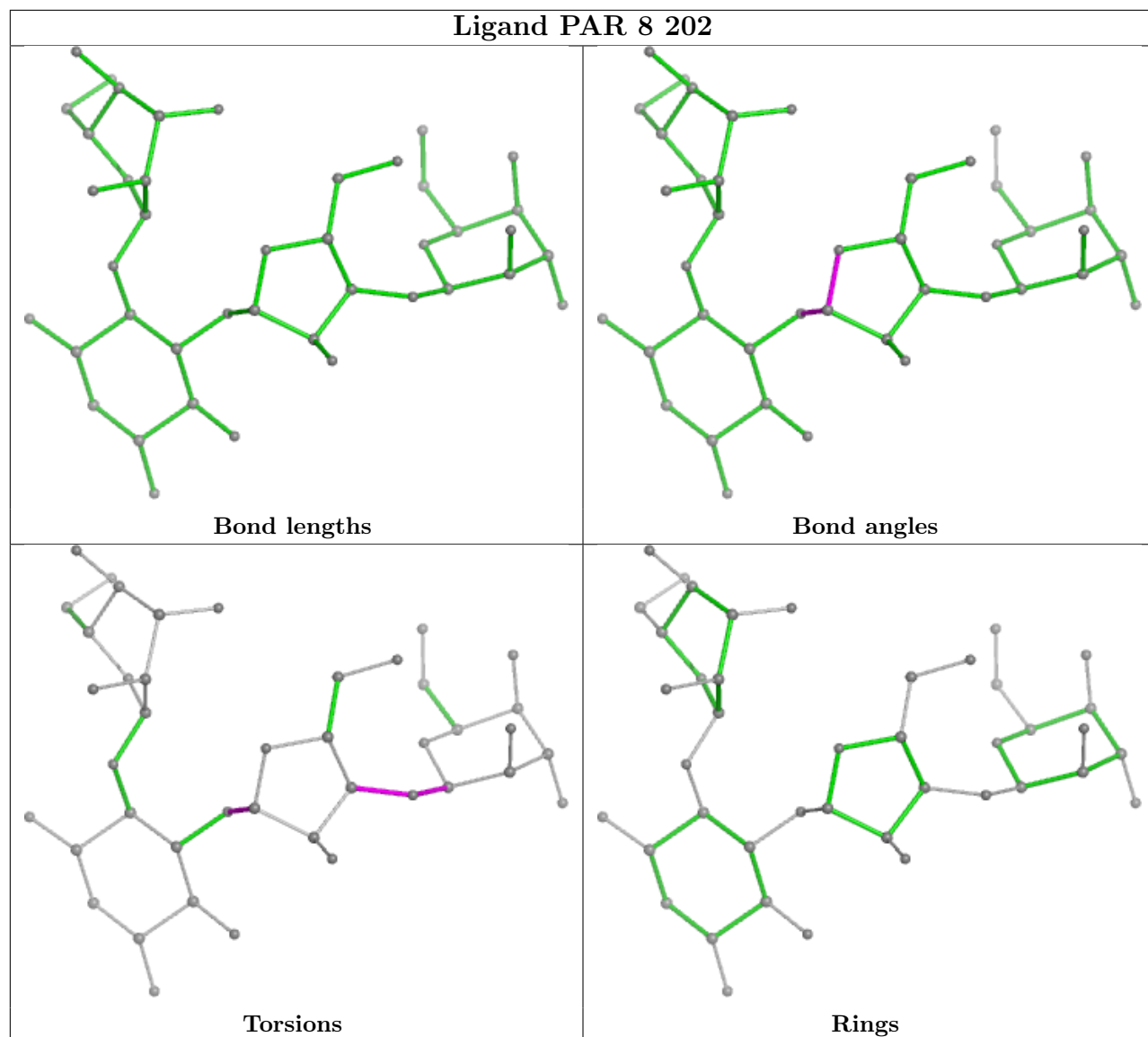


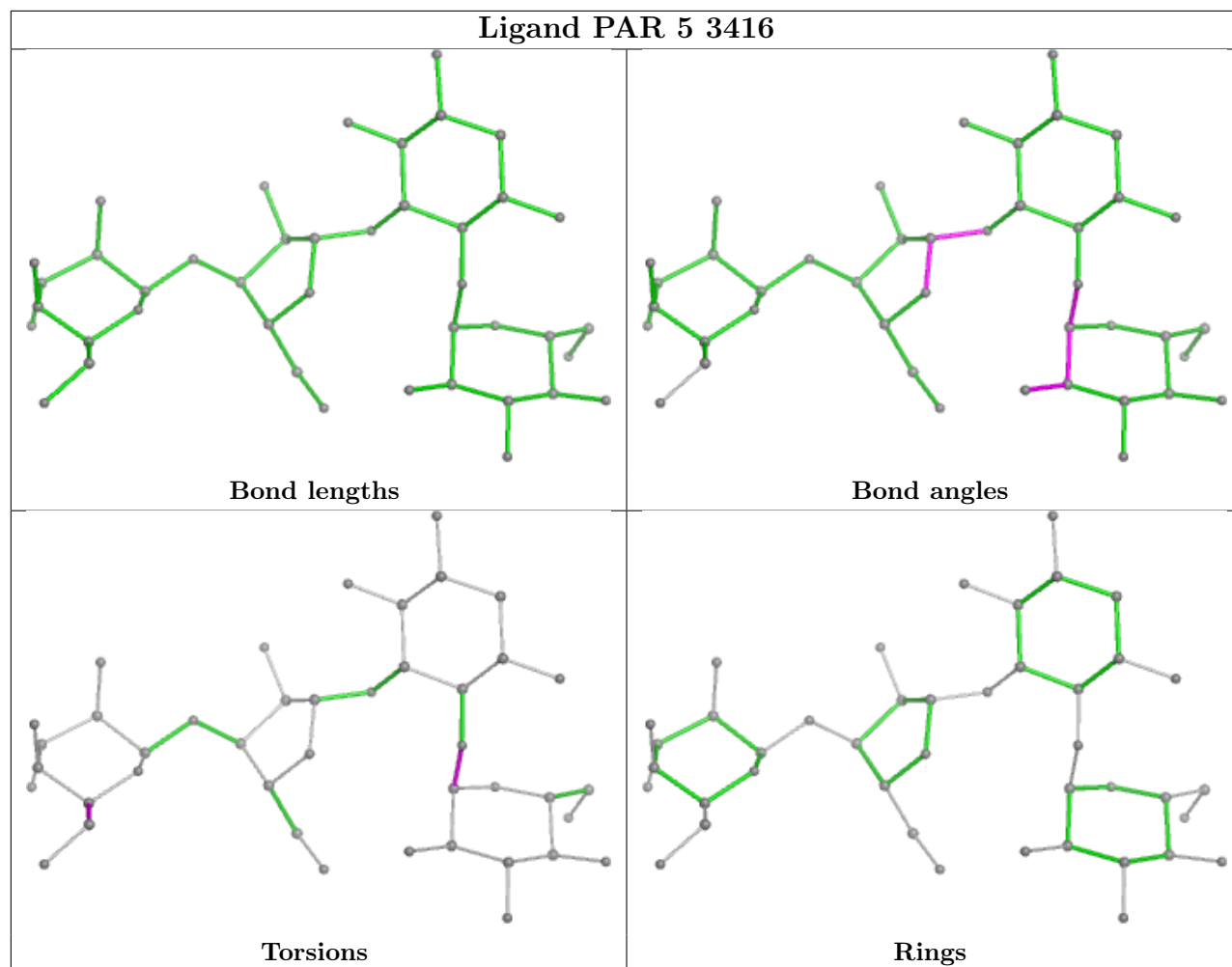


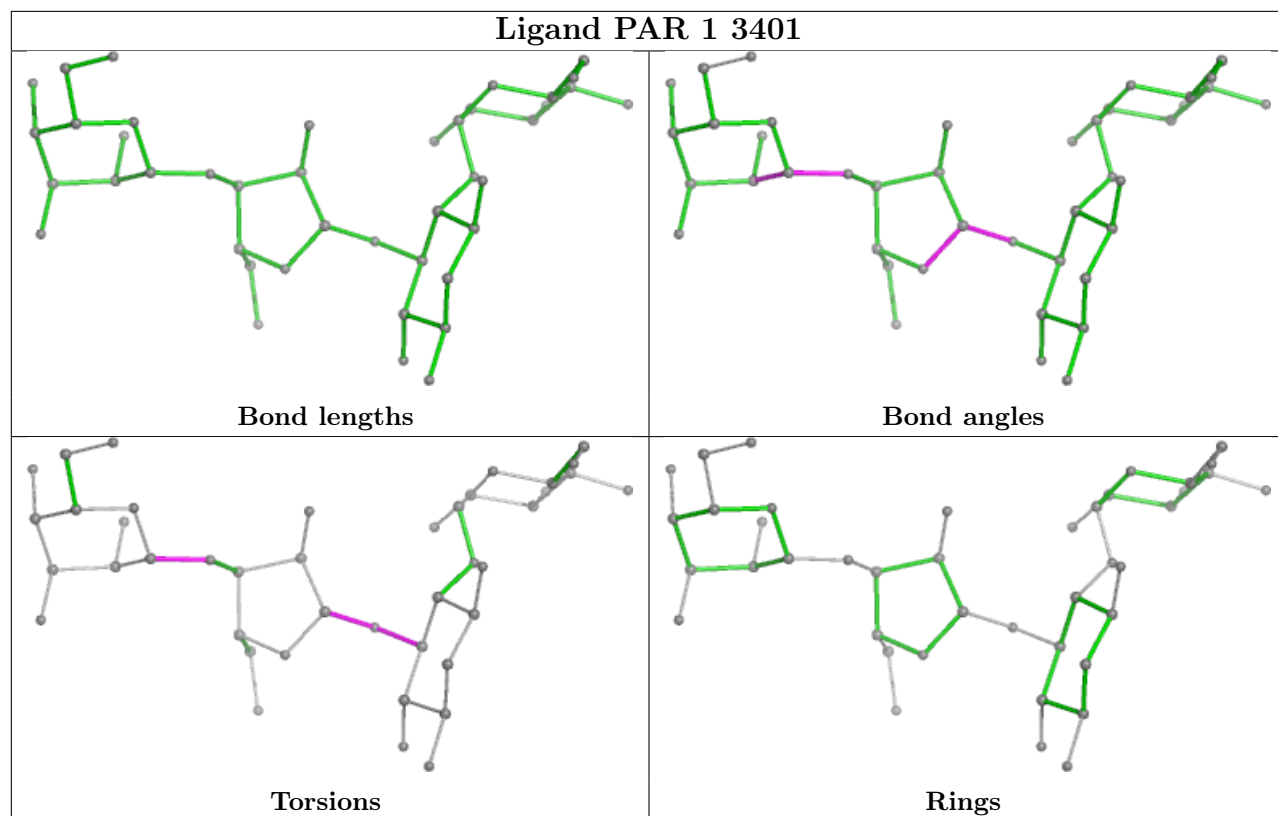


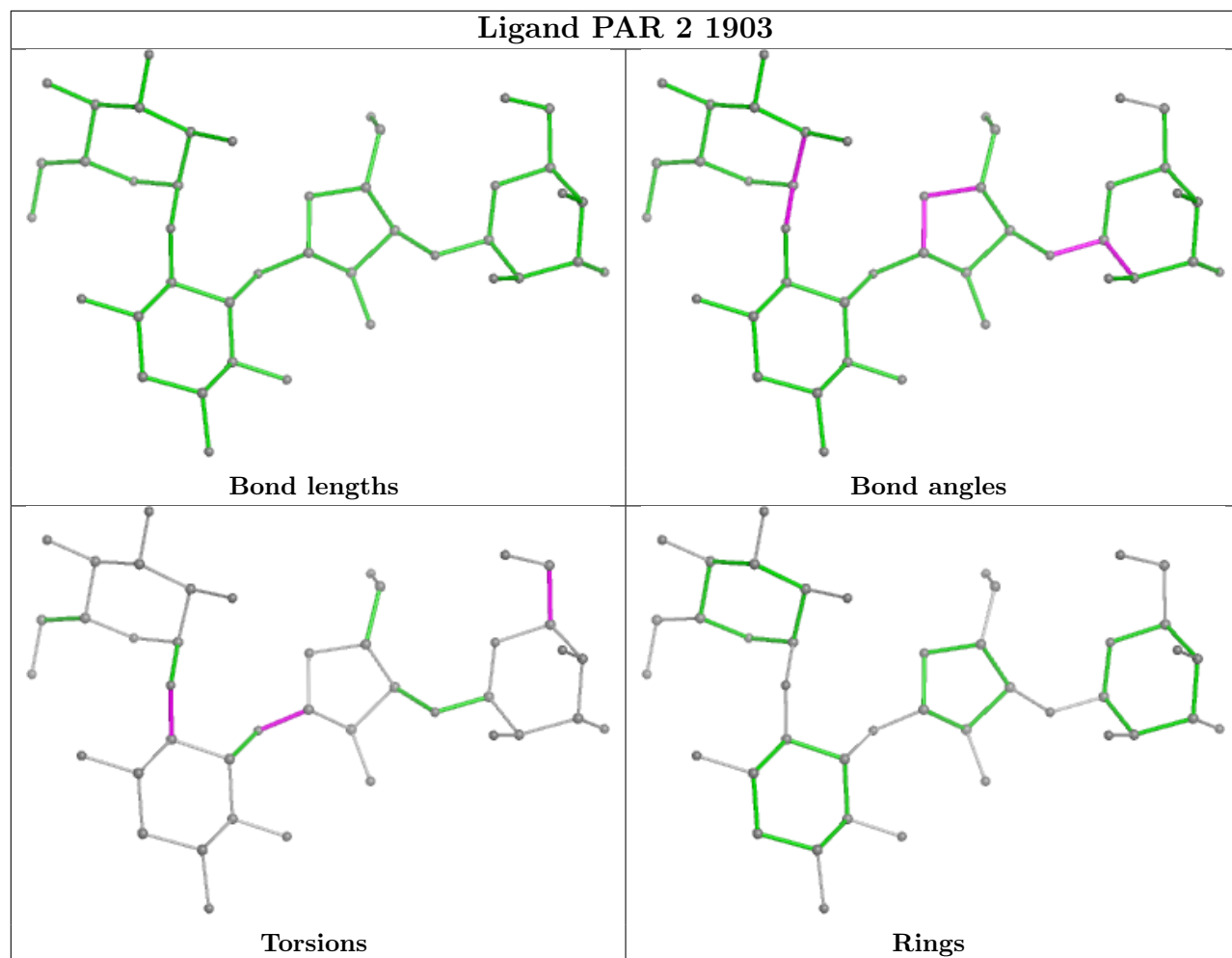


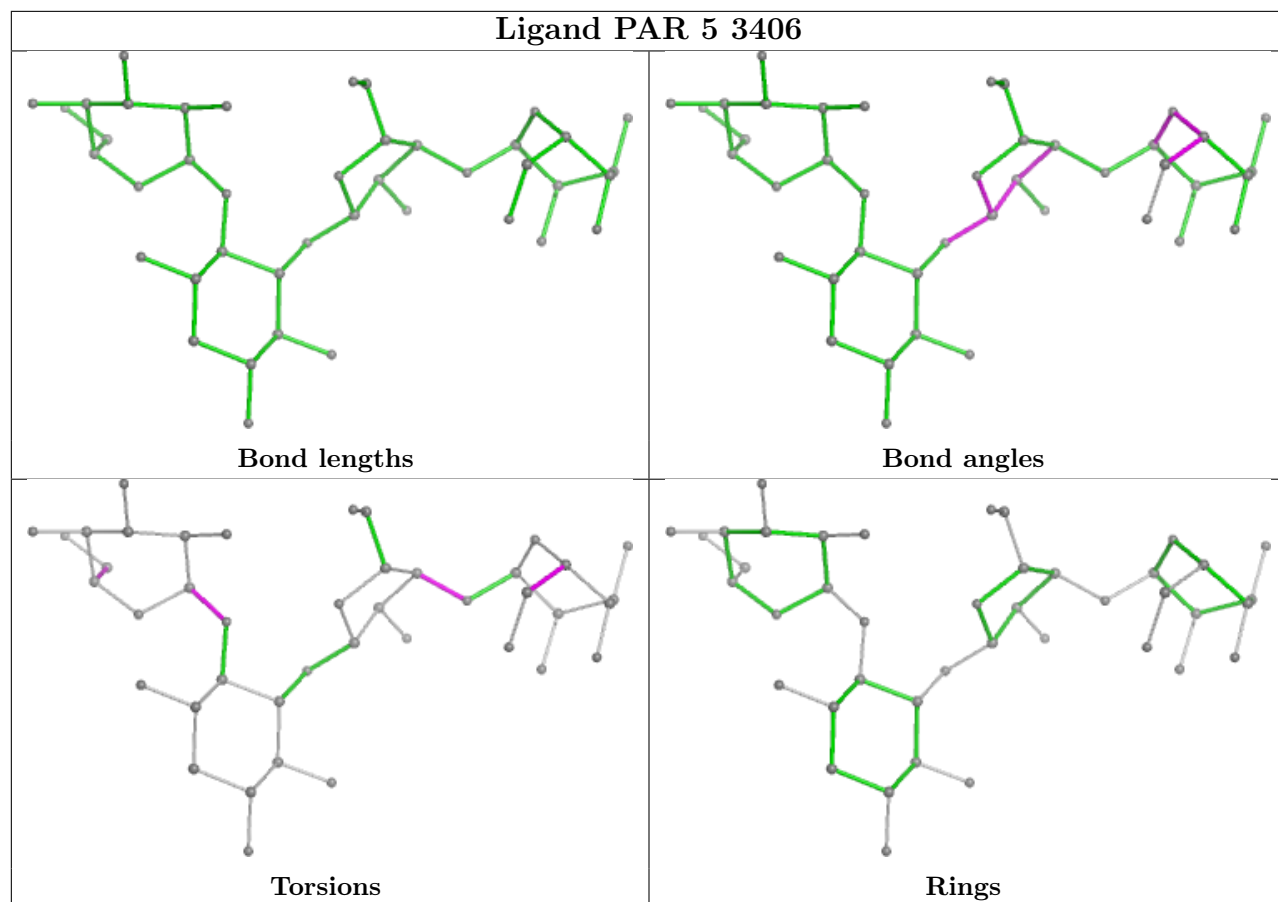


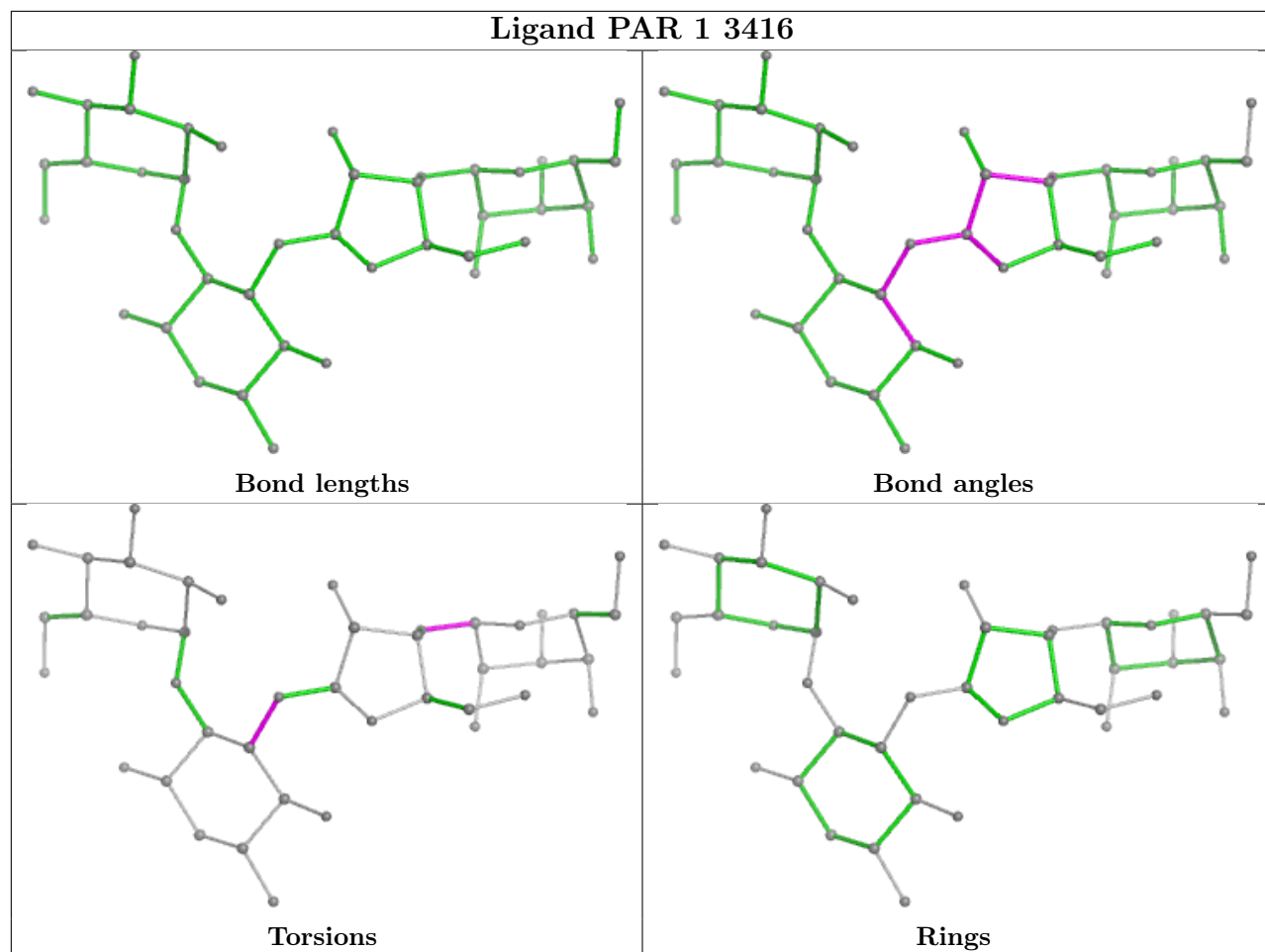


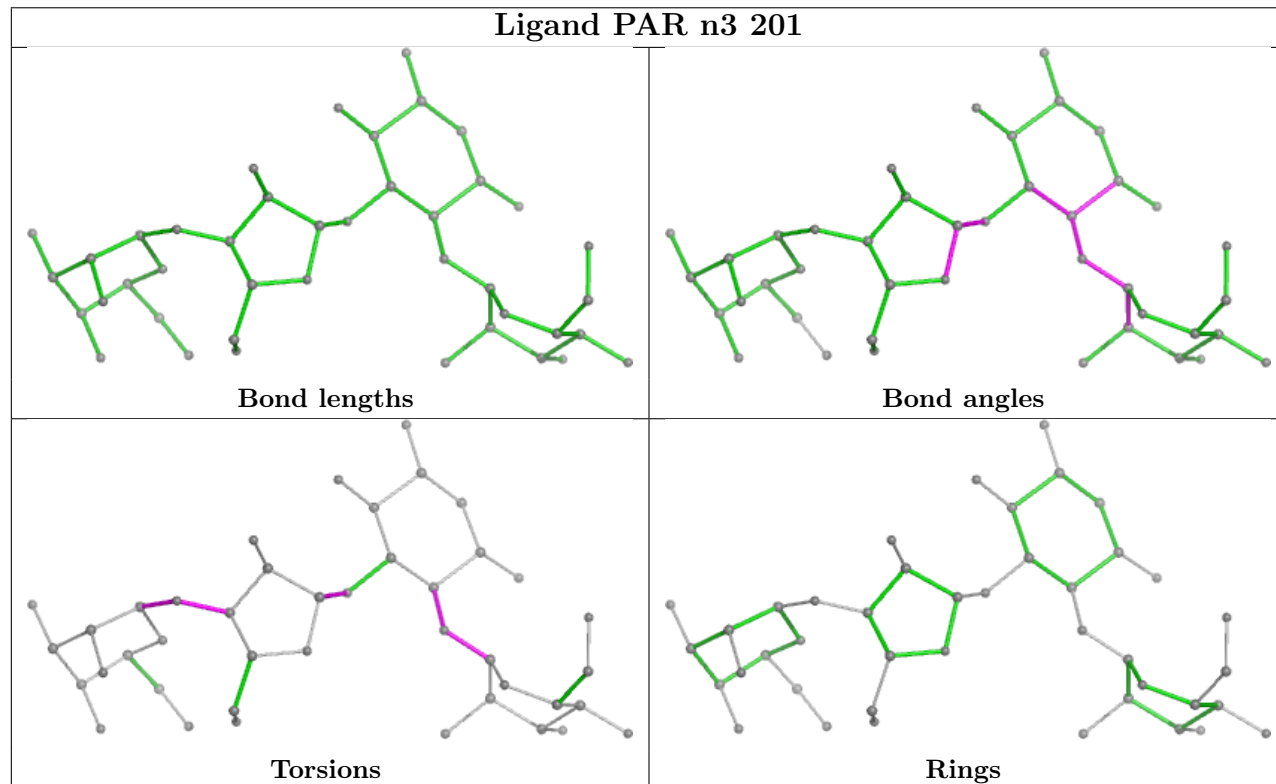
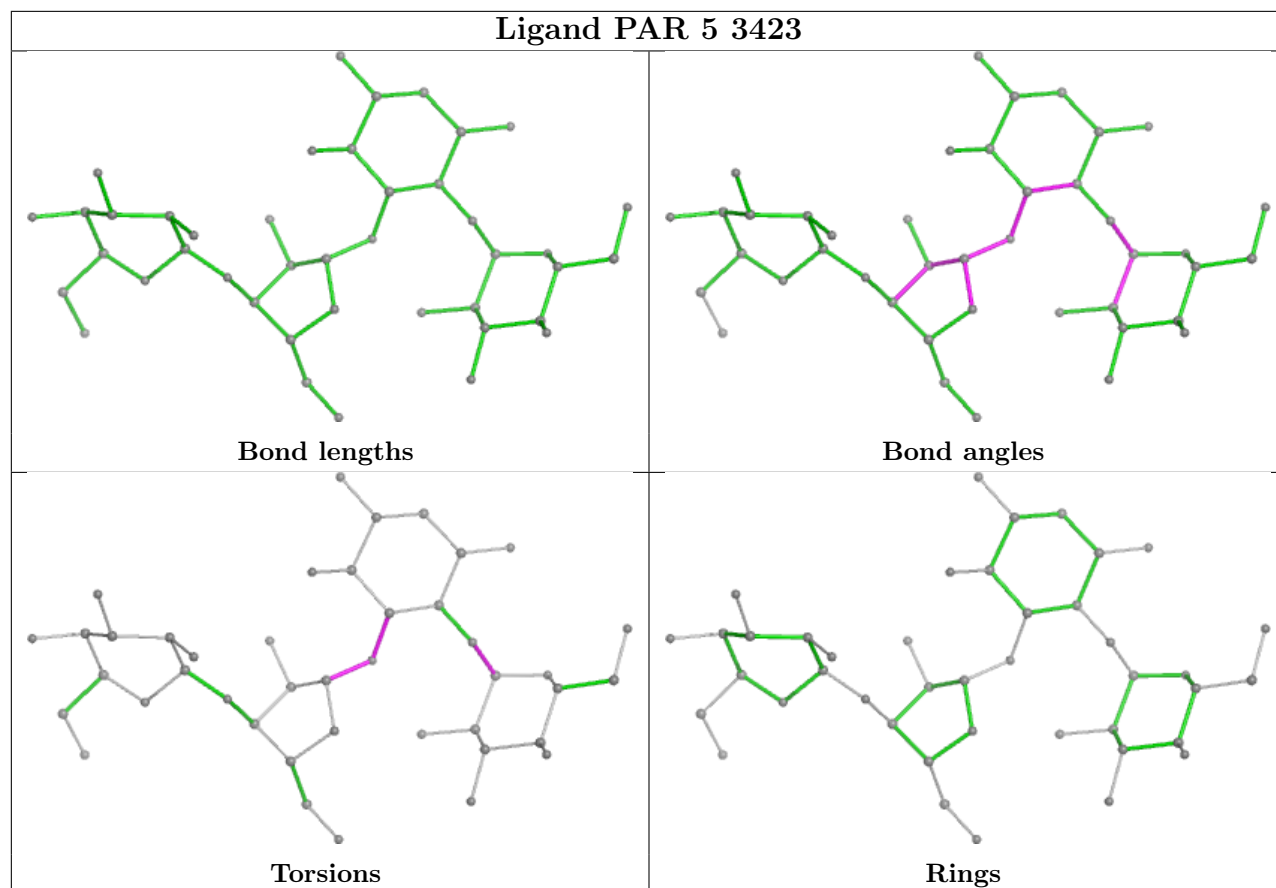


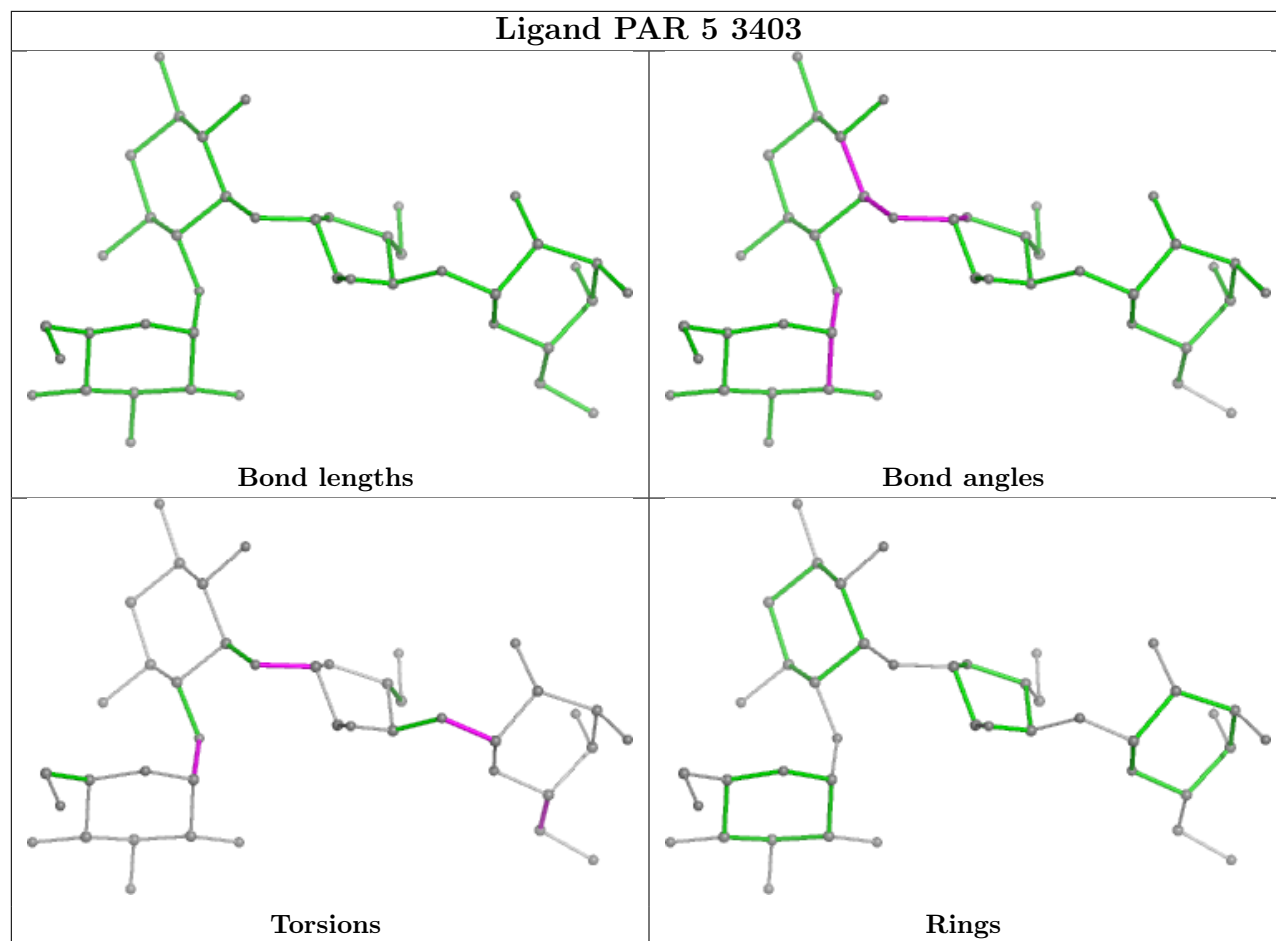


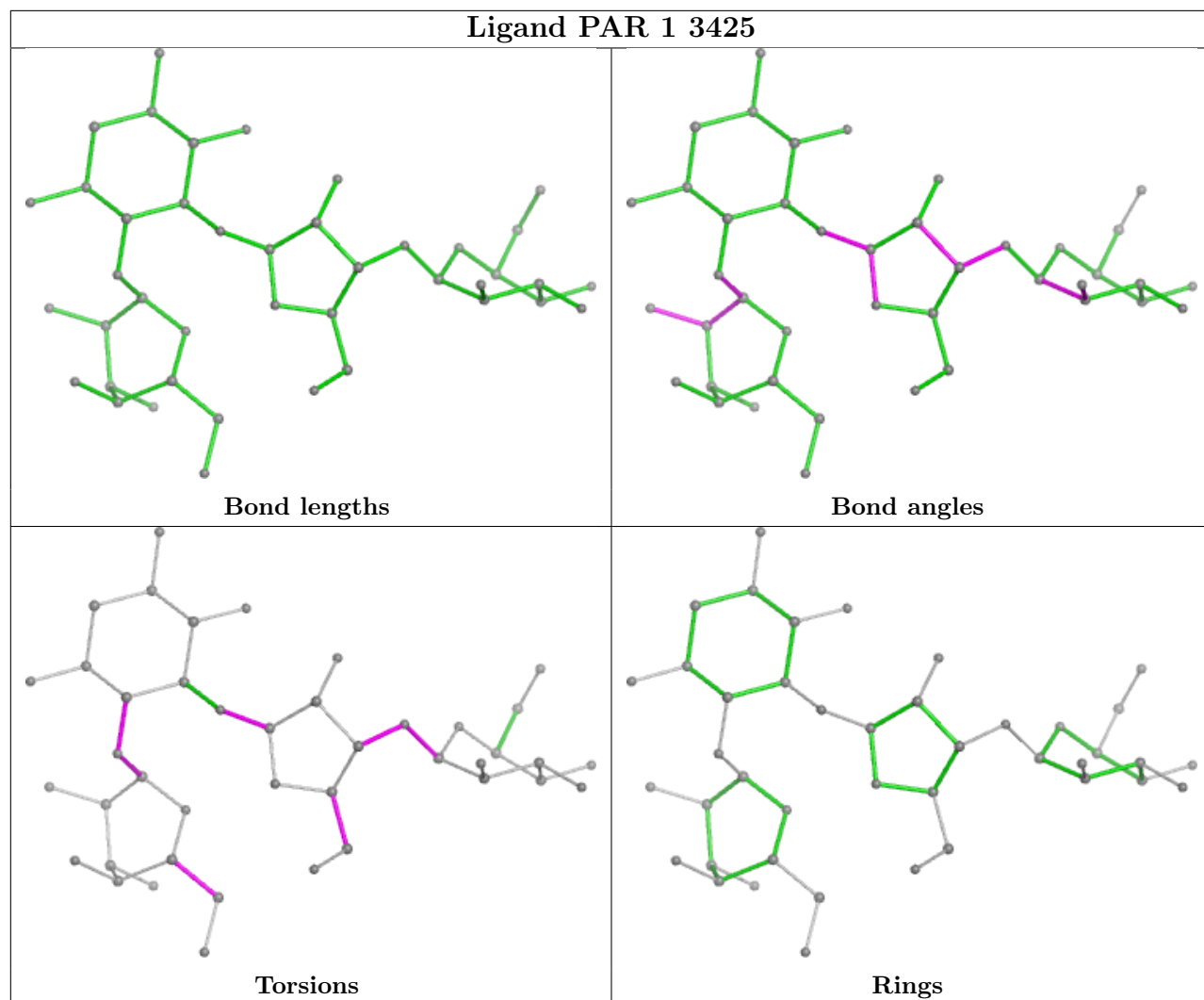


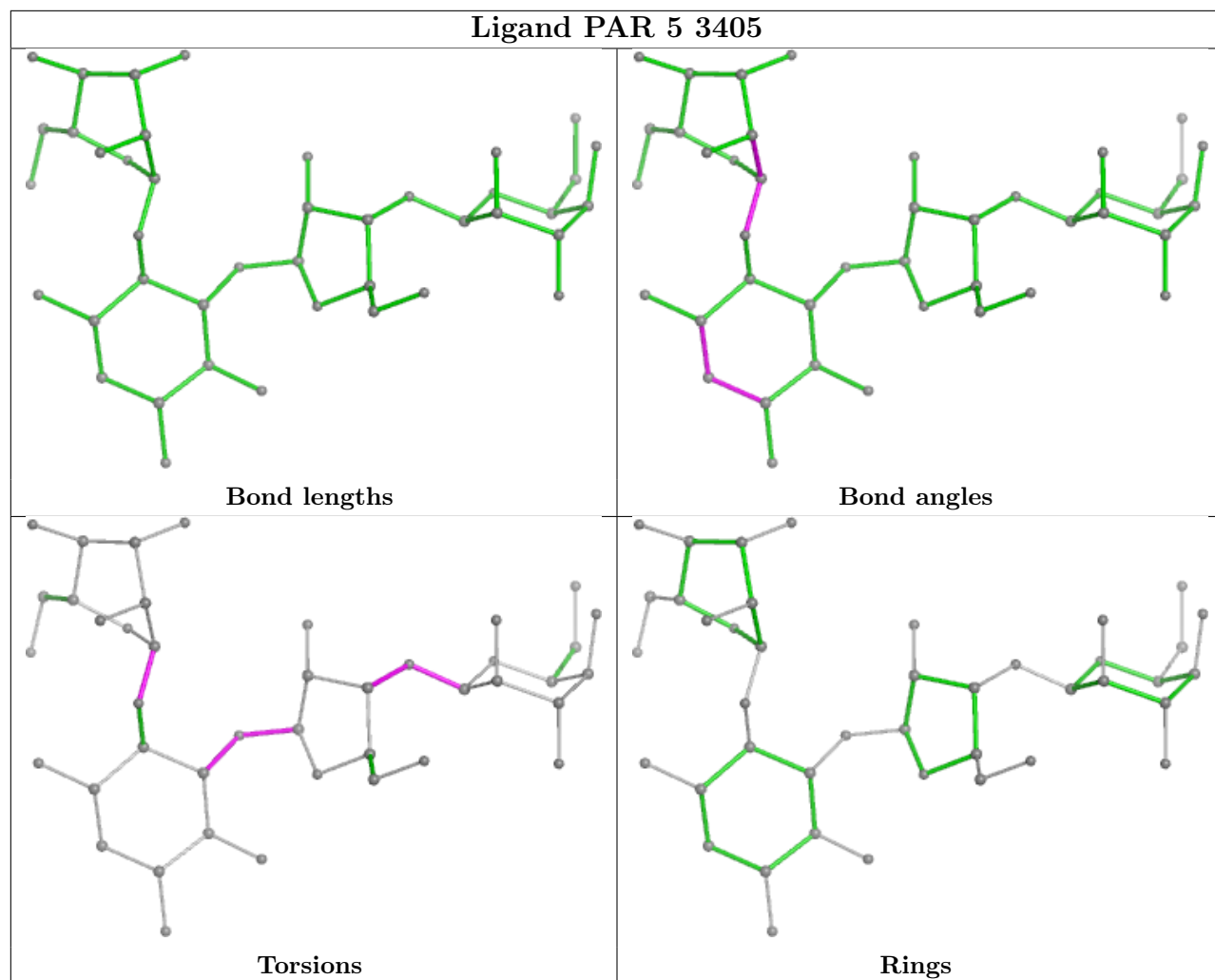


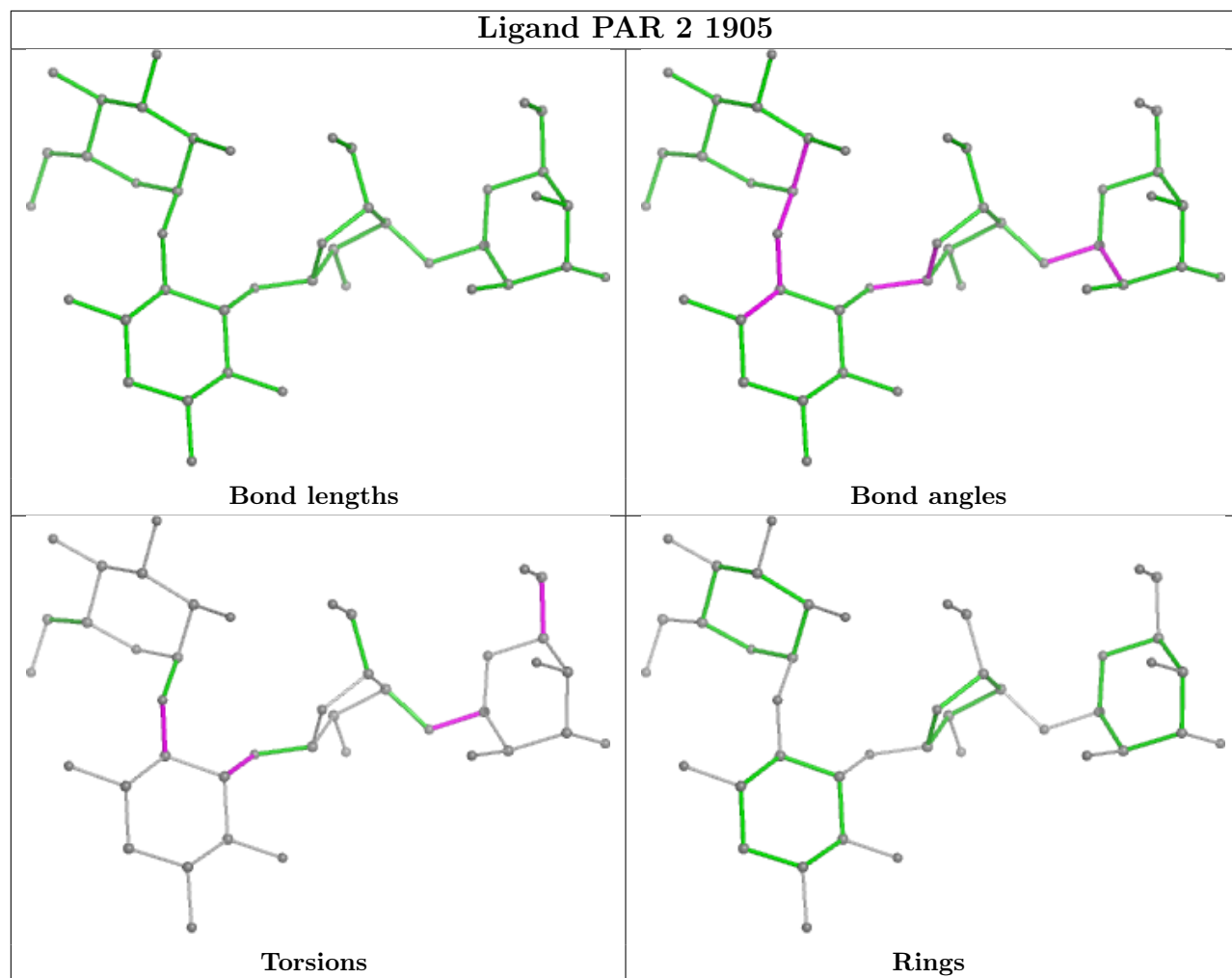


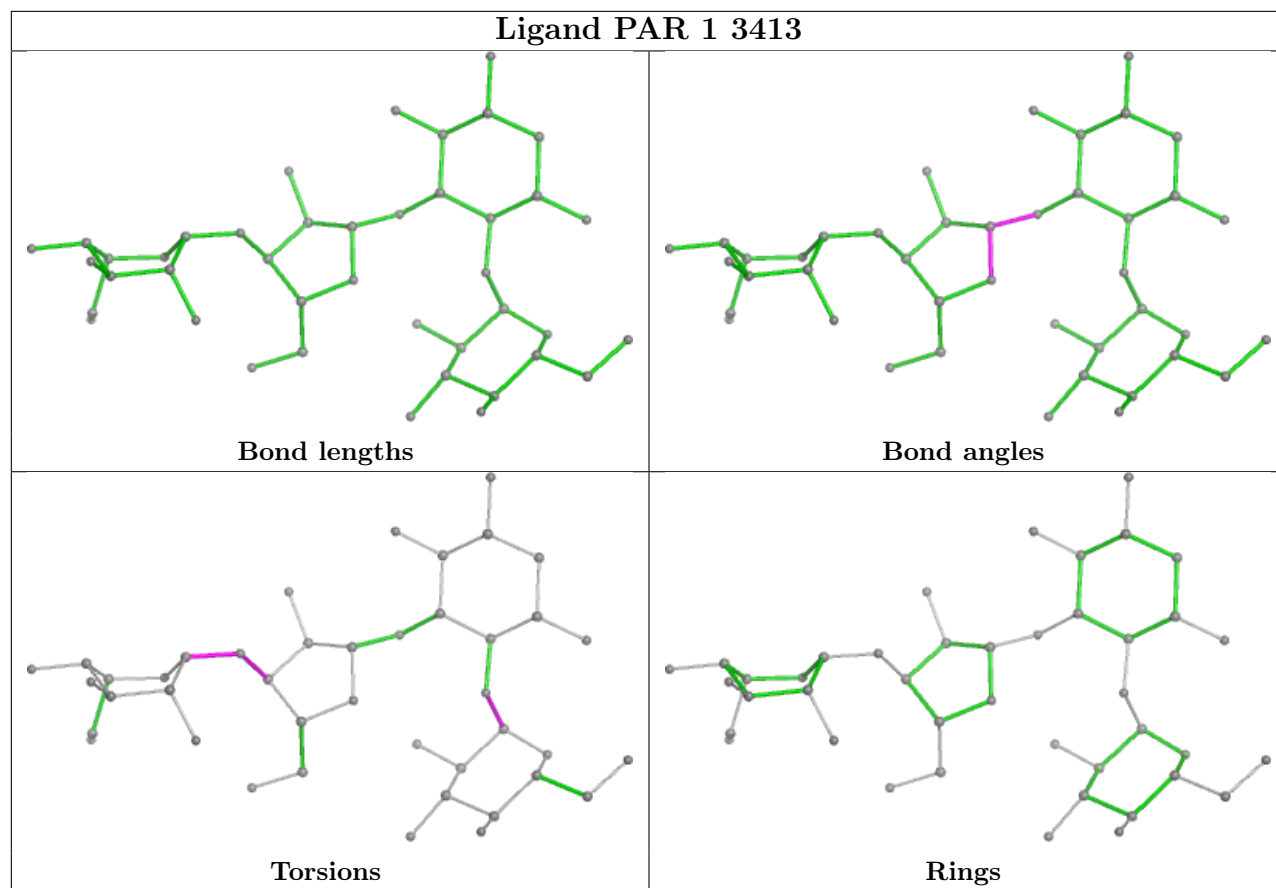


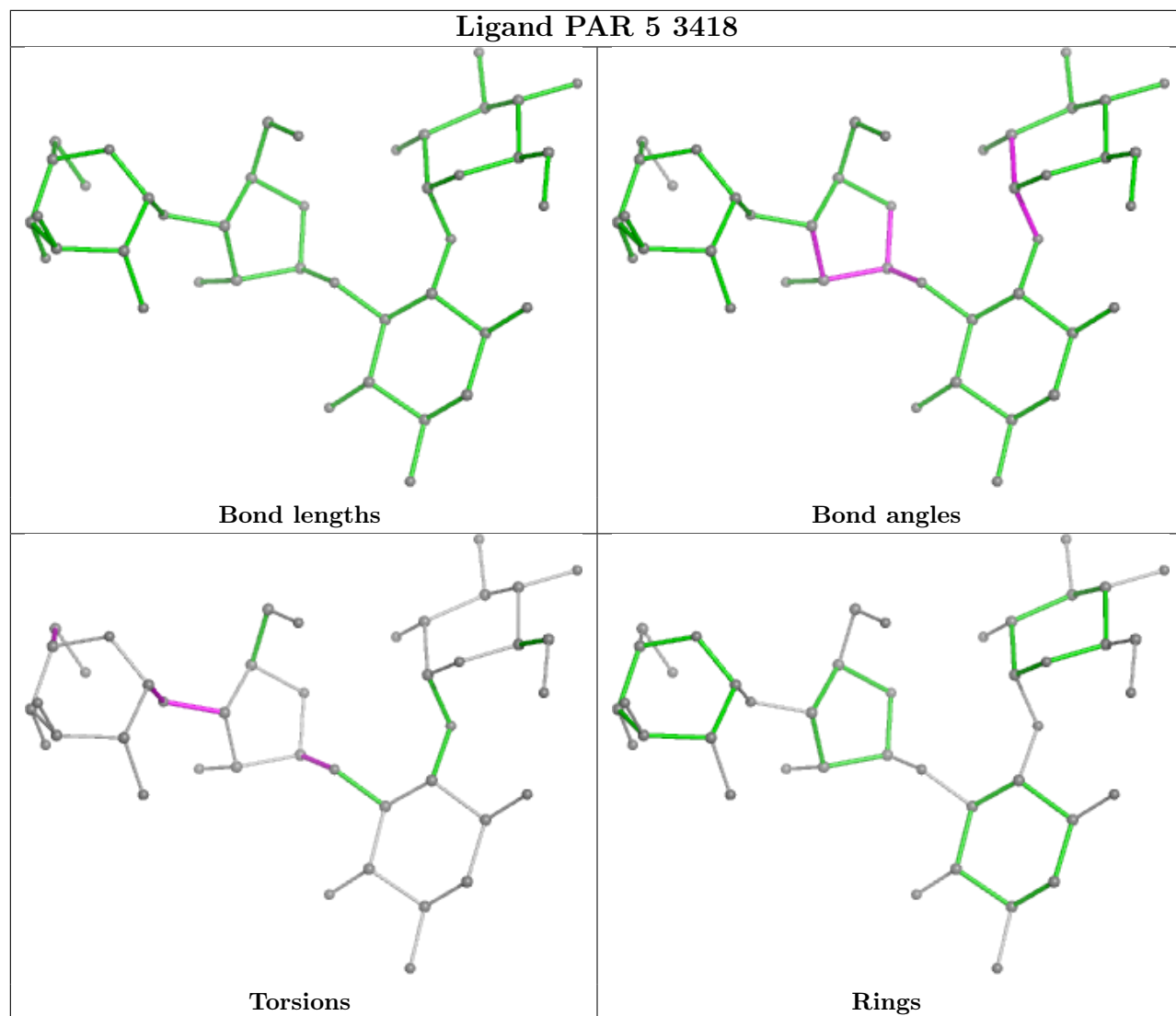


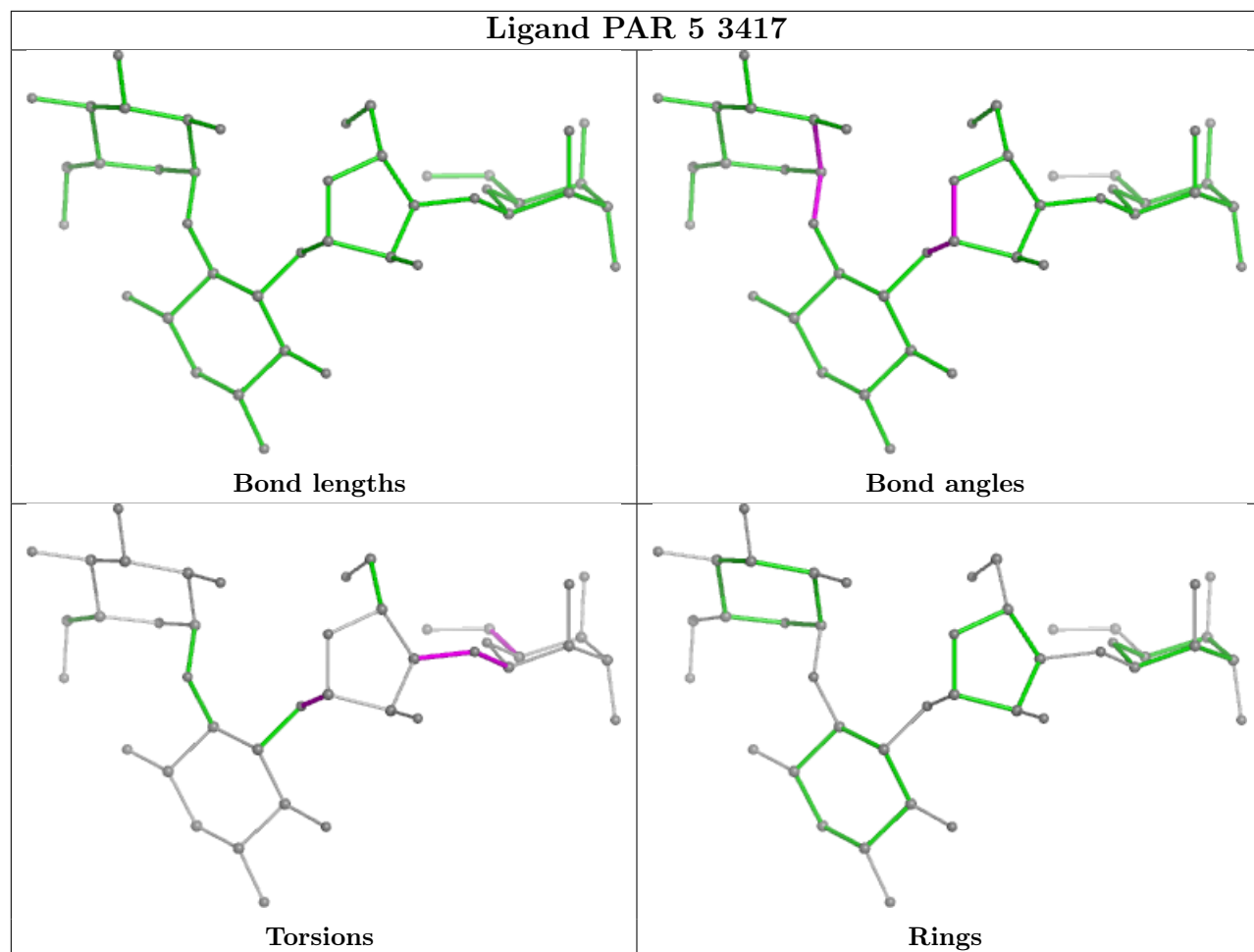


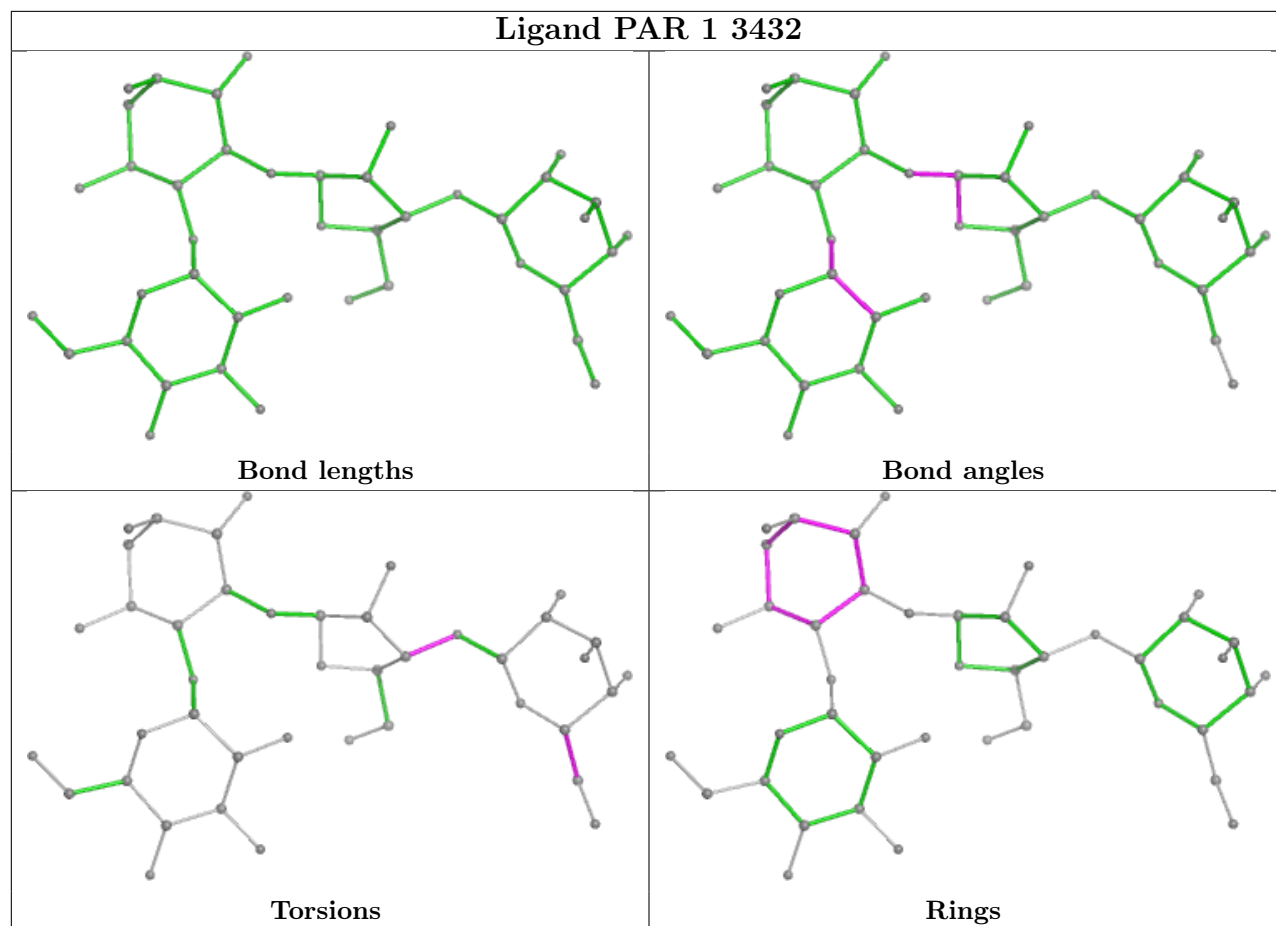


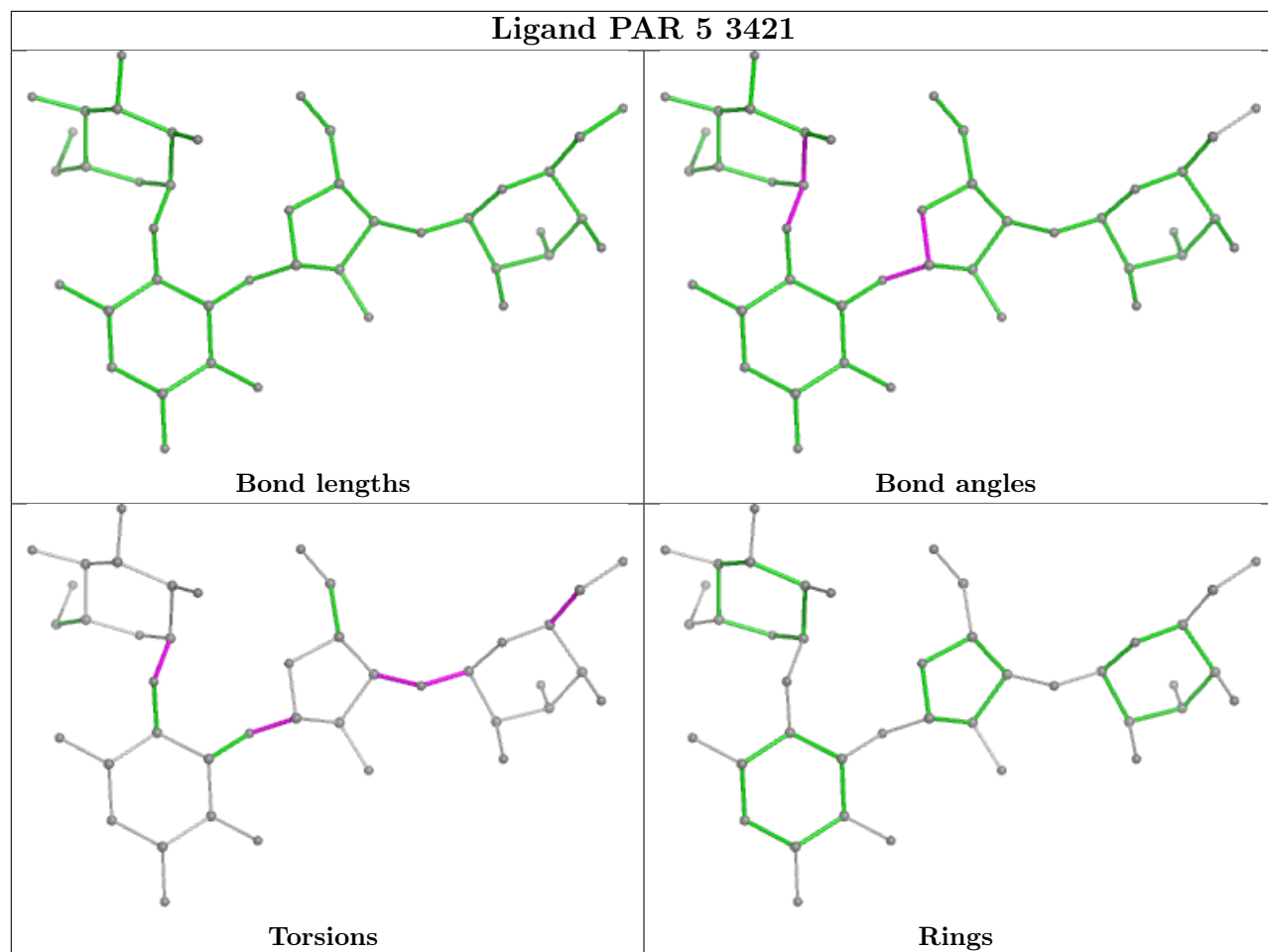


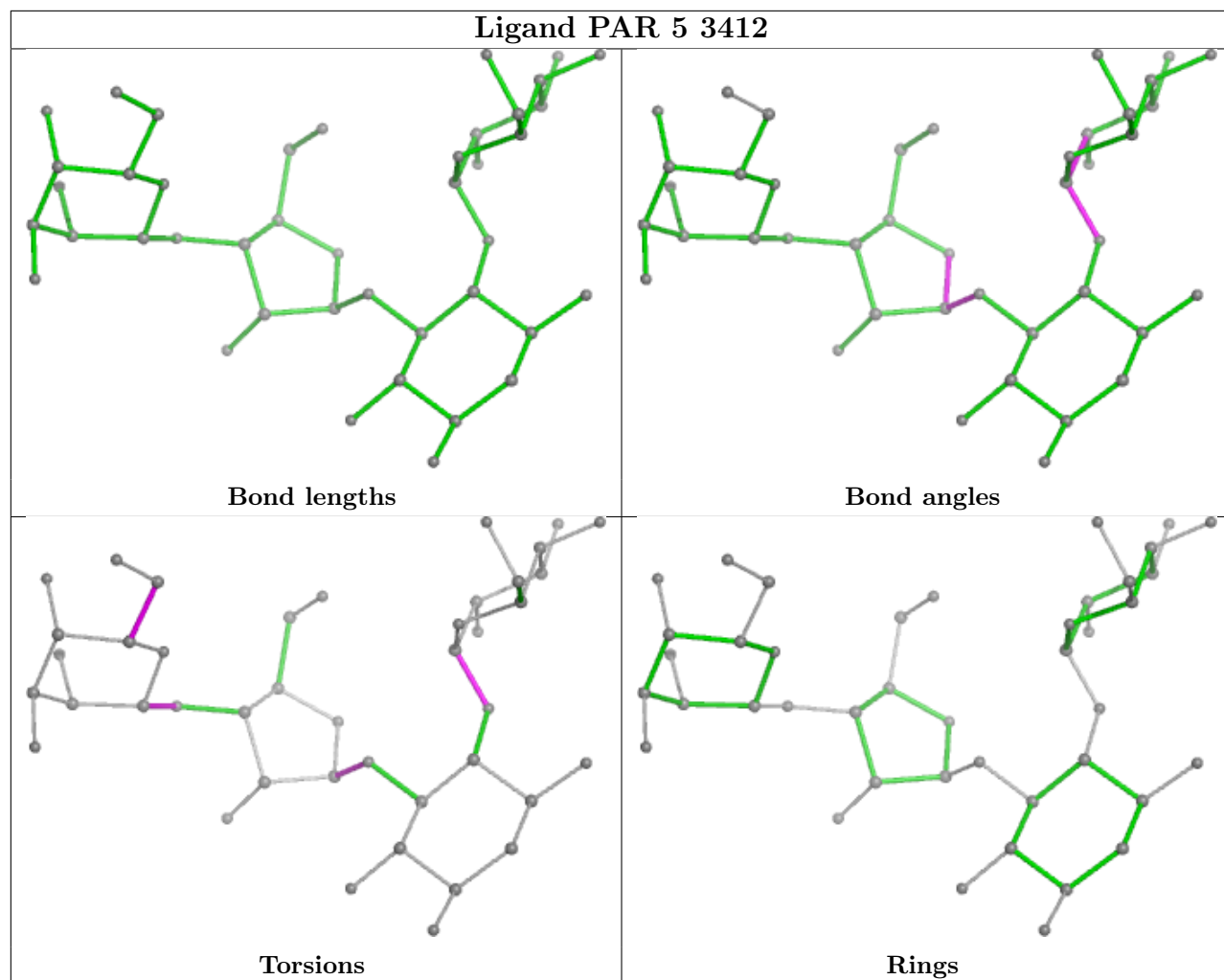


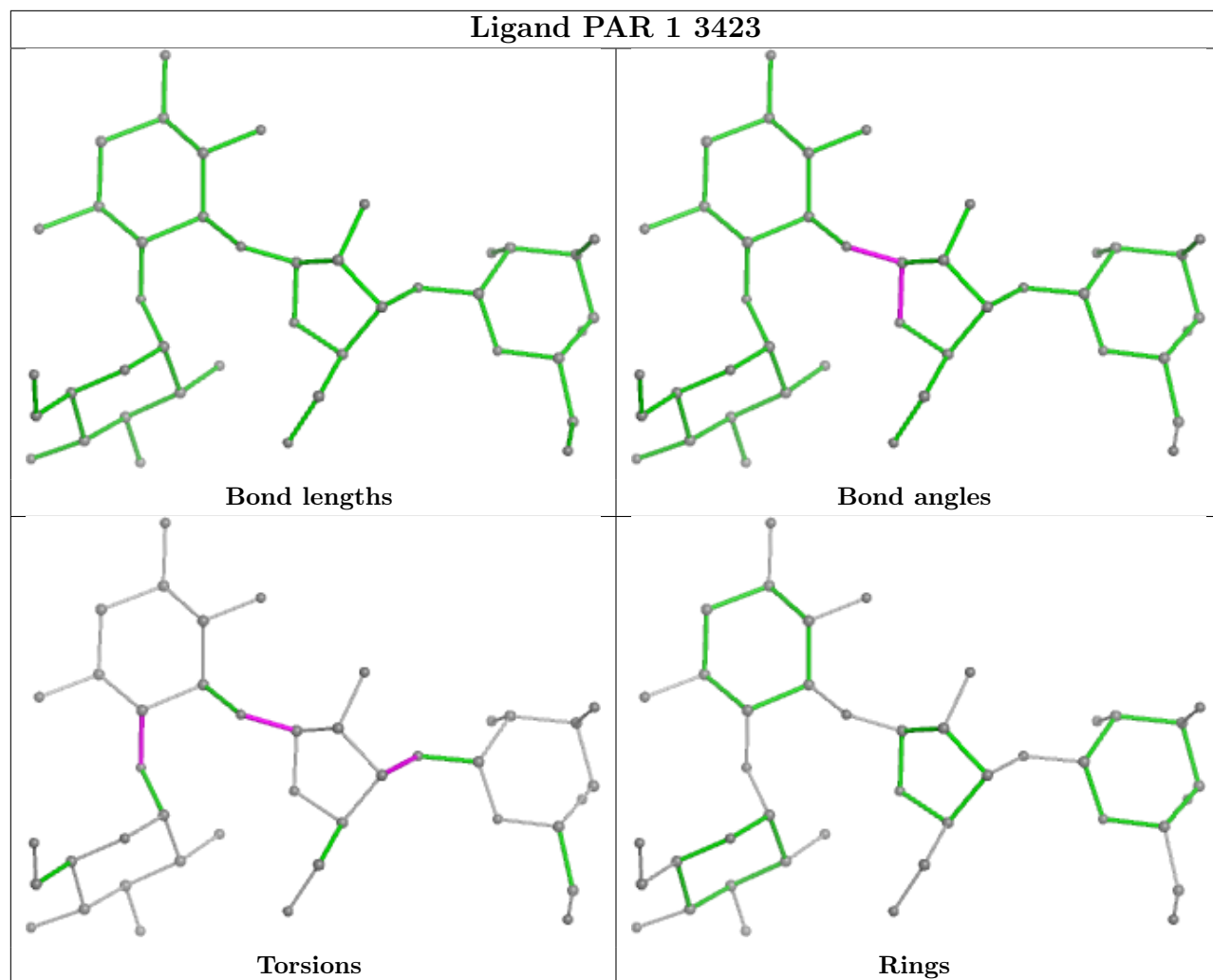


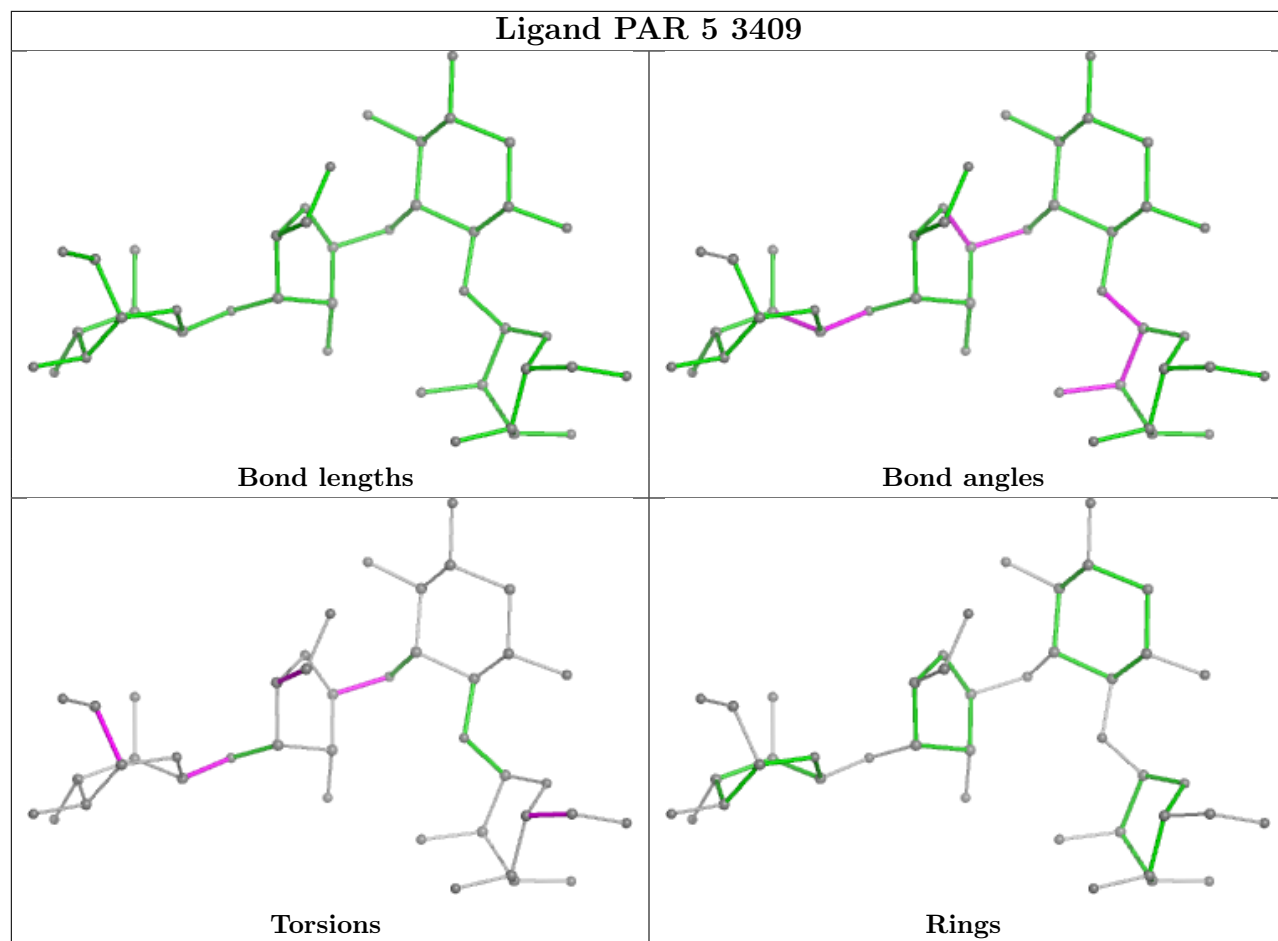


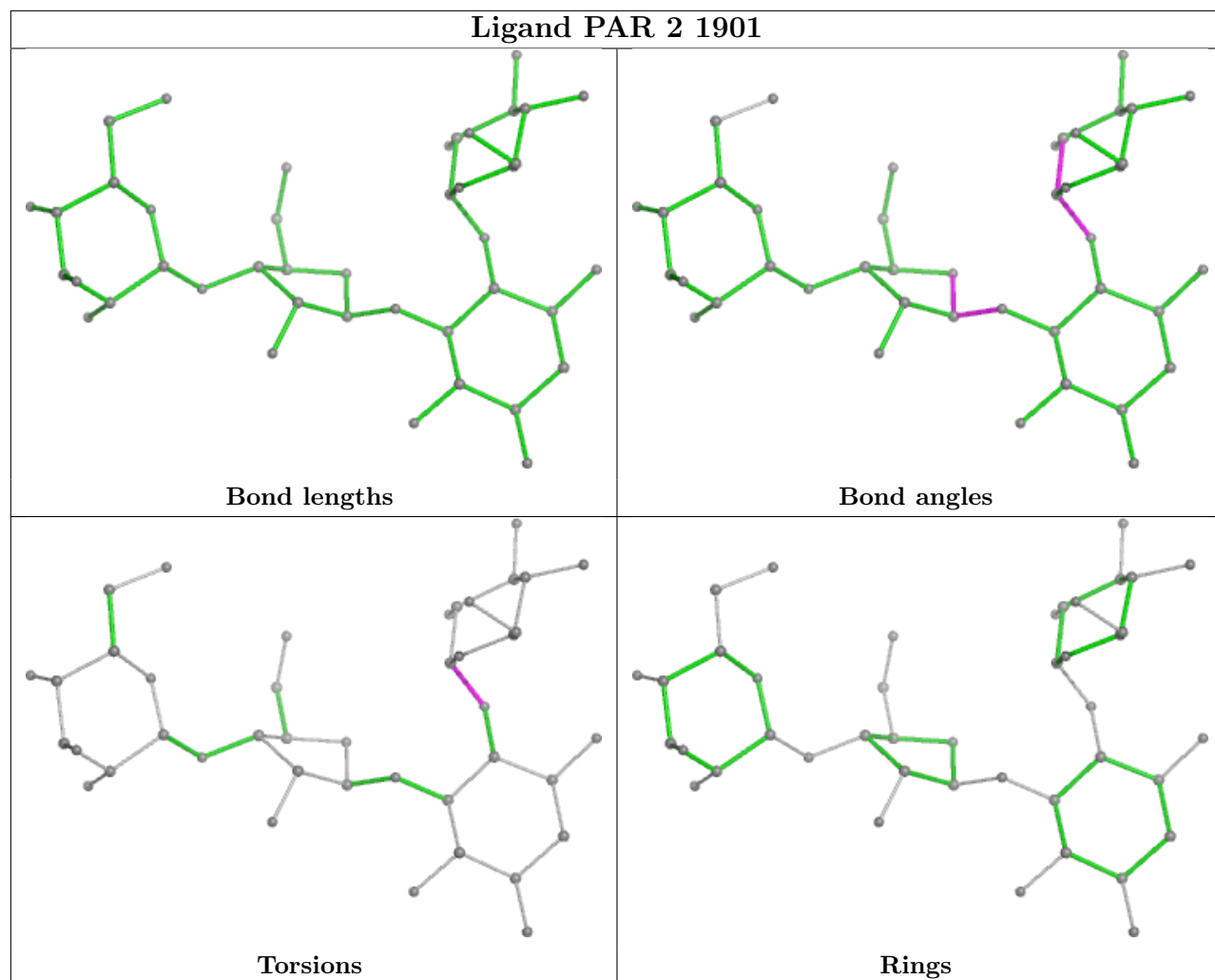


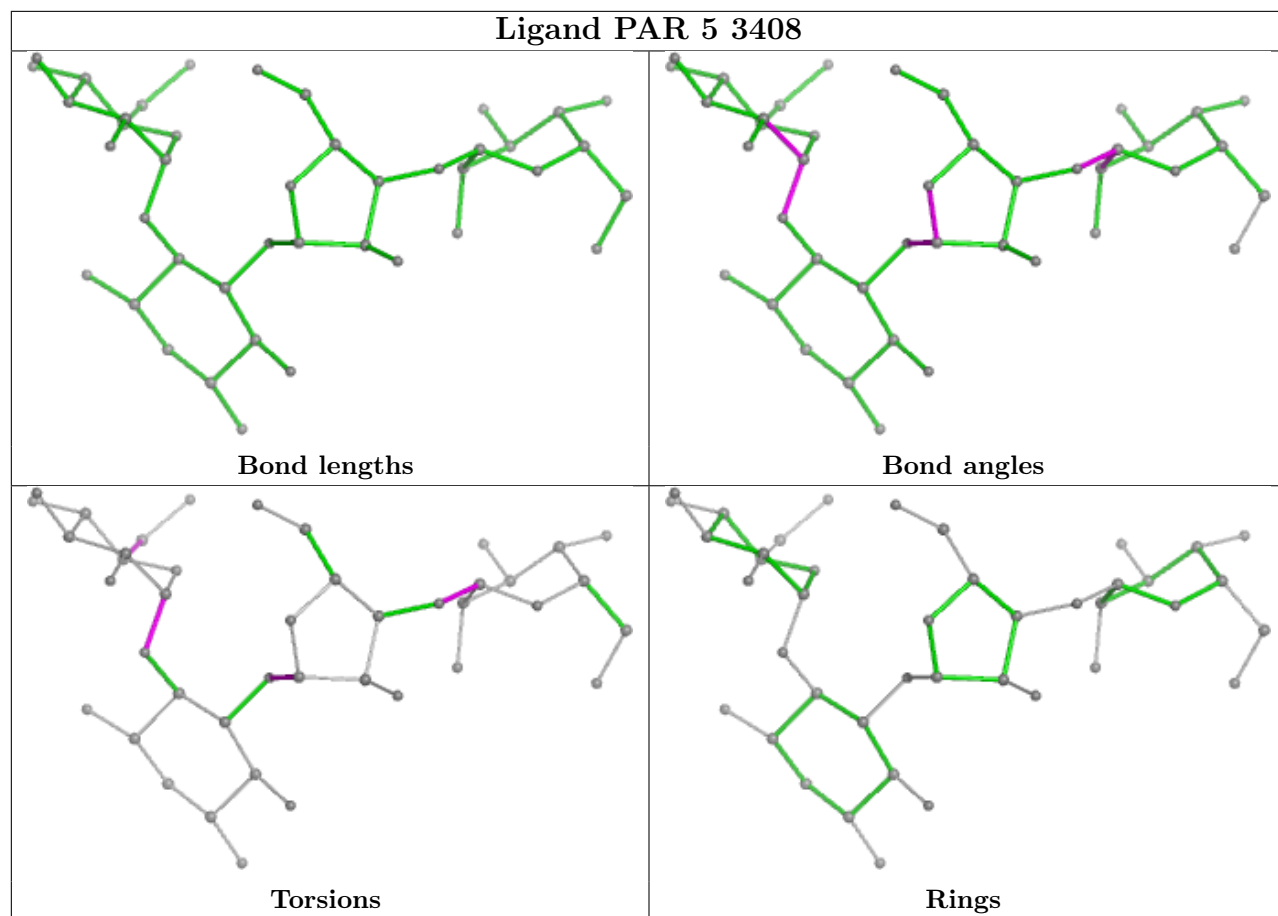


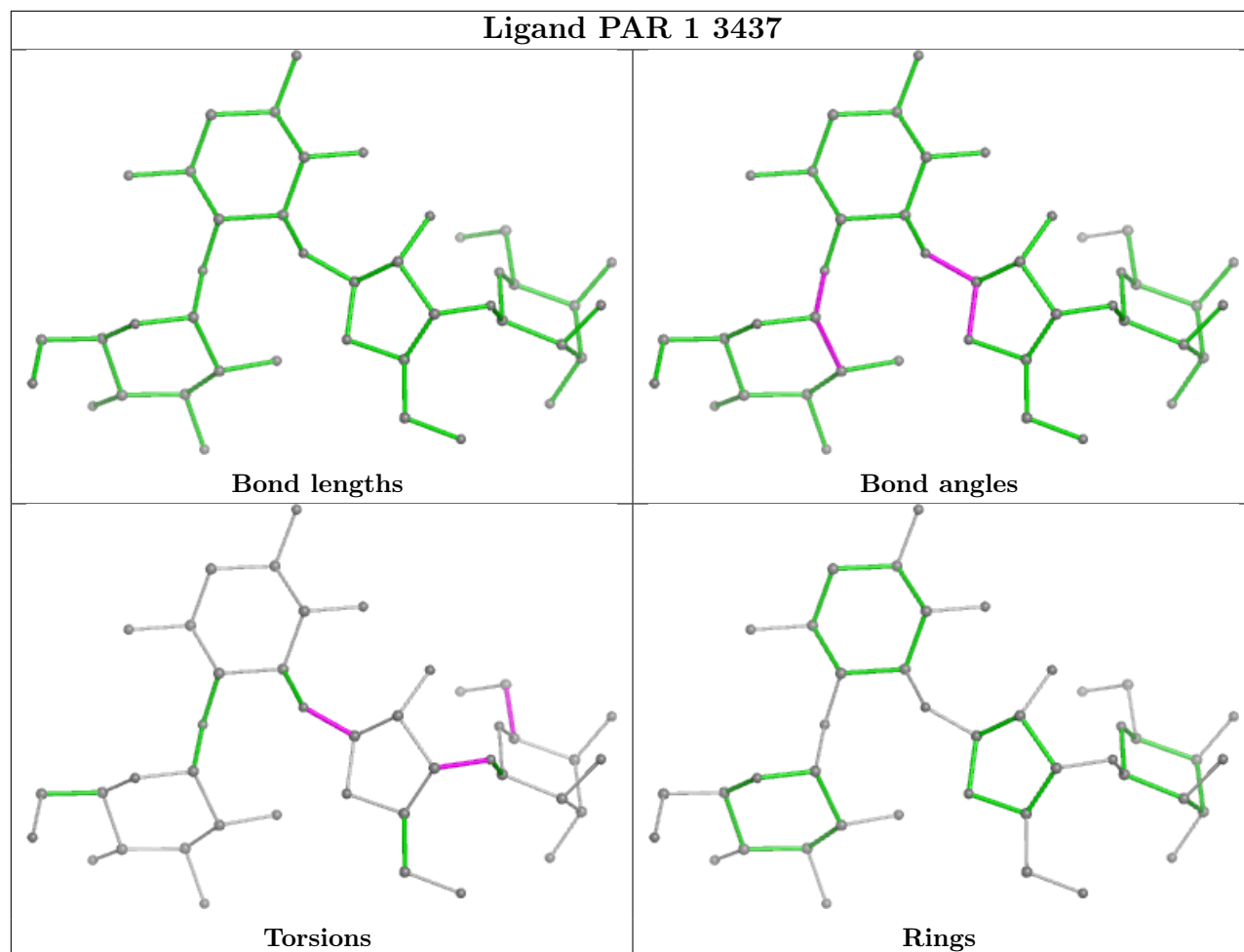


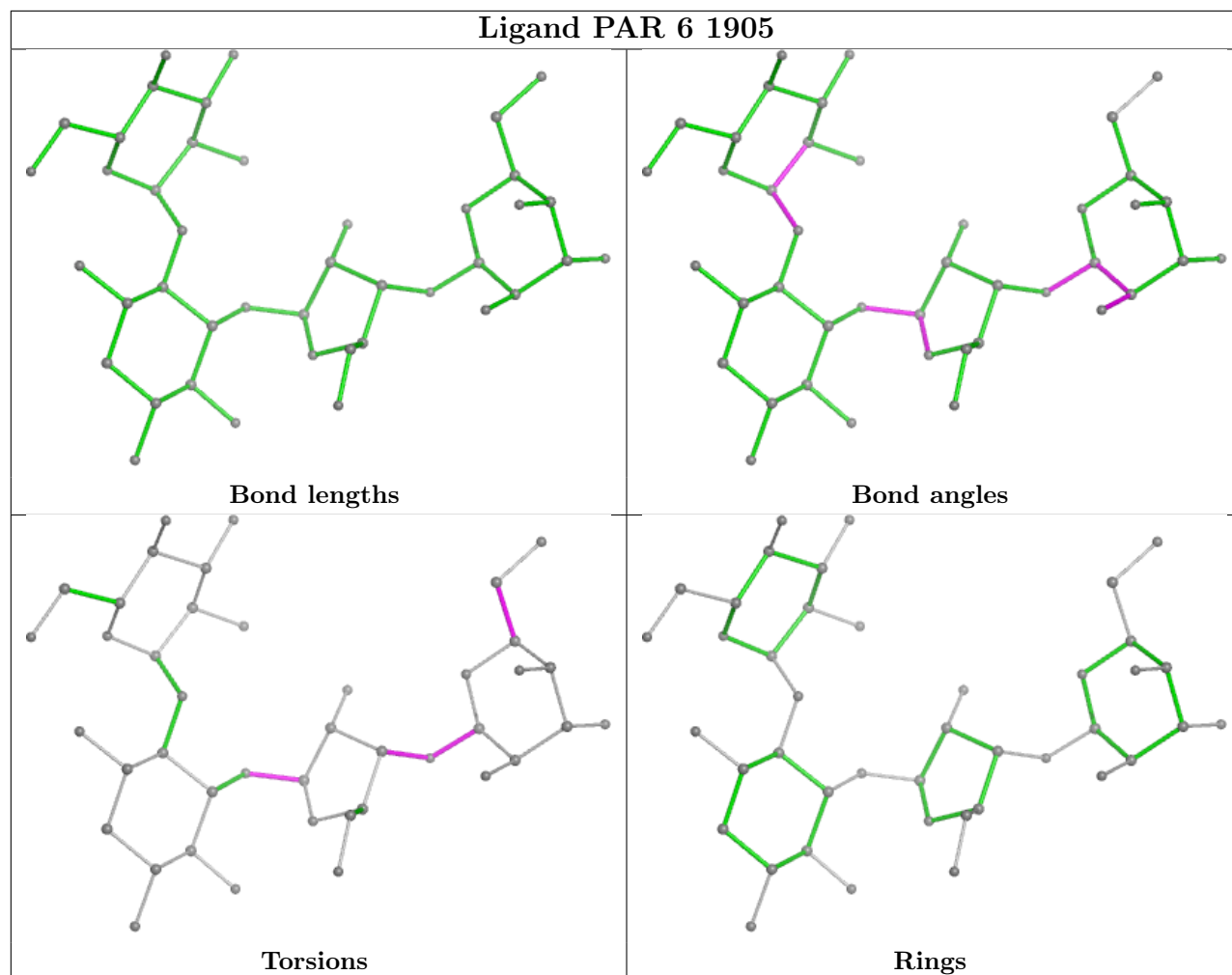


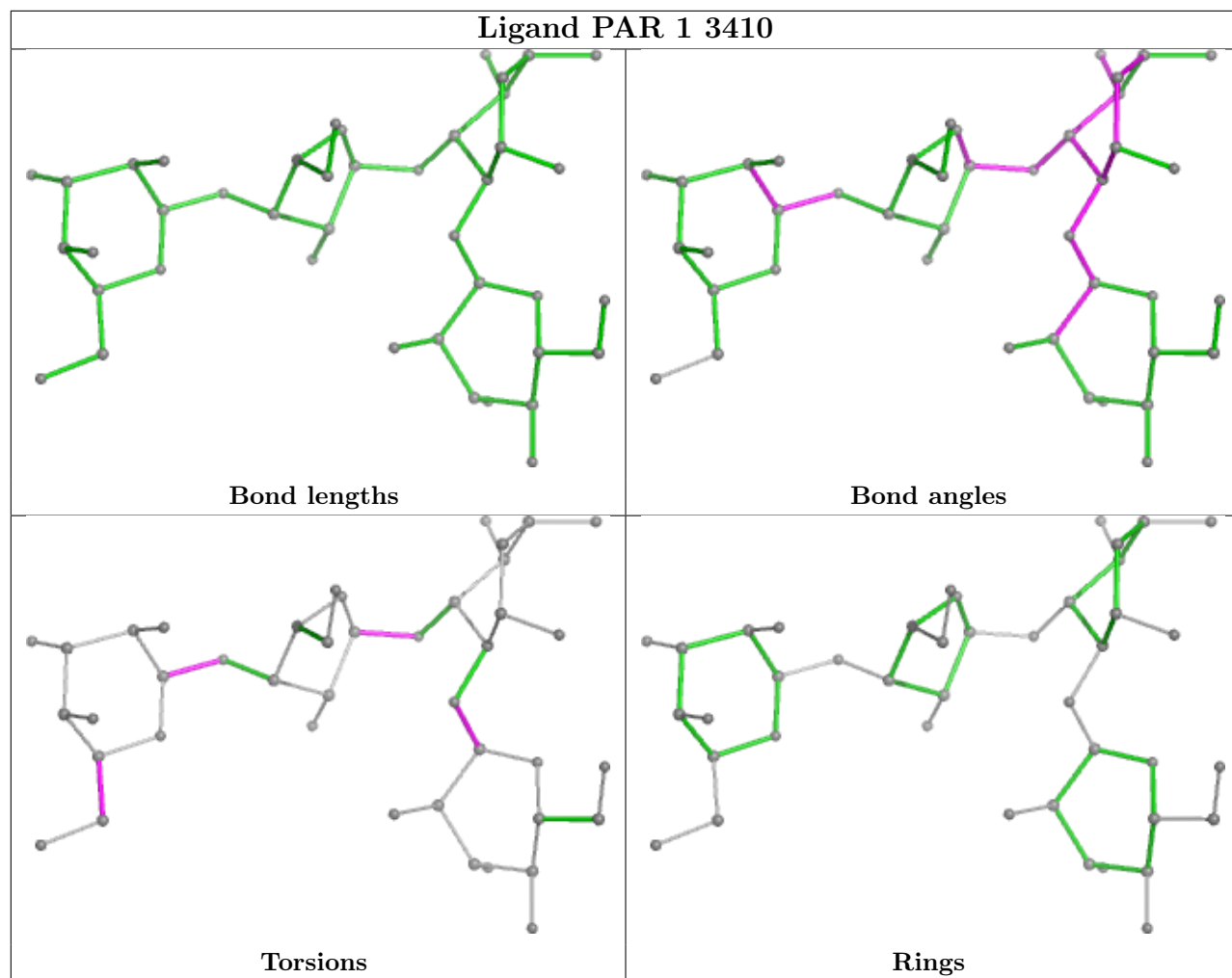


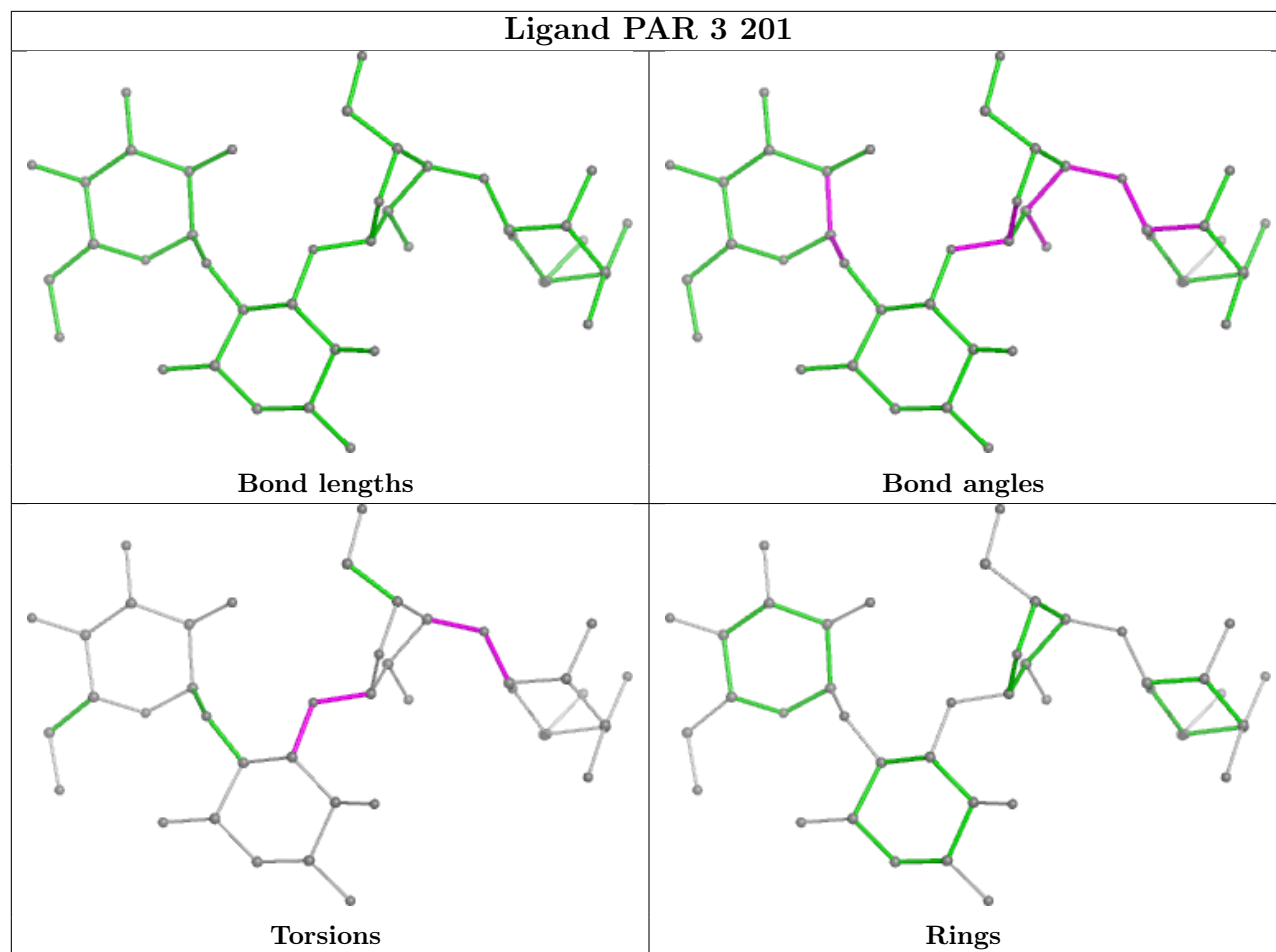


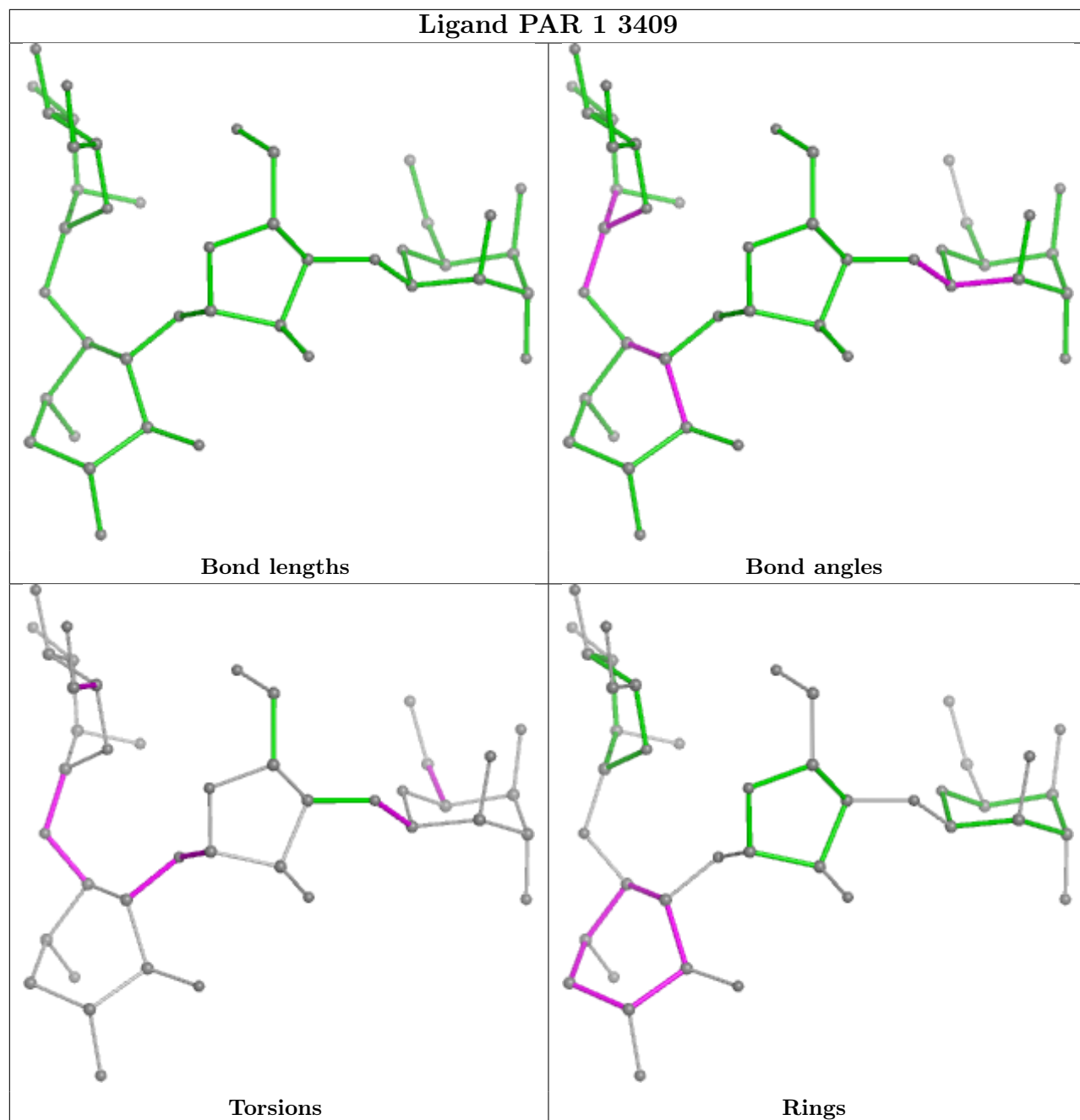


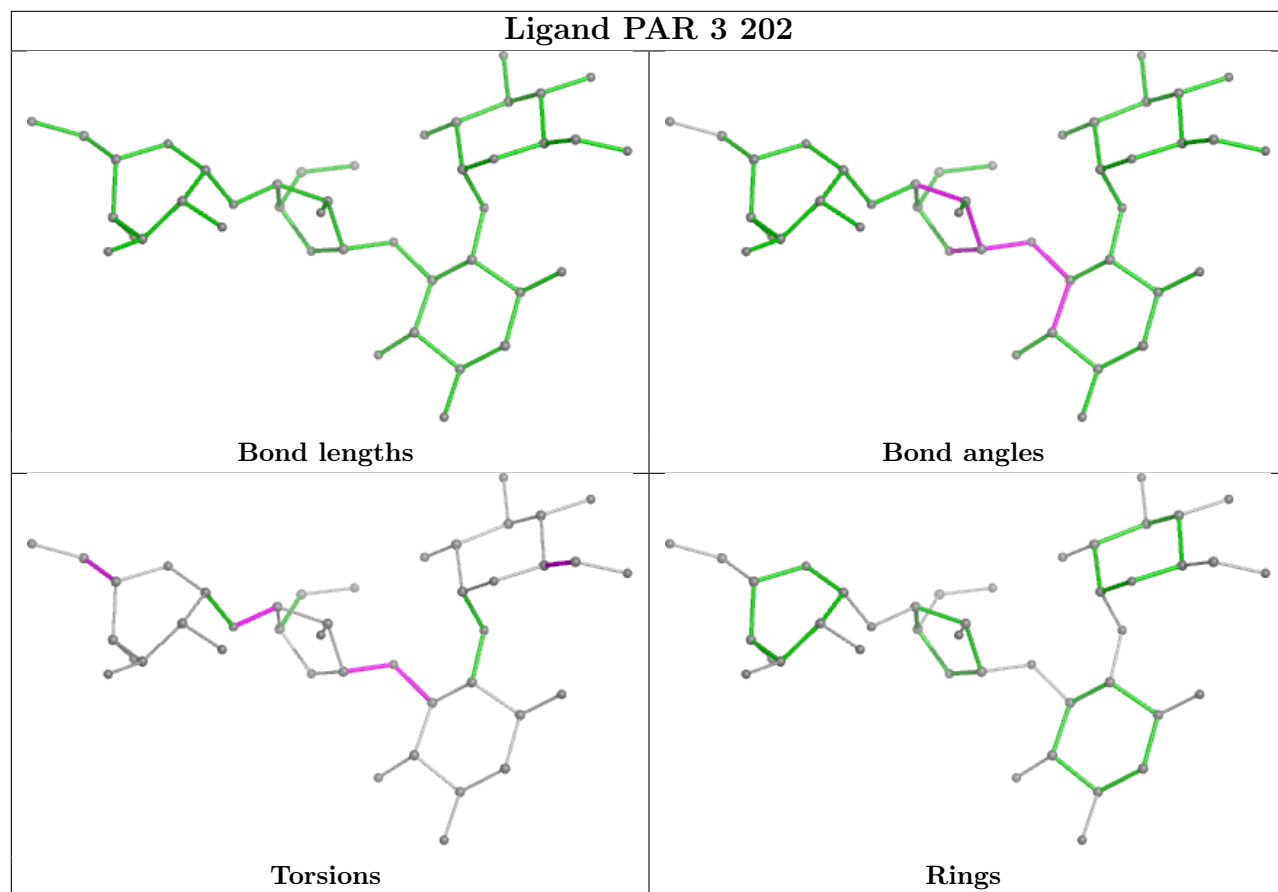


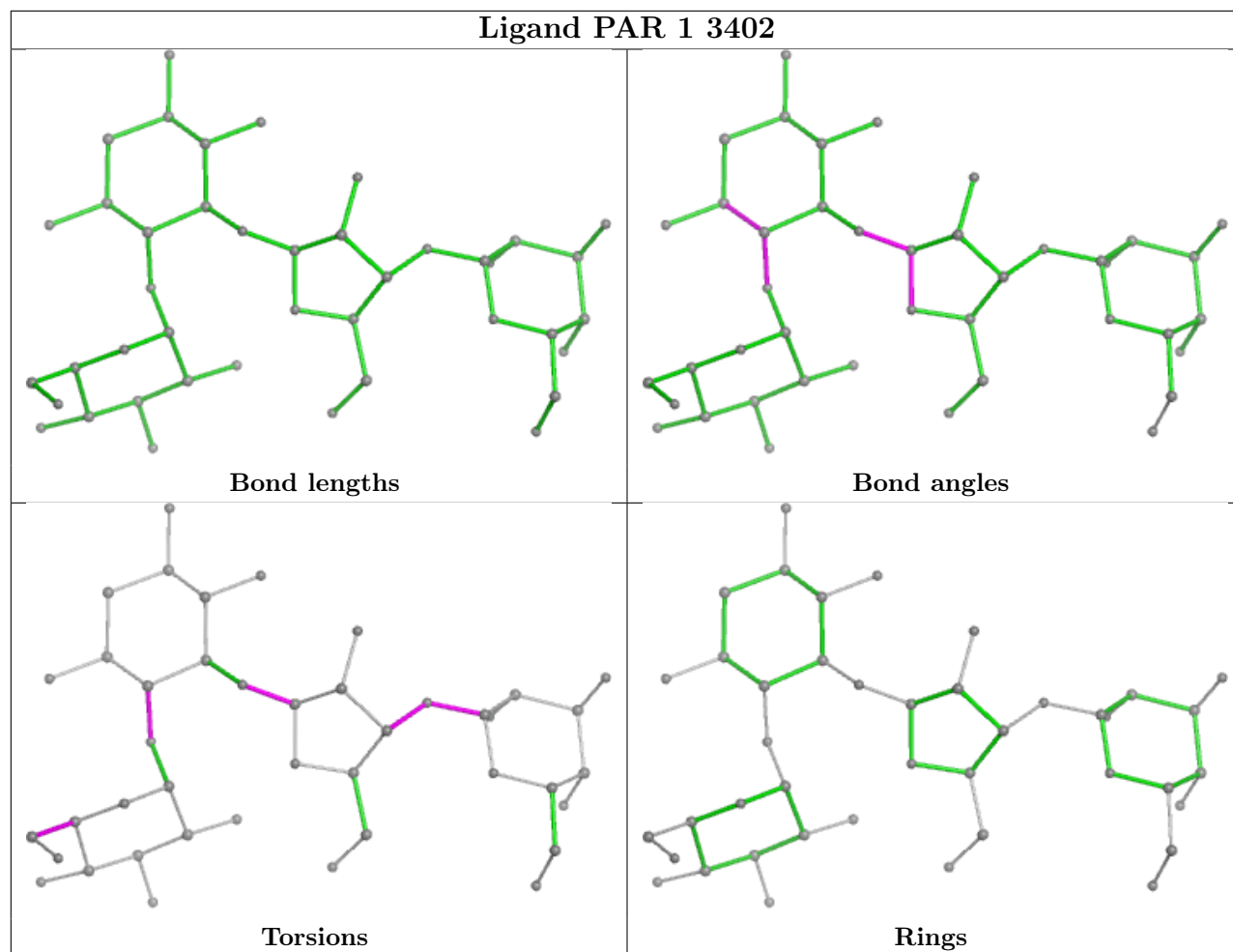


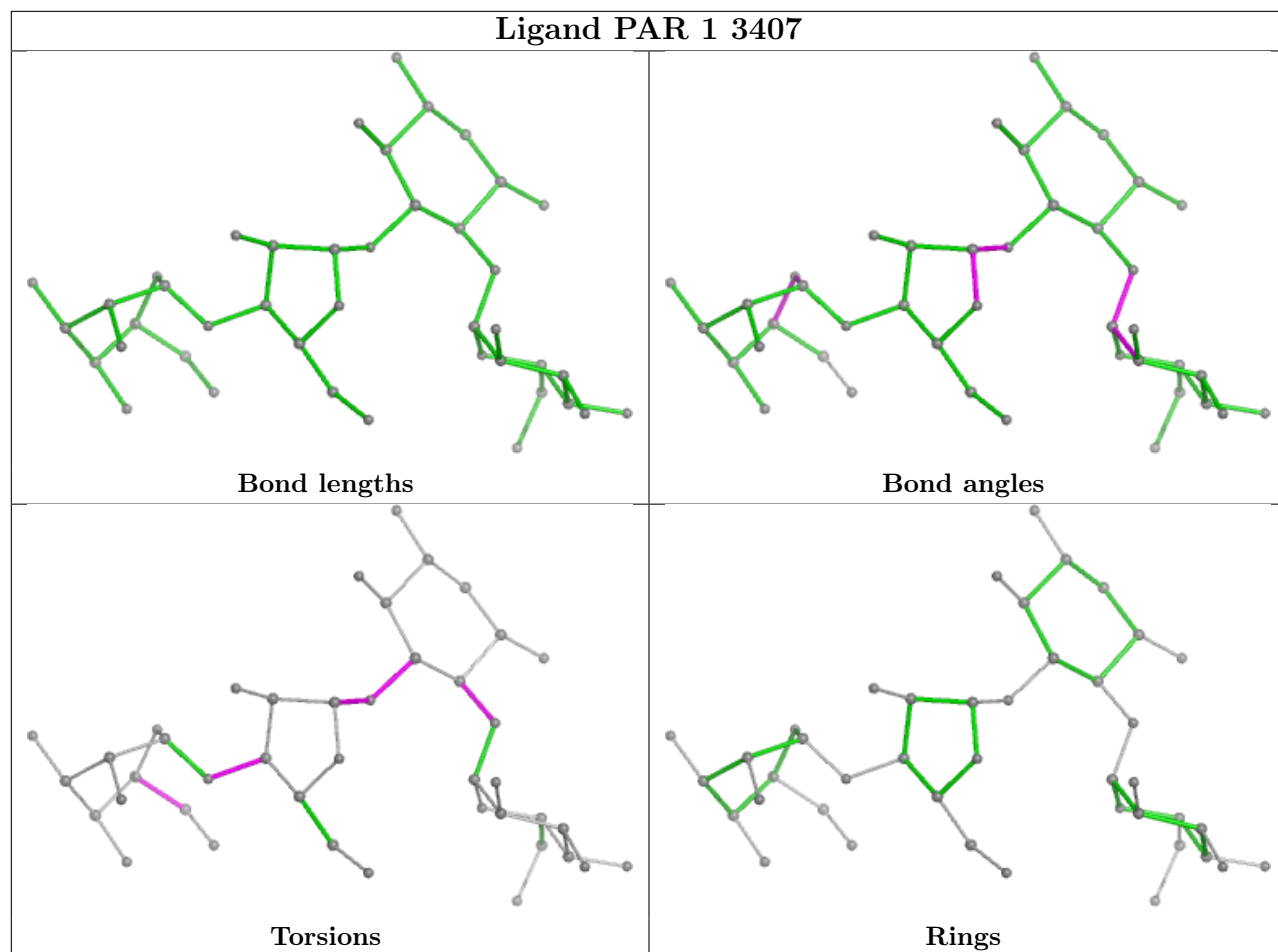


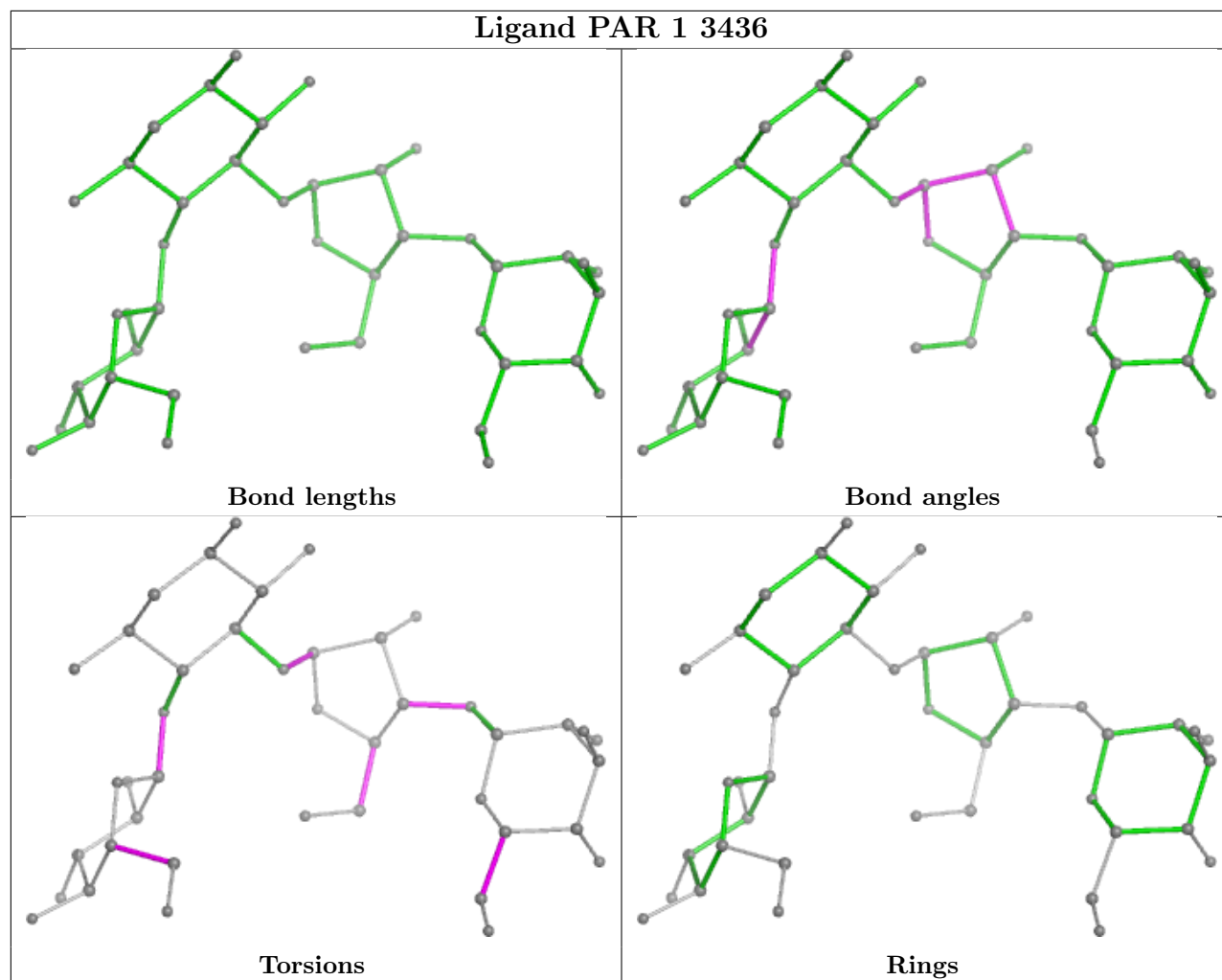


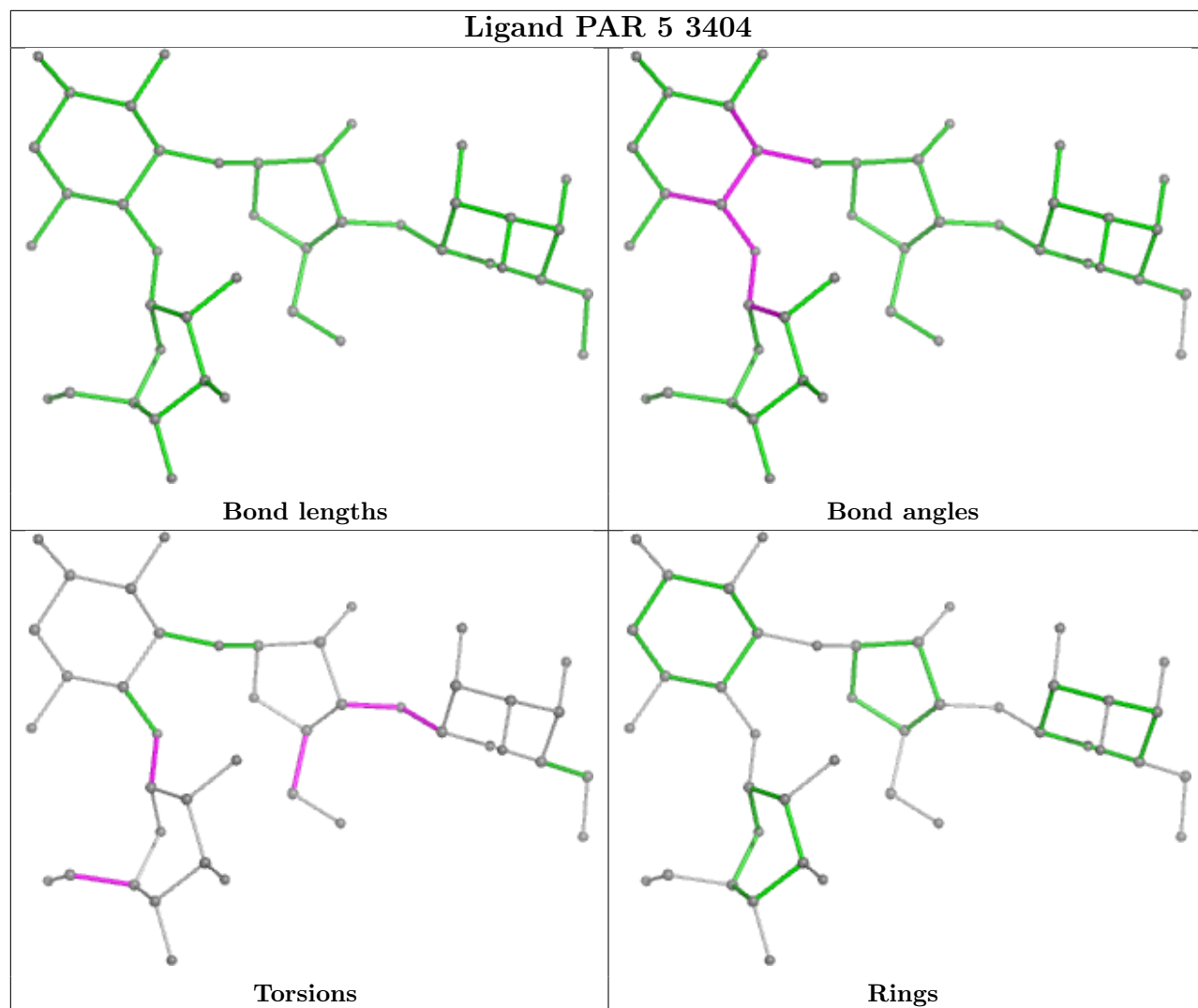


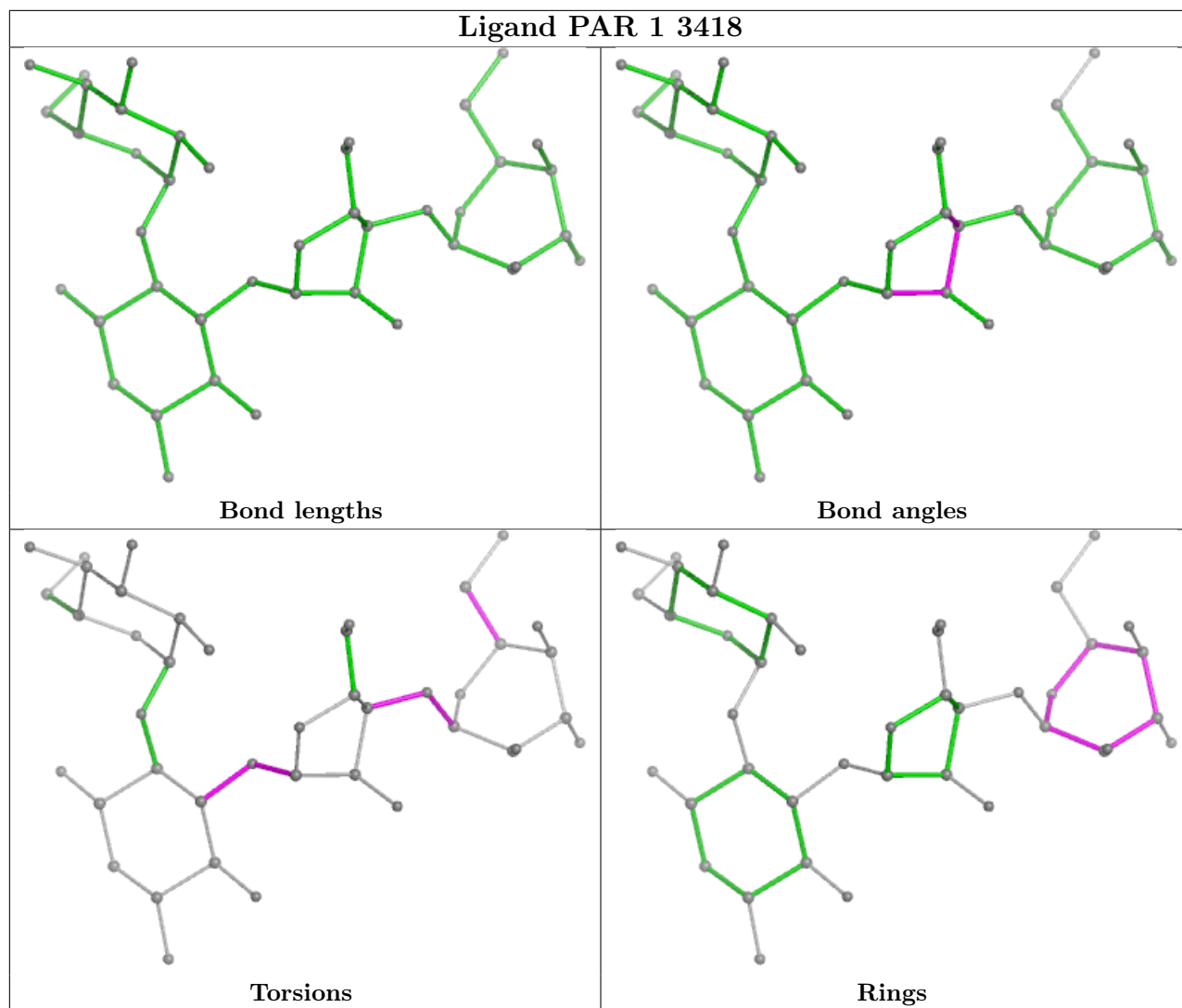


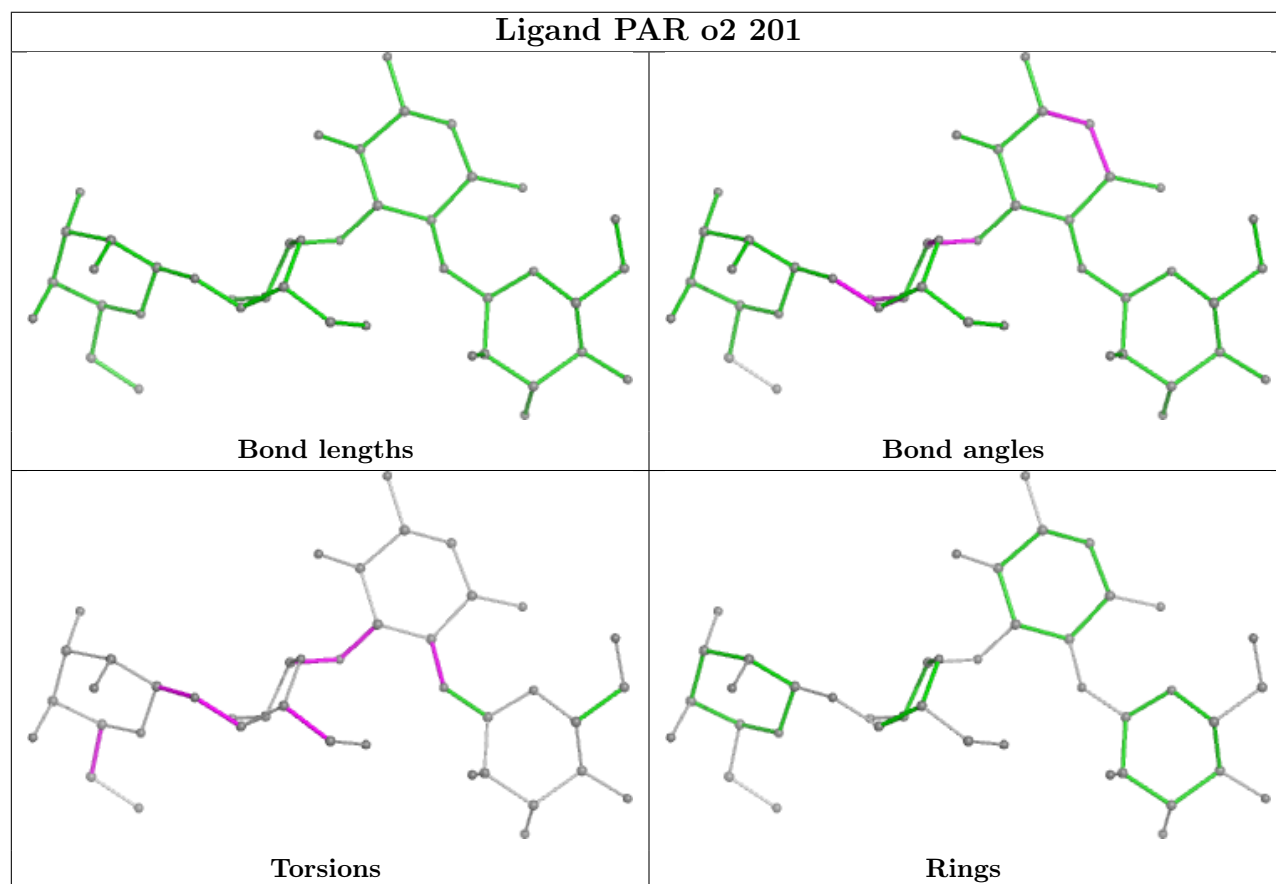
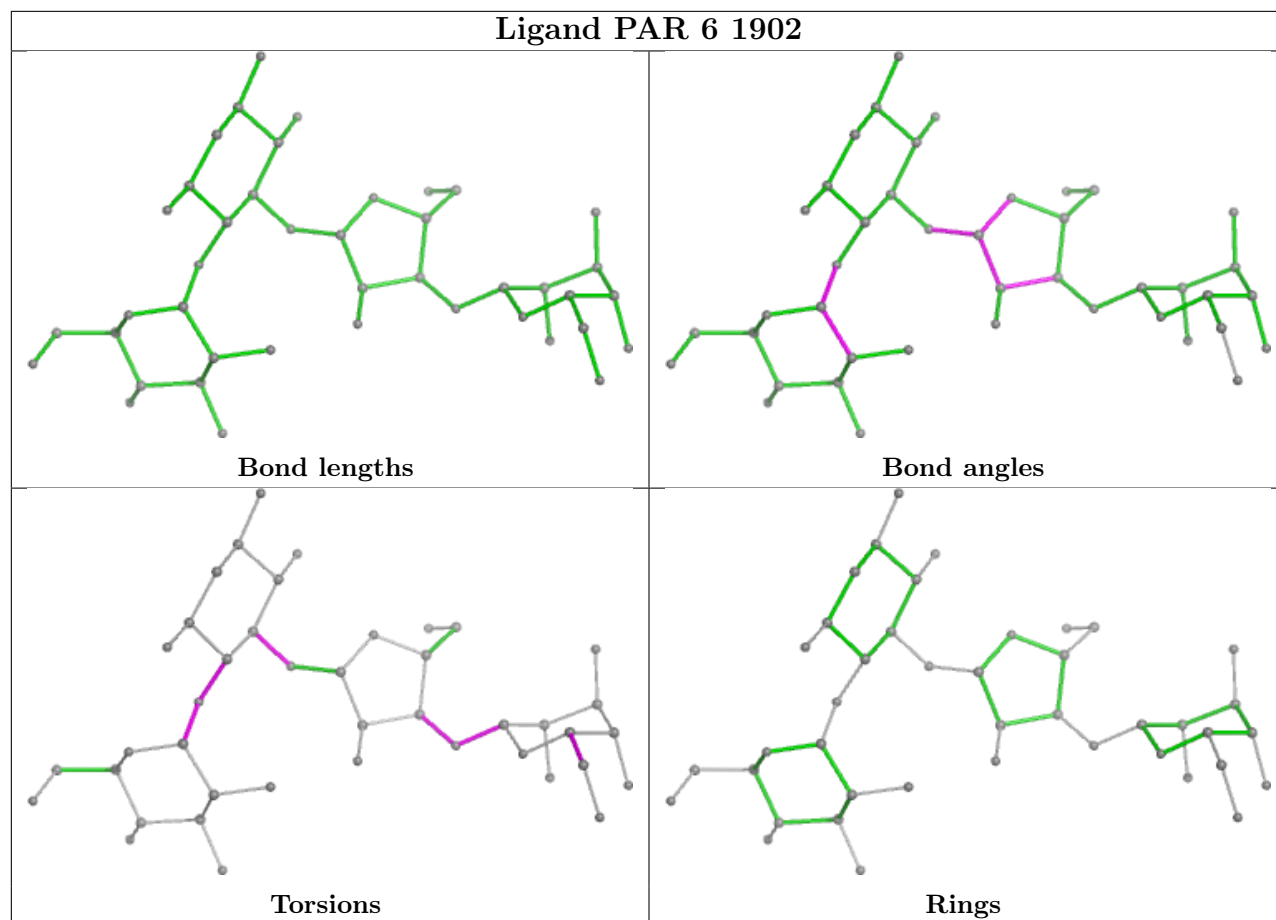


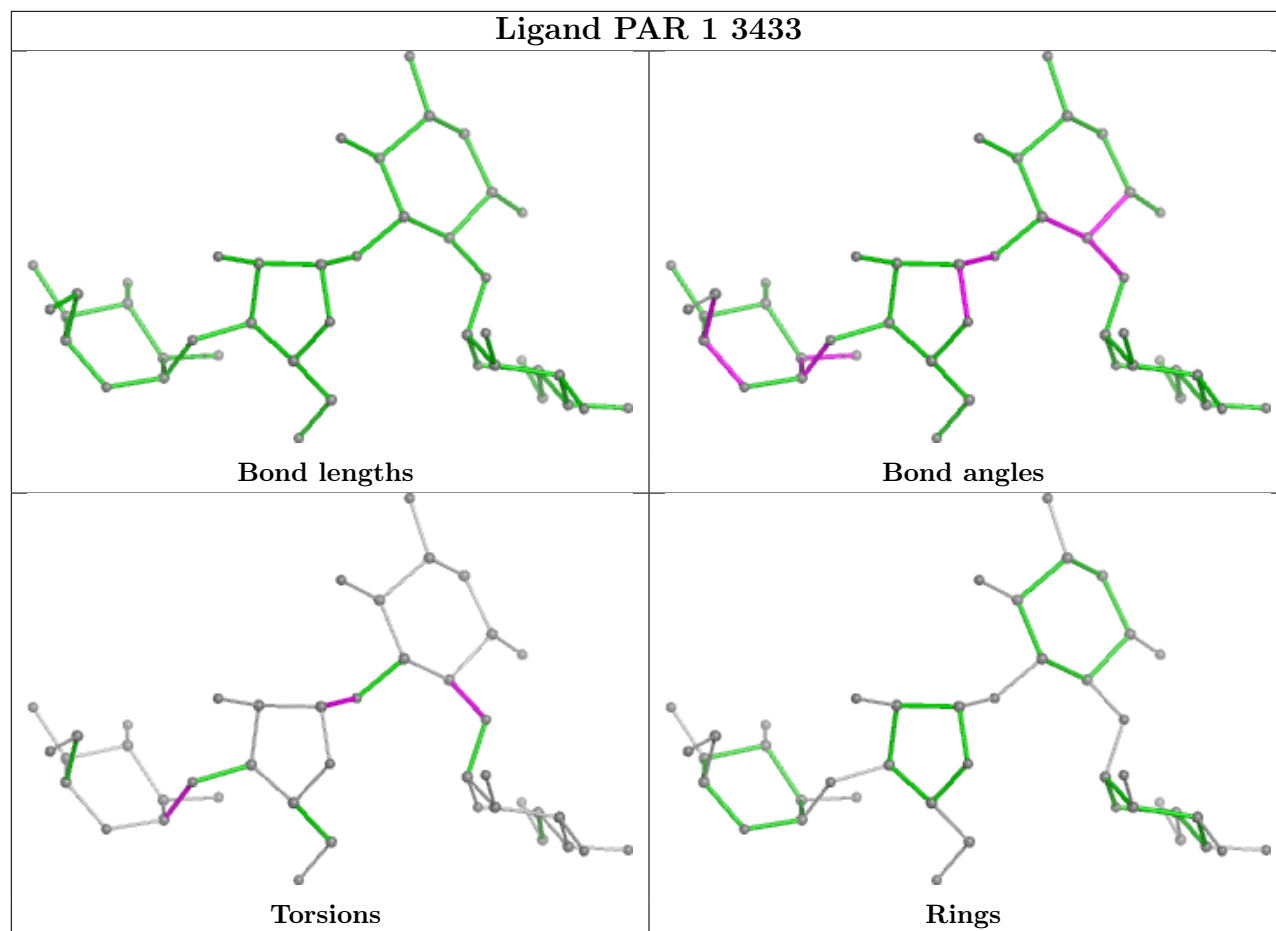


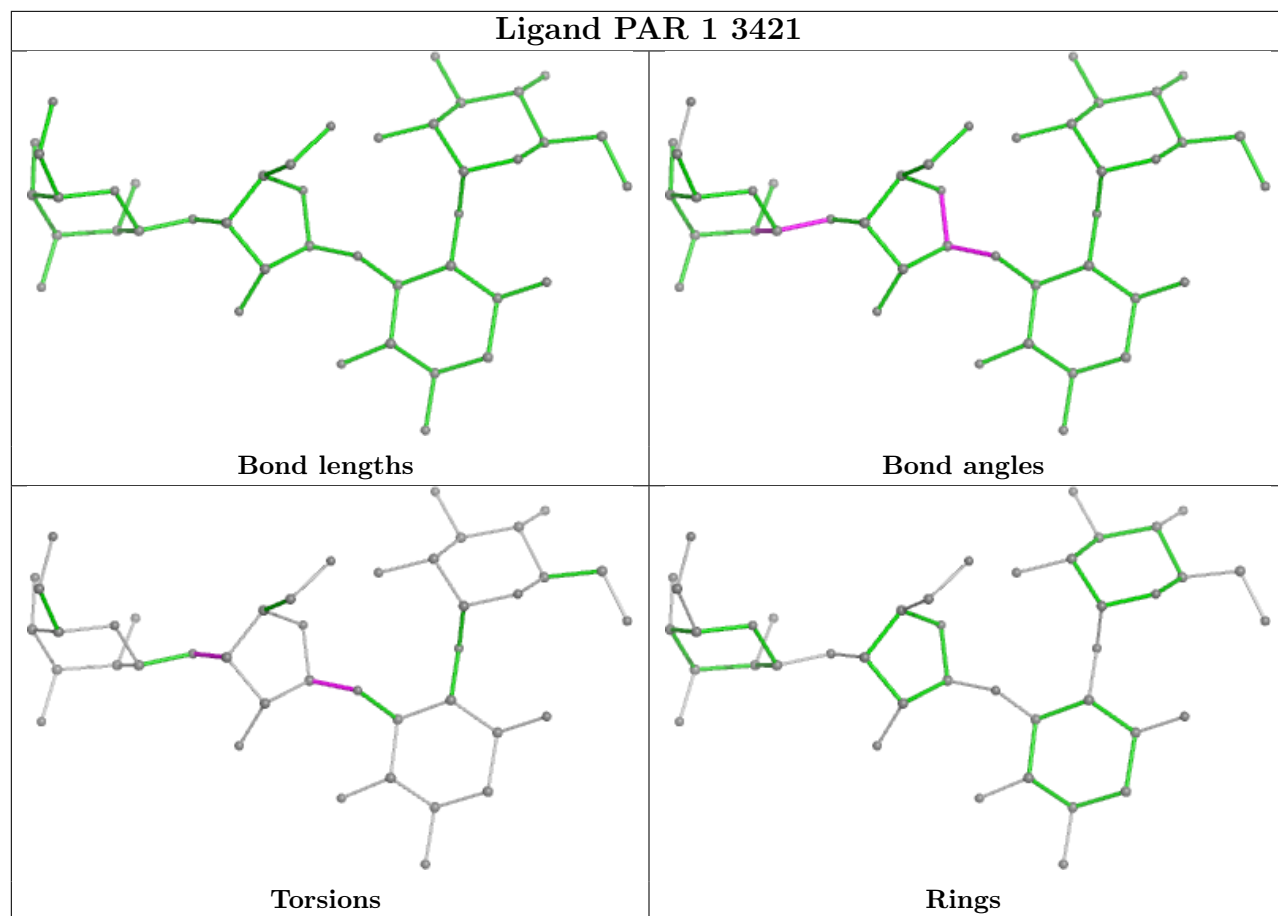


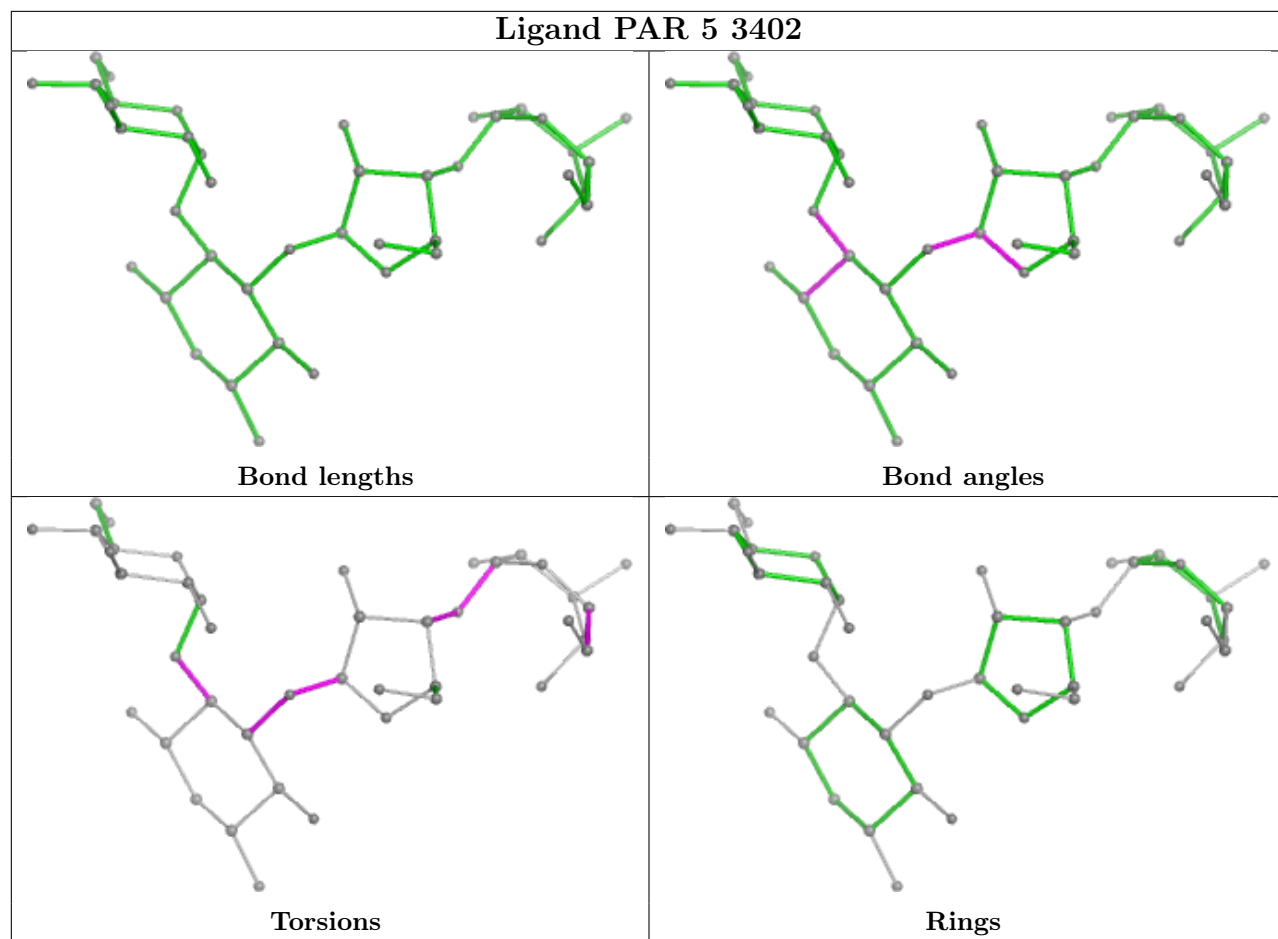


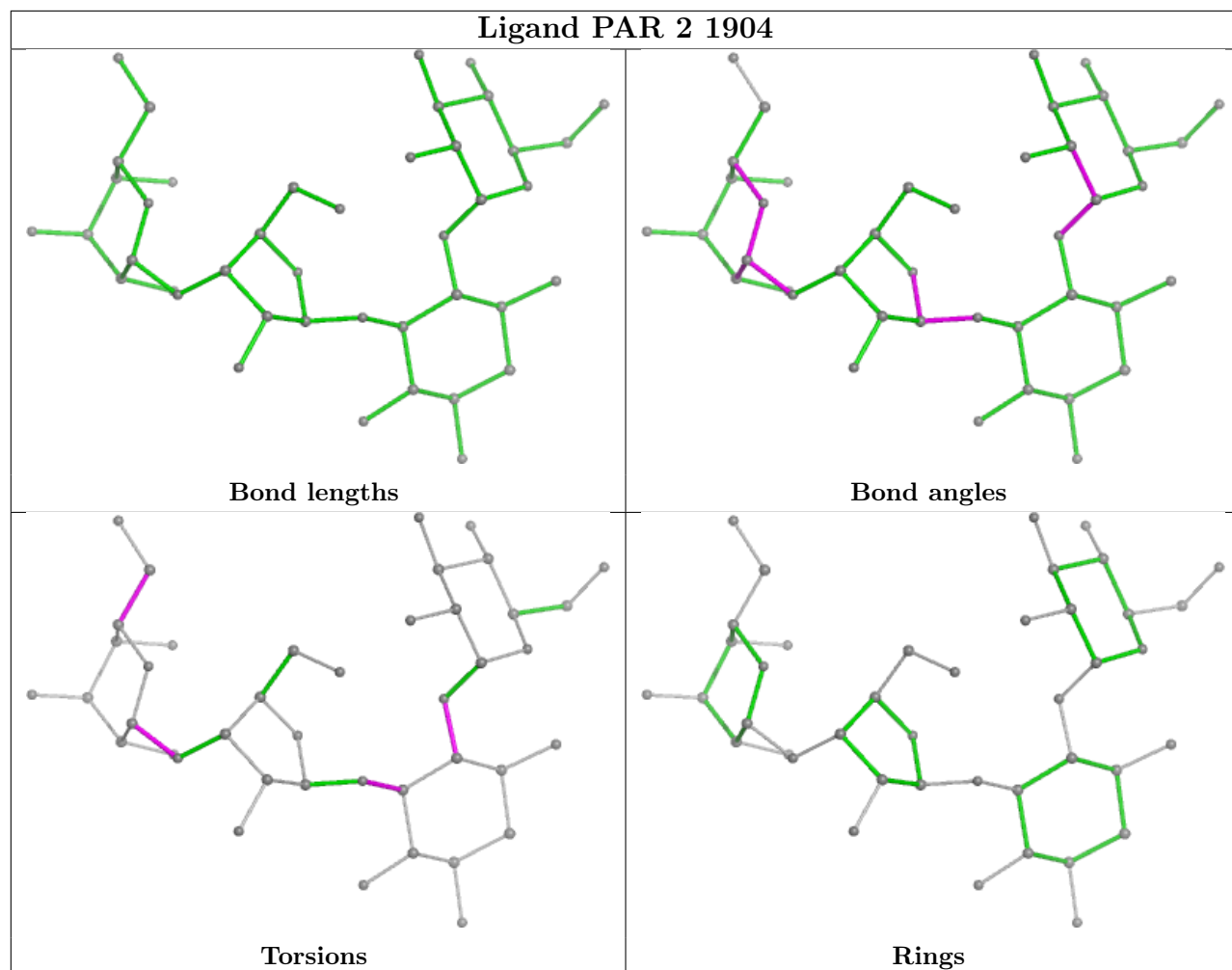


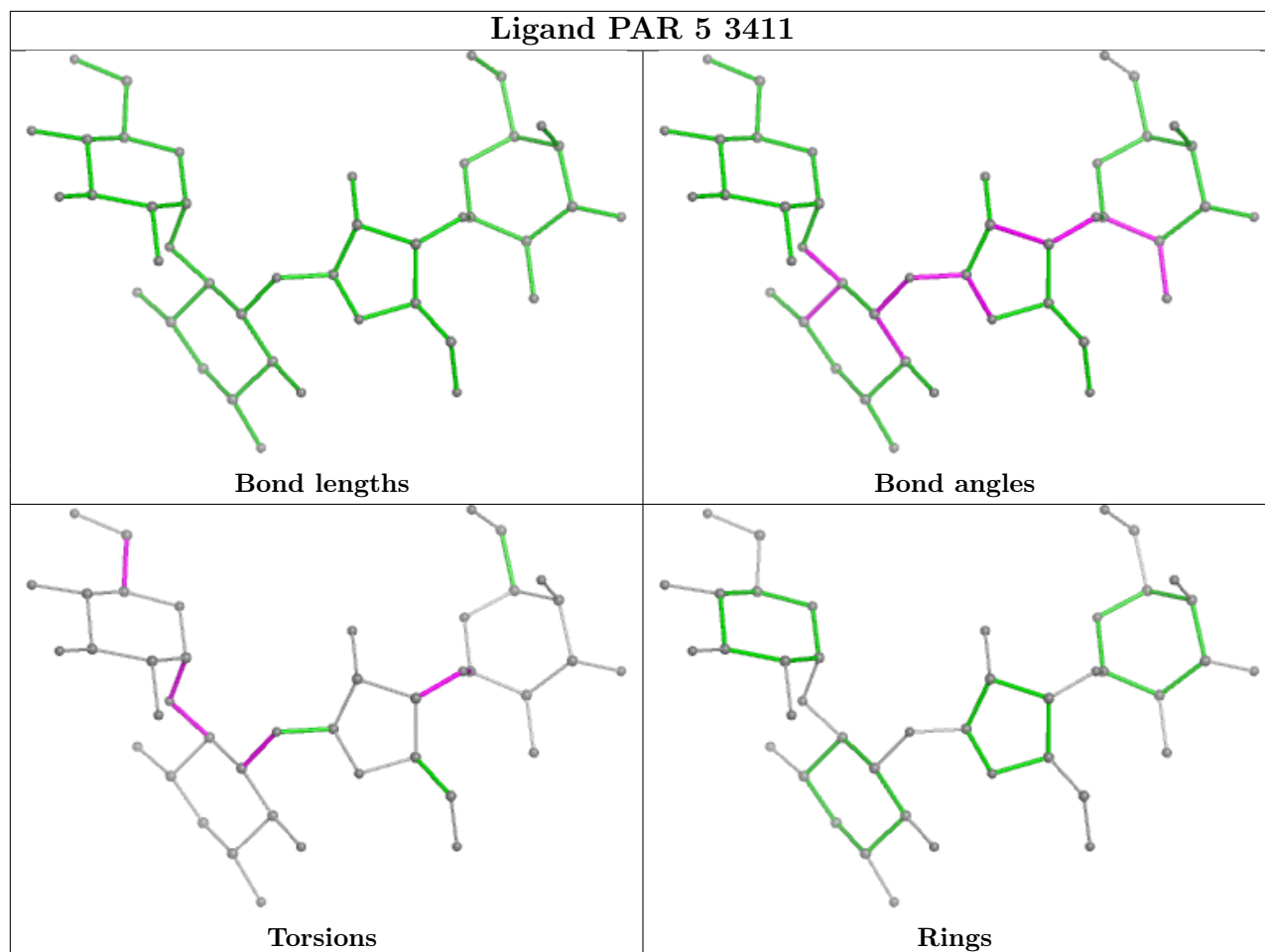


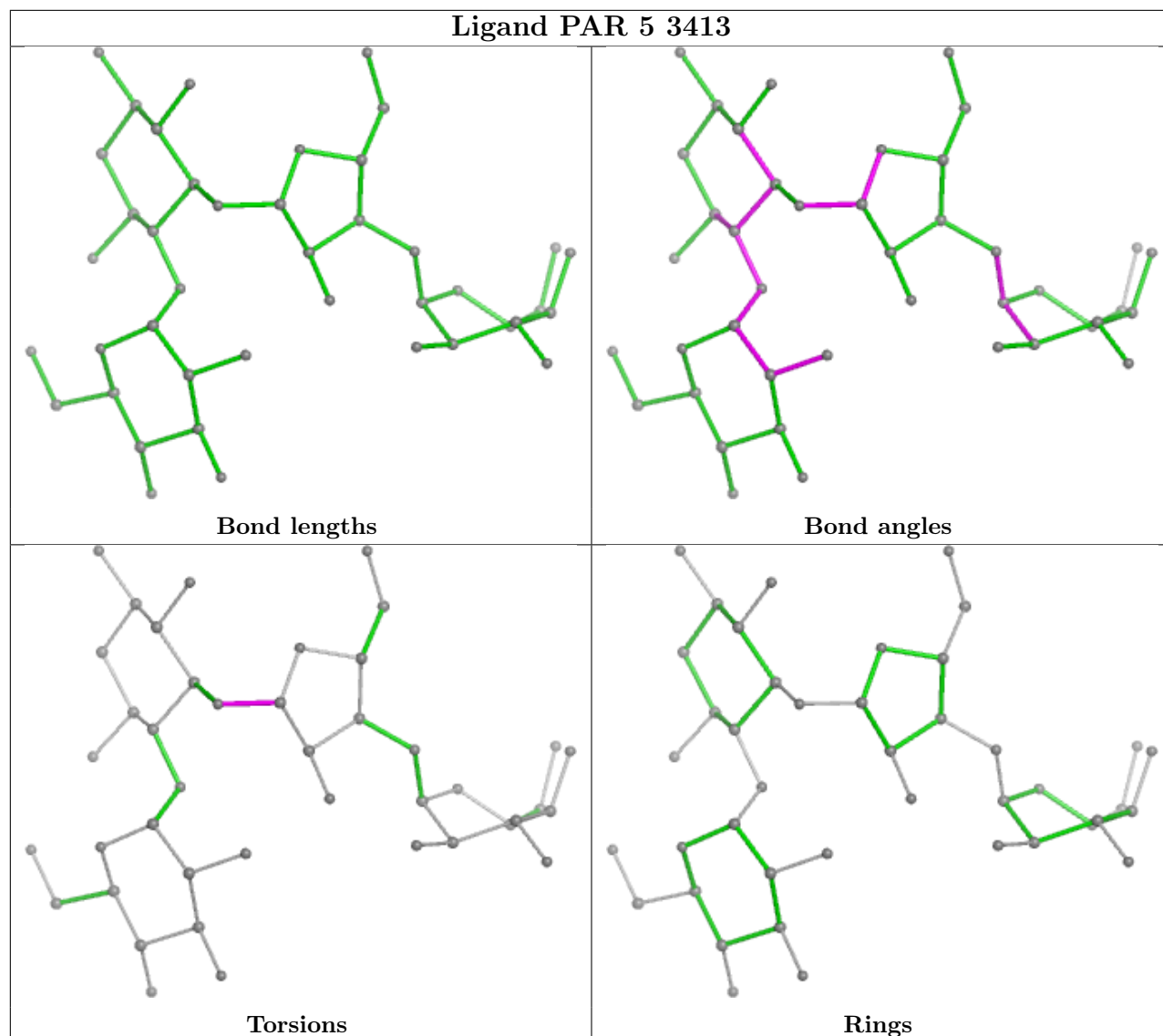


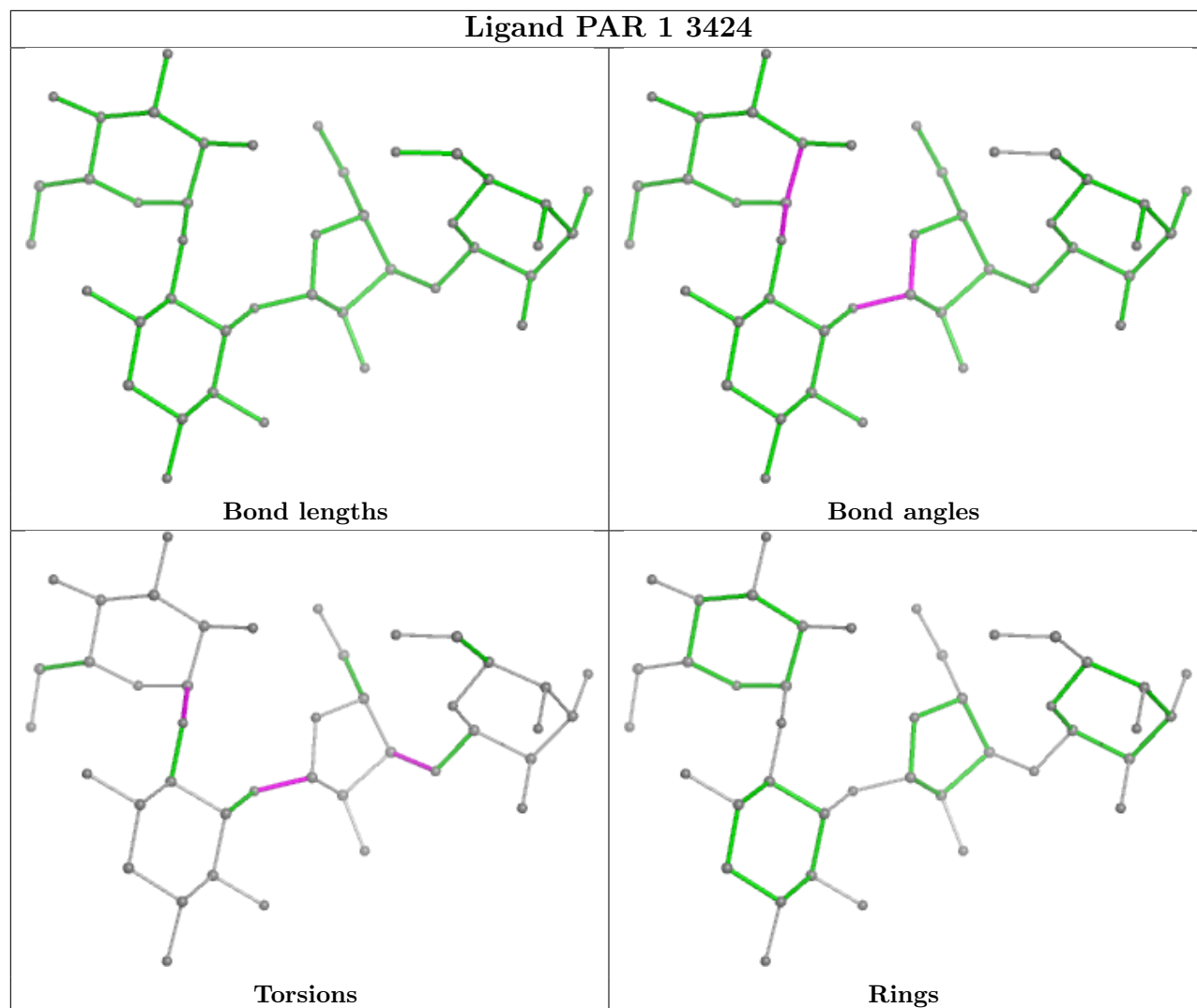


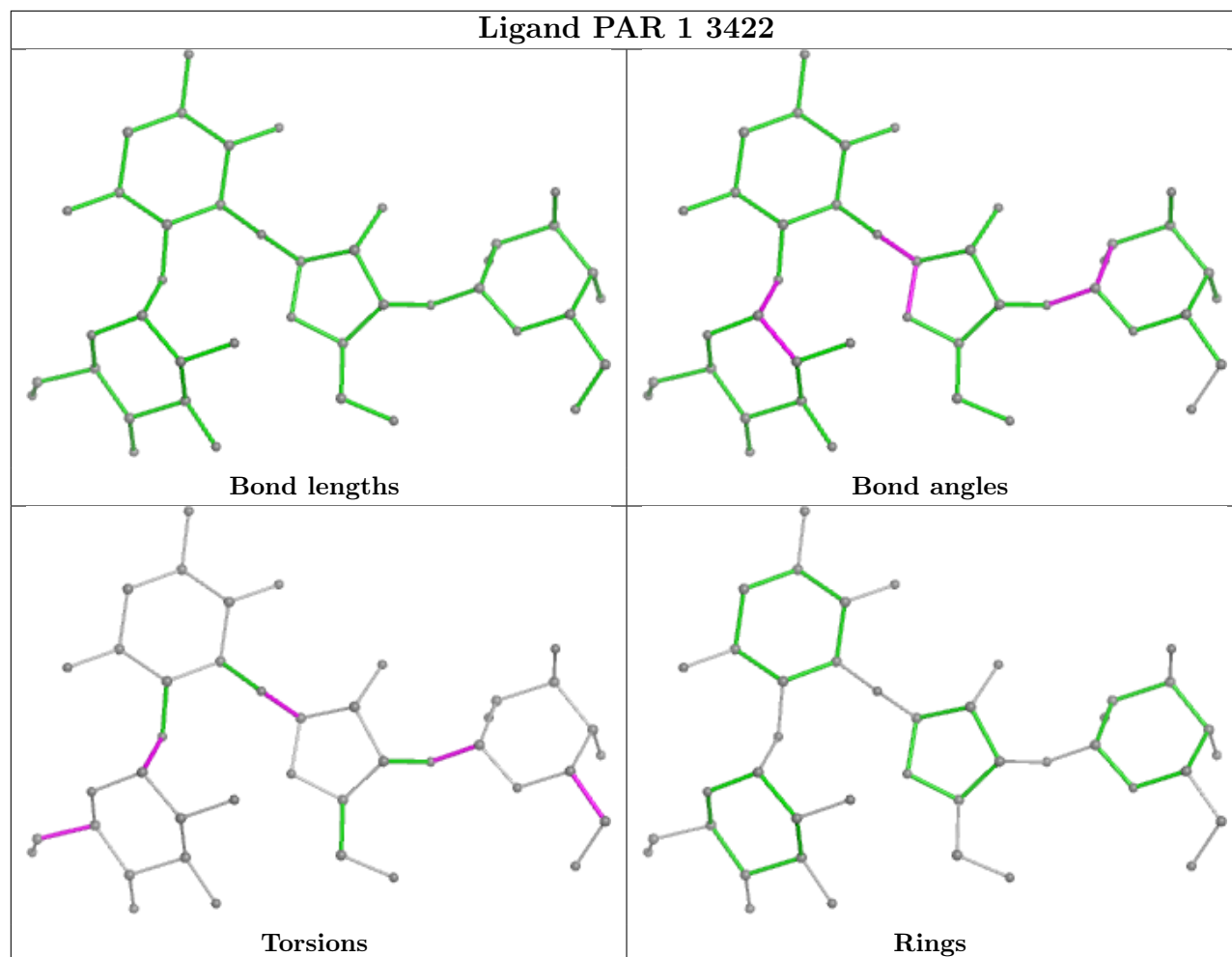


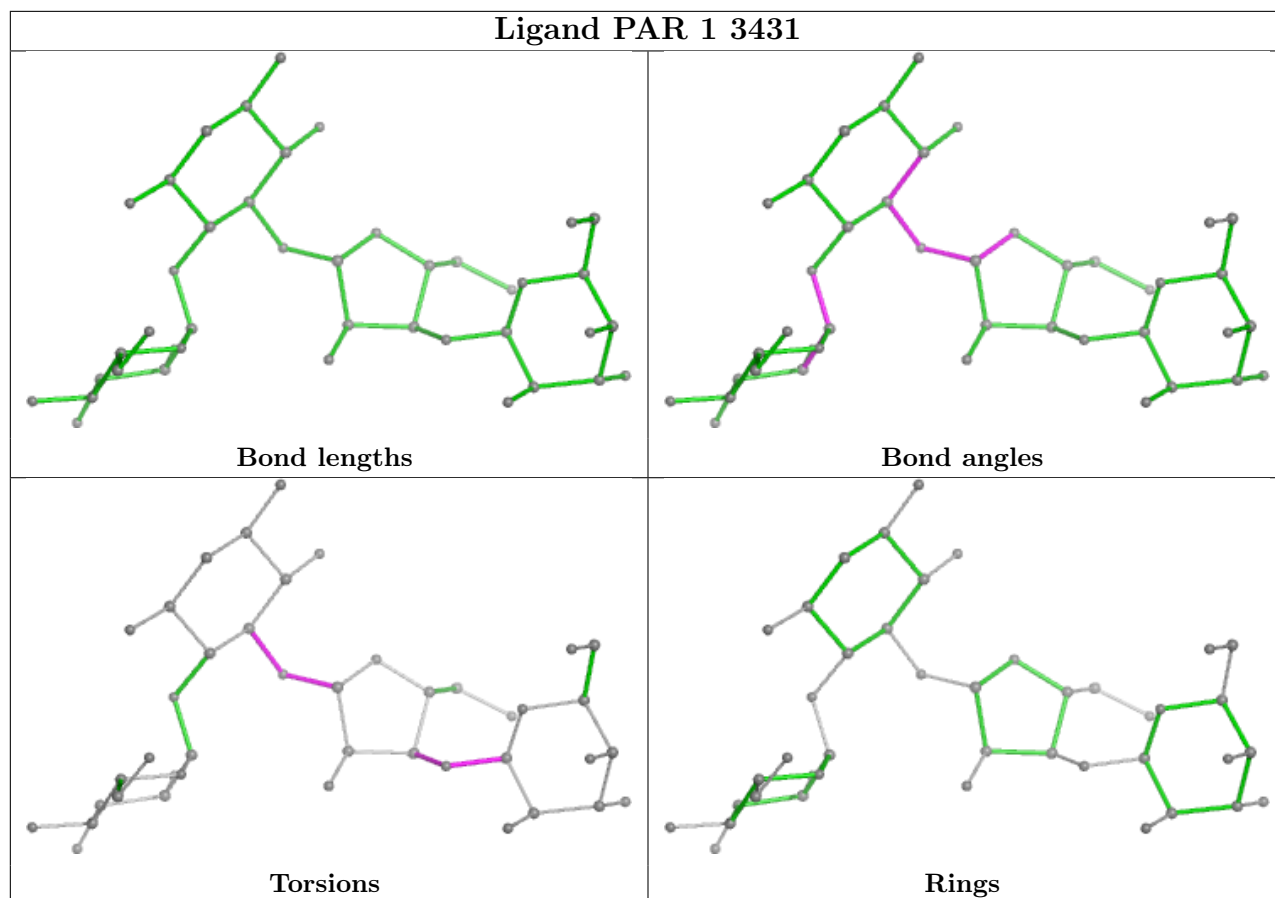












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	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	12	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	13	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	14	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	15	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	16	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	17	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	18	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	19	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 ²)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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	13	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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	12	301	1/1	0.96	0.13	53,53,53,53	0
81	MG	12	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	13	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	14	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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.