



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 11:25 AM JST

PDB ID : 8IUF
EMDB ID : EMD-35720
Title : Cryo-EM structure of Euglena gracilis super-complex I+III2+IV, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 2.81 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

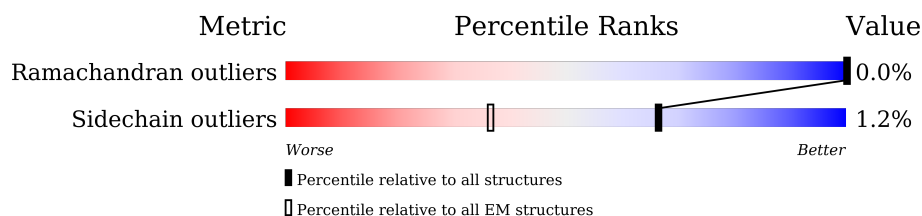
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


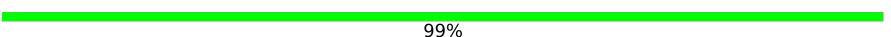
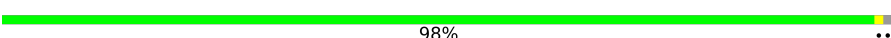


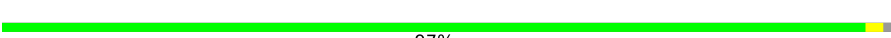



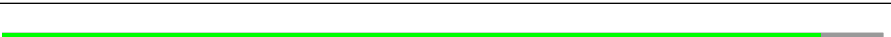
The reported resolution of this entry is 2.81 Å.

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.



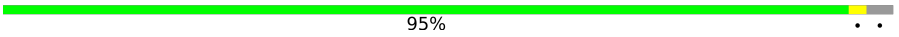
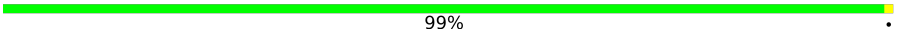


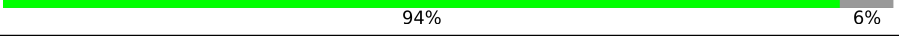

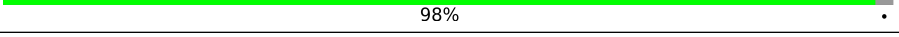

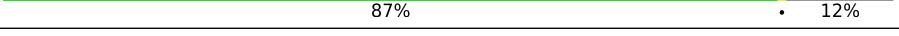
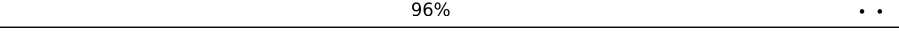
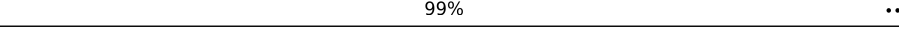
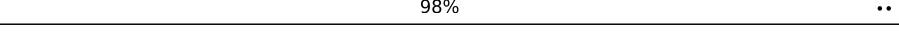

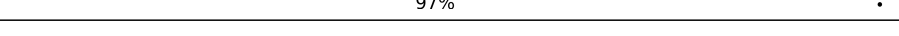
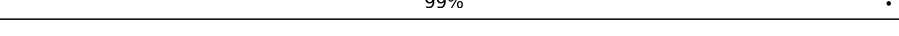
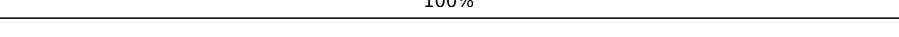
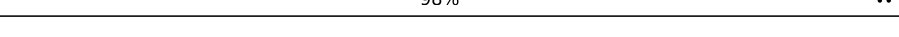

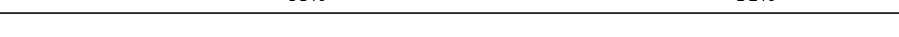






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1A	385	90%  9%
2	1B	527	99%  99%
3	2B	142	98%  98%
4	4A	246	83%  17%
5	4C	139	87%  12%
6	4D	174	97%  97%
7	4E	165	96%  96%
8	4F	75	100%  100%
9	4G	315	93%  6%
10	4H	221	92%  7%


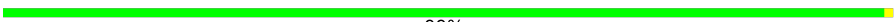












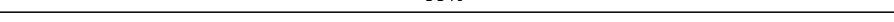

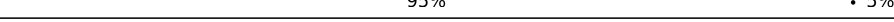


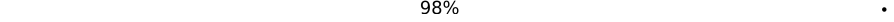
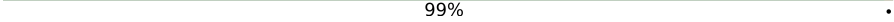

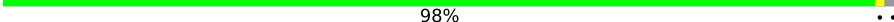
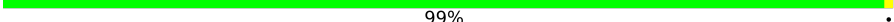

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Mol	Chain	Length	Quality of chain
11	4I	274	 95% . .
12	4J	88	 99% .
13	4L	171	 63% 37%
14	5B	174	 87% . 10%
15	5C	208	 94% 6%
16	6A	112	 81% 19%
17	6B	287	 98% .
18	7A	178	 92% . 7%
19	7C	171	 87% . 12%
20	A1	141	 96% . .
21	A2	193	 99% . .
22	A3	125	 98% . .
23	A5	184	 82% . 16%
24	A6	437	 97% .
25	A7	136	 99% .
26	A8	223	 100%
27	A9	489	 98% . .
28	AB	134	 66% 34%
29	AC	134	 68% . 31%
30	AL	281	 93% . 6%
31	AM	198	 93% 7%
32	AN	287	 100%
33	B2	145	 72% . 28%
34	B3	62	 98% .
35	B4	171	 100%

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Mol	Chain	Length	Quality of chain
36	B5	140	 100%
37	B6	91	 99%
38	B7	97	 99%
39	B8	176	 83% 16%
40	B9	158	 94% . .
41	BL	144	 99%
42	BM	112	 99%
43	C1	495	 99%
44	C2	196	 98%
45	C3	161	 98%
46	C4	185	 97%
47	DC	179	 93% . 7%
48	E1	483	 92% . 7%
49	E2	472	 99%
50	E3	594	 72% . 27%
51	E4	368	 95% . 5%
52	E5	290	 93% . 5%
53	E6	371	 91% . 8%
54	E7	246	 98%
55	E8	205	 99%
56	E9	178	 92% . 7%
57	EA	126	 98%
58	EB	101	 99%
59	EC	101	 84% 16%
60	ED	151	 89% . 9%

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Mol	Chain	Length	Quality of chain
61	FX	325	
62	G1	436	
63	G2	267	
64	G3	261	
65	N1	670	
66	N2	300	
67	N3	293	
67	N6	293	
68	N4	478	
69	N5	584	
70	QA	479	
70	Qa	479	
71	QB	474	
71	Qb	474	
72	QC	368	
72	Qc	368	
73	QD	243	
73	Qd	243	
74	QE	252	
74	Qe	252	
75	QF	72	
75	Qf	72	
76	QG	228	
76	Qg	228	
77	QH	85	

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Mol	Chain	Length	Quality of chain
77	Qh	85	100%
78	QI	70	99%
78	Qi	70	100%
79	QJ	154	95%
79	Qj	154	97%
80	QK	100	61% 39%
80	Qk	100	61% 39%
81	S2	395	98%
82	S3	277	89% 10%
83	S4	208	90% 9%
84	S5	122	99%
85	S6	147	98%
86	S7	207	95%
87	S8	212	85% 14%
88	V1	526	95%
89	V2	225	96%
90	A	12	100%
90	B	12	100%

2 Entry composition

There are 108 unique types of molecules in this entry. The entry contains 368218 atoms, of which 183093 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called NDUFS1a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	352	Total	C	H	N	O	S	0	0
			5501	1753	2700	488	537	23		

- Molecule 2 is a protein called NDUFS1b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1B	525	Total	C	H	N	O	S	1	0
			8357	2679	4159	743	765	11		

- Molecule 3 is a protein called ND2b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2B	140	Total	C	H	N	O	S	0	0
			2059	712	989	172	183	3		

- Molecule 4 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 5 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 6 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 7 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 8 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 9 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4G	297	Total	C	H	N	O	S	0	0
			4691	1478	2340	408	457	8		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4H	205	Total	C	H	N	O	S	0	0
			3250	1040	1644	260	306			

- Molecule 11 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 12 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 13 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	4L	108	Total	C	H	N	O	S	0	0
			1768	606	878	133	145	6		

- Molecule 14 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 15 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 16 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	6A	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		

- Molecule 17 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 18 is a protein called COX7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 19 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 20 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	A1	137	Total	C	H	N	O	S	0	0
			2097	684	1026	192	192	3		

- Molecule 21 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	A2	192	Total	C	H	N	O	S	0	0
			2967	942	1474	267	280	4		

- Molecule 22 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 23 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 24 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 25 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 26 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 27 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 28 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 29 is a protein called NDUFAB1-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 30 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 31 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 32 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 33 is a protein called NDUFB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 34 is a protein called NDUFB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 35 is a protein called NDUFB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 36 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 37 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 38 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 39 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 40 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 41 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 42 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 45 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 46 is a protein called NDUFC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 47 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 48 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 49 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 50 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 51 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 52 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 53 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	E6	342	Total	C	H	N	O	S	0	0
			5629	1839	2758	507	513	12		

- Molecule 54 is a protein called NDUEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- Molecule 55 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 56 is a protein called NDUEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	E9	165	Total	C	H	N	O	S	0	0
			2436	779	1224	213	217	3		

- Molecule 57 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 58 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 59 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 60 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 61 is a protein called NDUFEX.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 62 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	G1	426	Total	C	H	N	O	S	0	0
			6552	2115	3205	593	623	16		

- Molecule 63 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 64 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 65 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 66 is a protein called ND2a.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 67 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
67	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 68 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 69 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 70 is a protein called MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
70	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 71 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
71	Qb	423	Total	C	H	N	O	S	0	0
			6408	2057	3192	540	616	3		

- Molecule 72 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
72	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

- Molecule 73 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
73	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 74 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
74	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 75 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	QF	64	Total	C	H	N	O	S	0	0
			1014	325	499	91	93	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
75	Qf	64	Total	C	H	N	O	S	0	0
			1018	325	503	91	93	6		

- Molecule 76 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
76	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 77 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
77	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 78 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	QI	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		
78	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 79 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
79	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 80 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
80	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 81 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 82 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 83 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 84 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 85 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 86 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 87 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 88 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	V1	504	Total	C	H	N	O	S	0	0
			7724	2463	3827	680	727	27		

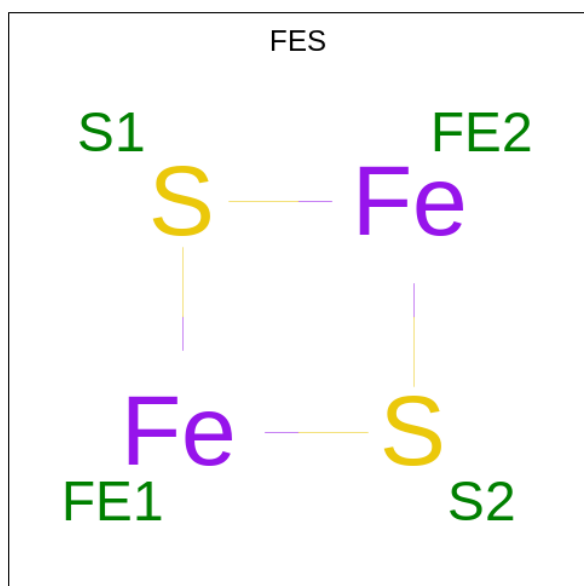
- Molecule 89 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	V2	225	Total	C	H	N	O	S	0	0
			3460	1124	1701	299	319	17		

- Molecule 90 is a protein called poly(UNK).

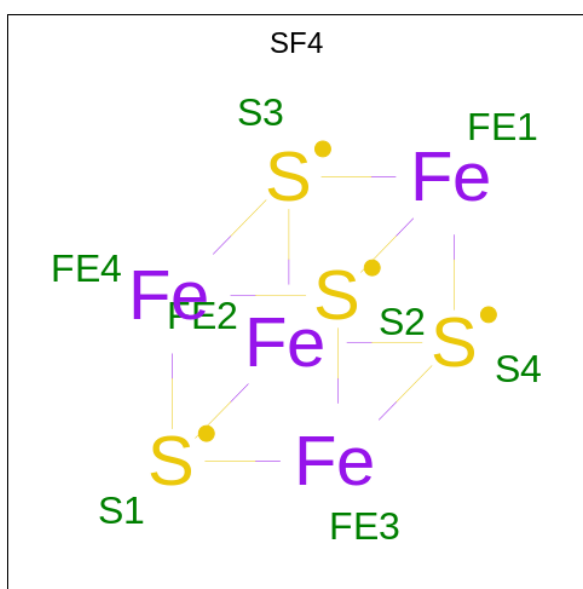
Mol	Chain	Residues	Atoms					AltConf	Trace
90	A	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
90	B	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- Molecule 91 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
91	1A	1	Total	Fe	S	0
			4	2	2	
91	QE	1	Total	Fe	S	0
			4	2	2	
91	Qe	1	Total	Fe	S	0
			4	2	2	
91	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 92 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).

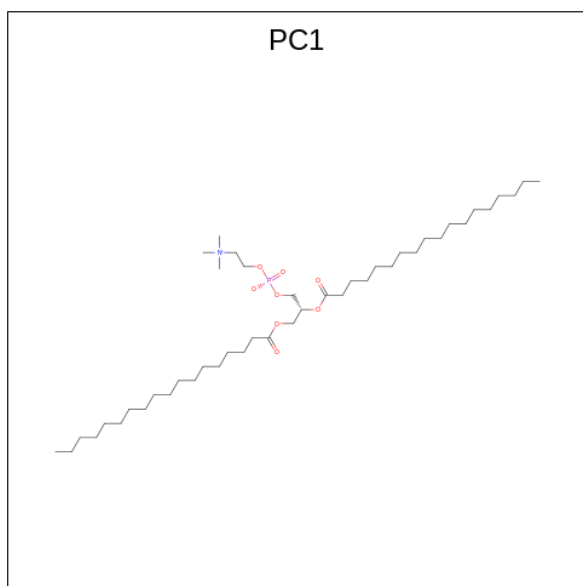


Mol	Chain	Residues	Atoms			AltConf
92	1A	1	Total	Fe	S	0
			8	4	4	
92	1A	1	Total	Fe	S	0
			8	4	4	
92	S7	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 93 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
93	1A	1	Total	K	0
			1	1	

- Molecule 94 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
94	4A	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
94	4A	1	Total	C	H	N	O	P	0
			112	36	66	1	8	1	
94	4E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
94	7A	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
94	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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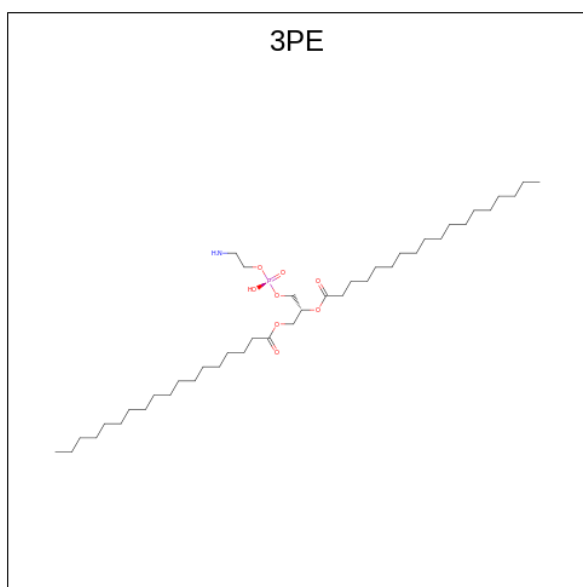
Mol	Chain	Residues	Atoms						AltConf
94	AM	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	AN	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B8	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
94	C1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
94	C3	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E4	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 73	C 23	H 40	N 1	O 8	P 1	0
94	E8	1	Total 64	C 20	H 34	N 1	O 8	P 1	0
94	E9	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
94	ED	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	ED	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
94	G2	1	Total 88	C 28	H 50	N 1	O 8	P 1	0
94	N1	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
94	N1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
94	N3	1	Total 103	C 32	H 61	N 1	O 8	P 1	0
94	N4	1	Total 91	C 29	H 52	N 1	O 8	P 1	0
94	N4	1	Total 73	C 23	H 40	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
94	N4	1	Total	C	H	N	O	P
			142	44	88	1	8	1
94	N5	1	Total	C	H	N	O	P
			82	26	46	1	8	1
94	QC	1	Total	C	H	N	O	P
			142	44	88	1	8	1
94	QD	1	Total	C	H	N	O	P
			67	21	36	1	8	1
94	QI	1	Total	C	H	N	O	P
			82	26	46	1	8	1
94	Qc	1	Total	C	H	N	O	P
			142	44	88	1	8	1
94	Qc	1	Total	C	H	N	O	P
			67	21	36	1	8	1
94	Qe	1	Total	C	H	N	O	P
			82	26	46	1	8	1
94	Qg	1	Total	C	H	N	O	P
			58	18	30	1	8	1
94	Qj	1	Total	C	H	N	O	P
			142	44	88	1	8	1

- Molecule 95 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



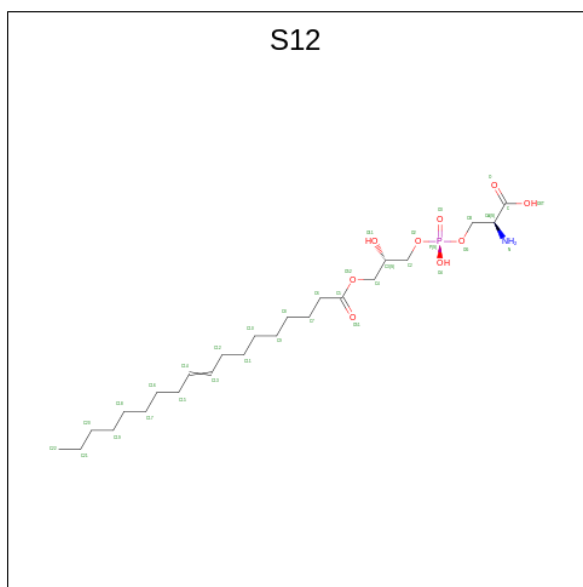
Mol	Chain	Residues	Atoms					AltConf
95	4D	1	Total	C	H	N	O	P
			79	25	44	1	8	1

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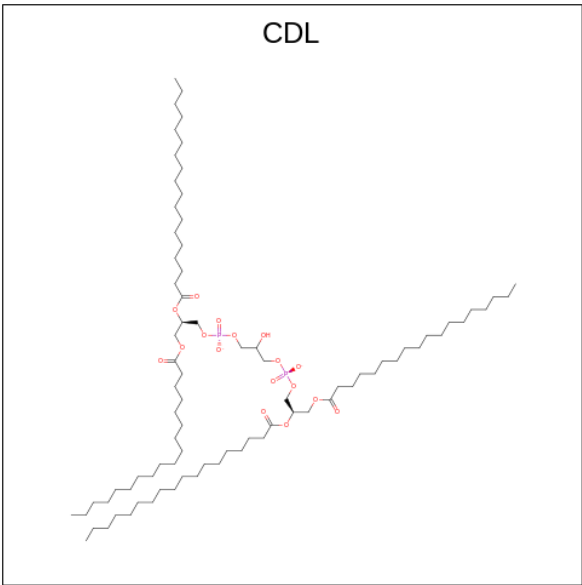
Mol	Chain	Residues	Atoms						AltConf
95	4D	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	7A	1	Total	C	H	N	O	P	0
			100	31	59	1	8	1	
95	B4	1	Total	C	H	N	O	P	0
			97	30	57	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	E9	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	N4	1	Total	C	H	N	O	P	0
			97	31	56	1	8	1	
95	N5	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 96 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (three-letter code: S12) (formula: C₂₄H₄₆NO₉P).



Mol	Chain	Residues	Atoms						AltConf
96	4D	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

- Molecule 97 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms					AltConf
97	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	7C	1	Total	C	H	O	P	0
			220	71	130	17	2	
97	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	A9	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	B8	1	Total	C	H	O	P	0
			157	51	87	17	2	
97	BM	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
97	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	C4	1	Total	C	H	O	P	0
			247	79	149	17	2	

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Mol	Chain	Residues	Atoms					AltConf
97	E4	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	E6	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
97	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	
97	N1	1	Total	C	H	O	P	0
			154	51	84	17	2	
97	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
97	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
97	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
97	QH	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
97	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
97	Qe	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	

- Molecule 98 is ZINC ION (three-letter code: ZN) (formula: Zn).

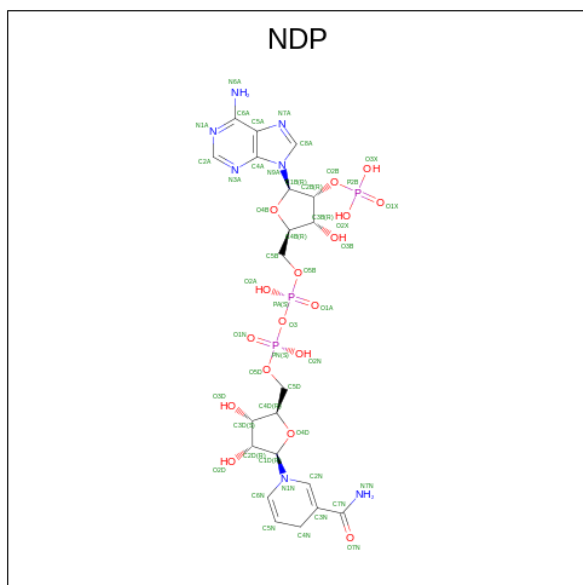
Mol	Chain	Residues	Atoms		AltConf
98	5B	1	Total	Zn	0
			1	1	
98	E7	1	Total	Zn	0
			1	1	

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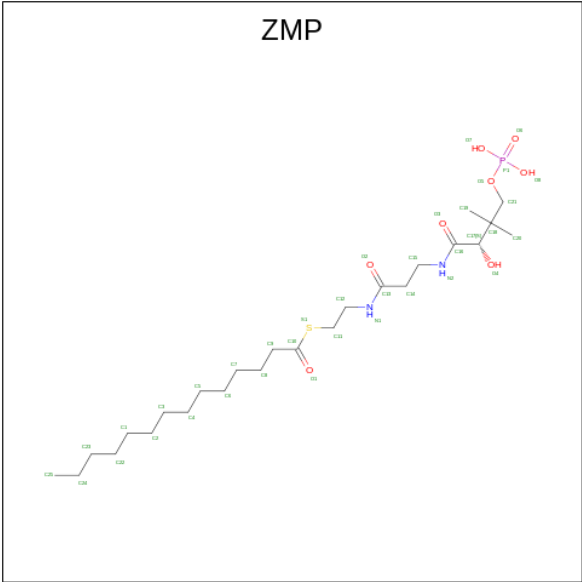
Mol	Chain	Residues	Atoms		AltConf
98	S6	1	Total	Zn	0
			1	1	

- Molecule 99 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



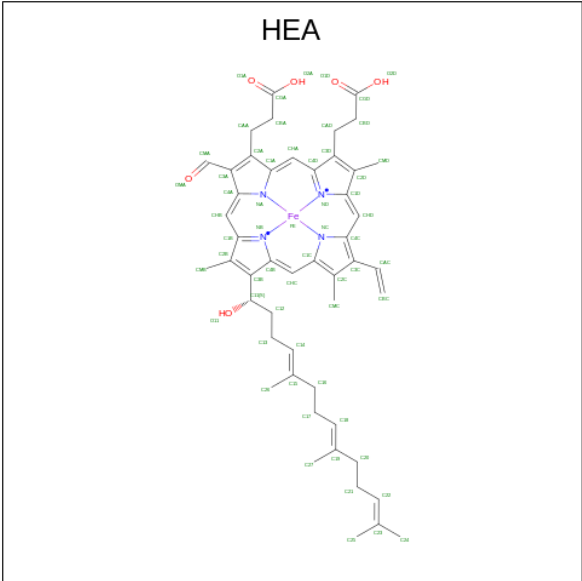
Mol	Chain	Residues	Atoms						AltConf
99	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 100 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
100	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
100	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 101 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

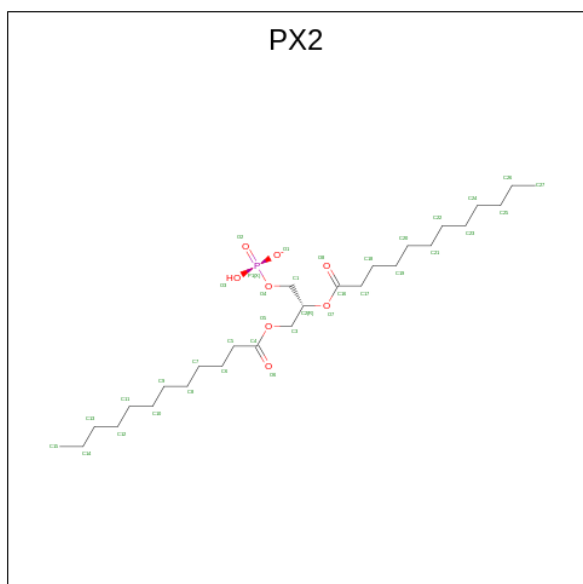
- Molecule 102 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
102	C1	1	Total	Cu	0
			1	1	
102	C2	2	Total	Cu	0
			2	2	

- Molecule 103 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
103	C1	1	Total	Mg	0
			1	1	

- Molecule 104 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: C₂₇H₅₂O₈P).



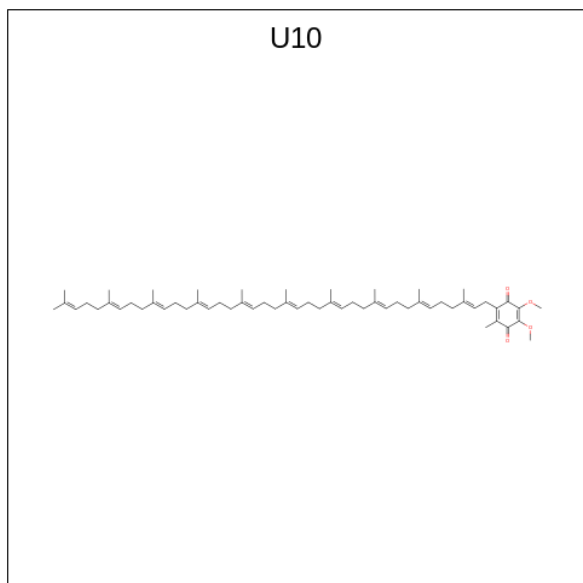
Mol	Chain	Residues	Atoms				AltConf
104	C2	1	Total	C	O	P	0
			36	27	8	1	

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Mol	Chain	Residues	Atoms				AltConf
104	QJ	1	Total	C	O	P	0
			36	27	8	1	
104	QJ	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 105 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

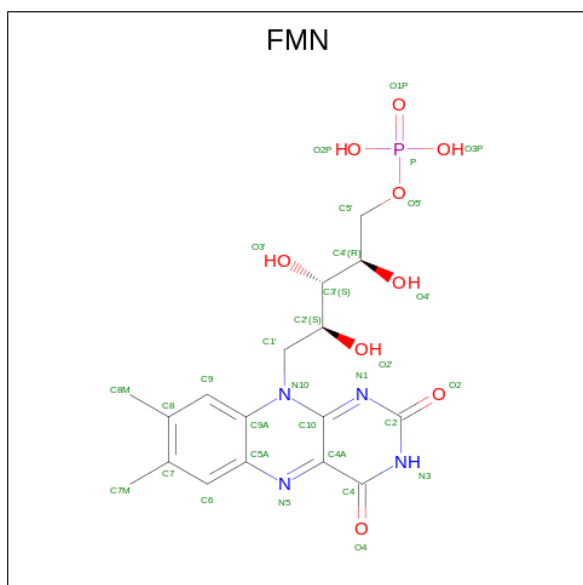


Mol	Chain	Residues	Atoms				AltConf
105	N4	1	Total	C	H	O	0
			98	39	55	4	

- Molecule 106 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
107	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
107	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 108 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



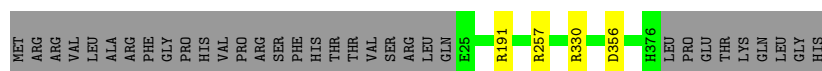
Mol	Chain	Residues	Atoms					AltConf
108	V1	1	Total	C	H	N	O	P
			50	17	19	4	9	1

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. 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. 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.

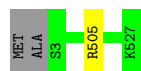
- Molecule 1: NDUFS1a

Chain 1A:  90% 9%



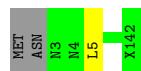
- Molecule 2: NDUFS1b

Chain 1B:  99%




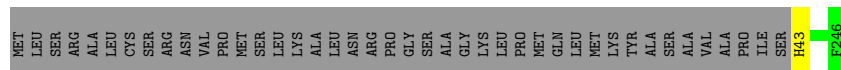
- Molecule 3: ND2b

Chain 2B:  98%



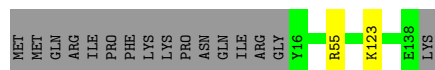
- Molecule 4: COXEG1

Chain 4A:  83% 17%



- Molecule 5: COXEG3

Chain 4C:  87% 12%



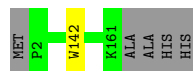
- Molecule 6: COXEG4

Chain 4D:  97%



- Molecule 7: COXEG5

Chain 4E: 96%



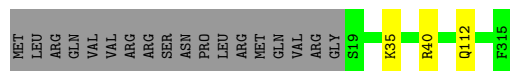
- Molecule 8: COXEG6

Chain 4F: 100%

There are no outlier residues recorded for this chain.

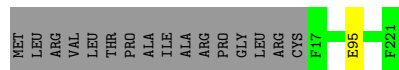
- Molecule 9: COXEG7

Chain 4G: 93%



- Molecule 10: COXEG8

Chain 4H: 92%



- Molecule 11: COXEG9

Chain 4I: 95%



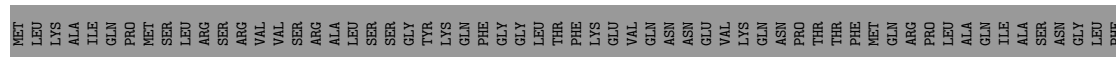
- Molecule 12: COXEG10

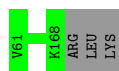
Chain 4J: 99%



- Molecule 13: ND4L

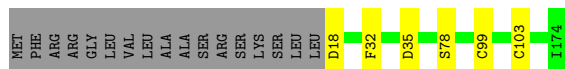
Chain 4L: 63%





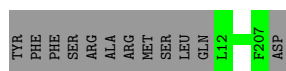
- Molecule 14: COX5b-2

Chain 5B: 87% 10%



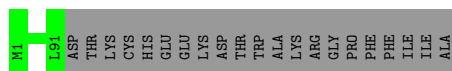
- Molecule 15: COX5c

Chain 5C: 94% 6%



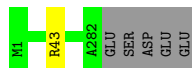
- Molecule 16: COX6a

Chain 6A: 81% 19%



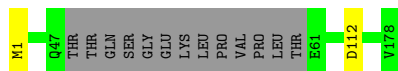
- Molecule 17: COX6b-1

Chain 6B: 98% 2%



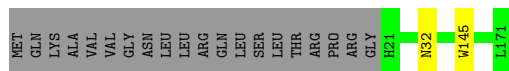
- Molecule 18: COX7a

Chain 7A: 92% 7%



- Molecule 19: COX7c

Chain 7C: 87% 12%



- Molecule 20: NDUFA1

Chain A1: 96% 4%



- Molecule 21: NDUFA2

Chain A2: 99% ..



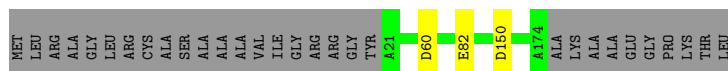
- Molecule 22: NDUFA3

Chain A3: 98% ..



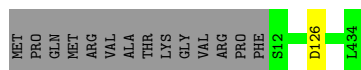
- Molecule 23: NDUFA5

Chain A5: 82% 16%



- Molecule 24: NDUFA6

Chain A6: 97% .



- Molecule 25: NDUFA7

Chain A7: 99% .



- Molecule 26: NDUFA8

Chain A8: 100%



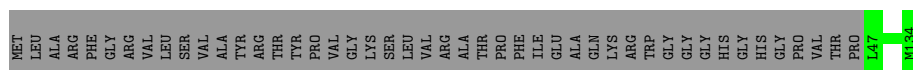
- Molecule 27: NDUFA9

Chain A9: 98% ..



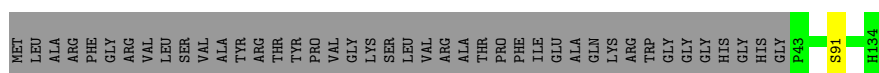
- Molecule 28: NDUFAB1-alpha

Chain AB: 66% 34%



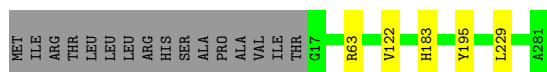
- Molecule 29: NDUFAB1-beta

Chain AC: 68% • 31%



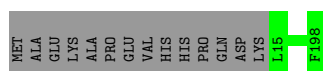
- Molecule 30: NDUFA12

Chain AL: 93% • 6%



- Molecule 31: NDUFA13

Chain AM: 93% 7%



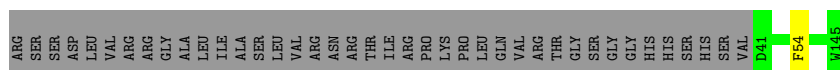
- Molecule 32: NDUFA11

Chain AN: 100%

There are no outlier residues recorded for this chain.

- Molecule 33: NDUFB2

Chain B2: 72% • 28%



- Molecule 34: NDUFB3

Chain B3: 98% •



Chain BM: 99%



- Molecule 43: Cytochrome c oxidase subunit 1

Chain C1: 99%



- Molecule 44: Cytochrome c oxidase subunit 2

Chain C2: 98%



- Molecule 45: Putative NADH dehydrogenase subunit 6

Chain C3: 98%



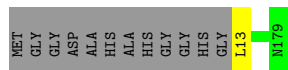
- Molecule 46: NDUFC2

Chain C4: 97%



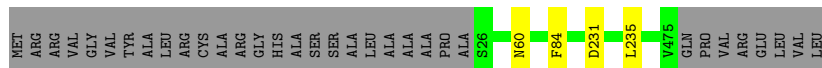
- Molecule 47: COX4

Chain DC: 93% 7%



- Molecule 48: NDUEG1

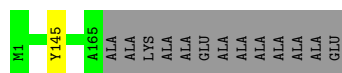
Chain E1: 92% 7%



- Molecule 49: NDUEG2

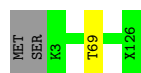
Chain E2: 99%

Chain E9:  92% • 7%



- Molecule 57: NDUEG10

Chain EA:  98% ••



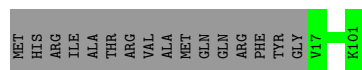
- Molecule 58: NDUEG11

Chain EB:  99% •



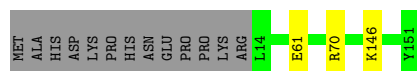
- Molecule 59: NDUEG11

Chain EC:  84% 16%



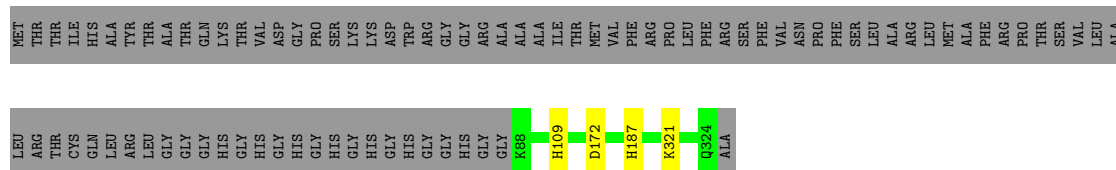
- Molecule 60: NDUEG13

Chain ED:  89% • 9%



- Molecule 61: NDUFX

Chain FX:  72% • 27%

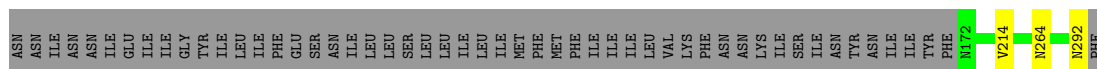


- Molecule 62: NDUCA1

Chain G1:  96% ••

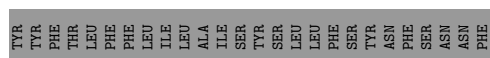
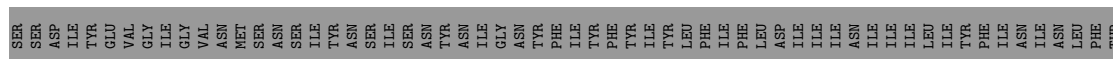
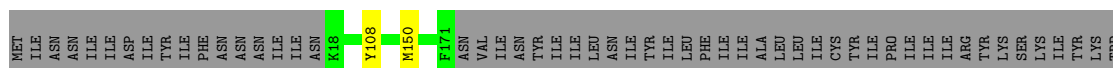


- Molecule 63: NDUCA2



- Molecule 67: ND3

Chain N6: 52% 47%



- Molecule 68: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 99%



- Molecule 69: ND5

Chain N5: 99%



- Molecule 70: MPP-beta

Chain QA: 98%



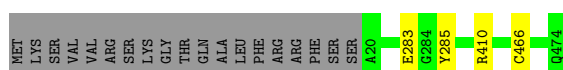
- Molecule 70: MPP-beta

Chain Qa: 99%




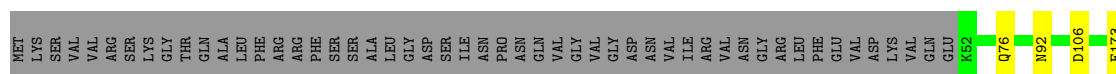
- Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain QB: 95%



- Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

Chain Qb:  88% 11%



- Molecule 72: Cytochrome b

Chain QC:  98% ..



- Molecule 72: Cytochrome b

Chain Qc:  98% ..



- Molecule 73: Cytochrome c1, heme protein

Chain QD:  98% ..



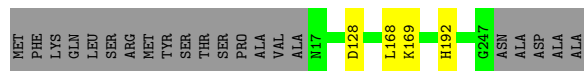
- Molecule 73: Cytochrome c1, heme protein

Chain Qd:  97% ..



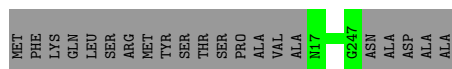
- Molecule 74: UQCRFS1

Chain QE:  90% 8%

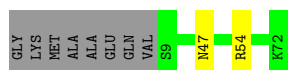
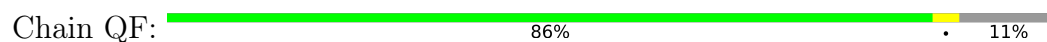


- Molecule 74: UQCRFS1

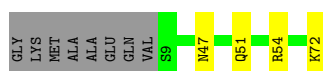
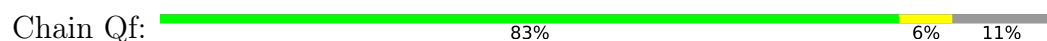
Chain Qe:  92% 8%



- Molecule 75: UQCRH



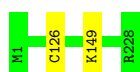
- Molecule 75: UQCRH



- Molecule 76: UQCRB



- Molecule 76: UQCRB



- Molecule 77: UQCRQ



There are no outlier residues recorded for this chain.

- Molecule 77: UQCRQ



There are no outlier residues recorded for this chain.

- Molecule 78: UQCR9



- Molecule 78: UQCR9

Chain Qi:  100%

There are no outlier residues recorded for this chain.

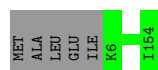
- Molecule 79: UQCR10

Chain QJ:  95%



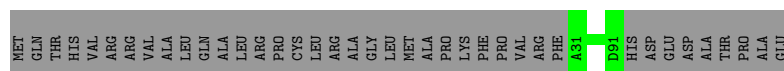
- Molecule 79: UQCR10

Chain Qj:  97%



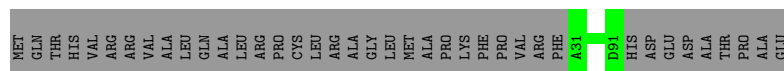
- Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK:  61%  39%



- Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain Qk:  61%  39%



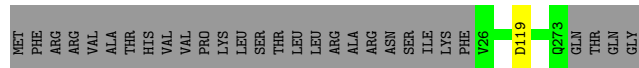
- Molecule 81: NDUFS2

Chain S2:  98%



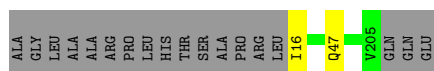
- Molecule 82: NDUFS3

Chain S3:  89%  10%



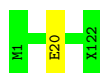
- Molecule 83: NDUFS4

Chain S4:  90% 9%



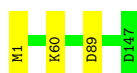
• Molecule 84: NDUFS5

Chain S5:  99%



• Molecule 85: NDUFS6

Chain S6:  98%



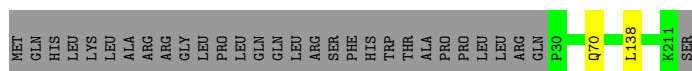
• Molecule 86: NDUFS7

Chain S7:  95%



• Molecule 87: NDUFS8

Chain S8:  85% 14%



• Molecule 88: NDUFV1

Chain V1:  95%



• Molecule 89: NDUFV2

Chain V2:  96%



• Molecule 90: poly(UNK)

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 90: poly(UNK)

Chain B:

100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	345048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, PX2, MG, SF4, K, S12, CU, NDP, CDL, 3PE, ZMP, FMN, HEC, FES, 2MR, HEA, ZN, U10, HEM

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	1A	0.37	0/2858	0.54	0/3878
2	1B	0.35	0/4306	0.51	0/5854
3	2B	0.37	0/958	0.47	0/1306
4	4A	0.29	0/1650	0.44	0/2235
5	4C	0.33	0/1051	0.46	0/1432
6	4D	0.30	0/1379	0.50	0/1867
7	4E	0.28	0/1376	0.45	0/1864
8	4F	0.35	0/641	0.43	0/867
9	4G	0.31	0/2391	0.50	0/3240
10	4H	0.31	0/1640	0.44	0/2224
11	4I	0.36	0/2255	0.50	0/3059
12	4J	0.34	0/736	0.50	0/1008
13	4L	0.37	0/924	0.46	0/1261
14	5B	0.42	1/1294 (0.1%)	0.51	0/1759
15	5C	0.39	0/1616	0.47	0/2192
16	6A	0.30	0/777	0.45	0/1055
17	6B	0.31	0/2343	0.45	0/3174
18	7A	0.31	0/1359	0.51	0/1835
19	7C	0.38	0/1299	0.47	0/1777
20	A1	0.31	0/1108	0.48	0/1511
21	A2	0.31	0/1530	0.51	0/2089
22	A3	0.35	0/1079	0.54	0/1453
23	A5	0.34	0/1282	0.51	0/1737
24	A6	0.32	0/3395	0.51	0/4608
25	A7	0.35	0/1194	0.56	0/1619
26	A8	0.32	0/1879	0.47	0/2543
27	A9	0.35	0/3920	0.52	0/5335
28	AB	0.32	0/704	0.44	0/951
29	AC	0.35	0/736	0.45	0/1000
30	AL	0.36	0/2317	0.55	0/3136
31	AM	0.34	0/1533	0.49	0/2079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AN	0.34	0/2382	0.49	0/3249
33	B2	0.36	0/947	0.44	0/1291
34	B3	0.37	0/326	0.52	0/441
35	B4	0.36	0/1419	0.50	0/1922
36	B5	0.35	0/1111	0.52	0/1505
37	B6	0.38	0/803	0.48	0/1087
38	B7	0.35	0/877	0.54	0/1172
39	B8	0.37	0/1273	0.46	0/1733
40	B9	0.36	0/1274	0.49	0/1728
41	BL	0.36	0/1266	0.51	0/1710
42	BM	0.34	0/876	0.55	0/1192
43	C1	0.38	0/4054	0.50	0/5516
44	C2	0.36	0/1620	0.51	0/2207
45	C3	0.35	0/1416	0.45	0/1945
46	C4	0.34	0/1592	0.49	0/2158
47	DC	0.36	0/1410	0.51	0/1914
48	E1	0.32	0/3596	0.49	0/4879
49	E2	0.30	0/3658	0.49	0/4983
50	E3	0.29	0/3320	0.47	0/4520
51	E4	0.32	0/2850	0.49	0/3884
52	E5	0.26	0/2004	0.50	0/2721
53	E6	0.33	0/2954	0.49	0/4004
54	E7	0.31	0/1931	0.50	0/2618
55	E8	0.36	0/1747	0.51	0/2367
56	E9	0.27	0/1239	0.47	0/1690
57	EA	0.35	0/858	0.46	0/1163
58	EB	0.31	0/650	0.52	0/863
59	EC	0.31	0/676	0.46	0/925
60	ED	0.32	0/1176	0.51	0/1590
61	FX	0.37	0/2035	0.49	0/2763
62	G1	0.35	0/3443	0.52	0/4686
63	G2	0.33	0/1832	0.54	0/2476
64	G3	0.32	0/1957	0.54	0/2646
65	N1	0.36	0/2672	0.47	0/3639
66	N2	0.42	0/2582	0.45	0/3530
67	N3	0.40	0/1068	0.45	0/1456
67	N6	0.33	0/1275	0.46	0/1730
68	N4	0.38	0/4105	0.46	0/5594
69	N5	0.38	0/4963	0.48	0/6758
70	QA	0.34	0/3838	0.52	0/5193
70	Qa	0.32	0/3838	0.51	0/5193
71	QB	0.33	0/3532	0.48	0/4805
71	Qb	0.34	0/3288	0.48	0/4474

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
72	QC	0.37	0/3058	0.48	0/4178
72	Qc	0.37	0/3058	0.47	0/4178
73	QD	0.37	0/2027	0.49	0/2760
73	Qd	0.36	0/2027	0.51	0/2760
74	QE	0.31	0/1842	0.51	0/2502
74	Qe	0.30	0/1842	0.51	0/2502
75	QF	0.28	0/526	0.41	0/702
75	Qf	0.27	0/526	0.40	0/702
76	QG	0.39	0/1987	0.54	0/2696
76	Qg	0.38	0/1987	0.54	0/2696
77	QH	0.34	0/717	0.55	0/966
77	Qh	0.33	0/717	0.56	0/966
78	QI	0.38	0/251	0.44	0/340
78	Qi	0.35	0/251	0.43	0/340
79	QJ	0.31	0/1243	0.52	0/1693
79	Qj	0.30	0/1243	0.51	0/1693
80	QK	0.34	0/498	0.48	0/677
80	Qk	0.34	0/498	0.47	0/677
81	S2	0.40	0/3244	0.54	0/4403
82	S3	0.39	0/2112	0.54	0/2874
83	S4	0.34	0/1573	0.59	0/2107
84	S5	0.31	0/960	0.47	0/1291
85	S6	0.35	0/1232	0.53	0/1659
86	S7	0.40	0/1558	0.53	0/2120
87	S8	0.40	0/1485	0.53	0/2010
88	V1	0.32	0/3990	0.51	0/5394
89	V2	0.33	0/1787	0.49	0/2428
All	All	0.35	1/183502 (0.0%)	0.50	0/249182

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5B	99	CYS	CB-SG	5.40	1.91	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	1A	350/385 (91%)	333 (95%)	17 (5%)	0	100	100
2	1B	523/527 (99%)	509 (97%)	14 (3%)	0	100	100
3	2B	112/142 (79%)	102 (91%)	10 (9%)	0	100	100
4	4A	202/246 (82%)	197 (98%)	5 (2%)	0	100	100
5	4C	121/139 (87%)	119 (98%)	2 (2%)	0	100	100
6	4D	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
7	4E	158/165 (96%)	155 (98%)	3 (2%)	0	100	100
8	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
9	4G	295/315 (94%)	288 (98%)	7 (2%)	0	100	100
10	4H	203/221 (92%)	195 (96%)	8 (4%)	0	100	100
11	4I	263/274 (96%)	256 (97%)	7 (3%)	0	100	100
12	4J	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
13	4L	106/171 (62%)	105 (99%)	1 (1%)	0	100	100
14	5B	155/174 (89%)	152 (98%)	3 (2%)	0	100	100
15	5C	194/208 (93%)	187 (96%)	7 (4%)	0	100	100
16	6A	89/112 (80%)	82 (92%)	7 (8%)	0	100	100
17	6B	280/287 (98%)	276 (99%)	4 (1%)	0	100	100
18	7A	161/178 (90%)	158 (98%)	3 (2%)	0	100	100
19	7C	149/171 (87%)	146 (98%)	3 (2%)	0	100	100
20	A1	135/141 (96%)	126 (93%)	9 (7%)	0	100	100
21	A2	190/193 (98%)	187 (98%)	3 (2%)	0	100	100
22	A3	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
23	A5	152/184 (83%)	147 (97%)	5 (3%)	0	100	100
24	A6	421/437 (96%)	396 (94%)	25 (6%)	0	100	100
25	A7	134/136 (98%)	128 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	A8	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
27	A9	482/489 (99%)	462 (96%)	20 (4%)	0	100	100
28	AB	86/134 (64%)	86 (100%)	0	0	100	100
29	AC	90/134 (67%)	90 (100%)	0	0	100	100
30	AL	263/281 (94%)	249 (95%)	14 (5%)	0	100	100
31	AM	182/198 (92%)	178 (98%)	4 (2%)	0	100	100
32	AN	285/287 (99%)	279 (98%)	6 (2%)	0	100	100
33	B2	103/145 (71%)	103 (100%)	0	0	100	100
34	B3	32/62 (52%)	30 (94%)	2 (6%)	0	100	100
35	B4	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
36	B5	132/140 (94%)	130 (98%)	2 (2%)	0	100	100
37	B6	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
38	B7	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
39	B8	145/176 (82%)	142 (98%)	3 (2%)	0	100	100
40	B9	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
41	BL	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
42	BM	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
43	C1	493/495 (100%)	474 (96%)	19 (4%)	0	100	100
44	C2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
45	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
46	C4	181/185 (98%)	175 (97%)	6 (3%)	0	100	100
47	DC	165/179 (92%)	156 (94%)	9 (6%)	0	100	100
48	E1	448/483 (93%)	431 (96%)	17 (4%)	0	100	100
49	E2	464/472 (98%)	447 (96%)	17 (4%)	0	100	100
50	E3	430/594 (72%)	419 (97%)	11 (3%)	0	100	100
51	E4	349/368 (95%)	339 (97%)	10 (3%)	0	100	100
52	E5	266/290 (92%)	246 (92%)	19 (7%)	1 (0%)	30	59
53	E6	340/371 (92%)	336 (99%)	4 (1%)	0	100	100
54	E7	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
55	E8	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
56	E9	163/178 (92%)	149 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
58	EB	73/101 (72%)	73 (100%)	0	0	100	100
59	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
60	ED	136/151 (90%)	132 (97%)	4 (3%)	0	100	100
61	FX	235/325 (72%)	224 (95%)	11 (5%)	0	100	100
62	G1	424/436 (97%)	408 (96%)	16 (4%)	0	100	100
63	G2	234/267 (88%)	221 (94%)	13 (6%)	0	100	100
64	G3	253/261 (97%)	238 (94%)	15 (6%)	0	100	100
65	N1	308/670 (46%)	292 (95%)	16 (5%)	0	100	100
66	N2	294/300 (98%)	274 (93%)	20 (7%)	0	100	100
67	N3	119/293 (41%)	116 (98%)	2 (2%)	1 (1%)	16	42
67	N6	152/293 (52%)	145 (95%)	7 (5%)	0	100	100
68	N4	476/478 (100%)	462 (97%)	14 (3%)	0	100	100
69	N5	582/584 (100%)	560 (96%)	22 (4%)	0	100	100
70	QA	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
70	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
71	QB	453/474 (96%)	443 (98%)	10 (2%)	0	100	100
71	Qb	421/474 (89%)	410 (97%)	11 (3%)	0	100	100
72	QC	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
72	Qc	362/368 (98%)	353 (98%)	9 (2%)	0	100	100
73	QD	239/243 (98%)	224 (94%)	15 (6%)	0	100	100
73	Qd	239/243 (98%)	215 (90%)	24 (10%)	0	100	100
74	QE	229/252 (91%)	218 (95%)	11 (5%)	0	100	100
74	Qe	229/252 (91%)	215 (94%)	14 (6%)	0	100	100
75	QF	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
75	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
76	QG	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
76	Qg	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
77	QH	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
77	Qh	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
78	QI	28/70 (40%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Qi	28/70 (40%)	28 (100%)	0	0	100	100
79	QJ	147/154 (96%)	143 (97%)	4 (3%)	0	100	100
79	Qj	147/154 (96%)	138 (94%)	9 (6%)	0	100	100
80	QK	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
80	Qk	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
81	S2	391/395 (99%)	373 (95%)	18 (5%)	0	100	100
82	S3	246/277 (89%)	235 (96%)	11 (4%)	0	100	100
83	S4	188/208 (90%)	179 (95%)	9 (5%)	0	100	100
84	S5	110/122 (90%)	105 (96%)	5 (4%)	0	100	100
85	S6	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
86	S7	195/207 (94%)	187 (96%)	8 (4%)	0	100	100
87	S8	180/212 (85%)	174 (97%)	6 (3%)	0	100	100
88	V1	502/526 (95%)	477 (95%)	25 (5%)	0	100	100
89	V2	220/225 (98%)	212 (96%)	8 (4%)	0	100	100
All	All	22046/24488 (90%)	21217 (96%)	827 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	E5	288	THR
67	N3	214	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	1A	310/340 (91%)	306 (99%)	4 (1%)	65	88
2	1B	453/454 (100%)	452 (100%)	1 (0%)	92	97
3	2B	109/111 (98%)	108 (99%)	1 (1%)	75	92
4	4A	173/207 (84%)	172 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4C	112/127 (88%)	110 (98%)	2 (2%)	54	82
6	4D	146/147 (99%)	142 (97%)	4 (3%)	40	72
7	4E	142/145 (98%)	141 (99%)	1 (1%)	81	94
8	4F	62/62 (100%)	62 (100%)	0	100	100
9	4G	247/264 (94%)	244 (99%)	3 (1%)	67	89
10	4H	176/189 (93%)	175 (99%)	1 (1%)	84	94
11	4I	230/238 (97%)	225 (98%)	5 (2%)	47	78
12	4J	75/75 (100%)	74 (99%)	1 (1%)	65	88
13	4L	96/151 (64%)	96 (100%)	0	100	100
14	5B	134/148 (90%)	129 (96%)	5 (4%)	29	61
15	5C	167/178 (94%)	167 (100%)	0	100	100
16	6A	79/97 (81%)	79 (100%)	0	100	100
17	6B	238/243 (98%)	237 (100%)	1 (0%)	89	96
18	7A	138/150 (92%)	136 (99%)	2 (1%)	62	86
19	7C	135/152 (89%)	133 (98%)	2 (2%)	60	85
20	A1	115/118 (98%)	113 (98%)	2 (2%)	56	83
21	A2	159/160 (99%)	158 (99%)	1 (1%)	84	94
22	A3	104/104 (100%)	103 (99%)	1 (1%)	73	91
23	A5	134/152 (88%)	131 (98%)	3 (2%)	47	78
24	A6	346/358 (97%)	345 (100%)	1 (0%)	91	97
25	A7	119/119 (100%)	118 (99%)	1 (1%)	79	93
26	A8	196/196 (100%)	195 (100%)	1 (0%)	86	95
27	A9	420/424 (99%)	416 (99%)	4 (1%)	73	91
28	AB	79/114 (69%)	79 (100%)	0	100	100
29	AC	80/111 (72%)	79 (99%)	1 (1%)	65	88
30	AL	228/242 (94%)	223 (98%)	5 (2%)	47	78
31	AM	156/168 (93%)	156 (100%)	0	100	100
32	AN	241/241 (100%)	241 (100%)	0	100	100
33	B2	97/131 (74%)	96 (99%)	1 (1%)	73	91
34	B3	30/31 (97%)	30 (100%)	0	100	100
35	B4	144/144 (100%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	B5	108/108 (100%)	108 (100%)	0	100	100
37	B6	82/82 (100%)	81 (99%)	1 (1%)	67	89
38	B7	93/93 (100%)	92 (99%)	1 (1%)	70	90
39	B8	127/148 (86%)	126 (99%)	1 (1%)	79	93
40	B9	132/139 (95%)	129 (98%)	3 (2%)	45	77
41	BL	132/132 (100%)	130 (98%)	2 (2%)	60	85
42	BM	93/93 (100%)	92 (99%)	1 (1%)	70	90
43	C1	438/438 (100%)	434 (99%)	4 (1%)	75	92
44	C2	178/178 (100%)	175 (98%)	3 (2%)	56	83
45	C3	155/155 (100%)	152 (98%)	3 (2%)	52	81
46	C4	166/167 (99%)	163 (98%)	3 (2%)	54	82
47	DC	148/153 (97%)	147 (99%)	1 (1%)	81	94
48	E1	381/404 (94%)	377 (99%)	4 (1%)	73	91
49	E2	379/385 (98%)	378 (100%)	1 (0%)	91	97
50	E3	339/460 (74%)	334 (98%)	5 (2%)	60	85
51	E4	302/317 (95%)	299 (99%)	3 (1%)	73	91
52	E5	200/205 (98%)	196 (98%)	4 (2%)	50	80
53	E6	293/314 (93%)	290 (99%)	3 (1%)	73	91
54	E7	192/192 (100%)	188 (98%)	4 (2%)	48	79
55	E8	179/179 (100%)	176 (98%)	3 (2%)	56	83
56	E9	115/118 (98%)	114 (99%)	1 (1%)	75	92
57	EA	84/86 (98%)	83 (99%)	1 (1%)	67	89
58	EB	70/70 (100%)	69 (99%)	1 (1%)	62	86
59	EC	73/86 (85%)	73 (100%)	0	100	100
60	ED	121/133 (91%)	118 (98%)	3 (2%)	42	74
61	FX	212/276 (77%)	208 (98%)	4 (2%)	52	81
62	G1	356/365 (98%)	348 (98%)	8 (2%)	47	78
63	G2	192/214 (90%)	189 (98%)	3 (2%)	58	84
64	G3	202/202 (100%)	199 (98%)	3 (2%)	60	85
65	N1	295/639 (46%)	289 (98%)	6 (2%)	50	80
66	N2	285/289 (99%)	283 (99%)	2 (1%)	81	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	N3	116/281 (41%)	114 (98%)	2 (2%)	56	83
67	N6	147/281 (52%)	145 (99%)	2 (1%)	62	86
68	N4	455/455 (100%)	448 (98%)	7 (2%)	60	85
69	N5	546/546 (100%)	538 (98%)	8 (2%)	60	85
70	QA	400/401 (100%)	394 (98%)	6 (2%)	60	85
70	Qa	400/401 (100%)	397 (99%)	3 (1%)	79	93
71	QB	369/386 (96%)	365 (99%)	4 (1%)	70	90
71	Qb	342/386 (89%)	337 (98%)	5 (2%)	60	85
72	QC	337/341 (99%)	334 (99%)	3 (1%)	75	92
72	Qc	337/341 (99%)	334 (99%)	3 (1%)	75	92
73	QD	206/207 (100%)	202 (98%)	4 (2%)	52	81
73	Qd	206/207 (100%)	201 (98%)	5 (2%)	44	76
74	QE	193/209 (92%)	189 (98%)	4 (2%)	48	79
74	Qe	193/209 (92%)	193 (100%)	0	100	100
75	QF	58/63 (92%)	56 (97%)	2 (3%)	32	64
75	Qf	58/63 (92%)	54 (93%)	4 (7%)	13	35
76	QG	207/207 (100%)	204 (99%)	3 (1%)	62	86
76	Qg	207/207 (100%)	205 (99%)	2 (1%)	73	91
77	QH	71/71 (100%)	71 (100%)	0	100	100
77	Qh	71/71 (100%)	71 (100%)	0	100	100
78	QI	27/27 (100%)	26 (96%)	1 (4%)	29	61
78	Qi	27/27 (100%)	27 (100%)	0	100	100
79	QJ	124/128 (97%)	122 (98%)	2 (2%)	58	84
79	Qj	124/128 (97%)	124 (100%)	0	100	100
80	QK	50/82 (61%)	50 (100%)	0	100	100
80	Qk	50/82 (61%)	50 (100%)	0	100	100
81	S2	335/336 (100%)	331 (99%)	4 (1%)	67	89
82	S3	224/250 (90%)	223 (100%)	1 (0%)	89	96
83	S4	159/172 (92%)	157 (99%)	2 (1%)	65	88
84	S5	102/102 (100%)	101 (99%)	1 (1%)	73	91
85	S6	130/130 (100%)	127 (98%)	3 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
86	S7	165/171 (96%)	161 (98%)	4 (2%)	44	76
87	S8	160/187 (86%)	158 (99%)	2 (1%)	65	88
88	V1	412/427 (96%)	407 (99%)	5 (1%)	67	89
89	V2	190/190 (100%)	182 (96%)	8 (4%)	25	57
All	All	19190/20883 (92%)	18953 (99%)	237 (1%)	66	89

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	G1	28	ARG
86	S7	157	TYR
68	N4	123	ILE
86	S7	116	ASP
89	V2	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
68	N4	157	ASN
70	Qa	398	GLN
68	N4	321	ASN
71	QB	133	ASN
72	Qc	231	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	2MR	S2	154	81	10,12,13	2.39	2 (20%)	5,13,15	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	2MR	S2	154	81	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	S2	154	2MR	CZ-NH2	5.07	1.44	1.33
81	S2	154	2MR	CZ-NE	4.97	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	S2	154	2MR	CG-CD-NE-CZ
81	S2	154	2MR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 116 ligands modelled in this entry, 8 are monoatomic - leaving 108 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	$\# Z > 2$
94	PC1	E9	202	-	34,34,53	0.36	0	40,42,61	0.42	0
99	NDP	A9	501	-	45,52,52	0.63	0	53,80,80	0.63	1 (1%)
97	CDL	AL	302	-	67,67,99	0.37	0	73,79,111	0.33	0
97	CDL	BM	201	-	57,57,99	0.39	0	63,69,111	0.36	0
94	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.32	0
91	FES	1A	401	1	0,4,4	-	-	-	-	-
104	PX2	C2	201	-	35,35,35	0.98	4 (11%)	39,40,40	1.07	2 (5%)
94	PC1	N1	703	-	39,39,53	0.34	0	45,47,61	0.29	0
94	PC1	B5	202	-	53,53,53	0.30	0	59,61,61	0.28	0
97	CDL	C4	201	-	93,93,99	0.32	0	99,105,111	0.36	0
94	PC1	4E	201	-	34,34,53	0.37	0	40,42,61	0.34	0
94	PC1	N4	505	-	53,53,53	0.30	0	59,61,61	0.29	0
94	PC1	Qe	303	-	35,35,53	0.36	0	41,43,61	0.34	0
97	CDL	Qh	101	-	64,64,99	0.38	0	70,76,111	0.33	0
94	PC1	N1	702	-	48,48,53	0.31	0	54,56,61	0.28	0
94	PC1	A1	202	-	30,30,53	0.38	0	36,38,61	0.34	0
94	PC1	G2	301	-	37,37,53	0.35	0	43,45,61	0.31	0
97	CDL	E7	301	-	67,67,99	0.37	0	73,79,111	0.33	0
97	CDL	QJ	203	-	57,57,99	0.40	0	63,69,111	0.32	0
97	CDL	Qc	405	-	53,53,99	0.41	0	59,65,111	0.35	0
95	3PE	N4	503	-	40,40,50	0.35	0	43,45,55	0.32	0
92	SF4	1A	402	1	0,12,12	-	-	-	-	-
106	HEM	QC	402	72	41,50,50	1.29	4 (9%)	45,82,82	1.76	10 (22%)
92	SF4	S8	301	87	0,12,12	-	-	-	-	-
105	U10	N4	504	-	43,43,63	2.39	15 (34%)	52,55,79	1.84	14 (26%)
95	3PE	N5	602	-	50,50,50	0.32	0	53,55,55	0.35	0
95	3PE	B4	201	-	39,39,50	0.34	0	42,44,55	0.36	0
94	PC1	B5	201	-	53,53,53	0.29	0	59,61,61	0.33	0
92	SF4	S8	302	87	0,12,12	-	-	-	-	-
91	FES	QE	301	74	0,4,4	-	-	-	-	-
94	PC1	Qc	404	-	30,30,53	0.40	0	36,38,61	0.44	0
97	CDL	AM	202	-	71,71,99	0.36	0	77,83,111	0.32	0
94	PC1	Qc	401	-	53,53,53	0.30	0	59,61,61	0.32	0
97	CDL	C4	203	-	97,97,99	0.32	0	103,109,111	0.34	0
95	3PE	4D	202	-	50,50,50	0.31	0	53,55,55	0.36	0
106	HEM	Qc	402	72	41,50,50	1.23	5 (12%)	45,82,82	1.75	8 (17%)
97	CDL	7C	201	-	89,89,99	0.32	0	95,101,111	0.30	0
107	HEC	Qd	301	73	32,50,50	2.03	4 (12%)	24,82,82	2.22	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
97	CDL	AL	303	-	63,63,99	0.38	0	69,75,111	0.33	0
95	3PE	7A	202	-	40,40,50	0.35	0	43,45,55	0.31	0
95	3PE	E9	201	-	50,50,50	0.30	0	53,55,55	0.28	0
97	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.36	0
106	HEM	Qc	403	72	41,50,50	1.28	5 (12%)	45,82,82	1.73	10 (22%)
94	PC1	A9	502	-	32,32,53	0.39	0	38,40,61	0.34	0
91	FES	Qe	301	74	0,4,4	-	-	-	-	-
97	CDL	C4	202	-	68,68,99	0.36	0	74,80,111	0.37	0
97	CDL	B3	101	-	64,64,99	0.38	0	70,76,111	0.33	0
95	3PE	C1	506	-	39,39,50	0.36	0	42,44,55	0.35	0
94	PC1	Qj	201	-	53,53,53	0.31	0	59,61,61	0.30	0
108	FMN	V1	601	-	33,33,33	0.36	0	48,50,50	0.43	0
107	HEC	QD	301	73	32,50,50	2.07	4 (12%)	24,82,82	2.32	15 (62%)
97	CDL	QD	302	-	68,68,99	0.37	0	74,80,111	0.36	0
97	CDL	A9	504	-	63,63,99	0.39	0	69,75,111	0.35	0
94	PC1	QI	101	-	35,35,53	0.36	0	41,43,61	0.40	0
94	PC1	N3	301	-	41,41,53	0.34	0	47,49,61	0.34	0
97	CDL	QH	102	-	59,59,99	0.38	0	65,71,111	0.35	0
95	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.34	0
101	HEA	C1	502	43	57,67,67	2.04	15 (26%)	61,103,103	2.62	23 (37%)
95	3PE	C1	507	-	39,39,50	0.35	0	42,44,55	0.38	0
94	PC1	N4	502	-	32,32,53	0.37	0	38,40,61	0.38	0
94	PC1	A1	201	-	48,48,53	0.32	0	54,56,61	0.35	0
94	PC1	E4	402	-	50,50,53	0.30	0	56,58,61	0.29	0
91	FES	V2	301	89	0,4,4	-	-	-	-	-
97	CDL	N1	701	-	69,69,99	0.37	0	75,81,111	0.32	0
106	HEM	QC	401	72	41,50,50	1.24	5 (12%)	45,82,82	1.70	7 (15%)
94	PC1	AN	301	-	47,47,53	0.31	0	53,55,61	0.30	0
94	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.28	0
94	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.34	0
94	PC1	AM	204	-	47,47,53	0.32	0	53,55,61	0.26	0
94	PC1	A9	503	-	32,32,53	0.38	0	38,40,61	0.36	0
94	PC1	E8	303	-	32,32,53	0.37	0	38,40,61	0.35	0
92	SF4	S7	301	86	0,12,12	-	-	-	-	-
104	PX2	QJ	202	-	35,35,35	0.98	3 (8%)	39,40,40	1.08	2 (5%)
97	CDL	B8	302	-	69,69,99	0.36	0	75,81,111	0.31	0
100	ZMP	AC	201	29	29,35,36	0.83	1 (3%)	34,42,45	1.09	3 (8%)
94	PC1	AM	203	-	48,48,53	0.31	0	54,56,61	0.32	0
94	PC1	4A	301	-	46,46,53	0.32	0	52,54,61	0.31	0
97	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
97	CDL	QC	403	-	55,55,99	0.41	0	61,67,111	0.33	0
94	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
97	CDL	EA	201	-	58,58,99	0.40	0	64,70,111	0.39	0
97	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.27	0
94	PC1	AL	301	-	49,49,53	0.32	0	55,57,61	0.29	0
94	PC1	C3	201	-	50,50,53	0.31	0	56,58,61	0.30	0
97	CDL	EA	202	-	54,54,99	0.40	0	60,66,111	0.37	0
104	PX2	QJ	201	-	35,35,35	0.99	3 (8%)	39,40,40	1.05	2 (5%)
94	PC1	7A	201	-	35,35,53	0.37	0	41,43,61	0.35	0
92	SF4	1A	403	1	0,12,12	-	-	-	-	-
94	PC1	N5	601	-	35,35,53	0.35	0	41,43,61	0.30	0
97	CDL	E6	401	-	57,57,99	0.39	0	63,69,111	0.45	0
97	CDL	AM	201	-	71,71,99	0.36	0	77,83,111	0.32	0
94	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.32	0
97	CDL	QH	101	-	75,75,99	0.36	0	81,87,111	0.32	0
97	CDL	E4	401	-	71,71,99	0.36	0	77,83,111	0.38	0
94	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.30	0
94	PC1	QD	303	-	30,30,53	0.39	0	36,38,61	0.38	0
97	CDL	Qe	302	-	59,59,99	0.38	0	65,71,111	0.34	0
101	HEA	C1	501	43	57,67,67	2.00	18 (31%)	61,103,103	2.59	27 (44%)
97	CDL	N5	603	-	92,92,99	0.31	0	98,104,111	0.31	0
94	PC1	N4	501	-	38,38,53	0.33	0	44,46,61	0.29	0
94	PC1	QC	404	-	53,53,53	0.30	0	59,61,61	0.33	0
100	ZMP	AB	201	28	29,35,36	0.77	1 (3%)	34,42,45	1.21	5 (14%)
94	PC1	ED	201	-	53,53,53	0.30	0	59,61,61	0.31	0
96	S12	4D	203	-	33,34,34	0.78	0	36,40,40	0.97	3 (8%)
97	CDL	A3	201	-	57,57,99	0.39	0	63,69,111	0.37	0
94	PC1	ED	202	-	40,40,53	0.33	0	46,48,61	0.33	0
94	PC1	B8	301	-	36,36,53	0.35	0	42,44,61	0.47	0
92	SF4	V1	602	88	0,12,12	-	-	-	-	-

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
94	PC1	E9	202	-	-	8/38/38/57	-
99	NDP	A9	501	-	-	10/30/77/77	0/5/5/5
97	CDL	AL	302	-	-	10/78/78/110	-
97	CDL	BM	201	-	-	7/68/68/110	-
94	PC1	E8	304	-	-	11/33/33/57	-
91	FES	1A	401	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
104	PX2	C2	201	-	-	20/37/37/37	-
94	PC1	N1	703	-	-	17/43/43/57	-
94	PC1	B5	202	-	-	19/57/57/57	-
97	CDL	C4	201	-	-	23/104/104/110	-
94	PC1	4E	201	-	-	13/38/38/57	-
94	PC1	N4	505	-	-	13/57/57/57	-
94	PC1	Qe	303	-	-	6/39/39/57	-
97	CDL	Qh	101	-	-	18/75/75/110	-
94	PC1	N1	702	-	-	14/52/52/57	-
94	PC1	A1	202	-	-	7/34/34/57	-
94	PC1	G2	301	-	-	9/41/41/57	-
97	CDL	E7	301	-	-	18/78/78/110	-
97	CDL	QJ	203	-	-	19/68/68/110	-
97	CDL	Qc	405	-	-	15/64/64/110	-
95	3PE	N4	503	-	-	8/44/44/54	-
92	SF4	1A	402	1	-	-	0/6/5/5
106	HEM	QC	402	72	-	4/12/54/54	-
92	SF4	S8	301	87	-	-	0/6/5/5
105	U10	N4	504	-	-	10/39/63/87	0/1/1/1
95	3PE	N5	602	-	-	11/54/54/54	-
95	3PE	B4	201	-	-	16/43/43/54	-
94	PC1	B5	201	-	-	15/57/57/57	-
92	SF4	S8	302	87	-	-	0/6/5/5
94	PC1	Qc	404	-	-	12/34/34/57	-
91	FES	QE	301	74	-	-	0/1/1/1
97	CDL	AM	202	-	-	20/82/82/110	-
94	PC1	Qc	401	-	-	17/57/57/57	-
97	CDL	C4	203	-	-	25/108/108/110	-
95	3PE	4D	202	-	-	21/54/54/54	-
106	HEM	Qc	402	72	-	5/12/54/54	-
97	CDL	7C	201	-	-	25/100/100/110	-
107	HEC	Qd	301	73	-	5/10/54/54	-
97	CDL	AL	303	-	-	15/74/74/110	-
95	3PE	7A	202	-	-	7/44/44/54	-
95	3PE	E9	201	-	-	8/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	CDL	Qj	202	-	-	19/58/58/110	-
106	HEM	Qc	403	72	-	4/12/54/54	-
94	PC1	A9	502	-	-	13/36/36/57	-
97	CDL	C4	202	-	-	10/79/79/110	-
91	FES	Qe	301	74	-	-	0/1/1/1
97	CDL	B3	101	-	-	10/75/75/110	-
95	3PE	C1	506	-	-	16/43/43/54	-
94	PC1	Qj	201	-	-	16/57/57/57	-
108	FMN	V1	601	-	-	3/18/18/18	0/3/3/3
107	HEC	QD	301	73	-	2/10/54/54	-
97	CDL	QD	302	-	-	15/79/79/110	-
97	CDL	A9	504	-	-	25/74/74/110	-
94	PC1	QI	101	-	-	3/39/39/57	-
94	PC1	N3	301	-	-	8/45/45/57	-
97	CDL	QH	102	-	-	19/70/70/110	-
95	3PE	4D	201	-	-	11/38/38/54	-
101	HEA	C1	502	43	-	16/32/76/76	-
95	3PE	C1	507	-	-	11/43/43/54	-
94	PC1	N4	502	-	-	10/36/36/57	-
94	PC1	A1	201	-	-	15/52/52/57	-
94	PC1	E4	402	-	-	9/54/54/57	-
91	FES	V2	301	89	-	-	0/1/1/1
97	CDL	N1	701	-	-	24/80/80/110	-
106	HEM	QC	401	72	-	6/12/54/54	-
94	PC1	AN	301	-	-	9/51/51/57	-
94	PC1	E8	301	-	-	13/57/57/57	-
94	PC1	Qg	301	-	-	3/31/31/57	-
94	PC1	AM	204	-	-	10/51/51/57	-
94	PC1	A9	503	-	-	6/36/36/57	-
94	PC1	E8	303	-	-	6/36/36/57	-
92	SF4	S7	301	86	-	-	0/6/5/5
104	PX2	QJ	202	-	-	24/37/37/37	-
97	CDL	B8	302	-	-	13/80/80/110	-
100	ZMP	AC	201	29	-	18/40/42/43	-
94	PC1	AM	203	-	-	18/52/52/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	PC1	4A	301	-	-	8/50/50/57	-
97	CDL	4E	202	-	-	20/82/82/110	-
97	CDL	QC	403	-	-	17/66/66/110	-
94	PC1	4A	302	-	-	21/49/49/57	-
97	CDL	EA	201	-	-	14/69/69/110	-
97	CDL	Qd	302	-	-	27/110/110/110	-
94	PC1	AL	301	-	-	12/53/53/57	-
94	PC1	C3	201	-	-	9/54/54/57	-
97	CDL	EA	202	-	-	17/65/65/110	-
104	PX2	QJ	201	-	-	19/37/37/37	-
94	PC1	7A	201	-	-	14/39/39/57	-
92	SF4	1A	403	1	-	-	0/6/5/5
94	PC1	N5	601	-	-	9/39/39/57	-
97	CDL	E6	401	-	-	23/68/68/110	-
97	CDL	AM	201	-	-	14/82/82/110	-
94	PC1	C1	505	-	-	10/53/53/57	-
97	CDL	QH	101	-	-	20/86/86/110	-
97	CDL	E4	401	-	-	14/82/82/110	-
94	PC1	E8	302	-	-	13/57/57/57	-
94	PC1	QD	303	-	-	11/34/34/57	-
97	CDL	Qe	302	-	-	12/70/70/110	-
101	HEA	C1	501	43	-	15/32/76/76	-
97	CDL	N5	603	-	-	30/103/103/110	-
94	PC1	N4	501	-	-	13/42/42/57	-
94	PC1	QC	404	-	-	8/57/57/57	-
100	ZMP	AB	201	28	-	20/40/42/43	-
94	PC1	ED	201	-	-	11/57/57/57	-
96	S12	4D	203	-	-	14/38/38/38	-
97	CDL	A3	201	-	-	7/68/68/110	-
94	PC1	ED	202	-	-	16/44/44/57	-
94	PC1	B8	301	-	-	8/40/40/57	-
92	SF4	V1	602	88	-	-	0/6/5/5

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
105	N4	504	U10	C6-C1	10.22	1.53	1.35
107	QD	301	HEC	C3C-C2C	-6.60	1.33	1.40
107	QD	301	HEC	C2B-C3B	-6.60	1.33	1.40
107	Qd	301	HEC	C3C-C2C	-6.57	1.33	1.40
107	Qd	301	HEC	C2B-C3B	-6.28	1.34	1.40

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	502	HEA	CAD-CBD-CGD	-8.14	96.09	113.60
101	C1	501	HEA	CAD-CBD-CGD	-6.75	99.07	113.60
101	C1	501	HEA	C2B-C1B-NB	5.67	116.68	109.88
101	C1	501	HEA	C3D-C4D-ND	5.42	115.60	110.36
101	C1	502	HEA	C13-C12-C11	-5.29	106.40	114.35

There are no chirality outliers.

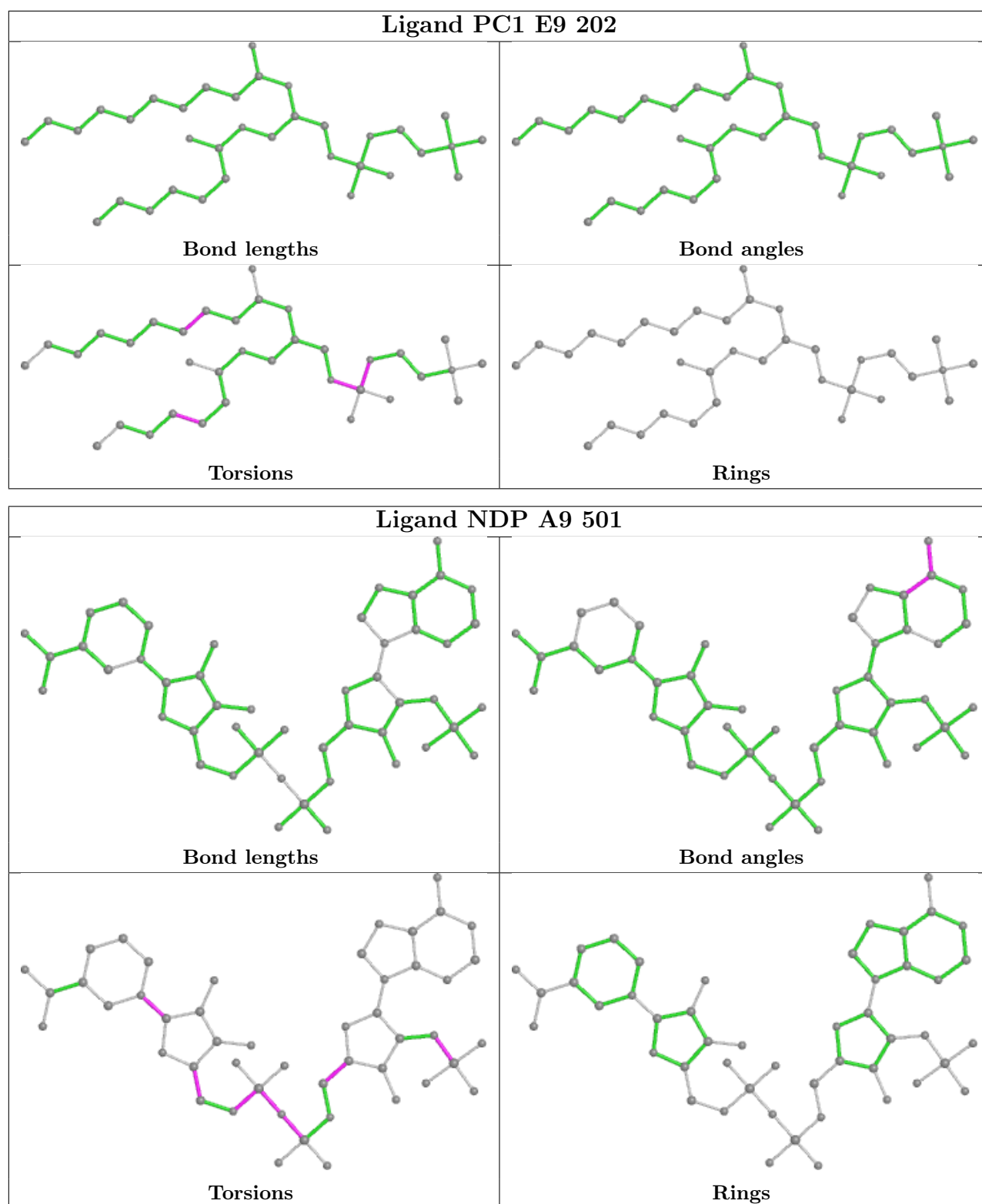
5 of 1312 torsion outliers are listed below:

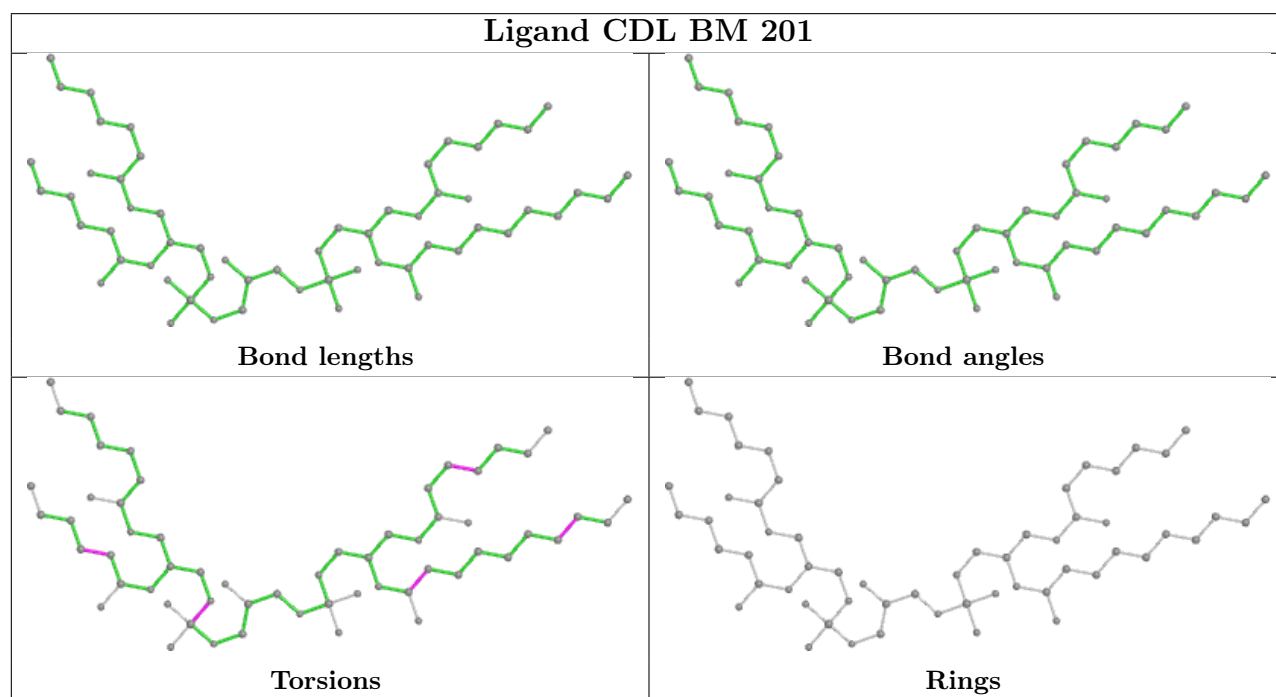
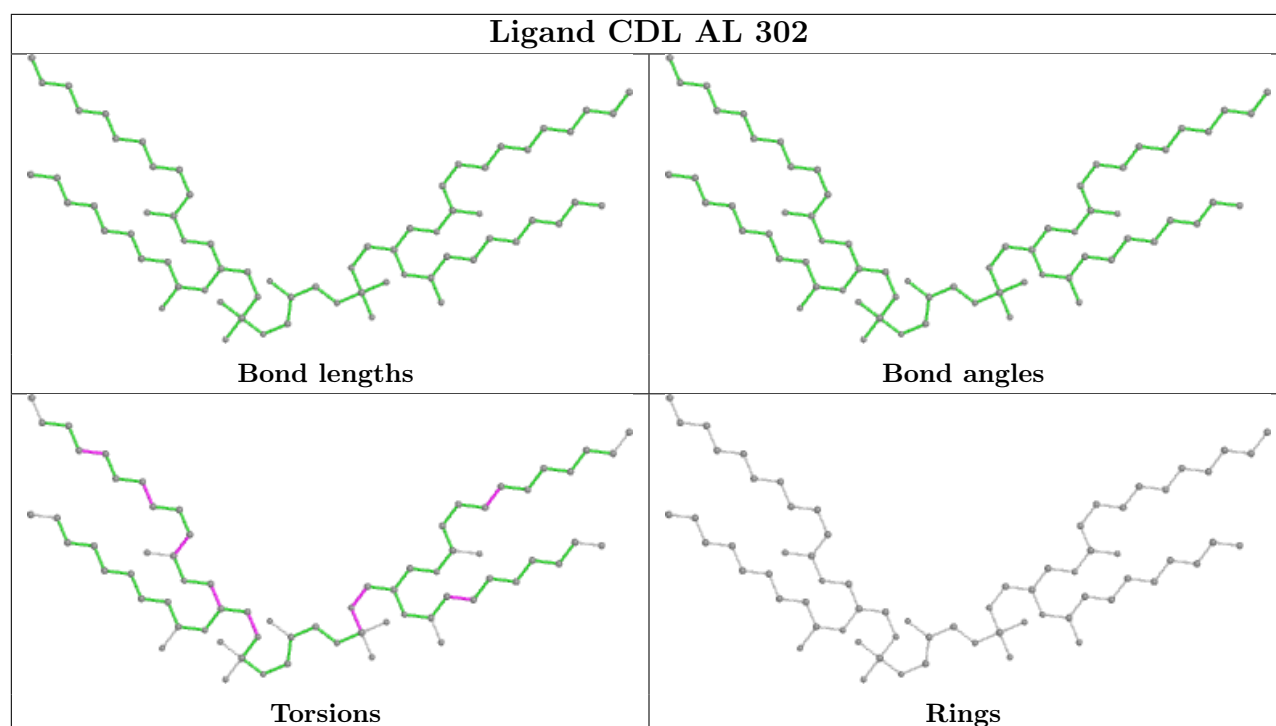
Mol	Chain	Res	Type	Atoms
94	4A	301	PC1	C11-O13-P-O12
94	4A	301	PC1	C1-O11-P-O14
94	4A	302	PC1	C11-O13-P-O14
94	4A	302	PC1	C1-O11-P-O12
94	4A	302	PC1	O21-C2-C3-O31

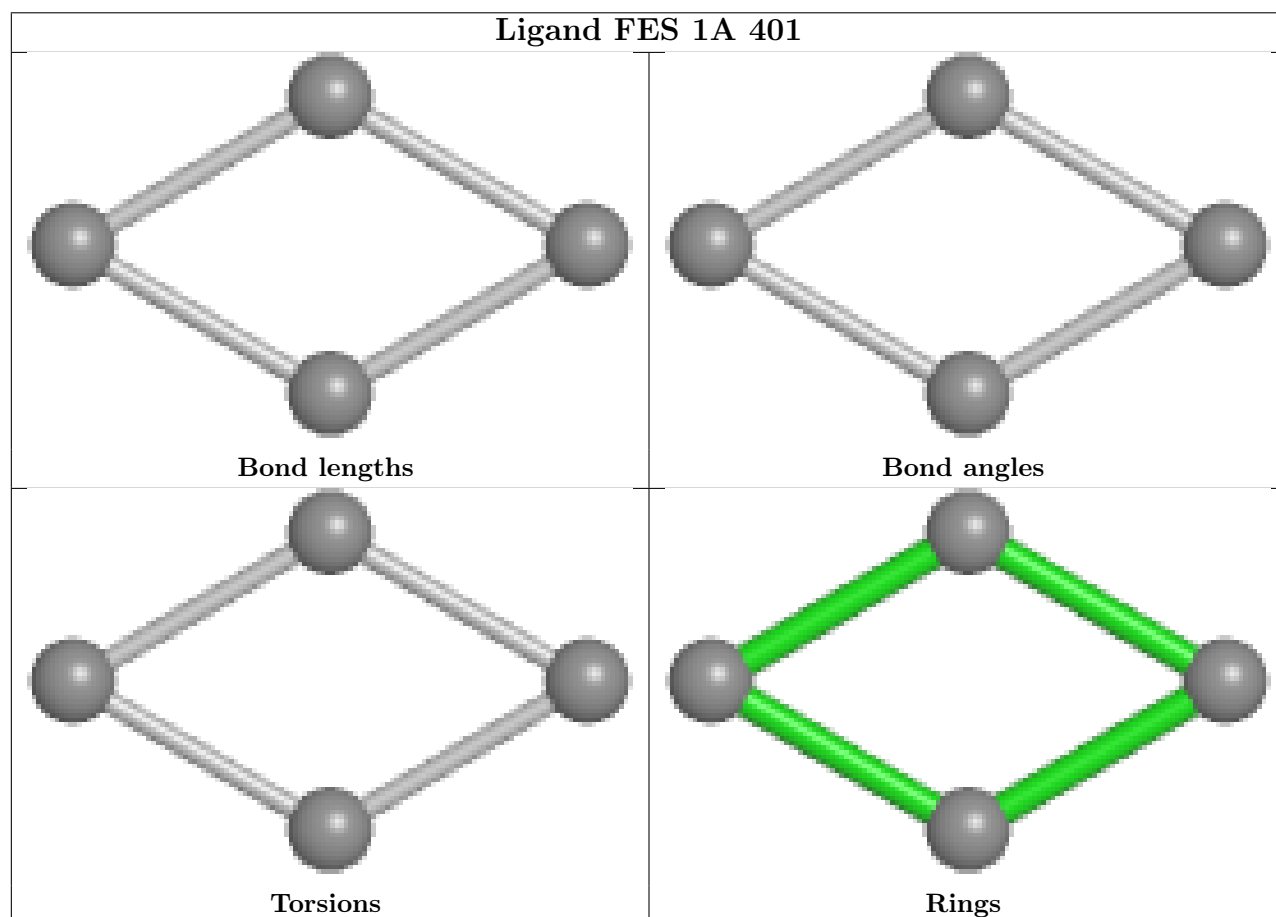
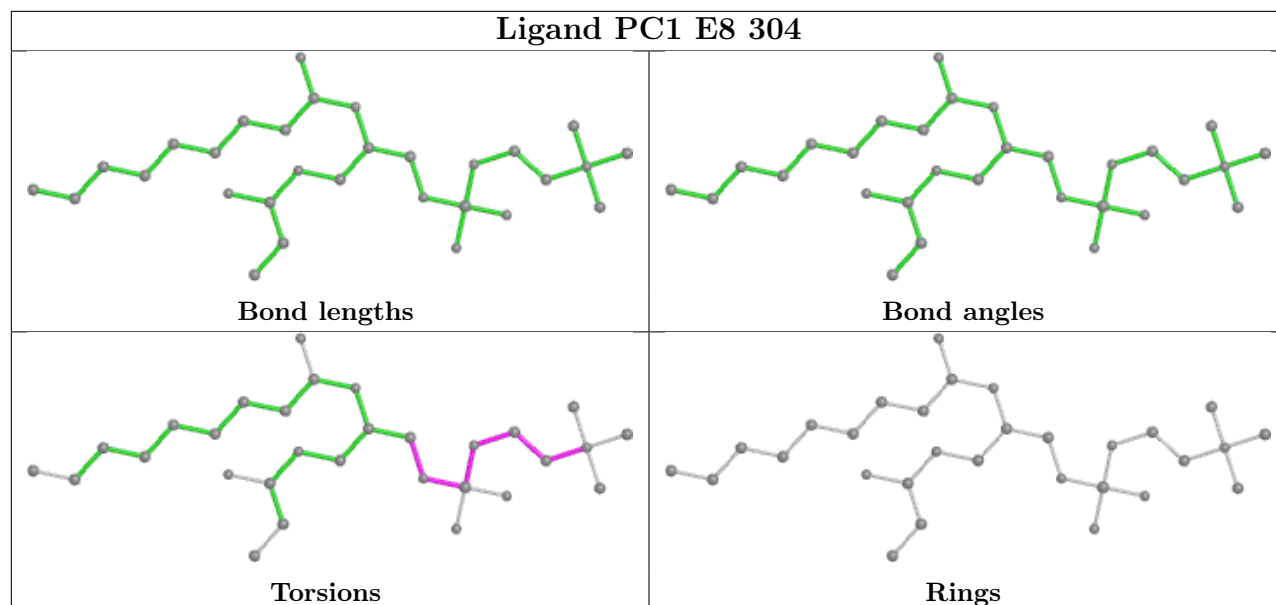
There are no ring outliers.

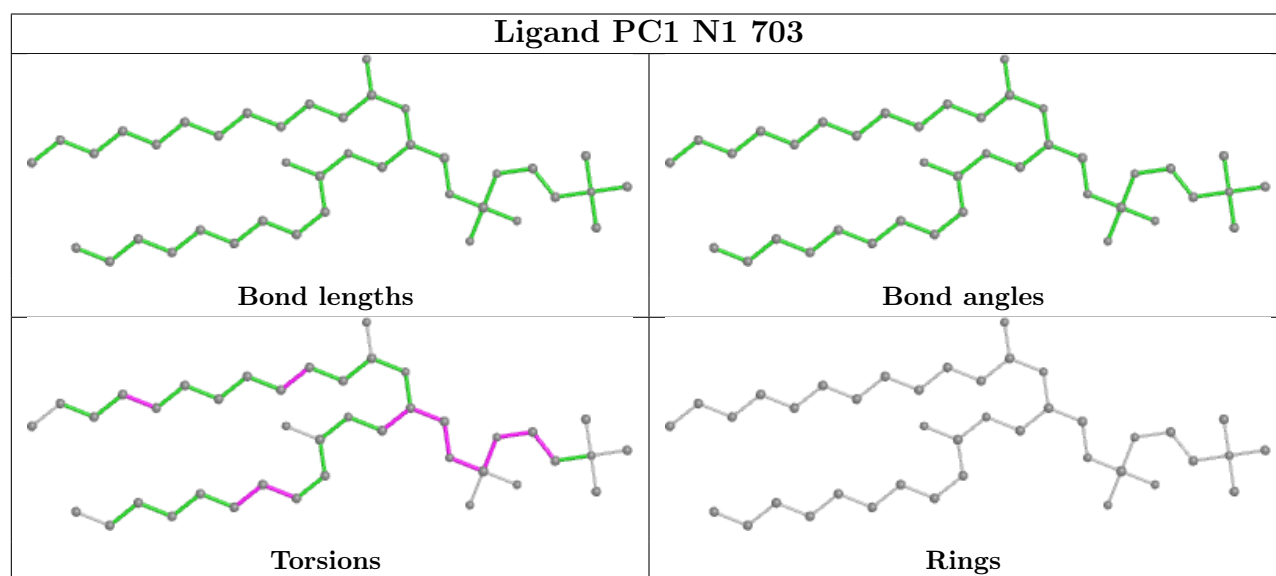
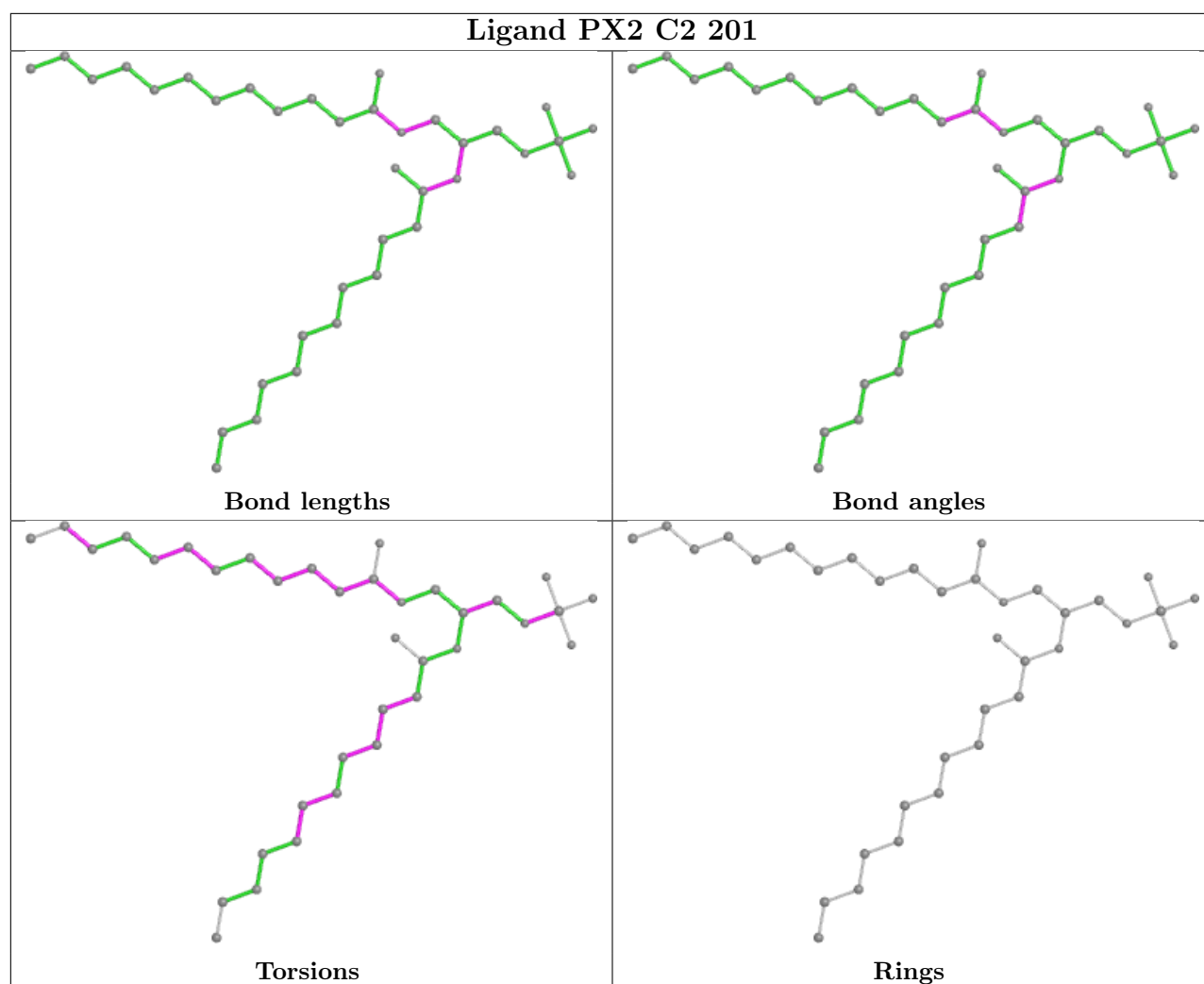
No monomer is involved in short contacts.

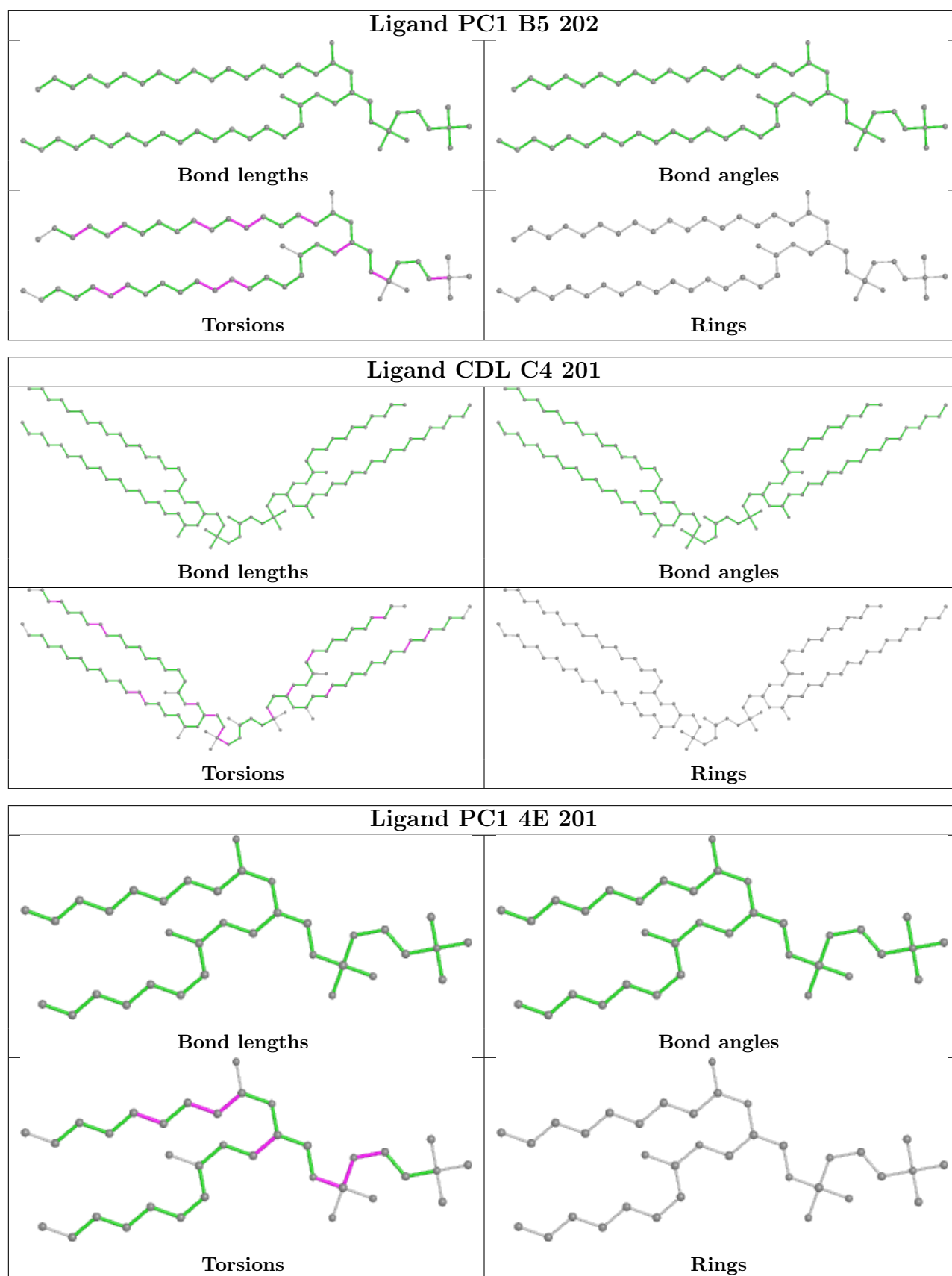
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

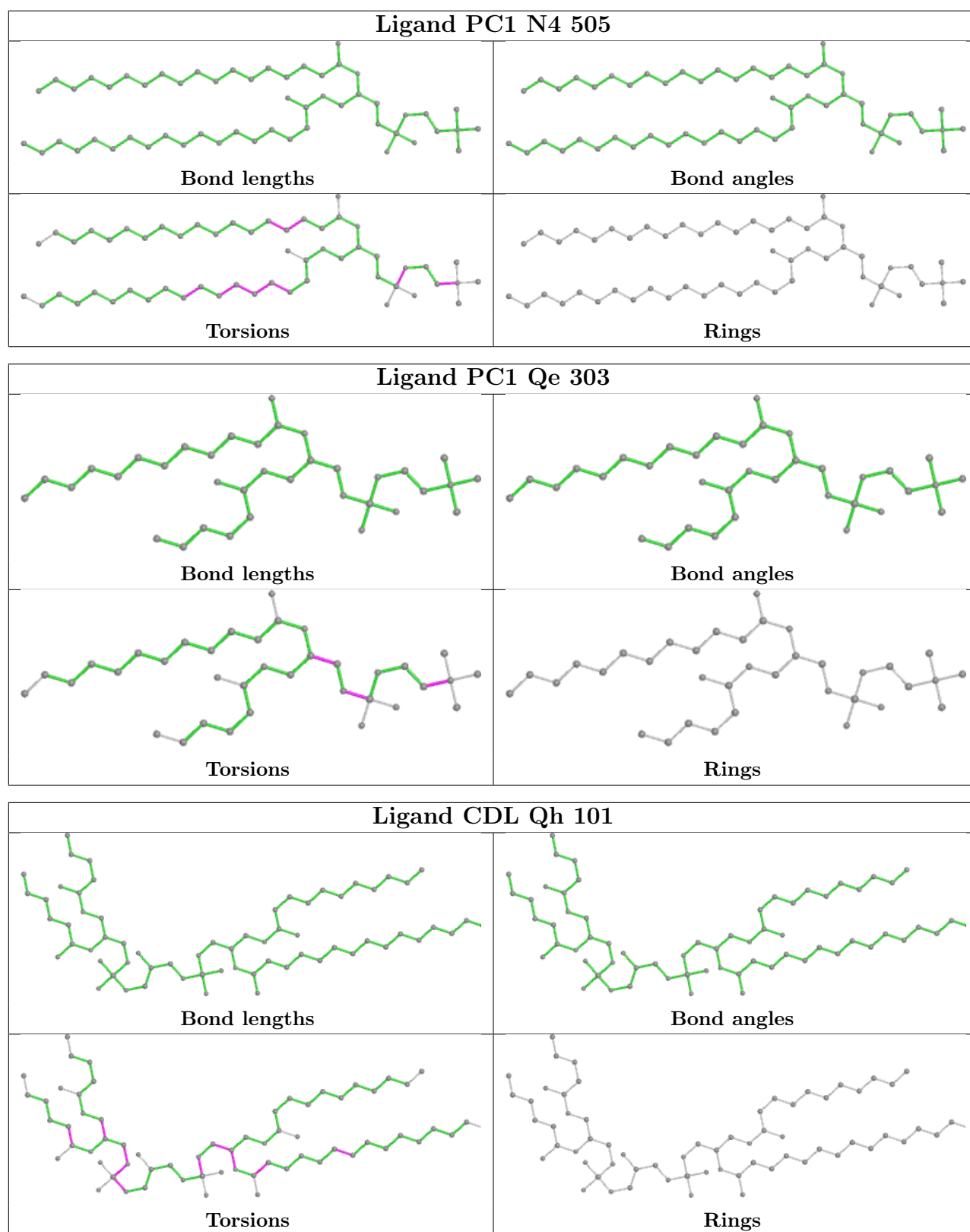


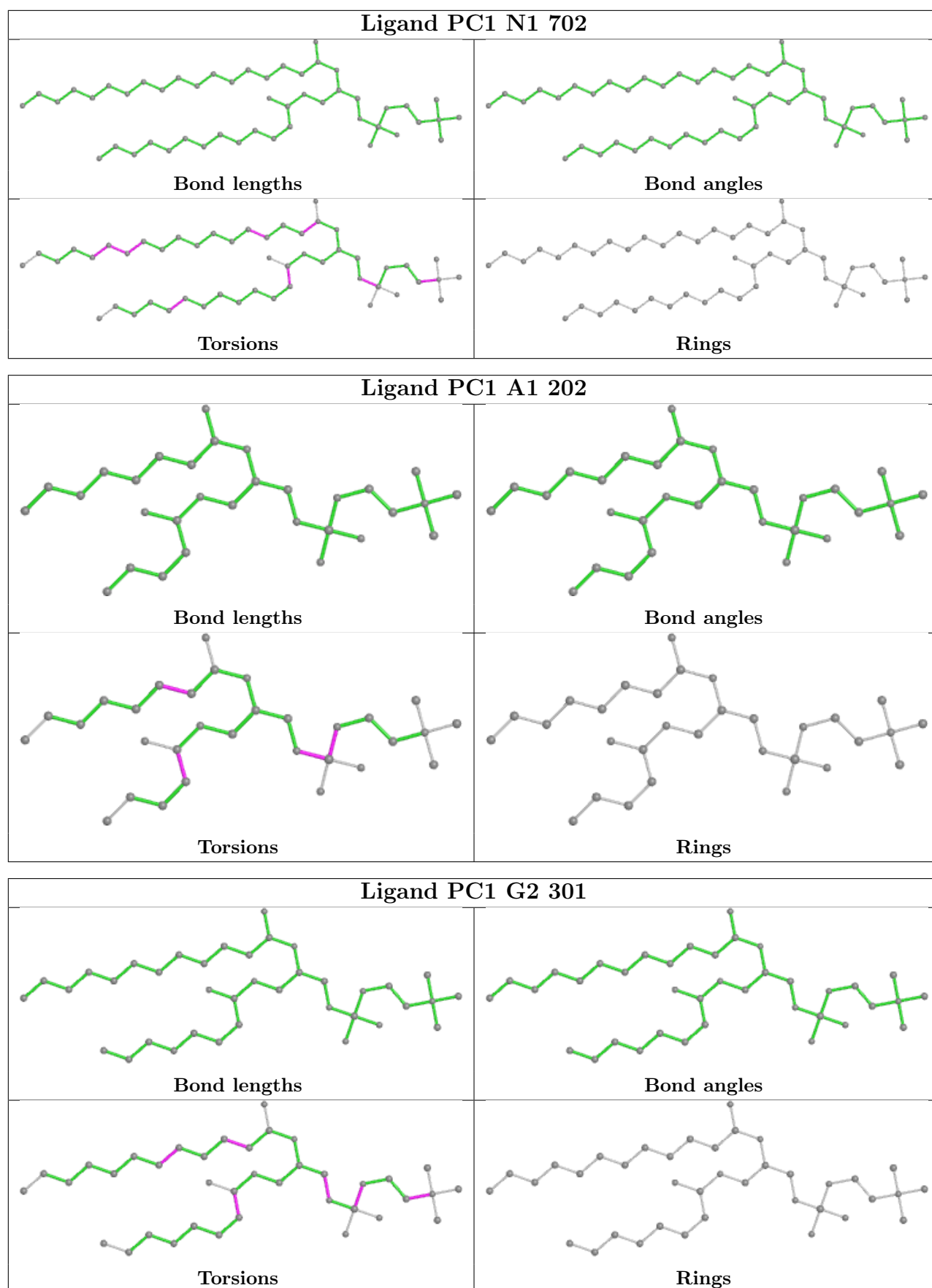


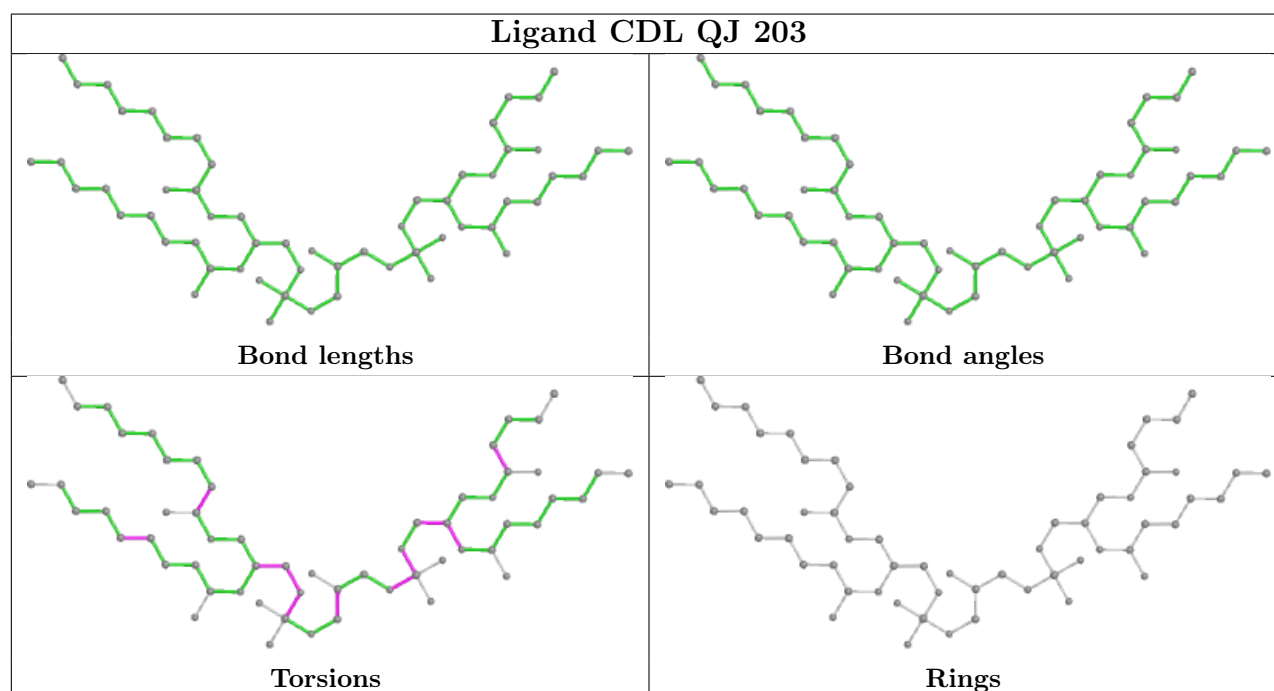
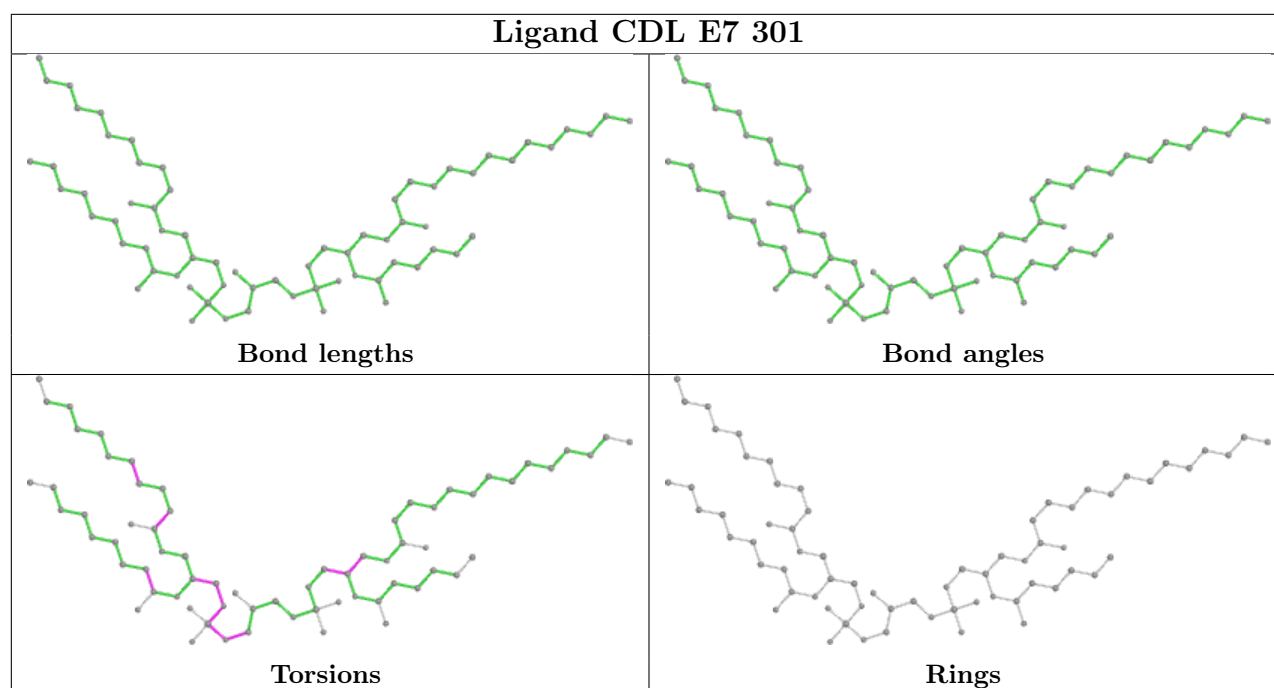


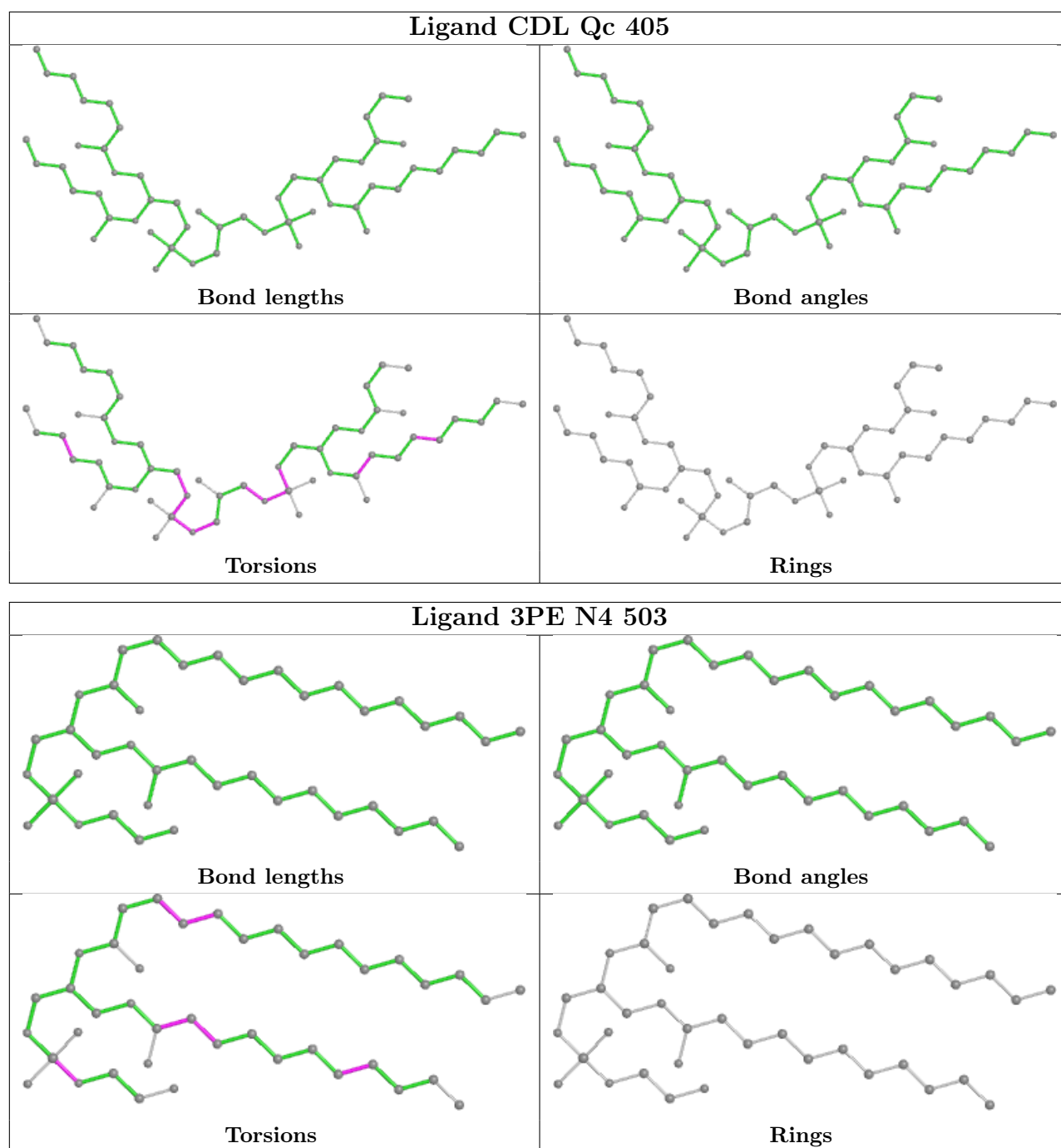


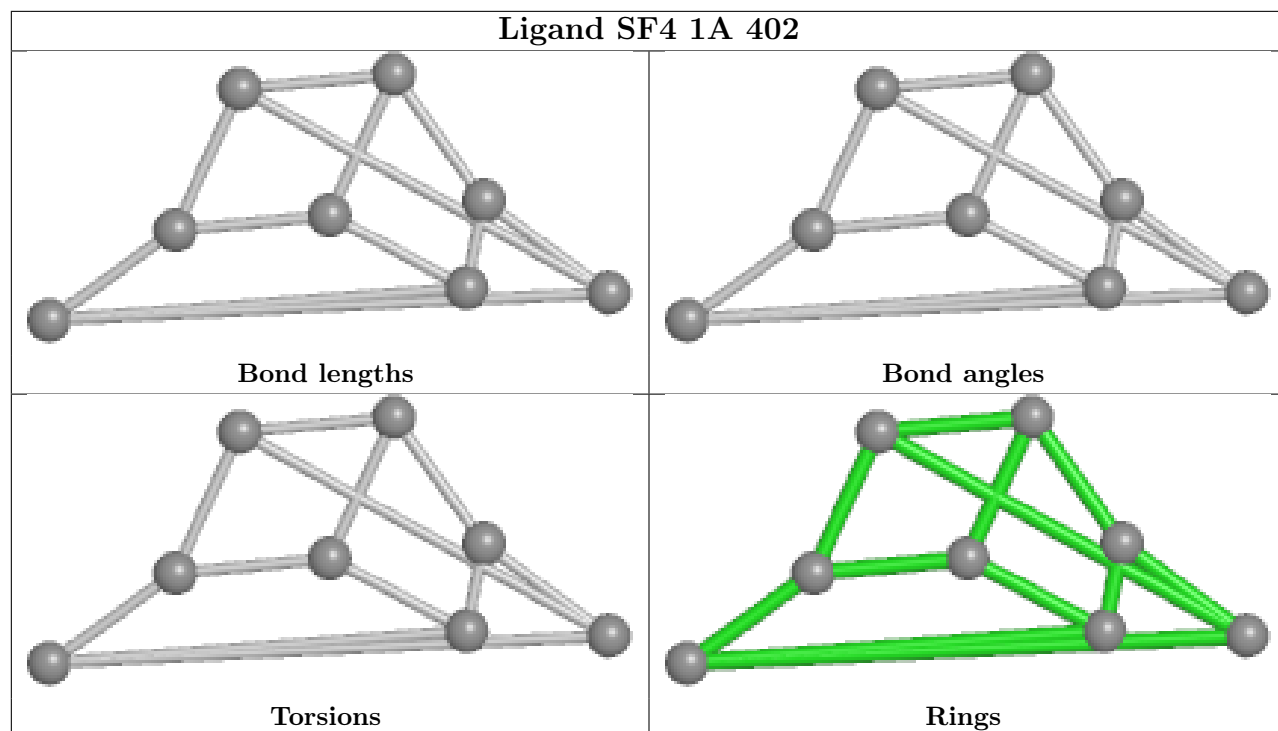


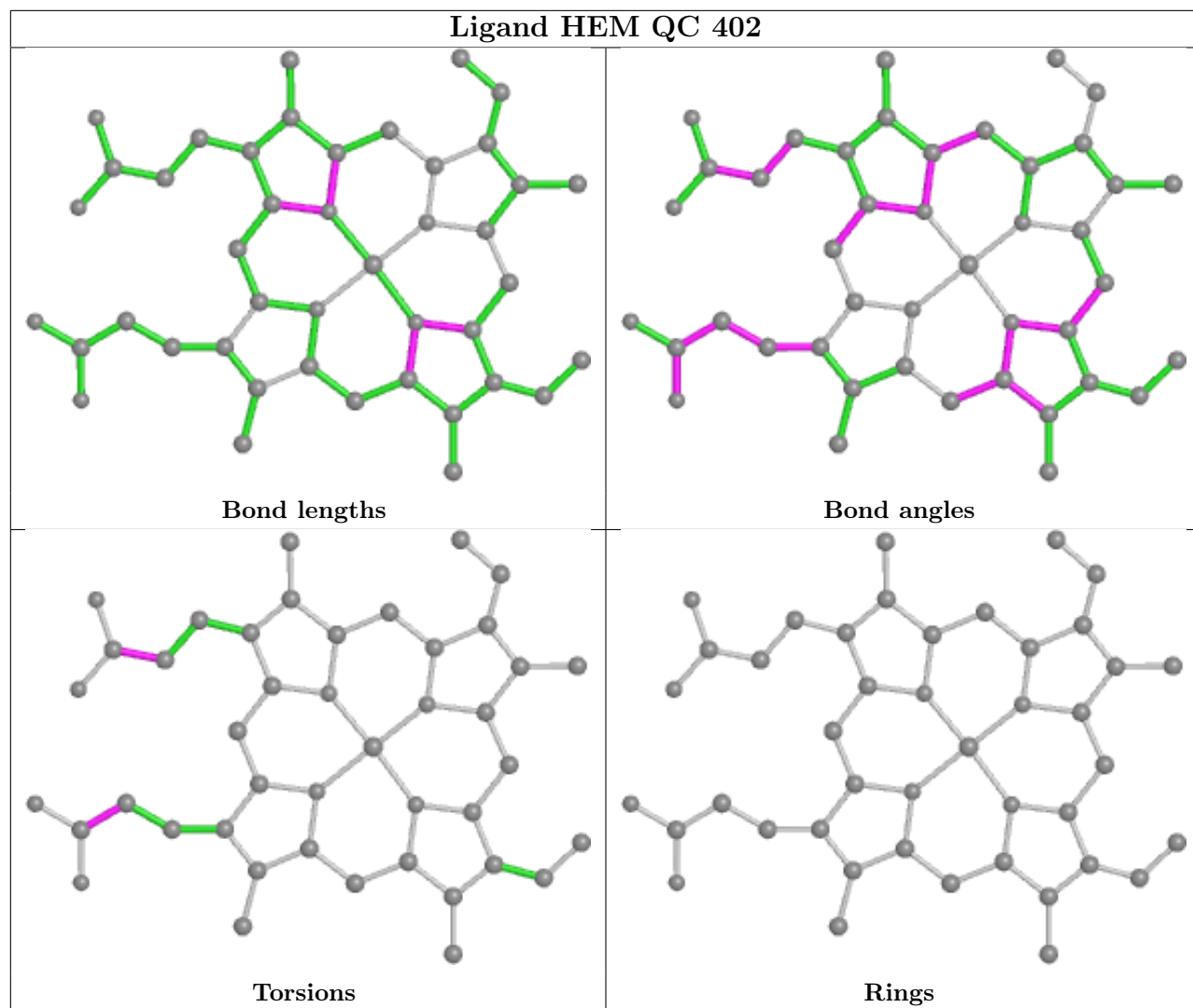


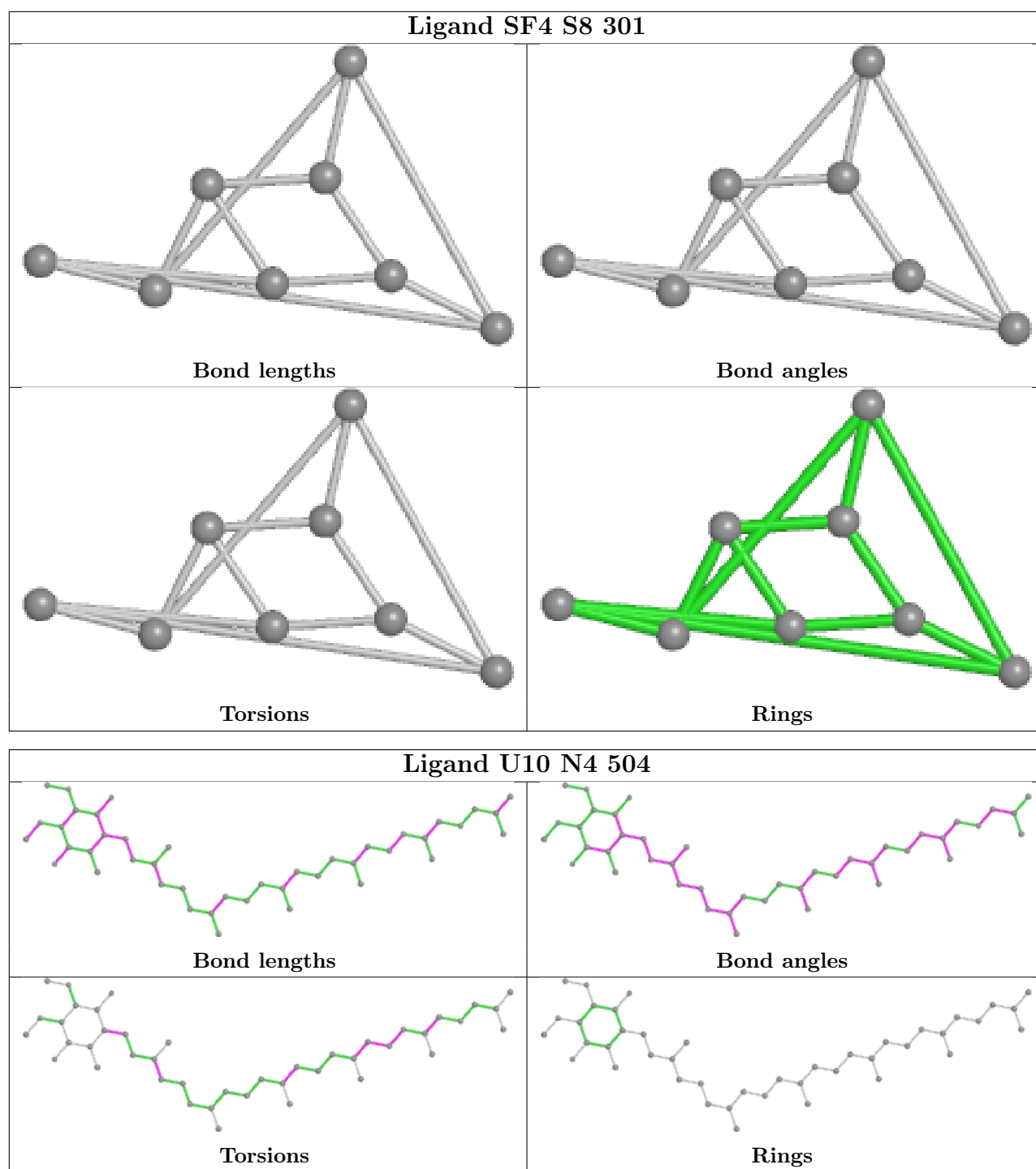


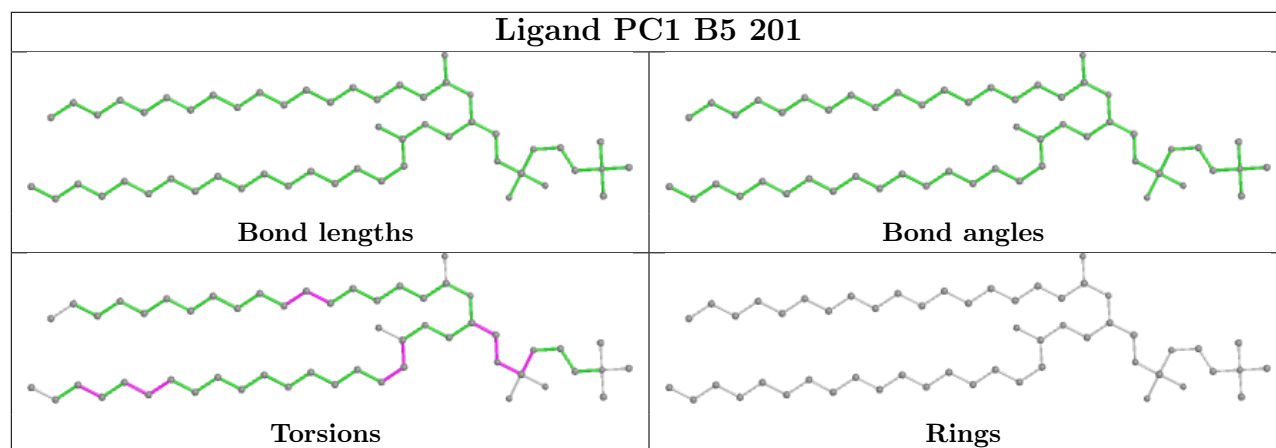
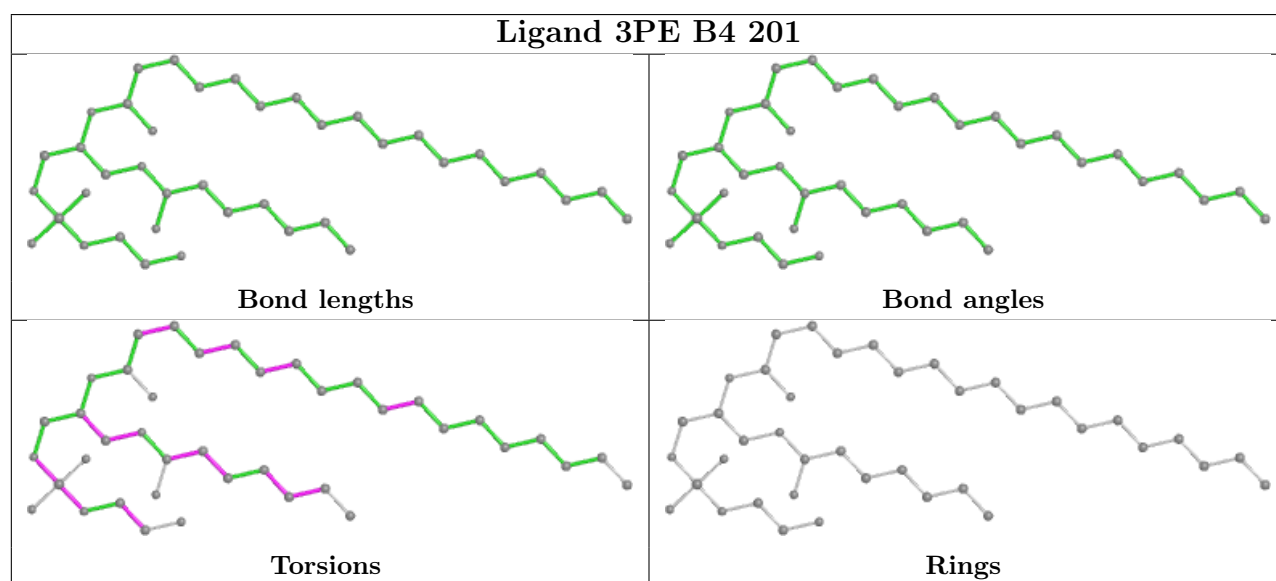
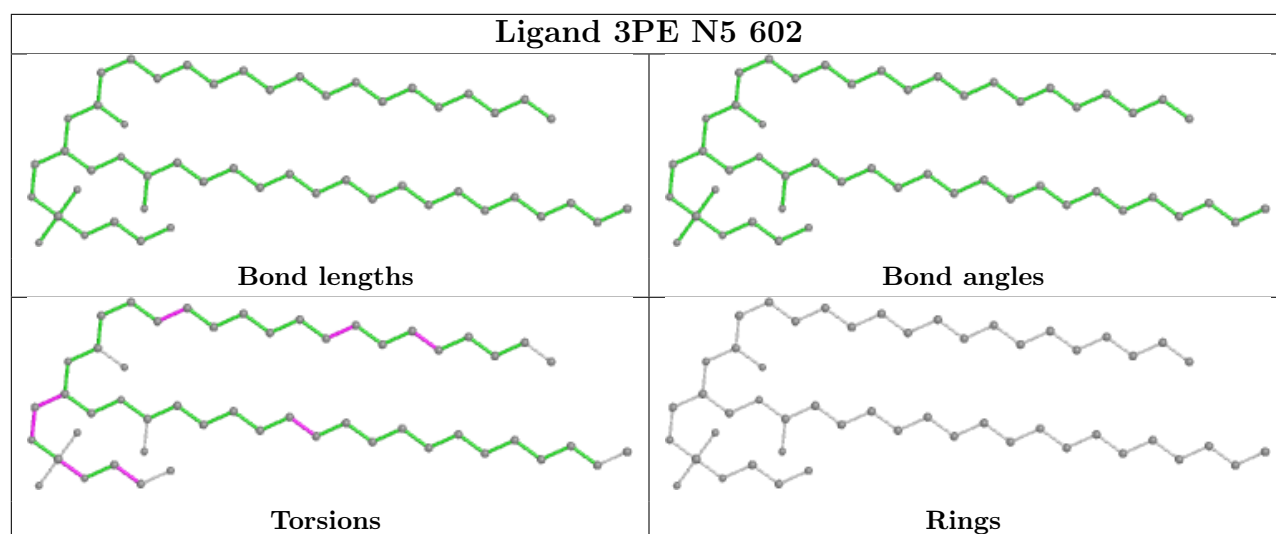


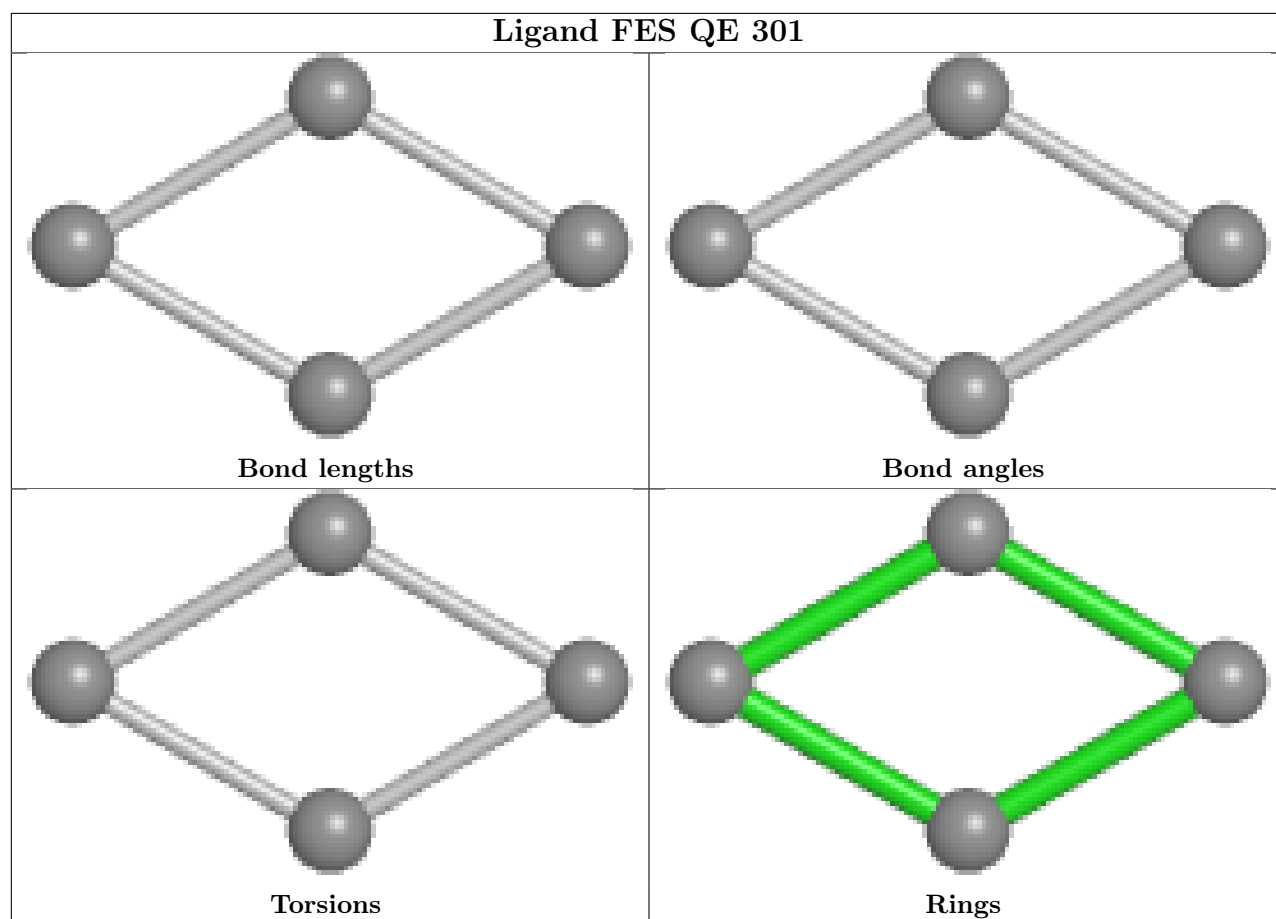
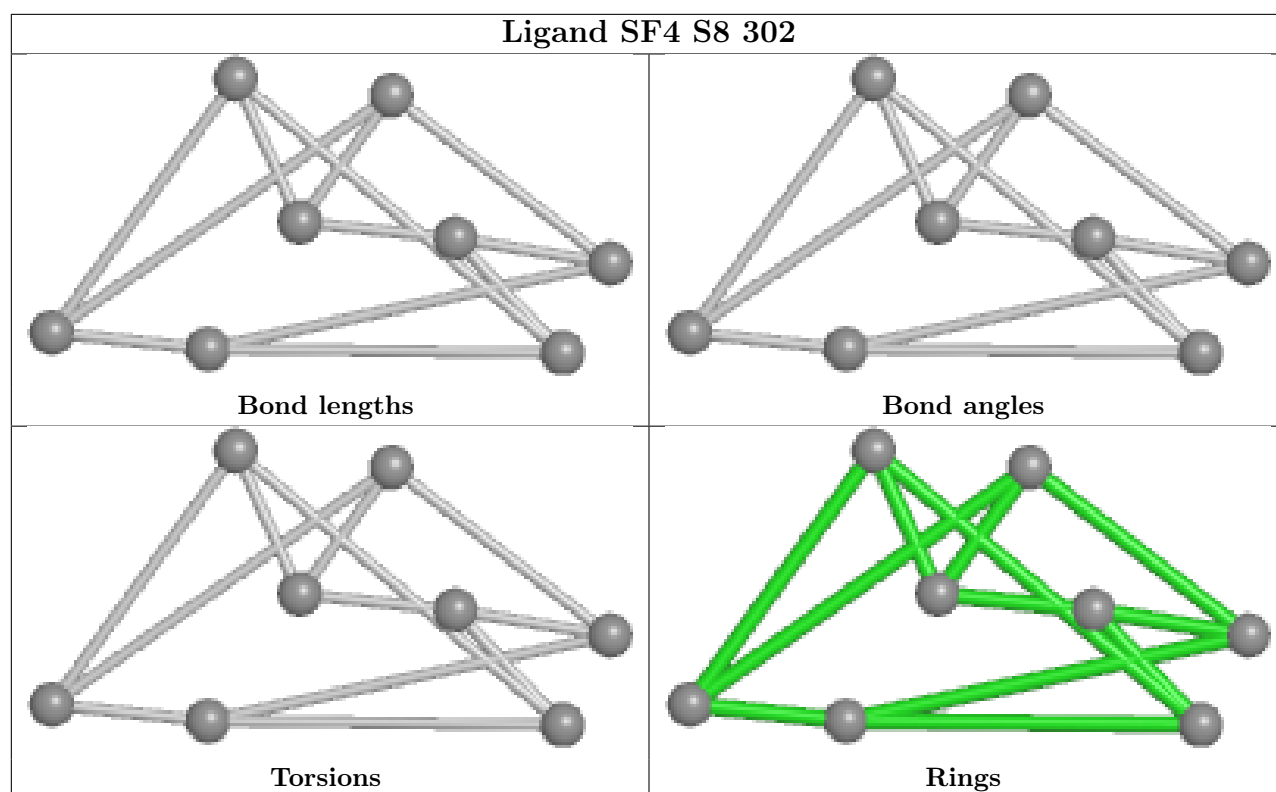


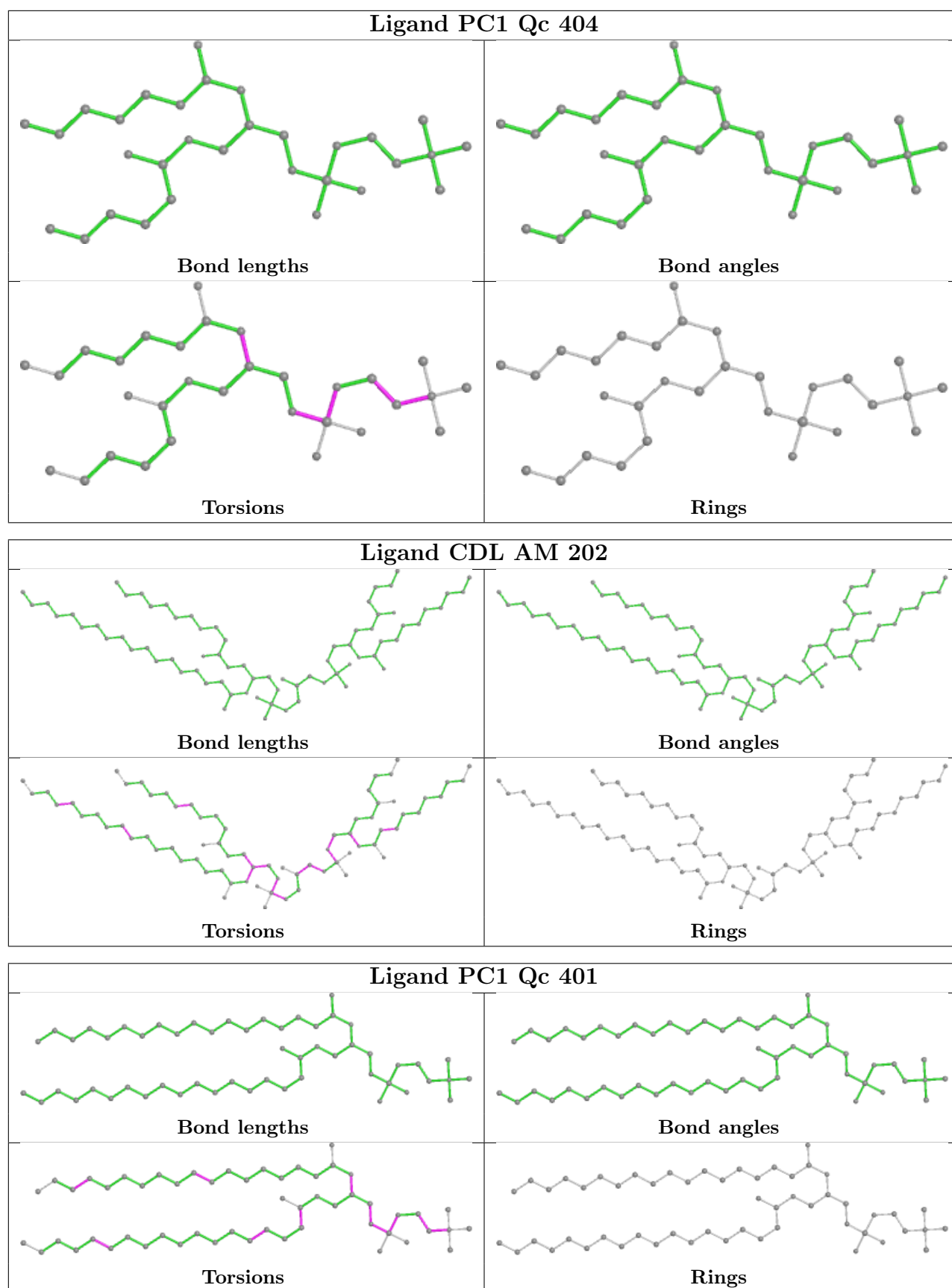


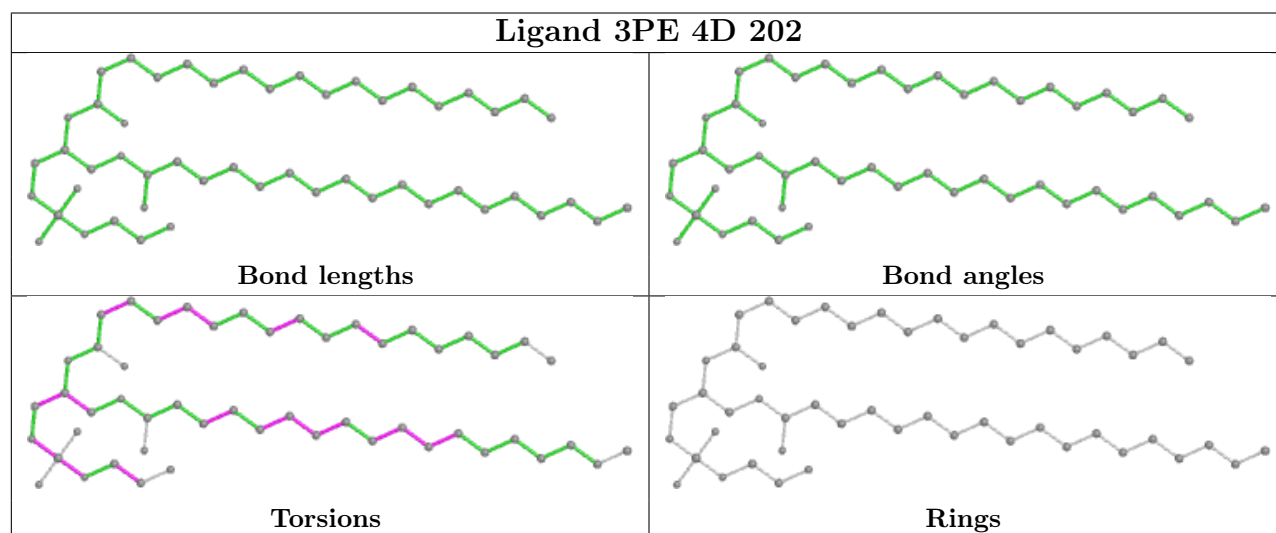
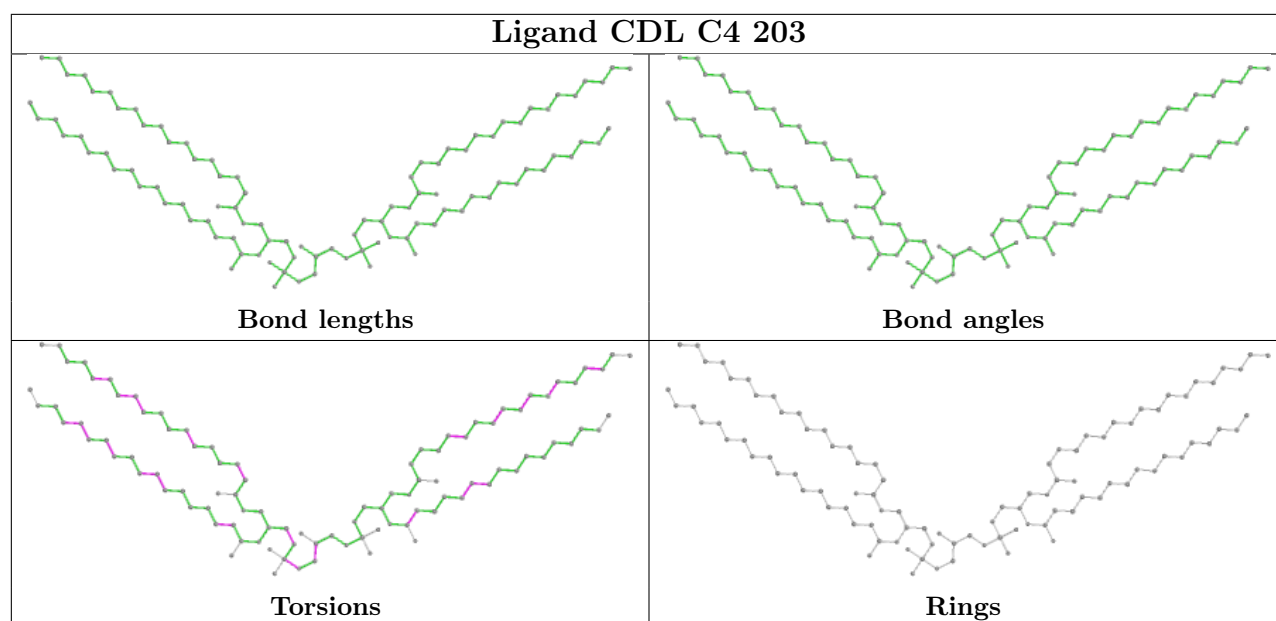


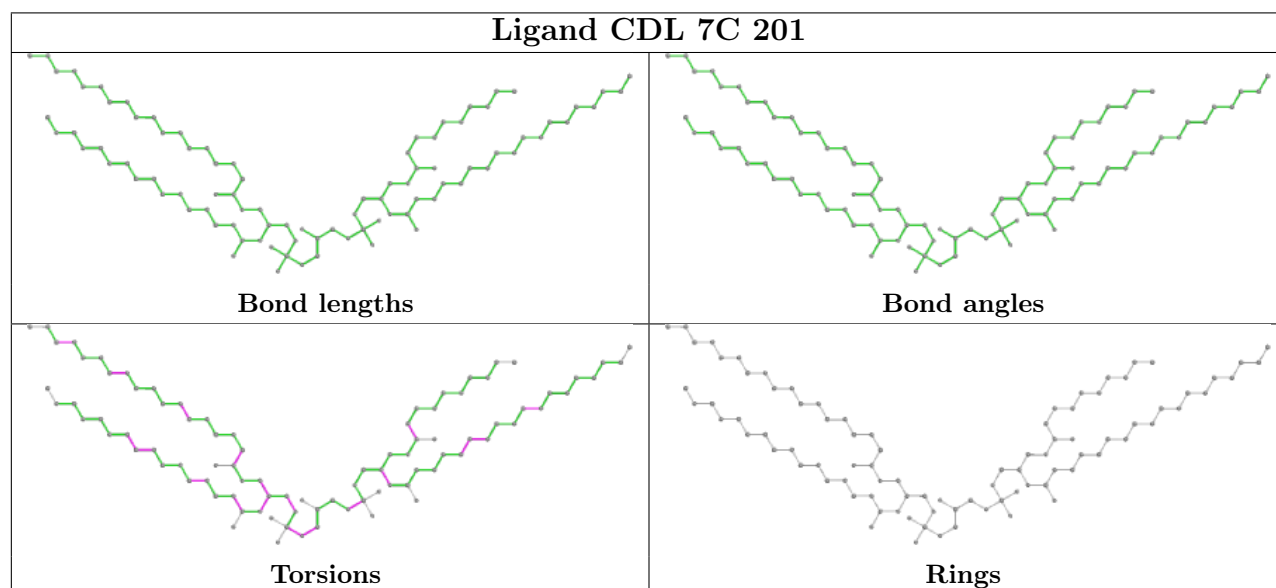
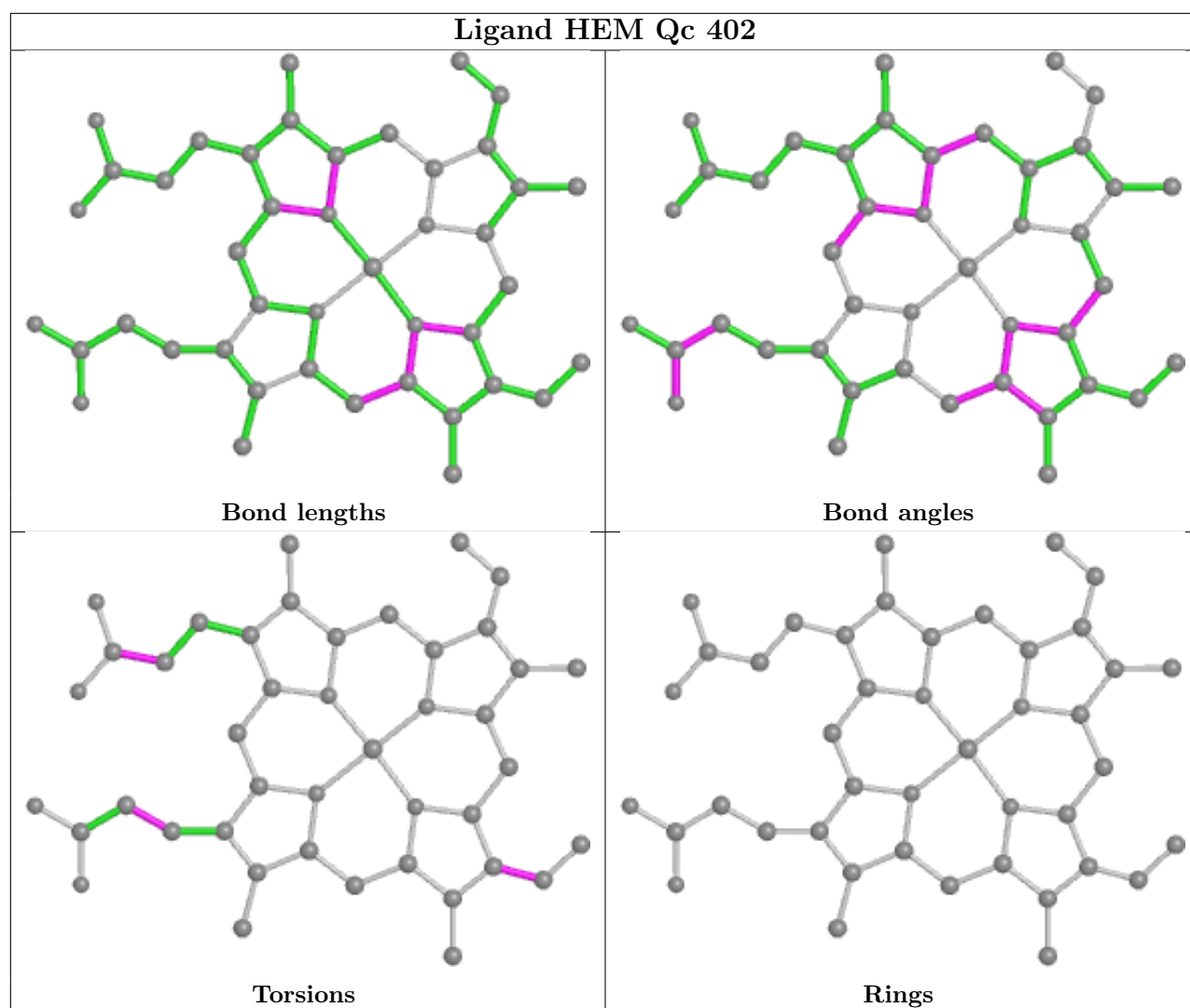


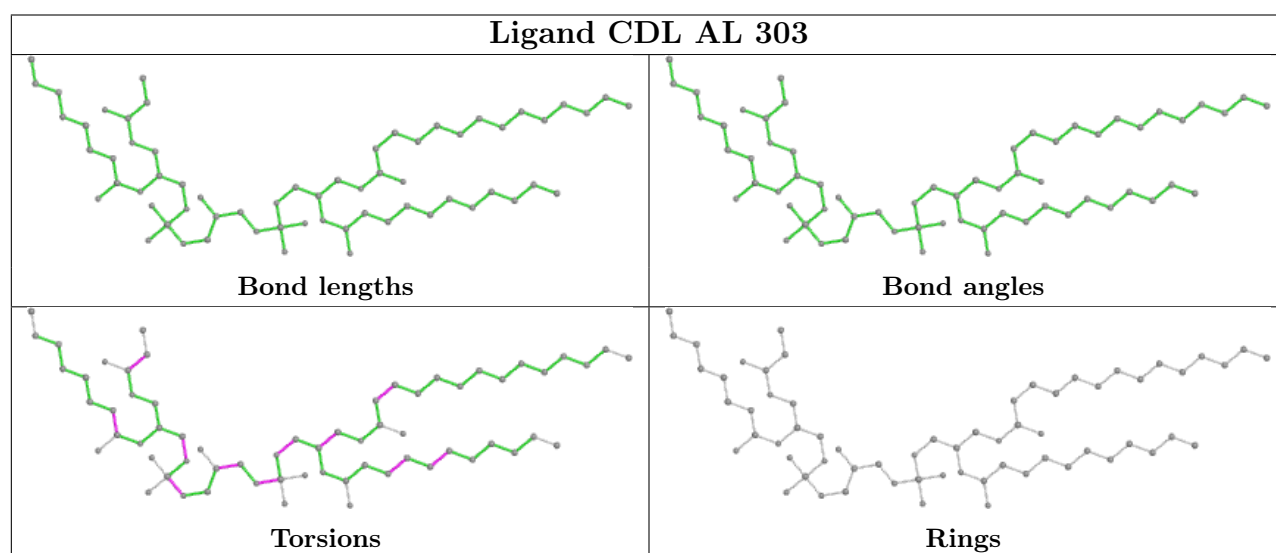
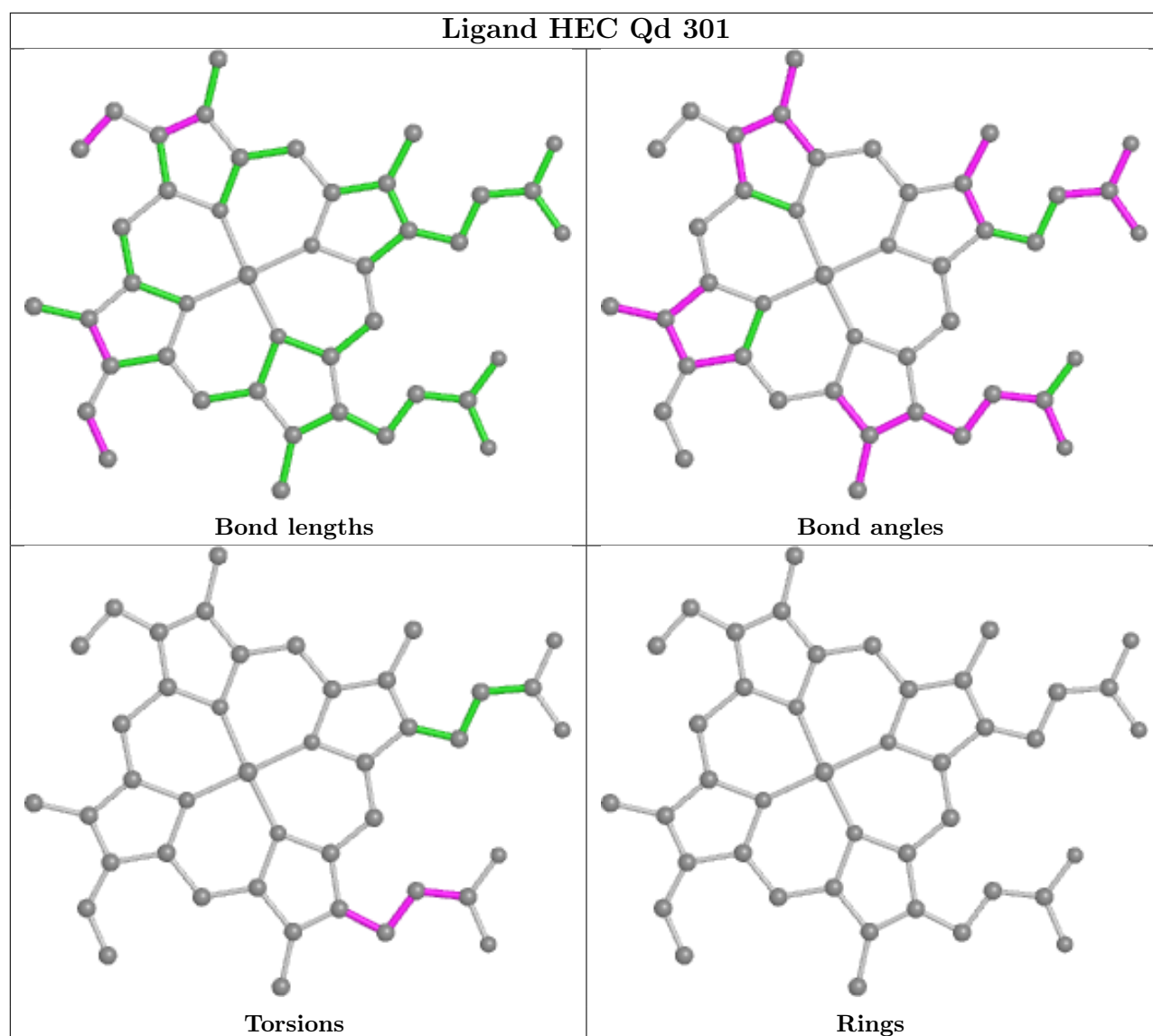


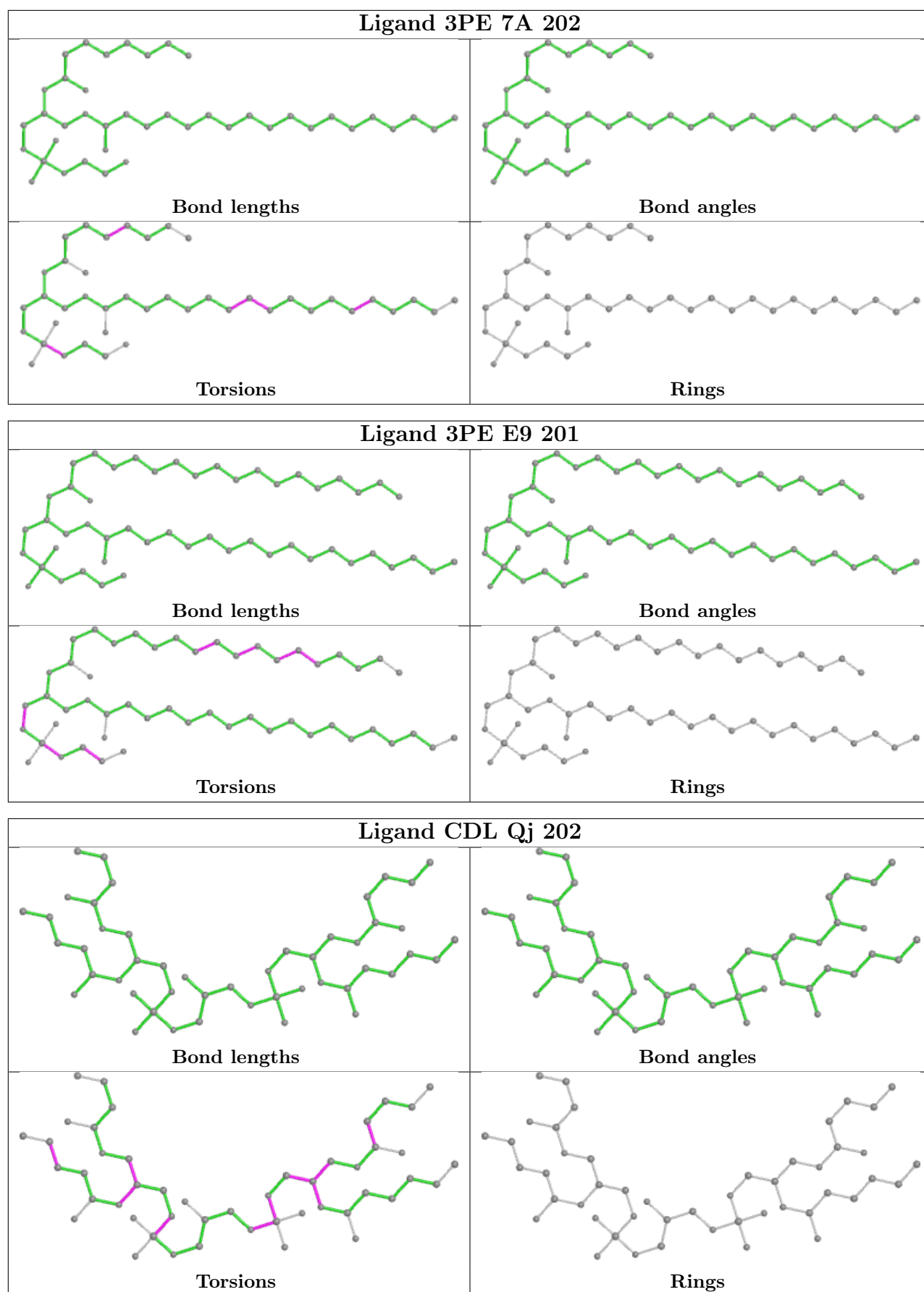


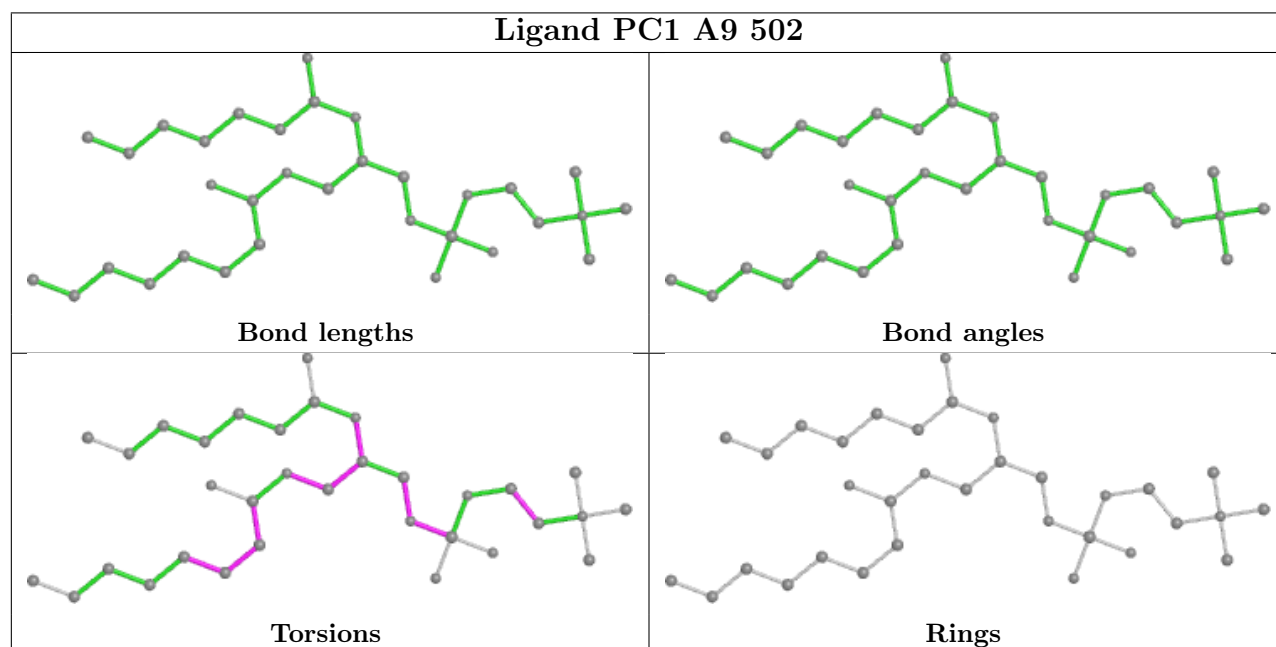
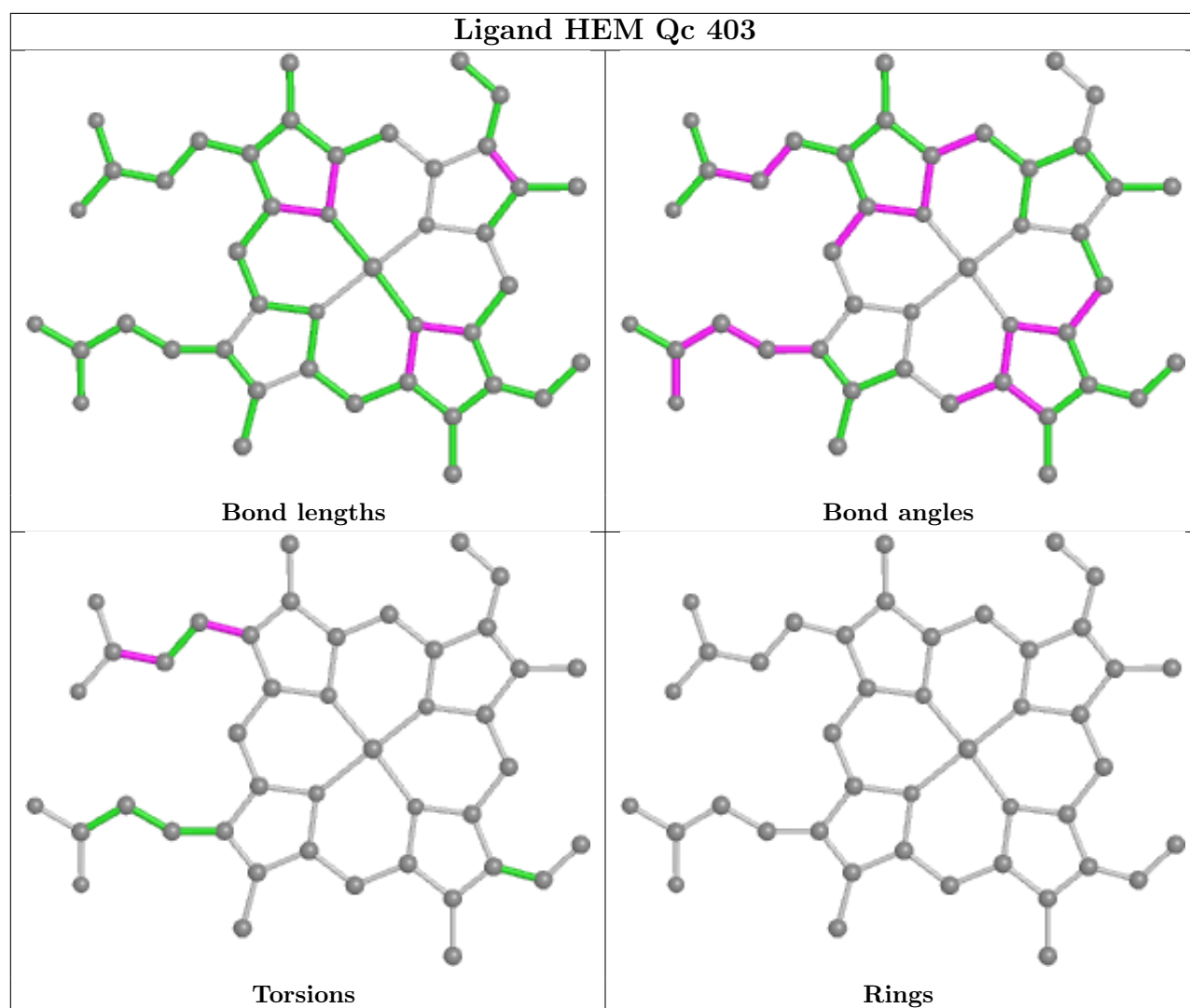


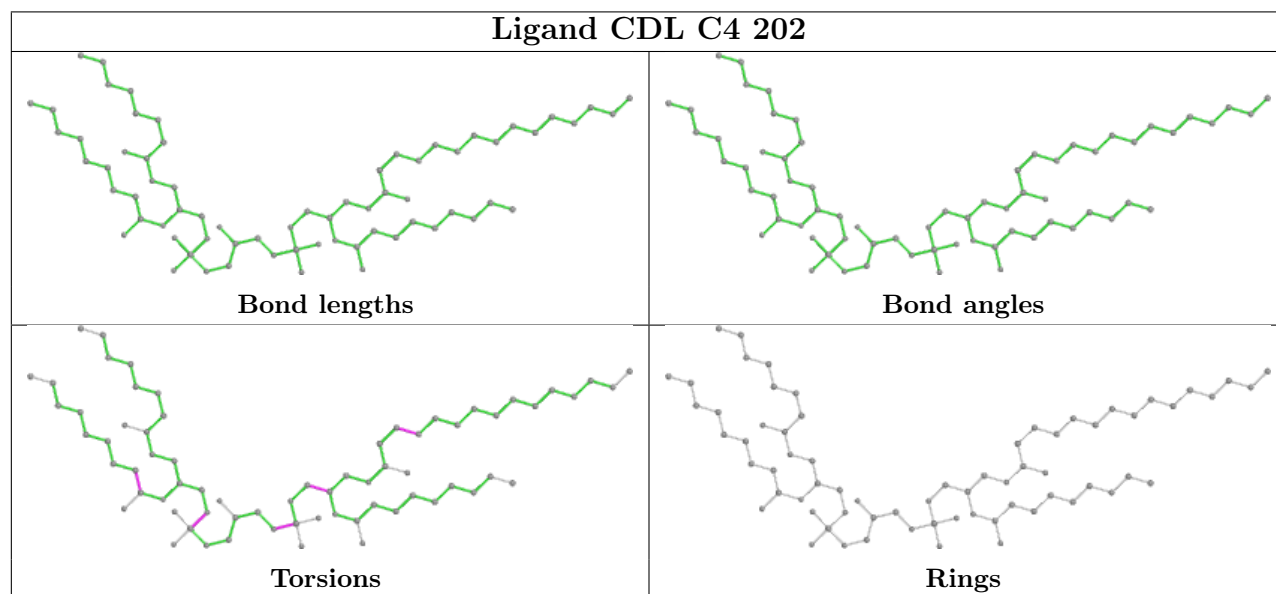
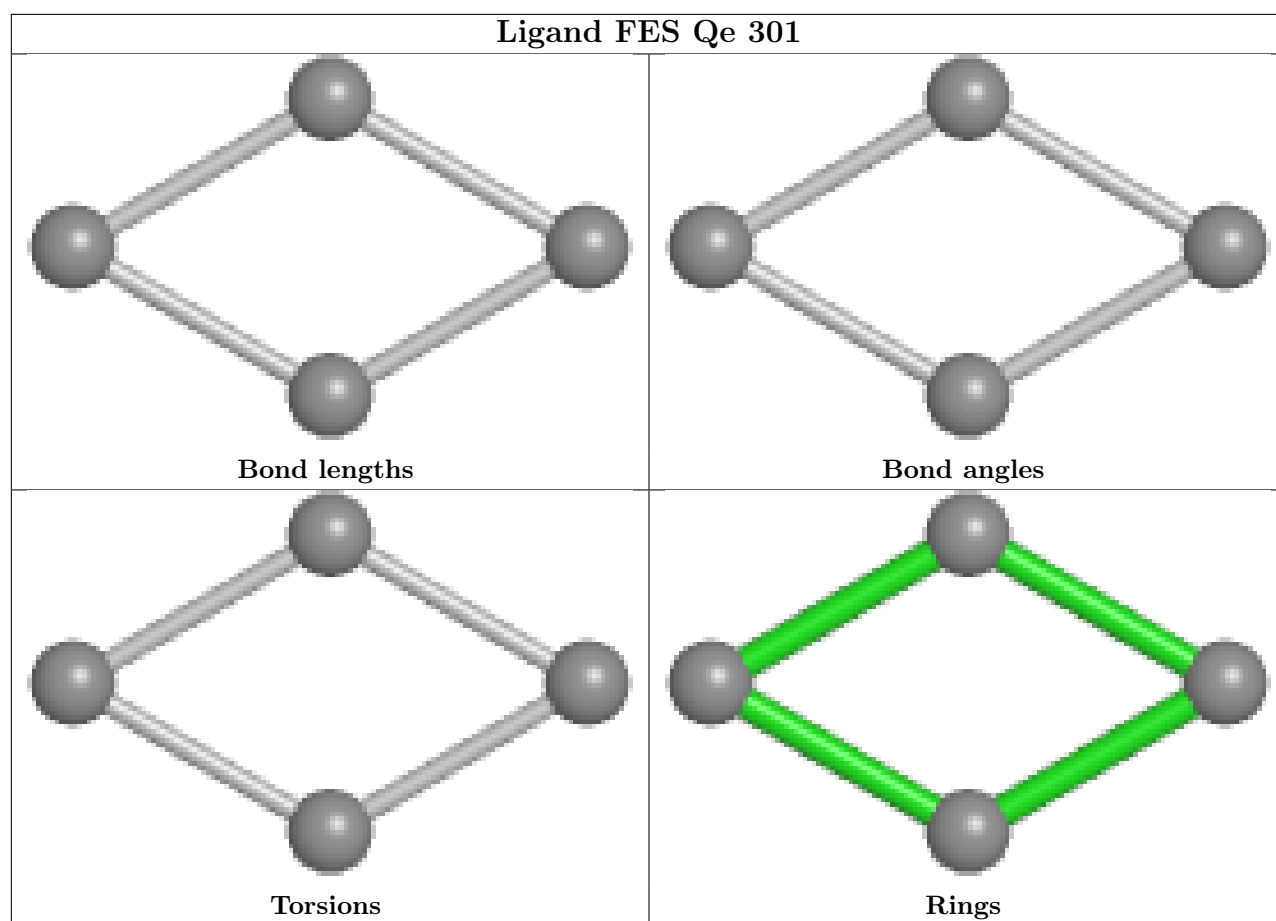


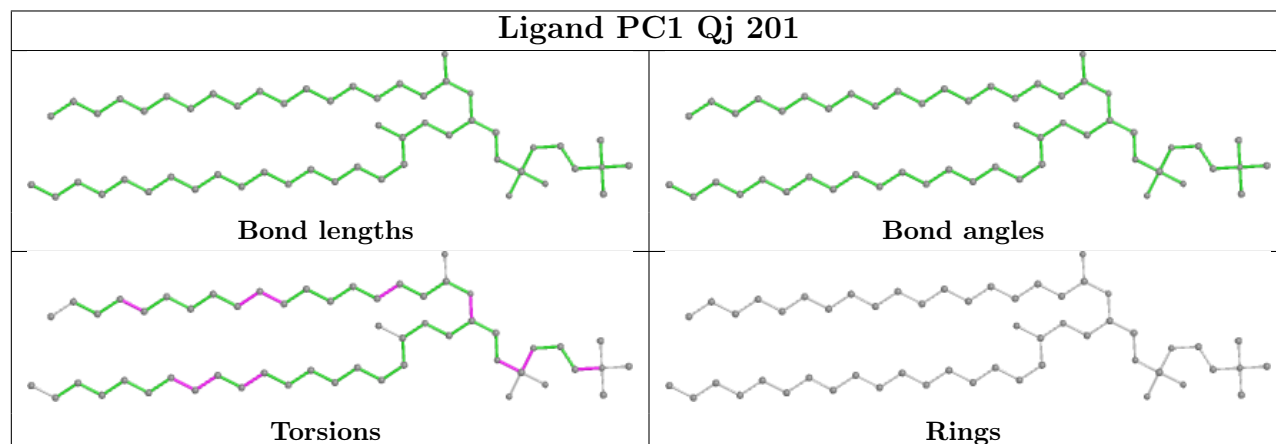
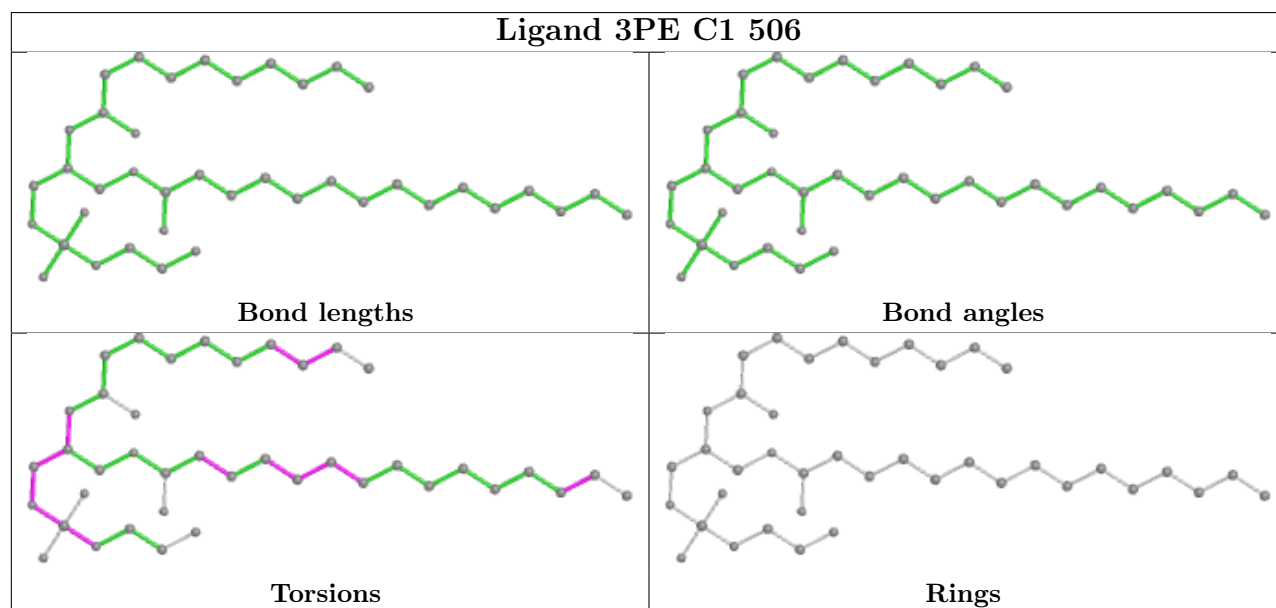
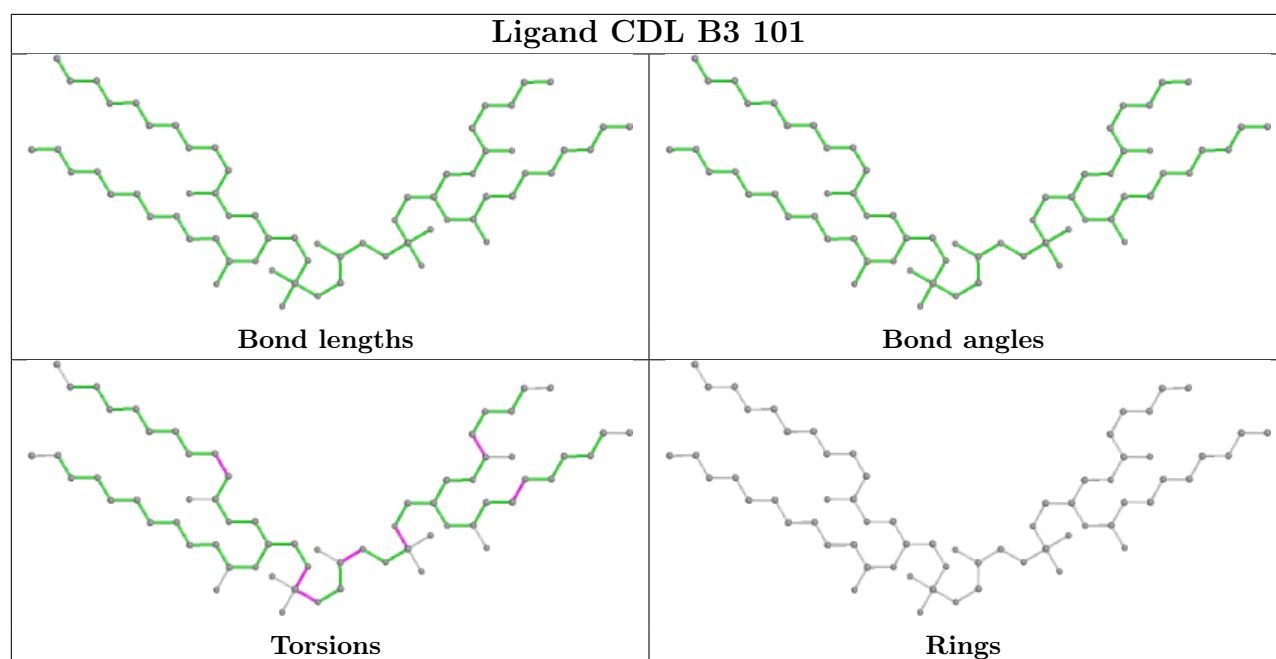




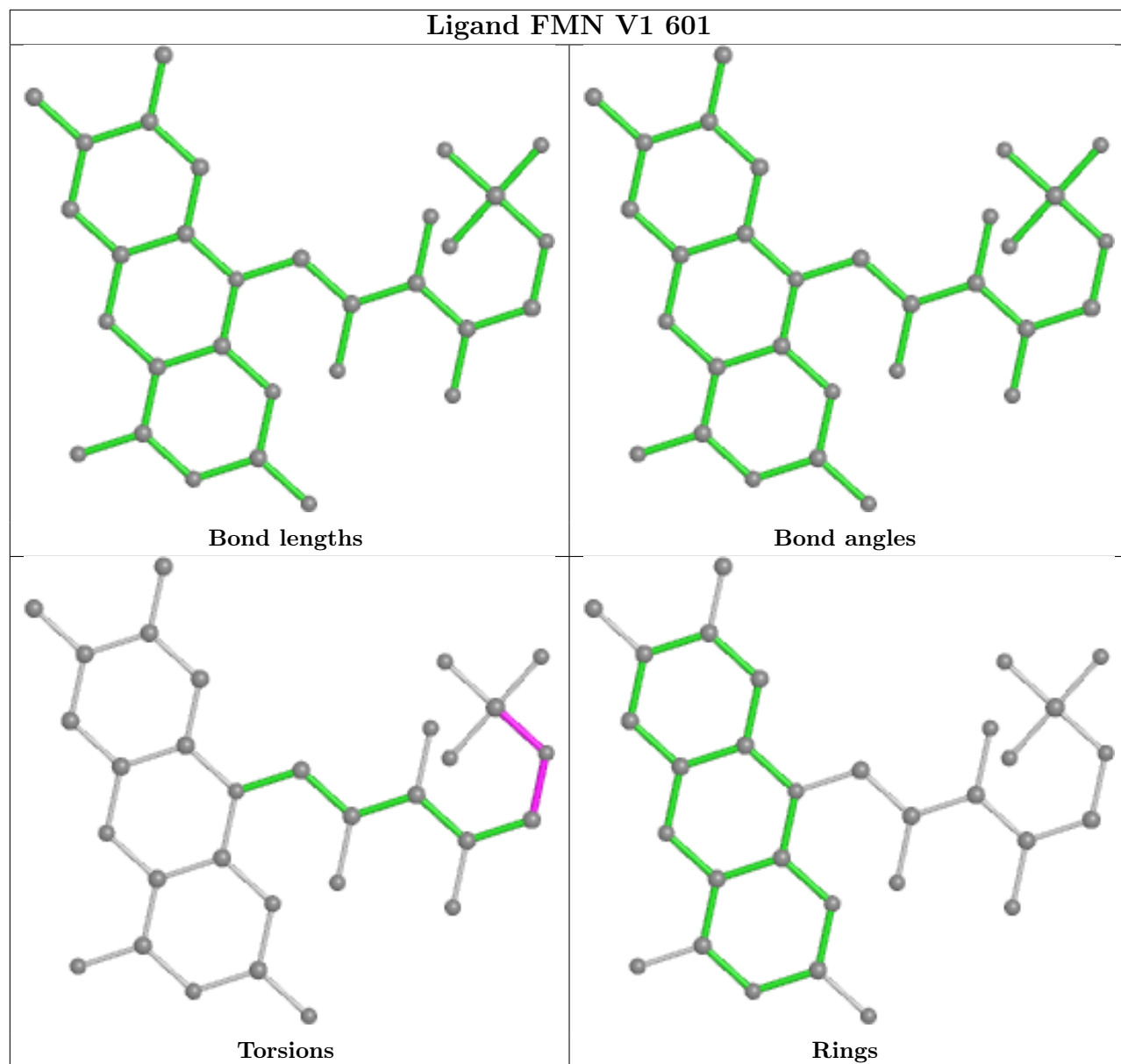




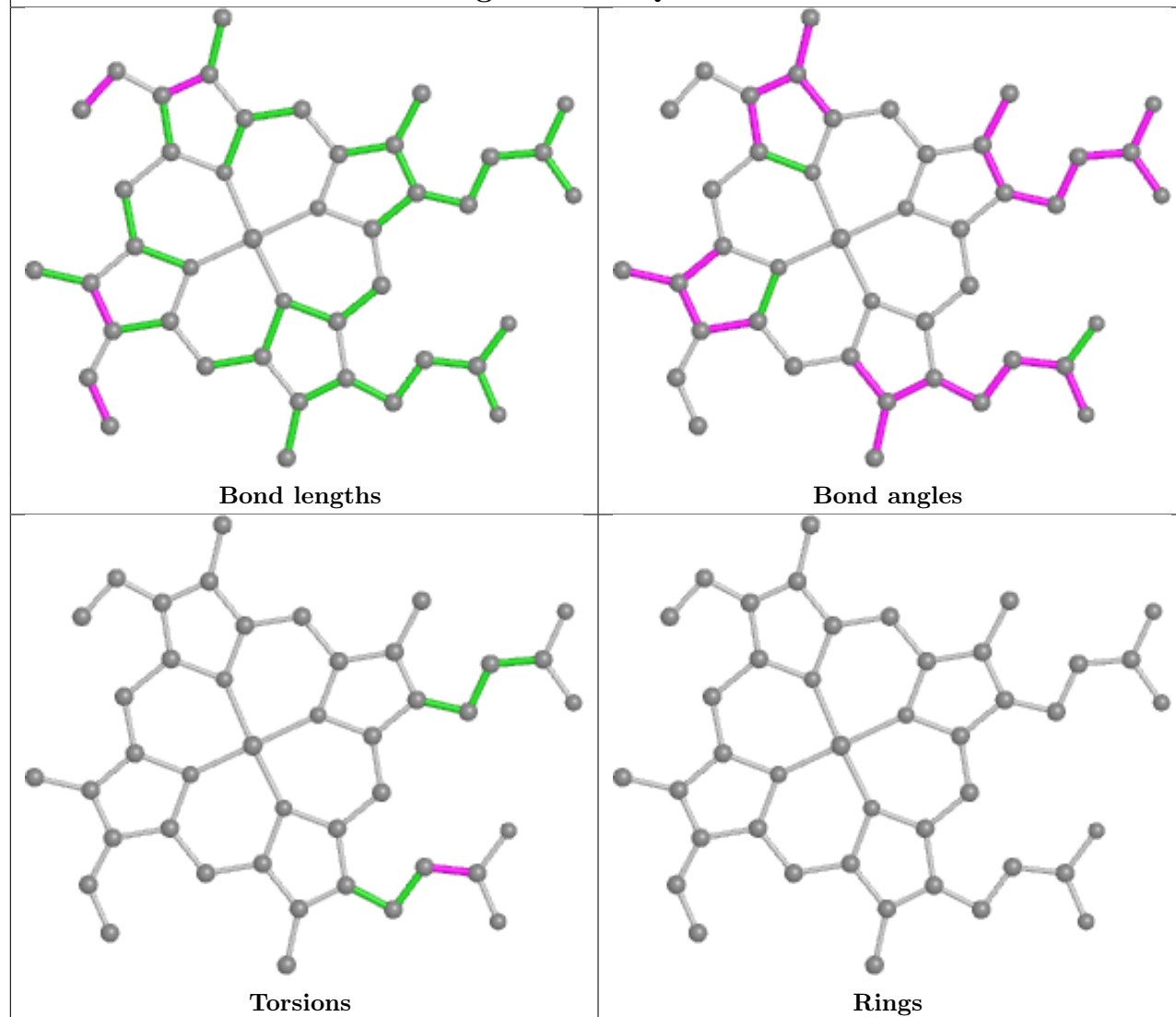




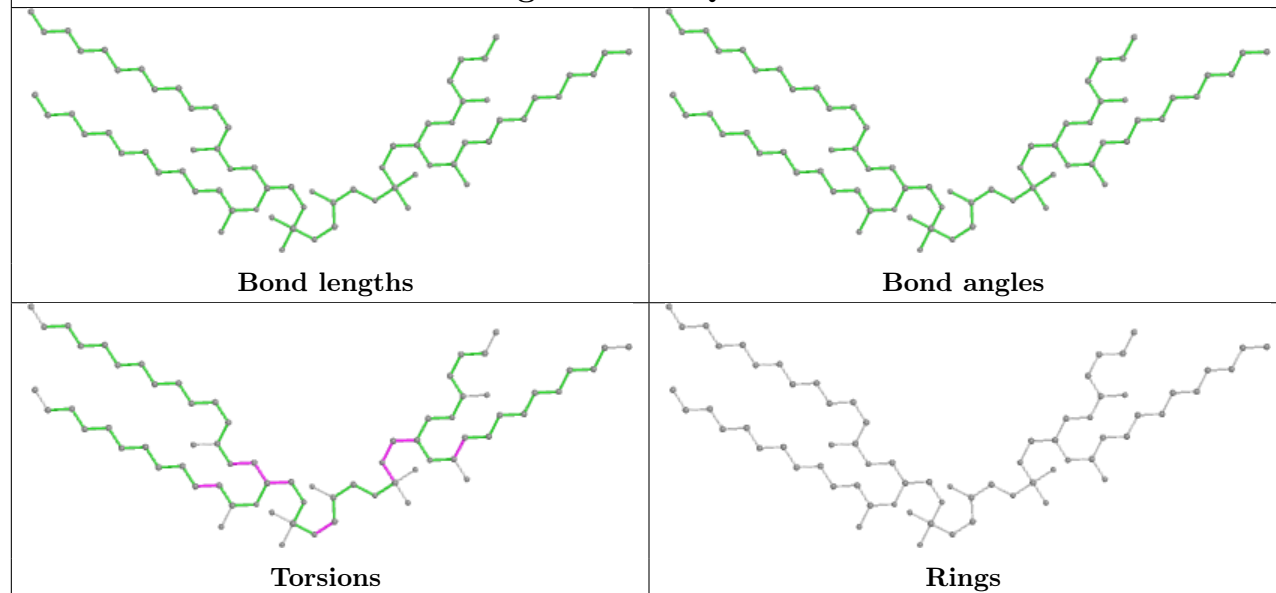
Ligand FMN V1 601

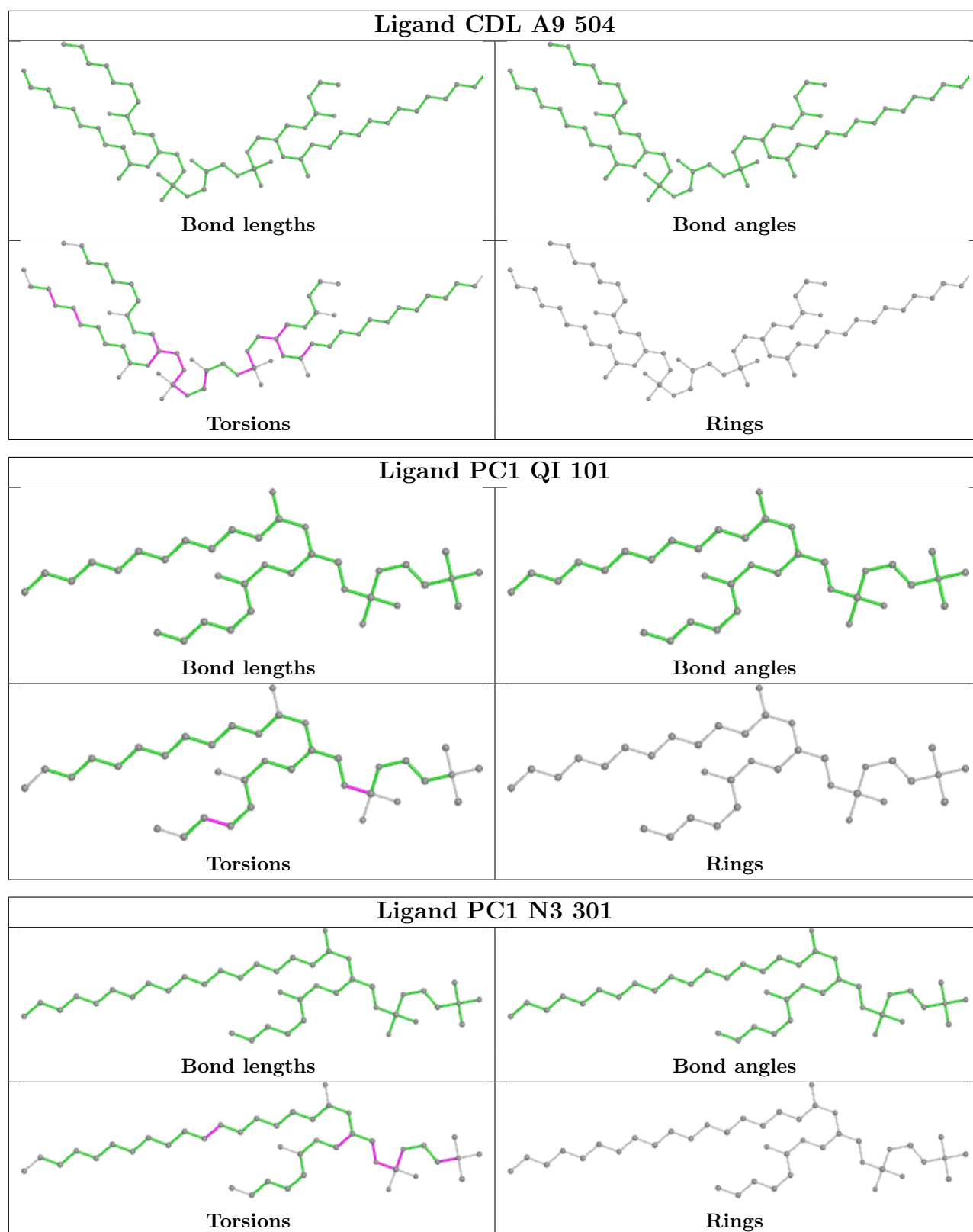


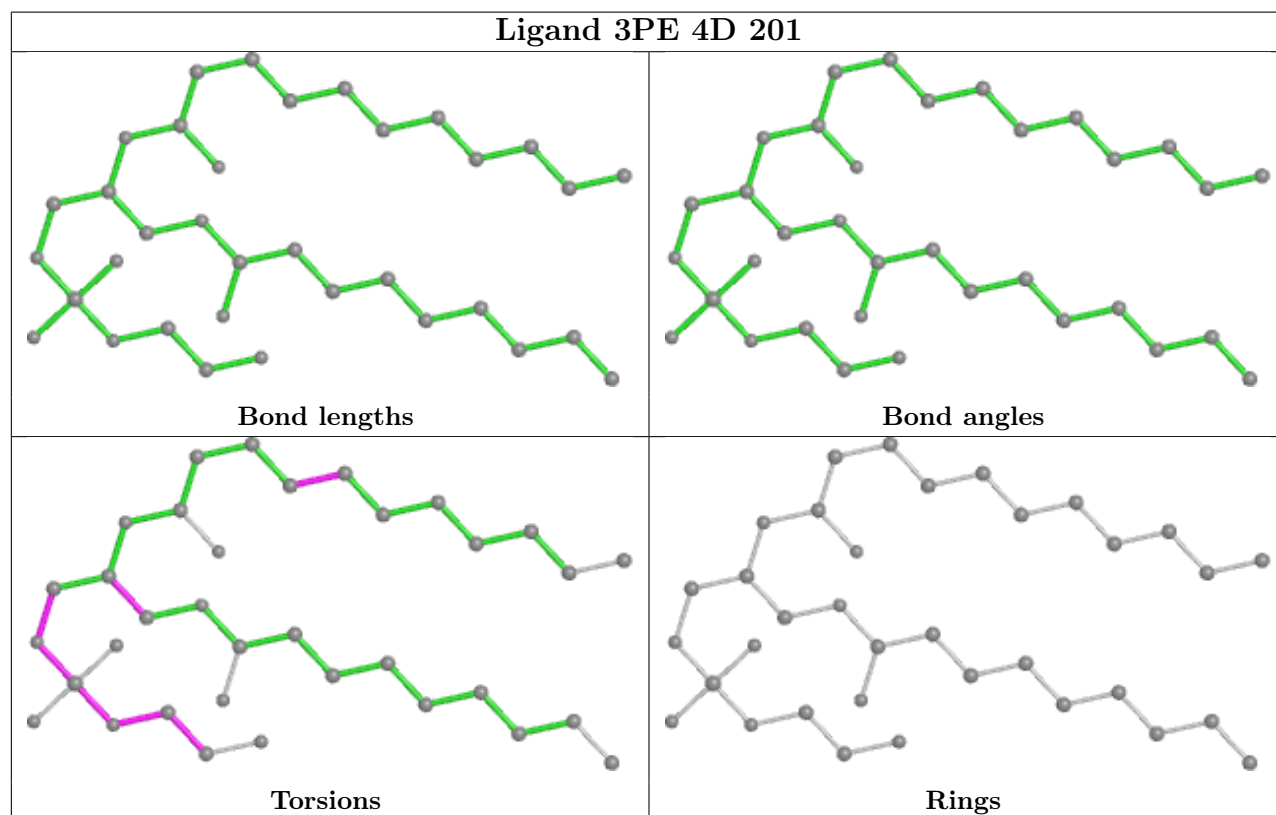
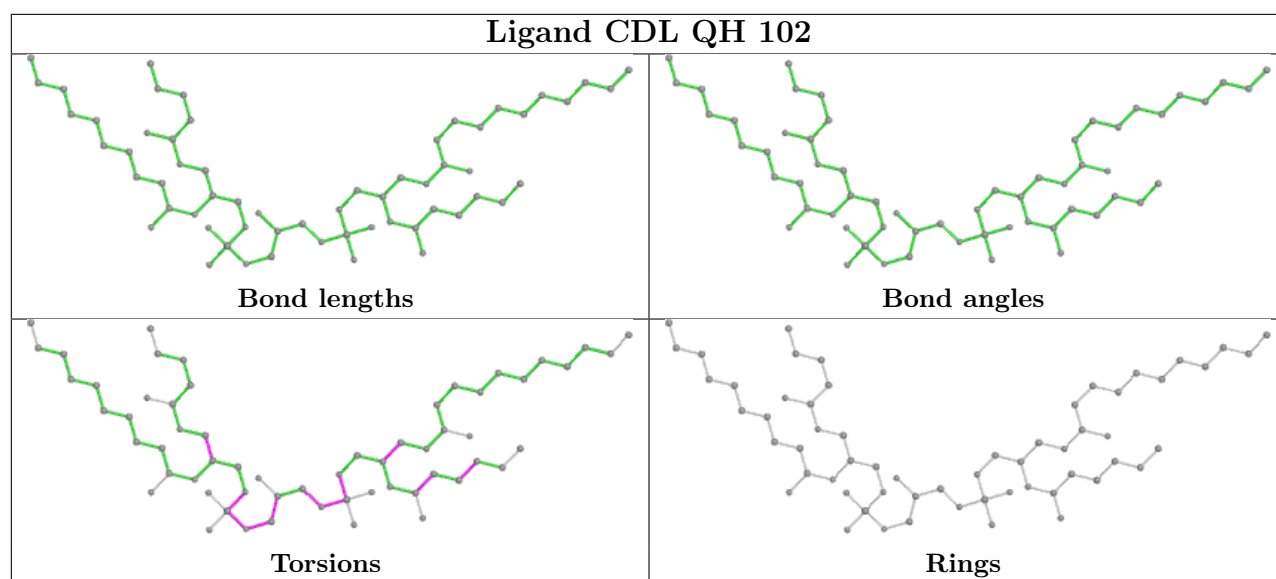
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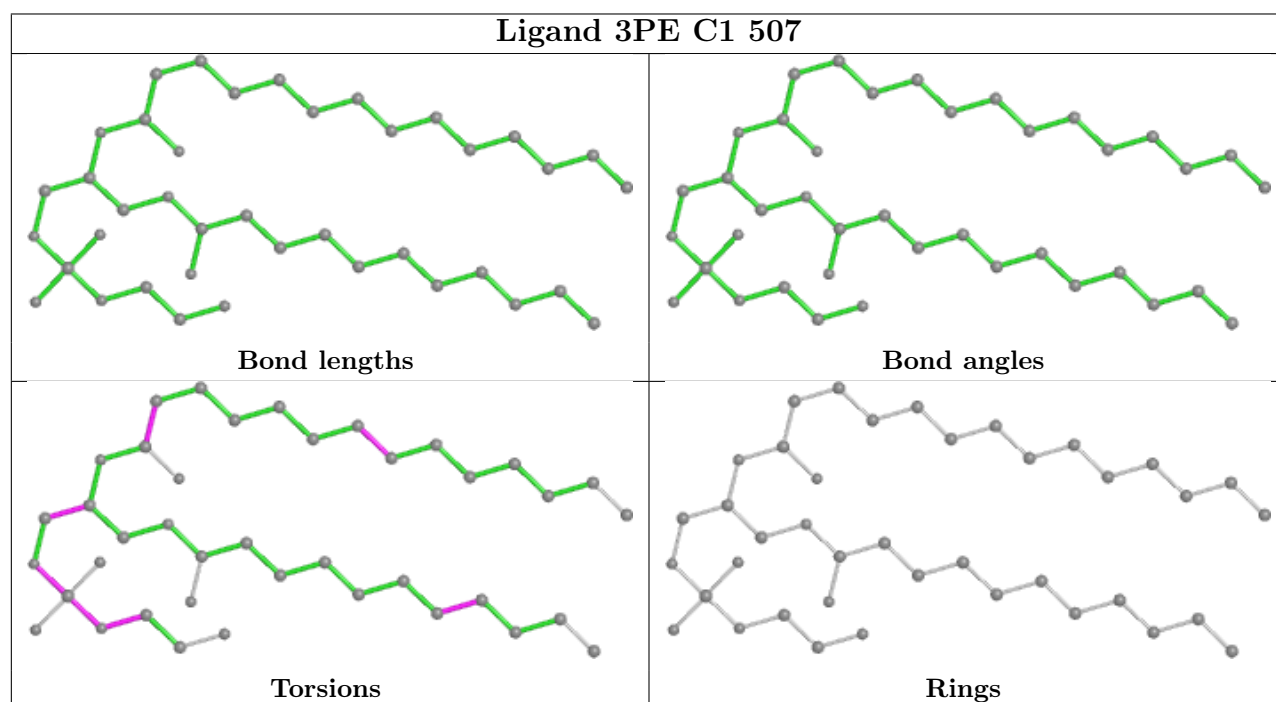
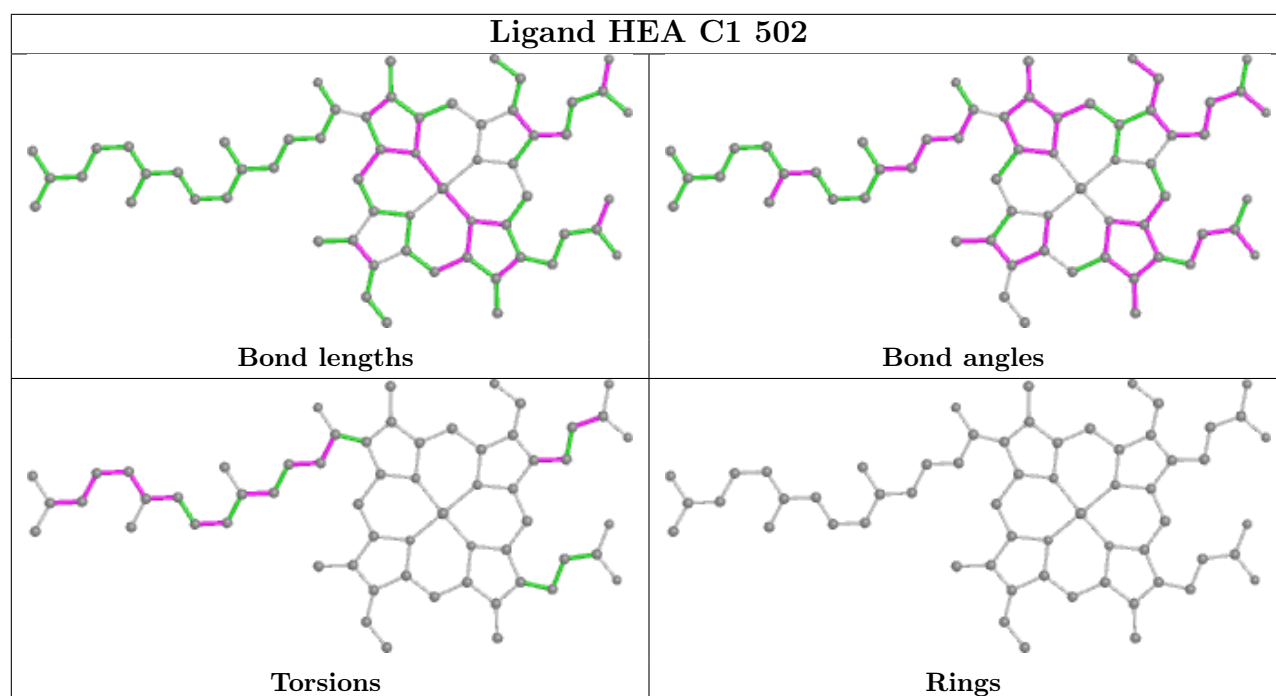


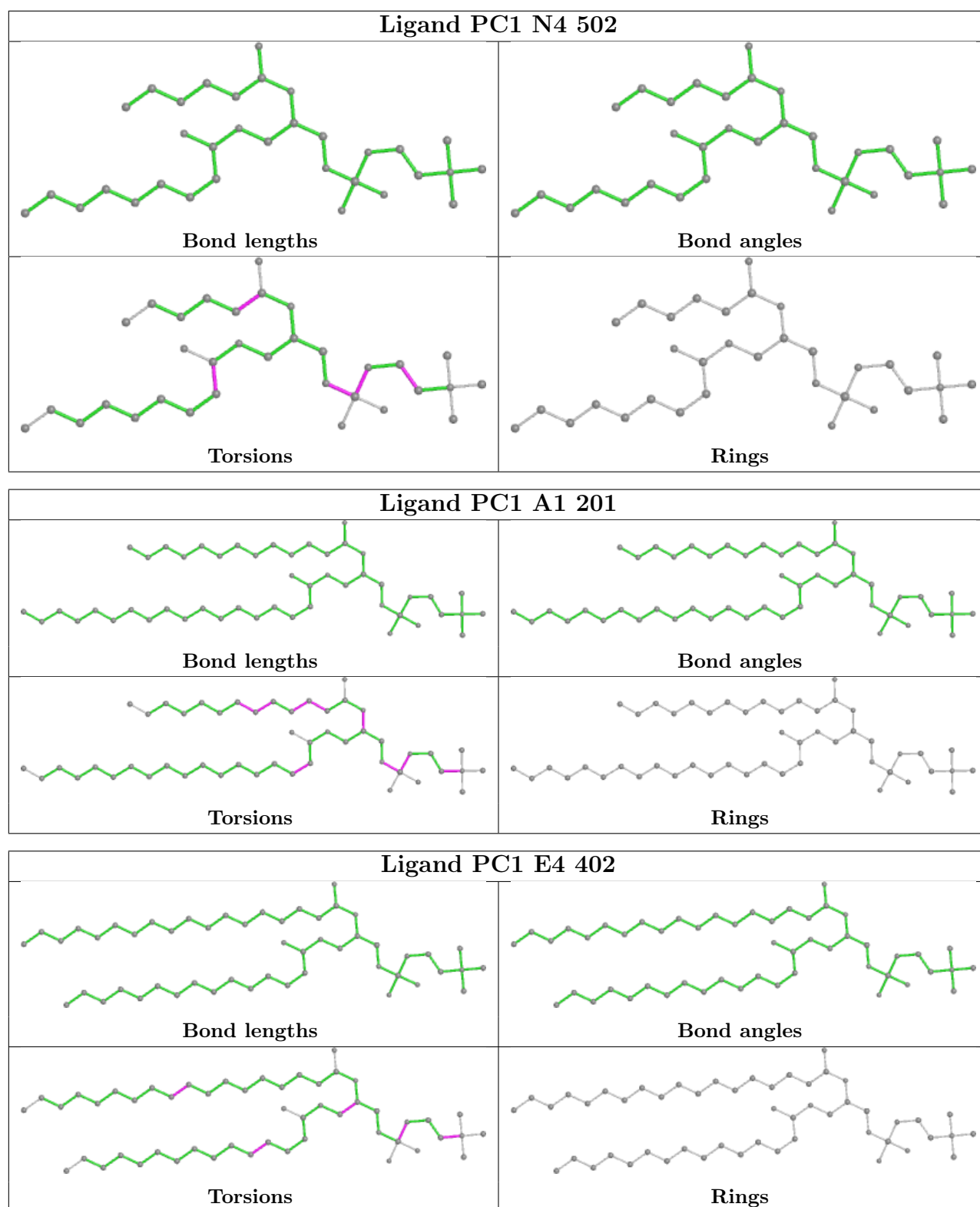
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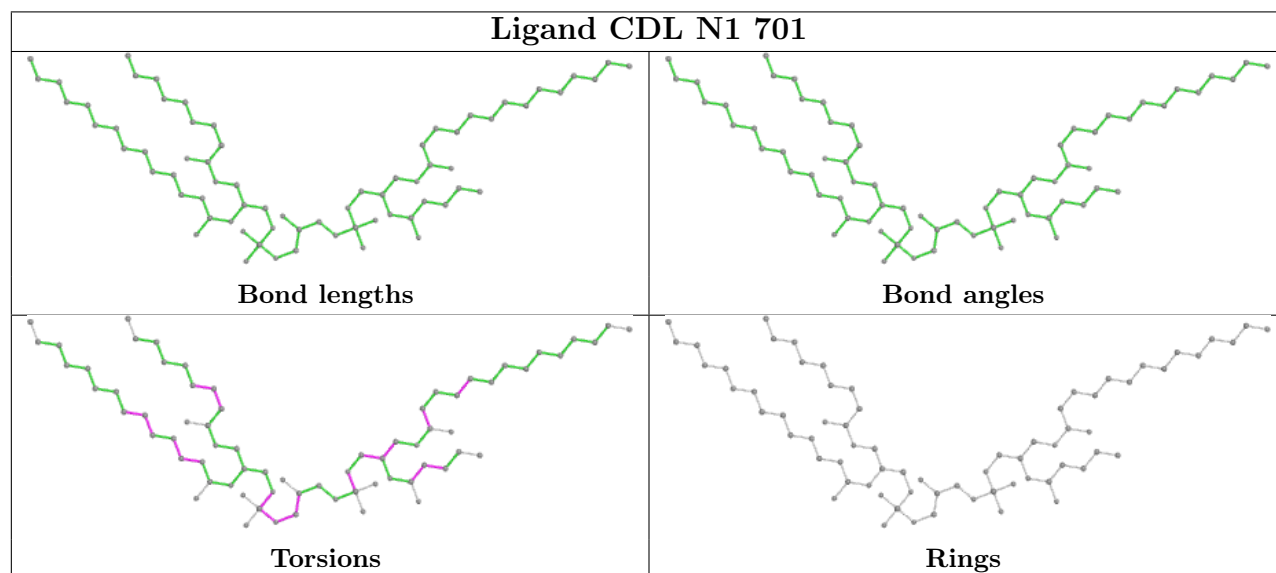
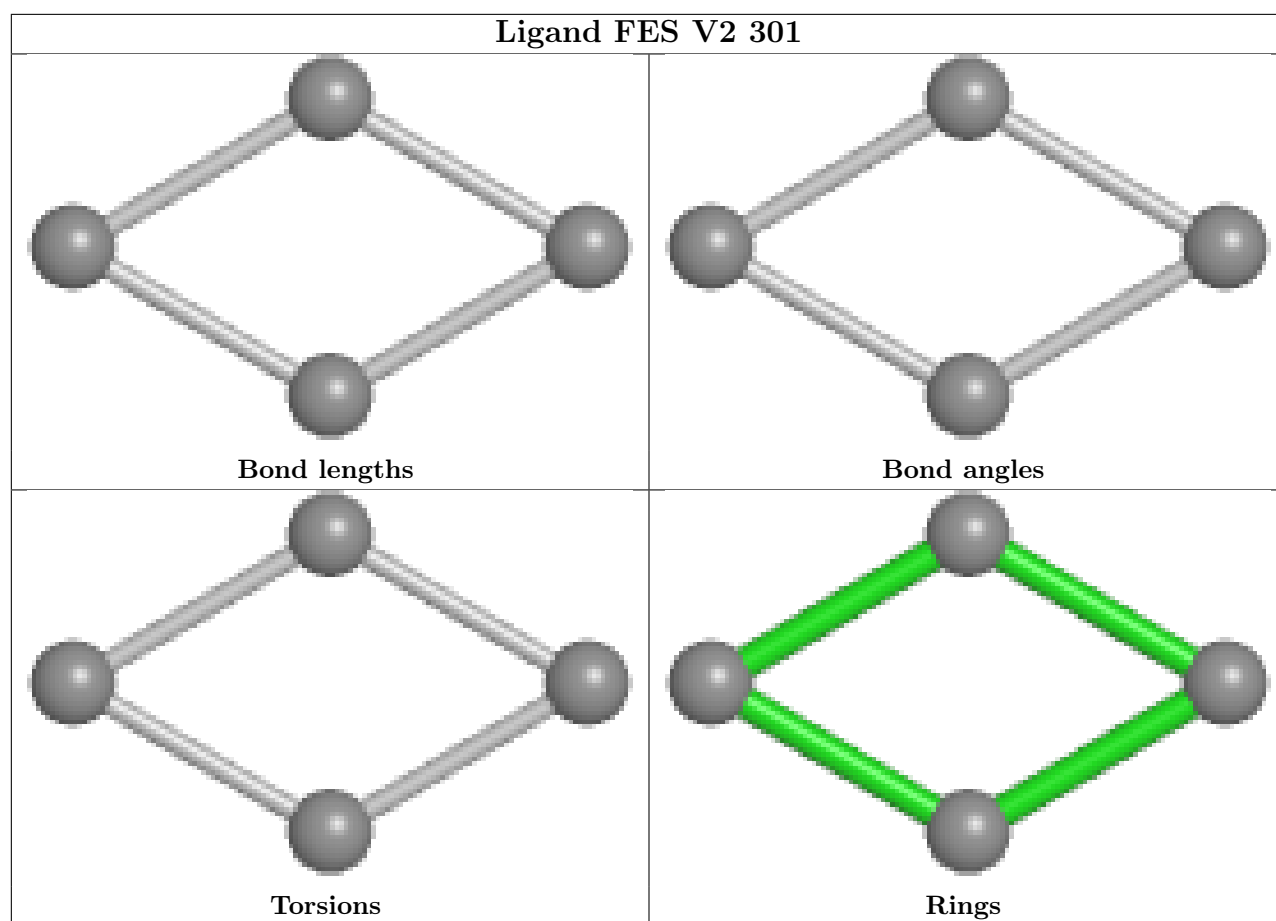




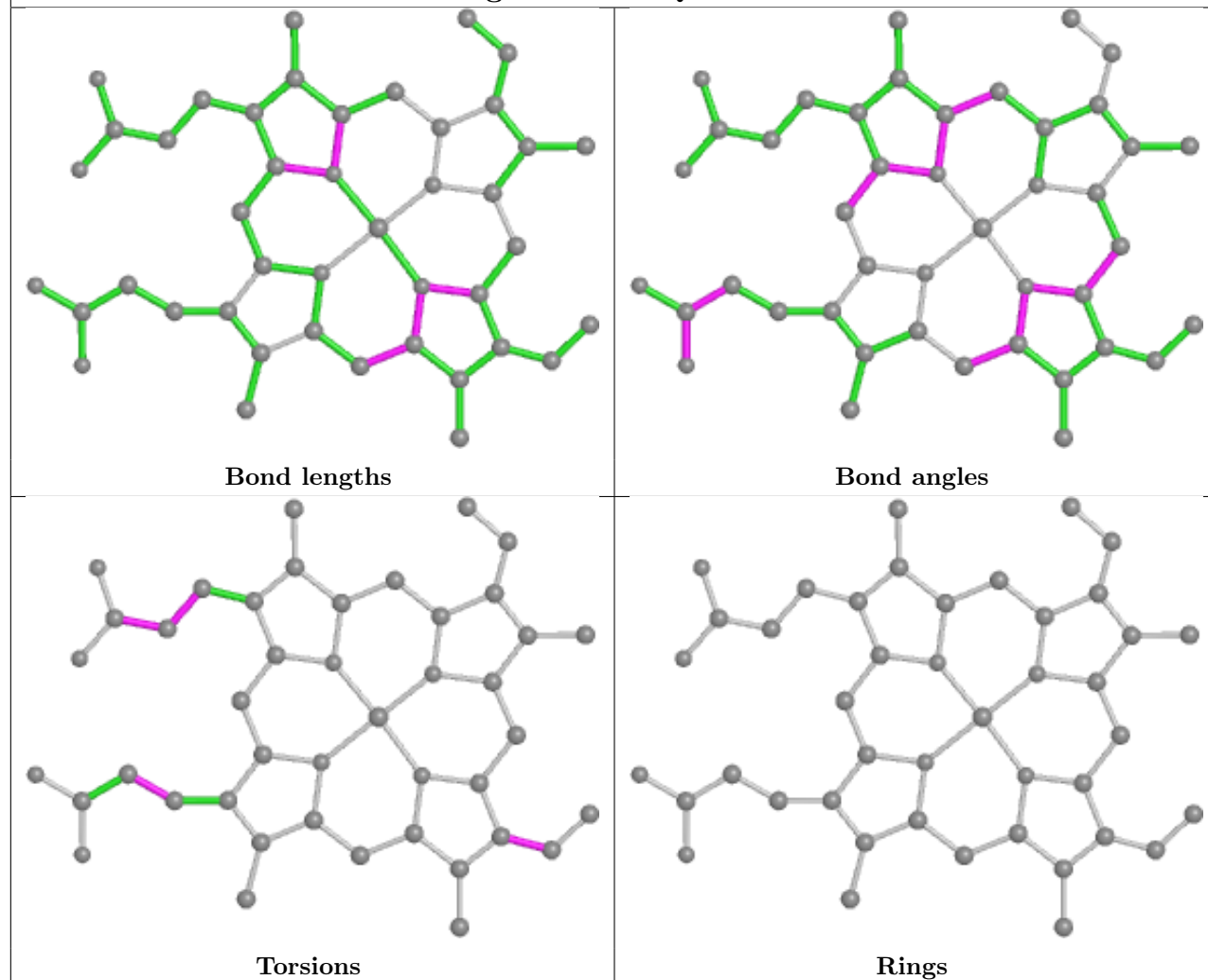




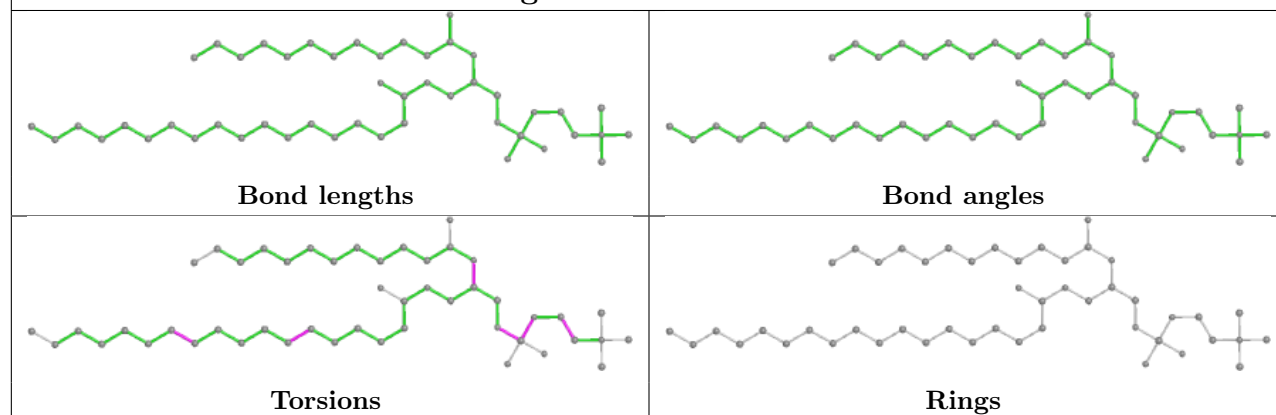


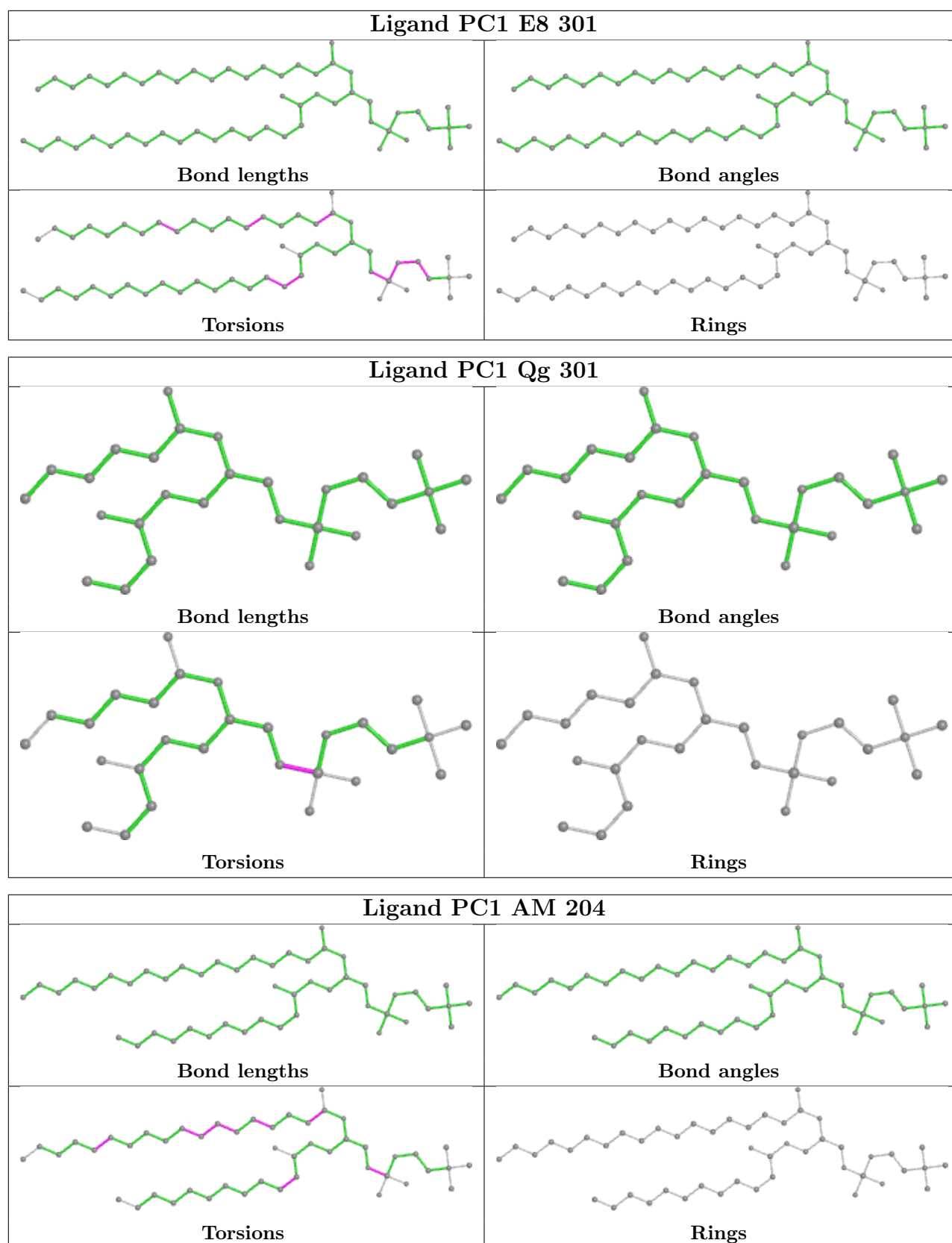


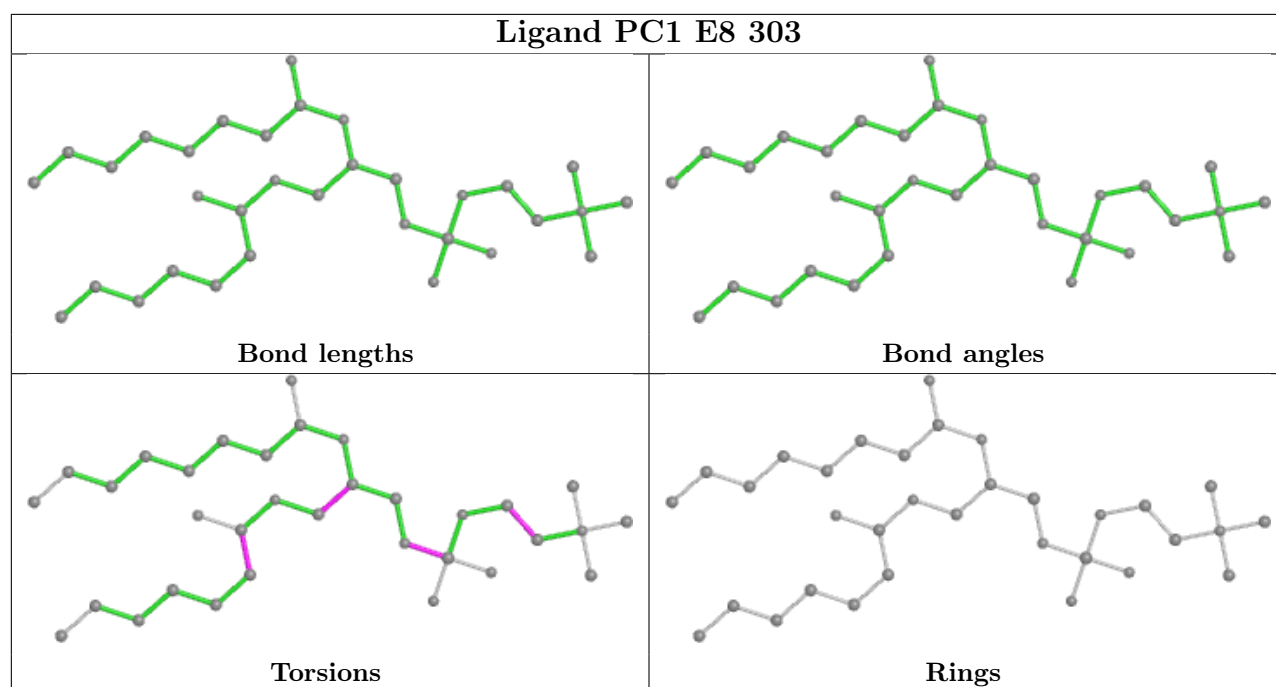
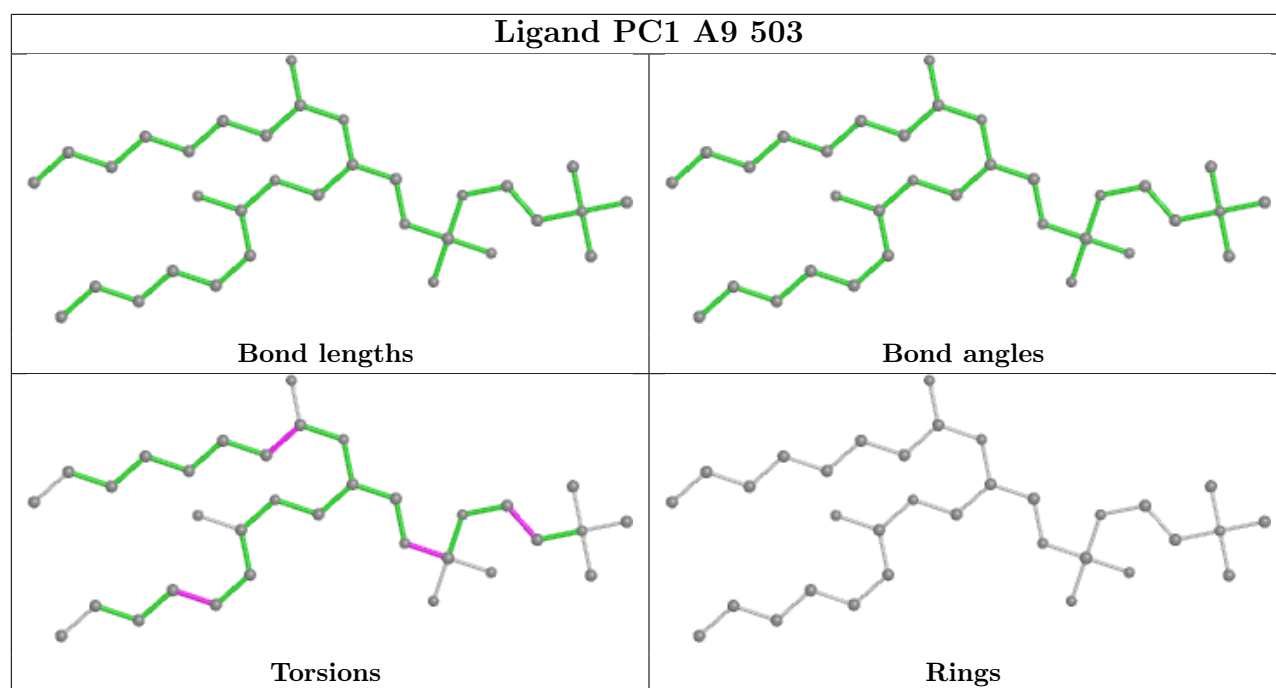
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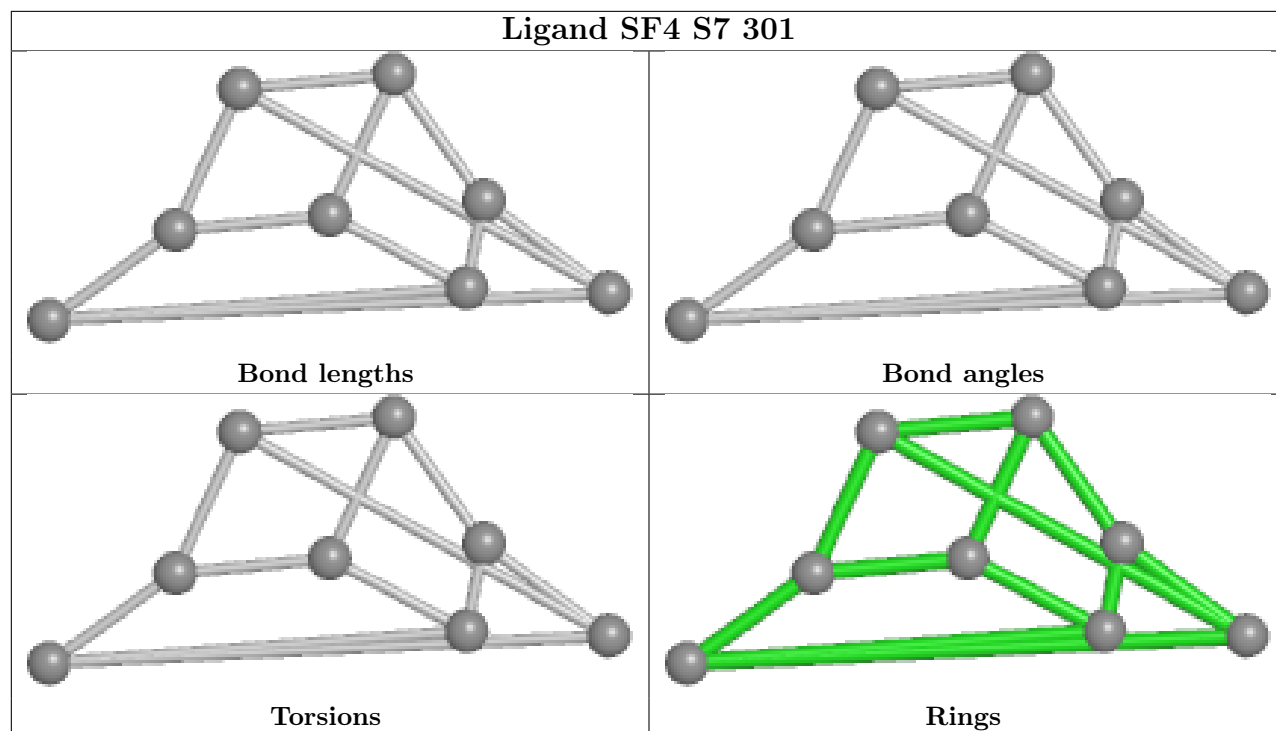
Ligand PC1 AN 301



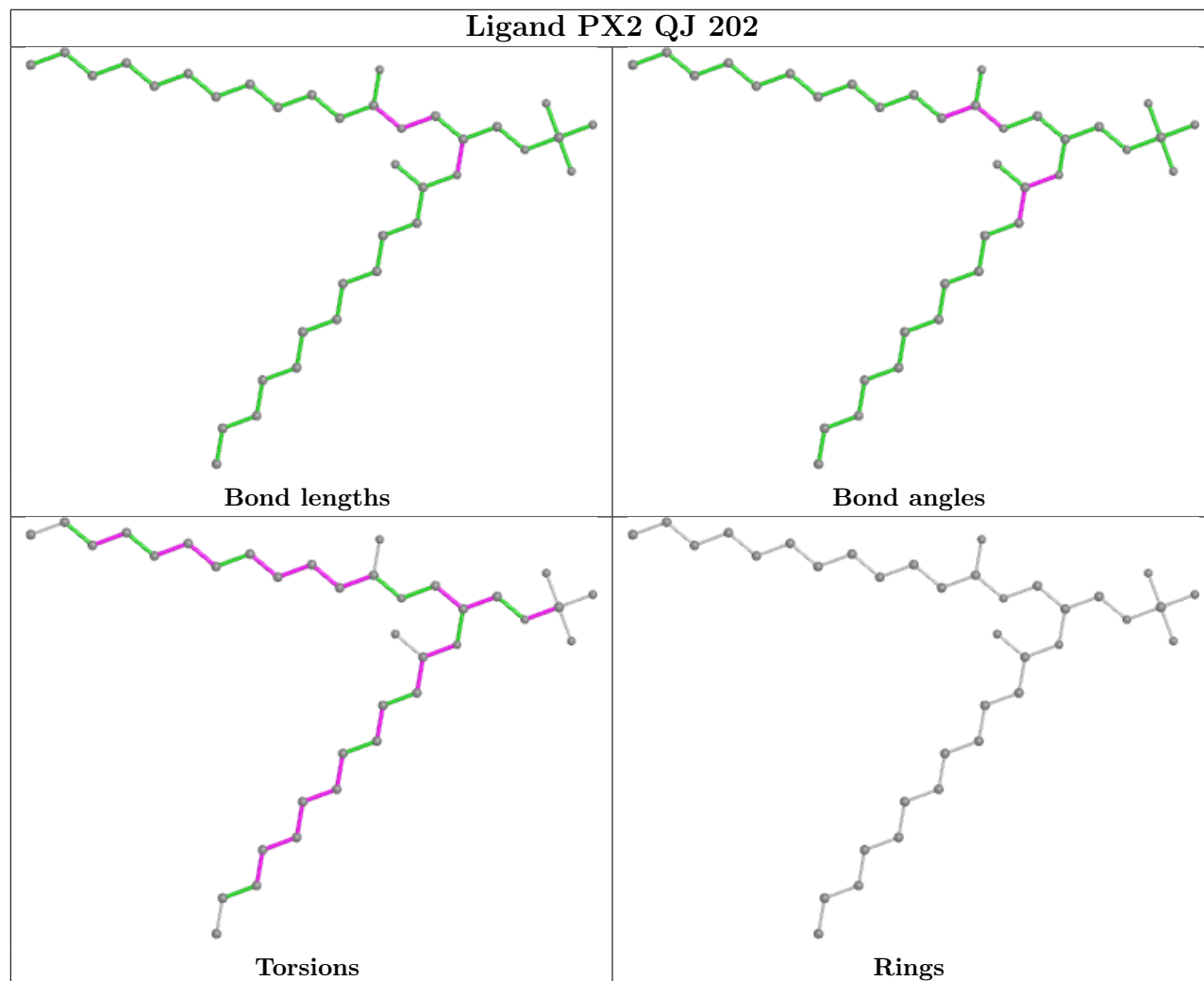


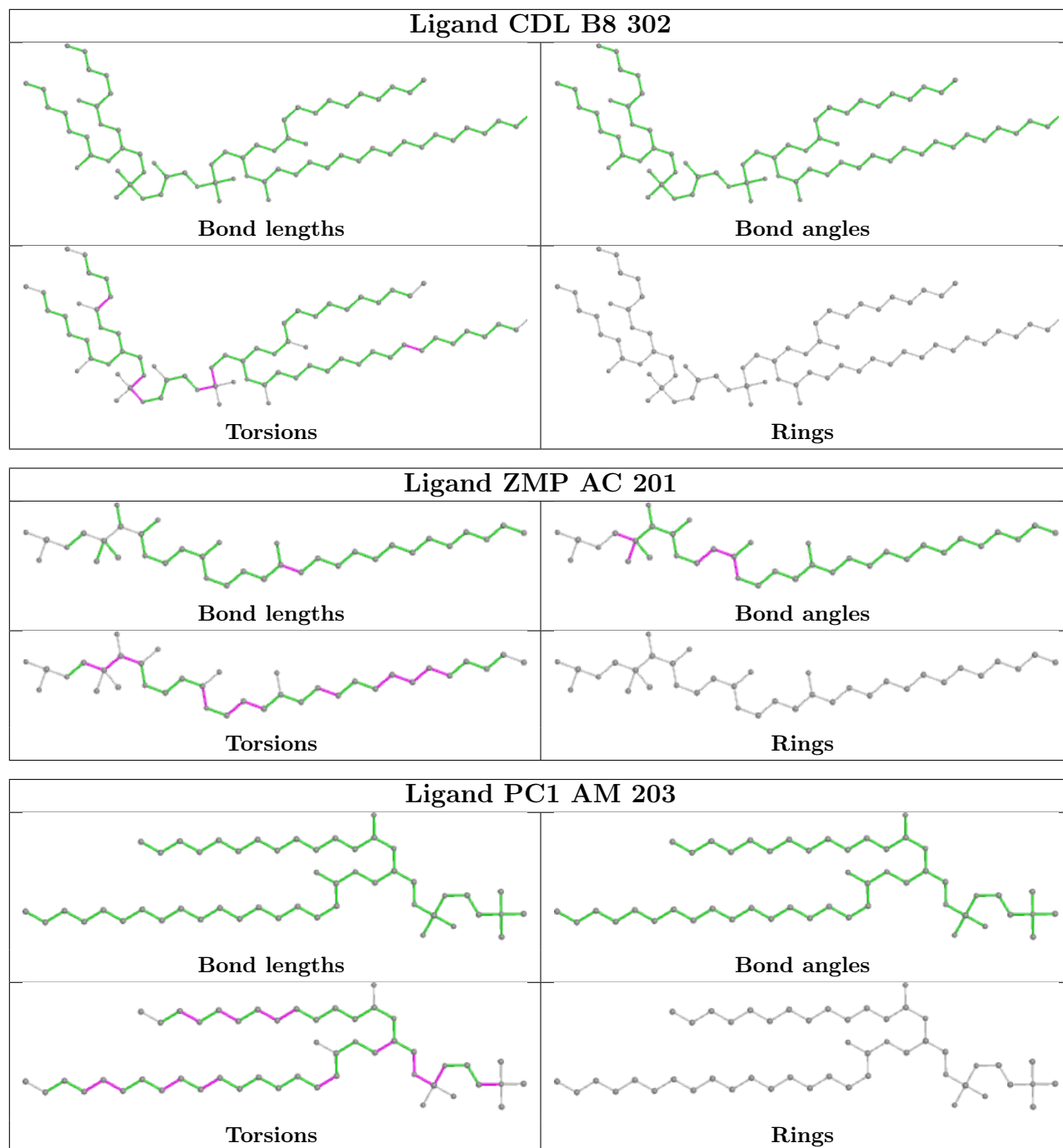


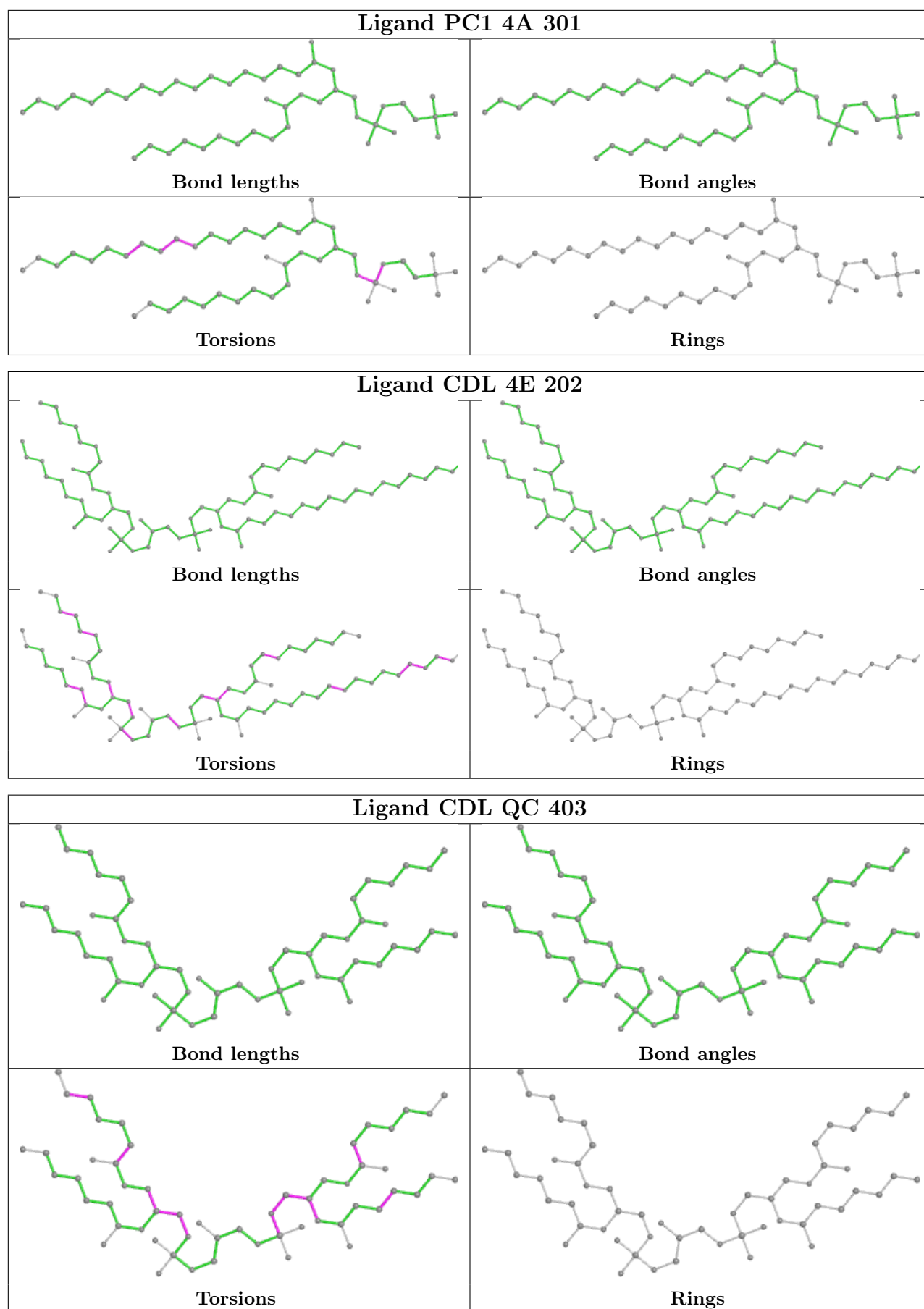
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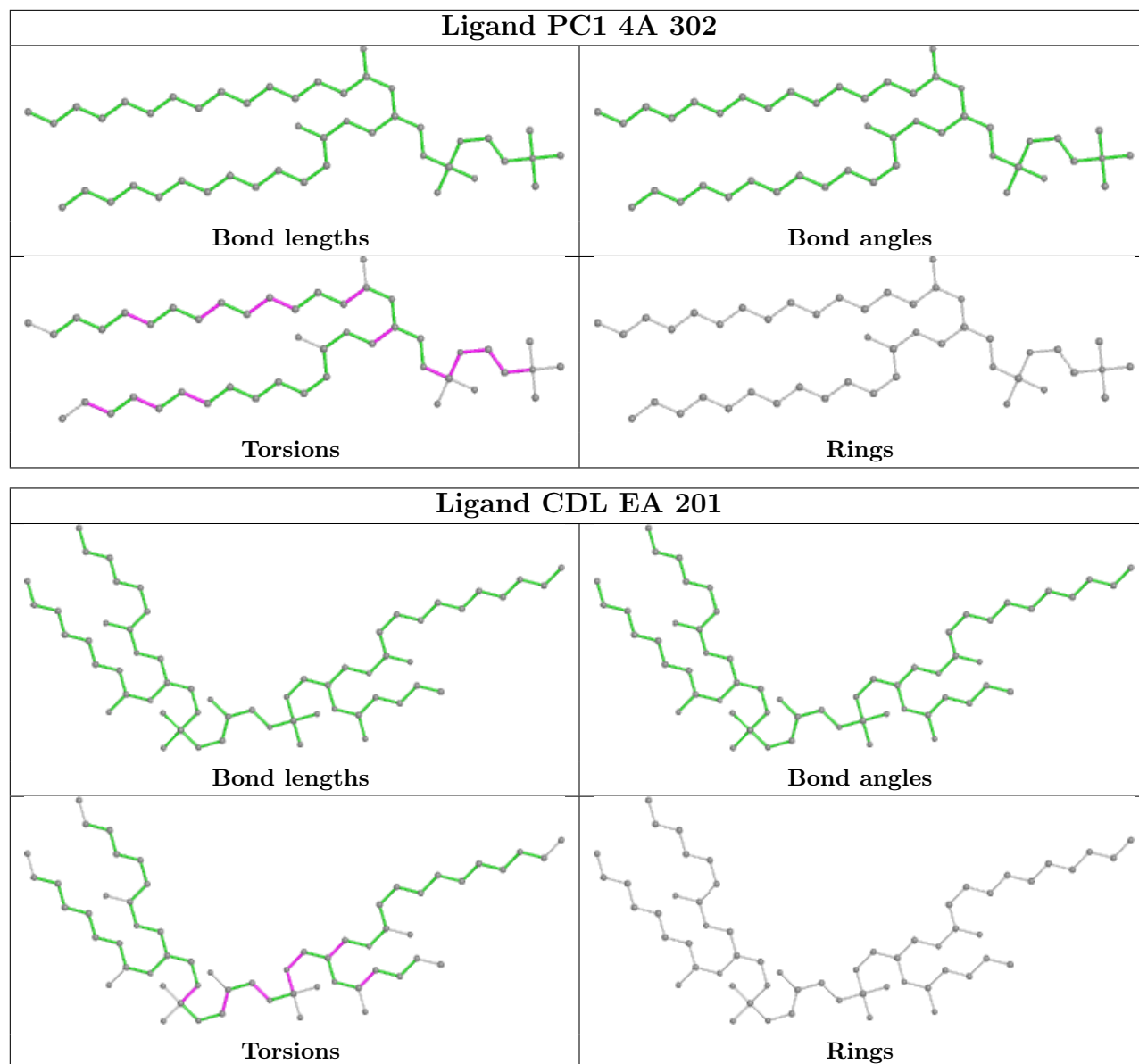


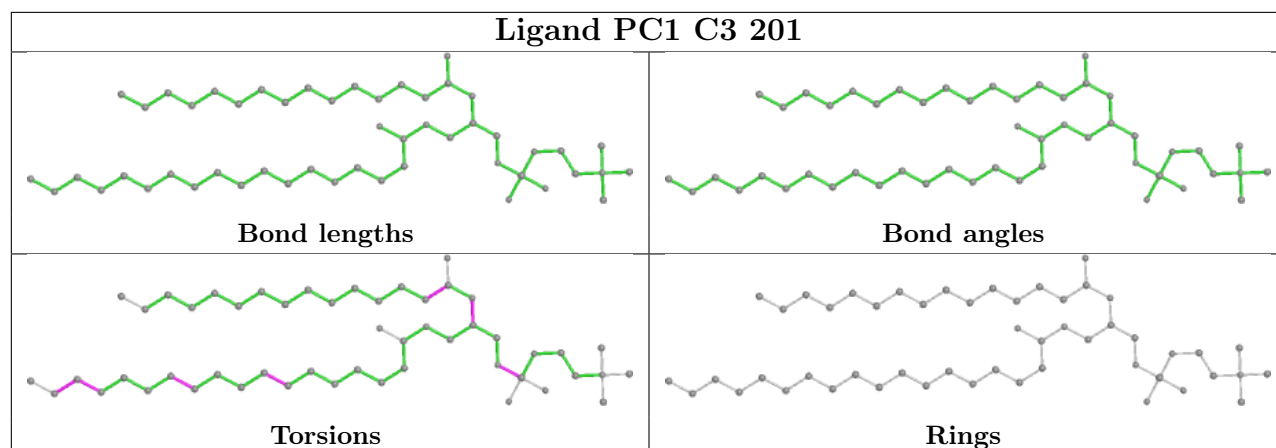
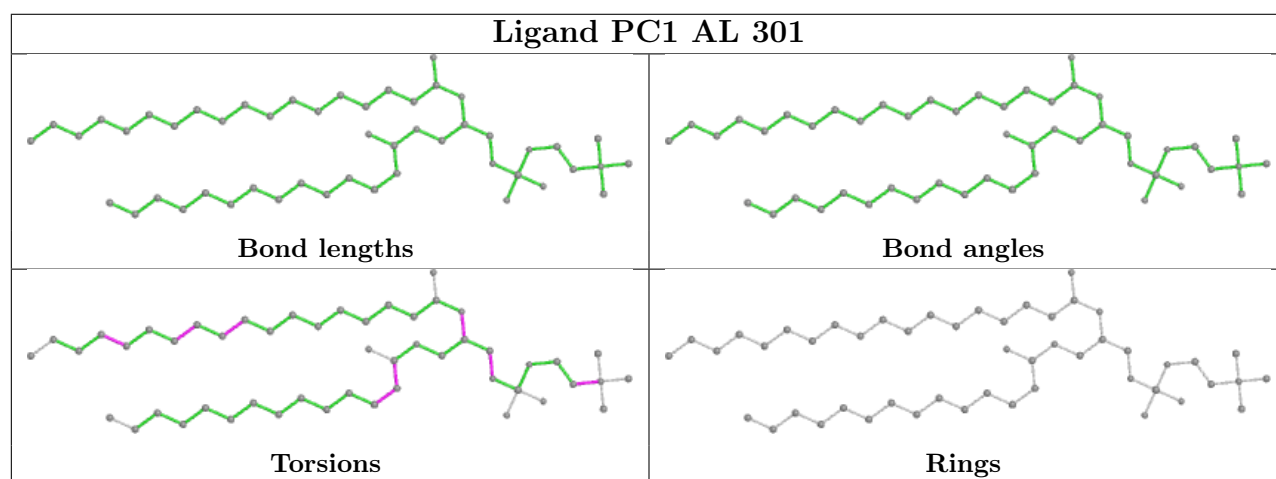
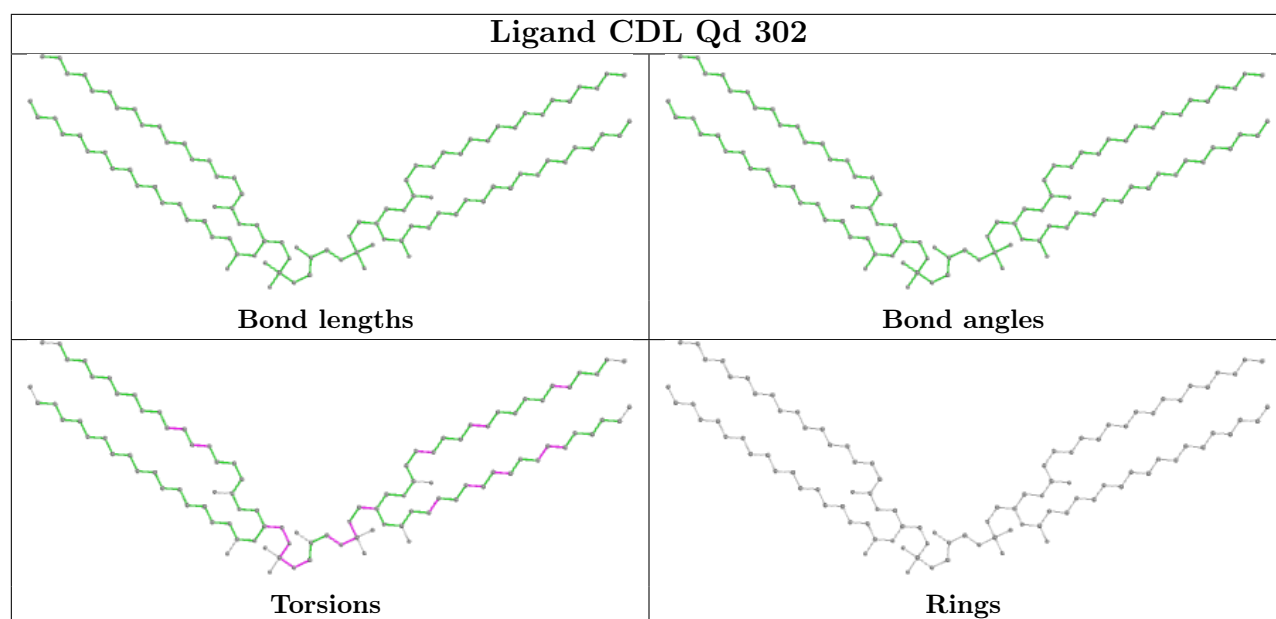
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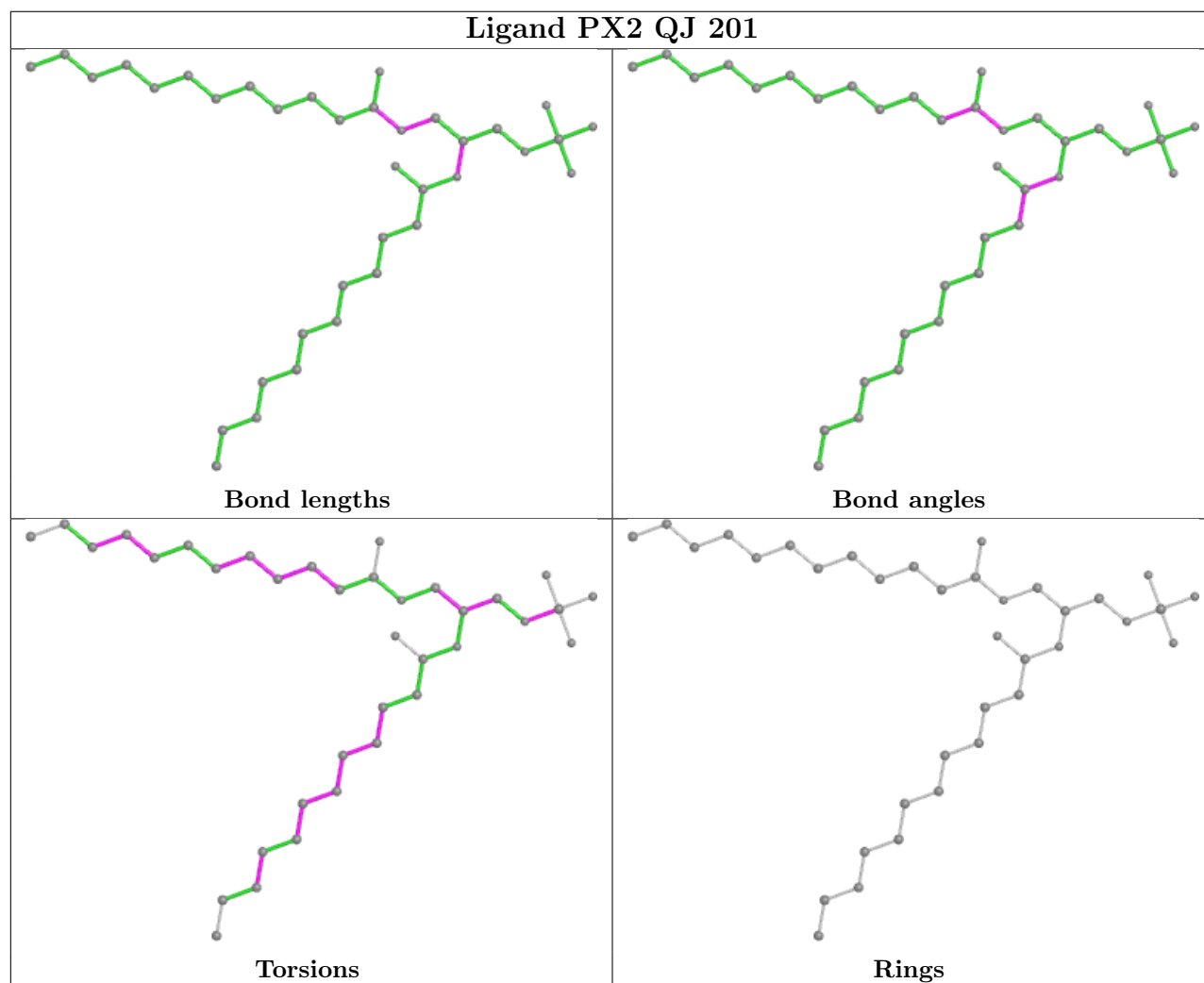
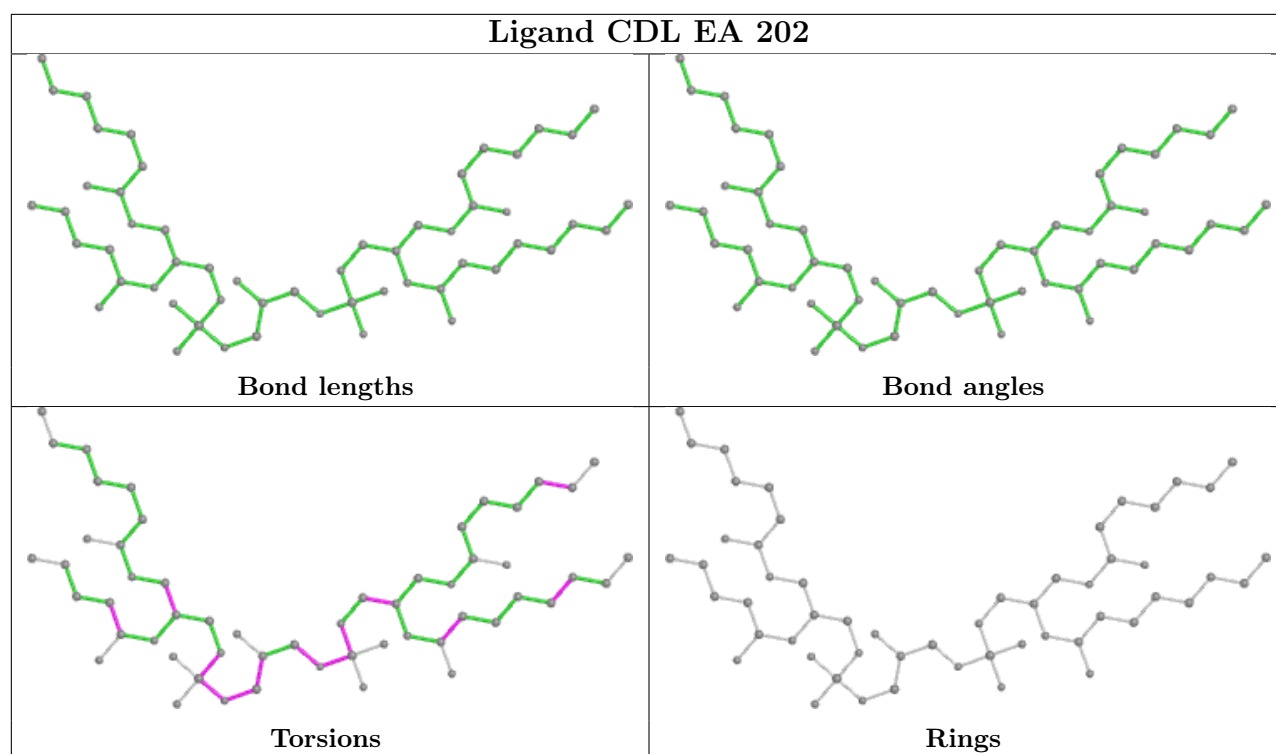


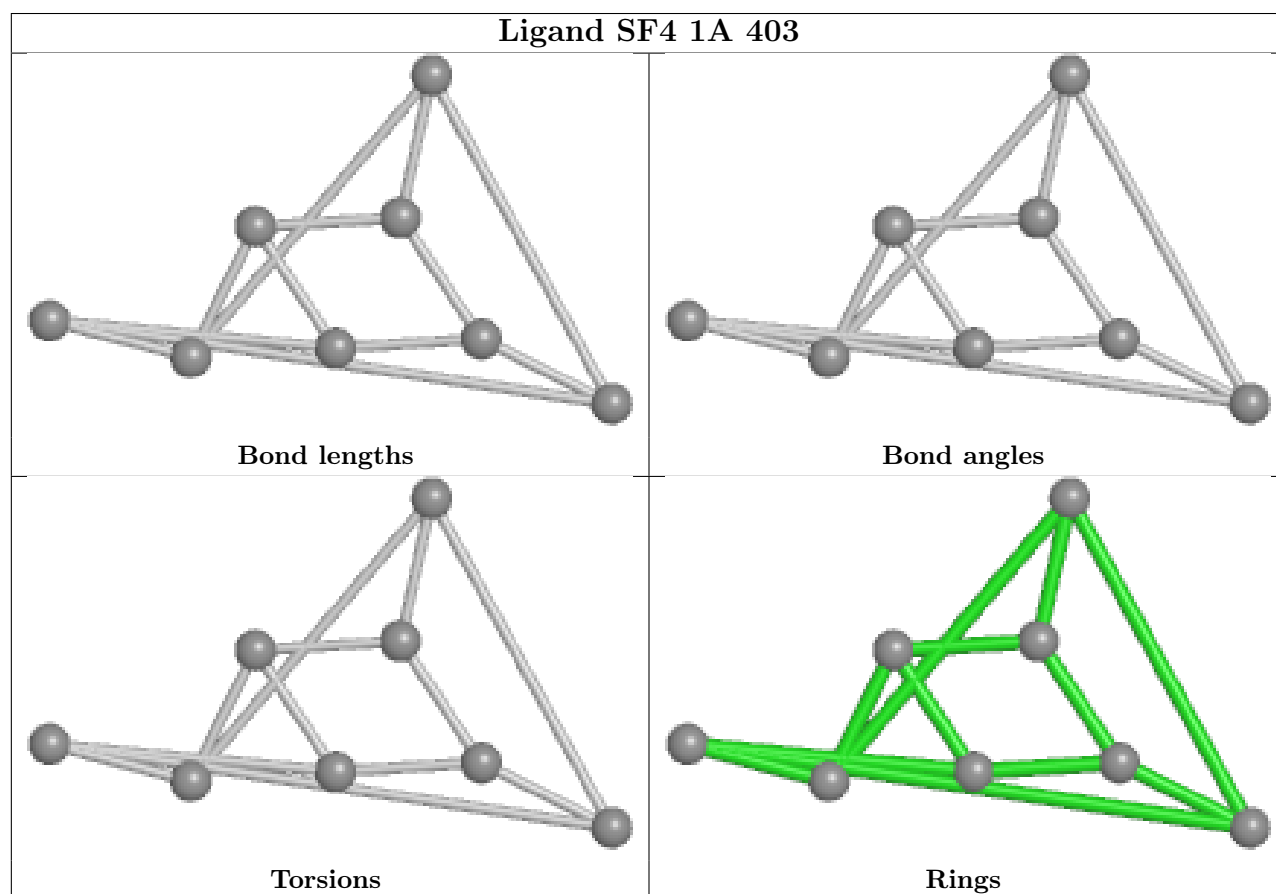
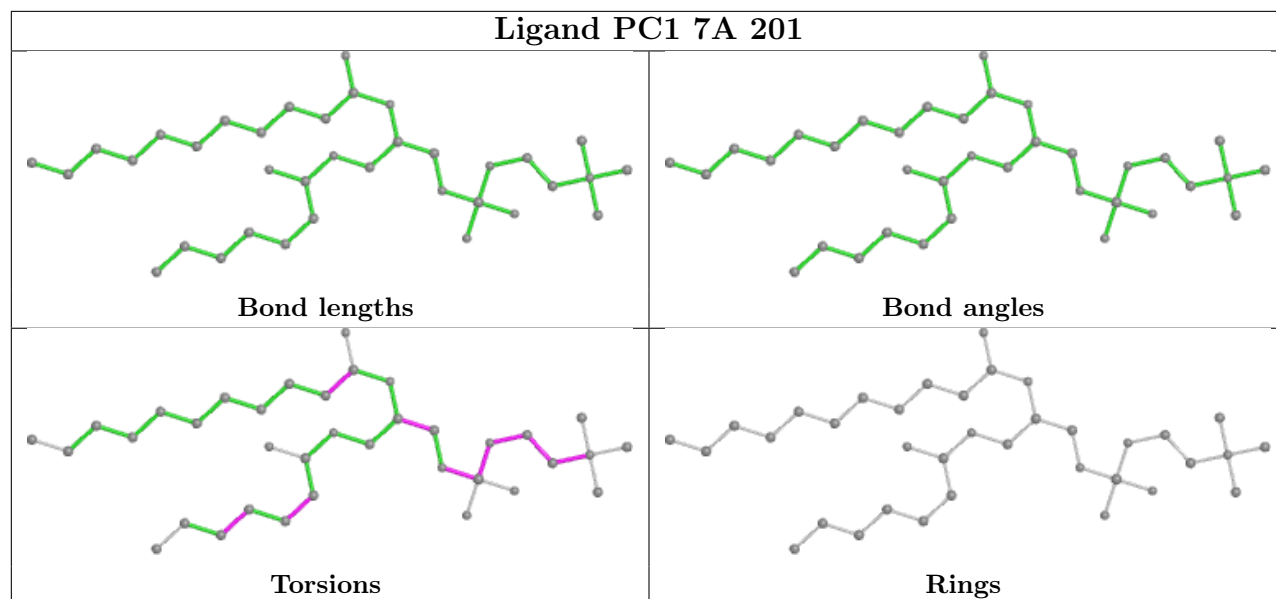


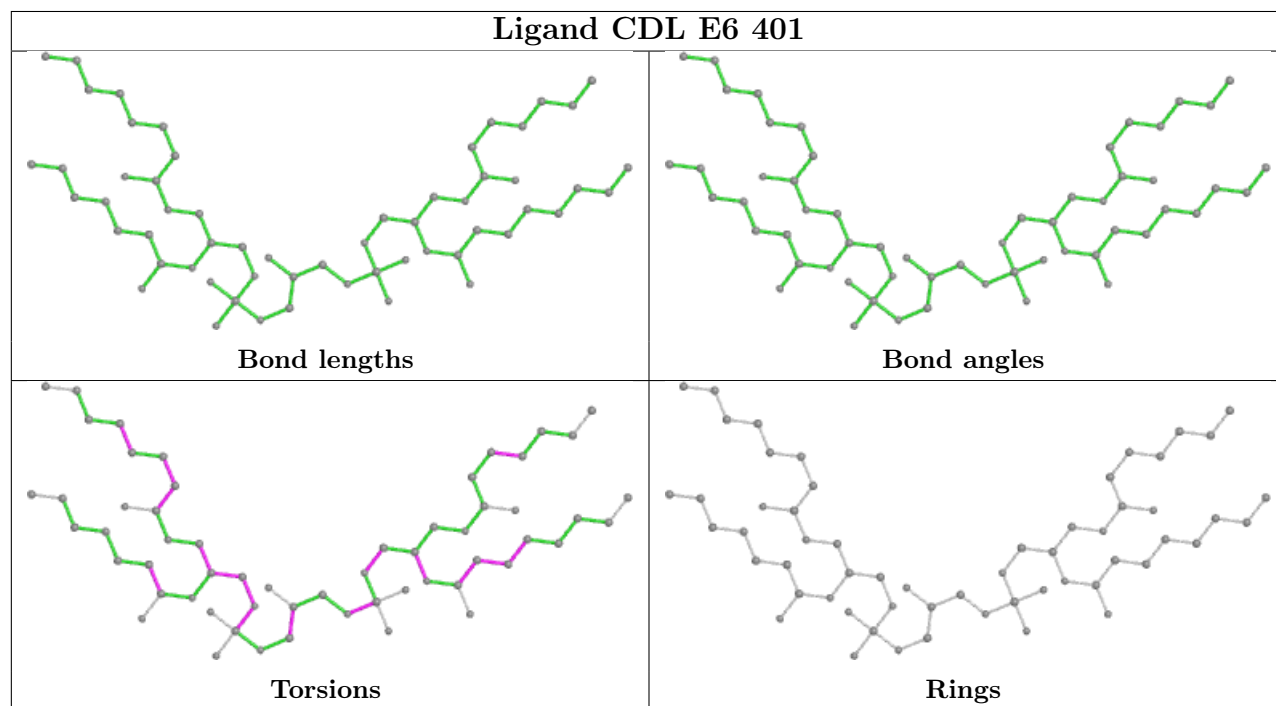
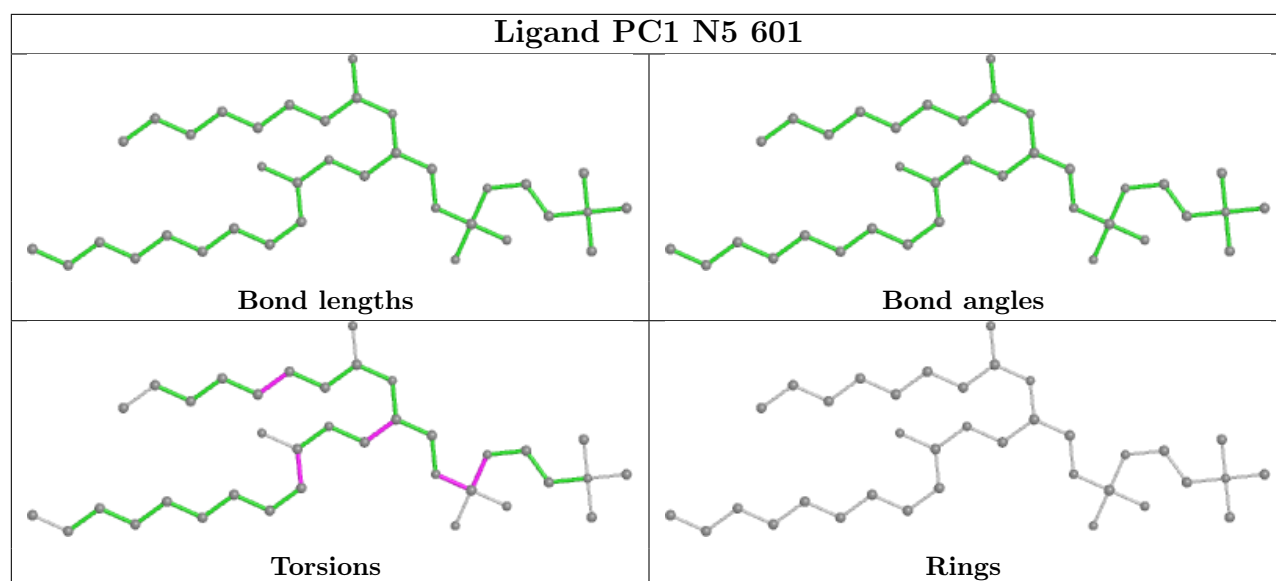


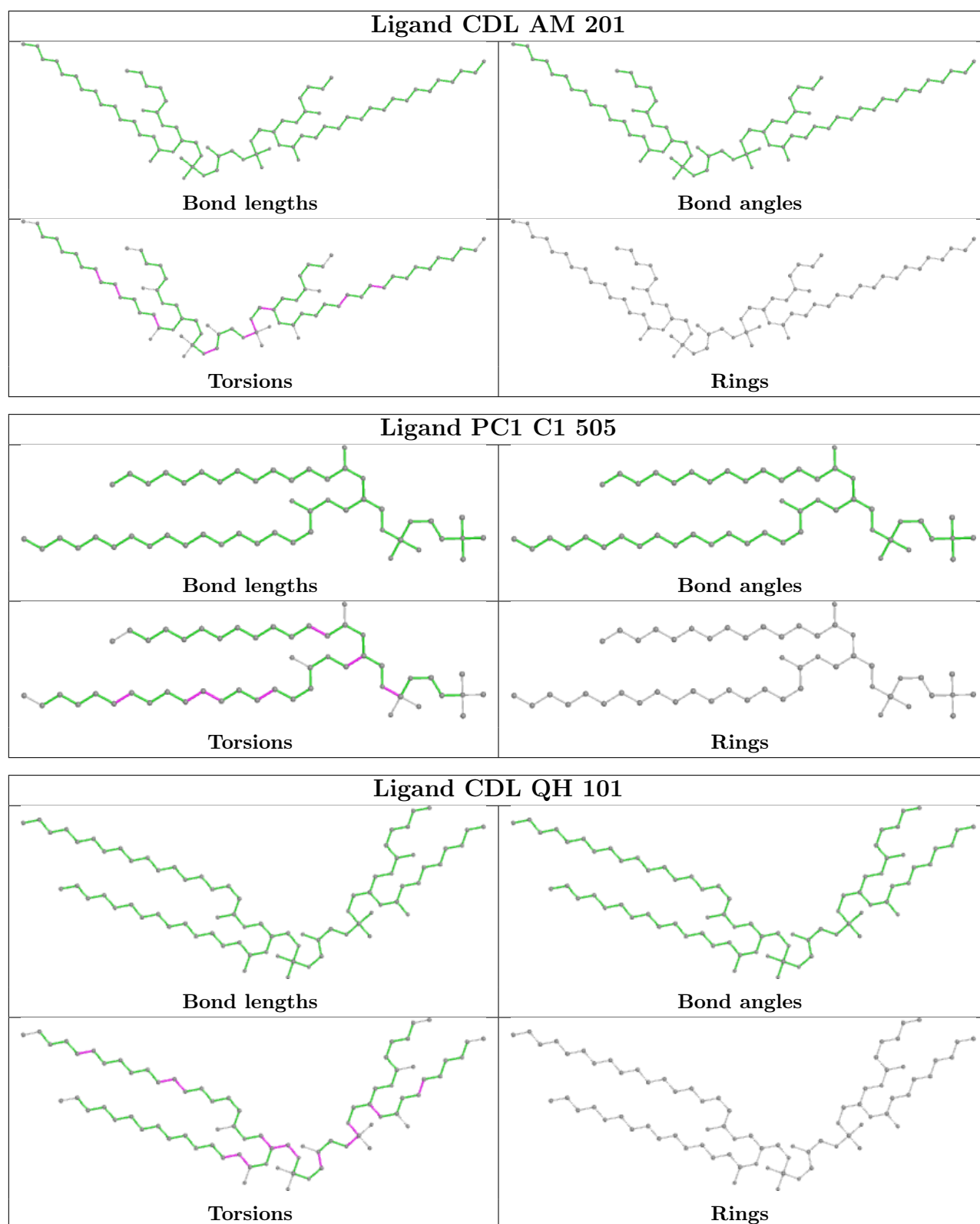


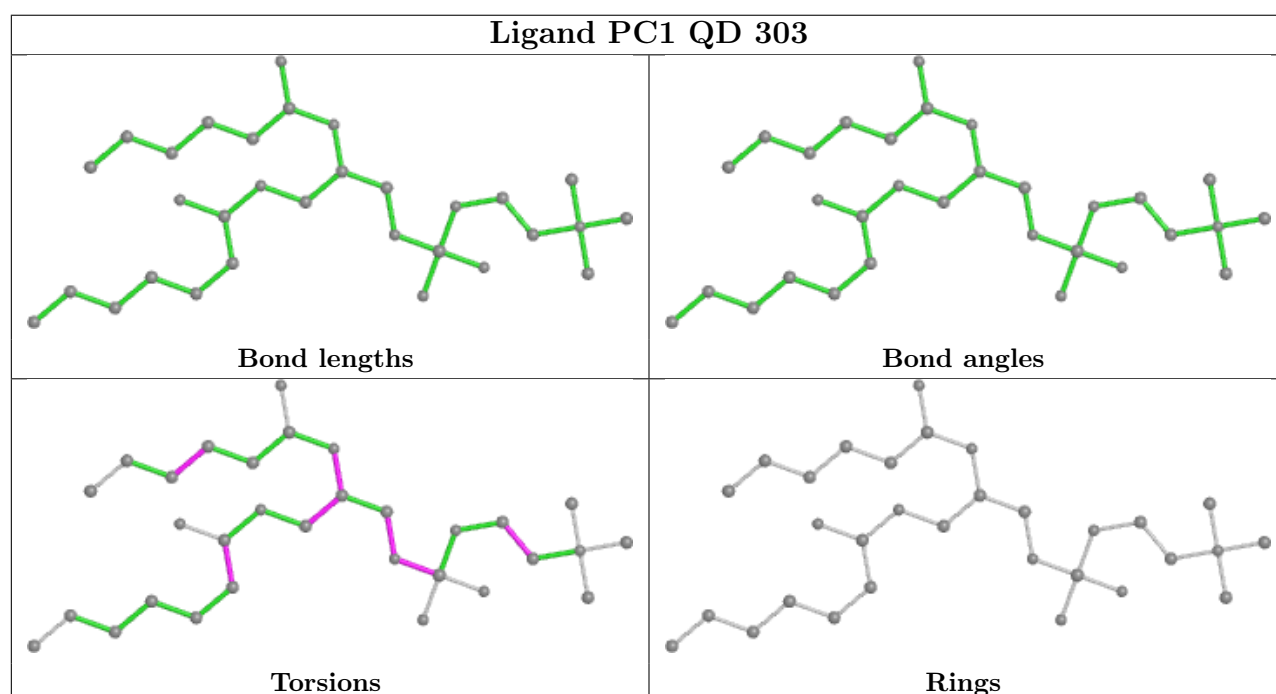
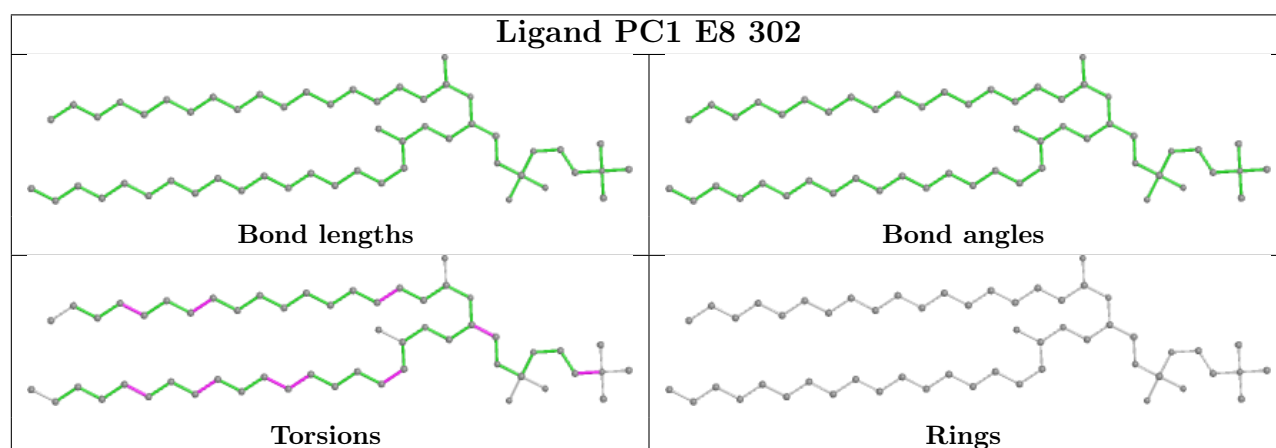
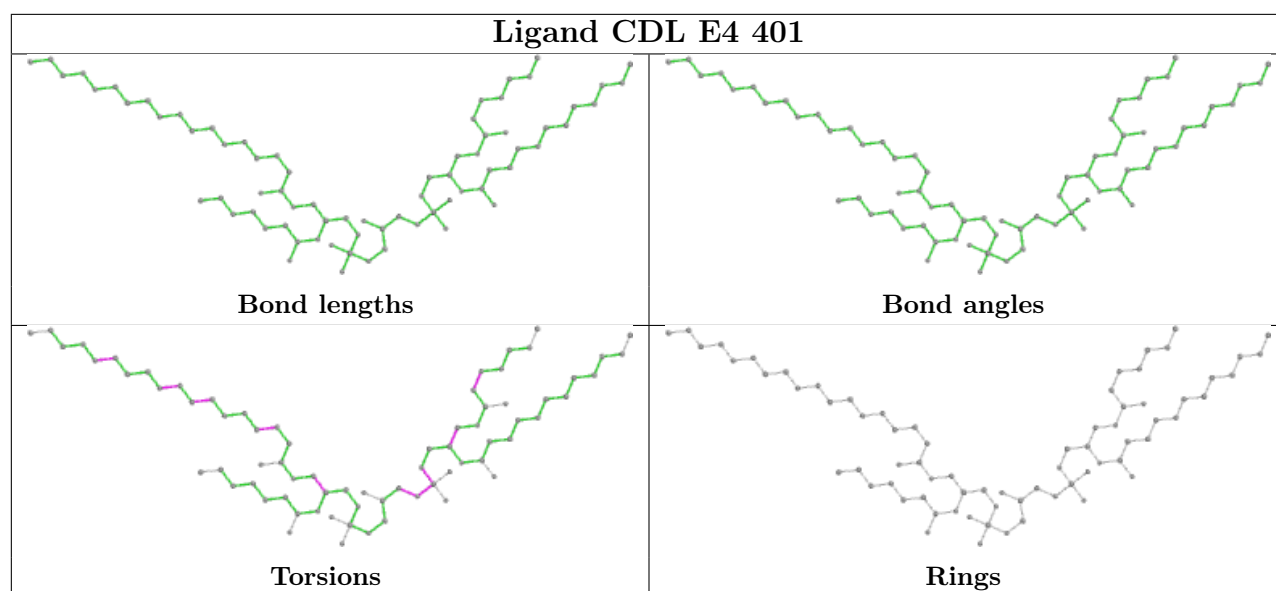


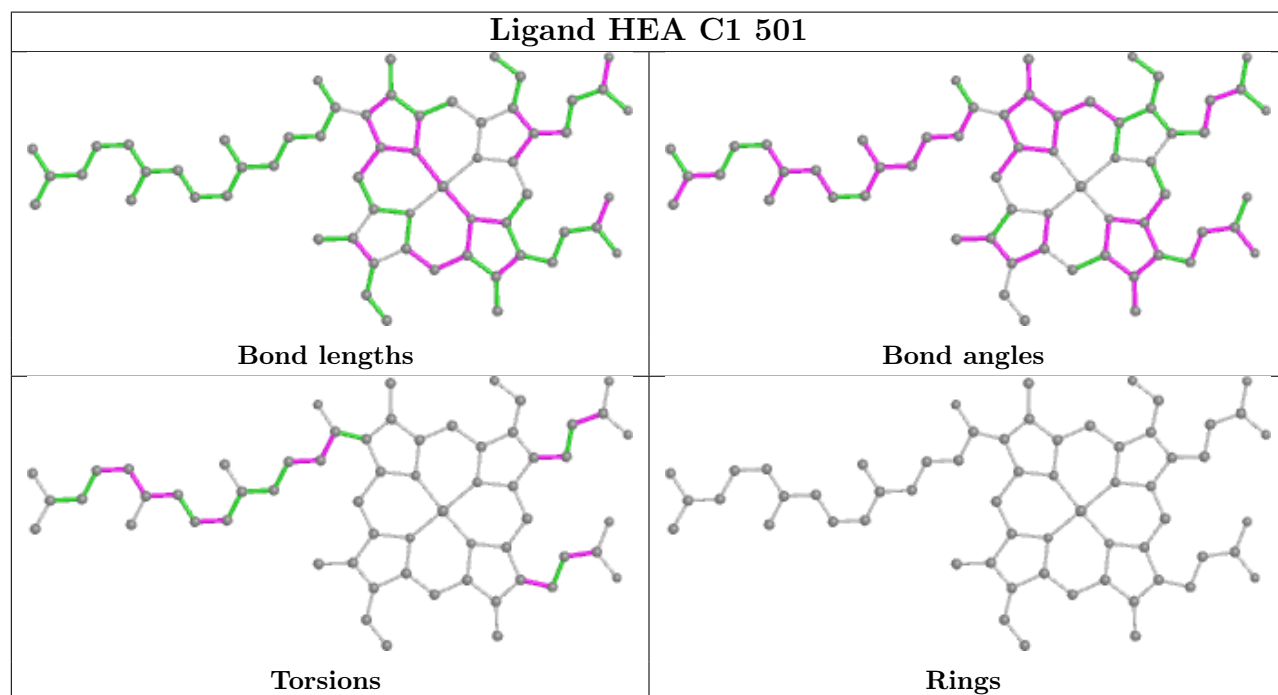
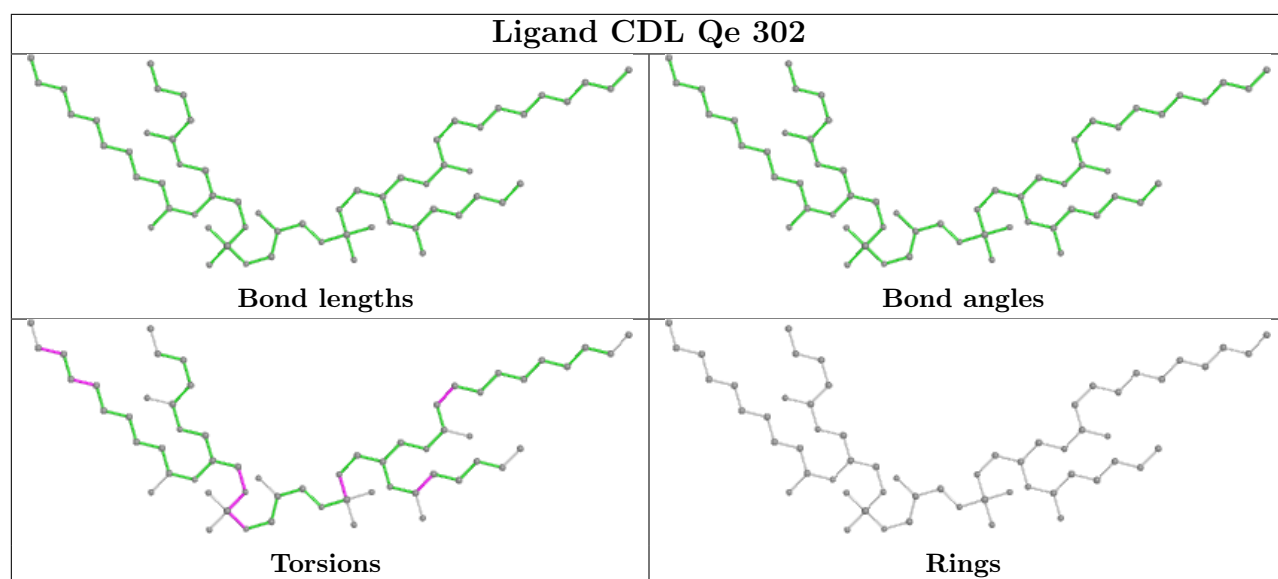


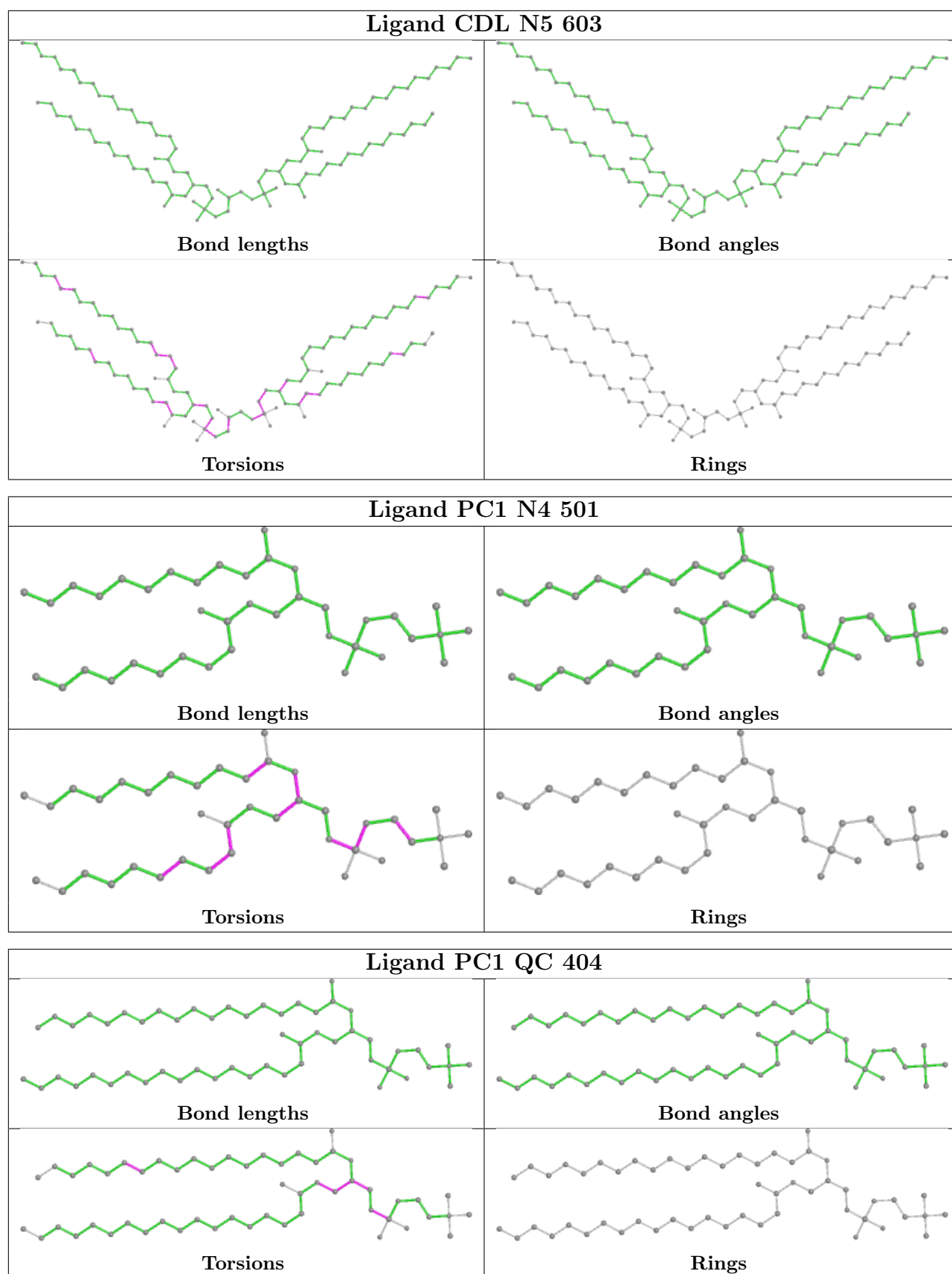


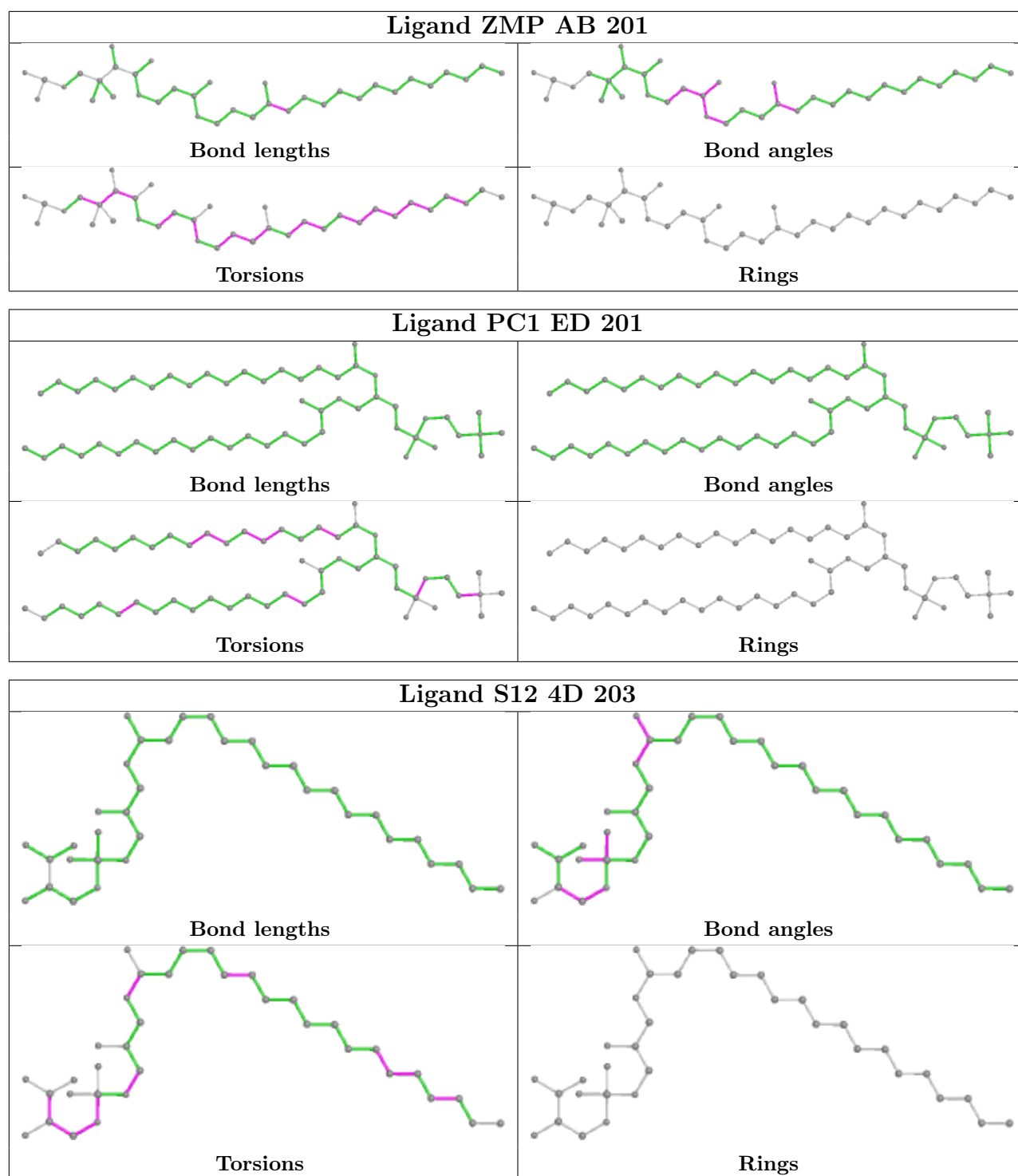


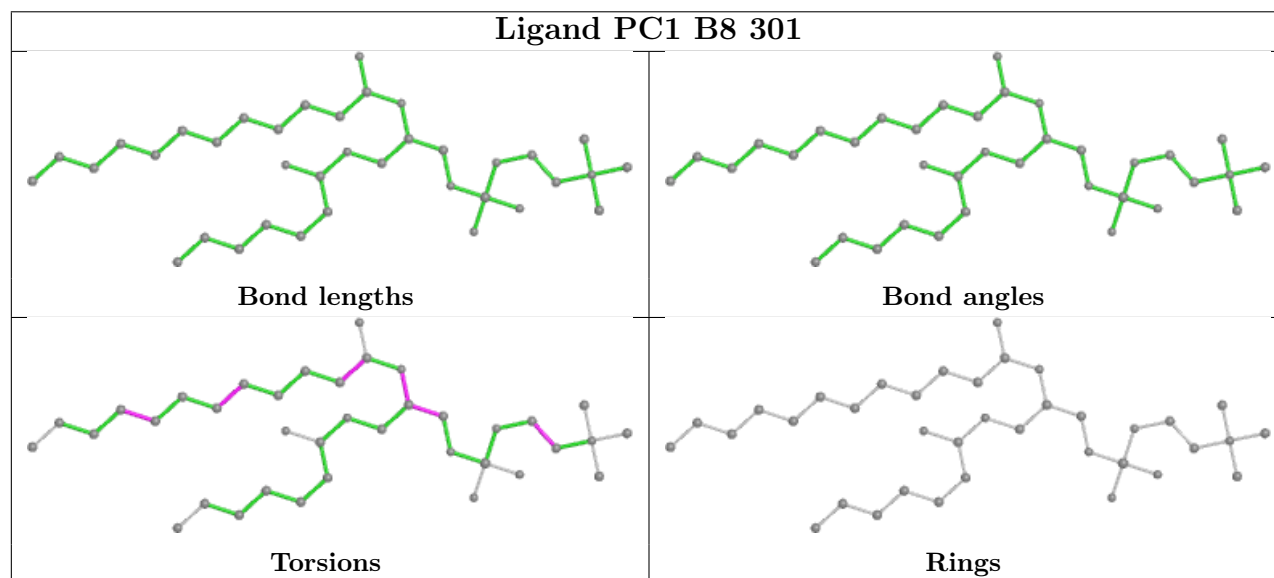
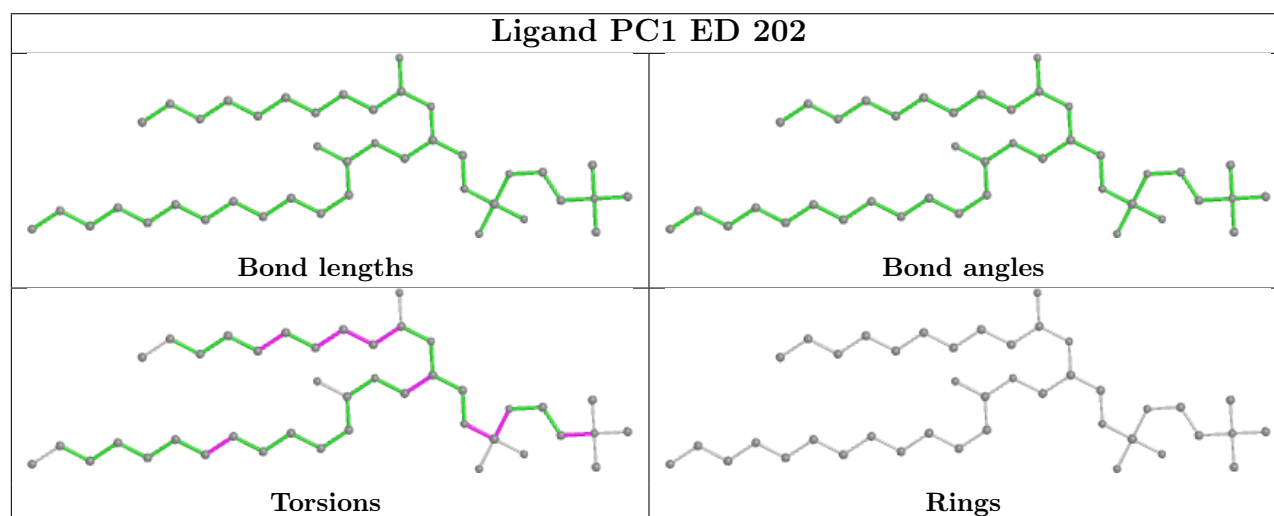
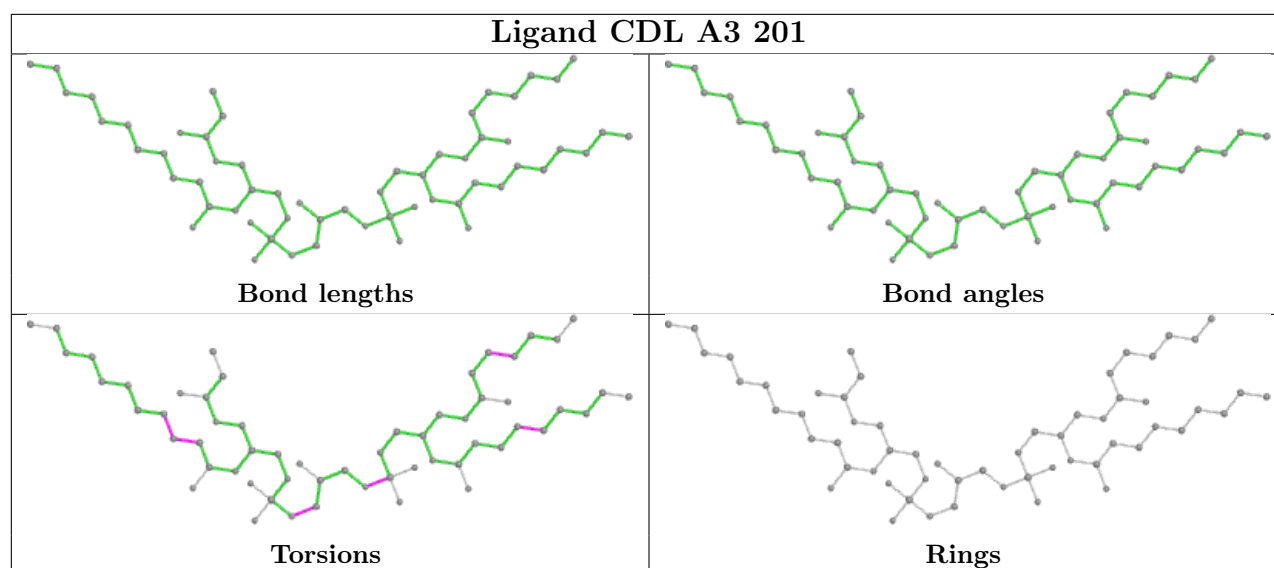


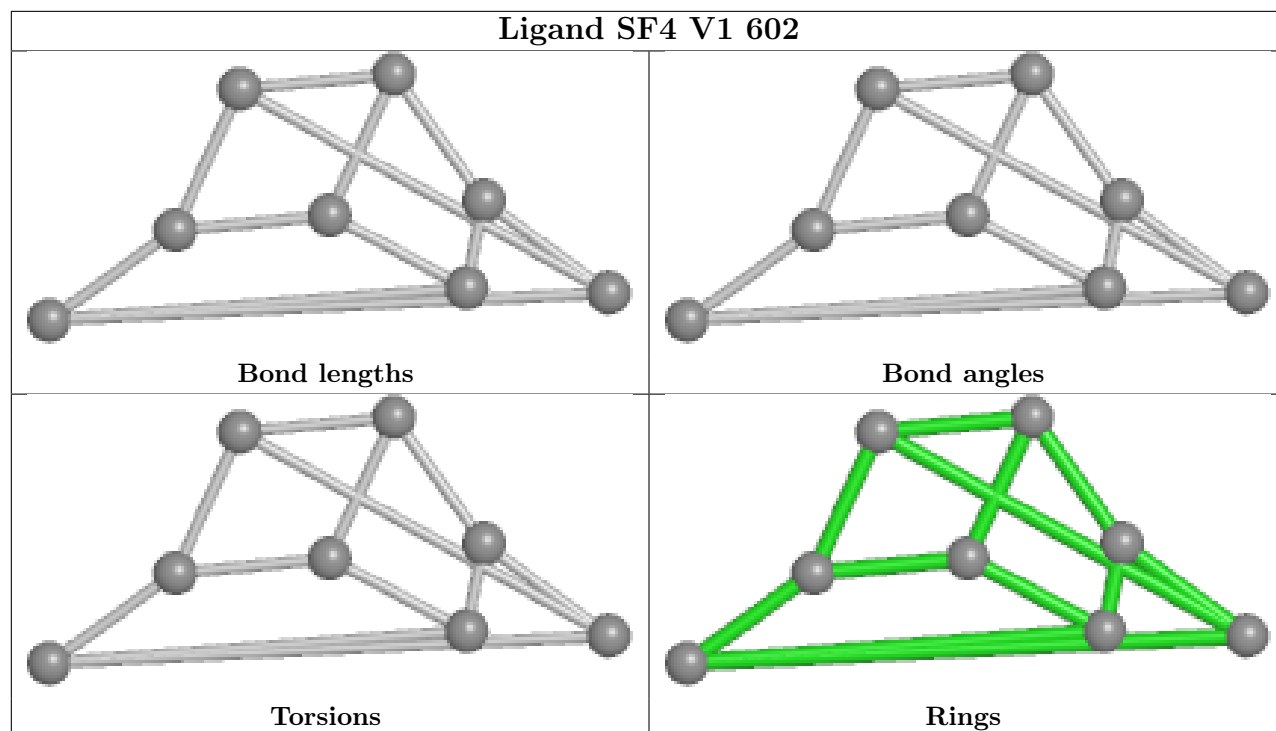












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.