



Full wwPDB EM Validation 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 Full wwPDB EM Validation 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

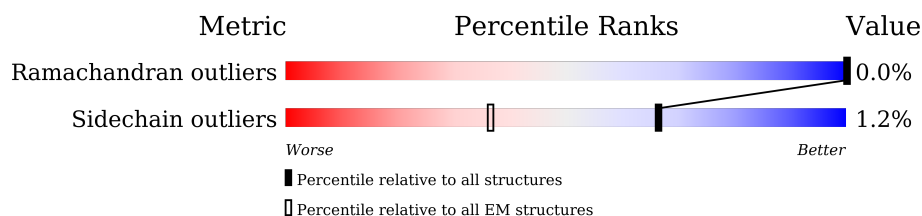
1 Overall quality at a glance

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.



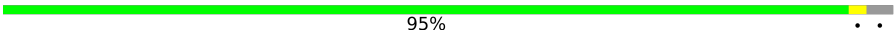
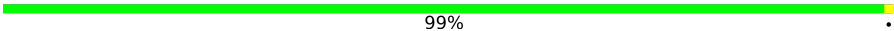




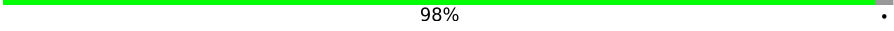


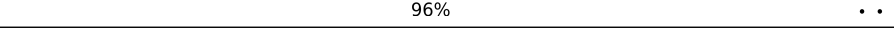
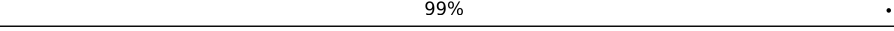
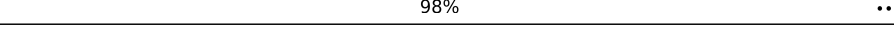

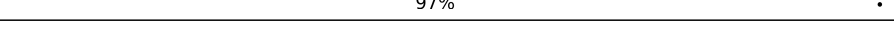
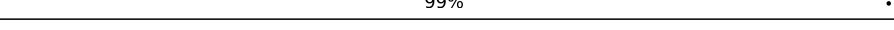
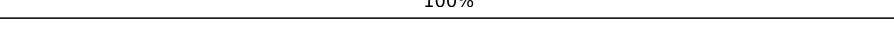
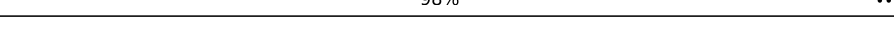


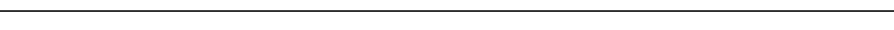

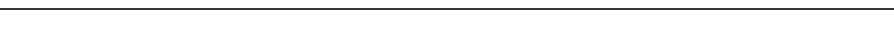
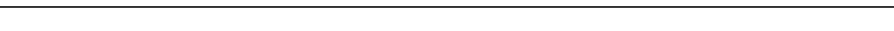


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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%
3	2B	142	98% ..
4	4A	246	83% 17%
5	4C	139	87% 12%
6	4D	174	97% ..
7	4E	165	96% ..
8	4F	75	100%
9	4G	315	93% 6%
10	4H	221	92% 7%


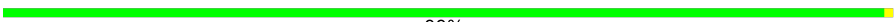












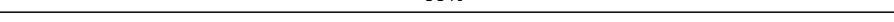

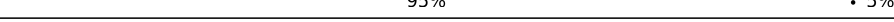


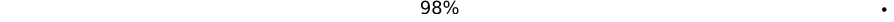
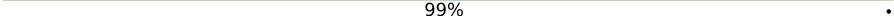

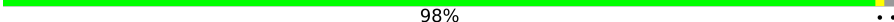
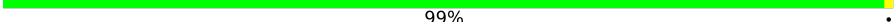

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Mol	Chain	Length	Quality of chain
11	4I	274	95% 
12	4J	88	99% 
13	4L	171	63% 
14	5B	174	87% 
15	5C	208	94% 
16	6A	112	81% 
17	6B	287	98% 
18	7A	178	92% 
19	7C	171	87% 
20	A1	141	96% 
21	A2	193	99% 
22	A3	125	98% 
23	A5	184	82% 
24	A6	437	97% 
25	A7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

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		

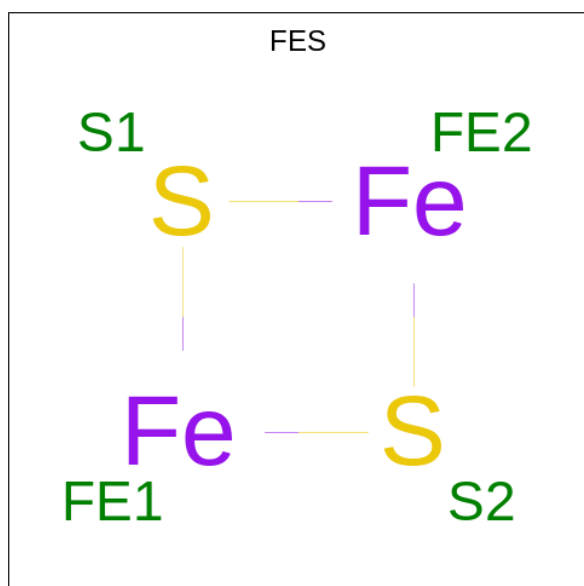
- Molecule 89 is a protein called NDUFV2.

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).

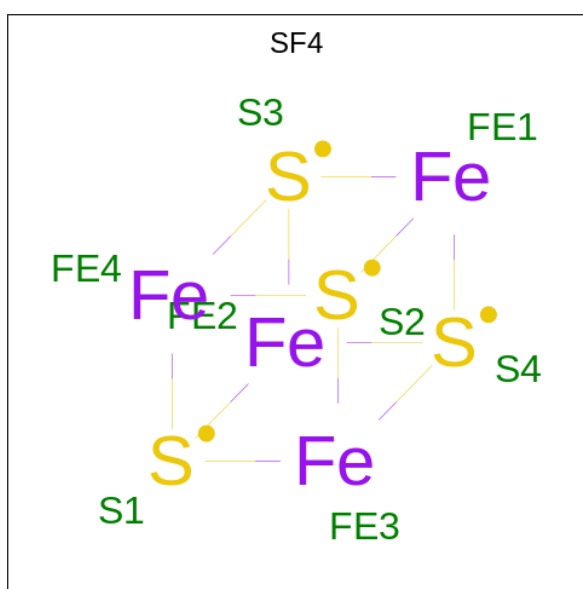
Mol	Chain	Residues	Atoms					AltConf	Trace
90	A	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
90	B	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- 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).

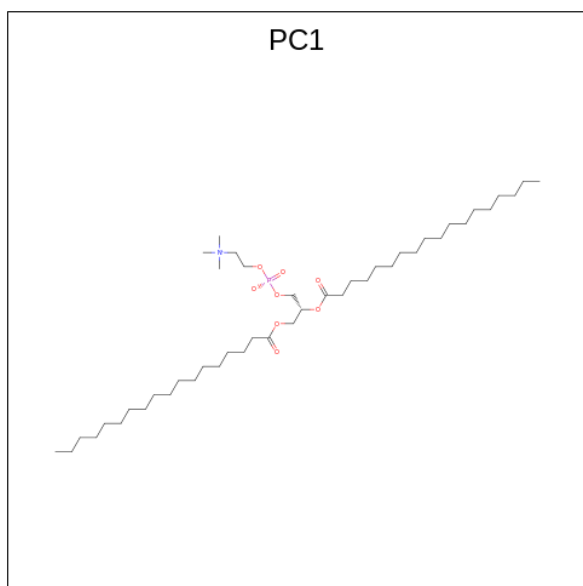


Mol	Chain	Residues	Atoms			AltConf
92	1A	1	Total	Fe	S	0
			8	4	4	
92	1A	1	Total	Fe	S	0
			8	4	4	
92	S7	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	V1	1	Total	Fe	S	0
			8	4	4	

- 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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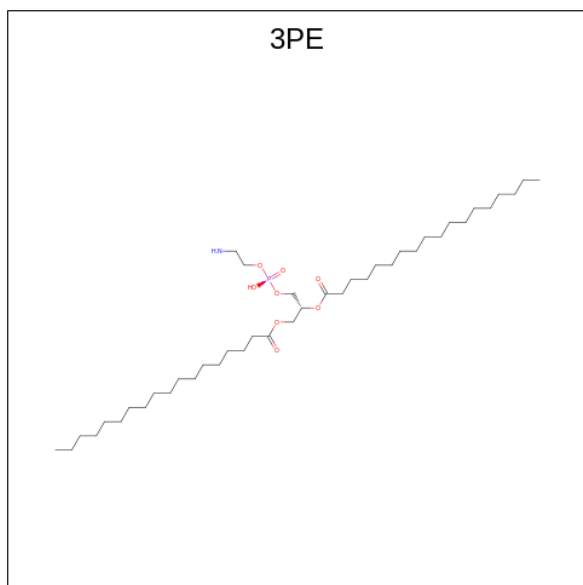
Mol	Chain	Residues	Atoms						AltConf
94	AM	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	AN	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B8	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
94	C1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
94	C3	1	Total 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 142	C 44	H 88	N 1	O 8	P 1	0
94	N5	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	QC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	QD	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	QI	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	Qc	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	Qe	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qg	1	Total 58	C 18	H 30	N 1	O 8	P 1	0
94	Qj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

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



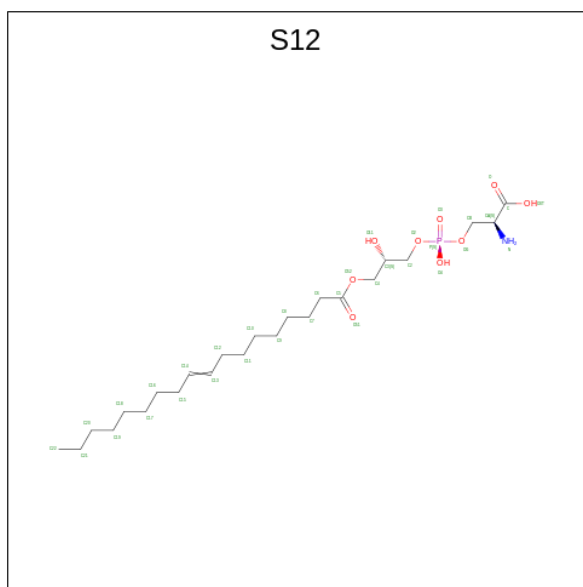
Mol	Chain	Residues	Atoms					AltConf	
95	4D	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	

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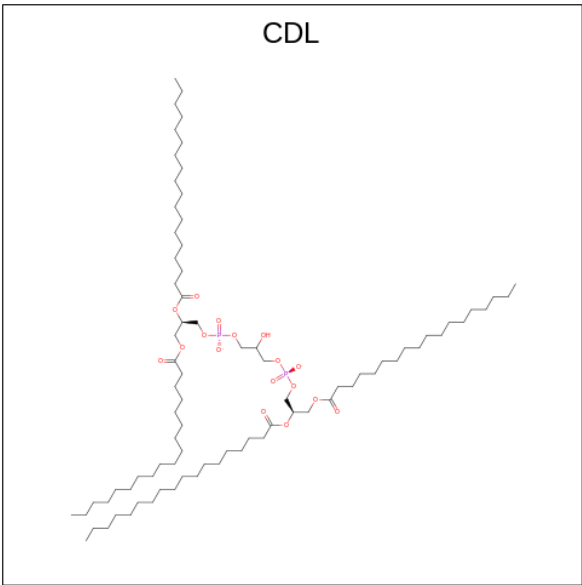
Mol	Chain	Residues	Atoms						AltConf
95	4D	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	7A	1	Total	C	H	N	O	P	0
			100	31	59	1	8	1	
95	B4	1	Total	C	H	N	O	P	0
			97	30	57	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	E9	1	Total	C	H	N	O	P	0
			133	41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

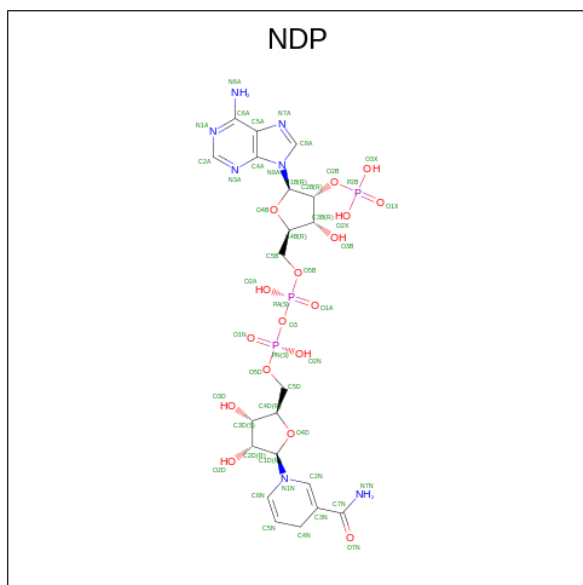
Mol	Chain	Residues	Atoms		AltConf
98	5B	1	Total	Zn	0
			1	1	
98	E7	1	Total	Zn	0
			1	1	

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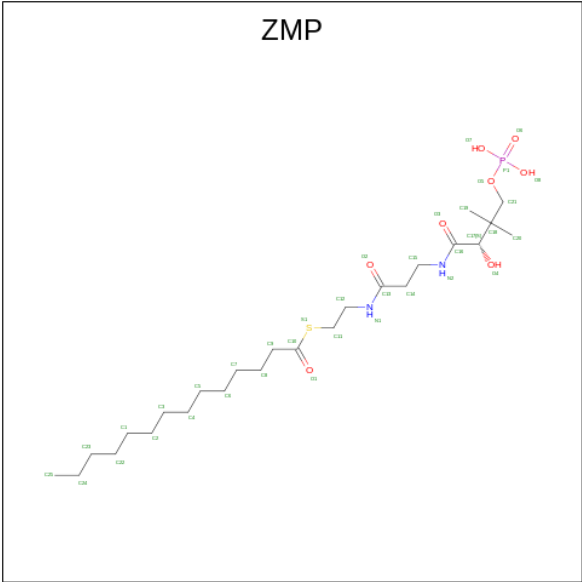
Mol	Chain	Residues	Atoms		AltConf
98	S6	1	Total	Zn	0
			1	1	

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



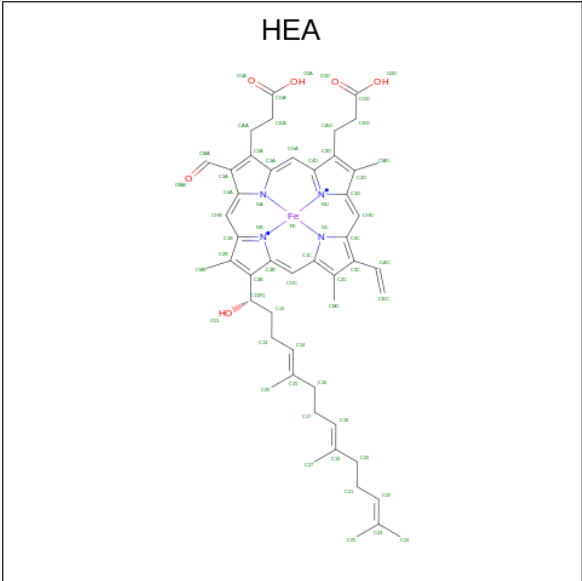
Mol	Chain	Residues	Atoms					AltConf	
99	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 100 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)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
			36	25	2	7	1	1
100	AC	1	Total	C	N	O	P	S
			36	25	2	7	1	1

- Molecule 101 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

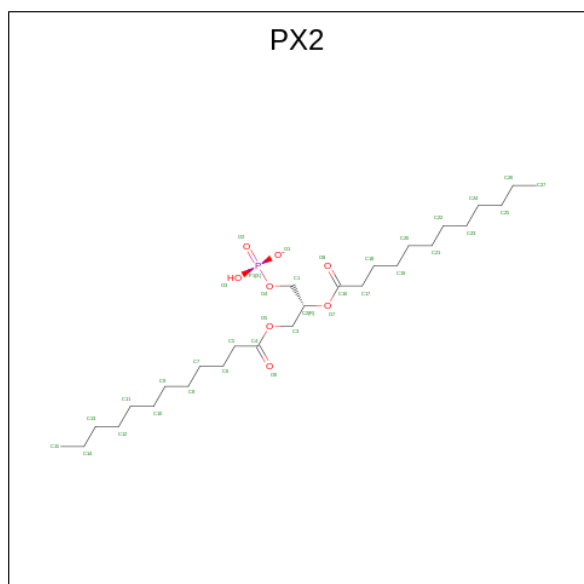
- Molecule 102 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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).



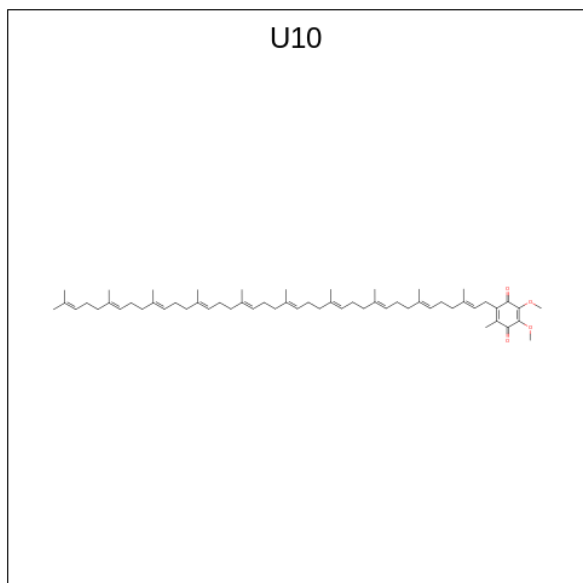
Mol	Chain	Residues	Atoms				AltConf
104	C2	1	Total	C	O	P	0
			36	27	8	1	

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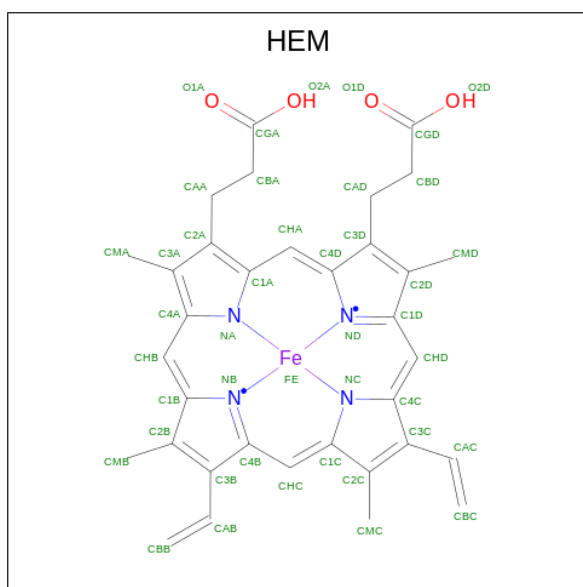
Mol	Chain	Residues	Atoms				AltConf
104	QJ	1	Total	C	O	P	0
			36	27	8	1	
104	QJ	1	Total	C	O	P	0
			36	27	8	1	

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



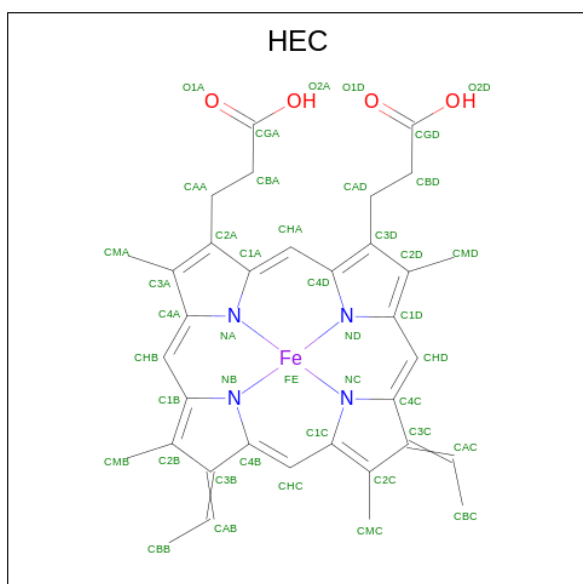
Mol	Chain	Residues	Atoms				AltConf
105	N4	1	Total	C	H	O	0
			98	39	55	4	

- 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).



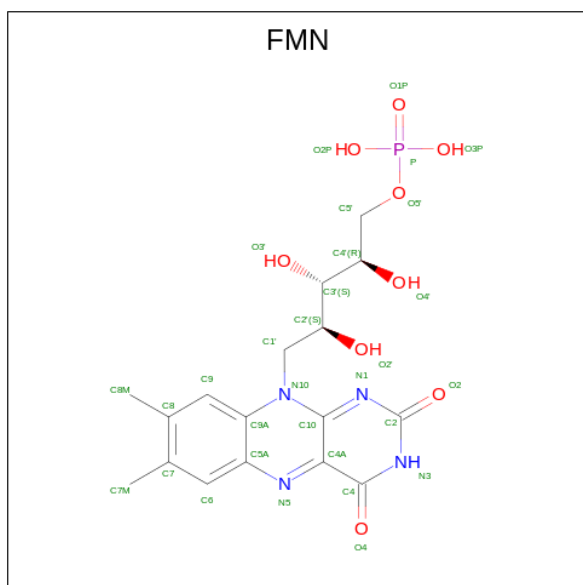
Mol	Chain	Residues	Atoms					AltConf
106	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
106	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
106	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
106	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 107 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (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).

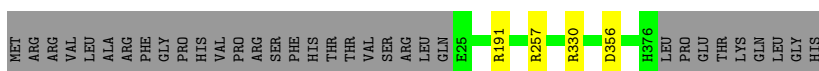


3 Residue-property plots [i](#)

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.

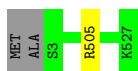
- Molecule 1: NDUFS1a

Chain 1A:  90% 9%



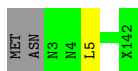
- Molecule 2: NDUFS1b

Chain 1B:  99%




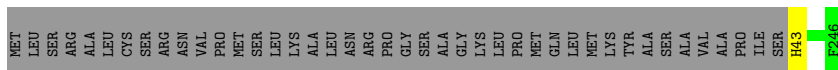
- Molecule 3: ND2b

Chain 2B:  98%




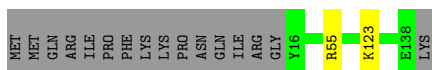
- Molecule 4: COXEG1

Chain 4A:  83% 17%



- Molecule 5: COXEG3

Chain 4C:  87% 12%



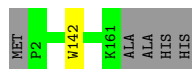
- Molecule 6: COXEG4

Chain 4D:  97%



- Molecule 7: COXEG5

Chain 4E: 96%



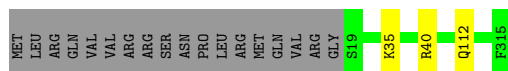
- Molecule 8: COXEG6

Chain 4F: 100%

There are no outlier residues recorded for this chain.

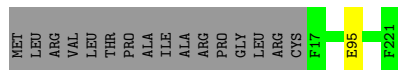
- Molecule 9: COXEG7

Chain 4G: 93%



- Molecule 10: COXEG8

Chain 4H: 92%



- Molecule 11: COXEG9

Chain 4I: 95%



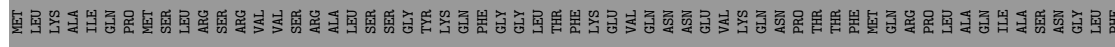
- Molecule 12: COXEG10

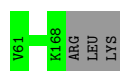
Chain 4J: 99%



- Molecule 13: ND4L

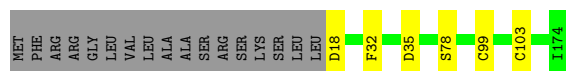
Chain 4L: 63%





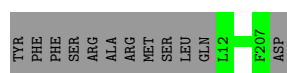
- Molecule 14: COX5b-2

Chain 5B: 87% 10%



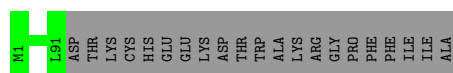
- Molecule 15: COX5c

Chain 5C: 94% 6%



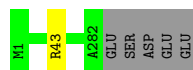
- Molecule 16: COX6a

Chain 6A: 81% 19%



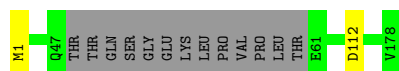
- Molecule 17: COX6b-1

Chain 6B: 98% 2%



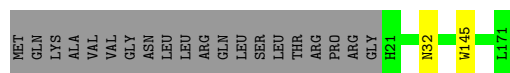
- Molecule 18: COX7a

Chain 7A: 92% 7%



- Molecule 19: COX7c

Chain 7C: 87% 12%



- Molecule 20: NDUFA1

Chain A1: 96% 4%



- Molecule 21: NDUFA2

Chain A2: 99% ..



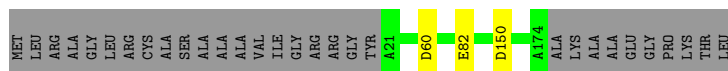
- Molecule 22: NDUFA3

Chain A3: 98% ..



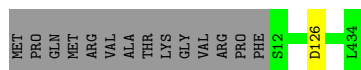
- Molecule 23: NDUFA5

Chain A5: 82% 16%



- Molecule 24: NDUFA6

Chain A6: 97% .



- Molecule 25: NDUFA7

Chain A7: 99% .



- Molecule 26: NDUFA8

Chain A8: 100%



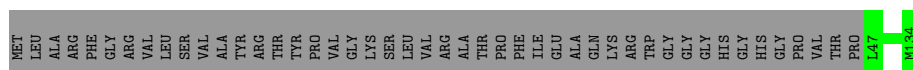
- Molecule 27: NDUFA9

Chain A9: 98% ..



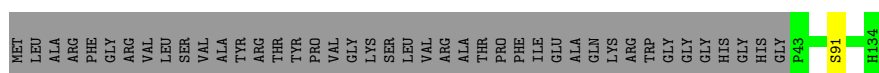
- Molecule 28: NDUFAB1-alpha

Chain AB: 66% 34%



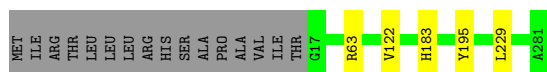
- Molecule 29: NDUFAB1-beta

Chain AC: 68% • 31%



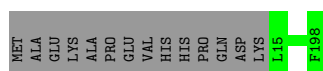
- Molecule 30: NDUFA12

Chain AL: 93% • 6%



- Molecule 31: NDUFA13

Chain AM: 93% 7%



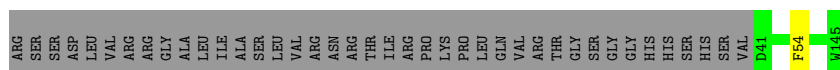
- Molecule 32: NDUFA11

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%



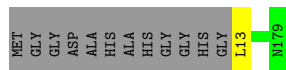
- Molecule 46: NDUFC2

Chain C4: 97%



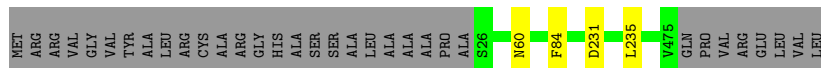
- Molecule 47: COX4

Chain DC: 93% 7%



- Molecule 48: NDUEG1

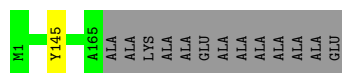
Chain E1: 92% 7%



- Molecule 49: NDUEG2

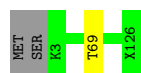
Chain E2: 99%

Chain E9:  92% • 7%



- Molecule 57: NDUEG10

Chain EA:  98% ••




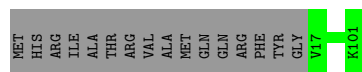
- Molecule 58: NDUEG11

Chain EB:  99% •



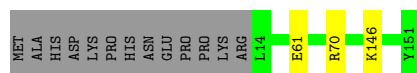
- Molecule 59: NDUEG11

Chain EC:  84% 16%



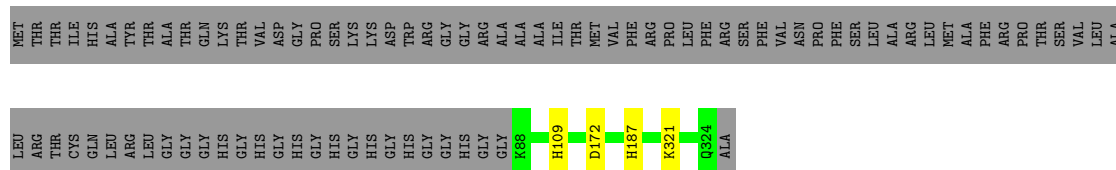
- Molecule 60: NDUEG13

Chain ED:  89% • 9%



- Molecule 61: NDUFX

Chain FX:  72% • 27%

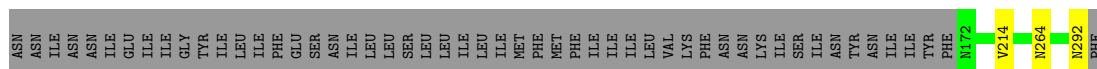


- Molecule 62: NDUCA1

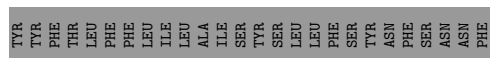
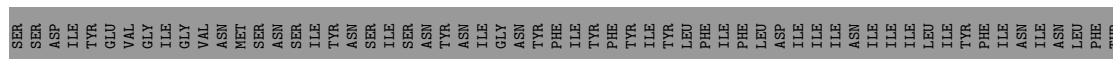
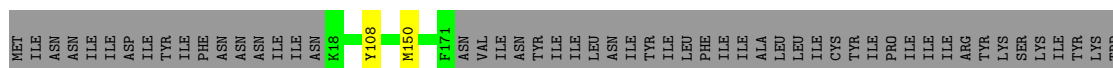
Chain G1:  96% ••



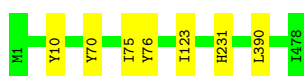
- Molecule 63: NDUCA2



- Molecule 67: ND3



- Molecule 68: NADH-ubiquinone oxidoreductase chain 4



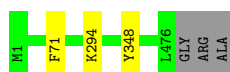
- Molecule 69: ND5



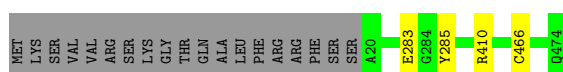
- Molecule 70: MPP-beta




- Molecule 70: MPP-beta

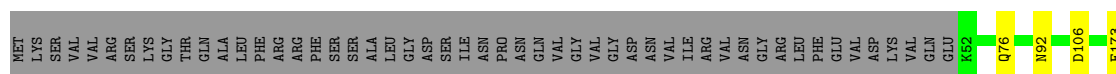


- Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



- 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% ..



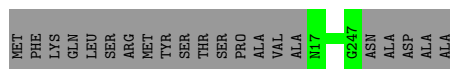
- Molecule 74: UQCRFS1

Chain QE:  90% 8%

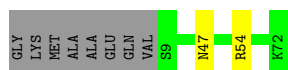
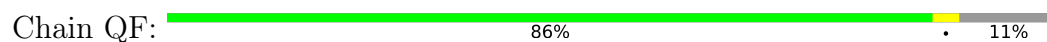


- Molecule 74: UQCRFS1

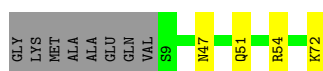
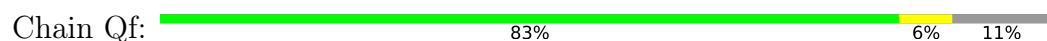
Chain Qe:  92% 8%



• Molecule 75: UQCRH



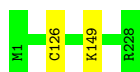
• Molecule 75: UQCRH



• 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.

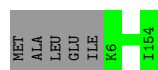
- Molecule 79: UQCR10

Chain QJ:  95%



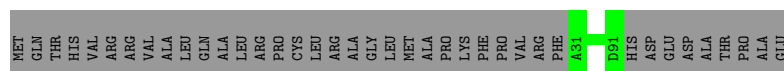
- Molecule 79: UQCR10

Chain Qj:  97%



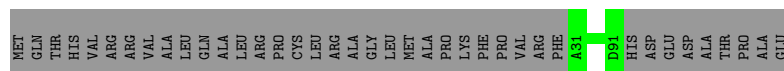
- Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

Chain QK:  61%  39%



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

Chain Qk:  61%  39%



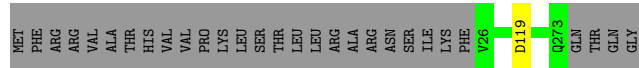
- Molecule 81: NDUFS2

Chain S2:  98%



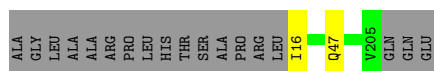
- Molecule 82: NDUFS3

Chain S3:  89%  10%



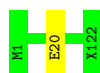
- Molecule 83: NDUFS4

Chain S4:  90% 9%



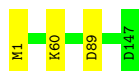
• Molecule 84: NDUFS5

Chain S5:  99%



• Molecule 85: NDUFS6

Chain S6:  98%



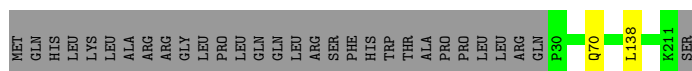
• Molecule 86: NDUFS7

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

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	191	ARG
1	1A	257	ARG
1	1A	330	ARG
1	1A	356	ASP
2	1B	505	ARG
3	2B	5	LEU
4	4A	43	HIS
5	4C	55	ARG
5	4C	123	LYS
6	4D	81	ILE
6	4D	125	HIS
6	4D	149	GLU
6	4D	170	VAL
7	4E	142	TRP
9	4G	35	LYS
9	4G	40	ARG
9	4G	112	GLN
10	4H	95	GLU
11	4I	18	LEU
11	4I	91	PHE
11	4I	130	ARG
11	4I	211	ARG
11	4I	266	ARG
12	4J	29	THR
14	5B	18	ASP
14	5B	32	PHE
14	5B	35	ASP
14	5B	78	SER
14	5B	103	CYS
17	6B	43	ARG
18	7A	1	MET
18	7A	112	ASP

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Mol	Chain	Res	Type
19	7C	32	ASN
19	7C	145	TRP
20	A1	37	HIS
20	A1	60	ASN
21	A2	163	ASP
22	A3	53	ARG
23	A5	60	ASP
23	A5	82	GLU
23	A5	150	ASP
24	A6	126	ASP
25	A7	22	GLN
26	A8	96	GLN
27	A9	115	ARG
27	A9	139	TYR
27	A9	180	TYR
27	A9	269	ASP
29	AC	91	SER
30	AL	63	ARG
30	AL	122	VAL
30	AL	183	HIS
30	AL	195	TYR
30	AL	229	LEU
33	B2	54	PHE
37	B6	25	ARG
38	B7	4	ASP
39	B8	107	LEU
40	B9	21	SER
40	B9	93	PHE
40	B9	130	GLN
41	BL	32	ARG
41	BL	95	ARG
42	BM	30	HIS
43	C1	139	LEU
43	C1	416	PHE
43	C1	465	PHE
43	C1	466	HIS
44	C2	60	TRP
44	C2	75	SER
44	C2	144	SER
45	C3	132	ASP
45	C3	135	LEU
45	C3	156	HIS

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Mol	Chain	Res	Type
46	C4	43	ASP
46	C4	131	PHE
46	C4	145	LEU
47	DC	13	LEU
48	E1	60	ASN
48	E1	84	PHE
48	E1	231	ASP
48	E1	235	LEU
49	E2	28	LEU
50	E3	20	GLN
50	E3	50	ASP
50	E3	107	HIS
50	E3	356	ASP
50	E3	376	VAL
51	E4	142	GLN
51	E4	304	ARG
51	E4	332	ASP
52	E5	49	ASP
52	E5	223	ASP
52	E5	263	ARG
52	E5	266	LEU
53	E6	204	GLN
53	E6	286	ARG
53	E6	306	ARG
54	E7	4	LEU
54	E7	149	LEU
54	E7	169	THR
54	E7	175	TYR
55	E8	1	MET
55	E8	79	LYS
55	E8	133	ASP
56	E9	145	TYR
57	EA	69	THR
58	EB	61	GLN
60	ED	61	GLU
60	ED	70	ARG
60	ED	146	LYS
61	FX	109	HIS
61	FX	172	ASP
61	FX	187	HIS
61	FX	321	LYS
62	G1	28	ARG

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Mol	Chain	Res	Type
62	G1	35	SER
62	G1	123	PHE
62	G1	251	ASP
62	G1	266	ARG
62	G1	321	HIS
62	G1	384	ASP
62	G1	413	ASN
63	G2	71	GLN
63	G2	108	ARG
63	G2	138	ASP
64	G3	37	ARG
64	G3	103	ARG
64	G3	133	ASP
65	N1	378	LEU
65	N1	437	CYS
65	N1	557	TYR
65	N1	622	PHE
65	N1	648	TYR
65	N1	652	PHE
66	N2	44	PHE
66	N2	155	SER
67	N3	264	ASN
67	N3	292	ASN
68	N4	10	TYR
68	N4	70	TYR
68	N4	75	ILE
68	N4	76	TYR
68	N4	123	ILE
68	N4	231	HIS
68	N4	390	LEU
69	N5	85	TYR
69	N5	260	THR
69	N5	349	LYS
69	N5	367	ASP
69	N5	377	HIS
69	N5	393	LEU
69	N5	533	HIS
69	N5	540	ASP
67	N6	108	TYR
67	N6	150	MET
70	QA	22	ARG
70	QA	71	PHE

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Mol	Chain	Res	Type
70	QA	255	ASN
70	QA	348	TYR
70	QA	430	ASP
70	QA	476	LEU
71	QB	283	GLU
71	QB	285	TYR
71	QB	410	ARG
71	QB	466	CYS
72	QC	173	TYR
72	QC	329	CYS
72	QC	361	PHE
73	QD	33	TYR
73	QD	142	GLN
73	QD	199	ASP
73	QD	241	ASN
74	QE	128	ASP
74	QE	168	LEU
74	QE	169	LYS
74	QE	192	HIS
75	QF	47	ASN
75	QF	54	ARG
76	QG	126	CYS
76	QG	138	GLN
76	QG	228	ARG
78	QI	2	LEU
79	QJ	6	LYS
79	QJ	135	LEU
70	Qa	71	PHE
70	Qa	294	LYS
70	Qa	348	TYR
71	Qb	76	GLN
71	Qb	92	ASN
71	Qb	106	ASP
71	Qb	173	GLU
71	Qb	285	TYR
72	Qc	191	HIS
72	Qc	329	CYS
72	Qc	361	PHE
73	Qd	18	PHE
73	Qd	33	TYR
73	Qd	76	LYS
73	Qd	82	ARG

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Mol	Chain	Res	Type
73	Qd	96	ASN
75	Qf	47	ASN
75	Qf	51	GLN
75	Qf	54	ARG
75	Qf	72	LYS
76	Qg	126	CYS
76	Qg	149	LYS
81	S2	33	GLU
81	S2	147	TYR
81	S2	187	ARG
81	S2	357	ARG
82	S3	119	ASP
83	S4	16	ILE
83	S4	47	GLN
84	S5	20	GLU
85	S6	1	MET
85	S6	60	LYS
85	S6	89	ASP
86	S7	86	CYS
86	S7	116	ASP
86	S7	147	SER
86	S7	157	TYR
87	S8	70	GLN
87	S8	138	LEU
88	V1	103	LYS
88	V1	278	CYS
88	V1	386	CYS
88	V1	426	CYS
88	V1	502	ASN
89	V2	108	MET
89	V2	120	CYS
89	V2	133	ASP
89	V2	139	CYS
89	V2	152	MET
89	V2	156	SER
89	V2	212	ASP
89	V2	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (340) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	76	HIS

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Mol	Chain	Res	Type
1	1A	80	ASN
1	1A	82	ASN
1	1A	128	GLN
1	1A	204	ASN
1	1A	326	ASN
2	1B	158	ASN
2	1B	242	ASN
2	1B	265	ASN
2	1B	291	HIS
2	1B	315	ASN
2	1B	332	ASN
2	1B	387	HIS
2	1B	500	HIS
2	1B	507	HIS
3	2B	4	ASN
3	2B	99	HIS
3	2B	102	ASN
4	4A	67	HIS
4	4A	131	GLN
4	4A	161	HIS
4	4A	196	HIS
4	4A	242	GLN
6	4D	94	GLN
6	4D	118	HIS
9	4G	22	ASN
9	4G	112	GLN
9	4G	141	ASN
10	4H	101	ASN
11	4I	62	HIS
11	4I	153	ASN
11	4I	167	HIS
11	4I	223	HIS
13	4L	106	HIS
14	5B	91	HIS
14	5B	131	HIS
14	5B	137	ASN
15	5C	22	GLN
15	5C	24	ASN
15	5C	32	ASN
15	5C	48	HIS
17	6B	252	HIS
18	7A	101	ASN

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Mol	Chain	Res	Type
18	7A	106	HIS
18	7A	132	HIS
19	7C	112	HIS
19	7C	120	GLN
19	7C	134	GLN
20	A1	47	ASN
20	A1	60	ASN
20	A1	67	GLN
20	A1	121	HIS
20	A1	132	HIS
21	A2	12	HIS
21	A2	113	HIS
21	A2	115	HIS
21	A2	123	ASN
21	A2	183	GLN
22	A3	28	GLN
22	A3	58	HIS
24	A6	88	ASN
24	A6	107	HIS
24	A6	134	ASN
24	A6	180	ASN
24	A6	282	ASN
25	A7	22	GLN
25	A7	56	GLN
25	A7	92	GLN
25	A7	124	GLN
26	A8	23	HIS
26	A8	27	GLN
26	A8	52	HIS
26	A8	54	HIS
26	A8	83	ASN
26	A8	96	GLN
27	A9	79	GLN
27	A9	165	GLN
27	A9	174	GLN
27	A9	190	GLN
27	A9	242	HIS
27	A9	288	ASN
27	A9	368	GLN
27	A9	394	HIS
28	AB	52	HIS
29	AC	110	HIS

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Mol	Chain	Res	Type
30	AL	20	GLN
30	AL	39	GLN
30	AL	107	GLN
30	AL	133	GLN
30	AL	201	HIS
30	AL	219	HIS
31	AM	25	GLN
31	AM	104	GLN
32	AN	20	HIS
32	AN	154	GLN
34	B3	5	ASN
34	B3	6	HIS
35	B4	69	GLN
35	B4	80	ASN
35	B4	92	HIS
36	B5	98	HIS
36	B5	100	GLN
37	B6	19	ASN
37	B6	62	GLN
39	B8	61	HIS
39	B8	63	ASN
39	B8	91	GLN
39	B8	113	ASN
39	B8	156	GLN
40	B9	20	GLN
40	B9	112	ASN
41	BL	3	GLN
42	BM	99	GLN
43	C1	18	HIS
43	C1	108	ASN
43	C1	192	ASN
43	C1	194	ASN
43	C1	299	HIS
43	C1	423	HIS
43	C1	439	HIS
43	C1	466	HIS
44	C2	90	ASN
44	C2	98	ASN
44	C2	105	ASN
45	C3	8	ASN
45	C3	124	HIS
45	C3	126	ASN

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Mol	Chain	Res	Type
45	C3	130	ASN
46	C4	10	GLN
46	C4	75	ASN
46	C4	76	GLN
46	C4	95	ASN
47	DC	29	GLN
47	DC	54	HIS
48	E1	44	HIS
48	E1	105	GLN
48	E1	192	GLN
48	E1	204	ASN
48	E1	227	HIS
48	E1	363	ASN
49	E2	18	HIS
49	E2	58	ASN
49	E2	99	GLN
49	E2	153	HIS
49	E2	169	HIS
49	E2	219	HIS
49	E2	321	HIS
49	E2	344	GLN
50	E3	99	GLN
50	E3	106	ASN
50	E3	160	GLN
50	E3	232	HIS
50	E3	244	HIS
50	E3	303	ASN
50	E3	313	HIS
50	E3	355	GLN
50	E3	365	GLN
51	E4	25	GLN
51	E4	146	ASN
51	E4	162	HIS
51	E4	233	GLN
51	E4	358	HIS
52	E5	255	ASN
53	E6	49	GLN
53	E6	57	ASN
53	E6	214	GLN
53	E6	219	GLN
53	E6	222	GLN
53	E6	328	GLN

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Mol	Chain	Res	Type
53	E6	335	ASN
54	E7	1	GLN
54	E7	166	HIS
54	E7	246	GLN
55	E8	19	ASN
55	E8	67	HIS
55	E8	89	HIS
55	E8	127	ASN
56	E9	33	HIS
57	EA	49	HIS
58	EB	78	GLN
59	EC	97	HIS
60	ED	28	ASN
60	ED	38	ASN
60	ED	71	HIS
60	ED	139	HIS
61	FX	95	HIS
61	FX	124	HIS
61	FX	133	GLN
61	FX	150	HIS
61	FX	324	GLN
62	G1	49	HIS
62	G1	105	HIS
62	G1	117	ASN
62	G1	150	GLN
62	G1	191	HIS
62	G1	208	HIS
62	G1	314	ASN
62	G1	321	HIS
62	G1	391	HIS
62	G1	401	GLN
62	G1	404	GLN
62	G1	413	ASN
63	G2	36	HIS
63	G2	71	GLN
63	G2	222	GLN
64	G3	174	GLN
64	G3	206	HIS
65	N1	402	ASN
65	N1	409	GLN
65	N1	440	ASN
65	N1	476	HIS

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Mol	Chain	Res	Type
65	N1	487	ASN
65	N1	537	ASN
66	N2	4	ASN
66	N2	6	ASN
66	N2	23	GLN
66	N2	76	ASN
66	N2	82	HIS
66	N2	89	ASN
66	N2	208	ASN
66	N2	209	HIS
66	N2	294	ASN
67	N3	172	ASN
67	N3	219	ASN
67	N3	222	ASN
67	N3	264	ASN
67	N3	292	ASN
68	N4	26	ASN
68	N4	59	ASN
68	N4	112	ASN
68	N4	140	ASN
68	N4	157	ASN
68	N4	200	HIS
68	N4	209	ASN
68	N4	231	HIS
68	N4	254	HIS
68	N4	283	ASN
68	N4	304	HIS
68	N4	321	ASN
68	N4	339	HIS
68	N4	359	ASN
68	N4	385	ASN
68	N4	422	ASN
68	N4	475	HIS
69	N5	49	ASN
69	N5	95	ASN
69	N5	101	ASN
69	N5	127	ASN
69	N5	202	ASN
69	N5	345	HIS
69	N5	373	ASN
69	N5	377	HIS
69	N5	572	HIS

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Mol	Chain	Res	Type
67	N6	121	ASN
67	N6	165	ASN
70	QA	30	ASN
70	QA	70	HIS
70	QA	167	HIS
70	QA	255	ASN
70	QA	268	GLN
71	QB	133	ASN
71	QB	199	HIS
71	QB	289	HIS
71	QB	329	GLN
71	QB	405	ASN
72	QC	33	GLN
72	QC	56	HIS
72	QC	194	ASN
72	QC	203	ASN
72	QC	204	ASN
73	QD	50	HIS
76	QG	2	ASN
76	QG	21	GLN
76	QG	96	HIS
76	QG	105	GLN
76	QG	196	HIS
76	QG	205	HIS
77	QH	40	GLN
79	QJ	116	HIS
70	Qa	29	GLN
70	Qa	30	ASN
70	Qa	66	ASN
70	Qa	167	HIS
70	Qa	268	GLN
70	Qa	285	GLN
70	Qa	333	ASN
70	Qa	398	GLN
71	Qb	133	ASN
71	Qb	199	HIS
71	Qb	218	ASN
71	Qb	289	HIS
71	Qb	329	GLN
71	Qb	405	ASN
71	Qb	413	GLN
71	Qb	474	GLN

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Mol	Chain	Res	Type
72	Qc	33	GLN
72	Qc	56	HIS
72	Qc	73	HIS
72	Qc	203	ASN
72	Qc	204	ASN
72	Qc	231	ASN
73	Qd	16	GLN
73	Qd	96	ASN
74	Qe	172	GLN
75	Qf	47	ASN
76	Qg	2	ASN
76	Qg	16	ASN
76	Qg	96	HIS
76	Qg	125	HIS
76	Qg	196	HIS
77	Qh	40	GLN
79	Qj	116	HIS
81	S2	50	HIS
81	S2	278	GLN
81	S2	344	GLN
81	S2	372	GLN
82	S3	99	GLN
82	S3	153	HIS
82	S3	173	HIS
82	S3	208	ASN
83	S4	39	ASN
84	S5	75	GLN
85	S6	85	HIS
85	S6	91	ASN
85	S6	136	GLN
86	S7	27	GLN
86	S7	31	GLN
86	S7	37	GLN
86	S7	50	HIS
86	S7	93	GLN
86	S7	159	HIS
86	S7	169	ASN
87	S8	70	GLN
87	S8	82	ASN
88	V1	42	GLN
88	V1	50	GLN
88	V1	245	ASN

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Mol	Chain	Res	Type
88	V1	381	ASN
88	V1	502	ASN
89	V2	149	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
101	C1	502	HEA	C3B-C2B	5.40	1.46	1.34
101	C1	501	HEA	C3B-C2B	4.80	1.45	1.34
101	C1	502	HEA	C3A-C2A	4.46	1.46	1.40
101	C1	502	HEA	C4B-NB	-4.45	1.32	1.40
101	C1	501	HEA	C3D-C2D	4.23	1.45	1.36
101	C1	502	HEA	CHC-C4B	4.22	1.45	1.35
101	C1	501	HEA	C1D-ND	-4.14	1.33	1.40
101	C1	501	HEA	CHC-C4B	4.09	1.45	1.35
105	N4	504	U10	C4-C3	4.08	1.52	1.36
101	C1	501	HEA	CHD-C1D	4.05	1.45	1.35
101	C1	502	HEA	C3C-C2C	4.00	1.45	1.40
101	C1	502	HEA	C3D-C2D	3.98	1.45	1.36
101	C1	502	HEA	C1D-ND	-3.98	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
106	QC	401	HEM	C4D-ND	-3.87	1.33	1.40
106	QC	402	HEM	C4D-ND	-3.87	1.33	1.40
101	C1	501	HEA	C3C-C2C	3.87	1.45	1.40
101	C1	502	HEA	CHD-C1D	3.82	1.44	1.35
101	C1	501	HEA	C4B-NB	-3.80	1.33	1.40
106	Qc	402	HEM	C4D-ND	-3.74	1.33	1.40
106	Qc	403	HEM	C4D-ND	-3.63	1.34	1.40
101	C1	501	HEA	C3A-C2A	3.63	1.45	1.40
107	QD	301	HEC	CBC-CAC	-3.46	1.36	1.49
107	Qd	301	HEC	CBC-CAC	-3.46	1.36	1.49
106	QC	402	HEM	C1B-NB	-3.39	1.34	1.40
100	AC	201	ZMP	C9-C10	-3.27	1.47	1.50
106	QC	401	HEM	C1B-NB	-3.23	1.34	1.40
105	N4	504	U10	C7-C6	3.23	1.56	1.51
106	Qc	403	HEM	C1B-NB	-3.21	1.34	1.40
101	C1	502	HEA	C1B-NB	-3.08	1.32	1.38
106	Qc	402	HEM	C1B-NB	-3.06	1.35	1.40
105	N4	504	U10	C7-C8	2.99	1.55	1.50
101	C1	501	HEA	C1B-NB	-2.91	1.32	1.38
101	C1	502	HEA	CAA-C2A	-2.90	1.47	1.52
104	QJ	202	PX2	O7-C2	-2.81	1.39	1.46
101	C1	501	HEA	C4B-C3B	2.81	1.49	1.44
100	AB	201	ZMP	C9-C10	-2.80	1.48	1.50
105	N4	504	U10	C31-C29	2.72	1.56	1.51
104	QJ	201	PX2	O7-C2	-2.70	1.39	1.46
101	C1	501	HEA	C4D-ND	-2.68	1.33	1.38
101	C1	501	HEA	FE-ND	2.67	2.10	1.96
101	C1	502	HEA	FE-ND	2.66	2.10	1.96
106	QC	402	HEM	C1D-ND	-2.65	1.33	1.38
105	N4	504	U10	C6-C5	2.65	1.54	1.46
105	N4	504	U10	O5-C5	-2.63	1.17	1.23
106	Qc	403	HEM	C1D-ND	-2.61	1.33	1.38
101	C1	502	HEA	O2D-CGD	-2.61	1.22	1.30
104	C2	201	PX2	O7-C2	-2.61	1.40	1.46
105	N4	504	U10	C16-C14	2.59	1.56	1.51
101	C1	501	HEA	CAA-C2A	-2.58	1.47	1.52
106	Qc	402	HEM	C1D-ND	-2.58	1.33	1.38
101	C1	502	HEA	C4D-ND	-2.57	1.33	1.38
101	C1	501	HEA	O2D-CGD	-2.52	1.22	1.30
106	QC	401	HEM	C1D-ND	-2.52	1.33	1.38
107	QD	301	HEC	CBB-CAB	-2.51	1.40	1.49
101	C1	501	HEA	FE-NB	2.50	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
101	C1	502	HEA	O2A-CGA	-2.48	1.22	1.30
101	C1	501	HEA	O2A-CGA	-2.48	1.22	1.30
107	Qd	301	HEC	CBB-CAB	-2.42	1.40	1.49
101	C1	502	HEA	FE-NB	2.37	2.08	1.96
104	QJ	202	PX2	O5-C4	2.32	1.40	1.33
104	QJ	201	PX2	O5-C3	-2.31	1.39	1.45
105	N4	504	U10	C26-C24	2.29	1.56	1.51
105	N4	504	U10	O2-C2	-2.28	1.18	1.23
104	QJ	201	PX2	O5-C4	2.26	1.39	1.33
105	N4	504	U10	O3-C3M	-2.24	1.40	1.45
106	Qc	403	HEM	C4B-NB	-2.23	1.34	1.38
105	N4	504	U10	C21-C19	2.19	1.55	1.51
101	C1	501	HEA	C4C-CHD	2.19	1.47	1.41
104	C2	201	PX2	O5-C4	2.18	1.39	1.33
104	C2	201	PX2	O5-C3	-2.17	1.40	1.45
106	QC	401	HEM	C4B-NB	-2.17	1.34	1.38
106	QC	402	HEM	C4B-NB	-2.15	1.34	1.38
106	Qc	402	HEM	CHB-C1B	2.14	1.40	1.35
104	C2	201	PX2	O7-C16	2.14	1.40	1.34
105	N4	504	U10	C36-C34	2.11	1.56	1.50
101	C1	501	HEA	C2A-C1A	2.11	1.47	1.42
106	QC	401	HEM	CHB-C1B	2.10	1.40	1.35
105	N4	504	U10	C27-C28	2.06	1.57	1.50
105	N4	504	U10	C11-C9	2.06	1.55	1.51
104	QJ	202	PX2	O5-C3	-2.04	1.40	1.45
106	Qc	402	HEM	C4B-NB	-2.03	1.34	1.38
106	Qc	403	HEM	C3C-C2C	-2.00	1.37	1.40

All (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
106	Qc	402	HEM	CHC-C4B-NB	5.22	130.10	124.43
101	C1	502	HEA	C3D-C4D-ND	5.09	115.28	110.36
106	QC	401	HEM	CHC-C4B-NB	5.09	129.96	124.43
101	C1	502	HEA	C1D-C2D-C3D	-5.07	101.63	106.96
101	C1	501	HEA	CAA-CBA-CGA	-4.96	99.84	113.76
106	QC	402	HEM	CHC-C4B-NB	4.92	129.78	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	502	HEA	CAA-CBA-CGA	-4.91	100.01	113.76
101	C1	502	HEA	C2D-C1D-ND	4.84	115.57	109.84
101	C1	502	HEA	C2B-C1B-NB	4.61	115.40	109.88
101	C1	501	HEA	C13-C12-C11	-4.50	107.59	114.35
106	Qc	403	HEM	CHC-C4B-NB	4.49	129.31	124.43
105	N4	504	U10	C7-C6-C5	4.46	123.85	118.48
101	C1	501	HEA	C1D-C2D-C3D	-4.39	102.34	106.96
101	C1	502	HEA	C3B-C4B-NB	4.38	115.02	109.84
101	C1	501	HEA	CHB-C1B-C2B	-4.36	118.16	124.98
104	C2	201	PX2	O7-C16-C17	4.34	120.85	111.50
101	C1	501	HEA	C3B-C4B-NB	4.33	114.97	109.84
105	N4	504	U10	C15-C14-C16	4.28	122.47	115.27
107	QD	301	HEC	CMD-C2D-C1D	-4.18	122.04	128.46
104	QJ	201	PX2	O7-C16-C17	4.17	120.48	111.50
101	C1	501	HEA	CHA-C4D-C3D	-4.15	118.74	124.84
106	QC	402	HEM	CHB-C1B-NB	4.14	129.50	124.38
101	C1	501	HEA	C2D-C1D-ND	4.14	114.74	109.84
101	C1	502	HEA	CHB-C1B-C2B	-4.12	118.54	124.98
105	N4	504	U10	C30-C29-C31	4.09	122.14	115.27
104	QJ	202	PX2	O7-C16-C17	3.96	120.04	111.50
101	C1	502	HEA	C3C-C4C-NC	3.93	114.29	109.21
106	Qc	402	HEM	CHB-C1B-NB	3.92	129.22	124.38
105	N4	504	U10	C15-C14-C13	-3.81	113.90	123.68
106	Qc	403	HEM	C4D-ND-C1D	3.79	108.99	105.07
106	Qc	403	HEM	CHB-C1B-NB	3.74	129.00	124.38
101	C1	502	HEA	CMC-C2C-C3C	3.69	131.59	124.68
101	C1	502	HEA	C4B-C3B-C2B	-3.64	101.19	107.41
101	C1	501	HEA	CMC-C2C-C3C	3.64	131.49	124.68
101	C1	501	HEA	C4B-C3B-C2B	-3.61	101.24	107.41
107	QD	301	HEC	CMC-C2C-C3C	3.61	130.06	125.82
107	Qd	301	HEC	CMD-C2D-C1D	-3.58	122.95	128.46
106	QC	401	HEM	CHB-C1B-NB	3.58	128.81	124.38
106	QC	402	HEM	C4D-ND-C1D	3.57	108.77	105.07
106	Qc	402	HEM	C4D-ND-C1D	3.50	108.69	105.07
106	Qc	402	HEM	C1B-NB-C4B	3.49	108.68	105.07
101	C1	501	HEA	CHC-C4B-NB	-3.46	120.11	124.38
106	QC	401	HEM	C4D-ND-C1D	3.42	108.60	105.07
107	Qd	301	HEC	CMC-C2C-C3C	3.39	129.81	125.82
101	C1	501	HEA	C3C-C4C-NC	3.39	113.59	109.21
106	QC	401	HEM	C1B-NB-C4B	3.38	108.56	105.07
107	Qd	301	HEC	CMB-C2B-C1B	-3.35	123.31	128.46
101	C1	502	HEA	CHA-C4D-C3D	-3.32	119.96	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
106	Qc	403	HEM	CHA-C4D-ND	3.24	128.38	124.38
107	Qd	301	HEC	CMB-C2B-C3B	3.23	129.62	125.82
105	N4	504	U10	C22-C23-C24	-3.20	119.96	127.66
106	QC	401	HEM	CHA-C4D-ND	3.14	128.26	124.38
106	Qc	403	HEM	CHD-C1D-ND	3.10	127.80	124.43
106	Qc	402	HEM	CHA-C4D-ND	3.08	128.19	124.38
100	AB	201	ZMP	C14-C13-N1	3.07	121.59	116.42
107	Qd	301	HEC	C4C-C3C-C2C	3.03	109.62	106.35
106	Qc	403	HEM	CAD-CBD-CGD	-2.99	107.17	113.60
107	QD	301	HEC	C4C-C3C-C2C	2.95	109.54	106.35
107	QD	301	HEC	CMC-C2C-C1C	-2.93	123.97	128.46
100	AC	201	ZMP	C20-C18-C21	2.91	112.98	108.23
104	QJ	202	PX2	O5-C4-C5	2.90	121.02	111.91
107	Qd	301	HEC	CBD-CAD-C3D	2.90	117.57	112.62
105	N4	504	U10	C7-C8-C9	-2.90	121.97	126.79
106	QC	402	HEM	C1B-NB-C4B	2.88	108.05	105.07
100	AB	201	ZMP	C15-C14-C13	-2.84	107.63	112.36
107	QD	301	HEC	O1D-CGD-CBD	-2.84	113.97	123.08
96	4D	203	S12	OG-CB-CA	2.83	110.53	108.06
107	QD	301	HEC	CMB-C2B-C1B	-2.82	124.12	128.46
106	QC	402	HEM	CBA-CAA-C2A	-2.80	107.84	112.62
107	Qd	301	HEC	O1D-CGD-CBD	-2.79	114.10	123.08
101	C1	501	HEA	CMB-C2B-C1B	-2.79	120.80	125.04
107	Qd	301	HEC	CMC-C2C-C1C	-2.79	124.18	128.46
105	N4	504	U10	C25-C24-C26	2.75	119.89	115.27
106	QC	402	HEM	CHA-C4D-ND	2.72	127.75	124.38
105	N4	504	U10	C20-C19-C21	2.71	119.84	115.27
106	Qc	403	HEM	C1B-NB-C4B	2.71	107.87	105.07
106	QC	402	HEM	CHD-C1D-ND	2.70	127.36	124.43
105	N4	504	U10	C10-C9-C11	2.67	119.77	115.27
101	C1	502	HEA	CMB-C2B-C1B	-2.67	120.97	125.04
101	C1	501	HEA	CMB-C2B-C3B	2.65	135.40	130.34
107	QD	301	HEC	CBD-CAD-C3D	2.65	117.15	112.62
105	N4	504	U10	C27-C28-C29	-2.63	121.33	127.66
101	C1	501	HEA	C13-C14-C15	-2.61	121.37	127.66
104	QJ	201	PX2	O5-C4-C5	2.59	120.04	111.91
107	QD	301	HEC	CMB-C2B-C3B	2.58	128.85	125.82
107	QD	301	HEC	CMA-C3A-C2A	2.55	129.75	124.94
101	C1	501	HEA	CMD-C2D-C1D	2.54	128.91	125.04
101	C1	502	HEA	CMB-C2B-C3B	2.54	135.19	130.34
107	QD	301	HEC	O1A-CGA-CBA	-2.54	114.92	123.08
101	C1	502	HEA	C27-C19-C18	-2.52	117.20	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	501	HEA	C1B-C2B-C3B	-2.51	103.80	106.80
96	4D	203	S12	O4-P-O3	2.51	124.65	112.24
101	C1	502	HEA	CAA-C2A-C3A	2.50	133.02	126.86
104	C2	201	PX2	O5-C4-C5	2.49	119.72	111.91
106	QC	402	HEM	CHB-C1B-C2B	-2.49	119.84	126.72
101	C1	502	HEA	C1B-C2B-C3B	-2.47	103.84	106.80
100	AB	201	ZMP	O1-C10-C9	-2.47	121.07	123.99
101	C1	501	HEA	C27-C19-C20	2.47	119.42	115.27
101	C1	501	HEA	C17-C18-C19	-2.45	121.76	127.66
106	Qc	403	HEM	CHB-C1B-C2B	-2.44	119.98	126.72
101	C1	501	HEA	C4D-C3D-C2D	-2.42	103.37	106.90
107	QD	301	HEC	CBA-CAA-C2A	2.41	116.67	112.60
107	QD	301	HEC	CMD-C2D-C3D	2.41	129.48	124.94
101	C1	502	HEA	O1D-CGD-CBD	-2.38	115.44	123.08
106	QC	401	HEM	CHD-C1D-ND	2.30	126.94	124.43
105	N4	504	U10	C6-C1-C2	2.30	121.00	119.18
107	QD	301	HEC	O2A-CGA-O1A	2.28	128.99	123.30
101	C1	502	HEA	O1A-CGA-CBA	-2.28	115.77	123.08
105	N4	504	U10	C11-C12-C13	-2.26	104.45	111.88
99	A9	501	NDP	C5A-C6A-N6A	2.25	123.77	120.35
101	C1	502	HEA	C13-C14-C15	-2.19	122.39	127.66
107	Qd	301	HEC	O1A-CGA-CBA	-2.19	116.06	123.08
100	AB	201	ZMP	O2-C13-C14	-2.18	118.02	122.02
106	Qc	402	HEM	CHD-C1D-ND	2.18	126.80	124.43
106	QC	402	HEM	O2A-CGA-CBA	2.18	121.03	114.03
107	Qd	301	HEC	O2A-CGA-O1A	2.18	128.73	123.30
106	Qc	403	HEM	CBA-CAA-C2A	-2.18	108.91	112.62
100	AC	201	ZMP	C15-C14-C13	-2.18	108.73	112.36
100	AB	201	ZMP	C12-N1-C13	2.16	126.84	122.84
100	AC	201	ZMP	C14-C13-N1	2.15	120.05	116.42
107	Qd	301	HEC	CMA-C3A-C2A	2.15	129.00	124.94
106	Qc	403	HEM	O2A-CGA-CBA	2.15	120.93	114.03
107	QD	301	HEC	C1D-C2D-C3D	2.14	108.48	107.00
107	QD	301	HEC	C2B-C3B-C4B	2.14	108.66	106.35
106	QC	402	HEM	CAD-CBD-CGD	-2.13	109.03	113.60
107	Qd	301	HEC	C2B-C3B-C4B	2.12	108.64	106.35
101	C1	502	HEA	OMA-CMA-C3A	-2.11	120.30	124.91
101	C1	501	HEA	C4A-CHB-C1B	2.11	125.34	122.56
106	Qc	402	HEM	CHB-C1B-C2B	-2.10	120.92	126.72
106	QC	401	HEM	O2A-CGA-CBA	2.10	120.76	114.03
101	C1	501	HEA	O1D-CGD-CBD	-2.08	116.38	123.08
101	C1	501	HEA	C27-C19-C18	-2.08	118.35	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
105	N4	504	U10	C10-C9-C8	-2.06	118.39	123.68
96	4D	203	S12	O52-C5-O51	-2.03	118.46	123.59
101	C1	501	HEA	C25-C23-C22	-2.03	116.79	122.65
107	Qd	301	HEC	CMD-C2D-C3D	2.02	128.74	124.94
101	C1	502	HEA	CMD-C2D-C1D	2.02	128.11	125.04
106	Qc	402	HEM	O2A-CGA-CBA	2.01	120.48	114.03
101	C1	501	HEA	C26-C15-C16	2.01	118.65	115.27
105	N4	504	U10	C32-C33-C34	-2.00	120.91	127.75

There are no chirality outliers.

All (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
94	4E	201	PC1	C11-O13-P-O12
94	4E	201	PC1	C1-O11-P-O12
94	4E	201	PC1	C1-O11-P-O14
94	4E	201	PC1	O21-C2-C3-O31
94	7A	201	PC1	C11-O13-P-O12
94	7A	201	PC1	C11-O13-P-O14
94	A1	201	PC1	C11-O13-P-O14
94	A1	202	PC1	C11-O13-P-O12
94	A1	202	PC1	C11-O13-P-O14
94	A1	202	PC1	C11-O13-P-O11
94	A1	202	PC1	C1-O11-P-O13
94	A9	502	PC1	C1-O11-P-O12
94	A9	502	PC1	C1-O11-P-O14
94	A9	503	PC1	C1-O11-P-O12
94	A9	503	PC1	O13-C11-C12-N
94	AM	203	PC1	C1-O11-P-O14
94	AM	204	PC1	C1-O11-P-O12
94	AM	204	PC1	C1-O11-P-O14
94	AM	204	PC1	C1-O11-P-O13
94	AN	301	PC1	C1-O11-P-O12
94	AN	301	PC1	C1-O11-P-O14
94	B5	201	PC1	C11-O13-P-O12
94	B5	201	PC1	C11-O13-P-O14
94	B5	201	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
94	B5	202	PC1	C1-O11-P-O12
94	B5	202	PC1	C1-O11-P-O14
94	B5	202	PC1	C1-O11-P-O13
94	C1	505	PC1	C1-O11-P-O12
94	C1	505	PC1	C1-O11-P-O14
94	C1	505	PC1	C1-O11-P-O13
94	E4	402	PC1	C11-O13-P-O11
94	E8	301	PC1	C1-O11-P-O12
94	E8	301	PC1	C1-O11-P-O14
94	E8	301	PC1	C1-O11-P-O13
94	E8	304	PC1	C11-O13-P-O12
94	E8	304	PC1	C11-O13-P-O14
94	E8	304	PC1	C11-O13-P-O11
94	E8	304	PC1	C2-C1-O11-P
94	E9	202	PC1	C11-O13-P-O12
94	E9	202	PC1	C11-O13-P-O14
94	E9	202	PC1	C11-O13-P-O11
94	E9	202	PC1	C1-O11-P-O12
94	E9	202	PC1	C1-O11-P-O14
94	E9	202	PC1	C1-O11-P-O13
94	ED	202	PC1	C11-O13-P-O12
94	ED	202	PC1	C1-O11-P-O14
94	ED	202	PC1	C1-O11-P-O13
94	N1	702	PC1	C1-O11-P-O12
94	N1	702	PC1	C1-O11-P-O14
94	N1	703	PC1	C11-O13-P-O12
94	N1	703	PC1	C11-O13-P-O14
94	N1	703	PC1	C1-O11-P-O14
94	N1	703	PC1	O13-C11-C12-N
94	N1	703	PC1	C2-C1-O11-P
94	N1	703	PC1	O21-C2-C3-O31
94	N4	501	PC1	C11-O13-P-O14
94	N4	501	PC1	C1-O11-P-O12
94	N4	502	PC1	C11-O13-P-O12
94	N4	505	PC1	C11-O13-P-O12
94	N4	505	PC1	C11-O13-P-O14
94	N4	505	PC1	C11-O13-P-O11
94	N5	601	PC1	C1-O11-P-O14
94	QC	404	PC1	C1-O11-P-O14
94	QD	303	PC1	C1-O11-P-O12
94	QD	303	PC1	C1-O11-P-O14
94	QD	303	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
94	QI	101	PC1	C1-O11-P-O12
94	Qc	401	PC1	C1-O11-P-O12
94	Qc	401	PC1	C1-O11-P-O14
94	Qc	401	PC1	C1-O11-P-O13
94	Qc	401	PC1	O13-C11-C12-N
94	Qc	404	PC1	C11-O13-P-O12
94	Qc	404	PC1	C11-O13-P-O14
94	Qc	404	PC1	C11-O13-P-O11
94	Qg	301	PC1	C1-O11-P-O12
94	Qg	301	PC1	C1-O11-P-O14
94	Qg	301	PC1	C1-O11-P-O13
94	Qj	201	PC1	C11-O13-P-O12
94	Qj	201	PC1	C11-O13-P-O14
94	Qj	201	PC1	C11-O13-P-O11
94	Qj	201	PC1	C1-O11-P-O14
95	4D	201	3PE	C11-O13-P-O11
95	4D	201	3PE	C11-O13-P-O12
95	4D	201	3PE	C11-O13-P-O14
95	4D	202	3PE	C1-O11-P-O13
95	4D	202	3PE	O13-C11-C12-N
95	7A	202	3PE	C11-O13-P-O11
95	7A	202	3PE	C11-O13-P-O12
95	B4	201	3PE	C11-O13-P-O14
95	B4	201	3PE	O13-C11-C12-N
95	C1	506	3PE	C11-O13-P-O12
95	C1	506	3PE	C11-O13-P-O14
95	C1	506	3PE	C2-C1-O11-P
95	E9	201	3PE	C11-O13-P-O11
95	E9	201	3PE	C11-O13-P-O14
95	E9	201	3PE	O13-C11-C12-N
95	N4	503	3PE	C11-O13-P-O11
95	N4	503	3PE	C11-O13-P-O12
95	N4	503	3PE	C11-O13-P-O14
95	N5	602	3PE	C11-O13-P-O11
95	N5	602	3PE	C11-O13-P-O12
95	N5	602	3PE	C11-O13-P-O14
95	N5	602	3PE	O13-C11-C12-N
96	4D	203	S12	O-C-CA-CB
96	4D	203	S12	OXT-C-CA-CB
96	4D	203	S12	CA-CB-OG-P
97	4E	202	CDL	CA2-OA2-PA1-OA3
97	4E	202	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
97	7C	201	CDL	CA2-OA2-PA1-OA3
97	7C	201	CDL	CB2-OB2-PB2-OB3
97	7C	201	CDL	CB2-OB2-PB2-OB4
97	7C	201	CDL	CB2-OB2-PB2-OB5
97	A9	504	CDL	O1-C1-CA2-OA2
97	A9	504	CDL	CA3-OA5-PA1-OA3
97	A9	504	CDL	CA3-OA5-PA1-OA4
97	A9	504	CDL	CB2-OB2-PB2-OB3
97	A9	504	CDL	CB2-OB2-PB2-OB4
97	A9	504	CDL	CB2-OB2-PB2-OB5
97	AM	201	CDL	CB2-OB2-PB2-OB3
97	AM	201	CDL	CB2-OB2-PB2-OB4
97	AM	201	CDL	CB3-OB5-PB2-OB2
97	AM	202	CDL	CA2-OA2-PA1-OA5
97	AM	202	CDL	CA3-OA5-PA1-OA4
97	B3	101	CDL	CA3-OA5-PA1-OA4
97	B8	302	CDL	CA2-OA2-PA1-OA5
97	B8	302	CDL	CA3-OA5-PA1-OA3
97	B8	302	CDL	CA3-OA5-PA1-OA4
97	B8	302	CDL	CB2-OB2-PB2-OB4
97	B8	302	CDL	CB3-OB5-PB2-OB3
97	C4	201	CDL	CA2-OA2-PA1-OA3
97	C4	201	CDL	CB3-OB5-PB2-OB3
97	C4	201	CDL	CB3-OB5-PB2-OB4
97	C4	202	CDL	CA3-OA5-PA1-OA2
97	C4	202	CDL	CA3-OA5-PA1-OA3
97	C4	202	CDL	CA3-OA5-PA1-OA4
97	C4	202	CDL	CB2-OB2-PB2-OB4
97	C4	203	CDL	CA2-OA2-PA1-OA3
97	C4	203	CDL	CA2-OA2-PA1-OA4
97	C4	203	CDL	CA2-OA2-PA1-OA5
97	E4	401	CDL	CB2-OB2-PB2-OB3
97	E4	401	CDL	CB2-OB2-PB2-OB4
97	E4	401	CDL	CB2-OB2-PB2-OB5
97	E6	401	CDL	CA3-OA5-PA1-OA2
97	E6	401	CDL	CA3-OA5-PA1-OA3
97	E6	401	CDL	CA4-CA3-OA5-PA1
97	E6	401	CDL	OA6-CA4-CA6-OA8
97	E7	301	CDL	C1-CA2-OA2-PA1
97	E7	301	CDL	CA2-OA2-PA1-OA3
97	E7	301	CDL	CA2-OA2-PA1-OA4
97	E7	301	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
97	E7	301	CDL	CA3-OA5-PA1-OA2
97	EA	201	CDL	O1-C1-CA2-OA2
97	EA	201	CDL	CB2-C1-CA2-OA2
97	EA	201	CDL	CA3-OA5-PA1-OA3
97	EA	201	CDL	CA3-OA5-PA1-OA4
97	EA	202	CDL	CB3-OB5-PB2-OB2
97	N1	701	CDL	CA2-OA2-PA1-OA4
97	N1	701	CDL	CB3-OB5-PB2-OB2
97	N5	603	CDL	CA3-OA5-PA1-OA4
97	N5	603	CDL	CB2-OB2-PB2-OB3
97	N5	603	CDL	CB2-OB2-PB2-OB4
97	QC	403	CDL	CB3-OB5-PB2-OB3
97	QD	302	CDL	CB3-OB5-PB2-OB2
97	QD	302	CDL	CB3-OB5-PB2-OB3
97	QD	302	CDL	CB3-OB5-PB2-OB4
97	QH	101	CDL	CB2-OB2-PB2-OB3
97	QH	101	CDL	CB2-OB2-PB2-OB4
97	QH	101	CDL	CB3-OB5-PB2-OB3
97	QJ	203	CDL	CA3-OA5-PA1-OA4
97	QJ	203	CDL	CB2-OB2-PB2-OB3
97	QJ	203	CDL	CB2-OB2-PB2-OB4
97	QJ	203	CDL	CB3-OB5-PB2-OB3
97	Qc	405	CDL	CA3-OA5-PA1-OA3
97	Qc	405	CDL	CA3-OA5-PA1-OA4
97	Qc	405	CDL	CB2-OB2-PB2-OB4
97	Qc	405	CDL	CB3-OB5-PB2-OB4
97	Qd	302	CDL	CA2-OA2-PA1-OA4
97	Qd	302	CDL	CA3-OA5-PA1-OA3
97	Qd	302	CDL	CA3-OA5-PA1-OA4
97	Qd	302	CDL	CB2-OB2-PB2-OB3
97	Qd	302	CDL	CB3-OB5-PB2-OB2
97	Qd	302	CDL	CB3-OB5-PB2-OB3
97	Qe	302	CDL	CB3-OB5-PB2-OB2
97	Qe	302	CDL	CB3-OB5-PB2-OB3
97	Qe	302	CDL	CB3-OB5-PB2-OB4
97	Qh	101	CDL	CA3-OA5-PA1-OA3
97	Qh	101	CDL	CA3-OA5-PA1-OA4
97	Qh	101	CDL	CB3-OB5-PB2-OB3
97	Qj	202	CDL	CA3-OA5-PA1-OA2
97	Qj	202	CDL	CA3-OA5-PA1-OA3
97	Qj	202	CDL	CB2-OB2-PB2-OB3
97	Qj	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
99	A9	501	NDP	C5D-O5D-PN-O1N
100	AB	201	ZMP	C16-C17-C18-C21
100	AB	201	ZMP	O1-C10-S1-C11
100	AB	201	ZMP	C7-C8-C9-C10
100	AC	201	ZMP	C19-C18-C21-O5
100	AC	201	ZMP	C20-C18-C21-O5
100	AC	201	ZMP	C17-C18-C21-O5
101	C1	501	HEA	C1A-C2A-CAA-CBA
101	C1	501	HEA	C3A-C2A-CAA-CBA
101	C1	501	HEA	C2D-C3D-CAD-CBD
101	C1	501	HEA	C4D-C3D-CAD-CBD
101	C1	501	HEA	C19-C20-C21-C22
101	C1	502	HEA	C1A-C2A-CAA-CBA
101	C1	502	HEA	C3A-C2A-CAA-CBA
101	C1	502	HEA	C11-C12-C13-C14
101	C1	502	HEA	C13-C14-C15-C16
101	C1	502	HEA	C13-C14-C15-C26
101	C1	502	HEA	C15-C16-C17-C18
101	C1	502	HEA	C17-C18-C19-C20
101	C1	502	HEA	C17-C18-C19-C27
101	C1	502	HEA	C19-C20-C21-C22
104	C2	201	PX2	C1-O4-P1-O1
104	C2	201	PX2	C1-O4-P1-O2
104	C2	201	PX2	C1-O4-P1-O3
104	QJ	201	PX2	C1-O4-P1-O1
104	QJ	201	PX2	C1-O4-P1-O2
104	QJ	201	PX2	C1-O4-P1-O3
104	QJ	202	PX2	C1-O4-P1-O1
104	QJ	202	PX2	C1-O4-P1-O2
104	QJ	202	PX2	C1-O4-P1-O3
104	QJ	202	PX2	C17-C16-O7-C2
105	N4	504	U10	C1-C6-C7-C8
105	N4	504	U10	C5-C6-C7-C8
108	V1	601	FMN	C5'-O5'-P-O2P
108	V1	601	FMN	C5'-O5'-P-O3P
96	4D	203	S12	O51-C5-O52-C4
104	QJ	202	PX2	O8-C16-O7-C2
100	AB	201	ZMP	C14-C13-N1-C12
100	AC	201	ZMP	C14-C13-N1-C12
96	4D	203	S12	C6-C5-O52-C4
101	C1	501	HEA	C17-C18-C19-C27
100	AC	201	ZMP	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
101	C1	501	HEA	C17-C18-C19-C20
94	A1	201	PC1	C11-C12-N-C13
97	EA	202	CDL	O1-C1-CA2-OA2
97	QH	101	CDL	O1-C1-CA2-OA2
101	C1	502	HEA	C21-C22-C23-C25
100	AC	201	ZMP	C1-C2-C3-C4
97	Qh	101	CDL	CA4-CA3-OA5-PA1
105	N4	504	U10	C30-C29-C31-C32
105	N4	504	U10	C28-C29-C31-C32
94	B8	301	PC1	C27-C28-C29-C2A
100	AB	201	ZMP	O2-C13-N1-C12
100	AC	201	ZMP	O2-C13-N1-C12
97	B3	101	CDL	CA7-C31-C32-C33
97	QH	101	CDL	CB2-C1-CA2-OA2
97	QH	102	CDL	CB2-C1-CA2-OA2
94	7A	201	PC1	C11-C12-N-C15
94	Qc	404	PC1	C11-C12-N-C13
101	C1	502	HEA	C21-C22-C23-C24
97	E7	301	CDL	OB5-CB3-CB4-OB6
97	AL	303	CDL	O1-C1-CB2-OB2
97	AM	202	CDL	O1-C1-CB2-OB2
97	QH	102	CDL	O1-C1-CA2-OA2
94	C1	505	PC1	O21-C2-C3-O31
95	4D	202	3PE	O21-C2-C3-O31
94	A1	201	PC1	C22-C23-C24-C25
106	QC	401	HEM	C2A-CAA-CBA-CGA
106	Qc	402	HEM	C2A-CAA-CBA-CGA
97	C4	201	CDL	CB7-C71-C72-C73
94	C1	505	PC1	C21-C22-C23-C24
94	ED	202	PC1	C21-C22-C23-C24
97	AL	302	CDL	CB5-C51-C52-C53
97	AM	202	CDL	CB5-C51-C52-C53
94	E4	402	PC1	C11-C12-N-C13
94	G2	301	PC1	C11-C12-N-C15
97	C4	203	CDL	CA5-C11-C12-C13
104	QJ	202	PX2	C17-C18-C19-C20
94	QI	101	PC1	C32-C33-C34-C35
94	A9	502	PC1	C2-C3-O31-C31
97	QH	101	CDL	CA5-C11-C12-C13
97	N1	701	CDL	O1-C1-CA2-OA2
97	AM	201	CDL	C53-C54-C55-C56
104	QJ	202	PX2	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
94	4A	301	PC1	C11-O13-P-O11
94	4A	302	PC1	C11-O13-P-O11
94	4A	302	PC1	C1-O11-P-O13
94	4E	201	PC1	C11-O13-P-O11
94	4E	201	PC1	C1-O11-P-O13
94	7A	201	PC1	C11-O13-P-O11
94	A1	201	PC1	C11-O13-P-O11
94	A1	201	PC1	C1-O11-P-O13
94	A9	502	PC1	C1-O11-P-O13
94	A9	503	PC1	C1-O11-P-O13
94	AN	301	PC1	C1-O11-P-O13
94	B5	201	PC1	C11-O13-P-O11
94	E8	301	PC1	C11-O13-P-O11
94	E8	303	PC1	C1-O11-P-O13
94	E8	304	PC1	C1-O11-P-O13
94	ED	202	PC1	C11-O13-P-O11
94	G2	301	PC1	C11-O13-P-O11
94	N1	702	PC1	C1-O11-P-O13
94	N1	703	PC1	C11-O13-P-O11
94	N1	703	PC1	C1-O11-P-O13
94	N4	501	PC1	C11-O13-P-O11
94	N4	501	PC1	C1-O11-P-O13
94	N4	502	PC1	C1-O11-P-O13
94	N5	601	PC1	C11-O13-P-O11
94	N5	601	PC1	C1-O11-P-O13
94	QC	404	PC1	C1-O11-P-O13
94	Qc	404	PC1	C1-O11-P-O13
95	4D	201	3PE	C1-O11-P-O13
95	4D	202	3PE	C11-O13-P-O11
95	C1	506	3PE	C11-O13-P-O11
95	C1	507	3PE	C11-O13-P-O11
97	4E	202	CDL	CA2-OA2-PA1-OA5
97	7C	201	CDL	CA2-OA2-PA1-OA5
97	A9	504	CDL	CA2-OA2-PA1-OA5
97	A9	504	CDL	CA3-OA5-PA1-OA2
97	A9	504	CDL	CB3-OB5-PB2-OB2
97	AM	201	CDL	CB2-OB2-PB2-OB5
97	AM	202	CDL	CA3-OA5-PA1-OA2
97	B8	302	CDL	CA3-OA5-PA1-OA2
97	B8	302	CDL	CB2-OB2-PB2-OB5
97	B8	302	CDL	CB3-OB5-PB2-OB2
97	BM	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
97	C4	201	CDL	CA2-OA2-PA1-OA5
97	C4	201	CDL	CA3-OA5-PA1-OA2
97	C4	201	CDL	CB3-OB5-PB2-OB2
97	C4	202	CDL	CB2-OB2-PB2-OB5
97	E4	401	CDL	CB3-OB5-PB2-OB2
97	EA	201	CDL	CA3-OA5-PA1-OA2
97	EA	201	CDL	CB3-OB5-PB2-OB2
97	N1	701	CDL	CA2-OA2-PA1-OA5
97	N5	603	CDL	CA2-OA2-PA1-OA5
97	N5	603	CDL	CA3-OA5-PA1-OA2
97	N5	603	CDL	CB2-OB2-PB2-OB5
97	QH	101	CDL	CB2-OB2-PB2-OB5
97	QH	101	CDL	CB3-OB5-PB2-OB2
97	QH	102	CDL	CA3-OA5-PA1-OA2
97	QH	102	CDL	CB2-OB2-PB2-OB5
97	QJ	203	CDL	CA3-OA5-PA1-OA2
97	QJ	203	CDL	CB2-OB2-PB2-OB5
97	QJ	203	CDL	CB3-OB5-PB2-OB2
97	Qc	405	CDL	CA3-OA5-PA1-OA2
97	Qc	405	CDL	CB2-OB2-PB2-OB5
97	Qd	302	CDL	CA2-OA2-PA1-OA5
97	Qd	302	CDL	CA3-OA5-PA1-OA2
97	Qd	302	CDL	CB2-OB2-PB2-OB5
97	Qh	101	CDL	CA3-OA5-PA1-OA2
97	Qh	101	CDL	CB3-OB5-PB2-OB2
97	Qj	202	CDL	CB2-OB2-PB2-OB5
104	QJ	201	PX2	C4-C5-C6-C7
95	4D	202	3PE	C27-C28-C29-C2A
97	AL	303	CDL	CB7-C71-C72-C73
97	AL	303	CDL	CA2-C1-CB2-OB2
97	N1	701	CDL	CB2-C1-CA2-OA2
94	4A	302	PC1	C11-C12-N-C13
94	4A	302	PC1	C11-C12-N-C14
94	7A	201	PC1	C11-C12-N-C13
94	A1	201	PC1	C11-C12-N-C14
94	E8	302	PC1	C11-C12-N-C14
94	Qc	404	PC1	C11-C12-N-C14
94	ED	201	PC1	C28-C29-C2A-C2B
97	Qd	302	CDL	C75-C76-C77-C78
94	A9	503	PC1	C32-C33-C34-C35
94	AM	203	PC1	C24-C25-C26-C27
94	B5	201	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
94	N4	505	PC1	C35-C36-C37-C38
100	AB	201	ZMP	C3-C4-C5-C6
104	QJ	201	PX2	C6-C7-C8-C9
94	E9	202	PC1	C32-C33-C34-C35
97	4E	202	CDL	C62-C63-C64-C65
104	QJ	202	PX2	C21-C22-C23-C24
97	QH	102	CDL	C1-CB2-OB2-PB2
97	Qc	405	CDL	C1-CA2-OA2-PA1
94	B5	202	PC1	C2C-C2D-C2E-C2F
94	B5	202	PC1	C2E-C2F-C2G-C2H
96	4D	203	S12	C16-C17-C18-C19
97	4E	202	CDL	C56-C57-C58-C59
97	N1	701	CDL	C11-C12-C13-C14
97	N1	701	CDL	C13-C14-C15-C16
96	4D	203	S12	C15-C16-C17-C18
96	4D	203	S12	C18-C19-C20-C21
104	QJ	201	PX2	C10-C11-C12-C13
95	B4	201	3PE	C31-C32-C33-C34
96	4D	203	S12	C11-C10-C9-C8
100	AC	201	ZMP	C22-C1-C2-C3
101	C1	501	HEA	C27-C19-C20-C21
94	AM	203	PC1	C25-C26-C27-C28
97	E6	401	CDL	CA7-C31-C32-C33
94	AM	204	PC1	C23-C24-C25-C26
97	AL	302	CDL	C32-C33-C34-C35
97	B3	101	CDL	C51-C52-C53-C54
104	QJ	202	PX2	C6-C7-C8-C9
97	QH	101	CDL	C41-C42-C43-C44
104	QJ	202	PX2	C22-C23-C24-C25
94	7A	201	PC1	C31-C32-C33-C34
94	ED	201	PC1	C21-C22-C23-C24
95	C1	506	3PE	C31-C32-C33-C34
97	A3	201	CDL	CA5-C11-C12-C13
94	N4	505	PC1	C22-C23-C24-C25
94	N4	505	PC1	C32-C33-C34-C35
97	E4	401	CDL	C37-C38-C39-C40
104	QJ	201	PX2	C11-C12-C13-C14
104	QJ	201	PX2	C20-C21-C22-C23
94	4A	302	PC1	C11-C12-N-C15
94	A1	201	PC1	C11-C12-N-C15
94	ED	202	PC1	C11-C12-N-C13
101	C1	501	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
105	N4	504	U10	C24-C26-C27-C28
97	AL	303	CDL	C51-C52-C53-C54
100	AB	201	ZMP	C1-C2-C3-C4
104	C2	201	PX2	C11-C10-C9-C8
94	E4	402	PC1	C33-C34-C35-C36
94	N1	703	PC1	C22-C23-C24-C25
95	N5	602	3PE	C35-C36-C37-C38
94	Qj	201	PC1	C2D-C2E-C2F-C2G
104	QJ	201	PX2	C5-C6-C7-C8
100	AC	201	ZMP	S1-C11-C12-N1
94	AM	204	PC1	C2C-C2D-C2E-C2F
94	N3	301	PC1	C26-C27-C28-C29
97	N1	701	CDL	CB3-CB4-CB6-OB8
97	Qh	101	CDL	CA3-CA4-CA6-OA8
94	A1	201	PC1	C31-C32-C33-C34
94	B5	201	PC1	C31-C32-C33-C34
101	C1	502	HEA	C27-C19-C20-C21
94	QC	404	PC1	C2-C3-O31-C31
97	QJ	203	CDL	C12-C13-C14-C15
104	QJ	201	PX2	C21-C22-C23-C24
97	4E	202	CDL	C31-C32-C33-C34
95	C1	506	3PE	C33-C34-C35-C36
95	7A	202	3PE	C36-C37-C38-C39
95	C1	507	3PE	C36-C37-C38-C39
97	QH	101	CDL	C51-C52-C53-C54
94	N1	702	PC1	C2B-C2C-C2D-C2E
97	QH	102	CDL	C51-C52-C53-C54
97	Qd	302	CDL	C1-CB2-OB2-PB2
94	E9	202	PC1	C22-C23-C24-C25
97	AM	202	CDL	C33-C34-C35-C36
100	AB	201	ZMP	C22-C1-C2-C3
94	7A	201	PC1	C11-C12-N-C14
94	AM	203	PC1	C11-C12-N-C13
94	B5	202	PC1	C11-C12-N-C13
94	ED	201	PC1	C11-C12-N-C14
94	N1	702	PC1	C11-C12-N-C15
94	N3	301	PC1	C11-C12-N-C15
94	Qc	401	PC1	C11-C12-N-C13
94	Qc	404	PC1	C11-C12-N-C15
94	Qe	303	PC1	C11-C12-N-C15
97	C4	203	CDL	CA7-C31-C32-C33
97	7C	201	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
97	N5	603	CDL	C42-C43-C44-C45
97	7C	201	CDL	C12-C13-C14-C15
97	AL	302	CDL	C35-C36-C37-C38
95	E9	201	3PE	C27-C28-C29-C2A
104	QJ	201	PX2	C7-C8-C9-C10
94	AL	301	PC1	C31-C32-C33-C34
95	4D	202	3PE	C21-C22-C23-C24
97	N5	603	CDL	CA7-C31-C32-C33
94	AM	203	PC1	C39-C3A-C3B-C3C
97	E6	401	CDL	C32-C33-C34-C35
100	AB	201	ZMP	C1-C22-C23-C24
94	4A	301	PC1	C27-C28-C29-C2A
95	N5	602	3PE	C2C-C2D-C2E-C2F
94	4E	201	PC1	C21-C22-C23-C24
94	B5	202	PC1	C21-C22-C23-C24
97	C4	201	CDL	C51-C52-C53-C54
104	C2	201	PX2	C5-C6-C7-C8
94	N4	505	PC1	C37-C38-C39-C3A
100	AB	201	ZMP	C6-C7-C8-C9
100	AB	201	ZMP	C13-C14-C15-N2
97	B8	302	CDL	C58-C59-C60-C61
97	QC	403	CDL	OA5-CA3-CA4-OA6
97	Qd	302	CDL	OA5-CA3-CA4-OA6
97	A3	201	CDL	C71-C72-C73-C74
97	C4	201	CDL	C59-C60-C61-C62
94	G2	301	PC1	C21-C22-C23-C24
104	QJ	201	PX2	C19-C20-C21-C22
104	QJ	201	PX2	C23-C24-C25-C26
94	E4	402	PC1	O21-C2-C3-O31
97	AL	303	CDL	OB6-CB4-CB6-OB8
97	QD	302	CDL	OA6-CA4-CA6-OA8
94	Qj	201	PC1	C3A-C3B-C3C-C3D
94	E4	402	PC1	C11-C12-N-C14
94	E4	402	PC1	C11-C12-N-C15
94	E8	302	PC1	C11-C12-N-C15
94	ED	202	PC1	C11-C12-N-C14
94	G2	301	PC1	C11-C12-N-C13
94	G2	301	PC1	C11-C12-N-C14
94	AN	301	PC1	C35-C36-C37-C38
104	QJ	202	PX2	C9-C10-C11-C12
94	N1	702	PC1	C37-C38-C39-C3A
95	4D	202	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
104	QJ	202	PX2	C19-C20-C21-C22
97	AM	201	CDL	C56-C57-C58-C59
106	Qc	403	HEM	C4D-C3D-CAD-CBD
97	EA	202	CDL	C53-C54-C55-C56
97	C4	203	CDL	C76-C77-C78-C79
94	4A	301	PC1	C1-O11-P-O13
94	N4	502	PC1	C11-O13-P-O11
94	Qj	201	PC1	C1-O11-P-O13
95	B4	201	3PE	C11-O13-P-O11
97	Qe	302	CDL	CA3-OA5-PA1-OA2
94	B5	202	PC1	C24-C25-C26-C27
97	Qe	302	CDL	CB7-C71-C72-C73
97	4E	202	CDL	C1-CB2-OB2-PB2
97	A3	201	CDL	C1-CA2-OA2-PA1
97	AL	302	CDL	CB4-CB3-OB5-PB2
97	EA	201	CDL	C1-CB2-OB2-PB2
97	Qd	302	CDL	C33-C34-C35-C36
95	C1	506	3PE	O11-C1-C2-C3
97	QD	302	CDL	OA5-CA3-CA4-CA6
97	QJ	203	CDL	OB5-CB3-CB4-CB6
97	Qh	101	CDL	OB5-CB3-CB4-CB6
97	QH	101	CDL	C35-C36-C37-C38
94	4A	302	PC1	C38-C39-C3A-C3B
94	ED	201	PC1	C24-C25-C26-C27
94	ED	201	PC1	C25-C26-C27-C28
97	N5	603	CDL	C17-C18-C19-C20
100	AC	201	ZMP	C6-C7-C8-C9
94	A1	201	PC1	C21-C22-C23-C24
97	4E	202	CDL	CA5-C11-C12-C13
95	7A	202	3PE	C23-C24-C25-C26
97	A9	504	CDL	CB2-C1-CA2-OA2
97	EA	202	CDL	CB2-C1-CA2-OA2
104	QJ	201	PX2	C18-C19-C20-C21
97	N5	603	CDL	CB5-C51-C52-C53
97	QD	302	CDL	CA5-C11-C12-C13
97	B3	101	CDL	O1-C1-CB2-OB2
94	E8	302	PC1	C11-C12-N-C13
94	ED	202	PC1	C11-C12-N-C15
94	4A	302	PC1	C1-C2-C3-O31
94	4E	201	PC1	C1-C2-C3-O31
94	A9	502	PC1	C1-C2-C3-O31
94	B5	202	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
94	C1	505	PC1	C1-C2-C3-O31
94	E4	402	PC1	C1-C2-C3-O31
94	QC	404	PC1	C1-C2-C3-O31
97	AL	302	CDL	CA3-CA4-CA6-OA8
97	E6	401	CDL	CA3-CA4-CA6-OA8
97	QH	102	CDL	CA3-CA4-CA6-OA8
104	QJ	201	PX2	C1-C2-C3-O5
95	4D	202	3PE	C3A-C3B-C3C-C3D
97	C4	201	CDL	C14-C15-C16-C17
94	AM	204	PC1	C31-C32-C33-C34
94	AM	204	PC1	C27-C28-C29-C2A
94	B8	301	PC1	C24-C25-C26-C27
94	Qc	401	PC1	C27-C28-C29-C2A
104	C2	201	PX2	C4-C5-C6-C7
104	C2	201	PX2	C16-C17-C18-C19
100	AB	201	ZMP	O3-C16-C17-O4
97	7C	201	CDL	C39-C40-C41-C42
101	C1	501	HEA	C18-C19-C20-C21
94	Qj	201	PC1	C22-C23-C24-C25
97	BM	201	CDL	C55-C56-C57-C58
104	QJ	202	PX2	C11-C12-C13-C14
97	A9	504	CDL	CB6-CB4-OB6-CB5
94	E8	302	PC1	C39-C3A-C3B-C3C
97	C4	201	CDL	C61-C62-C63-C64
97	A3	201	CDL	C52-C53-C54-C55
95	N5	602	3PE	O11-C1-C2-O21
94	B8	301	PC1	O21-C21-C22-C23
94	AM	203	PC1	C11-C12-N-C14
94	B5	202	PC1	C11-C12-N-C15
94	ED	201	PC1	C11-C12-N-C15
94	N1	702	PC1	C11-C12-N-C13
94	N3	301	PC1	C11-C12-N-C14
97	N1	701	CDL	CA7-C31-C32-C33
94	AM	203	PC1	C37-C38-C39-C3A
94	C3	201	PC1	C3E-C3F-C3G-C3H
94	N5	601	PC1	C22-C23-C24-C25
94	ED	202	PC1	O21-C2-C3-O31
97	Qh	101	CDL	OA6-CA4-CA6-OA8
104	QJ	201	PX2	O7-C2-C3-O5
94	N1	703	PC1	C27-C28-C29-C2A
95	4D	202	3PE	C23-C24-C25-C26
95	N4	503	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
94	E8	302	PC1	C22-C23-C24-C25
94	A1	202	PC1	C21-C22-C23-C24
94	QD	303	PC1	C22-C23-C24-C25
106	Qc	403	HEM	C2D-C3D-CAD-CBD
94	E4	402	PC1	C28-C29-C2A-C2B
94	E8	301	PC1	C24-C25-C26-C27
94	E8	302	PC1	C2D-C2E-C2F-C2G
95	N4	503	3PE	C22-C23-C24-C25
97	E6	401	CDL	C51-C52-C53-C54
104	C2	201	PX2	C12-C13-C14-C15
94	Qc	401	PC1	C11-C12-N-C14
94	E8	302	PC1	O11-C1-C2-C3
95	4D	202	3PE	O11-C1-C2-C3
95	N5	602	3PE	O11-C1-C2-C3
97	E7	301	CDL	OA5-CA3-CA4-CA6
97	E7	301	CDL	OB5-CB3-CB4-CB6
97	N1	701	CDL	OB5-CB3-CB4-CB6
97	QC	403	CDL	OA5-CA3-CA4-CA6
97	Qd	302	CDL	OA5-CA3-CA4-CA6
97	Qd	302	CDL	OB5-CB3-CB4-CB6
104	C2	201	PX2	O4-C1-C2-C3
104	QJ	201	PX2	O4-C1-C2-C3
94	Qc	401	PC1	C3C-C3D-C3E-C3F
94	QC	404	PC1	C2B-C2C-C2D-C2E
97	4E	202	CDL	C33-C34-C35-C36
97	7C	201	CDL	C34-C35-C36-C37
97	C4	203	CDL	C38-C39-C40-C41
97	BM	201	CDL	CA5-C11-C12-C13
95	4D	202	3PE	C32-C33-C34-C35
95	4D	202	3PE	C24-C25-C26-C27
94	Qj	201	PC1	C37-C38-C39-C3A
104	QJ	201	PX2	C17-C18-C19-C20
97	BM	201	CDL	C71-C72-C73-C74
94	E8	302	PC1	C31-C32-C33-C34
95	B4	201	3PE	C33-C34-C35-C36
97	A3	201	CDL	C11-C12-C13-C14
94	N3	301	PC1	C2-C1-O11-P
94	E8	302	PC1	C2A-C2B-C2C-C2D
97	A9	504	CDL	C15-C16-C17-C18
94	ED	202	PC1	C24-C25-C26-C27
94	AM	203	PC1	C3C-C3D-C3E-C3F
94	N1	702	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
94	N4	501	PC1	C1-C2-C3-O31
94	QD	303	PC1	C1-C2-C3-O31
95	4D	202	3PE	C1-C2-C3-O31
95	B4	201	3PE	C1-C2-C3-O31
97	AM	202	CDL	CA3-CA4-CA6-OA8
97	E7	301	CDL	CB3-CB4-CB6-OB8
97	QD	302	CDL	CA3-CA4-CA6-OA8
97	QH	102	CDL	CB3-CB4-CB6-OB8
94	E8	301	PC1	C31-C32-C33-C34
100	AC	201	ZMP	N2-C16-C17-C18
94	B5	202	PC1	C11-C12-N-C14
94	N1	702	PC1	C11-C12-N-C14
94	N3	301	PC1	C11-C12-N-C13
94	Qe	303	PC1	C11-C12-N-C13
97	Qc	405	CDL	C11-C12-C13-C14
94	AN	301	PC1	C11-O13-P-O11
95	4D	202	3PE	C34-C35-C36-C37
97	7C	201	CDL	C58-C59-C60-C61
94	B5	201	PC1	O11-C1-C2-O21
94	N1	703	PC1	O11-C1-C2-O21
97	4E	202	CDL	OB5-CB3-CB4-OB6
97	QJ	203	CDL	OB5-CB3-CB4-OB6
97	Qd	302	CDL	OB5-CB3-CB4-OB6
97	Qj	202	CDL	OB5-CB3-CB4-OB6
104	QJ	201	PX2	O4-C1-C2-O7
97	N5	603	CDL	CA5-C11-C12-C13
94	AL	301	PC1	C28-C29-C2A-C2B
104	C2	201	PX2	C18-C19-C20-C21
97	B8	302	CDL	C32-C31-CA7-OA8
94	B5	202	PC1	O21-C2-C3-O31
94	N4	501	PC1	O21-C2-C3-O31
97	4E	202	CDL	OA6-CA4-CA6-OA8
97	E4	401	CDL	OA6-CA4-CA6-OA8
97	QH	102	CDL	OB6-CB4-CB6-OB8
97	Qj	202	CDL	OA6-CA4-CA6-OA8
97	C4	203	CDL	C19-C20-C21-C22
97	B3	101	CDL	CA2-C1-CB2-OB2
104	C2	201	PX2	O5-C4-C5-C6
94	B5	201	PC1	C2-C1-O11-P
94	Qc	401	PC1	C2-C1-O11-P
95	4D	201	3PE	C2-C1-O11-P
95	N5	602	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
97	AM	202	CDL	CB4-CB3-OB5-PB2
97	E6	401	CDL	CB4-CB3-OB5-PB2
97	EA	202	CDL	C1-CA2-OA2-PA1
97	N5	603	CDL	CB4-CB3-OB5-PB2
108	V1	601	FMN	C4'-C5'-O5'-P
94	E8	304	PC1	C11-C12-N-C15
95	B4	201	3PE	C21-C22-C23-C24
97	N1	701	CDL	CA5-C11-C12-C13
97	N5	603	CDL	C81-C82-C83-C84
100	AB	201	ZMP	C2-C3-C4-C5
97	C4	203	CDL	C21-C22-C23-C24
97	E7	301	CDL	C32-C33-C34-C35
94	7A	201	PC1	O11-C1-C2-C3
94	B8	301	PC1	O11-C1-C2-C3
94	N1	703	PC1	O11-C1-C2-C3
97	EA	202	CDL	OB5-CB3-CB4-CB6
97	QD	302	CDL	OB5-CB3-CB4-CB6
97	QH	101	CDL	OA5-CA3-CA4-CA6
97	Qj	202	CDL	OB5-CB3-CB4-CB6
94	C3	201	PC1	C3F-C3G-C3H-C3I
94	C1	505	PC1	C3B-C3C-C3D-C3E
94	Qc	401	PC1	C33-C34-C35-C36
97	N1	701	CDL	C14-C15-C16-C17
94	AM	203	PC1	C11-C12-N-C15
94	ED	201	PC1	C11-C12-N-C13
104	C2	201	PX2	C5-C4-O5-C3
94	N5	601	PC1	O31-C31-C32-C33
106	QC	401	HEM	C2B-C3B-CAB-CBB
106	Qc	402	HEM	C2B-C3B-CAB-CBB
104	C2	201	PX2	C9-C10-C11-C12
94	A9	502	PC1	C2-C1-O11-P
94	AM	203	PC1	C2-C1-O11-P
94	AM	203	PC1	C1-C2-C3-O31
94	E8	303	PC1	C1-C2-C3-O31
94	N1	703	PC1	C1-C2-C3-O31
94	N3	301	PC1	C1-C2-C3-O31
94	QD	303	PC1	C2-C1-O11-P
97	A9	504	CDL	CA4-CA3-OA5-PA1
97	AM	201	CDL	C1-CA2-OA2-PA1
97	C4	201	CDL	CB3-CB4-CB6-OB8
97	E4	401	CDL	CA3-CA4-CA6-OA8
97	EA	201	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
97	EA	202	CDL	CA3-CA4-CA6-OA8
97	QC	403	CDL	CA4-CA3-OA5-PA1
97	QH	102	CDL	C1-CA2-OA2-PA1
94	7A	201	PC1	O11-C1-C2-O21
94	B8	301	PC1	O11-C1-C2-O21
95	C1	506	3PE	O11-C1-C2-O21
97	E7	301	CDL	OA5-CA3-CA4-OA6
97	N1	701	CDL	OB5-CB3-CB4-OB6
97	QD	302	CDL	OB5-CB3-CB4-OB6
97	Qh	101	CDL	OB5-CB3-CB4-OB6
104	C2	201	PX2	O4-C1-C2-O7
94	ED	202	PC1	C22-C23-C24-C25
95	B4	201	3PE	C25-C26-C27-C28
94	A1	201	PC1	C25-C26-C27-C28
94	B5	202	PC1	C3B-C3C-C3D-C3E
104	C2	201	PX2	O6-C4-O5-C3
94	C1	505	PC1	C36-C37-C38-C39
100	AB	201	ZMP	C16-C17-C18-C19
100	AB	201	ZMP	C16-C17-C18-C20
100	AC	201	ZMP	C16-C17-C18-C19
94	A9	502	PC1	O21-C2-C3-O31
94	AM	203	PC1	O21-C2-C3-O31
94	QC	404	PC1	O21-C2-C3-O31
95	B4	201	3PE	O21-C2-C3-O31
97	A9	504	CDL	OB6-CB4-CB6-OB8
97	AL	302	CDL	OA6-CA4-CA6-OA8
97	AM	202	CDL	OA6-CA4-CA6-OA8
97	C4	201	CDL	OB6-CB4-CB6-OB8
97	EA	202	CDL	OA6-CA4-CA6-OA8
97	QH	102	CDL	OA6-CA4-CA6-OA8
94	Qc	401	PC1	C11-C12-N-C15
94	Qe	303	PC1	C11-C12-N-C14
99	A9	501	NDP	C5D-O5D-PN-O3
97	AM	202	CDL	C17-C18-C19-C20
97	7C	201	CDL	C54-C55-C56-C57
97	Qd	302	CDL	C60-C61-C62-C63
94	A9	502	PC1	C31-C32-C33-C34
94	N4	505	PC1	C23-C24-C25-C26
99	A9	501	NDP	PN-O3-PA-O1A
94	ED	202	PC1	C35-C36-C37-C38
97	E4	401	CDL	C31-C32-C33-C34
96	4D	203	S12	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
95	7A	202	3PE	C3C-C3D-C3E-C3F
100	AC	201	ZMP	C2-C3-C4-C5
94	Qc	401	PC1	C11-O13-P-O11
95	C1	507	3PE	C1-O11-P-O13
97	E6	401	CDL	CB2-OB2-PB2-OB5
97	N1	701	CDL	CA3-OA5-PA1-OA2
97	Qc	405	CDL	CB3-OB5-PB2-OB2
97	Qj	202	CDL	CB3-OB5-PB2-OB2
97	E6	401	CDL	O1-C1-CA2-OA2
94	AL	301	PC1	C2-C1-O11-P
96	4D	203	S12	C3-C2-O2-P
97	7C	201	CDL	CA4-CA3-OA5-PA1
97	AL	303	CDL	CB4-CB3-OB5-PB2
97	AM	202	CDL	C1-CB2-OB2-PB2
97	C4	203	CDL	CA4-CA3-OA5-PA1
97	QD	302	CDL	C1-CA2-OA2-PA1
97	Qc	405	CDL	CA4-CA3-OA5-PA1
94	4A	302	PC1	C11-O13-P-O12
94	4E	201	PC1	C11-O13-P-O14
94	A1	201	PC1	C1-O11-P-O12
94	A1	201	PC1	C1-O11-P-O14
94	A1	202	PC1	C1-O11-P-O12
94	AL	301	PC1	C11-C12-N-C14
94	B5	201	PC1	C1-O11-P-O12
94	E4	402	PC1	C11-O13-P-O12
94	E8	301	PC1	C11-O13-P-O14
94	E8	303	PC1	C1-O11-P-O14
94	E8	304	PC1	C1-O11-P-O14
94	E8	304	PC1	C11-C12-N-C13
94	ED	202	PC1	C11-O13-P-O14
94	G2	301	PC1	C11-O13-P-O14
94	N1	703	PC1	C1-O11-P-O12
94	N4	501	PC1	C11-O13-P-O12
94	N4	502	PC1	C11-O13-P-O14
94	N4	502	PC1	C1-O11-P-O14
94	N5	601	PC1	C11-O13-P-O14
94	N5	601	PC1	C1-O11-P-O12
94	QC	404	PC1	C1-O11-P-O12
94	Qc	404	PC1	C1-O11-P-O12
94	Qc	404	PC1	C1-O11-P-O14
95	4D	201	3PE	C1-O11-P-O12
95	4D	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
95	4D	202	3PE	C1-O11-P-O12
95	4D	202	3PE	C11-O13-P-O14
95	7A	202	3PE	C11-O13-P-O14
95	C1	507	3PE	C11-O13-P-O12
95	C1	507	3PE	C11-O13-P-O14
97	7C	201	CDL	CA2-OA2-PA1-OA4
97	A9	504	CDL	CA2-OA2-PA1-OA3
97	A9	504	CDL	CB3-OB5-PB2-OB3
97	AM	201	CDL	CB3-OB5-PB2-OB4
97	AM	202	CDL	CA2-OA2-PA1-OA4
97	B8	302	CDL	CA2-OA2-PA1-OA4
97	BM	201	CDL	CA3-OA5-PA1-OA3
97	C4	201	CDL	CA2-OA2-PA1-OA4
97	C4	201	CDL	CA3-OA5-PA1-OA3
97	E4	401	CDL	CB3-OB5-PB2-OB4
97	E7	301	CDL	CA3-OA5-PA1-OA4
97	EA	201	CDL	CB3-OB5-PB2-OB3
97	EA	201	CDL	CB3-OB5-PB2-OB4
97	EA	202	CDL	CB3-OB5-PB2-OB4
97	N1	701	CDL	CB3-OB5-PB2-OB4
97	N5	603	CDL	CA2-OA2-PA1-OA3
97	N5	603	CDL	CA2-OA2-PA1-OA4
97	N5	603	CDL	CA3-OA5-PA1-OA3
97	QH	101	CDL	CB3-OB5-PB2-OB4
97	QH	102	CDL	CA3-OA5-PA1-OA3
97	QH	102	CDL	CA3-OA5-PA1-OA4
97	QH	102	CDL	CB2-OB2-PB2-OB3
97	Qd	302	CDL	CB2-OB2-PB2-OB4
97	Qh	101	CDL	CA2-OA2-PA1-OA3
97	Qh	101	CDL	CB3-OB5-PB2-OB4
97	Qj	202	CDL	CB2-OB2-PB2-OB4
97	Qj	202	CDL	CB3-OB5-PB2-OB4
99	A9	501	NDP	C5D-O5D-PN-O2N
94	B5	201	PC1	O11-C1-C2-C3
94	Qe	303	PC1	O11-C1-C2-C3
97	4E	202	CDL	OB5-CB3-CB4-CB6
97	AM	202	CDL	OA5-CA3-CA4-CA6
97	C4	202	CDL	OB5-CB3-CB4-CB6
95	N4	503	3PE	O31-C31-C32-C33
104	C2	201	PX2	C21-C22-C23-C24
104	QJ	202	PX2	C11-C10-C9-C8
94	E8	301	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
94	E8	304	PC1	C12-C11-O13-P
94	N1	703	PC1	C12-C11-O13-P
95	C1	507	3PE	C12-C11-O13-P
101	C1	502	HEA	C3B-C11-C12-C13
95	B4	201	3PE	C2-C3-O31-C31
104	C2	201	PX2	C6-C7-C8-C9
94	E8	302	PC1	O11-C1-C2-O21
94	Qe	303	PC1	O11-C1-C2-O21
95	4D	202	3PE	O11-C1-C2-O21
97	C4	201	CDL	OA5-CA3-CA4-OA6
97	E6	401	CDL	OA5-CA3-CA4-OA6
97	EA	202	CDL	OB5-CB3-CB4-OB6
97	QD	302	CDL	OA5-CA3-CA4-OA6
97	QH	101	CDL	OA5-CA3-CA4-OA6
99	A9	501	NDP	O4D-C4D-C5D-O5D
107	Qd	301	HEC	C3D-CAD-CBD-CGD
97	C4	203	CDL	C73-C74-C75-C76
94	N4	505	PC1	C11-C12-N-C13
97	C4	203	CDL	C80-C81-C82-C83
94	4A	302	PC1	O13-C11-C12-N
94	7A	201	PC1	O13-C11-C12-N
94	A9	502	PC1	O13-C11-C12-N
94	AN	301	PC1	O13-C11-C12-N
94	B8	301	PC1	O13-C11-C12-N
94	E8	301	PC1	O13-C11-C12-N
94	E8	303	PC1	O13-C11-C12-N
94	E8	304	PC1	O13-C11-C12-N
94	ED	201	PC1	C3B-C3C-C3D-C3E
94	N4	501	PC1	O13-C11-C12-N
94	N4	502	PC1	O13-C11-C12-N
94	QD	303	PC1	O13-C11-C12-N
94	Qc	404	PC1	O13-C11-C12-N
97	AL	303	CDL	CB3-CB4-CB6-OB8
97	N5	603	CDL	CB3-CB4-CB6-OB8
107	Qd	301	HEC	C2D-C3D-CAD-CBD
107	Qd	301	HEC	C4D-C3D-CAD-CBD
94	QD	303	PC1	O21-C2-C3-O31
97	E7	301	CDL	OB6-CB4-CB6-OB8
97	N1	701	CDL	OB6-CB4-CB6-OB8
97	N5	603	CDL	OB6-CB4-CB6-OB8
94	B5	202	PC1	C25-C26-C27-C28
97	4E	202	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
97	Qd	302	CDL	C59-C60-C61-C62
97	Qd	302	CDL	C56-C57-C58-C59
100	AC	201	ZMP	O3-C16-C17-O4
97	C4	203	CDL	C54-C55-C56-C57
97	E4	401	CDL	CB7-C71-C72-C73
94	AL	301	PC1	C11-C12-N-C15
94	Qj	201	PC1	C11-C12-N-C13
94	4A	301	PC1	C2A-C2B-C2C-C2D
94	B5	201	PC1	C25-C26-C27-C28
97	4E	202	CDL	C71-C72-C73-C74
97	C4	202	CDL	C71-C72-C73-C74
94	4A	302	PC1	C3A-C3B-C3C-C3D
94	AM	204	PC1	C25-C26-C27-C28
94	B5	202	PC1	C35-C36-C37-C38
94	N4	501	PC1	C31-C32-C33-C34
94	C1	505	PC1	C37-C38-C39-C3A
94	C3	201	PC1	C36-C37-C38-C39
100	AB	201	ZMP	C19-C18-C21-O5
94	Qj	201	PC1	C27-C28-C29-C2A
95	4D	202	3PE	C2A-C2B-C2C-C2D
94	B5	202	PC1	C3C-C3D-C3E-C3F
94	A9	502	PC1	C1-C2-O21-C21
94	AN	301	PC1	C1-C2-O21-C21
94	N4	501	PC1	C3-C2-O21-C21
94	Qj	201	PC1	C3-C2-O21-C21
97	A9	504	CDL	CA6-CA4-OA6-CA5
97	Qj	202	CDL	CA6-CA4-OA6-CA5
97	Qj	202	CDL	CB3-CB4-OB6-CB5
94	N4	505	PC1	C34-C35-C36-C37
101	C1	501	HEA	C11-C12-C13-C14
97	QH	101	CDL	C34-C35-C36-C37
97	QJ	203	CDL	C32-C31-CA7-OA8
94	4A	302	PC1	C26-C27-C28-C29
97	QC	403	CDL	CB4-CB3-OB5-PB2
97	C4	202	CDL	OB5-CB3-CB4-OB6
97	N5	603	CDL	OA5-CA3-CA4-OA6
97	AL	302	CDL	C32-C31-CA7-OA8
99	A9	501	NDP	O4D-C1D-N1N-C6N
95	C1	506	3PE	C35-C36-C37-C38
94	AM	203	PC1	C29-C2A-C2B-C2C
97	N1	701	CDL	C31-C32-C33-C34
97	QD	302	CDL	CA4-CA6-OA8-CA7

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Mol	Chain	Res	Type	Atoms
95	4D	201	3PE	O21-C2-C3-O31
97	EA	201	CDL	OB6-CB4-CB6-OB8
97	AM	201	CDL	C15-C16-C17-C18
94	AM	203	PC1	C11-O13-P-O11
94	AM	203	PC1	C1-O11-P-O13
94	C3	201	PC1	C1-O11-P-O13
94	ED	201	PC1	C11-O13-P-O11
94	N3	301	PC1	C1-O11-P-O13
94	Qe	303	PC1	C1-O11-P-O13
95	B4	201	3PE	C1-O11-P-O13
95	C1	506	3PE	C1-O11-P-O13
96	4D	203	S12	CB-OG-P-O2
97	AL	303	CDL	CA2-OA2-PA1-OA5
97	AL	303	CDL	CB2-OB2-PB2-OB5
97	B3	101	CDL	CB3-OB5-PB2-OB2
97	EA	202	CDL	CA2-OA2-PA1-OA5
97	EA	202	CDL	CB2-OB2-PB2-OB5
97	QC	403	CDL	CB3-OB5-PB2-OB2
97	QH	102	CDL	CA2-OA2-PA1-OA5
97	Qe	302	CDL	CA2-OA2-PA1-OA5
95	B4	201	3PE	C34-C35-C36-C37
97	C4	203	CDL	C53-C54-C55-C56
97	C4	203	CDL	C78-C79-C80-C81
97	A9	504	CDL	CB3-CB4-CB6-OB8
94	C3	201	PC1	C3A-C3B-C3C-C3D
104	C2	201	PX2	C17-C18-C19-C20
104	C2	201	PX2	C20-C21-C22-C23
101	C1	502	HEA	C20-C21-C22-C23
95	4D	201	3PE	C23-C24-C25-C26
99	A9	501	NDP	PA-O3-PN-O1N
97	N5	603	CDL	C32-C33-C34-C35
94	G2	301	PC1	C2-C1-O11-P
97	7C	201	CDL	C1-CA2-OA2-PA1
97	E4	401	CDL	C1-CB2-OB2-PB2
97	N1	701	CDL	C1-CA2-OA2-PA1
107	Qd	301	HEC	CAD-CBD-CGD-O1D
100	AB	201	ZMP	C4-C5-C6-C7
94	B5	201	PC1	C3E-C3F-C3G-C3H
97	C4	203	CDL	C34-C35-C36-C37
94	E8	304	PC1	C11-C12-N-C14
94	4E	201	PC1	C23-C24-C25-C26
97	AM	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
97	E6	401	CDL	OA5-CA3-CA4-CA6
97	A9	504	CDL	OA5-CA3-CA4-OA6
97	AM	201	CDL	OB5-CB3-CB4-OB6
106	Qc	402	HEM	C4B-C3B-CAB-CBB
94	B5	202	PC1	C36-C37-C38-C39
94	B8	301	PC1	O22-C21-C22-C23
95	C1	506	3PE	C26-C27-C28-C29
97	E4	401	CDL	C35-C36-C37-C38
106	QC	401	HEM	CAD-CBD-CGD-O1D
94	E8	303	PC1	O21-C2-C3-O31
97	E7	301	CDL	CA4-CA3-OA5-PA1
97	EA	201	CDL	CB4-CB3-OB5-PB2
97	EA	202	CDL	C1-CB2-OB2-PB2
97	QD	302	CDL	CB4-CB3-OB5-PB2
97	Qc	405	CDL	C1-CB2-OB2-PB2
97	Qd	302	CDL	CA4-CA3-OA5-PA1
97	Qe	302	CDL	CA4-CA3-OA5-PA1
94	AM	204	PC1	C26-C27-C28-C29
100	AB	201	ZMP	S1-C11-C12-N1
106	Qc	402	HEM	CAD-CBD-CGD-O1D
95	4D	202	3PE	C36-C37-C38-C39
95	N4	503	3PE	C23-C24-C25-C26
94	4A	302	PC1	C29-C2A-C2B-C2C
106	QC	402	HEM	CAD-CBD-CGD-O2D
94	7A	201	PC1	C33-C34-C35-C36
106	QC	401	HEM	C3D-CAD-CBD-CGD
94	Qc	401	PC1	C2E-C2F-C2G-C2H
107	QD	301	HEC	CAD-CBD-CGD-O1D
97	Qd	302	CDL	C35-C36-C37-C38
94	N5	601	PC1	C1-C2-C3-O31
97	C4	203	CDL	C41-C42-C43-C44
106	QC	402	HEM	CAD-CBD-CGD-O1D
106	Qc	403	HEM	CAD-CBD-CGD-O1D
94	E8	302	PC1	C35-C36-C37-C38
97	C4	201	CDL	C13-C14-C15-C16
94	A1	201	PC1	C1-C2-O21-C21
94	AL	301	PC1	C1-C2-O21-C21
94	B8	301	PC1	C3-C2-O21-C21
94	QD	303	PC1	C3-C2-O21-C21
94	Qc	404	PC1	C1-C2-O21-C21
95	C1	506	3PE	C3-C2-O21-C21
97	7C	201	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
97	7C	201	CDL	CB3-CB4-OB6-CB5
97	AM	202	CDL	CA6-CA4-OA6-CA5
97	AM	202	CDL	CB3-CB4-OB6-CB5
97	E6	401	CDL	CB6-CB4-OB6-CB5
97	QC	403	CDL	CB3-CB4-OB6-CB5
97	QH	101	CDL	CB3-CB4-OB6-CB5
97	QJ	203	CDL	CB3-CB4-OB6-CB5
97	Qh	101	CDL	CB3-CB4-OB6-CB5
97	Qj	202	CDL	CA3-CA4-OA6-CA5
94	AL	301	PC1	C11-C12-N-C13
94	N3	301	PC1	C11-O13-P-O11
94	7A	201	PC1	O21-C21-C22-C23
94	N1	702	PC1	O31-C31-C32-C33
106	QC	401	HEM	CAD-CBD-CGD-O2D
106	Qc	402	HEM	CAD-CBD-CGD-O2D
94	N1	702	PC1	C23-C24-C25-C26
95	E9	201	3PE	C2-C1-O11-P
97	7C	201	CDL	C32-C31-CA7-OA8
107	Qd	301	HEC	CAD-CBD-CGD-O2D
95	C1	507	3PE	O11-C1-C2-C3
97	C4	201	CDL	OA5-CA3-CA4-CA6
94	E8	301	PC1	C32-C33-C34-C35
107	QD	301	HEC	CAD-CBD-CGD-O2D
104	QJ	202	PX2	C5-C6-C7-C8
99	A9	501	NDP	O4B-C4B-C5B-O5B
95	B4	201	3PE	C29-C2A-C2B-C2C
97	N1	701	CDL	CB5-C51-C52-C53
97	4E	202	CDL	C64-C65-C66-C67
100	AB	201	ZMP	C12-C11-S1-C10
100	AC	201	ZMP	C12-C11-S1-C10
97	A9	504	CDL	OA6-CA4-CA6-OA8
97	E6	401	CDL	CB5-C51-C52-C53
97	E4	401	CDL	C41-C42-C43-C44
95	7A	202	3PE	C37-C38-C39-C3A
105	N4	504	U10	C26-C27-C28-C29
95	N4	503	3PE	C31-C32-C33-C34
97	AM	202	CDL	CA2-C1-CB2-OB2
97	7C	201	CDL	C53-C54-C55-C56
97	C4	203	CDL	C83-C84-C85-C86
97	Qe	302	CDL	C14-C15-C16-C17
104	QJ	202	PX2	C23-C24-C25-C26
97	AL	302	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
94	AM	203	PC1	C27-C28-C29-C2A
97	AL	303	CDL	CA4-CA3-OA5-PA1
94	4A	301	PC1	C28-C29-C2A-C2B
94	Qj	201	PC1	C39-C3A-C3B-C3C
97	Qc	405	CDL	C52-C51-CB5-OB6
94	AL	301	PC1	C2D-C2E-C2F-C2G
94	ED	202	PC1	C1-C2-C3-O31
95	4D	202	3PE	C35-C36-C37-C38
97	QC	403	CDL	CA3-CA4-CA6-OA8
94	E8	302	PC1	C3C-C3D-C3E-C3F
94	Qj	201	PC1	C28-C29-C2A-C2B
95	E9	201	3PE	C2C-C2D-C2E-C2F
104	QJ	202	PX2	C20-C21-C22-C23
95	B4	201	3PE	C23-C24-C25-C26
97	Qe	302	CDL	C16-C17-C18-C19
97	N5	603	CDL	C58-C59-C60-C61
97	C4	201	CDL	C77-C78-C79-C80
97	QC	403	CDL	OB5-CB3-CB4-OB6
104	QJ	202	PX2	O4-C1-C2-O7
94	4A	302	PC1	C24-C25-C26-C27
95	E9	201	3PE	C29-C2A-C2B-C2C
97	N5	603	CDL	OA5-CA3-CA4-CA6
94	AM	204	PC1	O21-C21-C22-C23
95	4D	201	3PE	O13-C11-C12-N
97	QH	101	CDL	CA4-CA3-OA5-PA1
97	QJ	203	CDL	CA4-CA3-OA5-PA1
104	QJ	202	PX2	O7-C2-C3-O5
97	E7	301	CDL	C12-C11-CA5-OA6
99	A9	501	NDP	C3D-C4D-C5D-O5D
99	A9	501	NDP	C2B-O2B-P2B-O1X
100	AC	201	ZMP	N2-C16-C17-O4
97	C4	202	CDL	C12-C11-CA5-OA6
97	E6	401	CDL	C12-C11-CA5-OA6
105	N4	504	U10	C12-C11-C9-C10
97	QH	102	CDL	CB3-OB5-PB2-OB2
94	N4	505	PC1	C11-C12-N-C14
94	N4	505	PC1	C11-C12-N-C15
94	Qj	201	PC1	C11-C12-N-C14
94	Qj	201	PC1	C11-C12-N-C15
97	E6	401	CDL	C32-C31-CA7-OA8
97	Qd	302	CDL	C51-C52-C53-C54
95	C1	506	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
97	7C	201	CDL	C16-C17-C18-C19
97	C4	203	CDL	O1-C1-CA2-OA2
97	N1	701	CDL	C72-C71-CB7-OB8
101	C1	501	HEA	CAD-CBD-CGD-O1D
94	C3	201	PC1	C1-C2-O21-C21
94	C3	201	PC1	C3-C2-O21-C21
94	Qc	401	PC1	C3-C2-O21-C21
97	AM	202	CDL	CB6-CB4-OB6-CB5
97	E6	401	CDL	CB3-CB4-OB6-CB5
95	C1	507	3PE	C26-C27-C28-C29
95	N5	602	3PE	C23-C24-C25-C26
94	A9	502	PC1	C32-C33-C34-C35
94	4A	302	PC1	O21-C21-C22-C23
94	N4	502	PC1	O31-C31-C32-C33
105	N4	504	U10	C20-C19-C21-C22
94	ED	201	PC1	C27-C28-C29-C2A
94	N4	502	PC1	O21-C21-C22-C23
97	E7	301	CDL	C32-C31-CA7-OA8
97	EA	201	CDL	C52-C51-CB5-OB6
97	Qh	101	CDL	C52-C51-CB5-OB6
97	QC	403	CDL	C51-C52-C53-C54
97	4E	202	CDL	CA3-CA4-CA6-OA8
97	4E	202	CDL	CB3-CB4-CB6-OB8
97	Qd	302	CDL	C1-CA2-OA2-PA1
104	QJ	202	PX2	C1-C2-C3-O5
97	C4	201	CDL	C38-C39-C40-C41
97	B8	302	CDL	C32-C31-CA7-OA9
94	QC	404	PC1	O11-C1-C2-O21
94	N1	702	PC1	O21-C21-C22-C23
97	7C	201	CDL	C72-C71-CB7-OB8
97	AL	303	CDL	C12-C11-CA5-OA6
97	QC	403	CDL	C32-C31-CA7-OA8
95	C1	506	3PE	C27-C28-C29-C2A
106	QC	402	HEM	CAA-CBA-CGA-O1A
106	Qc	403	HEM	CAD-CBD-CGD-O2D
97	AL	303	CDL	C53-C54-C55-C56
106	QC	401	HEM	C4B-C3B-CAB-CBB
104	QJ	202	PX2	O7-C16-C17-C18
101	C1	501	HEA	CAD-CBD-CGD-O2D
106	QC	402	HEM	CAA-CBA-CGA-O2A
97	C4	203	CDL	C39-C40-C41-C42
97	QC	403	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
100	AC	201	ZMP	C16-C17-C18-C20
97	A9	504	CDL	OA5-CA3-CA4-CA6
97	A9	504	CDL	OB5-CB3-CB4-CB6
97	QJ	203	CDL	OA5-CA3-CA4-CA6
94	A9	503	PC1	O21-C21-C22-C23
94	ED	202	PC1	O21-C21-C22-C23
97	N1	701	CDL	C52-C51-CB5-OB6
94	G2	301	PC1	C24-C25-C26-C27
97	7C	201	CDL	OA6-CA4-CA6-OA8
97	E4	401	CDL	OB6-CB4-CB6-OB8
97	QC	403	CDL	OA6-CA4-CA6-OA8
97	QH	101	CDL	OA6-CA4-CA6-OA8
97	Qj	202	CDL	OB6-CB4-CB6-OB8
94	E8	302	PC1	C36-C37-C38-C39
94	E8	301	PC1	O21-C21-C22-C23
95	C1	507	3PE	O21-C21-C22-C23
97	B3	101	CDL	C72-C71-CB7-OB8
104	QJ	202	PX2	O5-C4-C5-C6
97	4E	202	CDL	C61-C62-C63-C64
101	C1	501	HEA	CAA-CBA-CGA-O2A
94	4E	201	PC1	O21-C21-C22-C23
94	A9	502	PC1	O31-C31-C32-C33
94	Qc	401	PC1	O31-C31-C32-C33
97	AM	201	CDL	C12-C11-CA5-OA6
97	QC	403	CDL	C72-C71-CB7-OB8
97	C4	201	CDL	CA4-CA6-OA8-CA7
94	4A	302	PC1	C36-C37-C38-C39
105	N4	504	U10	C18-C19-C21-C22
97	4E	202	CDL	C12-C11-CA5-OA6
97	Qj	202	CDL	C72-C71-CB7-OB8
97	7C	201	CDL	C17-C18-C19-C20
97	Qc	405	CDL	C52-C53-C54-C55
94	N1	703	PC1	C32-C33-C34-C35
94	AL	301	PC1	O31-C31-C32-C33
97	E6	401	CDL	C52-C51-CB5-OB6
94	N4	505	PC1	C33-C34-C35-C36
97	Qj	202	CDL	C11-C12-C13-C14
97	Qe	302	CDL	C52-C51-CB5-OB6
97	Qd	302	CDL	C71-C72-C73-C74
97	C4	202	CDL	C12-C11-CA5-OA7
94	E8	301	PC1	C29-C2A-C2B-C2C
95	C1	506	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
97	QD	302	CDL	C52-C51-CB5-OB6
94	C1	505	PC1	C33-C34-C35-C36
97	N5	603	CDL	C41-C42-C43-C44
97	E6	401	CDL	C12-C11-CA5-OA7
97	E6	401	CDL	C32-C31-CA7-OA9
97	E6	401	CDL	C52-C51-CB5-OB7
95	4D	202	3PE	C39-C3A-C3B-C3C
97	4E	202	CDL	C12-C11-CA5-OA7
94	N1	702	PC1	C2A-C2B-C2C-C2D
94	N5	601	PC1	O32-C31-C32-C33
97	E7	301	CDL	C12-C11-CA5-OA7
97	EA	201	CDL	C52-C51-CB5-OB7
97	Qd	302	CDL	C54-C55-C56-C57
94	A9	503	PC1	O22-C21-C22-C23
94	N1	702	PC1	O22-C21-C22-C23
104	C2	201	PX2	O6-C4-C5-C6
94	B5	202	PC1	C27-C28-C29-C2A
95	E9	201	3PE	C2B-C2C-C2D-C2E
105	N4	504	U10	C25-C24-C26-C27
97	N5	603	CDL	C12-C11-CA5-OA6
97	QJ	203	CDL	C72-C71-CB7-OB8
97	AL	302	CDL	CA4-CA3-OA5-PA1
94	N4	502	PC1	O32-C31-C32-C33
97	N1	701	CDL	C72-C71-CB7-OB9
97	Qj	202	CDL	C72-C71-CB7-OB9
94	4A	301	PC1	C1-O11-P-O12
94	7A	201	PC1	C1-O11-P-O14
94	AN	301	PC1	C11-O13-P-O12
94	QI	101	PC1	C1-O11-P-O14
95	B4	201	3PE	C11-O13-P-O12
95	C1	506	3PE	C1-O11-P-O14
96	4D	203	S12	CB-OG-P-O3
97	A3	201	CDL	CB2-OB2-PB2-OB3
97	A3	201	CDL	CB2-OB2-PB2-OB4
97	AL	302	CDL	CB3-OB5-PB2-OB3
97	AL	303	CDL	CA2-OA2-PA1-OA3
97	AM	202	CDL	CB3-OB5-PB2-OB3
97	B3	101	CDL	CA2-OA2-PA1-OA3
97	B3	101	CDL	CA3-OA5-PA1-OA3
97	B8	302	CDL	CB3-OB5-PB2-OB4
97	EA	202	CDL	CA3-OA5-PA1-OA3
97	N5	603	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
97	N5	603	CDL	CB3-OB5-PB2-OB4
97	QH	102	CDL	CB3-OB5-PB2-OB3
97	QJ	203	CDL	CB3-OB5-PB2-OB4
97	Qc	405	CDL	CA2-OA2-PA1-OA3
97	Qc	405	CDL	CB3-OB5-PB2-OB3
97	Qe	302	CDL	CA3-OA5-PA1-OA3
94	B5	202	PC1	C34-C35-C36-C37
95	N5	602	3PE	C29-C2A-C2B-C2C
97	EA	202	CDL	C73-C74-C75-C76
94	E8	301	PC1	O22-C21-C22-C23
94	ED	202	PC1	O22-C21-C22-C23
97	7C	201	CDL	C72-C71-CB7-OB9
97	N1	701	CDL	C52-C51-CB5-OB7
104	QJ	202	PX2	O8-C16-C17-C18
97	7C	201	CDL	C12-C11-CA5-OA6
94	A1	201	PC1	C24-C25-C26-C27
94	4A	302	PC1	O22-C21-C22-C23
94	N4	502	PC1	O22-C21-C22-C23
95	C1	507	3PE	O22-C21-C22-C23
97	B3	101	CDL	C72-C71-CB7-OB9
97	E7	301	CDL	C32-C31-CA7-OA9
100	AB	201	ZMP	C20-C18-C21-O5
97	N5	603	CDL	C31-C32-C33-C34
101	C1	502	HEA	O11-C11-C12-C13
97	AL	303	CDL	C12-C11-CA5-OA7
97	QC	403	CDL	C32-C31-CA7-OA9
94	AL	301	PC1	C2A-C2B-C2C-C2D
94	A1	202	PC1	O31-C31-C32-C33
94	B5	201	PC1	C3B-C3C-C3D-C3E
94	4A	302	PC1	C12-C11-O13-P
94	4E	201	PC1	C12-C11-O13-P
94	7A	201	PC1	C12-C11-O13-P
94	A1	201	PC1	C3-C2-O21-C21
94	AL	301	PC1	C3-C2-O21-C21
94	Qc	401	PC1	C1-C2-O21-C21
94	Qc	404	PC1	C3-C2-O21-C21
95	4D	201	3PE	C12-C11-O13-P
97	7C	201	CDL	CA6-CA4-OA6-CA5
97	AM	202	CDL	CA3-CA4-OA6-CA5
97	QC	403	CDL	CB6-CB4-OB6-CB5
97	QJ	203	CDL	CB6-CB4-OB6-CB5
97	Qh	101	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
97	Qj	202	CDL	CB6-CB4-OB6-CB5
100	AC	201	ZMP	O3-C16-C17-C18
101	C1	501	HEA	C3B-C11-C12-C13
94	A9	502	PC1	O32-C31-C32-C33
94	Qc	401	PC1	O32-C31-C32-C33
97	QC	403	CDL	C72-C71-CB7-OB9
97	C4	203	CDL	C52-C51-CB5-OB6
97	QH	101	CDL	C12-C11-CA5-OA6
97	C4	201	CDL	C39-C40-C41-C42
94	B5	201	PC1	C3C-C3D-C3E-C3F
94	N1	703	PC1	C33-C34-C35-C36
94	N4	501	PC1	O31-C31-C32-C33
97	Qh	101	CDL	C12-C11-CA5-OA6
97	C4	201	CDL	C43-C44-C45-C46
94	ED	201	PC1	C32-C33-C34-C35
97	Qh	101	CDL	C54-C55-C56-C57
97	AM	201	CDL	C12-C11-CA5-OA7
94	4A	302	PC1	C23-C24-C25-C26
94	G2	301	PC1	O31-C31-C32-C33
94	N4	501	PC1	O21-C21-C22-C23
94	QD	303	PC1	O31-C31-C32-C33
97	BM	201	CDL	C52-C51-CB5-OB6
97	EA	202	CDL	C52-C51-CB5-OB6
97	N5	603	CDL	C52-C51-CB5-OB6
97	QH	102	CDL	C52-C51-CB5-OB6
97	N5	603	CDL	CB2-C1-CA2-OA2
97	QJ	203	CDL	CB2-C1-CA2-OA2
94	N4	501	PC1	C33-C34-C35-C36
97	AM	202	CDL	C22-C23-C24-C25
97	C4	203	CDL	C16-C17-C18-C19
97	N1	701	CDL	C72-C73-C74-C75
94	AL	301	PC1	O32-C31-C32-C33
104	QJ	202	PX2	O6-C4-C5-C6
97	A9	504	CDL	C13-C14-C15-C16
96	4D	203	S12	OXT-C-CA-N
95	C1	507	3PE	O11-C1-C2-O21
94	4E	201	PC1	O22-C21-C22-C23
94	C3	201	PC1	O22-C21-C22-C23
97	BM	201	CDL	C52-C51-CB5-OB7
97	N5	603	CDL	C12-C11-CA5-OA7
97	QD	302	CDL	C52-C51-CB5-OB7
97	QH	101	CDL	C12-C11-CA5-OA7

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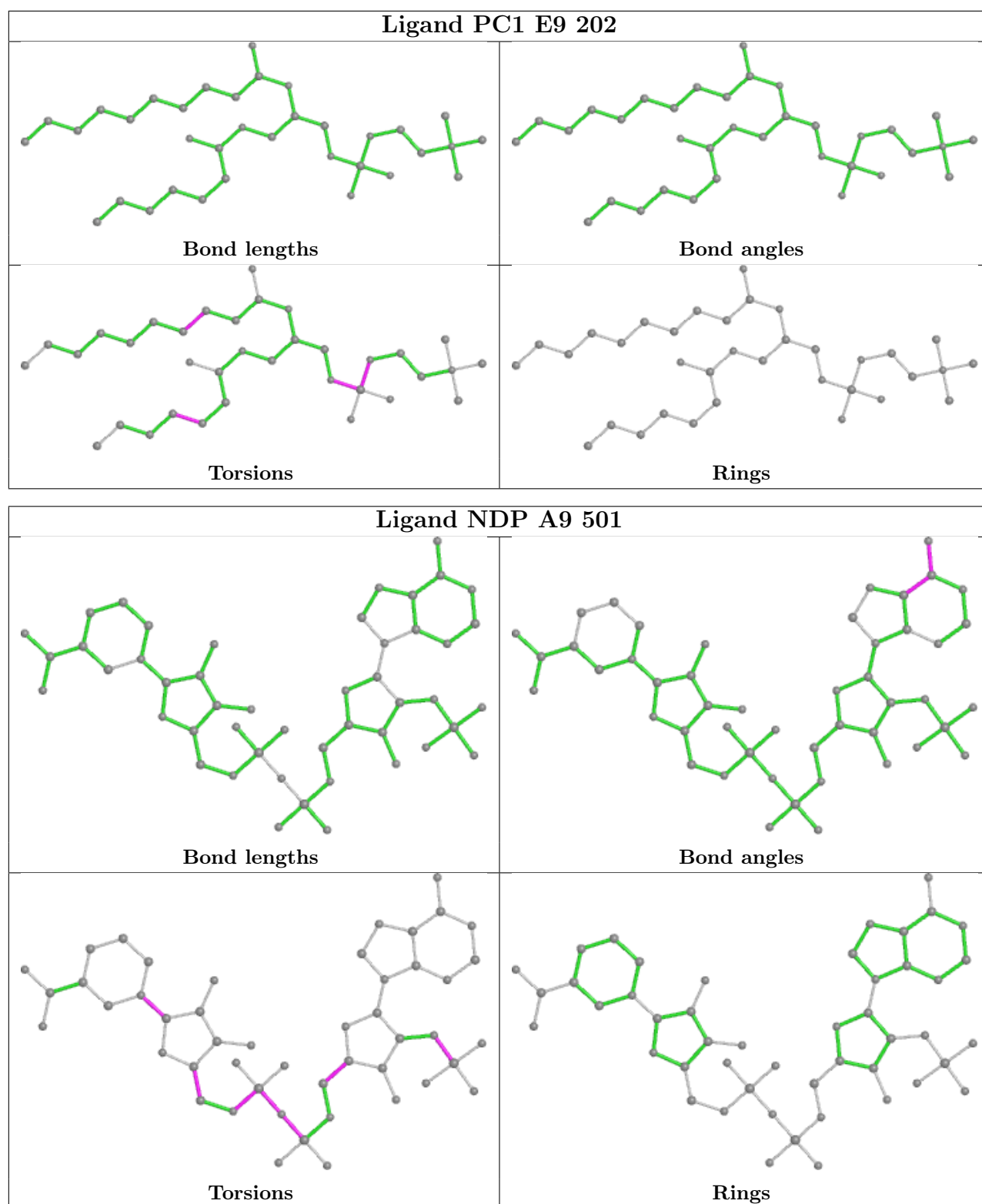
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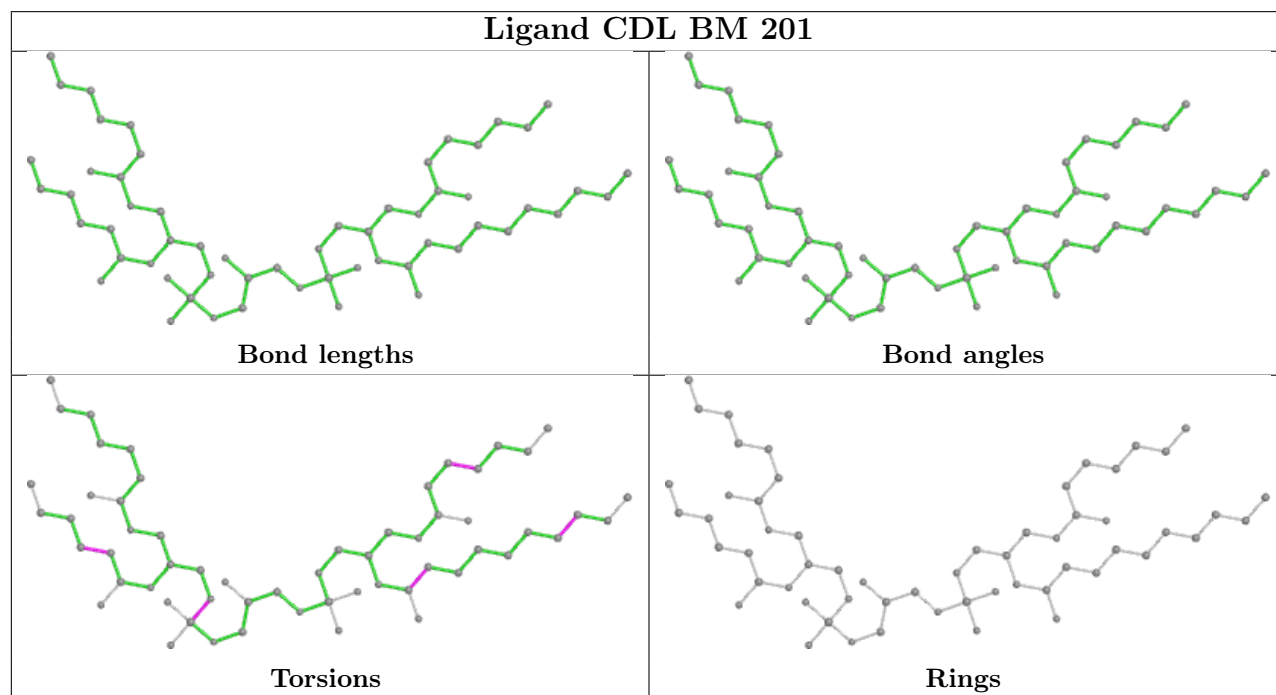
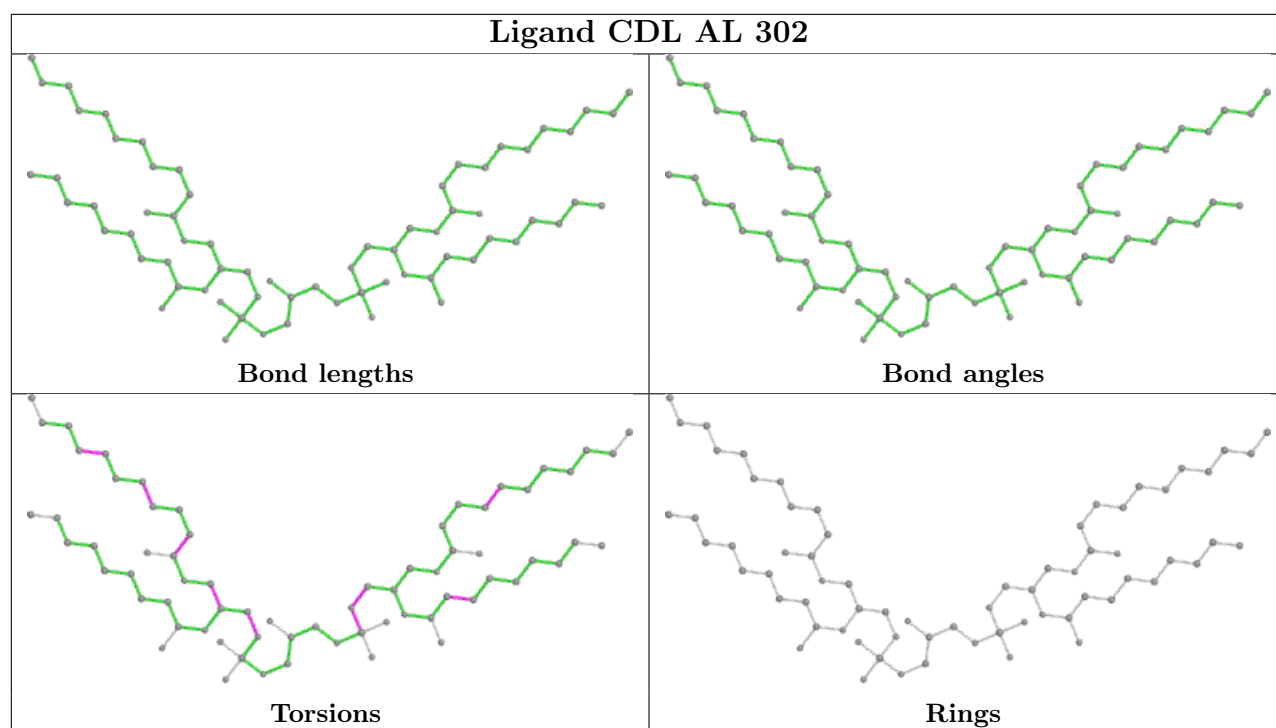
Mol	Chain	Res	Type	Atoms
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95	B4	201	3PE	O31-C31-C32-C33
97	C4	203	CDL	C15-C16-C17-C18
94	AN	301	PC1	C3A-C3B-C3C-C3D
97	AL	303	CDL	C32-C31-CA7-OA8
94	AM	203	PC1	C31-C32-C33-C34
94	QD	303	PC1	O32-C31-C32-C33
97	C4	203	CDL	C52-C51-CB5-OB7
97	QH	102	CDL	C52-C51-CB5-OB7
97	AM	201	CDL	C13-C14-C15-C16
94	C3	201	PC1	O21-C21-C22-C23
97	A9	504	CDL	C52-C51-CB5-OB6
97	A9	504	CDL	C52-C51-CB5-OB7
97	QJ	203	CDL	C72-C71-CB7-OB9
97	Qe	302	CDL	C52-C51-CB5-OB7
97	C4	203	CDL	C22-C23-C24-C25
97	Qd	302	CDL	C81-C82-C83-C84
94	AM	203	PC1	C3D-C3E-C3F-C3G
101	C1	502	HEA	CAA-CBA-CGA-O2A
97	Qh	101	CDL	C12-C11-CA5-OA7
97	E6	401	CDL	C71-C72-C73-C74
94	E8	303	PC1	O31-C31-C32-C33
97	EA	202	CDL	C12-C11-CA5-OA6

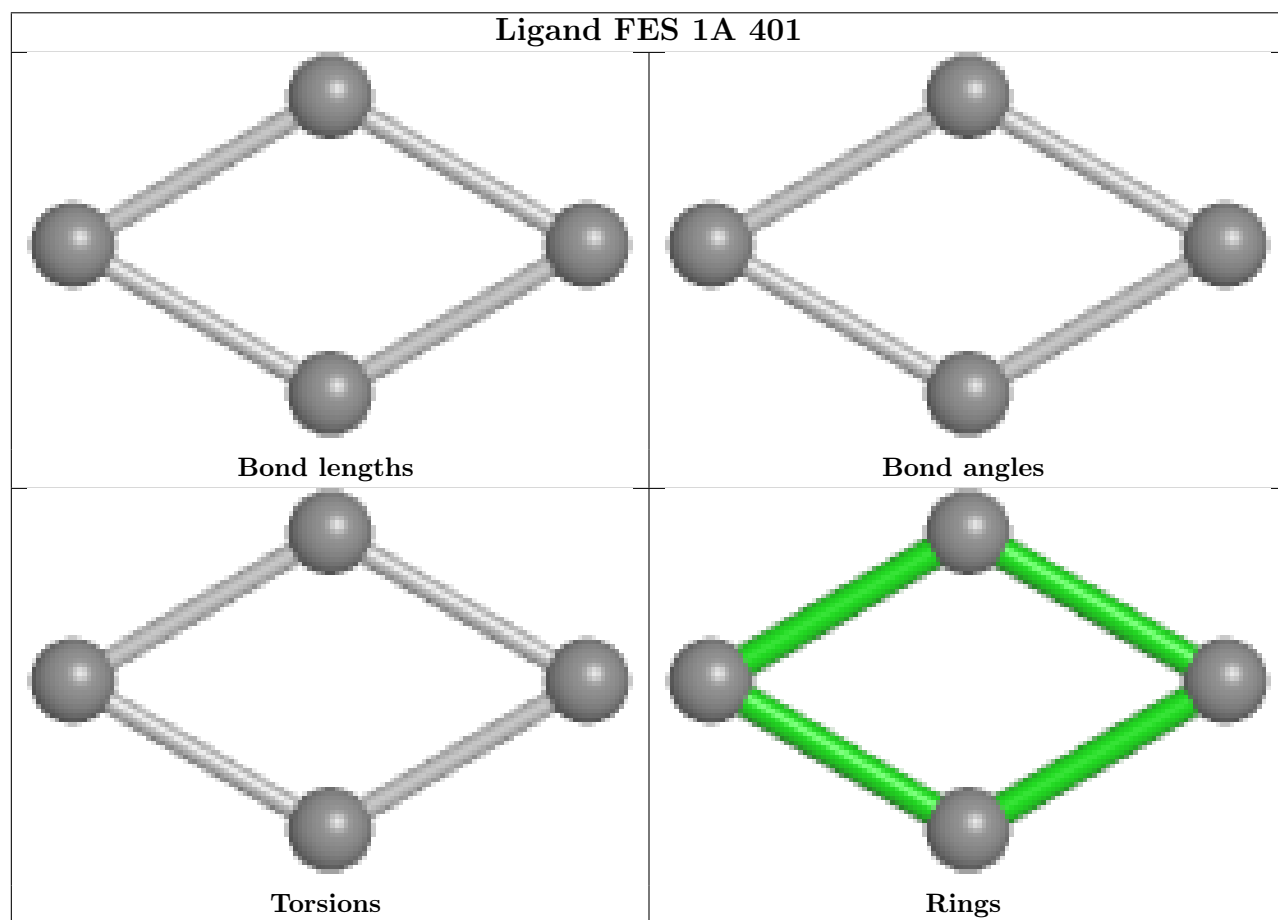
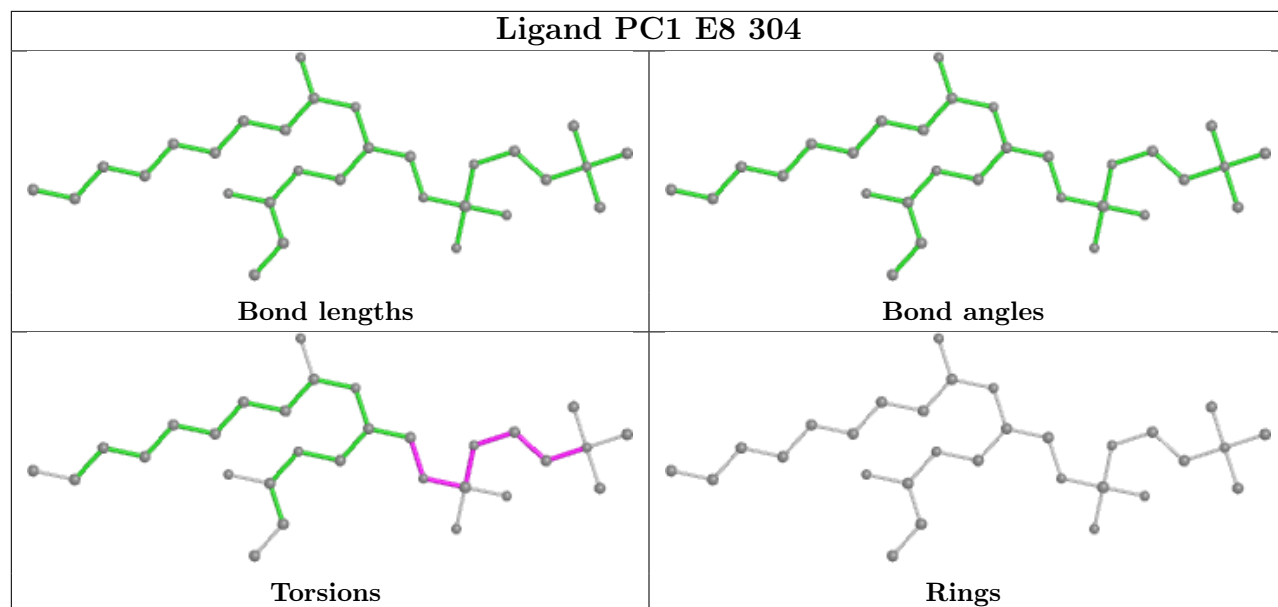
There are no ring outliers.

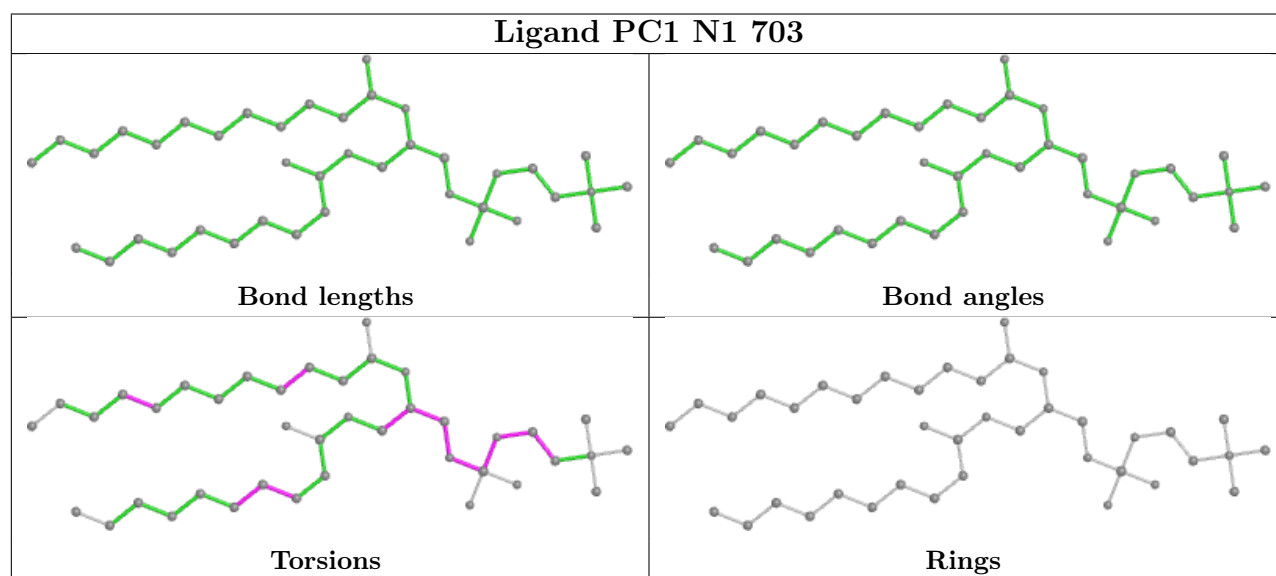
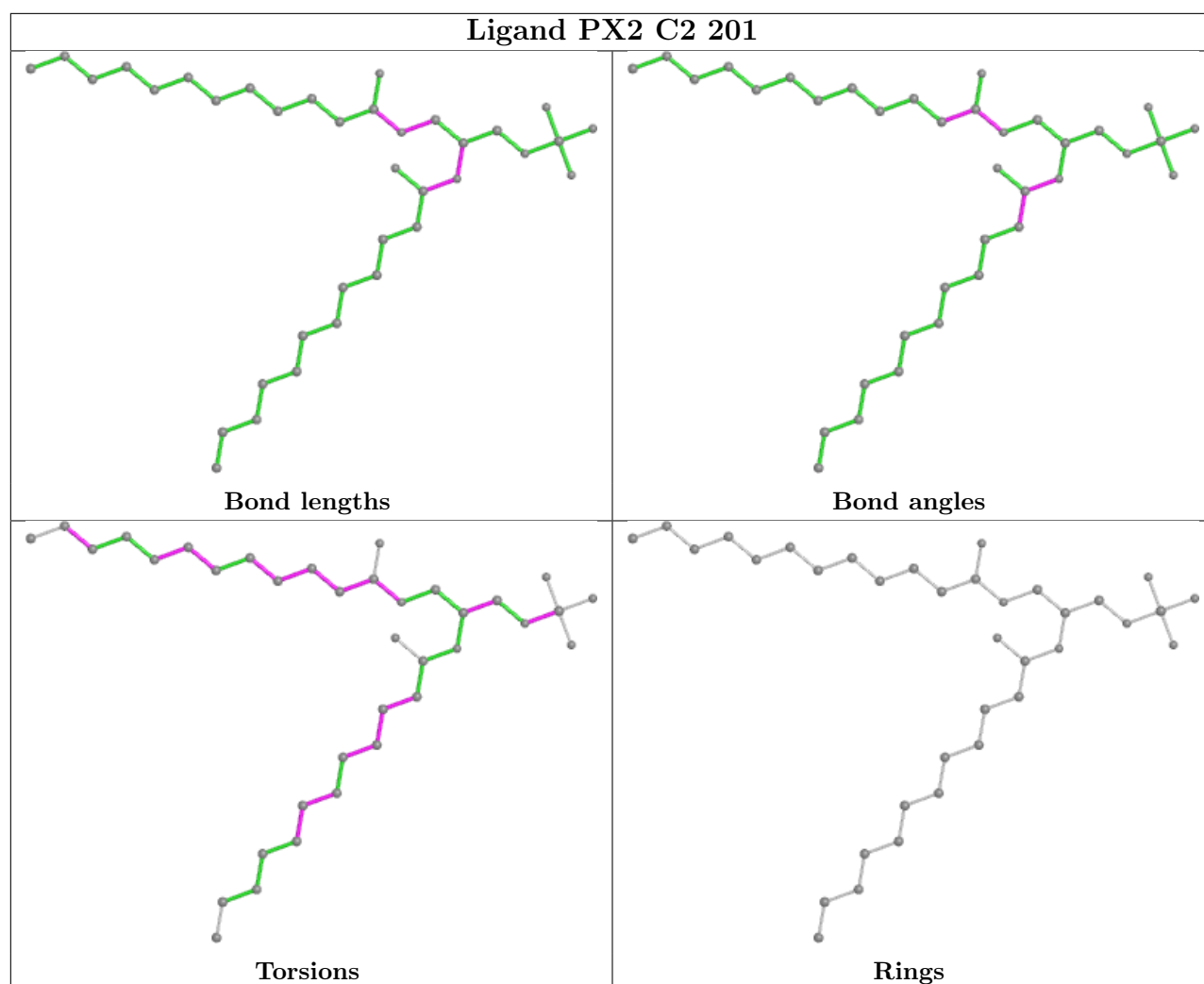
No monomer is involved in short contacts.

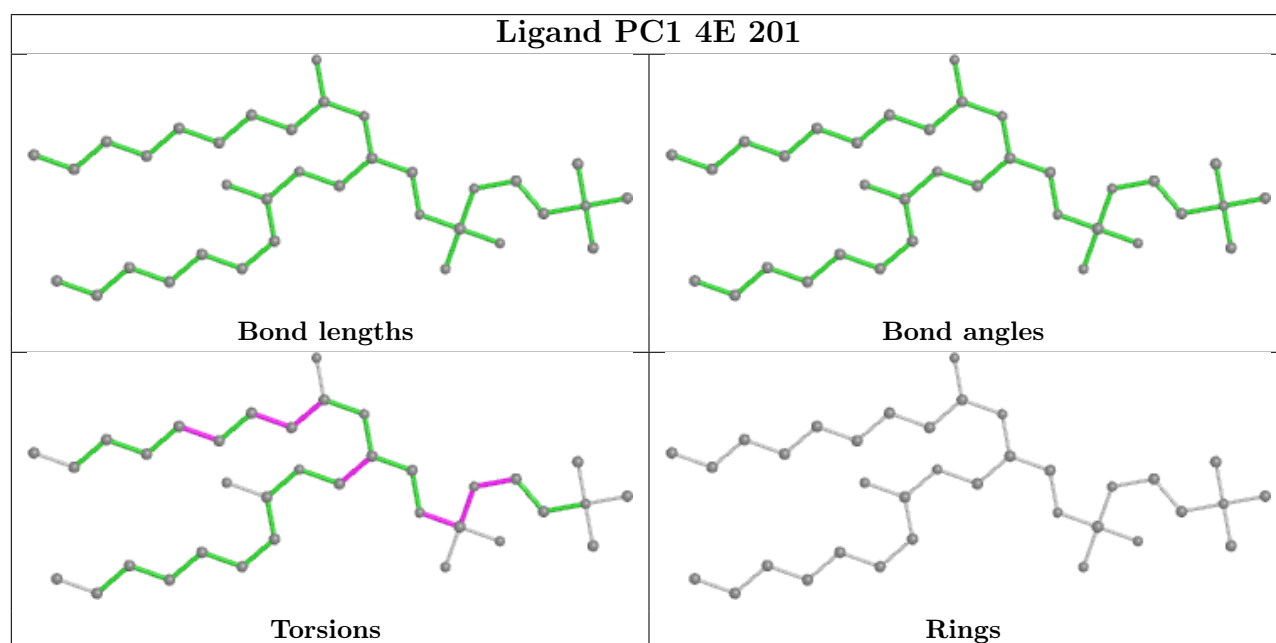
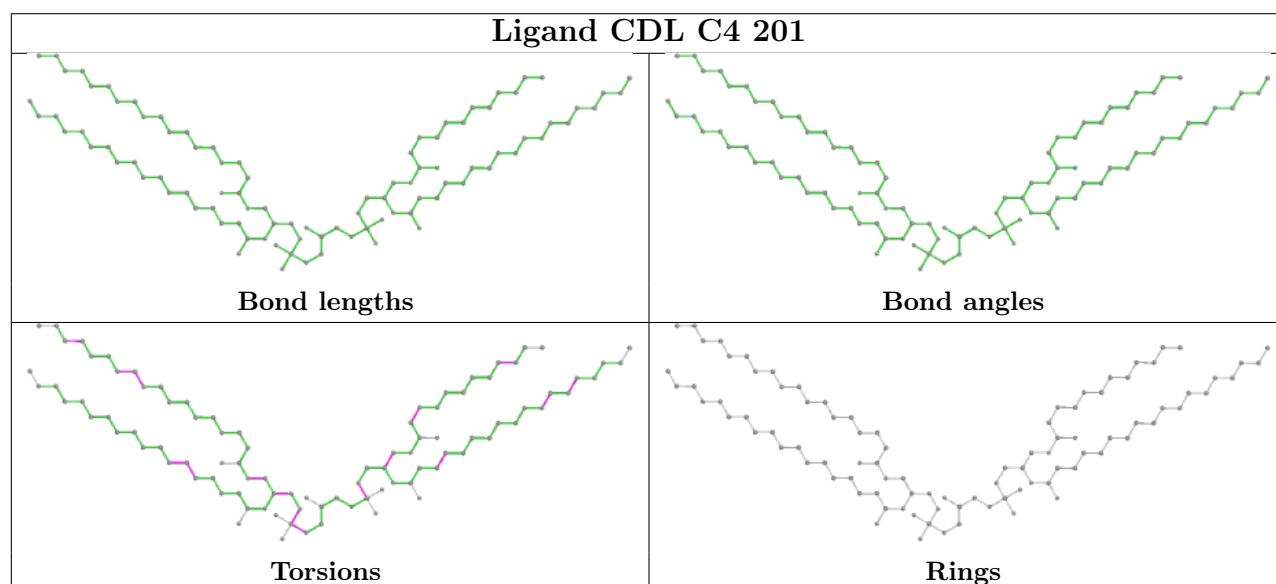
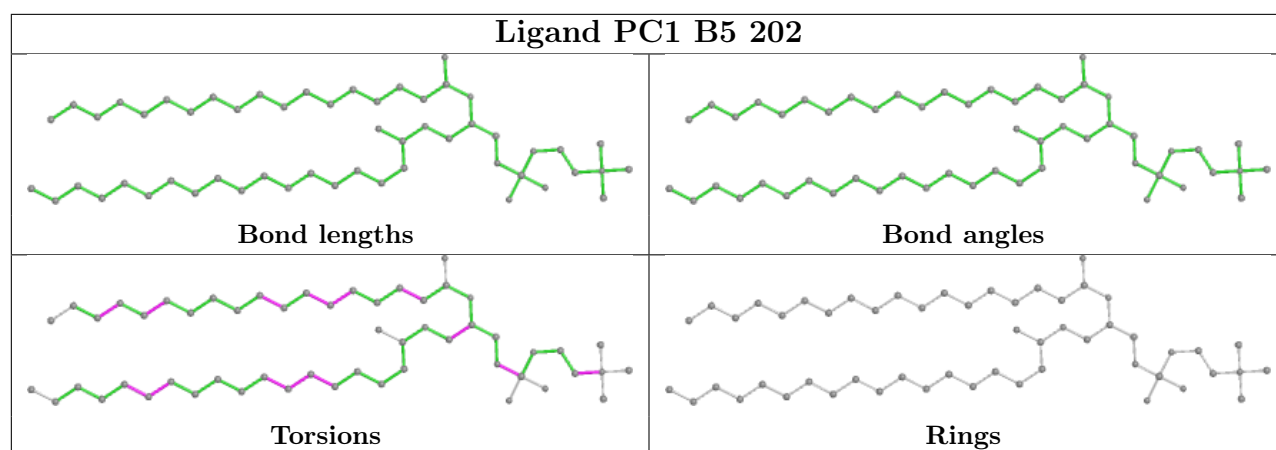
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

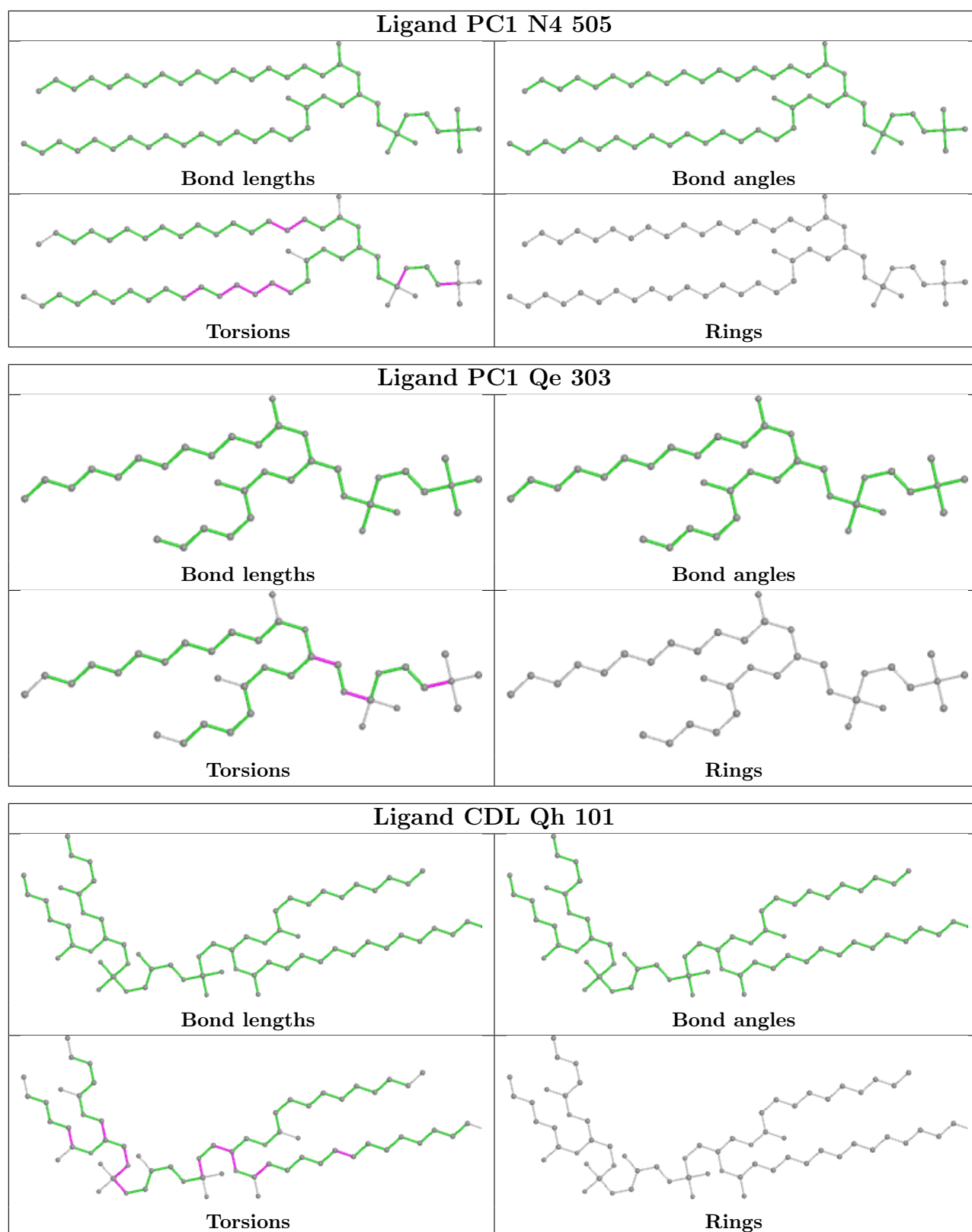


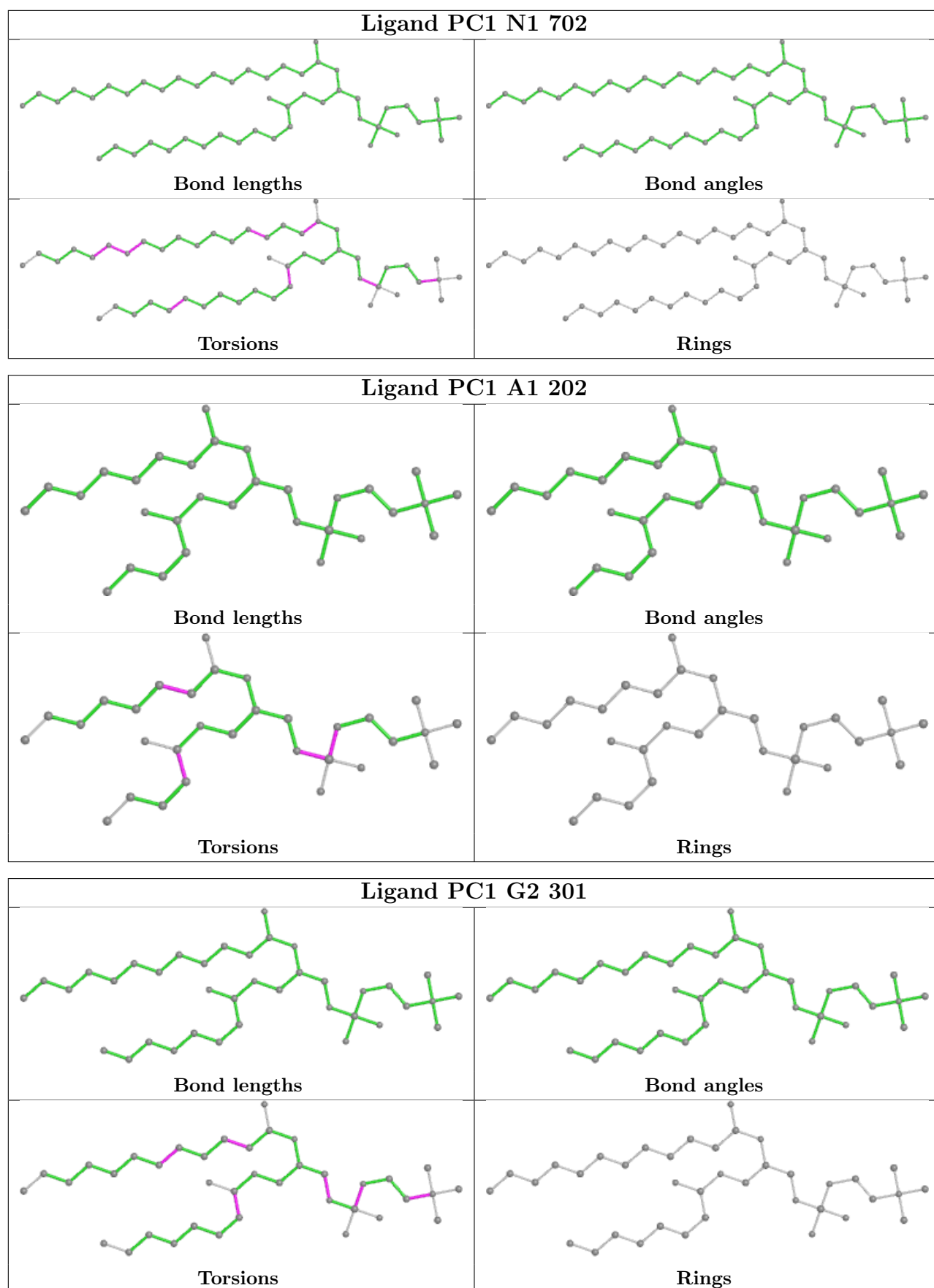


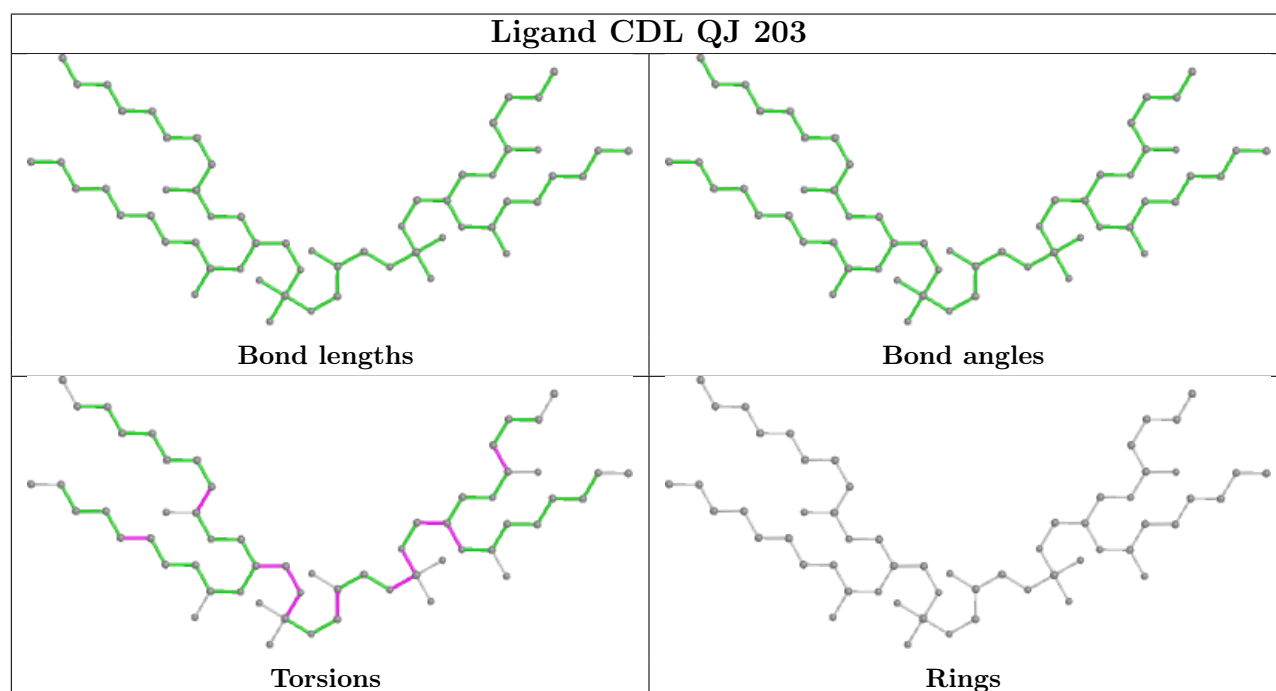
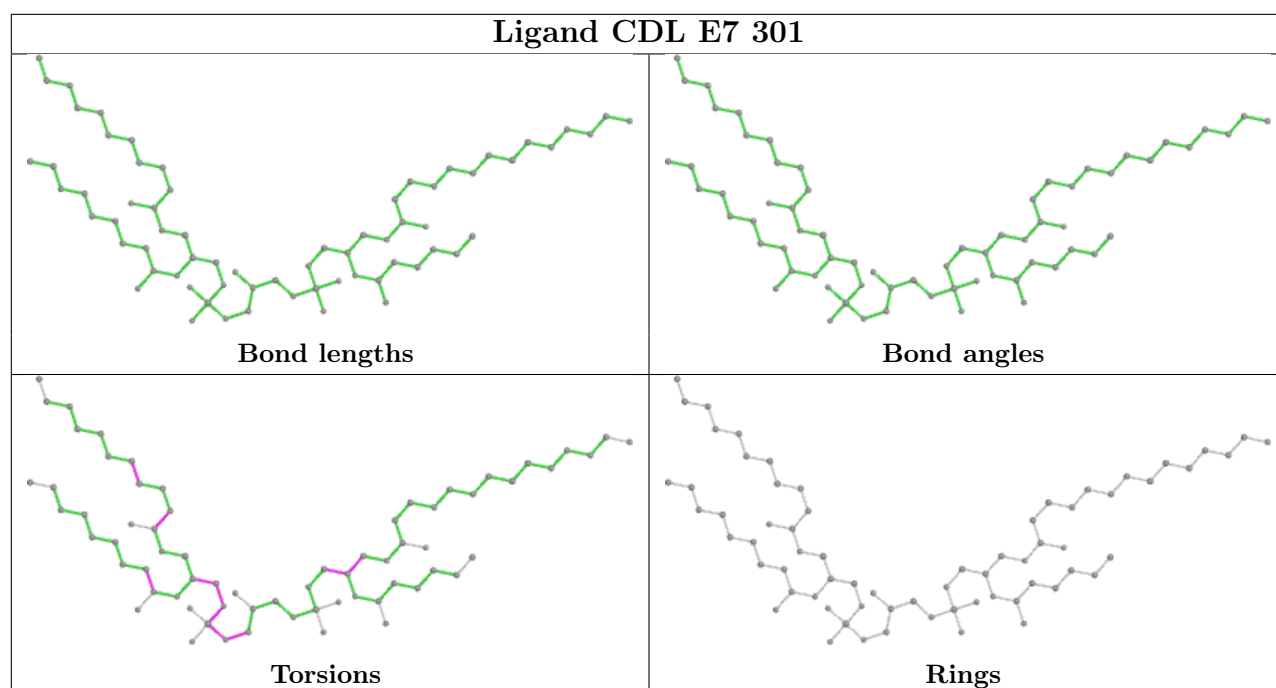


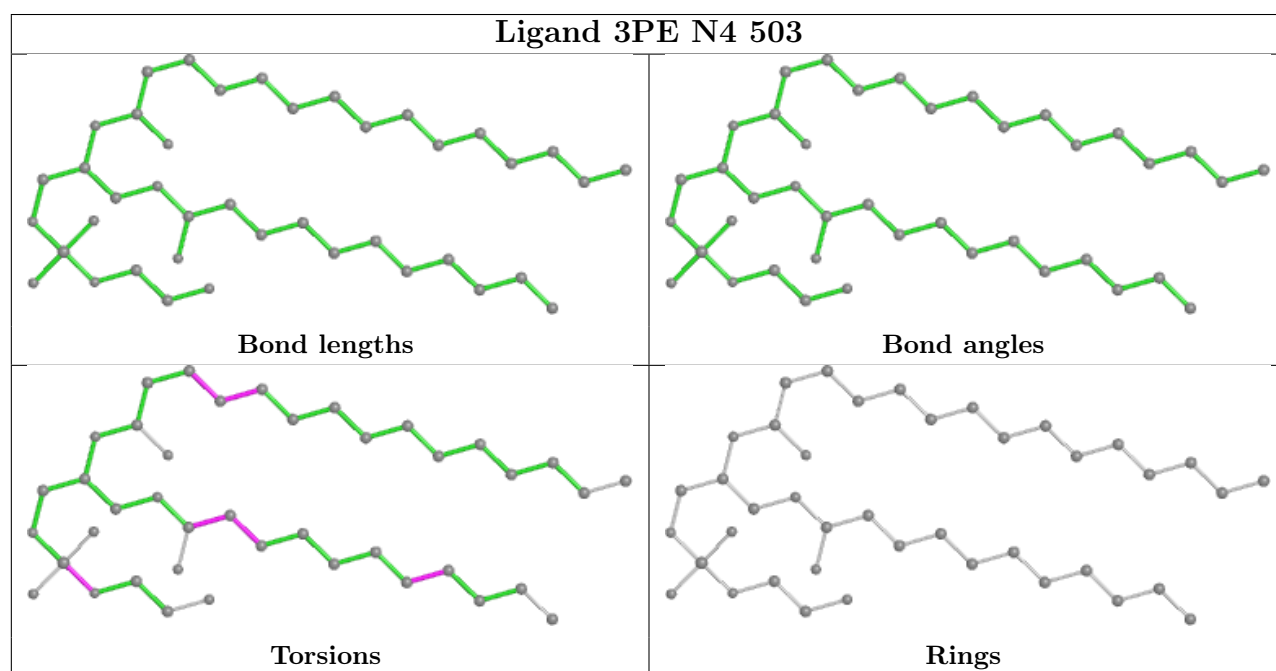
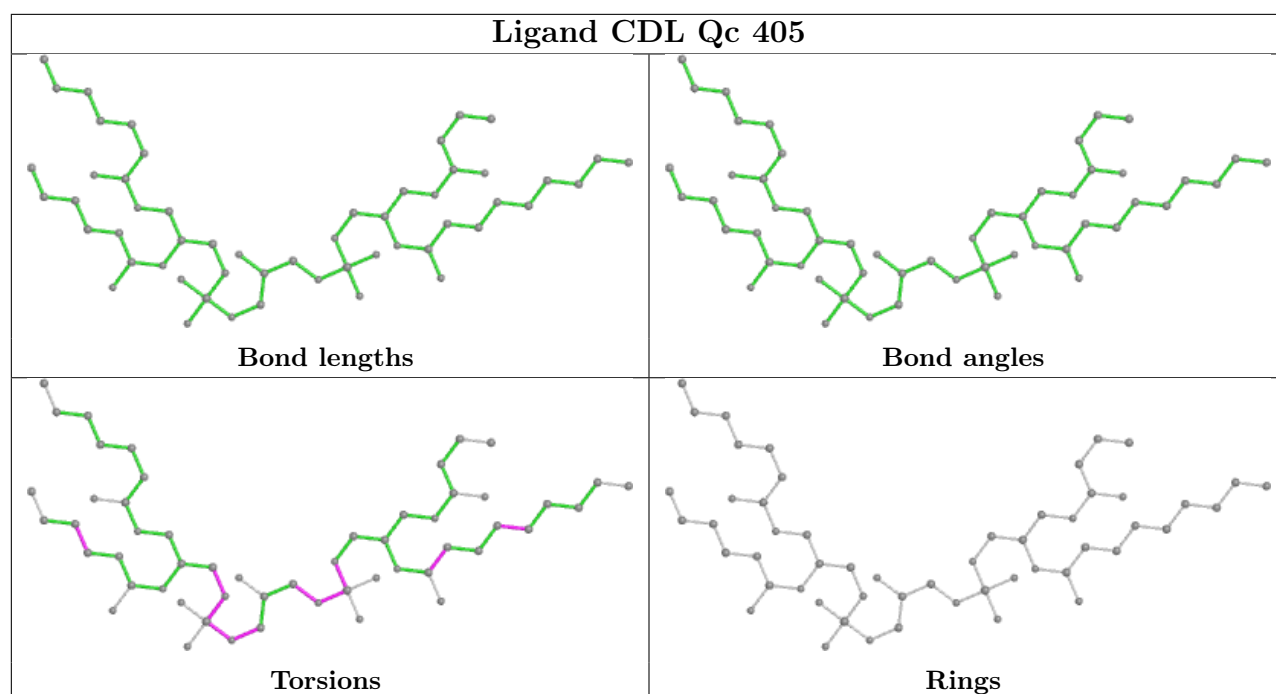


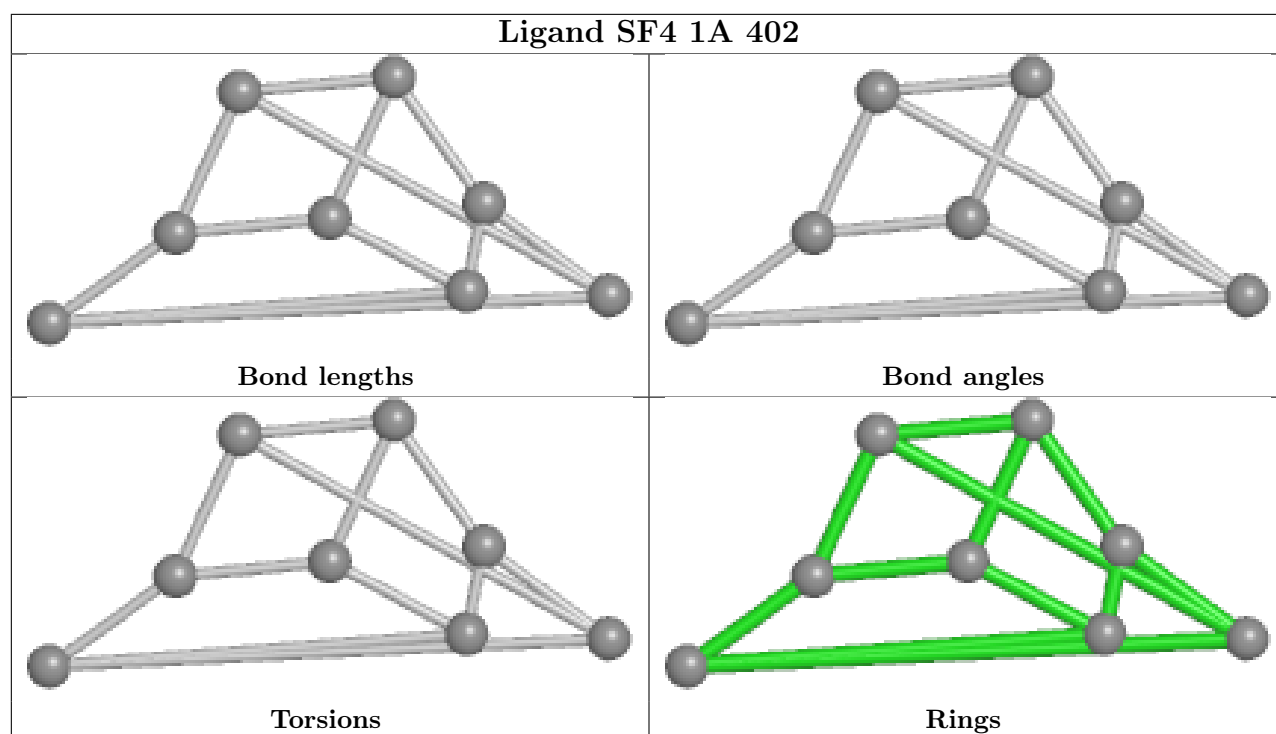


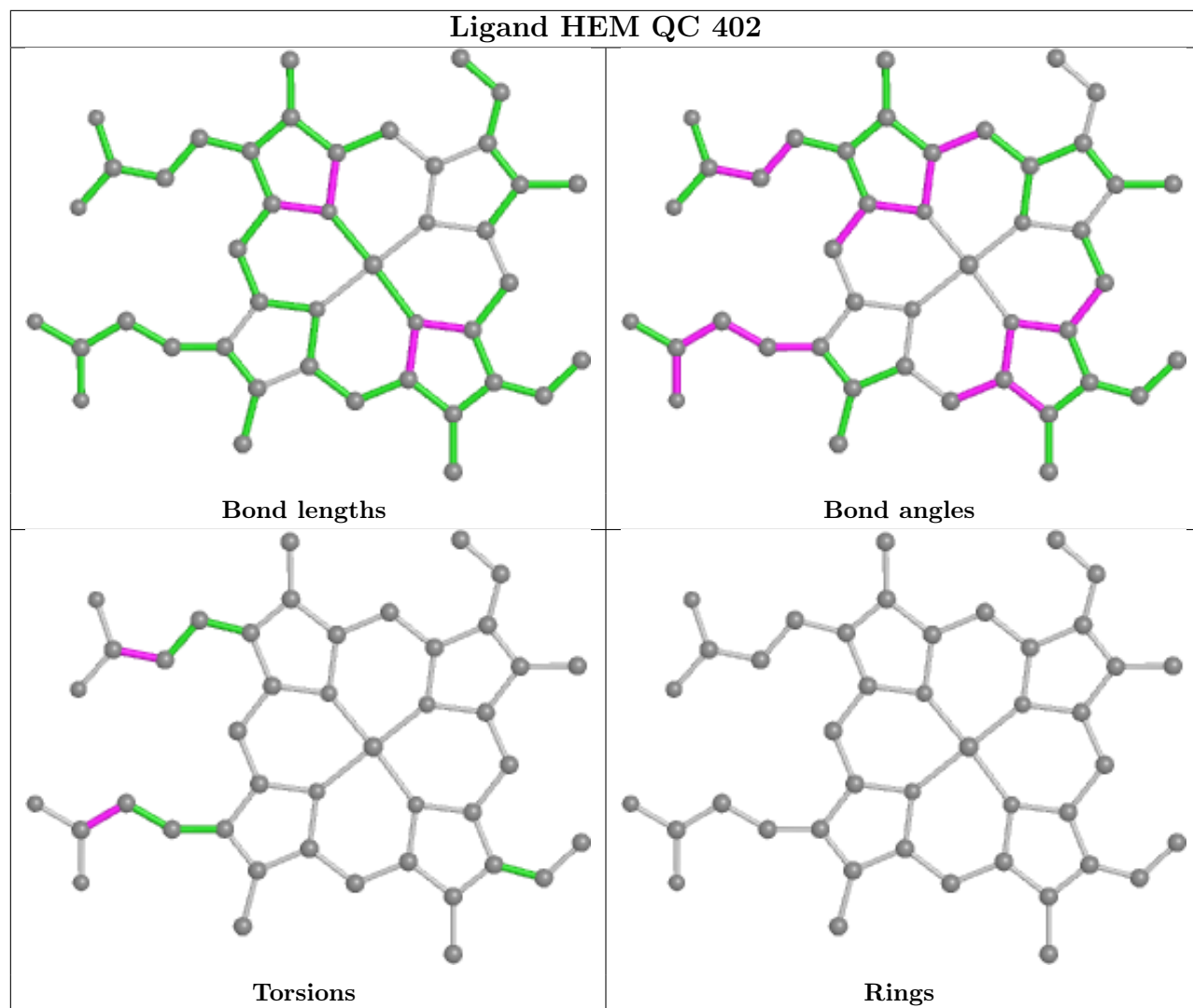


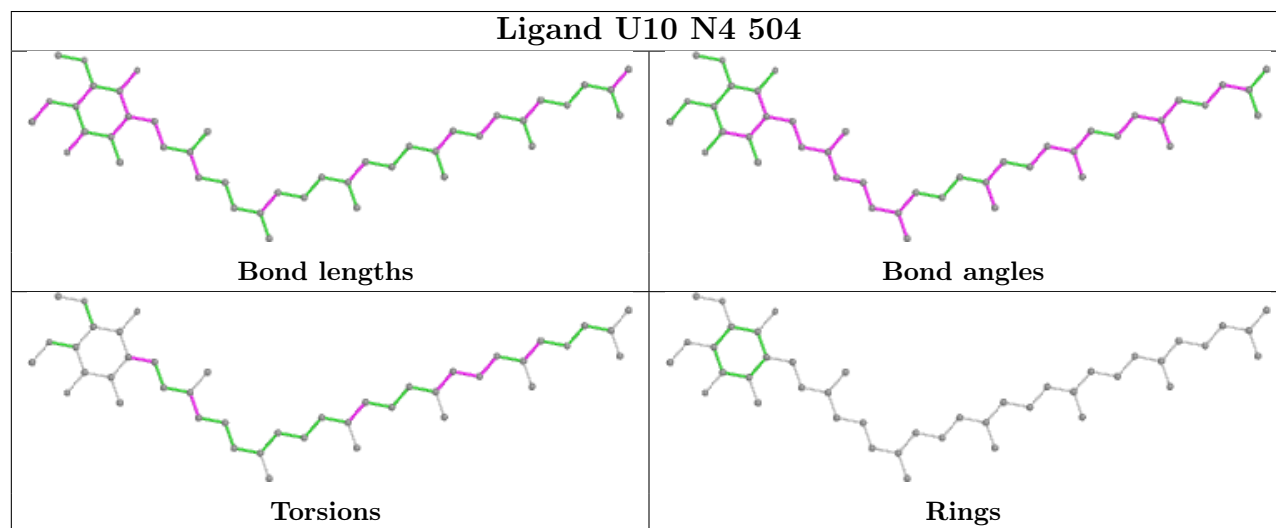
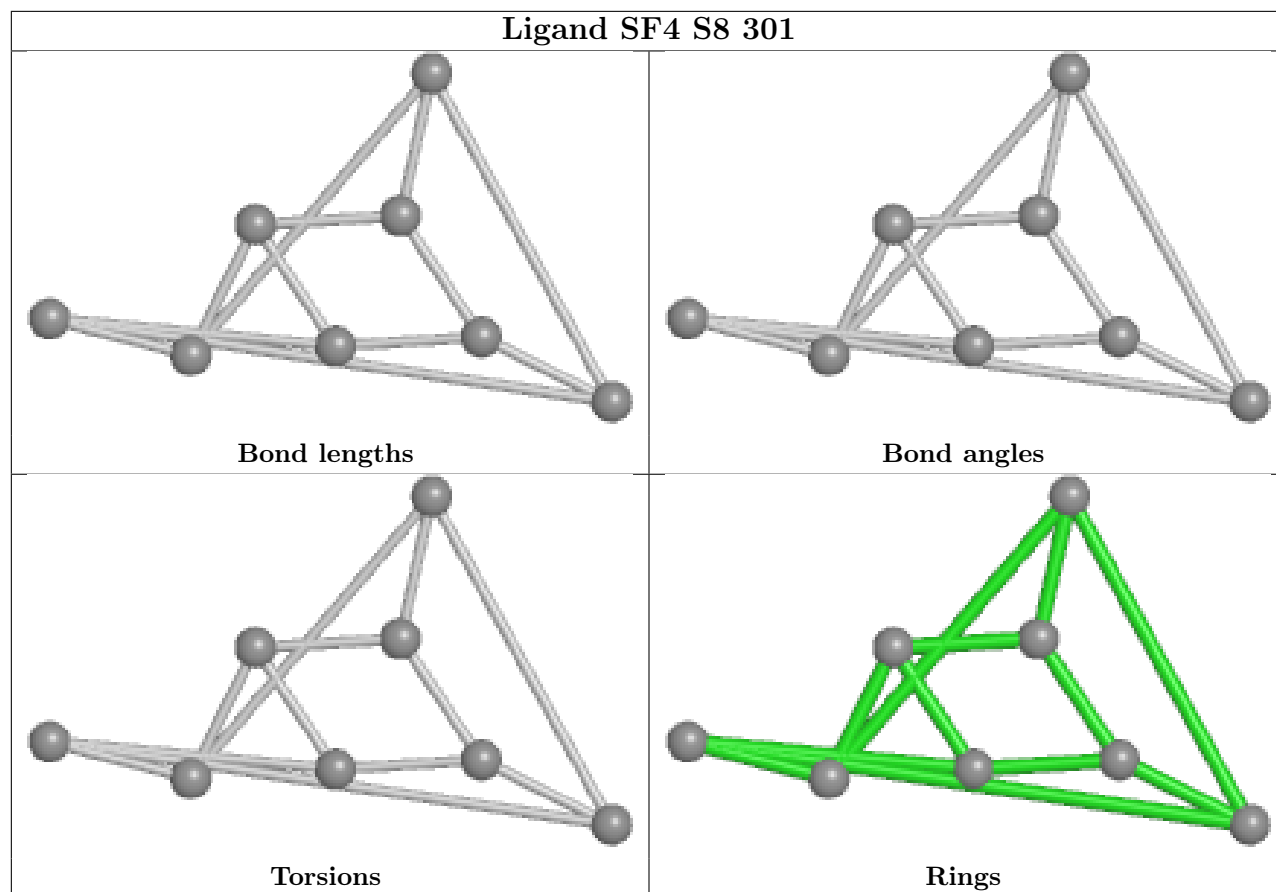


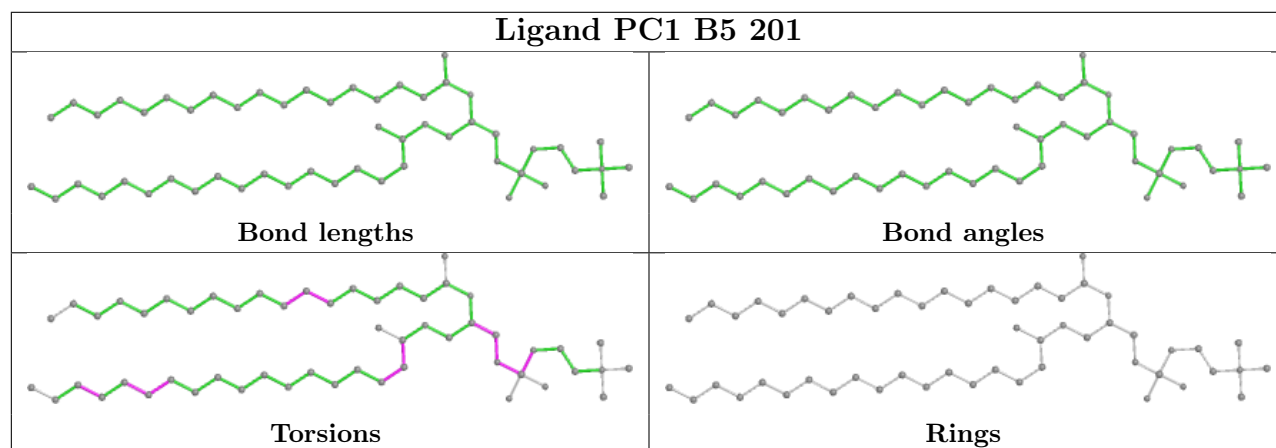
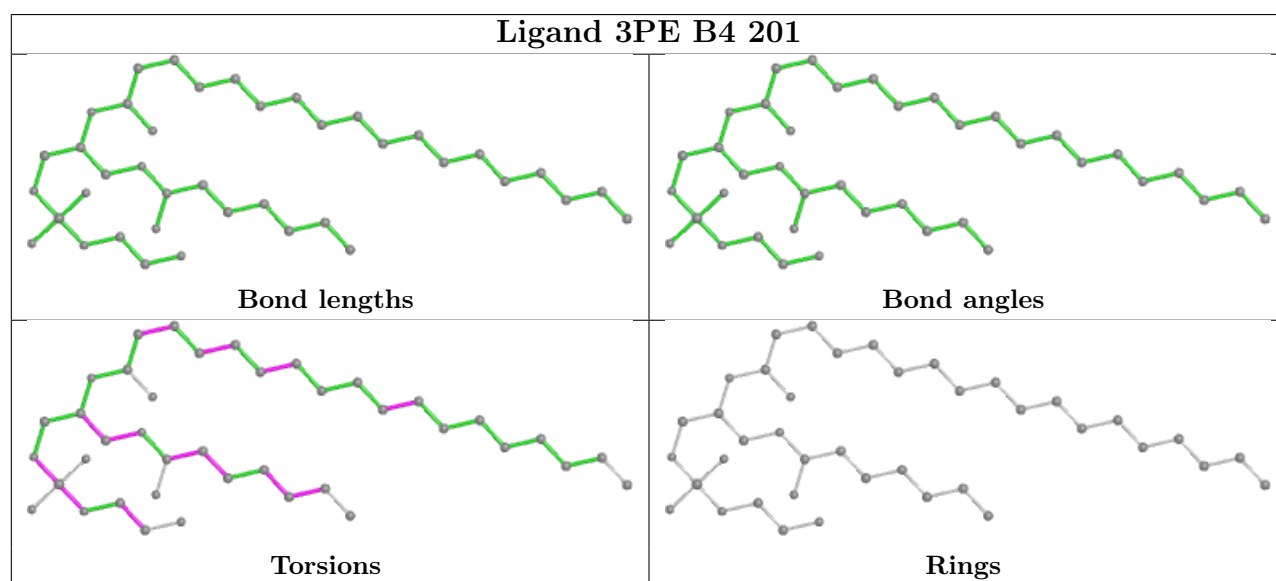
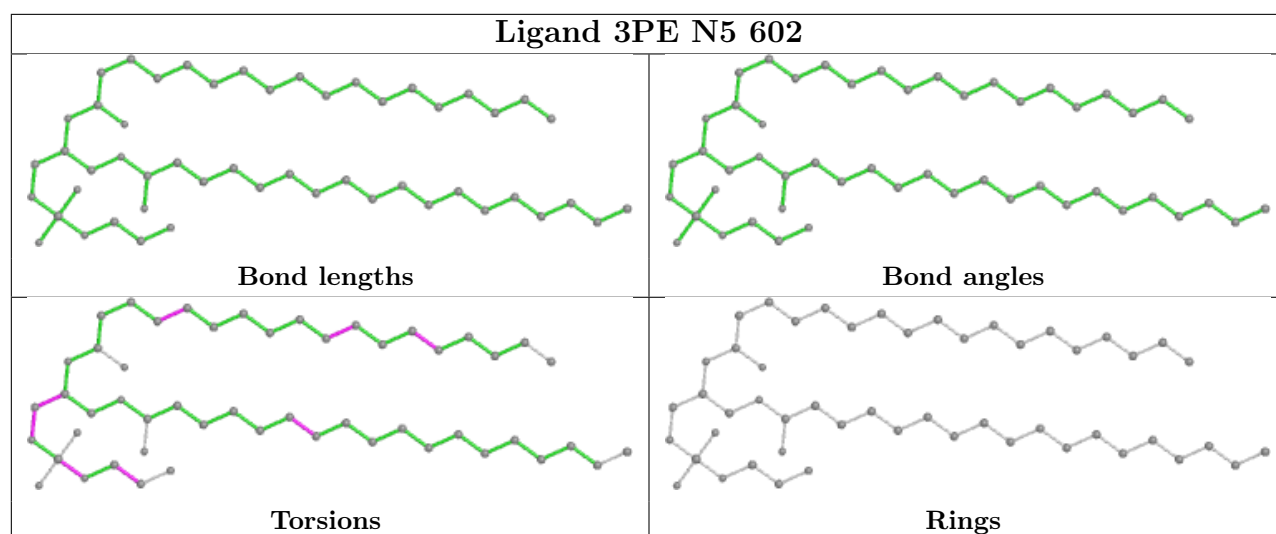


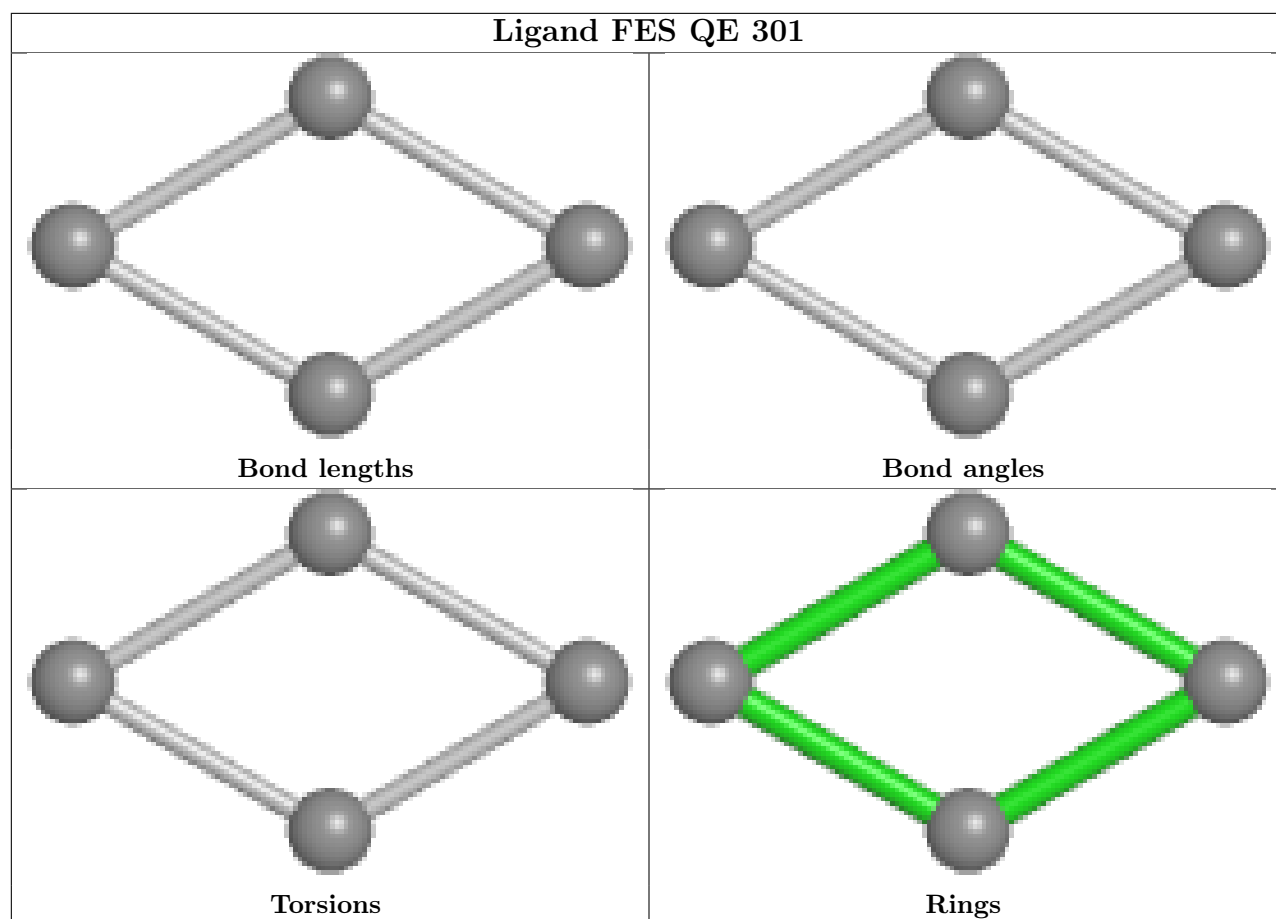
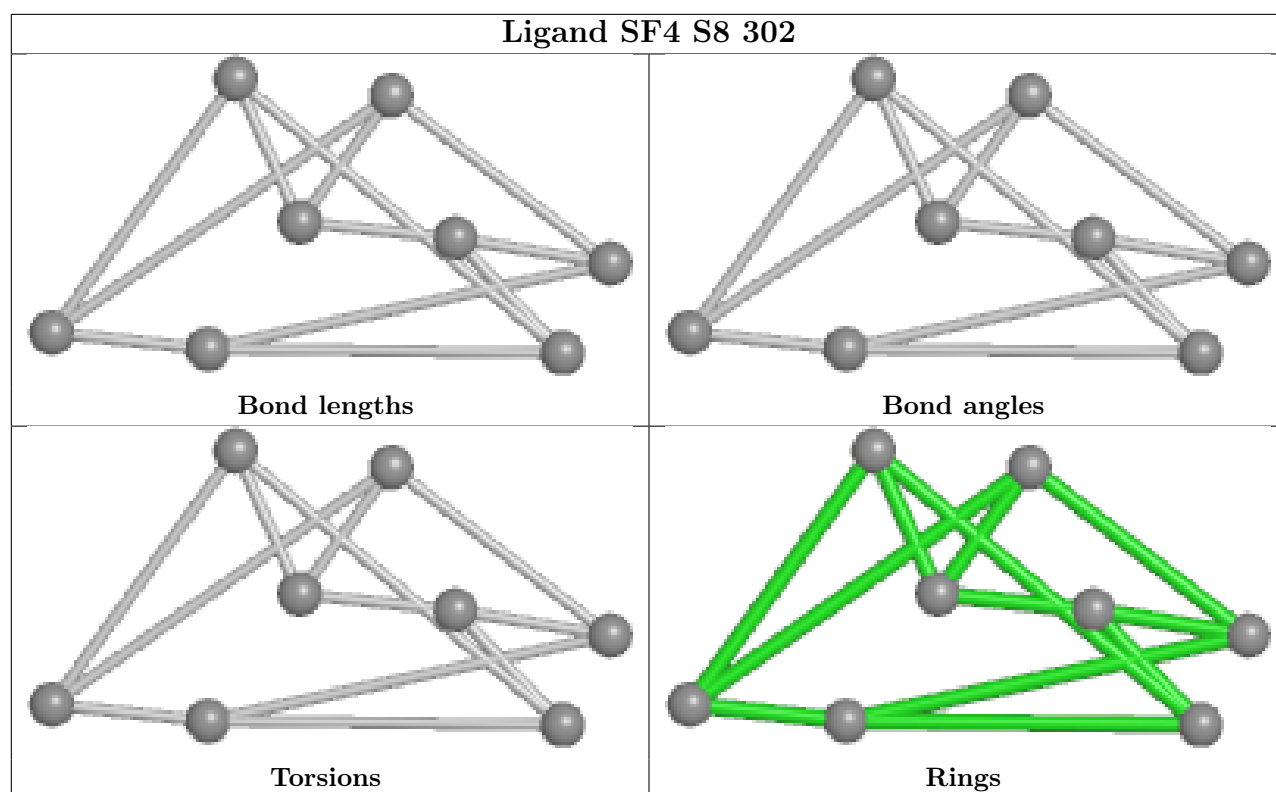


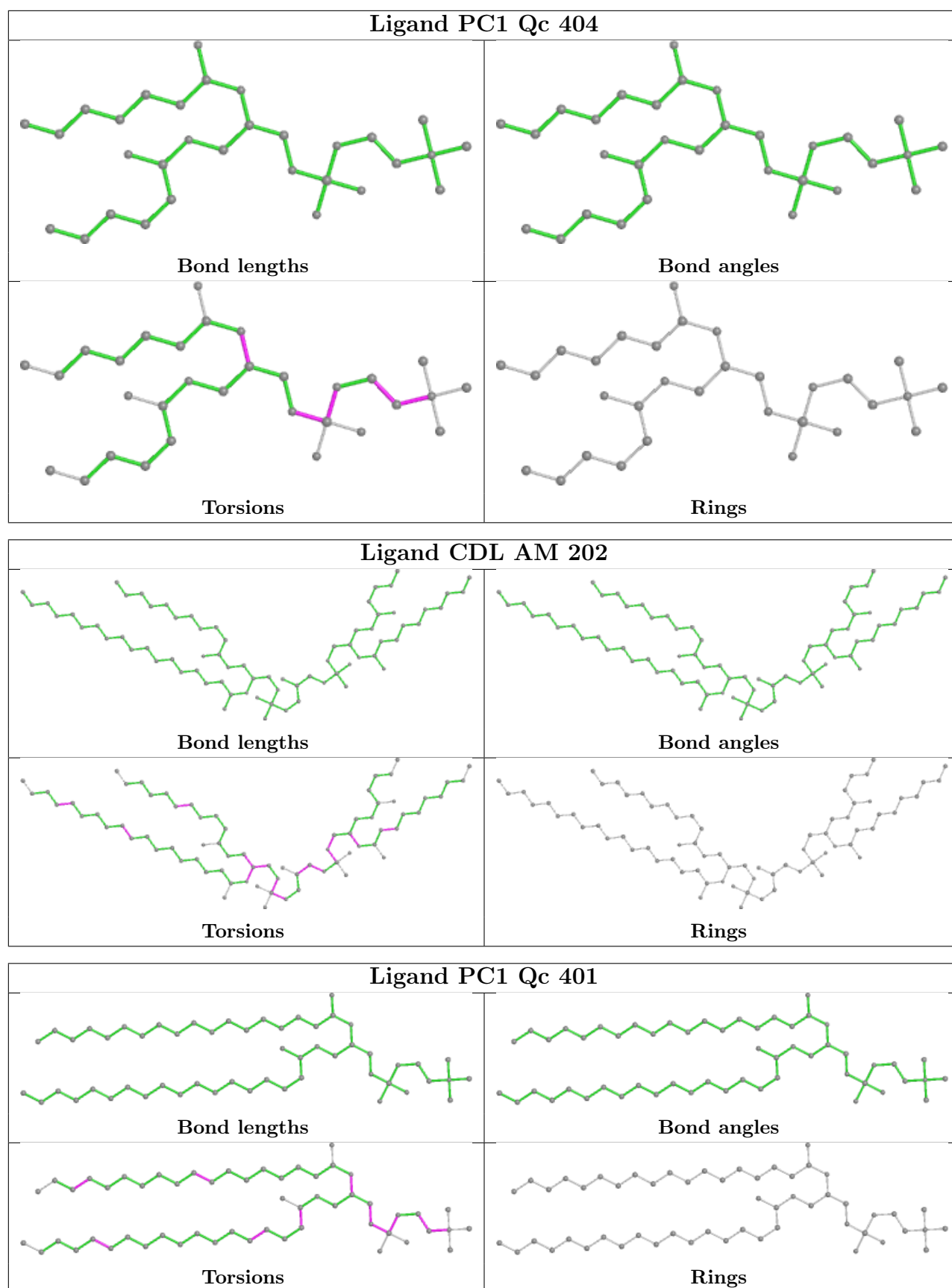


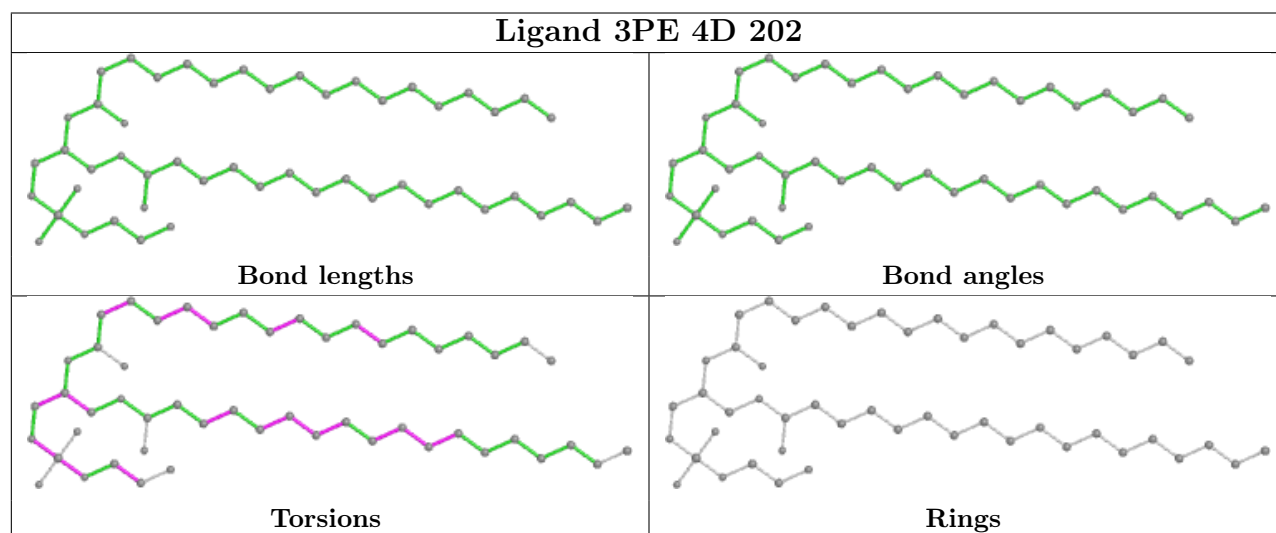
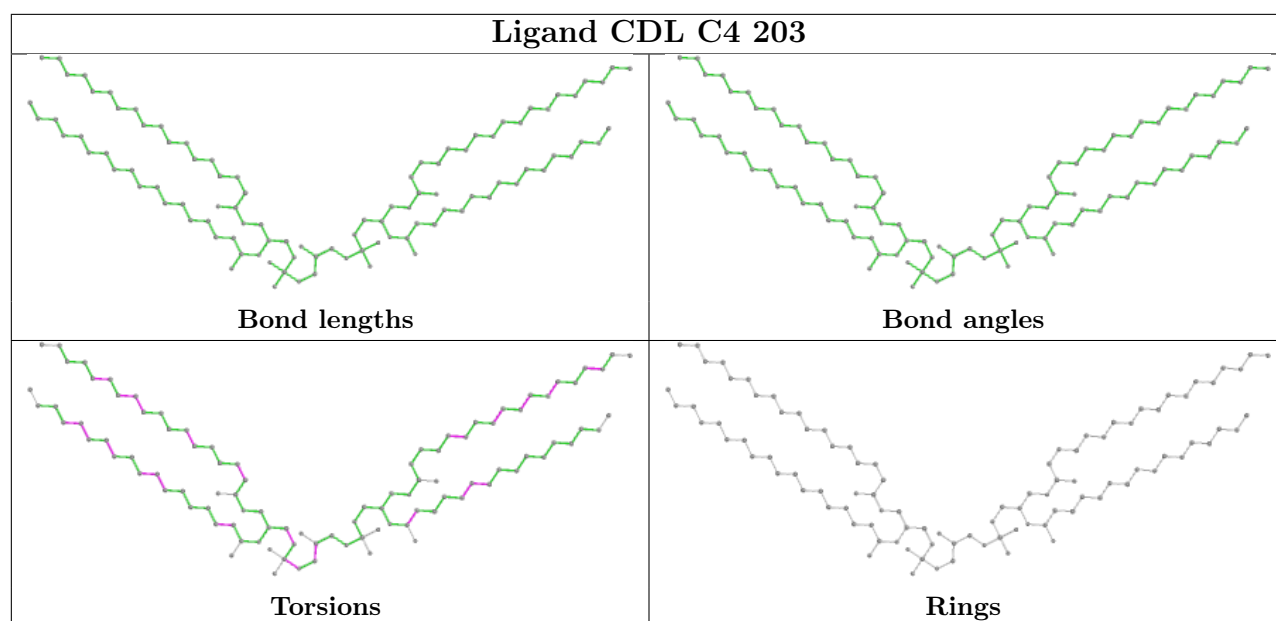


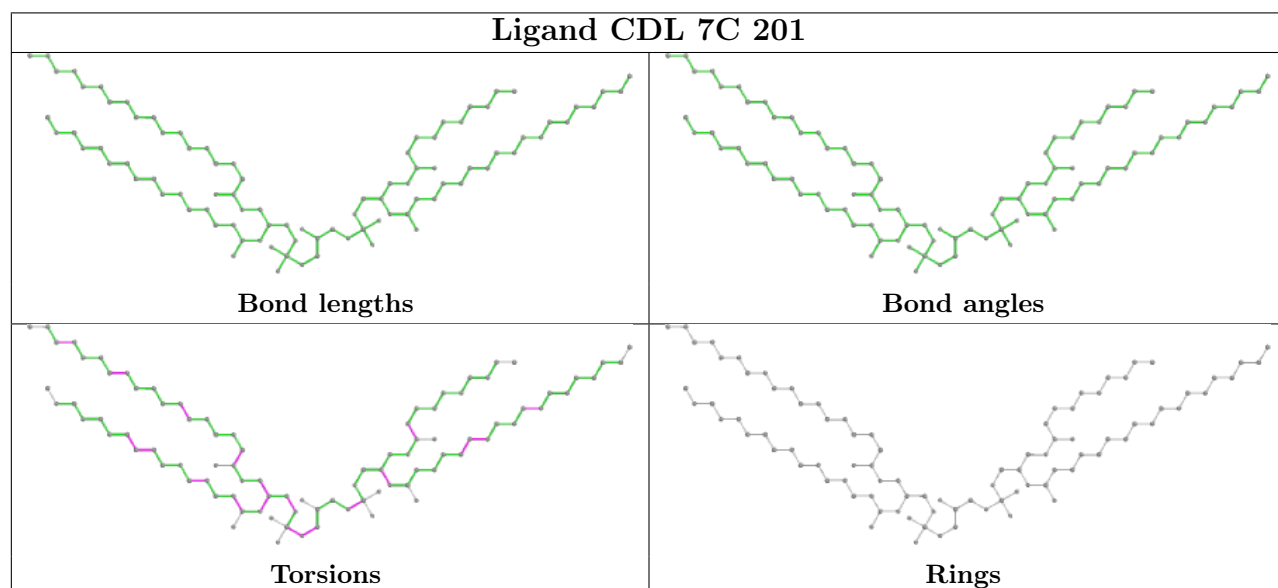
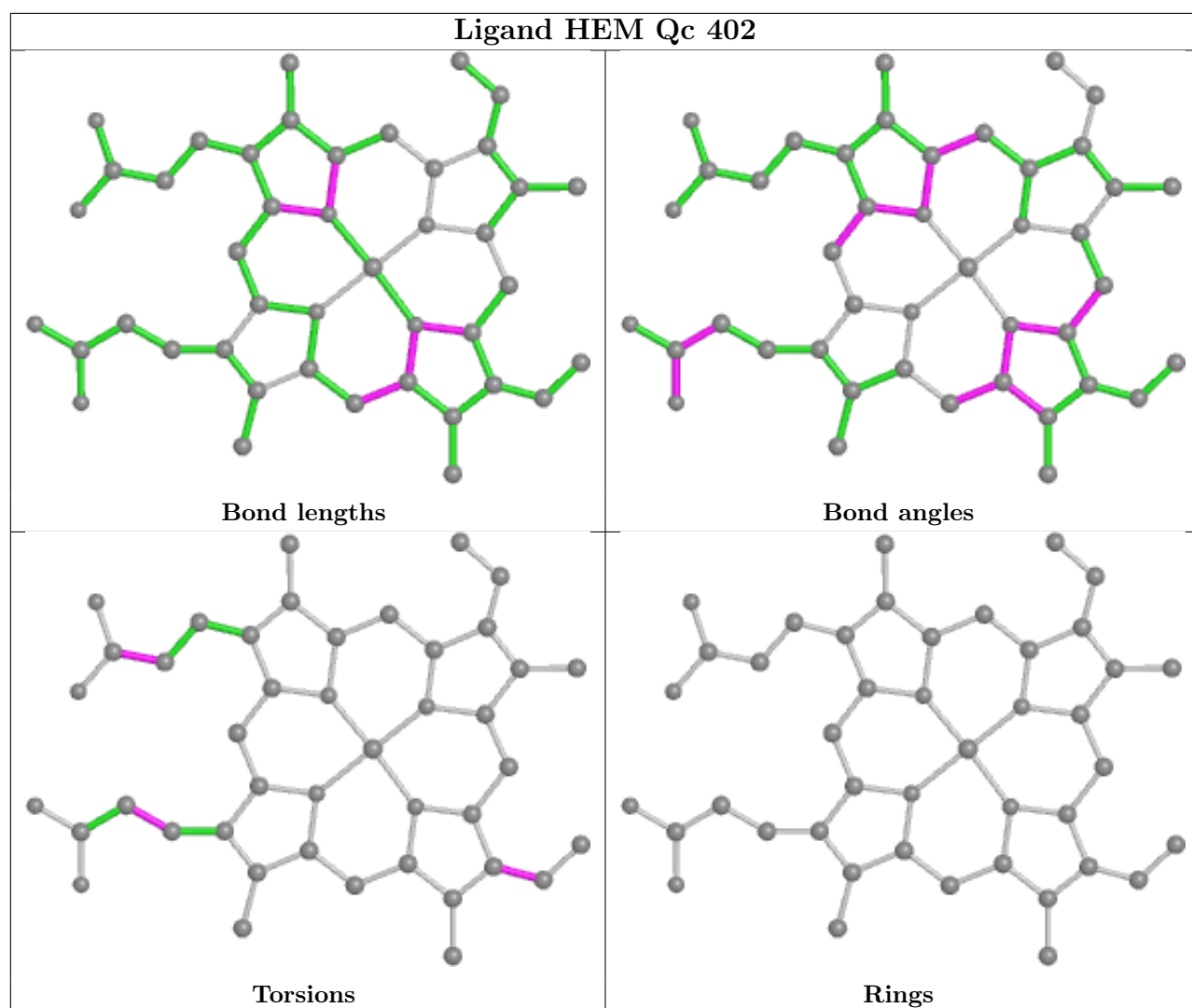


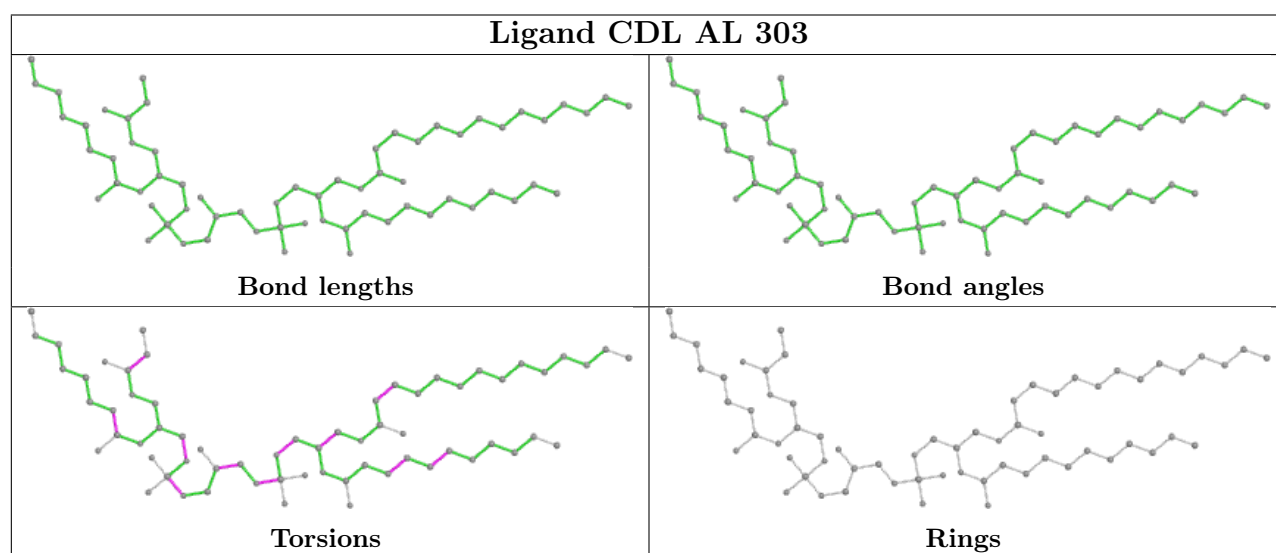
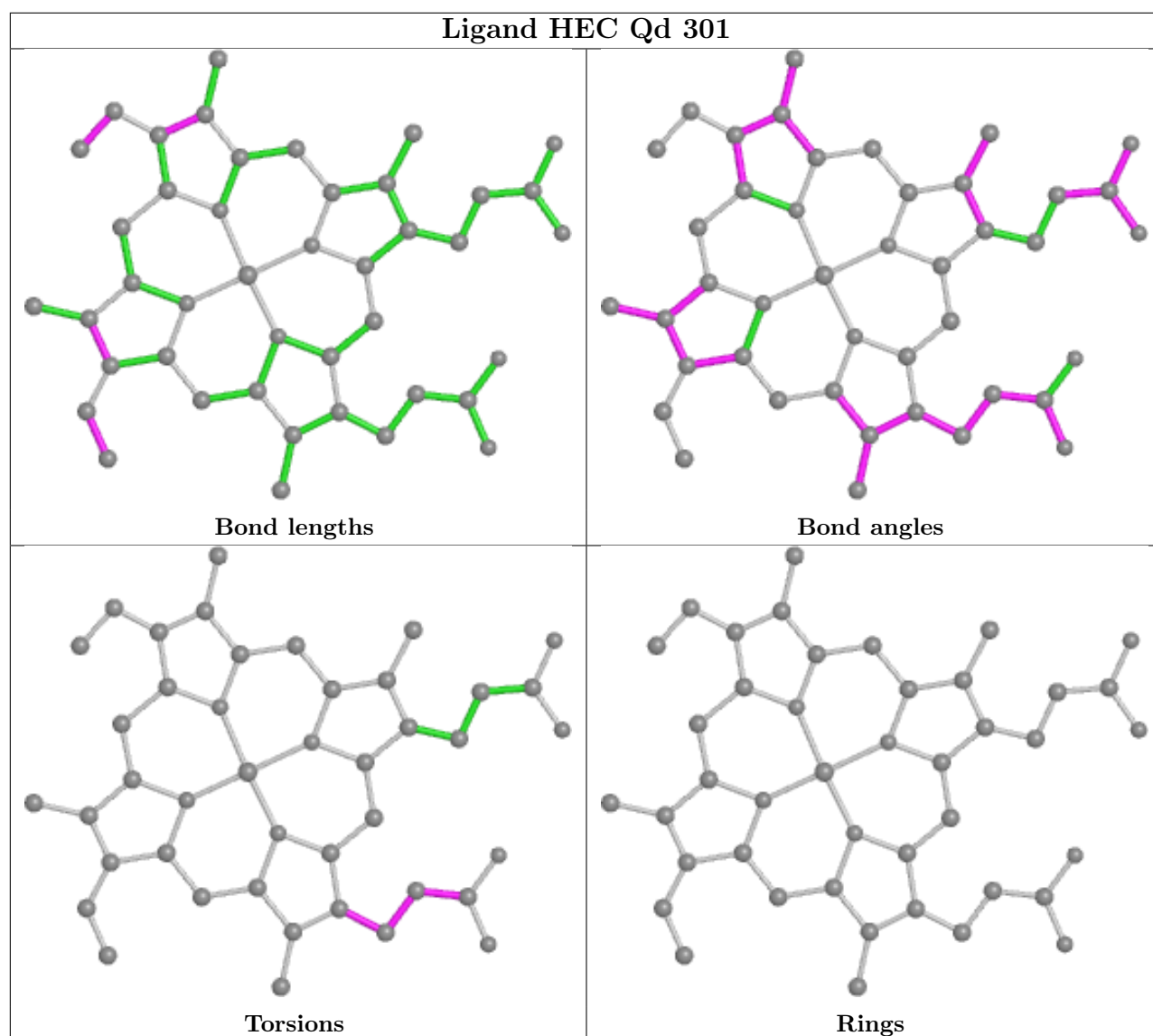


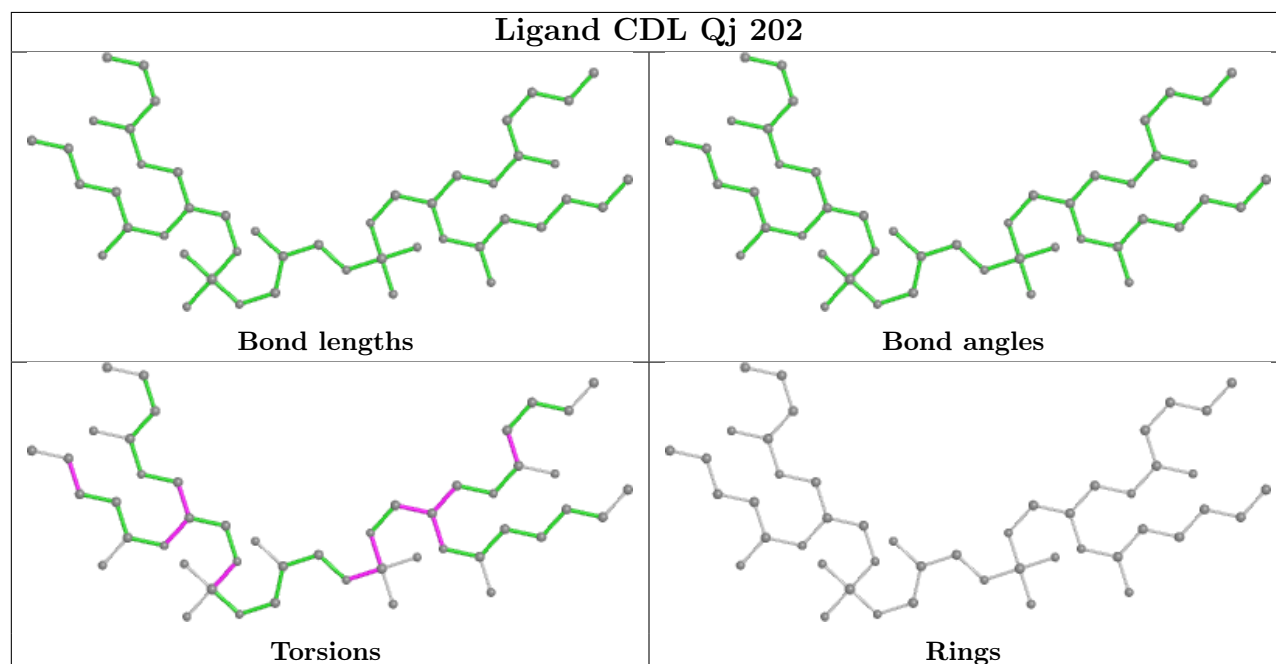
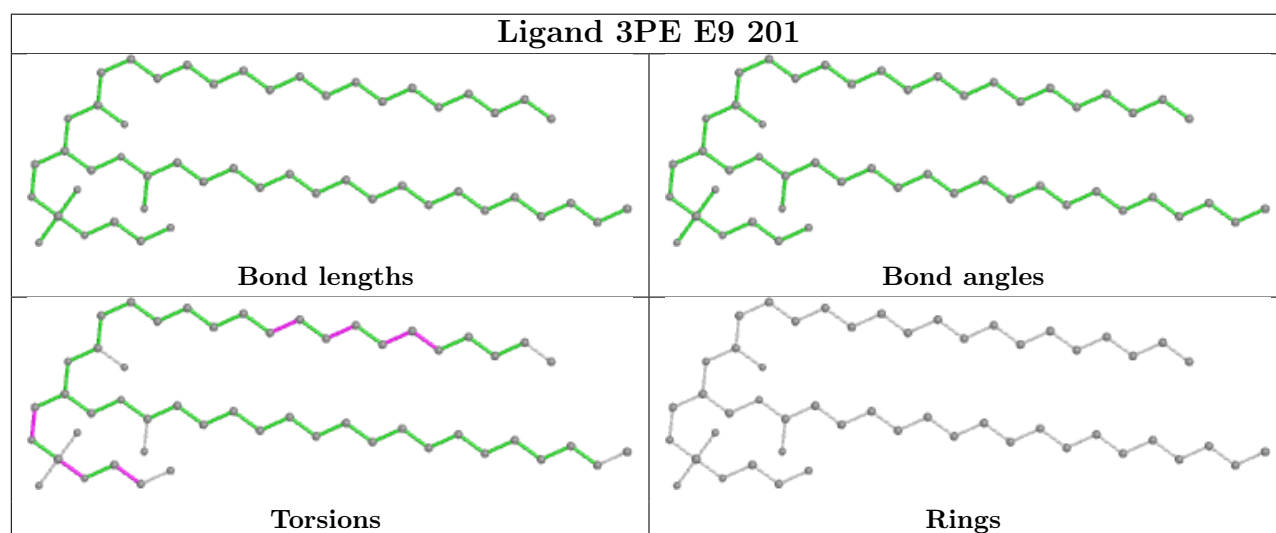
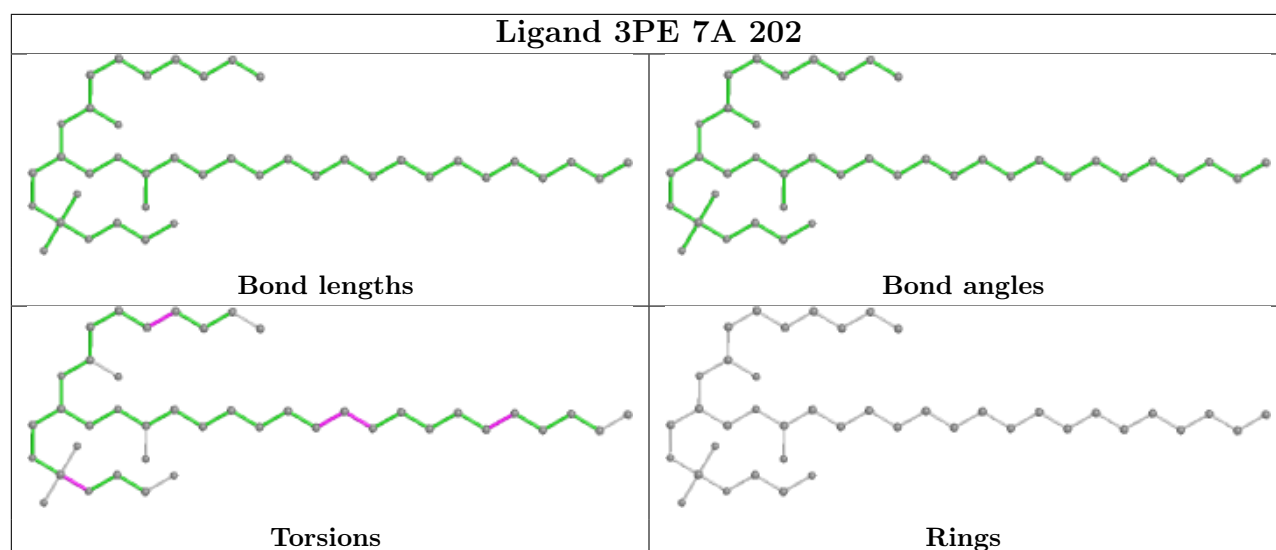




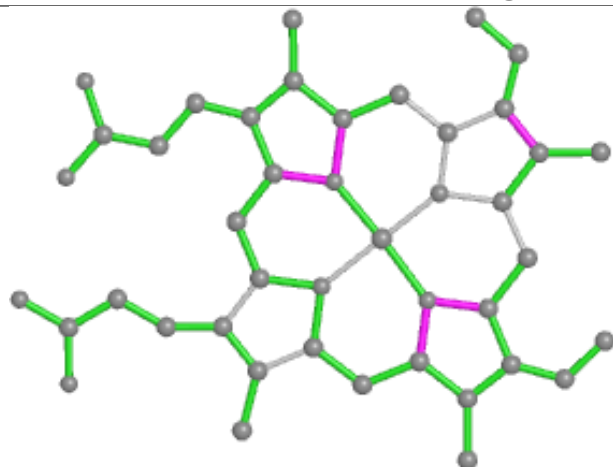




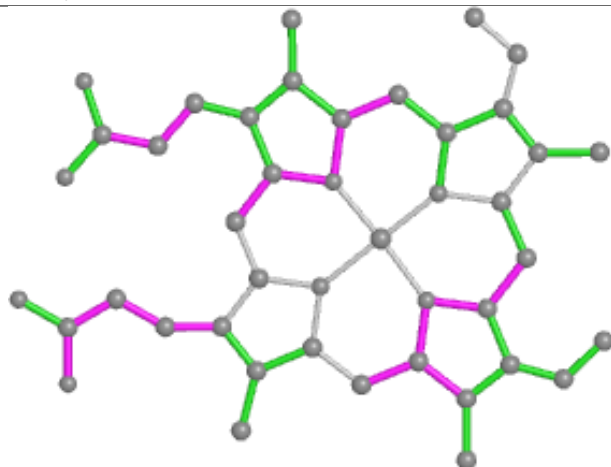




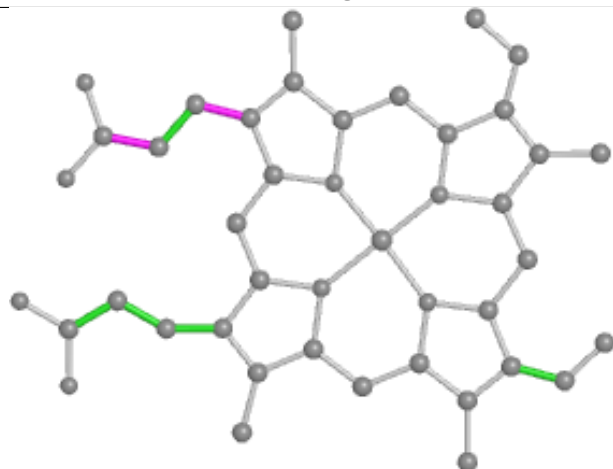
Ligand HEM Qc 403



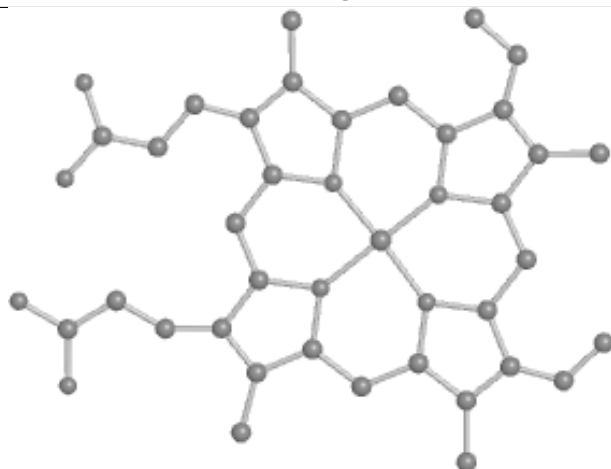
Bond lengths



Bond angles

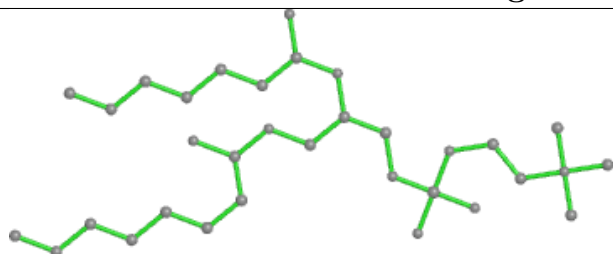


Torsions

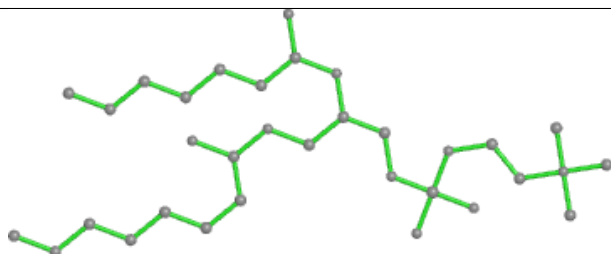


Rings

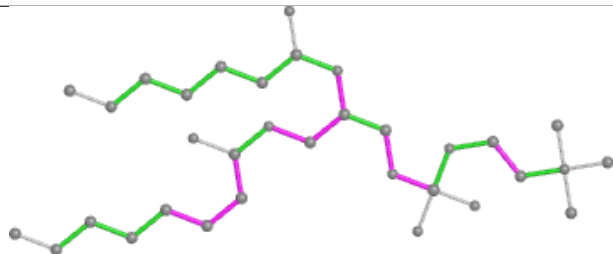
Ligand PC1 A9 502



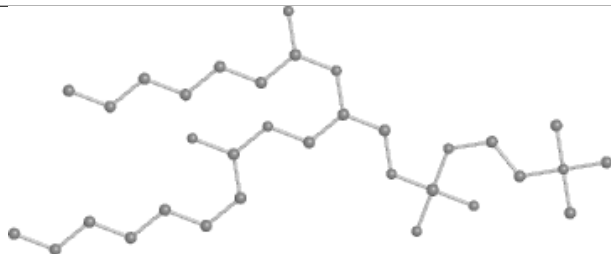
Bond lengths



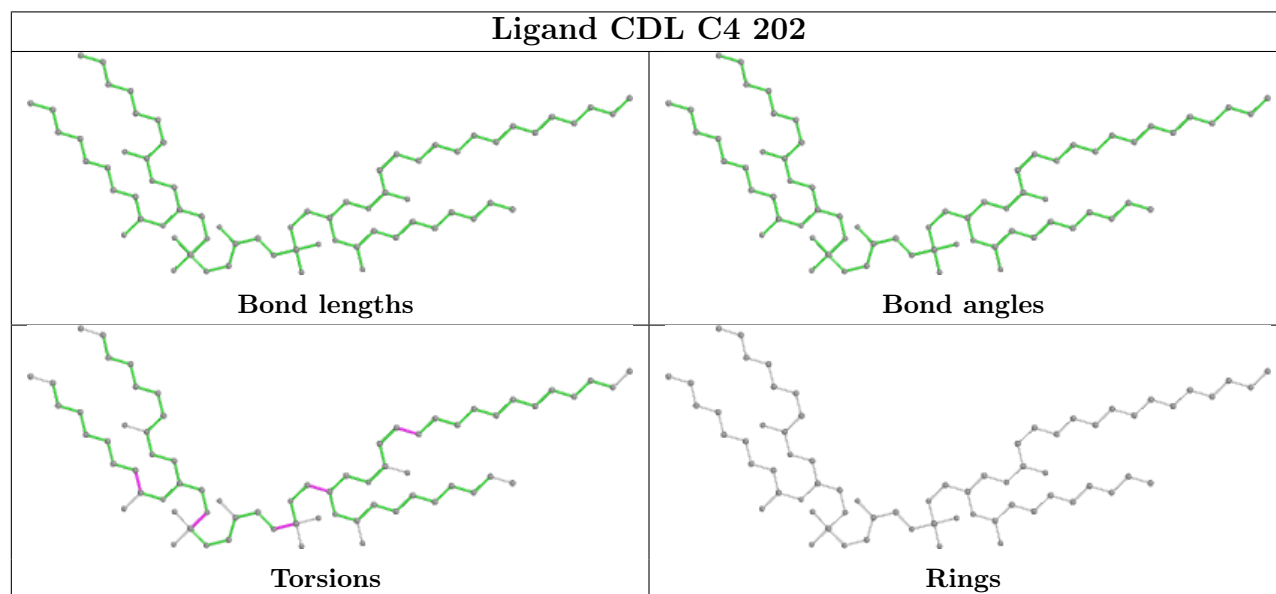
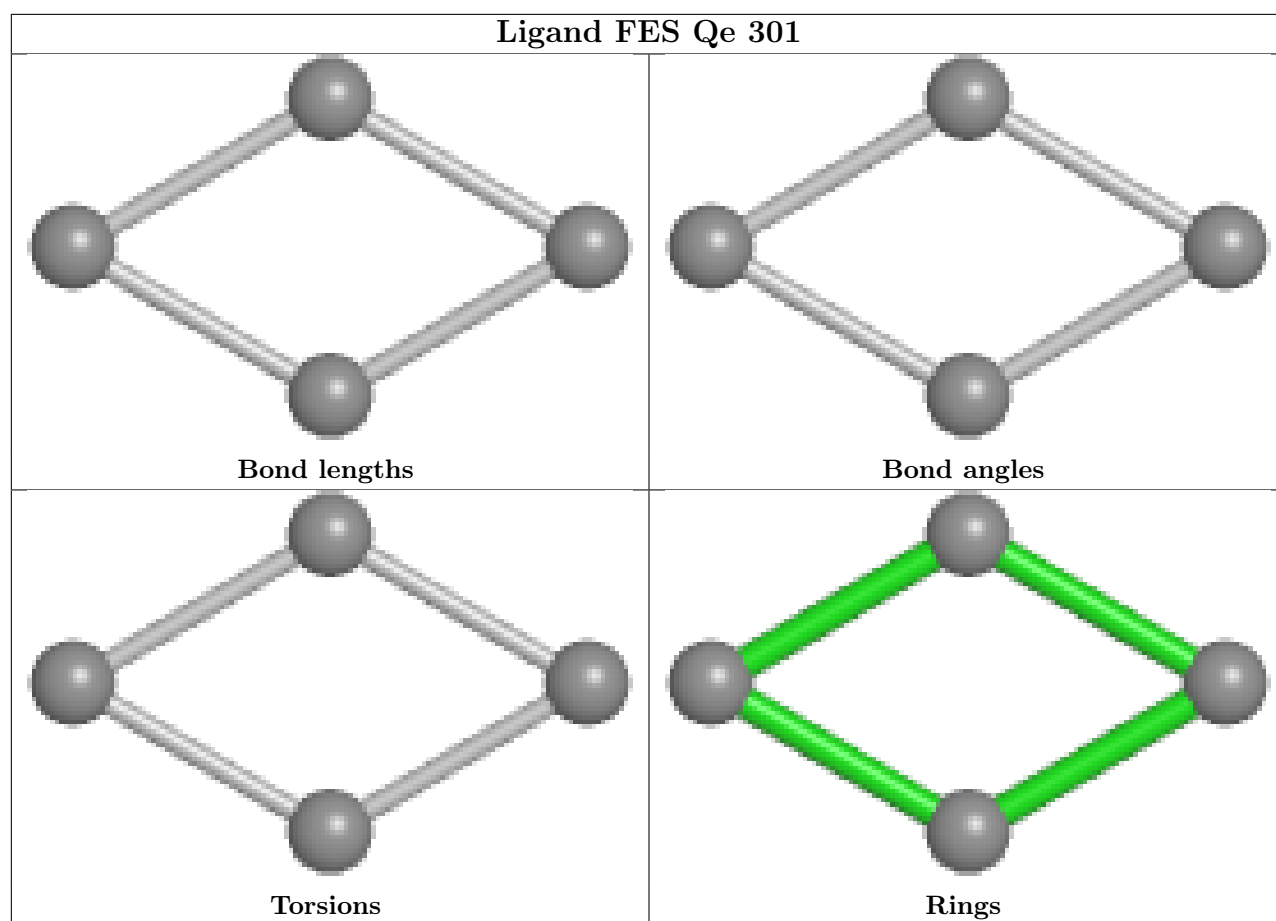
Bond angles

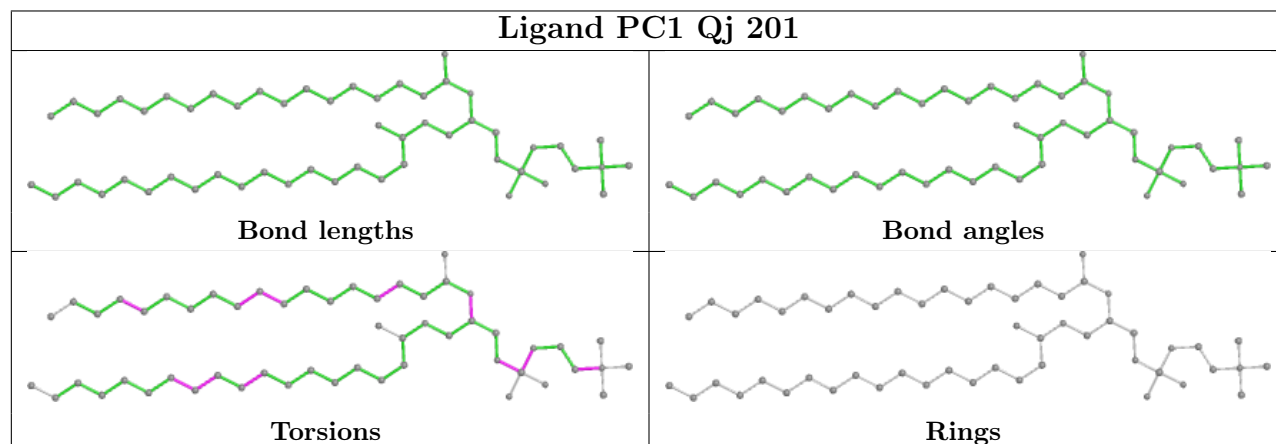
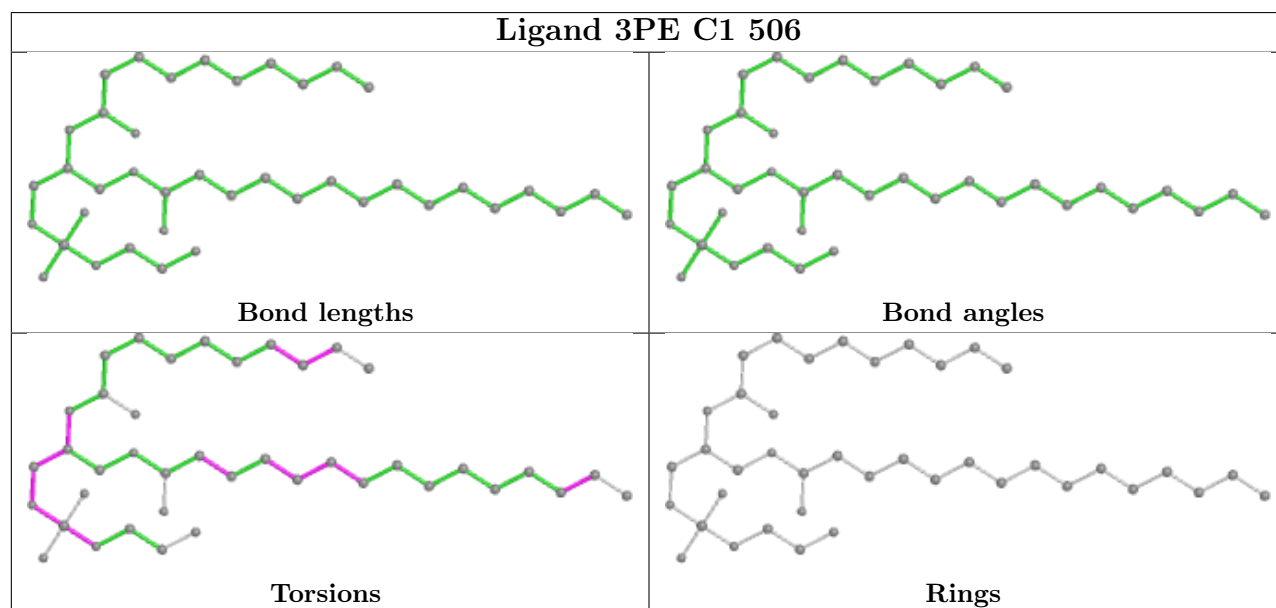
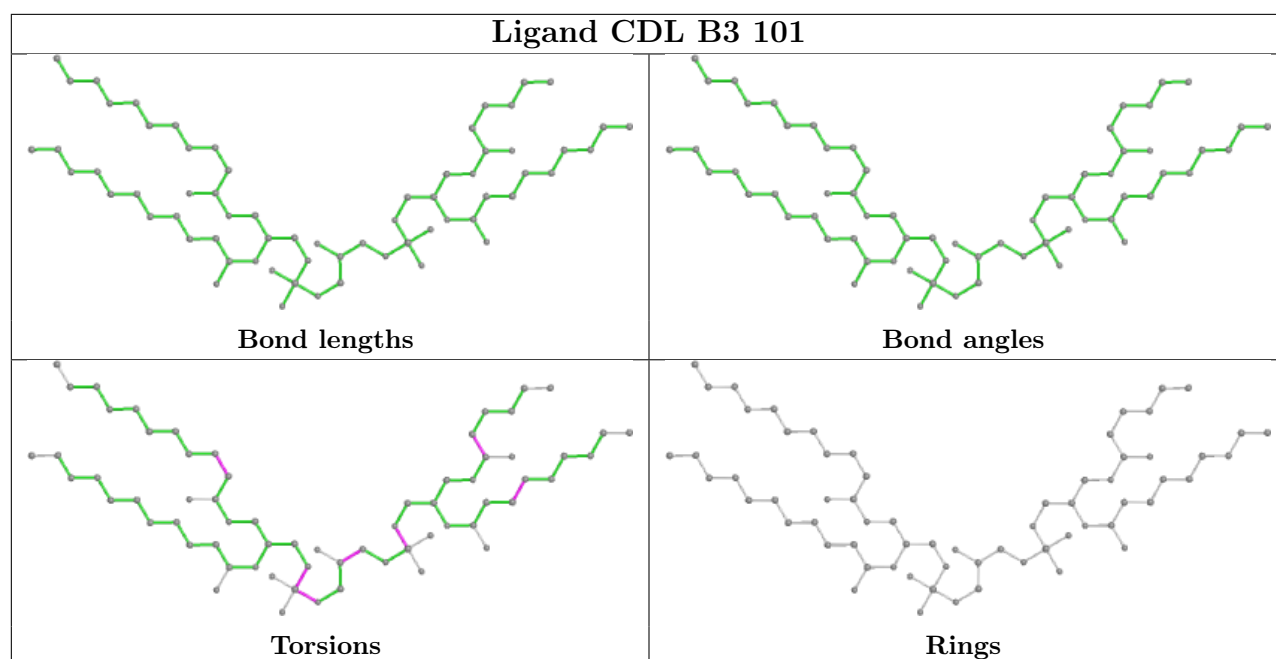


Torsions

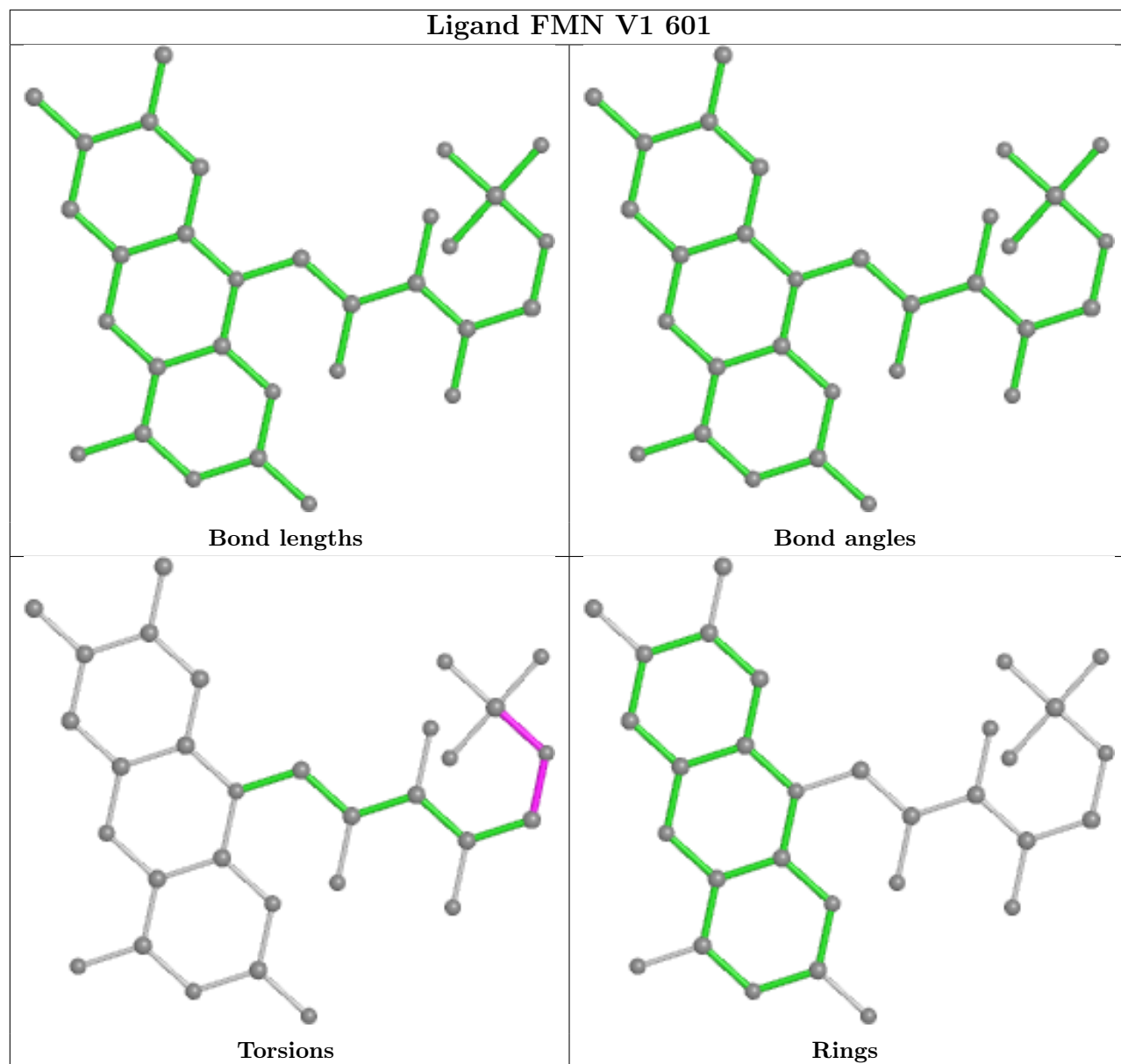


Rings

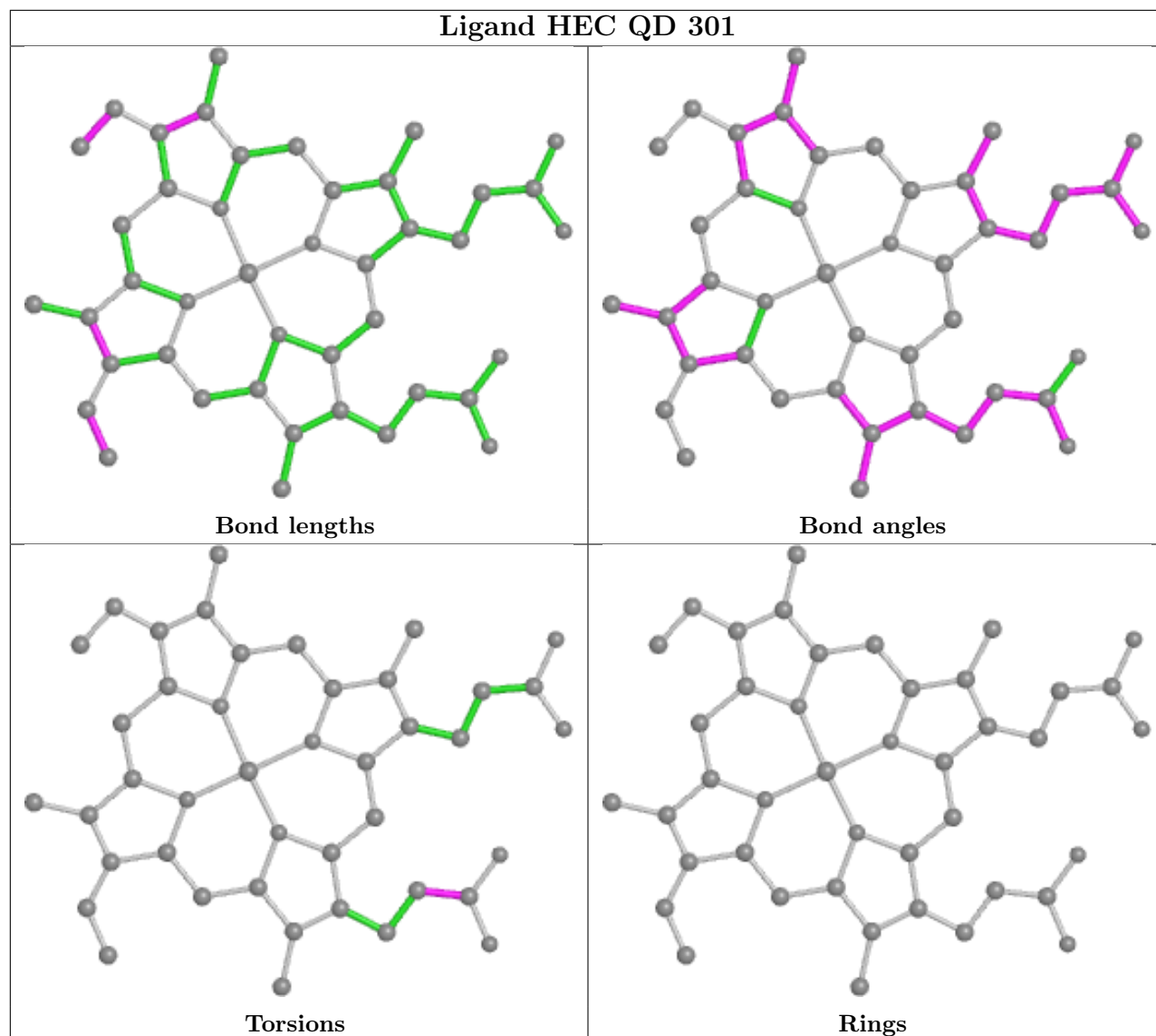




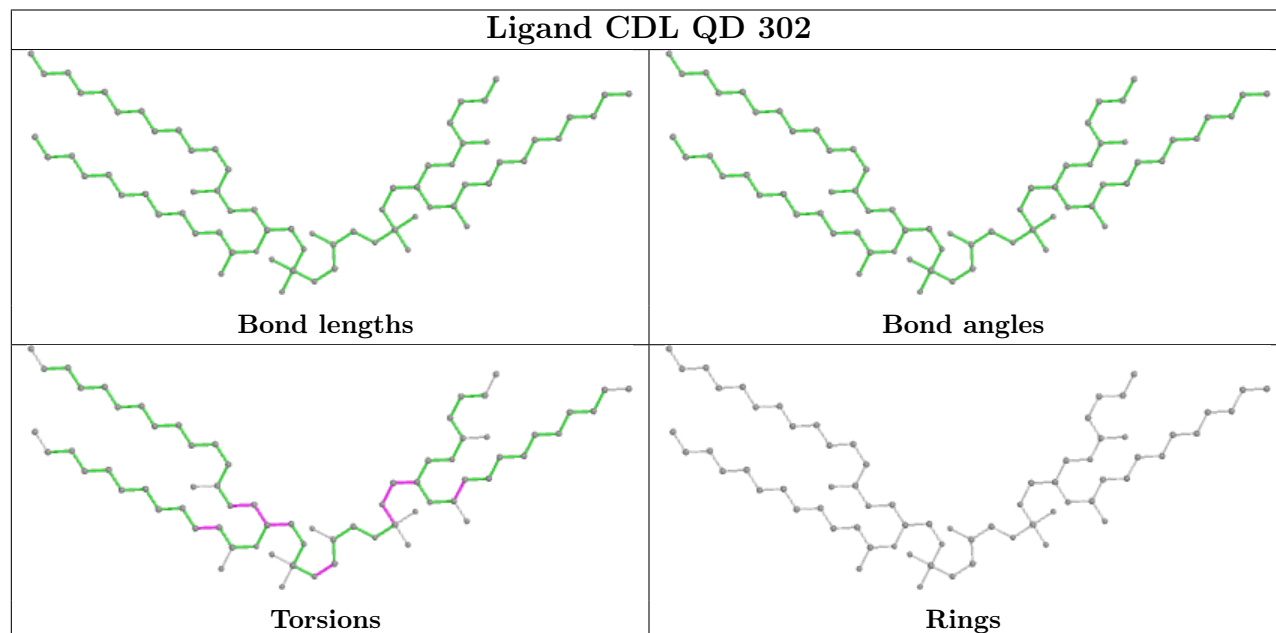
Ligand FMN V1 601

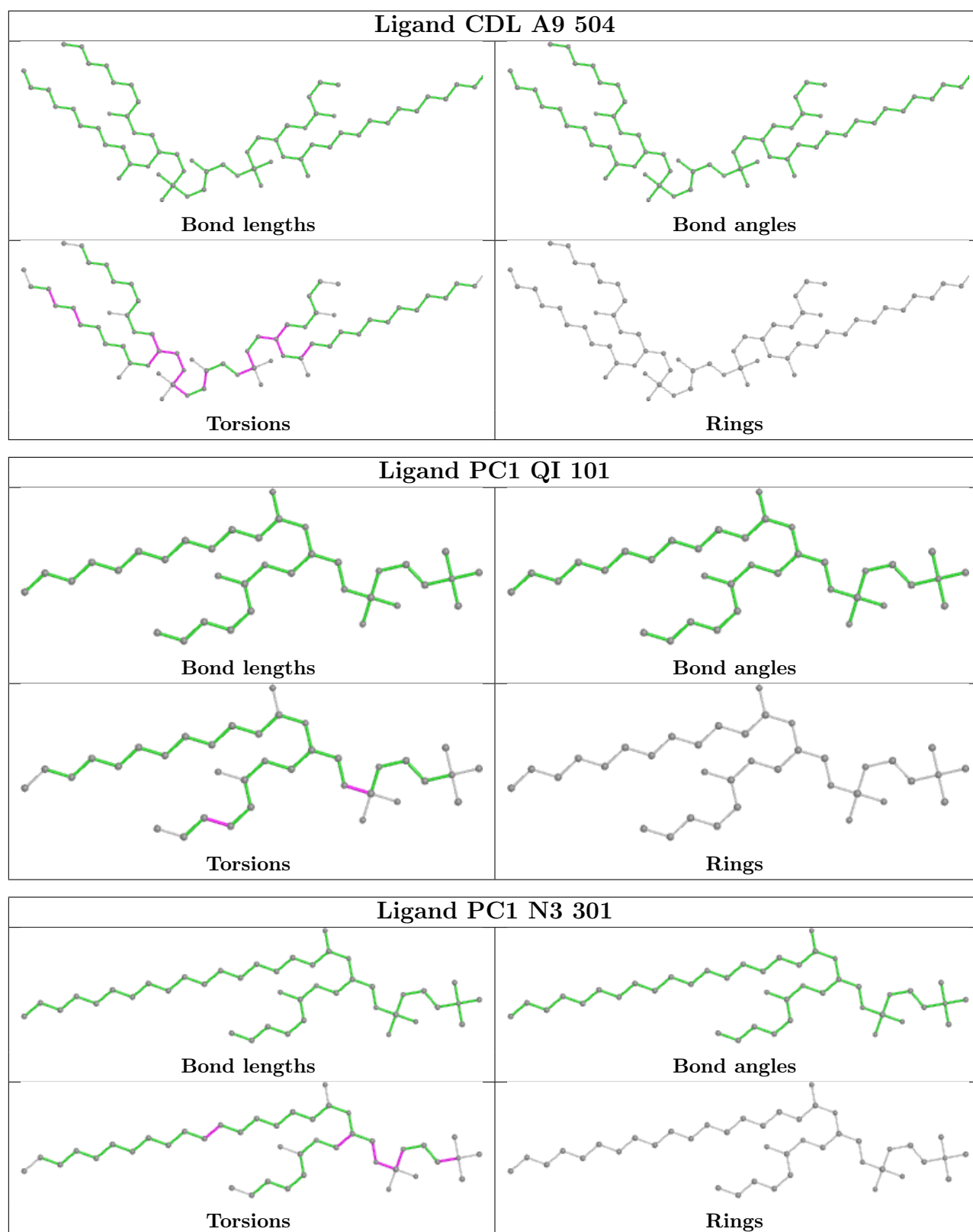


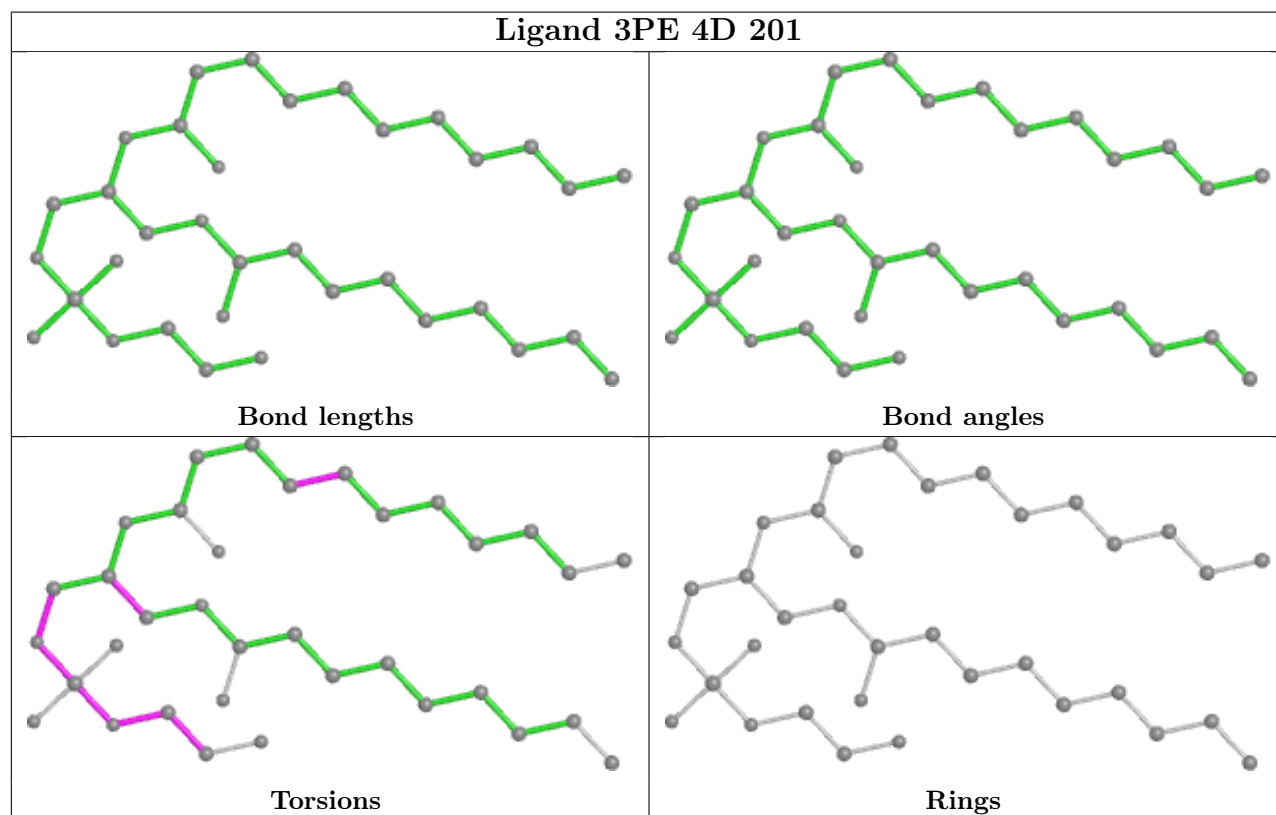
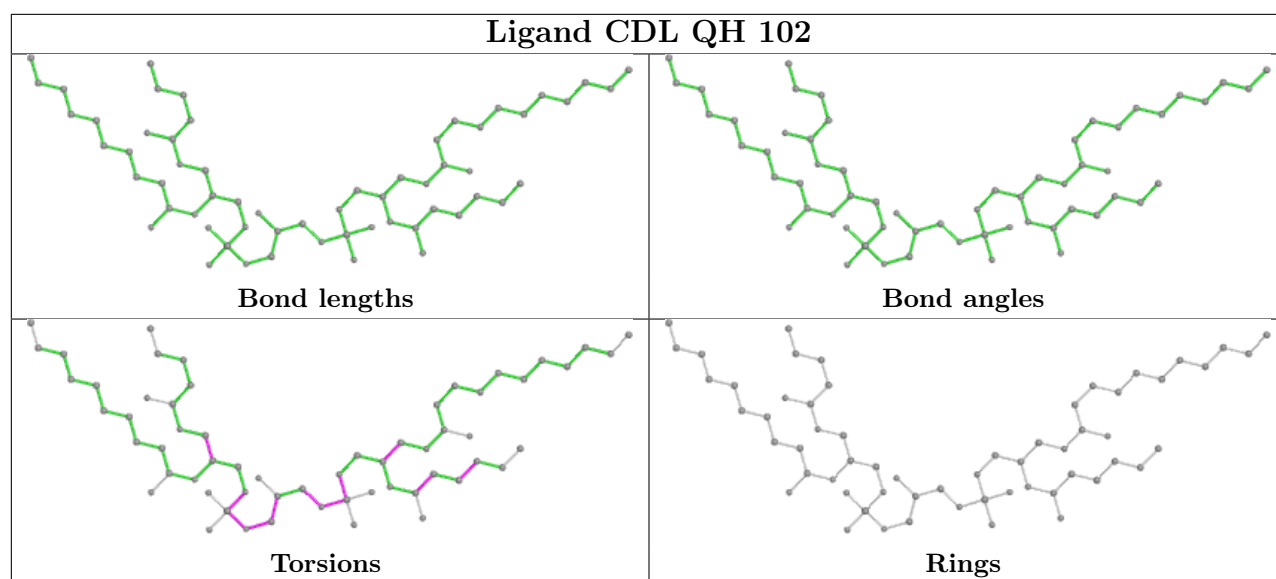
Ligand HEC QD 301

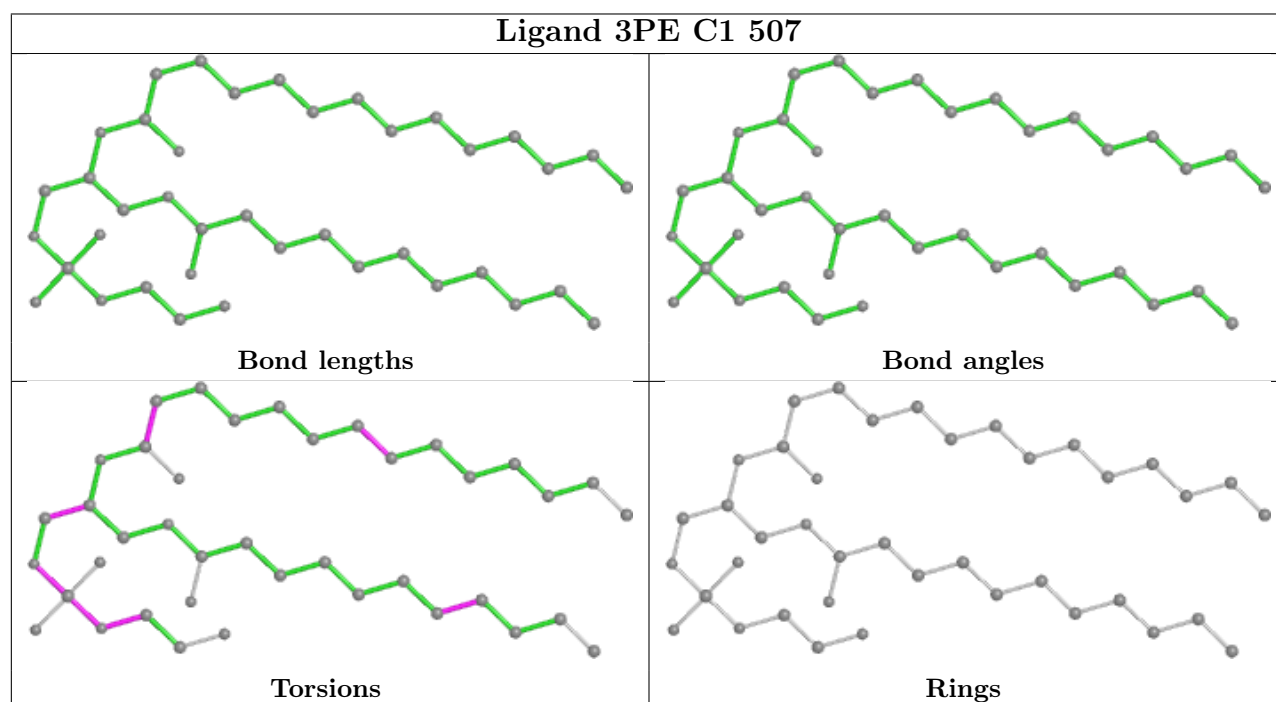
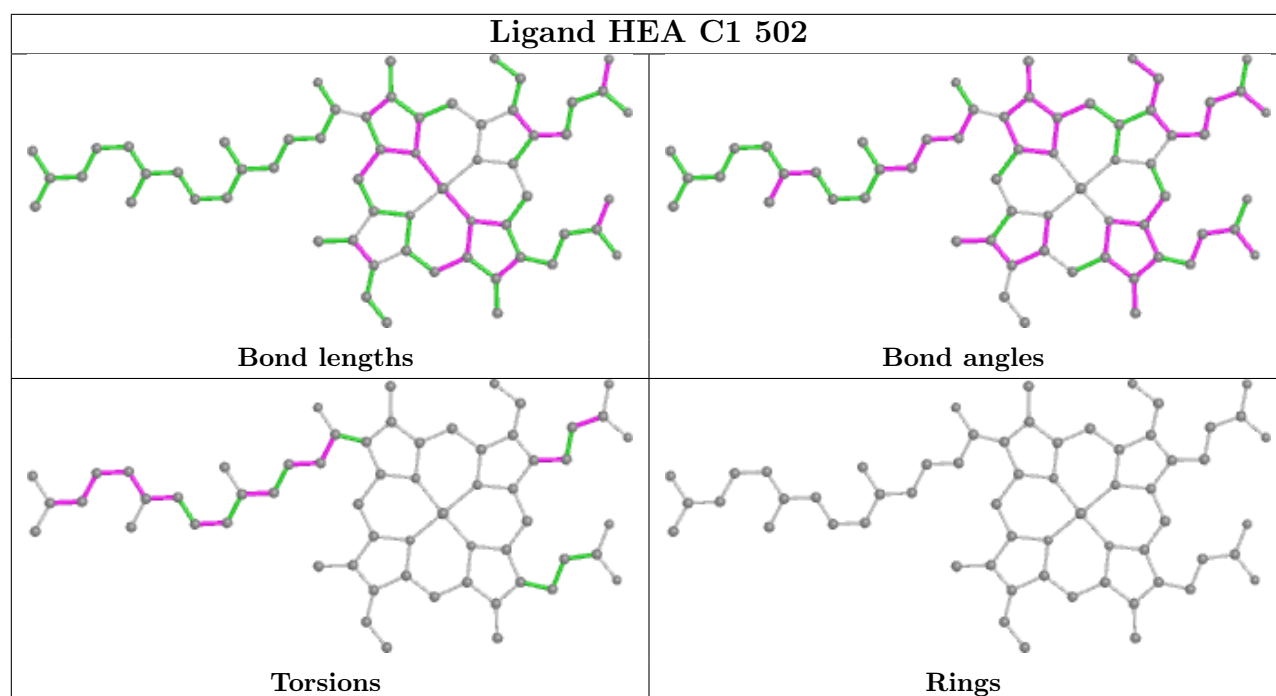


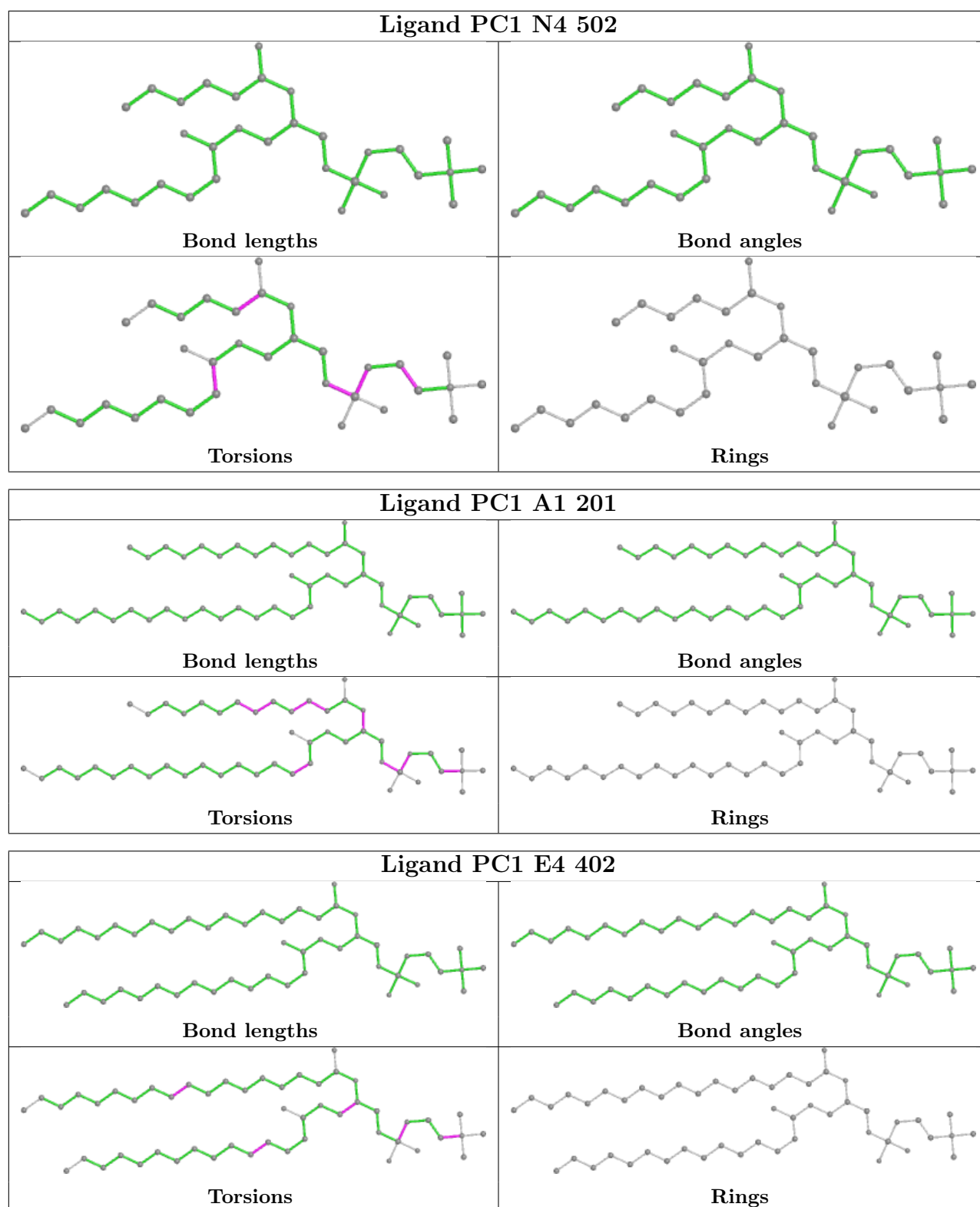
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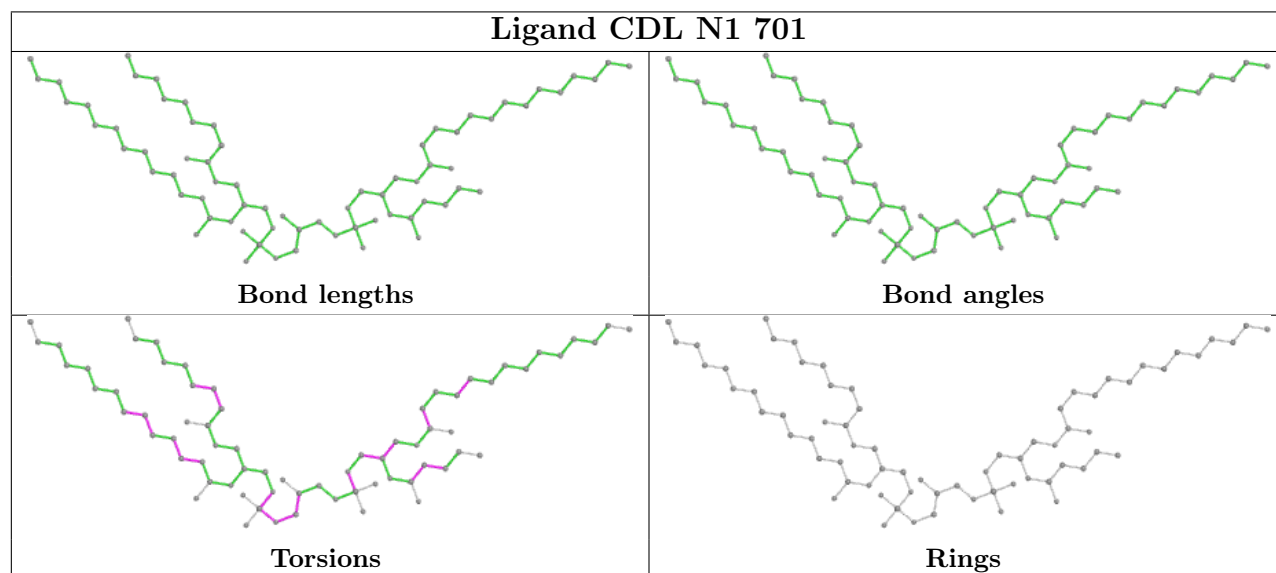
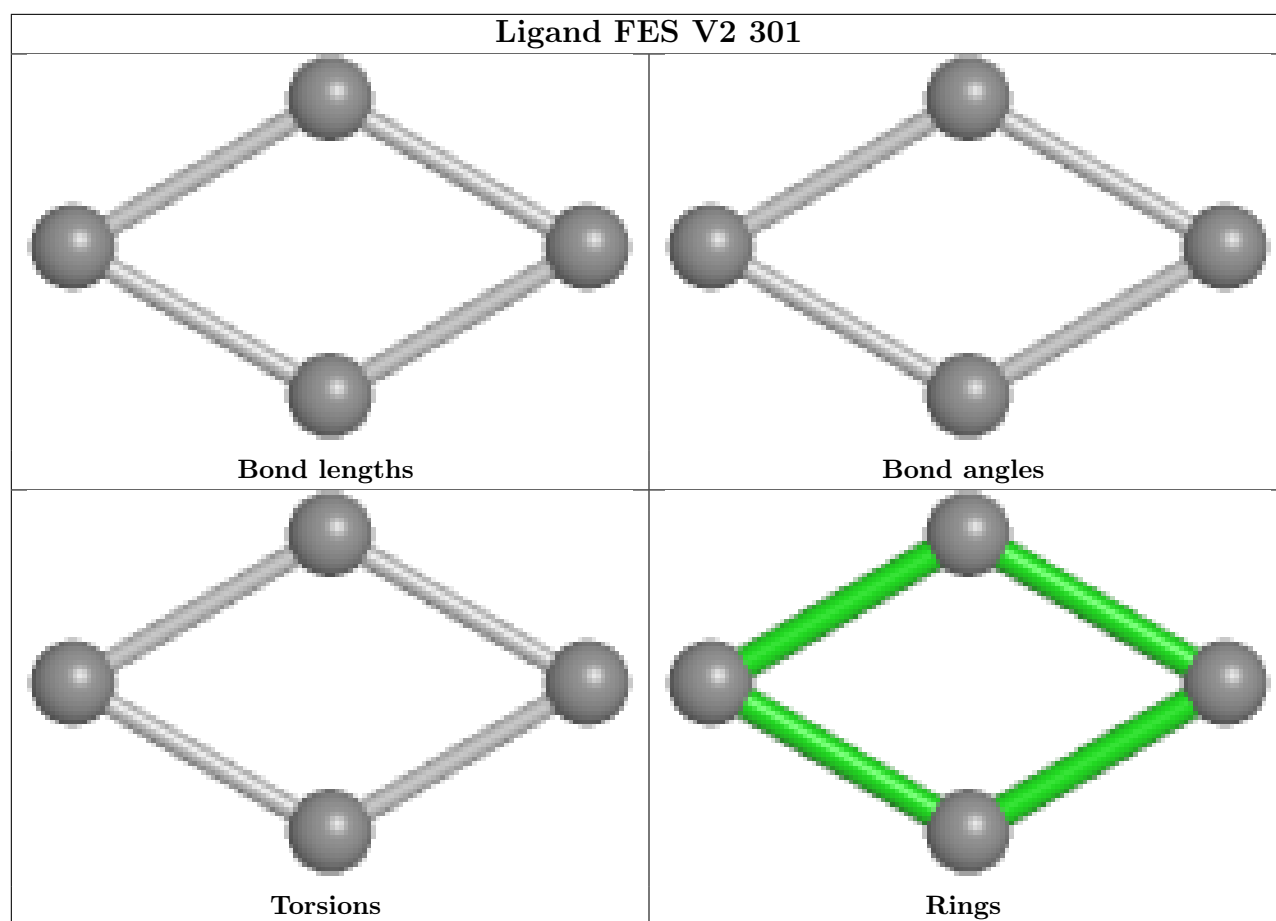




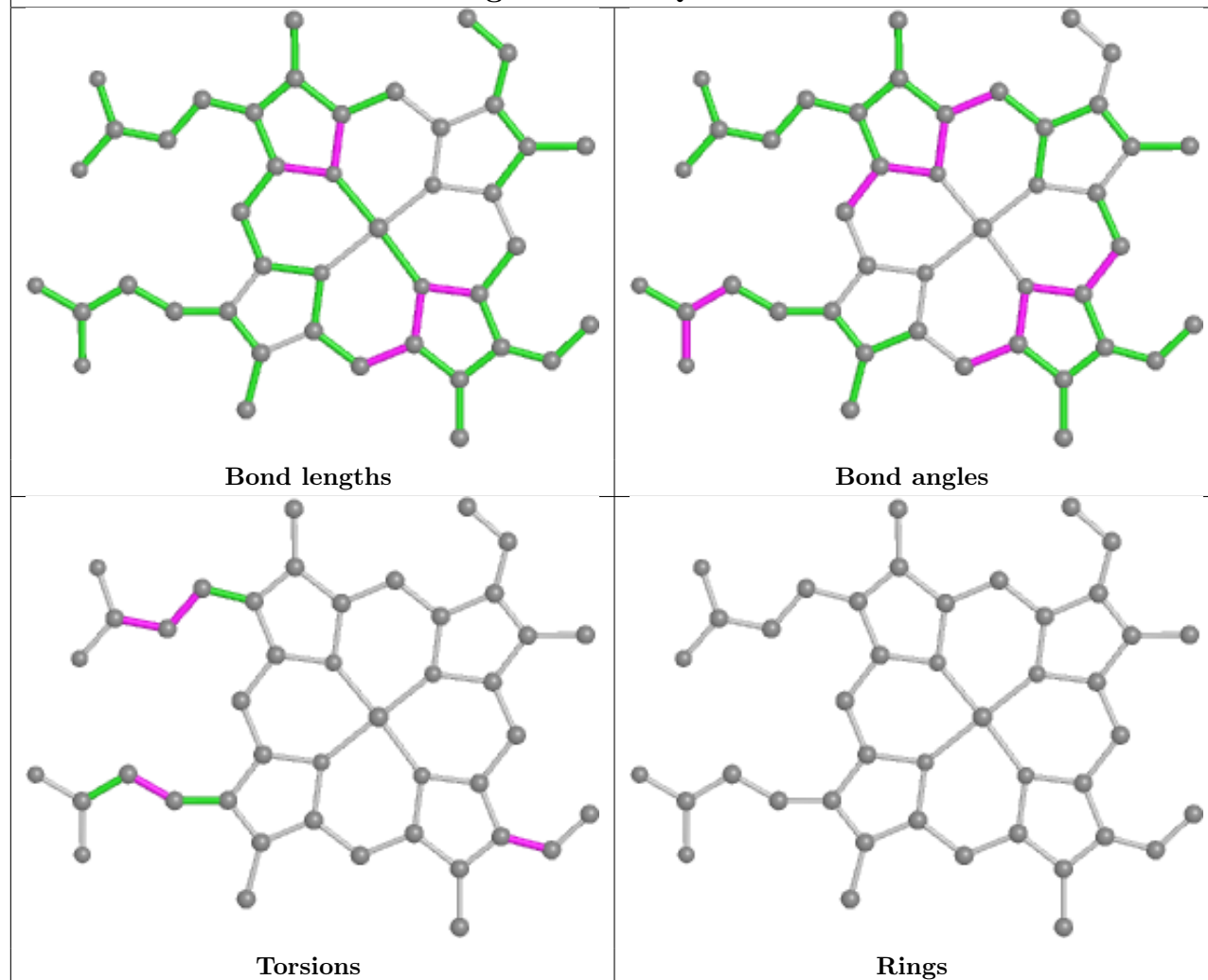




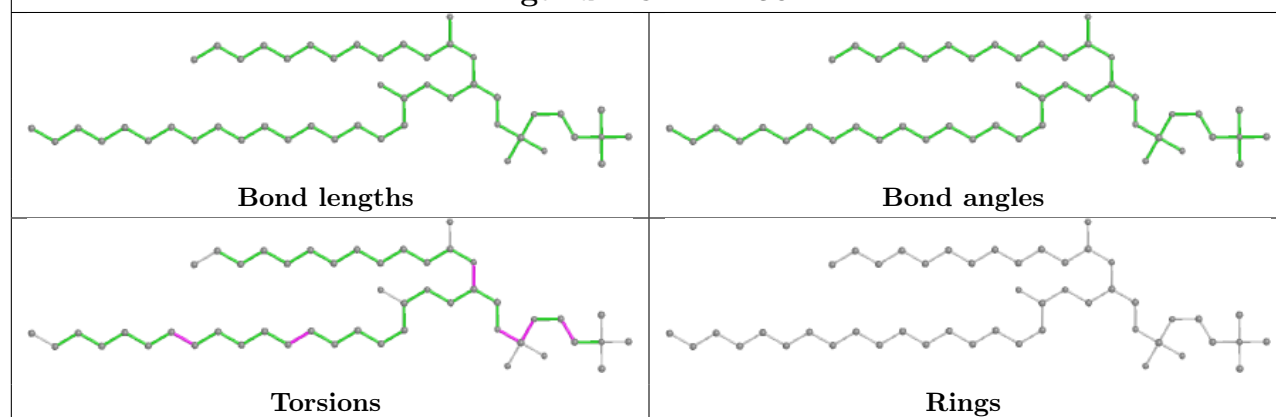


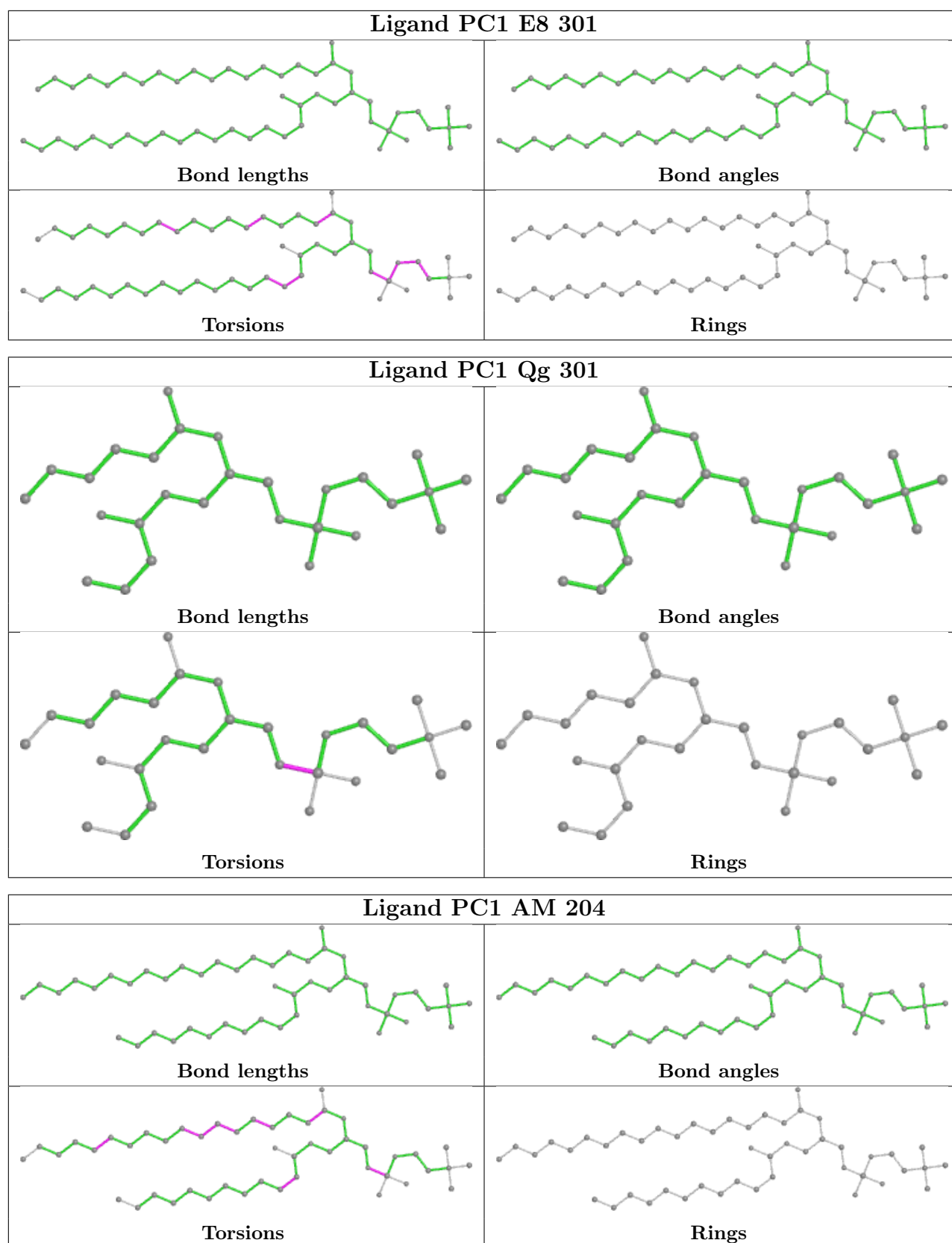


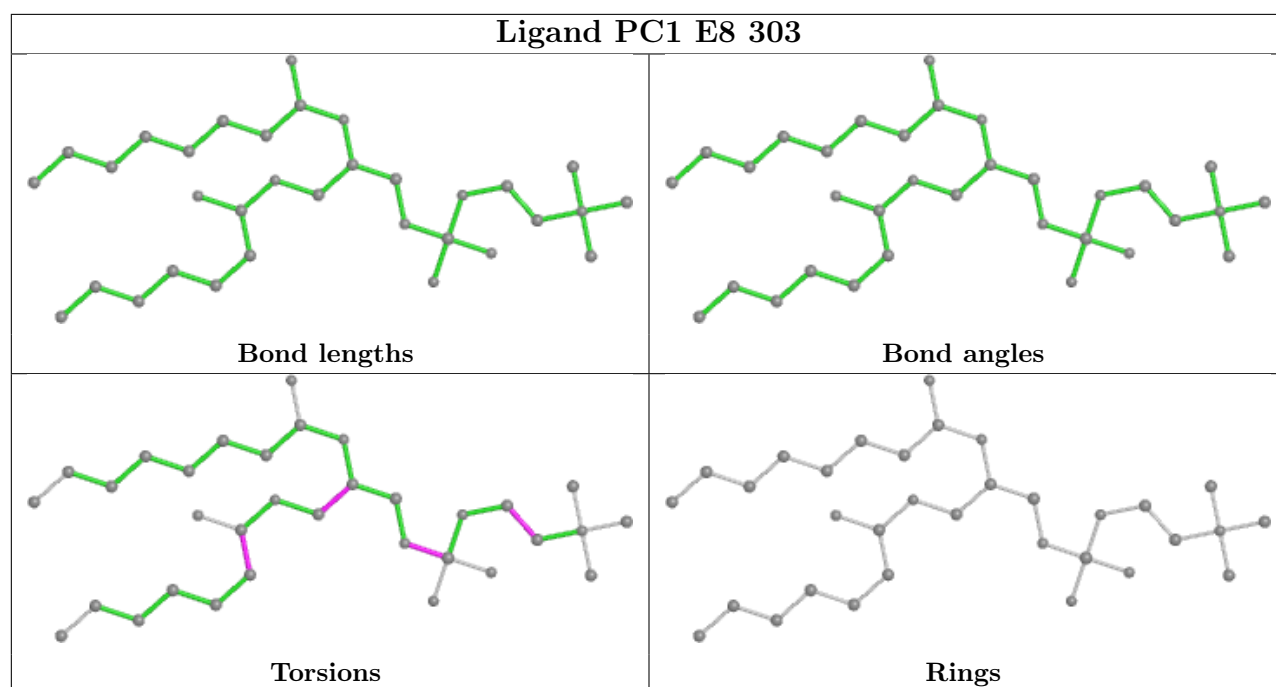
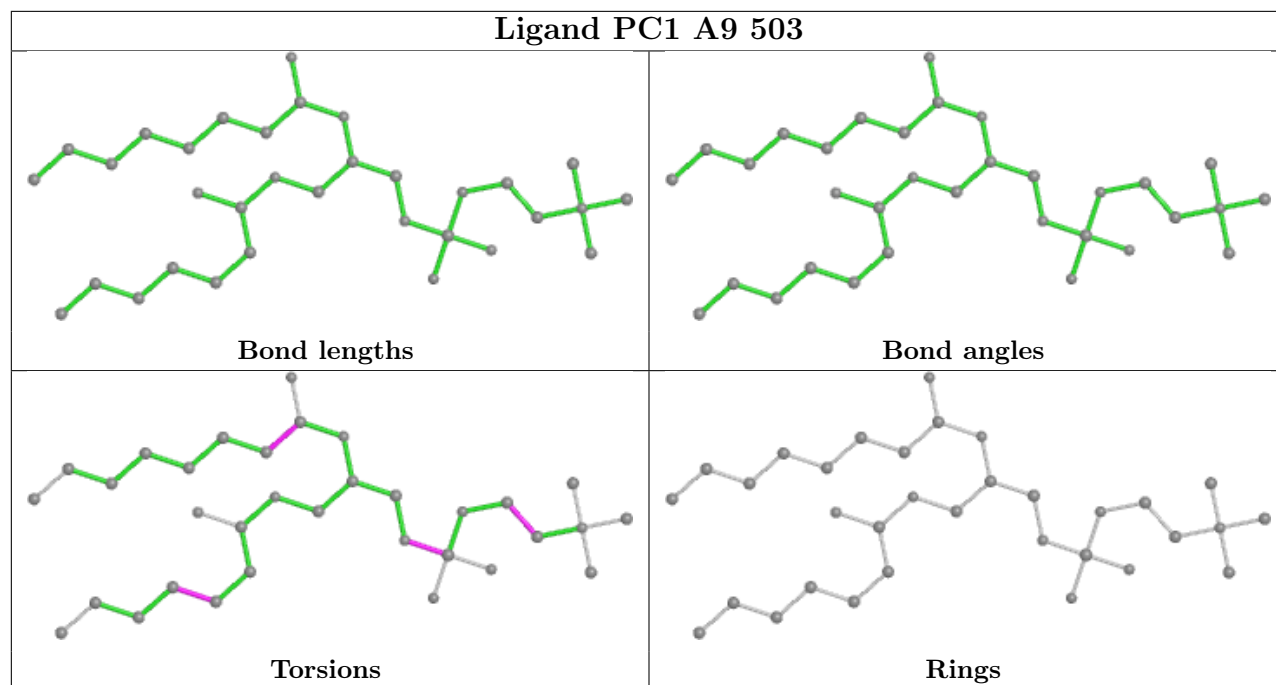
Ligand HEM QC 401



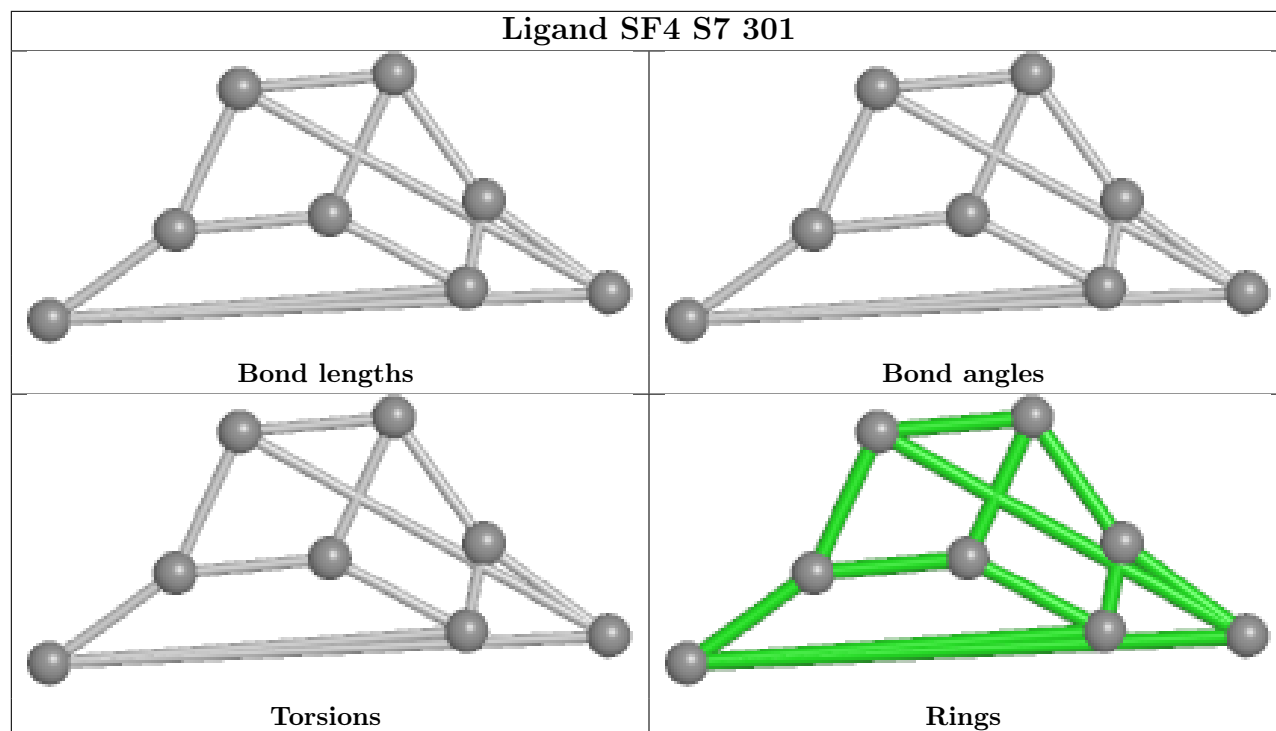
Ligand PC1 AN 301



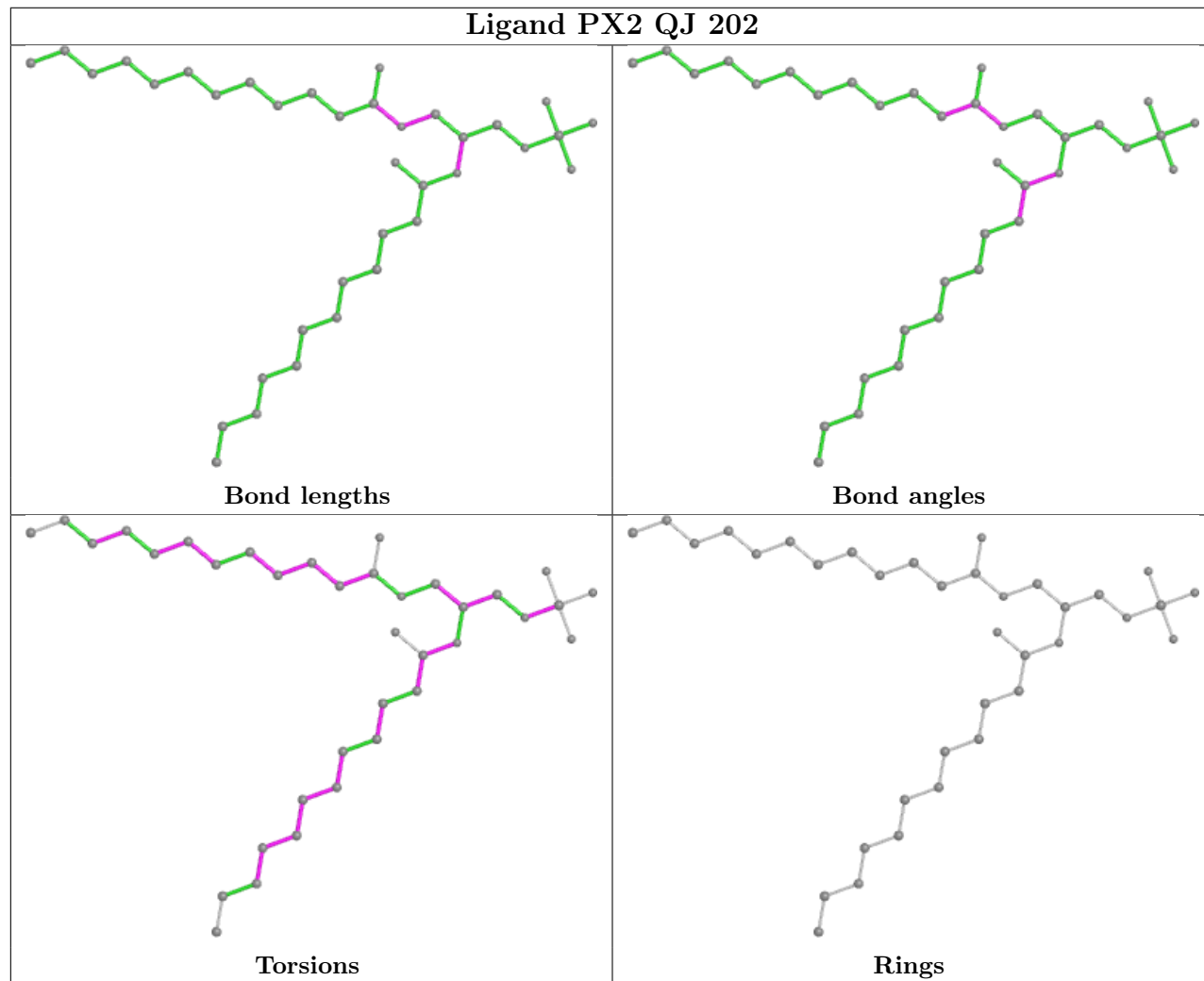


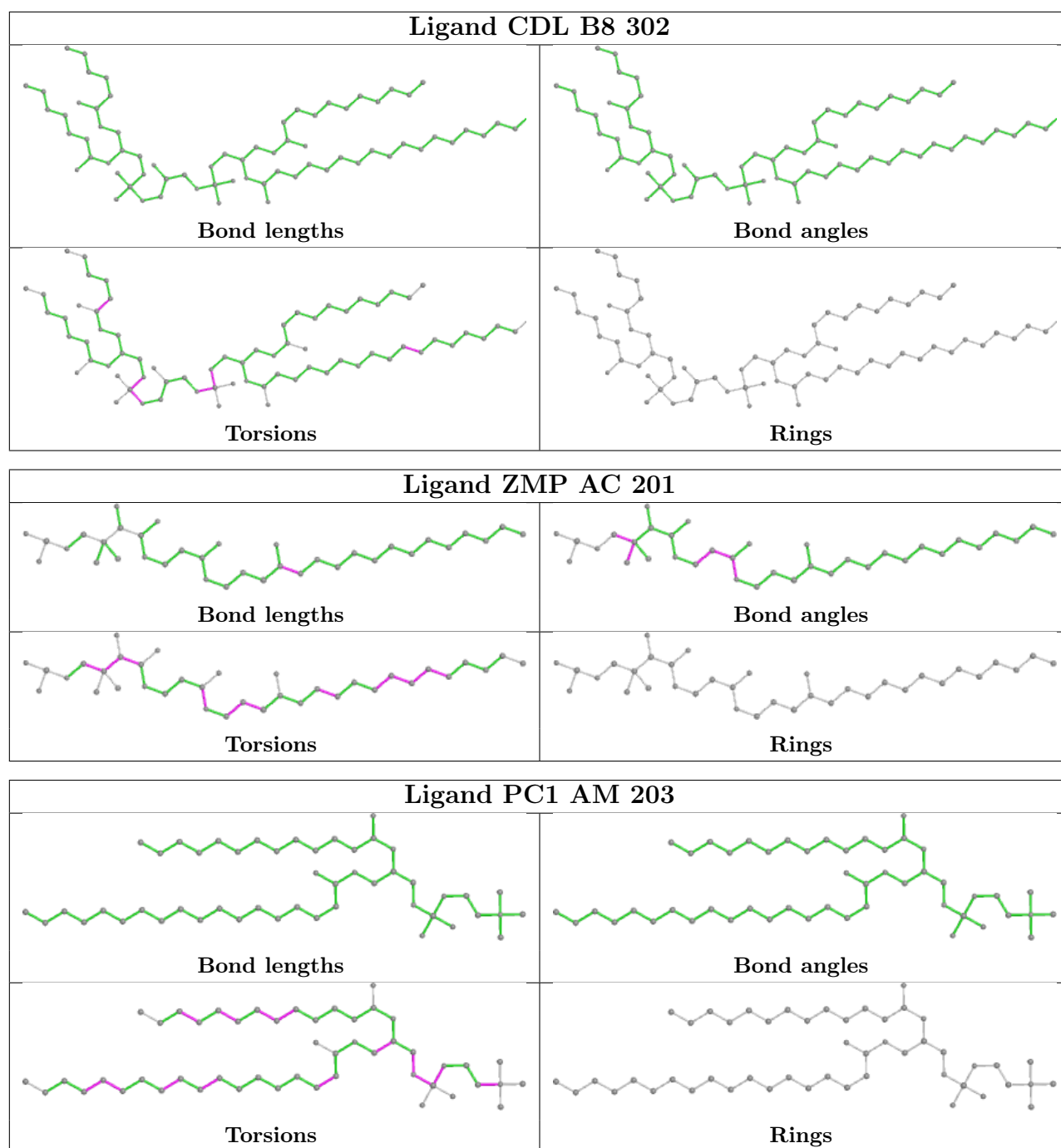


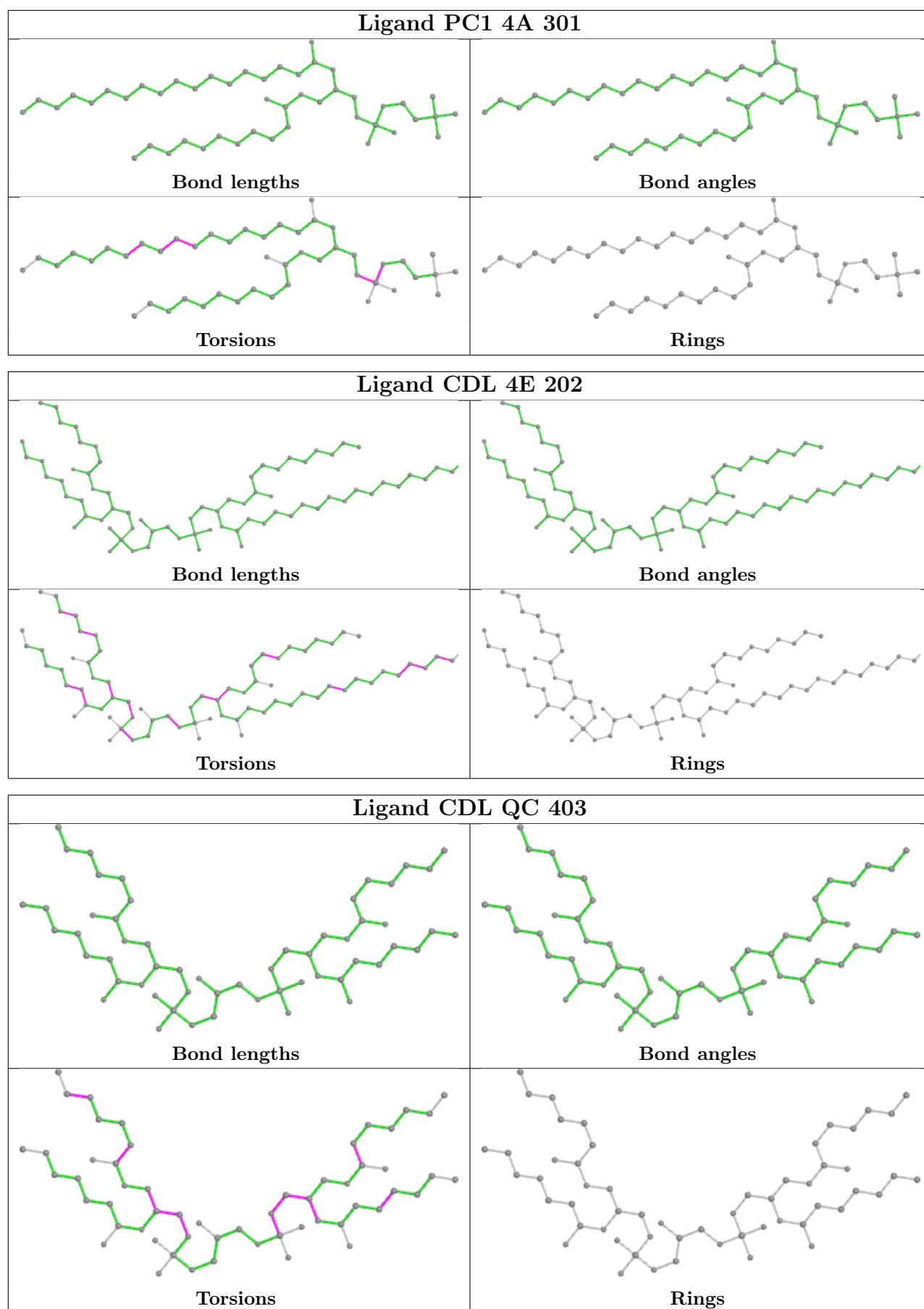
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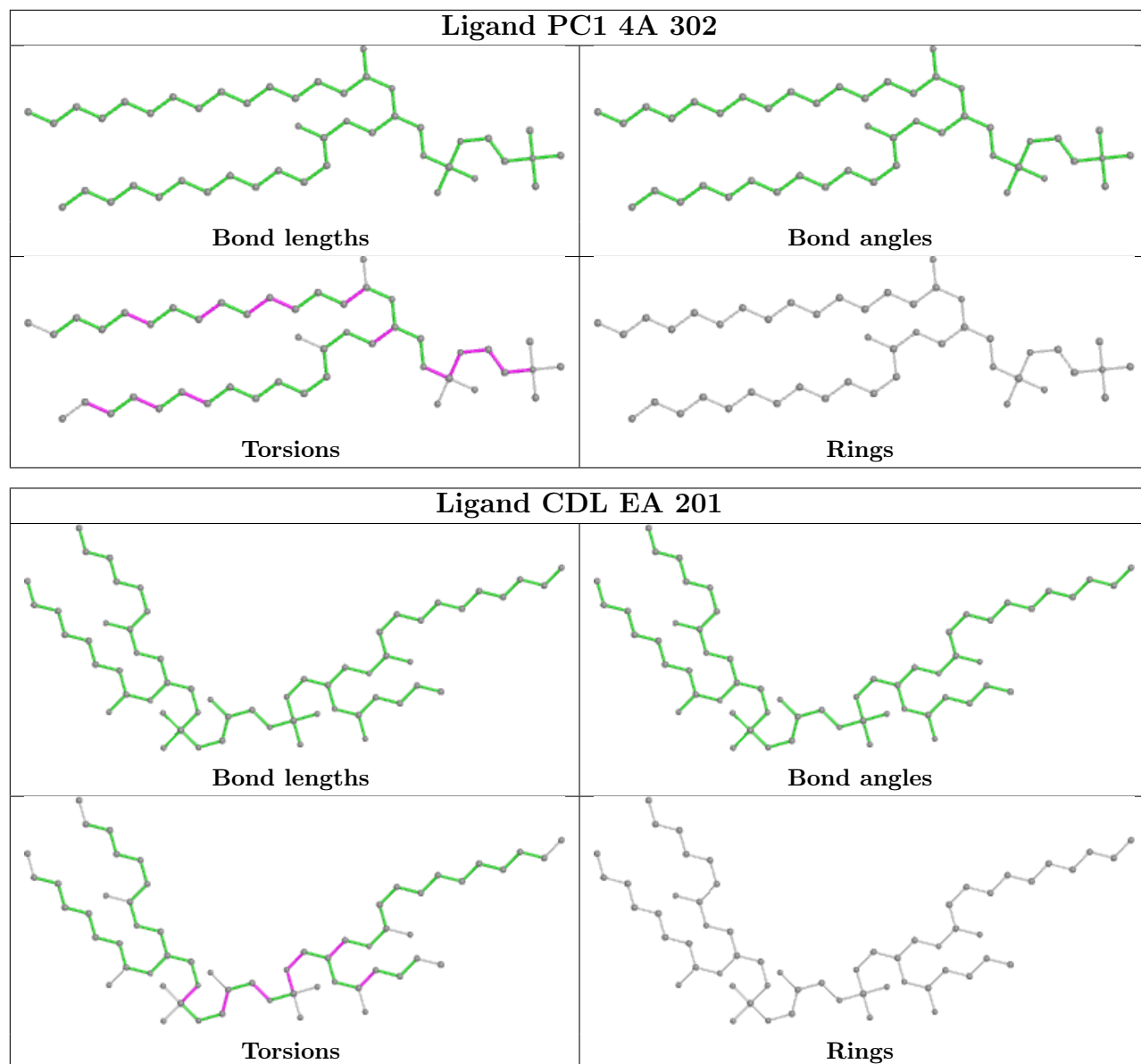


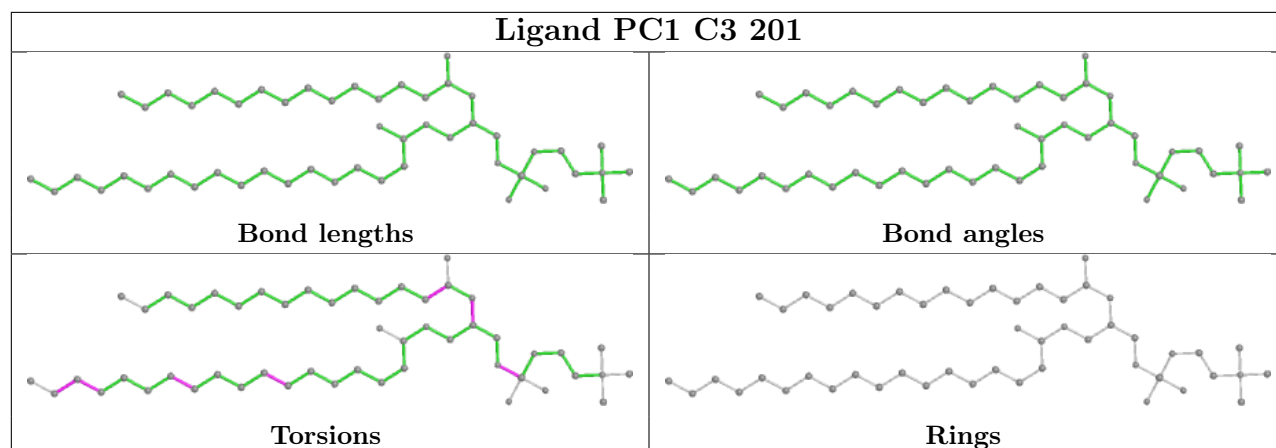
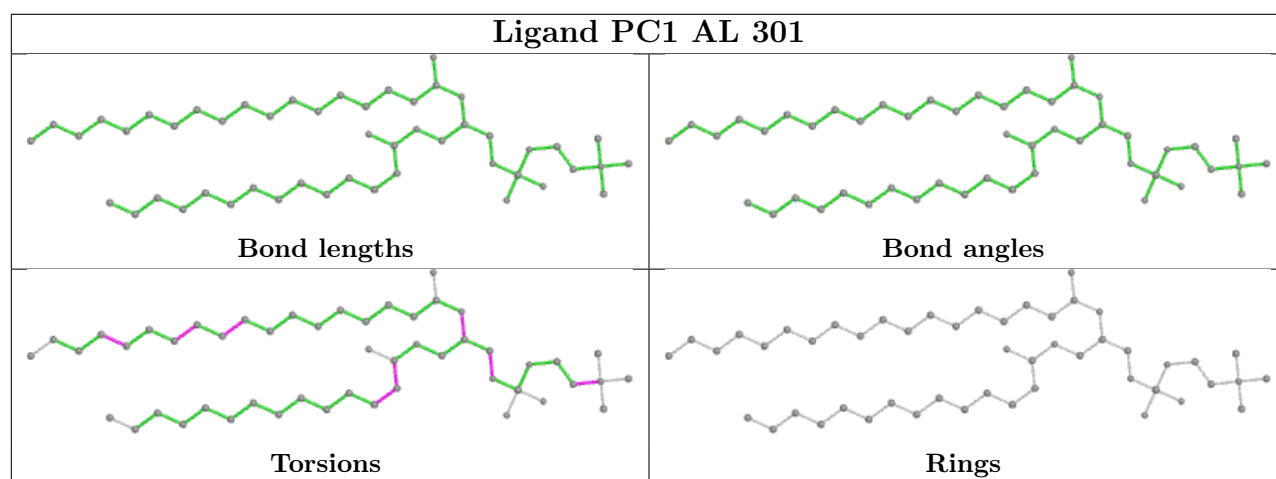
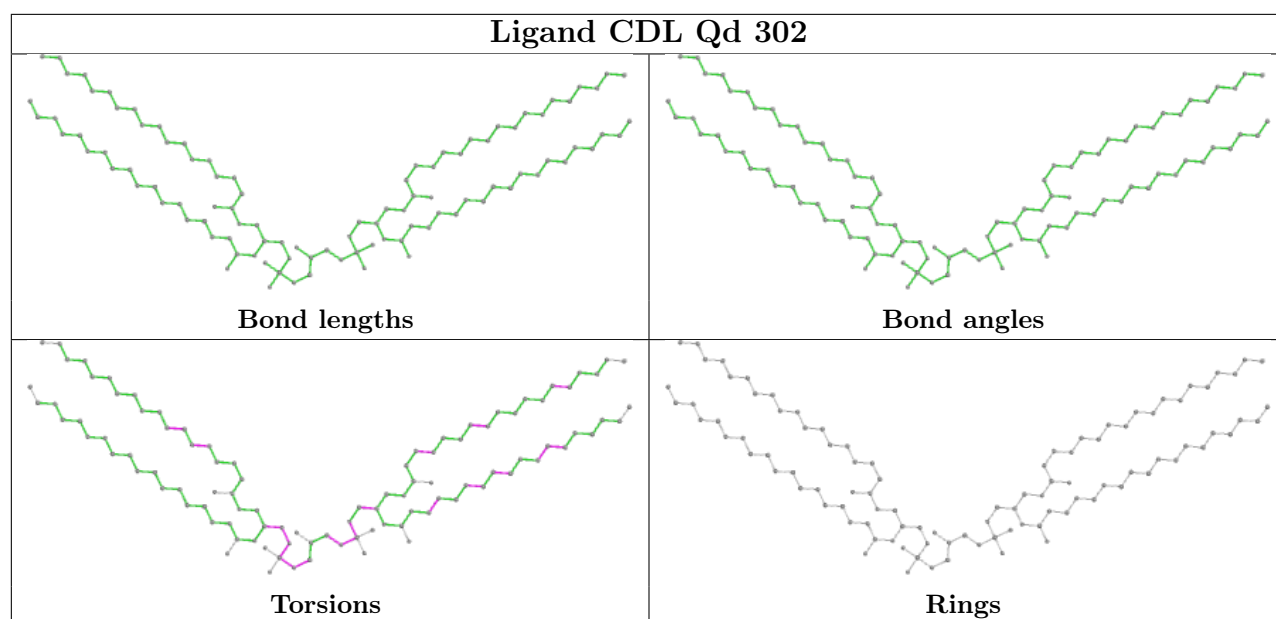
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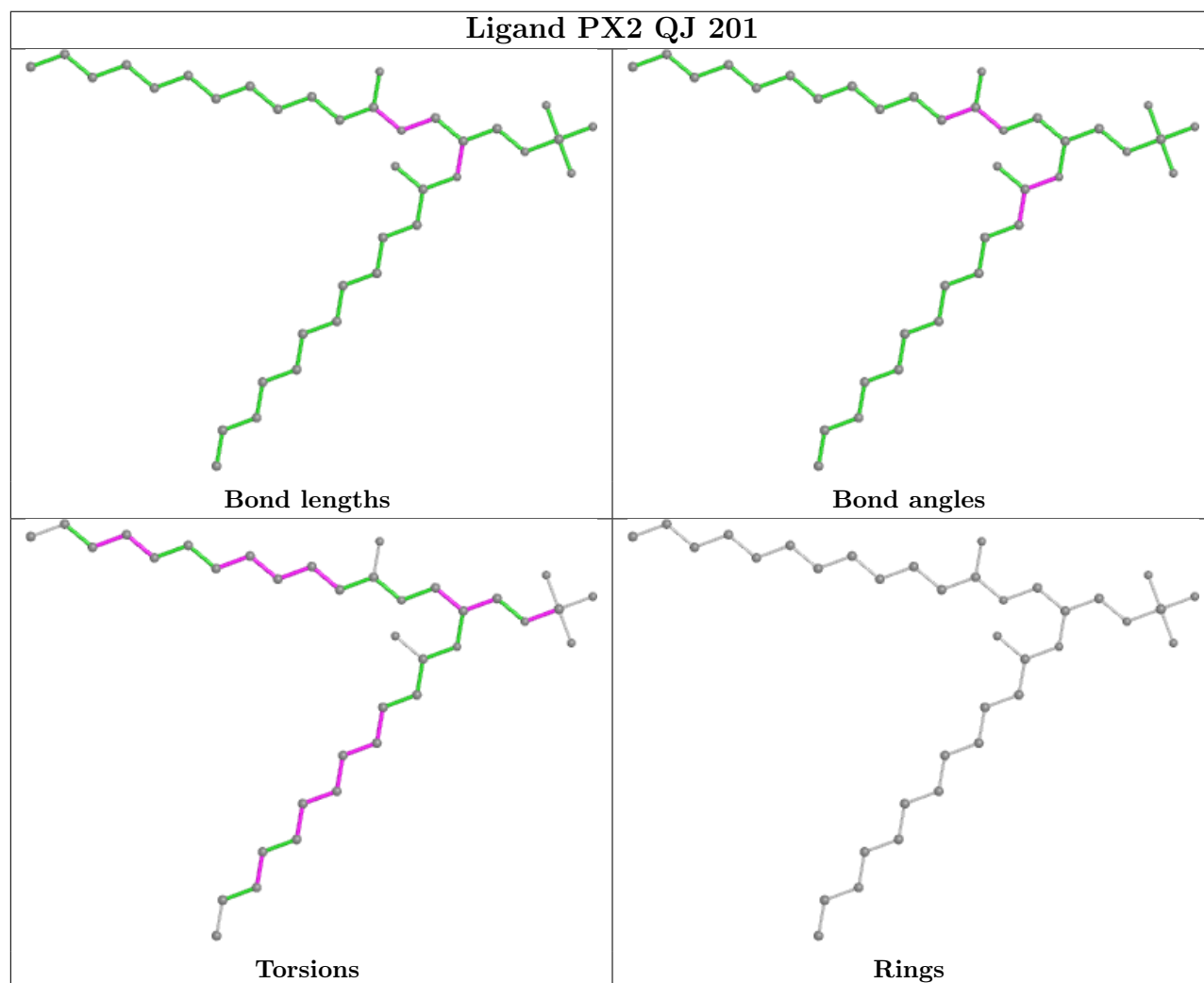
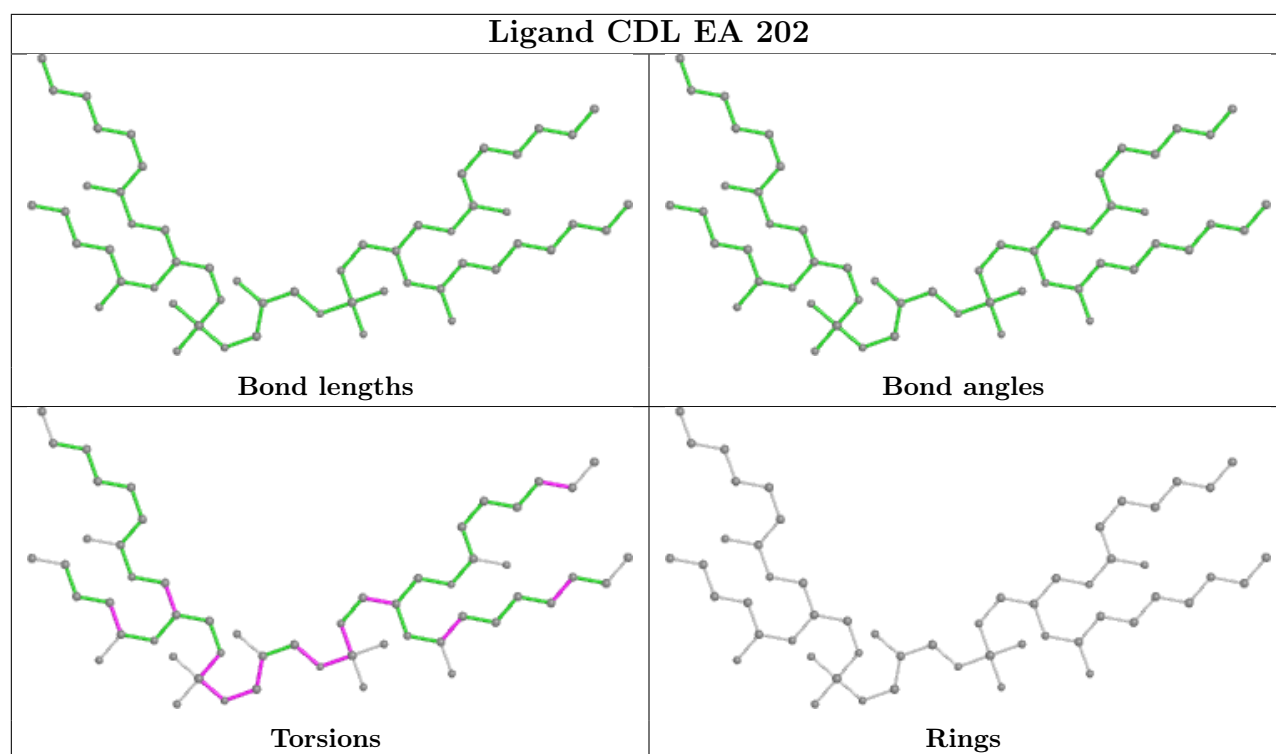


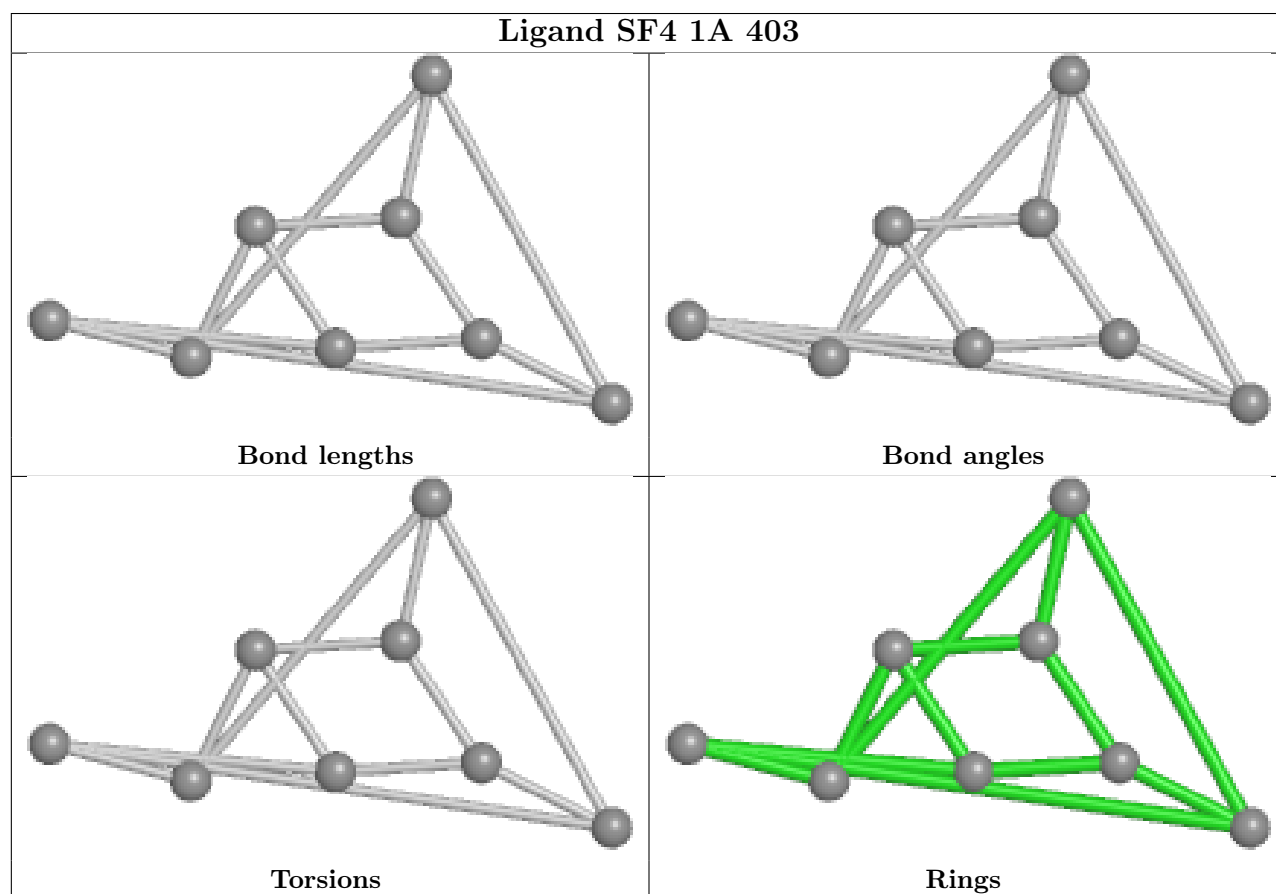
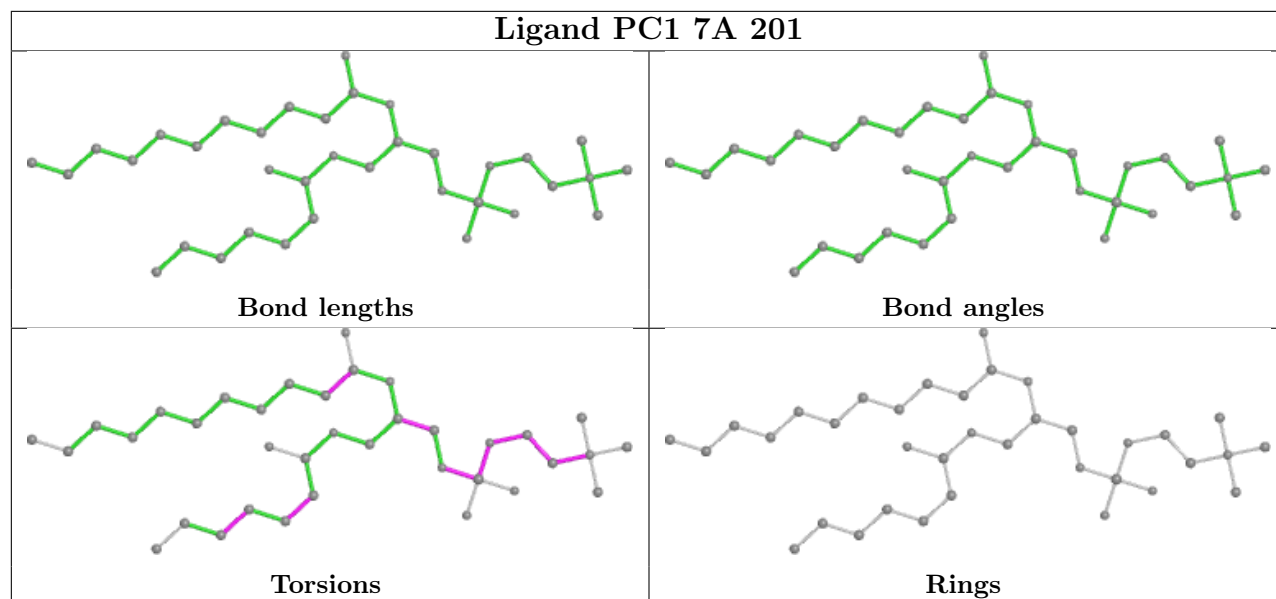


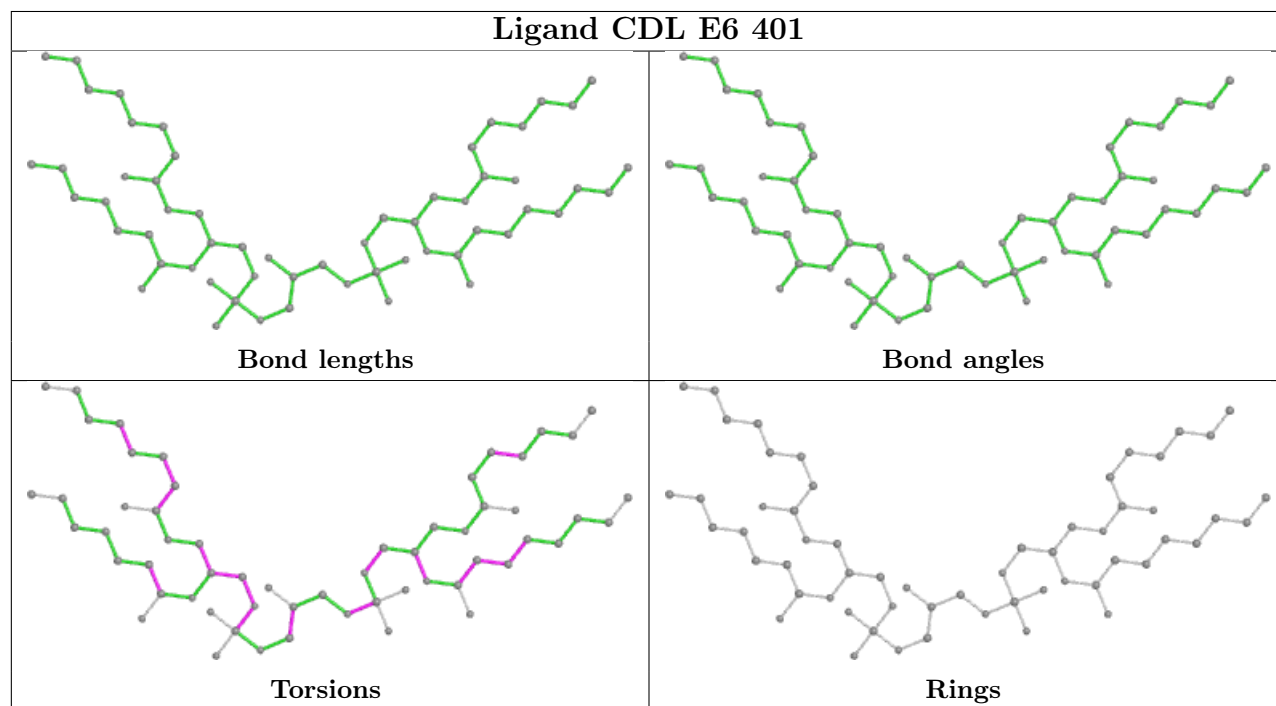
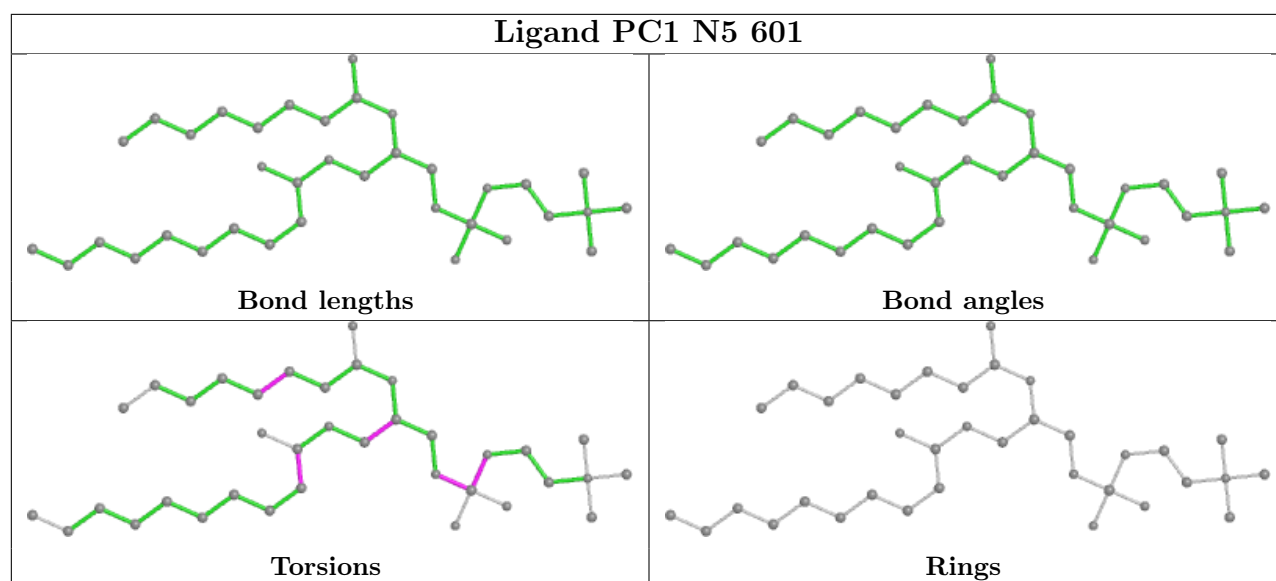


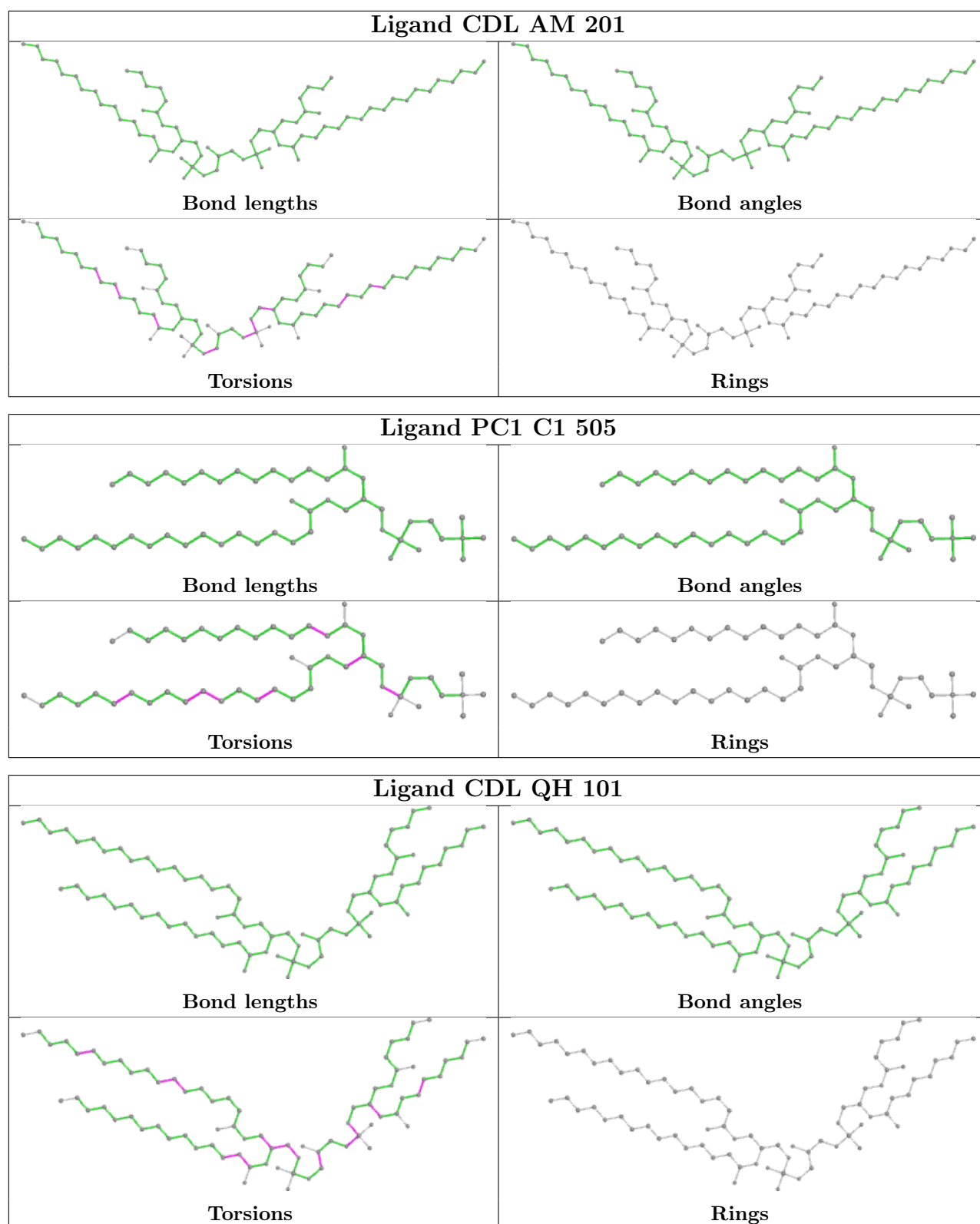


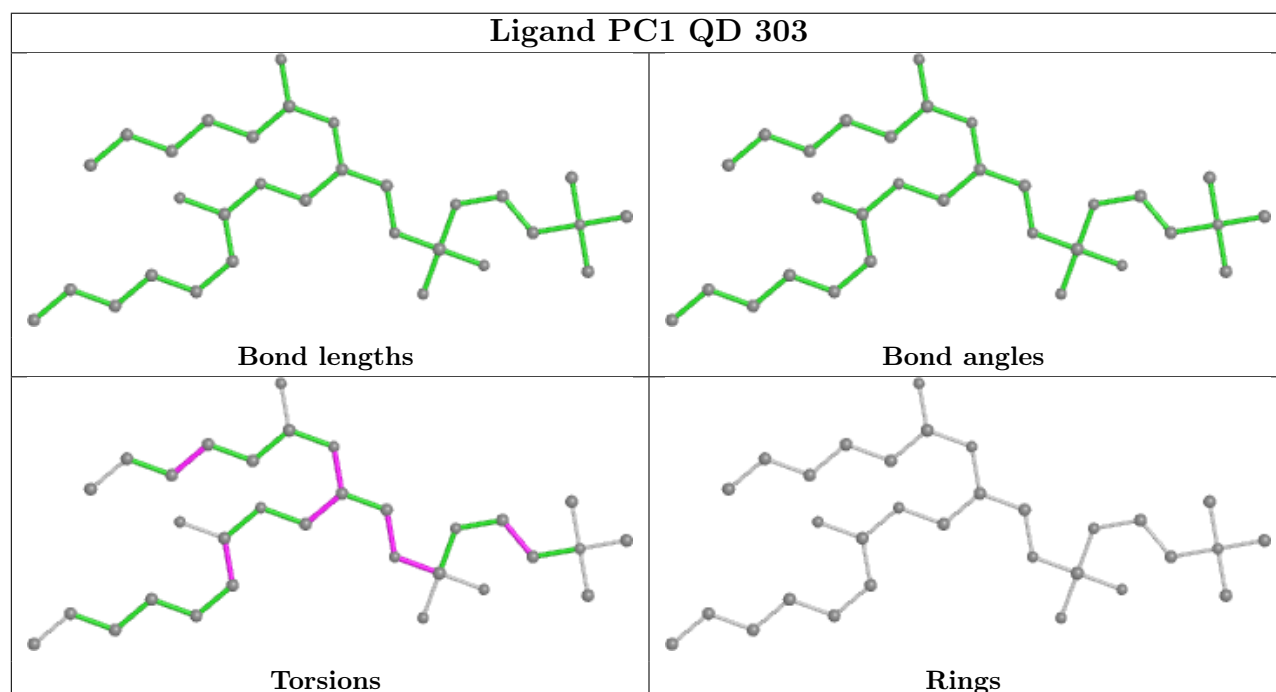
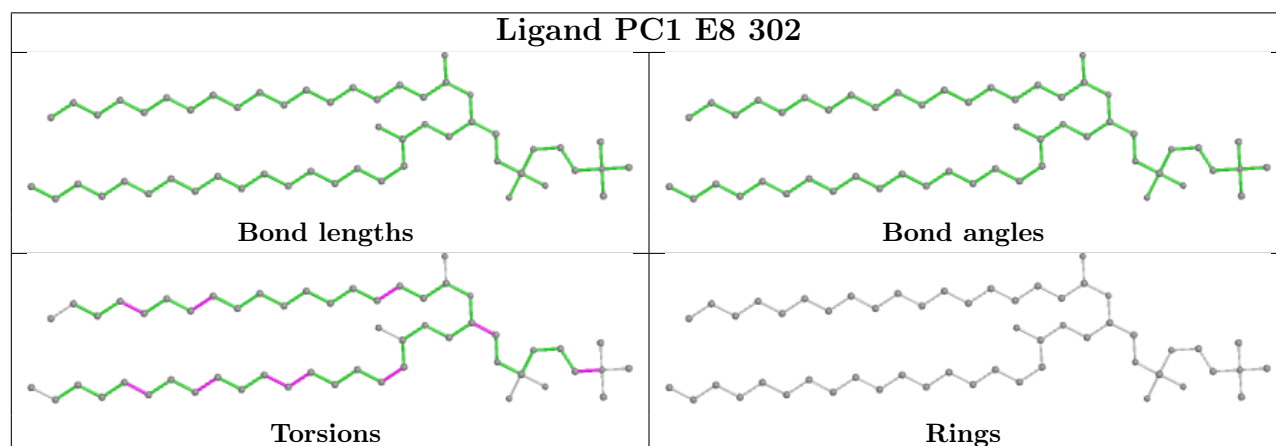
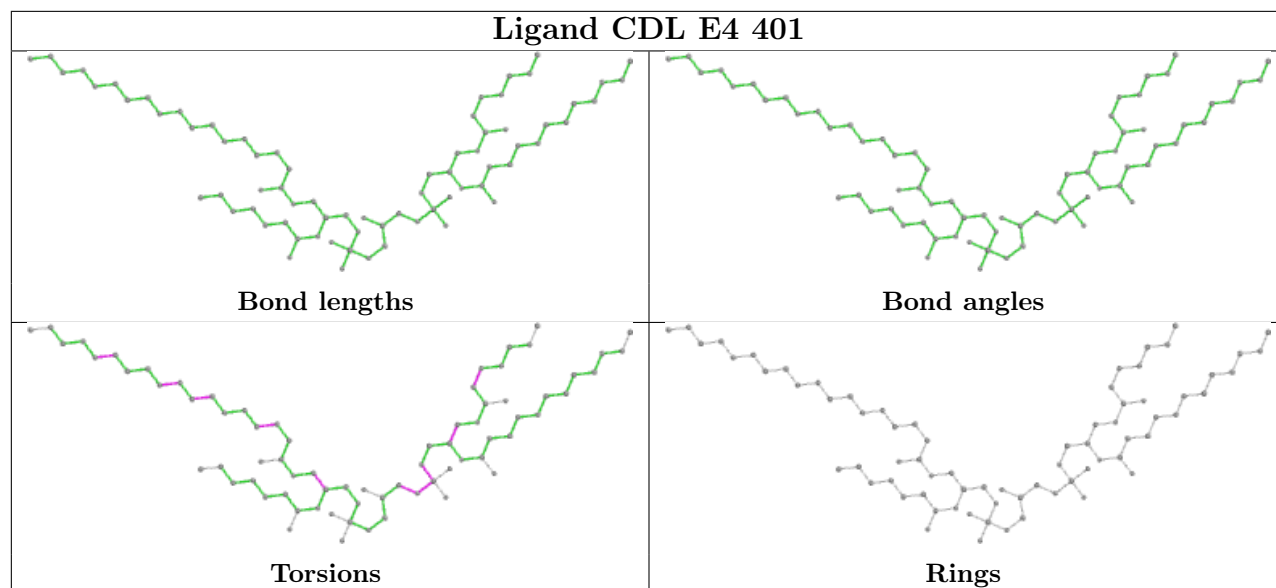


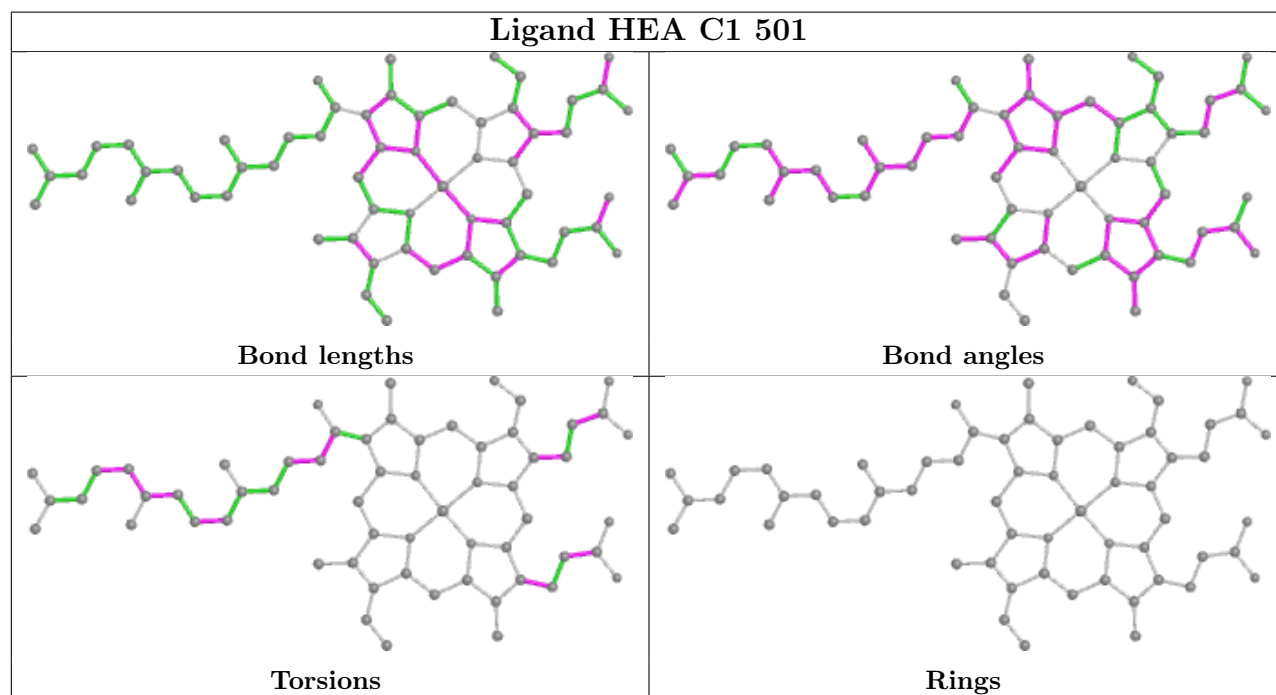
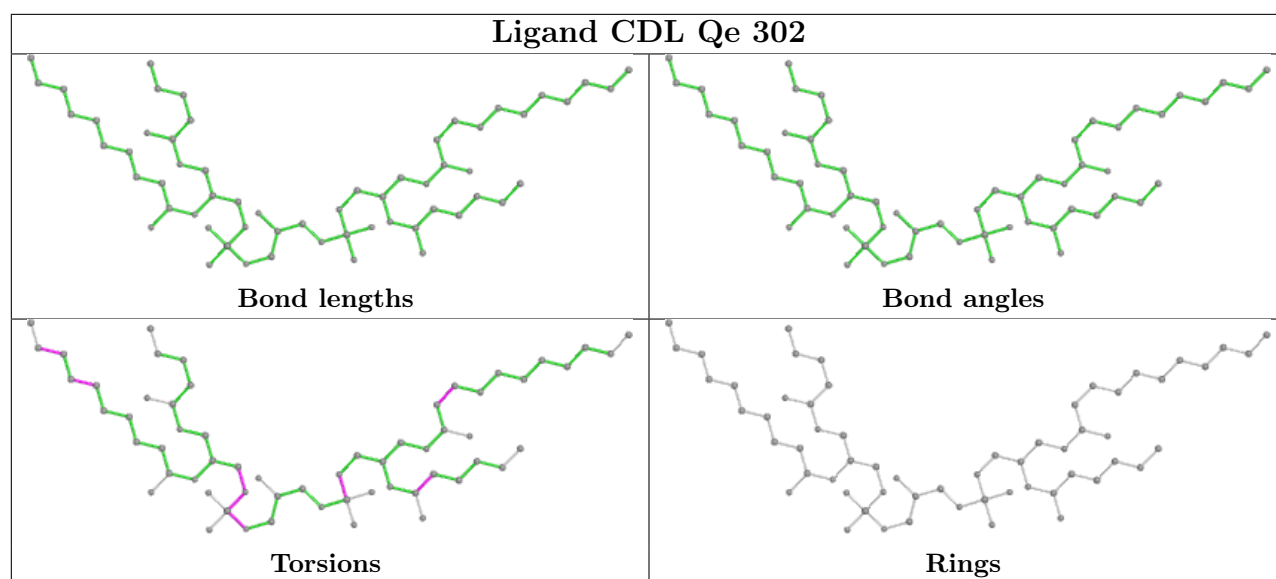


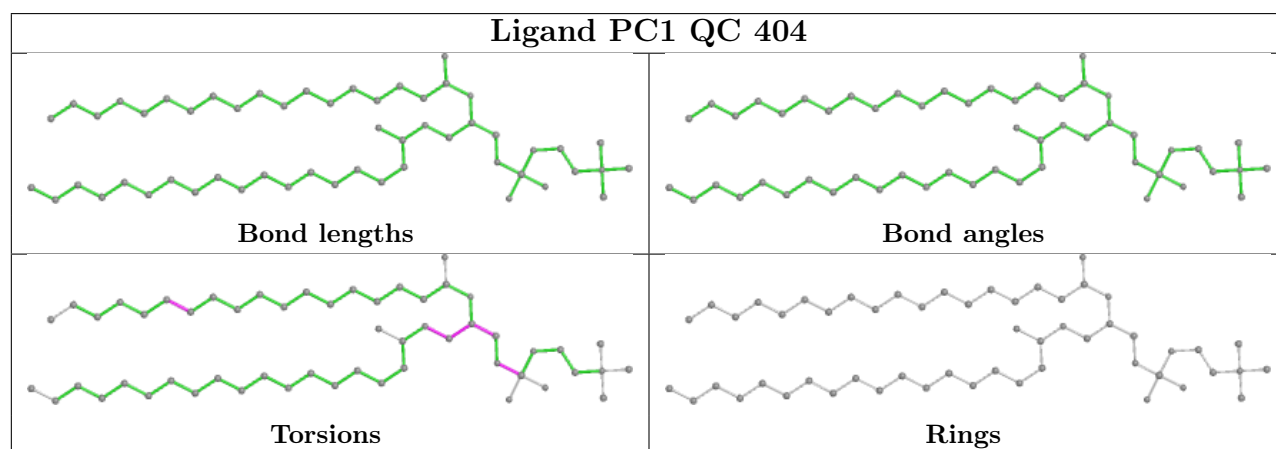
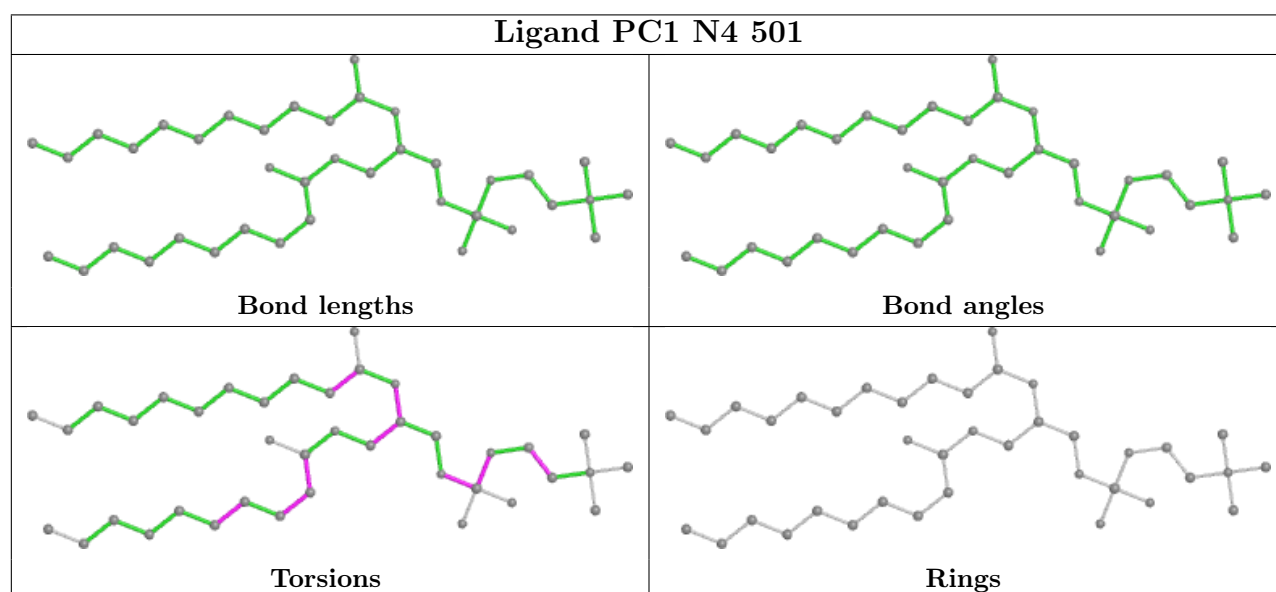
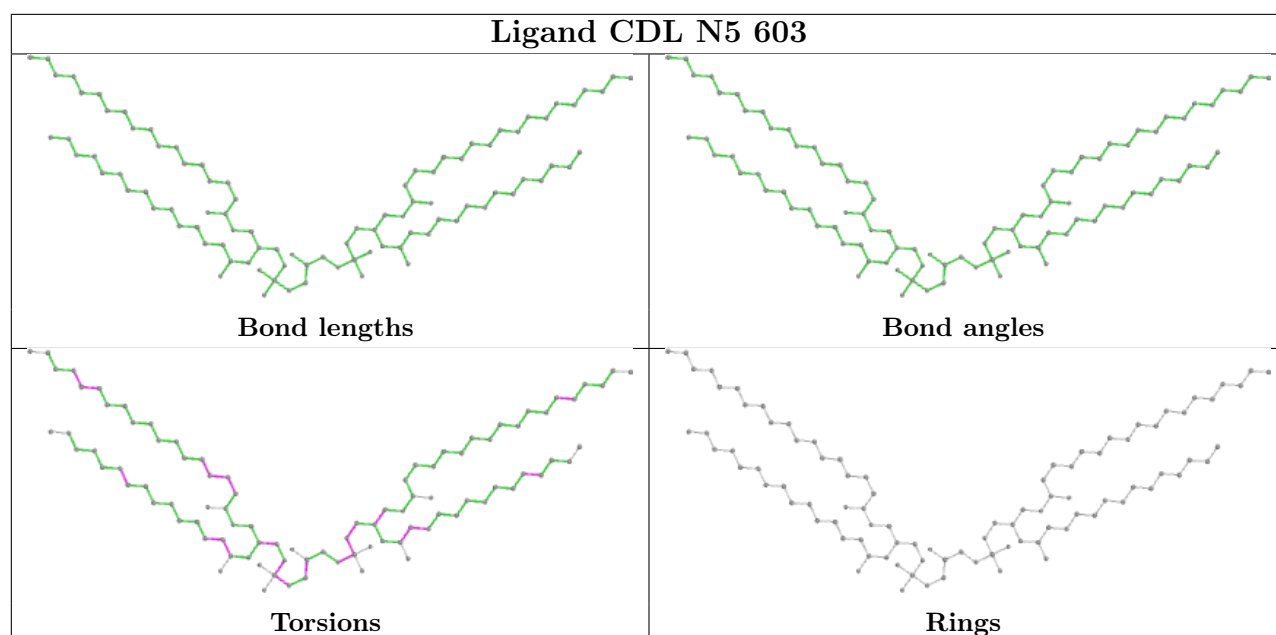


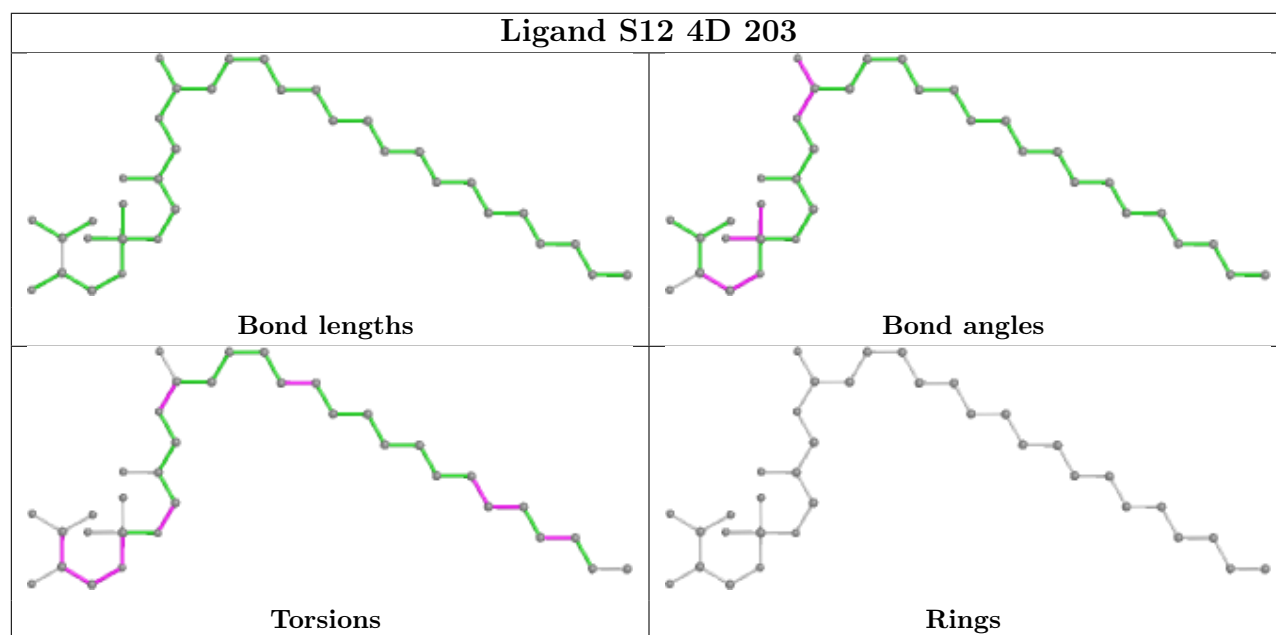
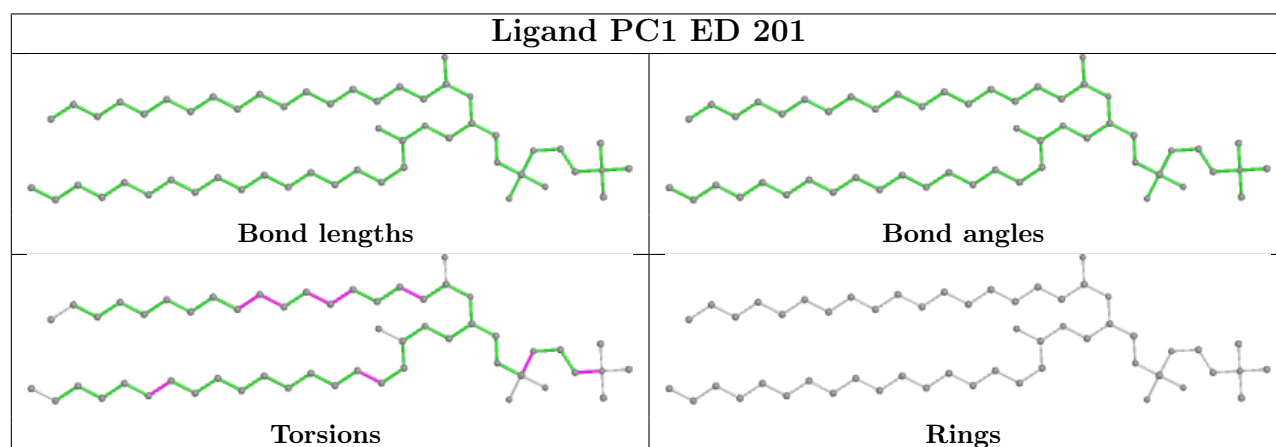
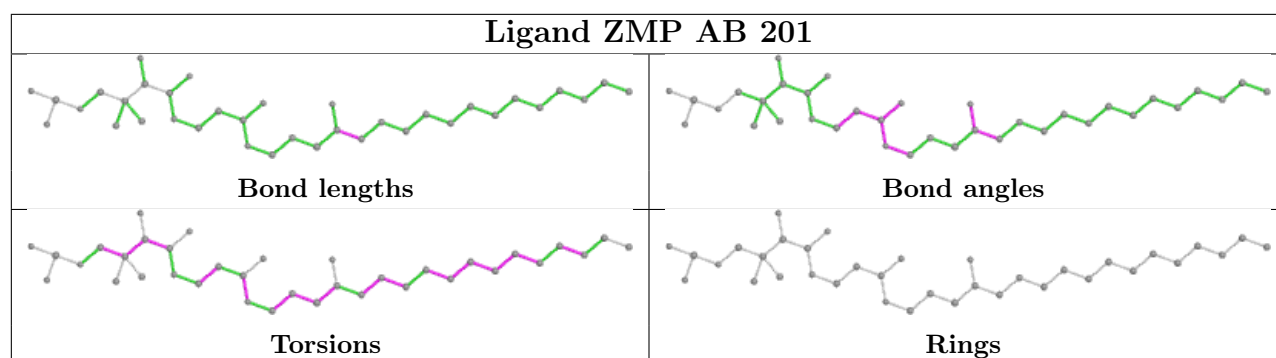


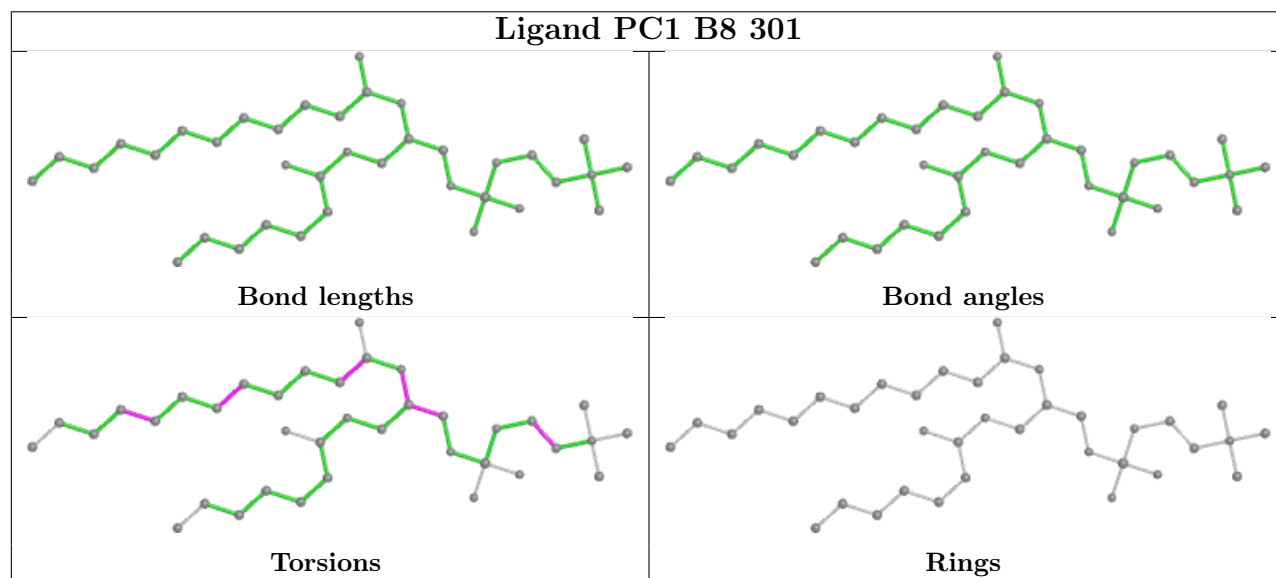
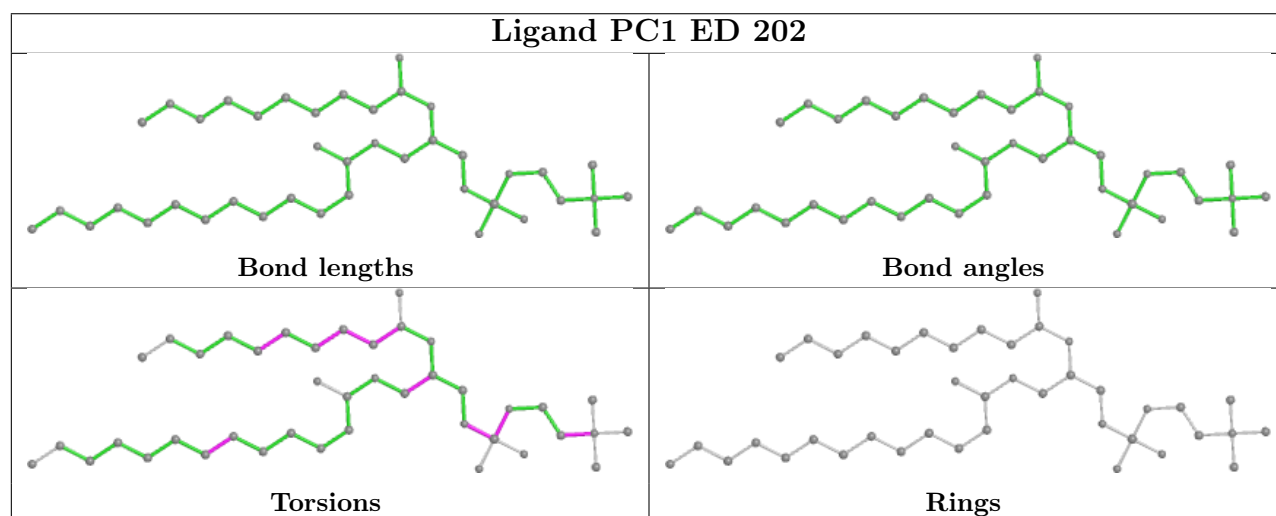
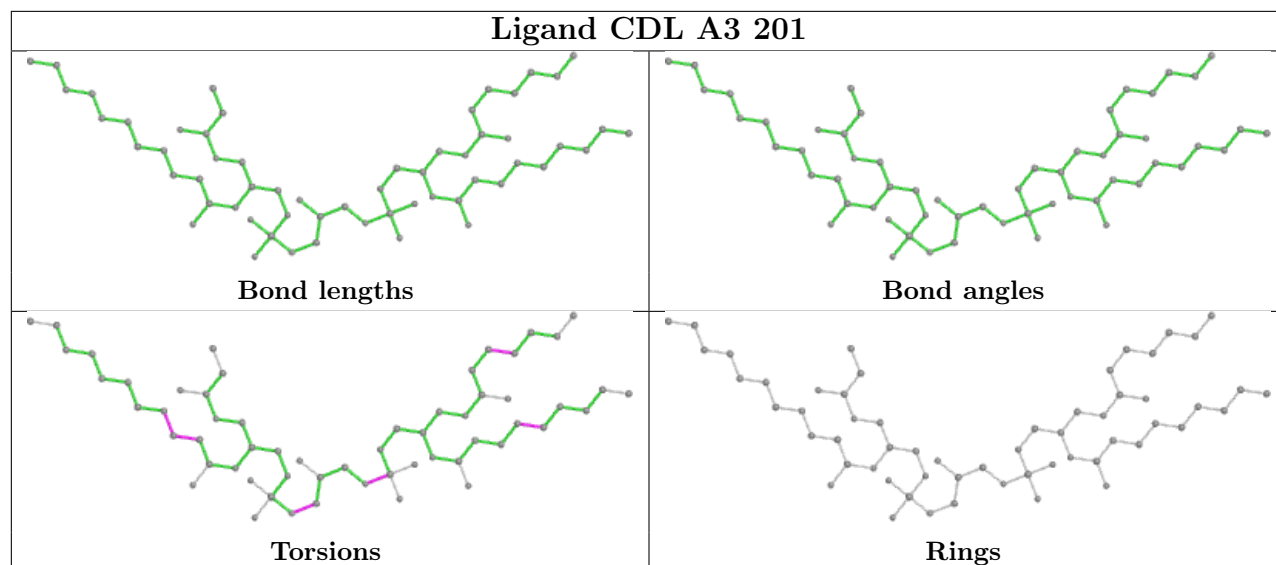


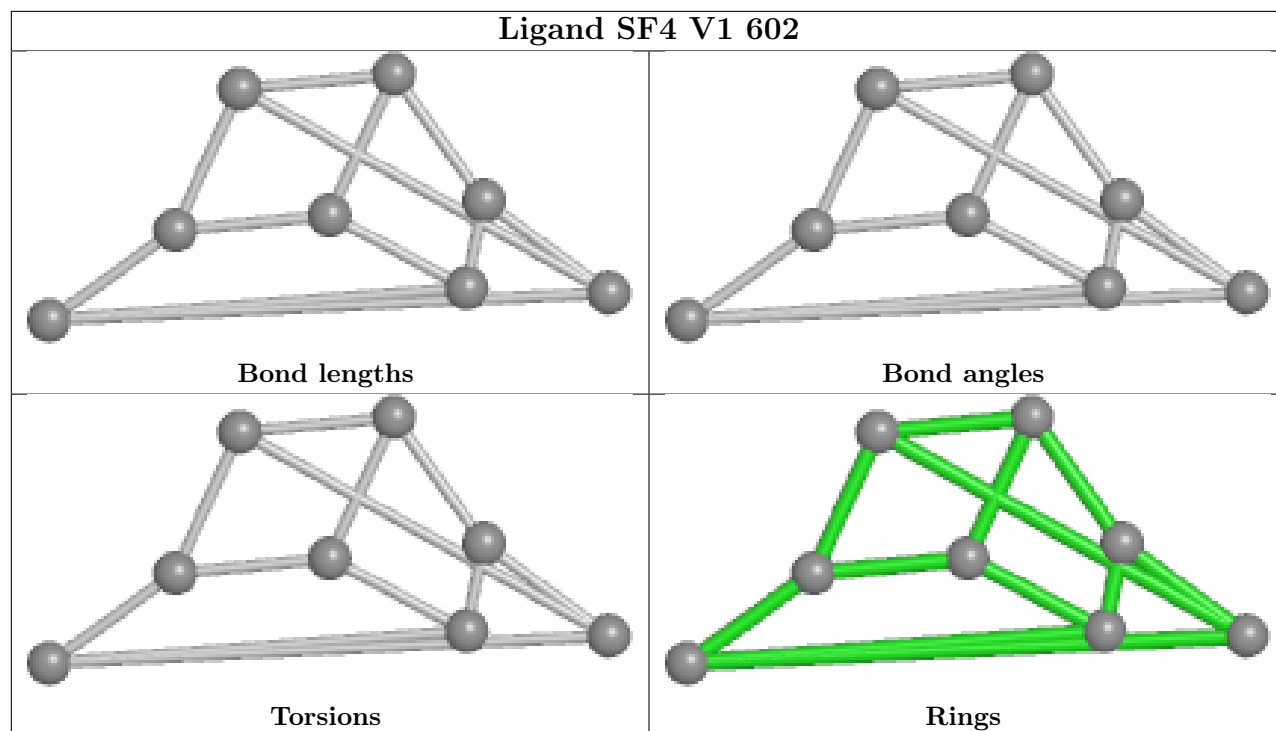












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.