



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 06:26 AM JST

PDB ID : 8GYM
EMDB ID : EMD-34373
Title : Cryo-EM structure of Tetrahymena thermophila respiratory mega-complex
MC IV2+(I+III2+II)2
Authors : Wu, M.C.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on : 2022-09-23
Resolution : 2.96 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:

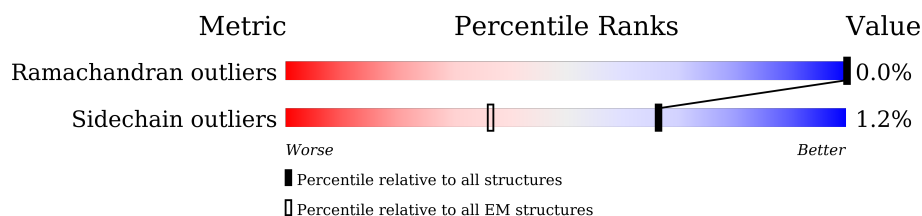
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.96 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.




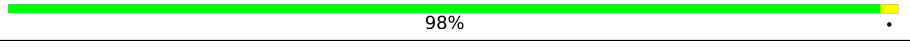
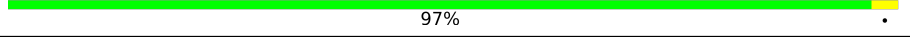
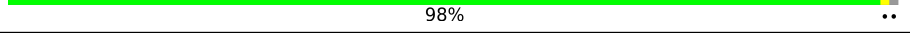
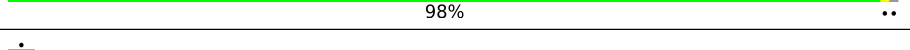
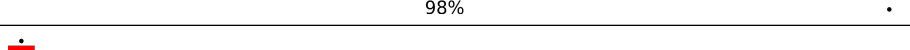
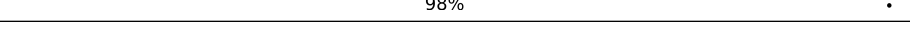

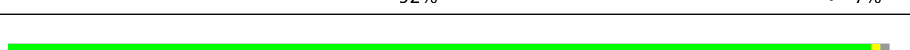

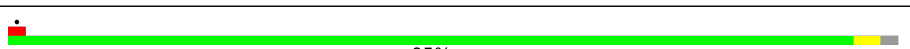
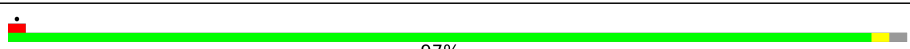


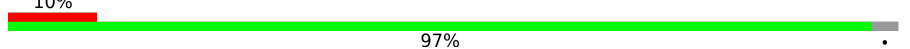
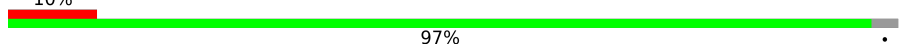






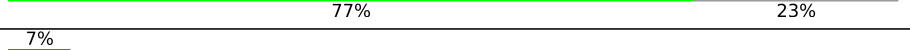


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1T	72	 96%
1	1t	72	 96%
2	2E	322	 6% 98%
2	2e	322	 6% 98%
3	2F	296	 72% 27%
3	2f	296	 72% 27%
4	2G	198	 99%
4	2g	198	 99%
5	2H	195	 52% 48%

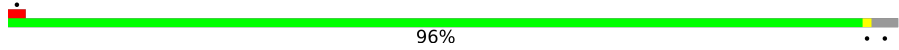
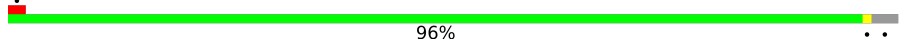
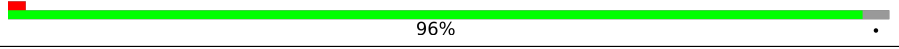
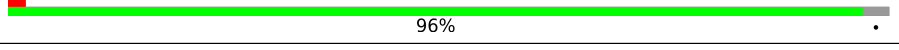
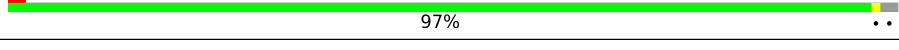
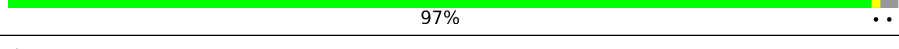
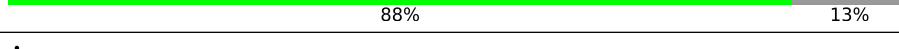
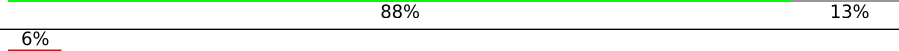
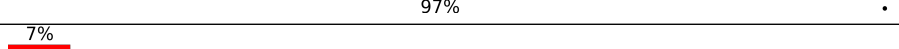
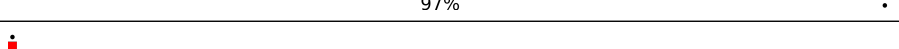
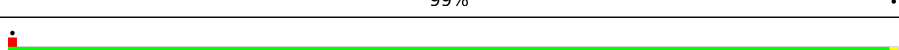
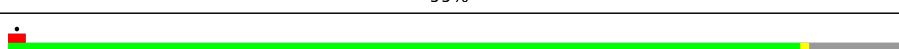
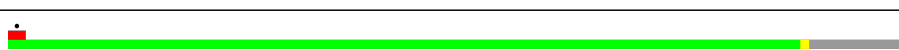







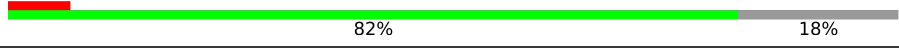
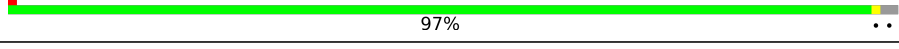
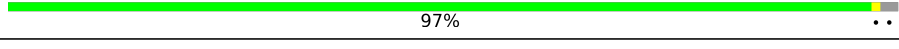
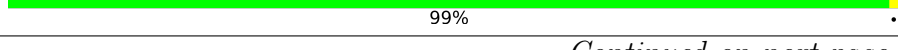

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	2h	195	
6	2I	114	
6	2i	114	
7	2J	103	
7	2j	103	
8	2K	93	
8	2k	93	
9	2L	89	
9	2l	89	
10	2M	76	
10	2m	76	
11	2N	62	
11	2n	62	
12	2O	46	
12	2o	46	
13	2T	72	
13	2t	72	
14	3T	93	
14	3t	93	
15	4A	127	
15	4a	127	
16	4T	68	
16	4t	68	
17	5T	81	
17	5t	81	

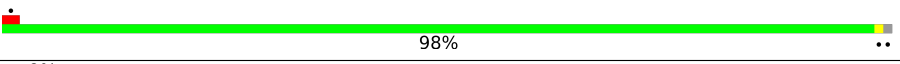
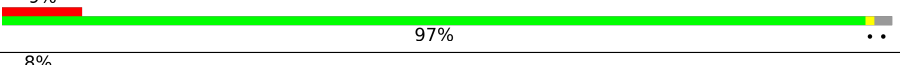
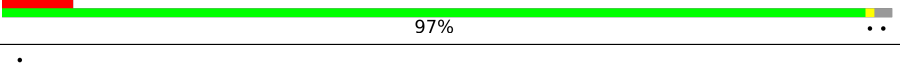


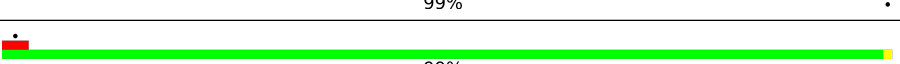
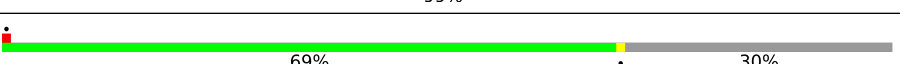
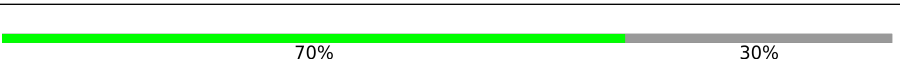
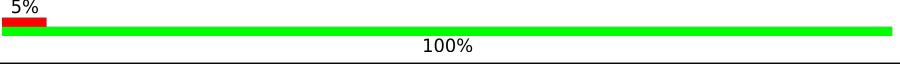
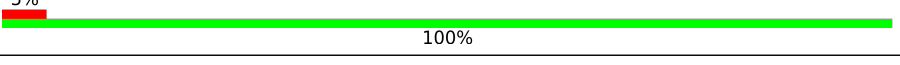
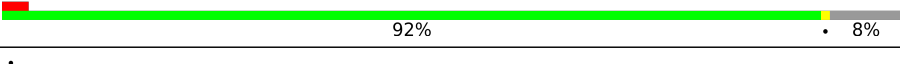
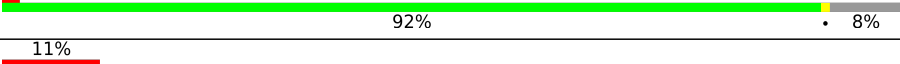
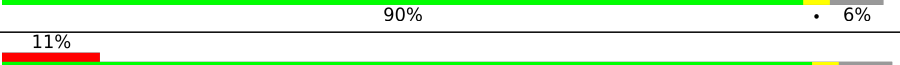
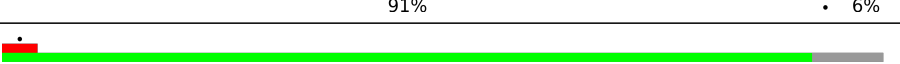
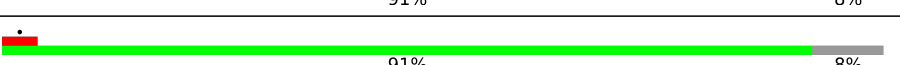


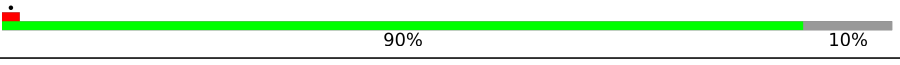
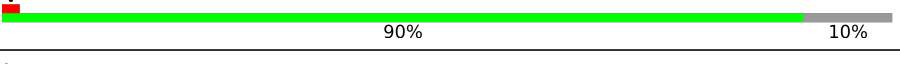


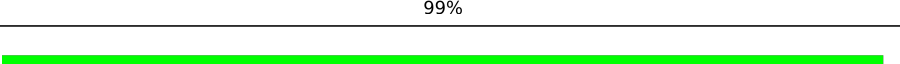
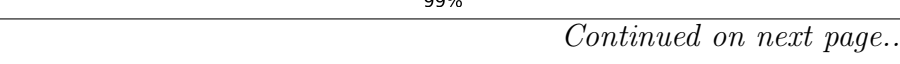


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	6A	130	
18	6a	130	
19	6B	230	
19	6b	230	
20	6C	103	
20	6c	103	
21	6L	88	
21	6l	88	
22	6T	72	
22	6t	72	
23	7A	133	
23	7a	133	
24	7C	236	
24	7c	236	
25	7L	990	
25	7l	990	
26	A	490	
26	a	490	
27	B	473	
27	b	473	
28	BP	462	
28	bp	462	
29	C1	688	
29	c1	688	
30	C2	604	

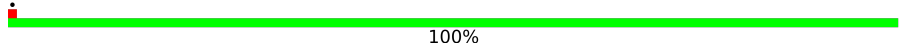
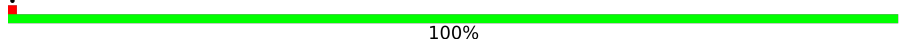
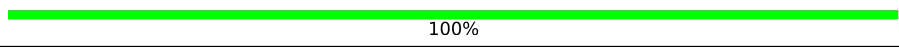
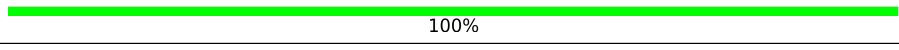
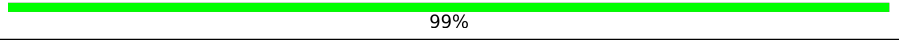
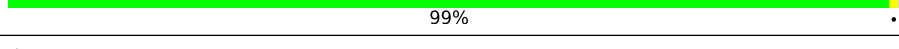
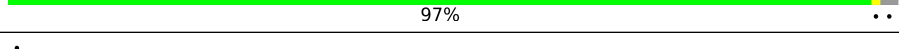
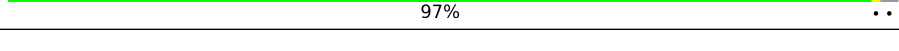
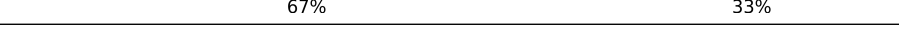
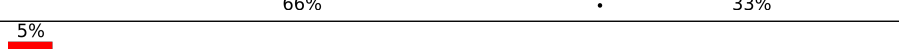
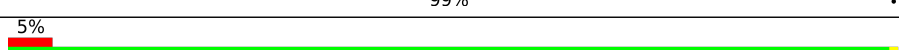
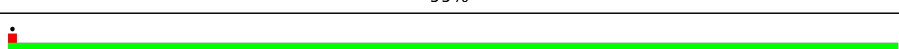
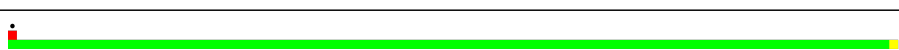
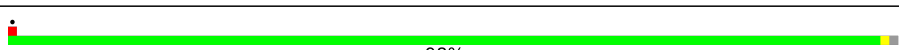
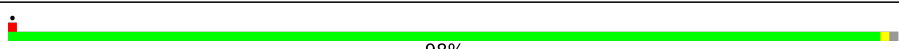
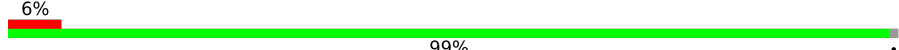
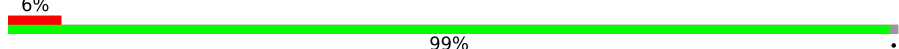
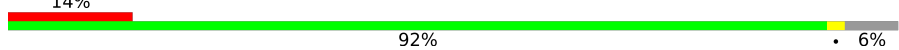
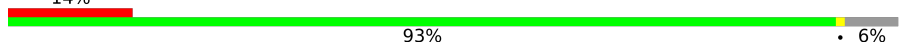

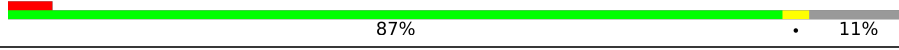
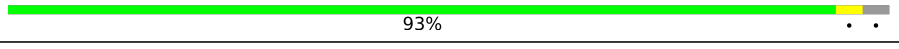
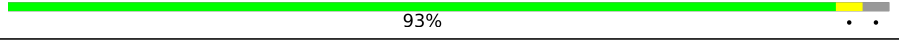
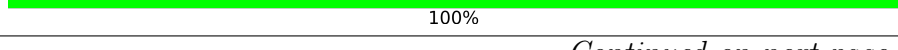

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	c2	604	
31	C3	594	
31	c3	594	
32	D	402	
32	d	402	
33	E	385	
33	e	385	
34	F	348	
34	f	348	
35	FS	188	
35	fs	188	
36	G	318	
36	g	318	
37	H	318	
37	h	318	
38	I	252	
38	i	252	
39	J	234	
39	j	234	
40	K	231	
40	k	231	
41	L	222	
41	l	222	
42	M	220	
42	m	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
43	M1	346	 100%
43	m1	346	 100%
44	M2	318	 100%
44	m2	318	 100%
45	M3	330	 99%
45	m3	330	 99%
46	N	210	 97%
46	n	210	 97%
47	O	193	 67% 33%
47	o	193	 66% 33%
48	P	175	 99%
48	p	175	 99%
49	Q	173	 100%
49	q	173	 99%
50	R	173	 98%
50	r	173	 98%
51	S	170	 99%
51	s	170	 99%
52	SA	636	 92% 6%
52	sa	636	 93% 6%
53	SB	312	 86% 11%
53	sb	312	 87% 11%
54	SC	60	 93%
54	sc	60	 93%
55	SD	44	 100%

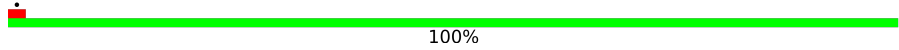
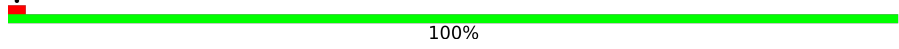
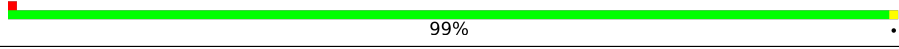
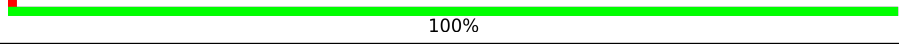
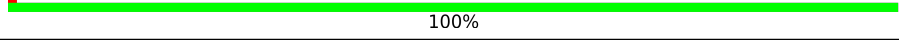
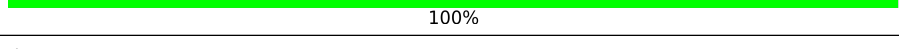
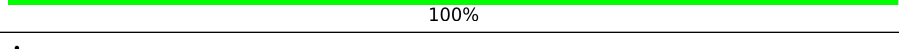
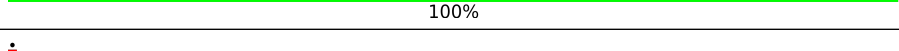
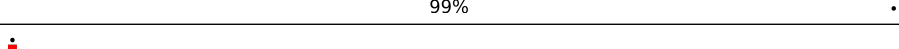
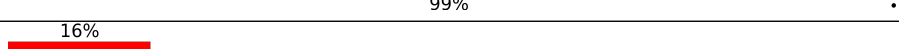
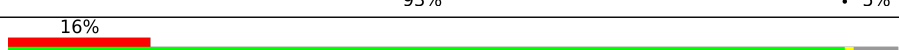
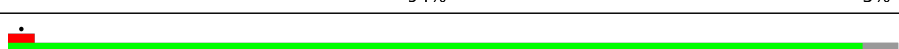
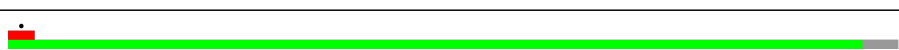

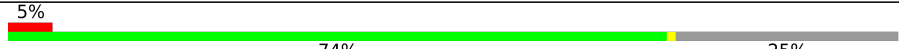
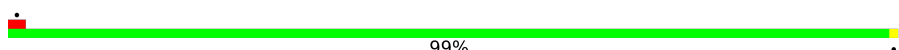
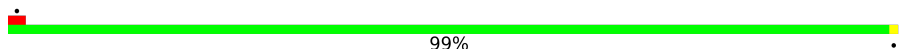
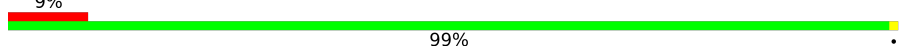
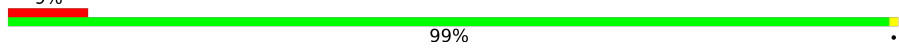

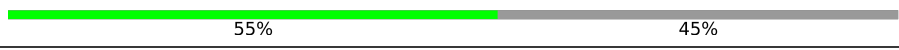
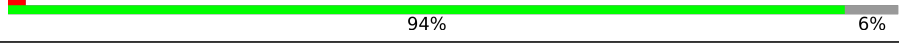
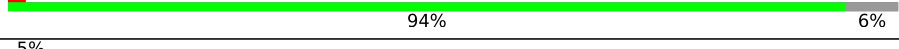


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	sd	44	100%
56	T	158	98%
56	t	158	98%
57	U	154	98%
57	u	154	98%
58	V	149	98%
58	v	149	98%
59	VB	637	86% 13%
59	vb	637	86% 13%
60	W	124	98%
60	w	124	98%
61	X	122	99%
61	x	122	99%
62	Y	105	99%
62	y	105	99%
63	Y0	89	100%
63	y0	89	100%
64	Y5	190	8% 100%
64	y5	190	8% 100%
65	Y7	453	7% 75% 24%
65	y7	453	7% 75% 24%
66	Z	90	6% 94%
66	z	90	6% 94%
67	Z1	100	97%
67	z1	100	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
68	1B	59	 100%
68	1b	59	 100%
69	2B	178	 99%
69	2b	178	 100%
70	4L	116	 100%
70	4l	116	 100%
71	5B	100	 100%
71	5b	100	 100%
72	A1	94	 99%
72	a1	94	 99%
73	A2	103	 16% 93% 5%
73	a2	103	 16% 94% 5%
74	A3	135	 96%
74	a3	135	 96%
75	A5	206	 5% 74% 25%
75	a5	206	 5% 74% 25%
76	A6	172	 99%
76	a6	172	 99%
77	A7	282	 9% 99%
77	a7	282	 9% 99%
78	A8	238	 55% 45%
78	a8	238	 55% 45%
79	A9	362	 94% 6%
79	a9	362	 94% 6%
80	AB	138	 5% 80% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
80	ab	138	
81	AC	133	
81	ac	133	
82	AL	194	
82	al	194	
83	AM	175	
83	am	175	
84	AN	231	
84	an	231	
85	B2	126	
85	b2	126	
86	B3	83	
86	b3	83	
87	B4	147	
87	b4	147	
88	B6	129	
88	b6	129	
89	B7	120	
89	b7	120	
90	B8	207	
90	b8	207	
91	B9	189	
91	b9	189	
92	BL	188	
92	bl	188	

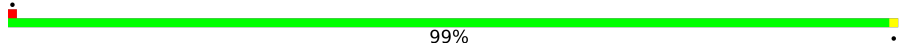

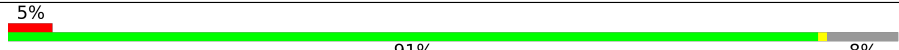
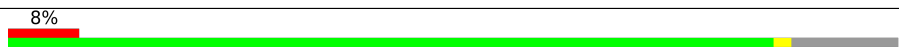

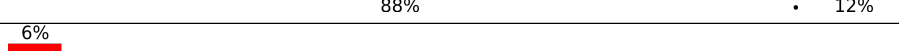
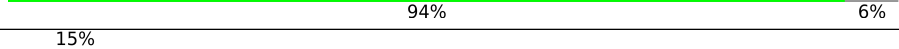
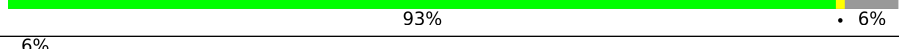
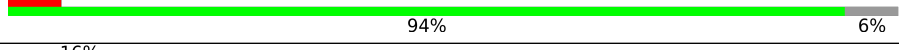
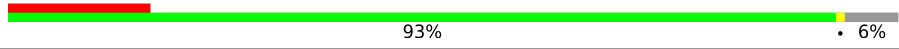
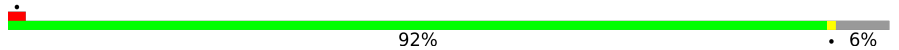
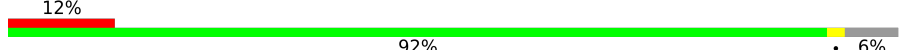
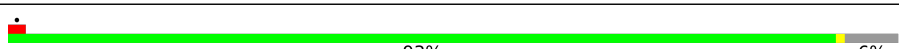

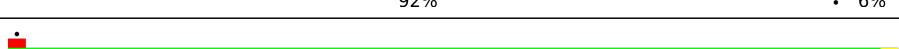
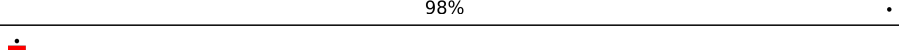
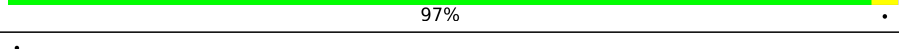
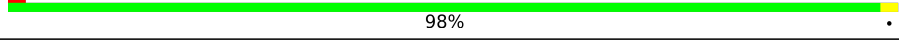
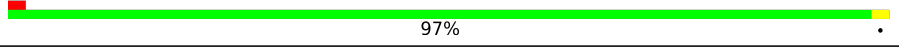
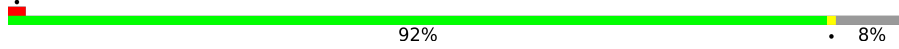
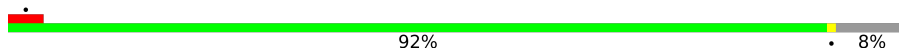
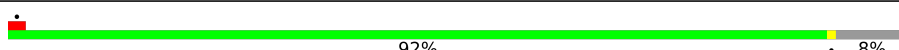

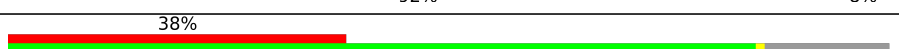
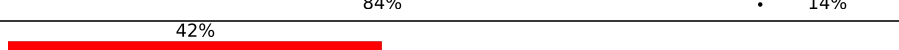
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
93	BM	214	
93	bm	214	
94	C4	102	
94	c4	102	
95	FX	172	
95	fx	172	
96	G1	257	
96	g1	257	
97	G2	233	
97	g2	233	
98	G3	346	
98	g3	346	
99	J1	317	
99	j1	317	
100	N1	284	
100	n1	284	
101	N2	360	
101	n2	360	
102	N3	121	
102	n3	121	
103	N4	505	
103	n4	505	
104	N5	750	
104	n5	750	
105	N6	255	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
105	n6	255	
106	P1	251	
106	p1	251	
107	P2	189	
107	p2	189	
108	QA	482	
108	Qa	482	
108	qA	482	
108	qa	482	
109	QB	513	
109	Qb	513	
109	qB	513	
109	qb	513	
110	QC	426	
110	Qc	426	
110	qC	426	
110	qc	426	
111	QD	319	
111	Qd	319	
111	qD	319	
111	qd	319	
112	QE	269	
112	Qe	269	
112	qE	269	
112	qe	269	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
113	QF	90	11% 98% ..
113	Qf	90	30% 89% 11%
113	qF	90	11% 98% ..
113	qf	90	31% 89% 11%
114	QG	328	21% 98% .
114	Qg	328	20% 98% ..
114	qG	328	21% 98% .
114	qg	328	20% 98% ..
115	QH	130	98% ..
115	Qh	130	. 99% .
115	qH	130	. 98% ..
115	qh	130	. 99% .
116	QI	119	. 95% . .
116	Qi	119	12% 95% . .
116	qI	119	. 94% . .
116	qi	119	12% 95% . .
117	QJ	62	5% 90% 10%
117	Qj	62	11% 92% . 6%
117	qJ	62	5% 90% 10%
117	qj	62	11% 92% . 6%
118	QL	41	15% 78% 22%
118	Ql	41	7% 78% 22%
118	qL	41	15% 78% 22%
118	ql	41	7% 78% 22%
119	QM	17	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
119	Qm	17	100%
119	U2	17	100%
119	qM	17	100%
119	qm	17	100%
119	u2	17	100%
120	S1	718	9% 95% . .
120	s1	718	8% 95% . .
121	S2	442	. 97% .
121	s2	442	. 98% .
122	S3	198	. 98% .
122	s3	198	. 98% .
123	S4	185	11% 96% . .
123	s4	185	11% 96% . .
124	S5	94	6% 96% . .
124	s5	94	6% 97% . .
125	S6	132	12% 68% . 30%
125	s6	132	11% 69% . 30%
126	S7	162	. 95% . .
126	s7	162	. 96% . .
127	S8	236	92% 8%
127	s8	236	92% 8%
128	T1	516	21% 96% . .
128	t1	516	21% 96% . .
129	T2	333	57% 82% . 16%
129	t2	333	57% 82% . 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
130	T3	311	
130	t3	311	
131	T4	212	
131	t4	212	
132	T5	205	
132	t5	205	
133	T6	144	
133	t6	144	
134	T7	143	
134	t7	143	
135	T8	135	
135	t8	135	
136	T9	136	
136	t9	136	
137	TA	127	
137	ta	127	
138	TB	113	
138	tb	113	
139	TC	93	
139	tc	93	
140	TD	73	
140	td	73	
141	TE	71	
141	te	71	
142	TF	236	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
142	tf	236	
143	TG	135	
143	tg	135	
144	TH	124	
144	th	124	
145	TX	166	
145	tx	166	
146	V1	474	
146	v1	474	
147	V2	274	
147	v2	274	
148	X1	150	
148	x1	150	
149	C	212	
149	c	212	
150	U1	92	
150	u1	92	

2 Entry composition

There are 171 unique types of molecules in this entry. The entry contains 568568 atoms, of which 0 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 Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1t	70	Total	C	N	O	S	0	0
			540	329	98	109	4		
1	1T	70	Total	C	N	O	S	0	0
			540	329	98	109	4		

- Molecule 2 is a protein called NmrA domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2e	321	Total	C	N	O	S	0	0
			2560	1623	449	487	1		
2	2E	321	Total	C	N	O	S	0	0
			2560	1623	449	487	1		

- Molecule 3 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2f	217	Total	C	N	O	S	0	0
			1803	1166	305	328	4		
3	2F	217	Total	C	N	O	S	0	0
			1803	1166	305	328	4		

- Molecule 4 is a protein called SDHTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2g	198	Total	C	N	O	S	0	0
			1671	1083	276	307	5		
4	2G	198	Total	C	N	O	S	0	0
			1671	1083	276	307	5		

- Molecule 5 is a protein called Dipthamide synthesis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2h	102	Total	C	N	O	S	0	0
			801	497	139	157	8		
5	2H	102	Total	C	N	O	S	0	0
			801	497	139	157	8		

- Molecule 6 is a protein called DUF4885 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2i	114	Total	C	N	O	S	0	0
			915	580	153	180	2		
6	2I	114	Total	C	N	O	S	0	0
			915	580	153	180	2		

- Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2j	102	Total	C	N	O	S	0	0
			839	549	139	149	2		
7	2J	102	Total	C	N	O	S	0	0
			839	549	139	149	2		

- Molecule 8 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2k	93	Total	C	N	O	S	0	0
			795	530	129	134	2		
8	2K	93	Total	C	N	O	S	0	0
			795	530	129	134	2		

- Molecule 9 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2l	83	Total	C	N	O	S	0	0
			722	467	120	134	1		
9	2L	83	Total	C	N	O	S	0	0
			722	467	120	134	1		

- Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2m	75	Total	C	N	O	S	0	0
			640	412	116	110	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2M	75	Total	C	N	O	S	0	0
			640	412	116	110	2		

- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2n	61	Total	C	N	O	S	0	0
			505	341	78	84	2		
11	2N	61	Total	C	N	O	S	0	0
			505	341	78	84	2		

- Molecule 12 is a protein called SDHTT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2o	42	Total	C	N	O	S	0	0
			356	239	59	56	2		
12	2O	42	Total	C	N	O	S	0	0
			356	239	59	56	2		

- Molecule 13 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2t	70	Total	C	N	O	S	0	0
			567	353	100	110	4		
13	2T	70	Total	C	N	O	S	0	0
			567	353	100	110	4		

- Molecule 14 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3t	83	Total	C	N	O	S	0	0
			655	412	109	128	6		
14	3T	83	Total	C	N	O	S	0	0
			655	412	109	128	6		

- Molecule 15 is a protein called Phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4a	100	Total	C	N	O	S	0	0
			816	519	144	151	2		
15	4A	100	Total	C	N	O	S	0	0
			816	519	144	151	2		

- Molecule 16 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4t	57	Total	C	N	O	S	0	0
			481	308	80	90	3		
16	4T	57	Total	C	N	O	S	0	0
			481	308	80	90	3		

- Molecule 17 is a protein called Cullin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5t	62	Total	C	N	O	S	0	0
			506	322	89	93	2		
17	5T	62	Total	C	N	O	S	0	0
			506	322	89	93	2		

- Molecule 18 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6a	126	Total	C	N	O	S	0	0
			1083	698	184	199	2		
18	6A	126	Total	C	N	O	S	0	0
			1083	698	184	199	2		

- Molecule 19 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6b	222	Total	C	N	O	S	0	0
			1912	1238	312	349	13		
19	6B	222	Total	C	N	O	S	0	0
			1912	1238	312	349	13		

- Molecule 20 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6c	101	Total	C	N	O	S	0	0
			891	580	158	150	3		
20	6C	101	Total	C	N	O	S	0	0
			891	580	158	150	3		

- Molecule 21 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6l	77	Total	C	N	O	S	0	0
			636	407	108	115	6		
21	6L	77	Total	C	N	O	S	0	0
			636	407	108	115	6		

- Molecule 22 is a protein called Annexin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6t	70	Total	C	N	O	S	0	0
			561	362	90	105	4		
22	6T	70	Total	C	N	O	S	0	0
			561	362	90	105	4		

- Molecule 23 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7a	133	Total	C	N	O	S	0	0
			1166	769	197	199	1		
23	7A	133	Total	C	N	O	S	0	0
			1166	769	197	199	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7c	211	Total	C	N	O	P S	0	0
			1825	1163	299	354	1 8		
24	7C	211	Total	C	N	O	P S	0	0
			1825	1163	299	354	1 8		

- Molecule 25 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7l	131	Total	C	N	O	S	0	0
			1078	698	175	196	9		
25	7L	131	Total	C	N	O	S	0	0
			1078	698	175	196	9		

- Molecule 26 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	449	Total	C	N	O	S	0	0
			3756	2408	638	701	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	449	Total	C	N	O	S	0	0
			3756	2408	638	701	9		

- Molecule 27 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	428	Total	C	N	O	S	0	0
			3398	2164	593	638	3		
27	B	428	Total	C	N	O	S	0	0
			3398	2164	593	638	3		

- Molecule 28 is a protein called Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	bp	381	Total	C	N	O	S	0	0
			2920	1858	493	567	2		
28	BP	381	Total	C	N	O	S	0	0
			2920	1858	493	567	2		

- Molecule 29 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	674	Total	C	N	O	S	0	0
			5576	3730	910	900	36		
29	C1	674	Total	C	N	O	S	0	0
			5576	3730	910	900	36		

- Molecule 30 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c2	599	Total	C	N	O	S	0	0
			5094	3322	881	880	11		
30	C2	599	Total	C	N	O	S	0	0
			5094	3322	881	880	11		

- Molecule 31 is a protein called Ymf68.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c3	582	Total	C	N	O	S	0	0
			5084	3451	787	838	8		
31	C3	582	Total	C	N	O	S	0	0
			5084	3451	787	838	8		

- Molecule 32 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	289	Total	C	N	O	S	0	0
			2366	1523	400	438	5		
32	D	289	Total	C	N	O	S	0	0
			2366	1523	400	438	5		

- Molecule 33 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	384	Total	C	N	O	S	0	0
			3176	2045	549	575	7		
33	E	384	Total	C	N	O	S	0	0
			3176	2045	549	575	7		

- Molecule 34 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	243	Total	C	N	O	S	0	0
			2024	1304	335	380	5		
34	F	243	Total	C	N	O	S	0	0
			2024	1304	335	380	5		

- Molecule 35 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	fs	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		
35	FS	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	293	Total	C	N	O	S	0	0
			2442	1555	410	465	12		
36	G	293	Total	C	N	O	S	0	0
			2442	1555	410	465	12		

- Molecule 37 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	298	Total	C	N	O	S	0	0
			2369	1500	409	450	10		
37	H	298	Total	C	N	O	S	0	0
			2369	1500	409	450	10		

- Molecule 38 is a protein called COXTT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	231	Total	C	N	O	S	0	0
			1943	1253	340	346	4		
38	I	231	Total	C	N	O	S	0	0
			1943	1253	340	346	4		

- Molecule 39 is a protein called COXTT10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		
39	J	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		
40	K	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		

- Molecule 41 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		
41	L	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		

- Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	219	Total	C	N	O	S	0	0
			1872	1218	315	328	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
42	M	219	Total	C	N	O	S	0	0
			1872	1218	315	328	11		

- Molecule 43 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		
43	M1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		

- Molecule 44 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m2	318	Total	C	N	O	S	0	0
			2558	1665	440	449	4		
44	M2	318	Total	C	N	O	S	0	0
			2558	1665	440	449	4		

- Molecule 45 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		
45	M3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		

- Molecule 46 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		
46	N	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		

- Molecule 47 is a protein called Mobilization protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	129	Total	C	N	O	S	0	0
			1081	675	191	209	6		
47	O	129	Total	C	N	O	S	0	0
			1081	675	191	209	6		

- Molecule 48 is a protein called YfIT domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	175	Total	C	N	O	S	0	0
			1410	889	247	273	1		
48	P	175	Total	C	N	O	S	0	0
			1410	889	247	273	1		

- Molecule 49 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		
49	Q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		

- Molecule 50 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	172	Total	C	N	O	S	0	0
			1407	921	231	252	3		
50	R	172	Total	C	N	O	S	0	0
			1407	921	231	252	3		

- Molecule 51 is a protein called Complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	169	Total	C	N	O	S	0	0
			1388	878	243	263	4		
51	S	169	Total	C	N	O	S	0	0
			1388	878	243	263	4		

- Molecule 52 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sa	599	Total	C	N	O	S	0	0
			4624	2907	825	866	26		
52	SA	599	Total	C	N	O	S	0	0
			4624	2907	825	866	26		

- Molecule 53 is a protein called Succinate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sb	279	Total	C	N	O	S	0	0
			2260	1437	385	417	21		
53	SB	279	Total	C	N	O	S	0	0
			2260	1437	385	417	21		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	sc	58	Total	C	N	O	S	0	0
			481	314	85	82			
54	SC	58	Total	C	N	O	S	0	0
			481	314	85	82			

- Molecule 55 is a protein called SDHD.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	sd	44	Total	C	N	O	S	0	0
			393	271	60	60	2		
55	SD	44	Total	C	N	O	S	0	0
			393	271	60	60	2		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	156	Total	C	N	O	S	0	0
			1315	858	230	223	4		
56	T	156	Total	C	N	O	S	0	0
			1315	858	230	223	4		

- Molecule 57 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	u	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		
57	U	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		

- Molecule 58 is a protein called COXTT22.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	v	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
58	V	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		

- Molecule 59 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	vb	555	Total	C	N	O	P S	0	0
			4630	2918	779	914	2 17		
59	VB	555	Total	C	N	O	P S	0	0
			4630	2918	779	914	2 17		

- Molecule 60 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	w	123	Total	C	N	O	S	0	0
			1096	716	183	193	4		
60	W	123	Total	C	N	O	S	0	0
			1096	716	183	193	4		

- Molecule 61 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	x	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		
61	X	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		

- Molecule 62 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		
62	Y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		

- Molecule 63 is a protein called Ymf70.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	y0	89	Total	C	N	O	S	0	0
			775	535	115	123	2		
63	Y0	89	Total	C	N	O	S	0	0
			775	535	115	123	2		

- Molecule 64 is a protein called Ymf75.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	y5	190	Total	C	N	O	S	0	0
			1659	1141	249	265	4		
64	Y5	190	Total	C	N	O	S	0	0
			1659	1141	249	265	4		

- Molecule 65 is a protein called Ymf67.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	y7	343	Total	C	N	O	S	0	0
			2938	1964	468	500	6		
65	Y7	343	Total	C	N	O	S	0	0
			2938	1964	468	500	6		

- Molecule 66 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	z	87	Total	C	N	O	0	0
			717	459	130	128		
66	Z	87	Total	C	N	O	0	0
			717	459	130	128		

- Molecule 67 is a protein called COXTT28.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	z1	97	Total	C	N	O	S	0	0
			766	489	135	140	2		
67	Z1	97	Total	C	N	O	S	0	0
			766	489	135	140	2		

- Molecule 68 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	1b	59	Total	C	N	O	S	0	0
			516	362	78	73	3		
68	1B	59	Total	C	N	O	S	0	0
			516	362	78	73	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1b	49	VAL	LEU	conflict	UNP Q09FB0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1b	56	THR	SER	conflict	UNP Q09FB0
1B	49	VAL	LEU	conflict	UNP Q09FB0
1B	56	THR	SER	conflict	UNP Q09FB0

- Molecule 69 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	2b	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		
69	2B	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		

- Molecule 70 is a protein called Ymf58.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	4l	116	Total	C	N	O	S	0	0
			957	648	142	163	4		
70	4L	116	Total	C	N	O	S	0	0
			957	648	142	163	4		

- Molecule 71 is a protein called Ymf57.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5b	100	Total	C	N	O	S	0	0
			888	620	128	137	3		
71	5B	100	Total	C	N	O	S	0	0
			888	620	128	137	3		

- Molecule 72 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	a1	93	Total	C	N	O	0	0
			806	531	139	136		
72	A1	93	Total	C	N	O	0	0
			806	531	139	136		

- Molecule 73 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	a2	98	Total	C	N	O	S	0	0
			811	512	146	151	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
73	A2	98	Total	C	N	O	S	0	0
			811	512	146	151	2		

- Molecule 74 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a3	129	Total	C	N	O	S	0	0
			1077	697	195	182	3		
74	A3	129	Total	C	N	O	S	0	0
			1077	697	195	182	3		

- Molecule 75 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	a5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		
75	A5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		

- Molecule 76 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	a6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		
76	A6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		

- Molecule 77 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	a7	282	Total	C	N	O	S	0	0
			2347	1478	413	453	3		
77	A7	282	Total	C	N	O	S	0	0
			2347	1478	413	453	3		

- Molecule 78 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		
78	A8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		

- Molecule 79 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	a9	340	Total	C	N	O	S	0	0
			2736	1747	479	498	12		
79	A9	340	Total	C	N	O	S	0	0
			2736	1747	479	498	12		

- Molecule 80 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	ab	112	Total	C	N	O		0	0
			926	586	158	182			
80	AB	112	Total	C	N	O		0	0
			926	586	158	182			

- Molecule 81 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ac	98	Total	C	N	O	S	0	0
			806	513	134	158	1		
81	AC	98	Total	C	N	O	S	0	0
			806	513	134	158	1		

- Molecule 82 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	al	193	Total	C	N	O	S	0	0
			1612	1019	303	285	5		
82	AL	193	Total	C	N	O	S	0	0
			1612	1019	303	285	5		

- Molecule 83 is a protein called NDUA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	am	160	Total	C	N	O	S	0	0
			1349	858	256	227	8		
83	AM	160	Total	C	N	O	S	0	0
			1349	858	256	227	8		

- Molecule 84 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	an	231	Total	C	N	O	S	0	0
			1879	1219	317	336	7		
84	AN	231	Total	C	N	O	S	0	0
			1879	1219	317	336	7		

- Molecule 85 is a protein called NDUB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	b2	120	Total	C	N	O	S	0	0
			966	621	167	175	3		
85	B2	120	Total	C	N	O	S	0	0
			966	621	167	175	3		

- Molecule 86 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	b3	69	Total	C	N	O	S	0	0
			602	396	105	100	1		
86	B3	69	Total	C	N	O	S	0	0
			602	396	105	100	1		

- Molecule 87 is a protein called NDUB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	b4	115	Total	C	N	O	S	0	0
			976	641	156	175	4		
87	B4	115	Total	C	N	O	S	0	0
			976	641	156	175	4		

- Molecule 88 is a protein called NDUB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	b6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		
88	B6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		

- Molecule 89 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	b7	116	Total	C	N	O	S	0	0
			941	595	163	177	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
89	B7	116	Total	C	N	O	S	0	0
			941	595	163	177	6		

- Molecule 90 is a protein called NDUB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	b8	175	Total	C	N	O	S	0	0
			1456	936	248	266	6		
90	B8	175	Total	C	N	O	S	0	0
			1456	936	248	266	6		

- Molecule 91 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	b9	188	Total	C	N	O	S	0	0
			1596	1032	255	304	5		
91	B9	188	Total	C	N	O	S	0	0
			1596	1032	255	304	5		

- Molecule 92 is a protein called NDUB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	bl	175	Total	C	N	O	S	0	0
			1461	925	264	268	4		
92	BL	175	Total	C	N	O	S	0	0
			1461	925	264	268	4		

- Molecule 93 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	bm	164	Total	C	N	O	S	0	0
			1321	834	223	259	5		
93	BM	164	Total	C	N	O	S	0	0
			1321	834	223	259	5		

- Molecule 94 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	c4	102	Total	C	N	O	S	0	0
			850	553	139	150	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
94	C4	102	Total	C	N	O	S	0	0
			850	553	139	150	8		

- Molecule 95 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	fx	146	Total	C	N	O	S	0	0
			1162	722	207	223	10		
95	FX	146	Total	C	N	O	S	0	0
			1162	722	207	223	10		

- Molecule 96 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	g1	229	Total	C	N	O	S	0	0
			1773	1113	305	350	5		
96	G1	229	Total	C	N	O	S	0	0
			1773	1113	305	350	5		

- Molecule 97 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	g2	230	Total	C	N	O	S	0	0
			1762	1106	315	334	7		
97	G2	230	Total	C	N	O	S	0	0
			1762	1106	315	334	7		

- Molecule 98 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	g3	346	Total	C	N	O	S	0	0
			2804	1766	481	549	8		
98	G3	346	Total	C	N	O	S	0	0
			2804	1766	481	549	8		

- Molecule 99 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	j1	265	Total	C	N	O	S	0	0
			2170	1375	402	390	3		
99	J1	265	Total	C	N	O	S	0	0
			2170	1375	402	390	3		

- Molecule 100 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	n1	283	Total	C	N	O	S	0	0
			2305	1581	334	378	12		
100	N1	283	Total	C	N	O	S	0	0
			2305	1581	334	378	12		

- Molecule 101 is a protein called Ymf65.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	n2	360	Total	C	N	O	S	0	0
			3073	2134	436	495	8		
101	N2	360	Total	C	N	O	S	0	0
			3073	2134	436	495	8		

- Molecule 102 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	n3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		
102	N3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		

- Molecule 103 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	n4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		
103	N4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		

- Molecule 104 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	n5	709	Total	C	N	O	S	0	0
			5908	4044	850	998	16		
104	N5	709	Total	C	N	O	S	0	0
			5908	4044	850	998	16		

- Molecule 105 is a protein called Ymf62.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	n6	255	Total	C	N	O	S	0	0
			2168	1483	306	374	5		
105	N6	255	Total	C	N	O	S	0	0
			2168	1483	306	374	5		

- Molecule 106 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	p1	230	Total	C	N	O	S	0	0
			1908	1241	322	340	5		
106	P1	230	Total	C	N	O	S	0	0
			1908	1241	322	340	5		

- Molecule 107 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	p2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		
107	P2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		

- Molecule 108 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	qA	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	qa	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	QA	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	Qa	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		

- Molecule 109 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	qB	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		
109	qb	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		
109	QB	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
109	Qb	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		

- Molecule 110 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	qC	426	Total	C	N	O	S	0	0
			3589	2417	541	609	22		
110	qc	425	Total	C	N	O	S	0	0
			3580	2411	539	608	22		
110	QC	426	Total	C	N	O	S	0	0
			3589	2417	541	609	22		
110	Qc	425	Total	C	N	O	S	0	0
			3580	2411	539	608	22		

- Molecule 111 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	qD	295	Total	C	N	O	S	0	0
			2489	1627	418	431	13		
111	qd	295	Total	C	N	O	S	0	0
			2489	1627	418	431	13		
111	QD	295	Total	C	N	O	S	0	0
			2489	1627	418	431	13		
111	Qd	295	Total	C	N	O	S	0	0
			2489	1627	418	431	13		

- Molecule 112 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	qE	230	Total	C	N	O	S	0	0
			1559	971	294	292	2		
112	qe	219	Total	C	N	O	S	0	0
			1471	917	278	274	2		
112	QE	230	Total	C	N	O	S	0	0
			1559	971	294	292	2		
112	Qe	219	Total	C	N	O	S	0	0
			1471	917	278	274	2		

- Molecule 113 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	qF	89	Total	C	N	O	S	0	0
			702	439	125	129	9		
113	qf	80	Total	C	N	O	S	0	0
			630	393	112	116	9		
113	QF	89	Total	C	N	O	S	0	0
			702	439	125	129	9		
113	Qf	80	Total	C	N	O	S	0	0
			630	393	112	116	9		

- Molecule 114 is a protein called Sulphotransf domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	qG	327	Total	C	N	O	S	0	0
			2767	1789	482	490	6		
114	qg	326	Total	C	N	O	S	0	0
			2760	1784	481	489	6		
114	QG	327	Total	C	N	O	S	0	0
			2767	1789	482	490	6		
114	Qg	326	Total	C	N	O	S	0	0
			2760	1784	481	489	6		

- Molecule 115 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	qH	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	qh	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	QH	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	Qh	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		

- Molecule 116 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	qI	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
116	qi	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
116	QI	114	Total	C	N	O	S	0	0
			971	651	161	158	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
116	Qi	114	Total	C	N	O	S	0	0
			971	651	161	158	1		

- Molecule 117 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	qJ	56	Total	C	N	O	S	0	0
			481	329	73	77	2		
117	qj	58	Total	C	N	O	S	0	0
			501	341	79	79	2		
117	QJ	56	Total	C	N	O	S	0	0
			481	329	73	77	2		
117	Qj	58	Total	C	N	O	S	0	0
			501	341	79	79	2		

- Molecule 118 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	qL	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	ql	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	QL	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	Ql	32	Total	C	N	O	S	0	0
			266	181	41	42	2		

- Molecule 119 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
119	qM	17	Total	C	N	O	0	0
			85	51	17	17		
119	qm	17	Total	C	N	O	0	0
			85	51	17	17		
119	Qm	17	Total	C	N	O	0	0
			85	51	17	17		
119	u2	17	Total	C	N	O	0	0
			85	51	17	17		
119	U2	17	Total	C	N	O	0	0
			85	51	17	17		
119	QM	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 120 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	s1	689	Total	C	N	O	S	0	0
			5410	3414	937	1031	28		
120	S1	689	Total	C	N	O	S	0	0
			5410	3414	937	1031	28		

- Molecule 121 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	s2	442	Total	C	N	O	S	0	0
			3598	2291	624	659	24		
121	S2	442	Total	C	N	O	S	0	0
			3598	2291	624	659	24		

- Molecule 122 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	s3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		
122	S3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		

- Molecule 123 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	s4	182	Total	C	N	O	S	0	0
			1500	952	268	272	8		
123	S4	182	Total	C	N	O	S	0	0
			1500	952	268	272	8		

- Molecule 124 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	s5	93	Total	C	N	O	S	0	0
			756	480	129	141	6		
124	S5	93	Total	C	N	O	S	0	0
			756	480	129	141	6		

- Molecule 125 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	s6	92	Total	C	N	O	S	0	0
			738	464	131	139	4		
125	S6	92	Total	C	N	O	S	0	0
			738	464	131	139	4		

- Molecule 126 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	s7	161	Total	C	N	O	S	0	0
			1278	822	220	226	10		
126	S7	161	Total	C	N	O	S	0	0
			1278	822	220	226	10		

- Molecule 127 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	s8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		
127	S8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		

- Molecule 128 is a protein called Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	t1	502	Total	C	N	O	S	0	0
			4059	2600	698	748	13		
128	T1	502	Total	C	N	O	S	0	0
			4059	2600	698	748	13		

- Molecule 129 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	t2	279	Total	C	N	O	S	0	0
			2180	1386	375	418	1		
129	T2	279	Total	C	N	O	S	0	0
			2180	1386	375	418	1		

- Molecule 130 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	t3	310	Total	C	N	O	S	0	0
			2479	1576	432	464	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
130	T3	310	Total	C	N	O	S	0	0
			2479	1576	432	464	7		

- Molecule 131 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
131	t4	198	Total	C	N	O	S	0	0
			1644	1068	284	289	3		
131	T4	198	Total	C	N	O	S	0	0
			1644	1068	284	289	3		

- Molecule 132 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	t5	141	Total	C	N	O	S	0	0
			1138	730	202	204	2		
132	T5	141	Total	C	N	O	S	0	0
			1138	730	202	204	2		

- Molecule 133 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	t6	109	Total	C	N	O	S	0	0
			903	562	161	174	6		
133	T6	109	Total	C	N	O	S	0	0
			903	562	161	174	6		

- Molecule 134 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
134	t7	142	Total	C	N	O	S	0	0
			1187	770	202	209	6		
134	T7	142	Total	C	N	O	S	0	0
			1187	770	202	209	6		

- Molecule 135 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
135	t8	131	Total	C	N	O	0	0
			1084	705	191	188		
135	T8	131	Total	C	N	O	0	0
			1084	705	191	188		

- Molecule 136 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	t9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		
136	T9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		

- Molecule 137 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
137	ta	102	Total	C	N	O	S	0	0
			854	553	141	155	5		
137	TA	102	Total	C	N	O	S	0	0
			854	553	141	155	5		

- Molecule 138 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
138	tb	96	Total	C	N	O		0	0
			801	515	139	147			
138	TB	96	Total	C	N	O		0	0
			801	515	139	147			

- Molecule 139 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
139	tc	92	Total	C	N	O	S	0	0
			789	497	146	145	1		
139	TC	92	Total	C	N	O	S	0	0
			789	497	146	145	1		

- Molecule 140 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
140	td	72	Total	C	N	O		0	0
			616	403	110	103			
140	TD	72	Total	C	N	O		0	0
			616	403	110	103			

- Molecule 141 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
141	te	50	Total	C	N	O	S	0	0
			420	282	64	72	2		
141	TE	50	Total	C	N	O	S	0	0
			420	282	64	72	2		

- Molecule 142 is a protein called NDUTT15.

Mol	Chain	Residues	Atoms					AltConf	Trace
142	tf	216	Total	C	N	O	S	0	0
			1789	1150	304	327	8		
142	TF	216	Total	C	N	O	S	0	0
			1789	1150	304	327	8		

- Molecule 143 is a protein called NDUTT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
143	tg	134	Total	C	N	O	S	0	0
			1081	683	194	203	1		
143	TG	134	Total	C	N	O	S	0	0
			1081	683	194	203	1		

- Molecule 144 is a protein called NDUTT17.

Mol	Chain	Residues	Atoms					AltConf	Trace
144	th	124	Total	C	N	O	S	0	0
			996	639	178	177	2		
144	TH	124	Total	C	N	O	S	0	0
			996	639	178	177	2		

- Molecule 145 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
145	tx	144	Total	C	N	O	S	0	0
			1206	767	205	227	7		
145	TX	144	Total	C	N	O	S	0	0
			1206	767	205	227	7		

- Molecule 146 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
146	v1	442	Total	C	N	O	S	0	0
			3410	2146	600	640	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
146	V1	442	Total	C	N	O	S	0	0
			3410	2146	600	640	24		

- Molecule 147 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
147	v2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		
147	V2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		

- Molecule 148 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
148	x1	149	Total	C	N	O	0	0
			1227	800	213	214		
148	X1	149	Total	C	N	O	0	0
			1227	800	213	214		

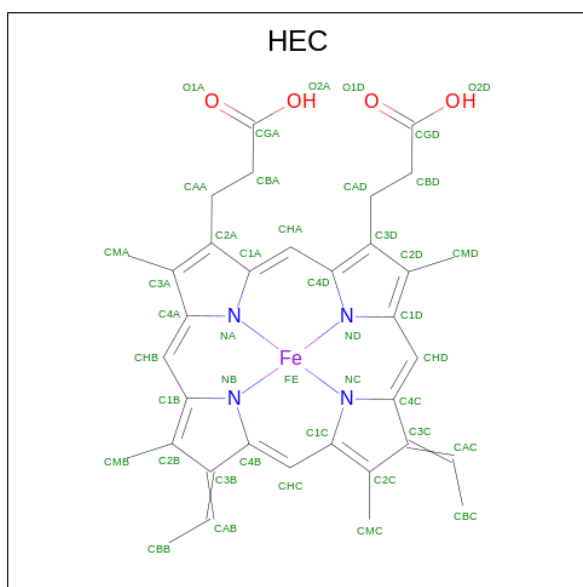
- Molecule 149 is a protein called COXTT3.

Mol	Chain	Residues	Atoms				AltConf	Trace
149	C	203	Total	C	N	O	0	0
			1368	851	246	271		
149	c	203	Total	C	N	O	0	0
			1368	851	246	271		

- Molecule 150 is a protein called Unknown peptide.

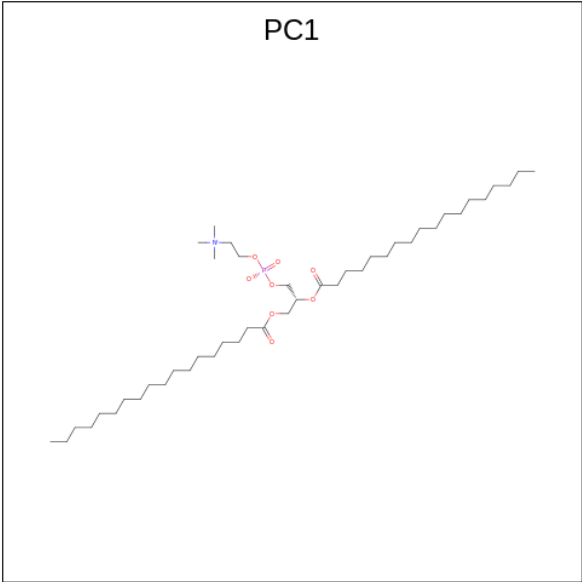
Mol	Chain	Residues	Atoms				AltConf	Trace
150	u1	92	Total	C	N	O	0	0
			460	276	92	92		
150	U1	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 151 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
151	2e	1	Total 43	C 34	Fe 1	N 4	O 4	0
151	qD	1	Total 43	C 34	Fe 1	N 4	O 4	0
151	qd	1	Total 43	C 34	Fe 1	N 4	O 4	0
151	2E	1	Total 43	C 34	Fe 1	N 4	O 4	0
151	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
151	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 152 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
152	2f	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	2f	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	2f	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2g	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	2j	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	6a	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	6c	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	7a	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	7c	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	c1	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	c1	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	c1	1	Total	C	N	O	P	0
			38	28	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	c1	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c2	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	c3	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c3	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	f	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	fs	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	i	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	j	1	Total	C	N	O	P	0
			37	27	1	8	1	
152	m	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	m	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	m	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	m1	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	m1	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	m2	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	m2	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	m2	1	Total	C	N	O	P	0
			46	36	1	8	1	
152	n	1	Total	C	N	O	P	0
			41	31	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	n	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	n	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	v	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	v	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	w	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	w	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	w	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	5b	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	al	1	Total	C	N	O	P	0
			26	16	1	8	1	
152	am	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	an	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	b9	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	c4	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	j1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	n1	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	n3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	n5	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	n5	1	Total	C	N	O	P	0
			53	43	1	8	1	
152	n5	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	n5	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	n6	1	Total	C	N	O	P	0
			54	44	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	p1	1	Total 40	C 30	N 1	O 8	P 1	0
152	qB	1	Total 44	C 34	N 1	O 8	P 1	0
152	qC	1	Total 38	C 28	N 1	O 8	P 1	0
152	qC	1	Total 50	C 40	N 1	O 8	P 1	0
152	qC	1	Total 36	C 26	N 1	O 8	P 1	0
152	qE	1	Total 24	C 14	N 1	O 8	P 1	0
152	qE	1	Total 39	C 29	N 1	O 8	P 1	0
152	qE	1	Total 28	C 18	N 1	O 8	P 1	0
152	qG	1	Total 32	C 22	N 1	O 8	P 1	0
152	qI	1	Total 30	C 20	N 1	O 8	P 1	0
152	qI	1	Total 43	C 33	N 1	O 8	P 1	0
152	qJ	1	Total 38	C 28	N 1	O 8	P 1	0
152	qb	1	Total 43	C 33	N 1	O 8	P 1	0
152	qc	1	Total 38	C 28	N 1	O 8	P 1	0
152	qc	1	Total 47	C 37	N 1	O 8	P 1	0
152	qe	1	Total 33	C 23	N 1	O 8	P 1	0
152	qe	1	Total 43	C 33	N 1	O 8	P 1	0
152	qg	1	Total 32	C 22	N 1	O 8	P 1	0
152	qi	1	Total 30	C 20	N 1	O 8	P 1	0
152	qi	1	Total 42	C 32	N 1	O 8	P 1	0
152	qj	1	Total 36	C 26	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	s8	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	t1	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	t4	1	Total	C	N	O	P	0
			48	38	1	8	1	
152	t4	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	tc	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	tc	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	te	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2F	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	2F	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	2F	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2G	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	2J	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	6A	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	6C	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	7A	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	7C	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	C1	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	C1	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	C1	1	Total	C	N	O	P	0
			38	28	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	C1	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C2	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	C3	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	D	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	F	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	FS	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	J	1	Total	C	N	O	P	0
			37	27	1	8	1	
152	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	M1	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	M2	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	M2	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	M2	1	Total	C	N	O	P	0
			46	36	1	8	1	
152	N	1	Total	C	N	O	P	0
			41	31	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	N	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	N	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	V	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	W	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	W	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	5B	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	AL	1	Total	C	N	O	P	0
			26	16	1	8	1	
152	AM	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	AN	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	B9	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	C4	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	J1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	N1	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	N3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	N5	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	N5	1	Total	C	N	O	P	0
			53	43	1	8	1	
152	N5	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	N5	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	

Continued on next page...

Continued from previous page...

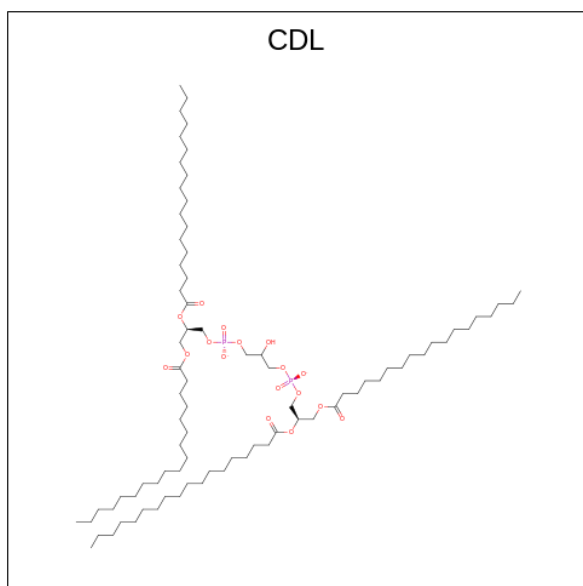
Mol	Chain	Residues	Atoms					AltConf
152	P1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	QB	1	Total	C	N	O	P	0
			44	34	1	8	1	
152	QC	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	QC	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	QC	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	QE	1	Total	C	N	O	P	0
			24	14	1	8	1	
152	QE	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	QG	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	QI	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	QI	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	QJ	1	Total	C	N	O	P	0
			28	18	1	8	1	
152	QJ	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	Qb	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	Qc	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	Qc	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	Qe	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	Qe	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	Qg	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	Qi	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	Qi	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	Qj	1	Total	C	N	O	P	0
			36	26	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
152	S8	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	T1	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	T4	1	Total	C	N	O	P	0
			48	38	1	8	1	
152	T4	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	TC	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	TC	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	TE	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 153 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
153	2g	1	Total	C	O	P	0
			89	70	17	2	
153	2g	1	Total	C	O	P	0
			55	36	17	2	
153	2g	1	Total	C	O	P	0
			63	44	17	2	
153	2k	1	Total	C	O	P	0
			98	79	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	2m	1	Total	C	O	P	0
			96	77	17	2	
153	2o	1	Total	C	O	P	0
			50	31	17	2	
153	6a	1	Total	C	O	P	0
			74	55	17	2	
153	6c	1	Total	C	O	P	0
			75	56	17	2	
153	6c	1	Total	C	O	P	0
			82	63	17	2	
153	7a	1	Total	C	O	P	0
			100	81	17	2	
153	7a	1	Total	C	O	P	0
			62	43	17	2	
153	7c	1	Total	C	O	P	0
			85	66	17	2	
153	7c	1	Total	C	O	P	0
			51	32	17	2	
153	a	1	Total	C	O	P	0
			51	32	17	2	
153	a	1	Total	C	O	P	0
			94	75	17	2	
153	a	1	Total	C	O	P	0
			82	63	17	2	
153	b	1	Total	C	O	P	0
			62	43	17	2	
153	c1	1	Total	C	O	P	0
			79	60	17	2	
153	c1	1	Total	C	O	P	0
			65	46	17	2	
153	c1	1	Total	C	O	P	0
			63	44	17	2	
153	c1	1	Total	C	O	P	0
			95	76	17	2	
153	c3	1	Total	C	O	P	0
			68	49	17	2	
153	e	1	Total	C	O	P	0
			60	41	17	2	
153	e	1	Total	C	O	P	0
			72	53	17	2	
153	e	1	Total	C	O	P	0
			63	44	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	f	1	Total 100	C 81	O 17	P 2	0
153	fs	1	Total 47	C 28	O 17	P 2	0
153	i	1	Total 77	C 58	O 17	P 2	0
153	i	1	Total 75	C 56	O 17	P 2	0
153	j	1	Total 70	C 51	O 17	P 2	0
153	l	1	Total 74	C 55	O 17	P 2	0
153	m	1	Total 64	C 45	O 17	P 2	0
153	m	1	Total 83	C 64	O 17	P 2	0
153	m	1	Total 64	C 45	O 17	P 2	0
153	m	1	Total 66	C 47	O 17	P 2	0
153	m1	1	Total 66	C 47	O 17	P 2	0
153	m1	1	Total 91	C 72	O 17	P 2	0
153	m1	1	Total 57	C 38	O 17	P 2	0
153	m2	1	Total 54	C 35	O 17	P 2	0
153	m2	1	Total 66	C 47	O 17	P 2	0
153	m2	1	Total 74	C 55	O 17	P 2	0
153	m3	1	Total 63	C 44	O 17	P 2	0
153	m3	1	Total 55	C 36	O 17	P 2	0
153	n	1	Total 84	C 65	O 17	P 2	0
153	q	1	Total 63	C 44	O 17	P 2	0
153	q	1	Total 72	C 53	O 17	P 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	q	1	Total	C	O	P	0
			86	67	17	2	
153	r	1	Total	C	O	P	0
			65	46	17	2	
153	sd	1	Total	C	O	P	0
			76	57	17	2	
153	t	1	Total	C	O	P	0
			59	40	17	2	
153	t	1	Total	C	O	P	0
			75	56	17	2	
153	t	1	Total	C	O	P	0
			71	52	17	2	
153	t	1	Total	C	O	P	0
			90	71	17	2	
153	u	1	Total	C	O	P	0
			60	41	17	2	
153	vb	1	Total	C	O	P	0
			62	43	17	2	
153	vb	1	Total	C	O	P	0
			67	48	17	2	
153	w	1	Total	C	O	P	0
			84	65	17	2	
153	y5	1	Total	C	O	P	0
			70	51	17	2	
153	y7	1	Total	C	O	P	0
			65	46	17	2	
153	z	1	Total	C	O	P	0
			67	48	17	2	
153	2b	1	Total	C	O	P	0
			87	68	17	2	
153	5b	1	Total	C	O	P	0
			81	62	17	2	
153	a1	1	Total	C	O	P	0
			67	48	17	2	
153	a9	1	Total	C	O	P	0
			76	57	17	2	
153	a9	1	Total	C	O	P	0
			87	68	17	2	
153	al	1	Total	C	O	P	0
			53	34	17	2	
153	am	1	Total	C	O	P	0
			56	37	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	an	1	Total	C	O	P	0
			87	68	17	2	
153	b3	1	Total	C	O	P	0
			58	39	17	2	
153	b3	1	Total	C	O	P	0
			82	63	17	2	
153	b4	1	Total	C	O	P	0
			37	18	17	2	
153	b8	1	Total	C	O	P	0
			69	50	17	2	
153	bm	1	Total	C	O	P	0
			86	67	17	2	
153	c4	1	Total	C	O	P	0
			98	79	17	2	
153	n5	1	Total	C	O	P	0
			90	71	17	2	
153	n6	1	Total	C	O	P	0
			90	71	17	2	
153	p1	1	Total	C	O	P	0
			63	44	17	2	
153	p1	1	Total	C	O	P	0
			58	39	17	2	
153	qB	1	Total	C	O	P	0
			68	49	17	2	
153	qC	1	Total	C	O	P	0
			64	45	17	2	
153	qC	1	Total	C	O	P	0
			56	37	17	2	
153	qD	1	Total	C	O	P	0
			61	42	17	2	
153	qG	1	Total	C	O	P	0
			86	67	17	2	
153	qH	1	Total	C	O	P	0
			94	75	17	2	
153	qI	1	Total	C	O	P	0
			71	52	17	2	
153	qb	1	Total	C	O	P	0
			68	49	17	2	
153	qc	1	Total	C	O	P	0
			64	45	17	2	
153	qc	1	Total	C	O	P	0
			56	37	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	qc	1	Total	C	O	P	0
			47	28	17	2	
153	qg	1	Total	C	O	P	0
			100	81	17	2	
153	qi	1	Total	C	O	P	0
			71	52	17	2	
153	t1	1	Total	C	O	P	0
			55	36	17	2	
153	t5	1	Total	C	O	P	0
			96	77	17	2	
153	t7	1	Total	C	O	P	0
			73	54	17	2	
153	td	1	Total	C	O	P	0
			66	47	17	2	
153	te	1	Total	C	O	P	0
			53	34	17	2	
153	th	1	Total	C	O	P	0
			84	65	17	2	
153	2G	1	Total	C	O	P	0
			89	70	17	2	
153	2G	1	Total	C	O	P	0
			55	36	17	2	
153	2G	1	Total	C	O	P	0
			63	44	17	2	
153	2K	1	Total	C	O	P	0
			98	79	17	2	
153	2M	1	Total	C	O	P	0
			96	77	17	2	
153	2O	1	Total	C	O	P	0
			50	31	17	2	
153	6A	1	Total	C	O	P	0
			74	55	17	2	
153	6C	1	Total	C	O	P	0
			75	56	17	2	
153	6C	1	Total	C	O	P	0
			82	63	17	2	
153	7A	1	Total	C	O	P	0
			100	81	17	2	
153	7A	1	Total	C	O	P	0
			62	43	17	2	
153	7C	1	Total	C	O	P	0
			85	66	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	7C	1	Total	C	O	P	0
			51	32	17	2	
153	A	1	Total	C	O	P	0
			51	32	17	2	
153	A	1	Total	C	O	P	0
			94	75	17	2	
153	B	1	Total	C	O	P	0
			62	43	17	2	
153	C1	1	Total	C	O	P	0
			79	60	17	2	
153	C1	1	Total	C	O	P	0
			65	46	17	2	
153	C1	1	Total	C	O	P	0
			63	44	17	2	
153	C1	1	Total	C	O	P	0
			95	76	17	2	
153	C3	1	Total	C	O	P	0
			68	49	17	2	
153	E	1	Total	C	O	P	0
			60	41	17	2	
153	E	1	Total	C	O	P	0
			72	53	17	2	
153	E	1	Total	C	O	P	0
			63	44	17	2	
153	F	1	Total	C	O	P	0
			100	81	17	2	
153	FS	1	Total	C	O	P	0
			47	28	17	2	
153	I	1	Total	C	O	P	0
			77	58	17	2	
153	I	1	Total	C	O	P	0
			75	56	17	2	
153	J	1	Total	C	O	P	0
			70	51	17	2	
153	L	1	Total	C	O	P	0
			74	55	17	2	
153	M	1	Total	C	O	P	0
			66	47	17	2	
153	M	1	Total	C	O	P	0
			64	45	17	2	
153	M	1	Total	C	O	P	0
			83	64	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	M	1	Total	C	O	P	0
			64	45	17	2	
153	M1	1	Total	C	O	P	0
			66	47	17	2	
153	M1	1	Total	C	O	P	0
			91	72	17	2	
153	M1	1	Total	C	O	P	0
			57	38	17	2	
153	M2	1	Total	C	O	P	0
			54	35	17	2	
153	M2	1	Total	C	O	P	0
			66	47	17	2	
153	M2	1	Total	C	O	P	0
			74	55	17	2	
153	M3	1	Total	C	O	P	0
			63	44	17	2	
153	M3	1	Total	C	O	P	0
			55	36	17	2	
153	N	1	Total	C	O	P	0
			84	65	17	2	
153	Q	1	Total	C	O	P	0
			63	44	17	2	
153	Q	1	Total	C	O	P	0
			72	53	17	2	
153	R	1	Total	C	O	P	0
			65	46	17	2	
153	SD	1	Total	C	O	P	0
			76	57	17	2	
153	T	1	Total	C	O	P	0
			59	40	17	2	
153	T	1	Total	C	O	P	0
			75	56	17	2	
153	T	1	Total	C	O	P	0
			71	52	17	2	
153	T	1	Total	C	O	P	0
			90	71	17	2	
153	U	1	Total	C	O	P	0
			60	41	17	2	
153	VB	1	Total	C	O	P	0
			62	43	17	2	
153	VB	1	Total	C	O	P	0
			86	67	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	VB	1	Total	C	O	P	0
			82	63	17	2	
153	VB	1	Total	C	O	P	0
			67	48	17	2	
153	W	1	Total	C	O	P	0
			84	65	17	2	
153	Y5	1	Total	C	O	P	0
			70	51	17	2	
153	Y7	1	Total	C	O	P	0
			65	46	17	2	
153	Z	1	Total	C	O	P	0
			67	48	17	2	
153	2B	1	Total	C	O	P	0
			87	68	17	2	
153	5B	1	Total	C	O	P	0
			81	62	17	2	
153	A1	1	Total	C	O	P	0
			66	47	17	2	
153	A1	1	Total	C	O	P	0
			67	48	17	2	
153	A9	1	Total	C	O	P	0
			76	57	17	2	
153	A9	1	Total	C	O	P	0
			87	68	17	2	
153	AL	1	Total	C	O	P	0
			53	34	17	2	
153	AM	1	Total	C	O	P	0
			56	37	17	2	
153	AN	1	Total	C	O	P	0
			87	68	17	2	
153	B3	1	Total	C	O	P	0
			58	39	17	2	
153	B3	1	Total	C	O	P	0
			82	63	17	2	
153	B4	1	Total	C	O	P	0
			37	18	17	2	
153	B8	1	Total	C	O	P	0
			69	50	17	2	
153	BM	1	Total	C	O	P	0
			86	67	17	2	
153	C4	1	Total	C	O	P	0
			98	79	17	2	

Continued on next page...

Continued from previous page...

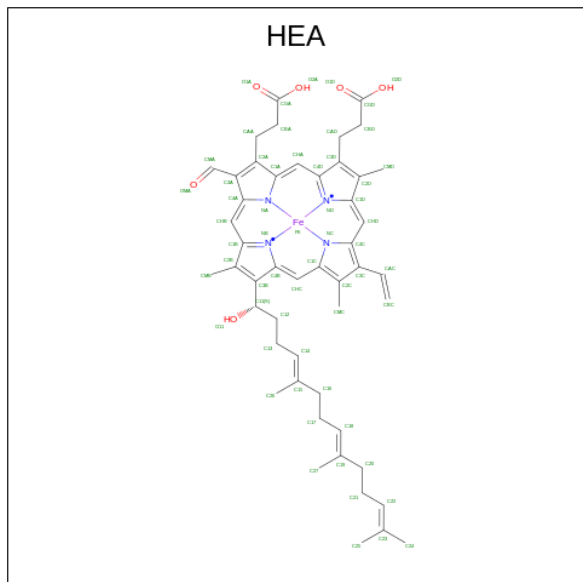
Mol	Chain	Residues	Atoms				AltConf
153	N5	1	Total	C	O	P	0
			90	71	17	2	
153	N6	1	Total	C	O	P	0
			90	71	17	2	
153	P1	1	Total	C	O	P	0
			63	44	17	2	
153	P1	1	Total	C	O	P	0
			58	39	17	2	
153	QB	1	Total	C	O	P	0
			68	49	17	2	
153	QC	1	Total	C	O	P	0
			64	45	17	2	
153	QC	1	Total	C	O	P	0
			56	37	17	2	
153	QD	1	Total	C	O	P	0
			61	42	17	2	
153	QG	1	Total	C	O	P	0
			86	67	17	2	
153	QH	1	Total	C	O	P	0
			94	75	17	2	
153	QI	1	Total	C	O	P	0
			71	52	17	2	
153	Qb	1	Total	C	O	P	0
			68	49	17	2	
153	Qc	1	Total	C	O	P	0
			64	45	17	2	
153	Qc	1	Total	C	O	P	0
			56	37	17	2	
153	Qc	1	Total	C	O	P	0
			47	28	17	2	
153	Qg	1	Total	C	O	P	0
			100	81	17	2	
153	Qi	1	Total	C	O	P	0
			71	52	17	2	
153	T1	1	Total	C	O	P	0
			55	36	17	2	
153	T5	1	Total	C	O	P	0
			96	77	17	2	
153	T7	1	Total	C	O	P	0
			73	54	17	2	
153	TE	1	Total	C	O	P	0
			53	34	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
153	TH	1	Total	C	O	P	0
			84	65	17	2	
153	C	1	Total	C	O	P	0
			64	45	17	2	
153	c	1	Total	C	O	P	0
			64	45	17	2	
153	u1	1	Total	C	O	P	0
			57	38	17	2	
153	U1	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 154 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
154	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

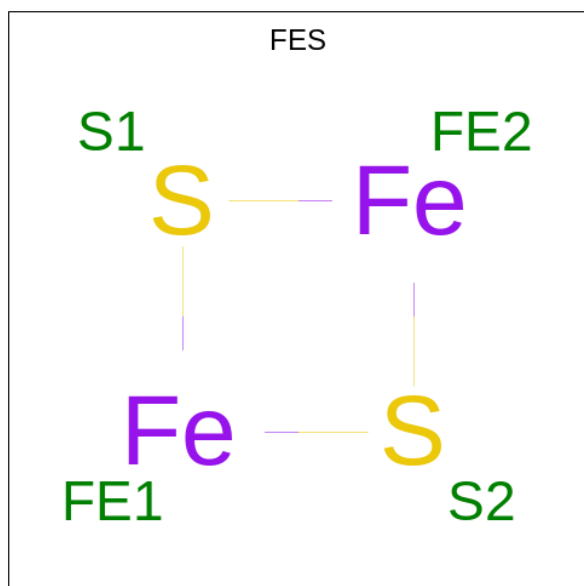
- Molecule 155 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
155	c1	1	Total 1	Cu 1	0
155	c2	2	Total 2	Cu 2	0
155	C1	1	Total 1	Cu 1	0
155	C2	2	Total 2	Cu 2	0

- Molecule 156 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
156	c1	1	Total 1	Mg 1	0
156	C1	1	Total 1	Mg 1	0

- Molecule 157 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



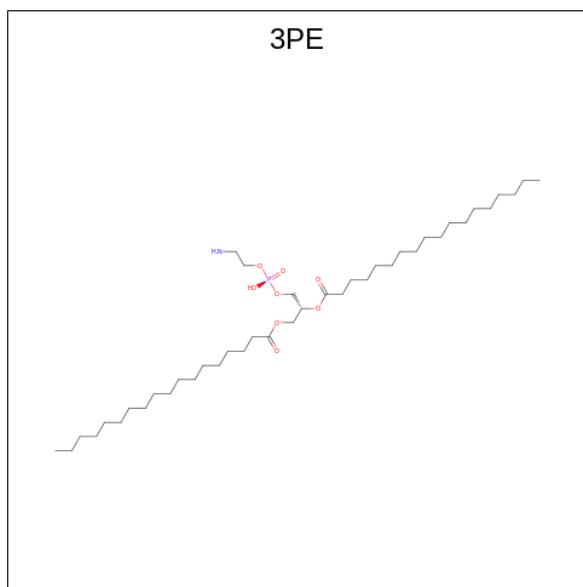
Mol	Chain	Residues	Atoms			AltConf
157	fs	1	Total 4	Fe 2	S 2	0
157	fs	1	Total 4	Fe 2	S 2	0
157	sb	1	Total 4	Fe 2	S 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
157	fx	1	Total 4	Fe 2	S 2	0
157	qE	1	Total 4	Fe 2	S 2	0
157	qe	1	Total 4	Fe 2	S 2	0
157	s1	1	Total 4	Fe 2	S 2	0
157	v2	1	Total 4	Fe 2	S 2	0
157	FS	1	Total 4	Fe 2	S 2	0
157	FS	1	Total 4	Fe 2	S 2	0
157	SB	1	Total 4	Fe 2	S 2	0
157	FX	1	Total 4	Fe 2	S 2	0
157	QE	1	Total 4	Fe 2	S 2	0
157	Qe	1	Total 4	Fe 2	S 2	0
157	S1	1	Total 4	Fe 2	S 2	0
157	V2	1	Total 4	Fe 2	S 2	0

- Molecule 158 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
158	i	1	Total	C	N	O	P	0
			32	22	1	8	1	
158	m2	1	Total	C	N	O	P	0
			31	21	1	8	1	
158	m3	1	Total	C	N	O	P	0
			38	28	1	8	1	
158	sc	1	Total	C	N	O	P	0
			40	30	1	8	1	
158	vb	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	w	1	Total	C	N	O	P	0
			34	24	1	8	1	
158	y5	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	a3	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	a3	1	Total	C	N	O	P	0
			44	34	1	8	1	
158	an	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	an	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	an	1	Total	C	N	O	P	0
			33	23	1	8	1	
158	an	1	Total	C	N	O	P	0
			29	19	1	8	1	
158	b4	1	Total	C	N	O	P	0
			48	38	1	8	1	

Continued on next page...

Continued from previous page...

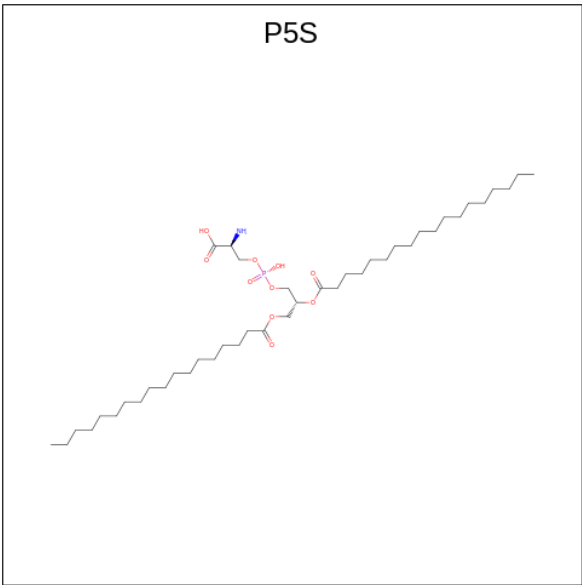
Mol	Chain	Residues	Atoms					AltConf
158	bm	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	c4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	g2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	n4	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	n5	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	s8	1	Total	C	N	O	P	0
			41	31	1	8	1	
158	t4	1	Total	C	N	O	P	0
			25	15	1	8	1	
158	t8	1	Total	C	N	O	P	0
			47	37	1	8	1	
158	t8	1	Total	C	N	O	P	0
			39	29	1	8	1	
158	ta	1	Total	C	N	O	P	0
			26	16	1	8	1	
158	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
158	M2	1	Total	C	N	O	P	0
			31	21	1	8	1	
158	M3	1	Total	C	N	O	P	0
			38	28	1	8	1	
158	SC	1	Total	C	N	O	P	0
			40	30	1	8	1	
158	VB	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
158	Y5	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	A3	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	A3	1	Total	C	N	O	P	0
			44	34	1	8	1	
158	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	

Continued on next page...

Continued from previous page...

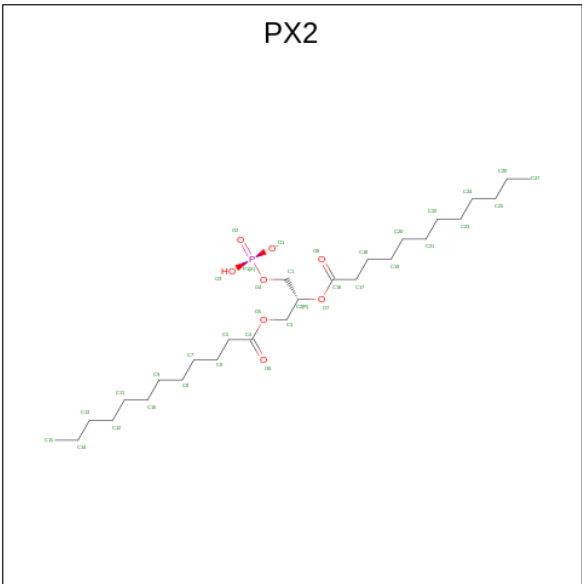
Mol	Chain	Residues	Atoms					AltConf
158	AN	1	Total	C	N	O	P	0
			33	23	1	8	1	
158	AN	1	Total	C	N	O	P	0
			29	19	1	8	1	
158	B4	1	Total	C	N	O	P	0
			48	38	1	8	1	
158	BM	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	C4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	G2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	N4	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	N5	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	S8	1	Total	C	N	O	P	0
			41	31	1	8	1	
158	T4	1	Total	C	N	O	P	0
			25	15	1	8	1	
158	T8	1	Total	C	N	O	P	0
			47	37	1	8	1	
158	T8	1	Total	C	N	O	P	0
			39	29	1	8	1	
158	TA	1	Total	C	N	O	P	0
			26	16	1	8	1	

- Molecule 159 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy} (hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
159	m2	1	Total	C	N	O	P	0
			36	24	1	10	1	
159	M2	1	Total	C	N	O	P	0
			36	24	1	10	1	

- Molecule 160 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: C₂₇H₅₂O₈P).



Mol	Chain	Residues	Atoms				AltConf
160	r	1	Total	C	O	P	0
			33	24	8	1	

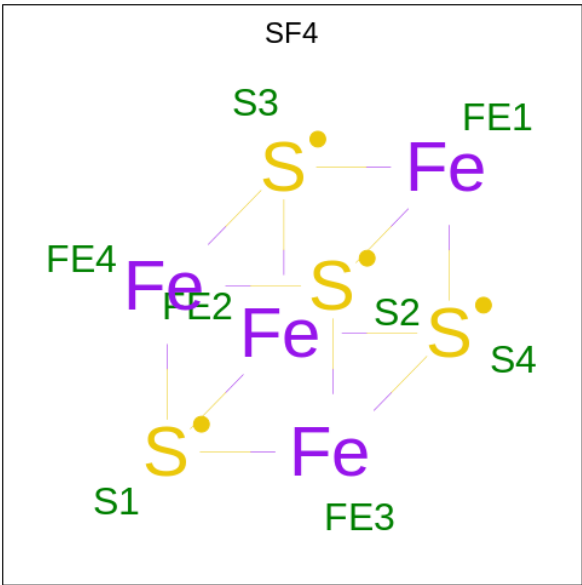
Continued on next page...

Mol	Chain	Residues	Atoms				AltConf
160	y5	1	Total 21	C 12	O 8	P 1	0
160	qh	1	Total 36	C 27	O 8	P 1	0
160	R	1	Total 33	C 24	O 8	P 1	0
160	Y5	1	Total 21	C 12	O 8	P 1	0
160	Qh	1	Total 36	C 27	O 8	P 1	0

- # FAD

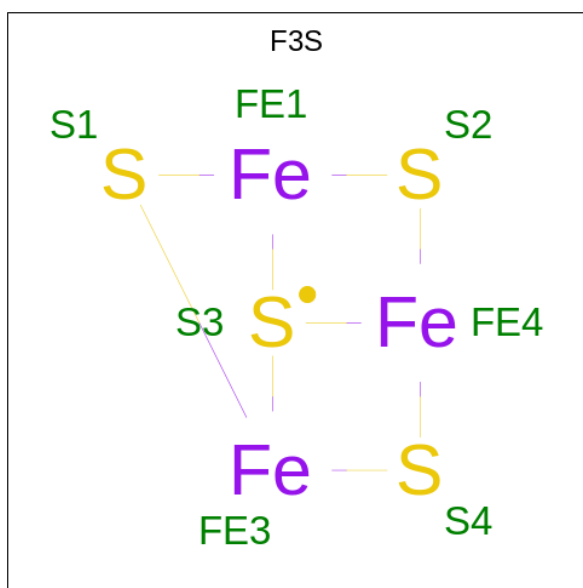
Mol	Chain	Residues	Atoms					AltConf
161	sa	1	Total 53	C 27	N 9	O 15	P 2	0
161	SA	1	Total 53	C 27	N 9	O 15	P 2	0

- 



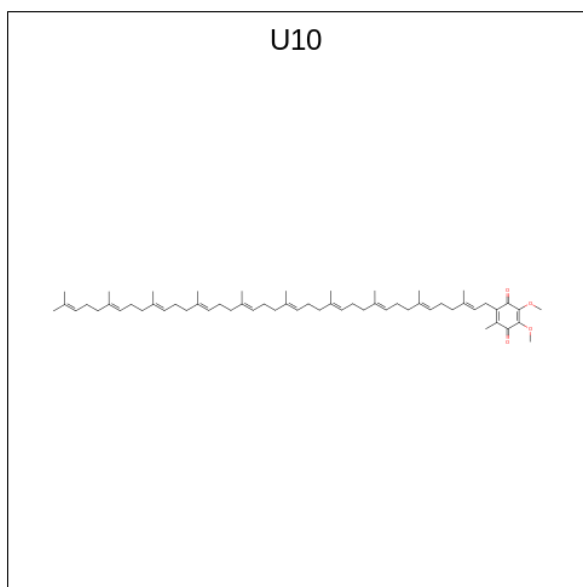
Mol	Chain	Residues	Atoms			AltConf
162	sb	1	Total	Fe	S	0
			8	4	4	
162	s1	1	Total	Fe	S	
			8	4	4	
162	s1	1	Total	Fe	S	0
			8	4	4	
162	s7	1	Total	Fe	S	
			8	4	4	
162	s8	1	Total	Fe	S	0
			8	4	4	
162	s8	1	Total	Fe	S	
			8	4	4	
162	v1	1	Total	Fe	S	0
			8	4	4	
162	SB	1	Total	Fe	S	
			8	4	4	
162	S1	1	Total	Fe	S	0
			8	4	4	
162	S1	1	Total	Fe	S	
			8	4	4	
162	S7	1	Total	Fe	S	0
			8	4	4	
162	S8	1	Total	Fe	S	
			8	4	4	
162	S8	1	Total	Fe	S	0
			8	4	4	
162	V1	1	Total	Fe	S	
			8	4	4	

- Molecule 163 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			AltConf
163	sb	1	Total	Fe	S	0
			7	3	4	
163	SB	1	Total	Fe	S	0
			7	3	4	

- Molecule 164 is UBIQUINONE-10 (three-letter code: U10) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$) (labeled as "Ligand of Interest" by depositor).

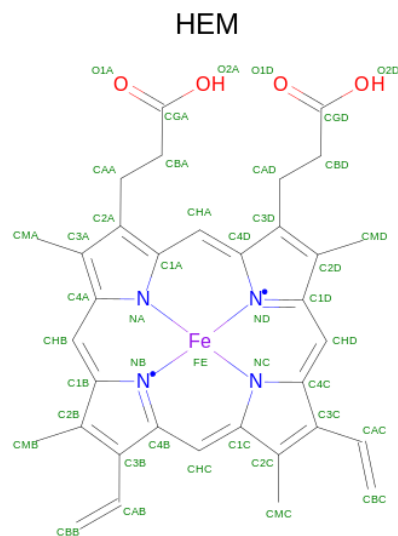


Mol	Chain	Residues	Atoms			AltConf
164	sc	1	Total	C	O	0
			63	59	4	
164	b8	1	Total	C	O	0
			63	59	4	
164	qC	1	Total	C	O	0
			29	25	4	
164	qc	1	Total	C		0
			26	26		
164	qc	1	Total	C	O	0
			29	25	4	
164	SC	1	Total	C	O	0
			63	59	4	
164	B8	1	Total	C	O	0
			63	59	4	
164	QC	1	Total	C	O	0
			29	25	4	
164	Qc	1	Total	C		0
			26	26		
164	Qc	1	Total	C	O	0
			29	25	4	

- Molecule 165 is ZINC ION (three-letter code: ZN) (formula: Zn).

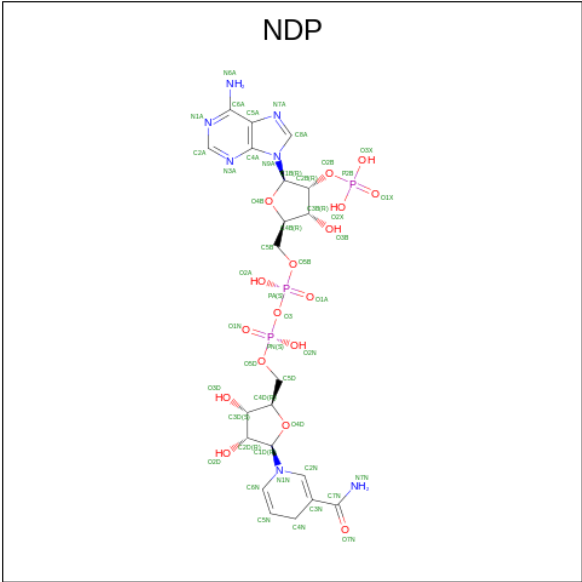
Mol	Chain	Residues	Atoms		AltConf
165	vb	2	Total	Zn	0
			2	2	
165	s6	1	Total	Zn	0
			1	1	
165	VB	2	Total	Zn	0
			2	2	
165	S6	1	Total	Zn	0
			1	1	

- Molecule 166 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



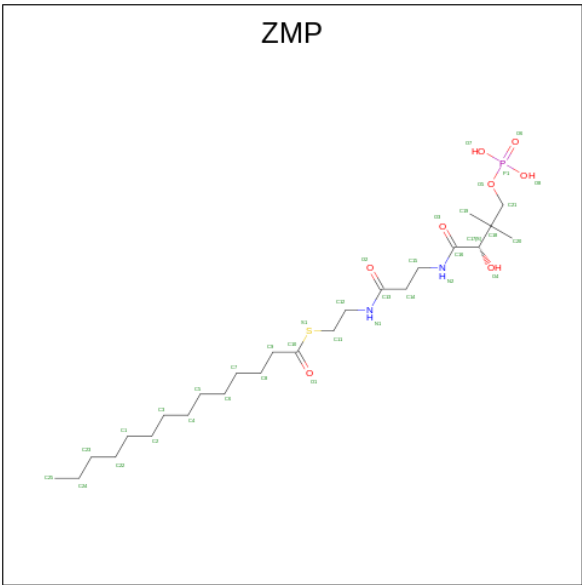
Mol	Chain	Residues	Atoms					AltConf
166	y5	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	qC	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	qC	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	Y5	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	QC	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0
166	Qc	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 167 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
167	a9	1	Total	C	N	O	P	0
			48	21	7	17	3	
167	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 168 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



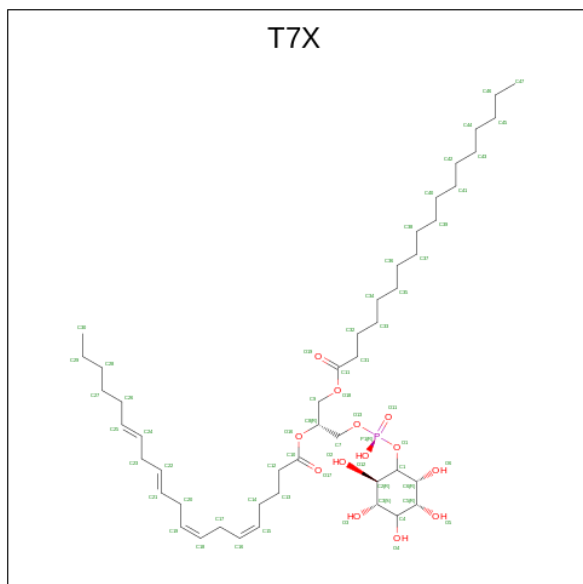
Mol	Chain	Residues	Atoms						AltConf
168	ab	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

Continued on next page...

Continued from previous page...

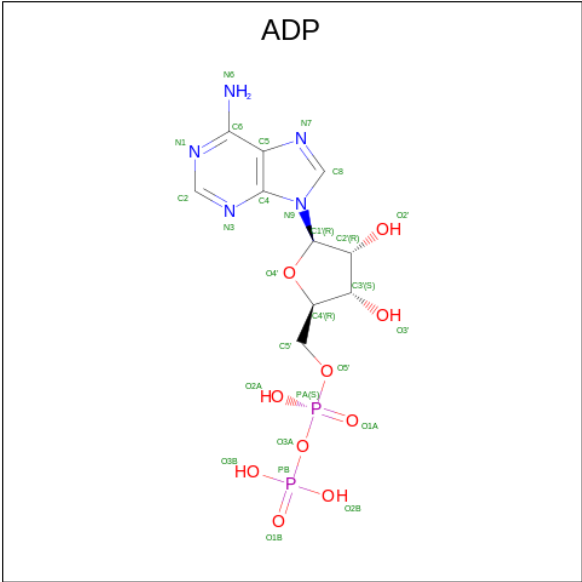
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
168	AB	1	37	25	2	8	1	1	0

- Molecule 169 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



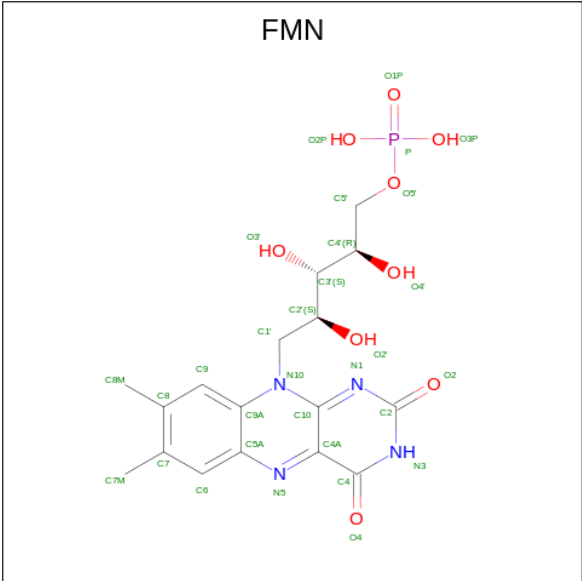
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
169	b6	1	55	41	13	1	0
169	B6	1	55	41	13	1	0

- Molecule 170 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
170	b9	1	Total	C	N	O	P	0
			27	10	5	10	2	
170	B9	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 171 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
171	v1	1	Total	C	N	O	P	0
			31	17	4	9	1	

Continued on next page...

Continued from previous page...

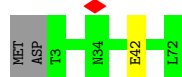
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
171	V1	1	31	17	4	9	1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

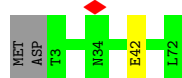
- Molecule 1: Tim10/DDP family zinc finger protein

Chain 1t:  96%



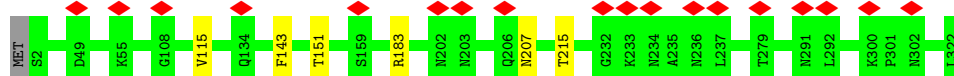
- Molecule 1: Tim10/DDP family zinc finger protein

Chain 1T:  96%



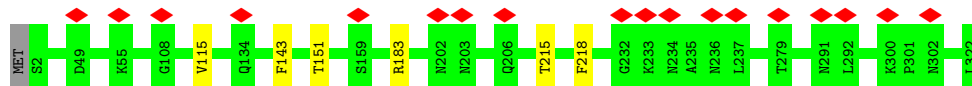
- Molecule 2: NmrA domain-containing protein

Chain 2e:  6% 98%



- Molecule 2: NmrA domain-containing protein

Chain 2E:  6% 98%



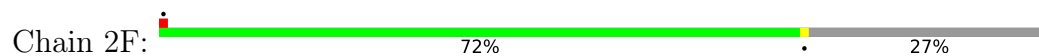
- Molecule 3: Transmembrane protein, putative

Chain 2f:  72% 27%





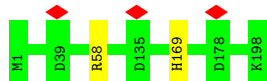
- Molecule 3: Transmembrane protein, putative



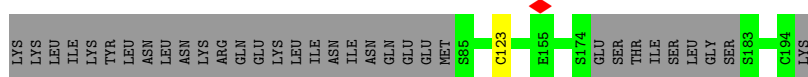
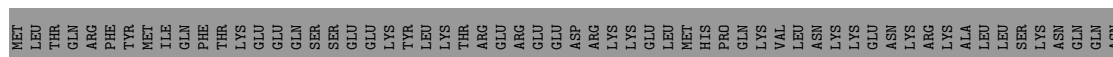
- Molecule 4: SDHTT3



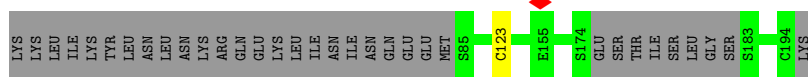
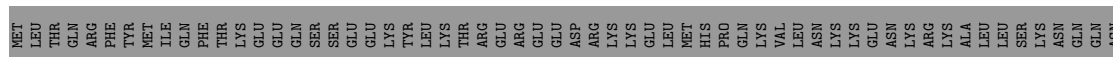
- Molecule 4: SDHTT3



- Molecule 5: Diphthamide synthesis protein



- Molecule 5: Diphthamide synthesis protein



- Molecule 6: DUF4885 domain-containing protein

Chain 2i:  97% .



- Molecule 6: DUF4885 domain-containing protein

Chain 2I:  98% .



- Molecule 7: Transmembrane protein, putative

Chain 2j:  98% ..



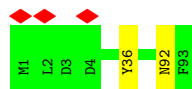
- Molecule 7: Transmembrane protein, putative

Chain 2J:  98% ..



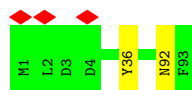
- Molecule 8: Transmembrane protein, putative

Chain 2k:  98% .



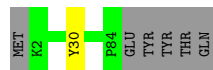
- Molecule 8: Transmembrane protein, putative

Chain 2K:  98% .



- Molecule 9: Transposase

Chain 2l:  92% . 7%



- Molecule 9: Transposase

Chain 2L:  91% • 7%



- Molecule 10: Transmembrane protein, putative

Chain 2m:  97% ..



- Molecule 10: Transmembrane protein, putative

Chain 2M:  97% ..



- Molecule 11: Transmembrane protein, putative

Chain 2n:  97% ..



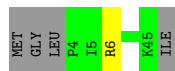
- Molecule 11: Transmembrane protein, putative

Chain 2N:  95% ..



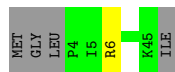
- Molecule 12: SDHTT11

Chain 2o:  89% • 9%



- Molecule 12: SDHTT11

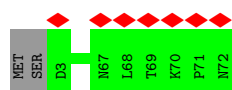
Chain 2O:  89% • 9%



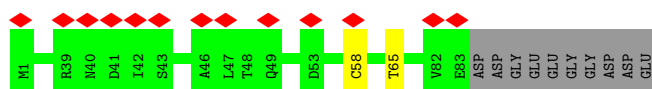
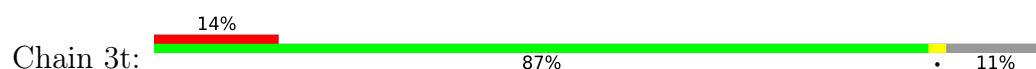
- Molecule 13: Zf-Tim10_DDP domain-containing protein



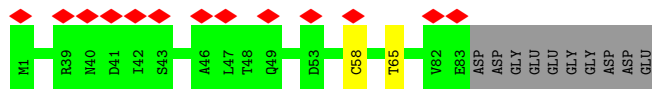
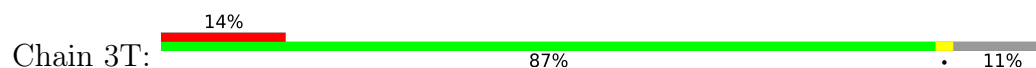
- Molecule 13: Zf-Tim10_DDP domain-containing protein



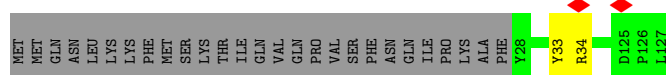
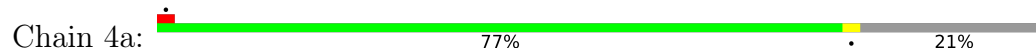
- Molecule 14: Zf-Tim10_DDP domain-containing protein



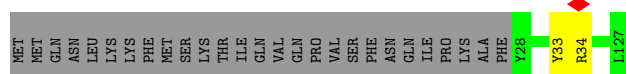
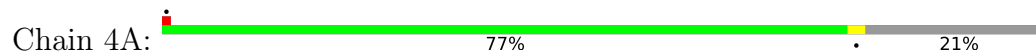
- Molecule 14: Zf-Tim10_DDP domain-containing protein



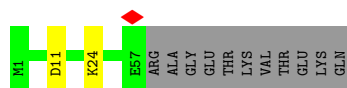
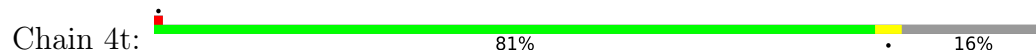
- Molecule 15: Phage protein



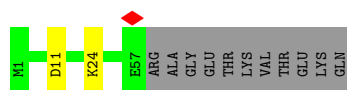
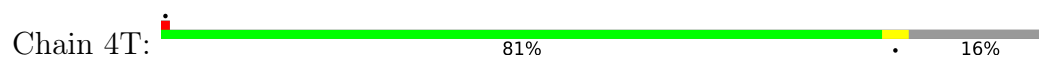
- Molecule 15: Phage protein



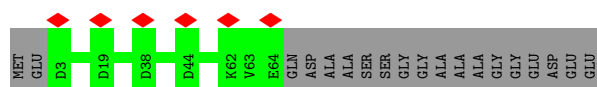
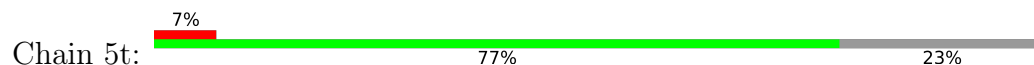
- Molecule 16: Transposase



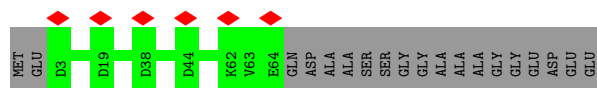
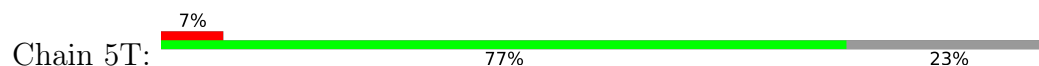
- Molecule 16: Transposase



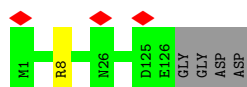
- Molecule 17: Cullin domain-containing protein



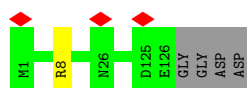
- Molecule 17: Cullin domain-containing protein



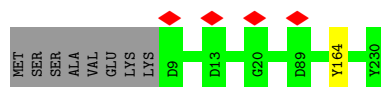
- Molecule 18: Transmembrane protein, putative



- Molecule 18: Transmembrane protein, putative

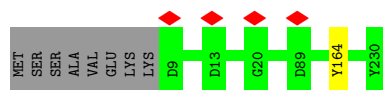


- Molecule 19: Structural protein

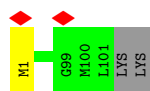


- Molecule 19: Structural protein

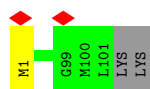




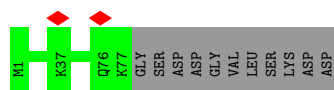
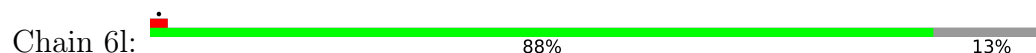
- Molecule 20: Transmembrane protein, putative



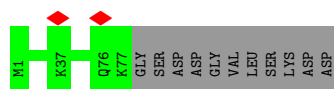
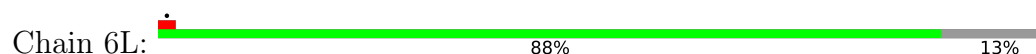
- Molecule 20: Transmembrane protein, putative



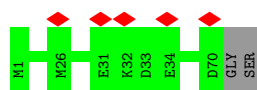
- Molecule 21: Decapping nuclease



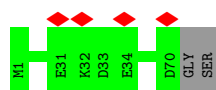
- Molecule 21: Decapping nuclease




- Molecule 22: Annexin



- Molecule 22: Annexin



- Molecule 23: Transmembrane protein, putative

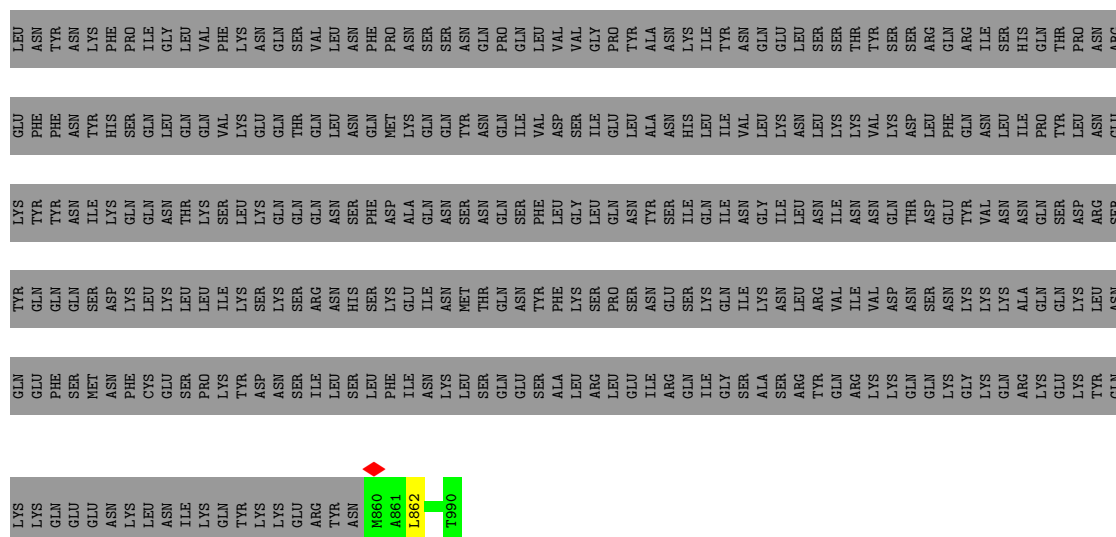
- Chain 7A: 

- [illegible]

- [illegible]

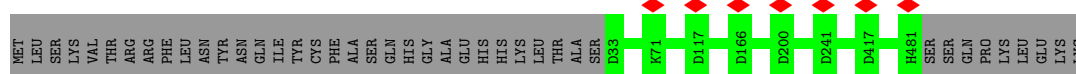
- [illegible]





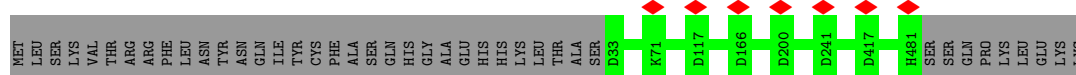
- Molecule 26: Transmembrane protein, putative

Chain a: 92% 8%



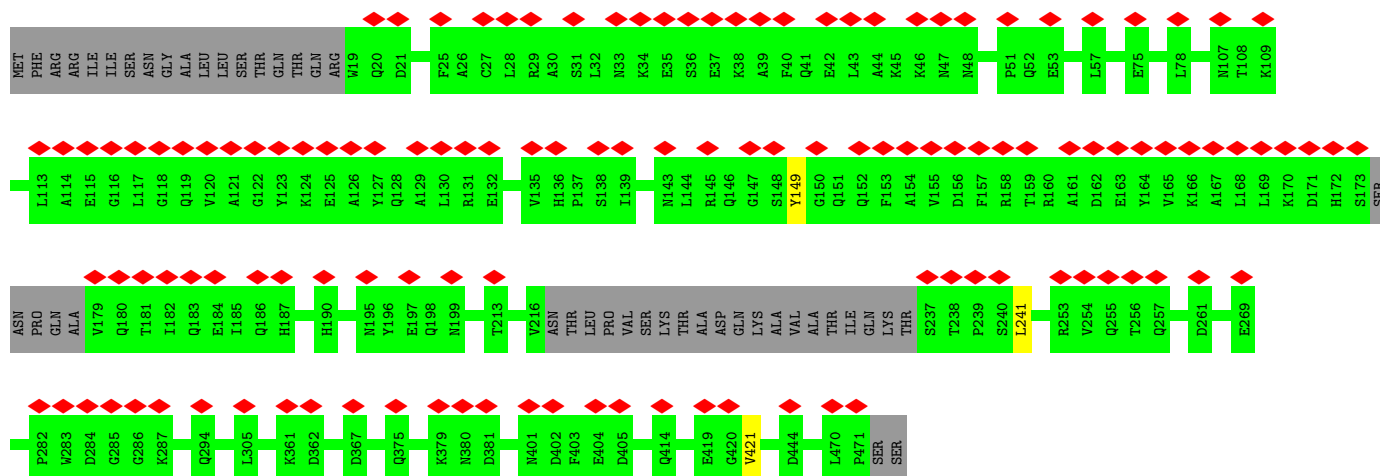
- Molecule 26: Transmembrane protein, putative

Chain A: 92% 8%



- Molecule 27: Protein phosphatase 2C, putative

Chain b: 27% 90% 10%



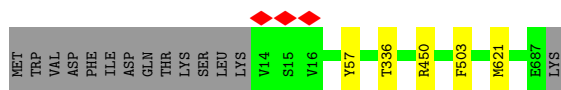
- Molecule 27: Protein phosphatase 2C, putative

[illegible]

- [illegible]

- [illegible]

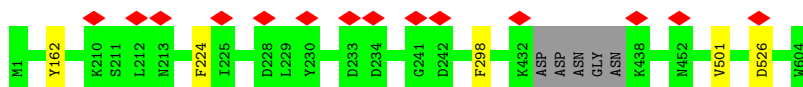
- Chain c1: 97% ..



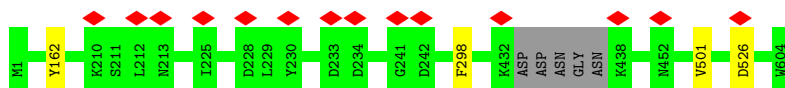
- Molecule 29: Cytochrome c oxidase subunit 1



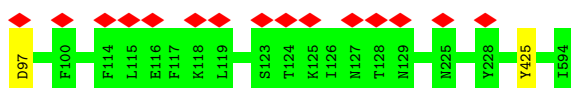
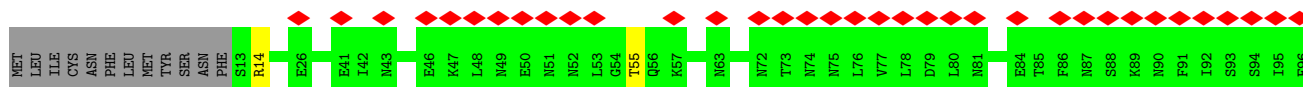
- Molecule 30: Cytochrome c oxidase subunit 2



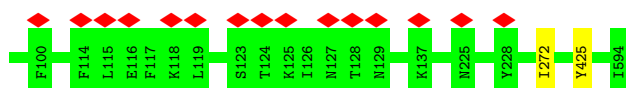
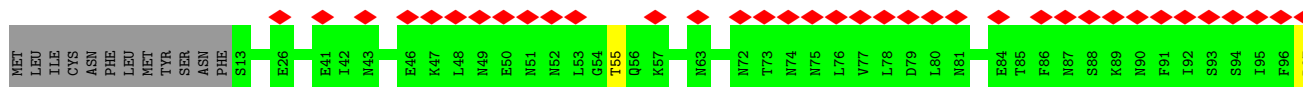
- Molecule 30: Cytochrome c oxidase subunit 2



- Molecule 31: Ymf68

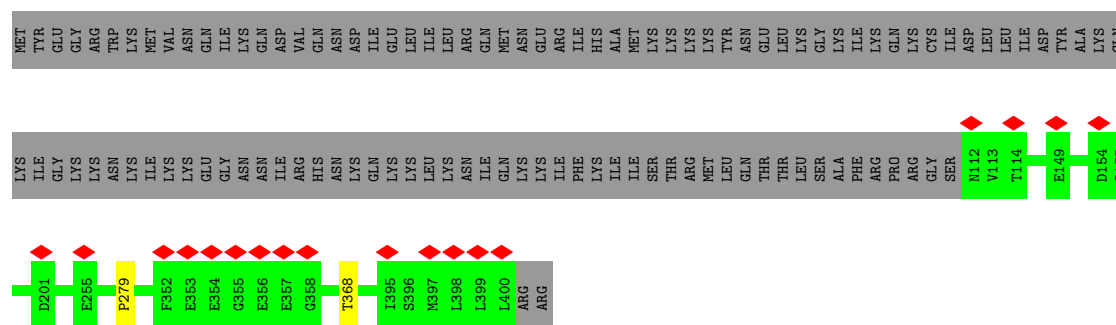


- Molecule 31: Ymf68



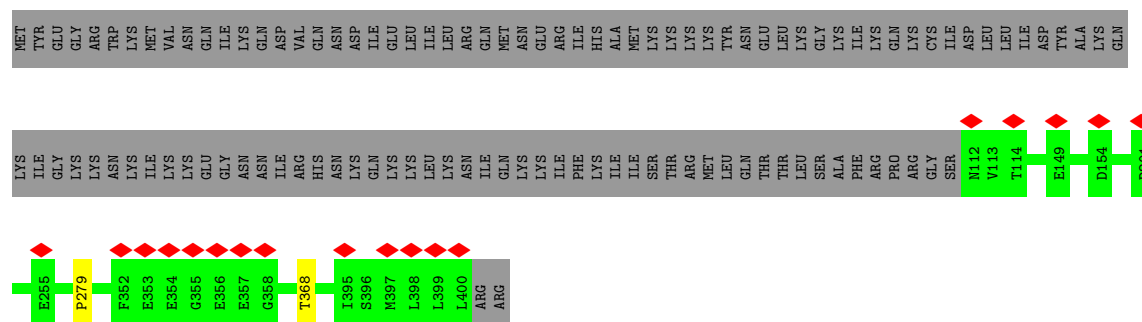
- Molecule 32: SURF1-like protein

Chain d:  71% 28%



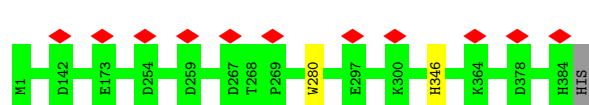
• Molecule 32: SURF1-like protein

Chain D:  71% 28%



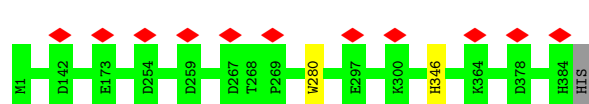
• Molecule 33: TraB family protein

Chain e:  99%



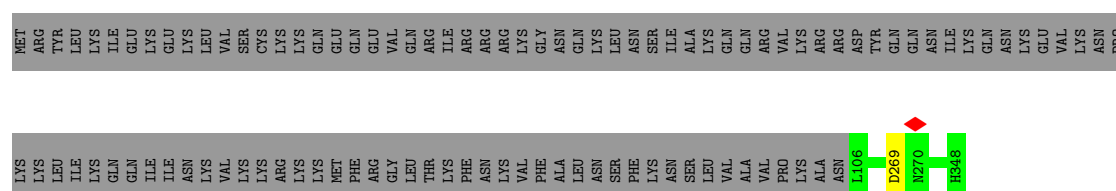
• Molecule 33: TraB family protein

Chain E:  99%

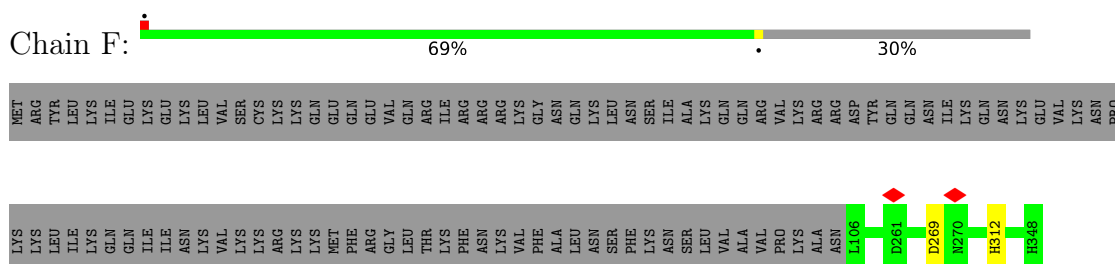


• Molecule 34: Transmembrane protein, putative

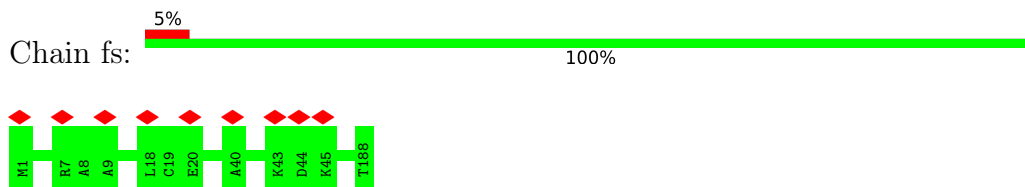
Chain f:  70% 30%



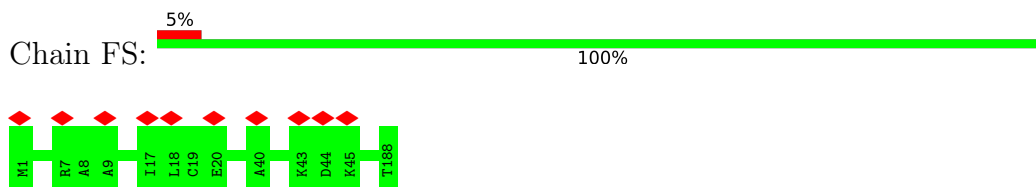
- Molecule 34: Transmembrane protein, putative



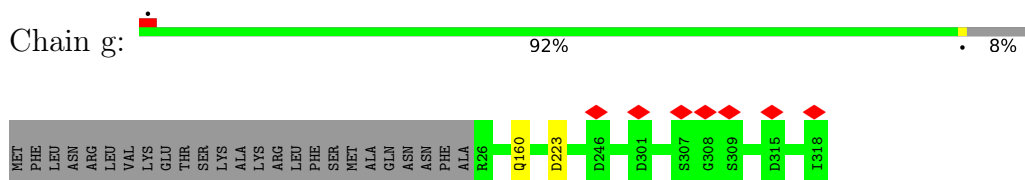
- Molecule 35: Iron-binding zinc finger CDGSH type protein



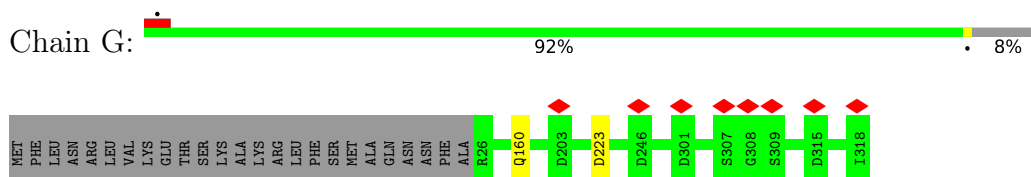
- Molecule 35: Iron-binding zinc finger CDGSH type protein



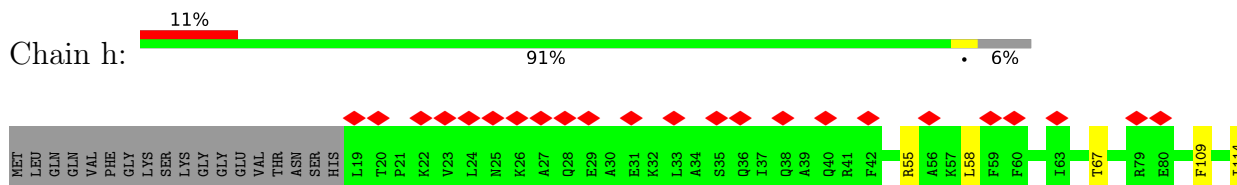
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

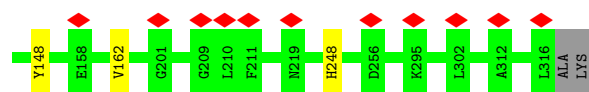


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

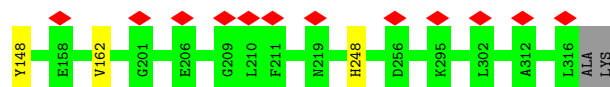
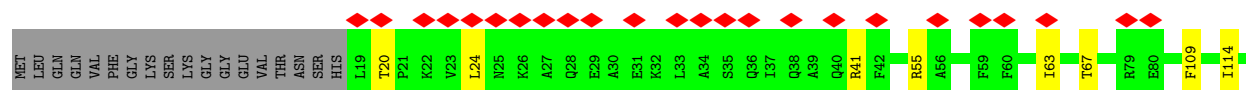
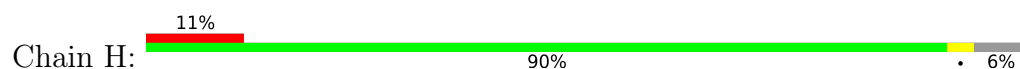


- Molecule 37: SURF1-like protein

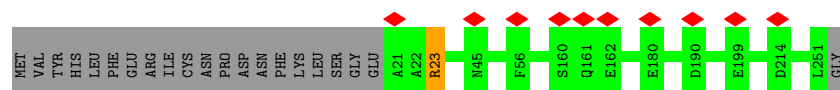




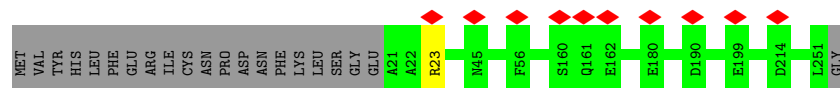
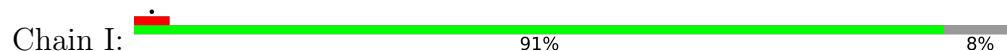
- Molecule 37: SURF1-like protein



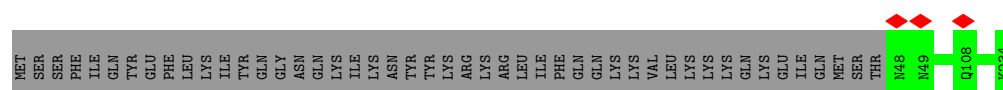
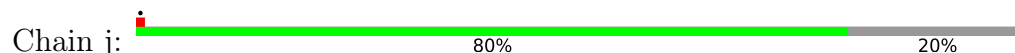
- Molecule 38: COXTT9



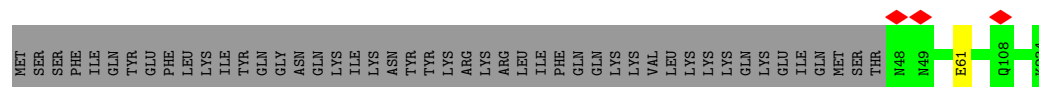
- Molecule 38: COXTT9



- Molecule 39: COXTT10

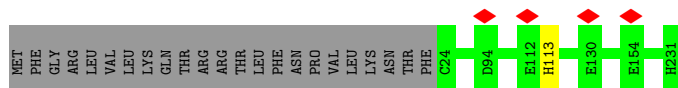


- Molecule 39: COXTT10

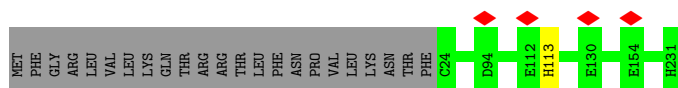
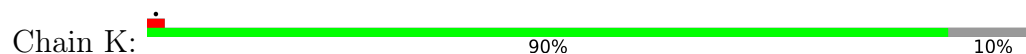


- Molecule 40: 39S ribosomal protein L9, mitochondrial

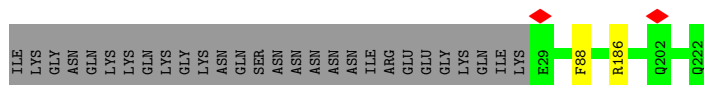
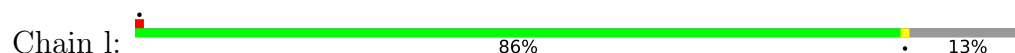




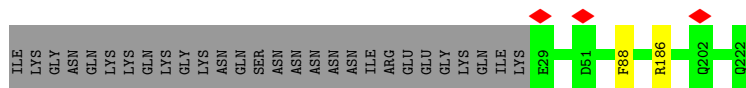
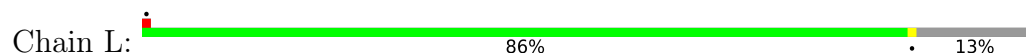
- Molecule 40: 39S ribosomal protein L9, mitochondrial



- Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 42: Transmembrane protein, putative



- Molecule 42: Transmembrane protein, putative



- Molecule 43: Oxoglutarate/malate translocator protein, putative



- Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain M1:  100%



- Molecule 44: 2-oxoglutarate/malate carrier protein

Chain m2:  100%



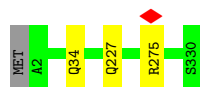
- Molecule 44: 2-oxoglutarate/malate carrier protein

Chain M2:  100%



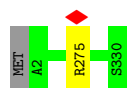
- Molecule 45: Carrier protein

Chain m3:  99%



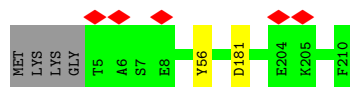
- Molecule 45: Carrier protein

Chain M3:  99%



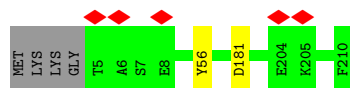
- Molecule 46: Transmembrane protein, putative

Chain n:  97%

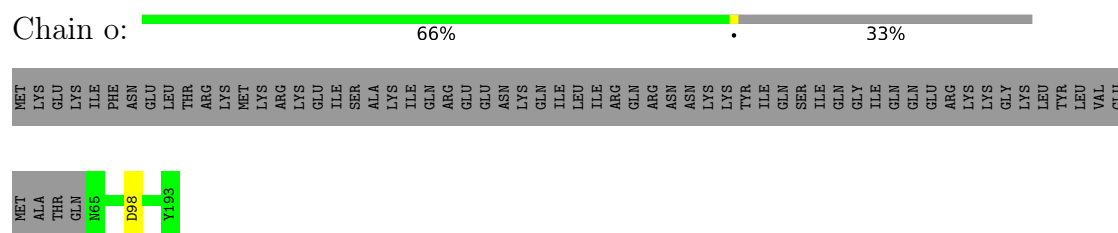


- Molecule 46: Transmembrane protein, putative

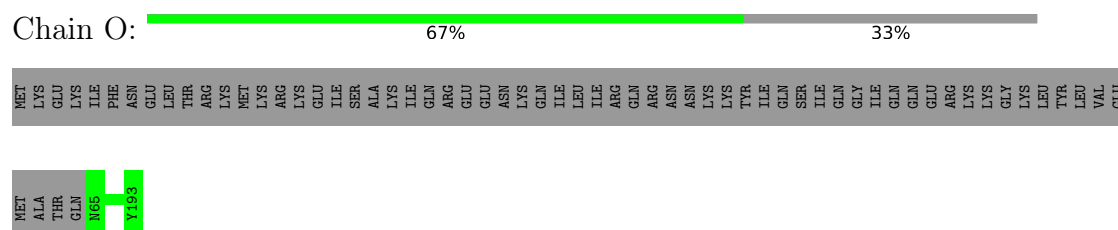
Chain N:  97%



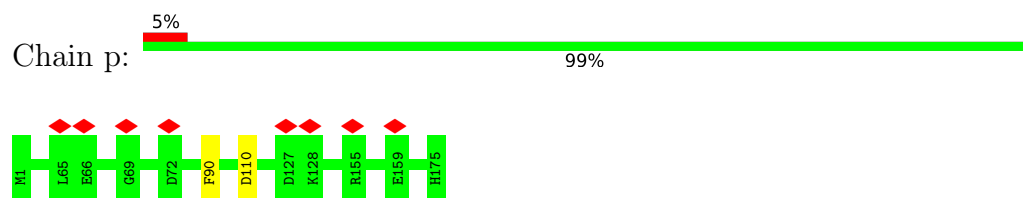
- Molecule 47: Mobilization protein



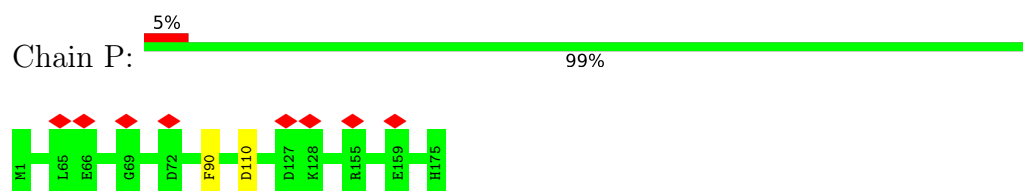
- Molecule 47: Mobilization protein



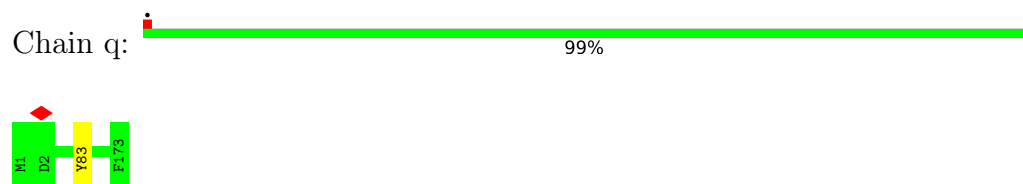
- Molecule 48: YffT domain-containing protein



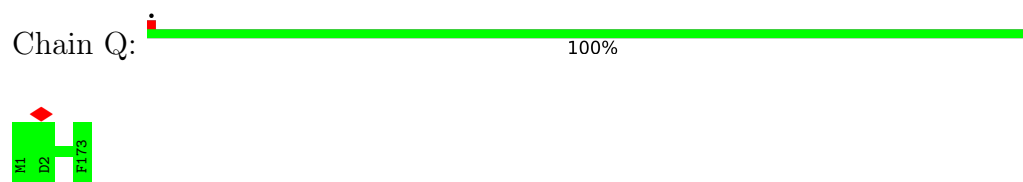
- Molecule 48: YffT domain-containing protein



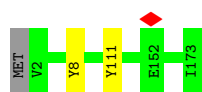
- Molecule 49: Transmembrane protein, putative



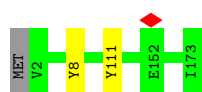
- Molecule 49: Transmembrane protein, putative



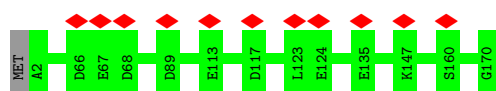
- Molecule 50: Transmembrane protein



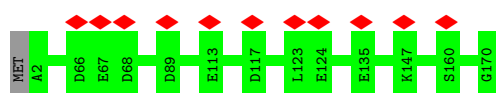
- Molecule 50: Transmembrane protein



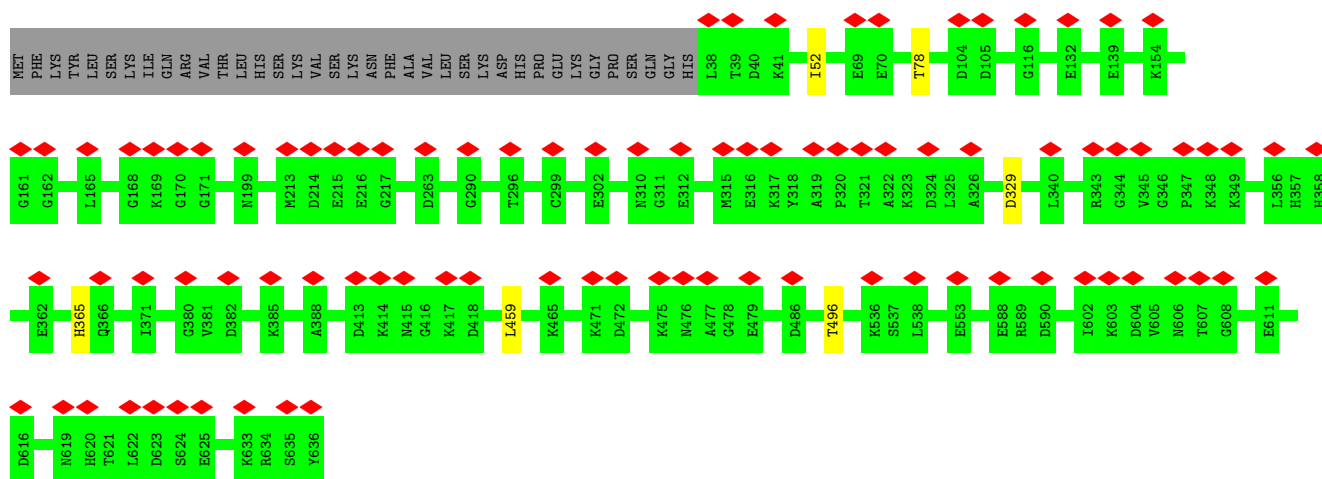
- Molecule 51: Complex III subunit VII



- Molecule 51: Complex III subunit VII

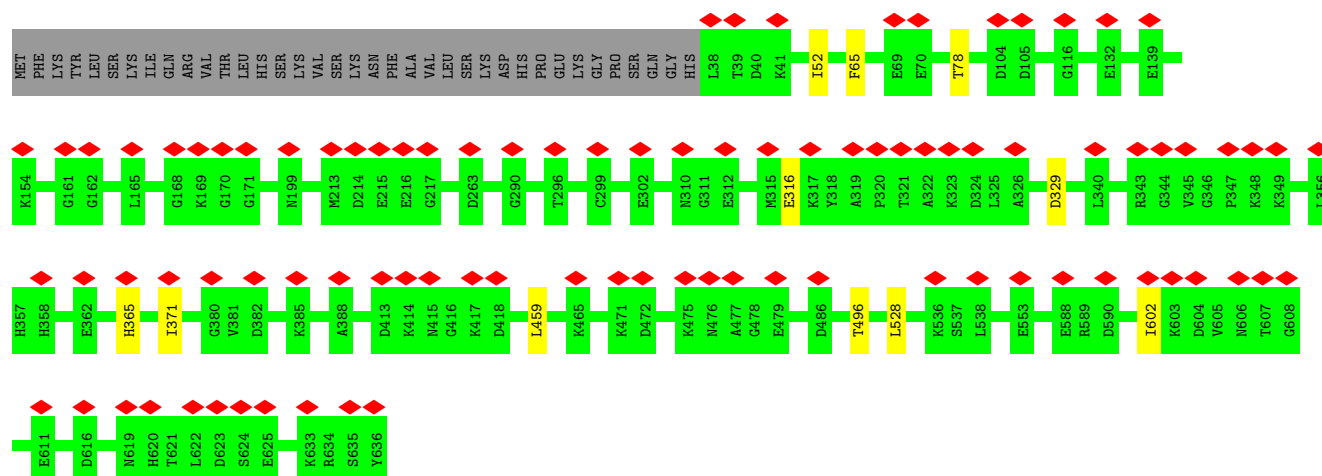


- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

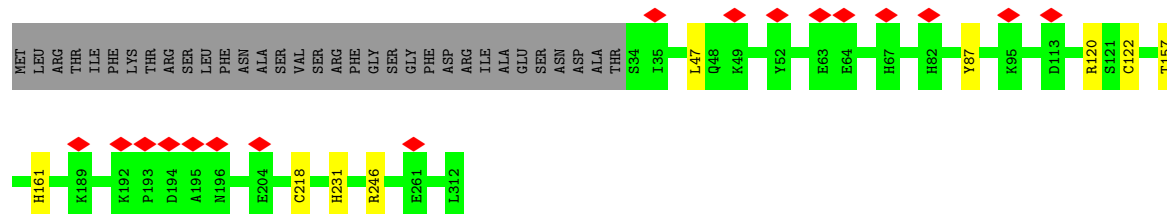
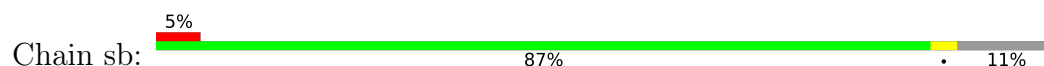


- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

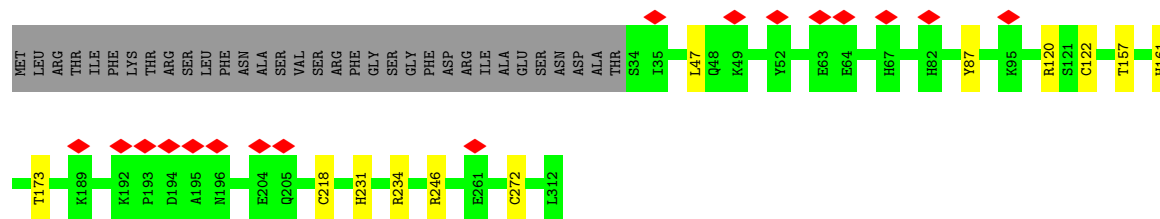
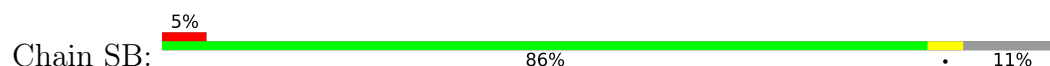




- Molecule 53: Succinate dehydrogenase (quinone)



- Molecule 53: Succinate dehydrogenase (quinone)



- Molecule 54: Cytochrome b-c1 complex subunit 8



- Molecule 54: Cytochrome b-c1 complex subunit 8



- Molecule 55: SDHD

Chain sd:  100%

There are no outlier residues recorded for this chain.

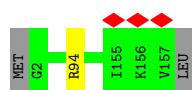
- Molecule 55: SDHD

Chain SD:  100%

There are no outlier residues recorded for this chain.

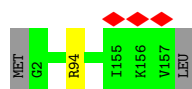
- Molecule 56: Transmembrane protein, putative

Chain t:  98% ..



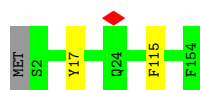
- Molecule 56: Transmembrane protein, putative

Chain T:  98% ..



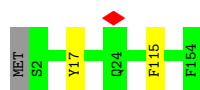
- Molecule 57: Transmembrane protein, putative

Chain u:  98% ..



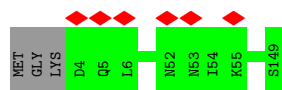
- Molecule 57: Transmembrane protein, putative

Chain U:  98% ..



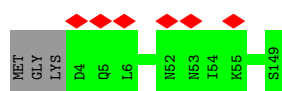
- Molecule 58: COXTT22

Chain v:  98% .



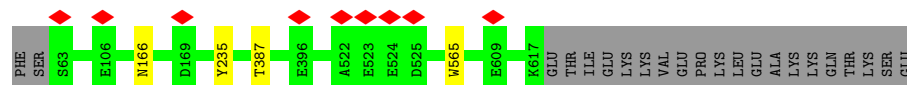
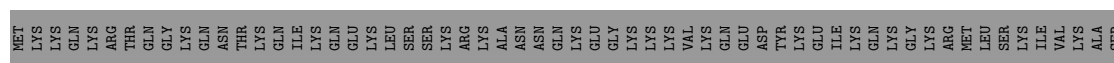
- Molecule 58: COXTT22

Chain V:  98%




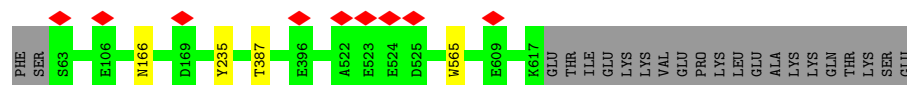
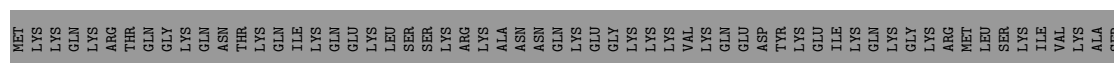
- Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain vb:  86%



- Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain VB:  86%



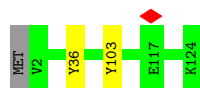
- Molecule 60: Transmembrane protein, putative

Chain w:  98%



- Molecule 60: Transmembrane protein, putative

Chain W:  98%



- Molecule 61: Transmembrane protein, putative

Chain x:  99%



- Molecule 61: Transmembrane protein, putative

Chain X:  99%



- Molecule 62: Lysozyme

Chain y:  99%



- Molecule 62: Lysozyme

Chain Y:  99%



- Molecule 63: Ymf70

Chain y0:  100%

There are no outlier residues recorded for this chain.

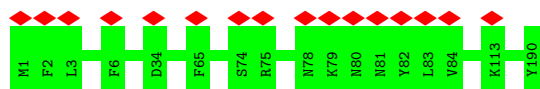
- Molecule 63: Ymf70

Chain Y0:  100%

There are no outlier residues recorded for this chain.

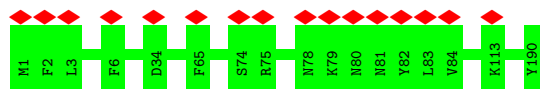
- Molecule 64: Ymf75

Chain y5:  8% 100%




- Molecule 64: Ymf75

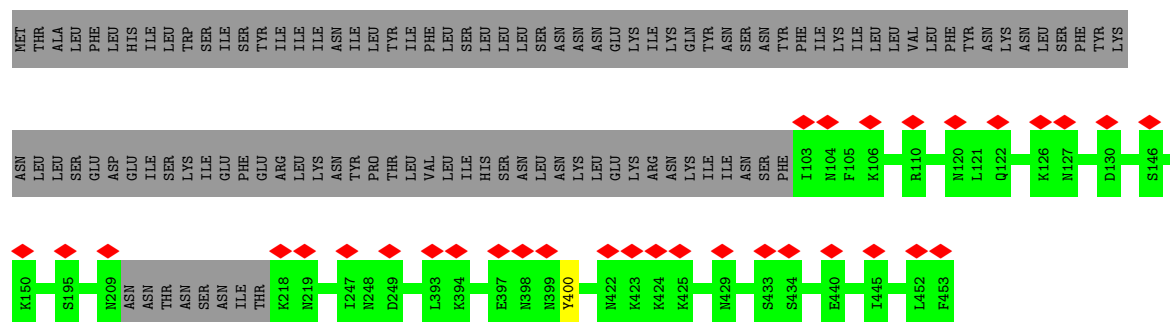
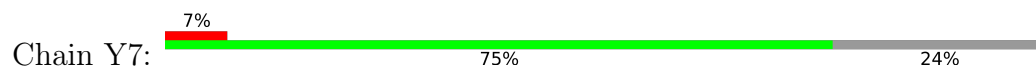
Chain Y5:  8% 100%



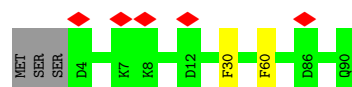
- Molecule 65: Ymf67

Chain y7:  7% 75% 24%

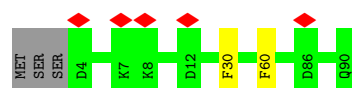
- Molecule 65: Ymf67



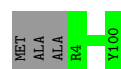
- Molecule 66: ABC transporter



- Molecule 66: ABC transporter

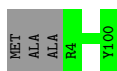


- Molecule 67: COXTT28



- Molecule 67: COXTT28





- Molecule 68: NADH dehydrogenase subunit 1

Chain 1b:  100%



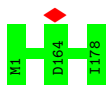
- Molecule 68: NADH dehydrogenase subunit 1

Chain 1B:  100%



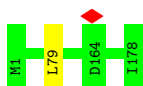
- Molecule 69: NADH dehydrogenase subunit 2

Chain 2b:  100%



- Molecule 69: NADH dehydrogenase subunit 2

Chain 2B:  99%



- Molecule 70: Ymf58

Chain 4l:  100%



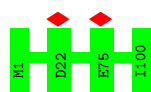
- Molecule 70: Ymf58

Chain 4L:  100%



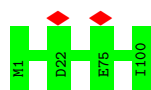
- Molecule 71: Ymf57

Chain 5b:  100%



- Molecule 71: Ymf57

Chain 5B:  100%



- Molecule 72: Transmembrane protein, putative

Chain a1:  99%



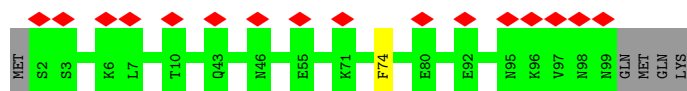
- Molecule 72: Transmembrane protein, putative

Chain A1:  99%



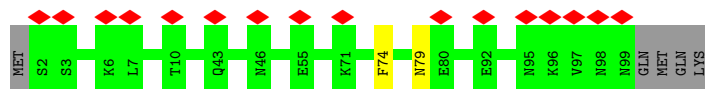
- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

Chain a2:  16% 94% 5%



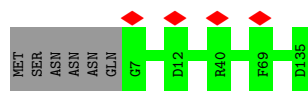
- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

Chain A2:  16% 93% 5%



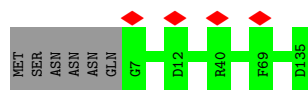
- Molecule 74: Transmembrane protein, putative

Chain a3:  96%




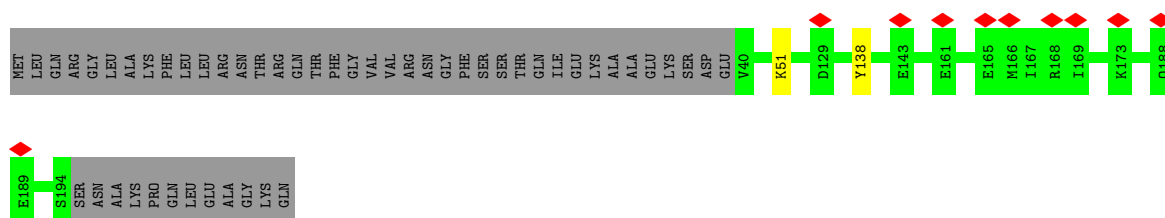
- Molecule 74: Transmembrane protein, putative

Chain A3:  96%




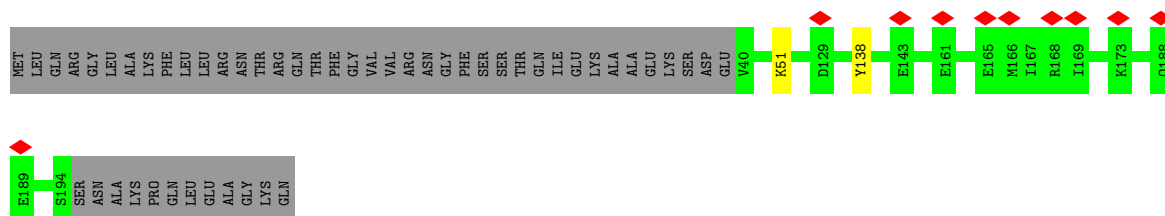
- Molecule 75: ETC complex I subunit motif protein

Chain a5:  5% 74% 25%



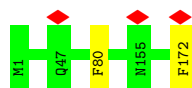
- Molecule 75: ETC complex I subunit motif protein

Chain A5:  5% 74% 25%



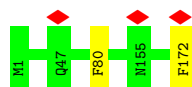
- Molecule 76: NADH dehydrogenase, putative

Chain a6:  99%



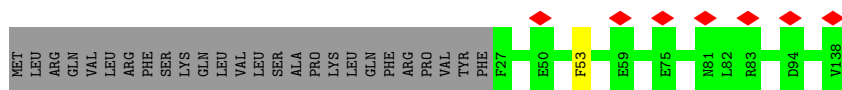
- Molecule 76: NADH dehydrogenase, putative

Chain A6:  99%

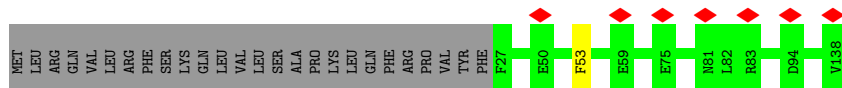
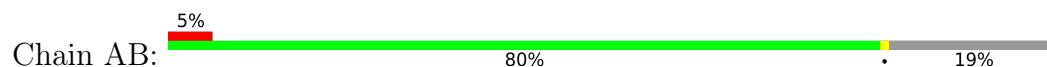


- Molecule 77: 37S ribosomal protein S25, mitochondrial

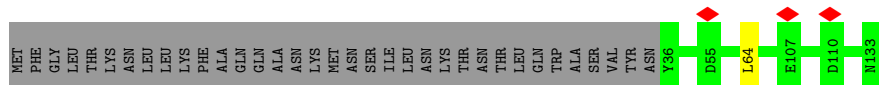
Chain a7:  9% 99%



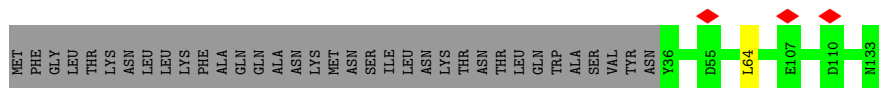
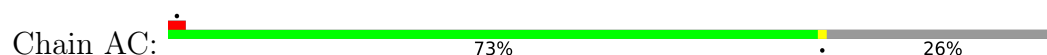
- Molecule 80: Acyl carrier protein



- Molecule 81: Acyl carrier protein



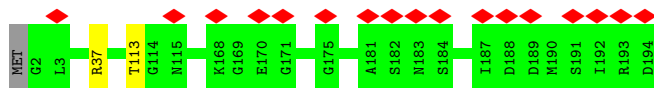
- Molecule 81: Acyl carrier protein



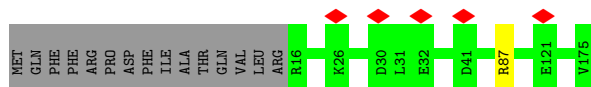
- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

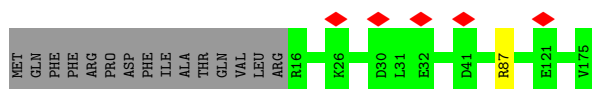


- Molecule 83: NDUA13



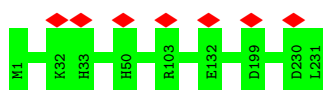
- Molecule 83: NDUA13

Chain AM:  91% 9%



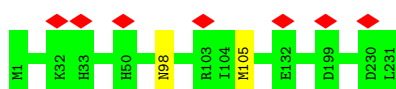
- Molecule 84: Transmembrane protein, putative

Chain an:  100%



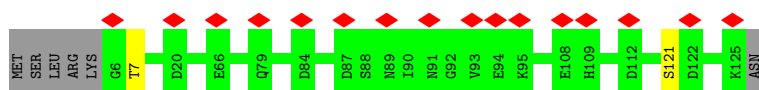
- Molecule 84: Transmembrane protein, putative

Chain AN:  99%



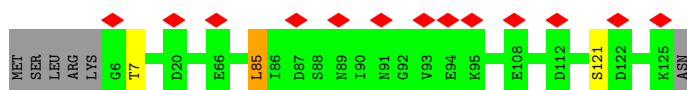
- Molecule 85: NDUB2

Chain b2:  13% 94% 5%




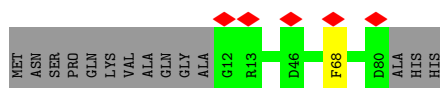
- Molecule 85: NDUB2

Chain B2:  10% 93% 5%




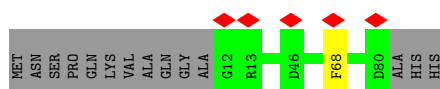
- Molecule 86: Transmembrane protein, putative

Chain b3:  6% 82% 17%




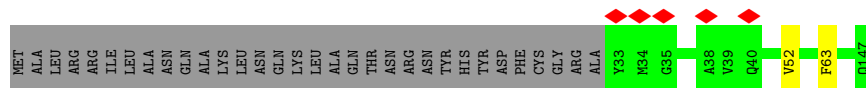
- Molecule 86: Transmembrane protein, putative

Chain B3:  6% 82% 17%




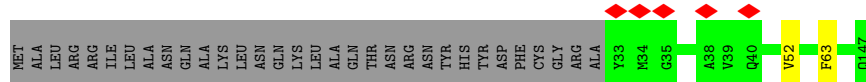
- Molecule 87: NDUB4

Chain b4:  77% 22%



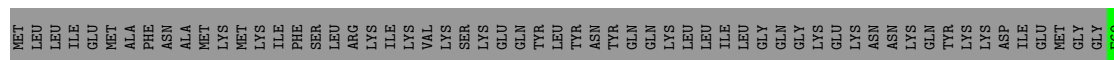
- Molecule 87: NDUB4

Chain B4:  77% 22%



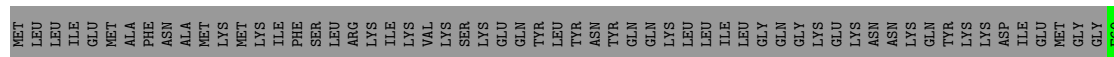
- Molecule 88: NDUB6

Chain b6:  54% 46%

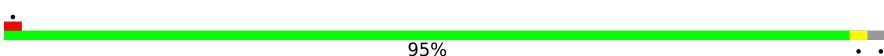


- Molecule 88: NDUB6

Chain B6:  54% 46%



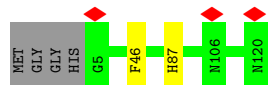
- Molecule 89: CHCH domain-containing protein

Chain b7:  95% . .

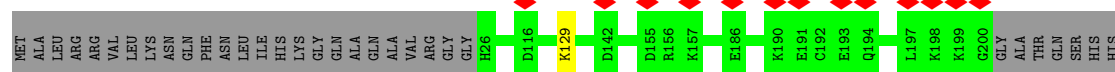
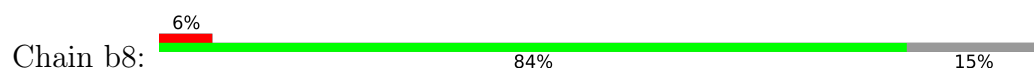


- Molecule 89: CHCH domain-containing protein

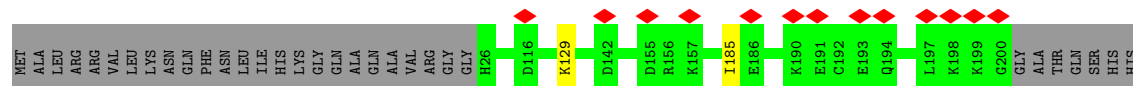
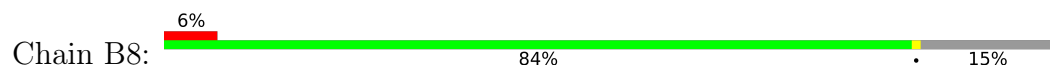
Chain B7:  95% . .



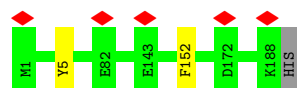
- Molecule 90: NDUB8



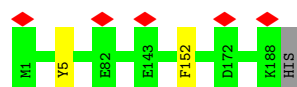
- Molecule 90: NDUB8



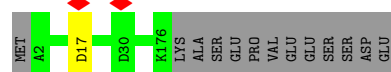
- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



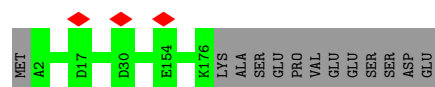
- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



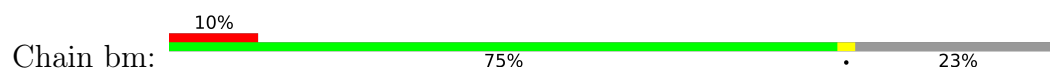
- Molecule 92: NDUB10

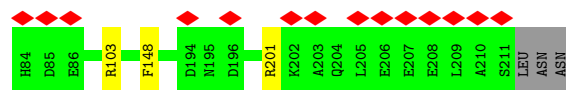
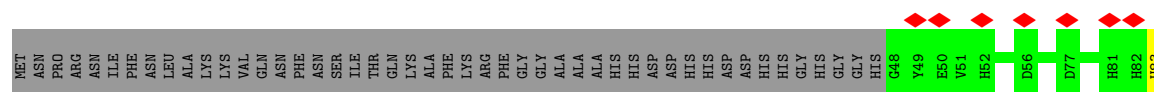


- Molecule 92: NDUB10

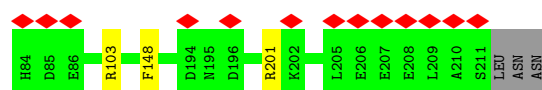
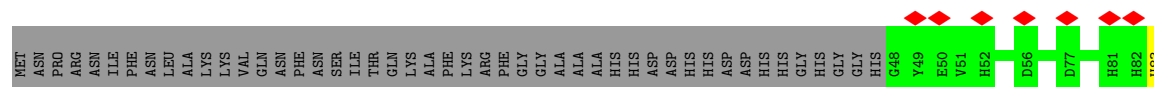
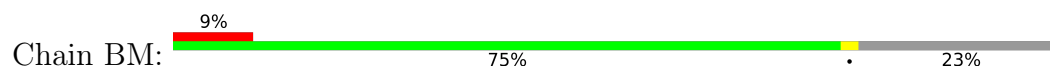


- Molecule 93: Transmembrane protein, putative





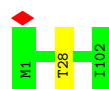
- Molecule 93: Transmembrane protein, putative



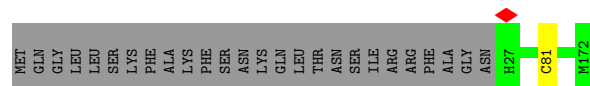
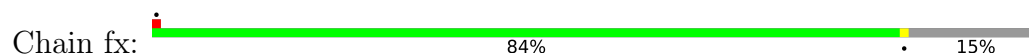
- Molecule 94: Complex I-MNLL



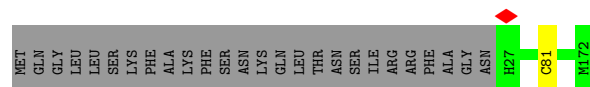
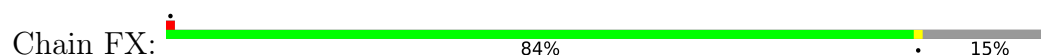
- Molecule 94: Complex I-MNLL




- Molecule 95: 2 iron, 2 sulfur cluster-binding protein

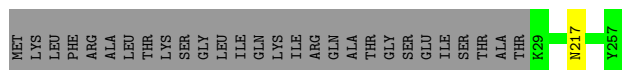


- Molecule 95: 2 iron, 2 sulfur cluster-binding protein




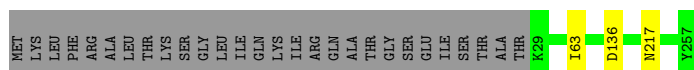
- Molecule 96: Gamma-carbonic anhydrase

Chain g1:  89% 11%



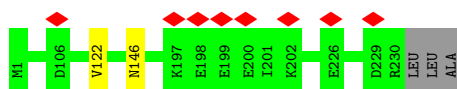
- Molecule 96: Gamma-carbonic anhydrase

Chain G1:  88% 11%



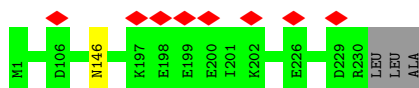
- Molecule 97: Gamma-carbonic anhydrase

Chain g2:  98% ..



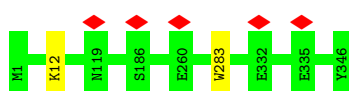
- Molecule 97: Gamma-carbonic anhydrase

Chain G2:  98% .



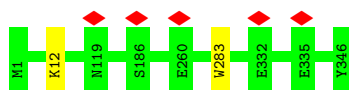
- Molecule 98: Transcription factor apfi protein, putative

Chain g3:  99% .




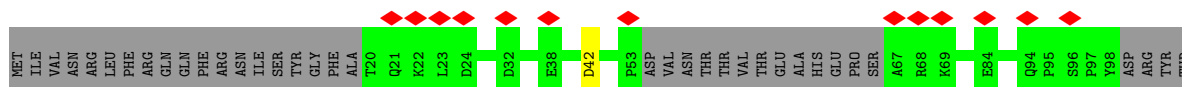
- Molecule 98: Transcription factor apfi protein, putative

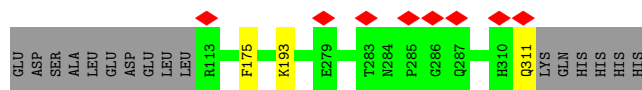
Chain G3:  99% .



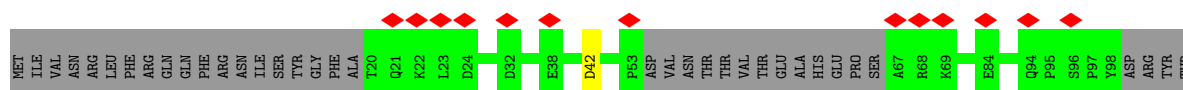
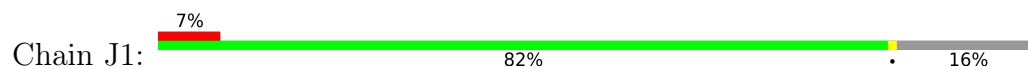
- Molecule 99: DnaJ domain protein

Chain j1:  7% 82% 16%

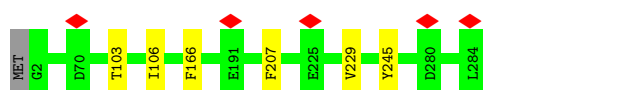




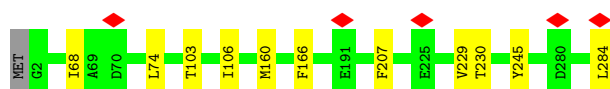
- Molecule 99: DnaJ domain protein



- Molecule 100: NADH-ubiquinone oxidoreductase chain 1



- Molecule 100: NADH-ubiquinone oxidoreductase chain 1



- Molecule 101: Ymf65

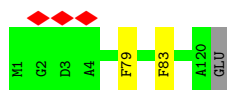


- Molecule 101: Ymf65

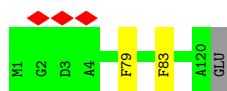


- Molecule 102: NADH-ubiquinone oxidoreductase chain 3





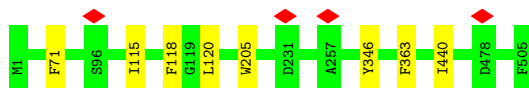
- Molecule 102: NADH-ubiquinone oxidoreductase chain 3



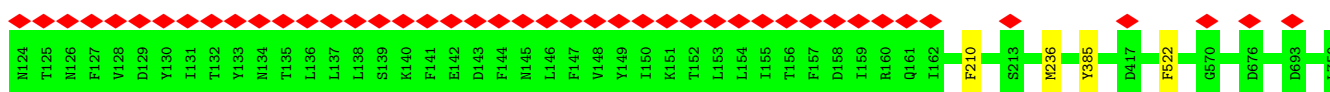
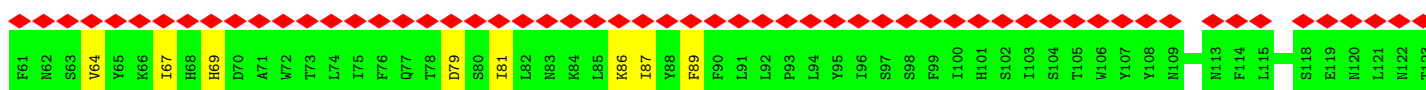
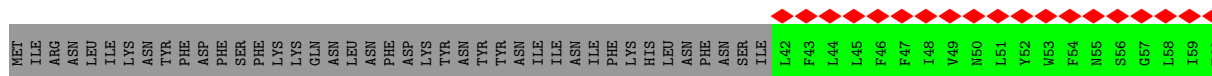
- Molecule 103: NADH-ubiquinone oxidoreductase chain 4



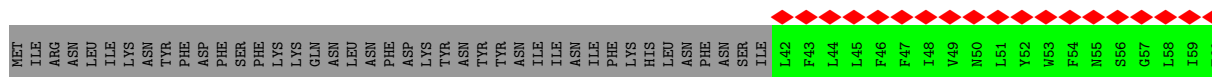
- Molecule 103: NADH-ubiquinone oxidoreductase chain 4

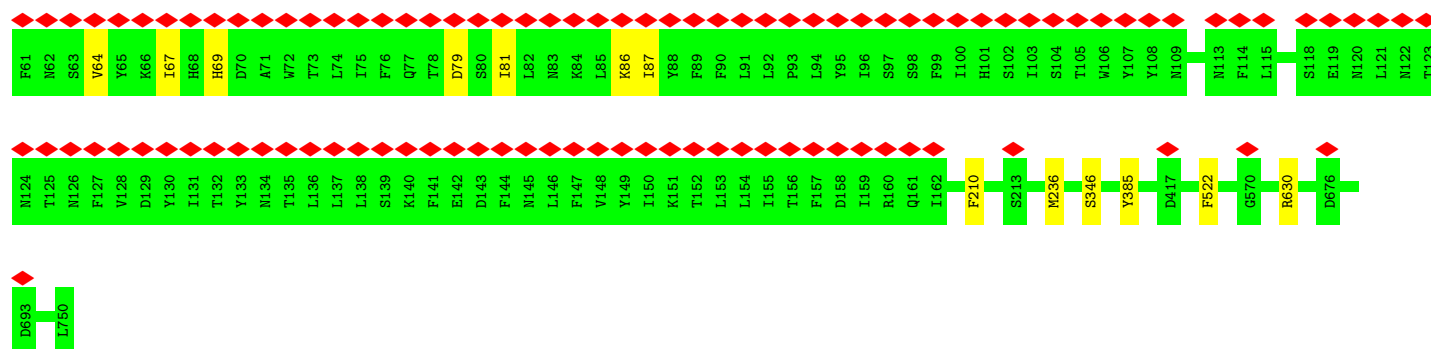


- Molecule 104: NADH dehydrogenase subunit 5



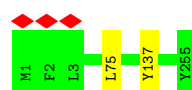
- Molecule 104: NADH dehydrogenase subunit 5





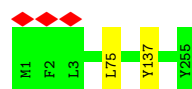
- Molecule 105: Ymf62

Chain n6: 99%



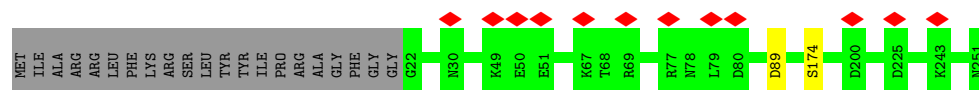
- Molecule 105: Ymf62

Chain N6: 99%



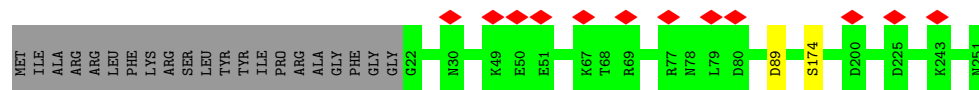
- Molecule 106: Transmembrane protein, putative

Chain p1: 91%



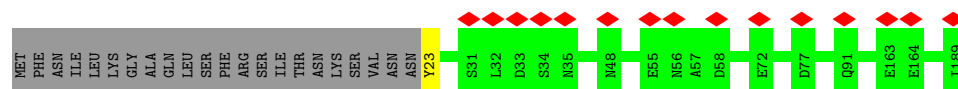
- Molecule 106: Transmembrane protein, putative

Chain P1: 91%

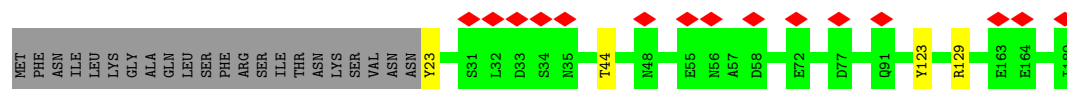
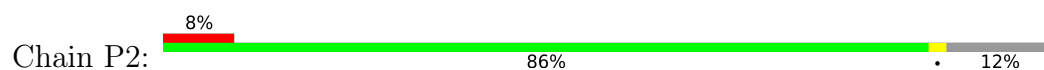


- Molecule 107: NDUPH2

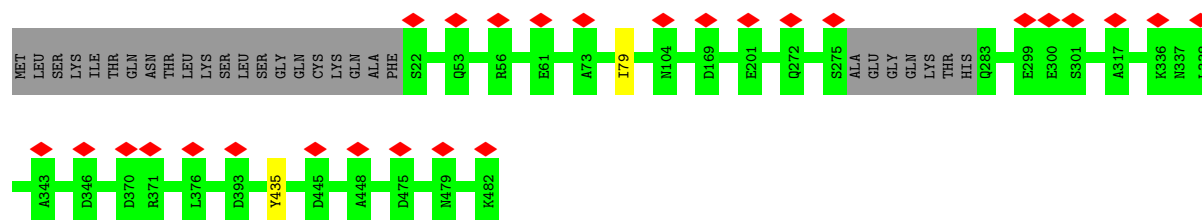
Chain p2: 88%



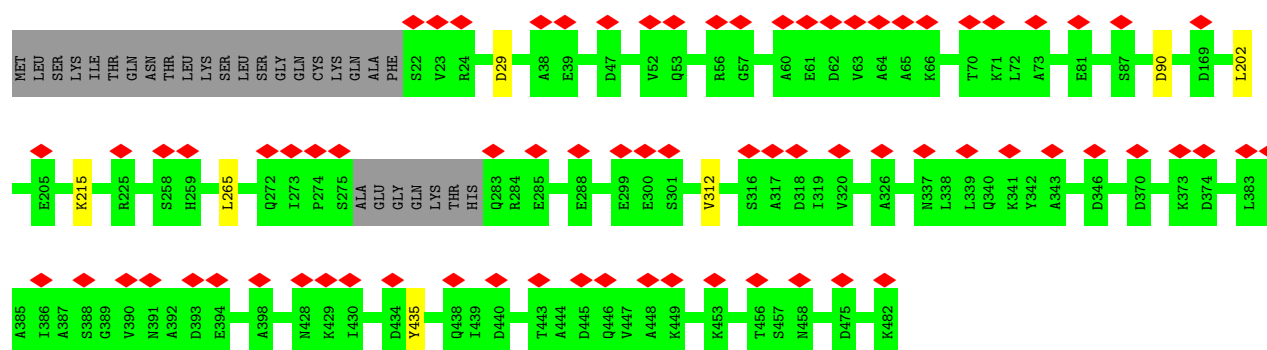
- Molecule 107: NDUPH2



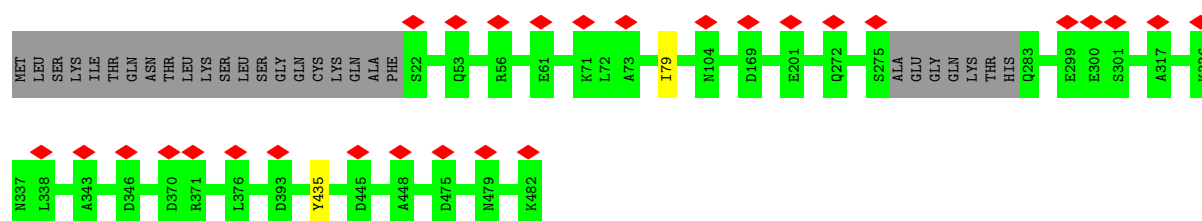
- Molecule 108: M16 family peptidase, putative



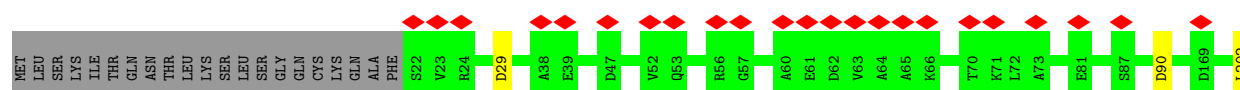
- Molecule 108: M16 family peptidase, putative

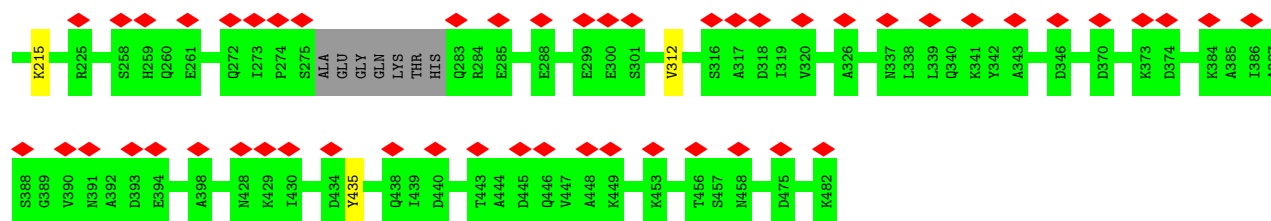


- Molecule 108: M16 family peptidase, putative



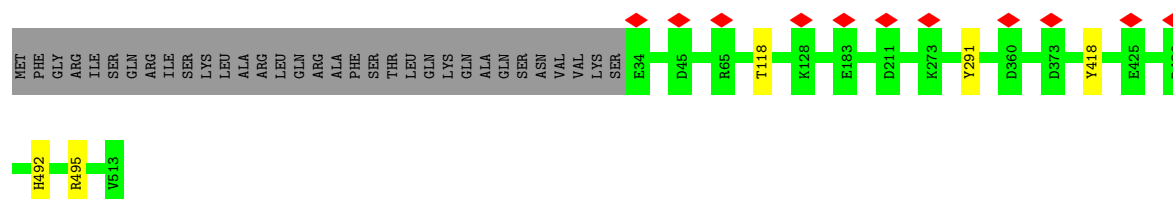
- Molecule 108: M16 family peptidase, putative





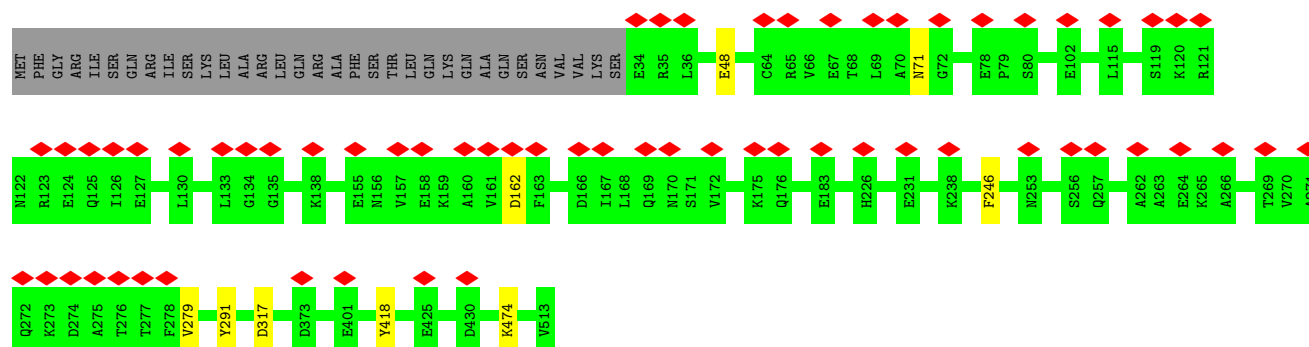
- Molecule 109: Peptidase M16 inactive domain protein

Chain qB: 93% • 6%



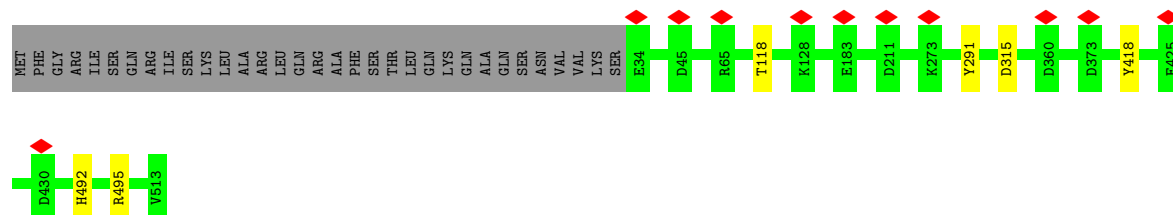
- Molecule 109: Peptidase M16 inactive domain protein

Chain qb: 12% 92% • 6%



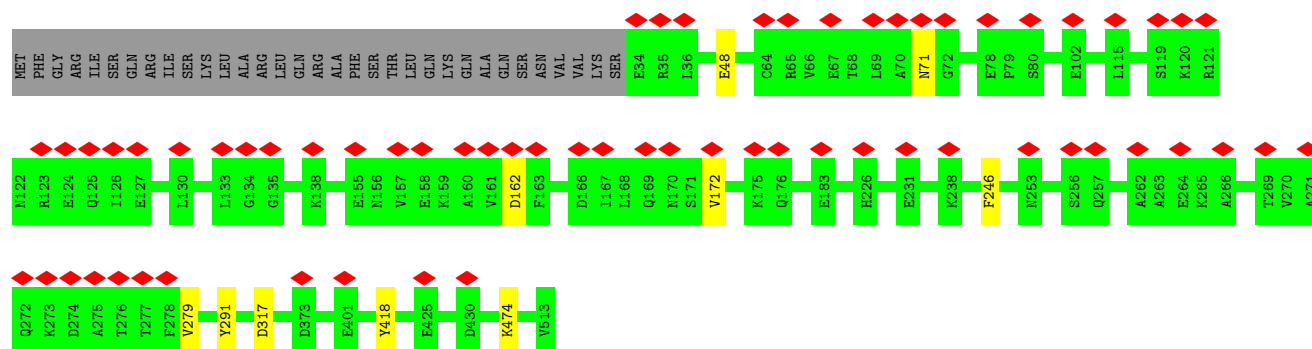
- Molecule 109: Peptidase M16 inactive domain protein

Chain QB: 12% 92% • 6%



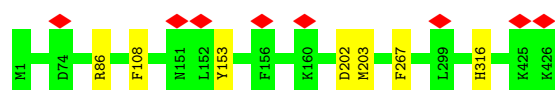
- Molecule 109: Peptidase M16 inactive domain protein

Chain Qb: 12% 92% • 6%



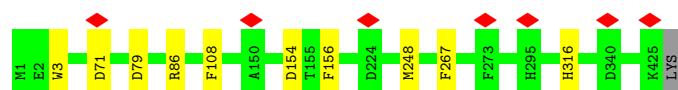
- Molecule 110: Apocytochrome b

Chain qC: 98%



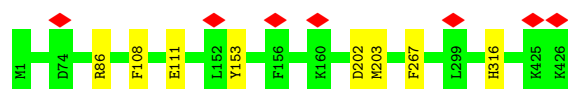
- Molecule 110: Apocytochrome b

Chain qc: 97%



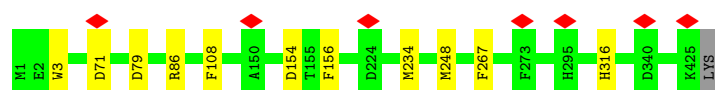
- Molecule 110: Apocytochrome b

Chain QC: 98%



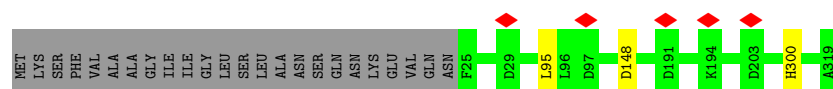
- Molecule 110: Apocytochrome b

Chain Qc: 97%



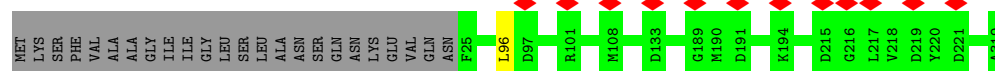
- Molecule 111: Cytochrome protein c1

Chain qD: 92% 8%



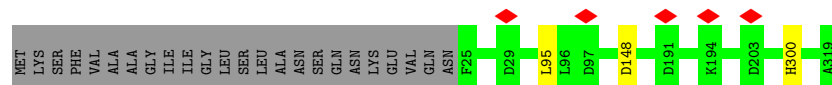
- Molecule 111: Cytochrome protein c1

Chain qd: 



• Molecule 111: Cytochrome protein c1

Chain QD: 




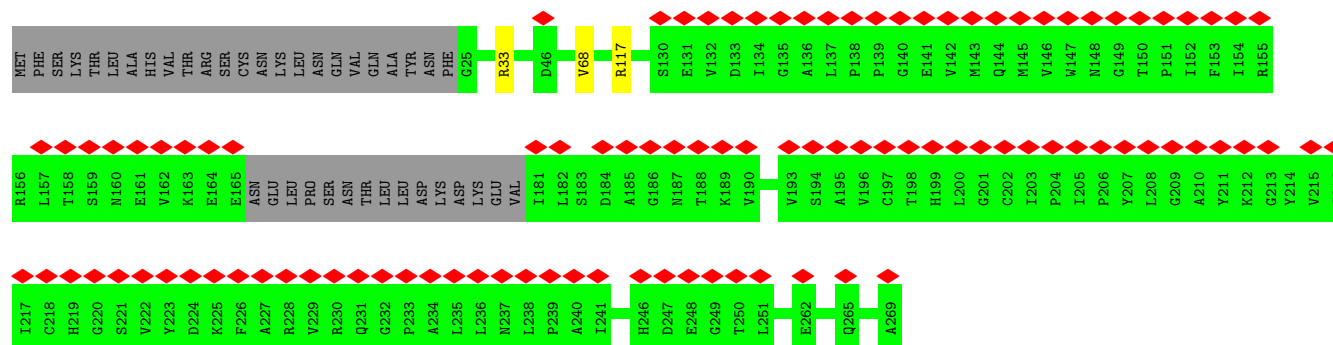
• Molecule 111: Cytochrome protein c1

Chain Qd: 




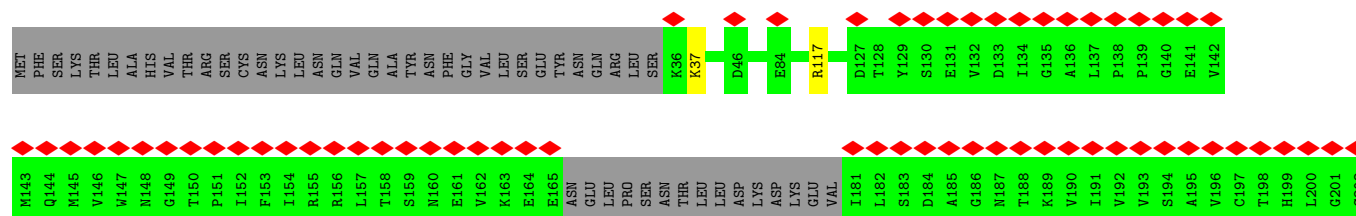
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit

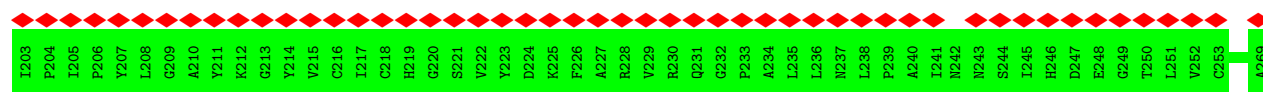
Chain qE: 



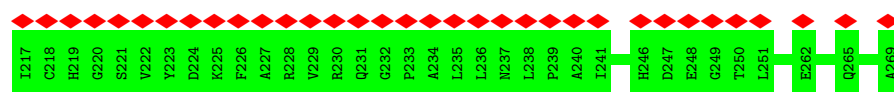
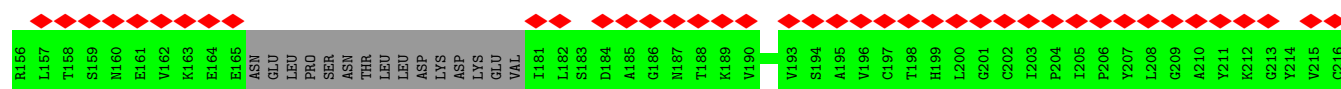
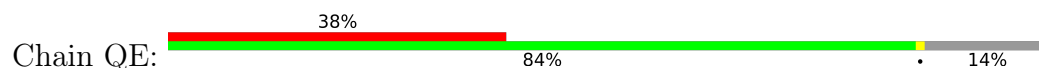
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit

Chain qe: 

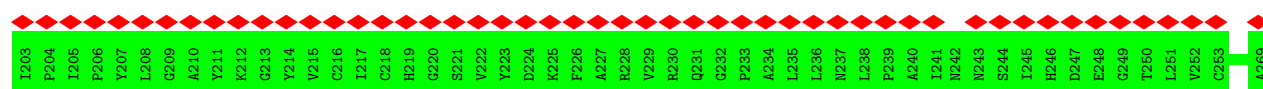
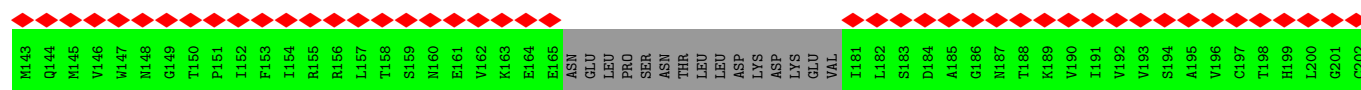
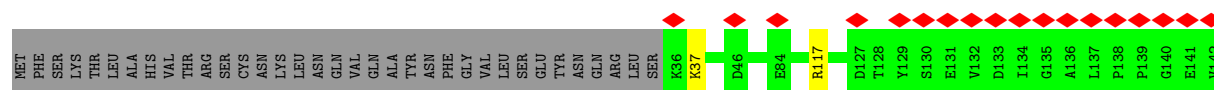
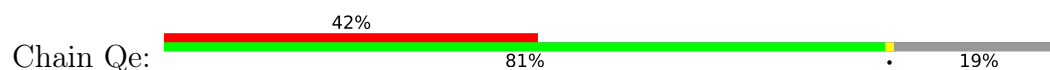




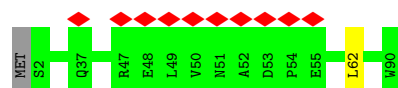
- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit



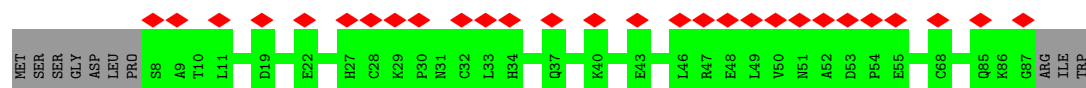
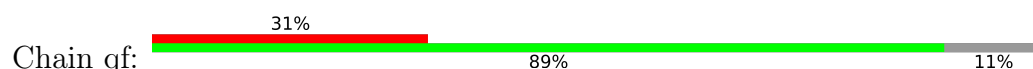
- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit



- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

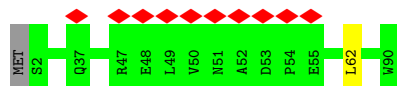


- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein




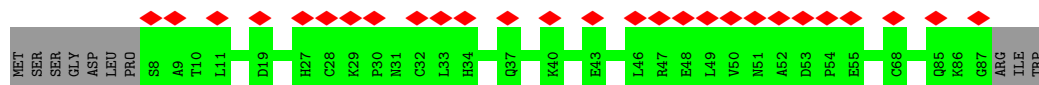
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain QF: 



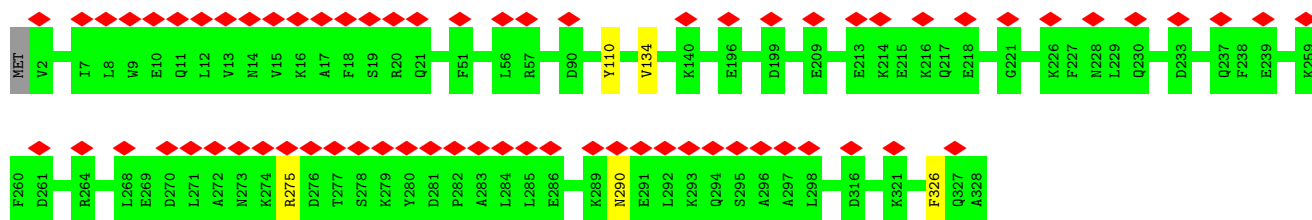
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain Qf: 



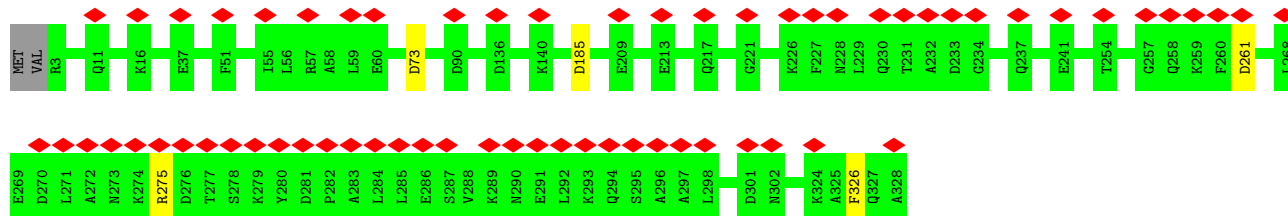
- Molecule 114: Sulphotransf domain-containing protein

Chain qG: 



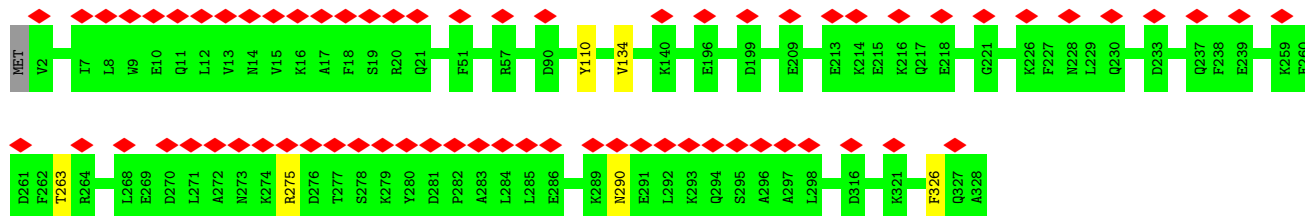
- Molecule 114: Sulphotransf domain-containing protein

Chain qg: 

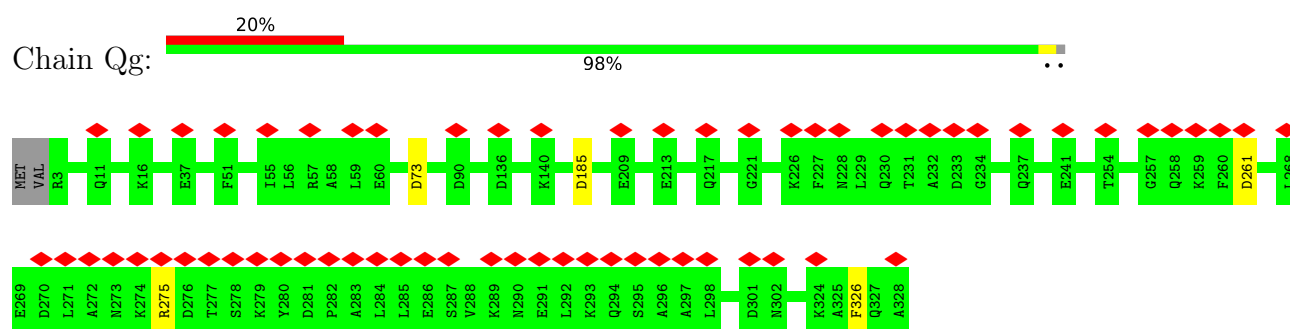


- Molecule 114: Sulphotransf domain-containing protein

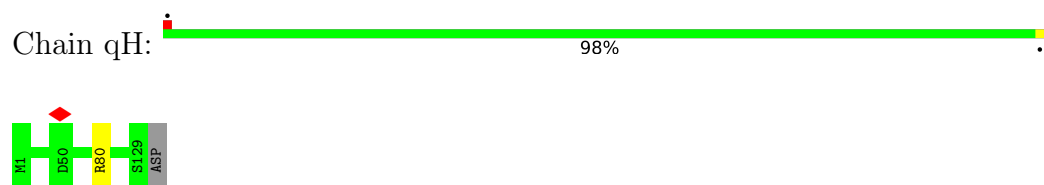
Chain QG: 



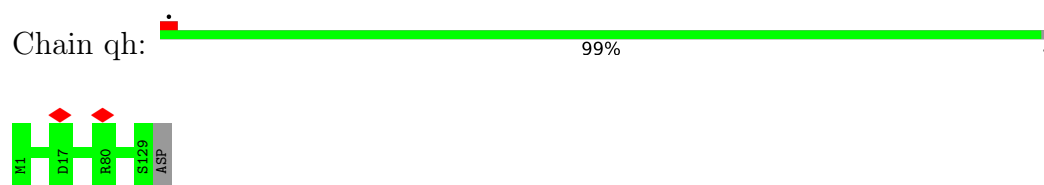
- Molecule 114: Sulphotransf domain-containing protein



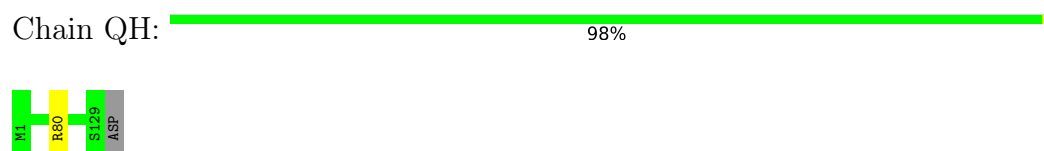
- Molecule 115: Transmembrane protein, putative



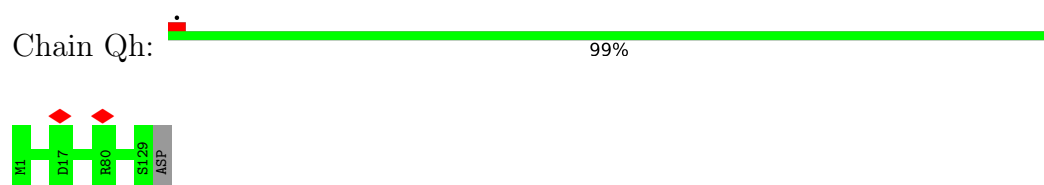
- Molecule 115: Transmembrane protein, putative



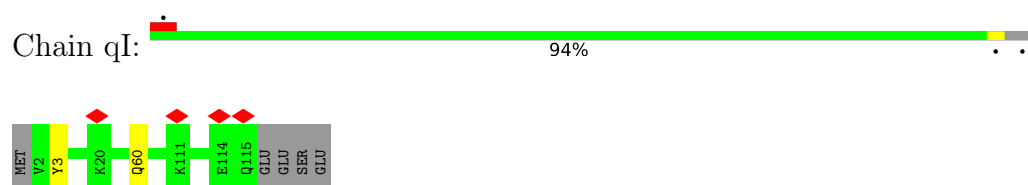
- Molecule 115: Transmembrane protein, putative



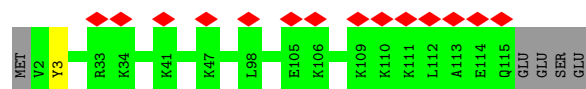
- Molecule 115: Transmembrane protein, putative



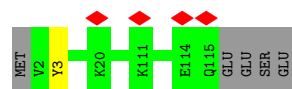
- Molecule 116: Transmembrane protein, putative



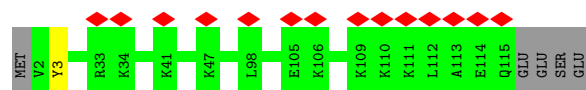
- Molecule 116: Transmembrane protein, putative



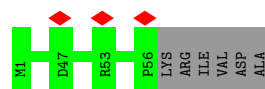
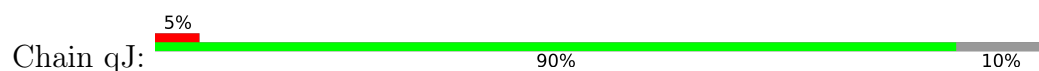
- Molecule 116: Transmembrane protein, putative



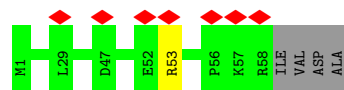
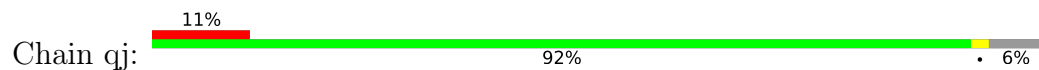
- Molecule 116: Transmembrane protein, putative



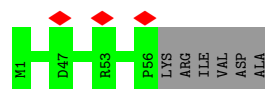
- Molecule 117: Transmembrane protein, putative



- Molecule 117: Transmembrane protein, putative



- Molecule 117: Transmembrane protein, putative

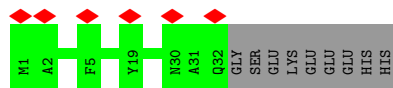
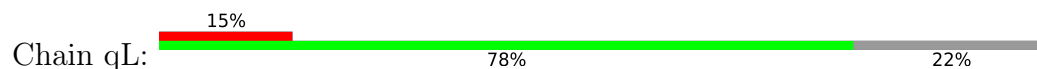


- Molecule 117: Transmembrane protein, putative

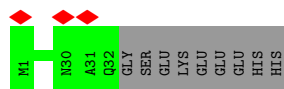
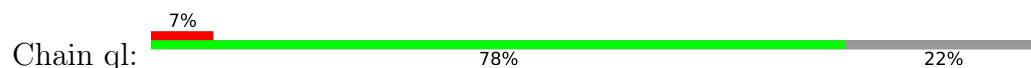




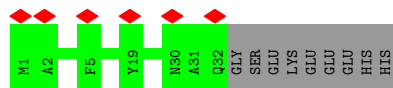
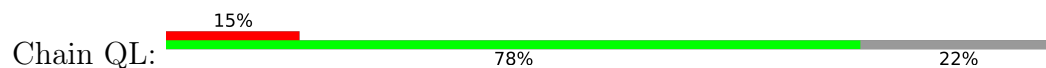
- Molecule 118: UQCRTT2



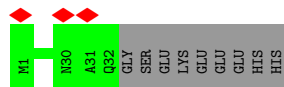
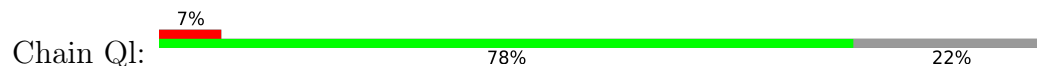
- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide

Chain u2:  100%

There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide

Chain U2:  100%

There are no outlier residues recorded for this chain.

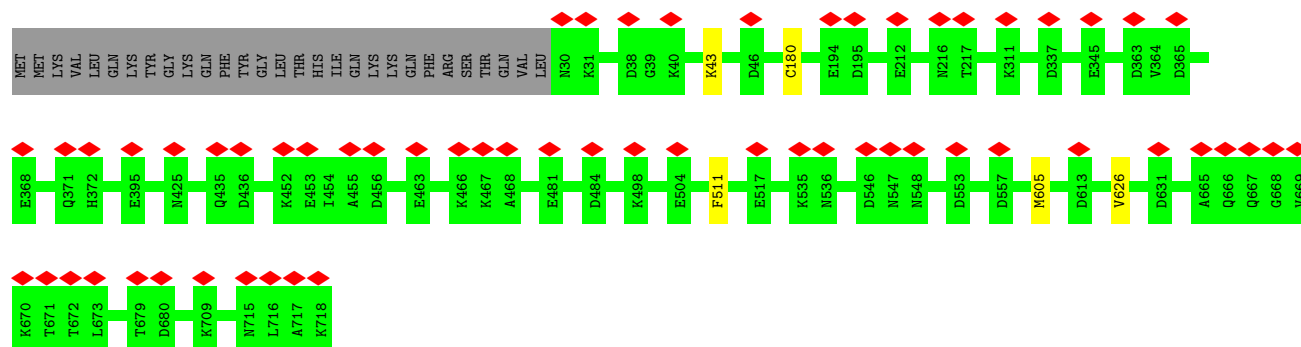
- Molecule 119: Unknown peptide

Chain QM:  100%

There are no outlier residues recorded for this chain.

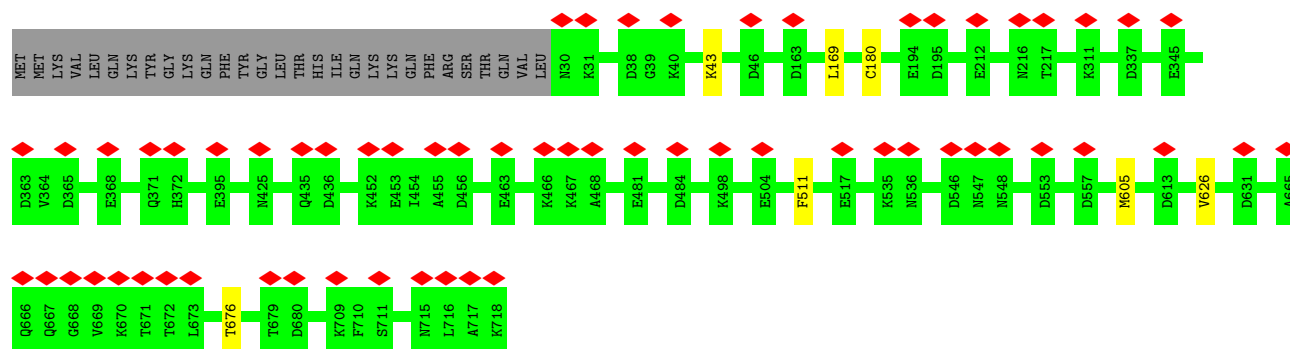
- Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain s1:  95%



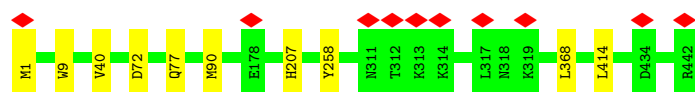
- Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain S1:  95%

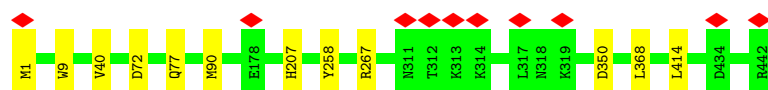


- Molecule 121: NADH dehydrogenase subunit 7

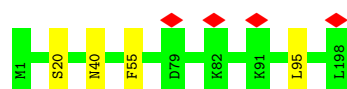
Chain s2:  98%



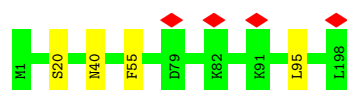
- Molecule 121: NADH dehydrogenase subunit 7



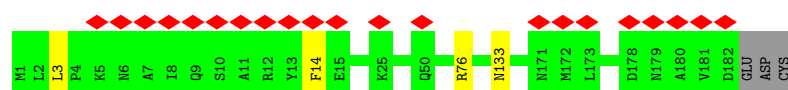
- Molecule 122: NADH dehydrogenase subunit 9



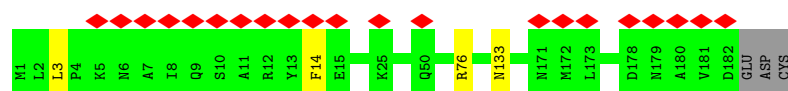
- Molecule 122: NADH dehydrogenase subunit 9



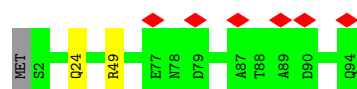
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



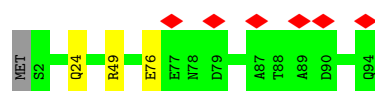
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



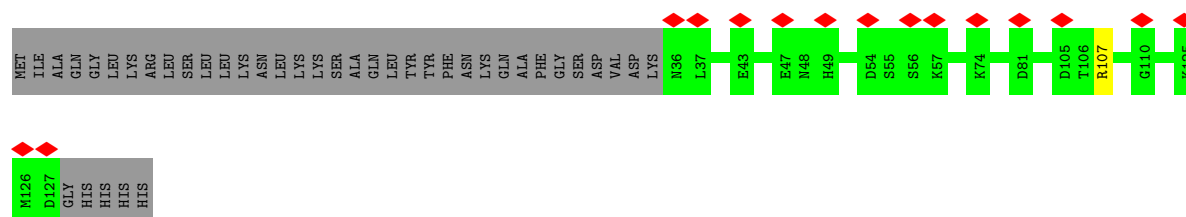
- Molecule 124: GRAM domain protein



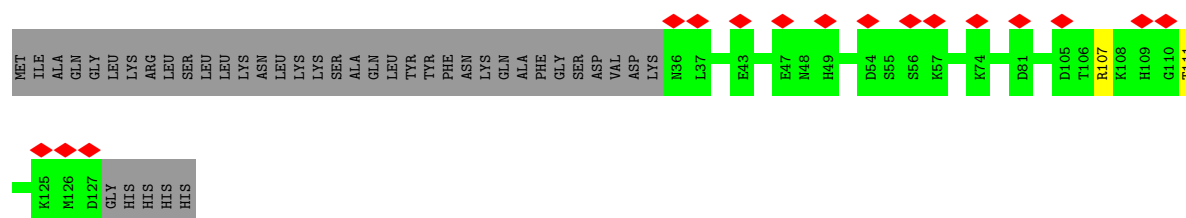
- Molecule 124: GRAM domain protein



- Molecule 125: Zinc-finger protein



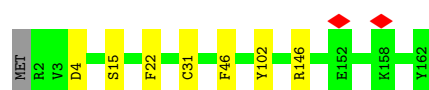
- Molecule 125: Zinc-finger protein



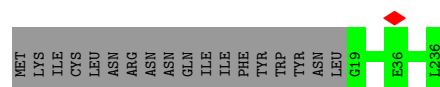
- Molecule 126: NADH dehydrogenase subunit 10



- Molecule 126: NADH dehydrogenase subunit 10

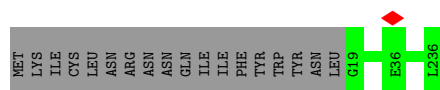


- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative



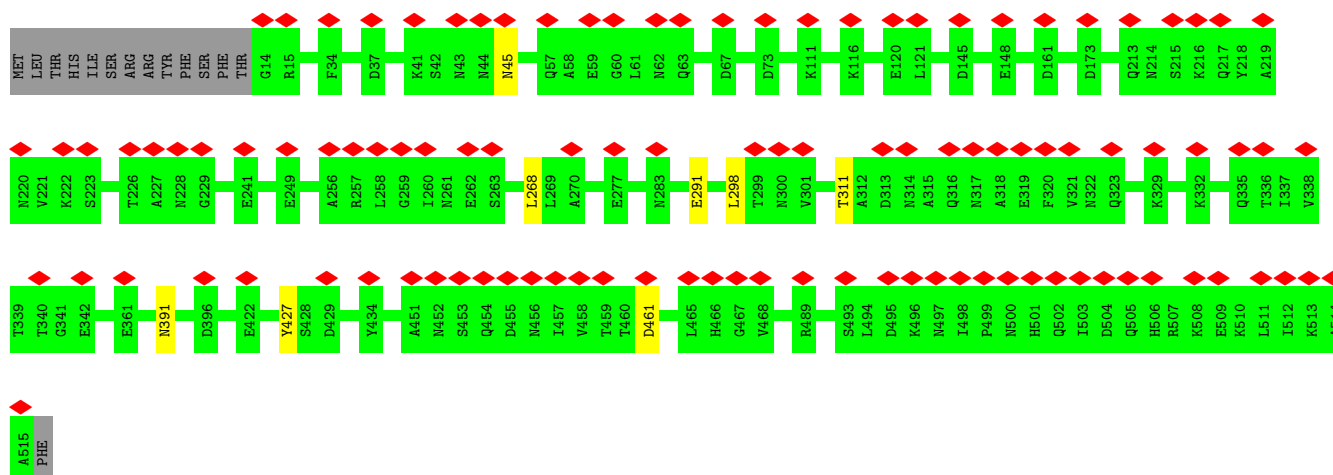
- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative

Chain S8: 



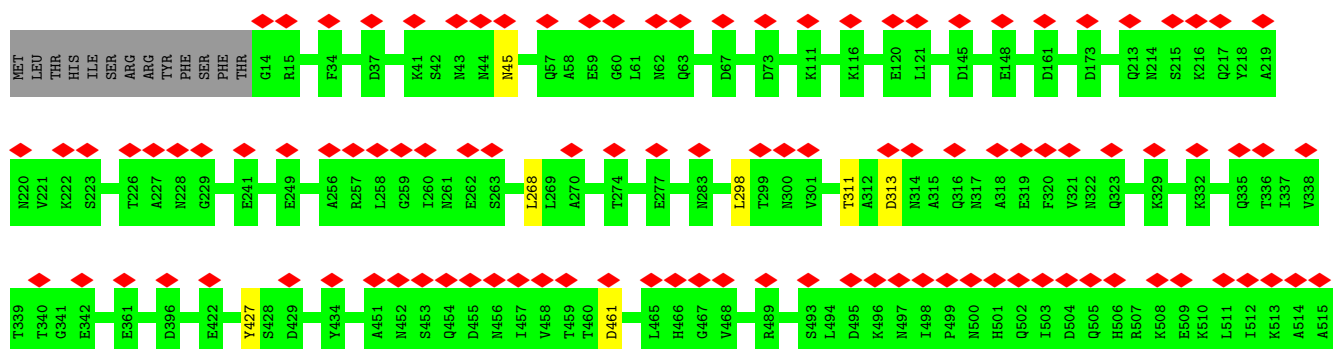
- Molecule 128: Lipid-A-disaccharide synthase

Chain t1: 




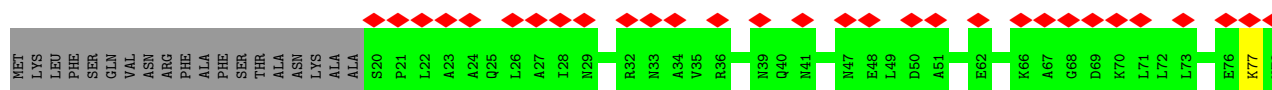
- Molecule 128: Lipid-A-disaccharide synthase

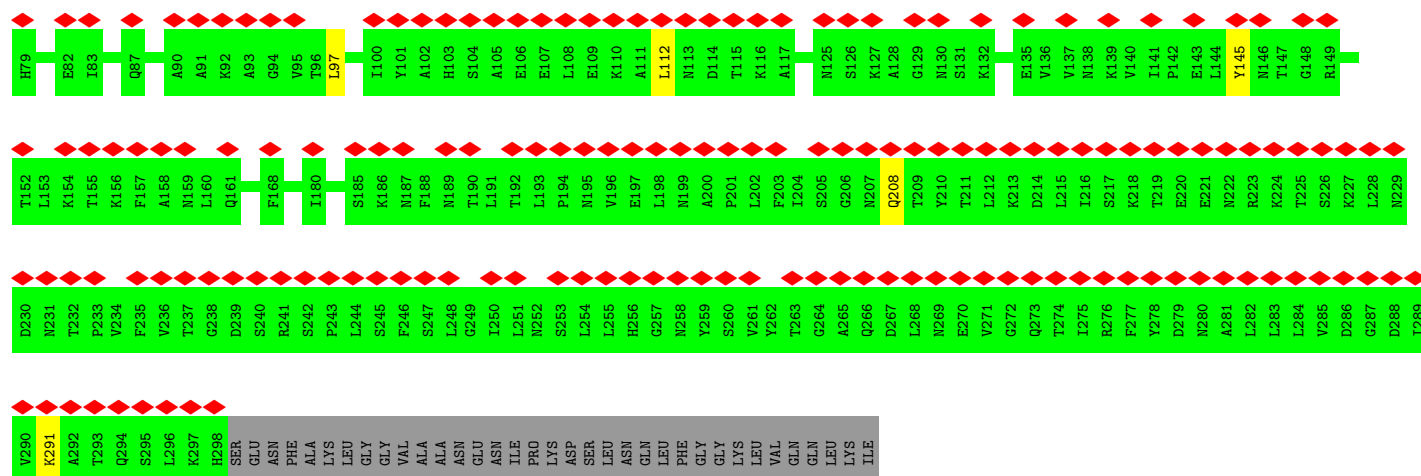
Chain T1: 



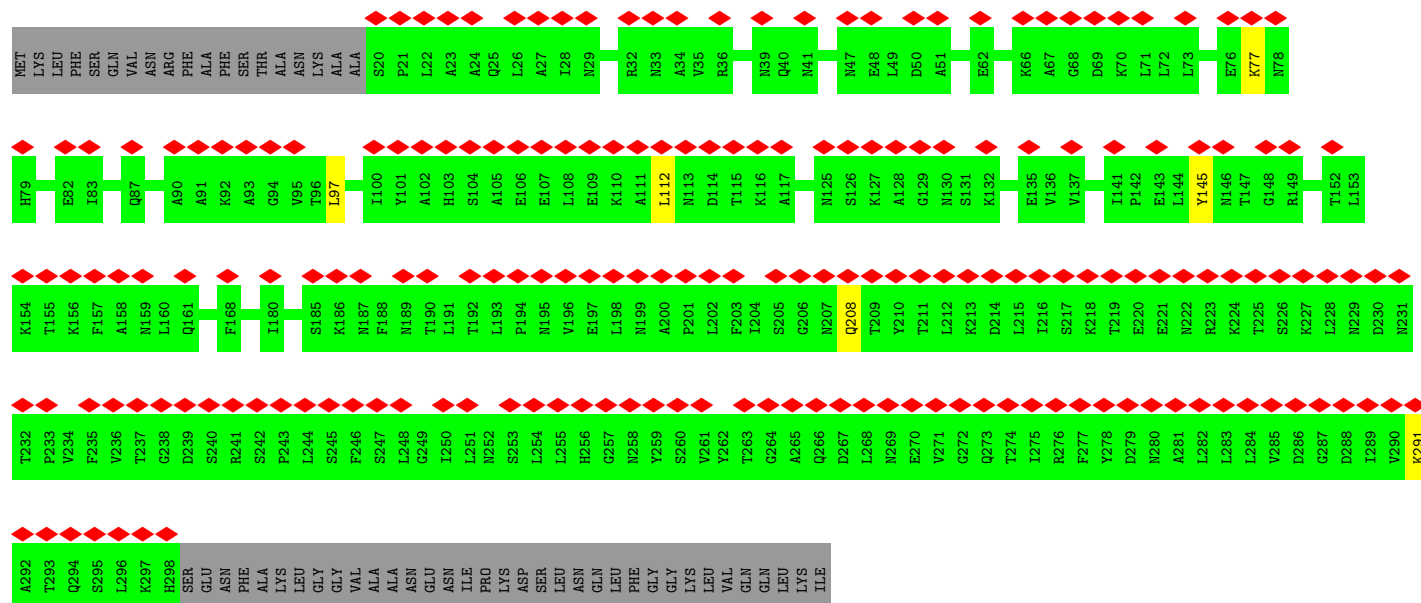
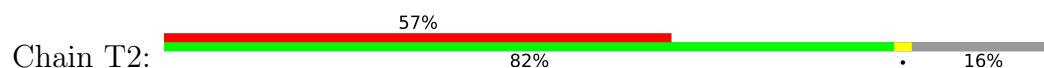
- Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

Chain t2: 

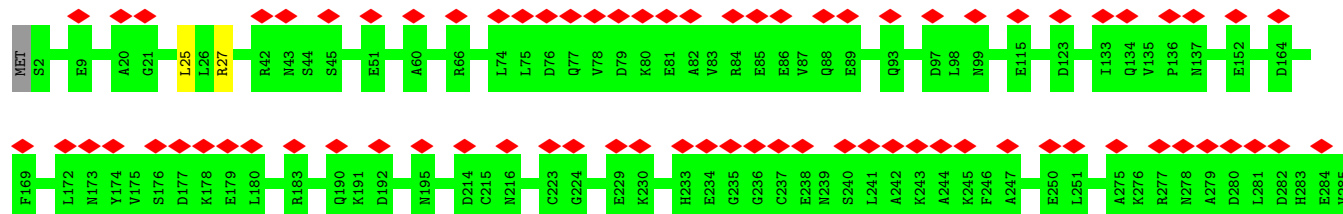


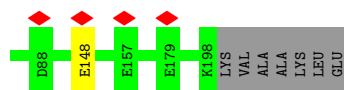


• Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

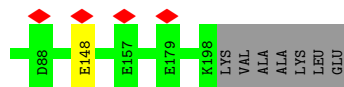
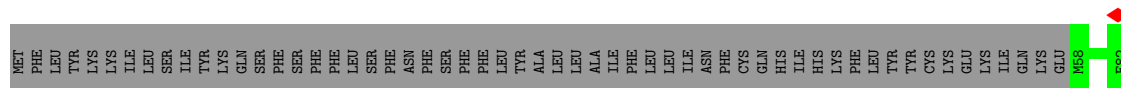


• Molecule 130: RNase III domain-containing protein

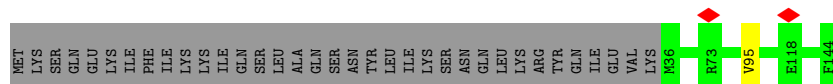
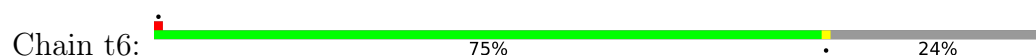




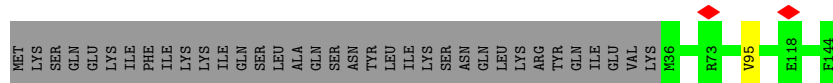
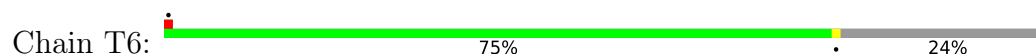
- Molecule 132: Transmembrane protein, putative



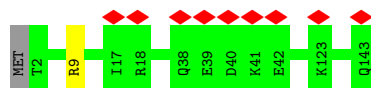
- Molecule 133: COX assembly mitochondrial protein



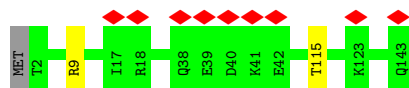
- Molecule 133: COX assembly mitochondrial protein



- Molecule 134: Transmembrane protein, putative

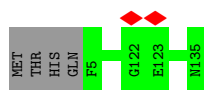


- Molecule 134: Transmembrane protein, putative

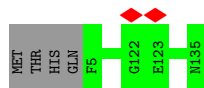


- Molecule 135: PH domain-containing protein

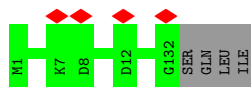




- Molecule 135: PH domain-containing protein



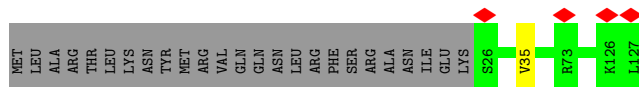
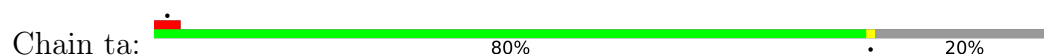
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



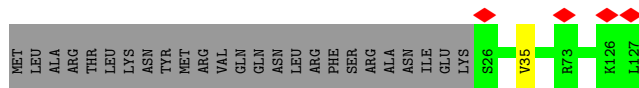
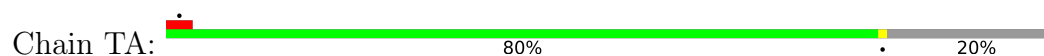
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



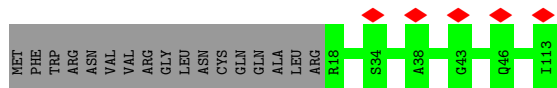
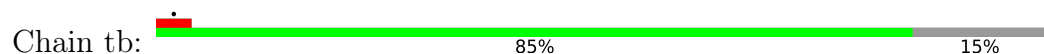
- Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4




- Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

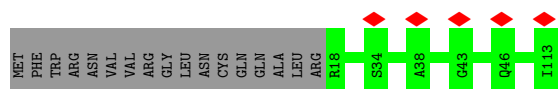


- Molecule 138: Transmembrane protein, putative



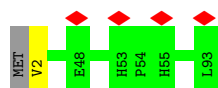
- Molecule 138: Transmembrane protein, putative

Chain TB:  85% 15%



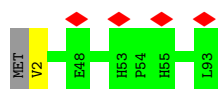
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain tc:  98% ..



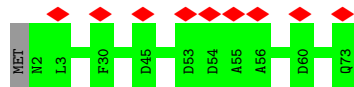
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain TC:  98% ..



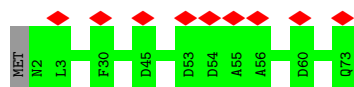
- Molecule 140: Transmembrane protein, putative

Chain td:  12% 99% .



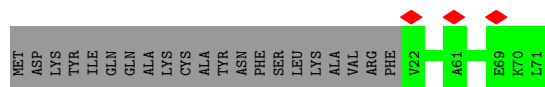
- Molecule 140: Transmembrane protein, putative

Chain TD:  12% 99% .



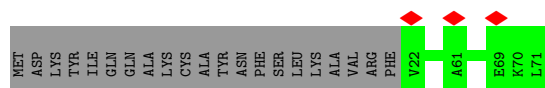
- Molecule 141: Transmembrane protein, putative

Chain te:  70% 30%

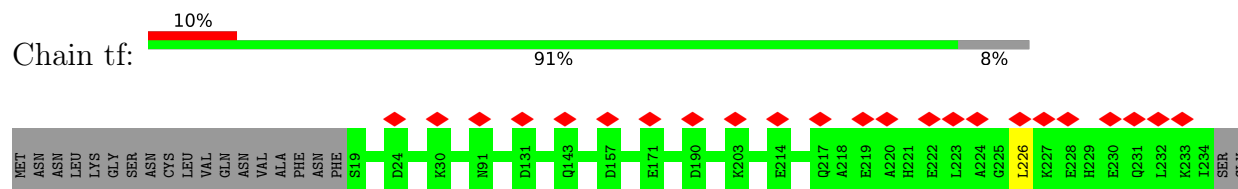


- Molecule 141: Transmembrane protein, putative

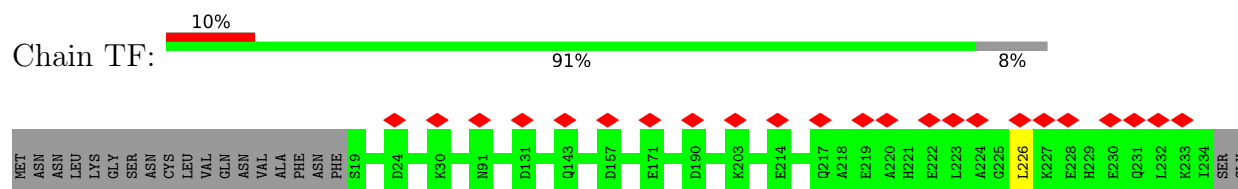
Chain TE:  70% 30%



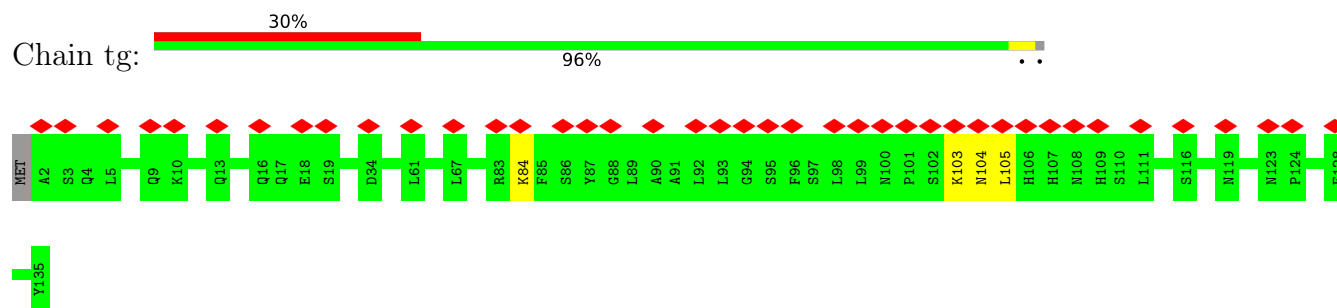
• Molecule 142: NDUTT15



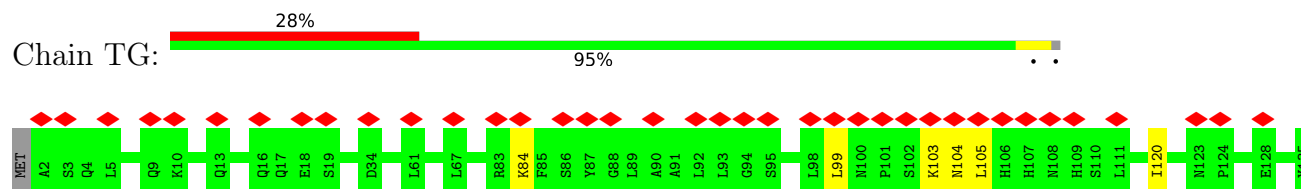
• Molecule 142: NDUTT15



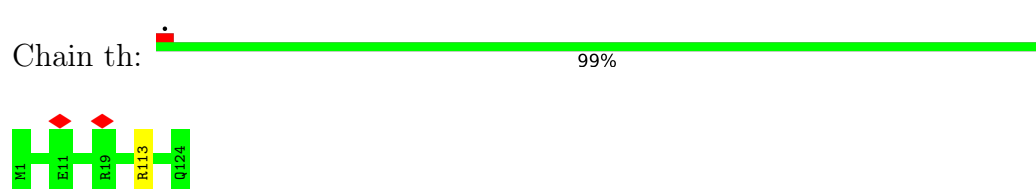
• Molecule 143: NDUTT16



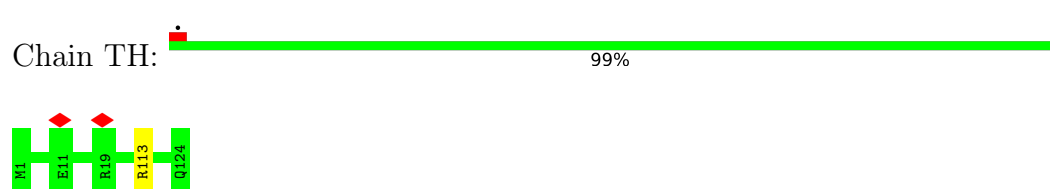
• Molecule 143: NDUTT16



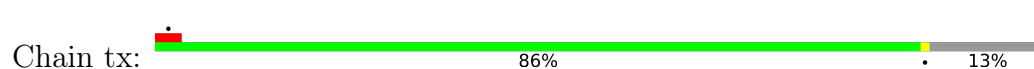
• Molecule 144: NDUTT17

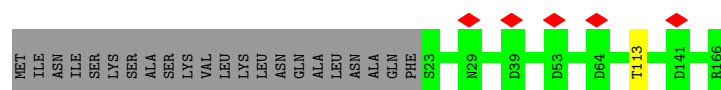


• Molecule 144: NDUTT17

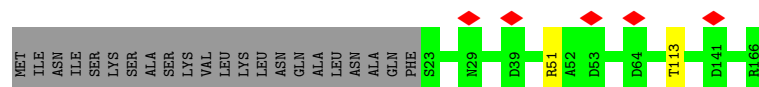


• Molecule 145: Thioredoxin

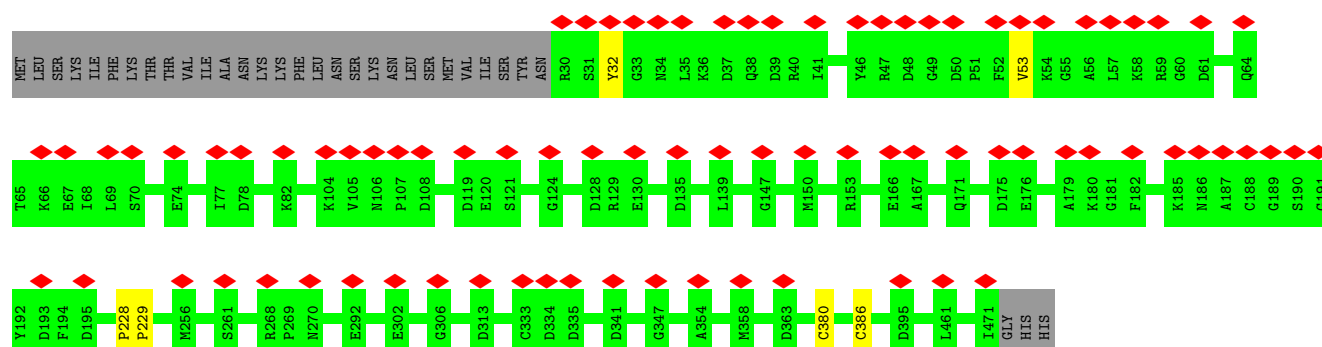




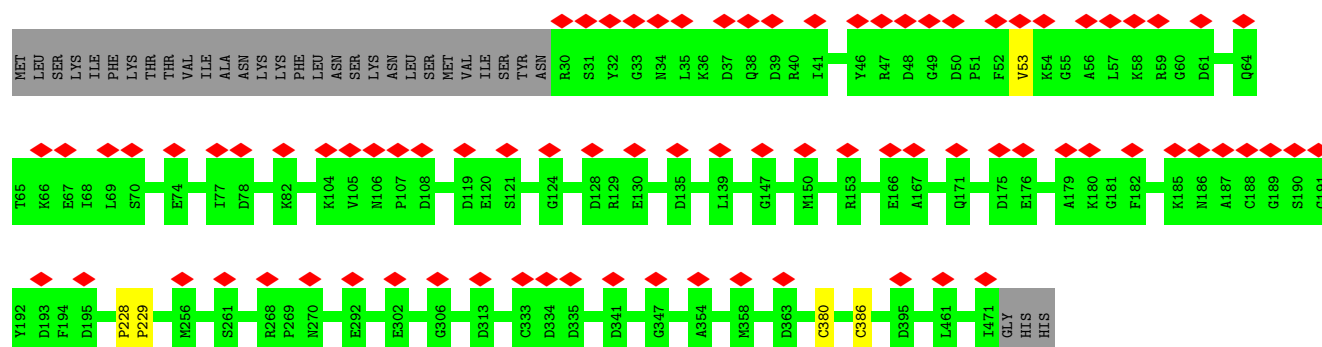
- Molecule 145: Thioredoxin



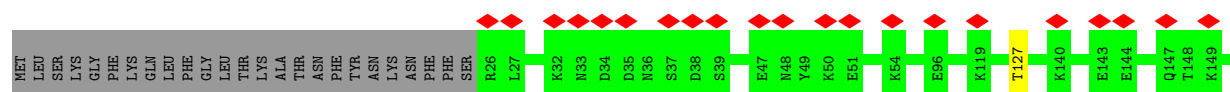
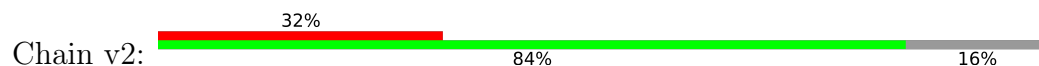
- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

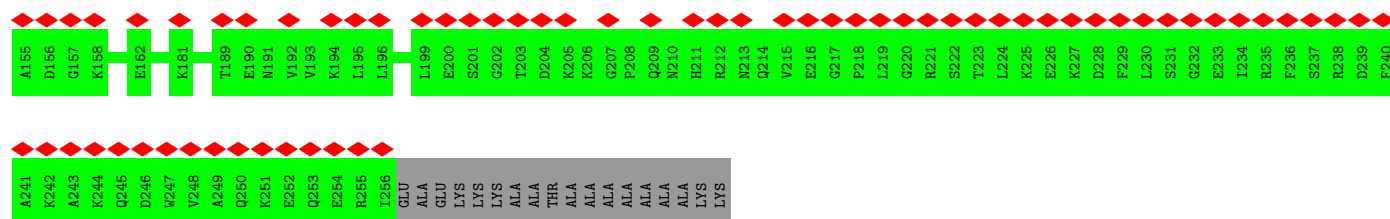


- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

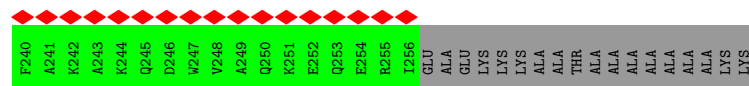
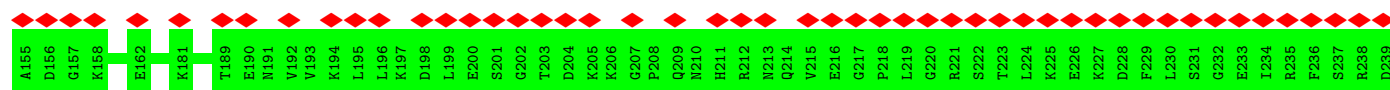
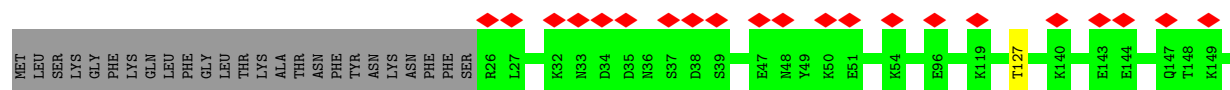
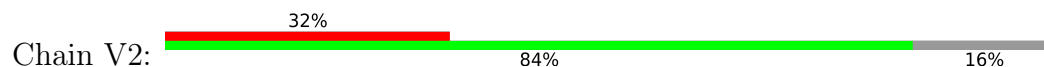


- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit

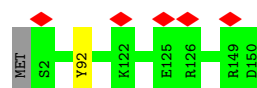




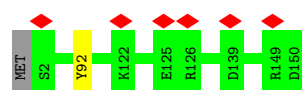
- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit



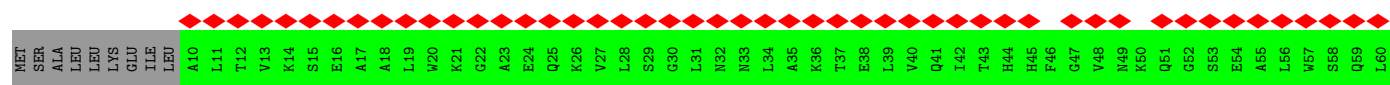
- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

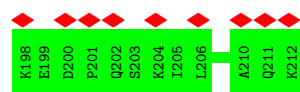


- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

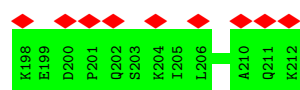
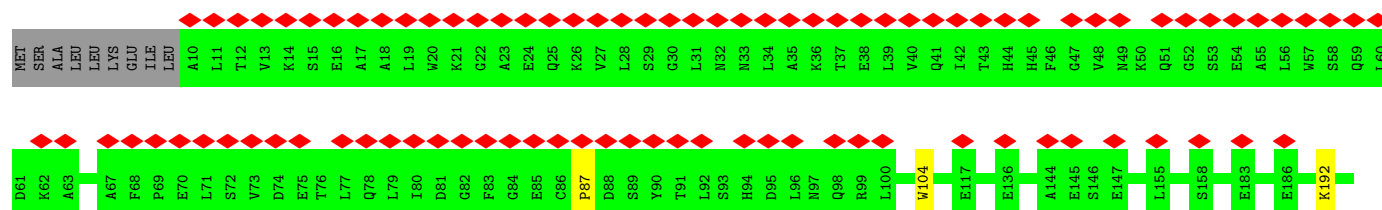


- Molecule 149: COXTT3





- Molecule 149: COXTT3



- Molecule 150: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 150: Unknown peptide



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97688	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 ($e^-/\text{\AA}^2$)	61.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	140000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	60.050	Depositor
Minimum map value	-23.470	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.045	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	781.2, 781.2, 781.2	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN, FAD, HEC, HEA, 3PE, ZMP, SF4, NDP, U10, HEM, P5S, CDL, CU, TPO, FES, MG, SEP, PX2, ADP, PC1, F3S, T7X

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	1T	0.25	0/546	0.39	0/735
1	1t	0.25	0/546	0.38	0/735
2	2E	0.25	0/2614	0.45	0/3553
2	2e	0.25	0/2614	0.45	0/3553
3	2F	0.27	0/1848	0.45	0/2500
3	2f	0.27	0/1848	0.45	0/2500
4	2G	0.26	0/1716	0.40	0/2317
4	2g	0.26	0/1716	0.40	0/2317
5	2H	0.25	0/812	0.42	0/1090
5	2h	0.25	0/812	0.42	0/1090
6	2I	0.28	0/930	0.42	0/1244
6	2i	0.27	0/930	0.42	0/1244
7	2J	0.27	0/866	0.39	0/1176
7	2j	0.27	0/866	0.39	0/1176
8	2K	0.30	0/821	0.46	0/1112
8	2k	0.30	0/821	0.46	0/1112
9	2L	0.27	0/738	0.43	0/990
9	2l	0.27	0/738	0.43	0/990
10	2M	0.25	0/660	0.48	0/895
10	2m	0.26	0/660	0.47	0/895
11	2N	0.28	0/521	0.49	0/708
11	2n	0.28	0/521	0.49	0/708
12	2O	0.28	0/367	0.45	0/496
12	2o	0.28	0/367	0.45	0/496
13	2T	0.24	0/574	0.43	0/772
13	2t	0.24	0/574	0.43	0/772
14	3T	0.25	0/662	0.42	0/888
14	3t	0.25	0/662	0.42	0/888
15	4A	0.25	0/836	0.47	0/1133
15	4a	0.24	0/836	0.47	0/1133
16	4T	0.26	0/491	0.41	0/662

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	4t	0.26	0/491	0.41	0/662
17	5T	0.26	0/514	0.41	0/693
17	5t	0.26	0/514	0.41	0/693
18	6A	0.26	0/1116	0.43	0/1512
18	6a	0.26	0/1116	0.43	0/1512
19	6B	0.26	0/1976	0.45	0/2673
19	6b	0.26	0/1976	0.45	0/2673
20	6C	0.28	0/926	0.48	0/1256
20	6c	0.28	0/926	0.47	0/1256
21	6L	0.26	0/649	0.42	0/871
21	6l	0.25	0/649	0.42	0/871
22	6T	0.25	0/573	0.38	0/770
22	6t	0.25	0/573	0.39	0/770
23	7A	0.26	0/1206	0.46	0/1631
23	7a	0.26	0/1206	0.46	0/1631
24	7C	0.25	0/1881	0.43	0/2558
24	7c	0.25	0/1881	0.43	0/2558
25	7L	0.25	0/1107	0.43	0/1505
25	7l	0.25	0/1107	0.43	0/1505
26	A	0.26	0/3874	0.45	0/5273
26	a	0.26	0/3874	0.45	0/5273
27	B	0.24	0/3453	0.43	0/4671
27	b	0.24	0/3453	0.43	0/4671
28	BP	0.26	0/2988	0.47	0/4052
28	bp	0.26	0/2988	0.47	0/4052
29	C1	0.27	0/5765	0.45	0/7819
29	c1	0.27	0/5765	0.45	0/7819
30	C2	0.25	0/5244	0.46	0/7107
30	c2	0.25	0/5244	0.47	0/7107
31	C3	0.27	0/5256	0.43	0/7142
31	c3	0.27	0/5256	0.43	0/7142
32	D	0.26	0/2430	0.47	0/3303
32	d	0.26	0/2430	0.47	0/3303
33	E	0.25	0/3266	0.45	0/4435
33	e	0.25	0/3266	0.45	0/4435
34	F	0.25	0/2077	0.44	0/2824
34	f	0.25	0/2077	0.44	0/2824
35	FS	0.27	0/1562	0.46	0/2123
35	fs	0.27	0/1562	0.46	0/2123
36	G	0.26	0/2517	0.46	0/3433
36	g	0.26	0/2517	0.46	0/3433
37	H	0.26	0/2423	0.46	0/3279
37	h	0.26	0/2423	0.46	0/3279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	I	0.25	0/2001	0.44	0/2702
38	i	0.25	0/2001	0.44	0/2702
39	J	0.24	0/1621	0.45	0/2201
39	j	0.24	0/1621	0.45	0/2201
40	K	0.24	0/1755	0.42	0/2376
40	k	0.24	0/1755	0.43	0/2376
41	L	0.26	0/1718	0.44	0/2333
41	l	0.26	0/1718	0.45	0/2333
42	M	0.26	0/1941	0.44	0/2637
42	m	0.26	0/1941	0.44	0/2637
43	M1	0.26	0/2958	0.46	0/4013
43	m1	0.26	0/2958	0.46	0/4013
44	M2	0.25	0/2629	0.46	0/3564
44	m2	0.25	0/2629	0.46	0/3564
45	M3	0.26	0/2689	0.44	0/3657
45	m3	0.26	0/2689	0.44	0/3657
46	N	0.26	0/1770	0.42	0/2391
46	n	0.26	0/1770	0.42	0/2391
47	O	0.25	0/1098	0.44	0/1477
47	o	0.25	0/1098	0.44	0/1477
48	P	0.25	0/1436	0.44	0/1941
48	p	0.25	0/1436	0.44	0/1941
49	Q	0.26	0/1478	0.46	0/2005
49	q	0.26	0/1478	0.46	0/2005
50	R	0.25	0/1441	0.43	0/1952
50	r	0.25	0/1441	0.43	0/1952
51	S	0.25	0/1409	0.44	0/1900
51	s	0.25	0/1409	0.43	0/1900
52	SA	0.25	0/4722	0.49	0/6385
52	sa	0.25	0/4722	0.49	0/6385
53	SB	0.25	0/2315	0.46	0/3136
53	sb	0.26	0/2315	0.46	0/3136
54	SC	0.27	0/493	0.47	0/664
54	sc	0.27	0/493	0.47	0/664
55	SD	0.28	0/404	0.40	0/542
55	sd	0.28	0/404	0.40	0/542
56	T	0.25	0/1359	0.44	0/1842
56	t	0.26	0/1359	0.45	0/1842
57	U	0.26	0/1335	0.45	0/1794
57	u	0.26	0/1335	0.45	0/1794
58	V	0.25	0/1277	0.46	0/1735
58	v	0.25	0/1277	0.46	0/1735
59	VB	0.26	0/4712	0.45	0/6357

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
59	vb	0.26	0/4712	0.45	0/6357
60	W	0.25	0/1136	0.45	0/1545
60	w	0.25	0/1136	0.45	0/1545
61	X	0.25	0/1043	0.43	0/1413
61	x	0.25	0/1043	0.43	0/1413
62	Y	0.27	0/882	0.45	0/1192
62	y	0.27	0/882	0.45	0/1192
63	Y0	0.27	0/801	0.43	0/1087
63	y0	0.27	0/801	0.43	0/1087
64	Y5	0.27	0/1708	0.39	0/2306
64	y5	0.27	0/1708	0.39	0/2306
65	Y7	0.26	0/3012	0.40	0/4072
65	y7	0.26	0/3012	0.40	0/4072
66	Z	0.25	0/737	0.45	0/995
66	z	0.25	0/737	0.44	0/995
67	Z1	0.26	0/781	0.44	0/1053
67	z1	0.26	0/781	0.44	0/1053
68	1B	0.27	0/536	0.42	0/727
68	1b	0.27	0/536	0.42	0/727
69	2B	0.27	0/1520	0.40	0/2058
69	2b	0.27	0/1520	0.39	0/2058
70	4L	0.25	0/982	0.41	0/1335
70	4l	0.25	0/982	0.41	0/1335
71	5B	0.27	0/915	0.40	0/1224
71	5b	0.27	0/915	0.40	0/1224
72	A1	0.26	0/834	0.50	0/1132
72	a1	0.26	0/834	0.50	0/1132
73	A2	0.25	0/826	0.46	0/1116
73	a2	0.25	0/826	0.46	0/1116
74	A3	0.25	0/1115	0.45	0/1507
74	a3	0.25	0/1115	0.45	0/1507
75	A5	0.24	0/1336	0.44	0/1797
75	a5	0.24	0/1336	0.44	0/1797
76	A6	0.26	0/1459	0.47	0/1965
76	a6	0.26	0/1459	0.47	0/1965
77	A7	0.24	0/2408	0.46	0/3269
77	a7	0.24	0/2408	0.46	0/3269
78	A8	0.25	0/1099	0.40	0/1477
78	a8	0.25	0/1099	0.41	0/1477
79	A9	0.26	0/2807	0.45	0/3801
79	a9	0.26	0/2807	0.45	0/3801
80	AB	0.24	0/942	0.42	0/1272
80	ab	0.24	0/942	0.42	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
81	AC	0.25	0/822	0.45	0/1114
81	ac	0.25	0/822	0.45	0/1114
82	AL	0.24	0/1667	0.47	0/2256
82	al	0.24	0/1667	0.47	0/2256
83	AM	0.24	0/1379	0.48	0/1841
83	am	0.24	0/1379	0.48	0/1841
84	AN	0.25	0/1935	0.42	0/2616
84	an	0.25	0/1935	0.42	0/2616
85	B2	0.25	0/991	0.45	1/1333 (0.1%)
85	b2	0.25	0/991	0.42	0/1333
86	B3	0.24	0/621	0.47	0/840
86	b3	0.25	0/621	0.47	0/840
87	B4	0.26	0/1015	0.40	0/1381
87	b4	0.27	0/1015	0.40	0/1381
88	B6	0.26	0/623	0.40	0/850
88	b6	0.26	0/623	0.40	0/850
89	B7	0.25	0/968	0.41	0/1307
89	b7	0.25	0/968	0.41	0/1307
90	B8	0.25	0/1494	0.45	0/2016
90	b8	0.25	0/1494	0.45	0/2016
91	B9	0.26	0/1644	0.43	0/2224
91	b9	0.26	0/1644	0.43	0/2224
92	BL	0.25	0/1489	0.47	0/2000
92	bl	0.25	0/1489	0.47	0/2000
93	BM	0.24	0/1351	0.42	0/1829
93	bm	0.24	0/1351	0.42	0/1829
94	C4	0.27	0/873	0.45	0/1175
94	c4	0.27	0/873	0.45	0/1175
95	FX	0.25	0/1186	0.49	0/1607
95	fx	0.25	0/1186	0.48	0/1607
96	G1	0.25	0/1810	0.46	0/2465
96	g1	0.26	0/1810	0.46	0/2465
97	G2	0.25	0/1793	0.49	0/2438
97	g2	0.25	0/1793	0.49	0/2438
98	G3	0.26	0/2865	0.46	0/3877
98	g3	0.26	0/2865	0.46	0/3877
99	J1	0.25	0/2219	0.46	0/2988
99	j1	0.25	0/2219	0.45	0/2988
100	N1	0.26	0/2376	0.41	0/3234
100	n1	0.26	0/2376	0.41	0/3234
101	N2	0.27	0/3173	0.39	0/4312
101	n2	0.27	0/3173	0.39	0/4312
102	N3	0.27	0/1051	0.37	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
102	n3	0.27	0/1051	0.37	0/1429
103	N4	0.27	0/4303	0.40	0/5844
103	n4	0.27	0/4303	0.40	0/5844
104	N5	0.27	0/6098	0.40	0/8297
104	n5	0.27	0/6098	0.40	0/8297
105	N6	0.27	0/2232	0.39	0/3035
105	n6	0.27	0/2232	0.39	0/3035
106	P1	0.26	0/1963	0.46	0/2658
106	p1	0.26	0/1963	0.47	0/2658
107	P2	0.26	0/1454	0.45	0/1970
107	p2	0.26	0/1454	0.45	0/1970
108	QA	0.25	0/3569	0.45	0/4835
108	Qa	0.25	0/3569	0.45	0/4835
108	qA	0.25	0/3569	0.45	0/4835
108	qa	0.25	0/3569	0.45	0/4835
109	QB	0.26	0/3921	0.48	0/5325
109	Qb	0.25	0/3921	0.48	0/5325
109	qB	0.26	0/3921	0.48	0/5325
109	qb	0.26	0/3921	0.48	0/5325
110	QC	0.27	0/3715	0.42	0/5046
110	Qc	0.27	0/3706	0.41	0/5035
110	qC	0.27	0/3715	0.42	0/5046
110	qc	0.27	0/3706	0.41	0/5035
111	QD	0.27	0/2580	0.47	0/3491
111	Qd	0.27	0/2580	0.46	0/3491
111	qD	0.28	0/2580	0.47	0/3491
111	qd	0.27	0/2580	0.46	0/3491
112	QE	0.25	0/1588	0.48	0/2162
112	Qe	0.25	0/1499	0.47	0/2042
112	qE	0.25	0/1588	0.48	0/2162
112	qe	0.25	0/1499	0.47	0/2042
113	QF	0.24	0/716	0.45	0/969
113	Qf	0.24	0/641	0.44	0/866
113	qF	0.24	0/716	0.46	0/969
113	qf	0.24	0/641	0.44	0/866
114	QG	0.26	0/2845	0.47	0/3839
114	Qg	0.26	0/2838	0.46	0/3829
114	qG	0.26	0/2845	0.47	0/3839
114	qg	0.25	0/2838	0.46	0/3829
115	QH	0.26	0/1133	0.49	0/1524
115	Qh	0.26	0/1133	0.49	0/1524
115	qH	0.26	0/1133	0.49	0/1524
115	qh	0.26	0/1133	0.48	0/1524

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
116	QI	0.25	0/1005	0.40	0/1365
116	Qi	0.26	0/1005	0.40	0/1365
116	qI	0.25	0/1005	0.40	0/1365
116	qi	0.25	0/1005	0.40	0/1365
117	QJ	0.26	0/502	0.41	0/687
117	Qj	0.26	0/522	0.44	0/712
117	qJ	0.26	0/502	0.41	0/687
117	qj	0.26	0/522	0.44	0/712
118	QL	0.25	0/273	0.38	0/371
118	Ql	0.26	0/273	0.37	0/371
118	qL	0.25	0/273	0.39	0/371
118	ql	0.26	0/273	0.37	0/371
120	S1	0.25	0/5518	0.47	0/7476
120	s1	0.25	0/5518	0.47	0/7476
121	S2	0.26	0/3680	0.47	0/4969
121	s2	0.26	0/3680	0.47	0/4969
122	S3	0.26	0/1718	0.44	0/2319
122	s3	0.26	0/1718	0.44	0/2319
123	S4	0.25	0/1543	0.48	0/2088
123	s4	0.25	0/1543	0.48	0/2088
124	S5	0.25	0/775	0.43	0/1048
124	s5	0.26	0/775	0.43	0/1048
125	S6	0.25	0/755	0.45	0/1022
125	s6	0.25	0/755	0.44	0/1022
126	S7	0.26	0/1311	0.50	0/1779
126	s7	0.26	0/1311	0.50	0/1779
127	S8	0.26	0/1867	0.47	0/2538
127	s8	0.26	0/1867	0.47	0/2538
128	T1	0.26	0/4153	0.44	0/5618
128	t1	0.26	0/4153	0.44	0/5618
129	T2	0.24	0/2224	0.44	0/3022
129	t2	0.24	0/2224	0.44	0/3022
130	T3	0.24	0/2527	0.43	0/3423
130	t3	0.24	0/2527	0.43	0/3423
131	T4	0.25	0/1689	0.41	0/2284
131	t4	0.25	0/1689	0.41	0/2284
132	T5	0.24	0/1163	0.46	0/1574
132	t5	0.25	0/1163	0.46	0/1574
133	T6	0.25	0/923	0.43	0/1239
133	t6	0.25	0/923	0.43	0/1239
134	T7	0.26	0/1223	0.45	0/1648
134	t7	0.26	0/1223	0.45	0/1648
135	T8	0.24	0/1112	0.44	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
135	t8	0.24	0/1112	0.44	0/1507
136	T9	0.25	0/1088	0.46	0/1458
136	t9	0.26	0/1088	0.46	0/1458
137	TA	0.26	0/877	0.42	0/1181
137	ta	0.26	0/877	0.42	0/1181
138	TB	0.27	0/825	0.44	0/1115
138	tb	0.27	0/825	0.44	0/1115
139	TC	0.26	0/811	0.44	0/1093
139	tc	0.26	0/811	0.44	0/1093
140	TD	0.24	0/634	0.45	0/855
140	td	0.24	0/634	0.45	0/855
141	TE	0.27	0/432	0.41	0/583
141	te	0.27	0/432	0.42	0/583
142	TF	0.24	0/1828	0.43	0/2472
142	tf	0.24	0/1828	0.43	0/2472
143	TG	0.24	0/1101	0.45	0/1486
143	tg	0.24	0/1101	0.44	0/1486
144	TH	0.25	0/1015	0.47	0/1366
144	th	0.25	0/1015	0.46	0/1366
145	TX	0.25	0/1235	0.45	0/1662
145	tx	0.25	0/1235	0.45	0/1662
146	V1	0.25	0/3485	0.49	1/4713 (0.0%)
146	v1	0.25	0/3485	0.49	1/4713 (0.0%)
147	V2	0.24	0/1895	0.44	0/2559
147	v2	0.24	0/1895	0.44	0/2559
148	X1	0.26	0/1261	0.47	0/1698
148	x1	0.26	0/1261	0.47	0/1698
149	C	0.24	0/1383	0.40	0/1880
149	c	0.24	0/1383	0.40	0/1880
All	All	0.26	0/556450	0.45	3/753536 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
146	V1	0	1
146	v1	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	B2	85	LEU	CA-CB-CG	6.86	131.08	115.30
146	v1	229	PRO	C-N-CA	-5.59	107.72	121.70
146	V1	229	PRO	C-N-CA	-5.52	107.91	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
146	V1	228	PRO	Peptide
146	v1	228	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1T	68/72 (94%)	68 (100%)	0	0	100	100
1	1t	68/72 (94%)	68 (100%)	0	0	100	100
2	2E	319/322 (99%)	300 (94%)	19 (6%)	0	100	100
2	2e	319/322 (99%)	300 (94%)	19 (6%)	0	100	100
3	2F	215/296 (73%)	206 (96%)	9 (4%)	0	100	100
3	2f	215/296 (73%)	206 (96%)	9 (4%)	0	100	100
4	2G	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
4	2g	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
5	2H	98/195 (50%)	92 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2h	98/195 (50%)	92 (94%)	6 (6%)	0	100	100
6	2I	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
6	2i	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
7	2J	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
7	2j	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
8	2K	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
8	2k	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
9	2L	81/89 (91%)	80 (99%)	1 (1%)	0	100	100
9	2l	81/89 (91%)	80 (99%)	1 (1%)	0	100	100
10	2M	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
10	2m	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
11	2N	59/62 (95%)	52 (88%)	7 (12%)	0	100	100
11	2n	59/62 (95%)	52 (88%)	7 (12%)	0	100	100
12	2O	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
12	2o	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
13	2T	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
13	2t	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
14	3T	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
14	3t	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
15	4A	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
15	4a	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
16	4T	55/68 (81%)	54 (98%)	1 (2%)	0	100	100
16	4t	55/68 (81%)	54 (98%)	1 (2%)	0	100	100
17	5T	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
17	5t	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
18	6A	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
18	6a	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
19	6B	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
19	6b	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
20	6C	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
20	6c	99/103 (96%)	94 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	6L	75/88 (85%)	74 (99%)	1 (1%)	0	100	100
21	6l	75/88 (85%)	74 (99%)	1 (1%)	0	100	100
22	6T	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
22	6t	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
23	7A	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
23	7a	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
24	7C	208/236 (88%)	199 (96%)	9 (4%)	0	100	100
24	7c	208/236 (88%)	199 (96%)	9 (4%)	0	100	100
25	7L	129/990 (13%)	116 (90%)	13 (10%)	0	100	100
25	7l	129/990 (13%)	116 (90%)	13 (10%)	0	100	100
26	A	447/490 (91%)	429 (96%)	18 (4%)	0	100	100
26	a	447/490 (91%)	431 (96%)	16 (4%)	0	100	100
27	B	422/473 (89%)	411 (97%)	10 (2%)	1 (0%)	44	67
27	b	422/473 (89%)	408 (97%)	14 (3%)	0	100	100
28	BP	379/462 (82%)	348 (92%)	31 (8%)	0	100	100
28	bp	379/462 (82%)	349 (92%)	30 (8%)	0	100	100
29	C1	672/688 (98%)	648 (96%)	24 (4%)	0	100	100
29	c1	672/688 (98%)	648 (96%)	24 (4%)	0	100	100
30	C2	595/604 (98%)	572 (96%)	23 (4%)	0	100	100
30	c2	595/604 (98%)	573 (96%)	22 (4%)	0	100	100
31	C3	580/594 (98%)	557 (96%)	23 (4%)	0	100	100
31	c3	580/594 (98%)	558 (96%)	22 (4%)	0	100	100
32	D	287/402 (71%)	278 (97%)	9 (3%)	0	100	100
32	d	287/402 (71%)	279 (97%)	8 (3%)	0	100	100
33	E	382/385 (99%)	362 (95%)	20 (5%)	0	100	100
33	e	382/385 (99%)	365 (96%)	17 (4%)	0	100	100
34	F	241/348 (69%)	239 (99%)	2 (1%)	0	100	100
34	f	241/348 (69%)	239 (99%)	2 (1%)	0	100	100
35	FS	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
35	fs	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
36	G	291/318 (92%)	282 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	g	291/318 (92%)	282 (97%)	9 (3%)	0	100	100
37	H	296/318 (93%)	286 (97%)	10 (3%)	0	100	100
37	h	296/318 (93%)	289 (98%)	7 (2%)	0	100	100
38	I	229/252 (91%)	220 (96%)	9 (4%)	0	100	100
38	i	229/252 (91%)	222 (97%)	6 (3%)	1 (0%)	30	54
39	J	185/234 (79%)	183 (99%)	2 (1%)	0	100	100
39	j	185/234 (79%)	183 (99%)	2 (1%)	0	100	100
40	K	206/231 (89%)	198 (96%)	8 (4%)	0	100	100
40	k	206/231 (89%)	198 (96%)	8 (4%)	0	100	100
41	L	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
41	l	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
42	M	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
42	m	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
43	M1	344/346 (99%)	329 (96%)	15 (4%)	0	100	100
43	m1	344/346 (99%)	331 (96%)	13 (4%)	0	100	100
44	M2	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
44	m2	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
45	M3	327/330 (99%)	317 (97%)	10 (3%)	0	100	100
45	m3	327/330 (99%)	317 (97%)	10 (3%)	0	100	100
46	N	204/210 (97%)	199 (98%)	5 (2%)	0	100	100
46	n	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
47	O	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
47	o	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
48	P	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
48	p	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
49	Q	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
49	q	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
50	R	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
50	r	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
51	S	167/170 (98%)	163 (98%)	4 (2%)	0	100	100
51	s	167/170 (98%)	163 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	SA	597/636 (94%)	563 (94%)	34 (6%)	0	100	100
52	sa	597/636 (94%)	565 (95%)	32 (5%)	0	100	100
53	SB	277/312 (89%)	256 (92%)	21 (8%)	0	100	100
53	sb	277/312 (89%)	256 (92%)	21 (8%)	0	100	100
54	SC	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
54	sc	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
55	SD	42/44 (96%)	42 (100%)	0	0	100	100
55	sd	42/44 (96%)	42 (100%)	0	0	100	100
56	T	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
56	t	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
57	U	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
57	u	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
58	V	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
58	v	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
59	VB	551/637 (86%)	542 (98%)	9 (2%)	0	100	100
59	vb	551/637 (86%)	542 (98%)	9 (2%)	0	100	100
60	W	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
60	w	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
61	X	120/122 (98%)	120 (100%)	0	0	100	100
61	x	120/122 (98%)	120 (100%)	0	0	100	100
62	Y	103/105 (98%)	103 (100%)	0	0	100	100
62	y	103/105 (98%)	103 (100%)	0	0	100	100
63	Y0	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
63	y0	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
64	Y5	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
64	y5	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
65	Y7	339/453 (75%)	326 (96%)	13 (4%)	0	100	100
65	y7	339/453 (75%)	325 (96%)	14 (4%)	0	100	100
66	Z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
66	z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
67	Z1	95/100 (95%)	95 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	z1	95/100 (95%)	95 (100%)	0	0	100	100
68	1B	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
68	1b	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
69	2B	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
69	2b	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
70	4L	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
70	4l	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
71	5B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
71	5b	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
72	A1	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
72	a1	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
73	A2	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
73	a2	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
74	A3	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
74	a3	127/135 (94%)	123 (97%)	4 (3%)	0	100	100
75	A5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
75	a5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
76	A6	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
76	a6	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
77	A7	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
77	a7	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
78	A8	130/238 (55%)	130 (100%)	0	0	100	100
78	a8	130/238 (55%)	130 (100%)	0	0	100	100
79	A9	338/362 (93%)	321 (95%)	17 (5%)	0	100	100
79	a9	338/362 (93%)	321 (95%)	17 (5%)	0	100	100
80	AB	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
80	ab	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
81	AC	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
81	ac	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
82	AL	191/194 (98%)	181 (95%)	10 (5%)	0	100	100
82	al	191/194 (98%)	182 (95%)	9 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	AM	158/175 (90%)	155 (98%)	3 (2%)	0	100	100
83	am	158/175 (90%)	155 (98%)	3 (2%)	0	100	100
84	AN	229/231 (99%)	223 (97%)	6 (3%)	0	100	100
84	an	229/231 (99%)	223 (97%)	6 (3%)	0	100	100
85	B2	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
85	b2	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
86	B3	67/83 (81%)	66 (98%)	1 (2%)	0	100	100
86	b3	67/83 (81%)	66 (98%)	1 (2%)	0	100	100
87	B4	113/147 (77%)	112 (99%)	1 (1%)	0	100	100
87	b4	113/147 (77%)	112 (99%)	1 (1%)	0	100	100
88	B6	68/129 (53%)	68 (100%)	0	0	100	100
88	b6	68/129 (53%)	68 (100%)	0	0	100	100
89	B7	114/120 (95%)	114 (100%)	0	0	100	100
89	b7	114/120 (95%)	114 (100%)	0	0	100	100
90	B8	173/207 (84%)	171 (99%)	2 (1%)	0	100	100
90	b8	173/207 (84%)	171 (99%)	2 (1%)	0	100	100
91	B9	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
91	b9	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
92	BL	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
92	bl	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
93	BM	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
93	bm	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
94	C4	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
94	c4	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
95	FX	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
95	fx	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
96	G1	227/257 (88%)	222 (98%)	5 (2%)	0	100	100
96	g1	227/257 (88%)	222 (98%)	5 (2%)	0	100	100
97	G2	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
97	g2	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
98	G3	344/346 (99%)	335 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
98	g3	344/346 (99%)	335 (97%)	9 (3%)	0	100	100
99	J1	259/317 (82%)	255 (98%)	4 (2%)	0	100	100
99	j1	259/317 (82%)	255 (98%)	4 (2%)	0	100	100
100	N1	281/284 (99%)	269 (96%)	11 (4%)	1 (0%)	30	54
100	n1	281/284 (99%)	268 (95%)	12 (4%)	1 (0%)	30	54
101	N2	358/360 (99%)	348 (97%)	10 (3%)	0	100	100
101	n2	358/360 (99%)	350 (98%)	8 (2%)	0	100	100
102	N3	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
102	n3	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
103	N4	503/505 (100%)	495 (98%)	8 (2%)	0	100	100
103	n4	503/505 (100%)	496 (99%)	7 (1%)	0	100	100
104	N5	707/750 (94%)	677 (96%)	30 (4%)	0	100	100
104	n5	707/750 (94%)	678 (96%)	29 (4%)	0	100	100
105	N6	253/255 (99%)	245 (97%)	8 (3%)	0	100	100
105	n6	253/255 (99%)	245 (97%)	8 (3%)	0	100	100
106	P1	228/251 (91%)	218 (96%)	10 (4%)	0	100	100
106	p1	228/251 (91%)	219 (96%)	9 (4%)	0	100	100
107	P2	165/189 (87%)	160 (97%)	5 (3%)	0	100	100
107	p2	165/189 (87%)	160 (97%)	5 (3%)	0	100	100
108	QA	450/482 (93%)	437 (97%)	13 (3%)	0	100	100
108	Qa	450/482 (93%)	434 (96%)	16 (4%)	0	100	100
108	qA	450/482 (93%)	438 (97%)	12 (3%)	0	100	100
108	qa	450/482 (93%)	433 (96%)	17 (4%)	0	100	100
109	QB	478/513 (93%)	463 (97%)	15 (3%)	0	100	100
109	Qb	478/513 (93%)	454 (95%)	24 (5%)	0	100	100
109	qB	478/513 (93%)	463 (97%)	15 (3%)	0	100	100
109	qb	478/513 (93%)	453 (95%)	25 (5%)	0	100	100
110	QC	424/426 (100%)	404 (95%)	20 (5%)	0	100	100
110	Qc	423/426 (99%)	405 (96%)	18 (4%)	0	100	100
110	qC	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
110	qc	423/426 (99%)	405 (96%)	18 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
111	QD	293/319 (92%)	279 (95%)	14 (5%)	0	100	100
111	Qd	293/319 (92%)	276 (94%)	17 (6%)	0	100	100
111	qD	293/319 (92%)	282 (96%)	11 (4%)	0	100	100
111	qd	293/319 (92%)	275 (94%)	18 (6%)	0	100	100
112	QE	226/269 (84%)	216 (96%)	10 (4%)	0	100	100
112	Qe	215/269 (80%)	204 (95%)	11 (5%)	0	100	100
112	qE	226/269 (84%)	216 (96%)	10 (4%)	0	100	100
112	qe	215/269 (80%)	205 (95%)	10 (5%)	0	100	100
113	QF	87/90 (97%)	87 (100%)	0	0	100	100
113	Qf	78/90 (87%)	76 (97%)	2 (3%)	0	100	100
113	qF	87/90 (97%)	87 (100%)	0	0	100	100
113	qf	78/90 (87%)	76 (97%)	2 (3%)	0	100	100
114	QG	325/328 (99%)	313 (96%)	12 (4%)	0	100	100
114	Qg	324/328 (99%)	316 (98%)	8 (2%)	0	100	100
114	qG	325/328 (99%)	312 (96%)	13 (4%)	0	100	100
114	qg	324/328 (99%)	316 (98%)	8 (2%)	0	100	100
115	QH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
115	Qh	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
115	qH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
115	qh	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
116	QI	112/119 (94%)	108 (96%)	4 (4%)	0	100	100
116	Qi	112/119 (94%)	111 (99%)	1 (1%)	0	100	100
116	qI	112/119 (94%)	108 (96%)	4 (4%)	0	100	100
116	qi	112/119 (94%)	110 (98%)	2 (2%)	0	100	100
117	QJ	54/62 (87%)	54 (100%)	0	0	100	100
117	Qj	56/62 (90%)	53 (95%)	3 (5%)	0	100	100
117	qJ	54/62 (87%)	54 (100%)	0	0	100	100
117	qj	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
118	QL	30/41 (73%)	30 (100%)	0	0	100	100
118	Ql	30/41 (73%)	30 (100%)	0	0	100	100
118	qL	30/41 (73%)	30 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
118	ql	30/41 (73%)	30 (100%)	0	0	100	100
120	S1	687/718 (96%)	661 (96%)	26 (4%)	0	100	100
120	s1	687/718 (96%)	662 (96%)	25 (4%)	0	100	100
121	S2	440/442 (100%)	424 (96%)	16 (4%)	0	100	100
121	s2	440/442 (100%)	423 (96%)	17 (4%)	0	100	100
122	S3	196/198 (99%)	193 (98%)	3 (2%)	0	100	100
122	s3	196/198 (99%)	193 (98%)	3 (2%)	0	100	100
123	S4	180/185 (97%)	172 (96%)	8 (4%)	0	100	100
123	s4	180/185 (97%)	172 (96%)	8 (4%)	0	100	100
124	S5	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
124	s5	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
125	S6	90/132 (68%)	84 (93%)	6 (7%)	0	100	100
125	s6	90/132 (68%)	85 (94%)	5 (6%)	0	100	100
126	S7	159/162 (98%)	152 (96%)	7 (4%)	0	100	100
126	s7	159/162 (98%)	151 (95%)	8 (5%)	0	100	100
127	S8	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
127	s8	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
128	T1	500/516 (97%)	482 (96%)	18 (4%)	0	100	100
128	t1	500/516 (97%)	481 (96%)	19 (4%)	0	100	100
129	T2	277/333 (83%)	268 (97%)	8 (3%)	1 (0%)	30	54
129	t2	277/333 (83%)	267 (96%)	9 (3%)	1 (0%)	30	54
130	T3	308/311 (99%)	304 (99%)	4 (1%)	0	100	100
130	t3	308/311 (99%)	304 (99%)	4 (1%)	0	100	100
131	T4	196/212 (92%)	194 (99%)	2 (1%)	0	100	100
131	t4	196/212 (92%)	194 (99%)	2 (1%)	0	100	100
132	T5	139/205 (68%)	136 (98%)	3 (2%)	0	100	100
132	t5	139/205 (68%)	136 (98%)	3 (2%)	0	100	100
133	T6	107/144 (74%)	103 (96%)	4 (4%)	0	100	100
133	t6	107/144 (74%)	103 (96%)	4 (4%)	0	100	100
134	T7	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
134	t7	140/143 (98%)	138 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
135	T8	129/135 (96%)	128 (99%)	1 (1%)	0	100	100
135	t8	129/135 (96%)	128 (99%)	1 (1%)	0	100	100
136	T9	130/136 (96%)	128 (98%)	2 (2%)	0	100	100
136	t9	130/136 (96%)	128 (98%)	2 (2%)	0	100	100
137	TA	100/127 (79%)	96 (96%)	4 (4%)	0	100	100
137	ta	100/127 (79%)	95 (95%)	5 (5%)	0	100	100
138	TB	94/113 (83%)	94 (100%)	0	0	100	100
138	tb	94/113 (83%)	94 (100%)	0	0	100	100
139	TC	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
139	tc	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
140	TD	70/73 (96%)	70 (100%)	0	0	100	100
140	td	70/73 (96%)	70 (100%)	0	0	100	100
141	TE	48/71 (68%)	43 (90%)	5 (10%)	0	100	100
141	te	48/71 (68%)	43 (90%)	5 (10%)	0	100	100
142	TF	214/236 (91%)	212 (99%)	2 (1%)	0	100	100
142	tf	214/236 (91%)	212 (99%)	2 (1%)	0	100	100
143	TG	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
143	tg	132/135 (98%)	132 (100%)	0	0	100	100
144	TH	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
144	th	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
145	TX	142/166 (86%)	141 (99%)	1 (1%)	0	100	100
145	tx	142/166 (86%)	141 (99%)	1 (1%)	0	100	100
146	V1	440/474 (93%)	424 (96%)	16 (4%)	0	100	100
146	v1	440/474 (93%)	424 (96%)	16 (4%)	0	100	100
147	V2	229/274 (84%)	219 (96%)	10 (4%)	0	100	100
147	v2	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
148	X1	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
148	x1	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
149	C	201/212 (95%)	192 (96%)	8 (4%)	1 (0%)	25	50
149	c	201/212 (95%)	192 (96%)	8 (4%)	1 (0%)	25	50
All	All	65386/73196 (89%)	63252 (97%)	2126 (3%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
129	t2	77	LYS
129	T2	77	LYS
149	C	87	PRO
149	c	87	PRO
100	n1	229	VAL
27	B	238	THR
100	N1	229	VAL
38	i	23	ARG

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	1T	61/63 (97%)	60 (98%)	1 (2%)	58	77
1	1t	61/63 (97%)	60 (98%)	1 (2%)	58	77
2	2E	286/287 (100%)	280 (98%)	6 (2%)	48	70
2	2e	286/287 (100%)	280 (98%)	6 (2%)	48	70
3	2F	193/268 (72%)	189 (98%)	4 (2%)	48	70
3	2f	193/268 (72%)	189 (98%)	4 (2%)	48	70
4	2G	181/181 (100%)	179 (99%)	2 (1%)	70	83
4	2g	181/181 (100%)	179 (99%)	2 (1%)	70	83
5	2H	93/184 (50%)	92 (99%)	1 (1%)	70	83
5	2h	93/184 (50%)	92 (99%)	1 (1%)	70	83
6	2I	97/97 (100%)	95 (98%)	2 (2%)	48	70
6	2i	97/97 (100%)	94 (97%)	3 (3%)	35	59
7	2J	85/86 (99%)	84 (99%)	1 (1%)	67	82
7	2j	85/86 (99%)	84 (99%)	1 (1%)	67	82
8	2K	85/85 (100%)	83 (98%)	2 (2%)	44	68
8	2k	85/85 (100%)	83 (98%)	2 (2%)	44	68
9	2L	77/83 (93%)	75 (97%)	2 (3%)	41	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	2l	77/83 (93%)	76 (99%)	1 (1%)	65	80
10	2M	66/67 (98%)	65 (98%)	1 (2%)	60	78
10	2m	66/67 (98%)	65 (98%)	1 (2%)	60	78
11	2N	55/56 (98%)	53 (96%)	2 (4%)	30	55
11	2n	55/56 (98%)	54 (98%)	1 (2%)	54	75
12	2O	37/40 (92%)	36 (97%)	1 (3%)	40	64
12	2o	37/40 (92%)	36 (97%)	1 (3%)	40	64
13	2T	65/67 (97%)	65 (100%)	0	100	100
13	2t	65/67 (97%)	65 (100%)	0	100	100
14	3T	76/83 (92%)	74 (97%)	2 (3%)	41	65
14	3t	76/83 (92%)	74 (97%)	2 (3%)	41	65
15	4A	87/113 (77%)	85 (98%)	2 (2%)	45	69
15	4a	87/113 (77%)	85 (98%)	2 (2%)	45	69
16	4T	54/63 (86%)	52 (96%)	2 (4%)	29	54
16	4t	54/63 (86%)	52 (96%)	2 (4%)	29	54
17	5T	56/66 (85%)	56 (100%)	0	100	100
17	5t	56/66 (85%)	56 (100%)	0	100	100
18	6A	114/116 (98%)	113 (99%)	1 (1%)	75	86
18	6a	114/116 (98%)	113 (99%)	1 (1%)	75	86
19	6B	200/207 (97%)	199 (100%)	1 (0%)	86	93
19	6b	200/207 (97%)	199 (100%)	1 (0%)	86	93
20	6C	86/88 (98%)	85 (99%)	1 (1%)	67	82
20	6c	86/88 (98%)	85 (99%)	1 (1%)	67	82
21	6L	72/81 (89%)	72 (100%)	0	100	100
21	6l	72/81 (89%)	72 (100%)	0	100	100
22	6T	62/63 (98%)	62 (100%)	0	100	100
22	6t	62/63 (98%)	62 (100%)	0	100	100
23	7A	120/120 (100%)	119 (99%)	1 (1%)	79	88
23	7a	120/120 (100%)	119 (99%)	1 (1%)	79	88
24	7C	198/218 (91%)	196 (99%)	2 (1%)	73	85
24	7c	198/218 (91%)	196 (99%)	2 (1%)	73	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	7L	122/943 (13%)	121 (99%)	1 (1%)	79	88
25	7I	122/943 (13%)	121 (99%)	1 (1%)	79	88
26	A	410/447 (92%)	410 (100%)	0	100	100
26	a	410/447 (92%)	410 (100%)	0	100	100
27	B	374/413 (91%)	370 (99%)	4 (1%)	70	83
27	b	374/413 (91%)	371 (99%)	3 (1%)	79	88
28	BP	308/386 (80%)	308 (100%)	0	100	100
28	bp	308/386 (80%)	308 (100%)	0	100	100
29	C1	599/613 (98%)	593 (99%)	6 (1%)	73	85
29	c1	599/613 (98%)	594 (99%)	5 (1%)	79	88
30	C2	565/569 (99%)	561 (99%)	4 (1%)	81	90
30	c2	565/569 (99%)	560 (99%)	5 (1%)	75	86
31	C3	553/565 (98%)	549 (99%)	4 (1%)	81	90
31	c3	553/565 (98%)	549 (99%)	4 (1%)	81	90
32	D	253/358 (71%)	251 (99%)	2 (1%)	79	88
32	d	253/358 (71%)	250 (99%)	3 (1%)	67	82
33	E	342/343 (100%)	340 (99%)	2 (1%)	84	91
33	e	342/343 (100%)	340 (99%)	2 (1%)	84	91
34	F	219/318 (69%)	217 (99%)	2 (1%)	75	86
34	f	219/318 (69%)	218 (100%)	1 (0%)	86	93
35	FS	164/164 (100%)	164 (100%)	0	100	100
35	fs	164/164 (100%)	164 (100%)	0	100	100
36	G	267/289 (92%)	265 (99%)	2 (1%)	81	90
36	g	267/289 (92%)	265 (99%)	2 (1%)	81	90
37	H	256/272 (94%)	245 (96%)	11 (4%)	25	49
37	h	256/272 (94%)	248 (97%)	8 (3%)	35	59
38	I	200/219 (91%)	199 (100%)	1 (0%)	86	93
38	i	200/219 (91%)	199 (100%)	1 (0%)	86	93
39	J	170/216 (79%)	169 (99%)	1 (1%)	84	91
39	j	170/216 (79%)	170 (100%)	0	100	100
40	K	191/213 (90%)	190 (100%)	1 (0%)	86	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	k	191/213 (90%)	190 (100%)	1 (0%)	86	93
41	L	181/206 (88%)	179 (99%)	2 (1%)	70	83
41	l	181/206 (88%)	179 (99%)	2 (1%)	70	83
42	M	198/199 (100%)	197 (100%)	1 (0%)	86	93
42	m	198/199 (100%)	197 (100%)	1 (0%)	86	93
43	M1	294/294 (100%)	293 (100%)	1 (0%)	91	96
43	m1	294/294 (100%)	293 (100%)	1 (0%)	91	96
44	M2	260/260 (100%)	259 (100%)	1 (0%)	89	95
44	m2	260/260 (100%)	259 (100%)	1 (0%)	89	95
45	M3	275/276 (100%)	274 (100%)	1 (0%)	89	95
45	m3	275/276 (100%)	272 (99%)	3 (1%)	70	83
46	N	178/181 (98%)	176 (99%)	2 (1%)	70	83
46	n	178/181 (98%)	176 (99%)	2 (1%)	70	83
47	O	120/180 (67%)	120 (100%)	0	100	100
47	o	120/180 (67%)	119 (99%)	1 (1%)	79	88
48	P	157/157 (100%)	155 (99%)	2 (1%)	65	80
48	p	157/157 (100%)	155 (99%)	2 (1%)	65	80
49	Q	157/157 (100%)	157 (100%)	0	100	100
49	q	157/157 (100%)	156 (99%)	1 (1%)	84	91
50	R	156/157 (99%)	154 (99%)	2 (1%)	65	80
50	r	156/157 (99%)	154 (99%)	2 (1%)	65	80
51	S	153/154 (99%)	153 (100%)	0	100	100
51	s	153/154 (99%)	153 (100%)	0	100	100
52	SA	481/515 (93%)	470 (98%)	11 (2%)	45	69
52	sa	481/515 (93%)	475 (99%)	6 (1%)	67	82
53	SB	255/283 (90%)	243 (95%)	12 (5%)	22	46
53	sb	255/283 (90%)	246 (96%)	9 (4%)	31	56
54	SC	49/51 (96%)	47 (96%)	2 (4%)	26	51
54	sc	49/51 (96%)	47 (96%)	2 (4%)	26	51
55	SD	43/43 (100%)	43 (100%)	0	100	100
55	sd	43/43 (100%)	43 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	T	137/139 (99%)	136 (99%)	1 (1%)	81	90
56	t	137/139 (99%)	136 (99%)	1 (1%)	81	90
57	U	137/138 (99%)	135 (98%)	2 (2%)	60	78
57	u	137/138 (99%)	135 (98%)	2 (2%)	60	78
58	V	133/135 (98%)	133 (100%)	0	100	100
58	v	133/135 (98%)	133 (100%)	0	100	100
59	VB	503/579 (87%)	500 (99%)	3 (1%)	84	91
59	vb	503/579 (87%)	500 (99%)	3 (1%)	84	91
60	W	112/113 (99%)	110 (98%)	2 (2%)	54	75
60	w	112/113 (99%)	110 (98%)	2 (2%)	54	75
61	X	105/105 (100%)	104 (99%)	1 (1%)	73	85
61	x	105/105 (100%)	104 (99%)	1 (1%)	73	85
62	Y	88/88 (100%)	87 (99%)	1 (1%)	70	83
62	y	88/88 (100%)	87 (99%)	1 (1%)	70	83
63	Y0	84/84 (100%)	84 (100%)	0	100	100
63	y0	84/84 (100%)	84 (100%)	0	100	100
64	Y5	185/185 (100%)	185 (100%)	0	100	100
64	y5	185/185 (100%)	185 (100%)	0	100	100
65	Y7	333/442 (75%)	332 (100%)	1 (0%)	91	96
65	y7	333/442 (75%)	332 (100%)	1 (0%)	91	96
66	Z	77/80 (96%)	75 (97%)	2 (3%)	41	65
66	z	77/80 (96%)	75 (97%)	2 (3%)	41	65
67	Z1	77/78 (99%)	77 (100%)	0	100	100
67	z1	77/78 (99%)	77 (100%)	0	100	100
68	1B	55/55 (100%)	55 (100%)	0	100	100
68	1b	55/55 (100%)	55 (100%)	0	100	100
69	2B	170/170 (100%)	169 (99%)	1 (1%)	84	91
69	2b	170/170 (100%)	170 (100%)	0	100	100
70	4L	108/108 (100%)	108 (100%)	0	100	100
70	4l	108/108 (100%)	108 (100%)	0	100	100
71	5B	98/98 (100%)	98 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	5b	98/98 (100%)	98 (100%)	0	100	100
72	A1	88/89 (99%)	88 (100%)	0	100	100
72	a1	88/89 (99%)	88 (100%)	0	100	100
73	A2	88/93 (95%)	86 (98%)	2 (2%)	45	69
73	a2	88/93 (95%)	87 (99%)	1 (1%)	70	83
74	A3	108/114 (95%)	108 (100%)	0	100	100
74	a3	108/114 (95%)	108 (100%)	0	100	100
75	A5	144/186 (77%)	142 (99%)	2 (1%)	62	79
75	a5	144/186 (77%)	142 (99%)	2 (1%)	62	79
76	A6	154/154 (100%)	152 (99%)	2 (1%)	65	80
76	a6	154/154 (100%)	152 (99%)	2 (1%)	65	80
77	A7	257/257 (100%)	255 (99%)	2 (1%)	79	88
77	a7	257/257 (100%)	255 (99%)	2 (1%)	79	88
78	A8	121/224 (54%)	121 (100%)	0	100	100
78	a8	121/224 (54%)	121 (100%)	0	100	100
79	A9	290/311 (93%)	290 (100%)	0	100	100
79	a9	290/311 (93%)	290 (100%)	0	100	100
80	AB	104/129 (81%)	103 (99%)	1 (1%)	73	85
80	ab	104/129 (81%)	103 (99%)	1 (1%)	73	85
81	AC	88/119 (74%)	87 (99%)	1 (1%)	70	83
81	ac	88/119 (74%)	87 (99%)	1 (1%)	70	83
82	AL	169/170 (99%)	167 (99%)	2 (1%)	67	82
82	al	169/170 (99%)	168 (99%)	1 (1%)	84	91
83	AM	142/156 (91%)	141 (99%)	1 (1%)	81	90
83	am	142/156 (91%)	141 (99%)	1 (1%)	81	90
84	AN	199/199 (100%)	197 (99%)	2 (1%)	73	85
84	an	199/199 (100%)	199 (100%)	0	100	100
85	B2	103/109 (94%)	100 (97%)	3 (3%)	37	61
85	b2	103/109 (94%)	101 (98%)	2 (2%)	52	73
86	B3	64/74 (86%)	63 (98%)	1 (2%)	58	77
86	b3	64/74 (86%)	63 (98%)	1 (2%)	58	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
87	B4	102/128 (80%)	100 (98%)	2 (2%)	50	72
87	b4	102/128 (80%)	100 (98%)	2 (2%)	50	72
88	B6	64/117 (55%)	64 (100%)	0	100	100
88	b6	64/117 (55%)	64 (100%)	0	100	100
89	B7	97/99 (98%)	95 (98%)	2 (2%)	48	70
89	b7	97/99 (98%)	95 (98%)	2 (2%)	48	70
90	B8	156/180 (87%)	154 (99%)	2 (1%)	65	80
90	b8	156/180 (87%)	155 (99%)	1 (1%)	84	91
91	B9	171/172 (99%)	169 (99%)	2 (1%)	67	82
91	b9	171/172 (99%)	169 (99%)	2 (1%)	67	82
92	BL	160/172 (93%)	160 (100%)	0	100	100
92	bl	160/172 (93%)	159 (99%)	1 (1%)	84	91
93	BM	142/182 (78%)	138 (97%)	4 (3%)	38	63
93	bm	142/182 (78%)	138 (97%)	4 (3%)	38	63
94	C4	89/89 (100%)	88 (99%)	1 (1%)	70	83
94	c4	89/89 (100%)	89 (100%)	0	100	100
95	FX	130/152 (86%)	129 (99%)	1 (1%)	79	88
95	fx	130/152 (86%)	129 (99%)	1 (1%)	79	88
96	G1	195/218 (89%)	192 (98%)	3 (2%)	60	78
96	g1	195/218 (89%)	194 (100%)	1 (0%)	86	93
97	G2	195/197 (99%)	194 (100%)	1 (0%)	86	93
97	g2	195/197 (99%)	193 (99%)	2 (1%)	73	85
98	G3	309/309 (100%)	307 (99%)	2 (1%)	84	91
98	g3	309/309 (100%)	307 (99%)	2 (1%)	84	91
99	J1	222/270 (82%)	218 (98%)	4 (2%)	54	75
99	j1	222/270 (82%)	218 (98%)	4 (2%)	54	75
100	N1	249/250 (100%)	239 (96%)	10 (4%)	27	51
100	n1	249/250 (100%)	244 (98%)	5 (2%)	50	72
101	N2	346/346 (100%)	338 (98%)	8 (2%)	45	69
101	n2	346/346 (100%)	341 (99%)	5 (1%)	62	79
102	N3	111/112 (99%)	109 (98%)	2 (2%)	54	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
102	n3	111/112 (99%)	109 (98%)	2 (2%)	54	75
103	N4	463/463 (100%)	455 (98%)	8 (2%)	56	76
103	n4	463/463 (100%)	455 (98%)	8 (2%)	56	76
104	N5	653/694 (94%)	640 (98%)	13 (2%)	50	72
104	n5	653/694 (94%)	641 (98%)	12 (2%)	54	75
105	N6	244/244 (100%)	242 (99%)	2 (1%)	79	88
105	n6	244/244 (100%)	242 (99%)	2 (1%)	79	88
106	P1	207/223 (93%)	205 (99%)	2 (1%)	73	85
106	p1	207/223 (93%)	205 (99%)	2 (1%)	73	85
107	P2	158/178 (89%)	154 (98%)	4 (2%)	42	66
107	p2	158/178 (89%)	157 (99%)	1 (1%)	84	91
108	QA	385/409 (94%)	383 (100%)	2 (0%)	86	93
108	Qa	385/409 (94%)	379 (98%)	6 (2%)	58	77
108	qA	385/409 (94%)	383 (100%)	2 (0%)	86	93
108	qa	385/409 (94%)	378 (98%)	7 (2%)	54	75
109	QB	411/440 (93%)	405 (98%)	6 (2%)	60	78
109	Qb	411/440 (93%)	401 (98%)	10 (2%)	44	68
109	qB	411/440 (93%)	406 (99%)	5 (1%)	67	82
109	qb	411/440 (93%)	402 (98%)	9 (2%)	47	69
110	QC	386/386 (100%)	378 (98%)	8 (2%)	48	70
110	Qc	385/386 (100%)	374 (97%)	11 (3%)	37	61
110	qC	386/386 (100%)	379 (98%)	7 (2%)	54	75
110	qc	385/386 (100%)	375 (97%)	10 (3%)	41	65
111	QD	255/274 (93%)	252 (99%)	3 (1%)	67	82
111	Qd	255/274 (93%)	253 (99%)	2 (1%)	79	88
111	qD	255/274 (93%)	252 (99%)	3 (1%)	67	82
111	qd	255/274 (93%)	254 (100%)	1 (0%)	89	95
112	QE	109/237 (46%)	106 (97%)	3 (3%)	38	63
112	Qe	99/237 (42%)	97 (98%)	2 (2%)	50	72
112	qE	109/237 (46%)	106 (97%)	3 (3%)	38	63
112	qe	99/237 (42%)	97 (98%)	2 (2%)	50	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
113	QF	80/81 (99%)	79 (99%)	1 (1%)	65	80
113	Qf	72/81 (89%)	72 (100%)	0	100	100
113	qF	80/81 (99%)	79 (99%)	1 (1%)	65	80
113	qf	72/81 (89%)	72 (100%)	0	100	100
114	QG	288/289 (100%)	282 (98%)	6 (2%)	48	70
114	Qg	287/289 (99%)	282 (98%)	5 (2%)	56	76
114	qG	288/289 (100%)	283 (98%)	5 (2%)	56	76
114	qg	287/289 (99%)	282 (98%)	5 (2%)	56	76
115	QH	117/118 (99%)	116 (99%)	1 (1%)	75	86
115	Qh	117/118 (99%)	117 (100%)	0	100	100
115	qH	117/118 (99%)	116 (99%)	1 (1%)	75	86
115	qh	117/118 (99%)	117 (100%)	0	100	100
116	QI	104/109 (95%)	103 (99%)	1 (1%)	73	85
116	Qi	104/109 (95%)	103 (99%)	1 (1%)	73	85
116	qI	104/109 (95%)	102 (98%)	2 (2%)	52	73
116	qi	104/109 (95%)	103 (99%)	1 (1%)	73	85
117	QJ	51/56 (91%)	51 (100%)	0	100	100
117	Qj	53/56 (95%)	52 (98%)	1 (2%)	52	73
117	qJ	51/56 (91%)	51 (100%)	0	100	100
117	qj	53/56 (95%)	52 (98%)	1 (2%)	52	73
118	QL	28/36 (78%)	28 (100%)	0	100	100
118	Ql	28/36 (78%)	28 (100%)	0	100	100
118	qL	28/36 (78%)	28 (100%)	0	100	100
118	ql	28/36 (78%)	28 (100%)	0	100	100
120	S1	590/617 (96%)	583 (99%)	7 (1%)	67	82
120	s1	590/617 (96%)	585 (99%)	5 (1%)	79	88
121	S2	399/399 (100%)	387 (97%)	12 (3%)	36	60
121	s2	399/399 (100%)	389 (98%)	10 (2%)	42	66
122	S3	191/191 (100%)	187 (98%)	4 (2%)	48	70
122	s3	191/191 (100%)	187 (98%)	4 (2%)	48	70
123	S4	160/163 (98%)	156 (98%)	4 (2%)	42	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
123	s4	160/163 (98%)	156 (98%)	4 (2%)	42	66
124	S5	82/83 (99%)	79 (96%)	3 (4%)	29	54
124	s5	82/83 (99%)	80 (98%)	2 (2%)	44	68
125	S6	82/116 (71%)	80 (98%)	2 (2%)	44	68
125	s6	82/116 (71%)	81 (99%)	1 (1%)	67	82
126	S7	136/137 (99%)	129 (95%)	7 (5%)	20	43
126	s7	136/137 (99%)	130 (96%)	6 (4%)	24	49
127	S8	197/215 (92%)	197 (100%)	0	100	100
127	s8	197/215 (92%)	197 (100%)	0	100	100
128	T1	440/454 (97%)	433 (98%)	7 (2%)	58	77
128	t1	440/454 (97%)	432 (98%)	8 (2%)	54	75
129	T2	237/280 (85%)	232 (98%)	5 (2%)	48	70
129	t2	237/280 (85%)	232 (98%)	5 (2%)	48	70
130	T3	272/275 (99%)	268 (98%)	4 (2%)	60	78
130	t3	272/275 (99%)	268 (98%)	4 (2%)	60	78
131	T4	178/190 (94%)	177 (99%)	1 (1%)	84	91
131	t4	178/190 (94%)	177 (99%)	1 (1%)	84	91
132	T5	119/179 (66%)	118 (99%)	1 (1%)	79	88
132	t5	119/179 (66%)	118 (99%)	1 (1%)	79	88
133	T6	97/131 (74%)	96 (99%)	1 (1%)	73	85
133	t6	97/131 (74%)	96 (99%)	1 (1%)	73	85
134	T7	124/125 (99%)	122 (98%)	2 (2%)	58	77
134	t7	124/125 (99%)	123 (99%)	1 (1%)	79	88
135	T8	118/122 (97%)	118 (100%)	0	100	100
135	t8	118/122 (97%)	118 (100%)	0	100	100
136	T9	118/122 (97%)	117 (99%)	1 (1%)	79	88
136	t9	118/122 (97%)	118 (100%)	0	100	100
137	TA	94/117 (80%)	93 (99%)	1 (1%)	70	83
137	ta	94/117 (80%)	93 (99%)	1 (1%)	70	83
138	TB	82/97 (84%)	82 (100%)	0	100	100
138	tb	82/97 (84%)	82 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
139	TC	83/84 (99%)	82 (99%)	1 (1%)	67	82
139	tc	83/84 (99%)	82 (99%)	1 (1%)	67	82
140	TD	64/65 (98%)	64 (100%)	0	100	100
140	td	64/65 (98%)	64 (100%)	0	100	100
141	TE	45/63 (71%)	45 (100%)	0	100	100
141	te	45/63 (71%)	45 (100%)	0	100	100
142	TF	195/212 (92%)	194 (100%)	1 (0%)	86	93
142	tf	195/212 (92%)	194 (100%)	1 (0%)	86	93
143	TG	121/122 (99%)	115 (95%)	6 (5%)	20	44
143	tg	121/122 (99%)	117 (97%)	4 (3%)	33	58
144	TH	108/108 (100%)	107 (99%)	1 (1%)	75	86
144	th	108/108 (100%)	107 (99%)	1 (1%)	75	86
145	TX	128/147 (87%)	126 (98%)	2 (2%)	58	77
145	tx	128/147 (87%)	127 (99%)	1 (1%)	79	88
146	V1	362/392 (92%)	359 (99%)	3 (1%)	79	88
146	v1	362/392 (92%)	358 (99%)	4 (1%)	70	83
147	V2	205/236 (87%)	204 (100%)	1 (0%)	86	93
147	v2	205/236 (87%)	204 (100%)	1 (0%)	86	93
148	X1	132/133 (99%)	131 (99%)	1 (1%)	79	88
148	x1	132/133 (99%)	131 (99%)	1 (1%)	79	88
149	C	106/178 (60%)	104 (98%)	2 (2%)	52	73
149	c	106/178 (60%)	104 (98%)	2 (2%)	52	73
All	All	58230/65244 (89%)	57534 (99%)	696 (1%)	66	82

All (696) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1t	42	GLU
2	2e	115	VAL
2	2e	143	PHE
2	2e	151	THR
2	2e	183	ARG
2	2e	207	ASN
2	2e	215	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2f	144	LEU
3	2f	181	PHE
3	2f	205	PHE
3	2f	243	TYR
4	2g	58	ARG
4	2g	169	HIS
5	2h	123	CYS
6	2i	42	GLN
6	2i	76	GLN
6	2i	81	ILE
7	2j	87	ASP
8	2k	36	TYR
8	2k	92	ASN
9	2l	30	TYR
10	2m	37	TYR
11	2n	34	VAL
12	2o	6	ARG
14	3t	58	CYS
14	3t	65	THR
15	4a	33	TYR
15	4a	34	ARG
16	4t	11	ASP
16	4t	24	LYS
18	6a	8	ARG
19	6b	164	TYR
20	6c	1	MET
23	7a	53	HIS
24	7c	106	TRP
24	7c	196	LYS
25	7l	862	LEU
27	b	149	TYR
27	b	241	LEU
27	b	421	VAL
29	c1	57	TYR
29	c1	336	THR
29	c1	450	ARG
29	c1	503	PHE
29	c1	621	MET
30	c2	162	TYR
30	c2	224	PHE
30	c2	298	PHE
30	c2	501	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	c2	526	ASP
31	c3	14	ARG
31	c3	55	THR
31	c3	97	ASP
31	c3	425	TYR
32	d	156	PRO
32	d	279	PRO
32	d	368	THR
33	e	280	TRP
33	e	346	HIS
34	f	269	ASP
36	g	160	GLN
36	g	223	ASP
37	h	55	ARG
37	h	58	LEU
37	h	67	THR
37	h	109	PHE
37	h	114	ILE
37	h	148	TYR
37	h	162	VAL
37	h	248	HIS
38	i	23	ARG
40	k	113	HIS
41	l	88	PHE
41	l	186	ARG
42	m	25	ASN
43	m1	164	ASP
44	m2	40	ARG
45	m3	34	GLN
45	m3	227	GLN
45	m3	275	ARG
46	n	56	TYR
46	n	181	ASP
47	o	98	ASP
48	p	90	PHE
48	p	110	ASP
49	q	83	TYR
50	r	8	TYR
50	r	111	TYR
52	sa	52	ILE
52	sa	78	THR
52	sa	329	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	sa	365	HIS
52	sa	459	LEU
52	sa	496	THR
53	sb	47	LEU
53	sb	87	TYR
53	sb	120	ARG
53	sb	122	CYS
53	sb	157	THR
53	sb	161	HIS
53	sb	218	CYS
53	sb	231	HIS
53	sb	246	ARG
54	sc	23	PHE
54	sc	26	ARG
56	t	94	ARG
57	u	17	TYR
57	u	115	PHE
59	vb	166	ASN
59	vb	235	TYR
59	vb	565	TRP
60	w	36	TYR
60	w	103	TYR
61	x	65	PHE
62	y	35	LYS
65	y7	400	TYR
66	z	30	PHE
66	z	60	PHE
73	a2	74	PHE
75	a5	51	LYS
75	a5	138	TYR
76	a6	80	PHE
76	a6	172	PHE
77	a7	101	ASN
77	a7	276	ARG
80	ab	53	PHE
81	ac	64	LEU
82	al	37	ARG
83	am	87	ARG
85	b2	7	THR
85	b2	121	SER
86	b3	68	PHE
87	b4	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
87	b4	63	PHE
89	b7	46	PHE
89	b7	87	HIS
90	b8	129	LYS
91	b9	5	TYR
91	b9	152	PHE
92	bl	17	ASP
93	bm	83	HIS
93	bm	103	ARG
93	bm	148	PHE
93	bm	201	ARG
95	fx	81	CYS
96	g1	217	ASN
97	g2	122	VAL
97	g2	146	ASN
98	g3	12	LYS
98	g3	283	TRP
99	j1	42	ASP
99	j1	175	PHE
99	j1	193	LYS
99	j1	311	GLN
100	n1	103	THR
100	n1	106	ILE
100	n1	166	PHE
100	n1	207	PHE
100	n1	245	TYR
101	n2	1	MET
101	n2	215	PHE
101	n2	221	THR
101	n2	268	TYR
101	n2	289	PHE
102	n3	79	PHE
102	n3	83	PHE
103	n4	71	PHE
103	n4	118	PHE
103	n4	120	LEU
103	n4	205	TRP
103	n4	224	THR
103	n4	346	TYR
103	n4	363	PHE
103	n4	479	LEU
104	n5	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
104	n5	67	ILE
104	n5	69	HIS
104	n5	79	ASP
104	n5	81	ILE
104	n5	86	LYS
104	n5	87	ILE
104	n5	89	PHE
104	n5	210	PHE
104	n5	236	MET
104	n5	385	TYR
104	n5	522	PHE
105	n6	75	LEU
105	n6	137	TYR
106	p1	89	ASP
106	p1	174	SER
107	p2	23	TYR
108	qA	79	ILE
108	qA	435	TYR
109	qB	118	THR
109	qB	291	TYR
109	qB	418	TYR
109	qB	492	HIS
109	qB	495	ARG
110	qC	86	ARG
110	qC	108	PHE
110	qC	153	TYR
110	qC	202	ASP
110	qC	203	MET
110	qC	267	PHE
110	qC	316	HIS
111	qD	95	LEU
111	qD	148	ASP
111	qD	300	HIS
112	qE	33	ARG
112	qE	68	VAL
112	qE	117	ARG
113	qF	62	LEU
114	qG	110	TYR
114	qG	134	VAL
114	qG	275	ARG
114	qG	290	ASN
114	qG	326	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
115	qH	80	ARG
116	qI	3	TYR
116	qI	60	GLN
108	qa	29	ASP
108	qa	90	ASP
108	qa	202	LEU
108	qa	215	LYS
108	qa	265	LEU
108	qa	312	VAL
108	qa	435	TYR
109	qb	48	GLU
109	qb	71	ASN
109	qb	162	ASP
109	qb	246	PHE
109	qb	279	VAL
109	qb	291	TYR
109	qb	317	ASP
109	qb	418	TYR
109	qb	474	LYS
110	qc	3	TRP
110	qc	71	ASP
110	qc	79	ASP
110	qc	86	ARG
110	qc	108	PHE
110	qc	154	ASP
110	qc	156	PHE
110	qc	248	MET
110	qc	267	PHE
110	qc	316	HIS
111	qd	96	LEU
112	qe	37	LYS
112	qe	117	ARG
114	qg	73	ASP
114	qg	185	ASP
114	qg	261	ASP
114	qg	275	ARG
114	qg	326	PHE
116	qi	3	TYR
117	qj	53	ARG
120	s1	43	LYS
120	s1	180	CYS
120	s1	511	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
120	s1	605	MET
120	s1	626	VAL
121	s2	1	MET
121	s2	9	TRP
121	s2	40	VAL
121	s2	72	ASP
121	s2	77	GLN
121	s2	90	MET
121	s2	207	HIS
121	s2	258	TYR
121	s2	368	LEU
121	s2	414	LEU
122	s3	20	SER
122	s3	40	ASN
122	s3	55	PHE
122	s3	95	LEU
123	s4	3	LEU
123	s4	14	PHE
123	s4	76	ARG
123	s4	133	ASN
124	s5	24	GLN
124	s5	49	ARG
125	s6	107	ARG
126	s7	4	ASP
126	s7	22	PHE
126	s7	31	CYS
126	s7	46	PHE
126	s7	102	TYR
126	s7	146	ARG
128	t1	45	ASN
128	t1	268	LEU
128	t1	291	GLU
128	t1	298	LEU
128	t1	311	THR
128	t1	391	ASN
128	t1	427	TYR
128	t1	461	ASP
129	t2	97	LEU
129	t2	112	LEU
129	t2	145	TYR
129	t2	208	GLN
129	t2	291	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
130	t3	25	LEU
130	t3	27	ARG
130	t3	297	VAL
130	t3	310	ARG
131	t4	57	HIS
132	t5	148	GLU
133	t6	95	VAL
134	t7	9	ARG
137	ta	35	VAL
139	tc	2	VAL
142	tf	226	LEU
143	tg	84	LYS
143	tg	103	LYS
143	tg	104	ASN
143	tg	105	LEU
144	th	113	ARG
145	tx	113	THR
146	v1	32	TYR
146	v1	53	VAL
146	v1	380	CYS
146	v1	386	CYS
147	v2	127	THR
148	x1	92	TYR
1	1T	42	GLU
2	2E	115	VAL
2	2E	143	PHE
2	2E	151	THR
2	2E	183	ARG
2	2E	215	THR
2	2E	218	PHE
3	2F	144	LEU
3	2F	181	PHE
3	2F	205	PHE
3	2F	243	TYR
4	2G	58	ARG
4	2G	169	HIS
5	2H	123	CYS
6	2I	76	GLN
6	2I	81	ILE
7	2J	87	ASP
8	2K	36	TYR
8	2K	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2L	4	ASP
9	2L	30	TYR
10	2M	37	TYR
11	2N	34	VAL
11	2N	43	GLN
12	2O	6	ARG
14	3T	58	CYS
14	3T	65	THR
15	4A	33	TYR
15	4A	34	ARG
16	4T	11	ASP
16	4T	24	LYS
18	6A	8	ARG
19	6B	164	TYR
20	6C	1	MET
23	7A	53	HIS
24	7C	106	TRP
24	7C	196	LYS
25	7L	862	LEU
27	B	103	ASN
27	B	149	TYR
27	B	241	LEU
27	B	421	VAL
29	C1	57	TYR
29	C1	183	GLN
29	C1	336	THR
29	C1	450	ARG
29	C1	503	PHE
29	C1	592	ASP
30	C2	162	TYR
30	C2	298	PHE
30	C2	501	VAL
30	C2	526	ASP
31	C3	55	THR
31	C3	97	ASP
31	C3	272	ILE
31	C3	425	TYR
32	D	279	PRO
32	D	368	THR
33	E	280	TRP
33	E	346	HIS
34	F	269	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	F	312	HIS
36	G	160	GLN
36	G	223	ASP
37	H	20	THR
37	H	24	LEU
37	H	41	ARG
37	H	55	ARG
37	H	63	ILE
37	H	67	THR
37	H	109	PHE
37	H	114	ILE
37	H	148	TYR
37	H	162	VAL
37	H	248	HIS
38	I	23	ARG
39	J	61	GLU
40	K	113	HIS
41	L	88	PHE
41	L	186	ARG
42	M	25	ASN
43	M1	164	ASP
44	M2	40	ARG
45	M3	275	ARG
46	N	56	TYR
46	N	181	ASP
48	P	90	PHE
48	P	110	ASP
50	R	8	TYR
50	R	111	TYR
52	SA	52	ILE
52	SA	65	PHE
52	SA	78	THR
52	SA	316	GLU
52	SA	329	ASP
52	SA	365	HIS
52	SA	371	ILE
52	SA	459	LEU
52	SA	496	THR
52	SA	528	LEU
52	SA	602	ILE
53	SB	47	LEU
53	SB	87	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	SB	120	ARG
53	SB	122	CYS
53	SB	157	THR
53	SB	161	HIS
53	SB	173	THR
53	SB	218	CYS
53	SB	231	HIS
53	SB	234	ARG
53	SB	246	ARG
53	SB	272	CYS
54	SC	23	PHE
54	SC	26	ARG
56	T	94	ARG
57	U	17	TYR
57	U	115	PHE
59	VB	166	ASN
59	VB	235	TYR
59	VB	565	TRP
60	W	36	TYR
60	W	103	TYR
61	X	65	PHE
62	Y	35	LYS
65	Y7	400	TYR
66	Z	30	PHE
66	Z	60	PHE
69	2B	79	LEU
73	A2	74	PHE
73	A2	79	ASN
75	A5	51	LYS
75	A5	138	TYR
76	A6	80	PHE
76	A6	172	PHE
77	A7	101	ASN
77	A7	276	ARG
80	AB	53	PHE
81	AC	64	LEU
82	AL	37	ARG
82	AL	113	THR
83	AM	87	ARG
84	AN	98	ASN
84	AN	105	MET
85	B2	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	B2	85	LEU
85	B2	121	SER
86	B3	68	PHE
87	B4	52	VAL
87	B4	63	PHE
89	B7	46	PHE
89	B7	87	HIS
90	B8	129	LYS
90	B8	185	ILE
91	B9	5	TYR
91	B9	152	PHE
93	BM	83	HIS
93	BM	103	ARG
93	BM	148	PHE
93	BM	201	ARG
94	C4	28	THR
95	FX	81	CYS
96	G1	63	ILE
96	G1	136	ASP
96	G1	217	ASN
97	G2	146	ASN
98	G3	12	LYS
98	G3	283	TRP
99	J1	42	ASP
99	J1	175	PHE
99	J1	193	LYS
99	J1	311	GLN
100	N1	68	ILE
100	N1	74	LEU
100	N1	103	THR
100	N1	106	ILE
100	N1	160	MET
100	N1	166	PHE
100	N1	207	PHE
100	N1	230	THR
100	N1	245	TYR
100	N1	284	LEU
101	N2	1	MET
101	N2	53	LYS
101	N2	215	PHE
101	N2	221	THR
101	N2	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
101	N2	268	TYR
101	N2	289	PHE
101	N2	332	ASP
102	N3	79	PHE
102	N3	83	PHE
103	N4	71	PHE
103	N4	115	ILE
103	N4	118	PHE
103	N4	120	LEU
103	N4	205	TRP
103	N4	346	TYR
103	N4	363	PHE
103	N4	440	ILE
104	N5	64	VAL
104	N5	67	ILE
104	N5	69	HIS
104	N5	79	ASP
104	N5	81	ILE
104	N5	86	LYS
104	N5	87	ILE
104	N5	210	PHE
104	N5	236	MET
104	N5	346	SER
104	N5	385	TYR
104	N5	522	PHE
104	N5	630	ARG
105	N6	75	LEU
105	N6	137	TYR
106	P1	89	ASP
106	P1	174	SER
107	P2	23	TYR
107	P2	44	THR
107	P2	123	TYR
107	P2	129	ARG
108	QA	79	ILE
108	QA	435	TYR
109	QB	118	THR
109	QB	291	TYR
109	QB	315	ASP
109	QB	418	TYR
109	QB	492	HIS
109	QB	495	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
110	QC	86	ARG
110	QC	108	PHE
110	QC	111	GLU
110	QC	153	TYR
110	QC	202	ASP
110	QC	203	MET
110	QC	267	PHE
110	QC	316	HIS
111	QD	95	LEU
111	QD	148	ASP
111	QD	300	HIS
112	QE	33	ARG
112	QE	68	VAL
112	QE	117	ARG
113	QF	62	LEU
114	QG	110	TYR
114	QG	134	VAL
114	QG	263	THR
114	QG	275	ARG
114	QG	290	ASN
114	QG	326	PHE
115	QH	80	ARG
116	QI	3	TYR
108	Qa	29	ASP
108	Qa	90	ASP
108	Qa	202	LEU
108	Qa	215	LYS
108	Qa	312	VAL
108	Qa	435	TYR
109	Qb	48	GLU
109	Qb	71	ASN
109	Qb	162	ASP
109	Qb	172	VAL
109	Qb	246	PHE
109	Qb	279	VAL
109	Qb	291	TYR
109	Qb	317	ASP
109	Qb	418	TYR
109	Qb	474	LYS
110	Qc	3	TRP
110	Qc	71	ASP
110	Qc	79	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
110	Qc	86	ARG
110	Qc	108	PHE
110	Qc	154	ASP
110	Qc	156	PHE
110	Qc	234	MET
110	Qc	248	MET
110	Qc	267	PHE
110	Qc	316	HIS
111	Qd	96	LEU
111	Qd	298	TYR
112	Qe	37	LYS
112	Qe	117	ARG
114	Qg	73	ASP
114	Qg	185	ASP
114	Qg	261	ASP
114	Qg	275	ARG
114	Qg	326	PHE
116	Qi	3	TYR
117	Qj	53	ARG
120	S1	43	LYS
120	S1	169	LEU
120	S1	180	CYS
120	S1	511	PHE
120	S1	605	MET
120	S1	626	VAL
120	S1	676	THR
121	S2	1	MET
121	S2	9	TRP
121	S2	40	VAL
121	S2	72	ASP
121	S2	77	GLN
121	S2	90	MET
121	S2	207	HIS
121	S2	258	TYR
121	S2	267	ARG
121	S2	350	ASP
121	S2	368	LEU
121	S2	414	LEU
122	S3	20	SER
122	S3	40	ASN
122	S3	55	PHE
122	S3	95	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
123	S4	3	LEU
123	S4	14	PHE
123	S4	76	ARG
123	S4	133	ASN
124	S5	24	GLN
124	S5	49	ARG
124	S5	76	GLU
125	S6	107	ARG
125	S6	111	THR
126	S7	4	ASP
126	S7	15	SER
126	S7	22	PHE
126	S7	31	CYS
126	S7	46	PHE
126	S7	102	TYR
126	S7	146	ARG
128	T1	45	ASN
128	T1	268	LEU
128	T1	298	LEU
128	T1	311	THR
128	T1	313	ASP
128	T1	427	TYR
128	T1	461	ASP
129	T2	97	LEU
129	T2	112	LEU
129	T2	145	TYR
129	T2	208	GLN
129	T2	291	LYS
130	T3	25	LEU
130	T3	27	ARG
130	T3	297	VAL
130	T3	310	ARG
131	T4	57	HIS
132	T5	148	GLU
133	T6	95	VAL
134	T7	9	ARG
134	T7	115	THR
136	T9	117	ARG
137	TA	35	VAL
139	TC	2	VAL
142	TF	226	LEU
143	TG	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
143	TG	99	LEU
143	TG	103	LYS
143	TG	104	ASN
143	TG	105	LEU
143	TG	120	ILE
144	TH	113	ARG
145	TX	51	ARG
145	TX	113	THR
146	V1	53	VAL
146	V1	380	CYS
146	V1	386	CYS
147	V2	127	THR
148	X1	92	TYR
149	C	104	TRP
149	C	192	LYS
149	c	104	TRP
149	c	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (977) such sidechains are listed below:

Mol	Chain	Res	Type
2	2e	10	ASN
2	2e	99	HIS
2	2e	120	ASN
2	2e	182	HIS
2	2e	252	ASN
3	2f	124	GLN
3	2f	140	GLN
3	2f	292	GLN
4	2g	41	HIS
4	2g	62	ASN
4	2g	96	GLN
4	2g	97	ASN
4	2g	99	HIS
4	2g	122	HIS
4	2g	123	ASN
4	2g	169	HIS
5	2h	91	GLN
5	2h	105	HIS
5	2h	110	ASN
5	2h	185	GLN
6	2i	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2i	42	GLN
6	2i	59	ASN
6	2i	61	GLN
6	2i	62	GLN
7	2j	2	ASN
7	2j	25	ASN
7	2j	40	ASN
7	2j	92	GLN
7	2j	101	HIS
9	2l	70	GLN
10	2m	17	GLN
10	2m	47	HIS
12	2o	14	HIS
13	2t	8	GLN
13	2t	24	GLN
13	2t	59	ASN
14	3t	40	ASN
17	5t	14	ASN
17	5t	47	GLN
18	6a	56	ASN
18	6a	112	HIS
19	6b	114	GLN
19	6b	157	GLN
19	6b	161	GLN
24	7c	103	GLN
24	7c	126	GLN
26	a	42	GLN
26	a	92	HIS
26	a	213	GLN
26	a	303	ASN
26	a	358	ASN
26	a	428	GLN
26	a	451	GLN
26	a	469	GLN
27	b	20	GLN
27	b	128	GLN
27	b	152	GLN
27	b	212	GLN
27	b	251	GLN
27	b	257	GLN
28	bp	129	ASN
28	bp	229	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	bp	386	GLN
29	c1	120	ASN
29	c1	327	HIS
29	c1	406	ASN
29	c1	571	GLN
29	c1	657	GLN
30	c2	4	ASN
30	c2	167	GLN
30	c2	239	ASN
31	c3	43	ASN
31	c3	129	ASN
31	c3	230	GLN
31	c3	306	GLN
31	c3	420	ASN
31	c3	472	ASN
31	c3	569	GLN
31	c3	591	ASN
32	d	305	GLN
32	d	321	ASN
33	e	33	ASN
34	f	267	ASN
34	f	304	ASN
35	fs	24	HIS
35	fs	87	ASN
35	fs	105	GLN
35	fs	160	HIS
36	g	67	ASN
36	g	72	ASN
36	g	98	ASN
36	g	138	GLN
36	g	277	GLN
36	g	293	GLN
37	h	38	GLN
37	h	105	GLN
37	h	232	HIS
38	i	49	ASN
38	i	220	GLN
38	i	240	HIS
39	j	57	HIS
39	j	108	GLN
39	j	193	GLN
39	j	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	30	GLN
40	k	95	GLN
40	k	182	GLN
40	k	193	HIS
40	k	217	ASN
40	k	230	ASN
41	l	169	ASN
41	l	170	GLN
41	l	178	HIS
42	m	10	ASN
42	m	25	ASN
42	m	79	HIS
42	m	94	GLN
42	m	106	GLN
42	m	184	HIS
42	m	200	HIS
42	m	214	HIS
43	m1	95	ASN
43	m1	208	GLN
44	m2	62	ASN
44	m2	80	GLN
44	m2	118	HIS
45	m3	17	ASN
45	m3	60	GLN
45	m3	185	GLN
46	n	23	HIS
46	n	101	GLN
47	o	65	ASN
47	o	86	GLN
47	o	105	GLN
47	o	129	GLN
48	p	36	ASN
48	p	44	ASN
48	p	75	GLN
48	p	117	ASN
48	p	135	GLN
49	q	70	HIS
49	q	118	ASN
49	q	132	GLN
51	s	48	GLN
51	s	55	ASN
51	s	96	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	sa	127	GLN
52	sa	172	GLN
52	sa	185	HIS
52	sa	189	HIS
52	sa	282	GLN
52	sa	284	HIS
52	sa	351	HIS
52	sa	366	GLN
52	sa	430	ASN
52	sa	526	GLN
52	sa	566	GLN
53	sb	84	GLN
53	sb	110	ASN
53	sb	133	ASN
53	sb	138	HIS
53	sb	178	GLN
53	sb	242	GLN
53	sb	289	GLN
54	sc	15	ASN
54	sc	16	ASN
55	sd	23	ASN
56	t	38	ASN
56	t	54	ASN
58	v	31	GLN
59	vb	164	GLN
59	vb	166	ASN
59	vb	216	HIS
59	vb	296	GLN
59	vb	339	ASN
59	vb	347	ASN
59	vb	485	ASN
59	vb	531	ASN
60	w	10	GLN
62	y	7	GLN
62	y	18	GLN
62	y	55	GLN
64	y5	70	ASN
64	y5	81	ASN
65	y7	129	ASN
65	y7	191	ASN
65	y7	194	ASN
65	y7	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
65	y7	309	GLN
65	y7	376	ASN
66	z	22	HIS
67	z1	10	ASN
67	z1	95	ASN
68	1b	34	GLN
69	2b	10	ASN
70	4l	99	GLN
70	4l	100	ASN
72	a1	68	HIS
72	a1	85	ASN
73	a2	24	GLN
73	a2	43	GLN
73	a2	93	GLN
73	a2	98	ASN
75	a5	121	GLN
75	a5	164	ASN
76	a6	110	GLN
77	a7	59	ASN
77	a7	63	HIS
77	a7	236	ASN
77	a7	260	HIS
78	a8	187	ASN
78	a8	196	ASN
78	a8	197	GLN
79	a9	23	GLN
79	a9	38	GLN
79	a9	139	ASN
79	a9	177	HIS
79	a9	239	ASN
79	a9	359	ASN
80	ab	28	GLN
80	ab	86	GLN
80	ab	98	GLN
82	al	10	GLN
82	al	40	HIS
82	al	53	GLN
82	al	73	ASN
82	al	86	GLN
82	al	156	GLN
83	am	97	ASN
84	an	12	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	an	29	HIS
84	an	106	GLN
84	an	150	GLN
84	an	158	ASN
85	b2	13	GLN
85	b2	71	HIS
85	b2	98	ASN
87	b4	40	GLN
88	b6	79	ASN
89	b7	25	GLN
89	b7	47	GLN
89	b7	78	HIS
89	b7	85	ASN
90	b8	109	GLN
91	b9	168	GLN
92	bl	114	HIS
92	bl	165	GLN
93	bm	169	ASN
94	c4	70	GLN
94	c4	100	ASN
95	fx	27	HIS
95	fx	29	HIS
95	fx	49	ASN
96	g1	70	ASN
96	g1	217	ASN
96	g1	243	ASN
97	g2	100	HIS
97	g2	125	ASN
97	g2	128	ASN
97	g2	146	ASN
97	g2	152	ASN
97	g2	170	ASN
98	g3	37	GLN
98	g3	104	GLN
98	g3	108	GLN
98	g3	114	GLN
98	g3	119	ASN
98	g3	120	GLN
98	g3	137	GLN
98	g3	142	ASN
98	g3	158	ASN
98	g3	306	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
98	g3	323	ASN
99	j1	21	GLN
99	j1	85	GLN
99	j1	287	GLN
99	j1	311	GLN
101	n2	30	ASN
101	n2	31	ASN
101	n2	54	GLN
101	n2	55	ASN
101	n2	106	ASN
101	n2	122	ASN
101	n2	308	ASN
102	n3	8	HIS
102	n3	114	ASN
103	n4	46	ASN
103	n4	56	ASN
103	n4	101	ASN
103	n4	107	ASN
103	n4	230	ASN
103	n4	462	ASN
104	n5	55	ASN
104	n5	101	HIS
104	n5	113	ASN
104	n5	145	ASN
104	n5	363	ASN
104	n5	670	ASN
104	n5	698	ASN
104	n5	718	ASN
105	n6	39	GLN
105	n6	118	ASN
105	n6	240	ASN
106	p1	44	HIS
106	p1	55	GLN
106	p1	150	ASN
106	p1	189	HIS
106	p1	205	GLN
106	p1	251	ASN
107	p2	91	GLN
107	p2	103	GLN
107	p2	125	GLN
107	p2	178	ASN
108	qA	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
108	qA	154	ASN
108	qA	283	GLN
108	qA	413	GLN
108	qA	446	GLN
108	qA	469	ASN
109	qB	71	ASN
109	qB	136	ASN
109	qB	170	ASN
109	qB	196	GLN
109	qB	301	ASN
109	qB	303	ASN
109	qB	485	HIS
109	qB	492	HIS
110	qC	31	ASN
110	qC	204	HIS
110	qC	209	ASN
110	qC	312	GLN
110	qC	328	ASN
110	qC	380	ASN
110	qC	383	ASN
110	qC	401	ASN
111	qD	312	GLN
112	qE	69	ASN
113	qF	15	GLN
113	qF	16	GLN
113	qF	51	ASN
114	qG	11	GLN
115	qH	35	ASN
115	qH	42	ASN
116	qI	26	GLN
116	qI	43	ASN
116	qI	67	GLN
116	qI	115	GLN
117	qJ	14	ASN
118	qL	30	ASN
108	qa	154	ASN
108	qa	188	GLN
108	qa	283	GLN
108	qa	296	ASN
108	qa	413	GLN
108	qa	423	ASN
108	qa	467	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
109	qb	71	ASN
109	qb	125	GLN
109	qb	136	ASN
109	qb	177	GLN
109	qb	196	GLN
109	qb	257	GLN
109	qb	303	ASN
109	qb	384	ASN
109	qb	407	ASN
109	qb	485	HIS
109	qb	492	HIS
110	qc	204	HIS
110	qc	312	GLN
111	qd	299	ASN
112	qe	39	HIS
112	qe	69	ASN
112	qe	80	HIS
112	qe	91	GLN
113	qf	15	GLN
113	qf	26	GLN
114	qg	11	GLN
114	qg	44	HIS
114	qg	294	GLN
114	qg	319	GLN
115	qh	15	HIS
115	qh	90	GLN
116	qi	26	GLN
116	qi	115	GLN
117	qj	14	ASN
118	ql	32	GLN
120	s1	57	ASN
120	s1	263	GLN
120	s1	371	GLN
120	s1	438	ASN
120	s1	490	ASN
120	s1	598	GLN
120	s1	666	GLN
120	s1	706	ASN
120	s1	712	ASN
120	s1	715	ASN
121	s2	19	ASN
121	s2	22	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
121	s2	182	ASN
121	s2	222	ASN
122	s3	2	GLN
122	s3	3	ASN
122	s3	87	ASN
122	s3	92	ASN
123	s4	94	HIS
123	s4	148	GLN
123	s4	171	ASN
124	s5	24	GLN
124	s5	52	GLN
124	s5	94	GLN
125	s6	70	GLN
125	s6	109	HIS
127	s8	27	HIS
127	s8	39	HIS
127	s8	81	GLN
128	t1	63	GLN
128	t1	104	GLN
128	t1	118	GLN
128	t1	146	GLN
128	t1	172	GLN
128	t1	273	ASN
128	t1	317	ASN
128	t1	327	ASN
128	t1	380	ASN
128	t1	497	ASN
128	t1	500	ASN
129	t2	25	GLN
129	t2	33	ASN
129	t2	125	ASN
129	t2	138	ASN
129	t2	161	GLN
129	t2	162	HIS
129	t2	222	ASN
129	t2	294	GLN
130	t3	56	GLN
130	t3	70	ASN
130	t3	73	GLN
130	t3	161	ASN
130	t3	272	HIS
131	t4	56	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
131	t4	72	ASN
131	t4	78	GLN
131	t4	94	HIS
131	t4	161	ASN
131	t4	206	GLN
132	t5	76	GLN
132	t5	178	GLN
132	t5	181	GLN
132	t5	187	GLN
133	t6	40	ASN
134	t7	44	GLN
134	t7	107	ASN
134	t7	143	GLN
135	t8	110	GLN
135	t8	115	HIS
137	ta	48	GLN
138	tb	24	ASN
138	tb	59	GLN
139	tc	17	ASN
139	tc	53	HIS
139	tc	55	HIS
139	tc	85	GLN
140	td	73	GLN
142	tf	84	ASN
142	tf	153	ASN
142	tf	217	GLN
142	tf	229	HIS
143	tg	6	GLN
143	tg	9	GLN
143	tg	16	GLN
143	tg	17	GLN
144	th	2	ASN
144	th	25	ASN
144	th	52	GLN
144	th	124	GLN
145	tx	107	GLN
145	tx	119	ASN
145	tx	156	GLN
146	v1	71	ASN
146	v1	137	HIS
146	v1	223	GLN
146	v1	414	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
146	v1	419	GLN
146	v1	470	GLN
147	v2	48	ASN
147	v2	81	ASN
147	v2	245	GLN
2	2E	10	ASN
2	2E	99	HIS
2	2E	120	ASN
2	2E	182	HIS
3	2F	124	GLN
3	2F	140	GLN
3	2F	292	GLN
4	2G	22	GLN
4	2G	41	HIS
4	2G	62	ASN
4	2G	96	GLN
4	2G	97	ASN
4	2G	99	HIS
4	2G	123	ASN
5	2H	91	GLN
5	2H	105	HIS
5	2H	110	ASN
5	2H	185	GLN
6	2I	32	ASN
6	2I	42	GLN
6	2I	59	ASN
6	2I	61	GLN
6	2I	62	GLN
7	2J	2	ASN
7	2J	25	ASN
7	2J	40	ASN
7	2J	92	GLN
7	2J	101	HIS
9	2L	70	GLN
10	2M	17	GLN
10	2M	47	HIS
12	2O	14	HIS
13	2T	8	GLN
13	2T	24	GLN
13	2T	59	ASN
14	3T	40	ASN
17	5T	14	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	5T	47	GLN
18	6A	56	ASN
18	6A	112	HIS
19	6B	114	GLN
19	6B	157	GLN
19	6B	161	GLN
24	7C	86	ASN
24	7C	103	GLN
24	7C	126	GLN
26	A	42	GLN
26	A	92	HIS
26	A	213	GLN
26	A	303	ASN
26	A	358	ASN
26	A	428	GLN
26	A	451	GLN
26	A	469	GLN
27	B	20	GLN
27	B	128	GLN
27	B	152	GLN
27	B	212	GLN
27	B	251	GLN
27	B	257	GLN
28	BP	129	ASN
28	BP	229	GLN
28	BP	386	GLN
29	C1	120	ASN
29	C1	327	HIS
29	C1	406	ASN
29	C1	571	GLN
29	C1	657	GLN
30	C2	4	ASN
30	C2	167	GLN
30	C2	239	ASN
31	C3	43	ASN
31	C3	129	ASN
31	C3	230	GLN
31	C3	297	GLN
31	C3	306	GLN
31	C3	418	ASN
31	C3	420	ASN
31	C3	472	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	C3	569	GLN
31	C3	591	ASN
32	D	305	GLN
33	E	33	ASN
33	E	235	ASN
33	E	346	HIS
34	F	267	ASN
34	F	304	ASN
34	F	325	ASN
35	FS	24	HIS
35	FS	87	ASN
35	FS	105	GLN
35	FS	160	HIS
36	G	67	ASN
36	G	72	ASN
36	G	98	ASN
36	G	138	GLN
36	G	293	GLN
37	H	38	GLN
37	H	105	GLN
37	H	232	HIS
38	I	49	ASN
38	I	220	GLN
38	I	240	HIS
39	J	57	HIS
39	J	108	GLN
39	J	193	GLN
40	K	30	GLN
40	K	95	GLN
40	K	182	GLN
40	K	193	HIS
40	K	217	ASN
40	K	230	ASN
41	L	53	ASN
41	L	169	ASN
41	L	170	GLN
41	L	178	HIS
42	M	10	ASN
42	M	25	ASN
42	M	79	HIS
42	M	94	GLN
42	M	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	M	184	HIS
42	M	200	HIS
42	M	214	HIS
43	M1	95	ASN
43	M1	208	GLN
44	M2	62	ASN
44	M2	80	GLN
44	M2	118	HIS
45	M3	17	ASN
45	M3	60	GLN
45	M3	185	GLN
46	N	23	HIS
46	N	101	GLN
47	O	65	ASN
47	O	86	GLN
47	O	105	GLN
47	O	129	GLN
48	P	36	ASN
48	P	44	ASN
48	P	75	GLN
48	P	117	ASN
48	P	135	GLN
49	Q	70	HIS
49	Q	118	ASN
49	Q	132	GLN
51	S	12	ASN
51	S	48	GLN
51	S	55	ASN
51	S	96	GLN
52	SA	127	GLN
52	SA	172	GLN
52	SA	185	HIS
52	SA	189	HIS
52	SA	282	GLN
52	SA	284	HIS
52	SA	351	HIS
52	SA	366	GLN
52	SA	430	ASN
52	SA	526	GLN
52	SA	566	GLN
53	SB	84	GLN
53	SB	110	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	SB	133	ASN
53	SB	138	HIS
53	SB	178	GLN
53	SB	242	GLN
53	SB	289	GLN
54	SC	16	ASN
55	SD	23	ASN
56	T	54	ASN
58	V	31	GLN
59	VB	164	GLN
59	VB	166	ASN
59	VB	216	HIS
59	VB	296	GLN
59	VB	339	ASN
59	VB	347	ASN
59	VB	485	ASN
59	VB	531	ASN
60	W	10	GLN
62	Y	7	GLN
62	Y	18	GLN
62	Y	55	GLN
64	Y5	70	ASN
65	Y7	129	ASN
65	Y7	191	ASN
65	Y7	309	GLN
65	Y7	376	ASN
66	Z	22	HIS
67	Z1	10	ASN
67	Z1	95	ASN
68	1B	34	GLN
69	2B	10	ASN
70	4L	99	GLN
70	4L	100	ASN
72	A1	68	HIS
72	A1	85	ASN
73	A2	24	GLN
73	A2	43	GLN
73	A2	93	GLN
73	A2	98	ASN
75	A5	121	GLN
75	A5	164	ASN
76	A6	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
77	A7	59	ASN
77	A7	63	HIS
77	A7	236	ASN
77	A7	260	HIS
78	A8	187	ASN
78	A8	196	ASN
78	A8	197	GLN
79	A9	23	GLN
79	A9	38	GLN
79	A9	139	ASN
79	A9	177	HIS
79	A9	239	ASN
79	A9	303	ASN
79	A9	359	ASN
80	AB	28	GLN
80	AB	86	GLN
80	AB	98	GLN
82	AL	10	GLN
82	AL	40	HIS
82	AL	53	GLN
82	AL	73	ASN
82	AL	86	GLN
82	AL	156	GLN
83	AM	97	ASN
84	AN	12	HIS
84	AN	29	HIS
84	AN	106	GLN
84	AN	150	GLN
84	AN	158	ASN
85	B2	13	GLN
85	B2	71	HIS
85	B2	98	ASN
87	B4	40	GLN
88	B6	79	ASN
89	B7	25	GLN
89	B7	47	GLN
89	B7	78	HIS
89	B7	85	ASN
90	B8	109	GLN
91	B9	168	GLN
92	BL	114	HIS
92	BL	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
93	BM	169	ASN
94	C4	70	GLN
95	FX	27	HIS
95	FX	29	HIS
95	FX	49	ASN
96	G1	70	ASN
96	G1	217	ASN
96	G1	243	ASN
97	G2	100	HIS
97	G2	125	ASN
97	G2	128	ASN
97	G2	146	ASN
97	G2	152	ASN
97	G2	170	ASN
98	G3	37	GLN
98	G3	104	GLN
98	G3	108	GLN
98	G3	114	GLN
98	G3	119	ASN
98	G3	120	GLN
98	G3	137	GLN
98	G3	142	ASN
98	G3	158	ASN
98	G3	306	GLN
98	G3	323	ASN
99	J1	21	GLN
99	J1	85	GLN
99	J1	287	GLN
99	J1	311	GLN
100	N1	282	ASN
101	N2	30	ASN
101	N2	31	ASN
101	N2	54	GLN
101	N2	55	ASN
101	N2	106	ASN
101	N2	122	ASN
101	N2	308	ASN
102	N3	8	HIS
102	N3	114	ASN
103	N4	46	ASN
103	N4	56	ASN
103	N4	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
103	N4	107	ASN
103	N4	230	ASN
103	N4	270	HIS
103	N4	462	ASN
104	N5	55	ASN
104	N5	101	HIS
104	N5	113	ASN
104	N5	145	ASN
104	N5	363	ASN
104	N5	670	ASN
104	N5	698	ASN
104	N5	718	ASN
105	N6	39	GLN
105	N6	118	ASN
105	N6	240	ASN
106	P1	44	HIS
106	P1	55	GLN
106	P1	150	ASN
106	P1	189	HIS
106	P1	251	ASN
107	P2	25	ASN
107	P2	91	GLN
107	P2	103	GLN
107	P2	125	GLN
107	P2	178	ASN
108	QA	125	ASN
108	QA	154	ASN
108	QA	283	GLN
108	QA	413	GLN
108	QA	446	GLN
109	QB	71	ASN
109	QB	136	ASN
109	QB	170	ASN
109	QB	196	GLN
109	QB	301	ASN
109	QB	303	ASN
109	QB	485	HIS
109	QB	492	HIS
110	QC	31	ASN
110	QC	204	HIS
110	QC	209	ASN
110	QC	312	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
110	QC	328	ASN
110	QC	380	ASN
110	QC	383	ASN
110	QC	401	ASN
111	QD	312	GLN
112	QE	69	ASN
113	QF	15	GLN
113	QF	16	GLN
113	QF	51	ASN
114	QG	11	GLN
115	QH	35	ASN
115	QH	42	ASN
116	QI	26	GLN
116	QI	43	ASN
116	QI	67	GLN
116	QI	115	GLN
117	QJ	14	ASN
118	QL	30	ASN
108	Qa	154	ASN
108	Qa	188	GLN
108	Qa	283	GLN
108	Qa	296	ASN
108	Qa	413	GLN
108	Qa	467	GLN
109	Qb	125	GLN
109	Qb	136	ASN
109	Qb	177	GLN
109	Qb	196	GLN
109	Qb	257	GLN
109	Qb	303	ASN
109	Qb	364	HIS
109	Qb	384	ASN
109	Qb	407	ASN
109	Qb	485	HIS
109	Qb	492	HIS
110	Qc	204	HIS
110	Qc	312	GLN
111	Qd	299	ASN
112	Qe	39	HIS
112	Qe	69	ASN
112	Qe	80	HIS
112	Qe	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
113	Qf	15	GLN
113	Qf	26	GLN
114	Qg	11	GLN
114	Qg	44	HIS
114	Qg	294	GLN
114	Qg	319	GLN
115	Qh	90	GLN
116	Qi	26	GLN
116	Qi	115	GLN
117	Qj	14	ASN
118	Ql	32	GLN
120	S1	57	ASN
120	S1	263	GLN
120	S1	371	GLN
120	S1	438	ASN
120	S1	490	ASN
120	S1	598	GLN
120	S1	666	GLN
120	S1	706	ASN
120	S1	712	ASN
120	S1	715	ASN
121	S2	22	GLN
121	S2	182	ASN
121	S2	222	ASN
122	S3	2	GLN
122	S3	3	ASN
122	S3	87	ASN
122	S3	92	ASN
123	S4	94	HIS
123	S4	148	GLN
123	S4	171	ASN
124	S5	24	GLN
124	S5	52	GLN
125	S6	70	GLN
125	S6	109	HIS
127	S8	27	HIS
127	S8	39	HIS
127	S8	81	GLN
128	T1	63	GLN
128	T1	104	GLN
128	T1	118	GLN
128	T1	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
128	T1	172	GLN
128	T1	273	ASN
128	T1	317	ASN
128	T1	327	ASN
128	T1	380	ASN
128	T1	497	ASN
128	T1	500	ASN
129	T2	25	GLN
129	T2	33	ASN
129	T2	125	ASN
129	T2	138	ASN
129	T2	161	GLN
129	T2	162	HIS
129	T2	222	ASN
129	T2	294	GLN
130	T3	56	GLN
130	T3	70	ASN
130	T3	73	GLN
130	T3	161	ASN
130	T3	272	HIS
131	T4	56	HIS
131	T4	72	ASN
131	T4	78	GLN
131	T4	94	HIS
131	T4	161	ASN
131	T4	206	GLN
132	T5	76	GLN
132	T5	178	GLN
132	T5	181	GLN
132	T5	187	GLN
133	T6	40	ASN
134	T7	44	GLN
134	T7	107	ASN
134	T7	143	GLN
135	T8	110	GLN
135	T8	115	HIS
137	TA	48	GLN
138	TB	24	ASN
138	TB	59	GLN
139	TC	17	ASN
139	TC	53	HIS
139	TC	55	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
139	TC	85	GLN
140	TD	73	GLN
142	TF	84	ASN
142	TF	153	ASN
142	TF	160	HIS
142	TF	217	GLN
142	TF	229	HIS
143	TG	6	GLN
143	TG	9	GLN
143	TG	17	GLN
144	TH	2	ASN
144	TH	25	ASN
144	TH	52	GLN
144	TH	124	GLN
145	TX	107	GLN
145	TX	119	ASN
145	TX	156	GLN
146	V1	71	ASN
146	V1	137	HIS
146	V1	223	GLN
146	V1	414	GLN
146	V1	419	GLN
146	V1	470	GLN
147	V2	48	ASN
147	V2	81	ASN
147	V2	245	GLN
149	C	97	ASN
149	C	172	GLN
149	C	184	GLN
149	c	97	ASN
149	c	172	GLN
149	c	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are 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$
59	SEP	VB	520	59	8,9,10	0.88	0	8,12,14	0.75	0
24	SEP	7C	120	24	8,9,10	0.87	0	8,12,14	0.67	0
59	TPO	VB	387	59	8,10,11	1.21	1 (12%)	10,14,16	1.05	0
24	SEP	7c	120	24	8,9,10	0.87	0	8,12,14	0.67	0
59	SEP	vb	520	59	8,9,10	0.88	0	8,12,14	0.76	0
59	TPO	vb	387	59	8,10,11	1.21	1 (12%)	10,14,16	1.05	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
59	SEP	VB	520	59	-	3/5/8/10	-
24	SEP	7C	120	24	-	3/5/8/10	-
59	TPO	VB	387	59	-	1/9/11/13	-
24	SEP	7c	120	24	-	3/5/8/10	-
59	SEP	vb	520	59	-	3/5/8/10	-
59	TPO	vb	387	59	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	VB	387	TPO	P-OG1	3.02	1.65	1.59
59	vb	387	TPO	P-OG1	3.01	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	7c	120	SEP	CB-OG-P-O1P
24	7c	120	SEP	CB-OG-P-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	7c	120	SEP	CB-OG-P-O3P
59	vb	387	TPO	O-C-CA-CB
59	vb	520	SEP	CB-OG-P-O1P
59	vb	520	SEP	CB-OG-P-O2P
59	vb	520	SEP	CB-OG-P-O3P
24	7C	120	SEP	CB-OG-P-O1P
24	7C	120	SEP	CB-OG-P-O2P
24	7C	120	SEP	CB-OG-P-O3P
59	VB	387	TPO	O-C-CA-CB
59	VB	520	SEP	CB-OG-P-O1P
59	VB	520	SEP	CB-OG-P-O2P
59	VB	520	SEP	CB-OG-P-O3P

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 510 ligands modelled in this entry, 14 are monoatomic - leaving 496 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	$\# Z > 2$
152	PC1	n5	803	-	52,52,53	0.29	0	58,60,61	0.29	0
153	CDL	T	201	-	58,58,99	0.38	0	64,70,111	0.32	0
152	PC1	c4	403	-	40,40,53	0.33	0	46,48,61	0.30	0
158	3PE	T8	602	-	38,38,50	0.34	0	41,43,55	0.36	0
157	FES	fs	201	35	0,4,4	-	-	-	-	-
153	CDL	QB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
158	3PE	bm	302	-	29,29,50	0.39	0	32,34,55	0.46	0
162	SF4	s7	201	126	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	c	301	-	63,63,99	0.37	0	69,75,111	0.43	0
153	CDL	u	201	-	59,59,99	0.38	0	65,71,111	0.32	0
153	CDL	2o	101	-	49,49,99	0.41	0	55,61,111	0.35	0
153	CDL	m1	404	-	90,90,99	0.32	0	96,102,111	0.28	0
153	CDL	N	304	-	83,83,99	0.33	0	89,95,111	0.32	0
152	PC1	B9	201	-	33,33,53	0.38	0	39,41,61	0.52	0
152	PC1	7C	303	-	42,42,53	0.32	0	48,50,61	0.32	0
153	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
152	PC1	t4	303	-	53,53,53	0.30	0	59,61,61	0.35	0
152	PC1	Qg	401	-	31,31,53	0.36	0	37,39,61	0.33	0
157	FES	QE	302	-	0,4,4	-	-	-	-	-
152	PC1	f	402	-	37,37,53	0.34	0	43,45,61	0.28	0
153	CDL	E	401	-	59,59,99	0.37	0	65,71,111	0.34	0
153	CDL	2b	201	-	86,86,99	0.32	0	92,98,111	0.36	0
153	CDL	q	203	-	85,85,99	0.33	0	91,97,111	0.31	0
153	CDL	qG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
153	CDL	A1	101	-	65,65,99	0.36	0	71,77,111	0.33	0
157	FES	V2	300	147	0,4,4	-	-	-	-	-
152	PC1	N	303	-	35,35,53	0.34	0	41,43,61	0.33	0
153	CDL	b4	201	-	36,36,99	0.43	0	42,48,111	0.40	0
152	PC1	m1	401	-	53,53,53	0.29	0	59,61,61	0.28	0
152	PC1	V	201	-	34,34,53	0.35	0	40,42,61	0.32	0
152	PC1	I	301	-	38,38,53	0.34	0	44,46,61	0.32	0
153	CDL	m	306	-	65,65,99	0.36	0	71,77,111	0.31	0
153	CDL	p1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	t1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
152	PC1	n5	804	-	38,38,53	0.33	0	44,46,61	0.32	0
152	PC1	6c	203	-	32,32,53	0.36	0	38,40,61	0.35	0
152	PC1	qc	509	-	46,46,53	0.31	0	52,54,61	0.34	0
153	CDL	a	502	-	50,50,99	0.41	0	56,62,111	0.47	0
153	CDL	B4	201	-	36,36,99	0.43	0	42,48,111	0.40	0
153	CDL	qH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
153	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.34	0
171	FMN	v1	501	-	33,33,33	0.20	0	48,50,50	0.42	0
152	PC1	qE	301	-	23,23,53	0.40	0	29,31,61	0.36	0
153	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.32	0
153	CDL	A9	402	-	75,75,99	0.34	0	81,87,111	0.35	0
152	PC1	fs	204	-	39,39,53	0.34	0	45,47,61	0.27	0
153	CDL	qB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
157	FES	FS	203	35	0,4,4	-	-	-	-	-
152	PC1	b9	201	-	33,33,53	0.38	0	39,41,61	0.52	0
153	CDL	6a	201	-	73,73,99	0.35	0	79,85,111	0.41	0
153	CDL	W	202	-	83,83,99	0.33	0	89,95,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	a	505	-	81,81,99	0.33	0	87,93,111	0.29	0
153	CDL	z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	TE	101	-	52,52,99	0.40	0	58,64,111	0.33	0
158	3PE	N5	802	-	35,35,50	0.36	0	38,40,55	0.31	0
153	CDL	q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
152	PC1	d	501	-	34,34,53	0.36	0	40,42,61	0.38	0
153	CDL	td	101	-	65,65,99	0.36	0	71,77,111	0.33	0
153	CDL	R	201	-	64,64,99	0.36	0	70,76,111	0.31	0
153	CDL	6c	202	-	81,81,99	0.32	0	87,93,111	0.30	0
152	PC1	qb	602	-	42,42,53	0.32	0	48,50,61	0.30	0
153	CDL	2k	101	-	97,97,99	0.31	0	103,109,111	0.35	0
167	NDP	a9	401	-	45,52,52	0.52	0	53,80,80	0.54	1 (1%)
171	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.42	0
153	CDL	qb	601	-	67,67,99	0.36	0	73,79,111	0.30	0
152	PC1	QG	401	-	31,31,53	0.37	0	37,39,61	0.40	0
152	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.34	0
153	CDL	2G	203	-	54,54,99	0.39	0	60,66,111	0.36	0
162	SF4	s8	302	127	0,12,12	-	-	-	-	-
152	PC1	m2	402	-	31,31,53	0.36	0	37,39,61	0.38	0
152	PC1	C3	606	-	48,48,53	0.31	0	54,56,61	0.35	0
152	PC1	n	302	-	31,31,53	0.36	0	37,39,61	0.32	0
153	CDL	a1	101	-	66,66,99	0.36	0	72,78,111	0.37	0
152	PC1	qg	401	-	31,31,53	0.36	0	37,39,61	0.33	0
153	CDL	U	201	-	59,59,99	0.38	0	65,71,111	0.32	0
153	CDL	2g	204	-	62,62,99	0.37	0	68,74,111	0.32	0
153	CDL	fs	203	-	46,46,99	0.42	0	52,58,111	0.35	0
153	CDL	7C	302	-	50,50,99	0.40	0	56,62,111	0.35	0
158	3PE	an	301	-	44,44,50	0.32	0	47,49,55	0.27	0
152	PC1	Qe	303	-	42,42,53	0.33	0	48,50,61	0.44	0
152	PC1	S8	301	-	29,29,53	0.38	0	35,37,61	0.33	0
153	CDL	E	403	-	62,62,99	0.37	0	68,74,111	0.30	0
152	PC1	N5	805	-	53,53,53	0.29	0	59,61,61	0.32	0
153	CDL	r	201	-	64,64,99	0.36	0	70,76,111	0.31	0
153	CDL	AN	302	-	86,86,99	0.32	0	92,98,111	0.29	0
152	PC1	qI	201	-	29,29,53	0.38	0	35,37,61	0.32	0
152	PC1	qC	508	-	35,35,53	0.35	0	41,43,61	0.34	0
152	PC1	Qc	506	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	N5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
154	HEA	c1	708	29	57,67,67	2.02	18 (31%)	61,103,103	2.76	26 (42%)
152	PC1	N1	301	-	35,35,53	0.35	0	41,43,61	0.33	0
169	T7X	b6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.08	4 (6%)
152	PC1	N	301	-	40,40,53	0.33	0	46,48,61	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	FS	201	-	39,39,53	0.34	0	45,47,61	0.27	0
170	ADP	b9	202	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
152	PC1	2f	301	-	46,46,53	0.32	0	52,54,61	0.50	0
158	3PE	g2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
164	U10	b8	301	-	63,63,63	2.15	21 (33%)	76,79,79	1.68	21 (27%)
153	CDL	C1	708	-	62,62,99	0.37	0	68,74,111	0.39	0
152	PC1	T4	301	-	47,47,53	0.31	0	53,55,61	0.36	0
152	PC1	Qb	602	-	42,42,53	0.32	0	48,50,61	0.30	0
153	CDL	qI	203	-	70,70,99	0.35	0	76,82,111	0.31	0
153	CDL	B3	101	-	57,57,99	0.38	0	63,69,111	0.32	0
153	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.29	0
153	CDL	Qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
158	3PE	AN	303	-	44,44,50	0.32	0	47,49,55	0.29	0
152	PC1	Qj	101	-	35,35,53	0.35	0	41,43,61	0.32	0
153	CDL	M	301	-	65,65,99	0.36	0	71,77,111	0.31	0
152	PC1	qC	507	-	49,49,53	0.30	0	55,57,61	0.30	0
157	FES	qe	302	-	0,4,4	-	-	-	-	-
158	3PE	S8	304	-	40,40,50	0.33	0	43,45,55	0.31	0
152	PC1	a	501	-	40,40,53	0.34	0	46,48,61	0.35	0
162	SF4	S8	302	127	0,12,12	-	-	-	-	-
157	FES	fs	202	35	0,4,4	-	-	-	-	-
153	CDL	QG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
153	CDL	e	401	-	59,59,99	0.37	0	65,71,111	0.34	0
152	PC1	C1	711	-	38,38,53	0.34	0	44,46,61	0.32	0
152	PC1	n5	805	-	53,53,53	0.29	0	59,61,61	0.32	0
153	CDL	AM	201	-	55,55,99	0.39	0	61,67,111	0.33	0
152	PC1	5B	202	-	46,46,53	0.32	0	52,54,61	0.28	0
152	PC1	v	201	-	34,34,53	0.35	0	40,42,61	0.31	0
164	U10	qc	507	-	29,29,63	2.68	11 (37%)	35,38,79	1.53	7 (20%)
151	HEC	qD	401	111	32,50,50	2.03	4 (12%)	24,82,82	2.31	14 (58%)
152	PC1	w	205	-	42,42,53	0.32	0	48,50,61	0.30	0
153	CDL	qD	402	-	60,60,99	0.37	0	66,72,111	0.31	0
153	CDL	6A	201	-	73,73,99	0.35	0	79,85,111	0.41	0
153	CDL	U1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
152	PC1	AN	304	-	35,35,53	0.36	0	41,43,61	0.33	0
153	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.34	0
157	FES	fx	201	95	0,4,4	-	-	-	-	-
152	PC1	w	204	-	33,33,53	0.36	0	39,41,61	0.34	0
152	PC1	AM	202	-	38,38,53	0.34	0	44,46,61	0.31	0
153	CDL	TH	200	-	83,83,99	0.32	0	89,95,111	0.28	0
153	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
158	3PE	ta	201	-	25,25,50	0.41	0	28,30,55	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.34	0
152	PC1	J1	400	-	39,39,53	0.33	0	45,47,61	0.33	0
153	CDL	t5	301	-	95,95,99	0.31	0	101,107,111	0.31	0
153	CDL	I	302	-	76,76,99	0.33	0	82,88,111	0.31	0
151	HEC	Qd	401	111	32,50,50	2.03	4 (12%)	24,82,82	2.27	14 (58%)
157	FES	FS	202	35	0,4,4	-	-	-	-	-
153	CDL	2M	101	-	95,95,99	0.31	0	101,107,111	0.30	0
158	3PE	an	306	-	28,28,50	0.40	0	31,33,55	0.42	0
153	CDL	2G	204	-	62,62,99	0.37	0	68,74,111	0.32	0
152	PC1	qj	101	-	35,35,53	0.35	0	41,43,61	0.32	0
153	CDL	QD	402	-	60,60,99	0.37	0	66,72,111	0.31	0
164	U10	SC	102	-	63,63,63	2.17	21 (33%)	76,79,79	1.65	20 (26%)
152	PC1	tc	102	-	46,46,53	0.31	0	52,54,61	0.30	0
153	CDL	C1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
153	CDL	B8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
166	HEM	QC	502	110	41,50,50	1.25	3 (7%)	45,82,82	1.67	10 (22%)
153	CDL	an	302	-	86,86,99	0.32	0	92,98,111	0.29	0
152	PC1	M2	402	-	31,31,53	0.36	0	37,39,61	0.38	0
153	CDL	AL	301	-	52,52,99	0.40	0	58,64,111	0.33	0
158	3PE	M3	402	-	37,37,50	0.35	0	40,42,55	0.31	0
158	3PE	T4	302	-	24,24,50	0.42	0	27,29,55	0.36	0
152	PC1	n5	801	-	51,51,53	0.30	0	57,59,61	0.29	0
152	PC1	C1	710	-	37,37,53	0.34	0	43,45,61	0.31	0
166	HEM	qC	501	110	41,50,50	1.22	4 (9%)	45,82,82	1.68	9 (20%)
152	PC1	C3	601	-	51,51,53	0.30	0	57,59,61	0.34	0
153	CDL	q	202	-	71,71,99	0.35	0	77,83,111	0.30	0
152	PC1	c3	606	-	48,48,53	0.31	0	54,56,61	0.35	0
152	PC1	M	303	-	44,44,53	0.32	0	50,52,61	0.37	0
152	PC1	F	401	-	37,37,53	0.34	0	43,45,61	0.28	0
152	PC1	m	301	-	44,44,53	0.32	0	50,52,61	0.37	0
158	3PE	an	305	-	32,32,50	0.37	0	35,37,55	0.34	0
158	3PE	n5	802	-	35,35,50	0.36	0	38,40,55	0.31	0
153	CDL	P1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
152	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.32	0
153	CDL	M3	401	-	62,62,99	0.37	0	68,74,111	0.32	0
152	PC1	al	302	-	25,25,53	0.40	0	31,33,61	0.37	0
158	3PE	G2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
152	PC1	M2	407	-	45,45,53	0.32	0	51,53,61	0.37	0
152	PC1	2f	303	-	31,31,53	0.37	0	37,39,61	0.31	0
152	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.30	0
164	U10	qc	501	-	25,25,63	2.22	5 (20%)	27,29,79	1.83	8 (29%)
158	3PE	I	304	-	31,31,50	0.37	0	34,36,55	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	vb	701	-	61,61,99	0.37	0	67,73,111	0.32	0
153	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.33	0
153	CDL	f	401	-	99,99,99	0.30	0	105,111,111	0.29	0
153	CDL	m2	404	-	73,73,99	0.35	0	79,85,111	0.34	0
157	FES	s1	803	120	0,4,4	-	-	-	-	-
153	CDL	qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
152	PC1	W	205	-	42,42,53	0.32	0	48,50,61	0.29	0
152	PC1	Qe	301	-	32,32,53	0.36	0	38,40,61	0.34	0
158	3PE	m2	408	-	30,30,50	0.38	0	33,35,55	0.36	0
152	PC1	P1	401	-	39,39,53	0.33	0	45,47,61	0.30	0
152	PC1	Qc	509	-	46,46,53	0.31	0	52,54,61	0.34	0
158	3PE	a3	201	-	44,44,50	0.33	0	47,49,55	0.55	1 (2%)
152	PC1	c3	605	-	38,38,53	0.33	0	44,46,61	0.32	0
152	PC1	v	202	-	48,48,53	0.31	0	54,56,61	0.32	0
152	PC1	w	201	-	48,48,53	0.30	0	54,56,61	0.29	0
158	3PE	AN	301	-	44,44,50	0.32	0	47,49,55	0.28	0
152	PC1	c2	703	-	35,35,53	0.35	0	41,43,61	0.31	0
152	PC1	6a	202	-	34,34,53	0.36	0	40,42,61	0.34	0
152	PC1	m1	403	-	41,41,53	0.33	0	47,49,61	0.38	0
153	CDL	Y5	201	-	69,69,99	0.35	0	75,81,111	0.30	0
152	PC1	qc	506	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	b3	102	-	81,81,99	0.33	0	87,93,111	0.30	0
152	PC1	qI	202	-	42,42,53	0.32	0	48,50,61	0.31	0
158	3PE	n4	601	-	35,35,50	0.35	0	38,40,55	0.36	0
162	SF4	v1	500	146	0,12,12	-	-	-	-	-
153	CDL	T1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
152	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.31	0
153	CDL	M3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
162	SF4	S1	802	120	0,12,12	-	-	-	-	-
158	3PE	t8	601	-	46,46,50	0.33	0	49,51,55	0.40	0
153	CDL	qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
152	PC1	qi	201	-	29,29,53	0.39	0	35,37,61	0.41	0
151	HEC	qd	401	111	32,50,50	2.03	4 (12%)	24,82,82	2.28	14 (58%)
152	PC1	qE	303	-	38,38,53	0.34	0	44,46,61	0.32	0
153	CDL	c1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
151	HEC	QD	401	111	32,50,50	2.02	4 (12%)	24,82,82	2.30	14 (58%)
153	CDL	BM	301	-	85,85,99	0.32	0	91,97,111	0.30	0
152	PC1	7a	202	-	44,44,53	0.31	0	50,52,61	0.31	0
152	PC1	p1	401	-	39,39,53	0.33	0	45,47,61	0.30	0
158	3PE	c4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
152	PC1	M2	405	-	53,53,53	0.30	0	59,61,61	0.26	0
153	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.31	0
153	CDL	B3	102	-	81,81,99	0.33	0	87,93,111	0.29	0
153	CDL	C1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
153	CDL	Qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
153	CDL	T	204	-	89,89,99	0.33	0	95,101,111	0.32	0
153	CDL	VB	706	-	66,66,99	0.36	0	72,78,111	0.30	0
152	PC1	n3	201	-	30,30,53	0.37	0	36,38,61	0.36	0
152	PC1	TC	101	-	41,41,53	0.32	0	47,49,61	0.28	0
153	CDL	VB	703	-	85,85,99	0.33	0	91,97,111	0.31	0
158	3PE	s8	304	-	40,40,50	0.33	0	43,45,55	0.31	0
166	HEM	y5	203	-	41,50,50	1.21	4 (9%)	45,82,82	1.70	7 (15%)
152	PC1	6A	202	-	34,34,53	0.36	0	40,42,61	0.34	0
153	CDL	7c	302	-	50,50,99	0.40	0	56,62,111	0.35	0
153	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
153	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
152	PC1	m2	407	-	45,45,53	0.32	0	51,53,61	0.37	0
170	ADP	B9	202	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
153	CDL	c4	401	-	97,97,99	0.30	0	103,109,111	0.31	0
152	PC1	2f	302	-	41,41,53	0.33	0	47,49,61	0.40	0
152	PC1	QE	303	-	38,38,53	0.34	0	44,46,61	0.32	0
153	CDL	qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
158	3PE	vb	705	-	27,27,50	0.39	0	30,32,55	0.34	0
153	CDL	a	504	-	93,93,99	0.31	0	99,105,111	0.27	0
152	PC1	QI	202	-	42,42,53	0.32	0	48,50,61	0.31	0
153	CDL	Qb	601	-	67,67,99	0.36	0	73,79,111	0.30	0
153	CDL	c3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
152	PC1	m	307	-	35,35,53	0.35	0	41,43,61	0.33	0
152	PC1	m2	405	-	53,53,53	0.30	0	59,61,61	0.26	0
153	CDL	y5	201	-	69,69,99	0.35	0	75,81,111	0.30	0
152	PC1	2j	201	-	41,41,53	0.33	0	47,49,61	0.36	0
153	CDL	u1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
153	CDL	m2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
153	CDL	a9	403	-	86,86,99	0.32	0	92,98,111	0.27	0
152	PC1	W	204	-	33,33,53	0.36	0	39,41,61	0.34	0
162	SF4	S8	303	127	0,12,12	-	-	-	-	-
153	CDL	qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
153	CDL	M	305	-	82,82,99	0.33	0	88,94,111	0.31	0
153	CDL	QC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
152	PC1	M	307	-	34,34,53	0.35	0	40,42,61	0.34	0
160	PX2	Y5	204	-	20,20,35	1.28	4 (20%)	24,25,40	1.25	2 (8%)
153	CDL	P1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
166	HEM	Qc	502	110	41,50,50	1.22	4 (9%)	45,82,82	1.67	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	D	501	-	34,34,53	0.36	0	40,42,61	0.38	0
153	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.33	0
161	FAD	sa	701	-	53,58,58	0.48	0	68,89,89	0.52	2 (2%)
158	3PE	BM	302	-	29,29,50	0.39	0	32,34,55	0.46	0
152	PC1	qJ	101	-	37,37,53	0.34	0	43,45,61	0.36	0
152	PC1	QC	508	-	35,35,53	0.35	0	41,43,61	0.34	0
153	CDL	2g	203	-	54,54,99	0.39	0	60,66,111	0.36	0
152	PC1	te	102	-	31,31,53	0.37	0	37,39,61	0.40	0
153	CDL	M1	404	-	90,90,99	0.32	0	96,102,111	0.28	0
164	U10	B8	301	-	63,63,63	2.15	21 (33%)	76,79,79	1.68	21 (27%)
153	CDL	SD	101	-	75,75,99	0.34	0	81,87,111	0.31	0
158	3PE	t4	302	-	24,24,50	0.42	0	27,29,55	0.36	0
153	CDL	A1	102	-	66,66,99	0.36	0	72,78,111	0.37	0
161	FAD	SA	701	-	53,58,58	0.48	0	68,89,89	0.52	2 (2%)
152	PC1	TC	102	-	46,46,53	0.31	0	52,54,61	0.30	0
152	PC1	s8	301	-	29,29,53	0.38	0	35,37,61	0.33	0
153	CDL	VB	705	-	81,81,99	0.33	0	87,93,111	0.29	0
153	CDL	e	402	-	71,71,99	0.35	0	77,83,111	0.35	0
153	CDL	bm	301	-	85,85,99	0.32	0	91,97,111	0.30	0
154	HEA	c1	702	29	57,67,67	2.04	17 (29%)	61,103,103	2.75	29 (47%)
153	CDL	6C	203	-	81,81,99	0.32	0	87,93,111	0.30	0
153	CDL	7A	201	-	99,99,99	0.30	0	105,111,111	0.28	0
157	FES	SB	401	53	0,4,4	-	-	-	-	-
158	3PE	M2	408	-	30,30,50	0.38	0	33,35,55	0.36	0
153	CDL	M2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
157	FES	qE	302	-	0,4,4	-	-	-	-	-
152	PC1	V	202	-	48,48,53	0.31	0	54,56,61	0.32	0
153	CDL	e	403	-	62,62,99	0.37	0	68,74,111	0.30	0
153	CDL	2g	201	-	88,88,99	0.32	0	94,100,111	0.28	0
153	CDL	VB	701	-	61,61,99	0.37	0	67,73,111	0.32	0
166	HEM	Qc	503	110	41,50,50	1.25	3 (7%)	45,82,82	1.70	10 (22%)
153	CDL	T5	301	-	95,95,99	0.31	0	101,107,111	0.31	0
152	PC1	W	201	-	48,48,53	0.30	0	54,56,61	0.29	0
158	3PE	AN	305	-	32,32,50	0.37	0	35,37,55	0.34	0
158	3PE	a3	202	-	43,43,50	0.32	0	46,48,55	0.29	0
169	T7X	B6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.08	4 (6%)
162	SF4	sb	402	53	0,12,12	-	-	-	-	-
157	FES	v2	300	147	0,4,4	-	-	-	-	-
152	PC1	n1	301	-	35,35,53	0.35	0	41,43,61	0.33	0
151	HEC	2e	401	2	32,50,50	2.04	4 (12%)	24,82,82	2.40	13 (54%)
153	CDL	QC	503	-	63,63,99	0.37	0	69,75,111	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	m	305	-	34,34,53	0.35	0	40,42,61	0.33	0
152	PC1	t1	602	-	32,32,53	0.36	0	38,40,61	0.34	0
152	PC1	7A	202	-	44,44,53	0.31	0	50,52,61	0.31	0
153	CDL	al	301	-	52,52,99	0.40	0	58,64,111	0.33	0
153	CDL	m3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
153	CDL	b8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
152	PC1	c1	704	-	48,48,53	0.31	0	54,56,61	0.27	0
159	P5S	M2	406	-	34,35,53	1.34	4 (11%)	38,42,60	1.04	2 (5%)
152	PC1	A	503	-	40,40,53	0.34	0	46,48,61	0.35	0
153	CDL	Q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
153	CDL	F	402	-	99,99,99	0.30	0	105,111,111	0.29	0
152	PC1	2F	301	-	46,46,53	0.32	0	52,54,61	0.50	0
152	PC1	C3	605	-	38,38,53	0.33	0	44,46,61	0.32	0
151	HEC	2E	401	2	32,50,50	2.10	6 (18%)	24,82,82	2.34	14 (58%)
160	PX2	r	202	-	32,32,35	1.02	4 (12%)	36,37,40	0.98	2 (5%)
153	CDL	M	306	-	63,63,99	0.36	0	69,75,111	0.32	0
160	PX2	y5	204	-	20,20,35	1.28	4 (20%)	24,25,40	1.26	2 (8%)
152	PC1	5b	202	-	46,46,53	0.32	0	52,54,61	0.28	0
153	CDL	C	301	-	63,63,99	0.37	0	69,75,111	0.43	0
153	CDL	n6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
152	PC1	Qi	201	-	29,29,53	0.39	0	35,37,61	0.41	0
152	PC1	c1	707	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	Qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
166	HEM	qc	502	110	41,50,50	1.23	4 (9%)	45,82,82	1.67	8 (17%)
152	PC1	qi	203	-	41,41,53	0.33	0	47,49,61	0.35	0
158	3PE	SC	101	-	39,39,50	0.34	0	42,44,55	0.30	0
153	CDL	m	303	-	82,82,99	0.33	0	88,94,111	0.30	0
152	PC1	C4	403	-	40,40,53	0.33	0	46,48,61	0.30	0
153	CDL	n5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
164	U10	sc	102	-	63,63,63	2.18	21 (33%)	76,79,79	1.64	20 (26%)
152	PC1	2F	303	-	31,31,53	0.37	0	37,39,61	0.31	0
152	PC1	M1	403	-	41,41,53	0.33	0	47,49,61	0.38	0
152	PC1	n	303	-	35,35,53	0.35	0	41,43,61	0.32	0
153	CDL	2G	201	-	88,88,99	0.32	0	94,100,111	0.28	0
158	3PE	m3	402	-	37,37,50	0.35	0	40,42,55	0.31	0
153	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.29	0
152	PC1	T4	303	-	53,53,53	0.30	0	59,61,61	0.35	0
158	3PE	sc	101	-	39,39,50	0.34	0	42,44,55	0.31	0
164	U10	qC	506	-	29,29,63	2.68	10 (34%)	35,38,79	1.55	7 (20%)
162	SF4	S1	801	120	0,12,12	-	-	-	-	-
158	3PE	A3	201	-	44,44,50	0.33	0	47,49,55	0.55	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
158	3PE	AN	306	-	28,28,50	0.40	0	31,33,55	0.42	0
153	CDL	c1	703	-	64,64,99	0.36	0	70,76,111	0.31	0
153	CDL	A	504	-	93,93,99	0.31	0	99,105,111	0.27	0
152	PC1	6C	201	-	32,32,53	0.36	0	38,40,61	0.35	0
152	PC1	am	202	-	38,38,53	0.33	0	44,46,61	0.32	0
163	F3S	SB	403	53	0,9,9	-	-	-		
157	FES	FX	201	95	0,4,4	-	-	-		
158	3PE	w	203	-	33,33,50	0.36	0	36,38,55	0.31	0
158	3PE	i	303	-	31,31,50	0.37	0	34,36,55	0.32	0
153	CDL	sd	101	-	75,75,99	0.34	0	81,87,111	0.31	0
152	PC1	2F	302	-	41,41,53	0.33	0	47,49,61	0.40	0
153	CDL	m3	401	-	62,62,99	0.37	0	68,74,111	0.32	0
153	CDL	am	201	-	55,55,99	0.39	0	61,67,111	0.33	0
158	3PE	Y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
152	PC1	C2	701	-	35,35,53	0.35	0	41,43,61	0.31	0
158	3PE	b4	202	-	47,47,50	0.32	0	50,52,55	0.28	0
152	PC1	2G	202	-	49,49,53	0.31	0	55,57,61	0.40	0
152	PC1	TE	102	-	31,31,53	0.37	0	37,39,61	0.40	0
153	CDL	t	204	-	89,89,99	0.33	0	95,101,111	0.32	0
153	CDL	7A	203	-	61,61,99	0.37	0	67,73,111	0.34	0
158	3PE	TA	201	-	25,25,50	0.41	0	28,30,55	0.40	0
152	PC1	c1	706	-	44,44,53	0.32	0	50,52,61	0.42	0
152	PC1	tc	101	-	41,41,53	0.32	0	47,49,61	0.28	0
153	CDL	i	301	-	76,76,99	0.33	0	82,88,111	0.31	0
153	CDL	QH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
152	PC1	C1	709	-	44,44,53	0.32	0	50,52,61	0.42	0
152	PC1	qB	602	-	43,43,53	0.32	0	49,51,61	0.29	0
160	PX2	Qh	201	-	35,35,35	0.98	4 (11%)	39,40,40	1.02	2 (5%)
153	CDL	2O	101	-	49,49,99	0.41	0	55,61,111	0.35	0
154	HEA	C1	703	29	57,67,67	2.08	17 (29%)	61,103,103	2.72	22 (36%)
163	F3S	sb	403	53	0,9,9	-	-	-		
153	CDL	M	304	-	63,63,99	0.37	0	69,75,111	0.31	0
152	PC1	a	503	-	40,40,53	0.34	0	46,48,61	0.35	0
152	PC1	qG	401	-	31,31,53	0.37	0	37,39,61	0.40	0
153	CDL	6C	202	-	74,74,99	0.34	0	80,86,111	0.32	0
153	CDL	m1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
153	CDL	b3	101	-	57,57,99	0.38	0	63,69,111	0.32	0
162	SF4	V1	500	146	0,12,12	-	-	-		
153	CDL	m	302	-	63,63,99	0.37	0	69,75,111	0.31	0
152	PC1	C1	706	-	48,48,53	0.31	0	54,56,61	0.27	0
153	CDL	T7	201	-	72,72,99	0.34	0	78,84,111	0.29	0
167	NDP	A9	401	-	45,52,52	0.52	0	53,80,80	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
164	U10	Qc	507	-	29,29,63	2.68	11 (37%)	35,38,79	1.53	7 (20%)
153	CDL	t7	201	-	72,72,99	0.35	0	78,84,111	0.29	0
158	3PE	B4	202	-	47,47,50	0.32	0	50,52,55	0.28	0
152	PC1	N5	801	-	51,51,53	0.30	0	57,59,61	0.29	0
168	ZMP	ab	201	80	33,36,36	0.67	1 (3%)	42,45,45	0.75	0
153	CDL	Q	202	-	71,71,99	0.35	0	77,83,111	0.30	0
153	CDL	A	502	-	50,50,99	0.41	0	56,62,111	0.47	0
164	U10	QC	506	-	29,29,63	2.68	10 (34%)	35,38,79	1.55	7 (20%)
152	PC1	n6	301	-	53,53,53	0.29	0	59,61,61	0.29	0
153	CDL	Y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
164	U10	Qc	501	-	25,25,63	2.22	5 (20%)	27,29,79	1.84	8 (29%)
153	CDL	qC	503	-	63,63,99	0.37	0	69,75,111	0.31	0
166	HEM	QC	501	110	41,50,50	1.22	4 (9%)	45,82,82	1.68	8 (17%)
153	CDL	Qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
152	PC1	c1	711	-	38,38,53	0.34	0	44,46,61	0.32	0
166	HEM	qc	503	110	41,50,50	1.25	3 (7%)	45,82,82	1.70	10 (22%)
152	PC1	QE	301	-	23,23,53	0.40	0	29,31,61	0.36	0
153	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
153	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
152	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.34	0
152	PC1	Qi	203	-	41,41,53	0.33	0	47,49,61	0.35	0
152	PC1	qE	304	-	27,27,53	0.39	0	33,35,61	0.43	0
153	CDL	7a	201	-	99,99,99	0.30	0	105,111,111	0.28	0
157	FES	Qe	302	-	0,4,4	-	-	-	-	-
153	CDL	2K	101	-	97,97,99	0.31	0	103,109,111	0.35	0
153	CDL	I	303	-	74,74,99	0.34	0	80,86,111	0.29	0
158	3PE	T8	601	-	46,46,50	0.33	0	49,51,55	0.40	0
152	PC1	N5	803	-	52,52,53	0.29	0	58,60,61	0.29	0
157	FES	sb	401	53	0,4,4	-	-	-	-	-
153	CDL	N6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
158	3PE	A3	202	-	43,43,50	0.32	0	46,48,55	0.29	0
158	3PE	VB	707	-	27,27,50	0.39	0	30,32,55	0.34	0
153	CDL	w	202	-	83,83,99	0.33	0	89,95,111	0.33	0
153	CDL	t	201	-	58,58,99	0.38	0	64,70,111	0.32	0
153	CDL	2B	201	-	86,86,99	0.32	0	92,98,111	0.36	0
153	CDL	y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
153	CDL	m	304	-	63,63,99	0.36	0	69,75,111	0.32	0
153	CDL	n	304	-	83,83,99	0.33	0	89,95,111	0.32	0
152	PC1	QI	201	-	29,29,53	0.38	0	35,37,61	0.32	0
152	PC1	qe	303	-	42,42,53	0.33	0	48,50,61	0.44	0
152	PC1	t4	301	-	47,47,53	0.31	0	53,55,61	0.36	0
153	CDL	a9	402	-	75,75,99	0.34	0	81,87,111	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	2g	202	-	49,49,53	0.31	0	55,57,61	0.40	0
158	3PE	an	303	-	44,44,50	0.32	0	47,49,55	0.29	0
153	CDL	FS	204	-	46,46,99	0.42	0	52,58,111	0.35	0
153	CDL	th	200	-	83,83,99	0.32	0	89,95,111	0.28	0
152	PC1	AL	302	-	25,25,53	0.40	0	31,33,61	0.37	0
159	P5S	m2	406	-	34,35,53	1.34	4 (11%)	38,42,60	1.04	2 (5%)
152	PC1	C3	602	-	38,38,53	0.34	0	44,46,61	0.30	0
152	PC1	QJ	102	-	37,37,53	0.34	0	43,45,61	0.36	0
153	CDL	C4	401	-	97,97,99	0.30	0	103,109,111	0.30	0
152	PC1	M	302	-	35,35,53	0.35	0	41,43,61	0.33	0
158	3PE	y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
153	CDL	Z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
158	3PE	W	203	-	33,33,50	0.36	0	36,38,55	0.31	0
152	PC1	A	501	-	40,40,53	0.34	0	46,48,61	0.35	0
158	3PE	t8	602	-	38,38,50	0.34	0	41,43,55	0.36	0
158	3PE	N4	601	-	35,35,50	0.35	0	38,40,55	0.36	0
153	CDL	7a	203	-	61,61,99	0.37	0	67,73,111	0.34	0
153	CDL	qC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
162	SF4	SB	402	53	0,12,12	-	-	-	-	-
152	PC1	QC	507	-	49,49,53	0.30	0	55,57,61	0.29	0
162	SF4	s1	801	120	0,12,12	-	-	-	-	-
152	PC1	QJ	101	-	27,27,53	0.39	0	33,35,61	0.43	0
160	PX2	R	202	-	32,32,35	1.01	4 (12%)	36,37,40	0.91	2 (5%)
152	PC1	M1	401	-	53,53,53	0.29	0	59,61,61	0.28	0
166	HEM	qC	502	110	41,50,50	1.25	3 (7%)	45,82,82	1.67	10 (22%)
152	PC1	j1	400	-	39,39,53	0.33	0	45,47,61	0.33	0
154	HEA	C1	702	29	57,67,67	2.03	16 (28%)	61,103,103	2.64	27 (44%)
152	PC1	n	301	-	40,40,53	0.33	0	46,48,61	0.29	0
168	ZMP	AB	201	80	33,36,36	0.67	1 (3%)	42,45,45	0.75	0
153	CDL	2m	101	-	95,95,99	0.31	0	101,107,111	0.30	0
153	CDL	6c	201	-	74,74,99	0.34	0	80,86,111	0.32	0
162	SF4	s1	802	120	0,12,12	-	-	-	-	-
153	CDL	QI	203	-	70,70,99	0.35	0	76,82,111	0.30	0
153	CDL	qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
153	CDL	Qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
153	CDL	C3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
160	PX2	qh	201	-	35,35,35	0.98	4 (11%)	39,40,40	0.99	2 (5%)
152	PC1	qC	505	-	37,37,53	0.34	0	43,45,61	0.29	0
153	CDL	te	101	-	52,52,99	0.40	0	58,64,111	0.33	0
153	CDL	c1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
152	PC1	N5	804	-	38,38,53	0.33	0	44,46,61	0.32	0
162	SF4	S7	201	126	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	5B	201	-	80,80,99	0.34	0	86,92,111	0.33	0
153	CDL	E	402	-	71,71,99	0.35	0	77,83,111	0.34	0
152	PC1	QC	505	-	37,37,53	0.34	0	43,45,61	0.29	0
153	CDL	p1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
153	CDL	m1	405	-	56,56,99	0.38	0	62,68,111	0.37	0
152	PC1	an	304	-	35,35,53	0.36	0	41,43,61	0.33	0
153	CDL	vb	704	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
152	PC1	2J	201	-	41,41,53	0.33	0	47,49,61	0.36	0
152	PC1	qe	301	-	32,32,53	0.36	0	38,40,61	0.34	0
152	PC1	N	302	-	31,31,53	0.36	0	37,39,61	0.32	0
153	CDL	A9	403	-	86,86,99	0.32	0	92,98,111	0.27	0
166	HEM	Y5	203	-	41,50,50	1.21	4 (9%)	45,82,82	1.70	7 (15%)
152	PC1	N3	201	-	30,30,53	0.37	0	36,38,61	0.36	0
152	PC1	N6	301	-	53,53,53	0.29	0	59,61,61	0.29	0
152	PC1	QB	602	-	43,43,53	0.32	0	49,51,61	0.29	0
153	CDL	t	203	-	70,70,99	0.35	0	76,82,111	0.32	0
157	FES	S1	803	120	0,4,4	-	-	-	-	-
152	PC1	i	304	-	38,38,53	0.34	0	44,46,61	0.32	0
153	CDL	M1	405	-	56,56,99	0.38	0	62,68,111	0.37	0
153	CDL	i	302	-	74,74,99	0.34	0	80,86,111	0.29	0
153	CDL	T	203	-	70,70,99	0.35	0	76,82,111	0.32	0
158	3PE	C4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
153	CDL	5b	201	-	80,80,99	0.34	0	86,92,111	0.33	0
162	SF4	s8	303	127	0,12,12	-	-	-	-	-
153	CDL	c1	709	-	62,62,99	0.37	0	68,74,111	0.39	0
152	PC1	T1	602	-	32,32,53	0.36	0	38,40,61	0.34	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
152	PC1	n5	803	-	-	9/56/56/57	-
153	CDL	T	201	-	-	12/69/69/110	-
152	PC1	c4	403	-	-	5/44/44/57	-
158	3PE	T8	602	-	-	11/42/42/54	-
157	FES	fs	201	35	-	-	0/1/1/1
153	CDL	QB	601	-	-	12/78/78/110	-
158	3PE	bm	302	-	-	8/33/33/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
162	SF4	s7	201	126	-	-	0/6/5/5
153	CDL	c	301	-	-	13/74/74/110	-
153	CDL	u	201	-	-	12/70/70/110	-
153	CDL	2o	101	-	-	19/60/60/110	-
153	CDL	m1	404	-	-	17/101/101/110	-
153	CDL	N	304	-	-	33/94/94/110	-
152	PC1	B9	201	-	-	13/37/37/57	-
152	PC1	7C	303	-	-	7/46/46/57	-
153	CDL	M2	403	-	-	19/76/76/110	-
152	PC1	t4	303	-	-	12/57/57/57	-
152	PC1	Qg	401	-	-	7/35/35/57	-
157	FES	QE	302	-	-	-	0/1/1/1
152	PC1	f	402	-	-	9/41/41/57	-
153	CDL	E	401	-	-	15/70/70/110	-
153	CDL	2b	201	-	-	17/97/97/110	-
153	CDL	q	203	-	-	16/96/96/110	-
153	CDL	qG	402	-	-	18/96/96/110	-
153	CDL	A1	101	-	-	17/76/76/110	-
157	FES	V2	300	147	-	-	0/1/1/1
152	PC1	N	303	-	-	6/39/39/57	-
153	CDL	b4	201	-	-	9/44/44/110	-
152	PC1	m1	401	-	-	14/57/57/57	-
152	PC1	V	201	-	-	4/38/38/57	-
152	PC1	I	301	-	-	10/42/42/57	-
153	CDL	m	306	-	-	15/76/76/110	-
153	CDL	p1	402	-	-	19/73/73/110	-
153	CDL	t1	601	-	-	12/65/65/110	-
152	PC1	n5	804	-	-	12/42/42/57	-
152	PC1	6c	203	-	-	8/36/36/57	-
152	PC1	qc	509	-	-	11/50/50/57	-
153	CDL	a	502	-	-	17/61/61/110	-
153	CDL	B4	201	-	-	9/44/44/110	-
153	CDL	qH	201	-	-	13/104/104/110	-
153	CDL	T	202	-	-	14/85/85/110	-
171	FMN	v1	501	-	-	2/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	qE	301	-	-	8/26/26/57	-
153	CDL	B	501	-	-	16/72/72/110	-
153	CDL	A9	402	-	-	17/86/86/110	-
152	PC1	fs	204	-	-	6/43/43/57	-
153	CDL	qB	601	-	-	12/78/78/110	-
157	FES	FS	203	35	-	-	0/1/1/1
152	PC1	b9	201	-	-	13/37/37/57	-
153	CDL	6a	201	-	-	21/84/84/110	-
153	CDL	W	202	-	-	17/94/94/110	-
153	CDL	a	505	-	-	20/92/92/110	-
153	CDL	z	101	-	-	13/77/77/110	-
153	CDL	TE	101	-	-	18/63/63/110	-
158	3PE	N5	802	-	-	7/39/39/54	-
153	CDL	q	201	-	-	13/73/73/110	-
152	PC1	d	501	-	-	15/38/38/57	-
153	CDL	td	101	-	-	18/76/76/110	-
153	CDL	R	201	-	-	25/75/75/110	-
153	CDL	6c	202	-	-	16/92/92/110	-
152	PC1	qb	602	-	-	8/46/46/57	-
153	CDL	2k	101	-	-	32/108/108/110	-
167	NDP	a9	401	-	-	8/30/77/77	0/5/5/5
171	FMN	V1	501	-	-	2/18/18/18	0/3/3/3
153	CDL	qb	601	-	-	9/78/78/110	-
152	PC1	QG	401	-	-	6/35/35/57	-
152	PC1	c3	601	-	-	10/55/55/57	-
153	CDL	2G	203	-	-	11/65/65/110	-
162	SF4	s8	302	127	-	-	0/6/5/5
152	PC1	m2	402	-	-	12/35/35/57	-
152	PC1	C3	606	-	-	7/52/52/57	-
152	PC1	n	302	-	-	10/35/35/57	-
153	CDL	a1	101	-	-	14/77/77/110	-
152	PC1	qg	401	-	-	6/35/35/57	-
153	CDL	U	201	-	-	12/70/70/110	-
153	CDL	2g	204	-	-	16/73/73/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	fs	203	-	-	11/57/57/110	-
153	CDL	7C	302	-	-	11/61/61/110	-
158	3PE	an	301	-	-	6/48/48/54	-
152	PC1	Qe	303	-	-	12/46/46/57	-
152	PC1	S8	301	-	-	9/33/33/57	-
153	CDL	E	403	-	-	13/73/73/110	-
152	PC1	N5	805	-	-	16/57/57/57	-
153	CDL	r	201	-	-	25/75/75/110	-
153	CDL	AN	302	-	-	18/97/97/110	-
152	PC1	qI	201	-	-	6/33/33/57	-
152	PC1	qC	508	-	-	10/39/39/57	-
152	PC1	Qc	506	-	-	15/41/41/57	-
153	CDL	N5	806	-	-	21/100/100/110	-
154	HEA	c1	708	29	-	15/32/76/76	-
152	PC1	N1	301	-	-	8/39/39/57	-
169	T7X	b6	201	-	-	25/50/74/80	0/1/1/1
152	PC1	N	301	-	-	5/44/44/57	-
152	PC1	FS	201	-	-	6/43/43/57	-
170	ADP	b9	202	-	-	4/12/32/32	0/3/3/3
152	PC1	2f	301	-	-	21/50/50/57	-
158	3PE	g2	301	-	-	15/54/54/54	-
164	U10	b8	301	-	-	13/63/87/87	0/1/1/1
153	CDL	C1	708	-	-	25/73/73/110	-
152	PC1	T4	301	-	-	18/51/51/57	-
152	PC1	Qb	602	-	-	8/46/46/57	-
153	CDL	qI	203	-	-	17/81/81/110	-
153	CDL	B3	101	-	-	14/68/68/110	-
153	CDL	j	301	-	-	16/80/80/110	-
153	CDL	Qc	508	-	-	12/57/57/110	-
158	3PE	AN	303	-	-	8/48/48/54	-
152	PC1	Qj	101	-	-	11/39/39/57	-
153	CDL	M	301	-	-	15/76/76/110	-
152	PC1	qC	507	-	-	12/53/53/57	-
157	FES	qe	302	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	S8	304	-	-	8/44/44/54	-
152	PC1	a	501	-	-	10/44/44/57	-
162	SF4	S8	302	127	-	-	0/6/5/5
157	FES	fs	202	35	-	-	0/1/1/1
153	CDL	QG	402	-	-	17/96/96/110	-
153	CDL	e	401	-	-	15/70/70/110	-
152	PC1	C1	711	-	-	12/42/42/57	-
152	PC1	n5	805	-	-	16/57/57/57	-
153	CDL	AM	201	-	-	12/66/66/110	-
152	PC1	5B	202	-	-	12/50/50/57	-
152	PC1	v	201	-	-	4/38/38/57	-
164	U10	qc	507	-	-	9/23/47/87	0/1/1/1
151	HEC	qD	401	111	-	4/10/54/54	-
152	PC1	w	205	-	-	6/46/46/57	-
153	CDL	qD	402	-	-	17/71/71/110	-
153	CDL	6A	201	-	-	21/84/84/110	-
153	CDL	U1	101	-	-	14/67/67/110	-
152	PC1	AN	304	-	-	9/39/39/57	-
153	CDL	t	202	-	-	14/85/85/110	-
157	FES	fx	201	95	-	-	0/1/1/1
152	PC1	w	204	-	-	7/37/37/57	-
152	PC1	AM	202	-	-	8/42/42/57	-
153	CDL	TH	200	-	-	17/94/94/110	-
153	CDL	M2	404	-	-	11/84/84/110	-
158	3PE	ta	201	-	-	10/29/29/54	-
152	PC1	C3	603	-	-	8/34/34/57	-
152	PC1	J1	400	-	-	10/43/43/57	-
153	CDL	t5	301	-	-	27/106/106/110	-
153	CDL	I	302	-	-	17/87/87/110	-
151	HEC	Qd	401	111	-	4/10/54/54	-
157	FES	FS	202	35	-	-	0/1/1/1
153	CDL	2M	101	-	-	17/106/106/110	-
158	3PE	an	306	-	-	6/32/32/54	-
153	CDL	2G	204	-	-	15/73/73/110	-
152	PC1	qj	101	-	-	11/39/39/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	QD	402	-	-	17/71/71/110	-
164	U10	SC	102	-	-	12/63/87/87	0/1/1/1
152	PC1	tc	102	-	-	15/50/50/57	-
153	CDL	C1	701	-	-	22/89/89/110	-
153	CDL	B8	302	-	-	11/79/79/110	-
166	HEM	QC	502	110	-	6/12/54/54	-
153	CDL	an	302	-	-	18/97/97/110	-
152	PC1	M2	402	-	-	12/35/35/57	-
153	CDL	AL	301	-	-	16/63/63/110	-
158	3PE	M3	402	-	-	8/41/41/54	-
158	3PE	T4	302	-	-	4/28/28/54	-
152	PC1	n5	801	-	-	11/55/55/57	-
152	PC1	C1	710	-	-	7/41/41/57	-
166	HEM	qC	501	110	-	5/12/54/54	-
152	PC1	C3	601	-	-	10/55/55/57	-
153	CDL	q	202	-	-	20/82/82/110	-
152	PC1	c3	606	-	-	7/52/52/57	-
152	PC1	M	303	-	-	15/48/48/57	-
152	PC1	F	401	-	-	9/41/41/57	-
152	PC1	m	301	-	-	15/48/48/57	-
158	3PE	an	305	-	-	5/36/36/54	-
158	3PE	n5	802	-	-	9/39/39/54	-
153	CDL	P1	402	-	-	19/73/73/110	-
152	PC1	7c	303	-	-	7/46/46/57	-
153	CDL	M3	401	-	-	8/73/73/110	-
152	PC1	al	302	-	-	2/29/29/57	-
158	3PE	G2	301	-	-	15/54/54/54	-
152	PC1	M2	407	-	-	10/49/49/57	-
152	PC1	2f	303	-	-	10/35/35/57	-
152	PC1	c3	602	-	-	13/42/42/57	-
164	U10	qc	501	-	-	9/28/28/87	-
158	3PE	I	304	-	-	9/35/35/54	-
153	CDL	vb	701	-	-	15/72/72/110	-
153	CDL	7C	301	-	-	23/95/95/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	f	401	-	-	17/110/110/110	-
153	CDL	m2	404	-	-	11/84/84/110	-
157	FES	s1	803	120	-	-	0/1/1/1
153	CDL	qc	505	-	-	17/66/66/110	-
152	PC1	W	205	-	-	6/46/46/57	-
152	PC1	Qe	301	-	-	6/36/36/57	-
158	3PE	m2	408	-	-	9/34/34/54	-
152	PC1	P1	401	-	-	10/43/43/57	-
152	PC1	Qc	509	-	-	11/50/50/57	-
158	3PE	a3	201	-	-	13/48/48/54	-
152	PC1	c3	605	-	-	3/42/42/57	-
152	PC1	v	202	-	-	13/52/52/57	-
152	PC1	w	201	-	-	16/52/52/57	-
158	3PE	AN	301	-	-	7/48/48/54	-
152	PC1	c2	703	-	-	11/39/39/57	-
152	PC1	6a	202	-	-	12/38/38/57	-
152	PC1	m1	403	-	-	7/45/45/57	-
153	CDL	Y5	201	-	-	15/80/80/110	-
152	PC1	qc	506	-	-	15/41/41/57	-
153	CDL	b3	102	-	-	21/92/92/110	-
152	PC1	qI	202	-	-	5/46/46/57	-
158	3PE	n4	601	-	-	10/39/39/54	-
162	SF4	v1	500	146	-	-	0/6/5/5
153	CDL	T1	601	-	-	12/65/65/110	-
152	PC1	J	302	-	-	7/40/40/57	-
153	CDL	M3	403	-	-	14/65/65/110	-
162	SF4	S1	802	120	-	-	0/6/5/5
158	3PE	t8	601	-	-	12/50/50/54	-
153	CDL	qc	504	-	-	21/74/74/110	-
152	PC1	qi	201	-	-	8/33/33/57	-
151	HEC	qd	401	111	-	4/10/54/54	-
152	PC1	qE	303	-	-	2/42/42/57	-
153	CDL	c1	701	-	-	22/89/89/110	-
151	HEC	QD	401	111	-	4/10/54/54	-
153	CDL	BM	301	-	-	24/96/96/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	7a	202	-	-	13/48/48/57	-
152	PC1	p1	401	-	-	10/43/43/57	-
158	3PE	c4	402	-	-	8/54/54/54	-
152	PC1	M2	405	-	-	9/57/57/57	-
153	CDL	b	501	-	-	16/72/72/110	-
152	PC1	j	302	-	-	7/40/40/57	-
153	CDL	B3	102	-	-	19/92/92/110	-
153	CDL	C1	712	-	-	16/105/105/110	-
153	CDL	Qc	505	-	-	17/66/66/110	-
153	CDL	T	204	-	-	30/100/100/110	-
153	CDL	VB	706	-	-	16/77/77/110	-
152	PC1	n3	201	-	-	4/34/34/57	-
152	PC1	TC	101	-	-	7/45/45/57	-
153	CDL	VB	703	-	-	17/96/96/110	-
158	3PE	s8	304	-	-	8/44/44/54	-
166	HEM	y5	203	-	-	6/12/54/54	-
152	PC1	6A	202	-	-	12/38/38/57	-
153	CDL	7c	302	-	-	11/61/61/110	-
153	CDL	m2	403	-	-	19/76/76/110	-
153	CDL	L	301	-	-	24/84/84/110	-
152	PC1	m2	407	-	-	10/49/49/57	-
170	ADP	B9	202	-	-	4/12/32/32	0/3/3/3
153	CDL	c4	401	-	-	23/108/108/110	-
152	PC1	2f	302	-	-	8/45/45/57	-
152	PC1	QE	303	-	-	2/42/42/57	-
153	CDL	qg	402	-	-	23/110/110/110	-
158	3PE	vb	705	-	-	10/31/31/54	-
153	CDL	a	504	-	-	15/104/104/110	-
152	PC1	QI	202	-	-	7/46/46/57	-
153	CDL	Qb	601	-	-	9/78/78/110	-
153	CDL	c3	604	-	-	7/78/78/110	-
152	PC1	m	307	-	-	12/39/39/57	-
152	PC1	m2	405	-	-	9/57/57/57	-
153	CDL	y5	201	-	-	15/80/80/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	2j	201	-	-	13/45/45/57	-
153	CDL	u1	101	-	-	14/67/67/110	-
153	CDL	m2	401	-	-	15/64/64/110	-
153	CDL	a9	403	-	-	20/97/97/110	-
152	PC1	W	204	-	-	7/37/37/57	-
162	SF4	S8	303	127	-	-	0/6/5/5
153	CDL	qi	202	-	-	14/81/81/110	-
153	CDL	M	305	-	-	11/93/93/110	-
153	CDL	QC	504	-	-	11/66/66/110	-
152	PC1	M	307	-	-	10/38/38/57	-
160	PX2	Y5	204	-	-	13/22/22/37	-
153	CDL	P1	403	-	-	15/68/68/110	-
166	HEM	Qc	502	110	-	2/12/54/54	-
152	PC1	D	501	-	-	15/38/38/57	-
153	CDL	7c	301	-	-	22/95/95/110	-
161	FAD	sa	701	-	-	10/30/50/50	0/6/6/6
158	3PE	BM	302	-	-	8/33/33/54	-
152	PC1	qJ	101	-	-	13/41/41/57	-
152	PC1	QC	508	-	-	10/39/39/57	-
153	CDL	2g	203	-	-	11/65/65/110	-
152	PC1	te	102	-	-	10/35/35/57	-
153	CDL	M1	404	-	-	17/101/101/110	-
164	U10	B8	301	-	-	12/63/87/87	0/1/1/1
153	CDL	SD	101	-	-	18/86/86/110	-
158	3PE	t4	302	-	-	4/28/28/54	-
153	CDL	A1	102	-	-	15/77/77/110	-
161	FAD	SA	701	-	-	10/30/50/50	0/6/6/6
152	PC1	TC	102	-	-	15/50/50/57	-
152	PC1	s8	301	-	-	9/33/33/57	-
153	CDL	VB	705	-	-	20/92/92/110	-
153	CDL	e	402	-	-	20/82/82/110	-
153	CDL	bm	301	-	-	23/96/96/110	-
154	HEA	c1	702	29	-	10/32/76/76	-
153	CDL	6C	203	-	-	16/92/92/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	7A	201	-	-	16/110/110/110	-
157	FES	SB	401	53	-	-	0/1/1/1
158	3PE	M2	408	-	-	9/34/34/54	-
153	CDL	M2	401	-	-	15/64/64/110	-
157	FES	qE	302	-	-	-	0/1/1/1
152	PC1	V	202	-	-	13/52/52/57	-
153	CDL	e	403	-	-	13/73/73/110	-
153	CDL	2g	201	-	-	19/99/99/110	-
153	CDL	VB	701	-	-	15/72/72/110	-
166	HEM	Qc	503	110	-	7/12/54/54	-
153	CDL	T5	301	-	-	27/106/106/110	-
152	PC1	W	201	-	-	16/52/52/57	-
158	3PE	AN	305	-	-	6/36/36/54	-
158	3PE	a3	202	-	-	12/47/47/54	-
169	T7X	B6	201	-	-	25/50/74/80	0/1/1/1
162	SF4	sb	402	53	-	-	0/6/5/5
157	FES	v2	300	147	-	-	0/1/1/1
152	PC1	n1	301	-	-	8/39/39/57	-
151	HEC	2e	401	2	-	7/10/54/54	-
153	CDL	QC	503	-	-	9/74/74/110	-
152	PC1	m	305	-	-	10/38/38/57	-
152	PC1	t1	602	-	-	13/36/36/57	-
152	PC1	7A	202	-	-	13/48/48/57	-
153	CDL	al	301	-	-	16/63/63/110	-
153	CDL	m3	403	-	-	14/65/65/110	-
153	CDL	b8	302	-	-	11/79/79/110	-
152	PC1	c1	704	-	-	14/52/52/57	-
159	P5S	M2	406	-	-	29/41/41/59	-
152	PC1	A	503	-	-	7/44/44/57	-
153	CDL	Q	201	-	-	13/73/73/110	-
153	CDL	F	402	-	-	19/110/110/110	-
152	PC1	2F	301	-	-	21/50/50/57	-
152	PC1	C3	605	-	-	3/42/42/57	-
151	HEC	2E	401	2	-	7/10/54/54	-
160	PX2	r	202	-	-	23/34/34/37	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	M	306	-	-	12/74/74/110	-
160	PX2	y5	204	-	-	12/22/22/37	-
152	PC1	5b	202	-	-	12/50/50/57	-
153	CDL	C	301	-	-	14/74/74/110	-
153	CDL	n6	302	-	-	19/100/100/110	-
152	PC1	Qi	201	-	-	8/33/33/57	-
152	PC1	c1	707	-	-	7/41/41/57	-
153	CDL	Qg	402	-	-	23/110/110/110	-
166	HEM	qc	502	110	-	2/12/54/54	-
152	PC1	qi	203	-	-	14/45/45/57	-
158	3PE	SC	101	-	-	10/43/43/54	-
153	CDL	m	303	-	-	11/93/93/110	-
152	PC1	C4	403	-	-	5/44/44/57	-
153	CDL	n5	806	-	-	21/100/100/110	-
164	U10	sc	102	-	-	12/63/87/87	0/1/1/1
152	PC1	2F	303	-	-	10/35/35/57	-
152	PC1	M1	403	-	-	7/45/45/57	-
152	PC1	n	303	-	-	7/39/39/57	-
153	CDL	2G	201	-	-	19/99/99/110	-
158	3PE	m3	402	-	-	8/41/41/54	-
153	CDL	J	301	-	-	16/80/80/110	-
152	PC1	T4	303	-	-	12/57/57/57	-
158	3PE	sc	101	-	-	10/43/43/54	-
164	U10	qC	506	-	-	6/23/47/87	0/1/1/1
162	SF4	S1	801	120	-	-	0/6/5/5
158	3PE	A3	201	-	-	12/48/48/54	-
158	3PE	AN	306	-	-	6/32/32/54	-
153	CDL	c1	703	-	-	8/75/75/110	-
153	CDL	A	504	-	-	15/104/104/110	-
152	PC1	6C	201	-	-	8/36/36/57	-
152	PC1	am	202	-	-	8/42/42/57	-
163	F3S	SB	403	53	-	-	0/3/3/3
157	FES	FX	201	95	-	-	0/1/1/1
158	3PE	w	203	-	-	15/37/37/54	-
158	3PE	i	303	-	-	9/35/35/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	sd	101	-	-	18/86/86/110	-
152	PC1	2F	302	-	-	8/45/45/57	-
153	CDL	m3	401	-	-	8/73/73/110	-
153	CDL	am	201	-	-	11/66/66/110	-
158	3PE	Y5	202	-	-	8/31/31/54	-
152	PC1	C2	701	-	-	11/39/39/57	-
158	3PE	b4	202	-	-	11/51/51/54	-
152	PC1	2G	202	-	-	12/53/53/57	-
152	PC1	TE	102	-	-	10/35/35/57	-
153	CDL	t	204	-	-	30/100/100/110	-
153	CDL	7A	203	-	-	12/72/72/110	-
158	3PE	TA	201	-	-	10/29/29/54	-
152	PC1	c1	706	-	-	8/48/48/57	-
152	PC1	tc	101	-	-	7/45/45/57	-
153	CDL	i	301	-	-	17/87/87/110	-
153	CDL	QH	201	-	-	13/104/104/110	-
152	PC1	C1	709	-	-	8/48/48/57	-
152	PC1	qB	602	-	-	6/47/47/57	-
160	PX2	Qh	201	-	-	21/37/37/37	-
153	CDL	2O	101	-	-	19/60/60/110	-
154	HEA	C1	703	29	-	13/32/76/76	-
163	F3S	sb	403	53	-	-	0/3/3/3
153	CDL	M	304	-	-	11/74/74/110	-
152	PC1	a	503	-	-	7/44/44/57	-
152	PC1	qG	401	-	-	6/35/35/57	-
153	CDL	6C	202	-	-	29/85/85/110	-
153	CDL	m1	402	-	-	15/76/76/110	-
153	CDL	b3	101	-	-	14/68/68/110	-
162	SF4	V1	500	146	-	-	0/6/5/5
153	CDL	m	302	-	-	11/74/74/110	-
152	PC1	C1	706	-	-	14/52/52/57	-
153	CDL	T7	201	-	-	17/83/83/110	-
167	NDP	A9	401	-	-	8/30/77/77	0/5/5/5
164	U10	Qc	507	-	-	9/23/47/87	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	t7	201	-	-	16/83/83/110	-
158	3PE	B4	202	-	-	11/51/51/54	-
152	PC1	N5	801	-	-	11/55/55/57	-
168	ZMP	ab	201	80	-	21/43/43/43	-
153	CDL	Q	202	-	-	20/82/82/110	-
153	CDL	A	502	-	-	16/61/61/110	-
164	U10	QC	506	-	-	5/23/47/87	0/1/1/1
152	PC1	n6	301	-	-	13/57/57/57	-
153	CDL	Y7	501	-	-	14/75/75/110	-
164	U10	Qc	501	-	-	9/28/28/87	-
153	CDL	qC	503	-	-	9/74/74/110	-
166	HEM	QC	501	110	-	5/12/54/54	-
153	CDL	Qi	202	-	-	14/81/81/110	-
152	PC1	c1	711	-	-	12/42/42/57	-
166	HEM	qc	503	110	-	7/12/54/54	-
152	PC1	QE	301	-	-	8/26/26/57	-
153	CDL	M1	402	-	-	15/76/76/110	-
153	CDL	C1	707	-	-	8/75/75/110	-
152	PC1	c3	603	-	-	8/34/34/57	-
152	PC1	Qi	203	-	-	14/45/45/57	-
152	PC1	qE	304	-	-	10/31/31/57	-
153	CDL	7a	201	-	-	16/110/110/110	-
157	FES	Qe	302	-	-	-	0/1/1/1
153	CDL	2K	101	-	-	32/108/108/110	-
153	CDL	I	303	-	-	14/85/85/110	-
158	3PE	T8	601	-	-	12/50/50/54	-
152	PC1	N5	803	-	-	9/56/56/57	-
158	3PE	A3	202	-	-	11/47/47/54	-
153	CDL	N6	302	-	-	18/100/100/110	-
157	FES	sb	401	53	-	-	0/1/1/1
158	3PE	VB	707	-	-	10/31/31/54	-
153	CDL	w	202	-	-	16/94/94/110	-
153	CDL	t	201	-	-	13/69/69/110	-
153	CDL	2B	201	-	-	17/97/97/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	y7	501	-	-	13/75/75/110	-
153	CDL	m	304	-	-	12/74/74/110	-
153	CDL	n	304	-	-	33/94/94/110	-
152	PC1	QI	201	-	-	6/33/33/57	-
152	PC1	qe	303	-	-	13/46/46/57	-
152	PC1	t4	301	-	-	18/51/51/57	-
153	CDL	a9	402	-	-	17/86/86/110	-
152	PC1	2g	202	-	-	12/53/53/57	-
158	3PE	an	303	-	-	8/48/48/54	-
153	CDL	FS	204	-	-	10/57/57/110	-
153	CDL	th	200	-	-	17/94/94/110	-
152	PC1	AL	302	-	-	2/29/29/57	-
159	P5S	m2	406	-	-	29/41/41/59	-
152	PC1	C3	602	-	-	13/42/42/57	-
152	PC1	QJ	102	-	-	13/41/41/57	-
153	CDL	C4	401	-	-	23/108/108/110	-
152	PC1	M	302	-	-	12/39/39/57	-
158	3PE	y5	202	-	-	8/31/31/54	-
153	CDL	Z	101	-	-	13/77/77/110	-
158	3PE	W	203	-	-	15/37/37/54	-
152	PC1	A	501	-	-	10/44/44/57	-
158	3PE	t8	602	-	-	11/42/42/54	-
158	3PE	N4	601	-	-	9/39/39/54	-
153	CDL	7a	203	-	-	12/72/72/110	-
153	CDL	qC	504	-	-	11/66/66/110	-
162	SF4	SB	402	53	-	-	0/6/5/5
152	PC1	QC	507	-	-	12/53/53/57	-
162	SF4	s1	801	120	-	-	0/6/5/5
152	PC1	QJ	101	-	-	10/31/31/57	-
160	PX2	R	202	-	-	19/34/34/37	-
152	PC1	M1	401	-	-	14/57/57/57	-
166	HEM	qC	502	110	-	6/12/54/54	-
152	PC1	j1	400	-	-	10/43/43/57	-
154	HEA	C1	702	29	-	11/32/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	n	301	-	-	5/44/44/57	-
168	ZMP	AB	201	80	-	21/43/43/43	-
153	CDL	2m	101	-	-	17/106/106/110	-
153	CDL	6c	201	-	-	29/85/85/110	-
162	SF4	s1	802	120	-	-	0/6/5/5
153	CDL	QI	203	-	-	17/81/81/110	-
153	CDL	qc	508	-	-	12/57/57/110	-
153	CDL	Qc	504	-	-	21/74/74/110	-
153	CDL	C3	604	-	-	6/78/78/110	-
160	PX2	qh	201	-	-	17/37/37/37	-
152	PC1	qC	505	-	-	12/41/41/57	-
153	CDL	te	101	-	-	20/63/63/110	-
153	CDL	c1	712	-	-	17/105/105/110	-
152	PC1	N5	804	-	-	12/42/42/57	-
162	SF4	S7	201	126	-	-	0/6/5/5
153	CDL	5B	201	-	-	18/91/91/110	-
153	CDL	E	402	-	-	20/82/82/110	-
152	PC1	QC	505	-	-	12/41/41/57	-
153	CDL	p1	403	-	-	15/68/68/110	-
153	CDL	m1	405	-	-	15/67/67/110	-
152	PC1	an	304	-	-	9/39/39/57	-
153	CDL	vb	704	-	-	17/77/77/110	-
153	CDL	l	301	-	-	23/84/84/110	-
152	PC1	2J	201	-	-	13/45/45/57	-
152	PC1	qe	301	-	-	6/36/36/57	-
152	PC1	N	302	-	-	10/35/35/57	-
153	CDL	A9	403	-	-	20/97/97/110	-
166	HEM	Y5	203	-	-	6/12/54/54	-
152	PC1	N3	201	-	-	4/34/34/57	-
152	PC1	N6	301	-	-	13/57/57/57	-
152	PC1	QB	602	-	-	6/47/47/57	-
153	CDL	t	203	-	-	23/81/81/110	-
157	FES	S1	803	120	-	-	0/1/1/1
152	PC1	i	304	-	-	10/42/42/57	-
153	CDL	M1	405	-	-	15/67/67/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	i	302	-	-	14/85/85/110	-
153	CDL	T	203	-	-	23/81/81/110	-
158	3PE	C4	402	-	-	8/54/54/54	-
153	CDL	5b	201	-	-	18/91/91/110	-
162	SF4	s8	303	127	-	-	0/6/5/5
153	CDL	c1	709	-	-	25/73/73/110	-
152	PC1	T1	602	-	-	13/36/36/57	-

All (312) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	sc	102	U10	C6-C1	10.31	1.54	1.35
164	SC	102	U10	C6-C1	10.29	1.54	1.35
164	qc	507	U10	C6-C1	10.17	1.53	1.35
164	Qc	507	U10	C6-C1	10.17	1.53	1.35
164	qC	506	U10	C6-C1	10.11	1.53	1.35
164	QC	506	U10	C6-C1	10.10	1.53	1.35
164	b8	301	U10	C6-C1	10.06	1.53	1.35
164	B8	301	U10	C6-C1	10.06	1.53	1.35
164	Qc	501	U10	C6-C1	8.66	1.53	1.33
164	qc	501	U10	C6-C1	8.66	1.53	1.33
151	2E	401	HEC	C2B-C3B	-6.75	1.33	1.40
151	Qd	401	HEC	C3C-C2C	-6.44	1.34	1.40
151	qd	401	HEC	C3C-C2C	-6.43	1.34	1.40
151	qD	401	HEC	C3C-C2C	-6.41	1.34	1.40
151	QD	401	HEC	C3C-C2C	-6.38	1.34	1.40
151	2e	401	HEC	C3C-C2C	-6.33	1.34	1.40
151	2e	401	HEC	C2B-C3B	-6.33	1.34	1.40
151	2E	401	HEC	C3C-C2C	-6.31	1.34	1.40
151	qD	401	HEC	C2B-C3B	-6.18	1.34	1.40
151	QD	401	HEC	C2B-C3B	-6.18	1.34	1.40
151	Qd	401	HEC	C2B-C3B	-6.13	1.34	1.40
151	qd	401	HEC	C2B-C3B	-6.12	1.34	1.40
154	C1	703	HEA	C4B-NB	-6.05	1.29	1.40
154	c1	702	HEA	C3B-C2B	5.49	1.47	1.34
154	C1	702	HEA	C3B-C2B	5.35	1.46	1.34
169	B6	201	T7X	P1-O1	5.35	1.74	1.60
169	b6	201	T7X	P1-O1	5.34	1.74	1.60
154	c1	708	HEA	C3B-C2B	5.34	1.46	1.34
154	c1	702	HEA	C3A-C2A	5.24	1.47	1.40
154	C1	703	HEA	C3D-C2D	4.88	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
154	c1	708	HEA	C3A-C2A	4.69	1.46	1.40
154	C1	703	HEA	CHC-C4B	4.64	1.46	1.35
154	C1	702	HEA	C3A-C2A	4.55	1.46	1.40
154	C1	703	HEA	C3C-C2C	4.51	1.46	1.40
154	C1	702	HEA	CHC-C4B	4.42	1.46	1.35
164	qc	507	U10	C4-C3	4.34	1.54	1.36
164	Qc	507	U10	C4-C3	4.34	1.54	1.36
154	C1	703	HEA	C3B-C2B	4.33	1.44	1.34
164	QC	506	U10	C4-C3	4.33	1.53	1.36
164	qC	506	U10	C4-C3	4.32	1.53	1.36
154	c1	702	HEA	CHC-C4B	4.26	1.45	1.35
164	B8	301	U10	C4-C3	4.23	1.53	1.36
164	b8	301	U10	C4-C3	4.23	1.53	1.36
154	C1	702	HEA	C3D-C2D	4.22	1.45	1.36
154	c1	708	HEA	CHC-C4B	4.22	1.45	1.35
154	c1	702	HEA	C3D-C2D	4.16	1.45	1.36
154	c1	702	HEA	CHD-C1D	4.15	1.45	1.35
164	sc	102	U10	C4-C3	4.15	1.53	1.36
164	SC	102	U10	C4-C3	4.15	1.53	1.36
154	C1	702	HEA	C1D-ND	-4.06	1.33	1.40
154	C1	703	HEA	CHD-C1D	4.00	1.45	1.35
154	c1	708	HEA	C1D-ND	-3.99	1.33	1.40
169	B6	201	T7X	O16-C10	3.98	1.45	1.34
169	b6	201	T7X	O16-C10	3.98	1.45	1.34
154	C1	703	HEA	C3A-C2A	3.95	1.45	1.40
154	c1	702	HEA	C4B-NB	-3.92	1.33	1.40
154	C1	702	HEA	C4B-NB	-3.91	1.33	1.40
154	c1	702	HEA	C1D-ND	-3.85	1.33	1.40
154	C1	702	HEA	CHD-C1D	3.85	1.44	1.35
154	C1	702	HEA	C3C-C2C	3.84	1.45	1.40
154	c1	708	HEA	C3D-C2D	3.82	1.44	1.36
154	c1	708	HEA	C4B-NB	-3.74	1.33	1.40
166	qC	502	HEM	C4D-ND	-3.66	1.34	1.40
166	QC	502	HEM	C4D-ND	-3.66	1.34	1.40
166	qC	501	HEM	C4D-ND	-3.64	1.34	1.40
166	QC	501	HEM	C4D-ND	-3.64	1.34	1.40
166	qc	503	HEM	C4D-ND	-3.60	1.34	1.40
166	Qc	503	HEM	C4D-ND	-3.60	1.34	1.40
154	c1	708	HEA	CHD-C1D	3.59	1.44	1.35
154	C1	703	HEA	C1B-NB	-3.58	1.31	1.38
166	qc	502	HEM	C4D-ND	-3.56	1.34	1.40
166	Qc	502	HEM	C4D-ND	-3.56	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	Y5	203	HEM	C4D-ND	-3.53	1.34	1.40
166	y5	203	HEM	C4D-ND	-3.53	1.34	1.40
169	b6	201	T7X	O18-C11	3.51	1.43	1.33
169	B6	201	T7X	O18-C11	3.51	1.43	1.33
151	2E	401	HEC	CBC-CAC	-3.46	1.36	1.49
154	c1	708	HEA	C4B-C3B	3.39	1.50	1.44
151	qD	401	HEC	CBC-CAC	-3.38	1.36	1.49
151	2e	401	HEC	CBC-CAC	-3.38	1.36	1.49
151	Qd	401	HEC	CBC-CAC	-3.37	1.36	1.49
151	qd	401	HEC	CBC-CAC	-3.37	1.36	1.49
151	QD	401	HEC	CBC-CAC	-3.36	1.36	1.49
154	c1	702	HEA	C3C-C2C	3.35	1.45	1.40
154	c1	708	HEA	C3C-C2C	3.20	1.44	1.40
159	M2	406	P5S	O19-C17	3.19	1.42	1.33
159	m2	406	P5S	O19-C17	3.19	1.42	1.33
169	b6	201	T7X	P1-O13	3.17	1.72	1.59
169	B6	201	T7X	P1-O13	3.16	1.72	1.59
166	qc	503	HEM	C1B-NB	-3.15	1.34	1.40
166	Qc	503	HEM	C1B-NB	-3.15	1.34	1.40
164	sc	102	U10	C7-C8	3.13	1.55	1.50
166	qc	502	HEM	C1B-NB	-3.12	1.34	1.40
166	Qc	502	HEM	C1B-NB	-3.12	1.34	1.40
164	SC	102	U10	C7-C8	3.11	1.55	1.50
166	QC	502	HEM	C1B-NB	-3.09	1.35	1.40
166	qC	502	HEM	C1B-NB	-3.09	1.35	1.40
166	qC	501	HEM	C1B-NB	-3.07	1.35	1.40
166	QC	501	HEM	C1B-NB	-3.07	1.35	1.40
154	C1	703	HEA	FE-ND	3.04	2.11	1.96
154	c1	708	HEA	FE-ND	3.00	2.11	1.96
154	C1	702	HEA	FE-ND	3.00	2.11	1.96
164	QC	506	U10	C7-C8	3.00	1.55	1.50
166	Y5	203	HEM	C1B-NB	-3.00	1.35	1.40
164	qC	506	U10	C7-C8	3.00	1.55	1.50
166	y5	203	HEM	C1B-NB	-3.00	1.35	1.40
164	SC	102	U10	C41-C39	2.98	1.57	1.51
164	sc	102	U10	C41-C39	2.98	1.57	1.51
164	b8	301	U10	C41-C39	2.95	1.57	1.51
164	B8	301	U10	C41-C39	2.95	1.57	1.51
164	Qc	507	U10	C7-C8	2.91	1.54	1.50
164	qc	507	U10	C7-C8	2.90	1.54	1.50
164	b8	301	U10	C7-C8	2.90	1.54	1.50
164	B8	301	U10	C7-C8	2.89	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	sc	102	U10	C7-C6	2.88	1.56	1.51
164	SC	102	U10	C7-C6	2.88	1.56	1.51
154	C1	702	HEA	CAA-C2A	-2.87	1.47	1.52
154	C1	702	HEA	C1B-NB	-2.85	1.32	1.38
169	B6	201	T7X	C12-C10	2.84	1.59	1.50
169	b6	201	T7X	C12-C10	2.84	1.59	1.50
164	SC	102	U10	C26-C24	2.83	1.57	1.51
164	sc	102	U10	C26-C24	2.83	1.57	1.51
164	qC	506	U10	C7-C6	2.80	1.56	1.51
164	QC	506	U10	C7-C6	2.80	1.56	1.51
164	b8	301	U10	C26-C24	2.80	1.57	1.51
164	B8	301	U10	C26-C24	2.80	1.57	1.51
154	c1	702	HEA	C1B-NB	-2.76	1.33	1.38
154	c1	702	HEA	CAA-C2A	-2.74	1.47	1.52
164	sc	102	U10	C31-C29	2.74	1.57	1.51
164	SC	102	U10	C31-C29	2.74	1.57	1.51
159	M2	406	P5S	O37-C38	2.71	1.41	1.34
159	m2	406	P5S	O37-C38	2.70	1.41	1.34
154	C1	702	HEA	C4D-ND	-2.67	1.33	1.38
154	c1	702	HEA	FE-ND	2.67	2.10	1.96
164	SC	102	U10	C21-C19	2.66	1.56	1.51
164	Qc	507	U10	C7-C6	2.65	1.55	1.51
164	qc	507	U10	C7-C6	2.65	1.55	1.51
164	sc	102	U10	C21-C19	2.65	1.56	1.51
164	B8	301	U10	C31-C29	2.65	1.56	1.51
164	b8	301	U10	C31-C29	2.65	1.56	1.51
164	B8	301	U10	C21-C19	2.62	1.56	1.51
154	c1	708	HEA	C4D-ND	-2.62	1.33	1.38
164	b8	301	U10	C21-C19	2.62	1.56	1.51
164	sc	102	U10	O5-C5	-2.60	1.17	1.23
166	qc	503	HEM	C1D-ND	-2.59	1.33	1.38
164	SC	102	U10	O5-C5	-2.59	1.17	1.23
166	QC	502	HEM	C1D-ND	-2.59	1.33	1.38
166	Qc	503	HEM	C1D-ND	-2.58	1.33	1.38
166	qC	502	HEM	C1D-ND	-2.58	1.33	1.38
160	qh	201	PX2	O7-C2	-2.57	1.40	1.46
160	Y5	204	PX2	O7-C2	-2.57	1.40	1.46
164	b8	301	U10	O5-C5	-2.56	1.17	1.23
154	C1	703	HEA	O2D-CGD	-2.56	1.22	1.30
164	B8	301	U10	O5-C5	-2.56	1.17	1.23
154	c1	702	HEA	FE-NB	2.56	2.09	1.96
160	Qh	201	PX2	O7-C2	-2.55	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
154	C1	703	HEA	CMC-C2C	-2.54	1.46	1.51
164	B8	301	U10	C7-C6	2.54	1.55	1.51
160	y5	204	PX2	O7-C2	-2.54	1.40	1.46
164	b8	301	U10	C7-C6	2.54	1.55	1.51
164	SC	102	U10	C46-C44	2.53	1.56	1.51
164	sc	102	U10	C46-C44	2.53	1.56	1.51
154	c1	708	HEA	CAA-C2A	-2.52	1.47	1.52
164	qc	501	U10	C21-C19	2.51	1.56	1.51
166	qc	502	HEM	C1D-ND	-2.51	1.33	1.38
166	Qc	502	HEM	C1D-ND	-2.51	1.33	1.38
164	Qc	501	U10	C21-C19	2.50	1.56	1.51
159	M2	406	P5S	O37-C2	-2.50	1.40	1.46
159	m2	406	P5S	O37-C2	-2.49	1.40	1.46
164	qc	507	U10	O5-C5	-2.49	1.17	1.23
164	Qc	507	U10	O5-C5	-2.49	1.18	1.23
164	qC	506	U10	O5-C5	-2.48	1.18	1.23
164	QC	506	U10	O5-C5	-2.48	1.18	1.23
166	qC	501	HEM	C1D-ND	-2.47	1.33	1.38
166	QC	501	HEM	C1D-ND	-2.47	1.33	1.38
170	B9	202	ADP	C5-C4	2.47	1.47	1.40
164	sc	102	U10	C36-C34	2.47	1.56	1.51
164	SC	102	U10	C36-C34	2.47	1.56	1.51
170	b9	202	ADP	C5-C4	2.47	1.47	1.40
166	y5	203	HEM	C1D-ND	-2.46	1.33	1.38
166	Y5	203	HEM	C1D-ND	-2.45	1.33	1.38
164	b8	301	U10	C46-C44	2.45	1.56	1.51
164	B8	301	U10	C46-C44	2.44	1.56	1.51
164	b8	301	U10	C36-C34	2.44	1.56	1.51
154	c1	702	HEA	O2D-CGD	-2.44	1.22	1.30
164	B8	301	U10	C36-C34	2.44	1.56	1.51
154	C1	702	HEA	O2D-CGD	-2.44	1.22	1.30
168	AB	201	ZMP	C9-C10	-2.43	1.48	1.50
154	C1	702	HEA	O2A-CGA	-2.42	1.22	1.30
154	c1	708	HEA	O2A-CGA	-2.42	1.22	1.30
168	ab	201	ZMP	C9-C10	-2.41	1.48	1.50
164	B8	301	U10	O2-C2	-2.40	1.18	1.23
154	C1	703	HEA	C1C-CHC	2.39	1.47	1.41
164	b8	301	U10	O2-C2	-2.39	1.18	1.23
164	Qc	507	U10	C11-C9	2.39	1.56	1.51
164	qc	507	U10	C11-C9	2.39	1.56	1.51
160	Y5	204	PX2	O5-C4	2.37	1.40	1.33
164	QC	506	U10	C6-C5	2.37	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	qC	506	U10	C6-C5	2.37	1.53	1.46
154	c1	702	HEA	C4D-ND	-2.36	1.33	1.38
164	b8	301	U10	C51-C49	2.36	1.56	1.51
164	B8	301	U10	C51-C49	2.36	1.56	1.51
160	R	202	PX2	O5-C4	2.36	1.40	1.33
160	y5	204	PX2	O5-C4	2.35	1.40	1.33
160	qh	201	PX2	O5-C4	2.35	1.40	1.33
164	SC	102	U10	C51-C49	2.35	1.56	1.51
154	c1	702	HEA	O2A-CGA	-2.35	1.22	1.30
164	sc	102	U10	C51-C49	2.35	1.56	1.51
160	r	202	PX2	O5-C4	2.35	1.40	1.33
154	c1	708	HEA	O2D-CGD	-2.35	1.22	1.30
164	B8	301	U10	C11-C9	2.34	1.56	1.51
164	QC	506	U10	C11-C9	2.34	1.56	1.51
164	b8	301	U10	C11-C9	2.34	1.56	1.51
164	qC	506	U10	C11-C9	2.34	1.56	1.51
164	sc	102	U10	O2-C2	-2.33	1.18	1.23
154	C1	703	HEA	C4B-C3B	2.33	1.48	1.44
160	Qh	201	PX2	O5-C4	2.33	1.40	1.33
164	SC	102	U10	O2-C2	-2.32	1.18	1.23
154	c1	708	HEA	FE-NB	2.32	2.08	1.96
164	SC	102	U10	O3-C3M	-2.31	1.39	1.45
164	sc	102	U10	O3-C3M	-2.31	1.39	1.45
151	2E	401	HEC	CAD-C3D	2.30	1.55	1.52
151	Qd	401	HEC	CBB-CAB	-2.29	1.41	1.49
151	qd	401	HEC	CBB-CAB	-2.28	1.41	1.49
151	qD	401	HEC	CBB-CAB	-2.28	1.41	1.49
160	R	202	PX2	O7-C2	-2.28	1.40	1.46
151	QD	401	HEC	CBB-CAB	-2.27	1.41	1.49
160	r	202	PX2	O7-C2	-2.26	1.40	1.46
164	QC	506	U10	O2-C2	-2.26	1.18	1.23
164	qc	507	U10	C6-C5	2.26	1.53	1.46
164	qC	506	U10	O2-C2	-2.26	1.18	1.23
164	Qc	507	U10	C6-C5	2.26	1.53	1.46
164	sc	102	U10	C6-C5	2.26	1.53	1.46
164	qc	507	U10	C16-C14	2.26	1.56	1.51
164	Qc	507	U10	C16-C14	2.26	1.56	1.51
164	B8	301	U10	C6-C5	2.26	1.53	1.46
154	c1	708	HEA	C1B-NB	-2.26	1.34	1.38
164	b8	301	U10	C6-C5	2.26	1.53	1.46
164	b8	301	U10	C16-C14	2.25	1.56	1.51
164	qc	501	U10	C11-C9	2.25	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	SC	102	U10	C16-C14	2.25	1.56	1.51
164	sc	102	U10	C16-C14	2.25	1.56	1.51
164	B8	301	U10	C16-C14	2.25	1.56	1.51
164	Qc	507	U10	O2-C2	-2.24	1.18	1.23
164	qc	507	U10	O2-C2	-2.24	1.18	1.23
164	SC	102	U10	C6-C5	2.24	1.52	1.46
164	Qc	501	U10	C11-C9	2.24	1.56	1.51
160	R	202	PX2	O7-C16	2.24	1.40	1.34
151	2E	401	HEC	CBB-CAB	-2.24	1.41	1.49
151	2e	401	HEC	CBB-CAB	-2.24	1.41	1.49
160	r	202	PX2	O7-C16	2.24	1.40	1.34
164	B8	301	U10	C27-C28	2.22	1.57	1.50
164	b8	301	U10	C27-C28	2.22	1.57	1.50
159	m2	406	P5S	P12-O16	2.20	1.68	1.59
164	SC	102	U10	C11-C9	2.20	1.55	1.51
159	M2	406	P5S	P12-O16	2.20	1.68	1.59
164	SC	102	U10	C27-C28	2.20	1.57	1.50
164	sc	102	U10	C27-C28	2.20	1.57	1.50
164	b8	301	U10	O3-C3M	-2.19	1.40	1.45
154	C1	703	HEA	O2A-CGA	-2.19	1.23	1.30
164	B8	301	U10	O3-C3M	-2.19	1.40	1.45
154	c1	708	HEA	C4C-CHD	2.17	1.47	1.41
164	qC	506	U10	C16-C14	2.17	1.55	1.51
164	sc	102	U10	C11-C9	2.17	1.55	1.51
164	QC	506	U10	C16-C14	2.17	1.55	1.51
151	2E	401	HEC	CMD-C2D	2.17	1.56	1.51
154	C1	703	HEA	C2A-C1A	2.16	1.47	1.42
164	qc	501	U10	C22-C23	2.16	1.57	1.50
164	Qc	501	U10	C22-C23	2.16	1.57	1.50
160	Qh	201	PX2	O5-C3	-2.16	1.40	1.45
154	C1	703	HEA	C1D-ND	-2.15	1.36	1.40
164	QC	506	U10	O3-C3M	-2.15	1.40	1.45
164	qC	506	U10	O3-C3M	-2.14	1.40	1.45
164	Qc	507	U10	O3-C3M	-2.13	1.40	1.45
164	qc	507	U10	O3-C3M	-2.13	1.40	1.45
154	C1	702	HEA	C4C-CHD	2.13	1.46	1.41
164	sc	102	U10	C22-C23	2.13	1.57	1.50
164	SC	102	U10	C22-C23	2.13	1.57	1.50
160	R	202	PX2	O5-C3	-2.12	1.40	1.45
160	r	202	PX2	O5-C3	-2.12	1.40	1.45
160	y5	204	PX2	O5-C3	-2.12	1.40	1.45
160	y5	204	PX2	O7-C16	2.12	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	b8	301	U10	C22-C23	2.11	1.57	1.50
164	B8	301	U10	C22-C23	2.11	1.57	1.50
154	C1	703	HEA	FE-NB	2.11	2.07	1.96
160	Y5	204	PX2	O5-C3	-2.11	1.40	1.45
160	Qh	201	PX2	O7-C16	2.10	1.40	1.34
160	Y5	204	PX2	O7-C16	2.09	1.40	1.34
166	y5	203	HEM	CHB-C1B	2.09	1.40	1.35
166	Y5	203	HEM	CHB-C1B	2.08	1.40	1.35
160	qh	201	PX2	O7-C16	2.08	1.40	1.34
164	SC	102	U10	C42-C43	2.08	1.57	1.50
164	sc	102	U10	C42-C43	2.08	1.57	1.50
160	qh	201	PX2	O5-C3	-2.07	1.40	1.45
154	c1	702	HEA	C4C-CHD	2.07	1.46	1.41
164	qc	507	U10	O4-C4M	-2.07	1.40	1.45
164	Qc	507	U10	O4-C4M	-2.07	1.40	1.45
166	QC	501	HEM	CHB-C1B	2.06	1.40	1.35
164	B8	301	U10	C42-C43	2.06	1.57	1.50
164	b8	301	U10	C42-C43	2.05	1.57	1.50
166	qC	501	HEM	CHB-C1B	2.05	1.40	1.35
154	C1	702	HEA	FE-NB	2.05	2.07	1.96
164	qc	501	U10	C16-C14	2.05	1.55	1.51
166	qc	502	HEM	CHB-C1B	2.05	1.40	1.35
164	Qc	501	U10	C16-C14	2.04	1.55	1.51
166	Qc	502	HEM	CHB-C1B	2.04	1.40	1.35
154	c1	708	HEA	CHB-C1B	2.02	1.46	1.41
164	b8	301	U10	O4-C4M	-2.02	1.40	1.45
164	B8	301	U10	O4-C4M	-2.01	1.40	1.45
154	c1	702	HEA	C1D-C2D	2.01	1.48	1.44
164	SC	102	U10	C17-C18	2.01	1.57	1.50
164	sc	102	U10	C17-C18	2.00	1.57	1.50

All (440) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
154	c1	702	HEA	CAD-CBD-CGD	-8.19	95.98	113.60
154	c1	708	HEA	CAD-CBD-CGD	-7.89	96.63	113.60
154	C1	702	HEA	CAD-CBD-CGD	-7.46	97.54	113.60
154	C1	703	HEA	CAD-CBD-CGD	-7.18	98.14	113.60
154	C1	703	HEA	C13-C12-C11	-6.58	104.46	114.35
154	c1	708	HEA	C13-C12-C11	-6.43	104.68	114.35
154	C1	703	HEA	C2B-C1B-NB	6.23	117.34	109.88
154	c1	702	HEA	C3D-C4D-ND	6.04	116.21	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
154	C1	703	HEA	CAA-CBA-CGA	-5.98	96.99	113.76
154	c1	708	HEA	C2B-C1B-NB	5.93	116.98	109.88
154	c1	702	HEA	C2D-C1D-ND	5.78	116.69	109.84
154	c1	708	HEA	CHB-C1B-C2B	-5.56	116.30	124.98
154	C1	703	HEA	CHB-C1B-C2B	-5.53	116.34	124.98
154	C1	702	HEA	C3B-C4B-NB	5.49	116.34	109.84
154	C1	702	HEA	C2B-C1B-NB	5.43	116.39	109.88
154	C1	702	HEA	CHB-C1B-C2B	-5.24	116.79	124.98
154	c1	702	HEA	C1D-C2D-C3D	-5.22	101.47	106.96
151	2e	401	HEC	CBD-CAD-C3D	4.95	121.07	112.62
154	C1	702	HEA	C3C-C4C-NC	4.81	115.43	109.21
154	c1	708	HEA	CAA-CBA-CGA	-4.78	100.35	113.76
166	y5	203	HEM	CHC-C4B-NB	4.77	129.61	124.43
166	Y5	203	HEM	CHC-C4B-NB	4.76	129.60	124.43
154	C1	703	HEA	C3C-C4C-NC	4.71	115.30	109.21
154	C1	702	HEA	C1D-C2D-C3D	-4.70	102.02	106.96
154	c1	708	HEA	CMC-C2C-C3C	4.66	133.39	124.68
154	c1	708	HEA	C3B-C4B-NB	4.60	115.29	109.84
154	c1	702	HEA	C2B-C1B-NB	4.52	115.30	109.88
151	2E	401	HEC	CBD-CAD-C3D	4.51	120.31	112.62
154	c1	702	HEA	CHA-C4D-C3D	-4.49	118.24	124.84
154	C1	702	HEA	C2D-C1D-ND	4.48	115.15	109.84
151	2e	401	HEC	CMD-C2D-C1D	-4.48	121.58	128.46
154	c1	702	HEA	CHB-C1B-C2B	-4.46	118.02	124.98
154	c1	702	HEA	C13-C12-C11	-4.43	107.69	114.35
166	qC	501	HEM	CHC-C4B-NB	4.43	129.24	124.43
166	QC	501	HEM	CHC-C4B-NB	4.42	129.24	124.43
166	qC	502	HEM	CHC-C4B-NB	4.41	129.22	124.43
166	QC	502	HEM	CHC-C4B-NB	4.41	129.22	124.43
154	c1	702	HEA	CAA-CBA-CGA	-4.40	101.42	113.76
166	qc	502	HEM	CHC-C4B-NB	4.38	129.19	124.43
166	Qc	502	HEM	CHC-C4B-NB	4.37	129.18	124.43
166	Qc	503	HEM	CHC-C4B-NB	4.36	129.17	124.43
166	qc	503	HEM	CHC-C4B-NB	4.36	129.17	124.43
154	C1	703	HEA	C1B-C2B-C3B	-4.32	101.63	106.80
169	B6	201	T7X	O16-C10-C12	4.25	120.66	111.50
169	b6	201	T7X	O16-C10-C12	4.24	120.65	111.50
154	C1	702	HEA	CAA-CBA-CGA	-4.22	101.92	113.76
154	c1	708	HEA	C3D-C4D-ND	4.19	114.41	110.36
151	qd	401	HEC	CMD-C2D-C1D	-4.15	122.08	128.46
151	Qd	401	HEC	CMD-C2D-C1D	-4.14	122.10	128.46
151	QD	401	HEC	CMD-C2D-C1D	-4.13	122.12	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
151	qD	401	HEC	CMD-C2D-C1D	-4.12	122.13	128.46
160	Qh	201	PX2	O7-C16-C17	4.08	120.29	111.50
166	qc	503	HEM	C4D-ND-C1D	4.06	109.26	105.07
160	y5	204	PX2	O7-C16-C17	4.06	120.24	111.50
154	C1	703	HEA	C2D-C1D-ND	4.05	114.64	109.84
166	Qc	503	HEM	C4D-ND-C1D	4.05	109.25	105.07
151	2E	401	HEC	CMD-C2D-C1D	-4.03	122.26	128.46
154	C1	703	HEA	C3B-C4B-NB	4.03	114.61	109.84
154	c1	708	HEA	C3C-C4C-NC	4.02	114.41	109.21
154	c1	702	HEA	C3C-C4C-NC	4.02	114.41	109.21
154	C1	703	HEA	C3D-C4D-ND	4.02	114.25	110.36
160	Y5	204	PX2	O7-C16-C17	4.01	120.13	111.50
154	C1	703	HEA	CMC-C2C-C3C	4.00	132.16	124.68
154	c1	708	HEA	C2D-C1D-ND	3.96	114.53	109.84
154	C1	702	HEA	C4B-C3B-C2B	-3.95	100.66	107.41
166	Y5	203	HEM	CHB-C1B-NB	3.89	129.18	124.38
166	y5	203	HEM	CHB-C1B-NB	3.88	129.17	124.38
160	qh	201	PX2	O7-C16-C17	3.88	119.86	111.50
166	qC	502	HEM	C4D-ND-C1D	3.87	109.07	105.07
154	C1	703	HEA	C1D-C2D-C3D	-3.87	102.89	106.96
151	Qd	401	HEC	CBD-CAD-C3D	3.86	119.21	112.62
151	qd	401	HEC	CBD-CAD-C3D	3.86	119.21	112.62
154	C1	702	HEA	C3D-C4D-ND	3.86	114.09	110.36
166	QC	502	HEM	C4D-ND-C1D	3.86	109.06	105.07
166	qc	503	HEM	CHB-C1B-NB	3.81	129.09	124.38
166	Qc	503	HEM	CHB-C1B-NB	3.81	129.09	124.38
151	qD	401	HEC	CBD-CAD-C3D	3.81	119.11	112.62
154	c1	708	HEA	C1D-C2D-C3D	-3.78	102.98	106.96
151	QD	401	HEC	CBD-CAD-C3D	3.75	119.02	112.62
166	Qc	502	HEM	CHB-C1B-NB	3.74	129.00	124.38
154	C1	702	HEA	CMC-C2C-C3C	3.73	131.66	124.68
166	qc	502	HEM	CHB-C1B-NB	3.73	128.99	124.38
159	m2	406	P5S	O37-C38-C39	3.71	119.50	111.50
159	M2	406	P5S	O37-C38-C39	3.71	119.49	111.50
164	Qc	501	U10	C12-C13-C14	-3.70	118.75	127.66
154	C1	702	HEA	C13-C12-C11	-3.68	108.81	114.35
166	qC	501	HEM	CHB-C1B-NB	3.68	128.93	124.38
160	r	202	PX2	O7-C16-C17	3.68	119.43	111.50
164	qc	501	U10	C12-C13-C14	-3.68	118.81	127.66
166	QC	501	HEM	CHB-C1B-NB	3.67	128.92	124.38
166	QC	502	HEM	CHB-C1B-NB	3.65	128.90	124.38
166	qC	502	HEM	CHB-C1B-NB	3.64	128.88	124.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
164	Qc	501	U10	C1M-C1-C2	3.63	120.14	115.98
164	Qc	507	U10	C7-C8-C9	-3.63	120.75	126.79
164	qc	507	U10	C7-C8-C9	-3.63	120.75	126.79
164	qc	501	U10	C1M-C1-C2	3.63	120.13	115.98
154	c1	708	HEA	CMB-C2B-C3B	3.56	137.14	130.34
151	qD	401	HEC	CMB-C2B-C3B	3.55	130.00	125.82
151	QD	401	HEC	CMB-C2B-C3B	3.54	129.98	125.82
154	c1	708	HEA	C1B-C2B-C3B	-3.53	102.58	106.80
151	2E	401	HEC	CMC-C2C-C3C	3.50	129.93	125.82
170	b9	202	ADP	PA-O3A-PB	-3.49	120.83	132.83
170	B9	202	ADP	PA-O3A-PB	-3.49	120.83	132.83
169	B6	201	T7X	C20-C19-C18	3.48	152.97	123.57
169	b6	201	T7X	C20-C19-C18	3.48	152.96	123.57
166	QC	501	HEM	C4D-ND-C1D	3.47	108.66	105.07
151	qD	401	HEC	CMB-C2B-C1B	-3.47	123.13	128.46
151	QD	401	HEC	CMB-C2B-C1B	-3.47	123.14	128.46
166	qC	501	HEM	C4D-ND-C1D	3.46	108.65	105.07
169	B6	201	T7X	C17-C16-C15	3.46	152.80	123.57
169	b6	201	T7X	C17-C16-C15	3.46	152.79	123.57
164	qc	507	U10	C20-C19-C21	3.46	119.94	115.98
154	c1	702	HEA	C3B-C4B-NB	3.46	113.93	109.84
164	Qc	507	U10	C20-C19-C21	3.45	119.93	115.98
151	2e	401	HEC	CMC-C2C-C3C	3.44	129.86	125.82
166	Qc	502	HEM	C4D-ND-C1D	3.43	108.61	105.07
166	qc	502	HEM	C4D-ND-C1D	3.43	108.61	105.07
166	y5	203	HEM	C4D-ND-C1D	3.42	108.60	105.07
166	Y5	203	HEM	C4D-ND-C1D	3.41	108.60	105.07
151	2E	401	HEC	CMB-C2B-C1B	-3.41	123.23	128.46
164	qC	506	U10	C12-C13-C14	-3.37	119.55	127.66
164	QC	506	U10	C12-C13-C14	-3.37	119.55	127.66
170	B9	202	ADP	C3'-C2'-C1'	3.35	106.03	100.98
170	b9	202	ADP	C3'-C2'-C1'	3.35	106.02	100.98
166	qc	502	HEM	C1B-NB-C4B	3.35	108.53	105.07
166	Qc	502	HEM	C1B-NB-C4B	3.34	108.53	105.07
151	2E	401	HEC	CMB-C2B-C3B	3.31	129.72	125.82
164	qC	506	U10	C20-C19-C21	3.31	119.76	115.98
164	QC	506	U10	C20-C19-C21	3.31	119.76	115.98
151	Qd	401	HEC	CMC-C2C-C3C	3.30	129.70	125.82
164	sc	102	U10	C37-C38-C39	-3.28	119.75	127.66
164	SC	102	U10	C37-C38-C39	-3.28	119.75	127.66
166	qC	501	HEM	C1B-NB-C4B	3.27	108.45	105.07
151	qd	401	HEC	CMB-C2B-C1B	-3.26	123.45	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
166	QC	501	HEM	C1B-NB-C4B	3.26	108.44	105.07
151	qd	401	HEC	CMB-C2B-C3B	3.25	129.64	125.82
151	qd	401	HEC	CMC-C2C-C3C	3.24	129.63	125.82
151	Qd	401	HEC	CMB-C2B-C1B	-3.23	123.50	128.46
164	B8	301	U10	C27-C28-C29	-3.22	119.89	127.66
164	b8	301	U10	C27-C28-C29	-3.22	119.90	127.66
164	B8	301	U10	C10-C9-C11	3.21	120.67	115.27
164	b8	301	U10	C10-C9-C11	3.21	120.67	115.27
164	sc	102	U10	C15-C14-C16	3.21	120.67	115.27
151	qD	401	HEC	CMC-C2C-C3C	3.19	129.57	125.82
151	QD	401	HEC	CMC-C2C-C3C	3.19	129.57	125.82
166	y5	203	HEM	C1B-NB-C4B	3.18	108.36	105.07
164	SC	102	U10	C15-C14-C16	3.18	120.62	115.27
164	B8	301	U10	C42-C43-C44	-3.18	120.00	127.66
166	Y5	203	HEM	C1B-NB-C4B	3.18	108.36	105.07
151	2e	401	HEC	CMB-C2B-C1B	-3.18	123.58	128.46
151	Qd	401	HEC	CMB-C2B-C3B	3.18	129.56	125.82
164	b8	301	U10	C42-C43-C44	-3.17	120.02	127.66
154	c1	708	HEA	C4B-C3B-C2B	-3.16	102.01	107.41
164	QC	506	U10	C7-C8-C9	-3.15	121.56	126.79
164	qC	506	U10	C7-C8-C9	-3.14	121.57	126.79
154	c1	702	HEA	C4B-C3B-C2B	-3.13	102.06	107.41
170	b9	202	ADP	N3-C2-N1	-3.13	123.78	128.68
170	B9	202	ADP	N3-C2-N1	-3.13	123.79	128.68
154	c1	708	HEA	CMB-C2B-C1B	-3.12	120.28	125.04
151	2e	401	HEC	CMB-C2B-C3B	3.11	129.48	125.82
154	C1	703	HEA	C26-C15-C16	3.11	120.50	115.27
164	b8	301	U10	C17-C18-C19	-3.11	120.18	127.66
164	B8	301	U10	C17-C18-C19	-3.10	120.19	127.66
164	Qc	501	U10	C17-C18-C19	-3.09	120.21	127.66
164	qc	501	U10	C17-C18-C19	-3.09	120.22	127.66
154	C1	702	HEA	C13-C14-C15	-3.07	120.26	127.66
164	sc	102	U10	C47-C48-C49	-3.07	120.28	127.66
154	c1	702	HEA	OMA-CMA-C3A	-3.07	118.23	124.91
164	SC	102	U10	C47-C48-C49	-3.07	120.28	127.66
154	c1	702	HEA	CMB-C2B-C1B	-3.05	120.39	125.04
160	R	202	PX2	O7-C16-C17	3.04	118.06	111.50
151	qD	401	HEC	C4C-C3C-C2C	3.04	109.64	106.35
166	QC	502	HEM	C1B-NB-C4B	3.03	108.20	105.07
166	qC	502	HEM	C1B-NB-C4B	3.02	108.20	105.07
164	qc	507	U10	C12-C13-C14	-3.02	120.39	127.66
164	Qc	507	U10	C12-C13-C14	-3.02	120.39	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
166	qc	503	HEM	C1B-NB-C4B	3.02	108.19	105.07
151	QD	401	HEC	C4C-C3C-C2C	3.02	109.61	106.35
166	qC	501	HEM	CHA-C4D-ND	3.01	128.10	124.38
166	Qc	503	HEM	C1B-NB-C4B	3.01	108.18	105.07
166	QC	501	HEM	CHA-C4D-ND	3.00	128.09	124.38
164	QC	506	U10	C17-C18-C19	-3.00	120.44	127.66
164	qC	506	U10	C17-C18-C19	-2.99	120.45	127.66
154	c1	708	HEA	C27-C19-C20	2.99	120.30	115.27
154	c1	702	HEA	CMC-C2C-C3C	2.99	130.27	124.68
154	c1	708	HEA	CHA-C4D-C3D	-2.99	120.45	124.84
154	c1	708	HEA	C26-C15-C16	2.98	120.28	115.27
164	qc	501	U10	C20-C19-C21	2.98	120.28	115.27
164	B8	301	U10	C35-C34-C36	2.97	120.27	115.27
164	b8	301	U10	C35-C34-C36	2.97	120.27	115.27
151	Qd	401	HEC	C4C-C3C-C2C	2.97	109.56	106.35
164	Qc	501	U10	C20-C19-C21	2.97	120.26	115.27
151	qd	401	HEC	C4C-C3C-C2C	2.95	109.54	106.35
154	C1	703	HEA	C13-C14-C15	-2.95	120.55	127.66
151	2e	401	HEC	CMC-C2C-C1C	-2.95	123.93	128.46
164	SC	102	U10	C27-C28-C29	-2.94	120.59	127.66
164	SC	102	U10	C12-C13-C14	-2.94	120.59	127.66
164	sc	102	U10	C12-C13-C14	-2.93	120.60	127.66
164	b8	301	U10	C37-C38-C39	-2.93	120.60	127.66
164	B8	301	U10	C37-C38-C39	-2.93	120.60	127.66
164	sc	102	U10	C27-C28-C29	-2.93	120.60	127.66
166	Y5	203	HEM	CHA-C4D-ND	2.93	128.00	124.38
166	y5	203	HEM	CHA-C4D-ND	2.92	127.99	124.38
164	B8	301	U10	C22-C23-C24	-2.92	120.64	127.66
164	b8	301	U10	C22-C23-C24	-2.92	120.64	127.66
151	2E	401	HEC	CMC-C2C-C1C	-2.92	123.98	128.46
166	qc	502	HEM	CHA-C4D-ND	2.91	127.98	124.38
166	Qc	502	HEM	CHA-C4D-ND	2.91	127.98	124.38
164	SC	102	U10	C32-C33-C34	-2.91	120.66	127.66
164	sc	102	U10	C32-C33-C34	-2.90	120.67	127.66
151	2E	401	HEC	O1D-CGD-CBD	-2.89	113.80	123.08
164	B8	301	U10	C32-C33-C34	-2.88	120.72	127.66
164	qC	506	U10	C10-C9-C11	2.88	120.12	115.27
164	b8	301	U10	C32-C33-C34	-2.88	120.72	127.66
164	SC	102	U10	C45-C44-C46	2.88	120.12	115.27
164	QC	506	U10	C10-C9-C11	2.88	120.12	115.27
164	qc	501	U10	C25-C24-C26	2.88	119.28	115.98
164	Qc	501	U10	C25-C24-C26	2.88	119.27	115.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
164	sc	102	U10	C45-C44-C46	2.87	120.11	115.27
154	C1	703	HEA	C27-C19-C20	2.87	120.11	115.27
164	sc	102	U10	C30-C29-C31	2.87	120.10	115.27
164	SC	102	U10	C30-C29-C31	2.86	120.09	115.27
164	b8	301	U10	C45-C44-C46	2.86	120.09	115.27
154	C1	703	HEA	C4B-C3B-C2B	-2.86	102.52	107.41
164	B8	301	U10	C45-C44-C46	2.85	120.07	115.27
164	sc	102	U10	C25-C24-C26	2.85	120.06	115.27
164	SC	102	U10	C25-C24-C26	2.85	120.06	115.27
154	c1	702	HEA	CMB-C2B-C3B	2.84	135.76	130.34
164	SC	102	U10	C22-C23-C24	-2.84	120.81	127.66
164	B8	301	U10	C50-C49-C51	2.84	120.05	115.27
164	b8	301	U10	C50-C49-C51	2.84	120.05	115.27
154	c1	702	HEA	C13-C14-C15	-2.83	120.84	127.66
164	sc	102	U10	C22-C23-C24	-2.83	120.84	127.66
164	sc	102	U10	C50-C49-C51	2.82	120.02	115.27
154	C1	702	HEA	C27-C19-C20	2.82	120.02	115.27
164	SC	102	U10	C40-C39-C41	2.82	120.02	115.27
164	SC	102	U10	C50-C49-C51	2.82	120.02	115.27
154	C1	702	HEA	CMB-C2B-C1B	-2.82	120.75	125.04
166	qC	502	HEM	CHA-C4D-ND	2.82	127.86	124.38
164	sc	102	U10	C40-C39-C41	2.82	120.01	115.27
164	Qc	507	U10	C1M-C1-C6	-2.82	119.81	124.40
164	qc	507	U10	C1M-C1-C6	-2.81	119.81	124.40
151	2e	401	HEC	O1D-CGD-CBD	-2.81	114.05	123.08
166	QC	502	HEM	CHA-C4D-ND	2.81	127.85	124.38
154	c1	702	HEA	C27-C19-C20	2.80	119.99	115.27
164	b8	301	U10	C47-C48-C49	-2.80	120.92	127.66
164	B8	301	U10	C47-C48-C49	-2.80	120.92	127.66
164	QC	506	U10	C1M-C1-C6	-2.80	119.84	124.40
164	qC	506	U10	C1M-C1-C6	-2.80	119.84	124.40
154	C1	703	HEA	CMB-C2B-C3B	2.77	135.63	130.34
164	Qc	507	U10	C17-C18-C19	-2.77	121.00	127.66
164	Qc	507	U10	C10-C9-C11	2.77	119.92	115.27
164	qc	507	U10	C10-C9-C11	2.76	119.92	115.27
164	qc	507	U10	C17-C18-C19	-2.76	121.01	127.66
164	B8	301	U10	C12-C13-C14	-2.76	121.01	127.66
164	b8	301	U10	C12-C13-C14	-2.76	121.02	127.66
164	SC	102	U10	C35-C34-C36	2.75	119.89	115.27
164	sc	102	U10	C35-C34-C36	2.75	119.89	115.27
154	c1	708	HEA	C17-C18-C19	-2.75	121.05	127.66
154	C1	702	HEA	CMB-C2B-C3B	2.73	135.55	130.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
166	Y5	203	HEM	CHD-C1D-ND	2.73	127.39	124.43
166	y5	203	HEM	CHD-C1D-ND	2.73	127.39	124.43
151	Qd	401	HEC	O1D-CGD-CBD	-2.72	114.33	123.08
151	qd	401	HEC	O1D-CGD-CBD	-2.72	114.33	123.08
164	SC	102	U10	C20-C19-C21	2.72	119.85	115.27
164	b8	301	U10	C25-C24-C26	2.72	119.84	115.27
164	sc	102	U10	C20-C19-C21	2.72	119.84	115.27
164	B8	301	U10	C25-C24-C26	2.72	119.84	115.27
151	QD	401	HEC	O1D-CGD-CBD	-2.71	114.38	123.08
151	qD	401	HEC	O1D-CGD-CBD	-2.71	114.39	123.08
160	qh	201	PX2	O5-C4-C5	2.70	120.38	111.91
164	B8	301	U10	C20-C19-C21	2.69	119.80	115.27
164	b8	301	U10	C20-C19-C21	2.69	119.80	115.27
166	qc	503	HEM	CHA-C4D-ND	2.69	127.70	124.38
151	2e	401	HEC	C1D-C2D-C3D	2.68	108.86	107.00
166	Qc	503	HEM	CHA-C4D-ND	2.67	127.68	124.38
160	y5	204	PX2	O5-C4-C5	2.67	120.29	111.91
154	c1	702	HEA	C17-C18-C19	-2.67	121.23	127.66
164	B8	301	U10	C40-C39-C41	2.65	119.73	115.27
164	b8	301	U10	C40-C39-C41	2.65	119.73	115.27
164	SC	102	U10	C17-C18-C19	-2.64	121.29	127.66
159	m2	406	P5S	O19-C17-C20	2.64	120.20	111.91
159	M2	406	P5S	O19-C17-C20	2.64	120.20	111.91
154	C1	703	HEA	C17-C18-C19	-2.64	121.30	127.66
164	qc	501	U10	C10-C9-C11	2.64	119.71	115.27
164	sc	102	U10	C17-C18-C19	-2.63	121.34	127.66
160	Y5	204	PX2	O5-C4-C5	2.62	120.13	111.91
164	sc	102	U10	C42-C43-C44	-2.62	121.36	127.66
164	SC	102	U10	C42-C43-C44	-2.61	121.37	127.66
161	SA	701	FAD	P-O3P-PA	-2.61	123.88	132.83
164	Qc	501	U10	C10-C9-C11	2.61	119.66	115.27
161	sa	701	FAD	P-O3P-PA	-2.60	123.89	132.83
160	r	202	PX2	O5-C4-C5	2.60	120.07	111.91
160	Qh	201	PX2	O5-C4-C5	2.60	120.07	111.91
154	C1	702	HEA	C17-C18-C19	-2.60	121.40	127.66
154	C1	702	HEA	C1B-C2B-C3B	-2.59	103.70	106.80
164	B8	301	U10	C30-C29-C31	2.58	119.61	115.27
154	c1	702	HEA	C4D-C3D-C2D	-2.57	103.15	106.90
164	b8	301	U10	C30-C29-C31	2.57	119.59	115.27
164	B8	301	U10	C7-C8-C9	-2.57	122.52	126.79
154	C1	702	HEA	CHA-C4D-C3D	-2.56	121.07	124.84
160	R	202	PX2	O5-C4-C5	2.55	119.92	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
154	c1	702	HEA	C26-C15-C16	2.55	119.57	115.27
151	Qd	401	HEC	CMC-C2C-C1C	-2.55	124.54	128.46
164	b8	301	U10	C7-C8-C9	-2.55	122.54	126.79
169	b6	201	T7X	O18-C11-C31	2.55	119.92	111.91
169	B6	201	T7X	O18-C11-C31	2.55	119.92	111.91
164	SC	102	U10	C7-C8-C9	-2.54	122.56	126.79
164	sc	102	U10	C7-C8-C9	-2.54	122.56	126.79
164	B8	301	U10	C15-C14-C16	2.54	119.55	115.27
164	b8	301	U10	C15-C14-C16	2.54	119.55	115.27
154	c1	702	HEA	C1D-ND-C4D	-2.54	102.45	105.07
151	2E	401	HEC	C4C-C3C-C2C	2.54	109.09	106.35
151	qd	401	HEC	CMC-C2C-C1C	-2.53	124.58	128.46
170	B9	202	ADP	C4-C5-N7	-2.52	106.77	109.40
164	Qc	501	U10	C15-C14-C16	2.52	119.51	115.27
154	c1	708	HEA	C13-C14-C15	-2.52	121.60	127.66
170	b9	202	ADP	C4-C5-N7	-2.51	106.78	109.40
164	qc	501	U10	C15-C14-C16	2.51	119.50	115.27
164	b8	301	U10	C1M-C1-C6	-2.49	120.33	124.40
164	B8	301	U10	C1M-C1-C6	-2.49	120.34	124.40
154	c1	702	HEA	C1B-C2B-C3B	-2.48	103.84	106.80
151	QD	401	HEC	CMC-C2C-C1C	-2.46	124.68	128.46
154	c1	702	HEA	CHC-C4B-NB	-2.46	121.34	124.38
154	C1	703	HEA	CMC-C2C-C1C	-2.46	124.69	128.46
154	c1	708	HEA	O1D-CGD-CBD	-2.45	115.19	123.08
151	qD	401	HEC	CMC-C2C-C1C	-2.45	124.69	128.46
164	qc	507	U10	C15-C14-C16	2.45	119.39	115.27
164	Qc	507	U10	C15-C14-C16	2.45	119.39	115.27
151	2e	401	HEC	CMD-C2D-C3D	2.45	129.55	124.94
154	c1	708	HEA	CHC-C4B-NB	-2.44	121.37	124.38
154	C1	702	HEA	C26-C15-C16	2.43	119.36	115.27
164	Qc	501	U10	C22-C23-C24	-2.43	121.81	127.66
166	Qc	502	HEM	CHD-C1D-ND	2.42	127.06	124.43
166	qc	502	HEM	CHD-C1D-ND	2.42	127.06	124.43
151	2e	401	HEC	C4C-C3C-C2C	2.42	108.96	106.35
164	qc	501	U10	C22-C23-C24	-2.41	121.85	127.66
166	qc	503	HEM	CHD-C1D-ND	2.41	127.05	124.43
166	Qc	503	HEM	CHD-C1D-ND	2.40	127.04	124.43
164	QC	506	U10	C15-C14-C16	2.40	119.31	115.27
151	qd	401	HEC	CMD-C2D-C3D	2.40	129.46	124.94
164	qC	506	U10	C15-C14-C16	2.39	119.30	115.27
151	Qd	401	HEC	CMD-C2D-C3D	2.38	129.44	124.94
151	qD	401	HEC	CMD-C2D-C3D	2.38	129.43	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
164	sc	102	U10	C56-C54-C55	2.38	119.86	114.60
151	QD	401	HEC	CMD-C2D-C3D	2.38	129.43	124.94
164	SC	102	U10	C56-C54-C55	2.38	119.86	114.60
167	a9	401	NDP	C5A-C6A-N6A	2.38	123.96	120.35
164	b8	301	U10	C56-C54-C55	2.37	119.84	114.60
164	B8	301	U10	C56-C54-C55	2.37	119.84	114.60
167	A9	401	NDP	C5A-C6A-N6A	2.35	123.93	120.35
166	qc	503	HEM	CHB-C1B-C2B	-2.35	120.23	126.72
166	Qc	503	HEM	CHB-C1B-C2B	-2.35	120.23	126.72
151	2e	401	HEC	O1A-CGA-CBA	-2.33	115.59	123.08
166	QC	501	HEM	CHD-C1D-ND	2.33	126.96	124.43
166	qC	501	HEM	CHD-C1D-ND	2.32	126.95	124.43
161	sa	701	FAD	C5A-C6A-N6A	2.32	123.87	120.35
166	Qc	503	HEM	C2C-C3C-C4C	2.32	108.52	106.90
161	SA	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
166	qc	503	HEM	C2C-C3C-C4C	2.30	108.51	106.90
151	qD	401	HEC	O1A-CGA-CBA	-2.30	115.69	123.08
151	2E	401	HEC	O2A-CGA-O1A	2.30	129.03	123.30
164	SC	102	U10	C10-C9-C11	2.29	119.12	115.27
166	qc	502	HEM	CAD-CBD-CGD	-2.28	108.69	113.60
151	QD	401	HEC	O1A-CGA-CBA	-2.28	115.75	123.08
154	c1	702	HEA	CHD-C1D-C2D	-2.28	120.42	126.72
151	qD	401	HEC	O2A-CGA-O1A	2.27	128.96	123.30
166	Qc	502	HEM	CAD-CBD-CGD	-2.27	108.71	113.60
151	2E	401	HEC	C1D-C2D-C3D	2.27	108.58	107.00
154	C1	702	HEA	C27-C19-C18	-2.27	117.86	123.68
154	C1	702	HEA	C4D-CHA-C1A	2.26	125.55	122.56
166	Y5	203	HEM	CHB-C1B-C2B	-2.26	120.47	126.72
166	y5	203	HEM	CHB-C1B-C2B	-2.26	120.48	126.72
151	QD	401	HEC	O2A-CGA-O1A	2.25	128.91	123.30
166	QC	502	HEM	CHB-C1B-C2B	-2.25	120.50	126.72
151	2e	401	HEC	O2A-CGA-O1A	2.25	128.90	123.30
166	QC	502	HEM	C2C-C3C-C4C	2.24	108.47	106.90
166	qC	502	HEM	CHB-C1B-C2B	-2.24	120.52	126.72
151	QD	401	HEC	C2B-C3B-C4B	2.24	108.77	106.35
151	2E	401	HEC	CMD-C2D-C3D	2.24	129.16	124.94
154	C1	702	HEA	CMD-C2D-C1D	2.24	128.44	125.04
151	qD	401	HEC	C2B-C3B-C4B	2.24	108.77	106.35
166	qC	502	HEM	C3C-C4C-NC	-2.23	106.73	110.94
166	QC	502	HEM	C3C-C4C-NC	-2.23	106.73	110.94
151	qd	401	HEC	O1A-CGA-CBA	-2.23	115.91	123.08
151	Qd	401	HEC	O1A-CGA-CBA	-2.23	115.91	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
166	Qc	502	HEM	CHB-C1B-C2B	-2.23	120.55	126.72
154	c1	702	HEA	C27-C19-C18	-2.23	117.96	123.68
166	qC	502	HEM	CAD-CBD-CGD	-2.23	108.81	113.60
166	qc	502	HEM	CHB-C1B-C2B	-2.22	120.58	126.72
166	qC	502	HEM	C2C-C3C-C4C	2.22	108.45	106.90
166	QC	502	HEM	CAD-CBD-CGD	-2.21	108.84	113.60
151	2E	401	HEC	O1A-CGA-CBA	-2.21	115.98	123.08
151	qd	401	HEC	CMA-C3A-C2A	2.21	129.10	124.94
166	qC	502	HEM	CHD-C1D-ND	2.20	126.83	124.43
166	QC	502	HEM	CHD-C1D-ND	2.20	126.82	124.43
151	Qd	401	HEC	CMA-C3A-C2A	2.20	129.09	124.94
166	qC	501	HEM	CHB-C1B-C2B	-2.20	120.65	126.72
154	c1	708	HEA	C4D-C3D-C2D	-2.19	103.70	106.90
166	QC	501	HEM	CHB-C1B-C2B	-2.19	120.66	126.72
154	C1	703	HEA	CMD-C2D-C1D	2.18	128.37	125.04
154	c1	702	HEA	CMD-C2D-C1D	2.18	128.37	125.04
154	c1	702	HEA	CAD-C3D-C2D	2.18	131.94	127.88
158	a3	201	3PE	O31-C3-C2	-2.18	102.08	108.43
158	A3	201	3PE	O31-C3-C2	-2.18	102.10	108.43
151	qd	401	HEC	C2B-C3B-C4B	2.18	108.70	106.35
164	sc	102	U10	C52-C53-C54	-2.17	120.32	127.75
164	SC	102	U10	C52-C53-C54	-2.17	120.32	127.75
154	C1	702	HEA	CHC-C4B-NB	-2.17	121.69	124.38
151	Qd	401	HEC	O2A-CGA-O1A	2.16	128.69	123.30
151	qd	401	HEC	O2A-CGA-O1A	2.16	128.69	123.30
151	Qd	401	HEC	C2B-C3B-C4B	2.16	108.69	106.35
166	qc	503	HEM	C3C-C4C-NC	-2.16	106.86	110.94
166	Qc	503	HEM	C3C-C4C-NC	-2.16	106.86	110.94
164	sc	102	U10	C10-C9-C11	2.16	118.91	115.27
151	qD	401	HEC	CMA-C3A-C2A	2.16	129.01	124.94
166	QC	501	HEM	CBA-CAA-C2A	-2.15	108.95	112.62
166	qC	501	HEM	CBA-CAA-C2A	-2.15	108.95	112.62
154	C1	702	HEA	OMA-CMA-C3A	-2.15	120.23	124.91
166	qc	503	HEM	CAD-CBD-CGD	-2.13	109.02	113.60
166	Qc	503	HEM	CAD-CBD-CGD	-2.13	109.02	113.60
151	QD	401	HEC	CMA-C3A-C2A	2.13	128.96	124.94
154	C1	702	HEA	C4B-NB-C1B	-2.13	102.88	105.07
154	c1	708	HEA	C27-C19-C18	-2.12	118.23	123.68
154	c1	708	HEA	CMD-C2D-C1D	2.12	128.26	125.04
154	c1	708	HEA	CHB-C1B-NB	2.11	126.72	124.43
151	Qd	401	HEC	C1D-C2D-C3D	2.11	108.46	107.00
154	C1	702	HEA	CHB-C1B-NB	2.10	126.72	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
151	qd	401	HEC	C1D-C2D-C3D	2.10	108.45	107.00
151	QD	401	HEC	C1D-C2D-C3D	2.09	108.45	107.00
164	B8	301	U10	C52-C53-C54	-2.09	120.61	127.75
164	b8	301	U10	C52-C53-C54	-2.09	120.62	127.75
154	C1	703	HEA	CHA-C4D-C3D	-2.08	121.78	124.84
151	qD	401	HEC	C1D-C2D-C3D	2.07	108.44	107.00
154	c1	702	HEA	CHB-C1B-NB	2.07	126.68	124.43
154	C1	703	HEA	C27-C19-C18	-2.05	118.42	123.68
151	2E	401	HEC	C2B-C3B-C4B	2.03	108.54	106.35
151	2E	401	HEC	CMA-C3A-C2A	2.02	128.76	124.94
166	qC	501	HEM	CAD-CBD-CGD	-2.02	109.26	113.60
151	2e	401	HEC	C2B-C3B-C4B	2.01	108.52	106.35

There are no chirality outliers.

All (5906) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
151	2e	401	HEC	C2D-C3D-CAD-CBD
151	2e	401	HEC	C4D-C3D-CAD-CBD
151	2E	401	HEC	C2D-C3D-CAD-CBD
151	2E	401	HEC	C4D-C3D-CAD-CBD
152	2f	301	PC1	C11-O13-P-O14
152	2f	301	PC1	C1-O11-P-O12
152	2f	301	PC1	C1-O11-P-O14
152	2f	301	PC1	C1-O11-P-O13
152	2f	302	PC1	C11-O13-P-O11
152	2j	201	PC1	C1-O11-P-O12
152	2j	201	PC1	C1-O11-P-O14
152	2j	201	PC1	O13-C11-C12-N
152	6a	202	PC1	C1-O11-P-O12
152	6a	202	PC1	C1-O11-P-O14
152	6c	203	PC1	C1-O11-P-O12
152	6c	203	PC1	C1-O11-P-O14
152	6c	203	PC1	C1-O11-P-O13
152	7a	202	PC1	C1-O11-P-O12
152	7a	202	PC1	C1-O11-P-O14
152	7a	202	PC1	C1-O11-P-O13
152	7c	303	PC1	C11-O13-P-O12
152	7c	303	PC1	C1-O11-P-O14
152	a	501	PC1	C11-O13-P-O12
152	a	501	PC1	C11-O13-P-O14
152	c1	704	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	c1	704	PC1	C1-O11-P-O12
152	c1	706	PC1	C11-O13-P-O12
152	c1	706	PC1	C1-O11-P-O14
152	c1	711	PC1	C11-O13-P-O14
152	c3	601	PC1	C1-O11-P-O14
152	c3	601	PC1	C2-C1-O11-P
152	c3	602	PC1	C1-O11-P-O12
152	c3	602	PC1	C1-O11-P-O14
152	c3	602	PC1	O21-C2-C3-O31
152	c3	603	PC1	C11-O13-P-O12
152	c3	606	PC1	C1-O11-P-O14
152	c3	606	PC1	C1-O11-P-O13
152	d	501	PC1	C11-O13-P-O14
152	d	501	PC1	C11-O13-P-O11
152	f	402	PC1	C11-O13-P-O14
152	f	402	PC1	C1-O11-P-O14
152	i	304	PC1	C1-O11-P-O12
152	i	304	PC1	C1-O11-P-O14
152	i	304	PC1	C1-O11-P-O13
152	j	302	PC1	C1-O11-P-O14
152	m	301	PC1	C11-O13-P-O12
152	m	301	PC1	C11-O13-P-O11
152	m	301	PC1	C1-O11-P-O13
152	m	305	PC1	C11-O13-P-O12
152	m	305	PC1	C1-O11-P-O12
152	m	305	PC1	C1-O11-P-O14
152	m	305	PC1	C1-O11-P-O13
152	m	305	PC1	O13-C11-C12-N
152	m	307	PC1	C11-O13-P-O12
152	m	307	PC1	C11-O13-P-O14
152	m	307	PC1	C11-O13-P-O11
152	m	307	PC1	C1-O11-P-O12
152	m	307	PC1	C1-O11-P-O14
152	m1	401	PC1	C11-O13-P-O12
152	m1	401	PC1	C11-O13-P-O14
152	m1	403	PC1	C1-O11-P-O12
152	m1	403	PC1	C1-O11-P-O14
152	m1	403	PC1	C1-O11-P-O13
152	m2	402	PC1	C11-O13-P-O12
152	m2	402	PC1	C1-O11-P-O14
152	m2	402	PC1	O13-C11-C12-N
152	m2	405	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	m2	405	PC1	C11-O13-P-O14
152	m2	407	PC1	C11-O13-P-O12
152	m2	407	PC1	C11-O13-P-O14
152	m2	407	PC1	C1-O11-P-O14
152	n	302	PC1	C11-O13-P-O12
152	v	202	PC1	C1-O11-P-O14
152	w	201	PC1	C11-O13-P-O12
152	w	201	PC1	C11-O13-P-O14
152	w	201	PC1	C1-O11-P-O14
152	w	204	PC1	C1-O11-P-O12
152	w	204	PC1	C1-O11-P-O14
152	w	204	PC1	C1-O11-P-O13
152	w	205	PC1	C11-O13-P-O12
152	w	205	PC1	C11-O13-P-O14
152	5b	202	PC1	C11-O13-P-O12
152	5b	202	PC1	C11-O13-P-O14
152	am	202	PC1	C11-O13-P-O12
152	am	202	PC1	C11-O13-P-O14
152	am	202	PC1	C11-O13-P-O11
152	am	202	PC1	C1-O11-P-O12
152	am	202	PC1	C1-O11-P-O14
152	am	202	PC1	C1-O11-P-O13
152	an	304	PC1	C1-O11-P-O12
152	an	304	PC1	C1-O11-P-O14
152	an	304	PC1	C1-O11-P-O13
152	b9	201	PC1	C11-O13-P-O12
152	b9	201	PC1	C1-O11-P-O14
152	b9	201	PC1	C1-O11-P-O13
152	c4	403	PC1	C11-O13-P-O12
152	j1	400	PC1	C1-O11-P-O12
152	j1	400	PC1	C1-O11-P-O14
152	j1	400	PC1	C1-O11-P-O13
152	n1	301	PC1	C1-O11-P-O12
152	n1	301	PC1	C1-O11-P-O14
152	n1	301	PC1	C1-O11-P-O13
152	n5	801	PC1	C11-O13-P-O14
152	n5	804	PC1	C11-O13-P-O12
152	n5	804	PC1	C11-O13-P-O14
152	n5	804	PC1	C1-O11-P-O12
152	n5	805	PC1	C11-O13-P-O12
152	n5	805	PC1	C1-O11-P-O13
152	n5	805	PC1	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	n6	301	PC1	C11-O13-P-O12
152	p1	401	PC1	C1-O11-P-O12
152	p1	401	PC1	C1-O11-P-O14
152	p1	401	PC1	C1-O11-P-O13
152	qB	602	PC1	C11-O13-P-O11
152	qC	505	PC1	C11-O13-P-O12
152	qC	505	PC1	C1-O11-P-O12
152	qC	505	PC1	C1-O11-P-O14
152	qC	507	PC1	C1-O11-P-O13
152	qC	508	PC1	C1-O11-P-O14
152	qE	301	PC1	C11-O13-P-O14
152	qE	301	PC1	C11-O13-P-O11
152	qE	304	PC1	C1-O11-P-O12
152	qE	304	PC1	C1-O11-P-O14
152	qG	401	PC1	C11-O13-P-O12
152	qG	401	PC1	C11-O13-P-O14
152	qG	401	PC1	C11-O13-P-O11
152	qI	201	PC1	C11-O13-P-O12
152	qI	201	PC1	C11-O13-P-O14
152	qJ	101	PC1	C11-O13-P-O12
152	qJ	101	PC1	C1-O11-P-O12
152	qJ	101	PC1	C1-O11-P-O14
152	qJ	101	PC1	C1-O11-P-O13
152	qJ	101	PC1	O13-C11-C12-N
152	qc	506	PC1	C11-O13-P-O12
152	qc	506	PC1	C11-O13-P-O14
152	qc	506	PC1	C1-O11-P-O12
152	qc	506	PC1	C1-O11-P-O14
152	qc	509	PC1	C1-O11-P-O14
152	qe	303	PC1	C11-O13-P-O14
152	qe	303	PC1	C1-O11-P-O12
152	qg	401	PC1	C11-O13-P-O12
152	qi	201	PC1	C1-O11-P-O12
152	qi	201	PC1	C1-O11-P-O14
152	qi	201	PC1	C1-O11-P-O13
152	qj	101	PC1	C11-O13-P-O12
152	qj	101	PC1	O11-C1-C2-O21
152	s8	301	PC1	C1-O11-P-O13
152	t1	602	PC1	C11-O13-P-O12
152	t1	602	PC1	C11-O13-P-O14
152	t4	301	PC1	C11-O13-P-O12
152	t4	301	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	t4	301	PC1	C1-O11-P-O12
152	t4	301	PC1	C1-O11-P-O14
152	t4	301	PC1	C1-O11-P-O13
152	t4	303	PC1	C11-O13-P-O12
152	t4	303	PC1	C11-O13-P-O14
152	t4	303	PC1	C11-O13-P-O11
152	tc	102	PC1	C11-O13-P-O14
152	tc	102	PC1	C1-O11-P-O12
152	te	102	PC1	C11-O13-P-O12
152	te	102	PC1	C1-O11-P-O14
152	2F	301	PC1	C11-O13-P-O14
152	2F	301	PC1	C1-O11-P-O12
152	2F	301	PC1	C1-O11-P-O14
152	2F	301	PC1	C1-O11-P-O13
152	2F	302	PC1	C11-O13-P-O11
152	2J	201	PC1	C1-O11-P-O12
152	2J	201	PC1	C1-O11-P-O14
152	2J	201	PC1	O13-C11-C12-N
152	6A	202	PC1	C1-O11-P-O12
152	6A	202	PC1	C1-O11-P-O14
152	6C	201	PC1	C1-O11-P-O12
152	6C	201	PC1	C1-O11-P-O14
152	6C	201	PC1	C1-O11-P-O13
152	7A	202	PC1	C1-O11-P-O12
152	7A	202	PC1	C1-O11-P-O14
152	7A	202	PC1	C1-O11-P-O13
152	7C	303	PC1	C11-O13-P-O12
152	7C	303	PC1	C1-O11-P-O14
152	A	501	PC1	C11-O13-P-O12
152	A	501	PC1	C11-O13-P-O14
152	C1	706	PC1	C11-O13-P-O12
152	C1	706	PC1	C1-O11-P-O12
152	C1	709	PC1	C11-O13-P-O12
152	C1	709	PC1	C1-O11-P-O14
152	C1	711	PC1	C11-O13-P-O14
152	C1	711	PC1	C11-O13-P-O11
152	C3	601	PC1	C1-O11-P-O14
152	C3	601	PC1	C2-C1-O11-P
152	C3	602	PC1	C1-O11-P-O12
152	C3	602	PC1	C1-O11-P-O14
152	C3	602	PC1	O21-C2-C3-O31
152	C3	603	PC1	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	C3	606	PC1	C1-O11-P-O14
152	C3	606	PC1	C1-O11-P-O13
152	D	501	PC1	C11-O13-P-O14
152	D	501	PC1	C11-O13-P-O11
152	F	401	PC1	C11-O13-P-O14
152	F	401	PC1	C1-O11-P-O14
152	I	301	PC1	C1-O11-P-O12
152	I	301	PC1	C1-O11-P-O14
152	I	301	PC1	C1-O11-P-O13
152	J	302	PC1	C1-O11-P-O14
152	M	302	PC1	C11-O13-P-O12
152	M	302	PC1	C11-O13-P-O14
152	M	302	PC1	C11-O13-P-O11
152	M	302	PC1	C1-O11-P-O12
152	M	302	PC1	C1-O11-P-O14
152	M	303	PC1	C11-O13-P-O12
152	M	303	PC1	C11-O13-P-O11
152	M	303	PC1	C1-O11-P-O13
152	M	307	PC1	C11-O13-P-O12
152	M	307	PC1	C1-O11-P-O12
152	M	307	PC1	C1-O11-P-O14
152	M	307	PC1	C1-O11-P-O13
152	M	307	PC1	O13-C11-C12-N
152	M1	401	PC1	C11-O13-P-O12
152	M1	401	PC1	C11-O13-P-O14
152	M1	403	PC1	C1-O11-P-O12
152	M1	403	PC1	C1-O11-P-O14
152	M1	403	PC1	C1-O11-P-O13
152	M2	402	PC1	C11-O13-P-O12
152	M2	402	PC1	C1-O11-P-O14
152	M2	402	PC1	O13-C11-C12-N
152	M2	405	PC1	C11-O13-P-O12
152	M2	405	PC1	C11-O13-P-O14
152	M2	407	PC1	C11-O13-P-O12
152	M2	407	PC1	C11-O13-P-O14
152	M2	407	PC1	C1-O11-P-O14
152	N	302	PC1	C11-O13-P-O12
152	V	202	PC1	C1-O11-P-O14
152	W	201	PC1	C11-O13-P-O12
152	W	201	PC1	C11-O13-P-O14
152	W	201	PC1	C1-O11-P-O14
152	W	204	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	W	204	PC1	C1-O11-P-O14
152	W	204	PC1	C1-O11-P-O13
152	W	205	PC1	C11-O13-P-O12
152	W	205	PC1	C11-O13-P-O14
152	5B	202	PC1	C11-O13-P-O12
152	5B	202	PC1	C11-O13-P-O14
152	AM	202	PC1	C11-O13-P-O12
152	AM	202	PC1	C11-O13-P-O14
152	AM	202	PC1	C11-O13-P-O11
152	AM	202	PC1	C1-O11-P-O12
152	AM	202	PC1	C1-O11-P-O14
152	AM	202	PC1	C1-O11-P-O13
152	AN	304	PC1	C1-O11-P-O12
152	AN	304	PC1	C1-O11-P-O14
152	AN	304	PC1	C1-O11-P-O13
152	B9	201	PC1	C11-O13-P-O12
152	B9	201	PC1	C1-O11-P-O14
152	B9	201	PC1	C1-O11-P-O13
152	C4	403	PC1	C11-O13-P-O12
152	J1	400	PC1	C1-O11-P-O12
152	J1	400	PC1	C1-O11-P-O14
152	J1	400	PC1	C1-O11-P-O13
152	N1	301	PC1	C1-O11-P-O12
152	N1	301	PC1	C1-O11-P-O14
152	N1	301	PC1	C1-O11-P-O13
152	N5	801	PC1	C11-O13-P-O14
152	N5	804	PC1	C11-O13-P-O12
152	N5	804	PC1	C11-O13-P-O14
152	N5	804	PC1	C1-O11-P-O12
152	N5	805	PC1	C11-O13-P-O12
152	N5	805	PC1	C1-O11-P-O13
152	N5	805	PC1	O21-C2-C3-O31
152	N6	301	PC1	C11-O13-P-O12
152	P1	401	PC1	C1-O11-P-O12
152	P1	401	PC1	C1-O11-P-O14
152	P1	401	PC1	C1-O11-P-O13
152	QB	602	PC1	C11-O13-P-O11
152	QC	505	PC1	C11-O13-P-O12
152	QC	505	PC1	C1-O11-P-O12
152	QC	505	PC1	C1-O11-P-O14
152	QC	507	PC1	C1-O11-P-O13
152	QC	508	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	QE	301	PC1	C11-O13-P-O14
152	QE	301	PC1	C11-O13-P-O11
152	QE	303	PC1	C1-O11-P-O14
152	QG	401	PC1	C11-O13-P-O12
152	QG	401	PC1	C11-O13-P-O14
152	QG	401	PC1	C11-O13-P-O11
152	QI	201	PC1	C11-O13-P-O12
152	QI	201	PC1	C11-O13-P-O14
152	QI	201	PC1	C1-O11-P-O14
152	QJ	101	PC1	C1-O11-P-O12
152	QJ	101	PC1	C1-O11-P-O14
152	QJ	102	PC1	C11-O13-P-O12
152	QJ	102	PC1	C1-O11-P-O12
152	QJ	102	PC1	C1-O11-P-O14
152	QJ	102	PC1	C1-O11-P-O13
152	QJ	102	PC1	O13-C11-C12-N
152	Qc	506	PC1	C11-O13-P-O12
152	Qc	506	PC1	C11-O13-P-O14
152	Qc	506	PC1	C1-O11-P-O12
152	Qc	506	PC1	C1-O11-P-O14
152	Qc	509	PC1	C1-O11-P-O14
152	Qe	303	PC1	C11-O13-P-O14
152	Qe	303	PC1	C1-O11-P-O12
152	Qg	401	PC1	C11-O13-P-O12
152	Qi	201	PC1	C1-O11-P-O12
152	Qi	201	PC1	C1-O11-P-O14
152	Qi	201	PC1	C1-O11-P-O13
152	Qj	101	PC1	C11-O13-P-O12
152	Qj	101	PC1	O11-C1-C2-O21
152	S8	301	PC1	C1-O11-P-O13
152	T1	602	PC1	C11-O13-P-O12
152	T1	602	PC1	C11-O13-P-O14
152	T4	301	PC1	C11-O13-P-O12
152	T4	301	PC1	C11-O13-P-O14
152	T4	301	PC1	C1-O11-P-O12
152	T4	301	PC1	C1-O11-P-O14
152	T4	301	PC1	C1-O11-P-O13
152	T4	303	PC1	C11-O13-P-O12
152	T4	303	PC1	C11-O13-P-O14
152	T4	303	PC1	C11-O13-P-O11
152	TC	102	PC1	C11-O13-P-O14
152	TC	102	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	TE	102	PC1	C11-O13-P-O12
152	TE	102	PC1	C1-O11-P-O14
153	2g	201	CDL	CB2-OB2-PB2-OB3
153	2g	201	CDL	CB2-OB2-PB2-OB4
153	2g	201	CDL	CB2-OB2-PB2-OB5
153	2g	201	CDL	CB3-OB5-PB2-OB3
153	2g	203	CDL	CA2-OA2-PA1-OA4
153	2g	203	CDL	CA3-OA5-PA1-OA2
153	2g	204	CDL	CA2-OA2-PA1-OA3
153	2g	204	CDL	CA2-OA2-PA1-OA4
153	2g	204	CDL	CA3-OA5-PA1-OA4
153	2g	204	CDL	CB3-OB5-PB2-OB4
153	2k	101	CDL	CA3-OA5-PA1-OA4
153	2k	101	CDL	CB2-OB2-PB2-OB3
153	2k	101	CDL	CB2-OB2-PB2-OB4
153	2k	101	CDL	CB3-OB5-PB2-OB3
153	2k	101	CDL	CB3-OB5-PB2-OB4
153	2m	101	CDL	CA3-OA5-PA1-OA2
153	2m	101	CDL	CA3-OA5-PA1-OA3
153	2m	101	CDL	CA3-OA5-PA1-OA4
153	2m	101	CDL	CB2-OB2-PB2-OB3
153	2m	101	CDL	CB2-OB2-PB2-OB4
153	2o	101	CDL	CA2-OA2-PA1-OA4
153	2o	101	CDL	CA3-OA5-PA1-OA3
153	2o	101	CDL	CA3-OA5-PA1-OA4
153	6a	201	CDL	CA2-OA2-PA1-OA3
153	6a	201	CDL	CA3-OA5-PA1-OA3
153	6a	201	CDL	CA3-OA5-PA1-OA4
153	6c	201	CDL	CB2-OB2-PB2-OB3
153	6c	201	CDL	CB2-OB2-PB2-OB5
153	6c	201	CDL	CB3-OB5-PB2-OB3
153	6c	201	CDL	CB3-OB5-PB2-OB4
153	6c	201	CDL	OB5-CB3-CB4-OB6
153	6c	202	CDL	CA2-OA2-PA1-OA3
153	6c	202	CDL	CB3-OB5-PB2-OB2
153	6c	202	CDL	CB3-OB5-PB2-OB3
153	7a	201	CDL	CA2-OA2-PA1-OA4
153	7a	201	CDL	CA3-OA5-PA1-OA3
153	7a	201	CDL	CB2-OB2-PB2-OB3
153	7a	203	CDL	CA2-OA2-PA1-OA3
153	7a	203	CDL	CB3-OB5-PB2-OB3
153	7c	301	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	7c	302	CDL	CA3-OA5-PA1-OA2
153	7c	302	CDL	CA3-OA5-PA1-OA3
153	7c	302	CDL	CB2-OB2-PB2-OB3
153	a	502	CDL	CA2-OA2-PA1-OA3
153	a	502	CDL	CB2-OB2-PB2-OB4
153	a	504	CDL	CA2-OA2-PA1-OA3
153	a	504	CDL	CA2-OA2-PA1-OA4
153	a	504	CDL	CB3-OB5-PB2-OB2
153	a	504	CDL	CB3-OB5-PB2-OB3
153	a	505	CDL	CB2-C1-CA2-OA2
153	b	501	CDL	CA2-OA2-PA1-OA3
153	b	501	CDL	CA2-OA2-PA1-OA4
153	b	501	CDL	CA2-OA2-PA1-OA5
153	b	501	CDL	CA3-OA5-PA1-OA2
153	b	501	CDL	CA3-OA5-PA1-OA3
153	b	501	CDL	CA3-OA5-PA1-OA4
153	c1	701	CDL	CA2-OA2-PA1-OA3
153	c1	701	CDL	CA2-OA2-PA1-OA4
153	c1	701	CDL	CA2-OA2-PA1-OA5
153	c1	701	CDL	CB2-OB2-PB2-OB3
153	c1	701	CDL	CB2-OB2-PB2-OB4
153	c1	701	CDL	CB3-OB5-PB2-OB2
153	c1	701	CDL	CB3-OB5-PB2-OB3
153	c1	703	CDL	CA3-OA5-PA1-OA3
153	c1	703	CDL	CB3-OB5-PB2-OB2
153	c1	703	CDL	CB3-OB5-PB2-OB3
153	c1	703	CDL	CB3-OB5-PB2-OB4
153	c1	709	CDL	C1-CA2-OA2-PA1
153	c1	709	CDL	CA2-OA2-PA1-OA4
153	c1	709	CDL	CB2-OB2-PB2-OB3
153	c1	709	CDL	CB2-OB2-PB2-OB4
153	c1	709	CDL	CB2-OB2-PB2-OB5
153	c1	709	CDL	CB3-OB5-PB2-OB3
153	c1	712	CDL	CB2-OB2-PB2-OB3
153	c3	604	CDL	CA2-OA2-PA1-OA3
153	c3	604	CDL	CA2-OA2-PA1-OA4
153	e	401	CDL	CA3-OA5-PA1-OA2
153	e	401	CDL	CA3-OA5-PA1-OA3
153	e	401	CDL	CA3-OA5-PA1-OA4
153	e	401	CDL	CB2-OB2-PB2-OB3
153	e	401	CDL	CB2-OB2-PB2-OB4
153	e	401	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	e	402	CDL	CA2-OA2-PA1-OA3
153	e	403	CDL	CB2-OB2-PB2-OB3
153	e	403	CDL	CB2-OB2-PB2-OB4
153	f	401	CDL	CB3-OB5-PB2-OB2
153	f	401	CDL	CB3-OB5-PB2-OB3
153	f	401	CDL	CB3-OB5-PB2-OB4
153	fs	203	CDL	CB3-OB5-PB2-OB3
153	fs	203	CDL	CB3-OB5-PB2-OB4
153	i	301	CDL	CA2-OA2-PA1-OA5
153	i	301	CDL	CA3-OA5-PA1-OA3
153	i	302	CDL	CA3-OA5-PA1-OA3
153	i	302	CDL	CB2-OB2-PB2-OB3
153	i	302	CDL	OB5-CB3-CB4-OB6
153	j	301	CDL	CA2-OA2-PA1-OA3
153	j	301	CDL	CA3-OA5-PA1-OA2
153	j	301	CDL	CB3-OB5-PB2-OB3
153	j	301	CDL	CB3-OB5-PB2-OB4
153	l	301	CDL	CA3-OA5-PA1-OA2
153	l	301	CDL	CB2-OB2-PB2-OB3
153	l	301	CDL	CB2-OB2-PB2-OB4
153	l	301	CDL	CB3-OB5-PB2-OB2
153	l	301	CDL	CB3-OB5-PB2-OB3
153	l	301	CDL	CB3-OB5-PB2-OB4
153	m	302	CDL	CA3-OA5-PA1-OA4
153	m	302	CDL	CB2-OB2-PB2-OB3
153	m	302	CDL	CB2-OB2-PB2-OB4
153	m	303	CDL	CA2-OA2-PA1-OA3
153	m	304	CDL	CA2-OA2-PA1-OA4
153	m	304	CDL	CA2-OA2-PA1-OA5
153	m	304	CDL	CA4-CA3-OA5-PA1
153	m	304	CDL	CB2-OB2-PB2-OB5
153	m	304	CDL	CB3-OB5-PB2-OB2
153	m	304	CDL	CB3-OB5-PB2-OB3
153	m	304	CDL	CB3-OB5-PB2-OB4
153	m	306	CDL	CA2-OA2-PA1-OA3
153	m	306	CDL	CA2-OA2-PA1-OA4
153	m	306	CDL	CA3-OA5-PA1-OA2
153	m	306	CDL	CA3-OA5-PA1-OA3
153	m	306	CDL	CA3-OA5-PA1-OA4
153	m	306	CDL	CB2-OB2-PB2-OB4
153	m1	404	CDL	CA2-OA2-PA1-OA5
153	m1	404	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	m1	404	CDL	CB2-OB2-PB2-OB4
153	m1	404	CDL	CB3-OB5-PB2-OB3
153	m1	404	CDL	CB3-OB5-PB2-OB4
153	m1	405	CDL	CA2-OA2-PA1-OA3
153	m1	405	CDL	CA2-OA2-PA1-OA5
153	m1	405	CDL	CA3-OA5-PA1-OA3
153	m1	405	CDL	CB2-OB2-PB2-OB4
153	m1	405	CDL	CB3-OB5-PB2-OB3
153	m2	401	CDL	CB2-OB2-PB2-OB3
153	m2	401	CDL	CB2-OB2-PB2-OB5
153	m2	403	CDL	CA3-OA5-PA1-OA4
153	m2	403	CDL	CB2-OB2-PB2-OB3
153	m2	403	CDL	CB2-OB2-PB2-OB4
153	m2	403	CDL	CB2-OB2-PB2-OB5
153	m2	403	CDL	CB3-OB5-PB2-OB2
153	m2	403	CDL	CB3-OB5-PB2-OB3
153	m2	403	CDL	CB3-OB5-PB2-OB4
153	m2	404	CDL	CA3-OA5-PA1-OA4
153	m3	401	CDL	CA2-OA2-PA1-OA3
153	m3	403	CDL	CA3-OA5-PA1-OA4
153	m3	403	CDL	CB3-OB5-PB2-OB2
153	m3	403	CDL	CB3-OB5-PB2-OB4
153	n	304	CDL	CA2-OA2-PA1-OA4
153	n	304	CDL	CA3-OA5-PA1-OA4
153	n	304	CDL	CB2-OB2-PB2-OB3
153	n	304	CDL	CB2-OB2-PB2-OB4
153	n	304	CDL	CB2-OB2-PB2-OB5
153	n	304	CDL	CB3-OB5-PB2-OB3
153	n	304	CDL	CB3-OB5-PB2-OB4
153	q	201	CDL	CB2-OB2-PB2-OB3
153	q	201	CDL	CB2-OB2-PB2-OB4
153	q	201	CDL	CB2-OB2-PB2-OB5
153	q	202	CDL	CB4-CB3-OB5-PB2
153	q	203	CDL	CA2-OA2-PA1-OA3
153	q	203	CDL	CA2-OA2-PA1-OA4
153	q	203	CDL	CA2-OA2-PA1-OA5
153	q	203	CDL	CA3-OA5-PA1-OA3
153	q	203	CDL	CA3-OA5-PA1-OA4
153	r	201	CDL	CA3-OA5-PA1-OA3
153	r	201	CDL	CA3-OA5-PA1-OA4
153	r	201	CDL	CB2-OB2-PB2-OB3
153	r	201	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	r	201	CDL	CB4-CB3-OB5-PB2
153	sd	101	CDL	CA2-OA2-PA1-OA3
153	sd	101	CDL	CB2-OB2-PB2-OB4
153	sd	101	CDL	CB2-OB2-PB2-OB5
153	sd	101	CDL	CB3-OB5-PB2-OB4
153	t	201	CDL	CA3-OA5-PA1-OA3
153	t	201	CDL	CB3-OB5-PB2-OB3
153	t	201	CDL	CB3-OB5-PB2-OB4
153	t	201	CDL	OB5-CB3-CB4-OB6
153	t	202	CDL	CA2-OA2-PA1-OA4
153	t	203	CDL	O1-C1-CB2-OB2
153	t	203	CDL	CB3-OB5-PB2-OB3
153	t	204	CDL	CA3-OA5-PA1-OA2
153	t	204	CDL	CA3-OA5-PA1-OA3
153	t	204	CDL	CB3-OB5-PB2-OB2
153	t	204	CDL	CB4-CB3-OB5-PB2
153	u	201	CDL	CA2-OA2-PA1-OA3
153	u	201	CDL	CA2-OA2-PA1-OA5
153	u	201	CDL	CA3-OA5-PA1-OA3
153	u	201	CDL	CA3-OA5-PA1-OA4
153	vb	701	CDL	CA2-OA2-PA1-OA3
153	vb	701	CDL	OA6-CA4-CA6-OA8
153	vb	704	CDL	CA2-OA2-PA1-OA3
153	vb	704	CDL	CA2-OA2-PA1-OA4
153	vb	704	CDL	CA2-OA2-PA1-OA5
153	vb	704	CDL	CB2-OB2-PB2-OB3
153	vb	704	CDL	CB2-OB2-PB2-OB4
153	vb	704	CDL	CB2-OB2-PB2-OB5
153	w	202	CDL	CB3-OB5-PB2-OB3
153	y5	201	CDL	CA3-OA5-PA1-OA4
153	y7	501	CDL	CA2-OA2-PA1-OA3
153	y7	501	CDL	CA2-OA2-PA1-OA4
153	y7	501	CDL	CA2-OA2-PA1-OA5
153	y7	501	CDL	CA3-OA5-PA1-OA3
153	z	101	CDL	CA2-OA2-PA1-OA3
153	z	101	CDL	CB3-OB5-PB2-OB4
153	2b	201	CDL	CB2-OB2-PB2-OB4
153	2b	201	CDL	CB3-OB5-PB2-OB4
153	5b	201	CDL	CA2-OA2-PA1-OA3
153	5b	201	CDL	CB2-OB2-PB2-OB4
153	5b	201	CDL	CB3-OB5-PB2-OB3
153	a1	101	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	a1	101	CDL	CA2-OA2-PA1-OA5
153	a1	101	CDL	CA3-OA5-PA1-OA2
153	a1	101	CDL	CA3-OA5-PA1-OA3
153	a1	101	CDL	CA3-OA5-PA1-OA4
153	a1	101	CDL	CB3-OB5-PB2-OB3
153	a9	402	CDL	CA3-OA5-PA1-OA3
153	a9	402	CDL	CB3-OB5-PB2-OB3
153	a9	403	CDL	CA2-OA2-PA1-OA3
153	a9	403	CDL	CA2-OA2-PA1-OA4
153	a9	403	CDL	CA2-OA2-PA1-OA5
153	a9	403	CDL	CA3-OA5-PA1-OA2
153	a9	403	CDL	CA3-OA5-PA1-OA3
153	a9	403	CDL	CA3-OA5-PA1-OA4
153	a9	403	CDL	CB2-OB2-PB2-OB3
153	a9	403	CDL	CB3-OB5-PB2-OB4
153	al	301	CDL	CA3-OA5-PA1-OA2
153	al	301	CDL	CB2-OB2-PB2-OB3
153	al	301	CDL	CB2-OB2-PB2-OB4
153	al	301	CDL	CB3-OB5-PB2-OB3
153	am	201	CDL	CA2-OA2-PA1-OA3
153	am	201	CDL	CA2-OA2-PA1-OA4
153	am	201	CDL	CB2-OB2-PB2-OB3
153	am	201	CDL	CB2-OB2-PB2-OB4
153	an	302	CDL	C1-CA2-OA2-PA1
153	an	302	CDL	CB2-OB2-PB2-OB4
153	b3	101	CDL	CB2-OB2-PB2-OB3
153	b3	101	CDL	CB2-OB2-PB2-OB4
153	b3	101	CDL	CB2-OB2-PB2-OB5
153	b3	102	CDL	CA2-OA2-PA1-OA3
153	b3	102	CDL	CA2-OA2-PA1-OA4
153	b3	102	CDL	CA2-OA2-PA1-OA5
153	b4	201	CDL	CA2-OA2-PA1-OA3
153	b8	302	CDL	CB3-OB5-PB2-OB3
153	bm	301	CDL	CA2-OA2-PA1-OA3
153	bm	301	CDL	CB3-OB5-PB2-OB4
153	c4	401	CDL	CA2-OA2-PA1-OA3
153	c4	401	CDL	CA2-OA2-PA1-OA4
153	c4	401	CDL	CA3-OA5-PA1-OA3
153	n5	806	CDL	CA2-OA2-PA1-OA3
153	n5	806	CDL	CA2-OA2-PA1-OA5
153	n5	806	CDL	CA3-OA5-PA1-OA3
153	n5	806	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	n6	302	CDL	CA2-OA2-PA1-OA3
153	n6	302	CDL	CA2-OA2-PA1-OA4
153	n6	302	CDL	CA3-OA5-PA1-OA3
153	n6	302	CDL	CB2-OB2-PB2-OB4
153	p1	402	CDL	CA2-OA2-PA1-OA3
153	p1	402	CDL	CB2-OB2-PB2-OB3
153	p1	402	CDL	CB3-OB5-PB2-OB2
153	p1	402	CDL	CB3-OB5-PB2-OB3
153	p1	402	CDL	CB3-OB5-PB2-OB4
153	p1	403	CDL	CA2-OA2-PA1-OA3
153	p1	403	CDL	CA2-OA2-PA1-OA4
153	p1	403	CDL	CA2-OA2-PA1-OA5
153	p1	403	CDL	CA3-OA5-PA1-OA4
153	qB	601	CDL	CA2-OA2-PA1-OA3
153	qB	601	CDL	CA2-OA2-PA1-OA4
153	qB	601	CDL	CA2-OA2-PA1-OA5
153	qC	504	CDL	CA3-OA5-PA1-OA3
153	qC	504	CDL	CB2-OB2-PB2-OB4
153	qC	504	CDL	CB3-OB5-PB2-OB4
153	qD	402	CDL	CA2-OA2-PA1-OA4
153	qD	402	CDL	CA3-OA5-PA1-OA3
153	qD	402	CDL	CB2-OB2-PB2-OB3
153	qD	402	CDL	CB2-OB2-PB2-OB4
153	qD	402	CDL	CB3-OB5-PB2-OB3
153	qG	402	CDL	CA2-OA2-PA1-OA3
153	qG	402	CDL	CA2-OA2-PA1-OA4
153	qG	402	CDL	CA2-OA2-PA1-OA5
153	qG	402	CDL	CA3-OA5-PA1-OA3
153	qG	402	CDL	CA3-OA5-PA1-OA4
153	qG	402	CDL	CB2-OB2-PB2-OB3
153	qH	201	CDL	O1-C1-CB2-OB2
153	qH	201	CDL	CA2-OA2-PA1-OA3
153	qH	201	CDL	CB2-OB2-PB2-OB3
153	qH	201	CDL	CB2-OB2-PB2-OB5
153	qH	201	CDL	CB3-OB5-PB2-OB3
153	qI	203	CDL	CA2-OA2-PA1-OA5
153	qI	203	CDL	CB2-OB2-PB2-OB5
153	qI	203	CDL	CB3-OB5-PB2-OB3
153	qc	504	CDL	CA2-OA2-PA1-OA3
153	qc	504	CDL	CA3-OA5-PA1-OA2
153	qc	504	CDL	CA3-OA5-PA1-OA3
153	qc	504	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qc	504	CDL	CB3-OB5-PB2-OB2
153	qc	504	CDL	CB3-OB5-PB2-OB3
153	qc	504	CDL	CB3-OB5-PB2-OB4
153	qc	505	CDL	CA2-OA2-PA1-OA3
153	qc	505	CDL	CA3-OA5-PA1-OA3
153	qc	505	CDL	CB2-OB2-PB2-OB3
153	qc	505	CDL	CB2-OB2-PB2-OB4
153	qc	505	CDL	CB3-OB5-PB2-OB2
153	qc	505	CDL	CB3-OB5-PB2-OB3
153	qc	505	CDL	CB3-OB5-PB2-OB4
153	qc	508	CDL	CA2-OA2-PA1-OA3
153	qg	402	CDL	CA3-OA5-PA1-OA2
153	qi	202	CDL	CA3-OA5-PA1-OA2
153	qi	202	CDL	CA3-OA5-PA1-OA3
153	qi	202	CDL	CA3-OA5-PA1-OA4
153	t1	601	CDL	CA3-OA5-PA1-OA3
153	t1	601	CDL	CB3-OB5-PB2-OB3
153	t1	601	CDL	CB3-OB5-PB2-OB4
153	t5	301	CDL	CA2-OA2-PA1-OA3
153	t5	301	CDL	CA2-OA2-PA1-OA4
153	t5	301	CDL	CA2-OA2-PA1-OA5
153	t5	301	CDL	CA3-OA5-PA1-OA3
153	t5	301	CDL	CB2-OB2-PB2-OB3
153	t5	301	CDL	CB3-OB5-PB2-OB3
153	t7	201	CDL	CA2-OA2-PA1-OA4
153	t7	201	CDL	CA2-OA2-PA1-OA5
153	t7	201	CDL	CB2-OB2-PB2-OB3
153	t7	201	CDL	CB2-OB2-PB2-OB4
153	t7	201	CDL	CB2-OB2-PB2-OB5
153	td	101	CDL	CA2-OA2-PA1-OA5
153	td	101	CDL	CB2-OB2-PB2-OB3
153	td	101	CDL	CB3-OB5-PB2-OB3
153	td	101	CDL	CB3-OB5-PB2-OB4
153	te	101	CDL	CB2-OB2-PB2-OB3
153	te	101	CDL	CB2-OB2-PB2-OB4
153	te	101	CDL	CB3-OB5-PB2-OB3
153	te	101	CDL	CB3-OB5-PB2-OB4
153	th	200	CDL	CA3-OA5-PA1-OA3
153	th	200	CDL	OA6-CA4-CA6-OA8
153	th	200	CDL	CB2-OB2-PB2-OB4
153	th	200	CDL	CB2-OB2-PB2-OB5
153	2G	201	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2G	201	CDL	CB2-OB2-PB2-OB4
153	2G	201	CDL	CB2-OB2-PB2-OB5
153	2G	201	CDL	CB3-OB5-PB2-OB3
153	2G	203	CDL	CA2-OA2-PA1-OA4
153	2G	203	CDL	CA3-OA5-PA1-OA2
153	2G	204	CDL	CA2-OA2-PA1-OA3
153	2G	204	CDL	CA2-OA2-PA1-OA4
153	2G	204	CDL	CA3-OA5-PA1-OA4
153	2G	204	CDL	CB3-OB5-PB2-OB4
153	2K	101	CDL	CA3-OA5-PA1-OA4
153	2K	101	CDL	CB2-OB2-PB2-OB3
153	2K	101	CDL	CB2-OB2-PB2-OB4
153	2K	101	CDL	CB3-OB5-PB2-OB3
153	2K	101	CDL	CB3-OB5-PB2-OB4
153	2M	101	CDL	CA3-OA5-PA1-OA2
153	2M	101	CDL	CA3-OA5-PA1-OA3
153	2M	101	CDL	CA3-OA5-PA1-OA4
153	2M	101	CDL	CB2-OB2-PB2-OB3
153	2M	101	CDL	CB2-OB2-PB2-OB4
153	2O	101	CDL	CA2-OA2-PA1-OA4
153	2O	101	CDL	CA3-OA5-PA1-OA3
153	2O	101	CDL	CA3-OA5-PA1-OA4
153	6A	201	CDL	CA2-OA2-PA1-OA3
153	6A	201	CDL	CA3-OA5-PA1-OA3
153	6A	201	CDL	CA3-OA5-PA1-OA4
153	6C	202	CDL	CB2-OB2-PB2-OB3
153	6C	202	CDL	CB2-OB2-PB2-OB5
153	6C	202	CDL	CB3-OB5-PB2-OB3
153	6C	202	CDL	CB3-OB5-PB2-OB4
153	6C	202	CDL	OB5-CB3-CB4-OB6
153	6C	203	CDL	CA2-OA2-PA1-OA3
153	6C	203	CDL	CB3-OB5-PB2-OB2
153	7A	201	CDL	CA2-OA2-PA1-OA4
153	7A	201	CDL	CA3-OA5-PA1-OA3
153	7A	201	CDL	CB2-OB2-PB2-OB3
153	7A	203	CDL	CA2-OA2-PA1-OA3
153	7A	203	CDL	CB3-OB5-PB2-OB3
153	7C	301	CDL	CB3-OB5-PB2-OB4
153	7C	302	CDL	CA3-OA5-PA1-OA2
153	7C	302	CDL	CA3-OA5-PA1-OA3
153	7C	302	CDL	CB2-OB2-PB2-OB3
153	A	502	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	A	502	CDL	CB2-OB2-PB2-OB4
153	A	504	CDL	CA2-OA2-PA1-OA3
153	A	504	CDL	CA2-OA2-PA1-OA4
153	A	504	CDL	CB3-OB5-PB2-OB2
153	A	504	CDL	CB3-OB5-PB2-OB3
153	B	501	CDL	CA2-OA2-PA1-OA3
153	B	501	CDL	CA2-OA2-PA1-OA4
153	B	501	CDL	CA2-OA2-PA1-OA5
153	B	501	CDL	CA3-OA5-PA1-OA2
153	B	501	CDL	CA3-OA5-PA1-OA3
153	B	501	CDL	CA3-OA5-PA1-OA4
153	C1	701	CDL	CA2-OA2-PA1-OA3
153	C1	701	CDL	CA2-OA2-PA1-OA4
153	C1	701	CDL	CA2-OA2-PA1-OA5
153	C1	701	CDL	CB2-OB2-PB2-OB3
153	C1	701	CDL	CB2-OB2-PB2-OB4
153	C1	701	CDL	CB3-OB5-PB2-OB2
153	C1	701	CDL	CB3-OB5-PB2-OB3
153	C1	707	CDL	CA3-OA5-PA1-OA3
153	C1	707	CDL	CB3-OB5-PB2-OB2
153	C1	707	CDL	CB3-OB5-PB2-OB3
153	C1	707	CDL	CB3-OB5-PB2-OB4
153	C1	708	CDL	C1-CA2-OA2-PA1
153	C1	708	CDL	CA2-OA2-PA1-OA4
153	C1	708	CDL	CB2-OB2-PB2-OB3
153	C1	708	CDL	CB2-OB2-PB2-OB4
153	C1	708	CDL	CB2-OB2-PB2-OB5
153	C1	708	CDL	CB3-OB5-PB2-OB3
153	C1	712	CDL	CB2-OB2-PB2-OB3
153	C3	604	CDL	CA2-OA2-PA1-OA3
153	C3	604	CDL	CA2-OA2-PA1-OA4
153	E	401	CDL	CA3-OA5-PA1-OA2
153	E	401	CDL	CA3-OA5-PA1-OA3
153	E	401	CDL	CA3-OA5-PA1-OA4
153	E	401	CDL	CB2-OB2-PB2-OB3
153	E	401	CDL	CB2-OB2-PB2-OB4
153	E	401	CDL	CB3-OB5-PB2-OB3
153	E	402	CDL	CA2-OA2-PA1-OA3
153	E	403	CDL	CB2-OB2-PB2-OB3
153	E	403	CDL	CB2-OB2-PB2-OB4
153	F	402	CDL	CB3-OB5-PB2-OB2
153	F	402	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	F	402	CDL	CB3-OB5-PB2-OB4
153	FS	204	CDL	CB3-OB5-PB2-OB3
153	FS	204	CDL	CB3-OB5-PB2-OB4
153	I	302	CDL	CA3-OA5-PA1-OA3
153	I	303	CDL	CA3-OA5-PA1-OA3
153	I	303	CDL	CB2-OB2-PB2-OB3
153	I	303	CDL	OB5-CB3-CB4-OB6
153	J	301	CDL	CA2-OA2-PA1-OA3
153	J	301	CDL	CA3-OA5-PA1-OA2
153	J	301	CDL	CB3-OB5-PB2-OB3
153	J	301	CDL	CB3-OB5-PB2-OB4
153	L	301	CDL	CA3-OA5-PA1-OA2
153	L	301	CDL	CB2-OB2-PB2-OB3
153	L	301	CDL	CB2-OB2-PB2-OB4
153	L	301	CDL	CB3-OB5-PB2-OB2
153	L	301	CDL	CB3-OB5-PB2-OB3
153	L	301	CDL	CB3-OB5-PB2-OB4
153	M	301	CDL	CA2-OA2-PA1-OA3
153	M	301	CDL	CA2-OA2-PA1-OA4
153	M	301	CDL	CA3-OA5-PA1-OA2
153	M	301	CDL	CA3-OA5-PA1-OA3
153	M	301	CDL	CA3-OA5-PA1-OA4
153	M	301	CDL	CB2-OB2-PB2-OB4
153	M	304	CDL	CA3-OA5-PA1-OA4
153	M	304	CDL	CB2-OB2-PB2-OB3
153	M	304	CDL	CB2-OB2-PB2-OB4
153	M	305	CDL	CA2-OA2-PA1-OA3
153	M	306	CDL	CA2-OA2-PA1-OA5
153	M	306	CDL	CA4-CA3-OA5-PA1
153	M	306	CDL	CB2-OB2-PB2-OB5
153	M	306	CDL	CB3-OB5-PB2-OB2
153	M	306	CDL	CB3-OB5-PB2-OB3
153	M	306	CDL	CB3-OB5-PB2-OB4
153	M1	404	CDL	CA2-OA2-PA1-OA5
153	M1	404	CDL	CB2-OB2-PB2-OB3
153	M1	404	CDL	CB2-OB2-PB2-OB4
153	M1	404	CDL	CB3-OB5-PB2-OB3
153	M1	405	CDL	CA2-OA2-PA1-OA3
153	M1	405	CDL	CA2-OA2-PA1-OA5
153	M1	405	CDL	CA3-OA5-PA1-OA3
153	M1	405	CDL	CB2-OB2-PB2-OB4
153	M1	405	CDL	CB3-OB5-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	M2	401	CDL	CB2-OB2-PB2-OB3
153	M2	401	CDL	CB2-OB2-PB2-OB5
153	M2	403	CDL	CA3-OA5-PA1-OA4
153	M2	403	CDL	CB2-OB2-PB2-OB3
153	M2	403	CDL	CB2-OB2-PB2-OB4
153	M2	403	CDL	CB2-OB2-PB2-OB5
153	M2	403	CDL	CB3-OB5-PB2-OB2
153	M2	403	CDL	CB3-OB5-PB2-OB3
153	M2	403	CDL	CB3-OB5-PB2-OB4
153	M2	404	CDL	CA3-OA5-PA1-OA4
153	M3	401	CDL	CA2-OA2-PA1-OA3
153	M3	403	CDL	CA3-OA5-PA1-OA2
153	M3	403	CDL	CB3-OB5-PB2-OB2
153	M3	403	CDL	CB3-OB5-PB2-OB4
153	N	304	CDL	CA2-OA2-PA1-OA4
153	N	304	CDL	CA3-OA5-PA1-OA4
153	N	304	CDL	CB2-OB2-PB2-OB3
153	N	304	CDL	CB2-OB2-PB2-OB4
153	N	304	CDL	CB2-OB2-PB2-OB5
153	N	304	CDL	CB3-OB5-PB2-OB3
153	N	304	CDL	CB3-OB5-PB2-OB4
153	Q	201	CDL	CB2-OB2-PB2-OB3
153	Q	201	CDL	CB2-OB2-PB2-OB4
153	Q	201	CDL	CB2-OB2-PB2-OB5
153	Q	202	CDL	CB4-CB3-OB5-PB2
153	R	201	CDL	CA3-OA5-PA1-OA3
153	R	201	CDL	CA3-OA5-PA1-OA4
153	R	201	CDL	CB2-OB2-PB2-OB3
153	R	201	CDL	CB3-OB5-PB2-OB2
153	R	201	CDL	CB4-CB3-OB5-PB2
153	SD	101	CDL	CA2-OA2-PA1-OA3
153	SD	101	CDL	CB2-OB2-PB2-OB4
153	SD	101	CDL	CB2-OB2-PB2-OB5
153	SD	101	CDL	CB3-OB5-PB2-OB4
153	T	201	CDL	CA3-OA5-PA1-OA3
153	T	201	CDL	CB3-OB5-PB2-OB3
153	T	201	CDL	CB3-OB5-PB2-OB4
153	T	201	CDL	OB5-CB3-CB4-OB6
153	T	202	CDL	CA2-OA2-PA1-OA4
153	T	203	CDL	O1-C1-CB2-OB2
153	T	203	CDL	CB3-OB5-PB2-OB3
153	T	204	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	T	204	CDL	CA3-OA5-PA1-OA3
153	T	204	CDL	CB3-OB5-PB2-OB2
153	T	204	CDL	CB4-CB3-OB5-PB2
153	U	201	CDL	CA2-OA2-PA1-OA3
153	U	201	CDL	CA2-OA2-PA1-OA5
153	U	201	CDL	CA3-OA5-PA1-OA3
153	U	201	CDL	CA3-OA5-PA1-OA4
153	VB	701	CDL	CA2-OA2-PA1-OA3
153	VB	701	CDL	OA6-CA4-CA6-OA8
153	VB	703	CDL	CA2-OA2-PA1-OA3
153	VB	703	CDL	CA2-OA2-PA1-OA4
153	VB	703	CDL	CA2-OA2-PA1-OA5
153	VB	703	CDL	CA3-OA5-PA1-OA3
153	VB	703	CDL	CA3-OA5-PA1-OA4
153	VB	705	CDL	CB2-C1-CA2-OA2
153	VB	706	CDL	CA2-OA2-PA1-OA3
153	VB	706	CDL	CA2-OA2-PA1-OA4
153	VB	706	CDL	CA2-OA2-PA1-OA5
153	VB	706	CDL	CB2-OB2-PB2-OB3
153	VB	706	CDL	CB2-OB2-PB2-OB4
153	VB	706	CDL	CB2-OB2-PB2-OB5
153	W	202	CDL	CB3-OB5-PB2-OB3
153	Y5	201	CDL	CA3-OA5-PA1-OA4
153	Y7	501	CDL	CA2-OA2-PA1-OA3
153	Y7	501	CDL	CA2-OA2-PA1-OA4
153	Y7	501	CDL	CA2-OA2-PA1-OA5
153	Y7	501	CDL	CA3-OA5-PA1-OA3
153	Z	101	CDL	CA2-OA2-PA1-OA3
153	Z	101	CDL	CB3-OB5-PB2-OB4
153	2B	201	CDL	CB2-OB2-PB2-OB4
153	2B	201	CDL	CB3-OB5-PB2-OB4
153	5B	201	CDL	CA2-OA2-PA1-OA3
153	5B	201	CDL	CB2-OB2-PB2-OB4
153	5B	201	CDL	CB3-OB5-PB2-OB3
153	A1	101	CDL	CA2-OA2-PA1-OA5
153	A1	101	CDL	CB2-OB2-PB2-OB3
153	A1	101	CDL	CB3-OB5-PB2-OB3
153	A1	101	CDL	CB3-OB5-PB2-OB4
153	A1	102	CDL	CA2-OA2-PA1-OA3
153	A1	102	CDL	CA2-OA2-PA1-OA5
153	A1	102	CDL	CA3-OA5-PA1-OA2
153	A1	102	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	A1	102	CDL	CA3-OA5-PA1-OA4
153	A1	102	CDL	CB3-OB5-PB2-OB3
153	A9	402	CDL	CA2-OA2-PA1-OA5
153	A9	402	CDL	CA3-OA5-PA1-OA3
153	A9	402	CDL	CB3-OB5-PB2-OB3
153	A9	403	CDL	CA2-OA2-PA1-OA3
153	A9	403	CDL	CA2-OA2-PA1-OA4
153	A9	403	CDL	CA3-OA5-PA1-OA2
153	A9	403	CDL	CA3-OA5-PA1-OA3
153	A9	403	CDL	CA3-OA5-PA1-OA4
153	A9	403	CDL	CB2-OB2-PB2-OB3
153	A9	403	CDL	CB3-OB5-PB2-OB4
153	AL	301	CDL	CA3-OA5-PA1-OA2
153	AL	301	CDL	CB2-OB2-PB2-OB3
153	AL	301	CDL	CB2-OB2-PB2-OB4
153	AL	301	CDL	CB3-OB5-PB2-OB3
153	AM	201	CDL	CA2-OA2-PA1-OA3
153	AM	201	CDL	CA2-OA2-PA1-OA4
153	AM	201	CDL	CB2-OB2-PB2-OB3
153	AM	201	CDL	CB2-OB2-PB2-OB4
153	AN	302	CDL	C1-CA2-OA2-PA1
153	AN	302	CDL	CB2-OB2-PB2-OB4
153	B3	101	CDL	CB2-OB2-PB2-OB3
153	B3	101	CDL	CB2-OB2-PB2-OB4
153	B3	101	CDL	CB2-OB2-PB2-OB5
153	B3	102	CDL	O1-C1-CA2-OA2
153	B3	102	CDL	CA2-OA2-PA1-OA3
153	B3	102	CDL	CA2-OA2-PA1-OA4
153	B3	102	CDL	CA2-OA2-PA1-OA5
153	B4	201	CDL	CA2-OA2-PA1-OA3
153	B8	302	CDL	CB3-OB5-PB2-OB3
153	BM	301	CDL	CA2-OA2-PA1-OA3
153	BM	301	CDL	CB3-OB5-PB2-OB4
153	C4	401	CDL	CA2-OA2-PA1-OA3
153	C4	401	CDL	CA2-OA2-PA1-OA4
153	C4	401	CDL	CA3-OA5-PA1-OA3
153	N5	806	CDL	CA2-OA2-PA1-OA3
153	N5	806	CDL	CA2-OA2-PA1-OA5
153	N5	806	CDL	CA3-OA5-PA1-OA3
153	N5	806	CDL	CB2-OB2-PB2-OB3
153	N6	302	CDL	CA2-OA2-PA1-OA3
153	N6	302	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	N6	302	CDL	CA3-OA5-PA1-OA3
153	N6	302	CDL	CB2-OB2-PB2-OB4
153	P1	402	CDL	CA2-OA2-PA1-OA3
153	P1	402	CDL	CB2-OB2-PB2-OB3
153	P1	402	CDL	CB3-OB5-PB2-OB2
153	P1	402	CDL	CB3-OB5-PB2-OB3
153	P1	402	CDL	CB3-OB5-PB2-OB4
153	P1	403	CDL	CA2-OA2-PA1-OA3
153	P1	403	CDL	CA2-OA2-PA1-OA4
153	P1	403	CDL	CA2-OA2-PA1-OA5
153	P1	403	CDL	CA3-OA5-PA1-OA4
153	QB	601	CDL	CA2-OA2-PA1-OA3
153	QB	601	CDL	CA2-OA2-PA1-OA4
153	QB	601	CDL	CA2-OA2-PA1-OA5
153	QC	504	CDL	CA3-OA5-PA1-OA3
153	QC	504	CDL	CB2-OB2-PB2-OB4
153	QC	504	CDL	CB3-OB5-PB2-OB4
153	QD	402	CDL	CA2-OA2-PA1-OA4
153	QD	402	CDL	CA3-OA5-PA1-OA3
153	QD	402	CDL	CB2-OB2-PB2-OB3
153	QD	402	CDL	CB2-OB2-PB2-OB4
153	QD	402	CDL	CB3-OB5-PB2-OB3
153	QG	402	CDL	CA2-OA2-PA1-OA3
153	QG	402	CDL	CA2-OA2-PA1-OA4
153	QG	402	CDL	CA2-OA2-PA1-OA5
153	QG	402	CDL	CA3-OA5-PA1-OA3
153	QG	402	CDL	CA3-OA5-PA1-OA4
153	QG	402	CDL	CB2-OB2-PB2-OB3
153	QH	201	CDL	O1-C1-CB2-OB2
153	QH	201	CDL	CA2-OA2-PA1-OA3
153	QH	201	CDL	CB2-OB2-PB2-OB3
153	QH	201	CDL	CB2-OB2-PB2-OB5
153	QH	201	CDL	CB3-OB5-PB2-OB3
153	QI	203	CDL	CA2-OA2-PA1-OA5
153	QI	203	CDL	CB3-OB5-PB2-OB3
153	Qc	504	CDL	CA2-OA2-PA1-OA3
153	Qc	504	CDL	CA3-OA5-PA1-OA2
153	Qc	504	CDL	CA3-OA5-PA1-OA3
153	Qc	504	CDL	CA3-OA5-PA1-OA4
153	Qc	504	CDL	CB3-OB5-PB2-OB2
153	Qc	504	CDL	CB3-OB5-PB2-OB3
153	Qc	504	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qc	505	CDL	CA2-OA2-PA1-OA3
153	Qc	505	CDL	CA3-OA5-PA1-OA3
153	Qc	505	CDL	CB2-OB2-PB2-OB3
153	Qc	505	CDL	CB2-OB2-PB2-OB4
153	Qc	505	CDL	CB3-OB5-PB2-OB2
153	Qc	505	CDL	CB3-OB5-PB2-OB3
153	Qc	505	CDL	CB3-OB5-PB2-OB4
153	Qc	508	CDL	CA2-OA2-PA1-OA3
153	Qg	402	CDL	CA3-OA5-PA1-OA2
153	Qi	202	CDL	CA3-OA5-PA1-OA2
153	Qi	202	CDL	CA3-OA5-PA1-OA3
153	Qi	202	CDL	CA3-OA5-PA1-OA4
153	T1	601	CDL	CA3-OA5-PA1-OA3
153	T1	601	CDL	CB3-OB5-PB2-OB3
153	T1	601	CDL	CB3-OB5-PB2-OB4
153	T5	301	CDL	CA2-OA2-PA1-OA3
153	T5	301	CDL	CA2-OA2-PA1-OA4
153	T5	301	CDL	CA2-OA2-PA1-OA5
153	T5	301	CDL	CA3-OA5-PA1-OA3
153	T5	301	CDL	CB2-OB2-PB2-OB3
153	T5	301	CDL	CB3-OB5-PB2-OB3
153	T7	201	CDL	CA2-OA2-PA1-OA4
153	T7	201	CDL	CA2-OA2-PA1-OA5
153	T7	201	CDL	CB2-OB2-PB2-OB3
153	T7	201	CDL	CB2-OB2-PB2-OB4
153	T7	201	CDL	CB2-OB2-PB2-OB5
153	TE	101	CDL	CB2-OB2-PB2-OB3
153	TE	101	CDL	CB2-OB2-PB2-OB4
153	TE	101	CDL	CB3-OB5-PB2-OB4
153	TH	200	CDL	CA3-OA5-PA1-OA3
153	TH	200	CDL	OA6-CA4-CA6-OA8
153	TH	200	CDL	CB2-OB2-PB2-OB4
153	TH	200	CDL	CB2-OB2-PB2-OB5
153	C	301	CDL	CB3-OB5-PB2-OB3
153	C	301	CDL	CB3-OB5-PB2-OB4
153	c	301	CDL	CB3-OB5-PB2-OB3
153	c	301	CDL	CB3-OB5-PB2-OB4
153	u1	101	CDL	CA2-OA2-PA1-OA4
153	u1	101	CDL	CB3-OB5-PB2-OB2
153	u1	101	CDL	CB3-OB5-PB2-OB3
153	U1	101	CDL	CA2-OA2-PA1-OA4
153	U1	101	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	U1	101	CDL	CB3-OB5-PB2-OB3
154	c1	702	HEA	C1A-C2A-CAA-CBA
154	c1	702	HEA	C3A-C2A-CAA-CBA
154	c1	702	HEA	C19-C20-C21-C22
154	c1	702	HEA	C21-C22-C23-C24
154	c1	708	HEA	C19-C20-C21-C22
154	C1	702	HEA	C1A-C2A-CAA-CBA
154	C1	702	HEA	C3A-C2A-CAA-CBA
154	C1	702	HEA	C19-C20-C21-C22
154	C1	702	HEA	C21-C22-C23-C24
154	C1	703	HEA	C19-C20-C21-C22
158	i	303	3PE	O13-C11-C12-N
158	m2	408	3PE	C1-O11-P-O12
158	m2	408	3PE	C1-O11-P-O14
158	m2	408	3PE	C11-O13-P-O14
158	m3	402	3PE	O13-C11-C12-N
158	sc	101	3PE	C1-O11-P-O12
158	sc	101	3PE	C1-O11-P-O13
158	sc	101	3PE	C1-O11-P-O14
158	sc	101	3PE	C11-O13-P-O12
158	sc	101	3PE	C11-O13-P-O14
158	sc	101	3PE	O13-C11-C12-N
158	vb	705	3PE	C1-O11-P-O12
158	w	203	3PE	C1-O11-P-O12
158	w	203	3PE	O13-C11-C12-N
158	y5	202	3PE	O13-C11-C12-N
158	a3	201	3PE	C11-O13-P-O12
158	a3	202	3PE	C11-O13-P-O11
158	a3	202	3PE	C11-O13-P-O12
158	a3	202	3PE	C11-O13-P-O14
158	a3	202	3PE	O13-C11-C12-N
158	an	303	3PE	O13-C11-C12-N
158	an	305	3PE	C11-O13-P-O11
158	an	306	3PE	C1-O11-P-O12
158	an	306	3PE	C1-O11-P-O14
158	b4	202	3PE	C11-O13-P-O11
158	b4	202	3PE	C11-O13-P-O14
158	bm	302	3PE	C11-O13-P-O12
158	bm	302	3PE	O13-C11-C12-N
158	c4	402	3PE	C11-O13-P-O12
158	c4	402	3PE	C12-C11-O13-P
158	g2	301	3PE	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	g2	301	3PE	O13-C11-C12-N
158	n4	601	3PE	C11-O13-P-O14
158	n5	802	3PE	C11-O13-P-O12
158	n5	802	3PE	C11-O13-P-O14
158	s8	304	3PE	C1-O11-P-O14
158	s8	304	3PE	O13-C11-C12-N
158	s8	304	3PE	O21-C2-C3-O31
158	t4	302	3PE	C11-O13-P-O12
158	t4	302	3PE	C11-O13-P-O14
158	t4	302	3PE	O13-C11-C12-N
158	t8	601	3PE	C1-O11-P-O12
158	t8	601	3PE	O13-C11-C12-N
158	t8	602	3PE	C11-O13-P-O12
158	t8	602	3PE	O13-C11-C12-N
158	t8	602	3PE	O21-C2-C3-O31
158	ta	201	3PE	C1-O11-P-O12
158	ta	201	3PE	C1-O11-P-O13
158	ta	201	3PE	C1-O11-P-O14
158	ta	201	3PE	C11-O13-P-O11
158	ta	201	3PE	C11-O13-P-O14
158	ta	201	3PE	O13-C11-C12-N
158	I	304	3PE	O13-C11-C12-N
158	M2	408	3PE	C1-O11-P-O12
158	M2	408	3PE	C1-O11-P-O14
158	M2	408	3PE	C11-O13-P-O14
158	M3	402	3PE	O13-C11-C12-N
158	SC	101	3PE	C1-O11-P-O12
158	SC	101	3PE	C1-O11-P-O13
158	SC	101	3PE	C1-O11-P-O14
158	SC	101	3PE	C11-O13-P-O12
158	SC	101	3PE	C11-O13-P-O14
158	VB	707	3PE	C1-O11-P-O12
158	W	203	3PE	C1-O11-P-O12
158	W	203	3PE	O13-C11-C12-N
158	Y5	202	3PE	O13-C11-C12-N
158	A3	201	3PE	C11-O13-P-O12
158	A3	202	3PE	C11-O13-P-O11
158	A3	202	3PE	C11-O13-P-O12
158	A3	202	3PE	C11-O13-P-O14
158	A3	202	3PE	O13-C11-C12-N
158	AN	303	3PE	O13-C11-C12-N
158	AN	305	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	AN	305	3PE	C11-O13-P-O12
158	AN	306	3PE	C1-O11-P-O12
158	AN	306	3PE	C1-O11-P-O14
158	B4	202	3PE	C11-O13-P-O11
158	B4	202	3PE	C11-O13-P-O14
158	BM	302	3PE	C11-O13-P-O12
158	BM	302	3PE	O13-C11-C12-N
158	C4	402	3PE	C11-O13-P-O12
158	C4	402	3PE	C12-C11-O13-P
158	G2	301	3PE	C1-O11-P-O14
158	G2	301	3PE	O13-C11-C12-N
158	N4	601	3PE	C11-O13-P-O14
158	N5	802	3PE	C11-O13-P-O12
158	N5	802	3PE	C11-O13-P-O14
158	S8	304	3PE	C1-O11-P-O14
158	S8	304	3PE	O13-C11-C12-N
158	S8	304	3PE	O21-C2-C3-O31
158	T4	302	3PE	C11-O13-P-O12
158	T4	302	3PE	C11-O13-P-O14
158	T4	302	3PE	O13-C11-C12-N
158	T8	601	3PE	C1-O11-P-O12
158	T8	601	3PE	O13-C11-C12-N
158	T8	602	3PE	C11-O13-P-O12
158	T8	602	3PE	O13-C11-C12-N
158	T8	602	3PE	O21-C2-C3-O31
158	TA	201	3PE	C1-O11-P-O12
158	TA	201	3PE	C1-O11-P-O13
158	TA	201	3PE	C1-O11-P-O14
158	TA	201	3PE	C11-O13-P-O11
158	TA	201	3PE	C11-O13-P-O14
158	TA	201	3PE	O13-C11-C12-N
159	m2	406	P5S	O-C-CA-CB
159	m2	406	P5S	OXT-C-CA-CB
159	m2	406	P5S	O19-C1-C2-O37
159	m2	406	P5S	C-CA-CB-OG
159	m2	406	P5S	N-CA-CB-OG
159	m2	406	P5S	CA-CB-OG-P12
159	m2	406	P5S	C3-O16-P12-OG
159	m2	406	P5S	C3-O16-P12-O13
159	m2	406	P5S	C3-O16-P12-O15
159	M2	406	P5S	O-C-CA-CB
159	M2	406	P5S	OXT-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
159	M2	406	P5S	O19-C1-C2-O37
159	M2	406	P5S	C-CA-CB-OG
159	M2	406	P5S	N-CA-CB-OG
159	M2	406	P5S	CA-CB-OG-P12
159	M2	406	P5S	C3-O16-P12-OG
159	M2	406	P5S	C3-O16-P12-O13
159	M2	406	P5S	C3-O16-P12-O15
160	r	202	PX2	C1-O4-P1-O1
160	r	202	PX2	C1-O4-P1-O3
160	y5	204	PX2	C1-O4-P1-O1
160	y5	204	PX2	C1-O4-P1-O2
160	y5	204	PX2	C1-O4-P1-O3
160	y5	204	PX2	O8-C16-O7-C2
160	y5	204	PX2	C17-C16-O7-C2
160	qh	201	PX2	C1-O4-P1-O1
160	qh	201	PX2	C1-O4-P1-O2
160	qh	201	PX2	C1-O4-P1-O3
160	R	202	PX2	C1-O4-P1-O1
160	R	202	PX2	C1-O4-P1-O2
160	R	202	PX2	C1-O4-P1-O3
160	Y5	204	PX2	C1-O4-P1-O1
160	Y5	204	PX2	C1-O4-P1-O2
160	Y5	204	PX2	C1-O4-P1-O3
160	Y5	204	PX2	C17-C16-O7-C2
160	Qh	201	PX2	C1-O4-P1-O1
160	Qh	201	PX2	C1-O4-P1-O2
160	Qh	201	PX2	C1-O4-P1-O3
160	Qh	201	PX2	O8-C16-O7-C2
160	Qh	201	PX2	C17-C16-O7-C2
161	sa	701	FAD	C5B-O5B-PA-O3P
161	sa	701	FAD	C2'-C3'-C4'-O4'
161	sa	701	FAD	O3'-C3'-C4'-O4'
161	SA	701	FAD	C5B-O5B-PA-O3P
161	SA	701	FAD	C2'-C3'-C4'-O4'
161	SA	701	FAD	O3'-C3'-C4'-O4'
164	sc	102	U10	C9-C11-C12-C13
164	sc	102	U10	C13-C14-C16-C17
164	sc	102	U10	C15-C14-C16-C17
164	sc	102	U10	C19-C21-C22-C23
164	sc	102	U10	C33-C34-C36-C37
164	sc	102	U10	C35-C34-C36-C37
164	b8	301	U10	C9-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
164	b8	301	U10	C13-C14-C16-C17
164	b8	301	U10	C15-C14-C16-C17
164	qc	501	U10	C12-C11-C9-C8
164	qc	501	U10	C12-C11-C9-C10
164	qc	501	U10	C23-C24-C26-C27
164	qc	507	U10	C18-C19-C21-C22
164	qc	507	U10	C20-C19-C21-C22
164	SC	102	U10	C9-C11-C12-C13
164	SC	102	U10	C13-C14-C16-C17
164	SC	102	U10	C15-C14-C16-C17
164	SC	102	U10	C19-C21-C22-C23
164	SC	102	U10	C33-C34-C36-C37
164	SC	102	U10	C35-C34-C36-C37
164	B8	301	U10	C9-C11-C12-C13
164	B8	301	U10	C13-C14-C16-C17
164	B8	301	U10	C15-C14-C16-C17
164	Qc	501	U10	C12-C11-C9-C10
164	Qc	501	U10	C23-C24-C26-C27
164	Qc	507	U10	C18-C19-C21-C22
164	Qc	507	U10	C20-C19-C21-C22
166	y5	203	HEM	C2B-C3B-CAB-CBB
166	Y5	203	HEM	C2B-C3B-CAB-CBB
168	ab	201	ZMP	C16-C17-C18-C21
168	ab	201	ZMP	C16-C17-C18-C19
168	ab	201	ZMP	C16-C17-C18-C20
168	ab	201	ZMP	C17-C16-N2-C15
168	ab	201	ZMP	C12-C11-S1-C10
168	ab	201	ZMP	C7-C8-C9-C10
168	AB	201	ZMP	C16-C17-C18-C21
168	AB	201	ZMP	C16-C17-C18-C19
168	AB	201	ZMP	C16-C17-C18-C20
168	AB	201	ZMP	C17-C16-N2-C15
168	AB	201	ZMP	C12-C11-S1-C10
168	AB	201	ZMP	C7-C8-C9-C10
169	b6	201	T7X	C7-O13-P1-O11
169	b6	201	T7X	C12-C10-O16-C8
169	b6	201	T7X	O17-C10-O16-C8
169	b6	201	T7X	C16-C17-C18-C19
169	B6	201	T7X	C7-O13-P1-O11
169	B6	201	T7X	C12-C10-O16-C8
169	B6	201	T7X	O17-C10-O16-C8
169	B6	201	T7X	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
170	b9	202	ADP	O4'-C4'-C5'-O5'
170	B9	202	ADP	O4'-C4'-C5'-O5'
154	c1	702	HEA	C21-C22-C23-C25
154	C1	702	HEA	C21-C22-C23-C25
160	Y5	204	PX2	O8-C16-O7-C2
168	ab	201	ZMP	C14-C13-N1-C12
168	AB	201	ZMP	C14-C13-N1-C12
164	sc	102	U10	C12-C11-C9-C10
164	SC	102	U10	C12-C11-C9-C10
164	Qc	501	U10	C12-C11-C9-C8
153	6c	201	CDL	O1-C1-CA2-OA2
153	a	505	CDL	O1-C1-CA2-OA2
153	b3	102	CDL	O1-C1-CA2-OA2
153	qg	402	CDL	O1-C1-CB2-OB2
153	6C	202	CDL	O1-C1-CA2-OA2
153	VB	705	CDL	O1-C1-CA2-OA2
153	Qg	402	CDL	O1-C1-CB2-OB2
168	ab	201	ZMP	O3-C16-N2-C15
168	AB	201	ZMP	O3-C16-N2-C15
159	m2	406	P5S	C41-C42-C43-C44
159	M2	406	P5S	C41-C42-C43-C44
159	m2	406	P5S	C23-C24-C25-C26
159	M2	406	P5S	C23-C24-C25-C26
161	sa	701	FAD	O4B-C4B-C5B-O5B
161	SA	701	FAD	O4B-C4B-C5B-O5B
152	qi	203	PC1	C2-C1-O11-P
152	Qi	203	PC1	C2-C1-O11-P
153	qD	402	CDL	CA4-CA3-OA5-PA1
153	QD	402	CDL	CA4-CA3-OA5-PA1
166	qC	501	HEM	C3D-CAD-CBD-CGD
166	qC	502	HEM	C3D-CAD-CBD-CGD
166	QC	501	HEM	C3D-CAD-CBD-CGD
166	QC	502	HEM	C3D-CAD-CBD-CGD
154	c1	702	HEA	C27-C19-C20-C21
154	c1	708	HEA	C27-C19-C20-C21
154	C1	702	HEA	C27-C19-C20-C21
154	C1	703	HEA	C27-C19-C20-C21
164	b8	301	U10	C35-C34-C36-C37
164	B8	301	U10	C35-C34-C36-C37
154	c1	702	HEA	C18-C19-C20-C21
154	c1	708	HEA	C18-C19-C20-C21
154	C1	702	HEA	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
154	C1	703	HEA	C18-C19-C20-C21
164	b8	301	U10	C33-C34-C36-C37
164	B8	301	U10	C33-C34-C36-C37
154	c1	702	HEA	C15-C16-C17-C18
154	c1	708	HEA	C15-C16-C17-C18
154	C1	702	HEA	C15-C16-C17-C18
154	C1	703	HEA	C15-C16-C17-C18
164	b8	301	U10	C19-C21-C22-C23
164	b8	301	U10	C24-C26-C27-C28
164	b8	301	U10	C29-C31-C32-C33
164	b8	301	U10	C44-C46-C47-C48
164	b8	301	U10	C49-C51-C52-C53
164	qc	501	U10	C14-C16-C17-C18
164	qc	501	U10	C19-C21-C22-C23
164	qc	507	U10	C9-C11-C12-C13
164	B8	301	U10	C19-C21-C22-C23
164	B8	301	U10	C24-C26-C27-C28
164	B8	301	U10	C29-C31-C32-C33
164	B8	301	U10	C44-C46-C47-C48
164	B8	301	U10	C49-C51-C52-C53
164	Qc	501	U10	C14-C16-C17-C18
164	Qc	501	U10	C19-C21-C22-C23
164	Qc	507	U10	C9-C11-C12-C13
168	ab	201	ZMP	O2-C13-N1-C12
168	AB	201	ZMP	O2-C13-N1-C12
161	sa	701	FAD	O3'-C3'-C4'-C5'
161	SA	701	FAD	O3'-C3'-C4'-C5'
161	sa	701	FAD	C2'-C3'-C4'-C5'
161	SA	701	FAD	C2'-C3'-C4'-C5'
159	m2	406	P5S	C17-C20-C21-C22
159	M2	406	P5S	C17-C20-C21-C22
153	2g	201	CDL	CA2-C1-CB2-OB2
153	6c	201	CDL	CB2-C1-CA2-OA2
153	t	203	CDL	CA2-C1-CB2-OB2
153	qg	402	CDL	CA2-C1-CB2-OB2
153	2G	201	CDL	CA2-C1-CB2-OB2
153	6C	202	CDL	CB2-C1-CA2-OA2
153	T	203	CDL	CA2-C1-CB2-OB2
153	Qg	402	CDL	CA2-C1-CB2-OB2
152	2f	303	PC1	C11-C12-N-C15
152	7a	202	PC1	C11-C12-N-C15
152	c2	703	PC1	C11-C12-N-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	c3	603	PC1	C11-C12-N-C13
152	c3	605	PC1	C11-C12-N-C13
152	fs	204	PC1	C11-C12-N-C13
152	n	301	PC1	C11-C12-N-C15
152	5b	202	PC1	C11-C12-N-C13
152	qB	602	PC1	C11-C12-N-C15
152	qb	602	PC1	C11-C12-N-C15
152	qj	101	PC1	C11-C12-N-C15
152	2F	303	PC1	C11-C12-N-C15
152	7A	202	PC1	C11-C12-N-C15
152	C2	701	PC1	C11-C12-N-C13
152	C3	603	PC1	C11-C12-N-C13
152	C3	605	PC1	C11-C12-N-C13
152	FS	201	PC1	C11-C12-N-C13
152	N	301	PC1	C11-C12-N-C15
152	5B	202	PC1	C11-C12-N-C13
152	QB	602	PC1	C11-C12-N-C15
152	QC	508	PC1	C11-C12-N-C13
152	Qb	602	PC1	C11-C12-N-C15
152	Qj	101	PC1	C11-C12-N-C15
160	r	202	PX2	C5-C4-O5-C3
160	Qh	201	PX2	C5-C4-O5-C3
153	c1	712	CDL	CB5-C51-C52-C53
153	C1	712	CDL	CB5-C51-C52-C53
153	a	505	CDL	OB5-CB3-CB4-OB6
153	al	301	CDL	OB5-CB3-CB4-OB6
153	VB	705	CDL	OB5-CB3-CB4-OB6
153	AL	301	CDL	OB5-CB3-CB4-OB6
153	2g	201	CDL	O1-C1-CB2-OB2
153	b3	101	CDL	O1-C1-CB2-OB2
153	2G	201	CDL	O1-C1-CB2-OB2
153	7c	301	CDL	CA5-C11-C12-C13
153	7C	301	CDL	CA5-C11-C12-C13
153	C1	708	CDL	CA7-C31-C32-C33
160	Qh	201	PX2	O6-C4-O5-C3
164	Qc	501	U10	C15-C14-C16-C17
164	sc	102	U10	C12-C11-C9-C8
164	SC	102	U10	C12-C11-C9-C8
160	Qh	201	PX2	C7-C8-C9-C10
152	w	204	PC1	C31-C32-C33-C34
152	W	204	PC1	C31-C32-C33-C34
152	QI	202	PC1	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	t7	201	CDL	CB7-C71-C72-C73
153	FS	204	CDL	CB7-C71-C72-C73
153	T7	201	CDL	CB7-C71-C72-C73
160	r	202	PX2	O6-C4-O5-C3
151	2e	401	HEC	C3D-CAD-CBD-CGD
151	2E	401	HEC	C3D-CAD-CBD-CGD
152	n	303	PC1	C31-C32-C33-C34
152	qC	507	PC1	C21-C22-C23-C24
152	N	303	PC1	C31-C32-C33-C34
152	QC	507	PC1	C21-C22-C23-C24
153	2g	201	CDL	CA5-C11-C12-C13
153	n6	302	CDL	CA5-C11-C12-C13
153	2G	201	CDL	CA5-C11-C12-C13
153	2B	201	CDL	CB7-C71-C72-C73
153	N6	302	CDL	CA5-C11-C12-C13
154	c1	702	HEA	C17-C18-C19-C27
154	C1	702	HEA	C17-C18-C19-C27
152	c3	602	PC1	C21-C22-C23-C24
152	qI	202	PC1	C31-C32-C33-C34
152	t4	303	PC1	C21-C22-C23-C24
152	C3	602	PC1	C21-C22-C23-C24
152	T4	303	PC1	C21-C22-C23-C24
153	7a	203	CDL	CA7-C31-C32-C33
153	fs	203	CDL	CB7-C71-C72-C73
153	2b	201	CDL	CB7-C71-C72-C73
153	te	101	CDL	CB5-C51-C52-C53
153	7A	203	CDL	CA7-C31-C32-C33
153	TE	101	CDL	CB5-C51-C52-C53
160	R	202	PX2	C4-C5-C6-C7
160	R	202	PX2	C16-C17-C18-C19
161	sa	701	FAD	C3B-C4B-C5B-O5B
161	SA	701	FAD	C3B-C4B-C5B-O5B
170	b9	202	ADP	C3'-C4'-C5'-O5'
170	B9	202	ADP	C3'-C4'-C5'-O5'
152	qC	507	PC1	C33-C34-C35-C36
152	QC	507	PC1	C33-C34-C35-C36
152	c2	703	PC1	C11-C12-N-C14
152	c3	602	PC1	C11-C12-N-C15
152	c3	603	PC1	C11-C12-N-C15
152	fs	204	PC1	C11-C12-N-C14
152	m	307	PC1	C11-C12-N-C13
152	m2	402	PC1	C11-C12-N-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	n	301	PC1	C11-C12-N-C14
152	w	205	PC1	C11-C12-N-C13
152	an	304	PC1	C11-C12-N-C14
152	j1	400	PC1	C11-C12-N-C15
152	n6	301	PC1	C11-C12-N-C15
152	qB	602	PC1	C11-C12-N-C13
152	qC	508	PC1	C11-C12-N-C13
152	qe	303	PC1	C11-C12-N-C14
152	qi	201	PC1	C11-C12-N-C14
152	qj	101	PC1	C11-C12-N-C13
152	C2	701	PC1	C11-C12-N-C14
152	C3	602	PC1	C11-C12-N-C15
152	C3	603	PC1	C11-C12-N-C15
152	FS	201	PC1	C11-C12-N-C14
152	M	302	PC1	C11-C12-N-C13
152	M2	402	PC1	C11-C12-N-C15
152	N	301	PC1	C11-C12-N-C14
152	W	205	PC1	C11-C12-N-C13
152	AN	304	PC1	C11-C12-N-C14
152	J1	400	PC1	C11-C12-N-C15
152	N6	301	PC1	C11-C12-N-C15
152	QB	602	PC1	C11-C12-N-C13
152	Qe	303	PC1	C11-C12-N-C14
152	Qi	201	PC1	C11-C12-N-C14
152	Qj	101	PC1	C11-C12-N-C13
152	6c	203	PC1	C21-C22-C23-C24
152	6C	201	PC1	C21-C22-C23-C24
153	c1	709	CDL	CA7-C31-C32-C33
153	e	403	CDL	CB7-C71-C72-C73
153	t	204	CDL	CA5-C11-C12-C13
153	qc	505	CDL	CA7-C31-C32-C33
153	th	200	CDL	CA5-C11-C12-C13
153	E	403	CDL	CB7-C71-C72-C73
153	T	204	CDL	CA5-C11-C12-C13
153	Qc	505	CDL	CA7-C31-C32-C33
153	TH	200	CDL	CA5-C11-C12-C13
160	qh	201	PX2	C16-C17-C18-C19
160	Y5	204	PX2	C16-C17-C18-C19
160	Qh	201	PX2	C16-C17-C18-C19
169	b6	201	T7X	C10-C12-C13-C14
169	B6	201	T7X	C10-C12-C13-C14
160	Qh	201	PX2	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qH	201	CDL	C12-C13-C14-C15
153	QH	201	CDL	C12-C13-C14-C15
160	y5	204	PX2	C16-C17-C18-C19
153	e	402	CDL	O1-C1-CA2-OA2
153	E	402	CDL	O1-C1-CA2-OA2
153	B3	101	CDL	O1-C1-CB2-OB2
153	qb	601	CDL	CB5-C51-C52-C53
153	Qb	601	CDL	CB5-C51-C52-C53
153	td	101	CDL	C14-C15-C16-C17
153	A1	101	CDL	C14-C15-C16-C17
168	ab	201	ZMP	C4-C5-C6-C7
168	AB	201	ZMP	C4-C5-C6-C7
152	2f	302	PC1	C1-O11-P-O13
152	2f	303	PC1	C11-O13-P-O11
152	2g	202	PC1	C11-O13-P-O11
152	2j	201	PC1	C11-O13-P-O11
152	2j	201	PC1	C1-O11-P-O13
152	6a	202	PC1	C1-O11-P-O13
152	7c	303	PC1	C11-O13-P-O11
152	a	501	PC1	C11-O13-P-O11
152	c1	706	PC1	C11-O13-P-O11
152	c1	706	PC1	C1-O11-P-O13
152	c1	707	PC1	C11-O13-P-O11
152	c1	711	PC1	C11-O13-P-O11
152	c3	601	PC1	C1-O11-P-O13
152	c3	602	PC1	C1-O11-P-O13
152	d	501	PC1	C1-O11-P-O13
152	f	402	PC1	C1-O11-P-O13
152	i	304	PC1	C11-O13-P-O11
152	j	302	PC1	C1-O11-P-O13
152	m	307	PC1	C1-O11-P-O13
152	m1	401	PC1	C11-O13-P-O11
152	m1	401	PC1	C1-O11-P-O13
152	m2	402	PC1	C11-O13-P-O11
152	m2	402	PC1	C1-O11-P-O13
152	m2	405	PC1	C11-O13-P-O11
152	m2	407	PC1	C11-O13-P-O11
152	n	302	PC1	C11-O13-P-O11
152	n	302	PC1	C1-O11-P-O13
152	v	201	PC1	C11-O13-P-O11
152	v	202	PC1	C11-O13-P-O11
152	v	202	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	w	201	PC1	C11-O13-P-O11
152	w	201	PC1	C1-O11-P-O13
152	w	205	PC1	C11-O13-P-O11
152	5b	202	PC1	C11-O13-P-O11
152	an	304	PC1	C11-O13-P-O11
152	b9	201	PC1	C11-O13-P-O11
152	c4	403	PC1	C11-O13-P-O11
152	j1	400	PC1	C11-O13-P-O11
152	n5	801	PC1	C11-O13-P-O11
152	n5	803	PC1	C11-O13-P-O11
152	n5	803	PC1	C1-O11-P-O13
152	n5	804	PC1	C11-O13-P-O11
152	n5	805	PC1	C11-O13-P-O11
152	n6	301	PC1	C11-O13-P-O11
152	qC	505	PC1	C11-O13-P-O11
152	qC	505	PC1	C1-O11-P-O13
152	qC	508	PC1	C1-O11-P-O13
152	qE	301	PC1	C1-O11-P-O13
152	qE	304	PC1	C1-O11-P-O13
152	qI	201	PC1	C11-O13-P-O11
152	qb	602	PC1	C11-O13-P-O11
152	qc	506	PC1	C11-O13-P-O11
152	qc	506	PC1	C1-O11-P-O13
152	qe	303	PC1	C1-O11-P-O13
152	qg	401	PC1	C11-O13-P-O11
152	qi	203	PC1	C1-O11-P-O13
152	qj	101	PC1	C11-O13-P-O11
152	t1	602	PC1	C11-O13-P-O11
152	t1	602	PC1	C1-O11-P-O13
152	t4	301	PC1	C11-O13-P-O11
152	t4	303	PC1	C1-O11-P-O13
152	tc	102	PC1	C11-O13-P-O11
152	tc	102	PC1	C1-O11-P-O13
152	te	102	PC1	C11-O13-P-O11
152	2F	302	PC1	C1-O11-P-O13
152	2F	303	PC1	C11-O13-P-O11
152	2G	202	PC1	C11-O13-P-O11
152	2J	201	PC1	C11-O13-P-O11
152	2J	201	PC1	C1-O11-P-O13
152	6A	202	PC1	C1-O11-P-O13
152	7C	303	PC1	C11-O13-P-O11
152	A	501	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	C1	709	PC1	C11-O13-P-O11
152	C1	709	PC1	C1-O11-P-O13
152	C1	710	PC1	C11-O13-P-O11
152	C3	601	PC1	C1-O11-P-O13
152	C3	602	PC1	C1-O11-P-O13
152	D	501	PC1	C1-O11-P-O13
152	F	401	PC1	C1-O11-P-O13
152	I	301	PC1	C11-O13-P-O11
152	J	302	PC1	C1-O11-P-O13
152	M	302	PC1	C1-O11-P-O13
152	M1	401	PC1	C11-O13-P-O11
152	M1	401	PC1	C1-O11-P-O13
152	M2	402	PC1	C11-O13-P-O11
152	M2	402	PC1	C1-O11-P-O13
152	M2	405	PC1	C11-O13-P-O11
152	M2	407	PC1	C11-O13-P-O11
152	N	302	PC1	C11-O13-P-O11
152	N	302	PC1	C1-O11-P-O13
152	V	201	PC1	C11-O13-P-O11
152	V	202	PC1	C11-O13-P-O11
152	V	202	PC1	C1-O11-P-O13
152	W	201	PC1	C11-O13-P-O11
152	W	201	PC1	C1-O11-P-O13
152	W	205	PC1	C11-O13-P-O11
152	5B	202	PC1	C11-O13-P-O11
152	AN	304	PC1	C11-O13-P-O11
152	B9	201	PC1	C11-O13-P-O11
152	C4	403	PC1	C11-O13-P-O11
152	J1	400	PC1	C11-O13-P-O11
152	N5	801	PC1	C11-O13-P-O11
152	N5	803	PC1	C11-O13-P-O11
152	N5	803	PC1	C1-O11-P-O13
152	N5	804	PC1	C11-O13-P-O11
152	N5	805	PC1	C11-O13-P-O11
152	N6	301	PC1	C11-O13-P-O11
152	QC	505	PC1	C11-O13-P-O11
152	QC	505	PC1	C1-O11-P-O13
152	QC	508	PC1	C1-O11-P-O13
152	QE	301	PC1	C1-O11-P-O13
152	QI	201	PC1	C11-O13-P-O11
152	QJ	101	PC1	C1-O11-P-O13
152	Qb	602	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	Qc	506	PC1	C11-O13-P-O11
152	Qc	506	PC1	C1-O11-P-O13
152	Qe	303	PC1	C1-O11-P-O13
152	Qg	401	PC1	C11-O13-P-O11
152	Qi	203	PC1	C1-O11-P-O13
152	Qj	101	PC1	C11-O13-P-O11
152	T1	602	PC1	C11-O13-P-O11
152	T1	602	PC1	C1-O11-P-O13
152	T4	301	PC1	C11-O13-P-O11
152	T4	303	PC1	C1-O11-P-O13
152	TC	102	PC1	C11-O13-P-O11
152	TC	102	PC1	C1-O11-P-O13
152	TE	102	PC1	C11-O13-P-O11
153	2g	201	CDL	CB3-OB5-PB2-OB2
153	2g	203	CDL	CA2-OA2-PA1-OA5
153	2g	204	CDL	CA2-OA2-PA1-OA5
153	2g	204	CDL	CA3-OA5-PA1-OA2
153	2g	204	CDL	CB3-OB5-PB2-OB2
153	2k	101	CDL	CA3-OA5-PA1-OA2
153	2k	101	CDL	CB2-OB2-PB2-OB5
153	2k	101	CDL	CB3-OB5-PB2-OB2
153	2m	101	CDL	CB2-OB2-PB2-OB5
153	2o	101	CDL	CA3-OA5-PA1-OA2
153	2o	101	CDL	CB2-OB2-PB2-OB5
153	6a	201	CDL	CA3-OA5-PA1-OA2
153	6a	201	CDL	CB3-OB5-PB2-OB2
153	6c	201	CDL	CB3-OB5-PB2-OB2
153	6c	202	CDL	CA2-OA2-PA1-OA5
153	6c	202	CDL	CA3-OA5-PA1-OA2
153	7a	201	CDL	CA3-OA5-PA1-OA2
153	7a	203	CDL	CA2-OA2-PA1-OA5
153	7c	301	CDL	CA3-OA5-PA1-OA2
153	7c	301	CDL	CB2-OB2-PB2-OB5
153	a	502	CDL	CA2-OA2-PA1-OA5
153	a	504	CDL	CA2-OA2-PA1-OA5
153	c1	701	CDL	CA3-OA5-PA1-OA2
153	c1	701	CDL	CB2-OB2-PB2-OB5
153	c1	703	CDL	CA3-OA5-PA1-OA2
153	c1	709	CDL	CA2-OA2-PA1-OA5
153	c1	709	CDL	CB3-OB5-PB2-OB2
153	c3	604	CDL	CA2-OA2-PA1-OA5
153	e	401	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	e	402	CDL	CB2-OB2-PB2-OB5
153	e	403	CDL	CB2-OB2-PB2-OB5
153	e	403	CDL	CB3-OB5-PB2-OB2
153	fs	203	CDL	CB3-OB5-PB2-OB2
153	i	302	CDL	CA3-OA5-PA1-OA2
153	i	302	CDL	CB2-OB2-PB2-OB5
153	j	301	CDL	CA2-OA2-PA1-OA5
153	j	301	CDL	CB3-OB5-PB2-OB2
153	l	301	CDL	CB2-OB2-PB2-OB5
153	m	302	CDL	CB2-OB2-PB2-OB5
153	m	306	CDL	CA2-OA2-PA1-OA5
153	m	306	CDL	CB2-OB2-PB2-OB5
153	m1	404	CDL	CB2-OB2-PB2-OB5
153	m1	404	CDL	CB3-OB5-PB2-OB2
153	m1	405	CDL	CB2-OB2-PB2-OB5
153	m2	401	CDL	CB3-OB5-PB2-OB2
153	m2	403	CDL	CA3-OA5-PA1-OA2
153	m2	404	CDL	CA3-OA5-PA1-OA2
153	m3	403	CDL	CA3-OA5-PA1-OA2
153	n	304	CDL	CA2-OA2-PA1-OA5
153	n	304	CDL	CA3-OA5-PA1-OA2
153	n	304	CDL	CB3-OB5-PB2-OB2
153	q	201	CDL	CB3-OB5-PB2-OB2
153	q	202	CDL	CB2-OB2-PB2-OB5
153	q	202	CDL	CB3-OB5-PB2-OB2
153	q	203	CDL	CA3-OA5-PA1-OA2
153	r	201	CDL	CA2-OA2-PA1-OA5
153	r	201	CDL	CA3-OA5-PA1-OA2
153	r	201	CDL	CB2-OB2-PB2-OB5
153	sd	101	CDL	CB3-OB5-PB2-OB2
153	t	201	CDL	CB3-OB5-PB2-OB2
153	t	203	CDL	CA2-OA2-PA1-OA5
153	t	203	CDL	CA3-OA5-PA1-OA2
153	u	201	CDL	CA3-OA5-PA1-OA2
153	u	201	CDL	CB3-OB5-PB2-OB2
153	vb	701	CDL	CA2-OA2-PA1-OA5
153	vb	701	CDL	CA3-OA5-PA1-OA2
153	vb	704	CDL	CA3-OA5-PA1-OA2
153	w	202	CDL	CA3-OA5-PA1-OA2
153	w	202	CDL	CB3-OB5-PB2-OB2
153	y7	501	CDL	CB2-OB2-PB2-OB5
153	z	101	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	z	101	CDL	CB3-OB5-PB2-OB2
153	2b	201	CDL	CB2-OB2-PB2-OB5
153	2b	201	CDL	CB3-OB5-PB2-OB2
153	5b	201	CDL	CA2-OA2-PA1-OA5
153	al	301	CDL	CA2-OA2-PA1-OA5
153	al	301	CDL	CB2-OB2-PB2-OB5
153	al	301	CDL	CB3-OB5-PB2-OB2
153	am	201	CDL	CA2-OA2-PA1-OA5
153	am	201	CDL	CB2-OB2-PB2-OB5
153	an	302	CDL	CB2-OB2-PB2-OB5
153	b3	101	CDL	CA3-OA5-PA1-OA2
153	b4	201	CDL	CA2-OA2-PA1-OA5
153	b8	302	CDL	CB3-OB5-PB2-OB2
153	bm	301	CDL	CA2-OA2-PA1-OA5
153	bm	301	CDL	CB3-OB5-PB2-OB2
153	c4	401	CDL	CA2-OA2-PA1-OA5
153	c4	401	CDL	CB2-OB2-PB2-OB5
153	n5	806	CDL	CB2-OB2-PB2-OB5
153	n6	302	CDL	CA2-OA2-PA1-OA5
153	n6	302	CDL	CB2-OB2-PB2-OB5
153	p1	402	CDL	CA3-OA5-PA1-OA2
153	qB	601	CDL	CB3-OB5-PB2-OB2
153	qC	503	CDL	CA3-OA5-PA1-OA2
153	qC	504	CDL	CA3-OA5-PA1-OA2
153	qC	504	CDL	CB2-OB2-PB2-OB5
153	qC	504	CDL	CB3-OB5-PB2-OB2
153	qD	402	CDL	CA2-OA2-PA1-OA5
153	qD	402	CDL	CB2-OB2-PB2-OB5
153	qG	402	CDL	CA3-OA5-PA1-OA2
153	qH	201	CDL	CA2-OA2-PA1-OA5
153	qI	203	CDL	CA3-OA5-PA1-OA2
153	qc	504	CDL	CA2-OA2-PA1-OA5
153	qc	505	CDL	CA3-OA5-PA1-OA2
153	qc	505	CDL	CB2-OB2-PB2-OB5
153	qg	402	CDL	CA2-OA2-PA1-OA5
153	qg	402	CDL	CB2-OB2-PB2-OB5
153	qg	402	CDL	CB3-OB5-PB2-OB2
153	qi	202	CDL	CB2-OB2-PB2-OB5
153	t1	601	CDL	CB3-OB5-PB2-OB2
153	t5	301	CDL	CB2-OB2-PB2-OB5
153	t7	201	CDL	CA3-OA5-PA1-OA2
153	td	101	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	te	101	CDL	CA2-OA2-PA1-OA5
153	te	101	CDL	CB2-OB2-PB2-OB5
153	te	101	CDL	CB3-OB5-PB2-OB2
153	th	200	CDL	CA3-OA5-PA1-OA2
153	th	200	CDL	CB3-OB5-PB2-OB2
153	2G	201	CDL	CB3-OB5-PB2-OB2
153	2G	203	CDL	CA2-OA2-PA1-OA5
153	2G	204	CDL	CA2-OA2-PA1-OA5
153	2G	204	CDL	CA3-OA5-PA1-OA2
153	2G	204	CDL	CB3-OB5-PB2-OB2
153	2K	101	CDL	CA3-OA5-PA1-OA2
153	2K	101	CDL	CB2-OB2-PB2-OB5
153	2K	101	CDL	CB3-OB5-PB2-OB2
153	2M	101	CDL	CB2-OB2-PB2-OB5
153	2O	101	CDL	CA3-OA5-PA1-OA2
153	2O	101	CDL	CB2-OB2-PB2-OB5
153	6A	201	CDL	CA3-OA5-PA1-OA2
153	6A	201	CDL	CB3-OB5-PB2-OB2
153	6C	202	CDL	CB3-OB5-PB2-OB2
153	6C	203	CDL	CA2-OA2-PA1-OA5
153	6C	203	CDL	CA3-OA5-PA1-OA2
153	7A	201	CDL	CA3-OA5-PA1-OA2
153	7A	203	CDL	CA2-OA2-PA1-OA5
153	7C	301	CDL	CA3-OA5-PA1-OA2
153	7C	301	CDL	CB2-OB2-PB2-OB5
153	A	502	CDL	CA2-OA2-PA1-OA5
153	A	504	CDL	CA2-OA2-PA1-OA5
153	C1	701	CDL	CA3-OA5-PA1-OA2
153	C1	701	CDL	CB2-OB2-PB2-OB5
153	C1	707	CDL	CA3-OA5-PA1-OA2
153	C1	708	CDL	CA2-OA2-PA1-OA5
153	C1	708	CDL	CB3-OB5-PB2-OB2
153	C3	604	CDL	CA2-OA2-PA1-OA5
153	E	401	CDL	CB2-OB2-PB2-OB5
153	E	402	CDL	CB2-OB2-PB2-OB5
153	E	403	CDL	CB2-OB2-PB2-OB5
153	FS	204	CDL	CB3-OB5-PB2-OB2
153	I	302	CDL	CA2-OA2-PA1-OA5
153	I	303	CDL	CA3-OA5-PA1-OA2
153	I	303	CDL	CB2-OB2-PB2-OB5
153	J	301	CDL	CA2-OA2-PA1-OA5
153	J	301	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	L	301	CDL	CB2-OB2-PB2-OB5
153	M	301	CDL	CA2-OA2-PA1-OA5
153	M	301	CDL	CB2-OB2-PB2-OB5
153	M	304	CDL	CB2-OB2-PB2-OB5
153	M1	404	CDL	CB2-OB2-PB2-OB5
153	M1	404	CDL	CB3-OB5-PB2-OB2
153	M1	405	CDL	CB2-OB2-PB2-OB5
153	M2	401	CDL	CB3-OB5-PB2-OB2
153	M2	403	CDL	CA3-OA5-PA1-OA2
153	M2	404	CDL	CA3-OA5-PA1-OA2
153	N	304	CDL	CA2-OA2-PA1-OA5
153	N	304	CDL	CA3-OA5-PA1-OA2
153	N	304	CDL	CB3-OB5-PB2-OB2
153	Q	201	CDL	CB3-OB5-PB2-OB2
153	Q	202	CDL	CB2-OB2-PB2-OB5
153	Q	202	CDL	CB3-OB5-PB2-OB2
153	R	201	CDL	CA2-OA2-PA1-OA5
153	R	201	CDL	CA3-OA5-PA1-OA2
153	SD	101	CDL	CB3-OB5-PB2-OB2
153	T	201	CDL	CB3-OB5-PB2-OB2
153	T	203	CDL	CA2-OA2-PA1-OA5
153	T	203	CDL	CA3-OA5-PA1-OA2
153	U	201	CDL	CA3-OA5-PA1-OA2
153	U	201	CDL	CB3-OB5-PB2-OB2
153	VB	701	CDL	CA2-OA2-PA1-OA5
153	VB	701	CDL	CA3-OA5-PA1-OA2
153	VB	703	CDL	CA3-OA5-PA1-OA2
153	VB	706	CDL	CA3-OA5-PA1-OA2
153	W	202	CDL	CA3-OA5-PA1-OA2
153	W	202	CDL	CB3-OB5-PB2-OB2
153	Y7	501	CDL	CB2-OB2-PB2-OB5
153	Z	101	CDL	CA2-OA2-PA1-OA5
153	Z	101	CDL	CB3-OB5-PB2-OB2
153	2B	201	CDL	CB2-OB2-PB2-OB5
153	2B	201	CDL	CB3-OB5-PB2-OB2
153	5B	201	CDL	CA2-OA2-PA1-OA5
153	A1	101	CDL	CB3-OB5-PB2-OB2
153	A9	403	CDL	CA2-OA2-PA1-OA5
153	AL	301	CDL	CA2-OA2-PA1-OA5
153	AL	301	CDL	CB2-OB2-PB2-OB5
153	AL	301	CDL	CB3-OB5-PB2-OB2
153	AM	201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AM	201	CDL	CB2-OB2-PB2-OB5
153	AN	302	CDL	CB2-OB2-PB2-OB5
153	B3	101	CDL	CA3-OA5-PA1-OA2
153	B3	102	CDL	CA3-OA5-PA1-OA2
153	B4	201	CDL	CA2-OA2-PA1-OA5
153	B8	302	CDL	CB3-OB5-PB2-OB2
153	BM	301	CDL	CA2-OA2-PA1-OA5
153	BM	301	CDL	CB3-OB5-PB2-OB2
153	C4	401	CDL	CA2-OA2-PA1-OA5
153	C4	401	CDL	CB2-OB2-PB2-OB5
153	N5	806	CDL	CA3-OA5-PA1-OA2
153	N5	806	CDL	CB2-OB2-PB2-OB5
153	N6	302	CDL	CA2-OA2-PA1-OA5
153	N6	302	CDL	CB2-OB2-PB2-OB5
153	P1	402	CDL	CA3-OA5-PA1-OA2
153	QB	601	CDL	CB3-OB5-PB2-OB2
153	QC	503	CDL	CA3-OA5-PA1-OA2
153	QC	504	CDL	CA3-OA5-PA1-OA2
153	QC	504	CDL	CB2-OB2-PB2-OB5
153	QC	504	CDL	CB3-OB5-PB2-OB2
153	QD	402	CDL	CA2-OA2-PA1-OA5
153	QD	402	CDL	CB2-OB2-PB2-OB5
153	QG	402	CDL	CA3-OA5-PA1-OA2
153	QH	201	CDL	CA2-OA2-PA1-OA5
153	QI	203	CDL	CA3-OA5-PA1-OA2
153	QI	203	CDL	CB2-OB2-PB2-OB5
153	Qc	504	CDL	CA2-OA2-PA1-OA5
153	Qc	504	CDL	CB2-OB2-PB2-OB5
153	Qc	505	CDL	CA3-OA5-PA1-OA2
153	Qc	505	CDL	CB2-OB2-PB2-OB5
153	Qg	402	CDL	CA2-OA2-PA1-OA5
153	Qg	402	CDL	CB2-OB2-PB2-OB5
153	Qg	402	CDL	CB3-OB5-PB2-OB2
153	Qi	202	CDL	CB2-OB2-PB2-OB5
153	T1	601	CDL	CB3-OB5-PB2-OB2
153	T5	301	CDL	CB2-OB2-PB2-OB5
153	T7	201	CDL	CA3-OA5-PA1-OA2
153	TE	101	CDL	CA2-OA2-PA1-OA5
153	TE	101	CDL	CB2-OB2-PB2-OB5
153	TE	101	CDL	CB3-OB5-PB2-OB2
153	TH	200	CDL	CA3-OA5-PA1-OA2
153	TH	200	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C	301	CDL	CB3-OB5-PB2-OB2
153	c	301	CDL	CB3-OB5-PB2-OB2
153	u1	101	CDL	CA2-OA2-PA1-OA5
153	u1	101	CDL	CA3-OA5-PA1-OA2
153	u1	101	CDL	CB2-OB2-PB2-OB5
153	U1	101	CDL	CA2-OA2-PA1-OA5
153	U1	101	CDL	CA3-OA5-PA1-OA2
153	U1	101	CDL	CB2-OB2-PB2-OB5
158	i	303	3PE	C1-O11-P-O13
158	m2	408	3PE	C1-O11-P-O13
158	m2	408	3PE	C11-O13-P-O11
158	sc	101	3PE	C11-O13-P-O11
158	vb	705	3PE	C11-O13-P-O11
158	y5	202	3PE	C1-O11-P-O13
158	y5	202	3PE	C11-O13-P-O11
158	a3	201	3PE	C11-O13-P-O11
158	an	306	3PE	C1-O11-P-O13
158	b4	202	3PE	C1-O11-P-O13
158	bm	302	3PE	C11-O13-P-O11
158	c4	402	3PE	C11-O13-P-O11
158	n4	601	3PE	C1-O11-P-O13
158	n5	802	3PE	C11-O13-P-O11
158	s8	304	3PE	C1-O11-P-O13
158	s8	304	3PE	C11-O13-P-O11
158	t4	302	3PE	C11-O13-P-O11
158	t8	601	3PE	C1-O11-P-O13
158	I	304	3PE	C1-O11-P-O13
158	M2	408	3PE	C1-O11-P-O13
158	M2	408	3PE	C11-O13-P-O11
158	SC	101	3PE	C11-O13-P-O11
158	VB	707	3PE	C11-O13-P-O11
158	Y5	202	3PE	C1-O11-P-O13
158	Y5	202	3PE	C11-O13-P-O11
158	A3	201	3PE	C11-O13-P-O11
158	AN	306	3PE	C1-O11-P-O13
158	B4	202	3PE	C1-O11-P-O13
158	BM	302	3PE	C11-O13-P-O11
158	C4	402	3PE	C11-O13-P-O11
158	N4	601	3PE	C1-O11-P-O13
158	N5	802	3PE	C11-O13-P-O11
158	S8	304	3PE	C1-O11-P-O13
158	S8	304	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	T4	302	3PE	C11-O13-P-O11
158	T8	601	3PE	C1-O11-P-O13
159	m2	406	P5S	CB-OG-P12-O16
159	M2	406	P5S	CB-OG-P12-O16
152	7c	303	PC1	C31-C32-C33-C34
152	n3	201	PC1	C31-C32-C33-C34
152	7C	303	PC1	C31-C32-C33-C34
160	qh	201	PX2	C5-C4-O5-C3
160	R	202	PX2	C5-C4-O5-C3
152	qC	507	PC1	C38-C39-C3A-C3B
152	QC	507	PC1	C38-C39-C3A-C3B
152	N3	201	PC1	C31-C32-C33-C34
153	y5	201	CDL	CB7-C71-C72-C73
153	Y5	201	CDL	CB7-C71-C72-C73
153	qH	201	CDL	CA2-C1-CB2-OB2
153	QH	201	CDL	CA2-C1-CB2-OB2
164	qc	501	U10	C15-C14-C16-C17
152	2f	303	PC1	C11-C12-N-C13
152	6a	202	PC1	C11-C12-N-C13
152	6a	202	PC1	C11-C12-N-C14
152	6a	202	PC1	C11-C12-N-C15
152	7a	202	PC1	C11-C12-N-C13
152	7a	202	PC1	C11-C12-N-C14
152	c3	605	PC1	C11-C12-N-C14
152	w	205	PC1	C11-C12-N-C14
152	n5	801	PC1	C11-C12-N-C13
152	qC	507	PC1	C11-C12-N-C13
152	qC	508	PC1	C11-C12-N-C15
152	qb	602	PC1	C11-C12-N-C13
152	2F	303	PC1	C11-C12-N-C13
152	6A	202	PC1	C11-C12-N-C13
152	6A	202	PC1	C11-C12-N-C14
152	7A	202	PC1	C11-C12-N-C13
152	C3	605	PC1	C11-C12-N-C14
152	W	205	PC1	C11-C12-N-C14
152	N5	801	PC1	C11-C12-N-C13
152	QC	507	PC1	C11-C12-N-C13
152	QC	508	PC1	C11-C12-N-C15
152	Qb	602	PC1	C11-C12-N-C13
153	vb	701	CDL	CA5-C11-C12-C13
153	VB	701	CDL	CA5-C11-C12-C13
152	c1	711	PC1	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
160	r	202	PX2	C17-C16-O7-C2
152	qi	203	PC1	C24-C25-C26-C27
152	t4	303	PC1	C37-C38-C39-C3A
152	C1	711	PC1	C33-C34-C35-C36
152	Qi	203	PC1	C24-C25-C26-C27
152	T4	303	PC1	C37-C38-C39-C3A
153	m	302	CDL	C31-C32-C33-C34
153	c4	401	CDL	C78-C79-C80-C81
153	M	304	CDL	C31-C32-C33-C34
153	C4	401	CDL	C78-C79-C80-C81
158	a3	201	3PE	C34-C35-C36-C37
158	A3	201	3PE	C34-C35-C36-C37
160	qh	201	PX2	C21-C22-C23-C24
153	n	304	CDL	C74-C75-C76-C77
153	N	304	CDL	C74-C75-C76-C77
169	b6	201	T7X	C39-C40-C41-C42
169	B6	201	T7X	C39-C40-C41-C42
160	r	202	PX2	O8-C16-O7-C2
153	q	203	CDL	C13-C14-C15-C16
153	w	202	CDL	C62-C63-C64-C65
153	VB	703	CDL	C13-C14-C15-C16
153	W	202	CDL	C62-C63-C64-C65
153	7a	203	CDL	CB4-CB3-OB5-PB2
153	m1	405	CDL	C1-CA2-OA2-PA1
153	b3	101	CDL	C1-CB2-OB2-PB2
153	7A	203	CDL	CB4-CB3-OB5-PB2
153	M1	405	CDL	C1-CA2-OA2-PA1
153	B3	101	CDL	C1-CB2-OB2-PB2
158	ta	201	3PE	C2-C1-O11-P
158	TA	201	3PE	C2-C1-O11-P
153	e	402	CDL	C57-C58-C59-C60
159	m2	406	P5S	C21-C22-C23-C24
159	M2	406	P5S	C21-C22-C23-C24
160	Qh	201	PX2	C21-C22-C23-C24
169	B6	201	T7X	C34-C35-C36-C37
153	m2	404	CDL	O1-C1-CB2-OB2
153	M2	404	CDL	O1-C1-CB2-OB2
152	c3	606	PC1	C22-C23-C24-C25
152	C3	606	PC1	C22-C23-C24-C25
152	M2	405	PC1	C22-C23-C24-C25
160	qh	201	PX2	C11-C12-C13-C14
169	b6	201	T7X	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	i	304	PC1	C21-C22-C23-C24
152	I	301	PC1	C21-C22-C23-C24
153	an	302	CDL	CB5-C51-C52-C53
153	C1	701	CDL	CA5-C11-C12-C13
153	AN	302	CDL	CB5-C51-C52-C53
152	c1	704	PC1	C3B-C3C-C3D-C3E
152	m2	405	PC1	C22-C23-C24-C25
152	C1	706	PC1	C3B-C3C-C3D-C3E
158	m3	402	3PE	C27-C28-C29-C2A
158	M3	402	3PE	C27-C28-C29-C2A
153	a9	403	CDL	C18-C19-C20-C21
153	E	402	CDL	C57-C58-C59-C60
153	A9	403	CDL	C18-C19-C20-C21
153	a	505	CDL	CB7-C71-C72-C73
153	c1	701	CDL	CA5-C11-C12-C13
153	n	304	CDL	CA5-C11-C12-C13
153	VB	705	CDL	CB7-C71-C72-C73
153	7c	301	CDL	C78-C79-C80-C81
153	m2	403	CDL	C11-C12-C13-C14
153	7C	301	CDL	C78-C79-C80-C81
153	M2	403	CDL	C11-C12-C13-C14
152	tc	101	PC1	C25-C26-C27-C28
152	M	302	PC1	C22-C23-C24-C25
153	qc	504	CDL	C54-C55-C56-C57
152	m	307	PC1	C22-C23-C24-C25
152	TC	101	PC1	C25-C26-C27-C28
153	m1	404	CDL	C54-C55-C56-C57
153	w	202	CDL	C58-C59-C60-C61
153	t5	301	CDL	C15-C16-C17-C18
153	M1	404	CDL	C54-C55-C56-C57
153	W	202	CDL	C58-C59-C60-C61
153	Qc	504	CDL	C54-C55-C56-C57
153	T5	301	CDL	C15-C16-C17-C18
153	N	304	CDL	CA5-C11-C12-C13
153	f	401	CDL	C39-C40-C41-C42
153	p1	402	CDL	C53-C54-C55-C56
153	qC	503	CDL	C75-C76-C77-C78
153	td	101	CDL	C17-C18-C19-C20
153	F	402	CDL	C39-C40-C41-C42
153	A1	101	CDL	C17-C18-C19-C20
153	A9	402	CDL	C77-C78-C79-C80
153	P1	402	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	QC	503	CDL	C75-C76-C77-C78
158	AN	303	3PE	C32-C33-C34-C35
152	a	503	PC1	C11-C12-N-C15
152	c2	703	PC1	C11-C12-N-C15
152	m1	401	PC1	C11-C12-N-C15
152	w	201	PC1	C11-C12-N-C13
152	5b	202	PC1	C11-C12-N-C14
152	5b	202	PC1	C11-C12-N-C15
152	qC	505	PC1	C11-C12-N-C14
152	qC	507	PC1	C11-C12-N-C14
152	qC	507	PC1	C11-C12-N-C15
152	6A	202	PC1	C11-C12-N-C15
152	7A	202	PC1	C11-C12-N-C14
152	A	503	PC1	C11-C12-N-C15
152	C2	701	PC1	C11-C12-N-C15
152	M1	401	PC1	C11-C12-N-C15
152	M2	402	PC1	C11-C12-N-C14
152	W	201	PC1	C11-C12-N-C13
152	5B	202	PC1	C11-C12-N-C14
152	5B	202	PC1	C11-C12-N-C15
152	QC	505	PC1	C11-C12-N-C14
152	QC	507	PC1	C11-C12-N-C14
152	QC	507	PC1	C11-C12-N-C15
164	sc	102	U10	C49-C51-C52-C53
164	SC	102	U10	C49-C51-C52-C53
153	a9	402	CDL	C77-C78-C79-C80
158	an	303	3PE	C32-C33-C34-C35
160	r	202	PX2	C21-C22-C23-C24
158	m2	408	3PE	O13-C11-C12-N
158	M2	408	3PE	O13-C11-C12-N
158	SC	101	3PE	O13-C11-C12-N
153	2k	101	CDL	C74-C75-C76-C77
153	m	303	CDL	C54-C55-C56-C57
158	g2	301	3PE	C2E-C2F-C2G-C2H
158	G2	301	3PE	C2E-C2F-C2G-C2H
160	R	202	PX2	O6-C4-O5-C3
153	2K	101	CDL	C74-C75-C76-C77
153	M	305	CDL	C54-C55-C56-C57
160	R	202	PX2	C5-C6-C7-C8
168	ab	201	ZMP	C6-C7-C8-C9
168	AB	201	ZMP	C6-C7-C8-C9
151	2e	401	HEC	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
151	2E	401	HEC	C2A-CAA-CBA-CGA
168	AB	201	ZMP	C3-C4-C5-C6
152	n6	301	PC1	C38-C39-C3A-C3B
152	Qi	203	PC1	C23-C24-C25-C26
153	c1	703	CDL	C53-C54-C55-C56
153	n5	806	CDL	C61-C62-C63-C64
153	2K	101	CDL	C56-C57-C58-C59
153	C1	707	CDL	C53-C54-C55-C56
153	N5	806	CDL	C61-C62-C63-C64
160	Qh	201	PX2	C5-C6-C7-C8
168	ab	201	ZMP	C3-C4-C5-C6
153	2G	203	CDL	CB3-CB4-CB6-OB8
153	B3	102	CDL	CA3-CA4-CA6-OA8
152	qi	203	PC1	C23-C24-C25-C26
152	N6	301	PC1	C38-C39-C3A-C3B
153	2k	101	CDL	C56-C57-C58-C59
160	r	202	PX2	C5-C6-C7-C8
152	w	204	PC1	C33-C34-C35-C36
152	W	204	PC1	C33-C34-C35-C36
169	b6	201	T7X	C31-C32-C33-C34
169	B6	201	T7X	C31-C32-C33-C34
164	b8	301	U10	C12-C11-C9-C8
164	B8	301	U10	C12-C11-C9-C8
152	p1	401	PC1	C32-C33-C34-C35
152	P1	401	PC1	C32-C33-C34-C35
152	qc	509	PC1	C37-C38-C39-C3A
160	qh	201	PX2	O6-C4-O5-C3
158	m3	402	3PE	C21-C22-C23-C24
152	Qc	509	PC1	C37-C38-C39-C3A
153	T5	301	CDL	C38-C39-C40-C41
153	r	201	CDL	O1-C1-CB2-OB2
153	R	201	CDL	O1-C1-CB2-OB2
153	c4	401	CDL	C34-C35-C36-C37
153	t5	301	CDL	C38-C39-C40-C41
153	n5	806	CDL	C57-C58-C59-C60
153	C1	712	CDL	C76-C77-C78-C79
153	Q	202	CDL	C11-C12-C13-C14
153	C4	401	CDL	C34-C35-C36-C37
153	N5	806	CDL	C57-C58-C59-C60
152	qc	506	PC1	C34-C35-C36-C37
153	q	202	CDL	C11-C12-C13-C14
153	b3	101	CDL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	B3	101	CDL	C11-C12-C13-C14
153	c1	712	CDL	C76-C77-C78-C79
153	c3	604	CDL	C54-C55-C56-C57
153	C3	604	CDL	C54-C55-C56-C57
152	Qc	506	PC1	C34-C35-C36-C37
153	b3	102	CDL	C14-C15-C16-C17
153	te	101	CDL	C52-C53-C54-C55
152	2f	303	PC1	C11-C12-N-C14
152	a	501	PC1	C11-C12-N-C13
152	c1	707	PC1	C11-C12-N-C14
152	c3	602	PC1	C11-C12-N-C13
152	c3	603	PC1	C11-C12-N-C14
152	c3	605	PC1	C11-C12-N-C15
152	fs	204	PC1	C11-C12-N-C15
152	m	307	PC1	C11-C12-N-C14
152	m2	402	PC1	C11-C12-N-C14
152	n	301	PC1	C11-C12-N-C13
152	n	302	PC1	C11-C12-N-C14
152	an	304	PC1	C11-C12-N-C15
152	j1	400	PC1	C11-C12-N-C13
152	j1	400	PC1	C11-C12-N-C14
152	qB	602	PC1	C11-C12-N-C14
152	qe	301	PC1	C11-C12-N-C14
152	qe	303	PC1	C11-C12-N-C13
152	qi	201	PC1	C11-C12-N-C15
152	qj	101	PC1	C11-C12-N-C14
152	t1	602	PC1	C11-C12-N-C13
152	2F	303	PC1	C11-C12-N-C14
152	2G	202	PC1	C11-C12-N-C13
152	A	501	PC1	C11-C12-N-C13
152	C1	710	PC1	C11-C12-N-C14
152	C3	602	PC1	C11-C12-N-C13
152	C3	603	PC1	C11-C12-N-C14
152	C3	605	PC1	C11-C12-N-C15
152	FS	201	PC1	C11-C12-N-C15
152	M	302	PC1	C11-C12-N-C14
152	N	301	PC1	C11-C12-N-C13
152	N	302	PC1	C11-C12-N-C14
152	AN	304	PC1	C11-C12-N-C13
152	AN	304	PC1	C11-C12-N-C15
152	J1	400	PC1	C11-C12-N-C13
152	J1	400	PC1	C11-C12-N-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	QB	602	PC1	C11-C12-N-C14
152	Qe	301	PC1	C11-C12-N-C14
152	Qe	303	PC1	C11-C12-N-C13
152	Qi	201	PC1	C11-C12-N-C15
152	Qj	101	PC1	C11-C12-N-C14
152	T1	602	PC1	C11-C12-N-C13
152	2f	301	PC1	C31-C32-C33-C34
152	2F	301	PC1	C31-C32-C33-C34
153	p1	402	CDL	CA5-C11-C12-C13
153	P1	402	CDL	CA5-C11-C12-C13
158	M3	402	3PE	C21-C22-C23-C24
153	B3	102	CDL	C14-C15-C16-C17
152	m1	401	PC1	C24-C25-C26-C27
159	m2	406	P5S	C38-C39-C40-C41
159	M2	406	P5S	C38-C39-C40-C41
152	6a	202	PC1	C24-C25-C26-C27
152	6A	202	PC1	C24-C25-C26-C27
152	M1	401	PC1	C24-C25-C26-C27
153	m	302	CDL	C52-C53-C54-C55
153	M	304	CDL	C52-C53-C54-C55
153	c1	701	CDL	C73-C74-C75-C76
153	C1	701	CDL	C73-C74-C75-C76
164	qc	507	U10	C15-C14-C16-C17
164	Qc	507	U10	C15-C14-C16-C17
164	qc	507	U10	C13-C14-C16-C17
164	Qc	507	U10	C13-C14-C16-C17
169	b6	201	T7X	C12-C13-C14-C15
160	R	202	PX2	O8-C16-O7-C2
153	6c	201	CDL	CB5-C51-C52-C53
153	2b	201	CDL	CB5-C51-C52-C53
153	2B	201	CDL	CB5-C51-C52-C53
158	a3	202	3PE	C31-C32-C33-C34
158	A3	202	3PE	C31-C32-C33-C34
160	y5	204	PX2	C5-C4-O5-C3
153	TE	101	CDL	C52-C53-C54-C55
168	AB	201	ZMP	C22-C23-C24-C25
153	t5	301	CDL	C59-C60-C61-C62
168	ab	201	ZMP	C22-C23-C24-C25
153	i	302	CDL	C36-C37-C38-C39
153	I	303	CDL	C36-C37-C38-C39
153	N5	806	CDL	C18-C19-C20-C21
158	SC	101	3PE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	6c	202	CDL	CB5-C51-C52-C53
153	n5	806	CDL	CA7-C31-C32-C33
153	2M	101	CDL	CA5-C11-C12-C13
153	6C	202	CDL	CB5-C51-C52-C53
152	qB	602	PC1	C24-C25-C26-C27
153	n5	806	CDL	C18-C19-C20-C21
153	2M	101	CDL	C71-C72-C73-C74
153	T5	301	CDL	C59-C60-C61-C62
158	sc	101	3PE	C33-C34-C35-C36
166	qC	502	HEM	C2B-C3B-CAB-CBB
166	qc	503	HEM	C2B-C3B-CAB-CBB
166	QC	502	HEM	C2B-C3B-CAB-CBB
166	Qc	503	HEM	C2B-C3B-CAB-CBB
152	QB	602	PC1	C24-C25-C26-C27
153	2m	101	CDL	C71-C72-C73-C74
153	m1	404	CDL	C72-C73-C74-C75
153	m	306	CDL	C11-C12-C13-C14
153	E	401	CDL	C13-C14-C15-C16
153	I	303	CDL	C54-C55-C56-C57
153	M1	404	CDL	C72-C73-C74-C75
153	B3	102	CDL	C72-C73-C74-C75
159	m2	406	P5S	C39-C38-O37-C2
159	M2	406	P5S	C39-C38-O37-C2
160	R	202	PX2	C17-C16-O7-C2
153	n5	806	CDL	OB5-CB3-CB4-OB6
153	qi	202	CDL	OB5-CB3-CB4-OB6
153	N5	806	CDL	OB5-CB3-CB4-OB6
153	Qi	202	CDL	OB5-CB3-CB4-OB6
158	c4	402	3PE	O11-C1-C2-O21
158	C4	402	3PE	O11-C1-C2-O21
153	b3	102	CDL	C76-C77-C78-C79
153	M	301	CDL	C11-C12-C13-C14
160	qh	201	PX2	C17-C18-C19-C20
166	y5	203	HEM	C4B-C3B-CAB-CBB
166	qC	502	HEM	C4B-C3B-CAB-CBB
166	qc	503	HEM	C4B-C3B-CAB-CBB
166	Y5	203	HEM	C4B-C3B-CAB-CBB
166	QC	502	HEM	C4B-C3B-CAB-CBB
166	Qc	503	HEM	C4B-C3B-CAB-CBB
153	b8	302	CDL	C55-C56-C57-C58
153	B3	102	CDL	C76-C77-C78-C79
153	B8	302	CDL	C55-C56-C57-C58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2m	101	CDL	O1-C1-CA2-OA2
153	2M	101	CDL	O1-C1-CA2-OA2
159	M2	406	P5S	O47-C38-O37-C2
153	6C	203	CDL	CB5-C51-C52-C53
152	c2	703	PC1	O21-C2-C3-O31
152	m2	407	PC1	O21-C2-C3-O31
152	C2	701	PC1	O21-C2-C3-O31
152	M2	407	PC1	O21-C2-C3-O31
153	a	502	CDL	OB6-CB4-CB6-OB8
153	m	306	CDL	OB6-CB4-CB6-OB8
153	2G	204	CDL	OA6-CA4-CA6-OA8
153	A	502	CDL	OB6-CB4-CB6-OB8
153	M	301	CDL	OB6-CB4-CB6-OB8
158	a3	202	3PE	O21-C2-C3-O31
158	g2	301	3PE	O21-C2-C3-O31
158	A3	202	3PE	O21-C2-C3-O31
158	G2	301	3PE	O21-C2-C3-O31
160	qh	201	PX2	O7-C2-C3-O5
153	2k	101	CDL	C38-C39-C40-C41
153	i	302	CDL	C54-C55-C56-C57
153	b3	102	CDL	C72-C73-C74-C75
153	2K	101	CDL	C38-C39-C40-C41
158	an	301	3PE	C22-C23-C24-C25
152	c3	602	PC1	C11-C12-N-C14
152	m	307	PC1	C11-C12-N-C15
152	m2	402	PC1	C11-C12-N-C13
152	w	201	PC1	C11-C12-N-C15
152	w	205	PC1	C11-C12-N-C15
152	an	304	PC1	C11-C12-N-C13
152	n5	801	PC1	C11-C12-N-C15
152	n6	301	PC1	C11-C12-N-C13
152	n6	301	PC1	C11-C12-N-C14
152	qC	508	PC1	C11-C12-N-C14
152	qJ	101	PC1	C11-C12-N-C15
152	qb	602	PC1	C11-C12-N-C14
152	qe	303	PC1	C11-C12-N-C15
152	qi	201	PC1	C11-C12-N-C13
152	C3	602	PC1	C11-C12-N-C14
152	M	302	PC1	C11-C12-N-C15
152	M2	402	PC1	C11-C12-N-C13
152	W	201	PC1	C11-C12-N-C15
152	W	205	PC1	C11-C12-N-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	N5	801	PC1	C11-C12-N-C15
152	N6	301	PC1	C11-C12-N-C13
152	N6	301	PC1	C11-C12-N-C14
152	QC	505	PC1	C11-C12-N-C15
152	QC	508	PC1	C11-C12-N-C14
152	Qb	602	PC1	C11-C12-N-C14
152	Qe	303	PC1	C11-C12-N-C15
152	Qi	201	PC1	C11-C12-N-C13
158	AN	301	3PE	C22-C23-C24-C25
169	b6	201	T7X	C38-C39-C40-C41
169	B6	201	T7X	C38-C39-C40-C41
169	B6	201	T7X	C12-C13-C14-C15
164	b8	301	U10	C12-C11-C9-C10
164	B8	301	U10	C12-C11-C9-C10
153	t	203	CDL	CB5-C51-C52-C53
153	y5	201	CDL	CA7-C31-C32-C33
153	T	203	CDL	CB5-C51-C52-C53
164	Qc	501	U10	C13-C14-C16-C17
153	6a	201	CDL	C34-C35-C36-C37
153	6A	201	CDL	C34-C35-C36-C37
158	C4	402	3PE	C33-C34-C35-C36
153	u	201	CDL	C13-C14-C15-C16
153	am	201	CDL	C34-C35-C36-C37
153	U	201	CDL	C13-C14-C15-C16
153	AM	201	CDL	C34-C35-C36-C37
158	c4	402	3PE	C33-C34-C35-C36
158	t8	601	3PE	C22-C23-C24-C25
153	Y5	201	CDL	CA7-C31-C32-C33
158	T8	601	3PE	C22-C23-C24-C25
160	y5	204	PX2	O6-C4-O5-C3
159	m2	406	P5S	O47-C38-O37-C2
153	6c	201	CDL	C15-C16-C17-C18
153	e	401	CDL	C13-C14-C15-C16
152	2f	301	PC1	C11-O13-P-O11
152	c1	704	PC1	C11-O13-P-O11
152	f	402	PC1	C11-O13-P-O11
152	w	204	PC1	C11-O13-P-O11
152	5b	202	PC1	C1-O11-P-O13
152	qc	509	PC1	C1-O11-P-O13
152	2F	301	PC1	C11-O13-P-O11
152	C1	706	PC1	C11-O13-P-O11
152	F	401	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	W	204	PC1	C11-O13-P-O11
152	5B	202	PC1	C1-O11-P-O13
152	Qc	509	PC1	C1-O11-P-O13
152	Qe	303	PC1	C11-O13-P-O11
153	6a	201	CDL	CA2-OA2-PA1-OA5
153	7a	201	CDL	CB2-OB2-PB2-OB5
153	7a	203	CDL	CB3-OB5-PB2-OB2
153	7c	302	CDL	CB2-OB2-PB2-OB5
153	a	502	CDL	CA3-OA5-PA1-OA2
153	i	301	CDL	CA3-OA5-PA1-OA2
153	m1	405	CDL	CA3-OA5-PA1-OA2
153	t	201	CDL	CA3-OA5-PA1-OA2
153	t	203	CDL	CB3-OB5-PB2-OB2
153	a9	402	CDL	CA2-OA2-PA1-OA5
153	a9	402	CDL	CA3-OA5-PA1-OA2
153	b3	102	CDL	CA3-OA5-PA1-OA2
153	b3	102	CDL	CB3-OB5-PB2-OB2
153	n5	806	CDL	CA3-OA5-PA1-OA2
153	p1	402	CDL	CA2-OA2-PA1-OA5
153	p1	402	CDL	CB2-OB2-PB2-OB5
153	p1	403	CDL	CA3-OA5-PA1-OA2
153	qH	201	CDL	CB3-OB5-PB2-OB2
153	qI	203	CDL	CB3-OB5-PB2-OB2
153	qc	504	CDL	CB2-OB2-PB2-OB5
153	qc	505	CDL	CA2-OA2-PA1-OA5
153	t5	301	CDL	CA3-OA5-PA1-OA2
153	td	101	CDL	CB2-OB2-PB2-OB5
153	th	200	CDL	CA2-OA2-PA1-OA5
153	6A	201	CDL	CA2-OA2-PA1-OA5
153	7A	201	CDL	CB2-OB2-PB2-OB5
153	7A	203	CDL	CB3-OB5-PB2-OB2
153	7C	301	CDL	CB3-OB5-PB2-OB2
153	7C	302	CDL	CB2-OB2-PB2-OB5
153	A	502	CDL	CA3-OA5-PA1-OA2
153	E	403	CDL	CB3-OB5-PB2-OB2
153	I	302	CDL	CA3-OA5-PA1-OA2
153	M1	405	CDL	CA3-OA5-PA1-OA2
153	R	201	CDL	CB2-OB2-PB2-OB5
153	T	201	CDL	CA3-OA5-PA1-OA2
153	T	203	CDL	CB3-OB5-PB2-OB2
153	A1	101	CDL	CB2-OB2-PB2-OB5
153	A9	402	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	A9	403	CDL	CB3-OB5-PB2-OB2
153	P1	402	CDL	CA2-OA2-PA1-OA5
153	P1	402	CDL	CB2-OB2-PB2-OB5
153	P1	403	CDL	CA3-OA5-PA1-OA2
153	QH	201	CDL	CB3-OB5-PB2-OB2
153	Qc	505	CDL	CA2-OA2-PA1-OA5
153	T5	301	CDL	CA3-OA5-PA1-OA2
153	TH	200	CDL	CA2-OA2-PA1-OA5
158	vb	705	3PE	C1-O11-P-O13
158	g2	301	3PE	C1-O11-P-O13
158	t8	602	3PE	C11-O13-P-O11
158	VB	707	3PE	C1-O11-P-O13
158	G2	301	3PE	C1-O11-P-O13
158	T8	602	3PE	C11-O13-P-O11
153	7a	201	CDL	C62-C63-C64-C65
153	7A	201	CDL	C62-C63-C64-C65
153	2m	101	CDL	CA5-C11-C12-C13
153	c1	712	CDL	CB7-C71-C72-C73
153	C1	712	CDL	CB7-C71-C72-C73
152	d	501	PC1	C2-C1-O11-P
152	m	301	PC1	C2-C1-O11-P
152	D	501	PC1	C2-C1-O11-P
152	M	303	PC1	C2-C1-O11-P
153	qB	601	CDL	CA4-CA3-OA5-PA1
153	QB	601	CDL	CA4-CA3-OA5-PA1
153	6C	202	CDL	C15-C16-C17-C18
152	n5	805	PC1	O11-C1-C2-C3
152	N5	805	PC1	O11-C1-C2-C3
153	6c	201	CDL	OB5-CB3-CB4-CB6
153	7a	203	CDL	OB5-CB3-CB4-CB6
153	f	401	CDL	OB5-CB3-CB4-CB6
153	i	301	CDL	OB5-CB3-CB4-CB6
153	sd	101	CDL	OA5-CA3-CA4-CA6
153	t	201	CDL	OB5-CB3-CB4-CB6
153	vb	701	CDL	OB5-CB3-CB4-CB6
153	c4	401	CDL	OB5-CB3-CB4-CB6
153	n5	806	CDL	OB5-CB3-CB4-CB6
153	qB	601	CDL	OB5-CB3-CB4-CB6
153	qb	601	CDL	OB5-CB3-CB4-CB6
153	6C	202	CDL	OB5-CB3-CB4-CB6
153	7A	203	CDL	OB5-CB3-CB4-CB6
153	F	402	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	I	302	CDL	OB5-CB3-CB4-CB6
153	N	304	CDL	OA5-CA3-CA4-CA6
153	SD	101	CDL	OA5-CA3-CA4-CA6
153	SD	101	CDL	OB5-CB3-CB4-CB6
153	T	201	CDL	OB5-CB3-CB4-CB6
153	VB	701	CDL	OB5-CB3-CB4-CB6
153	C4	401	CDL	OB5-CB3-CB4-CB6
153	N5	806	CDL	OB5-CB3-CB4-CB6
153	QB	601	CDL	OB5-CB3-CB4-CB6
153	Qb	601	CDL	OB5-CB3-CB4-CB6
153	u1	101	CDL	OB5-CB3-CB4-CB6
153	U1	101	CDL	OB5-CB3-CB4-CB6
158	c4	402	3PE	O11-C1-C2-C3
158	ta	201	3PE	O11-C1-C2-C3
158	C4	402	3PE	O11-C1-C2-C3
158	TA	201	3PE	O11-C1-C2-C3
154	C1	703	HEA	O11-C11-C12-C13
153	C4	401	CDL	CA7-C31-C32-C33
166	y5	203	HEM	C3D-CAD-CBD-CGD
153	t	204	CDL	C59-C60-C61-C62
153	T	204	CDL	C59-C60-C61-C62
153	a9	402	CDL	C33-C34-C35-C36
153	bm	301	CDL	C13-C14-C15-C16
153	n6	302	CDL	C51-C52-C53-C54
153	A9	402	CDL	C33-C34-C35-C36
153	AN	302	CDL	C80-C81-C82-C83
153	N6	302	CDL	C51-C52-C53-C54
158	b4	202	3PE	C24-C25-C26-C27
158	B4	202	3PE	C24-C25-C26-C27
160	qh	201	PX2	C22-C23-C24-C25
153	c4	401	CDL	CA7-C31-C32-C33
152	5b	202	PC1	C36-C37-C38-C39
152	5B	202	PC1	C36-C37-C38-C39
153	m1	404	CDL	C74-C75-C76-C77
153	an	302	CDL	C80-C81-C82-C83
153	M1	404	CDL	C74-C75-C76-C77
153	a9	403	CDL	CA2-C1-CB2-OB2
153	A9	403	CDL	CA2-C1-CB2-OB2
153	B3	102	CDL	CB2-C1-CA2-OA2
152	5b	202	PC1	C38-C39-C3A-C3B
152	t4	303	PC1	C27-C28-C29-C2A
152	5B	202	PC1	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	T	202	CDL	C75-C76-C77-C78
153	BM	301	CDL	C13-C14-C15-C16
168	AB	201	ZMP	C1-C22-C23-C24
169	b6	201	T7X	C36-C37-C38-C39
169	B6	201	T7X	C36-C37-C38-C39
152	T4	303	PC1	C27-C28-C29-C2A
153	bm	301	CDL	C77-C78-C79-C80
168	ab	201	ZMP	C1-C22-C23-C24
153	2k	101	CDL	C57-C58-C59-C60
153	q	203	CDL	C52-C53-C54-C55
152	a	503	PC1	C11-C12-N-C13
152	a	503	PC1	C11-C12-N-C14
152	w	201	PC1	C11-C12-N-C14
152	b9	201	PC1	C11-C12-N-C13
152	n5	801	PC1	C11-C12-N-C14
152	qC	505	PC1	C11-C12-N-C13
152	qC	505	PC1	C11-C12-N-C15
152	W	201	PC1	C11-C12-N-C14
152	B9	201	PC1	C11-C12-N-C13
152	N5	801	PC1	C11-C12-N-C14
152	QC	505	PC1	C11-C12-N-C13
152	2j	201	PC1	C1-C2-C3-O31
152	c3	602	PC1	C1-C2-C3-O31
152	s8	301	PC1	C1-C2-C3-O31
152	t1	602	PC1	C1-C2-C3-O31
152	tc	102	PC1	C1-C2-C3-O31
152	2J	201	PC1	C1-C2-C3-O31
152	S8	301	PC1	C1-C2-C3-O31
152	T1	602	PC1	C1-C2-C3-O31
152	TC	102	PC1	C1-C2-C3-O31
153	2g	201	CDL	C18-C19-C20-C21
153	2g	203	CDL	CB3-CB4-CB6-OB8
153	2g	204	CDL	CA3-CA4-CA6-OA8
153	6c	201	CDL	CA3-CA4-CA6-OA8
153	7c	302	CDL	CA3-CA4-CA6-OA8
153	b	501	CDL	CB3-CB4-CB6-OB8
153	t	202	CDL	C14-C15-C16-C17
153	a9	402	CDL	CB3-CB4-CB6-OB8
153	b3	102	CDL	CA3-CA4-CA6-OA8
153	bm	301	CDL	CA3-CA4-CA6-OA8
153	qc	504	CDL	CB3-CB4-CB6-OB8
153	th	200	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2G	204	CDL	CA3-CA4-CA6-OA8
153	6C	202	CDL	CA3-CA4-CA6-OA8
153	7C	301	CDL	CA3-CA4-CA6-OA8
153	B	501	CDL	CB3-CB4-CB6-OB8
153	E	403	CDL	C52-C53-C54-C55
153	T	202	CDL	C14-C15-C16-C17
153	VB	703	CDL	C52-C53-C54-C55
153	A9	402	CDL	CB3-CB4-CB6-OB8
153	BM	301	CDL	CA3-CA4-CA6-OA8
153	BM	301	CDL	C77-C78-C79-C80
153	Qc	504	CDL	CB3-CB4-CB6-OB8
153	TH	200	CDL	CA3-CA4-CA6-OA8
158	g2	301	3PE	C1-C2-C3-O31
158	s8	304	3PE	C1-C2-C3-O31
158	t8	602	3PE	C1-C2-C3-O31
158	G2	301	3PE	C1-C2-C3-O31
158	S8	304	3PE	C1-C2-C3-O31
158	T8	602	3PE	C1-C2-C3-O31
159	m2	406	P5S	O19-C1-C2-C3
159	M2	406	P5S	O19-C1-C2-C3
160	Y5	204	PX2	C1-C2-C3-O5
153	2b	201	CDL	C79-C80-C81-C82
153	2G	201	CDL	C18-C19-C20-C21
153	2K	101	CDL	C57-C58-C59-C60
158	c4	402	3PE	C2B-C2C-C2D-C2E
153	qi	202	CDL	C56-C57-C58-C59
153	2B	201	CDL	C79-C80-C81-C82
158	N4	601	3PE	C25-C26-C27-C28
160	r	202	PX2	C23-C24-C25-C26
160	R	202	PX2	C24-C25-C26-C27
153	e	403	CDL	C52-C53-C54-C55
153	w	202	CDL	C55-C56-C57-C58
153	W	202	CDL	C55-C56-C57-C58
153	Qi	202	CDL	C56-C57-C58-C59
152	d	501	PC1	O21-C21-C22-C23
152	D	501	PC1	O21-C21-C22-C23
153	6a	201	CDL	C32-C31-CA7-OA8
153	6A	201	CDL	C32-C31-CA7-OA8
153	Q	202	CDL	C12-C11-CA5-OA6
153	w	202	CDL	CA7-C31-C32-C33
153	t	202	CDL	C75-C76-C77-C78
158	C4	402	3PE	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
168	ab	201	ZMP	O3-C16-C17-O4
168	AB	201	ZMP	O3-C16-C17-O4
152	tc	101	PC1	C28-C29-C2A-C2B
153	a	504	CDL	CA5-C11-C12-C13
153	m	302	CDL	CB5-C51-C52-C53
153	A	504	CDL	CA5-C11-C12-C13
153	M	304	CDL	CB5-C51-C52-C53
153	W	202	CDL	CA7-C31-C32-C33
152	t4	303	PC1	C25-C26-C27-C28
152	T4	303	PC1	C25-C26-C27-C28
152	6A	202	PC1	C26-C27-C28-C29
152	TC	101	PC1	C28-C29-C2A-C2B
152	6a	202	PC1	C26-C27-C28-C29
153	BM	301	CDL	C40-C41-C42-C43
158	n4	601	3PE	C25-C26-C27-C28
154	c1	708	HEA	C11-C12-C13-C14
153	2b	201	CDL	C16-C17-C18-C19
153	2B	201	CDL	C16-C17-C18-C19
153	i	301	CDL	CB4-CB3-OB5-PB2
153	a9	402	CDL	CB4-CB3-OB5-PB2
153	I	302	CDL	CB4-CB3-OB5-PB2
153	A9	402	CDL	CB4-CB3-OB5-PB2
160	r	202	PX2	C1-O4-P1-O2
153	c4	401	CDL	C81-C82-C83-C84
153	C4	401	CDL	C81-C82-C83-C84
160	Y5	204	PX2	C5-C4-O5-C3
152	2g	202	PC1	O11-C1-C2-O21
152	t4	301	PC1	O11-C1-C2-O21
152	2G	202	PC1	O11-C1-C2-O21
152	T4	301	PC1	O11-C1-C2-O21
153	6c	201	CDL	OA5-CA3-CA4-OA6
153	c1	701	CDL	OB5-CB3-CB4-OB6
153	e	402	CDL	OB5-CB3-CB4-OB6
153	m1	402	CDL	OB5-CB3-CB4-OB6
153	n6	302	CDL	OB5-CB3-CB4-OB6
153	qC	503	CDL	OB5-CB3-CB4-OB6
153	qg	402	CDL	OB5-CB3-CB4-OB6
153	6C	202	CDL	OA5-CA3-CA4-OA6
153	C1	701	CDL	OB5-CB3-CB4-OB6
153	C1	712	CDL	OB5-CB3-CB4-OB6
153	E	402	CDL	OB5-CB3-CB4-OB6
153	M1	402	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	N6	302	CDL	OB5-CB3-CB4-OB6
153	Qg	402	CDL	OB5-CB3-CB4-OB6
158	bm	302	3PE	O11-C1-C2-O21
158	BM	302	3PE	O11-C1-C2-O21
153	m2	401	CDL	C32-C31-CA7-OA8
153	q	202	CDL	C12-C11-CA5-OA6
153	te	101	CDL	C32-C31-CA7-OA8
153	M2	401	CDL	C32-C31-CA7-OA8
152	2g	202	PC1	C11-C12-N-C13
152	a	501	PC1	C11-C12-N-C14
152	c1	707	PC1	C11-C12-N-C13
152	m1	401	PC1	C11-C12-N-C14
152	n	302	PC1	C11-C12-N-C13
152	qe	301	PC1	C11-C12-N-C15
152	t1	602	PC1	C11-C12-N-C15
152	A	501	PC1	C11-C12-N-C14
152	A	503	PC1	C11-C12-N-C13
152	M1	401	PC1	C11-C12-N-C14
152	N	302	PC1	C11-C12-N-C13
152	QJ	102	PC1	C11-C12-N-C15
152	Qe	301	PC1	C11-C12-N-C15
152	T1	602	PC1	C11-C12-N-C15
153	l	301	CDL	C55-C56-C57-C58
153	t1	601	CDL	C72-C73-C74-C75
153	t5	301	CDL	C78-C79-C80-C81
153	L	301	CDL	C55-C56-C57-C58
153	T5	301	CDL	C78-C79-C80-C81
166	Y5	203	HEM	C3D-CAD-CBD-CGD
153	m2	403	CDL	C52-C53-C54-C55
160	qh	201	PX2	C6-C7-C8-C9
160	Qh	201	PX2	C10-C11-C12-C13
158	a3	202	3PE	C21-C22-C23-C24
158	g2	301	3PE	C21-C22-C23-C24
158	A3	202	3PE	C21-C22-C23-C24
153	M2	403	CDL	C52-C53-C54-C55
152	m1	403	PC1	O21-C2-C3-O31
152	M1	403	PC1	O21-C2-C3-O31
153	2g	203	CDL	OB6-CB4-CB6-OB8
153	2g	204	CDL	OA6-CA4-CA6-OA8
153	2k	101	CDL	OA6-CA4-CA6-OA8
153	7c	302	CDL	OA6-CA4-CA6-OA8
153	m	303	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	b3	102	CDL	OA6-CA4-CA6-OA8
153	2G	203	CDL	OB6-CB4-CB6-OB8
153	2K	101	CDL	OA6-CA4-CA6-OA8
153	7C	302	CDL	OA6-CA4-CA6-OA8
153	M	305	CDL	OA6-CA4-CA6-OA8
153	B3	102	CDL	OA6-CA4-CA6-OA8
160	r	202	PX2	O7-C2-C3-O5
153	bm	301	CDL	C40-C41-C42-C43
158	G2	301	3PE	C21-C22-C23-C24
153	T1	601	CDL	C72-C73-C74-C75
152	n	303	PC1	O31-C31-C32-C33
153	TE	101	CDL	C32-C31-CA7-OA8
153	b3	102	CDL	C62-C63-C64-C65
153	B3	102	CDL	C62-C63-C64-C65
152	n	301	PC1	C22-C23-C24-C25
152	N	301	PC1	C22-C23-C24-C25
169	b6	201	T7X	C44-C45-C46-C47
169	B6	201	T7X	C44-C45-C46-C47
153	7C	302	CDL	C31-C32-C33-C34
153	QB	601	CDL	C12-C13-C14-C15
153	Qb	601	CDL	C71-C72-C73-C74
160	qh	201	PX2	C10-C11-C12-C13
153	7c	302	CDL	C31-C32-C33-C34
153	qI	203	CDL	C12-C13-C14-C15
153	qb	601	CDL	C71-C72-C73-C74
153	qB	601	CDL	C12-C13-C14-C15
153	QI	203	CDL	C12-C13-C14-C15
160	Qh	201	PX2	C19-C20-C21-C22
153	E	402	CDL	CB5-C51-C52-C53
167	a9	401	NDP	C2D-C1D-N1N-C6N
152	te	102	PC1	C32-C33-C34-C35
158	M3	402	3PE	C2A-C2B-C2C-C2D
158	B4	202	3PE	C3A-C3B-C3C-C3D
152	A	503	PC1	C11-C12-N-C14
152	C1	710	PC1	C11-C12-N-C13
152	2g	202	PC1	O11-C1-C2-C3
152	m	301	PC1	O11-C1-C2-C3
152	v	201	PC1	O11-C1-C2-C3
152	w	201	PC1	O11-C1-C2-C3
152	tc	102	PC1	O11-C1-C2-C3
152	2G	202	PC1	O11-C1-C2-C3
152	M	303	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	V	201	PC1	O11-C1-C2-C3
152	W	201	PC1	O11-C1-C2-C3
153	2g	203	CDL	OB5-CB3-CB4-CB6
153	2o	101	CDL	OB5-CB3-CB4-CB6
153	6c	201	CDL	OA5-CA3-CA4-CA6
153	6c	202	CDL	OB5-CB3-CB4-CB6
153	a	504	CDL	OB5-CB3-CB4-CB6
153	a	505	CDL	OB5-CB3-CB4-CB6
153	i	302	CDL	OB5-CB3-CB4-CB6
153	j	301	CDL	OB5-CB3-CB4-CB6
153	m2	401	CDL	OB5-CB3-CB4-CB6
153	n	304	CDL	OA5-CA3-CA4-CA6
153	n	304	CDL	OB5-CB3-CB4-CB6
153	q	202	CDL	OB5-CB3-CB4-CB6
153	r	201	CDL	OB5-CB3-CB4-CB6
153	sd	101	CDL	OB5-CB3-CB4-CB6
153	u	201	CDL	OB5-CB3-CB4-CB6
153	al	301	CDL	OB5-CB3-CB4-CB6
153	b3	101	CDL	OA5-CA3-CA4-CA6
153	qD	402	CDL	OB5-CB3-CB4-CB6
153	qG	402	CDL	OB5-CB3-CB4-CB6
153	qi	202	CDL	OB5-CB3-CB4-CB6
153	t5	301	CDL	OB5-CB3-CB4-CB6
153	2G	203	CDL	OB5-CB3-CB4-CB6
153	2G	204	CDL	OB5-CB3-CB4-CB6
153	2O	101	CDL	OB5-CB3-CB4-CB6
153	6C	203	CDL	OB5-CB3-CB4-CB6
153	A	504	CDL	OB5-CB3-CB4-CB6
153	I	303	CDL	OB5-CB3-CB4-CB6
153	J	301	CDL	OB5-CB3-CB4-CB6
153	M2	401	CDL	OB5-CB3-CB4-CB6
153	N	304	CDL	OB5-CB3-CB4-CB6
153	Q	202	CDL	OB5-CB3-CB4-CB6
153	R	201	CDL	OB5-CB3-CB4-CB6
153	T	204	CDL	OB5-CB3-CB4-CB6
153	U	201	CDL	OB5-CB3-CB4-CB6
153	VB	705	CDL	OB5-CB3-CB4-CB6
153	AL	301	CDL	OB5-CB3-CB4-CB6
153	B3	101	CDL	OA5-CA3-CA4-CA6
153	QD	402	CDL	OB5-CB3-CB4-CB6
153	QG	402	CDL	OB5-CB3-CB4-CB6
153	Qi	202	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	T5	301	CDL	OB5-CB3-CB4-CB6
160	r	202	PX2	O4-C1-C2-C3
153	sd	101	CDL	C71-C72-C73-C74
169	b6	201	T7X	C33-C34-C35-C36
169	B6	201	T7X	C33-C34-C35-C36
158	an	301	3PE	O13-C11-C12-N
158	n4	601	3PE	O13-C11-C12-N
158	AN	301	3PE	O13-C11-C12-N
158	N4	601	3PE	O13-C11-C12-N
152	7a	202	PC1	C22-C23-C24-C25
152	7A	202	PC1	C22-C23-C24-C25
153	t	202	CDL	C56-C57-C58-C59
158	m3	402	3PE	C2A-C2B-C2C-C2D
164	qc	501	U10	C13-C14-C16-C17
153	6c	201	CDL	CA7-C31-C32-C33
160	Y5	204	PX2	C17-C18-C19-C20
153	qG	402	CDL	C21-C22-C23-C24
158	b4	202	3PE	C3A-C3B-C3C-C3D
153	td	101	CDL	C72-C71-CB7-OB8
153	A1	101	CDL	C72-C71-CB7-OB8
153	al	301	CDL	CB7-C71-C72-C73
153	6C	202	CDL	CA7-C31-C32-C33
153	AL	301	CDL	CB7-C71-C72-C73
152	b9	201	PC1	C34-C35-C36-C37
152	TE	102	PC1	C32-C33-C34-C35
153	2g	201	CDL	C16-C17-C18-C19
153	vb	701	CDL	C73-C74-C75-C76
153	2G	201	CDL	C16-C17-C18-C19
153	VB	701	CDL	C73-C74-C75-C76
152	m1	403	PC1	C2-C1-O11-P
152	qE	304	PC1	C2-C1-O11-P
152	tc	102	PC1	C2-C1-O11-P
152	M1	403	PC1	C2-C1-O11-P
152	QJ	101	PC1	C2-C1-O11-P
152	TC	102	PC1	C2-C1-O11-P
153	7c	301	CDL	C1-CB2-OB2-PB2
153	m2	401	CDL	CB4-CB3-OB5-PB2
153	m3	403	CDL	CA4-CA3-OA5-PA1
153	q	201	CDL	C1-CA2-OA2-PA1
153	t	202	CDL	CA4-CA3-OA5-PA1
153	y5	201	CDL	CA4-CA3-OA5-PA1
153	b3	101	CDL	CA4-CA3-OA5-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qc	508	CDL	C1-CA2-OA2-PA1
153	7C	301	CDL	C1-CB2-OB2-PB2
153	M2	401	CDL	CB4-CB3-OB5-PB2
153	M3	403	CDL	CA4-CA3-OA5-PA1
153	Q	201	CDL	C1-CA2-OA2-PA1
153	T	202	CDL	CA4-CA3-OA5-PA1
153	Y5	201	CDL	CA4-CA3-OA5-PA1
153	B3	101	CDL	CA4-CA3-OA5-PA1
153	Qc	508	CDL	C1-CA2-OA2-PA1
168	ab	201	ZMP	S1-C11-C12-N1
168	AB	201	ZMP	S1-C11-C12-N1
152	qC	505	PC1	C22-C23-C24-C25
152	QC	505	PC1	C22-C23-C24-C25
153	p1	402	CDL	C74-C75-C76-C77
153	SD	101	CDL	C71-C72-C73-C74
153	P1	402	CDL	C74-C75-C76-C77
153	QG	402	CDL	C21-C22-C23-C24
152	am	202	PC1	C38-C39-C3A-C3B
152	B9	201	PC1	C34-C35-C36-C37
153	a	505	CDL	C64-C65-C66-C67
153	VB	705	CDL	C64-C65-C66-C67
152	M2	407	PC1	C38-C39-C3A-C3B
152	AM	202	PC1	C38-C39-C3A-C3B
153	m1	402	CDL	C54-C55-C56-C57
153	M1	402	CDL	C54-C55-C56-C57
160	r	202	PX2	C24-C25-C26-C27
152	c2	703	PC1	C1-C2-C3-O31
152	qC	508	PC1	C1-C2-C3-O31
152	qc	506	PC1	C1-C2-C3-O31
152	C2	701	PC1	C1-C2-C3-O31
152	C3	602	PC1	C1-C2-C3-O31
152	QC	508	PC1	C1-C2-C3-O31
152	Qc	506	PC1	C1-C2-C3-O31
153	2k	101	CDL	CA3-CA4-CA6-OA8
153	a	502	CDL	CB3-CB4-CB6-OB8
153	m	303	CDL	CA3-CA4-CA6-OA8
153	m	306	CDL	CB3-CB4-CB6-OB8
153	m1	402	CDL	CA3-CA4-CA6-OA8
153	m2	403	CDL	CA3-CA4-CA6-OA8
153	q	202	CDL	CB3-CB4-CB6-OB8
153	sd	101	CDL	CB3-CB4-CB6-OB8
153	t	201	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	t	204	CDL	CA3-CA4-CA6-OA8
153	b4	201	CDL	CB3-CB4-CB6-OB8
153	2K	101	CDL	CA3-CA4-CA6-OA8
153	7C	302	CDL	CA3-CA4-CA6-OA8
153	A	502	CDL	CB3-CB4-CB6-OB8
153	M	301	CDL	CB3-CB4-CB6-OB8
153	M	305	CDL	CA3-CA4-CA6-OA8
153	M1	402	CDL	CA3-CA4-CA6-OA8
153	M2	403	CDL	CA3-CA4-CA6-OA8
153	Q	202	CDL	CB3-CB4-CB6-OB8
153	SD	101	CDL	CB3-CB4-CB6-OB8
153	T	201	CDL	CB3-CB4-CB6-OB8
153	T	204	CDL	CA3-CA4-CA6-OA8
153	B4	201	CDL	CB3-CB4-CB6-OB8
158	a3	202	3PE	C1-C2-C3-O31
158	an	301	3PE	C1-C2-C3-O31
158	A3	202	3PE	C1-C2-C3-O31
158	AN	301	3PE	C1-C2-C3-O31
160	r	202	PX2	C1-C2-C3-O5
160	qh	201	PX2	C1-C2-C3-O5
152	m2	407	PC1	C38-C39-C3A-C3B
153	T	202	CDL	C56-C57-C58-C59
160	y5	204	PX2	C17-C18-C19-C20
152	b9	201	PC1	C36-C37-C38-C39
152	B9	201	PC1	C36-C37-C38-C39
159	M2	406	P5S	C39-C40-C41-C42
153	N5	806	CDL	CA7-C31-C32-C33
152	b9	201	PC1	C11-C12-N-C14
152	2G	202	PC1	C11-C12-N-C14
152	M1	401	PC1	C11-C12-N-C13
152	B9	201	PC1	C11-C12-N-C14
159	m2	406	P5S	C39-C40-C41-C42
153	t5	301	CDL	C76-C77-C78-C79
169	b6	201	T7X	C41-C42-C43-C44
152	7c	303	PC1	C1-O11-P-O13
152	m	305	PC1	C11-O13-P-O11
152	n5	804	PC1	C1-O11-P-O13
152	qe	303	PC1	C11-O13-P-O11
152	7C	303	PC1	C1-O11-P-O13
152	M	307	PC1	C11-O13-P-O11
152	M2	405	PC1	C1-O11-P-O13
152	N5	804	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2o	101	CDL	CB3-OB5-PB2-OB2
153	7c	301	CDL	CB3-OB5-PB2-OB2
153	a1	101	CDL	CB2-OB2-PB2-OB5
153	b3	101	CDL	CB3-OB5-PB2-OB2
153	2O	101	CDL	CB3-OB5-PB2-OB2
153	A1	102	CDL	CB2-OB2-PB2-OB5
153	B3	101	CDL	CB3-OB5-PB2-OB2
153	QI	203	CDL	CB3-OB5-PB2-OB2
169	b6	201	T7X	C19-C20-C21-C22
169	B6	201	T7X	C19-C20-C21-C22
153	m1	405	CDL	CA5-C11-C12-C13
153	bm	301	CDL	CA7-C31-C32-C33
153	M1	405	CDL	CA5-C11-C12-C13
160	Y5	204	PX2	O6-C4-O5-C3
167	A9	401	NDP	C2D-C1D-N1N-C6N
152	2F	301	PC1	C2C-C2D-C2E-C2F
153	T5	301	CDL	C76-C77-C78-C79
160	r	202	PX2	C17-C18-C19-C20
169	B6	201	T7X	C41-C42-C43-C44
152	n5	805	PC1	O11-C1-C2-O21
152	qc	509	PC1	O11-C1-C2-O21
152	N5	805	PC1	O11-C1-C2-O21
152	Qc	509	PC1	O11-C1-C2-O21
153	2g	204	CDL	OB5-CB3-CB4-OB6
153	2o	101	CDL	OB5-CB3-CB4-OB6
153	c1	709	CDL	OA5-CA3-CA4-OA6
153	c1	712	CDL	OB5-CB3-CB4-OB6
153	fs	203	CDL	OA5-CA3-CA4-OA6
153	n	304	CDL	OA5-CA3-CA4-OA6
153	t	204	CDL	OB5-CB3-CB4-OB6
153	u	201	CDL	OB5-CB3-CB4-OB6
153	b3	102	CDL	OB5-CB3-CB4-OB6
153	p1	402	CDL	OB5-CB3-CB4-OB6
153	2O	101	CDL	OB5-CB3-CB4-OB6
153	C1	708	CDL	OA5-CA3-CA4-OA6
153	FS	204	CDL	OA5-CA3-CA4-OA6
153	N	304	CDL	OA5-CA3-CA4-OA6
153	SD	101	CDL	OB5-CB3-CB4-OB6
153	T	204	CDL	OB5-CB3-CB4-OB6
153	U	201	CDL	OB5-CB3-CB4-OB6
153	P1	402	CDL	OB5-CB3-CB4-OB6
153	QC	503	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C	301	CDL	OB5-CB3-CB4-OB6
153	c	301	CDL	OB5-CB3-CB4-OB6
153	u1	101	CDL	OB5-CB3-CB4-OB6
153	U1	101	CDL	OB5-CB3-CB4-OB6
153	7a	201	CDL	C64-C65-C66-C67
153	7A	201	CDL	C64-C65-C66-C67
160	R	202	PX2	C17-C18-C19-C20
152	2f	301	PC1	C2C-C2D-C2E-C2F
153	y5	201	CDL	C12-C11-CA5-OA6
153	Y5	201	CDL	C12-C11-CA5-OA6
153	a9	403	CDL	O1-C1-CB2-OB2
153	P1	403	CDL	C34-C35-C36-C37
152	qC	508	PC1	O21-C2-C3-O31
152	QC	508	PC1	O21-C2-C3-O31
153	7c	301	CDL	OA6-CA4-CA6-OA8
153	m1	402	CDL	OA6-CA4-CA6-OA8
153	n	304	CDL	OB6-CB4-CB6-OB8
153	b4	201	CDL	OB6-CB4-CB6-OB8
153	bm	301	CDL	OA6-CA4-CA6-OA8
153	n5	806	CDL	OB6-CB4-CB6-OB8
153	qc	504	CDL	OB6-CB4-CB6-OB8
153	M1	402	CDL	OA6-CA4-CA6-OA8
153	N	304	CDL	OB6-CB4-CB6-OB8
153	B4	201	CDL	OB6-CB4-CB6-OB8
153	BM	301	CDL	OA6-CA4-CA6-OA8
153	N5	806	CDL	OB6-CB4-CB6-OB8
153	Qc	504	CDL	OB6-CB4-CB6-OB8
158	vb	705	3PE	O21-C2-C3-O31
158	w	203	3PE	O21-C2-C3-O31
158	a3	201	3PE	O21-C2-C3-O31
158	n5	802	3PE	O21-C2-C3-O31
158	VB	707	3PE	O21-C2-C3-O31
158	W	203	3PE	O21-C2-C3-O31
158	A3	201	3PE	O21-C2-C3-O31
158	N5	802	3PE	O21-C2-C3-O31
152	qC	505	PC1	C34-C35-C36-C37
158	ta	201	3PE	C21-C22-C23-C24
158	TA	201	3PE	C21-C22-C23-C24
153	p1	403	CDL	C34-C35-C36-C37
153	c1	709	CDL	CB2-C1-CA2-OA2
153	e	402	CDL	CB2-C1-CA2-OA2
153	an	302	CDL	CB2-C1-CA2-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C1	708	CDL	CB2-C1-CA2-OA2
153	AN	302	CDL	CB2-C1-CA2-OA2
153	C	301	CDL	CA2-C1-CB2-OB2
153	2k	101	CDL	C54-C55-C56-C57
153	2K	101	CDL	C54-C55-C56-C57
152	6c	203	PC1	C2-C1-O11-P
152	a	503	PC1	C2-C1-O11-P
152	w	201	PC1	C2-C1-O11-P
152	n1	301	PC1	C2-C1-O11-P
152	n5	804	PC1	C2-C1-O11-P
152	qC	507	PC1	C2-C1-O11-P
152	6C	201	PC1	C2-C1-O11-P
152	A	503	PC1	C2-C1-O11-P
152	W	201	PC1	C2-C1-O11-P
152	N1	301	PC1	C2-C1-O11-P
152	N5	804	PC1	C2-C1-O11-P
152	QC	507	PC1	C2-C1-O11-P
153	2g	203	CDL	C1-CB2-OB2-PB2
153	2k	101	CDL	CB4-CB3-OB5-PB2
153	2o	101	CDL	CB4-CB3-OB5-PB2
153	c1	709	CDL	CB4-CB3-OB5-PB2
153	e	402	CDL	C1-CA2-OA2-PA1
153	fs	203	CDL	CA4-CA3-OA5-PA1
153	m2	403	CDL	C1-CB2-OB2-PB2
153	m3	403	CDL	C1-CB2-OB2-PB2
153	t	203	CDL	CA4-CA3-OA5-PA1
153	t	203	CDL	C1-CB2-OB2-PB2
153	t	204	CDL	CA4-CA3-OA5-PA1
153	t	204	CDL	C1-CB2-OB2-PB2
153	vb	701	CDL	CB4-CB3-OB5-PB2
153	an	302	CDL	CA4-CA3-OA5-PA1
153	an	302	CDL	CB4-CB3-OB5-PB2
153	b3	101	CDL	C1-CA2-OA2-PA1
153	p1	402	CDL	C1-CA2-OA2-PA1
153	p1	403	CDL	CB4-CB3-OB5-PB2
153	qc	505	CDL	C1-CA2-OA2-PA1
153	qg	402	CDL	CA4-CA3-OA5-PA1
153	2K	101	CDL	CB4-CB3-OB5-PB2
153	2O	101	CDL	CB4-CB3-OB5-PB2
153	C1	708	CDL	CA4-CA3-OA5-PA1
153	C1	708	CDL	CB4-CB3-OB5-PB2
153	FS	204	CDL	CA4-CA3-OA5-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	M2	403	CDL	C1-CB2-OB2-PB2
153	M3	403	CDL	C1-CB2-OB2-PB2
153	T	203	CDL	CA4-CA3-OA5-PA1
153	T	203	CDL	C1-CB2-OB2-PB2
153	T	204	CDL	CA4-CA3-OA5-PA1
153	T	204	CDL	C1-CB2-OB2-PB2
153	VB	701	CDL	CB4-CB3-OB5-PB2
153	AN	302	CDL	CA4-CA3-OA5-PA1
153	AN	302	CDL	CB4-CB3-OB5-PB2
153	B3	101	CDL	C1-CA2-OA2-PA1
153	P1	402	CDL	C1-CA2-OA2-PA1
153	P1	403	CDL	CB4-CB3-OB5-PB2
153	Qc	505	CDL	C1-CA2-OA2-PA1
153	Qg	402	CDL	CA4-CA3-OA5-PA1
153	u1	101	CDL	CA4-CA3-OA5-PA1
153	U1	101	CDL	CA4-CA3-OA5-PA1
158	bm	302	3PE	C2-C1-O11-P
158	BM	302	3PE	C2-C1-O11-P
159	m2	406	P5S	C2-C3-O16-P12
159	M2	406	P5S	C2-C3-O16-P12
152	QC	505	PC1	C34-C35-C36-C37
152	TC	102	PC1	C35-C36-C37-C38
152	m	301	PC1	C11-C12-N-C13
152	m	305	PC1	C11-C12-N-C15
152	m2	405	PC1	C11-C12-N-C14
152	qE	304	PC1	C11-C12-N-C13
152	M	303	PC1	C11-C12-N-C13
152	M	307	PC1	C11-C12-N-C15
152	M2	405	PC1	C11-C12-N-C14
152	QJ	101	PC1	C11-C12-N-C13
153	6a	201	CDL	C36-C37-C38-C39
153	b3	102	CDL	C55-C56-C57-C58
153	R	201	CDL	C51-C52-C53-C54
153	q	202	CDL	C72-C71-CB7-OB8
153	Q	202	CDL	C72-C71-CB7-OB8
153	6A	201	CDL	C36-C37-C38-C39
152	tc	102	PC1	C35-C36-C37-C38
153	r	201	CDL	C51-C52-C53-C54
153	p1	403	CDL	C73-C74-C75-C76
153	td	101	CDL	C16-C17-C18-C19
153	T	204	CDL	C57-C58-C59-C60
153	A1	101	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	P1	403	CDL	C73-C74-C75-C76
152	qC	508	PC1	C31-C32-C33-C34
152	QC	508	PC1	C31-C32-C33-C34
153	c1	701	CDL	C15-C16-C17-C18
153	t	204	CDL	C57-C58-C59-C60
160	qh	201	PX2	C7-C8-C9-C10
153	m2	401	CDL	CA5-C11-C12-C13
153	M2	401	CDL	CA5-C11-C12-C13
153	C1	701	CDL	C15-C16-C17-C18
161	sa	701	FAD	PA-O3P-P-O5'
161	SA	701	FAD	PA-O3P-P-O5'
169	b6	201	T7X	C21-C22-C23-C24
169	B6	201	T7X	C21-C22-C23-C24
153	B3	102	CDL	C55-C56-C57-C58
152	qJ	101	PC1	O11-C1-C2-C3
152	qc	509	PC1	O11-C1-C2-C3
152	qj	101	PC1	O11-C1-C2-C3
152	QC	507	PC1	O11-C1-C2-C3
152	QJ	102	PC1	O11-C1-C2-C3
152	Qc	509	PC1	O11-C1-C2-C3
152	Qj	101	PC1	O11-C1-C2-C3
152	TC	102	PC1	O11-C1-C2-C3
153	2g	204	CDL	OB5-CB3-CB4-CB6
153	c1	701	CDL	OB5-CB3-CB4-CB6
153	m1	404	CDL	OB5-CB3-CB4-CB6
153	t	204	CDL	OB5-CB3-CB4-CB6
153	y7	501	CDL	OB5-CB3-CB4-CB6
153	a1	101	CDL	OB5-CB3-CB4-CB6
153	a9	403	CDL	OB5-CB3-CB4-CB6
153	b3	102	CDL	OB5-CB3-CB4-CB6
153	p1	402	CDL	OB5-CB3-CB4-CB6
153	qD	402	CDL	OA5-CA3-CA4-CA6
153	6C	202	CDL	OA5-CA3-CA4-CA6
153	C1	701	CDL	OB5-CB3-CB4-CB6
153	M1	404	CDL	OB5-CB3-CB4-CB6
153	Y7	501	CDL	OB5-CB3-CB4-CB6
153	B8	302	CDL	OB5-CB3-CB4-CB6
153	P1	402	CDL	OB5-CB3-CB4-CB6
153	QD	402	CDL	OA5-CA3-CA4-CA6
158	bm	302	3PE	O11-C1-C2-C3
158	n5	802	3PE	O11-C1-C2-C3
158	BM	302	3PE	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	N5	802	3PE	O11-C1-C2-C3
153	n6	302	CDL	O1-C1-CA2-OA2
153	A9	403	CDL	O1-C1-CB2-OB2
153	c1	701	CDL	C14-C15-C16-C17
152	V	202	PC1	C24-C25-C26-C27
153	C1	701	CDL	C14-C15-C16-C17
169	b6	201	T7X	C32-C33-C34-C35
152	v	202	PC1	C24-C25-C26-C27
153	I	302	CDL	C38-C39-C40-C41
152	n5	801	PC1	C26-C27-C28-C29
153	i	301	CDL	C38-C39-C40-C41
153	6C	203	CDL	C62-C63-C64-C65
169	B6	201	T7X	C32-C33-C34-C35
158	T8	602	3PE	C2A-C2B-C2C-C2D
168	ab	201	ZMP	N2-C16-C17-O4
168	AB	201	ZMP	N2-C16-C17-O4
153	BM	301	CDL	CA7-C31-C32-C33
152	N5	801	PC1	C26-C27-C28-C29
153	7C	301	CDL	C38-C39-C40-C41
158	t8	602	3PE	C2A-C2B-C2C-C2D
152	m1	401	PC1	C11-C12-N-C13
152	n	302	PC1	C11-C12-N-C15
152	N	302	PC1	C11-C12-N-C15
153	6c	202	CDL	C62-C63-C64-C65
153	7c	301	CDL	C38-C39-C40-C41
153	an	302	CDL	C78-C79-C80-C81
160	r	202	PX2	C1-C2-O7-C16
166	qC	501	HEM	C2B-C3B-CAB-CBB
166	QC	501	HEM	C2B-C3B-CAB-CBB
153	AN	302	CDL	C78-C79-C80-C81
152	t4	301	PC1	O31-C31-C32-C33
152	M1	401	PC1	C25-C26-C27-C28
153	m2	404	CDL	C75-C76-C77-C78
153	e	403	CDL	C76-C77-C78-C79
153	E	403	CDL	C76-C77-C78-C79
153	M2	404	CDL	C75-C76-C77-C78
152	tc	102	PC1	C34-C35-C36-C37
153	VB	706	CDL	C74-C75-C76-C77
152	m2	407	PC1	C1-C2-C3-O31
152	n5	805	PC1	C1-C2-C3-O31
152	p1	401	PC1	C2-C1-O11-P
152	qe	301	PC1	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	qg	401	PC1	C2-C1-O11-P
152	M2	407	PC1	C1-C2-C3-O31
152	N5	805	PC1	C1-C2-C3-O31
152	P1	401	PC1	C2-C1-O11-P
152	Qe	301	PC1	C1-C2-C3-O31
152	Qg	401	PC1	C2-C1-O11-P
153	6a	201	CDL	CB4-CB3-OB5-PB2
153	7c	301	CDL	CA3-CA4-CA6-OA8
153	7c	302	CDL	CB4-CB3-OB5-PB2
153	a	504	CDL	CB3-CB4-CB6-OB8
153	a	505	CDL	C1-CA2-OA2-PA1
153	c1	701	CDL	C1-CA2-OA2-PA1
153	c1	709	CDL	CA4-CA3-OA5-PA1
153	c3	604	CDL	CB4-CB3-OB5-PB2
153	j	301	CDL	C1-CA2-OA2-PA1
153	l	301	CDL	C1-CA2-OA2-PA1
153	m1	402	CDL	CB3-CB4-CB6-OB8
153	m2	403	CDL	C1-CA2-OA2-PA1
153	m2	404	CDL	CB4-CB3-OB5-PB2
153	n	304	CDL	C1-CB2-OB2-PB2
153	vb	701	CDL	CA3-CA4-CA6-OA8
153	b8	302	CDL	CA4-CA3-OA5-PA1
153	n5	806	CDL	C1-CB2-OB2-PB2
153	n5	806	CDL	CB3-CB4-CB6-OB8
153	qC	503	CDL	C1-CA2-OA2-PA1
153	qG	402	CDL	C1-CB2-OB2-PB2
153	td	101	CDL	CA4-CA3-OA5-PA1
153	2G	203	CDL	C1-CB2-OB2-PB2
153	6A	201	CDL	CB4-CB3-OB5-PB2
153	7C	302	CDL	CB4-CB3-OB5-PB2
153	A	504	CDL	CB3-CB4-CB6-OB8
153	C3	604	CDL	CB4-CB3-OB5-PB2
153	E	402	CDL	C1-CA2-OA2-PA1
153	L	301	CDL	C1-CA2-OA2-PA1
153	M1	402	CDL	CB3-CB4-CB6-OB8
153	M2	403	CDL	C1-CA2-OA2-PA1
153	M2	404	CDL	CB4-CB3-OB5-PB2
153	N	304	CDL	C1-CB2-OB2-PB2
153	VB	701	CDL	CA3-CA4-CA6-OA8
153	VB	705	CDL	C1-CA2-OA2-PA1
153	Z	101	CDL	CB3-CB4-CB6-OB8
153	A1	101	CDL	CA4-CA3-OA5-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	B8	302	CDL	CA4-CA3-OA5-PA1
153	N5	806	CDL	C1-CB2-OB2-PB2
153	N5	806	CDL	CB3-CB4-CB6-OB8
153	QC	503	CDL	C1-CA2-OA2-PA1
153	QG	402	CDL	C1-CB2-OB2-PB2
158	w	203	3PE	C1-C2-C3-O31
158	W	203	3PE	C1-C2-C3-O31
152	m1	401	PC1	C25-C26-C27-C28
152	TC	102	PC1	C34-C35-C36-C37
153	vb	704	CDL	C74-C75-C76-C77
152	2j	201	PC1	O11-C1-C2-O21
152	v	201	PC1	O11-C1-C2-O21
152	w	201	PC1	O11-C1-C2-O21
152	qJ	101	PC1	O11-C1-C2-O21
152	tc	102	PC1	O11-C1-C2-O21
152	2J	201	PC1	O11-C1-C2-O21
152	V	201	PC1	O11-C1-C2-O21
152	W	201	PC1	O11-C1-C2-O21
152	QJ	102	PC1	O11-C1-C2-O21
152	TC	102	PC1	O11-C1-C2-O21
153	2g	203	CDL	OB5-CB3-CB4-OB6
153	6c	202	CDL	OB5-CB3-CB4-OB6
153	c1	701	CDL	OA5-CA3-CA4-OA6
153	j	301	CDL	OB5-CB3-CB4-OB6
153	m	306	CDL	OB5-CB3-CB4-OB6
153	m1	404	CDL	OB5-CB3-CB4-OB6
153	m3	403	CDL	OB5-CB3-CB4-OB6
153	q	202	CDL	OB5-CB3-CB4-OB6
153	q	203	CDL	OB5-CB3-CB4-OB6
153	r	201	CDL	OB5-CB3-CB4-OB6
153	sd	101	CDL	OA5-CA3-CA4-OA6
153	sd	101	CDL	OB5-CB3-CB4-OB6
153	a1	101	CDL	OB5-CB3-CB4-OB6
153	b3	101	CDL	OA5-CA3-CA4-OA6
153	b8	302	CDL	OB5-CB3-CB4-OB6
153	p1	403	CDL	OB5-CB3-CB4-OB6
153	qG	402	CDL	OB5-CB3-CB4-OB6
153	qI	203	CDL	OB5-CB3-CB4-OB6
153	qc	508	CDL	OB5-CB3-CB4-OB6
153	2G	203	CDL	OB5-CB3-CB4-OB6
153	C1	701	CDL	OA5-CA3-CA4-OA6
153	J	301	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	M	301	CDL	OB5-CB3-CB4-OB6
153	M1	404	CDL	OB5-CB3-CB4-OB6
153	M3	403	CDL	OB5-CB3-CB4-OB6
153	Q	202	CDL	OB5-CB3-CB4-OB6
153	R	201	CDL	OB5-CB3-CB4-OB6
153	SD	101	CDL	OA5-CA3-CA4-OA6
153	VB	703	CDL	OB5-CB3-CB4-OB6
153	Y7	501	CDL	OB5-CB3-CB4-OB6
153	A1	102	CDL	OB5-CB3-CB4-OB6
153	B3	101	CDL	OA5-CA3-CA4-OA6
153	B8	302	CDL	OB5-CB3-CB4-OB6
153	P1	403	CDL	OB5-CB3-CB4-OB6
153	QG	402	CDL	OB5-CB3-CB4-OB6
153	Qc	508	CDL	OB5-CB3-CB4-OB6
158	n5	802	3PE	O11-C1-C2-O21
158	N5	802	3PE	O11-C1-C2-O21
159	m2	406	P5S	O37-C2-C3-O16
159	M2	406	P5S	O37-C2-C3-O16
152	C3	601	PC1	O31-C31-C32-C33
152	T4	301	PC1	O31-C31-C32-C33
152	T4	301	PC1	C35-C36-C37-C38
152	t4	301	PC1	C35-C36-C37-C38
152	Qb	602	PC1	C26-C27-C28-C29
153	m2	404	CDL	CA2-C1-CB2-OB2
153	E	402	CDL	CB2-C1-CA2-OA2
153	M2	404	CDL	CA2-C1-CB2-OB2
152	qe	303	PC1	C22-C23-C24-C25
152	2F	301	PC1	C25-C26-C27-C28
152	Qe	303	PC1	C22-C23-C24-C25
153	T	204	CDL	C19-C20-C21-C22
160	qh	201	PX2	C19-C20-C21-C22
152	2f	301	PC1	C25-C26-C27-C28
153	t	204	CDL	C19-C20-C21-C22
158	W	203	3PE	C35-C36-C37-C38
152	qc	506	PC1	O21-C2-C3-O31
152	s8	301	PC1	O21-C2-C3-O31
152	t4	303	PC1	O21-C2-C3-O31
152	Qc	506	PC1	O21-C2-C3-O31
152	S8	301	PC1	O21-C2-C3-O31
153	m2	403	CDL	OA6-CA4-CA6-OA8
153	m3	401	CDL	OA6-CA4-CA6-OA8
153	q	202	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	t	201	CDL	OB6-CB4-CB6-OB8
153	t	204	CDL	OA6-CA4-CA6-OA8
153	z	101	CDL	OB6-CB4-CB6-OB8
153	7C	301	CDL	OA6-CA4-CA6-OA8
153	L	301	CDL	OB6-CB4-CB6-OB8
153	M2	403	CDL	OA6-CA4-CA6-OA8
153	M3	401	CDL	OA6-CA4-CA6-OA8
153	Q	202	CDL	OB6-CB4-CB6-OB8
153	T	201	CDL	OB6-CB4-CB6-OB8
153	T	204	CDL	OA6-CA4-CA6-OA8
153	Z	101	CDL	OB6-CB4-CB6-OB8
160	Y5	204	PX2	O7-C2-C3-O5
153	BM	301	CDL	C15-C16-C17-C18
158	w	203	3PE	C35-C36-C37-C38
152	a	501	PC1	C11-C12-N-C15
152	f	402	PC1	C11-C12-N-C13
152	m	301	PC1	C11-C12-N-C15
152	m	305	PC1	C11-C12-N-C14
152	m2	405	PC1	C11-C12-N-C15
152	qJ	101	PC1	C11-C12-N-C14
152	s8	301	PC1	C11-C12-N-C13
152	t1	602	PC1	C11-C12-N-C14
152	F	401	PC1	C11-C12-N-C13
152	M	303	PC1	C11-C12-N-C15
152	QJ	102	PC1	C11-C12-N-C14
152	S8	301	PC1	C11-C12-N-C13
152	T1	602	PC1	C11-C12-N-C14
152	c2	703	PC1	C24-C25-C26-C27
152	N6	301	PC1	C31-C32-C33-C34
152	W	201	PC1	C33-C34-C35-C36
152	c3	601	PC1	O31-C31-C32-C33
152	c3	602	PC1	C25-C26-C27-C28
152	w	201	PC1	C33-C34-C35-C36
152	C3	602	PC1	C25-C26-C27-C28
153	l	301	CDL	C16-C17-C18-C19
153	6C	202	CDL	C12-C13-C14-C15
160	Qh	201	PX2	C17-C18-C19-C20
152	n6	301	PC1	C31-C32-C33-C34
152	C2	701	PC1	C24-C25-C26-C27
153	L	301	CDL	C16-C17-C18-C19
153	Qg	402	CDL	C83-C84-C85-C86
152	d	501	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	D	501	PC1	O31-C31-C32-C33
152	qb	602	PC1	C26-C27-C28-C29
153	qg	402	CDL	C83-C84-C85-C86
153	t7	201	CDL	CA5-C11-C12-C13
152	n	303	PC1	C33-C34-C35-C36
152	a	503	PC1	C27-C28-C29-C2A
153	bm	301	CDL	C15-C16-C17-C18
152	A	503	PC1	C27-C28-C29-C2A
153	5B	201	CDL	C38-C39-C40-C41
153	N6	302	CDL	C58-C59-C60-C61
152	m2	405	PC1	C1-O11-P-O13
152	m2	407	PC1	C1-O11-P-O13
152	qb	602	PC1	C1-O11-P-O13
152	M2	407	PC1	C1-O11-P-O13
152	Qb	602	PC1	C1-O11-P-O13
153	6c	201	CDL	CA2-OA2-PA1-OA5
153	a	502	CDL	CB2-OB2-PB2-OB5
153	e	401	CDL	CB3-OB5-PB2-OB2
153	e	402	CDL	CA2-OA2-PA1-OA5
153	f	401	CDL	CB2-OB2-PB2-OB5
153	m	302	CDL	CA3-OA5-PA1-OA2
153	m	303	CDL	CA2-OA2-PA1-OA5
153	m3	403	CDL	CB2-OB2-PB2-OB5
153	sd	101	CDL	CA2-OA2-PA1-OA5
153	t	201	CDL	CA2-OA2-PA1-OA5
153	t	202	CDL	CB3-OB5-PB2-OB2
153	a1	101	CDL	CB3-OB5-PB2-OB2
153	a9	403	CDL	CB3-OB5-PB2-OB2
153	n5	806	CDL	CB3-OB5-PB2-OB2
153	n6	302	CDL	CA3-OA5-PA1-OA2
153	qD	402	CDL	CA3-OA5-PA1-OA2
153	qG	402	CDL	CB2-OB2-PB2-OB5
153	qc	508	CDL	CA2-OA2-PA1-OA5
153	qc	508	CDL	CA3-OA5-PA1-OA2
153	qc	508	CDL	CB3-OB5-PB2-OB2
153	t1	601	CDL	CA3-OA5-PA1-OA2
153	6C	202	CDL	CA2-OA2-PA1-OA5
153	A	502	CDL	CB2-OB2-PB2-OB5
153	E	401	CDL	CB3-OB5-PB2-OB2
153	E	402	CDL	CA2-OA2-PA1-OA5
153	M	304	CDL	CA3-OA5-PA1-OA2
153	M	305	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	M3	403	CDL	CB2-OB2-PB2-OB5
153	SD	101	CDL	CA2-OA2-PA1-OA5
153	T	201	CDL	CA2-OA2-PA1-OA5
153	A1	102	CDL	CB3-OB5-PB2-OB2
153	N5	806	CDL	CB3-OB5-PB2-OB2
153	N6	302	CDL	CA3-OA5-PA1-OA2
153	QD	402	CDL	CA3-OA5-PA1-OA2
153	QG	402	CDL	CB2-OB2-PB2-OB5
153	Qc	508	CDL	CA2-OA2-PA1-OA5
153	Qc	508	CDL	CA3-OA5-PA1-OA2
153	Qc	508	CDL	CB3-OB5-PB2-OB2
153	T1	601	CDL	CA3-OA5-PA1-OA2
153	C	301	CDL	CA3-OA5-PA1-OA2
153	c	301	CDL	CA3-OA5-PA1-OA2
158	w	203	3PE	C11-O13-P-O11
158	an	301	3PE	C11-O13-P-O11
158	n4	601	3PE	C11-O13-P-O11
158	W	203	3PE	C11-O13-P-O11
158	AN	301	3PE	C11-O13-P-O11
158	N4	601	3PE	C11-O13-P-O11
167	a9	401	NDP	O4D-C1D-N1N-C6N
153	6c	201	CDL	C12-C13-C14-C15
153	5b	201	CDL	C38-C39-C40-C41
153	n6	302	CDL	C58-C59-C60-C61
153	A9	402	CDL	C31-C32-C33-C34
153	6a	201	CDL	O1-C1-CB2-OB2
153	6A	201	CDL	O1-C1-CB2-OB2
153	M	306	CDL	O1-C1-CB2-OB2
152	m2	407	PC1	C2-C1-O11-P
152	an	304	PC1	C2-C1-O11-P
152	tc	101	PC1	C2-C1-O11-P
152	M2	407	PC1	C2-C1-O11-P
152	AN	304	PC1	C2-C1-O11-P
152	TC	101	PC1	C2-C1-O11-P
153	a	505	CDL	CA4-CA3-OA5-PA1
153	f	401	CDL	CB4-CB3-OB5-PB2
153	l	301	CDL	CA4-CA3-OA5-PA1
153	l	301	CDL	CB4-CB3-OB5-PB2
153	m	302	CDL	C1-CA2-OA2-PA1
153	m	304	CDL	C1-CB2-OB2-PB2
153	m2	404	CDL	CA4-CA3-OA5-PA1
153	r	201	CDL	C1-CA2-OA2-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	w	202	CDL	CA4-CA3-OA5-PA1
153	y7	501	CDL	CB4-CB3-OB5-PB2
153	a9	403	CDL	C1-CA2-OA2-PA1
153	am	201	CDL	C1-CA2-OA2-PA1
153	p1	403	CDL	C1-CB2-OB2-PB2
153	qc	504	CDL	C1-CA2-OA2-PA1
153	qg	402	CDL	C1-CB2-OB2-PB2
153	t1	601	CDL	CB4-CB3-OB5-PB2
153	t7	201	CDL	C1-CA2-OA2-PA1
153	th	200	CDL	CB4-CB3-OB5-PB2
153	C1	701	CDL	C1-CA2-OA2-PA1
153	E	403	CDL	CB4-CB3-OB5-PB2
153	F	402	CDL	C1-CB2-OB2-PB2
153	F	402	CDL	CB4-CB3-OB5-PB2
153	J	301	CDL	C1-CA2-OA2-PA1
153	L	301	CDL	CB4-CB3-OB5-PB2
153	M	304	CDL	C1-CA2-OA2-PA1
153	M	306	CDL	C1-CB2-OB2-PB2
153	M2	404	CDL	CA4-CA3-OA5-PA1
153	R	201	CDL	C1-CA2-OA2-PA1
153	VB	705	CDL	CA4-CA3-OA5-PA1
153	W	202	CDL	CA4-CA3-OA5-PA1
153	Y7	501	CDL	CB4-CB3-OB5-PB2
153	A9	403	CDL	C1-CA2-OA2-PA1
153	P1	403	CDL	C1-CB2-OB2-PB2
153	Qc	504	CDL	C1-CA2-OA2-PA1
153	Qg	402	CDL	C1-CB2-OB2-PB2
153	T1	601	CDL	CB4-CB3-OB5-PB2
153	T7	201	CDL	C1-CA2-OA2-PA1
153	TH	200	CDL	CB4-CB3-OB5-PB2
158	y5	202	3PE	C2-C1-O11-P
158	t8	601	3PE	C2-C1-O11-P
158	Y5	202	3PE	C2-C1-O11-P
158	T8	601	3PE	C2-C1-O11-P
152	qg	401	PC1	C23-C24-C25-C26
153	a9	402	CDL	C31-C32-C33-C34
152	2f	301	PC1	C11-O13-P-O12
152	2f	302	PC1	C11-O13-P-O12
152	2f	302	PC1	C1-O11-P-O12
152	2f	302	PC1	C1-O11-P-O14
152	2f	303	PC1	C11-O13-P-O12
152	2f	303	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	2g	202	PC1	C11-O13-P-O14
152	2g	202	PC1	C11-C12-N-C14
152	2j	201	PC1	C11-O13-P-O14
152	c1	704	PC1	C11-O13-P-O14
152	c1	704	PC1	C1-O11-P-O14
152	c1	707	PC1	C11-O13-P-O14
152	c1	707	PC1	C11-C12-N-C15
152	c3	601	PC1	C1-O11-P-O12
152	c3	603	PC1	C11-O13-P-O14
152	d	501	PC1	C1-O11-P-O12
152	d	501	PC1	C1-O11-P-O14
152	f	402	PC1	C1-O11-P-O12
152	f	402	PC1	C11-C12-N-C14
152	i	304	PC1	C11-O13-P-O14
152	m	301	PC1	C11-O13-P-O14
152	m	301	PC1	C1-O11-P-O12
152	m	305	PC1	C11-O13-P-O14
152	m1	401	PC1	C1-O11-P-O12
152	m1	401	PC1	C1-O11-P-O14
152	m2	402	PC1	C11-O13-P-O14
152	m2	402	PC1	C1-O11-P-O12
152	n	302	PC1	C1-O11-P-O14
152	v	201	PC1	C11-O13-P-O14
152	v	202	PC1	C11-O13-P-O14
152	v	202	PC1	C1-O11-P-O12
152	an	304	PC1	C11-O13-P-O14
152	b9	201	PC1	C11-O13-P-O14
152	j1	400	PC1	C11-O13-P-O14
152	n5	801	PC1	C11-O13-P-O12
152	n5	803	PC1	C11-O13-P-O12
152	n5	803	PC1	C11-O13-P-O14
152	n5	803	PC1	C1-O11-P-O14
152	n5	804	PC1	C1-O11-P-O14
152	n5	805	PC1	C11-O13-P-O14
152	n5	805	PC1	C1-O11-P-O12
152	qB	602	PC1	C11-O13-P-O12
152	qC	507	PC1	C1-O11-P-O12
152	qC	508	PC1	C1-O11-P-O12
152	qE	301	PC1	C1-O11-P-O14
152	qE	303	PC1	C1-O11-P-O14
152	qE	304	PC1	C11-C12-N-C14
152	qc	509	PC1	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	qe	303	PC1	C11-O13-P-O12
152	qi	203	PC1	C1-O11-P-O14
152	qi	203	PC1	C11-C12-N-C13
152	s8	301	PC1	C1-O11-P-O12
152	t1	602	PC1	C1-O11-P-O14
152	t4	303	PC1	C1-O11-P-O14
152	tc	102	PC1	C11-O13-P-O12
152	2F	301	PC1	C11-O13-P-O12
152	2F	302	PC1	C11-O13-P-O12
152	2F	302	PC1	C1-O11-P-O12
152	2F	302	PC1	C1-O11-P-O14
152	2F	303	PC1	C11-O13-P-O12
152	2F	303	PC1	C11-O13-P-O14
152	2G	202	PC1	C11-O13-P-O14
152	2J	201	PC1	C11-O13-P-O14
152	C1	706	PC1	C11-O13-P-O14
152	C1	706	PC1	C1-O11-P-O14
152	C1	710	PC1	C11-O13-P-O14
152	C1	710	PC1	C11-C12-N-C15
152	C3	601	PC1	C1-O11-P-O12
152	C3	603	PC1	C11-O13-P-O14
152	D	501	PC1	C1-O11-P-O12
152	D	501	PC1	C1-O11-P-O14
152	F	401	PC1	C1-O11-P-O12
152	F	401	PC1	C11-C12-N-C14
152	I	301	PC1	C11-O13-P-O14
152	M	303	PC1	C11-O13-P-O14
152	M	303	PC1	C1-O11-P-O12
152	M	307	PC1	C11-O13-P-O14
152	M	307	PC1	C11-C12-N-C14
152	M1	401	PC1	C1-O11-P-O12
152	M1	401	PC1	C1-O11-P-O14
152	M2	402	PC1	C11-O13-P-O14
152	M2	402	PC1	C1-O11-P-O12
152	M2	405	PC1	C11-C12-N-C15
152	N	302	PC1	C1-O11-P-O14
152	V	201	PC1	C11-O13-P-O14
152	V	202	PC1	C11-O13-P-O14
152	V	202	PC1	C1-O11-P-O12
152	AN	304	PC1	C11-O13-P-O14
152	B9	201	PC1	C11-O13-P-O14
152	J1	400	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	N5	801	PC1	C11-O13-P-O12
152	N5	803	PC1	C11-O13-P-O12
152	N5	803	PC1	C11-O13-P-O14
152	N5	803	PC1	C1-O11-P-O14
152	N5	804	PC1	C1-O11-P-O14
152	N5	805	PC1	C11-O13-P-O14
152	N5	805	PC1	C1-O11-P-O12
152	QB	602	PC1	C11-O13-P-O12
152	QC	507	PC1	C1-O11-P-O12
152	QC	508	PC1	C1-O11-P-O12
152	QE	301	PC1	C1-O11-P-O14
152	QJ	101	PC1	C11-C12-N-C14
152	Qc	509	PC1	C1-O11-P-O12
152	Qe	303	PC1	C11-O13-P-O12
152	Qi	203	PC1	C1-O11-P-O14
152	Qi	203	PC1	C11-C12-N-C13
152	S8	301	PC1	C1-O11-P-O12
152	T1	602	PC1	C1-O11-P-O14
152	T4	303	PC1	C1-O11-P-O14
152	TC	101	PC1	C11-C12-N-C13
152	TC	102	PC1	C11-O13-P-O12
153	2g	201	CDL	CB3-OB5-PB2-OB4
153	2g	203	CDL	CA3-OA5-PA1-OA4
153	2g	204	CDL	CA3-OA5-PA1-OA3
153	2g	204	CDL	CB3-OB5-PB2-OB3
153	2k	101	CDL	CA3-OA5-PA1-OA3
153	2o	101	CDL	CB2-OB2-PB2-OB3
153	6a	201	CDL	CA2-OA2-PA1-OA4
153	6a	201	CDL	CB3-OB5-PB2-OB3
153	6c	202	CDL	CA3-OA5-PA1-OA3
153	7a	201	CDL	CA3-OA5-PA1-OA4
153	7a	201	CDL	CB2-OB2-PB2-OB4
153	7a	203	CDL	CA2-OA2-PA1-OA4
153	7c	301	CDL	CA3-OA5-PA1-OA3
153	7c	301	CDL	CB2-OB2-PB2-OB3
153	7c	301	CDL	CB2-OB2-PB2-OB4
153	7c	301	CDL	CB3-OB5-PB2-OB3
153	7c	302	CDL	CB2-OB2-PB2-OB4
153	a	502	CDL	CA2-OA2-PA1-OA4
153	a	504	CDL	CA3-OA5-PA1-OA3
153	c1	701	CDL	CA3-OA5-PA1-OA3
153	c1	703	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	c1	709	CDL	CB3-OB5-PB2-OB4
153	e	401	CDL	CB3-OB5-PB2-OB4
153	e	402	CDL	CB2-OB2-PB2-OB4
153	e	403	CDL	CB3-OB5-PB2-OB3
153	e	403	CDL	CB3-OB5-PB2-OB4
153	i	301	CDL	CA2-OA2-PA1-OA4
153	i	301	CDL	CA3-OA5-PA1-OA4
153	i	301	CDL	CB3-OB5-PB2-OB4
153	i	302	CDL	CA3-OA5-PA1-OA4
153	i	302	CDL	CB2-OB2-PB2-OB4
153	j	301	CDL	CA2-OA2-PA1-OA4
153	j	301	CDL	CA3-OA5-PA1-OA4
153	l	301	CDL	CA3-OA5-PA1-OA4
153	m	302	CDL	CA3-OA5-PA1-OA3
153	m	303	CDL	CA2-OA2-PA1-OA4
153	m	304	CDL	CA2-OA2-PA1-OA3
153	m	306	CDL	CB2-OB2-PB2-OB3
153	m1	404	CDL	CA2-OA2-PA1-OA4
153	m1	405	CDL	CB2-OB2-PB2-OB3
153	m1	405	CDL	CB3-OB5-PB2-OB4
153	m2	401	CDL	CB3-OB5-PB2-OB3
153	m2	401	CDL	CB3-OB5-PB2-OB4
153	m2	403	CDL	CA3-OA5-PA1-OA3
153	m3	403	CDL	CB3-OB5-PB2-OB3
153	n	304	CDL	CA3-OA5-PA1-OA3
153	q	201	CDL	CB3-OB5-PB2-OB3
153	q	202	CDL	CB2-OB2-PB2-OB3
153	q	202	CDL	CB3-OB5-PB2-OB4
153	r	201	CDL	CB2-OB2-PB2-OB4
153	r	201	CDL	CB3-OB5-PB2-OB4
153	sd	101	CDL	CB2-OB2-PB2-OB3
153	sd	101	CDL	CB3-OB5-PB2-OB3
153	t	201	CDL	CA3-OA5-PA1-OA4
153	t	203	CDL	CA2-OA2-PA1-OA3
153	t	203	CDL	CA3-OA5-PA1-OA3
153	t	203	CDL	CA3-OA5-PA1-OA4
153	t	203	CDL	CB3-OB5-PB2-OB4
153	t	204	CDL	CB3-OB5-PB2-OB4
153	u	201	CDL	CB3-OB5-PB2-OB3
153	vb	701	CDL	CA2-OA2-PA1-OA4
153	vb	704	CDL	CA3-OA5-PA1-OA3
153	vb	704	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	w	202	CDL	CA3-OA5-PA1-OA3
153	w	202	CDL	CB3-OB5-PB2-OB4
153	y7	501	CDL	CB2-OB2-PB2-OB3
153	z	101	CDL	CA2-OA2-PA1-OA4
153	z	101	CDL	CB3-OB5-PB2-OB3
153	5b	201	CDL	CA2-OA2-PA1-OA4
153	5b	201	CDL	CB3-OB5-PB2-OB4
153	a9	402	CDL	CA2-OA2-PA1-OA4
153	a9	403	CDL	CB3-OB5-PB2-OB3
153	al	301	CDL	CA2-OA2-PA1-OA3
153	al	301	CDL	CA3-OA5-PA1-OA4
153	al	301	CDL	CB3-OB5-PB2-OB4
153	an	302	CDL	CB3-OB5-PB2-OB3
153	b3	101	CDL	CA3-OA5-PA1-OA3
153	b3	102	CDL	CB3-OB5-PB2-OB3
153	b4	201	CDL	CA2-OA2-PA1-OA4
153	b8	302	CDL	CB3-OB5-PB2-OB4
153	bm	301	CDL	CA2-OA2-PA1-OA4
153	c4	401	CDL	CB2-OB2-PB2-OB3
153	n5	806	CDL	CA3-OA5-PA1-OA4
153	n5	806	CDL	CB2-OB2-PB2-OB4
153	n6	302	CDL	CA3-OA5-PA1-OA4
153	p1	402	CDL	CA2-OA2-PA1-OA4
153	p1	402	CDL	CA3-OA5-PA1-OA3
153	p1	402	CDL	CA3-OA5-PA1-OA4
153	p1	403	CDL	CA3-OA5-PA1-OA3
153	qB	601	CDL	CB3-OB5-PB2-OB3
153	qC	503	CDL	CA3-OA5-PA1-OA3
153	qC	504	CDL	CA3-OA5-PA1-OA4
153	qD	402	CDL	CA3-OA5-PA1-OA4
153	qH	201	CDL	CA2-OA2-PA1-OA4
153	qH	201	CDL	CB3-OB5-PB2-OB4
153	qI	203	CDL	CA2-OA2-PA1-OA4
153	qI	203	CDL	CA3-OA5-PA1-OA3
153	qI	203	CDL	CA3-OA5-PA1-OA4
153	qI	203	CDL	CB2-OB2-PB2-OB4
153	qc	504	CDL	CA2-OA2-PA1-OA4
153	qc	504	CDL	CB2-OB2-PB2-OB3
153	qc	504	CDL	CB2-OB2-PB2-OB4
153	qc	505	CDL	CA3-OA5-PA1-OA4
153	qg	402	CDL	CA2-OA2-PA1-OA3
153	qg	402	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qg	402	CDL	CA3-OA5-PA1-OA4
153	qg	402	CDL	CB2-OB2-PB2-OB3
153	qg	402	CDL	CB2-OB2-PB2-OB4
153	qg	402	CDL	CB3-OB5-PB2-OB3
153	qi	202	CDL	CB2-OB2-PB2-OB3
153	t5	301	CDL	CA3-OA5-PA1-OA4
153	t7	201	CDL	CA2-OA2-PA1-OA3
153	t7	201	CDL	CA3-OA5-PA1-OA3
153	td	101	CDL	CA2-OA2-PA1-OA4
153	td	101	CDL	CB2-OB2-PB2-OB4
153	te	101	CDL	CA2-OA2-PA1-OA3
153	th	200	CDL	CA2-OA2-PA1-OA3
153	th	200	CDL	CA2-OA2-PA1-OA4
153	th	200	CDL	CA3-OA5-PA1-OA4
153	th	200	CDL	CB2-OB2-PB2-OB3
153	th	200	CDL	CB3-OB5-PB2-OB3
153	2G	201	CDL	CB3-OB5-PB2-OB4
153	2G	203	CDL	CA3-OA5-PA1-OA4
153	2G	204	CDL	CA3-OA5-PA1-OA3
153	2K	101	CDL	CA3-OA5-PA1-OA3
153	2O	101	CDL	CB2-OB2-PB2-OB3
153	6A	201	CDL	CA2-OA2-PA1-OA4
153	6A	201	CDL	CB3-OB5-PB2-OB3
153	6C	203	CDL	CA3-OA5-PA1-OA3
153	6C	203	CDL	CB3-OB5-PB2-OB3
153	7A	201	CDL	CA3-OA5-PA1-OA4
153	7A	201	CDL	CB2-OB2-PB2-OB4
153	7A	203	CDL	CA2-OA2-PA1-OA4
153	7C	301	CDL	CA3-OA5-PA1-OA3
153	7C	301	CDL	CB2-OB2-PB2-OB3
153	7C	301	CDL	CB2-OB2-PB2-OB4
153	7C	301	CDL	CB3-OB5-PB2-OB3
153	7C	302	CDL	CB2-OB2-PB2-OB4
153	A	502	CDL	CA2-OA2-PA1-OA4
153	A	504	CDL	CA3-OA5-PA1-OA3
153	C1	701	CDL	CA3-OA5-PA1-OA3
153	C1	707	CDL	CA3-OA5-PA1-OA4
153	C1	708	CDL	CB3-OB5-PB2-OB4
153	E	401	CDL	CB3-OB5-PB2-OB4
153	E	402	CDL	CB2-OB2-PB2-OB4
153	E	403	CDL	CB3-OB5-PB2-OB3
153	E	403	CDL	CB3-OB5-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	I	302	CDL	CA2-OA2-PA1-OA4
153	I	302	CDL	CA3-OA5-PA1-OA4
153	I	302	CDL	CB3-OB5-PB2-OB4
153	I	303	CDL	CA3-OA5-PA1-OA4
153	I	303	CDL	CB2-OB2-PB2-OB4
153	J	301	CDL	CA2-OA2-PA1-OA4
153	J	301	CDL	CA3-OA5-PA1-OA4
153	L	301	CDL	CA3-OA5-PA1-OA4
153	M	301	CDL	CB2-OB2-PB2-OB3
153	M	304	CDL	CA3-OA5-PA1-OA3
153	M	305	CDL	CA2-OA2-PA1-OA4
153	M	306	CDL	CA2-OA2-PA1-OA3
153	M	306	CDL	CA2-OA2-PA1-OA4
153	M1	404	CDL	CA2-OA2-PA1-OA4
153	M1	404	CDL	CB3-OB5-PB2-OB4
153	M1	405	CDL	CA3-OA5-PA1-OA4
153	M1	405	CDL	CB2-OB2-PB2-OB3
153	M1	405	CDL	CB3-OB5-PB2-OB4
153	M2	401	CDL	CB3-OB5-PB2-OB3
153	M2	401	CDL	CB3-OB5-PB2-OB4
153	M2	403	CDL	CA3-OA5-PA1-OA3
153	M3	403	CDL	CA3-OA5-PA1-OA4
153	M3	403	CDL	CB3-OB5-PB2-OB3
153	N	304	CDL	CA3-OA5-PA1-OA3
153	Q	201	CDL	CB3-OB5-PB2-OB3
153	Q	202	CDL	CB2-OB2-PB2-OB3
153	Q	202	CDL	CB3-OB5-PB2-OB4
153	R	201	CDL	CB2-OB2-PB2-OB4
153	R	201	CDL	CB3-OB5-PB2-OB4
153	SD	101	CDL	CB2-OB2-PB2-OB3
153	SD	101	CDL	CB3-OB5-PB2-OB3
153	T	201	CDL	CA3-OA5-PA1-OA4
153	T	203	CDL	CA2-OA2-PA1-OA3
153	T	203	CDL	CA3-OA5-PA1-OA3
153	T	203	CDL	CA3-OA5-PA1-OA4
153	T	203	CDL	CB3-OB5-PB2-OB4
153	T	204	CDL	CB3-OB5-PB2-OB4
153	U	201	CDL	CB3-OB5-PB2-OB3
153	VB	701	CDL	CA2-OA2-PA1-OA4
153	VB	701	CDL	CB3-OB5-PB2-OB3
153	VB	706	CDL	CA3-OA5-PA1-OA3
153	VB	706	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	W	202	CDL	CA3-OA5-PA1-OA3
153	W	202	CDL	CB3-OB5-PB2-OB4
153	Y5	201	CDL	CA3-OA5-PA1-OA3
153	Y7	501	CDL	CB2-OB2-PB2-OB3
153	Z	101	CDL	CA2-OA2-PA1-OA4
153	Z	101	CDL	CB3-OB5-PB2-OB3
153	5B	201	CDL	CA2-OA2-PA1-OA4
153	A1	101	CDL	CA2-OA2-PA1-OA4
153	A1	101	CDL	CB2-OB2-PB2-OB4
153	A9	402	CDL	CA2-OA2-PA1-OA4
153	A9	402	CDL	CA3-OA5-PA1-OA4
153	A9	403	CDL	CB2-OB2-PB2-OB4
153	A9	403	CDL	CB3-OB5-PB2-OB3
153	AL	301	CDL	CA2-OA2-PA1-OA3
153	AL	301	CDL	CA3-OA5-PA1-OA4
153	AL	301	CDL	CB3-OB5-PB2-OB4
153	AN	302	CDL	CB3-OB5-PB2-OB3
153	B3	101	CDL	CA3-OA5-PA1-OA3
153	B4	201	CDL	CA2-OA2-PA1-OA4
153	B8	302	CDL	CB3-OB5-PB2-OB4
153	BM	301	CDL	CA2-OA2-PA1-OA4
153	C4	401	CDL	CB2-OB2-PB2-OB3
153	N5	806	CDL	CA3-OA5-PA1-OA4
153	N5	806	CDL	CB2-OB2-PB2-OB4
153	N6	302	CDL	CA3-OA5-PA1-OA4
153	P1	402	CDL	CA2-OA2-PA1-OA4
153	P1	402	CDL	CA3-OA5-PA1-OA3
153	P1	402	CDL	CA3-OA5-PA1-OA4
153	P1	403	CDL	CA3-OA5-PA1-OA3
153	QB	601	CDL	CB3-OB5-PB2-OB3
153	QC	503	CDL	CA3-OA5-PA1-OA3
153	QC	504	CDL	CA3-OA5-PA1-OA4
153	QD	402	CDL	CA3-OA5-PA1-OA4
153	QH	201	CDL	CA2-OA2-PA1-OA4
153	QH	201	CDL	CB3-OB5-PB2-OB4
153	QI	203	CDL	CA2-OA2-PA1-OA4
153	QI	203	CDL	CA3-OA5-PA1-OA3
153	QI	203	CDL	CA3-OA5-PA1-OA4
153	QI	203	CDL	CB2-OB2-PB2-OB4
153	Qc	504	CDL	CA2-OA2-PA1-OA4
153	Qc	504	CDL	CB2-OB2-PB2-OB3
153	Qc	504	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qc	505	CDL	CA3-OA5-PA1-OA4
153	Qg	402	CDL	CA2-OA2-PA1-OA3
153	Qg	402	CDL	CA2-OA2-PA1-OA4
153	Qg	402	CDL	CA3-OA5-PA1-OA4
153	Qg	402	CDL	CB2-OB2-PB2-OB3
153	Qg	402	CDL	CB2-OB2-PB2-OB4
153	Qg	402	CDL	CB3-OB5-PB2-OB3
153	Qi	202	CDL	CB2-OB2-PB2-OB3
153	T5	301	CDL	CA3-OA5-PA1-OA4
153	T7	201	CDL	CA2-OA2-PA1-OA3
153	T7	201	CDL	CA3-OA5-PA1-OA3
153	TE	101	CDL	CA2-OA2-PA1-OA3
153	TE	101	CDL	CB3-OB5-PB2-OB3
153	TH	200	CDL	CA2-OA2-PA1-OA3
153	TH	200	CDL	CA2-OA2-PA1-OA4
153	TH	200	CDL	CA3-OA5-PA1-OA4
153	TH	200	CDL	CB2-OB2-PB2-OB3
153	TH	200	CDL	CB3-OB5-PB2-OB3
153	u1	101	CDL	CA2-OA2-PA1-OA3
153	u1	101	CDL	CA3-OA5-PA1-OA3
153	u1	101	CDL	CB2-OB2-PB2-OB3
153	u1	101	CDL	CB2-OB2-PB2-OB4
153	U1	101	CDL	CA2-OA2-PA1-OA3
153	U1	101	CDL	CA3-OA5-PA1-OA3
153	U1	101	CDL	CB2-OB2-PB2-OB3
153	U1	101	CDL	CB2-OB2-PB2-OB4
158	i	303	3PE	C1-O11-P-O12
158	i	303	3PE	C1-O11-P-O14
158	m2	408	3PE	C11-O13-P-O12
158	vb	705	3PE	C1-O11-P-O14
158	vb	705	3PE	C11-O13-P-O12
158	vb	705	3PE	C11-O13-P-O14
158	w	203	3PE	C1-O11-P-O14
158	y5	202	3PE	C1-O11-P-O14
158	y5	202	3PE	C11-O13-P-O14
158	an	305	3PE	C11-O13-P-O12
158	an	305	3PE	C11-O13-P-O14
158	b4	202	3PE	C1-O11-P-O14
158	n4	601	3PE	C1-O11-P-O14
158	s8	304	3PE	C1-O11-P-O12
158	s8	304	3PE	C11-O13-P-O14
158	t8	602	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	I	304	3PE	C1-O11-P-O12
158	I	304	3PE	C1-O11-P-O14
158	M2	408	3PE	C11-O13-P-O12
158	VB	707	3PE	C1-O11-P-O14
158	VB	707	3PE	C11-O13-P-O12
158	VB	707	3PE	C11-O13-P-O14
158	Y5	202	3PE	C1-O11-P-O14
158	Y5	202	3PE	C11-O13-P-O14
158	AN	305	3PE	C11-O13-P-O14
158	B4	202	3PE	C1-O11-P-O14
158	N4	601	3PE	C1-O11-P-O14
158	S8	304	3PE	C1-O11-P-O12
158	S8	304	3PE	C11-O13-P-O14
158	T8	602	3PE	C11-O13-P-O14
159	m2	406	P5S	CB-OG-P12-O13
159	M2	406	P5S	CB-OG-P12-O13
161	sa	701	FAD	C5B-O5B-PA-O1A
161	sa	701	FAD	C5B-O5B-PA-O2A
161	SA	701	FAD	C5B-O5B-PA-O1A
161	SA	701	FAD	C5B-O5B-PA-O2A
153	e	402	CDL	CB5-C51-C52-C53
153	W	202	CDL	CB5-C51-C52-C53
153	T7	201	CDL	CA5-C11-C12-C13
152	2j	201	PC1	O11-C1-C2-C3
152	n1	301	PC1	O11-C1-C2-C3
152	qC	507	PC1	O11-C1-C2-C3
152	qi	203	PC1	O11-C1-C2-C3
152	t4	301	PC1	O11-C1-C2-C3
152	N1	301	PC1	O11-C1-C2-C3
152	Qi	203	PC1	O11-C1-C2-C3
152	T4	301	PC1	O11-C1-C2-C3
153	c1	701	CDL	OA5-CA3-CA4-CA6
153	e	401	CDL	OB5-CB3-CB4-CB6
153	e	402	CDL	OB5-CB3-CB4-CB6
153	fs	203	CDL	OA5-CA3-CA4-CA6
153	m	306	CDL	OB5-CB3-CB4-CB6
153	m3	403	CDL	OB5-CB3-CB4-CB6
153	q	203	CDL	OB5-CB3-CB4-CB6
153	t	203	CDL	OB5-CB3-CB4-CB6
153	z	101	CDL	OB5-CB3-CB4-CB6
153	b8	302	CDL	OB5-CB3-CB4-CB6
153	p1	403	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qC	503	CDL	OB5-CB3-CB4-CB6
153	qI	203	CDL	OB5-CB3-CB4-CB6
153	C1	701	CDL	OA5-CA3-CA4-CA6
153	E	401	CDL	OB5-CB3-CB4-CB6
153	E	402	CDL	OB5-CB3-CB4-CB6
153	FS	204	CDL	OA5-CA3-CA4-CA6
153	M	301	CDL	OB5-CB3-CB4-CB6
153	M3	403	CDL	OB5-CB3-CB4-CB6
153	T	203	CDL	OB5-CB3-CB4-CB6
153	VB	703	CDL	OB5-CB3-CB4-CB6
153	Z	101	CDL	OB5-CB3-CB4-CB6
153	A1	102	CDL	OB5-CB3-CB4-CB6
153	A9	403	CDL	OB5-CB3-CB4-CB6
153	B3	102	CDL	OB5-CB3-CB4-CB6
153	P1	403	CDL	OB5-CB3-CB4-CB6
153	QC	503	CDL	OB5-CB3-CB4-CB6
153	C	301	CDL	OB5-CB3-CB4-CB6
153	c	301	CDL	OB5-CB3-CB4-CB6
159	m2	406	P5S	C1-C2-C3-O16
159	M2	406	P5S	C1-C2-C3-O16
164	sc	102	U10	C39-C41-C42-C43
164	SC	102	U10	C39-C41-C42-C43
152	TC	101	PC1	C26-C27-C28-C29
153	I	302	CDL	C31-C32-C33-C34
153	6c	201	CDL	C32-C31-CA7-OA8
152	Qg	401	PC1	C23-C24-C25-C26
154	c1	708	HEA	O11-C11-C12-C13
152	2f	301	PC1	C12-C11-O13-P
152	c1	706	PC1	C12-C11-O13-P
152	d	501	PC1	C12-C11-O13-P
152	j	302	PC1	C12-C11-O13-P
152	v	202	PC1	C12-C11-O13-P
152	n5	805	PC1	C12-C11-O13-P
152	qc	506	PC1	C12-C11-O13-P
152	t1	602	PC1	C12-C11-O13-P
152	t4	301	PC1	C12-C11-O13-P
152	2F	301	PC1	C12-C11-O13-P
152	C1	709	PC1	C12-C11-O13-P
152	D	501	PC1	C12-C11-O13-P
152	J	302	PC1	C12-C11-O13-P
152	V	202	PC1	C12-C11-O13-P
152	N5	805	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	Qc	506	PC1	C12-C11-O13-P
152	T1	602	PC1	C12-C11-O13-P
152	T4	301	PC1	C12-C11-O13-P
154	c1	708	HEA	C3B-C11-C12-C13
154	C1	703	HEA	C3B-C11-C12-C13
158	y5	202	3PE	C12-C11-O13-P
158	Y5	202	3PE	C12-C11-O13-P
164	qC	506	U10	C18-C19-C21-C22
164	QC	506	U10	C18-C19-C21-C22
153	w	202	CDL	CB5-C51-C52-C53
153	6C	202	CDL	C32-C31-CA7-OA8
152	tc	101	PC1	C26-C27-C28-C29
153	n	304	CDL	C55-C56-C57-C58
153	N	304	CDL	C55-C56-C57-C58
153	q	201	CDL	CB5-C51-C52-C53
153	Q	201	CDL	CB5-C51-C52-C53
153	c4	401	CDL	C57-C58-C59-C60
153	c	301	CDL	CA2-C1-CB2-OB2
159	m2	406	P5S	C20-C21-C22-C23
159	M2	406	P5S	C20-C21-C22-C23
152	2f	301	PC1	O11-C1-C2-O21
152	m	301	PC1	O11-C1-C2-O21
152	qC	507	PC1	O11-C1-C2-O21
152	2F	301	PC1	O11-C1-C2-O21
152	M	303	PC1	O11-C1-C2-O21
152	QC	507	PC1	O11-C1-C2-O21
153	7a	201	CDL	OB5-CB3-CB4-OB6
153	7a	203	CDL	OB5-CB3-CB4-OB6
153	a	504	CDL	OB5-CB3-CB4-OB6
153	f	401	CDL	OB5-CB3-CB4-OB6
153	m2	401	CDL	OB5-CB3-CB4-OB6
153	m2	403	CDL	OB5-CB3-CB4-OB6
153	n	304	CDL	OB5-CB3-CB4-OB6
153	t	203	CDL	OB5-CB3-CB4-OB6
153	vb	701	CDL	OB5-CB3-CB4-OB6
153	y7	501	CDL	OB5-CB3-CB4-OB6
153	a9	403	CDL	OB5-CB3-CB4-OB6
153	c4	401	CDL	OB5-CB3-CB4-OB6
153	qB	601	CDL	OB5-CB3-CB4-OB6
153	qD	402	CDL	OA5-CA3-CA4-OA6
153	qD	402	CDL	OB5-CB3-CB4-OB6
153	qb	601	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	t5	301	CDL	OB5-CB3-CB4-OB6
153	2G	204	CDL	OB5-CB3-CB4-OB6
153	6C	203	CDL	OB5-CB3-CB4-OB6
153	7A	201	CDL	OB5-CB3-CB4-OB6
153	7A	203	CDL	OB5-CB3-CB4-OB6
153	A	504	CDL	OB5-CB3-CB4-OB6
153	F	402	CDL	OB5-CB3-CB4-OB6
153	M2	401	CDL	OB5-CB3-CB4-OB6
153	M2	403	CDL	OB5-CB3-CB4-OB6
153	N	304	CDL	OB5-CB3-CB4-OB6
153	T	203	CDL	OB5-CB3-CB4-OB6
153	VB	701	CDL	OB5-CB3-CB4-OB6
153	A1	102	CDL	OA5-CA3-CA4-OA6
153	A9	403	CDL	OB5-CB3-CB4-OB6
153	B3	102	CDL	OB5-CB3-CB4-OB6
153	C4	401	CDL	OB5-CB3-CB4-OB6
153	QB	601	CDL	OB5-CB3-CB4-OB6
153	QD	402	CDL	OA5-CA3-CA4-OA6
153	QD	402	CDL	OB5-CB3-CB4-OB6
153	T5	301	CDL	OB5-CB3-CB4-OB6
158	a3	201	3PE	O11-C1-C2-O21
158	A3	201	3PE	O11-C1-C2-O21
166	y5	203	HEM	C2A-CAA-CBA-CGA
166	Y5	203	HEM	C2A-CAA-CBA-CGA
171	v1	501	FMN	N10-C1'-C2'-O2'
171	V1	501	FMN	N10-C1'-C2'-O2'
168	ab	201	ZMP	C2-C3-C4-C5
153	2o	101	CDL	C72-C71-CB7-OB8
153	i	301	CDL	C31-C32-C33-C34
153	C4	401	CDL	C57-C58-C59-C60
153	2o	101	CDL	C12-C13-C14-C15
153	2O	101	CDL	C12-C13-C14-C15
153	B	501	CDL	C51-C52-C53-C54
168	AB	201	ZMP	C2-C3-C4-C5
152	2f	301	PC1	C11-C12-N-C15
152	c1	711	PC1	C11-C12-N-C15
152	qe	301	PC1	C11-C12-N-C13
152	tc	101	PC1	C11-C12-N-C13
152	2F	301	PC1	C11-C12-N-C15
152	A	501	PC1	C11-C12-N-C15
152	C1	711	PC1	C11-C12-N-C15
152	C3	601	PC1	C11-C12-N-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	Qe	301	PC1	C11-C12-N-C13
152	S8	301	PC1	C11-C12-N-C14
152	T4	301	PC1	C11-C12-N-C14
152	a	501	PC1	C31-C32-C33-C34
152	A	501	PC1	C31-C32-C33-C34
167	a9	401	NDP	C2D-C1D-N1N-C2N
152	2f	301	PC1	O13-C11-C12-N
152	2f	302	PC1	O13-C11-C12-N
152	2g	202	PC1	O13-C11-C12-N
152	6a	202	PC1	O13-C11-C12-N
152	6c	203	PC1	O13-C11-C12-N
152	7a	202	PC1	O13-C11-C12-N
152	7c	303	PC1	O13-C11-C12-N
152	c1	706	PC1	O13-C11-C12-N
152	c1	711	PC1	O13-C11-C12-N
152	c3	606	PC1	O13-C11-C12-N
152	d	501	PC1	O13-C11-C12-N
152	i	304	PC1	O13-C11-C12-N
152	m2	407	PC1	O13-C11-C12-N
152	n	303	PC1	O13-C11-C12-N
152	v	202	PC1	O13-C11-C12-N
152	am	202	PC1	O13-C11-C12-N
152	n3	201	PC1	O13-C11-C12-N
152	n5	803	PC1	O13-C11-C12-N
152	n5	804	PC1	O13-C11-C12-N
152	p1	401	PC1	O13-C11-C12-N
152	qE	301	PC1	O13-C11-C12-N
152	qE	303	PC1	O13-C11-C12-N
152	qc	506	PC1	O13-C11-C12-N
152	qc	509	PC1	O13-C11-C12-N
152	qg	401	PC1	O13-C11-C12-N
152	t4	301	PC1	O13-C11-C12-N
152	tc	102	PC1	O13-C11-C12-N
152	te	102	PC1	O13-C11-C12-N
152	2F	301	PC1	O13-C11-C12-N
152	2F	302	PC1	O13-C11-C12-N
152	2G	202	PC1	O13-C11-C12-N
152	6A	202	PC1	O13-C11-C12-N
152	6C	201	PC1	O13-C11-C12-N
152	7A	202	PC1	O13-C11-C12-N
152	7C	303	PC1	O13-C11-C12-N
152	C1	709	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	C1	711	PC1	O13-C11-C12-N
152	C3	606	PC1	O13-C11-C12-N
152	D	501	PC1	O13-C11-C12-N
152	I	301	PC1	O13-C11-C12-N
152	M2	407	PC1	O13-C11-C12-N
152	N	303	PC1	O13-C11-C12-N
152	V	202	PC1	O13-C11-C12-N
152	AM	202	PC1	O13-C11-C12-N
152	N3	201	PC1	O13-C11-C12-N
152	N5	803	PC1	O13-C11-C12-N
152	N5	804	PC1	O13-C11-C12-N
152	P1	401	PC1	O13-C11-C12-N
152	QE	301	PC1	O13-C11-C12-N
152	QE	303	PC1	O13-C11-C12-N
152	Qc	506	PC1	O13-C11-C12-N
152	Qc	509	PC1	O13-C11-C12-N
152	Qg	401	PC1	O13-C11-C12-N
152	T4	301	PC1	O13-C11-C12-N
152	TC	102	PC1	O13-C11-C12-N
152	TE	102	PC1	O13-C11-C12-N
153	l	301	CDL	CB3-CB4-CB6-OB8
153	n	304	CDL	CB3-CB4-CB6-OB8
153	z	101	CDL	CB3-CB4-CB6-OB8
153	L	301	CDL	CB3-CB4-CB6-OB8
153	N	304	CDL	CB3-CB4-CB6-OB8
158	a3	201	3PE	C1-C2-C3-O31
158	A3	201	3PE	C1-C2-C3-O31
152	2j	201	PC1	O21-C2-C3-O31
152	i	304	PC1	O21-C2-C3-O31
152	qe	301	PC1	O21-C2-C3-O31
152	I	301	PC1	O21-C2-C3-O31
152	T4	303	PC1	O21-C2-C3-O31
153	6c	201	CDL	OA6-CA4-CA6-OA8
153	l	301	CDL	OB6-CB4-CB6-OB8
153	sd	101	CDL	OB6-CB4-CB6-OB8
153	6C	202	CDL	OA6-CA4-CA6-OA8
153	SD	101	CDL	OB6-CB4-CB6-OB8
158	an	301	3PE	O21-C2-C3-O31
158	AN	301	3PE	O21-C2-C3-O31
152	n5	801	PC1	C21-C22-C23-C24
152	N5	801	PC1	C21-C22-C23-C24
160	r	202	PX2	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	T	201	CDL	C12-C11-CA5-OA6
152	T4	301	PC1	C28-C29-C2A-C2B
152	qc	509	PC1	C2-C1-O11-P
152	Qc	509	PC1	C2-C1-O11-P
153	2k	101	CDL	CA4-CA3-OA5-PA1
153	7c	302	CDL	C1-CA2-OA2-PA1
153	a	502	CDL	CA4-CA3-OA5-PA1
153	e	403	CDL	CB4-CB3-OB5-PB2
153	f	401	CDL	C1-CB2-OB2-PB2
153	5b	201	CDL	CA4-CA3-OA5-PA1
153	2K	101	CDL	CA4-CA3-OA5-PA1
153	7C	302	CDL	C1-CA2-OA2-PA1
153	A	502	CDL	CA4-CA3-OA5-PA1
153	L	301	CDL	CA4-CA3-OA5-PA1
153	5B	201	CDL	CA4-CA3-OA5-PA1
153	AM	201	CDL	C1-CA2-OA2-PA1
152	t4	301	PC1	C28-C29-C2A-C2B
152	qg	401	PC1	O21-C21-C22-C23
153	t	201	CDL	C12-C11-CA5-OA6
153	qi	202	CDL	C32-C31-CA7-OA8
153	2O	101	CDL	C72-C71-CB7-OB8
153	M2	401	CDL	C12-C11-CA5-OA6
169	B6	201	T7X	C35-C36-C37-C38
153	M	305	CDL	C81-C82-C83-C84
158	AN	306	3PE	C22-C23-C24-C25
168	AB	201	ZMP	C1-C2-C3-C4
158	an	306	3PE	C22-C23-C24-C25
168	ab	201	ZMP	C1-C2-C3-C4
169	b6	201	T7X	C35-C36-C37-C38
153	b	501	CDL	C51-C52-C53-C54
153	m	303	CDL	C81-C82-C83-C84
152	c3	603	PC1	O21-C21-C22-C23
152	N	303	PC1	O31-C31-C32-C33
152	Qg	401	PC1	O21-C21-C22-C23
153	m2	401	CDL	C12-C11-CA5-OA6
153	a9	403	CDL	C32-C31-CA7-OA8
153	A9	403	CDL	C32-C31-CA7-OA8
153	Qi	202	CDL	C32-C31-CA7-OA8
153	A	504	CDL	C59-C60-C61-C62
167	A9	401	NDP	O4D-C1D-N1N-C6N
153	u	201	CDL	C53-C54-C55-C56
153	A	504	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	U	201	CDL	C53-C54-C55-C56
153	Qg	402	CDL	CA7-C31-C32-C33
152	b9	201	PC1	C11-C12-N-C15
152	qJ	101	PC1	C11-C12-N-C13
152	qi	203	PC1	C11-C12-N-C14
152	s8	301	PC1	C11-C12-N-C14
152	2G	202	PC1	C11-C12-N-C15
152	B9	201	PC1	C11-C12-N-C15
152	QJ	102	PC1	C11-C12-N-C13
152	Qi	203	PC1	C11-C12-N-C14
153	a	504	CDL	C59-C60-C61-C62
152	n5	801	PC1	C27-C28-C29-C2A
153	a	504	CDL	C32-C33-C34-C35
153	m	304	CDL	O1-C1-CB2-OB2
153	N6	302	CDL	O1-C1-CA2-OA2
152	N5	801	PC1	C27-C28-C29-C2A
164	qC	506	U10	C2-C3-O3-C3M
164	qc	507	U10	C2-C3-O3-C3M
164	qc	507	U10	C5-C4-O4-C4M
164	QC	506	U10	C2-C3-O3-C3M
164	Qc	507	U10	C2-C3-O3-C3M
164	Qc	507	U10	C5-C4-O4-C4M
152	C3	603	PC1	O21-C21-C22-C23
153	f	401	CDL	C32-C31-CA7-OA8
153	t1	601	CDL	C72-C71-CB7-OB8
153	F	402	CDL	C32-C31-CA7-OA8
167	A9	401	NDP	C2D-C1D-N1N-C2N
153	f	401	CDL	C16-C17-C18-C19
153	F	402	CDL	C16-C17-C18-C19
153	N6	302	CDL	C12-C13-C14-C15
153	n6	302	CDL	C12-C13-C14-C15
168	ab	201	ZMP	C2-C1-C22-C23
152	2f	301	PC1	C1-C2-O21-C21
152	2f	302	PC1	C3-C2-O21-C21
152	b9	201	PC1	C1-C2-O21-C21
152	2F	301	PC1	C1-C2-O21-C21
152	2F	302	PC1	C3-C2-O21-C21
152	B9	201	PC1	C1-C2-O21-C21
153	a	502	CDL	CA3-CA4-OA6-CA5
153	A	502	CDL	CA3-CA4-OA6-CA5
160	R	202	PX2	C3-C2-O7-C16
152	2J	201	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	m1	402	CDL	OB5-CB3-CB4-CB6
153	qg	402	CDL	OB5-CB3-CB4-CB6
153	M1	402	CDL	OB5-CB3-CB4-CB6
153	QI	203	CDL	OB5-CB3-CB4-CB6
153	Qg	402	CDL	OB5-CB3-CB4-CB6
153	b3	102	CDL	CB2-C1-CA2-OA2
154	C1	703	HEA	C11-C12-C13-C14
153	qg	402	CDL	CA7-C31-C32-C33
153	T1	601	CDL	C72-C71-CB7-OB8
153	2g	201	CDL	C1-CB2-OB2-PB2
153	6c	201	CDL	C1-CA2-OA2-PA1
153	6c	201	CDL	CA4-CA3-OA5-PA1
153	b	501	CDL	C1-CA2-OA2-PA1
153	m	306	CDL	C1-CB2-OB2-PB2
153	n	304	CDL	CA4-CA3-OA5-PA1
153	b4	201	CDL	C1-CA2-OA2-PA1
153	6C	202	CDL	C1-CA2-OA2-PA1
153	N	304	CDL	CA4-CA3-OA5-PA1
153	QC	504	CDL	C1-CA2-OA2-PA1
152	n1	301	PC1	O11-C1-C2-O21
152	n5	804	PC1	O11-C1-C2-O21
152	N1	301	PC1	O11-C1-C2-O21
152	N5	804	PC1	O11-C1-C2-O21
153	i	301	CDL	OB5-CB3-CB4-OB6
153	a1	101	CDL	OA5-CA3-CA4-OA6
153	I	302	CDL	OB5-CB3-CB4-OB6
153	Z	101	CDL	OB5-CB3-CB4-OB6
153	QI	203	CDL	OB5-CB3-CB4-OB6
153	Qb	601	CDL	OB5-CB3-CB4-OB6
158	ta	201	3PE	O11-C1-C2-O21
158	TA	201	3PE	O11-C1-C2-O21
160	r	202	PX2	O4-C1-C2-O7
153	c1	712	CDL	C72-C73-C74-C75
153	m	304	CDL	C52-C51-CB5-OB6
153	b8	302	CDL	C72-C71-CB7-OB8
153	M	306	CDL	C52-C51-CB5-OB6
153	B8	302	CDL	C72-C71-CB7-OB8
152	2g	202	PC1	C11-C12-N-C15
152	c1	711	PC1	C11-C12-N-C13
152	m	301	PC1	C11-C12-N-C14
152	m2	405	PC1	C11-C12-N-C13
152	tc	101	PC1	C11-C12-N-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	C1	711	PC1	C11-C12-N-C13
152	C3	601	PC1	C11-C12-N-C15
152	M	303	PC1	C11-C12-N-C14
152	TC	101	PC1	C11-C12-N-C14
153	BM	301	CDL	C76-C77-C78-C79
153	t	204	CDL	C17-C18-C19-C20
154	c1	708	HEA	C2D-C3D-CAD-CBD
152	7c	303	PC1	C32-C33-C34-C35
152	7C	303	PC1	C32-C33-C34-C35
153	a	505	CDL	C32-C31-CA7-OA8
168	AB	201	ZMP	C2-C1-C22-C23
152	c1	704	PC1	C2A-C2B-C2C-C2D
153	l	301	CDL	C12-C13-C14-C15
152	C1	706	PC1	C2A-C2B-C2C-C2D
153	C1	712	CDL	C72-C73-C74-C75
153	6c	201	CDL	CA5-C11-C12-C13
158	w	203	3PE	C21-C22-C23-C24
158	W	203	3PE	C21-C22-C23-C24
153	T	204	CDL	C17-C18-C19-C20
153	VB	705	CDL	C34-C35-C36-C37
158	a3	201	3PE	O21-C21-C22-C23
158	A3	201	3PE	O21-C21-C22-C23
152	t1	602	PC1	O21-C2-C3-O31
152	tc	102	PC1	O21-C2-C3-O31
152	2J	201	PC1	O21-C2-C3-O31
152	Qe	301	PC1	O21-C2-C3-O31
152	T1	602	PC1	O21-C2-C3-O31
152	TC	102	PC1	O21-C2-C3-O31
153	b	501	CDL	OB6-CB4-CB6-OB8
153	m1	402	CDL	OB6-CB4-CB6-OB8
153	A	504	CDL	OB6-CB4-CB6-OB8
153	B	501	CDL	OB6-CB4-CB6-OB8
153	M1	402	CDL	OB6-CB4-CB6-OB8
153	a	505	CDL	C34-C35-C36-C37
153	n5	806	CDL	C31-C32-C33-C34
158	an	303	3PE	C27-C28-C29-C2A
158	AN	303	3PE	C27-C28-C29-C2A
152	7a	202	PC1	C11-O13-P-O11
152	c1	704	PC1	C1-O11-P-O13
152	c1	711	PC1	C1-O11-P-O13
152	c2	703	PC1	C1-O11-P-O13
152	n	303	PC1	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	n3	201	PC1	C11-O13-P-O11
152	qC	508	PC1	C11-O13-P-O11
152	7A	202	PC1	C11-O13-P-O11
152	C1	706	PC1	C1-O11-P-O13
152	C1	711	PC1	C1-O11-P-O13
152	C2	701	PC1	C1-O11-P-O13
152	N	303	PC1	C11-O13-P-O11
152	N3	201	PC1	C11-O13-P-O11
152	QC	508	PC1	C11-O13-P-O11
153	7a	203	CDL	CB2-OB2-PB2-OB5
153	a	505	CDL	CA2-OA2-PA1-OA5
153	a	505	CDL	CB2-OB2-PB2-OB5
153	b	501	CDL	CB3-OB5-PB2-OB2
153	c1	709	CDL	CA3-OA5-PA1-OA2
153	c1	712	CDL	CB2-OB2-PB2-OB5
153	e	403	CDL	CA2-OA2-PA1-OA5
153	fs	203	CDL	CA3-OA5-PA1-OA2
153	i	302	CDL	CB3-OB5-PB2-OB2
153	j	301	CDL	CB2-OB2-PB2-OB5
153	m	303	CDL	CB3-OB5-PB2-OB2
153	m1	405	CDL	CB3-OB5-PB2-OB2
153	m2	404	CDL	CA2-OA2-PA1-OA5
153	m3	401	CDL	CA2-OA2-PA1-OA5
153	q	201	CDL	CA2-OA2-PA1-OA5
153	q	201	CDL	CA3-OA5-PA1-OA2
153	sd	101	CDL	CA3-OA5-PA1-OA2
153	t	203	CDL	CB2-OB2-PB2-OB5
153	vb	701	CDL	CB3-OB5-PB2-OB2
153	y7	501	CDL	CA3-OA5-PA1-OA2
153	5b	201	CDL	CB3-OB5-PB2-OB2
153	an	302	CDL	CA3-OA5-PA1-OA2
153	b8	302	CDL	CA2-OA2-PA1-OA5
153	bm	301	CDL	CB2-OB2-PB2-OB5
153	c4	401	CDL	CA3-OA5-PA1-OA2
153	qC	503	CDL	CB3-OB5-PB2-OB2
153	qD	402	CDL	CB3-OB5-PB2-OB2
153	qb	601	CDL	CB3-OB5-PB2-OB2
153	t5	301	CDL	CB3-OB5-PB2-OB2
153	t7	201	CDL	CB3-OB5-PB2-OB2
153	7A	203	CDL	CB2-OB2-PB2-OB5
153	B	501	CDL	CB3-OB5-PB2-OB2
153	C1	708	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	C1	712	CDL	CB2-OB2-PB2-OB5
153	E	403	CDL	CA2-OA2-PA1-OA5
153	F	402	CDL	CB2-OB2-PB2-OB5
153	FS	204	CDL	CA3-OA5-PA1-OA2
153	I	303	CDL	CB3-OB5-PB2-OB2
153	J	301	CDL	CB2-OB2-PB2-OB5
153	M	305	CDL	CB3-OB5-PB2-OB2
153	M1	405	CDL	CB3-OB5-PB2-OB2
153	M2	404	CDL	CA2-OA2-PA1-OA5
153	M3	401	CDL	CA2-OA2-PA1-OA5
153	Q	201	CDL	CA2-OA2-PA1-OA5
153	Q	201	CDL	CA3-OA5-PA1-OA2
153	SD	101	CDL	CA3-OA5-PA1-OA2
153	T	202	CDL	CB3-OB5-PB2-OB2
153	T	203	CDL	CB2-OB2-PB2-OB5
153	VB	701	CDL	CB3-OB5-PB2-OB2
153	VB	705	CDL	CA2-OA2-PA1-OA5
153	VB	705	CDL	CB2-OB2-PB2-OB5
153	Y7	501	CDL	CA3-OA5-PA1-OA2
153	5B	201	CDL	CB3-OB5-PB2-OB2
153	AN	302	CDL	CA3-OA5-PA1-OA2
153	B8	302	CDL	CA2-OA2-PA1-OA5
153	BM	301	CDL	CB2-OB2-PB2-OB5
153	C4	401	CDL	CA3-OA5-PA1-OA2
153	QC	503	CDL	CB3-OB5-PB2-OB2
153	QD	402	CDL	CB3-OB5-PB2-OB2
153	Qb	601	CDL	CB3-OB5-PB2-OB2
153	T5	301	CDL	CB3-OB5-PB2-OB2
153	T7	201	CDL	CB3-OB5-PB2-OB2
153	C	301	CDL	CB2-OB2-PB2-OB5
153	c	301	CDL	CB2-OB2-PB2-OB5
158	i	303	3PE	C11-O13-P-O11
158	m3	402	3PE	C11-O13-P-O11
158	an	306	3PE	C11-O13-P-O11
158	I	304	3PE	C11-O13-P-O11
158	M3	402	3PE	C11-O13-P-O11
158	AN	306	3PE	C11-O13-P-O11
153	t7	201	CDL	CB5-C51-C52-C53
153	L	301	CDL	C12-C13-C14-C15
152	N6	301	PC1	C26-C27-C28-C29
153	a	505	CDL	C14-C15-C16-C17
153	N5	806	CDL	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	VB	705	CDL	C32-C31-CA7-OA8
153	6C	202	CDL	CA5-C11-C12-C13
153	VB	705	CDL	C14-C15-C16-C17
152	i	304	PC1	C1-C2-C3-O31
152	m1	403	PC1	C1-C2-C3-O31
152	I	301	PC1	C1-C2-C3-O31
152	M1	403	PC1	C1-C2-C3-O31
153	2g	201	CDL	CB3-CB4-CB6-OB8
153	m1	404	CDL	CB3-CB4-CB6-OB8
153	M1	404	CDL	CB3-CB4-CB6-OB8
164	Qc	501	U10	C20-C19-C21-C22
152	n6	301	PC1	C26-C27-C28-C29
153	bm	301	CDL	C22-C23-C24-C25
160	qh	201	PX2	C20-C21-C22-C23
153	Qi	202	CDL	CB7-C71-C72-C73
153	e	402	CDL	C51-C52-C53-C54
153	z	101	CDL	C31-C32-C33-C34
153	bm	301	CDL	C76-C77-C78-C79
152	2F	303	PC1	O31-C31-C32-C33
153	vb	704	CDL	C12-C11-CA5-OA6
153	VB	706	CDL	C12-C11-CA5-OA6
152	t4	301	PC1	C11-C12-N-C14
152	M2	405	PC1	C11-C12-N-C13
152	N5	805	PC1	C35-C36-C37-C38
164	qC	506	U10	C4-C3-O3-C3M
164	QC	506	U10	C4-C3-O3-C3M
153	qi	202	CDL	CB7-C71-C72-C73
152	n5	805	PC1	C35-C36-C37-C38
153	BM	301	CDL	C22-C23-C24-C25
159	M2	406	P5S	C40-C41-C42-C43
153	Z	101	CDL	C31-C32-C33-C34
159	m2	406	P5S	C40-C41-C42-C43
153	6a	201	CDL	C32-C31-CA7-OA9
153	6A	201	CDL	C32-C31-CA7-OA9
153	BM	301	CDL	C20-C21-C22-C23
153	bm	301	CDL	C20-C21-C22-C23
153	qc	504	CDL	C33-C34-C35-C36
159	m2	406	P5S	C42-C43-C44-C45
159	M2	406	P5S	C42-C43-C44-C45
152	S8	301	PC1	C2-C1-O11-P
153	a	505	CDL	CB4-CB3-OB5-PB2
153	b	501	CDL	CB4-CB3-OB5-PB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	c1	709	CDL	C1-CB2-OB2-PB2
153	e	403	CDL	C1-CA2-OA2-PA1
153	q	202	CDL	CA4-CA3-OA5-PA1
153	r	201	CDL	C1-CB2-OB2-PB2
153	vb	701	CDL	C1-CA2-OA2-PA1
153	p1	402	CDL	CA4-CA3-OA5-PA1
153	qC	504	CDL	C1-CA2-OA2-PA1
153	qD	402	CDL	CB4-CB3-OB5-PB2
153	qG	402	CDL	C1-CA2-OA2-PA1
153	t1	601	CDL	C1-CA2-OA2-PA1
153	2G	201	CDL	C1-CB2-OB2-PB2
153	6C	202	CDL	CA4-CA3-OA5-PA1
153	B	501	CDL	C1-CA2-OA2-PA1
153	B	501	CDL	CB4-CB3-OB5-PB2
153	C1	708	CDL	C1-CB2-OB2-PB2
153	E	403	CDL	C1-CA2-OA2-PA1
153	M	301	CDL	C1-CB2-OB2-PB2
153	Q	202	CDL	CA4-CA3-OA5-PA1
153	R	201	CDL	C1-CB2-OB2-PB2
153	VB	701	CDL	C1-CA2-OA2-PA1
153	VB	705	CDL	CB4-CB3-OB5-PB2
153	AL	301	CDL	C1-CA2-OA2-PA1
153	B4	201	CDL	C1-CA2-OA2-PA1
153	P1	402	CDL	CA4-CA3-OA5-PA1
153	QD	402	CDL	CB4-CB3-OB5-PB2
153	QG	402	CDL	C1-CA2-OA2-PA1
153	T1	601	CDL	C1-CA2-OA2-PA1
153	C	301	CDL	C1-CA2-OA2-PA1
153	C	301	CDL	CA4-CA3-OA5-PA1
153	c	301	CDL	C1-CA2-OA2-PA1
153	c	301	CDL	CA4-CA3-OA5-PA1
171	v1	501	FMN	C4'-C5'-O5'-P
171	V1	501	FMN	C4'-C5'-O5'-P
158	t8	602	3PE	C28-C29-C2A-C2B
153	n	304	CDL	C72-C71-CB7-OB8
153	N	304	CDL	C72-C71-CB7-OB8
160	Qh	201	PX2	C24-C25-C26-C27
153	Qc	504	CDL	C78-C79-C80-C81
152	TC	102	PC1	C3B-C3C-C3D-C3E
153	E	402	CDL	C51-C52-C53-C54
158	an	305	3PE	C33-C34-C35-C36
158	AN	305	3PE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	T8	602	3PE	C28-C29-C2A-C2B
164	qc	501	U10	C20-C19-C21-C22
152	v	202	PC1	C21-C22-C23-C24
152	V	202	PC1	C21-C22-C23-C24
160	r	202	PX2	O7-C16-C17-C18
152	tc	102	PC1	C3B-C3C-C3D-C3E
153	qc	504	CDL	C78-C79-C80-C81
153	Qc	504	CDL	C33-C34-C35-C36
169	b6	201	T7X	C31-C11-O18-C9
169	B6	201	T7X	C31-C11-O18-C9
169	B6	201	T7X	O19-C11-O18-C9
153	6C	203	CDL	C74-C75-C76-C77
166	qc	503	HEM	C3D-CAD-CBD-CGD
166	Qc	503	HEM	C3D-CAD-CBD-CGD
153	qc	504	CDL	C73-C74-C75-C76
153	Qc	504	CDL	C73-C74-C75-C76
169	b6	201	T7X	O19-C11-O18-C9
153	6C	202	CDL	C73-C74-C75-C76
160	R	202	PX2	C19-C20-C21-C22
152	c3	601	PC1	C11-C12-N-C13
152	qE	304	PC1	C11-C12-N-C15
152	QJ	101	PC1	C11-C12-N-C15
166	qc	503	HEM	CAD-CBD-CGD-O1D
153	c1	712	CDL	C53-C54-C55-C56
158	t8	602	3PE	C24-C25-C26-C27
158	T8	602	3PE	C24-C25-C26-C27
152	n5	805	PC1	C28-C29-C2A-C2B
152	N5	805	PC1	C28-C29-C2A-C2B
153	6c	201	CDL	C73-C74-C75-C76
153	2G	204	CDL	C51-C52-C53-C54
153	7A	201	CDL	CB5-C51-C52-C53
158	an	306	3PE	O13-C11-C12-N
158	b4	202	3PE	O13-C11-C12-N
158	AN	306	3PE	O13-C11-C12-N
158	B4	202	3PE	O13-C11-C12-N
153	7a	201	CDL	C37-C38-C39-C40
153	a	504	CDL	OA5-CA3-CA4-OA6
153	z	101	CDL	OB5-CB3-CB4-OB6
153	A	504	CDL	OA5-CA3-CA4-OA6
152	W	201	PC1	C3C-C3D-C3E-C3F
153	7A	201	CDL	C37-C38-C39-C40
153	C1	712	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	M1	402	CDL	C13-C14-C15-C16
152	m1	403	PC1	C2A-C2B-C2C-C2D
152	M1	403	PC1	C2A-C2B-C2C-C2D
153	6c	202	CDL	C74-C75-C76-C77
153	e	401	CDL	C16-C17-C18-C19
152	w	201	PC1	C3C-C3D-C3E-C3F
152	2F	301	PC1	C32-C33-C34-C35
153	2m	101	CDL	C20-C21-C22-C23
153	m1	402	CDL	C13-C14-C15-C16
153	C1	707	CDL	C71-C72-C73-C74
153	M2	401	CDL	C32-C31-CA7-OA9
166	Qc	503	HEM	CAD-CBD-CGD-O1D
152	J1	400	PC1	C32-C33-C34-C35
152	2f	301	PC1	C32-C33-C34-C35
153	c1	703	CDL	C71-C72-C73-C74
152	j1	400	PC1	C32-C33-C34-C35
152	N5	805	PC1	C36-C37-C38-C39
153	n	304	CDL	C51-C52-C53-C54
153	N	304	CDL	C51-C52-C53-C54
154	C1	703	HEA	CAA-CBA-CGA-O1A
153	6a	201	CDL	C71-C72-C73-C74
153	2M	101	CDL	C20-C21-C22-C23
153	Qc	504	CDL	C71-C72-C73-C74
158	w	203	3PE	C38-C39-C3A-C3B
153	n	304	CDL	CB5-C51-C52-C53
153	t	204	CDL	CB5-C51-C52-C53
153	N	304	CDL	CB5-C51-C52-C53
153	i	301	CDL	C39-C40-C41-C42
153	A9	403	CDL	C51-C52-C53-C54
152	c1	711	PC1	O21-C2-C3-O31
152	qG	401	PC1	O21-C2-C3-O31
152	QG	401	PC1	O21-C2-C3-O31
153	m1	404	CDL	OB6-CB4-CB6-OB8
153	te	101	CDL	OB6-CB4-CB6-OB8
153	M1	404	CDL	OB6-CB4-CB6-OB8
153	VB	706	CDL	C12-C11-CA5-OA7
153	B3	102	CDL	OB6-CB4-CB6-OB8
153	TE	101	CDL	OB6-CB4-CB6-OB8
153	a9	403	CDL	C51-C52-C53-C54
153	6A	201	CDL	C71-C72-C73-C74
153	I	302	CDL	C39-C40-C41-C42
158	W	203	3PE	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	T8	602	3PE	C27-C28-C29-C2A
152	m1	401	PC1	C31-C32-C33-C34
152	M1	401	PC1	C31-C32-C33-C34
153	T	204	CDL	CB5-C51-C52-C53
152	n5	805	PC1	C36-C37-C38-C39
153	qc	504	CDL	C71-C72-C73-C74
153	Y5	201	CDL	C71-C72-C73-C74
152	s8	301	PC1	C2-C1-O11-P
153	6c	201	CDL	C1-CB2-OB2-PB2
153	m	303	CDL	CB4-CB3-OB5-PB2
153	m1	402	CDL	C1-CA2-OA2-PA1
153	t	203	CDL	CB4-CB3-OB5-PB2
153	al	301	CDL	C1-CA2-OA2-PA1
153	c4	401	CDL	C1-CB2-OB2-PB2
153	t5	301	CDL	C1-CB2-OB2-PB2
153	6C	202	CDL	C1-CB2-OB2-PB2
153	M	305	CDL	CB4-CB3-OB5-PB2
153	M1	402	CDL	C1-CA2-OA2-PA1
153	T	203	CDL	CB4-CB3-OB5-PB2
153	C4	401	CDL	C1-CB2-OB2-PB2
153	T5	301	CDL	C1-CB2-OB2-PB2
152	d	501	PC1	O22-C21-C22-C23
152	D	501	PC1	O22-C21-C22-C23
153	m2	401	CDL	C32-C31-CA7-OA9
153	Q	202	CDL	C12-C11-CA5-OA7
152	2F	301	PC1	C11-C12-N-C14
152	S8	301	PC1	C11-C12-N-C15
169	b6	201	T7X	C13-C14-C15-C16
153	y5	201	CDL	C71-C72-C73-C74
160	y5	204	PX2	O5-C4-C5-C6
158	i	303	3PE	C25-C26-C27-C28
158	t8	602	3PE	C27-C28-C29-C2A
158	I	304	3PE	C25-C26-C27-C28
153	q	202	CDL	C12-C11-CA5-OA7
152	te	102	PC1	C23-C24-C25-C26
153	7c	301	CDL	C39-C40-C41-C42
154	C1	703	HEA	CAA-CBA-CGA-O2A
166	qc	503	HEM	CAA-CBA-CGA-O1A
166	Qc	503	HEM	CAA-CBA-CGA-O2A
153	7a	201	CDL	CB5-C51-C52-C53
153	Y5	201	CDL	CA5-C11-C12-C13
153	C4	401	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	V	202	PC1	C36-C37-C38-C39
153	sd	101	CDL	C14-C15-C16-C17
153	7C	301	CDL	C39-C40-C41-C42
166	qc	503	HEM	CAA-CBA-CGA-O2A
153	bm	301	CDL	C33-C34-C35-C36
153	c4	401	CDL	C74-C75-C76-C77
152	v	202	PC1	C36-C37-C38-C39
153	t	202	CDL	C13-C14-C15-C16
152	c1	711	PC1	C1-C2-C3-O31
152	C1	711	PC1	C1-C2-C3-O31
153	a	505	CDL	CB3-CB4-CB6-OB8
153	m1	405	CDL	CB3-CB4-CB6-OB8
153	2G	201	CDL	CB3-CB4-CB6-OB8
153	M1	405	CDL	CB3-CB4-CB6-OB8
153	VB	705	CDL	CB3-CB4-CB6-OB8
153	E	401	CDL	C16-C17-C18-C19
154	c1	708	HEA	CAA-CBA-CGA-O2A
166	qC	502	HEM	CAA-CBA-CGA-O1A
166	QC	502	HEM	CAA-CBA-CGA-O1A
166	Qc	503	HEM	CAA-CBA-CGA-O1A
169	B6	201	T7X	C13-C14-C15-C16
153	T	202	CDL	C13-C14-C15-C16
153	te	101	CDL	C32-C31-CA7-OA9
154	c1	708	HEA	C4D-C3D-CAD-CBD
153	QI	203	CDL	C52-C53-C54-C55
153	y5	201	CDL	CA5-C11-C12-C13
154	C1	703	HEA	CAD-CBD-CGD-O1D
166	qC	501	HEM	CAD-CBD-CGD-O1D
153	6c	201	CDL	C35-C36-C37-C38
153	i	301	CDL	C12-C13-C14-C15
153	qI	203	CDL	C52-C53-C54-C55
153	6C	202	CDL	C35-C36-C37-C38
152	TE	102	PC1	C23-C24-C25-C26
159	m2	406	P5S	OXT-C-CA-N
152	qc	506	PC1	C33-C34-C35-C36
153	I	302	CDL	C12-C13-C14-C15
158	g2	301	3PE	C33-C34-C35-C36
158	G2	301	3PE	C33-C34-C35-C36
166	QC	501	HEM	CAD-CBD-CGD-O1D
152	2g	202	PC1	C1-C2-O21-C21
152	c1	706	PC1	C3-C2-O21-C21
152	c3	601	PC1	C1-C2-O21-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	m	301	PC1	C3-C2-O21-C21
152	qE	304	PC1	C3-C2-O21-C21
152	qe	303	PC1	C3-C2-O21-C21
152	t4	301	PC1	C1-C2-O21-C21
152	te	102	PC1	C1-C2-O21-C21
152	2G	202	PC1	C1-C2-O21-C21
152	A	501	PC1	C3-C2-O21-C21
152	C1	709	PC1	C3-C2-O21-C21
152	C3	601	PC1	C1-C2-O21-C21
152	M	303	PC1	C3-C2-O21-C21
152	QJ	101	PC1	C3-C2-O21-C21
152	Qe	303	PC1	C3-C2-O21-C21
152	T4	301	PC1	C1-C2-O21-C21
152	TE	102	PC1	C1-C2-O21-C21
153	2k	101	CDL	CA3-CA4-OA6-CA5
153	6a	201	CDL	CA6-CA4-OA6-CA5
153	c1	709	CDL	CA3-CA4-OA6-CA5
153	e	402	CDL	CB6-CB4-OB6-CB5
153	m1	405	CDL	CB3-CB4-OB6-CB5
153	m2	404	CDL	CB3-CB4-OB6-CB5
153	m3	403	CDL	CB3-CB4-OB6-CB5
153	q	201	CDL	CB6-CB4-OB6-CB5
153	y7	501	CDL	CA6-CA4-OA6-CA5
153	5b	201	CDL	CA3-CA4-OA6-CA5
153	a1	101	CDL	CA3-CA4-OA6-CA5
153	a9	402	CDL	CB3-CB4-OB6-CB5
153	qi	202	CDL	CA6-CA4-OA6-CA5
153	2K	101	CDL	CA3-CA4-OA6-CA5
153	6A	201	CDL	CA6-CA4-OA6-CA5
153	C1	708	CDL	CA3-CA4-OA6-CA5
153	E	402	CDL	CB6-CB4-OB6-CB5
153	M1	405	CDL	CB3-CB4-OB6-CB5
153	M2	404	CDL	CB3-CB4-OB6-CB5
153	M3	403	CDL	CB3-CB4-OB6-CB5
153	Q	201	CDL	CB6-CB4-OB6-CB5
153	Y7	501	CDL	CA6-CA4-OA6-CA5
153	5B	201	CDL	CA3-CA4-OA6-CA5
153	A1	102	CDL	CA3-CA4-OA6-CA5
153	A9	402	CDL	CB3-CB4-OB6-CB5
153	Qi	202	CDL	CA6-CA4-OA6-CA5
153	C	301	CDL	CA3-CA4-OA6-CA5
153	c	301	CDL	CA3-CA4-OA6-CA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	a3	201	3PE	C1-C2-O21-C21
158	bm	302	3PE	C3-C2-O21-C21
158	t8	601	3PE	C3-C2-O21-C21
158	A3	201	3PE	C1-C2-O21-C21
158	BM	302	3PE	C3-C2-O21-C21
158	T8	601	3PE	C3-C2-O21-C21
153	n	304	CDL	C53-C54-C55-C56
153	N	304	CDL	C53-C54-C55-C56
152	c1	711	PC1	C11-C12-N-C14
152	f	402	PC1	C11-C12-N-C15
152	m	305	PC1	C11-C12-N-C13
152	qi	203	PC1	C11-C12-N-C15
152	s8	301	PC1	C11-C12-N-C15
152	tc	101	PC1	C11-C12-N-C15
152	C1	711	PC1	C11-C12-N-C14
152	C3	601	PC1	C11-C12-N-C14
152	F	401	PC1	C11-C12-N-C15
152	M	307	PC1	C11-C12-N-C13
152	Qi	203	PC1	C11-C12-N-C15
152	TC	101	PC1	C11-C12-N-C15
153	qB	601	CDL	C72-C71-CB7-OB8
153	QB	601	CDL	C72-C71-CB7-OB8
153	c1	712	CDL	C12-C13-C14-C15
153	t5	301	CDL	C56-C57-C58-C59
158	M2	408	3PE	C32-C33-C34-C35
152	2f	303	PC1	O31-C31-C32-C33
152	al	302	PC1	O31-C31-C32-C33
152	AL	302	PC1	O31-C31-C32-C33
153	T5	301	CDL	C56-C57-C58-C59
158	m2	408	3PE	C32-C33-C34-C35
152	te	102	PC1	C1-O11-P-O13
153	5b	201	CDL	CB2-OB2-PB2-OB5
153	a9	403	CDL	CB2-OB2-PB2-OB5
153	Y5	201	CDL	CA3-OA5-PA1-OA2
153	5B	201	CDL	CB2-OB2-PB2-OB5
158	w	203	3PE	C1-O11-P-O13
167	a9	401	NDP	O4D-C1D-N1N-C2N
153	2g	204	CDL	C52-C53-C54-C55
153	qi	202	CDL	C53-C54-C55-C56
153	C1	712	CDL	C12-C13-C14-C15
153	QI	203	CDL	C56-C57-C58-C59
153	Qi	202	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	d	501	PC1	C24-C25-C26-C27
152	D	501	PC1	C24-C25-C26-C27
153	qC	503	CDL	C74-C75-C76-C77
153	qI	203	CDL	C56-C57-C58-C59
153	BM	301	CDL	C75-C76-C77-C78
153	QC	503	CDL	C74-C75-C76-C77
152	Qc	506	PC1	C33-C34-C35-C36
158	a3	202	3PE	C32-C33-C34-C35
158	A3	202	3PE	C32-C33-C34-C35
160	R	202	PX2	C21-C22-C23-C24
152	6a	202	PC1	C31-C32-C33-C34
152	6A	202	PC1	C31-C32-C33-C34
153	2o	101	CDL	OA5-CA3-CA4-OA6
153	c1	709	CDL	OB5-CB3-CB4-OB6
153	C1	708	CDL	OB5-CB3-CB4-OB6
153	E	401	CDL	OB5-CB3-CB4-OB6
152	c4	403	PC1	O21-C21-C22-C23
152	C4	403	PC1	O21-C21-C22-C23
154	c1	708	HEA	CAA-CBA-CGA-O1A
166	qC	502	HEM	CAA-CBA-CGA-O2A
166	QC	501	HEM	CAD-CBD-CGD-O2D
166	QC	502	HEM	CAA-CBA-CGA-O2A
153	6c	202	CDL	C32-C33-C34-C35
153	bm	301	CDL	C75-C76-C77-C78
153	vb	704	CDL	C12-C11-CA5-OA7
153	6C	203	CDL	C32-C33-C34-C35
153	T	203	CDL	C20-C21-C22-C23
153	7a	201	CDL	OB5-CB3-CB4-CB6
153	c1	709	CDL	OB5-CB3-CB4-CB6
153	c1	712	CDL	OB5-CB3-CB4-CB6
153	t	202	CDL	OA5-CA3-CA4-CA6
153	vb	704	CDL	OB5-CB3-CB4-CB6
153	7A	201	CDL	OB5-CB3-CB4-CB6
153	C1	708	CDL	OB5-CB3-CB4-CB6
153	T	202	CDL	OA5-CA3-CA4-CA6
153	t	203	CDL	C20-C21-C22-C23
153	N6	302	CDL	C73-C74-C75-C76
153	Qg	402	CDL	C33-C34-C35-C36
151	qD	401	HEC	CAA-CBA-CGA-O1A
151	QD	401	HEC	CAA-CBA-CGA-O1A
166	qC	501	HEM	CAD-CBD-CGD-O2D
153	SD	101	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	A9	402	CDL	C73-C74-C75-C76
158	T8	601	3PE	C36-C37-C38-C39
158	t8	601	3PE	C36-C37-C38-C39
153	VB	705	CDL	CA5-C11-C12-C13
153	f	401	CDL	C81-C82-C83-C84
154	c1	708	HEA	CAD-CBD-CGD-O1D
152	N6	301	PC1	C28-C29-C2A-C2B
153	a9	402	CDL	C73-C74-C75-C76
153	n6	302	CDL	C73-C74-C75-C76
153	C1	712	CDL	C77-C78-C79-C80
153	F	402	CDL	C81-C82-C83-C84
152	2f	301	PC1	C11-C12-N-C14
153	qg	402	CDL	C33-C34-C35-C36
153	2M	101	CDL	C74-C75-C76-C77
151	qd	401	HEC	CAA-CBA-CGA-O1A
151	Qd	401	HEC	CAA-CBA-CGA-O1A
153	BM	301	CDL	C33-C34-C35-C36
152	C1	711	PC1	O21-C2-C3-O31
153	2g	201	CDL	OB6-CB4-CB6-OB8
153	a	504	CDL	OB6-CB4-CB6-OB8
153	b3	102	CDL	OB6-CB4-CB6-OB8
153	2G	201	CDL	OB6-CB4-CB6-OB8
153	a	505	CDL	CA5-C11-C12-C13
153	T7	201	CDL	CB5-C51-C52-C53
152	c1	706	PC1	O21-C21-C22-C23
152	C1	709	PC1	O21-C21-C22-C23
158	b4	202	3PE	C23-C24-C25-C26
166	qc	503	HEM	CAD-CBD-CGD-O2D
153	c1	712	CDL	C77-C78-C79-C80
167	A9	401	NDP	O4D-C1D-N1N-C2N
152	n6	301	PC1	C28-C29-C2A-C2B
153	m1	404	CDL	C22-C23-C24-C25
153	qc	504	CDL	C75-C76-C77-C78
153	M1	404	CDL	C22-C23-C24-C25
158	B4	202	3PE	C23-C24-C25-C26
164	qC	506	U10	C14-C16-C17-C18
164	QC	506	U10	C14-C16-C17-C18
151	QD	401	HEC	CAA-CBA-CGA-O2A
154	C1	703	HEA	CAD-CBD-CGD-O2D
166	Qc	503	HEM	CAD-CBD-CGD-O2D
153	P1	402	CDL	C52-C53-C54-C55
153	Qc	504	CDL	C75-C76-C77-C78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	p1	402	CDL	C52-C53-C54-C55
153	t5	301	CDL	C37-C38-C39-C40
169	B6	201	T7X	C43-C44-C45-C46
152	5B	202	PC1	C28-C29-C2A-C2B
153	T5	301	CDL	C37-C38-C39-C40
159	M2	406	P5S	OXT-C-CA-N
151	qD	401	HEC	CAA-CBA-CGA-O2A
153	bm	301	CDL	C73-C74-C75-C76
158	A3	201	3PE	C22-C23-C24-C25
153	I	302	CDL	C1-CB2-OB2-PB2
160	r	202	PX2	C2-C1-O4-P1
167	a9	401	NDP	PN-O3-PA-O1A
167	a9	401	NDP	PN-O3-PA-O2A
167	A9	401	NDP	PN-O3-PA-O1A
167	A9	401	NDP	PN-O3-PA-O2A
170	b9	202	ADP	PB-O3A-PA-O1A
170	B9	202	ADP	PB-O3A-PA-O1A
153	c1	712	CDL	C52-C51-CB5-OB6
152	C3	602	PC1	C22-C23-C24-C25
152	Qb	602	PC1	C24-C25-C26-C27
153	7C	301	CDL	C53-C54-C55-C56
153	j	301	CDL	O1-C1-CA2-OA2
152	c3	602	PC1	C22-C23-C24-C25
152	5b	202	PC1	C28-C29-C2A-C2B
153	2k	101	CDL	C55-C56-C57-C58
153	l	301	CDL	C71-C72-C73-C74
158	a3	201	3PE	C22-C23-C24-C25
152	i	304	PC1	C11-C12-N-C14
153	2K	101	CDL	C55-C56-C57-C58
153	7C	301	CDL	C77-C78-C79-C80
153	L	301	CDL	C54-C55-C56-C57
153	BM	301	CDL	C73-C74-C75-C76
152	n	303	PC1	O32-C31-C32-C33
152	c1	704	PC1	C26-C27-C28-C29
152	N6	301	PC1	C35-C36-C37-C38
153	7c	301	CDL	C53-C54-C55-C56
153	7c	301	CDL	C77-C78-C79-C80
153	C1	712	CDL	C52-C51-CB5-OB6
153	B8	302	CDL	C12-C11-CA5-OA6
152	C1	706	PC1	C26-C27-C28-C29
153	2m	101	CDL	C75-C76-C77-C78
158	b4	202	3PE	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
151	qd	401	HEC	CAA-CBA-CGA-O2A
152	m1	401	PC1	C2D-C2E-C2F-C2G
153	qc	508	CDL	C71-C72-C73-C74
158	B4	202	3PE	C26-C27-C28-C29
169	b6	201	T7X	C43-C44-C45-C46
152	n6	301	PC1	C35-C36-C37-C38
153	Qg	402	CDL	C56-C57-C58-C59
164	sc	102	U10	C20-C19-C21-C22
153	qg	402	CDL	C56-C57-C58-C59
151	2e	401	HEC	CAA-CBA-CGA-O2A
151	Qd	401	HEC	CAA-CBA-CGA-O2A
154	c1	708	HEA	CAD-CBD-CGD-O2D
153	TE	101	CDL	C32-C31-CA7-OA9
164	qC	506	U10	C1-C6-C7-C8
153	L	301	CDL	C71-C72-C73-C74
152	qb	602	PC1	C24-C25-C26-C27
152	N5	801	PC1	C35-C36-C37-C38
153	l	301	CDL	C54-C55-C56-C57
153	C1	712	CDL	C51-C52-C53-C54
153	Qc	508	CDL	C71-C72-C73-C74
153	b8	302	CDL	C12-C11-CA5-OA6
153	2M	101	CDL	C12-C11-CA5-OA6
158	y5	202	3PE	O21-C21-C22-C23
158	Y5	202	3PE	O21-C21-C22-C23
152	n5	801	PC1	C35-C36-C37-C38
152	M1	401	PC1	C2D-C2E-C2F-C2G
158	g2	301	3PE	C3C-C3D-C3E-C3F
158	G2	301	3PE	C3C-C3D-C3E-C3F
152	c3	601	PC1	O11-C1-C2-O21
152	C3	601	PC1	O11-C1-C2-O21
153	e	401	CDL	OB5-CB3-CB4-OB6
153	vb	704	CDL	OB5-CB3-CB4-OB6
153	qc	508	CDL	OA5-CA3-CA4-OA6
153	te	101	CDL	OB5-CB3-CB4-OB6
153	2O	101	CDL	OA5-CA3-CA4-OA6
153	Qc	508	CDL	OA5-CA3-CA4-OA6
153	TE	101	CDL	OB5-CB3-CB4-OB6
158	SC	101	3PE	O11-C1-C2-O21
154	C1	703	HEA	C2D-C3D-CAD-CBD
151	2E	401	HEC	CAA-CBA-CGA-O2A
153	6C	203	CDL	C53-C54-C55-C56
159	m2	406	P5S	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
159	m2	406	P5S	O37-C38-C39-C40
159	M2	406	P5S	O37-C38-C39-C40
160	R	202	PX2	O7-C16-C17-C18
153	t	204	CDL	CB7-C71-C72-C73
153	T	204	CDL	CB7-C71-C72-C73
152	m1	401	PC1	C29-C2A-C2B-C2C
153	n6	302	CDL	C13-C14-C15-C16
152	2j	201	PC1	C11-C12-N-C15
152	2J	201	PC1	C11-C12-N-C15
152	I	301	PC1	C11-C12-N-C14
152	M1	401	PC1	C29-C2A-C2B-C2C
159	M2	406	P5S	C25-C26-C27-C28
153	r	201	CDL	OA5-CA3-CA4-CA6
153	bm	301	CDL	OA5-CA3-CA4-CA6
153	n6	302	CDL	OB5-CB3-CB4-CB6
153	te	101	CDL	OB5-CB3-CB4-CB6
153	C1	712	CDL	OB5-CB3-CB4-CB6
153	R	201	CDL	OA5-CA3-CA4-CA6
153	VB	706	CDL	OB5-CB3-CB4-CB6
153	BM	301	CDL	OA5-CA3-CA4-CA6
153	N6	302	CDL	OB5-CB3-CB4-CB6
152	C1	711	PC1	O21-C21-C22-C23
153	2m	101	CDL	C12-C11-CA5-OA6
153	l	301	CDL	CA5-C11-C12-C13
164	SC	102	U10	C20-C19-C21-C22
153	6c	202	CDL	C53-C54-C55-C56
153	N6	302	CDL	C13-C14-C15-C16
158	c4	402	3PE	O13-C11-C12-N
158	C4	402	3PE	O13-C11-C12-N
152	C2	701	PC1	C23-C24-C25-C26
152	Qc	506	PC1	C31-C32-C33-C34
153	c1	709	CDL	C12-C11-CA5-OA6
153	b4	201	CDL	C72-C71-CB7-OB8
153	C1	708	CDL	C12-C11-CA5-OA6
153	B4	201	CDL	C72-C71-CB7-OB8
153	Y5	201	CDL	C12-C11-CA5-OA7
153	A1	101	CDL	C72-C71-CB7-OB9
152	qE	304	PC1	O21-C21-C22-C23
153	b3	102	CDL	C12-C11-CA5-OA6
153	7A	203	CDL	C32-C31-CA7-OA8
153	2k	101	CDL	C53-C54-C55-C56
153	2K	101	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2o	101	CDL	CA4-CA3-OA5-PA1
153	i	301	CDL	C1-CB2-OB2-PB2
153	2O	101	CDL	CA4-CA3-OA5-PA1
154	c1	708	HEA	C17-C18-C19-C27
154	C1	703	HEA	C17-C18-C19-C27
152	n1	301	PC1	O21-C2-C3-O31
152	N1	301	PC1	O21-C2-C3-O31
153	r	201	CDL	OB6-CB4-CB6-OB8
153	am	201	CDL	OB6-CB4-CB6-OB8
153	E	402	CDL	OB6-CB4-CB6-OB8
153	R	201	CDL	OB6-CB4-CB6-OB8
153	AM	201	CDL	OB6-CB4-CB6-OB8
153	m1	402	CDL	C53-C54-C55-C56
153	y5	201	CDL	C12-C11-CA5-OA7
153	M1	402	CDL	C53-C54-C55-C56
153	BM	301	CDL	C21-C22-C23-C24
152	c1	711	PC1	O21-C21-C22-C23
153	7a	203	CDL	C32-C31-CA7-OA8
153	f	401	CDL	C52-C51-CB5-OB6
153	m3	401	CDL	C72-C71-CB7-OB8
153	F	402	CDL	C52-C51-CB5-OB6
153	M3	401	CDL	C52-C51-CB5-OB6
160	R	202	PX2	O5-C4-C5-C6
160	Qh	201	PX2	C12-C13-C14-C15
153	L	301	CDL	CA5-C11-C12-C13
152	c2	703	PC1	C23-C24-C25-C26
153	c1	709	CDL	C76-C77-C78-C79
153	2b	201	CDL	C62-C63-C64-C65
153	2G	201	CDL	C11-C12-C13-C14
153	C1	712	CDL	C16-C17-C18-C19
153	2B	201	CDL	C62-C63-C64-C65
167	a9	401	NDP	C2B-O2B-P2B-O1X
167	A9	401	NDP	C2B-O2B-P2B-O1X
152	P1	401	PC1	O21-C21-C22-C23
152	QJ	101	PC1	O21-C21-C22-C23
153	c1	701	CDL	C32-C31-CA7-OA8
153	m2	403	CDL	C72-C71-CB7-OB8
153	m3	401	CDL	C52-C51-CB5-OB6
153	w	202	CDL	C72-C71-CB7-OB8
153	C1	701	CDL	C32-C31-CA7-OA8
153	M3	401	CDL	C72-C71-CB7-OB8
153	W	202	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	td	101	CDL	C72-C71-CB7-OB9
152	qC	507	PC1	C29-C2A-C2B-C2C
153	TH	200	CDL	C77-C78-C79-C80
158	g2	301	3PE	C2D-C2E-C2F-C2G
153	C1	708	CDL	C76-C77-C78-C79
152	c3	603	PC1	C11-O13-P-O11
152	c3	603	PC1	C1-O11-P-O13
152	C3	603	PC1	C1-O11-P-O13
153	a	502	CDL	CB3-OB5-PB2-OB2
153	a	505	CDL	CA3-OA5-PA1-OA2
153	m2	403	CDL	CA2-OA2-PA1-OA5
153	M2	403	CDL	CA2-OA2-PA1-OA5
168	ab	201	ZMP	C19-C18-C21-O5
168	AB	201	ZMP	C19-C18-C21-O5
153	2m	101	CDL	C74-C75-C76-C77
153	c1	712	CDL	C51-C52-C53-C54
153	Y5	201	CDL	C33-C34-C35-C36
158	G2	301	3PE	C25-C26-C27-C28
152	2F	301	PC1	C11-C12-N-C13
152	T4	301	PC1	C11-C12-N-C15
152	m2	402	PC1	O31-C31-C32-C33
152	p1	401	PC1	O21-C21-C22-C23
153	q	202	CDL	C52-C51-CB5-OB6
153	te	101	CDL	C12-C11-CA5-OA6
153	Q	202	CDL	C52-C51-CB5-OB6
153	TE	101	CDL	C12-C11-CA5-OA6
158	M3	402	3PE	O31-C31-C32-C33
153	2g	201	CDL	C11-C12-C13-C14
153	y5	201	CDL	C33-C34-C35-C36
153	bm	301	CDL	C21-C22-C23-C24
158	AN	303	3PE	C29-C2A-C2B-C2C
164	qC	506	U10	C5-C6-C7-C8
164	QC	506	U10	C5-C6-C7-C8
153	7C	301	CDL	C12-C13-C14-C15
158	an	303	3PE	C29-C2A-C2B-C2C
153	J	301	CDL	O1-C1-CA2-OA2
153	t	202	CDL	C12-C11-CA5-OA6
153	qi	202	CDL	C52-C51-CB5-OB6
153	FS	204	CDL	C12-C11-CA5-OA6
153	M2	403	CDL	C72-C71-CB7-OB8
153	T	202	CDL	C12-C11-CA5-OA6
153	B3	102	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qi	202	CDL	C52-C51-CB5-OB6
152	a	503	PC1	C24-C25-C26-C27
152	a	501	PC1	C3-C2-O21-C21
152	a	503	PC1	C3-C2-O21-C21
152	d	501	PC1	C3-C2-O21-C21
152	qG	401	PC1	C3-C2-O21-C21
152	qi	201	PC1	C1-C2-O21-C21
152	qi	203	PC1	C3-C2-O21-C21
152	t4	303	PC1	C1-C2-O21-C21
152	A	503	PC1	C3-C2-O21-C21
152	D	501	PC1	C3-C2-O21-C21
152	QG	401	PC1	C3-C2-O21-C21
152	Qi	201	PC1	C1-C2-O21-C21
152	Qi	203	PC1	C3-C2-O21-C21
152	T4	303	PC1	C1-C2-O21-C21
153	2k	101	CDL	CB3-CB4-OB6-CB5
153	2m	101	CDL	CB3-CB4-OB6-CB5
153	7c	301	CDL	CB6-CB4-OB6-CB5
153	m2	401	CDL	CB6-CB4-OB6-CB5
153	n	304	CDL	CA3-CA4-OA6-CA5
153	t	202	CDL	CA6-CA4-OA6-CA5
153	t	204	CDL	CA6-CA4-OA6-CA5
153	w	202	CDL	CA6-CA4-OA6-CA5
153	2b	201	CDL	CA3-CA4-OA6-CA5
153	2b	201	CDL	CB3-CB4-OB6-CB5
153	c4	401	CDL	CA6-CA4-OA6-CA5
153	qc	508	CDL	CB6-CB4-OB6-CB5
153	qg	402	CDL	CA6-CA4-OA6-CA5
153	t5	301	CDL	CB3-CB4-OB6-CB5
153	2K	101	CDL	CB3-CB4-OB6-CB5
153	2M	101	CDL	CB3-CB4-OB6-CB5
153	7C	301	CDL	CB6-CB4-OB6-CB5
153	M2	401	CDL	CB6-CB4-OB6-CB5
153	N	304	CDL	CA3-CA4-OA6-CA5
153	T	202	CDL	CA6-CA4-OA6-CA5
153	T	204	CDL	CA6-CA4-OA6-CA5
153	W	202	CDL	CA6-CA4-OA6-CA5
153	2B	201	CDL	CA3-CA4-OA6-CA5
153	2B	201	CDL	CA6-CA4-OA6-CA5
153	2B	201	CDL	CB3-CB4-OB6-CB5
153	C4	401	CDL	CA6-CA4-OA6-CA5
153	Qc	508	CDL	CB6-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qg	402	CDL	CA6-CA4-OA6-CA5
153	T5	301	CDL	CB3-CB4-OB6-CB5
160	y5	204	PX2	C1-C2-O7-C16
160	y5	204	PX2	C3-C2-O7-C16
166	qc	502	HEM	C2B-C3B-CAB-CBB
166	Qc	502	HEM	C2B-C3B-CAB-CBB
158	g2	301	3PE	C25-C26-C27-C28
152	2F	302	PC1	C2B-C2C-C2D-C2E
152	QC	507	PC1	C29-C2A-C2B-C2C
153	c1	712	CDL	C16-C17-C18-C19
158	m2	408	3PE	C35-C36-C37-C38
154	C1	702	HEA	C11-C12-C13-C14
152	2f	302	PC1	C2B-C2C-C2D-C2E
152	qe	303	PC1	C26-C27-C28-C29
152	C1	711	PC1	C22-C23-C24-C25
153	q	203	CDL	CA7-C31-C32-C33
152	qC	505	PC1	O31-C31-C32-C33
152	M2	402	PC1	O31-C31-C32-C33
153	VB	703	CDL	C52-C51-CB5-OB6
158	m3	402	3PE	O31-C31-C32-C33
160	r	202	PX2	O5-C4-C5-C6
158	M2	408	3PE	C35-C36-C37-C38
152	c1	711	PC1	C22-C23-C24-C25
153	7c	301	CDL	C12-C13-C14-C15
153	C4	401	CDL	C62-C63-C64-C65
152	2J	201	PC1	C31-C32-C33-C34
152	A	503	PC1	C24-C25-C26-C27
152	Qe	303	PC1	C26-C27-C28-C29
152	b9	201	PC1	O21-C21-C22-C23
152	qJ	101	PC1	O21-C21-C22-C23
152	qj	101	PC1	O31-C31-C32-C33
152	QJ	102	PC1	O21-C21-C22-C23
152	Qj	101	PC1	O31-C31-C32-C33
153	2g	201	CDL	C12-C11-CA5-OA6
153	2o	101	CDL	C32-C31-CA7-OA8
153	b	501	CDL	C32-C31-CA7-OA8
153	fs	203	CDL	C12-C11-CA5-OA6
153	i	301	CDL	C12-C11-CA5-OA6
153	q	203	CDL	C52-C51-CB5-OB6
153	5b	201	CDL	C72-C71-CB7-OB8
153	t7	201	CDL	C12-C11-CA5-OA6
153	2G	201	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	2K	101	CDL	C52-C51-CB5-OB6
153	2O	101	CDL	C32-C31-CA7-OA8
153	B	501	CDL	C32-C31-CA7-OA8
153	I	302	CDL	C12-C11-CA5-OA6
153	5B	201	CDL	C72-C71-CB7-OB8
153	Qg	402	CDL	C52-C51-CB5-OB6
158	vb	705	3PE	O21-C21-C22-C23
158	t8	601	3PE	O21-C21-C22-C23
158	VB	707	3PE	O21-C21-C22-C23
158	AN	303	3PE	O31-C31-C32-C33
158	T8	601	3PE	O21-C21-C22-C23
153	l	301	CDL	C11-C12-C13-C14
153	L	301	CDL	C11-C12-C13-C14
152	c1	704	PC1	C24-C25-C26-C27
152	C1	706	PC1	C24-C25-C26-C27
153	2M	101	CDL	C75-C76-C77-C78
153	6C	202	CDL	C11-C12-C13-C14
152	m2	405	PC1	C1-C2-C3-O31
152	al	302	PC1	C2-C1-O11-P
152	n1	301	PC1	C1-C2-C3-O31
152	M2	405	PC1	C1-C2-C3-O31
152	AL	302	PC1	C2-C1-O11-P
153	y7	501	CDL	C1-CB2-OB2-PB2
153	p1	403	CDL	CA3-CA4-CA6-OA8
153	Y7	501	CDL	C1-CB2-OB2-PB2
153	A1	101	CDL	C1-CB2-OB2-PB2
153	P1	403	CDL	CA3-CA4-CA6-OA8
158	vb	705	3PE	C1-C2-C3-O31
158	b4	202	3PE	C1-C2-C3-O31
158	B4	202	3PE	C1-C2-C3-O31
166	y5	203	HEM	CAA-CBA-CGA-O1A
166	Y5	203	HEM	CAA-CBA-CGA-O1A
153	6c	201	CDL	C11-C12-C13-C14
153	r	201	CDL	OA5-CA3-CA4-OA6
153	t	202	CDL	OA5-CA3-CA4-OA6
153	b4	201	CDL	OB5-CB3-CB4-OB6
153	R	201	CDL	OA5-CA3-CA4-OA6
153	T	202	CDL	OA5-CA3-CA4-OA6
153	VB	706	CDL	OB5-CB3-CB4-OB6
153	B4	201	CDL	OB5-CB3-CB4-OB6
152	7a	202	PC1	O21-C21-C22-C23
152	m	301	PC1	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	c4	403	PC1	O31-C31-C32-C33
152	qc	509	PC1	O31-C31-C32-C33
152	7A	202	PC1	O21-C21-C22-C23
152	M	303	PC1	O21-C21-C22-C23
152	B9	201	PC1	O21-C21-C22-C23
152	QC	505	PC1	O31-C31-C32-C33
152	Qc	509	PC1	O31-C31-C32-C33
153	2k	101	CDL	C52-C51-CB5-OB6
153	2k	101	CDL	C72-C71-CB7-OB8
153	m2	404	CDL	C52-C51-CB5-OB6
153	qg	402	CDL	C52-C51-CB5-OB6
153	2K	101	CDL	C72-C71-CB7-OB8
153	M2	404	CDL	C52-C51-CB5-OB6
153	T7	201	CDL	C12-C11-CA5-OA6
158	i	303	3PE	O21-C21-C22-C23
158	an	303	3PE	O31-C31-C32-C33
158	n4	601	3PE	O21-C21-C22-C23
158	I	304	3PE	O21-C21-C22-C23
158	N4	601	3PE	O21-C21-C22-C23
152	2f	301	PC1	C11-C12-N-C13
153	q	201	CDL	C55-C56-C57-C58
153	th	200	CDL	C77-C78-C79-C80
153	Q	201	CDL	C55-C56-C57-C58
152	2j	201	PC1	C31-C32-C33-C34
152	qc	506	PC1	C31-C32-C33-C34
152	2J	201	PC1	C22-C23-C24-C25
153	Y5	201	CDL	C37-C38-C39-C40
152	n5	803	PC1	C34-C35-C36-C37
153	b	501	CDL	C13-C14-C15-C16
153	q	202	CDL	C41-C42-C43-C44
153	B	501	CDL	C13-C14-C15-C16
153	Q	202	CDL	C41-C42-C43-C44
166	qC	501	HEM	C4B-C3B-CAB-CBB
166	qc	502	HEM	C4B-C3B-CAB-CBB
166	QC	501	HEM	C4B-C3B-CAB-CBB
166	Qc	502	HEM	C4B-C3B-CAB-CBB
158	a3	201	3PE	C32-C31-O31-C3
152	N5	803	PC1	C34-C35-C36-C37
158	g2	301	3PE	C34-C35-C36-C37
158	G2	301	3PE	C34-C35-C36-C37
152	qc	506	PC1	O21-C21-C22-C23
153	t	203	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qG	402	CDL	C52-C51-CB5-OB6
153	qI	203	CDL	C12-C11-CA5-OA6
153	qb	601	CDL	C72-C71-CB7-OB8
153	QG	402	CDL	C52-C51-CB5-OB6
153	Qb	601	CDL	C72-C71-CB7-OB8
151	2e	401	HEC	CAA-CBA-CGA-O1A
153	7a	201	CDL	C78-C79-C80-C81
153	t	204	CDL	C81-C82-C83-C84
152	Qj	101	PC1	C23-C24-C25-C26
153	6c	201	CDL	C56-C57-C58-C59
153	t	204	CDL	C76-C77-C78-C79
153	t	204	CDL	C78-C79-C80-C81
153	y5	201	CDL	C37-C38-C39-C40
153	qb	601	CDL	CA5-C11-C12-C13
153	an	302	CDL	O1-C1-CA2-OA2
153	AN	302	CDL	O1-C1-CA2-OA2
152	2j	201	PC1	C22-C23-C24-C25
153	7A	201	CDL	C78-C79-C80-C81
152	2g	202	PC1	O31-C31-C32-C33
152	c3	602	PC1	O21-C21-C22-C23
152	C3	602	PC1	O21-C21-C22-C23
152	QE	301	PC1	O31-C31-C32-C33
153	e	401	CDL	C72-C71-CB7-OB8
153	t	204	CDL	C52-C51-CB5-OB6
153	E	401	CDL	C72-C71-CB7-OB8
153	I	303	CDL	C52-C51-CB5-OB6
153	T	204	CDL	C52-C51-CB5-OB6
160	Y5	204	PX2	O5-C4-C5-C6
153	6C	202	CDL	C56-C57-C58-C59
158	A3	201	3PE	C32-C31-O31-C3
152	7a	202	PC1	C23-C24-C25-C26
153	c4	401	CDL	C62-C63-C64-C65
153	6C	203	CDL	C55-C56-C57-C58
153	T	204	CDL	C78-C79-C80-C81
152	qj	101	PC1	C23-C24-C25-C26
153	2K	101	CDL	C13-C14-C15-C16
153	QI	203	CDL	C16-C17-C18-C19
158	a3	201	3PE	C32-C33-C34-C35
153	t	204	CDL	OA5-CA3-CA4-CA6
153	qC	504	CDL	OB5-CB3-CB4-CB6
153	qc	508	CDL	OB5-CB3-CB4-CB6
153	QC	504	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qc	508	CDL	OB5-CB3-CB4-CB6
151	2E	401	HEC	CAA-CBA-CGA-O1A
152	N5	801	PC1	C2C-C2D-C2E-C2F
153	2k	101	CDL	C13-C14-C15-C16
153	2k	101	CDL	C51-C52-C53-C54
153	j	301	CDL	C16-C17-C18-C19
153	m1	402	CDL	C31-C32-C33-C34
153	qD	402	CDL	C72-C73-C74-C75
153	2K	101	CDL	C51-C52-C53-C54
153	7C	301	CDL	C43-C44-C45-C46
153	M1	402	CDL	C31-C32-C33-C34
153	QD	402	CDL	C72-C73-C74-C75
152	2f	303	PC1	O21-C21-C22-C23
152	qE	301	PC1	O31-C31-C32-C33
152	qI	202	PC1	O31-C31-C32-C33
152	qi	203	PC1	O31-C31-C32-C33
152	2F	303	PC1	O21-C21-C22-C23
152	6C	201	PC1	O21-C21-C22-C23
152	Qc	506	PC1	O21-C21-C22-C23
152	Qi	203	PC1	O31-C31-C32-C33
153	6a	201	CDL	C72-C71-CB7-OB8
153	a	505	CDL	C12-C11-CA5-OA6
153	l	301	CDL	C72-C71-CB7-OB8
153	6A	201	CDL	C72-C71-CB7-OB8
153	J	301	CDL	C72-C71-CB7-OB8
153	N	304	CDL	C12-C11-CA5-OA6
153	T	203	CDL	C32-C31-CA7-OA8
153	VB	705	CDL	C12-C11-CA5-OA6
153	2B	201	CDL	C12-C11-CA5-OA6
153	7c	301	CDL	C43-C44-C45-C46
153	J	301	CDL	C16-C17-C18-C19
158	A3	201	3PE	C32-C33-C34-C35
152	c1	704	PC1	O21-C2-C3-O31
152	j	302	PC1	O21-C2-C3-O31
152	C1	706	PC1	O21-C2-C3-O31
152	J	302	PC1	O21-C2-C3-O31
153	a	505	CDL	OB6-CB4-CB6-OB8
153	c1	709	CDL	C12-C11-CA5-OA7
153	e	402	CDL	OB6-CB4-CB6-OB8
153	r	201	CDL	OA6-CA4-CA6-OA8
153	b4	201	CDL	C72-C71-CB7-OB9
153	n6	302	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	qG	402	CDL	OA6-CA4-CA6-OA8
153	C1	708	CDL	C12-C11-CA5-OA7
153	R	201	CDL	OA6-CA4-CA6-OA8
153	VB	705	CDL	OB6-CB4-CB6-OB8
153	B4	201	CDL	C72-C71-CB7-OB9
153	QG	402	CDL	OA6-CA4-CA6-OA8
153	Qb	601	CDL	CA5-C11-C12-C13
152	qI	202	PC1	C2B-C2C-C2D-C2E
166	y5	203	HEM	CAA-CBA-CGA-O2A
166	Y5	203	HEM	CAA-CBA-CGA-O2A
152	7A	202	PC1	C23-C24-C25-C26
152	N	303	PC1	C33-C34-C35-C36
153	T	204	CDL	C76-C77-C78-C79
153	VB	703	CDL	CA7-C31-C32-C33
158	W	203	3PE	C25-C26-C27-C28
152	6a	202	PC1	O21-C21-C22-C23
152	6c	203	PC1	O21-C21-C22-C23
152	2G	202	PC1	O31-C31-C32-C33
152	N5	805	PC1	O31-C31-C32-C33
152	QI	202	PC1	O31-C31-C32-C33
153	2b	201	CDL	C12-C11-CA5-OA6
153	E	402	CDL	C12-C11-CA5-OA6
153	AN	302	CDL	C52-C51-CB5-OB6
153	QI	203	CDL	C12-C11-CA5-OA6
169	b6	201	T7X	O18-C11-C31-C32
152	n5	801	PC1	C2C-C2D-C2E-C2F
153	2g	204	CDL	C54-C55-C56-C57
153	6c	202	CDL	C55-C56-C57-C58
153	a	504	CDL	C71-C72-C73-C74
153	A	504	CDL	C71-C72-C73-C74
153	T	204	CDL	C81-C82-C83-C84
158	w	203	3PE	C25-C26-C27-C28
152	d	501	PC1	C11-C12-N-C14
152	D	501	PC1	C11-C12-N-C14
152	T4	301	PC1	C11-C12-N-C13
152	c2	703	PC1	C32-C33-C34-C35
152	QI	202	PC1	C2B-C2C-C2D-C2E
153	q	202	CDL	C72-C71-CB7-OB9
153	Q	202	CDL	C72-C71-CB7-OB9
152	6A	202	PC1	O21-C21-C22-C23
153	a	502	CDL	C52-C51-CB5-OB6
153	e	402	CDL	C12-C11-CA5-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	an	302	CDL	C52-C51-CB5-OB6
153	t5	301	CDL	C12-C11-CA5-OA6
153	L	301	CDL	C72-C71-CB7-OB8
153	Z	101	CDL	C52-C51-CB5-OB6
169	B6	201	T7X	O18-C11-C31-C32
152	C1	706	PC1	C3A-C3B-C3C-C3D
153	c4	401	CDL	C55-C56-C57-C58
153	qc	505	CDL	C31-C32-C33-C34
153	N5	806	CDL	C77-C78-C79-C80
152	2F	301	PC1	C21-C22-C23-C24
153	n5	806	CDL	C77-C78-C79-C80
164	qc	501	U10	C18-C19-C21-C22
164	Qc	501	U10	C18-C19-C21-C22
153	td	101	CDL	C1-CB2-OB2-PB2
153	Qb	601	CDL	C1-CA2-OA2-PA1
152	c1	704	PC1	C3A-C3B-C3C-C3D
152	C2	701	PC1	C32-C33-C34-C35
153	T	204	CDL	C11-C12-C13-C14
152	n5	804	PC1	O21-C21-C22-C23
152	n5	805	PC1	O31-C31-C32-C33
152	M	302	PC1	O21-C21-C22-C23
152	C4	403	PC1	O31-C31-C32-C33
152	N5	804	PC1	O21-C21-C22-C23
153	i	302	CDL	C52-C51-CB5-OB6
153	n	304	CDL	C12-C11-CA5-OA6
153	r	201	CDL	C12-C11-CA5-OA6
153	T5	301	CDL	C12-C11-CA5-OA6
158	sc	101	3PE	O31-C31-C32-C33
158	w	203	3PE	O21-C21-C22-C23
158	SC	101	3PE	O31-C31-C32-C33
158	W	203	3PE	O21-C21-C22-C23
152	2f	301	PC1	C21-C22-C23-C24
164	sc	102	U10	C29-C31-C32-C33
164	SC	102	U10	C29-C31-C32-C33
153	t	204	CDL	C11-C12-C13-C14
167	a9	401	NDP	O4B-C4B-C5B-O5B
167	A9	401	NDP	O4B-C4B-C5B-O5B
152	v	202	PC1	O31-C31-C32-C33
153	j	301	CDL	C72-C71-CB7-OB8
153	z	101	CDL	C52-C51-CB5-OB6
153	qc	505	CDL	C72-C71-CB7-OB8
153	A	502	CDL	C52-C51-CB5-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Qc	505	CDL	C72-C71-CB7-OB8
152	qj	101	PC1	O32-C31-C32-C33
153	2o	101	CDL	C32-C31-CA7-OA9
153	m3	401	CDL	C52-C51-CB5-OB7
170	b9	202	ADP	PB-O3A-PA-O2A
170	B9	202	ADP	PB-O3A-PA-O2A
153	th	200	CDL	C11-C12-C13-C14
153	AN	302	CDL	C53-C54-C55-C56
152	qE	304	PC1	O22-C21-C22-C23
153	2k	101	CDL	C52-C51-CB5-OB7
153	t7	201	CDL	C12-C11-CA5-OA7
153	2K	101	CDL	C52-C51-CB5-OB7
153	T7	201	CDL	C12-C11-CA5-OA7
153	T	203	CDL	C22-C23-C24-C25
153	Qc	505	CDL	C31-C32-C33-C34
152	fs	204	PC1	O21-C21-C22-C23
152	m	307	PC1	O21-C21-C22-C23
153	t	204	CDL	C72-C71-CB7-OB8
153	R	201	CDL	C12-C11-CA5-OA6
153	T	204	CDL	C72-C71-CB7-OB8
160	Qh	201	PX2	O5-C4-C5-C6
153	an	302	CDL	C53-C54-C55-C56
153	2m	101	CDL	C18-C19-C20-C21
153	t	203	CDL	C22-C23-C24-C25
153	TH	200	CDL	C11-C12-C13-C14
152	t4	301	PC1	C11-C12-N-C15
152	QC	505	PC1	O32-C31-C32-C33
152	Qj	101	PC1	O32-C31-C32-C33
153	w	202	CDL	C72-C71-CB7-OB9
153	2O	101	CDL	C32-C31-CA7-OA9
153	VB	703	CDL	C52-C51-CB5-OB7
153	W	202	CDL	C72-C71-CB7-OB9
153	B3	102	CDL	C12-C11-CA5-OA7
158	an	303	3PE	O32-C31-C32-C33
158	AN	303	3PE	O32-C31-C32-C33
152	c1	704	PC1	C28-C29-C2A-C2B
152	n5	803	PC1	C3A-C3B-C3C-C3D
152	C1	706	PC1	C28-C29-C2A-C2B
152	N5	803	PC1	C3A-C3B-C3C-C3D
158	an	303	3PE	C25-C26-C27-C28
153	e	402	CDL	C61-C62-C63-C64
153	6C	203	CDL	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	FS	201	PC1	O21-C21-C22-C23
152	V	202	PC1	O31-C31-C32-C33
153	6c	202	CDL	C34-C35-C36-C37
158	AN	303	3PE	C25-C26-C27-C28
152	qC	505	PC1	O32-C31-C32-C33
152	7A	202	PC1	O22-C21-C22-C23
153	2g	201	CDL	C12-C11-CA5-OA7
153	5b	201	CDL	C72-C71-CB7-OB9
153	2G	201	CDL	C12-C11-CA5-OA7
153	B	501	CDL	C32-C31-CA7-OA9
158	n4	601	3PE	O22-C21-C22-C23
152	c3	606	PC1	C25-C26-C27-C28
153	E	402	CDL	C61-C62-C63-C64
152	Qc	509	PC1	C31-C32-C33-C34
152	C3	606	PC1	C25-C26-C27-C28
152	7a	202	PC1	O22-C21-C22-C23
152	qc	509	PC1	O32-C31-C32-C33
152	Qc	509	PC1	O32-C31-C32-C33
153	b	501	CDL	C32-C31-CA7-OA9
153	c1	701	CDL	C32-C31-CA7-OA9
153	m2	404	CDL	C52-C51-CB5-OB7
153	q	202	CDL	C52-C51-CB5-OB7
153	q	203	CDL	C52-C51-CB5-OB7
153	te	101	CDL	C12-C11-CA5-OA7
153	C1	701	CDL	C32-C31-CA7-OA9
153	M2	404	CDL	C52-C51-CB5-OB7
153	M3	401	CDL	C52-C51-CB5-OB7
153	Q	202	CDL	C52-C51-CB5-OB7
153	TE	101	CDL	C12-C11-CA5-OA7
158	VB	707	3PE	O22-C21-C22-C23
160	R	202	PX2	O6-C4-C5-C6
152	n	302	PC1	O21-C21-C22-C23
152	N	302	PC1	O21-C21-C22-C23
153	2M	101	CDL	C18-C19-C20-C21
154	c1	708	HEA	C17-C18-C19-C20
152	7a	202	PC1	C26-C27-C28-C29
153	2k	101	CDL	C35-C36-C37-C38
158	G2	301	3PE	C2D-C2E-C2F-C2G
158	w	203	3PE	C31-C32-C33-C34
158	W	203	3PE	C31-C32-C33-C34
152	m2	402	PC1	O32-C31-C32-C33
153	2k	101	CDL	C72-C71-CB7-OB9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	i	301	CDL	C12-C11-CA5-OA7
153	b3	102	CDL	C12-C11-CA5-OA7
153	qb	601	CDL	C72-C71-CB7-OB9
153	qi	202	CDL	C52-C51-CB5-OB7
153	2K	101	CDL	C72-C71-CB7-OB9
153	F	402	CDL	C52-C51-CB5-OB7
153	I	302	CDL	C12-C11-CA5-OA7
153	5B	201	CDL	C72-C71-CB7-OB9
153	Qb	601	CDL	C72-C71-CB7-OB9
153	Qi	202	CDL	C52-C51-CB5-OB7
158	vb	705	3PE	O22-C21-C22-C23
158	N4	601	3PE	O22-C21-C22-C23
152	2f	301	PC1	C1-C2-C3-O31
152	2F	301	PC1	C1-C2-C3-O31
152	N1	301	PC1	C1-C2-C3-O31
153	m3	401	CDL	CA3-CA4-CA6-OA8
153	am	201	CDL	CB3-CB4-CB6-OB8
153	M3	401	CDL	CA3-CA4-CA6-OA8
153	A1	102	CDL	CB3-CB4-CB6-OB8
153	AM	201	CDL	CB3-CB4-CB6-OB8
158	n5	802	3PE	C1-C2-C3-O31
158	VB	707	3PE	C1-C2-C3-O31
158	N5	802	3PE	C1-C2-C3-O31
152	p1	401	PC1	O31-C31-C32-C33
153	F	402	CDL	C72-C71-CB7-OB8
152	7A	202	PC1	C26-C27-C28-C29
153	2g	201	CDL	C59-C60-C61-C62
153	2m	101	CDL	C58-C59-C60-C61
153	te	101	CDL	C54-C55-C56-C57
153	A9	402	CDL	C34-C35-C36-C37
158	W	203	3PE	C33-C34-C35-C36
152	C3	603	PC1	C11-O13-P-O11
152	TE	102	PC1	C1-O11-P-O13
153	y5	201	CDL	CA3-OA5-PA1-OA2
153	VB	705	CDL	CA3-OA5-PA1-OA2
153	A9	403	CDL	CB2-OB2-PB2-OB5
158	W	203	3PE	C1-O11-P-O13
152	Qe	303	PC1	C33-C34-C35-C36
153	n	304	CDL	C52-C53-C54-C55
153	qI	203	CDL	C16-C17-C18-C19
153	2K	101	CDL	C35-C36-C37-C38
153	2M	101	CDL	C58-C59-C60-C61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	Y7	501	CDL	O1-C1-CA2-OA2
152	qc	509	PC1	C31-C32-C33-C34
153	p1	403	CDL	CA5-C11-C12-C13
153	P1	403	CDL	CA5-C11-C12-C13
152	p1	401	PC1	O22-C21-C22-C23
152	6C	201	PC1	O22-C21-C22-C23
152	M2	402	PC1	O32-C31-C32-C33
152	C4	403	PC1	O32-C31-C32-C33
153	f	401	CDL	C52-C51-CB5-OB7
153	m3	401	CDL	C72-C71-CB7-OB9
153	M3	401	CDL	C72-C71-CB7-OB9
160	Qh	201	PX2	O6-C4-C5-C6
153	t	203	CDL	C13-C14-C15-C16
153	a9	402	CDL	C34-C35-C36-C37
153	2G	201	CDL	C59-C60-C61-C62
152	2G	202	PC1	C36-C37-C38-C39
153	N	304	CDL	C52-C53-C54-C55
158	w	203	3PE	C33-C34-C35-C36
152	t1	602	PC1	O21-C21-C22-C23
152	P1	401	PC1	O31-C31-C32-C33
152	T1	602	PC1	O21-C21-C22-C23
153	a	502	CDL	C12-C11-CA5-OA6
153	t1	601	CDL	C32-C31-CA7-OA8
153	A	502	CDL	C12-C11-CA5-OA6
153	VB	706	CDL	C72-C71-CB7-OB8
153	T1	601	CDL	C32-C31-CA7-OA8
158	a3	201	3PE	O31-C31-C32-C33
158	A3	201	3PE	O31-C31-C32-C33
153	q	202	CDL	C1-CB2-OB2-PB2
153	qb	601	CDL	C1-CA2-OA2-PA1
153	Q	202	CDL	C1-CB2-OB2-PB2
153	N5	806	CDL	CB4-CB3-OB5-PB2
152	2f	303	PC1	O22-C21-C22-C23
152	6a	202	PC1	O22-C21-C22-C23
152	n5	804	PC1	O22-C21-C22-C23
152	qE	301	PC1	O32-C31-C32-C33
152	qi	203	PC1	O32-C31-C32-C33
152	P1	401	PC1	O22-C21-C22-C23
152	QJ	101	PC1	O22-C21-C22-C23
152	Qi	203	PC1	O32-C31-C32-C33
153	i	302	CDL	C52-C51-CB5-OB7
153	t	204	CDL	C52-C51-CB5-OB7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	t	204	CDL	C72-C71-CB7-OB9
153	T	202	CDL	C12-C11-CA5-OA7
153	T	203	CDL	C32-C31-CA7-OA9
153	T	204	CDL	C52-C51-CB5-OB7
153	T	204	CDL	C72-C71-CB7-OB9
160	Y5	204	PX2	O6-C4-C5-C6
153	e	402	CDL	C31-C32-C33-C34
153	T	203	CDL	C13-C14-C15-C16
153	C4	401	CDL	C51-C52-C53-C54
152	qe	303	PC1	C33-C34-C35-C36
152	qi	203	PC1	C29-C2A-C2B-C2C
152	Qi	203	PC1	C29-C2A-C2B-C2C
153	5b	201	CDL	C32-C33-C34-C35
153	c4	401	CDL	C51-C52-C53-C54
153	E	402	CDL	C31-C32-C33-C34
160	R	202	PX2	C7-C8-C9-C10
152	c2	703	PC1	C1-O11-P-O14
152	c3	601	PC1	C11-C12-N-C14
152	c3	601	PC1	C11-C12-N-C15
152	f	402	PC1	C11-O13-P-O12
152	j	302	PC1	C11-O13-P-O12
152	j	302	PC1	C11-O13-P-O14
152	n	302	PC1	C1-O11-P-O12
152	n	303	PC1	C11-O13-P-O14
152	w	204	PC1	C11-O13-P-O14
152	5b	202	PC1	C1-O11-P-O14
152	n3	201	PC1	C11-O13-P-O14
152	n6	301	PC1	C1-O11-P-O14
152	qI	201	PC1	C1-O11-P-O14
152	qI	202	PC1	C11-O13-P-O14
152	qJ	101	PC1	C11-O13-P-O14
152	qb	602	PC1	C11-O13-P-O14
152	s8	301	PC1	C11-O13-P-O14
152	t4	301	PC1	C11-C12-N-C13
152	C2	701	PC1	C1-O11-P-O14
152	F	401	PC1	C11-O13-P-O12
152	J	302	PC1	C11-O13-P-O12
152	J	302	PC1	C11-O13-P-O14
152	N	302	PC1	C1-O11-P-O12
152	N	303	PC1	C11-O13-P-O14
152	W	204	PC1	C11-O13-P-O14
152	5B	202	PC1	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	N3	201	PC1	C11-O13-P-O14
152	N5	805	PC1	C11-C12-N-C14
152	N6	301	PC1	C1-O11-P-O14
152	QI	202	PC1	C11-O13-P-O14
152	QJ	102	PC1	C11-O13-P-O14
152	Qb	602	PC1	C11-O13-P-O14
152	S8	301	PC1	C11-O13-P-O14
153	2g	204	CDL	CB2-OB2-PB2-OB3
153	2k	101	CDL	CA2-OA2-PA1-OA3
153	2o	101	CDL	CA2-OA2-PA1-OA3
153	2o	101	CDL	CB3-OB5-PB2-OB3
153	6c	201	CDL	CA2-OA2-PA1-OA4
153	7a	201	CDL	CA2-OA2-PA1-OA3
153	7a	203	CDL	CB2-OB2-PB2-OB3
153	a	502	CDL	CA3-OA5-PA1-OA3
153	a	502	CDL	CB2-OB2-PB2-OB3
153	a	502	CDL	CB3-OB5-PB2-OB3
153	b	501	CDL	CB3-OB5-PB2-OB3
153	e	402	CDL	CA3-OA5-PA1-OA3
153	f	401	CDL	CB2-OB2-PB2-OB3
153	fs	203	CDL	CA3-OA5-PA1-OA3
153	i	301	CDL	CB3-OB5-PB2-OB3
153	i	302	CDL	CA2-OA2-PA1-OA3
153	m	302	CDL	CB3-OB5-PB2-OB3
153	m	303	CDL	CB3-OB5-PB2-OB3
153	m	304	CDL	CA3-OA5-PA1-OA3
153	m1	402	CDL	CA3-OA5-PA1-OA3
153	m1	405	CDL	CA3-OA5-PA1-OA4
153	m2	401	CDL	CA2-OA2-PA1-OA3
153	q	202	CDL	CA3-OA5-PA1-OA3
153	r	201	CDL	CA2-OA2-PA1-OA3
153	t	202	CDL	CA2-OA2-PA1-OA3
153	vb	701	CDL	CA3-OA5-PA1-OA3
153	vb	701	CDL	CB3-OB5-PB2-OB3
153	y5	201	CDL	CA3-OA5-PA1-OA3
153	5b	201	CDL	CB2-OB2-PB2-OB3
153	a1	101	CDL	CB2-OB2-PB2-OB3
153	a9	402	CDL	CA3-OA5-PA1-OA4
153	a9	402	CDL	CB3-OB5-PB2-OB4
153	a9	403	CDL	CB2-OB2-PB2-OB4
153	an	302	CDL	CA2-OA2-PA1-OA3
153	an	302	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	an	302	CDL	CA3-OA5-PA1-OA3
153	b3	101	CDL	CB3-OB5-PB2-OB3
153	b3	102	CDL	CA3-OA5-PA1-OA3
153	b8	302	CDL	CA2-OA2-PA1-OA3
153	qB	601	CDL	CA3-OA5-PA1-OA3
153	qB	601	CDL	CA3-OA5-PA1-OA4
153	qC	504	CDL	CA2-OA2-PA1-OA3
153	qc	505	CDL	CA2-OA2-PA1-OA4
153	t1	601	CDL	CA3-OA5-PA1-OA4
153	t5	301	CDL	CB2-OB2-PB2-OB4
153	te	101	CDL	CA3-OA5-PA1-OA3
153	2G	204	CDL	CB2-OB2-PB2-OB3
153	2K	101	CDL	CA2-OA2-PA1-OA3
153	2O	101	CDL	CA2-OA2-PA1-OA3
153	2O	101	CDL	CB3-OB5-PB2-OB3
153	6C	202	CDL	CA2-OA2-PA1-OA4
153	7A	201	CDL	CA2-OA2-PA1-OA3
153	7A	203	CDL	CB2-OB2-PB2-OB3
153	A	502	CDL	CA3-OA5-PA1-OA3
153	A	502	CDL	CB2-OB2-PB2-OB3
153	A	502	CDL	CB3-OB5-PB2-OB3
153	B	501	CDL	CB3-OB5-PB2-OB3
153	E	402	CDL	CA3-OA5-PA1-OA3
153	F	402	CDL	CB2-OB2-PB2-OB3
153	FS	204	CDL	CA3-OA5-PA1-OA3
153	I	302	CDL	CB3-OB5-PB2-OB3
153	I	303	CDL	CA2-OA2-PA1-OA3
153	M	304	CDL	CB3-OB5-PB2-OB3
153	M	305	CDL	CB3-OB5-PB2-OB3
153	M	306	CDL	CA3-OA5-PA1-OA3
153	M1	402	CDL	CA3-OA5-PA1-OA3
153	M2	401	CDL	CA2-OA2-PA1-OA3
153	Q	202	CDL	CA3-OA5-PA1-OA3
153	R	201	CDL	CA2-OA2-PA1-OA3
153	T	202	CDL	CA2-OA2-PA1-OA3
153	VB	701	CDL	CA3-OA5-PA1-OA3
153	VB	703	CDL	CB3-OB5-PB2-OB3
153	5B	201	CDL	CB2-OB2-PB2-OB3
153	5B	201	CDL	CB3-OB5-PB2-OB4
153	A1	102	CDL	CB2-OB2-PB2-OB3
153	A9	402	CDL	CB3-OB5-PB2-OB4
153	AN	302	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	AN	302	CDL	CA2-OA2-PA1-OA4
153	AN	302	CDL	CA3-OA5-PA1-OA3
153	B3	101	CDL	CB3-OB5-PB2-OB3
153	B3	102	CDL	CA3-OA5-PA1-OA3
153	B8	302	CDL	CA2-OA2-PA1-OA3
153	QB	601	CDL	CA3-OA5-PA1-OA3
153	QB	601	CDL	CA3-OA5-PA1-OA4
153	QC	504	CDL	CA2-OA2-PA1-OA3
153	Qc	505	CDL	CA2-OA2-PA1-OA4
153	T1	601	CDL	CA3-OA5-PA1-OA4
153	T5	301	CDL	CB2-OB2-PB2-OB4
153	T7	201	CDL	CB3-OB5-PB2-OB3
153	TE	101	CDL	CA3-OA5-PA1-OA3
153	u1	101	CDL	CA3-OA5-PA1-OA4
153	U1	101	CDL	CA3-OA5-PA1-OA4
158	an	305	3PE	C1-O11-P-O14
158	g2	301	3PE	C1-O11-P-O12
158	n5	802	3PE	C1-O11-P-O14
158	W	203	3PE	C1-O11-P-O14
158	AN	305	3PE	C1-O11-P-O12
158	AN	305	3PE	C1-O11-P-O14
158	G2	301	3PE	C1-O11-P-O12
153	q	201	CDL	CA5-C11-C12-C13
152	2g	202	PC1	C36-C37-C38-C39
152	c3	602	PC1	O22-C21-C22-C23
152	c4	403	PC1	O32-C31-C32-C33
152	n5	805	PC1	O32-C31-C32-C33
152	6A	202	PC1	O22-C21-C22-C23
152	C3	602	PC1	O22-C21-C22-C23
152	QE	301	PC1	O32-C31-C32-C33
152	Qc	506	PC1	O22-C21-C22-C23
153	a	505	CDL	C12-C11-CA5-OA7
153	t	202	CDL	C12-C11-CA5-OA7
153	an	302	CDL	C52-C51-CB5-OB7
153	qG	402	CDL	C52-C51-CB5-OB7
153	VB	705	CDL	C12-C11-CA5-OA7
153	QG	402	CDL	C52-C51-CB5-OB7
158	t8	601	3PE	O22-C21-C22-C23
152	qI	201	PC1	O31-C31-C32-C33
152	2F	301	PC1	O21-C21-C22-C23
153	6c	201	CDL	C52-C51-CB5-OB6
153	vb	704	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	6C	202	CDL	C52-C51-CB5-OB6
153	m2	403	CDL	OB5-CB3-CB4-CB6
153	M2	403	CDL	OB5-CB3-CB4-CB6
153	T	204	CDL	OA5-CA3-CA4-CA6
153	5B	201	CDL	C32-C33-C34-C35
160	r	202	PX2	C7-C8-C9-C10
151	qd	401	HEC	CAD-CBD-CGD-O2D
152	a	501	PC1	C23-C24-C25-C26
152	Qj	101	PC1	C33-C34-C35-C36
153	2G	204	CDL	C55-C56-C57-C58
152	6c	203	PC1	O22-C21-C22-C23
152	qc	506	PC1	O22-C21-C22-C23
152	2F	303	PC1	O22-C21-C22-C23
152	QI	202	PC1	O32-C31-C32-C33
153	t	203	CDL	C32-C31-CA7-OA9
153	I	303	CDL	C52-C51-CB5-OB7
153	J	301	CDL	C72-C71-CB7-OB9
158	M3	402	3PE	O32-C31-C32-C33
152	qj	101	PC1	C33-C34-C35-C36
153	AL	301	CDL	C72-C73-C74-C75
152	2f	301	PC1	O21-C21-C22-C23
152	C2	701	PC1	O31-C31-C32-C33
153	7c	301	CDL	C12-C11-CA5-OA6
153	f	401	CDL	C72-C71-CB7-OB8
153	qc	508	CDL	C32-C31-CA7-OA8
153	Qc	508	CDL	C32-C31-CA7-OA8
153	al	301	CDL	C72-C73-C74-C75
151	Qd	401	HEC	CAD-CBD-CGD-O2D
153	QH	201	CDL	C31-C32-C33-C34
152	b9	201	PC1	O22-C21-C22-C23
152	qI	202	PC1	O32-C31-C32-C33
152	B9	201	PC1	O22-C21-C22-C23
153	j	301	CDL	C72-C71-CB7-OB9
153	AN	302	CDL	C52-C51-CB5-OB7
153	Qg	402	CDL	C52-C51-CB5-OB7
158	w	203	3PE	O22-C21-C22-C23
158	I	304	3PE	O22-C21-C22-C23
158	T8	601	3PE	O22-C21-C22-C23
153	t7	201	CDL	C22-C23-C24-C25
153	C1	701	CDL	C11-C12-C13-C14
153	C4	401	CDL	C55-C56-C57-C58
153	T7	201	CDL	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
158	a3	202	3PE	C27-C28-C29-C2A
152	A	501	PC1	C23-C24-C25-C26
153	a9	402	CDL	C52-C51-CB5-OB6
153	qC	504	CDL	C72-C71-CB7-OB8
153	7C	301	CDL	C12-C11-CA5-OA6
153	QC	504	CDL	C72-C71-CB7-OB8
152	c1	704	PC1	C23-C24-C25-C26
153	q	203	CDL	C12-C13-C14-C15
153	y5	201	CDL	C35-C36-C37-C38
153	qH	201	CDL	C31-C32-C33-C34
153	qH	201	CDL	C56-C57-C58-C59
158	A3	202	3PE	C25-C26-C27-C28
152	N5	804	PC1	O22-C21-C22-C23
152	QJ	102	PC1	O22-C21-C22-C23
153	e	401	CDL	C72-C71-CB7-OB9
153	E	401	CDL	C72-C71-CB7-OB9
153	2B	201	CDL	C12-C11-CA5-OA7
158	i	303	3PE	O22-C21-C22-C23
158	m3	402	3PE	O32-C31-C32-C33
160	r	202	PX2	O6-C4-C5-C6
153	QH	201	CDL	C56-C57-C58-C59
158	a3	202	3PE	C25-C26-C27-C28
153	5b	201	CDL	C14-C15-C16-C17
153	N	304	CDL	C75-C76-C77-C78
153	5B	201	CDL	C14-C15-C16-C17
153	TE	101	CDL	C54-C55-C56-C57
158	A3	202	3PE	C27-C28-C29-C2A
158	BM	302	3PE	C33-C34-C35-C36
151	qd	401	HEC	CAD-CBD-CGD-O1D
166	QC	502	HEM	CAD-CBD-CGD-O2D
152	2f	303	PC1	C12-C11-O13-P
152	a	501	PC1	C1-C2-O21-C21
152	c3	606	PC1	C1-C2-O21-C21
152	c3	606	PC1	C3-C2-O21-C21
152	d	501	PC1	C1-C2-O21-C21
152	fs	204	PC1	C12-C11-O13-P
152	m	301	PC1	C1-C2-O21-C21
152	w	201	PC1	C12-C11-O13-P
152	5b	202	PC1	C12-C11-O13-P
152	j1	400	PC1	C12-C11-O13-P
152	n5	803	PC1	C12-C11-O13-P
152	qE	301	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	qG	401	PC1	C1-C2-O21-C21
152	qI	201	PC1	C12-C11-O13-P
152	qe	301	PC1	C12-C11-O13-P
152	qi	201	PC1	C3-C2-O21-C21
152	qi	203	PC1	C1-C2-O21-C21
152	t4	301	PC1	C3-C2-O21-C21
152	t4	303	PC1	C3-C2-O21-C21
152	tc	102	PC1	C12-C11-O13-P
152	te	102	PC1	C12-C11-O13-P
152	te	102	PC1	C3-C2-O21-C21
152	2F	303	PC1	C12-C11-O13-P
152	A	501	PC1	C1-C2-O21-C21
152	C3	606	PC1	C1-C2-O21-C21
152	C3	606	PC1	C3-C2-O21-C21
152	D	501	PC1	C1-C2-O21-C21
152	FS	201	PC1	C12-C11-O13-P
152	M	303	PC1	C1-C2-O21-C21
152	W	201	PC1	C12-C11-O13-P
152	5B	202	PC1	C12-C11-O13-P
152	J1	400	PC1	C12-C11-O13-P
152	N5	803	PC1	C12-C11-O13-P
152	QE	301	PC1	C12-C11-O13-P
152	QG	401	PC1	C1-C2-O21-C21
152	QI	201	PC1	C12-C11-O13-P
152	Qe	301	PC1	C12-C11-O13-P
152	Qi	201	PC1	C3-C2-O21-C21
152	Qi	203	PC1	C1-C2-O21-C21
152	T4	301	PC1	C3-C2-O21-C21
152	T4	303	PC1	C3-C2-O21-C21
152	TC	102	PC1	C12-C11-O13-P
152	TE	102	PC1	C12-C11-O13-P
152	TE	102	PC1	C3-C2-O21-C21
153	2k	101	CDL	CA6-CA4-OA6-CA5
153	2k	101	CDL	CB6-CB4-OB6-CB5
153	2m	101	CDL	CB6-CB4-OB6-CB5
153	6a	201	CDL	CB3-CB4-OB6-CB5
153	6a	201	CDL	CB6-CB4-OB6-CB5
153	7c	301	CDL	CB3-CB4-OB6-CB5
153	c1	709	CDL	CA6-CA4-OA6-CA5
153	c1	712	CDL	CB3-CB4-OB6-CB5
153	c1	712	CDL	CB6-CB4-OB6-CB5
153	m2	401	CDL	CB3-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	m3	403	CDL	CB6-CB4-OB6-CB5
153	n	304	CDL	CA6-CA4-OA6-CA5
153	q	201	CDL	CB3-CB4-OB6-CB5
153	t	202	CDL	CA3-CA4-OA6-CA5
153	t	204	CDL	CA3-CA4-OA6-CA5
153	w	202	CDL	CA3-CA4-OA6-CA5
153	2b	201	CDL	CA6-CA4-OA6-CA5
153	qc	508	CDL	CB3-CB4-OB6-CB5
153	t5	301	CDL	CB6-CB4-OB6-CB5
153	2K	101	CDL	CA6-CA4-OA6-CA5
153	2K	101	CDL	CB6-CB4-OB6-CB5
153	2M	101	CDL	CB6-CB4-OB6-CB5
153	6A	201	CDL	CB3-CB4-OB6-CB5
153	6A	201	CDL	CB6-CB4-OB6-CB5
153	7C	301	CDL	CB3-CB4-OB6-CB5
153	C1	708	CDL	CA6-CA4-OA6-CA5
153	C1	712	CDL	CB3-CB4-OB6-CB5
153	C1	712	CDL	CB6-CB4-OB6-CB5
153	M2	401	CDL	CB3-CB4-OB6-CB5
153	M3	403	CDL	CB6-CB4-OB6-CB5
153	N	304	CDL	CA6-CA4-OA6-CA5
153	Q	201	CDL	CB3-CB4-OB6-CB5
153	T	202	CDL	CA3-CA4-OA6-CA5
153	T	204	CDL	CA3-CA4-OA6-CA5
153	W	202	CDL	CA3-CA4-OA6-CA5
153	Qc	508	CDL	CB3-CB4-OB6-CB5
153	T5	301	CDL	CB6-CB4-OB6-CB5
153	C	301	CDL	CA6-CA4-OA6-CA5
153	C	301	CDL	CB6-CB4-OB6-CB5
153	c	301	CDL	CA6-CA4-OA6-CA5
153	c	301	CDL	CB6-CB4-OB6-CB5
158	b4	202	3PE	C12-C11-O13-P
158	t8	601	3PE	C1-C2-O21-C21
158	t8	602	3PE	C12-C11-O13-P
158	B4	202	3PE	C12-C11-O13-P
158	T8	601	3PE	C1-C2-O21-C21
158	T8	602	3PE	C12-C11-O13-P
153	A9	402	CDL	CA5-C11-C12-C13
152	2g	202	PC1	O32-C31-C32-C33
152	m	301	PC1	O22-C21-C22-C23
152	qJ	101	PC1	O22-C21-C22-C23
152	M	303	PC1	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
152	N5	805	PC1	O32-C31-C32-C33
153	2b	201	CDL	C12-C11-CA5-OA7
153	qI	203	CDL	C12-C11-CA5-OA7
153	qg	402	CDL	C52-C51-CB5-OB7
153	QI	203	CDL	C12-C11-CA5-OA7
158	W	203	3PE	O22-C21-C22-C23
153	c1	701	CDL	C11-C12-C13-C14
153	n	304	CDL	C75-C76-C77-C78
153	Y5	201	CDL	C35-C36-C37-C38
158	i	303	3PE	C23-C24-C25-C26
158	n4	601	3PE	C26-C27-C28-C29
158	I	304	3PE	C23-C24-C25-C26
152	c2	703	PC1	O31-C31-C32-C33
153	r	201	CDL	C52-C51-CB5-OB6
158	M3	402	3PE	O21-C21-C22-C23
153	y7	501	CDL	O1-C1-CA2-OA2
153	2G	201	CDL	C79-C80-C81-C82
151	Qd	401	HEC	CAD-CBD-CGD-O1D
153	Q	201	CDL	CA5-C11-C12-C13
153	e	402	CDL	C12-C11-CA5-OA7
152	2f	301	PC1	C2A-C2B-C2C-C2D
152	C1	706	PC1	C23-C24-C25-C26
153	2g	201	CDL	C79-C80-C81-C82
153	R	201	CDL	C72-C73-C74-C75
153	T5	301	CDL	C77-C78-C79-C80
152	c1	707	PC1	O31-C31-C32-C33
152	C1	710	PC1	O31-C31-C32-C33
153	q	203	CDL	C32-C31-CA7-OA8
153	c4	401	CDL	C72-C71-CB7-OB8
153	qG	402	CDL	C32-C31-CA7-OA8
153	td	101	CDL	C52-C51-CB5-OB6
153	5B	201	CDL	C52-C51-CB5-OB6
153	A1	101	CDL	C52-C51-CB5-OB6
153	A9	402	CDL	C52-C51-CB5-OB6
153	BM	301	CDL	C52-C51-CB5-OB6
158	g2	301	3PE	O21-C21-C22-C23
158	t8	601	3PE	O31-C31-C32-C33
158	G2	301	3PE	O21-C21-C22-C23
158	T8	601	3PE	O31-C31-C32-C33
152	w	201	PC1	C25-C26-C27-C28
153	6a	201	CDL	C17-C18-C19-C20
152	2F	301	PC1	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	e	402	CDL	C12-C13-C14-C15
153	6C	203	CDL	C61-C62-C63-C64
153	E	402	CDL	C12-C13-C14-C15
153	BM	301	CDL	C78-C79-C80-C81
153	l	301	CDL	C72-C71-CB7-OB9
153	6c	202	CDL	C61-C62-C63-C64
153	r	201	CDL	C72-C73-C74-C75
153	VB	703	CDL	C12-C13-C14-C15
153	C4	401	CDL	C79-C80-C81-C82
158	N4	601	3PE	C26-C27-C28-C29
152	n5	804	PC1	O31-C31-C32-C33
152	N5	804	PC1	O31-C31-C32-C33
152	N6	301	PC1	O31-C31-C32-C33
153	2g	203	CDL	C12-C11-CA5-OA6
153	7c	302	CDL	C12-C11-CA5-OA6
153	m1	402	CDL	C12-C11-CA5-OA6
153	m3	403	CDL	C12-C11-CA5-OA6
153	y5	201	CDL	C72-C71-CB7-OB8
153	2b	201	CDL	C72-C71-CB7-OB8
153	5b	201	CDL	C52-C51-CB5-OB6
153	am	201	CDL	C52-C51-CB5-OB6
153	2G	203	CDL	C12-C11-CA5-OA6
153	7C	302	CDL	C12-C11-CA5-OA6
153	C3	604	CDL	C12-C11-CA5-OA6
153	M3	403	CDL	C12-C11-CA5-OA6
153	U	201	CDL	C32-C31-CA7-OA8
153	Z	101	CDL	C32-C31-CA7-OA8
153	2B	201	CDL	C72-C71-CB7-OB8
153	A1	102	CDL	C72-C71-CB7-OB8
153	AL	301	CDL	C72-C71-CB7-OB8
153	AM	201	CDL	C52-C51-CB5-OB6
158	AN	301	3PE	O31-C31-C32-C33
158	AN	303	3PE	O21-C21-C22-C23
160	Qh	201	PX2	O7-C16-C17-C18
169	b6	201	T7X	O16-C10-C12-C13
169	B6	201	T7X	O16-C10-C12-C13
152	W	201	PC1	C25-C26-C27-C28
153	sd	101	CDL	C55-C56-C57-C58
153	c4	401	CDL	C79-C80-C81-C82
153	6A	201	CDL	C17-C18-C19-C20
153	W	202	CDL	C14-C15-C16-C17
158	bm	302	3PE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	c1	709	CDL	CB7-C71-C72-C73
153	a9	402	CDL	CA5-C11-C12-C13
153	C1	708	CDL	CB7-C71-C72-C73
153	bm	301	CDL	C52-C51-CB5-OB7
153	E	402	CDL	C12-C11-CA5-OA7
153	t5	301	CDL	C77-C78-C79-C80
153	c3	604	CDL	C1-CB2-OB2-PB2
153	t	201	CDL	C1-CB2-OB2-PB2
153	n5	806	CDL	CB4-CB3-OB5-PB2
153	t5	301	CDL	CB4-CB3-OB5-PB2
153	Y7	501	CDL	CA4-CA3-OA5-PA1
153	T5	301	CDL	CB4-CB3-OB5-PB2
153	m1	404	CDL	C15-C16-C17-C18
158	sc	101	3PE	O11-C1-C2-O21
152	fs	204	PC1	O22-C21-C22-C23
152	2G	202	PC1	O32-C31-C32-C33
152	FS	201	PC1	O22-C21-C22-C23
153	6a	201	CDL	C72-C71-CB7-OB9
153	a	502	CDL	C12-C11-CA5-OA7
153	td	101	CDL	C52-C51-CB5-OB7
153	N	304	CDL	C12-C11-CA5-OA7
169	B6	201	T7X	O19-C11-C31-C32
151	qD	401	HEC	CAD-CBD-CGD-O2D
151	QD	401	HEC	CAD-CBD-CGD-O2D
166	qC	502	HEM	CAD-CBD-CGD-O2D
153	w	202	CDL	C14-C15-C16-C17
153	M1	404	CDL	C15-C16-C17-C18
153	SD	101	CDL	C55-C56-C57-C58
152	n6	301	PC1	O31-C31-C32-C33
152	QI	201	PC1	O31-C31-C32-C33
152	Qg	401	PC1	O31-C31-C32-C33
153	c3	604	CDL	C12-C11-CA5-OA6
153	f	401	CDL	C12-C11-CA5-OA6
153	fs	203	CDL	C72-C71-CB7-OB8
153	t	203	CDL	C72-C71-CB7-OB8
153	u	201	CDL	C32-C31-CA7-OA8
153	z	101	CDL	C32-C31-CA7-OA8
153	a1	101	CDL	C72-C71-CB7-OB8
153	al	301	CDL	C72-C71-CB7-OB8
153	bm	301	CDL	C52-C51-CB5-OB6
153	c4	401	CDL	C12-C11-CA5-OA6
153	qC	503	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	F	402	CDL	C12-C11-CA5-OA6
153	M1	402	CDL	C12-C11-CA5-OA6
153	M3	403	CDL	C32-C31-CA7-OA8
153	R	201	CDL	C52-C51-CB5-OB6
153	T	204	CDL	C12-C11-CA5-OA6
153	VB	703	CDL	C32-C31-CA7-OA8
153	Y5	201	CDL	C72-C71-CB7-OB8
153	C4	401	CDL	C12-C11-CA5-OA6
153	C4	401	CDL	C72-C71-CB7-OB8
153	QC	503	CDL	C32-C31-CA7-OA8
153	QG	402	CDL	C32-C31-CA7-OA8
158	an	301	3PE	O31-C31-C32-C33
158	an	303	3PE	O21-C21-C22-C23
152	N	301	PC1	C25-C26-C27-C28
153	E	403	CDL	C72-C73-C74-C75
153	2B	201	CDL	C31-C32-C33-C34
153	2b	201	CDL	C31-C32-C33-C34
153	VB	706	CDL	C73-C74-C75-C76
153	2o	101	CDL	C52-C51-CB5-OB6
153	2O	101	CDL	C52-C51-CB5-OB6
153	m	303	CDL	CB7-C71-C72-C73
158	n5	802	3PE	C21-C22-C23-C24
152	n	302	PC1	O22-C21-C22-C23
152	v	202	PC1	O32-C31-C32-C33
152	p1	401	PC1	O32-C31-C32-C33
152	M	302	PC1	O22-C21-C22-C23
152	N	302	PC1	O22-C21-C22-C23
152	V	202	PC1	O32-C31-C32-C33
152	P1	401	PC1	O32-C31-C32-C33
153	2g	203	CDL	C12-C11-CA5-OA7
153	n	304	CDL	C12-C11-CA5-OA7
153	2b	201	CDL	C72-C71-CB7-OB9
153	5b	201	CDL	C52-C51-CB5-OB7
153	t1	601	CDL	C32-C31-CA7-OA9
153	2G	203	CDL	C12-C11-CA5-OA7
153	A	502	CDL	C12-C11-CA5-OA7
153	L	301	CDL	C72-C71-CB7-OB9
153	A1	101	CDL	C52-C51-CB5-OB7
158	AN	301	3PE	O32-C31-C32-C33
151	2E	401	HEC	CAD-CBD-CGD-O1D
154	C1	702	HEA	CAD-CBD-CGD-O1D
153	7a	201	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	vb	704	CDL	C73-C74-C75-C76
153	l	301	CDL	C12-C11-CA5-OA6
153	t	204	CDL	C12-C11-CA5-OA6
153	p1	403	CDL	C72-C71-CB7-OB8
153	L	301	CDL	C12-C11-CA5-OA6
153	M1	402	CDL	C52-C51-CB5-OB6
153	N	304	CDL	C52-C51-CB5-OB6
164	qc	507	U10	C4-C3-O3-C3M
164	qc	507	U10	C3-C4-O4-C4M
164	Qc	507	U10	C4-C3-O3-C3M
164	Qc	507	U10	C3-C4-O4-C4M
152	m	307	PC1	O22-C21-C22-C23
152	t1	602	PC1	O22-C21-C22-C23
152	N6	301	PC1	O32-C31-C32-C33
153	q	203	CDL	C32-C31-CA7-OA9
153	r	201	CDL	C12-C11-CA5-OA7
153	vb	704	CDL	C72-C71-CB7-OB9
153	qc	505	CDL	C72-C71-CB7-OB9
153	t5	301	CDL	C12-C11-CA5-OA7
153	6A	201	CDL	C72-C71-CB7-OB9
153	L	301	CDL	C12-C11-CA5-OA7
153	M1	402	CDL	C12-C11-CA5-OA7
153	R	201	CDL	C12-C11-CA5-OA7
153	VB	703	CDL	C32-C31-CA7-OA9
153	2B	201	CDL	C72-C71-CB7-OB9
153	BM	301	CDL	C52-C51-CB5-OB7
153	Qc	505	CDL	C72-C71-CB7-OB9
153	T1	601	CDL	C32-C31-CA7-OA9
153	T5	301	CDL	C12-C11-CA5-OA7
169	b6	201	T7X	O19-C11-C31-C32
151	2e	401	HEC	CAD-CBD-CGD-O1D
151	QD	401	HEC	CAD-CBD-CGD-O1D
154	c1	702	HEA	CAD-CBD-CGD-O1D
152	n	301	PC1	C25-C26-C27-C28
153	y5	201	CDL	C53-C54-C55-C56
153	te	101	CDL	C57-C58-C59-C60
153	7A	201	CDL	C16-C17-C18-C19
153	c1	709	CDL	O1-C1-CA2-OA2
153	C1	708	CDL	O1-C1-CA2-OA2
153	C	301	CDL	O1-C1-CB2-OB2
152	W	201	PC1	O31-C31-C32-C33
153	m1	402	CDL	C52-C51-CB5-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
153	m1	402	CDL	C72-C71-CB7-OB8
153	n	304	CDL	C52-C51-CB5-OB6
153	N6	302	CDL	C52-C51-CB5-OB6
153	P1	403	CDL	C72-C71-CB7-OB8
158	m3	402	3PE	O21-C21-C22-C23
153	e	403	CDL	C72-C73-C74-C75
153	qG	402	CDL	C33-C34-C35-C36
153	Y5	201	CDL	C53-C54-C55-C56
152	n6	301	PC1	O32-C31-C32-C33
152	T1	602	PC1	O22-C21-C22-C23
153	5B	201	CDL	C52-C51-CB5-OB7
158	g2	301	3PE	O22-C21-C22-C23
158	t8	601	3PE	O32-C31-C32-C33
152	j	302	PC1	C11-C12-N-C15
152	n5	805	PC1	C11-C12-N-C14
152	J	302	PC1	C11-C12-N-C15
151	qD	401	HEC	CAD-CBD-CGD-O1D
152	v	202	PC1	C38-C39-C3A-C3B
153	W	202	CDL	C56-C57-C58-C59
152	QI	202	PC1	C34-C35-C36-C37
158	a3	202	3PE	C29-C2A-C2B-C2C
153	M	305	CDL	CB7-C71-C72-C73
152	c1	707	PC1	O32-C31-C32-C33
152	C1	710	PC1	O32-C31-C32-C33
153	F	402	CDL	C72-C71-CB7-OB9
158	a3	201	3PE	O32-C31-C32-C33
158	G2	301	3PE	O22-C21-C22-C23
158	T8	601	3PE	O32-C31-C32-C33
160	Qh	201	PX2	O8-C16-C17-C18
164	b8	301	U10	C30-C29-C31-C32
152	qe	303	PC1	C2D-C2E-C2F-C2G
152	V	202	PC1	C38-C39-C3A-C3B
153	c1	712	CDL	C78-C79-C80-C81
153	7C	301	CDL	C58-C59-C60-C61
153	F	402	CDL	C31-C32-C33-C34
152	w	201	PC1	O31-C31-C32-C33
152	QI	202	PC1	O21-C21-C22-C23
153	m3	403	CDL	C32-C31-CA7-OA8
153	n6	302	CDL	C52-C51-CB5-OB6
153	td	101	CDL	C12-C11-CA5-OA6
153	T	203	CDL	C72-C71-CB7-OB8
153	AM	201	CDL	C72-C71-CB7-OB8

Continued on next page...

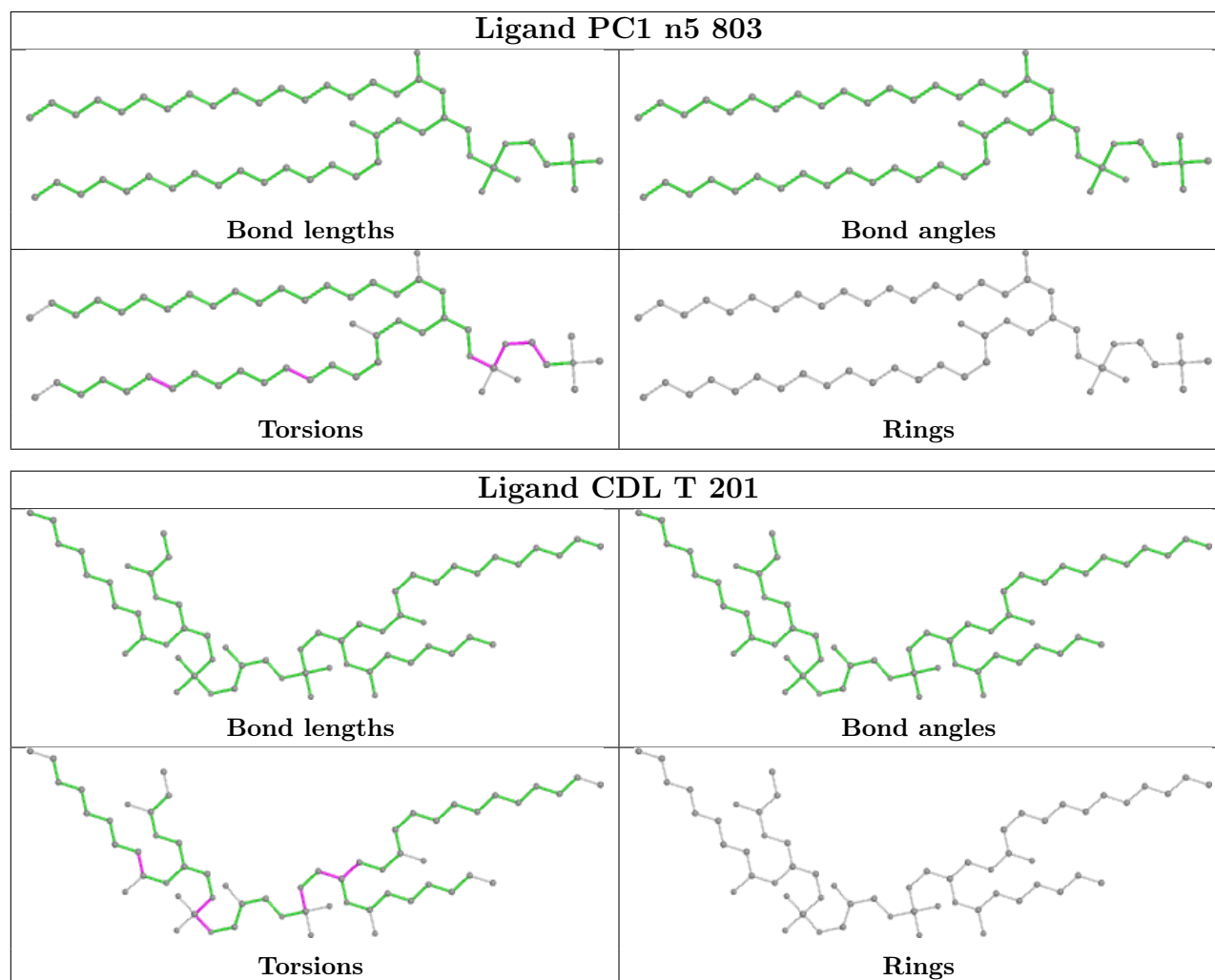
Continued from previous page...

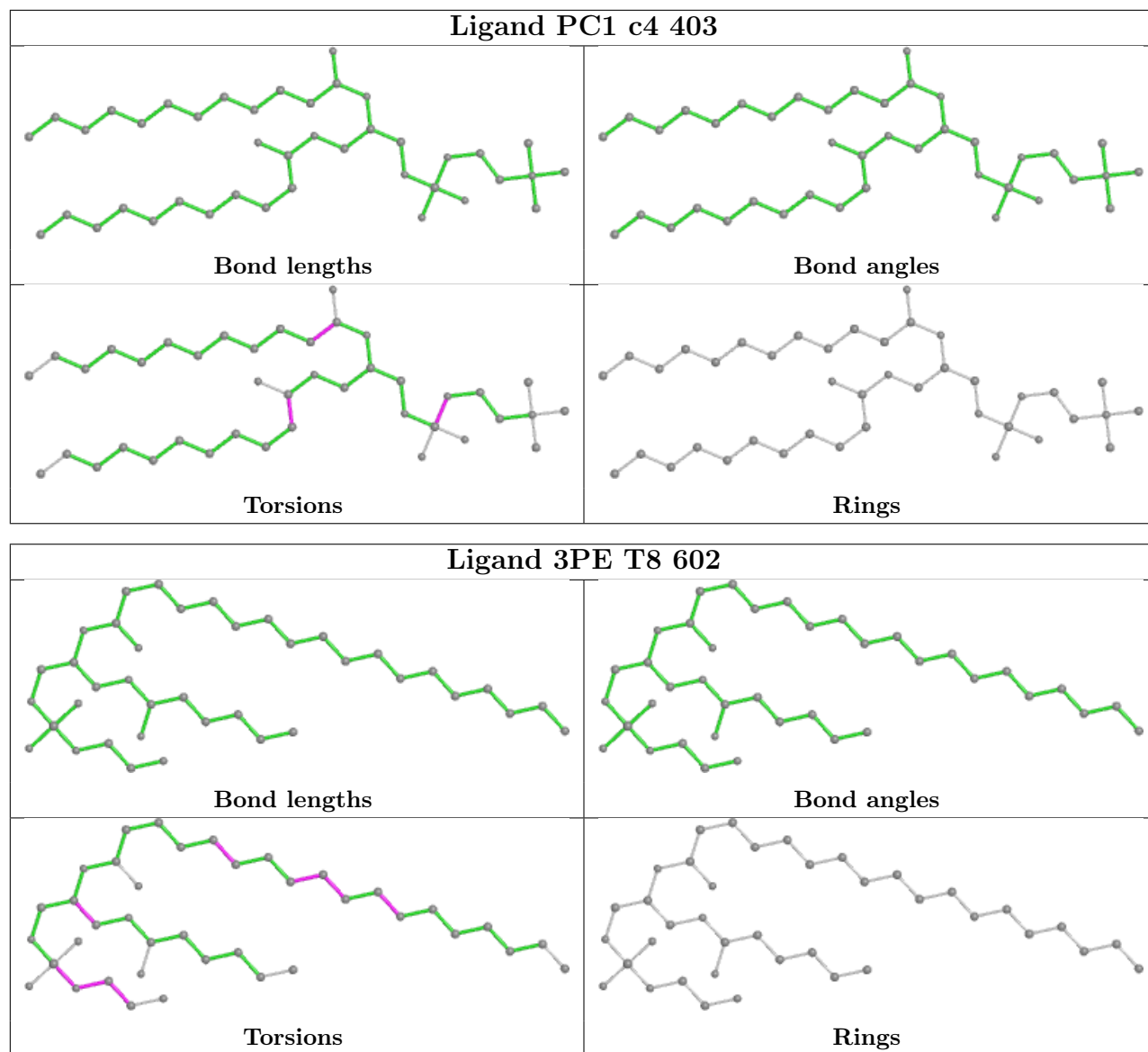
Mol	Chain	Res	Type	Atoms
158	n4	601	3PE	O31-C31-C32-C33

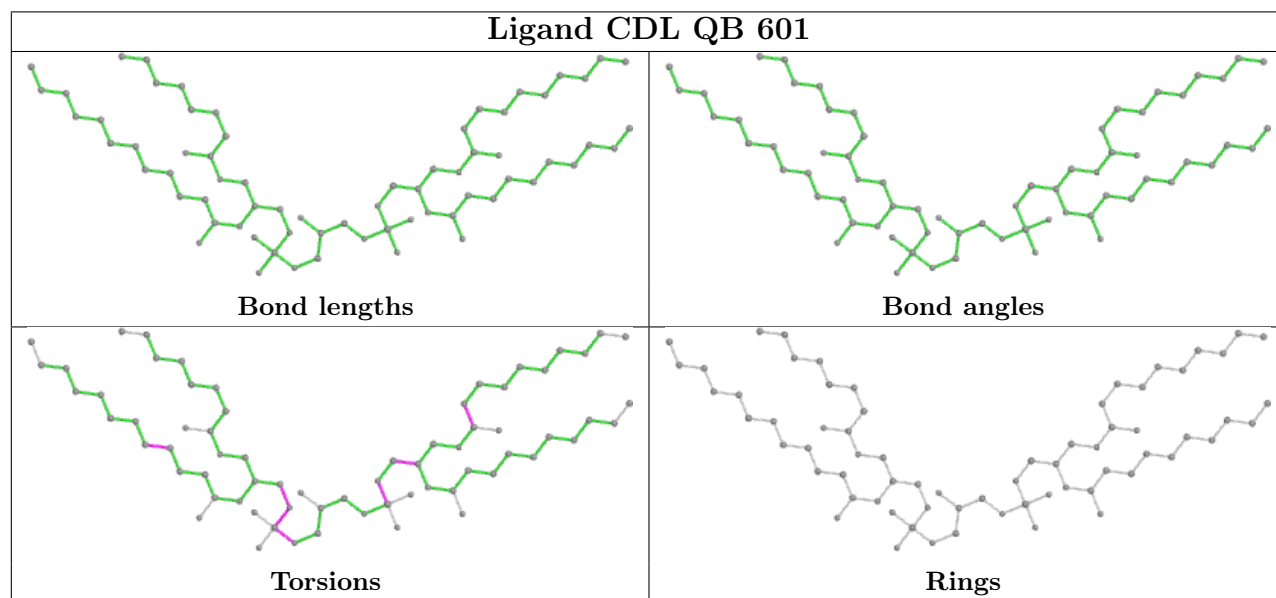
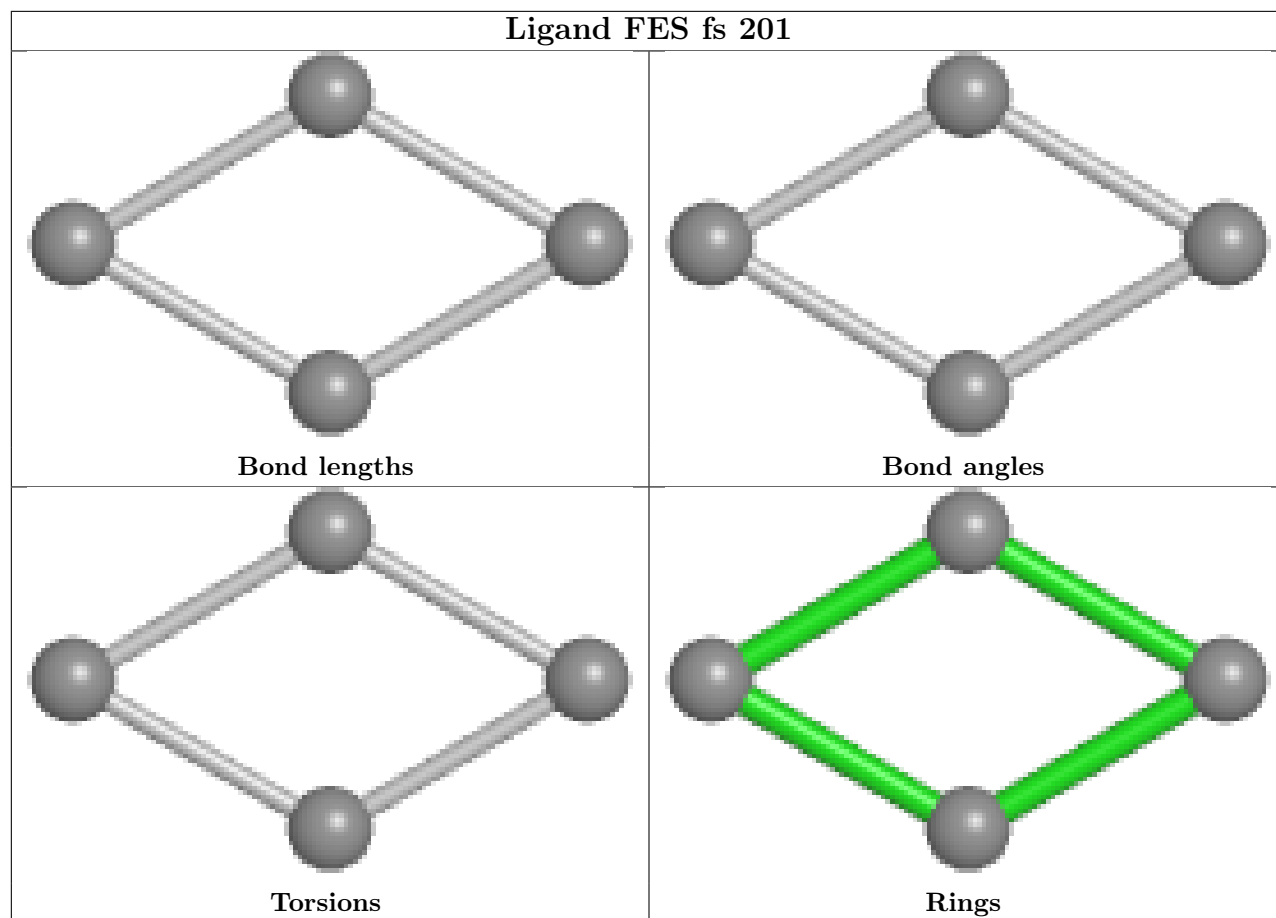
There are no ring outliers.

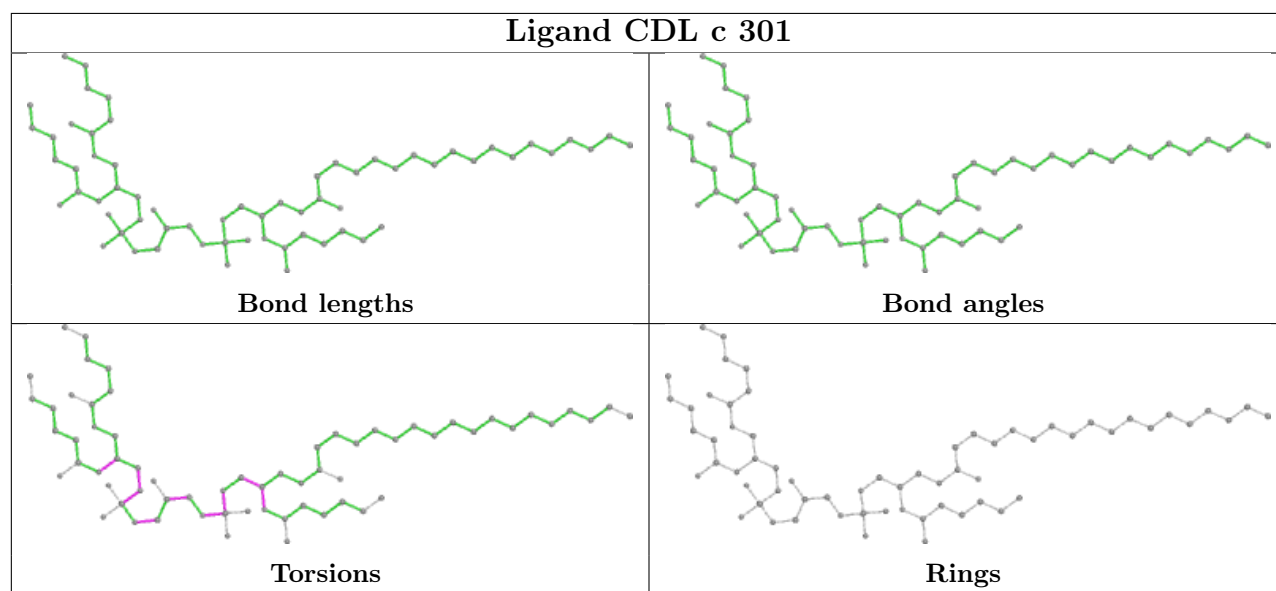
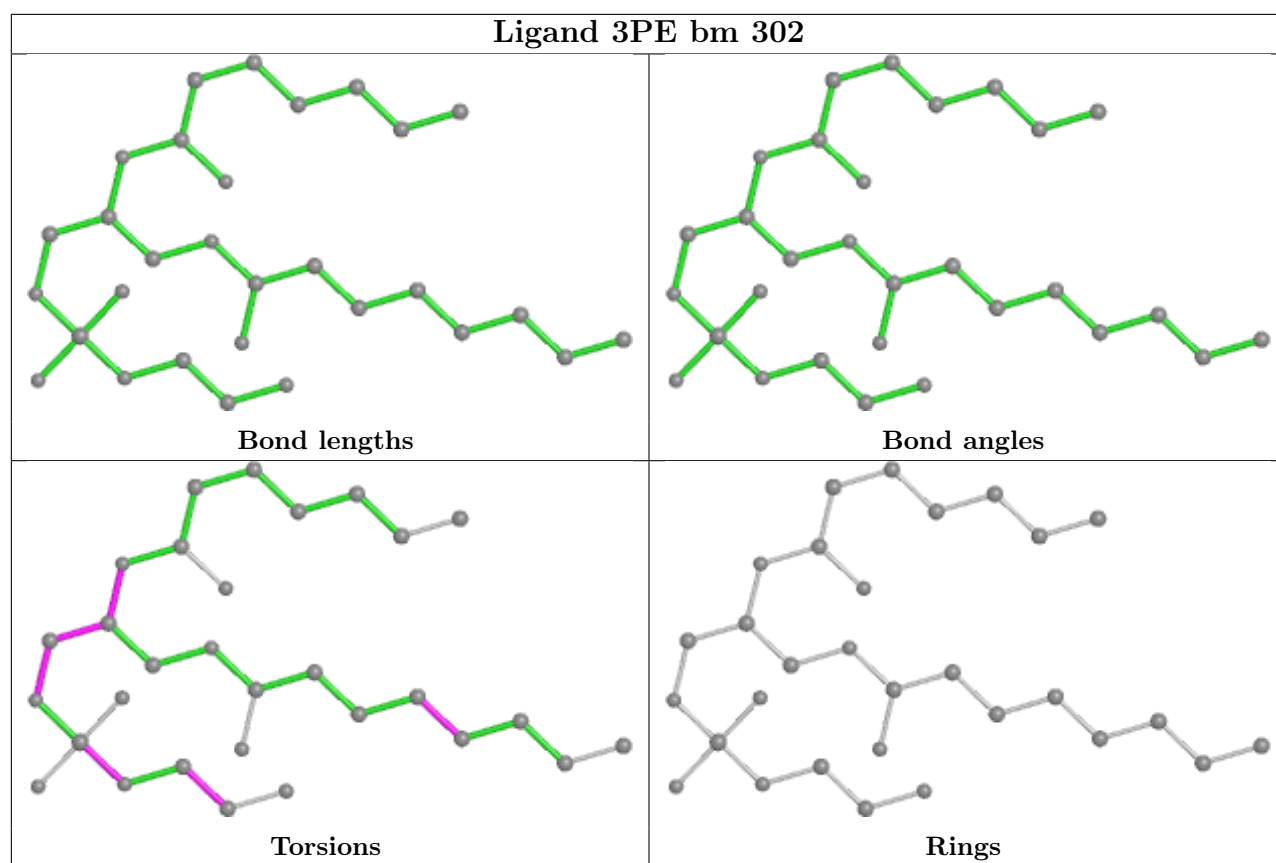
No monomer is involved in short contacts.

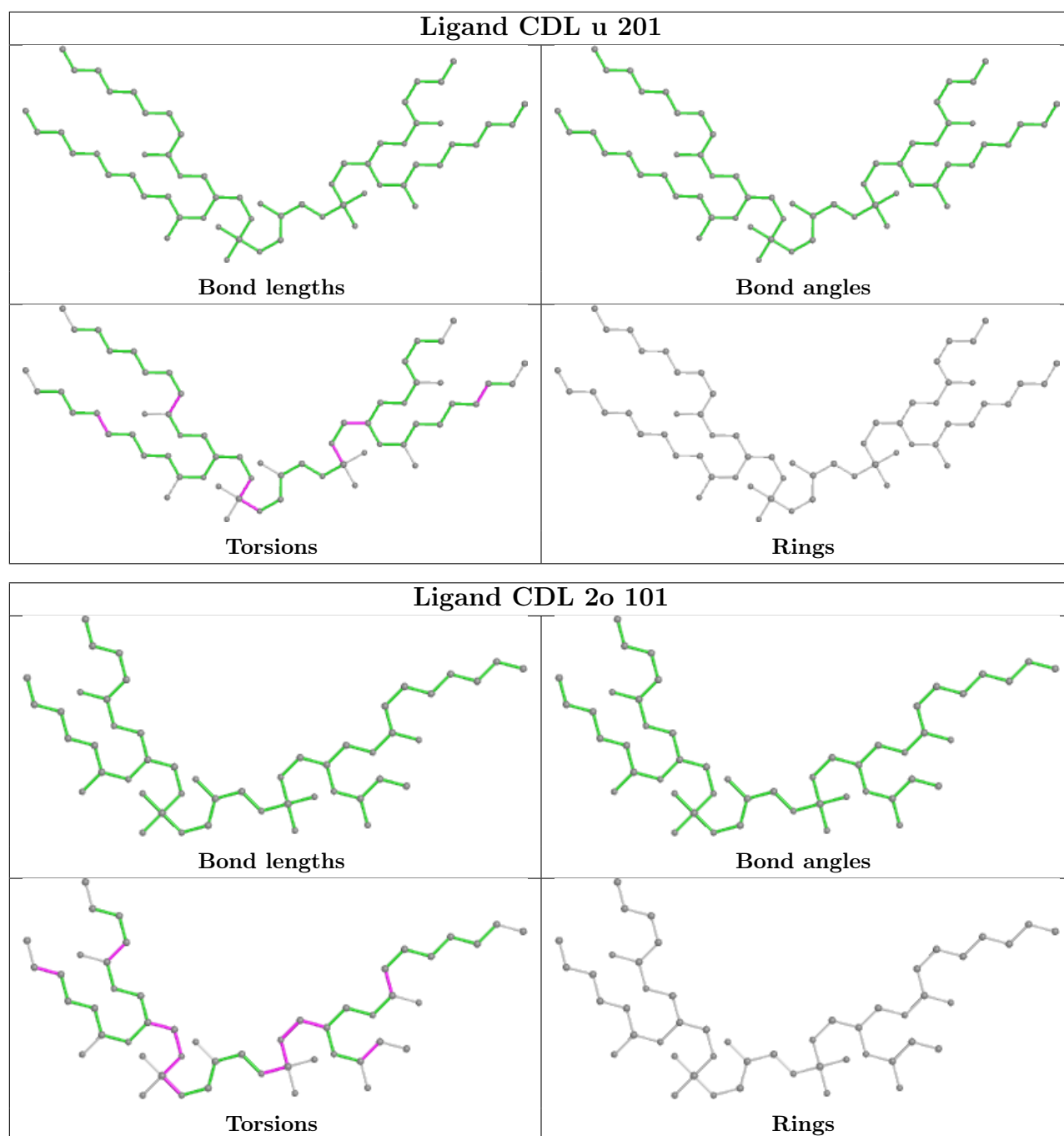
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

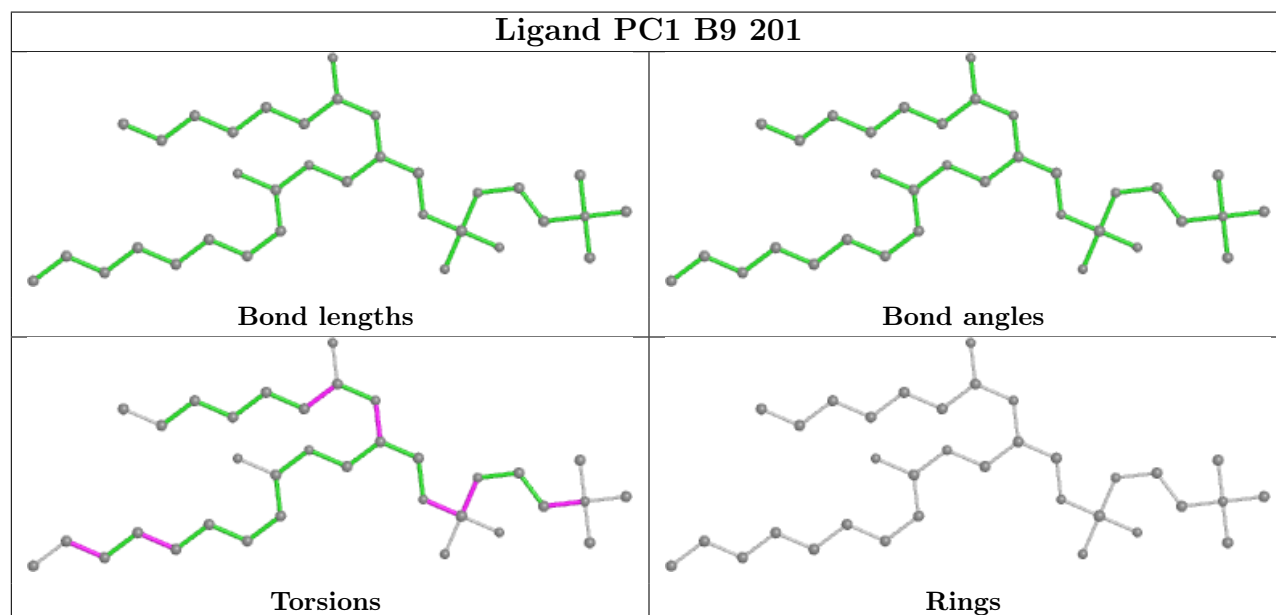
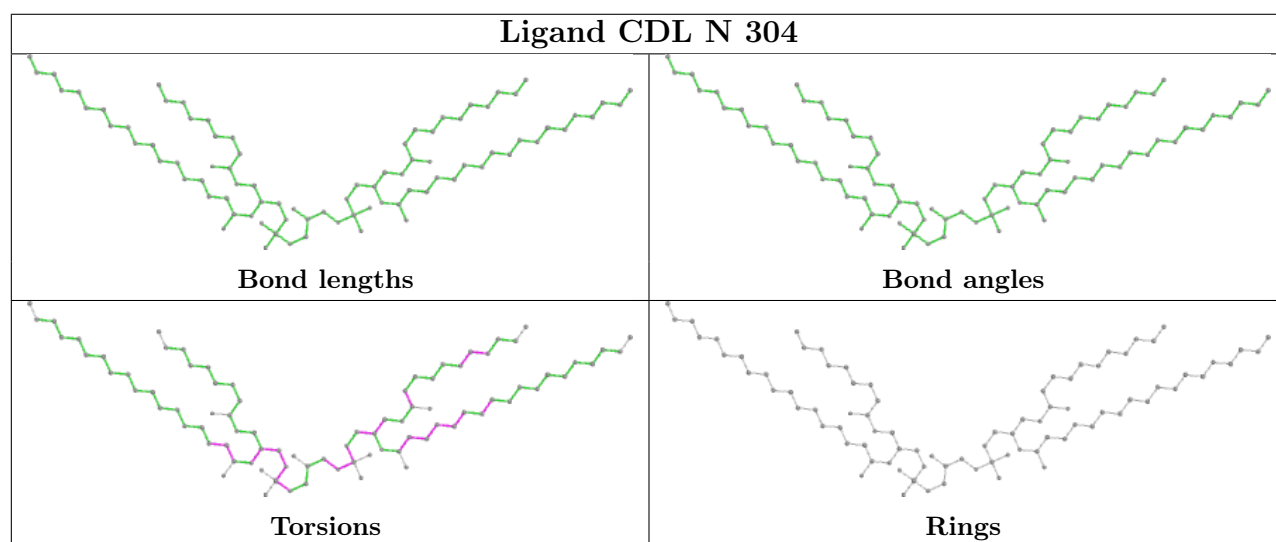
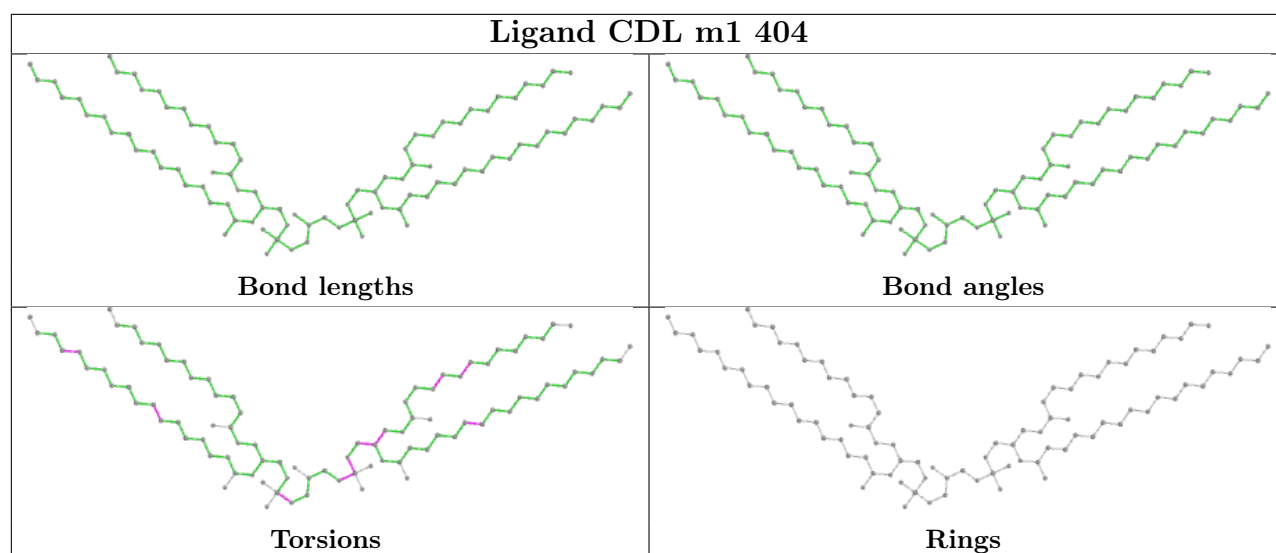


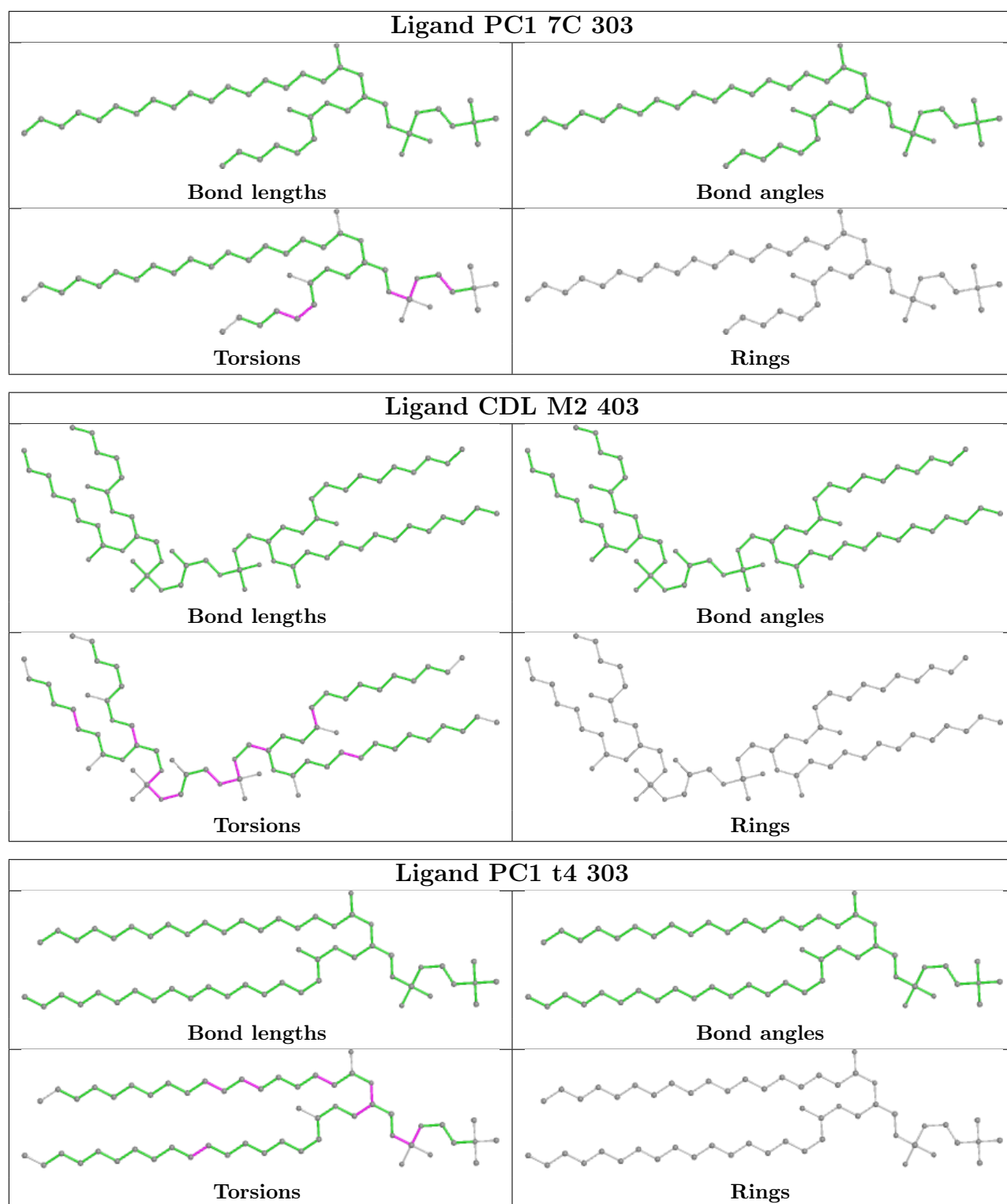


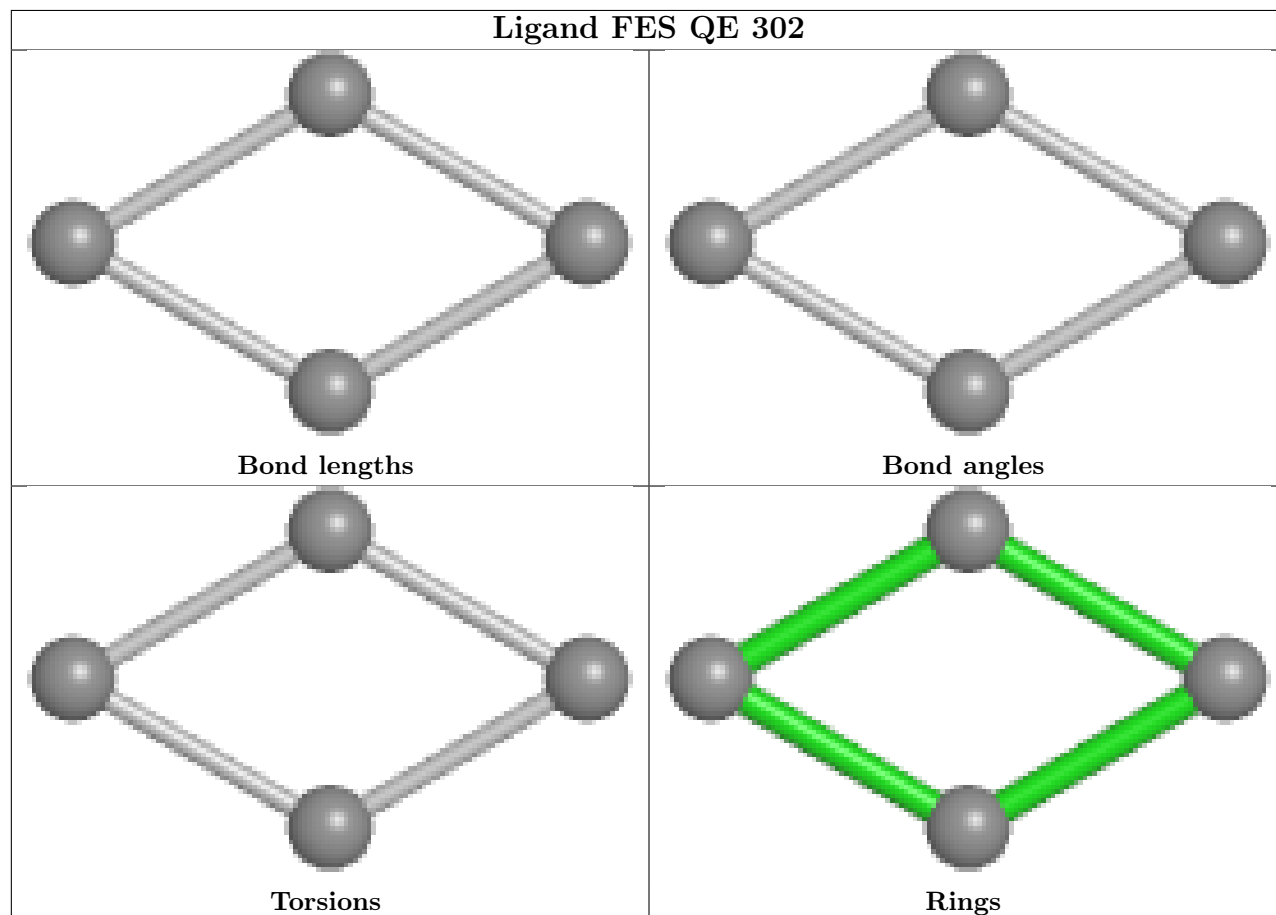
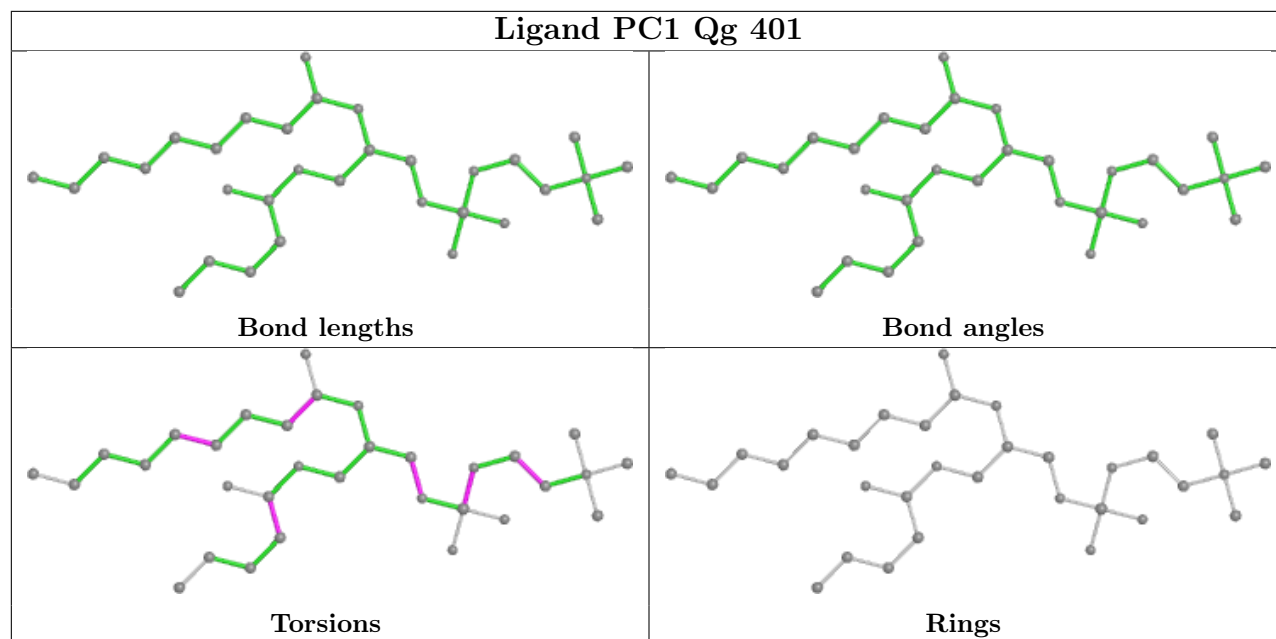


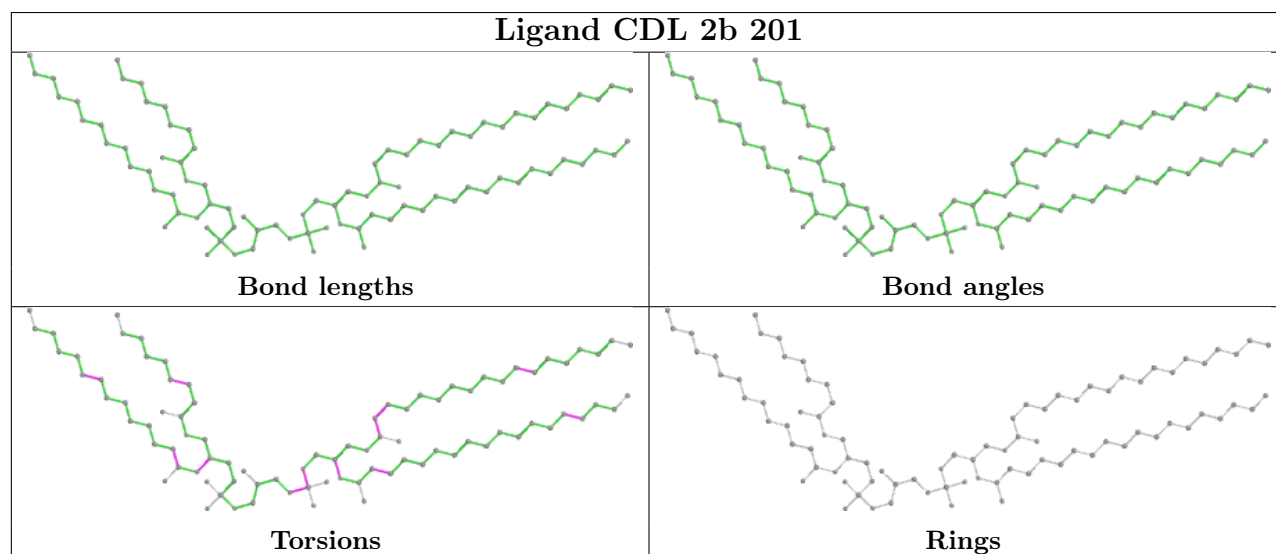
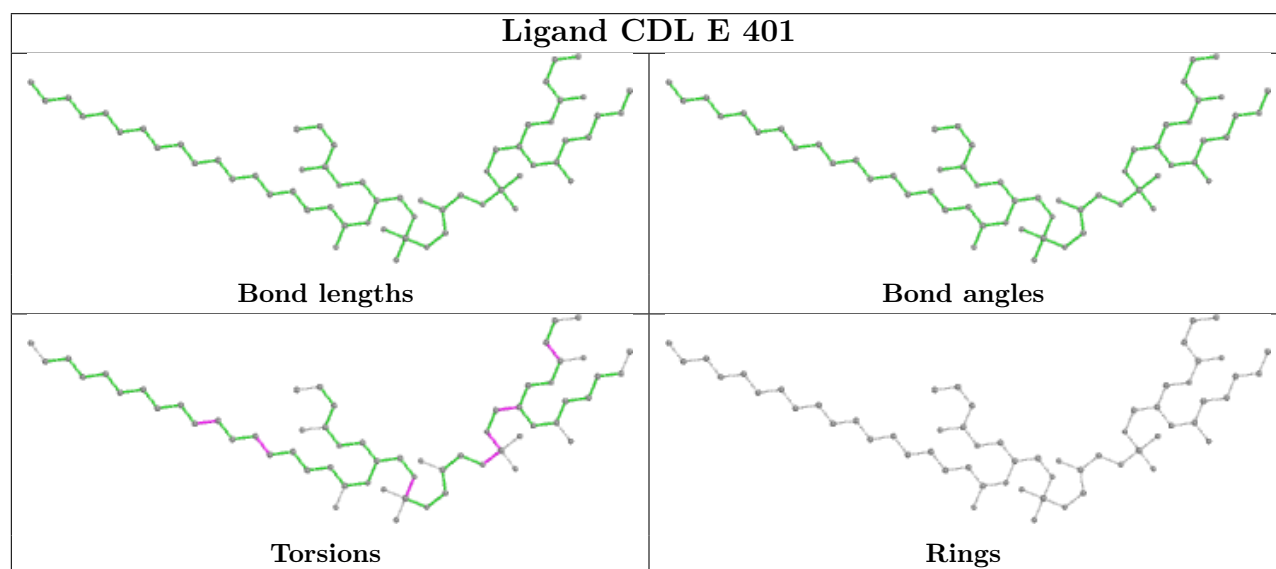
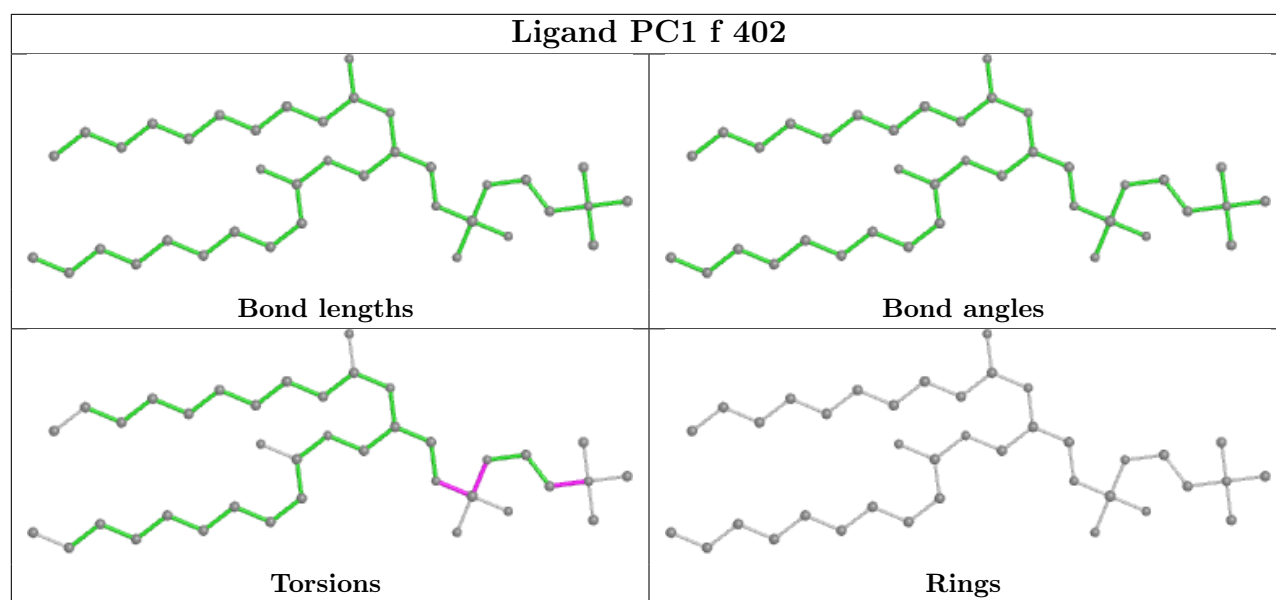


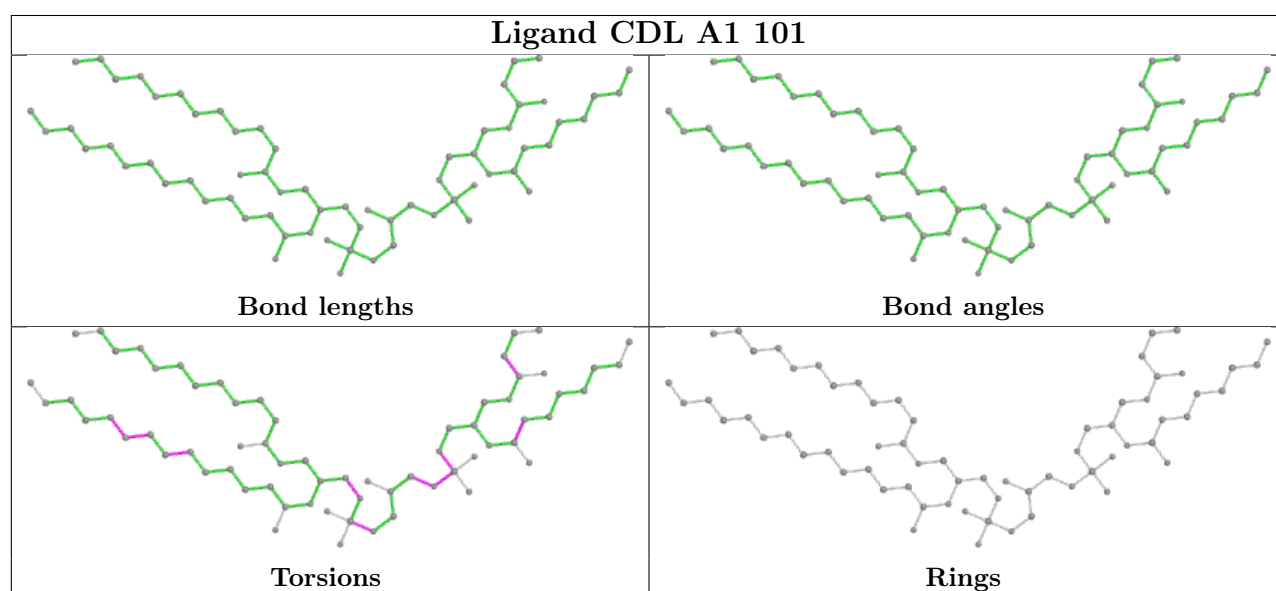
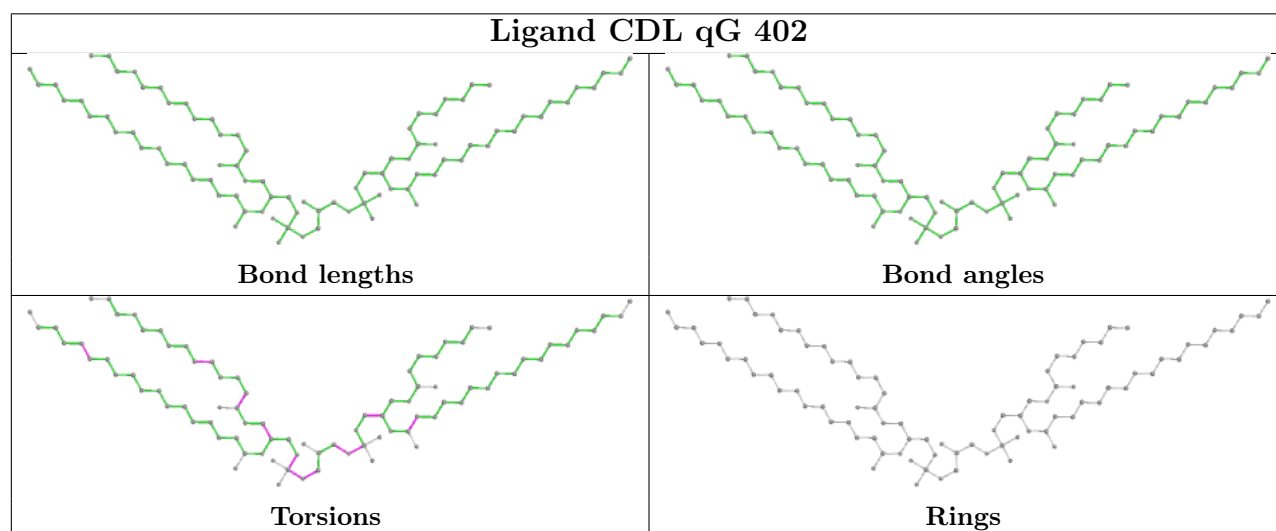
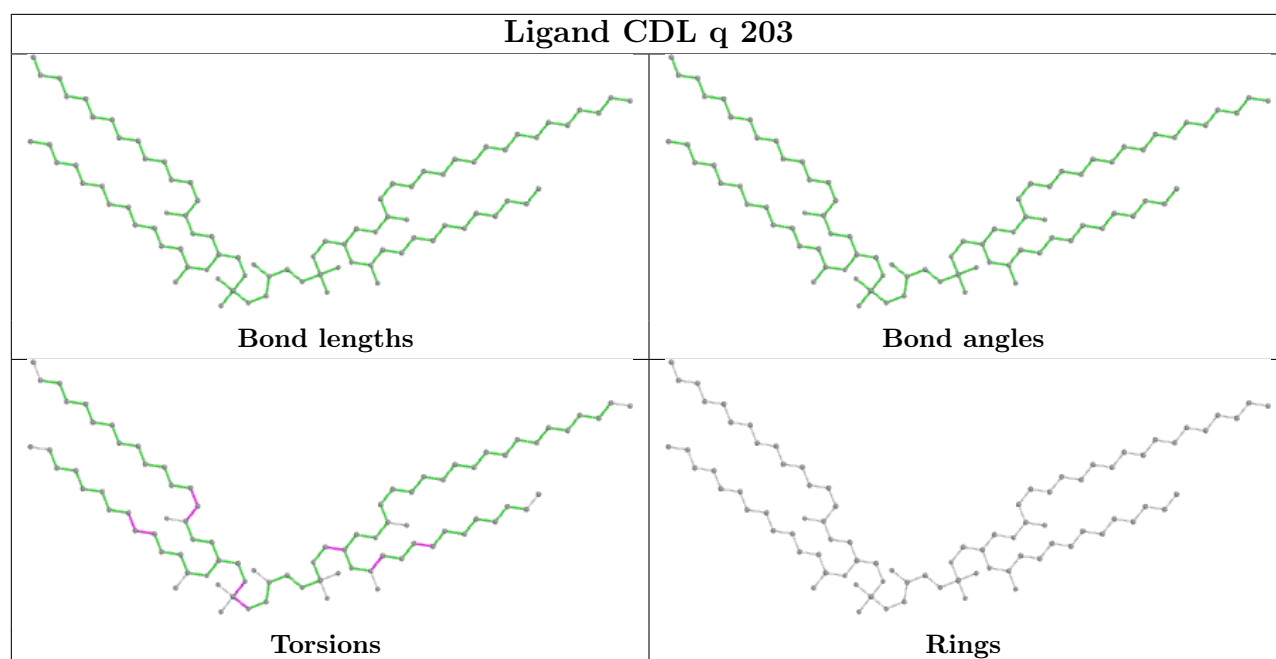


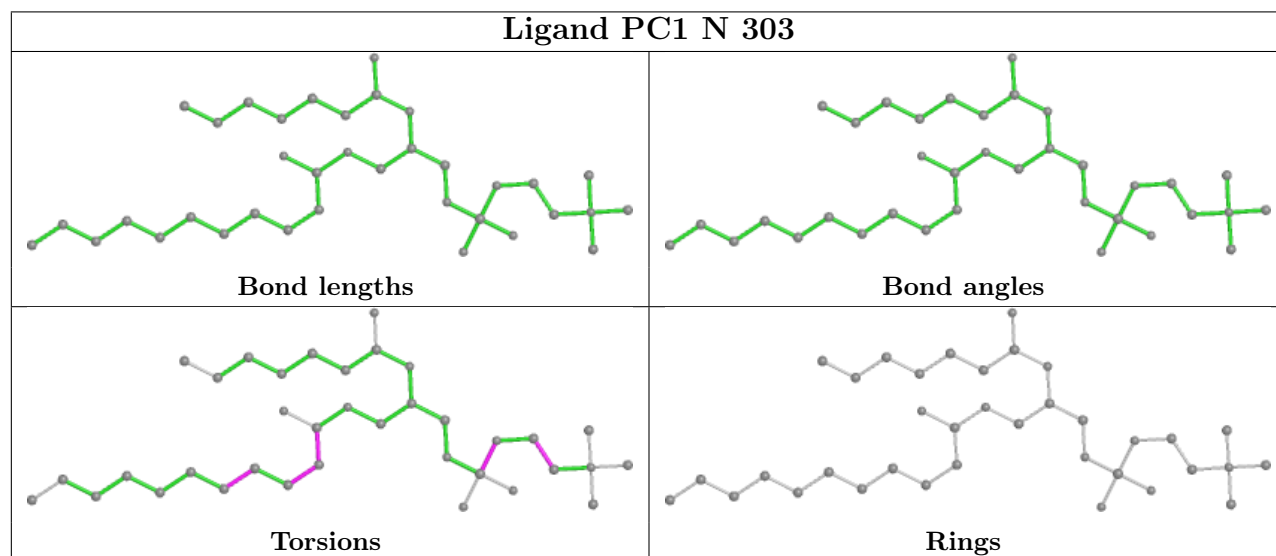
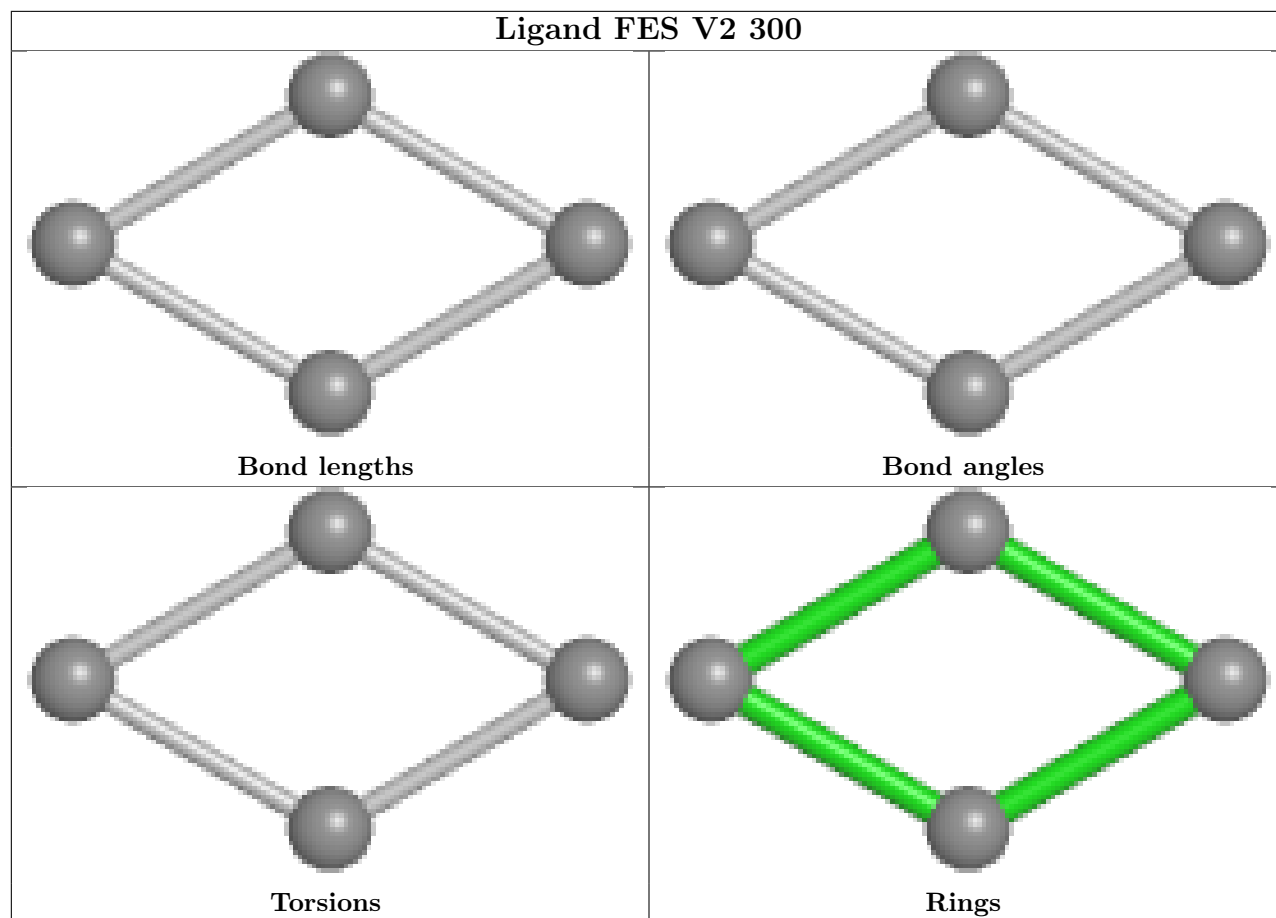


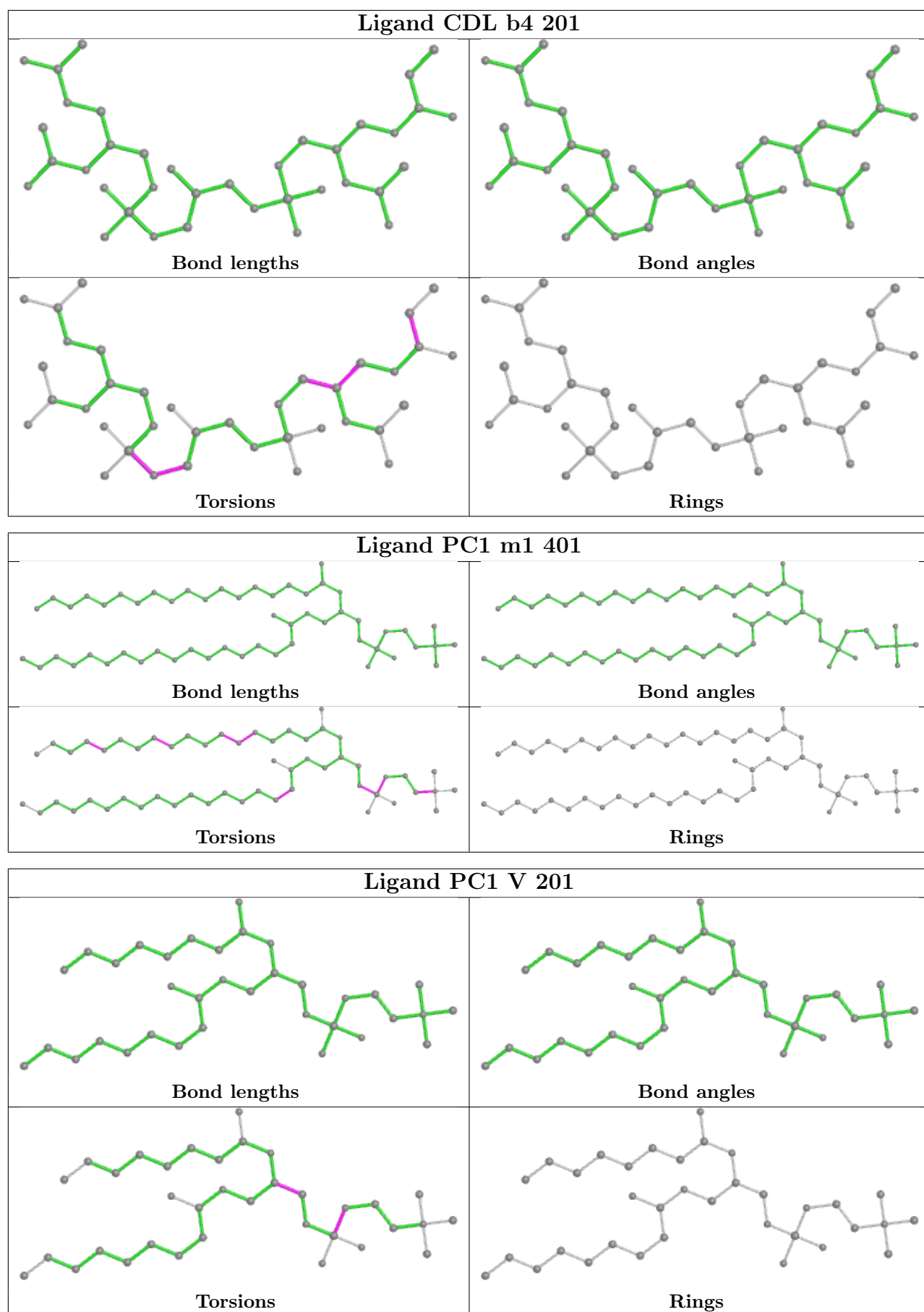


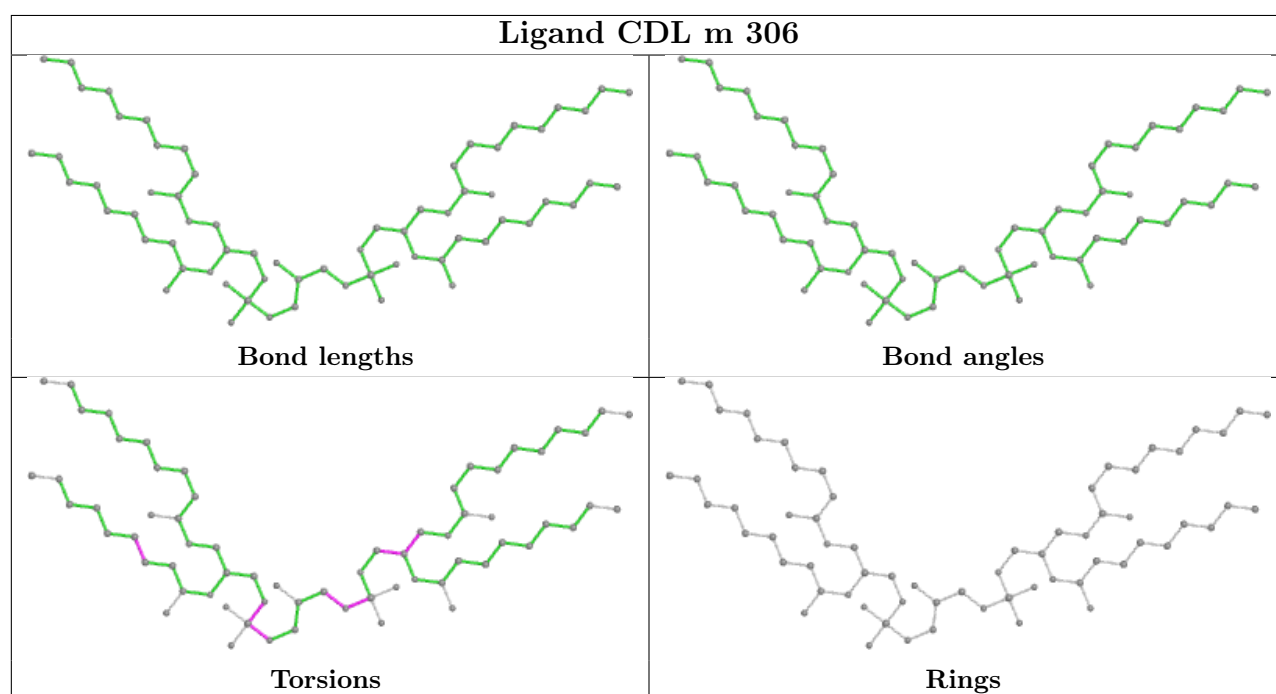
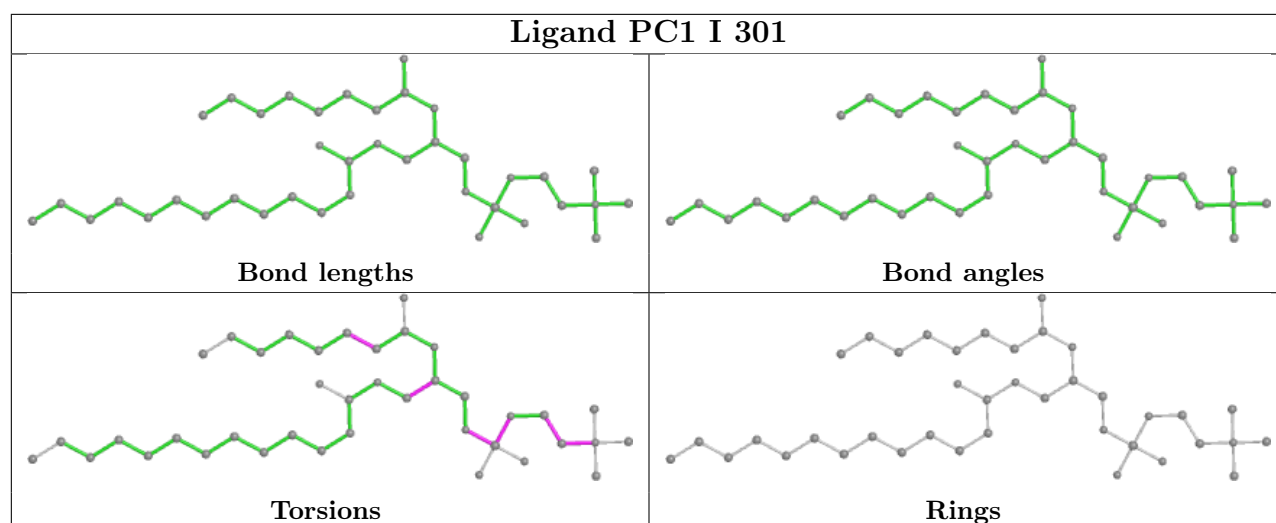


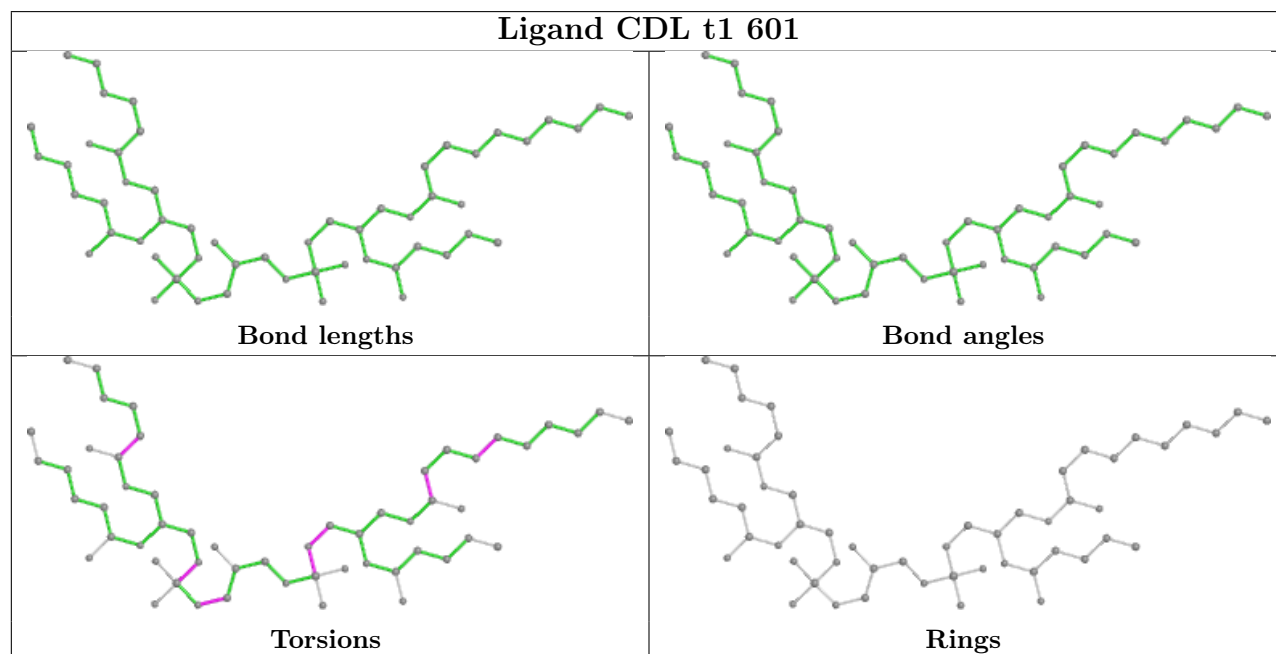
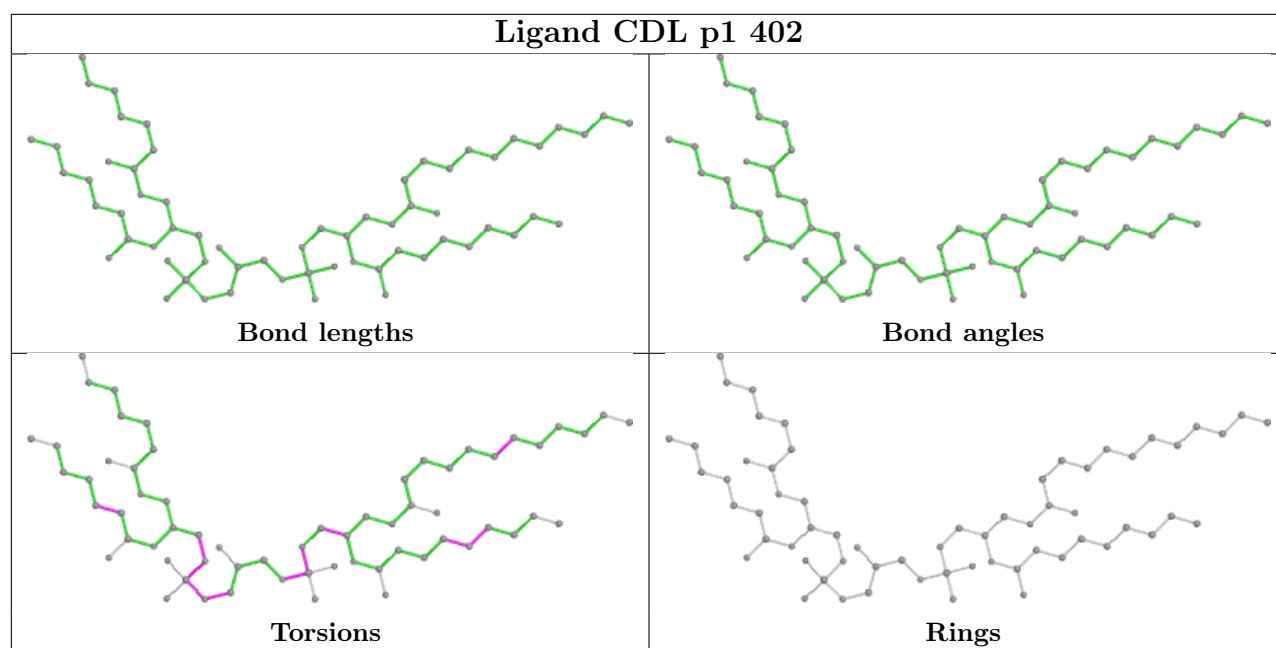


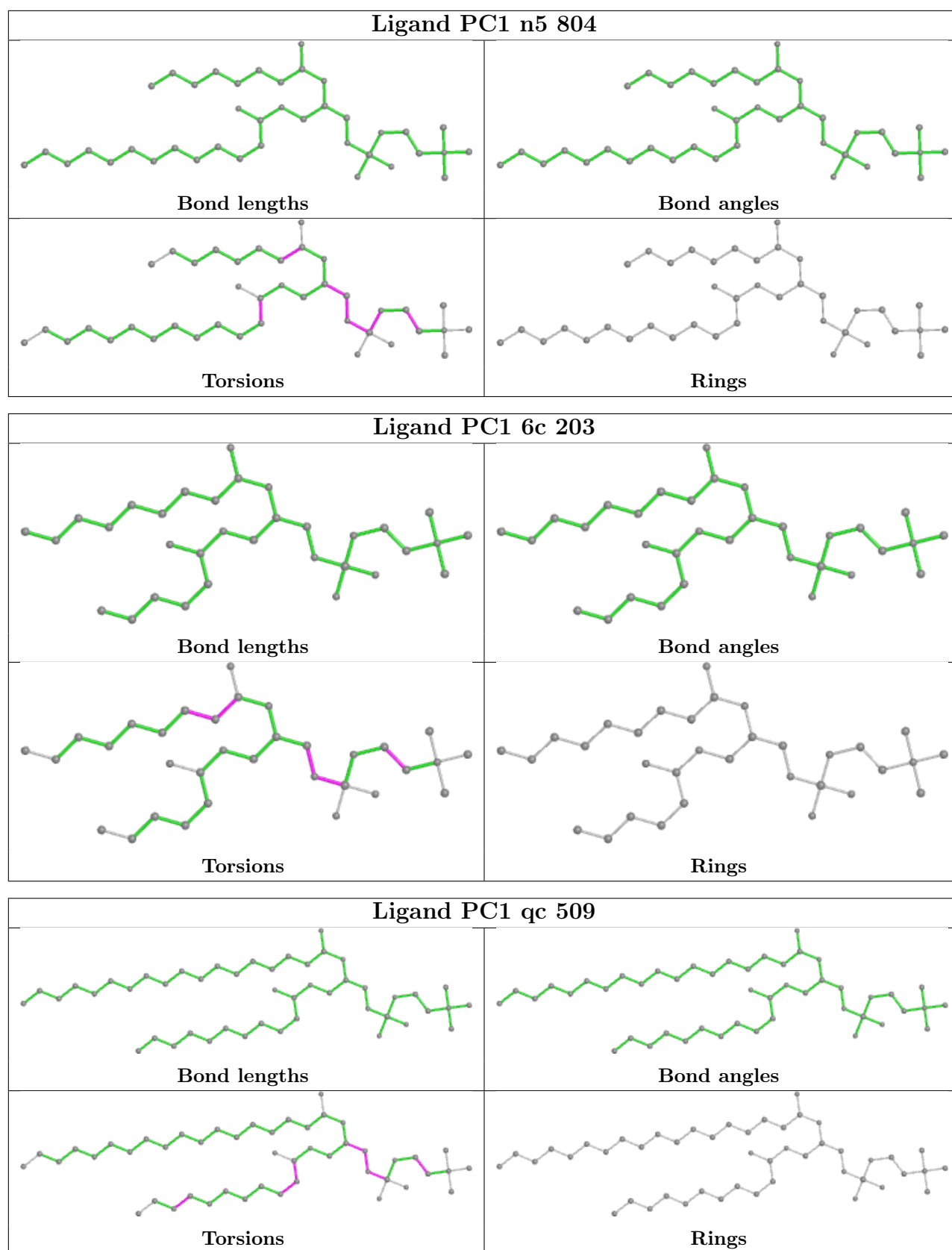


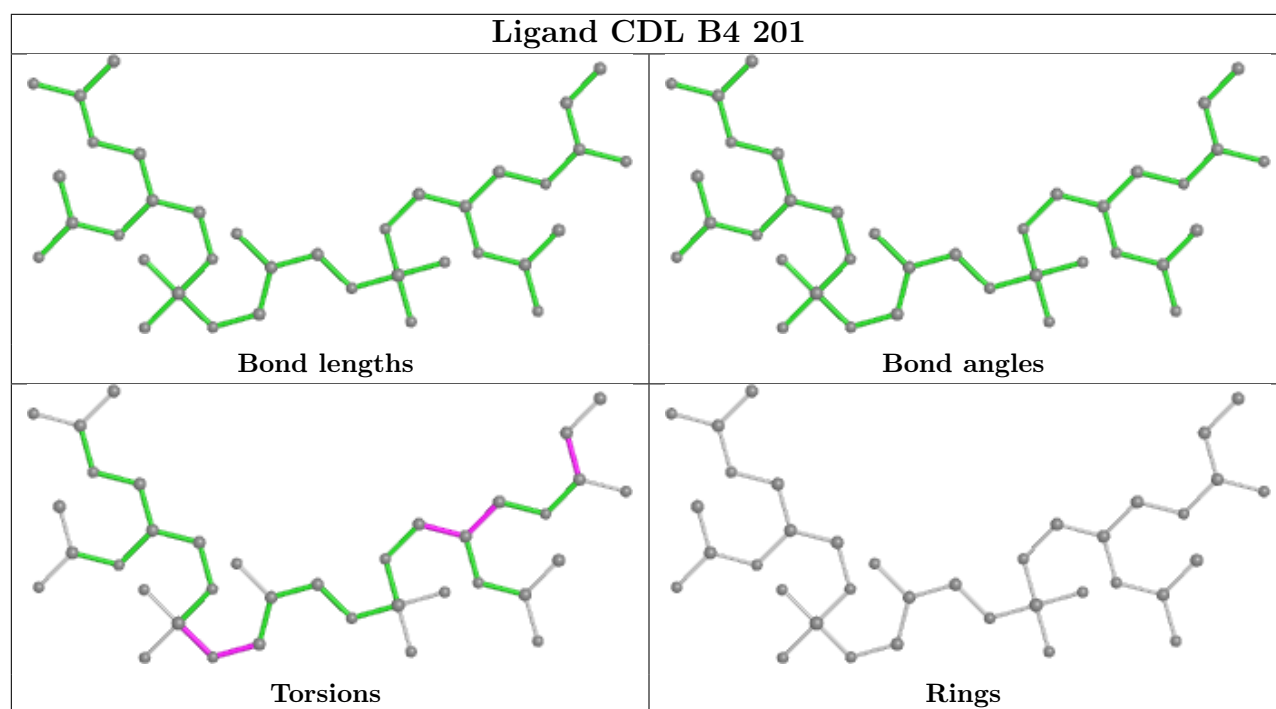
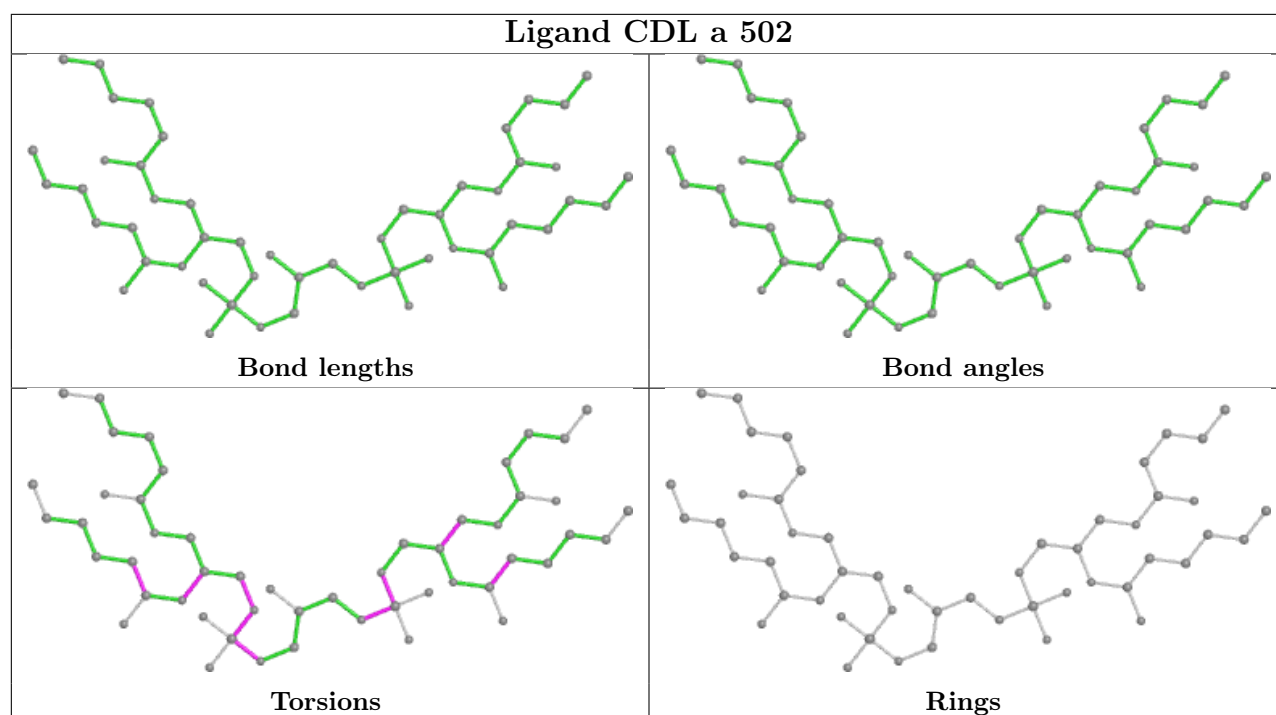


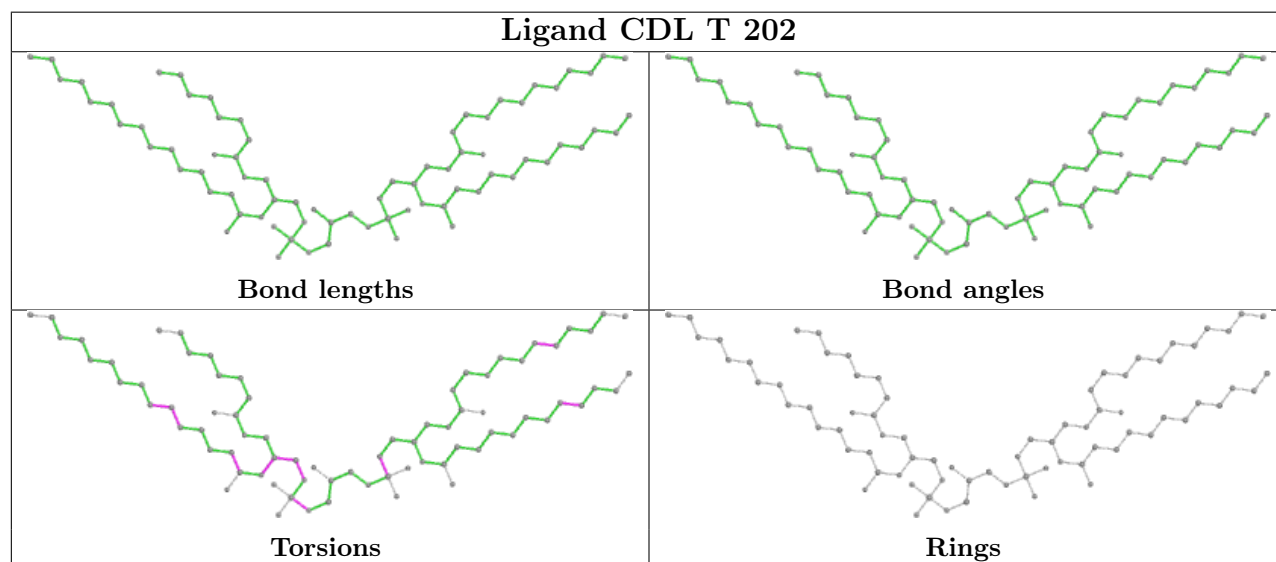
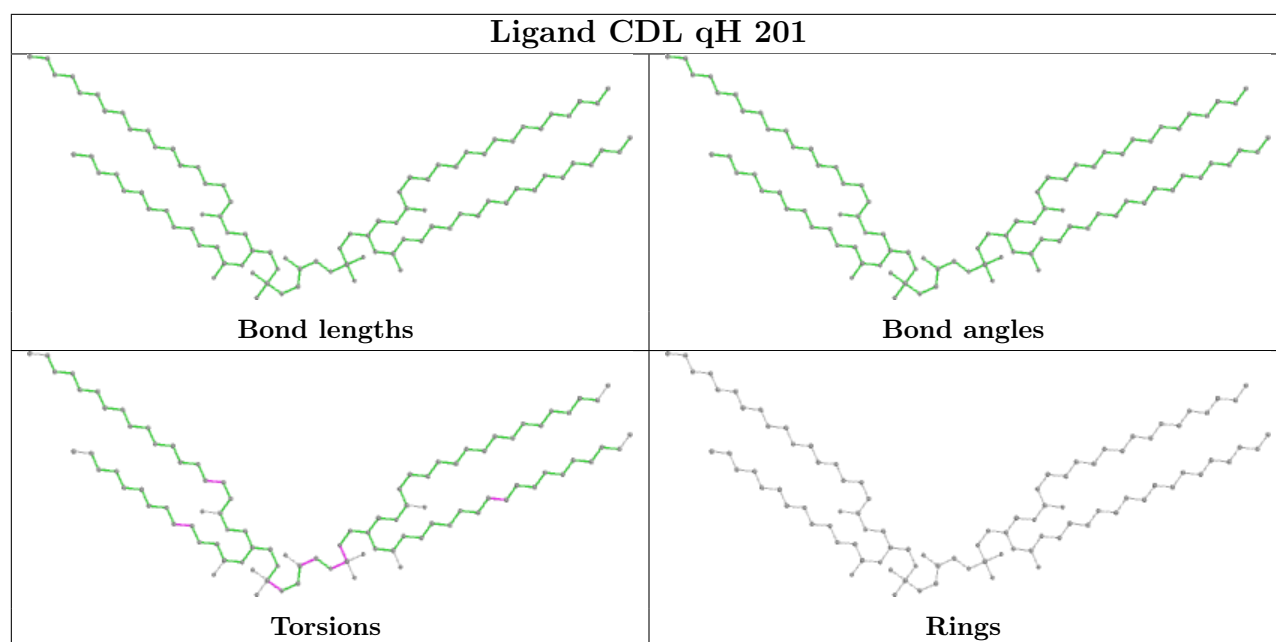


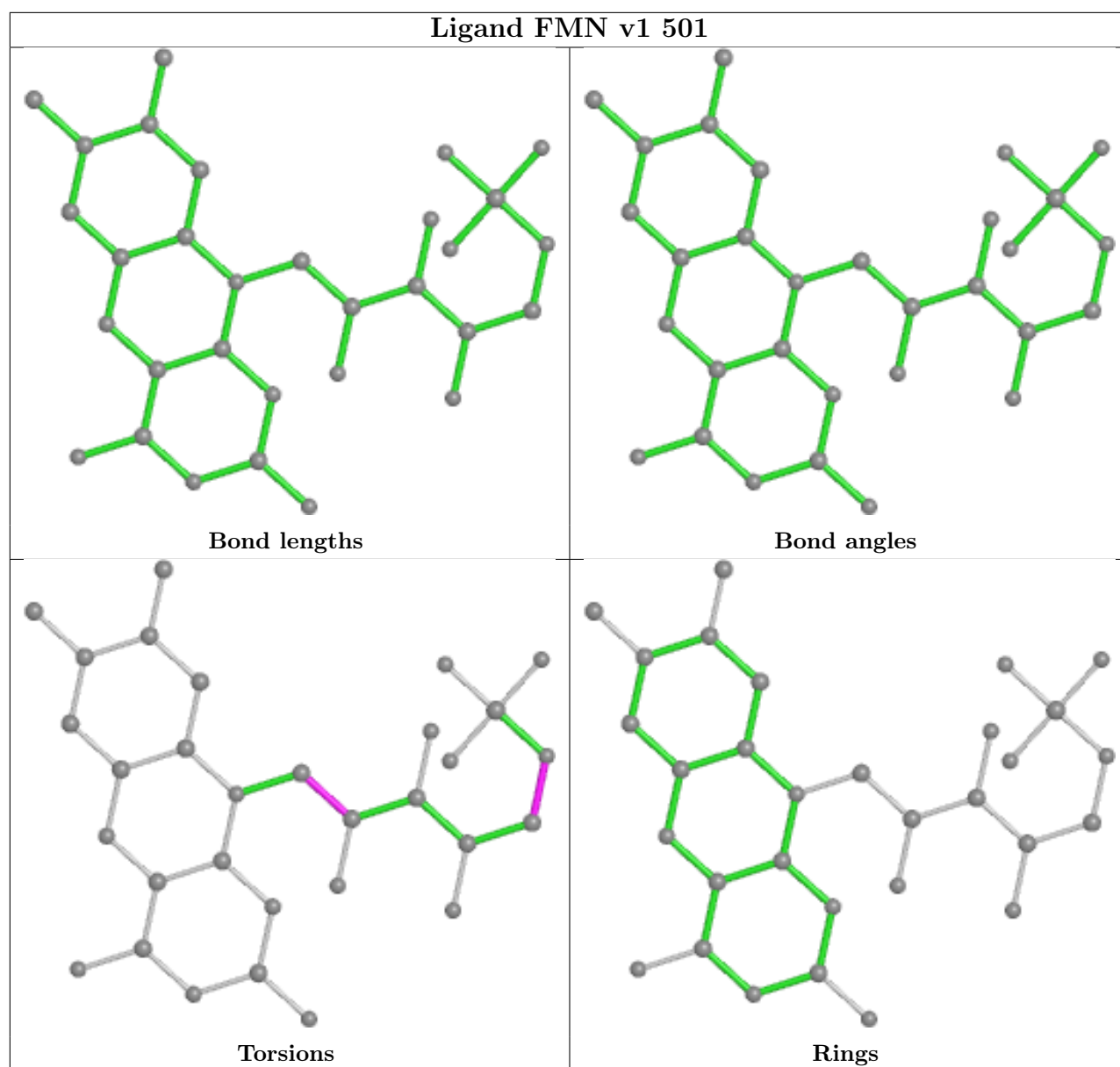


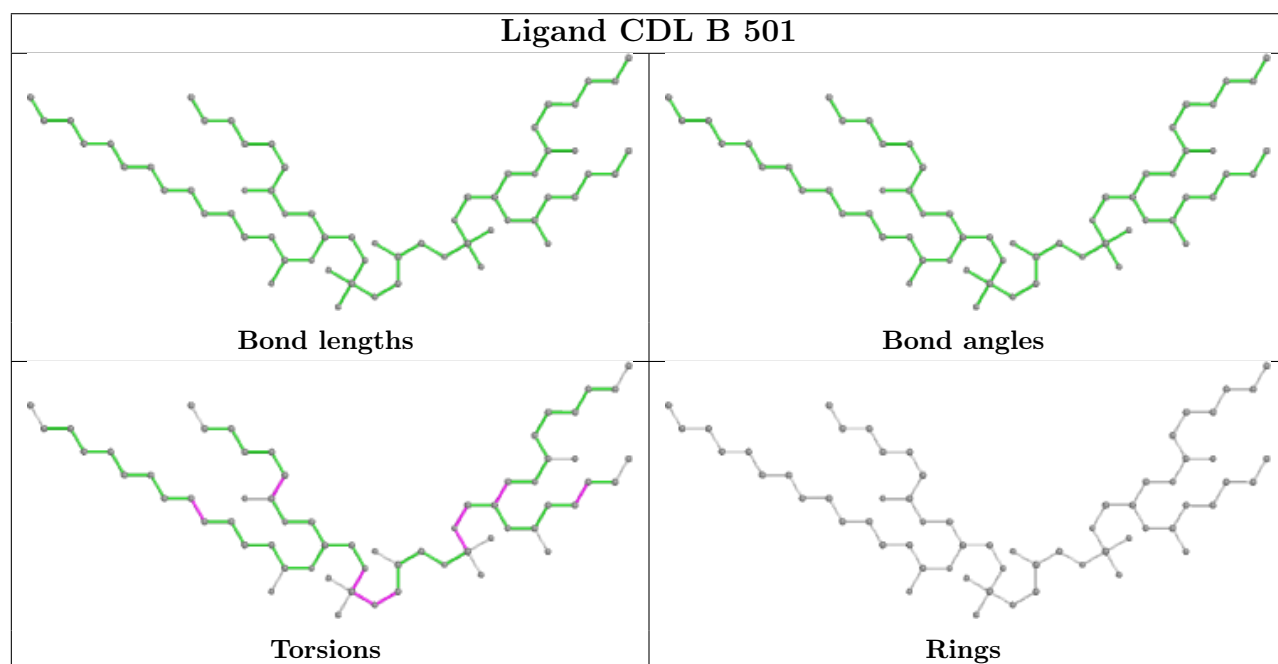
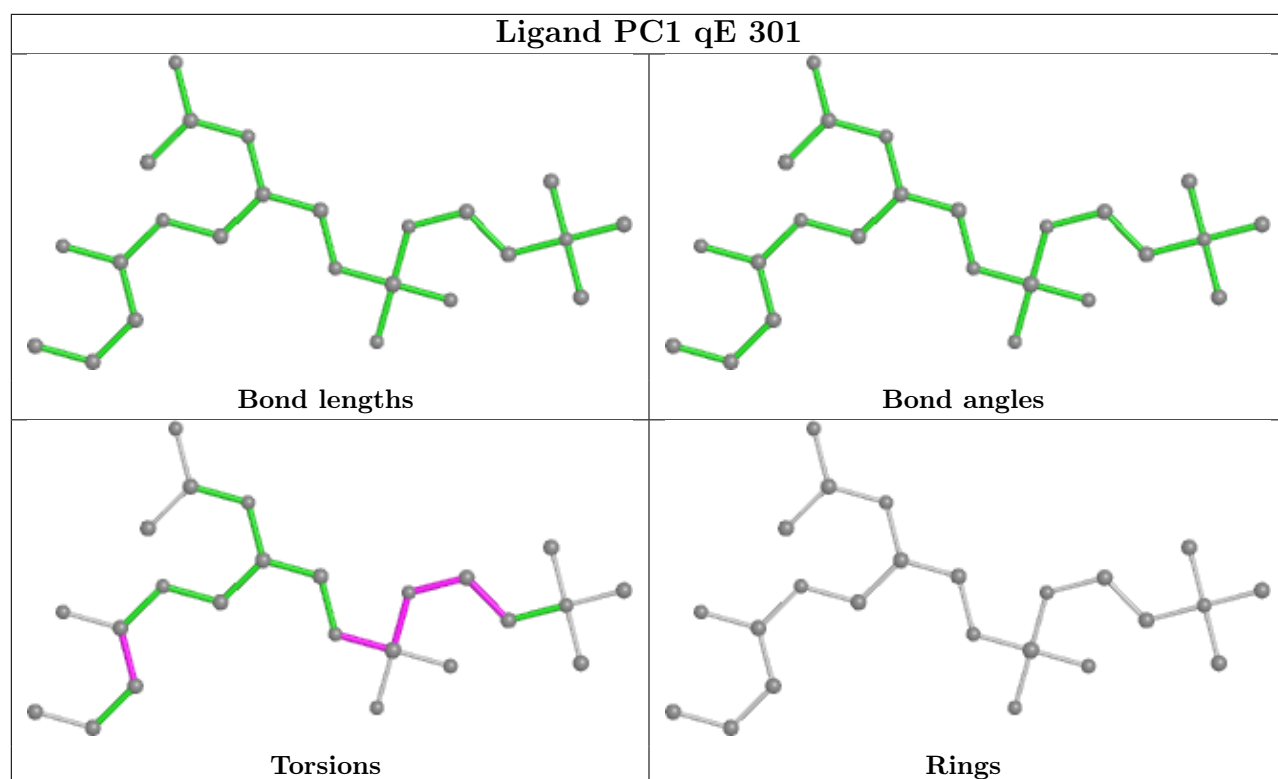




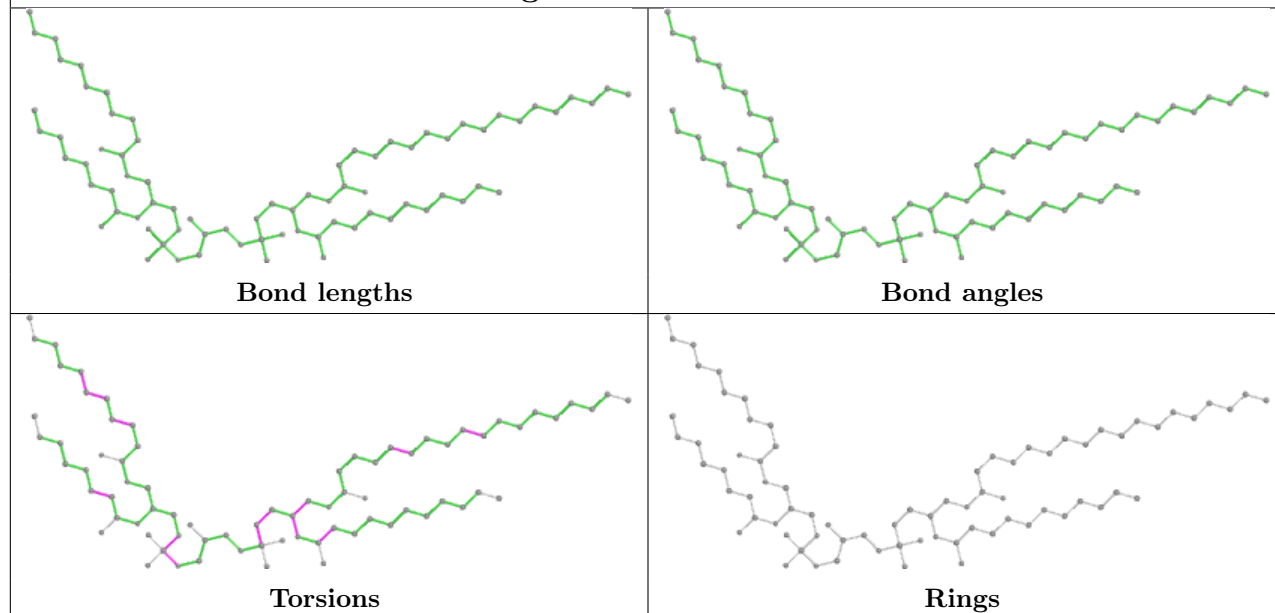




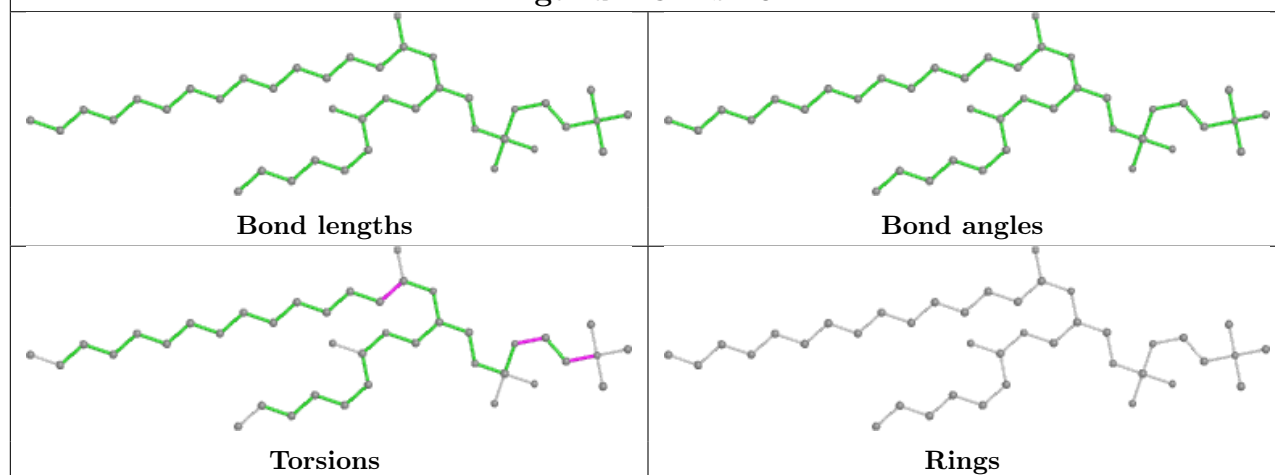




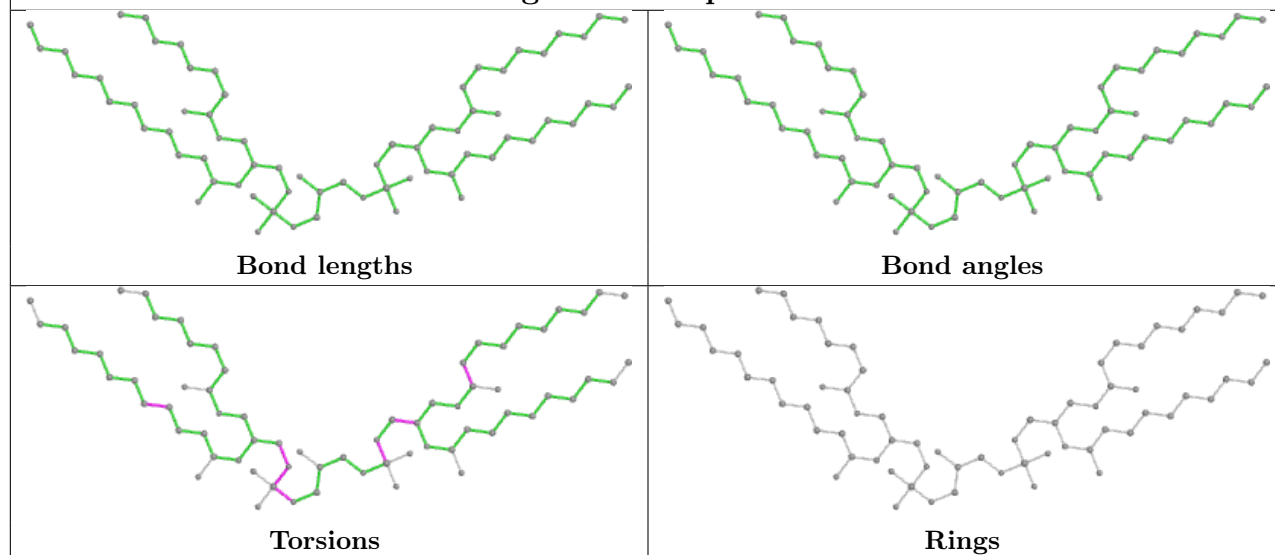
Ligand CDL A9 402

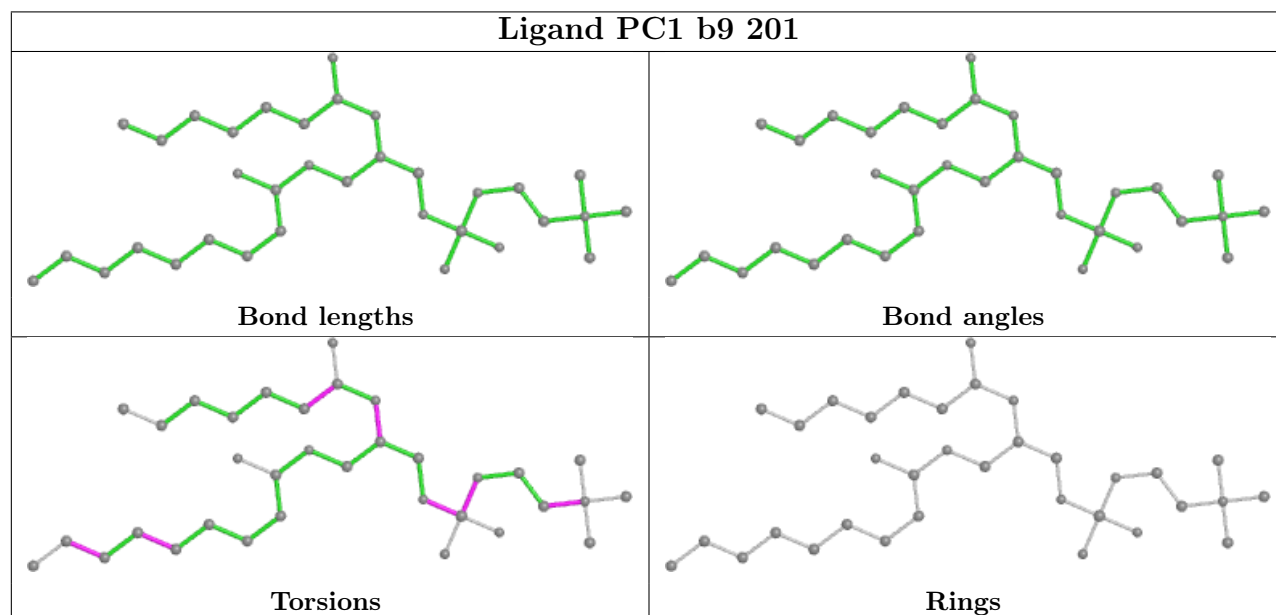
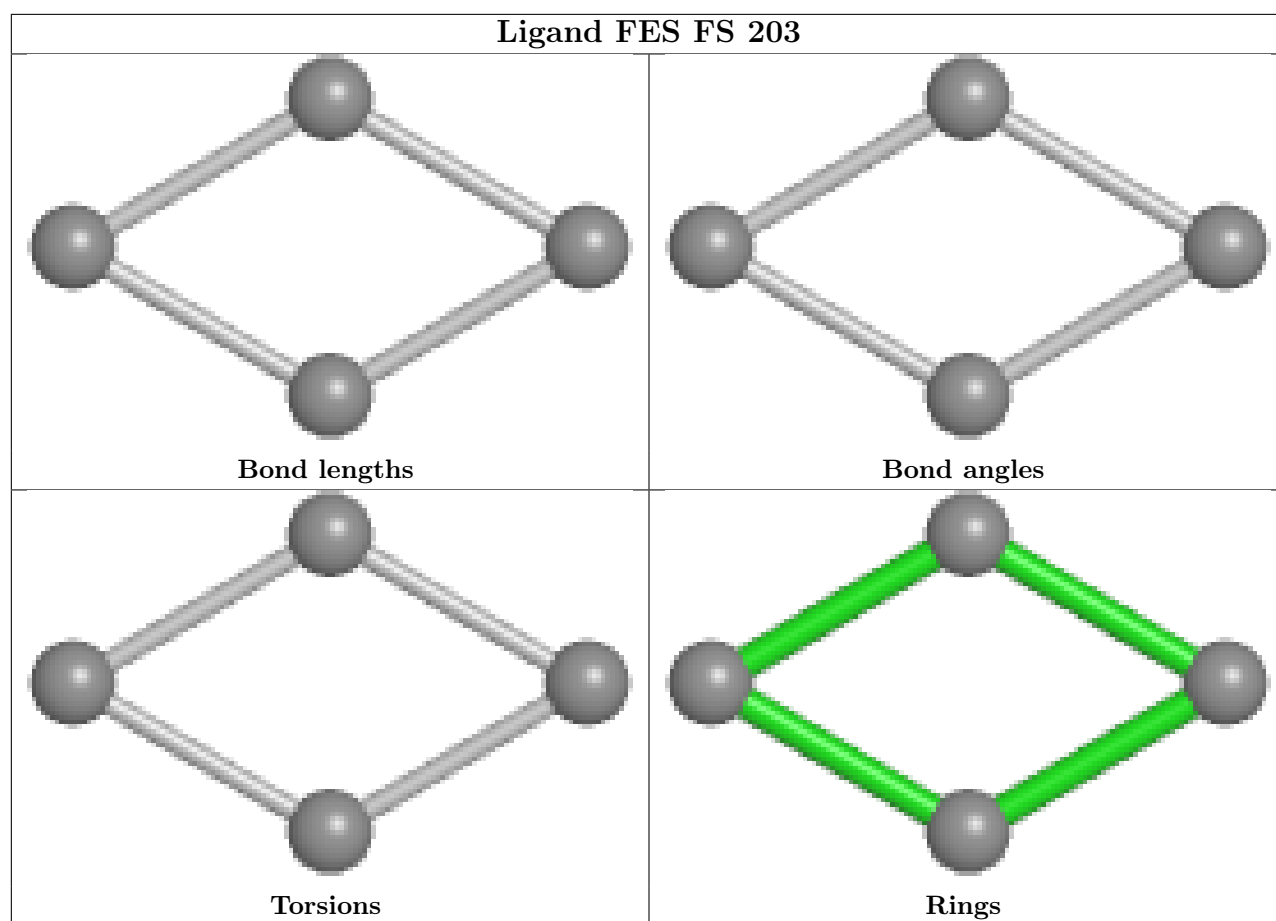


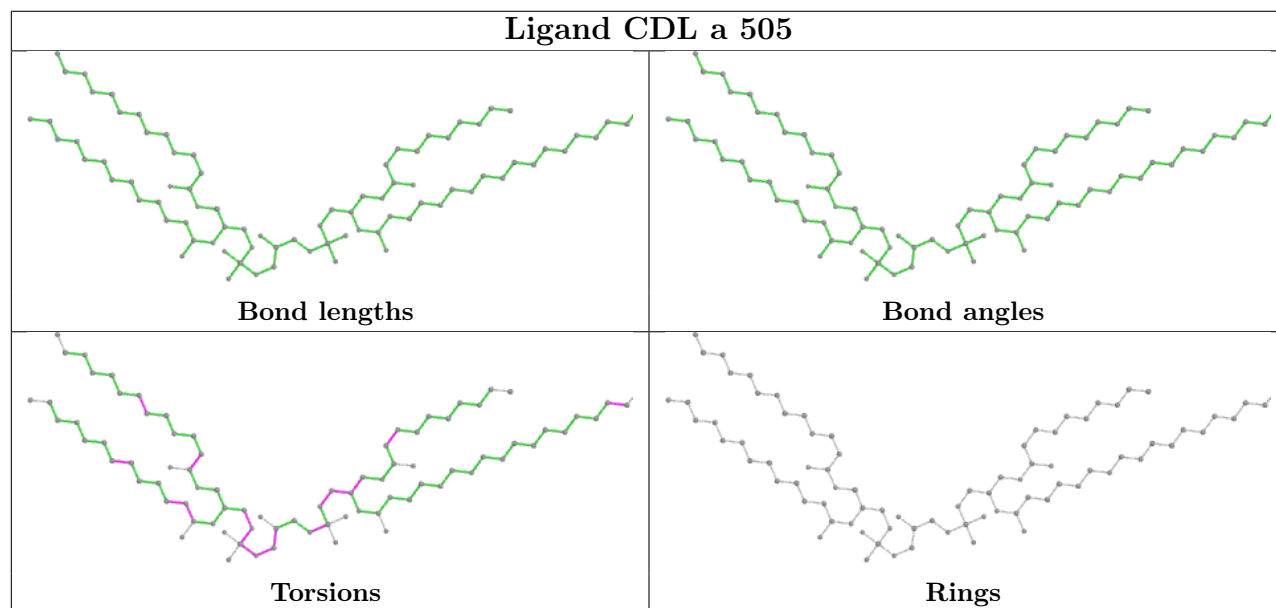
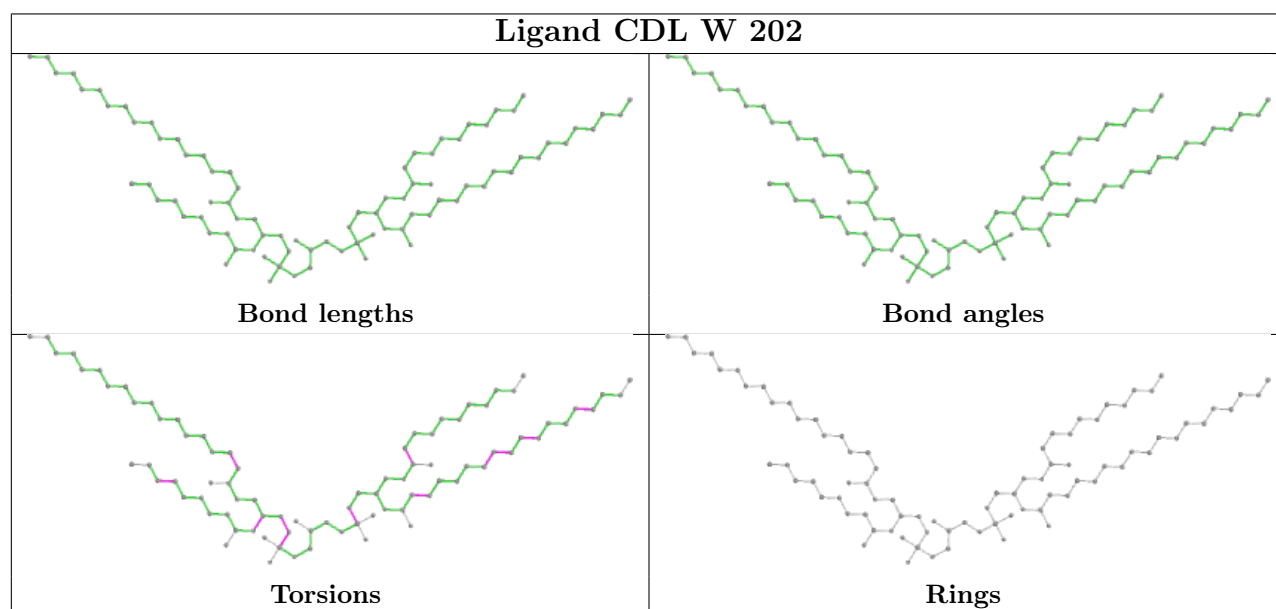
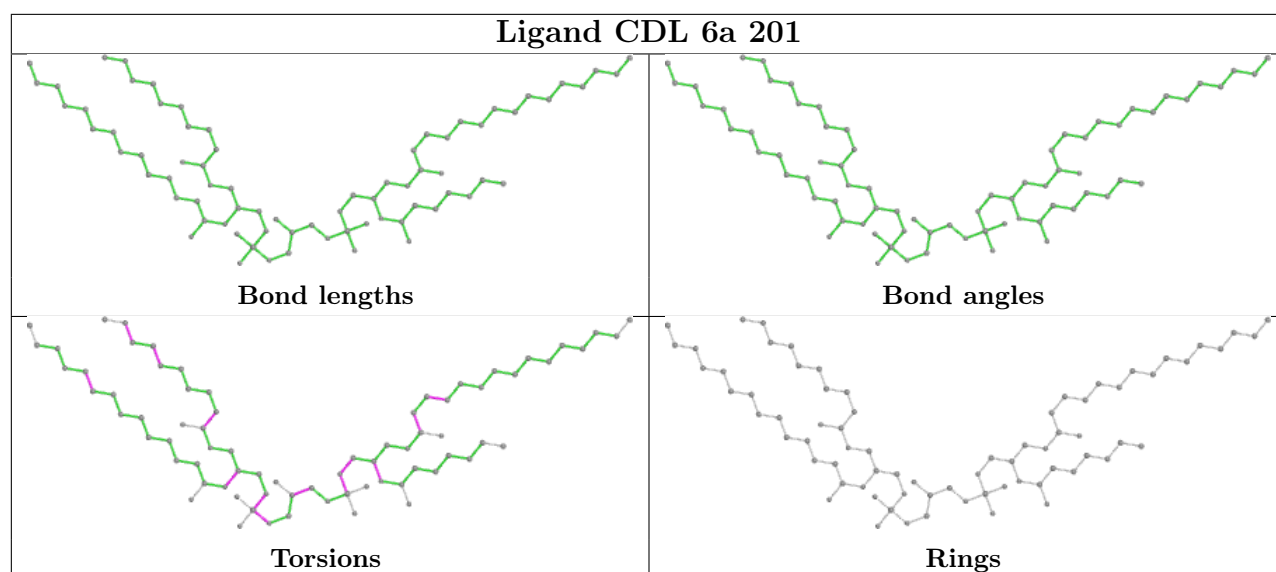
Ligand PC1 fs 204

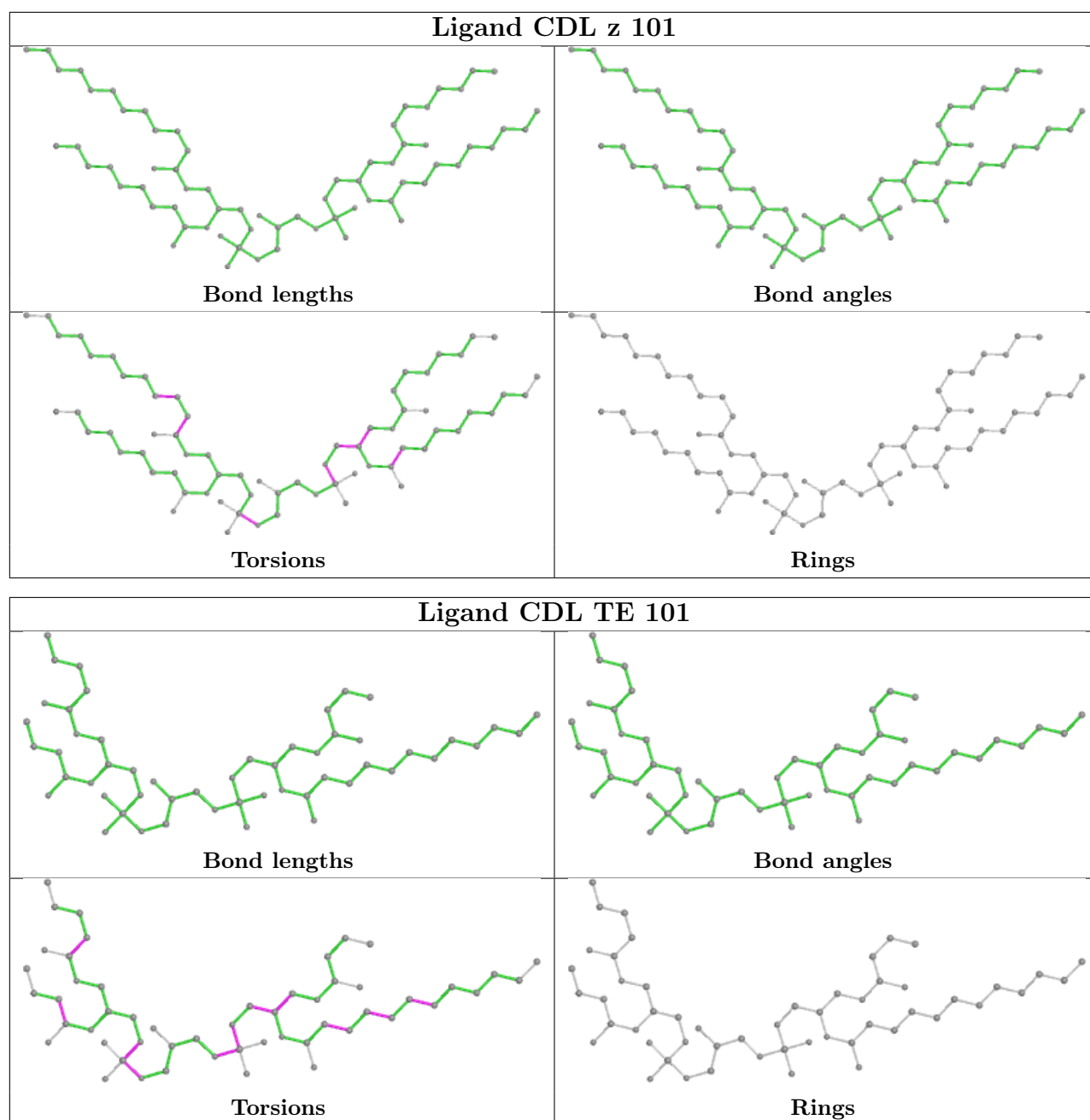


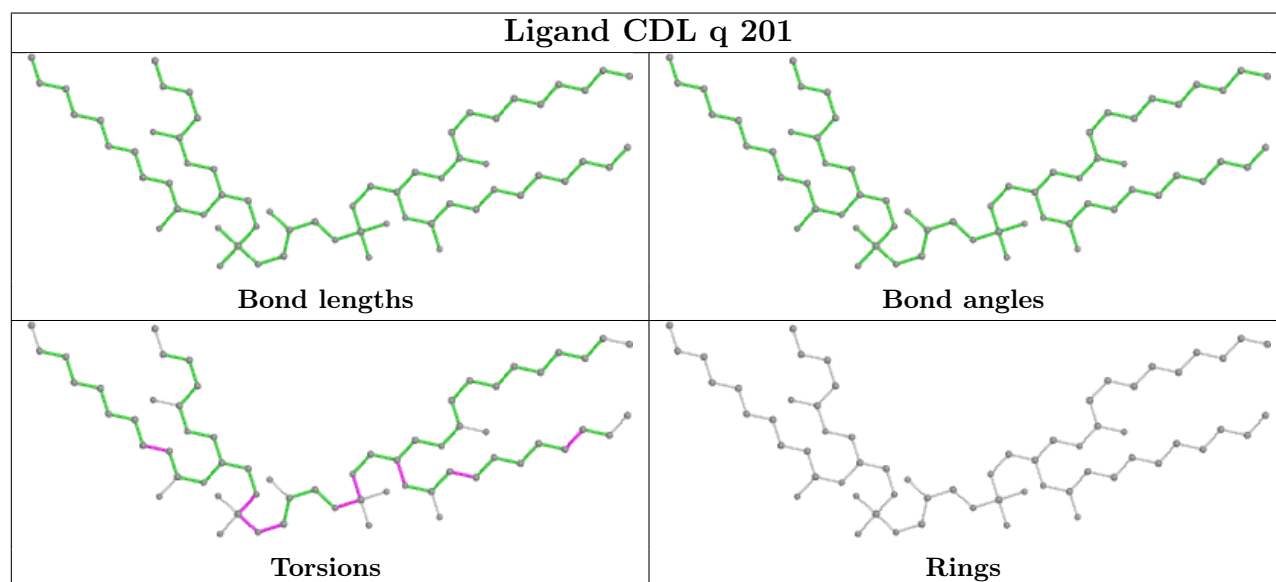
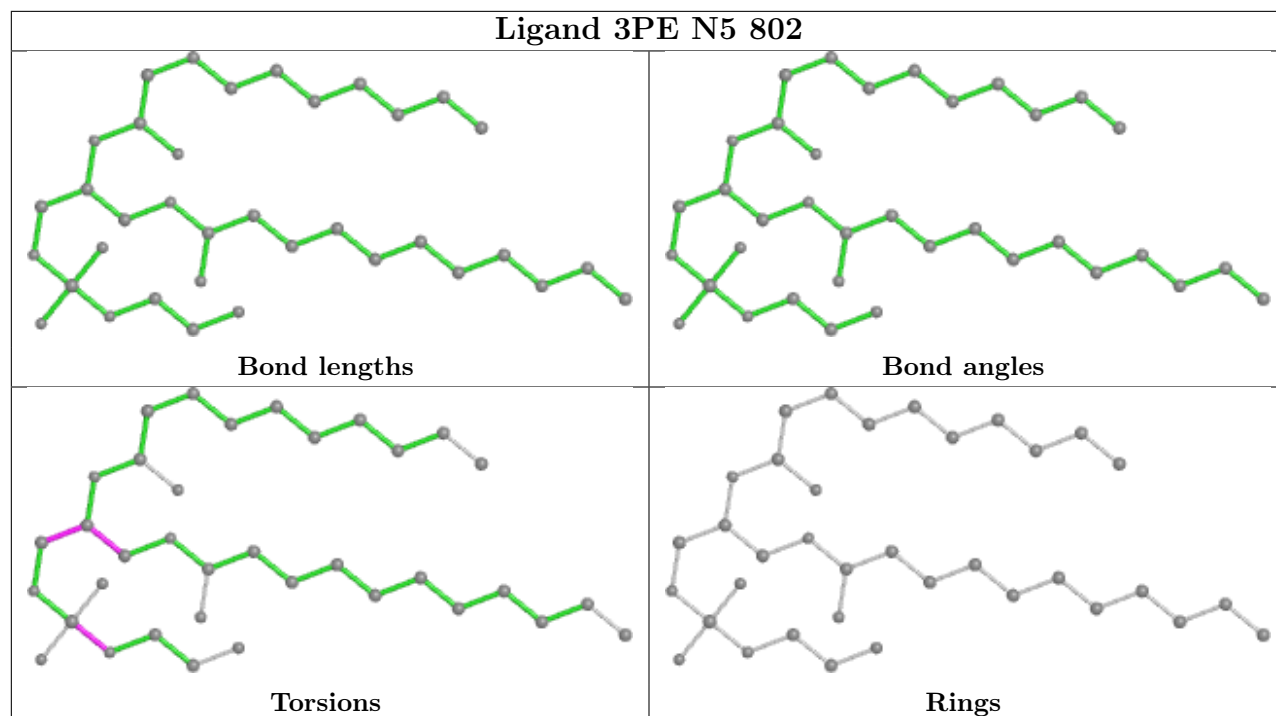
Ligand CDL qB 601

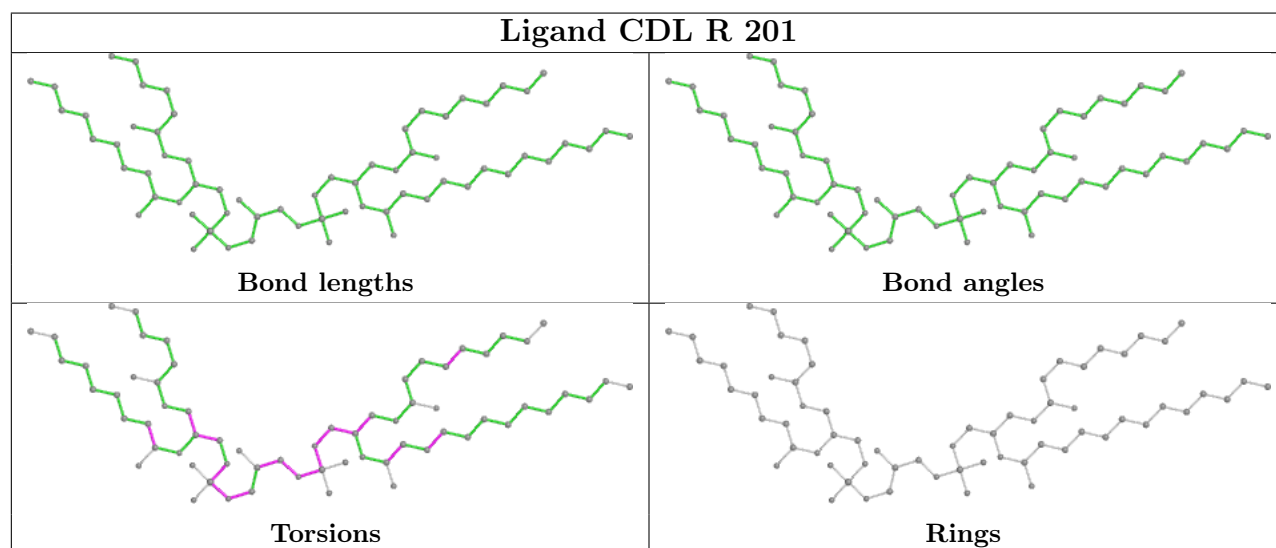
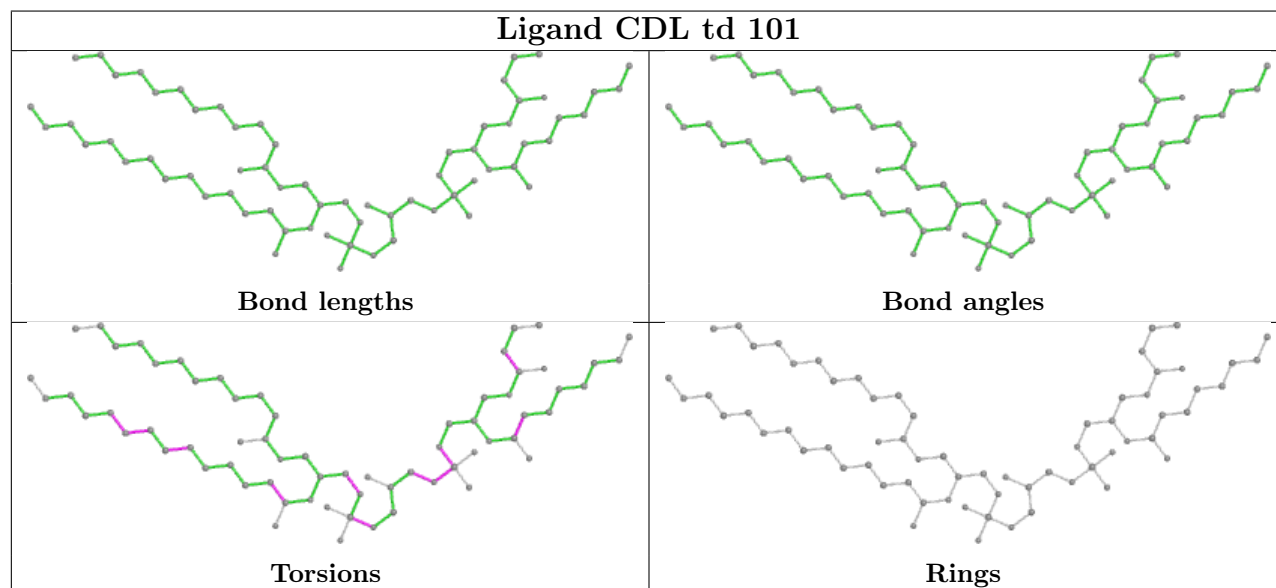
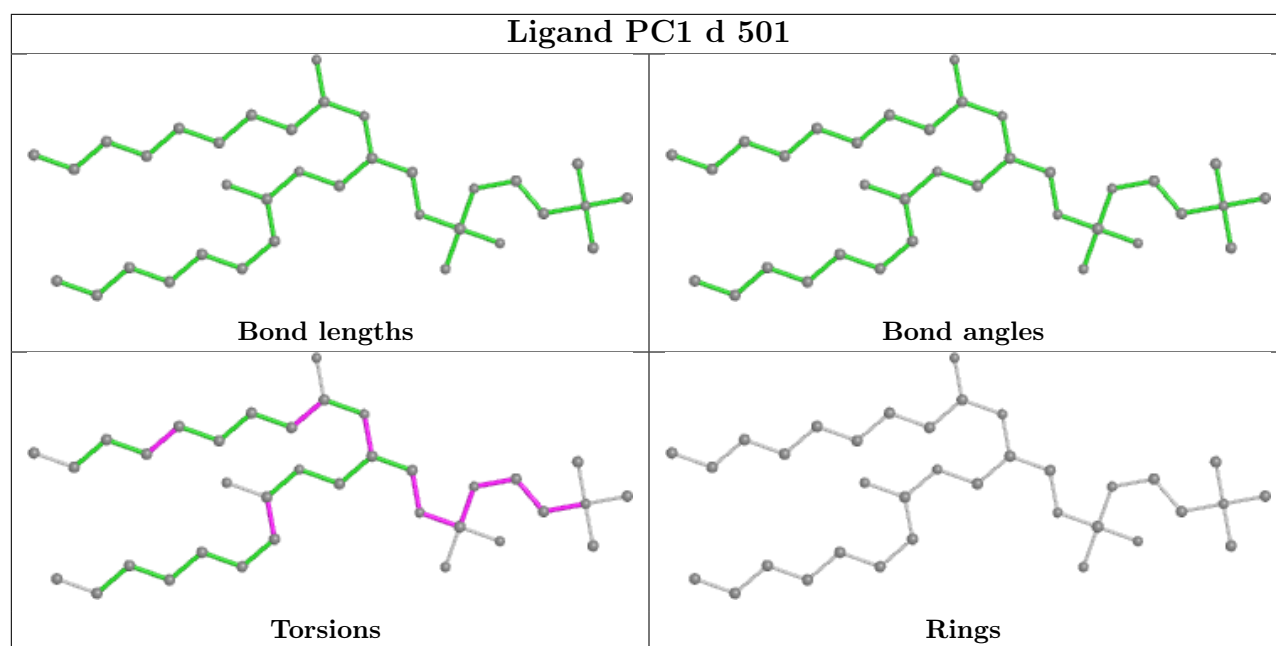


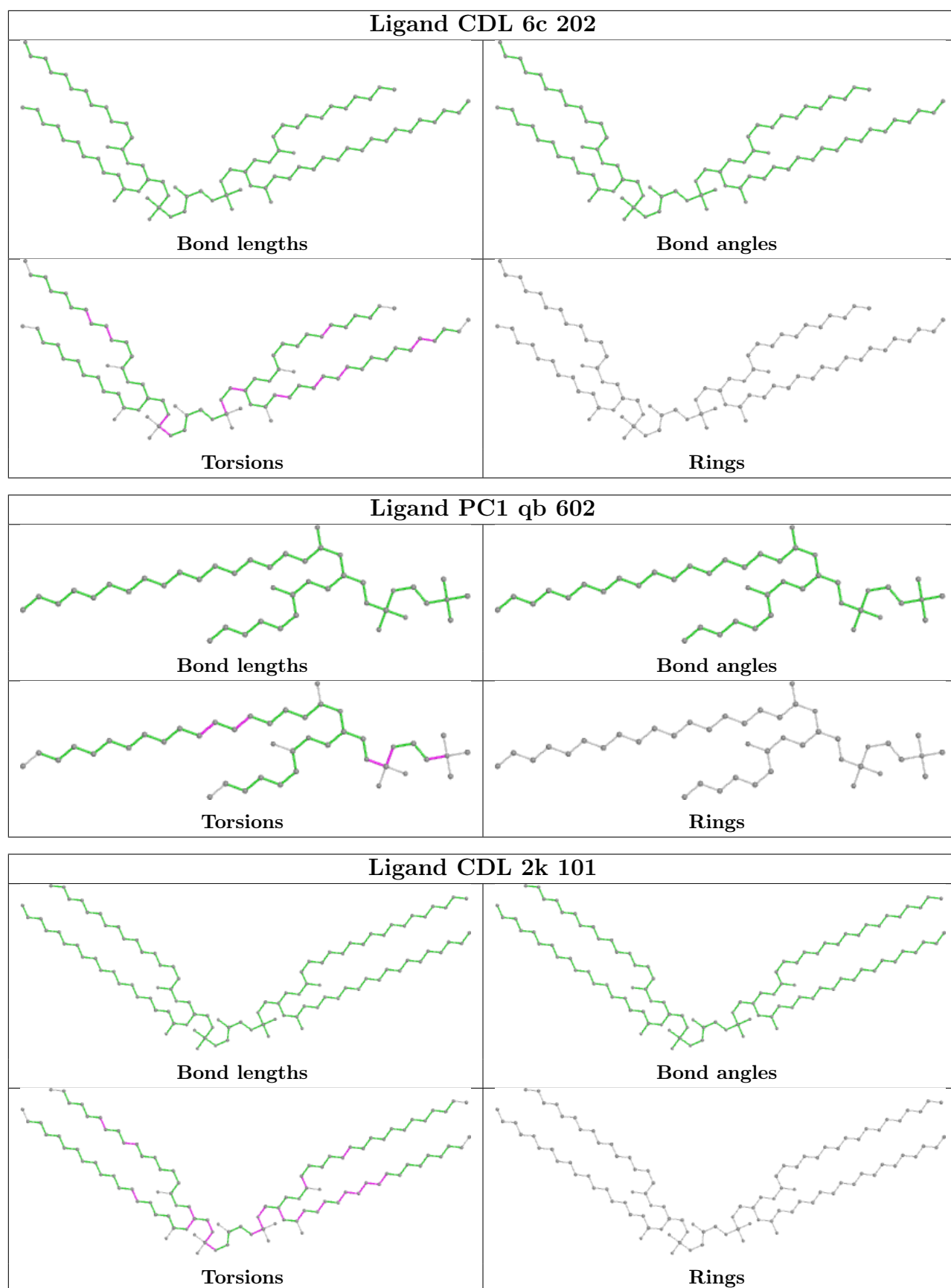


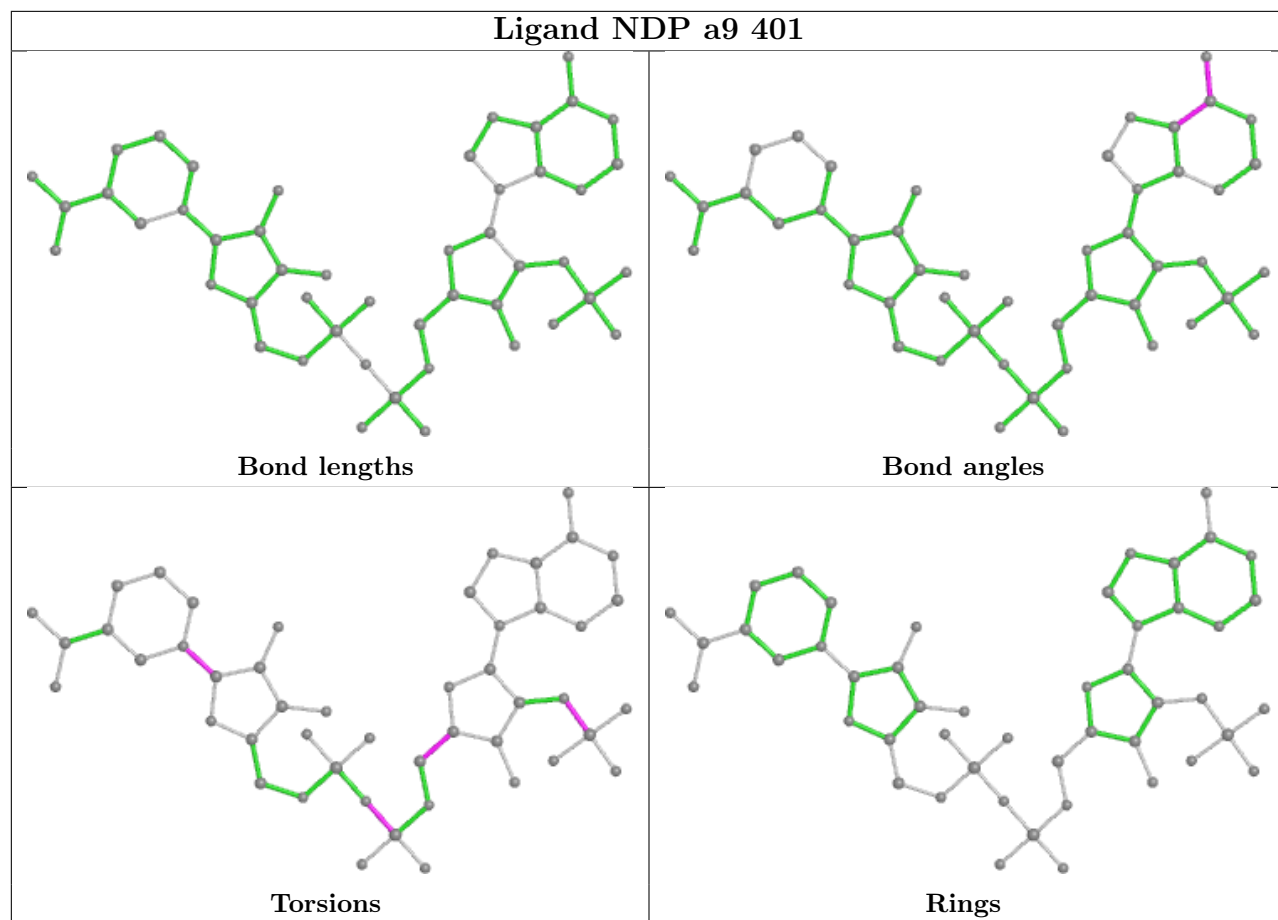




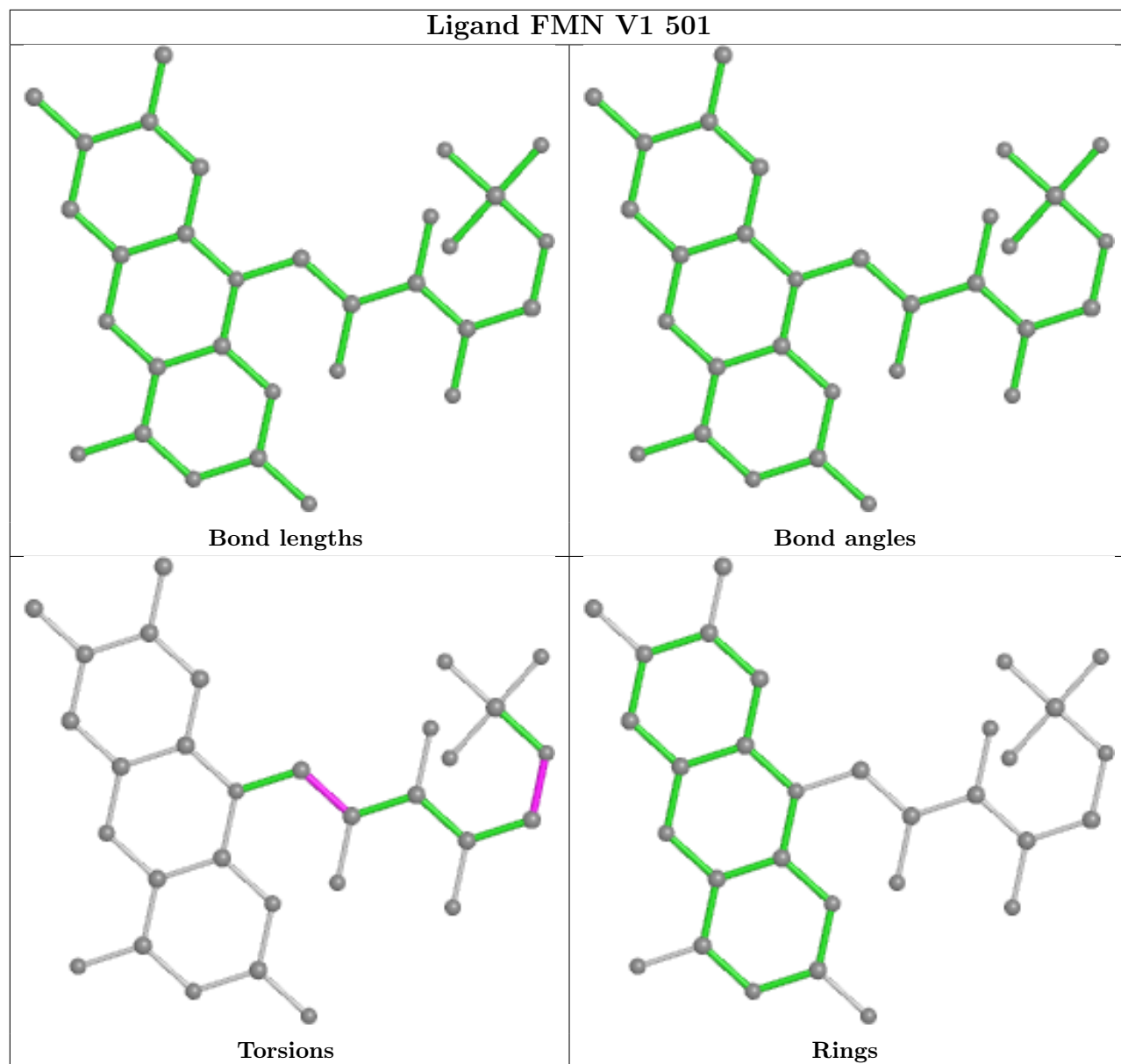


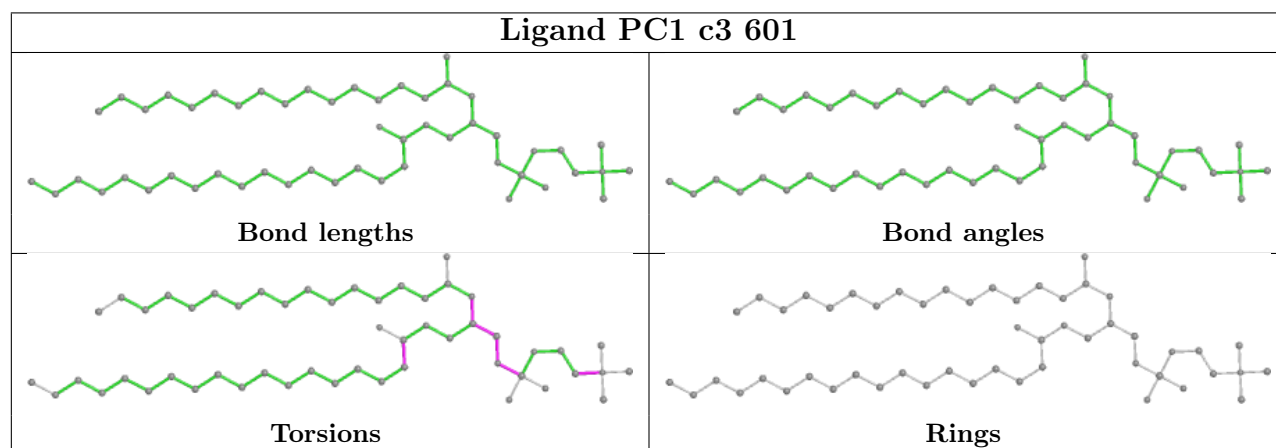
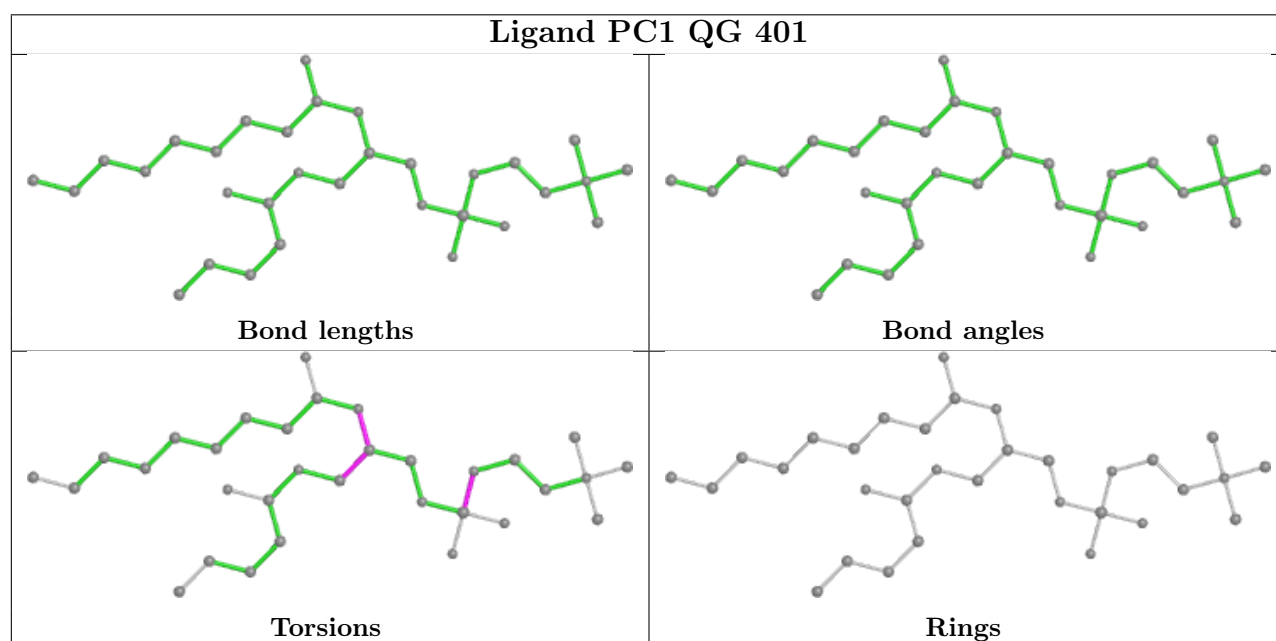
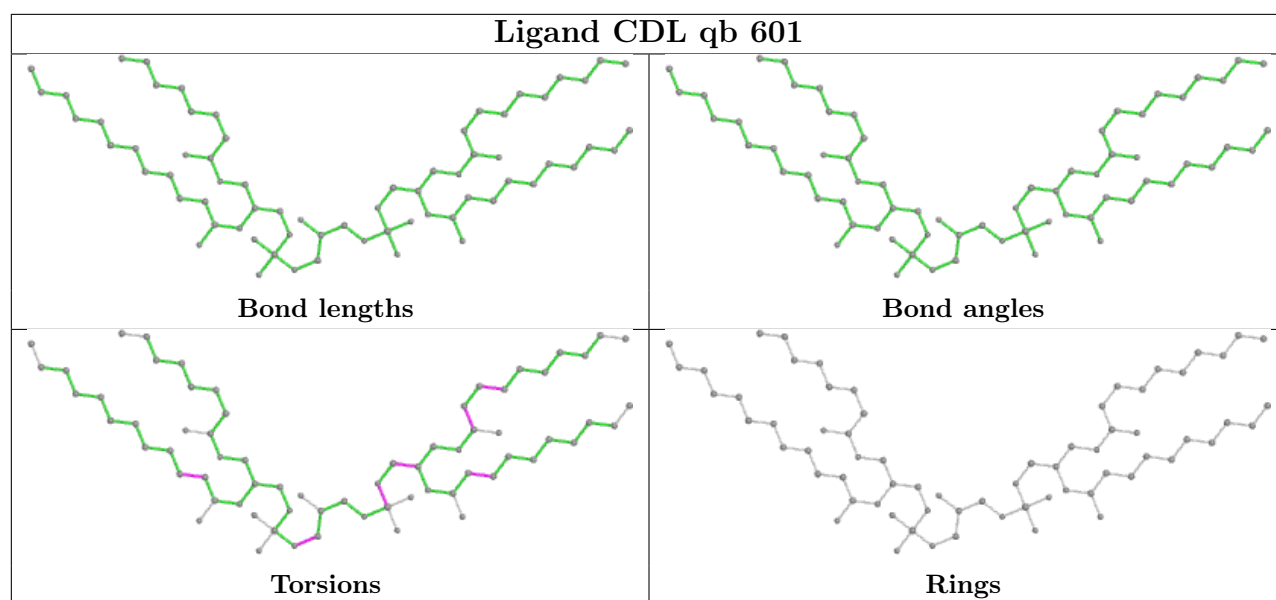


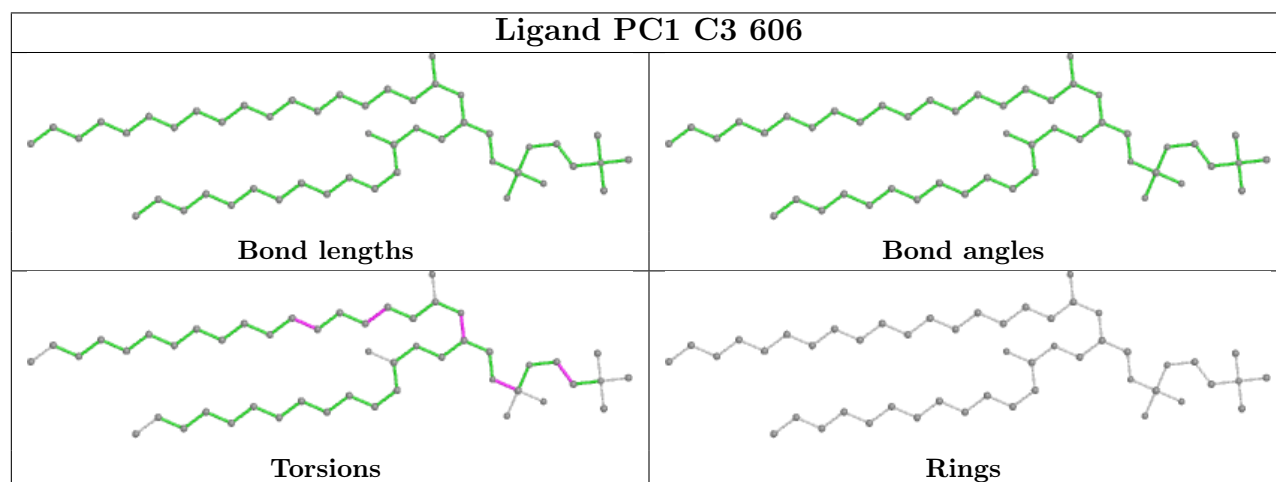
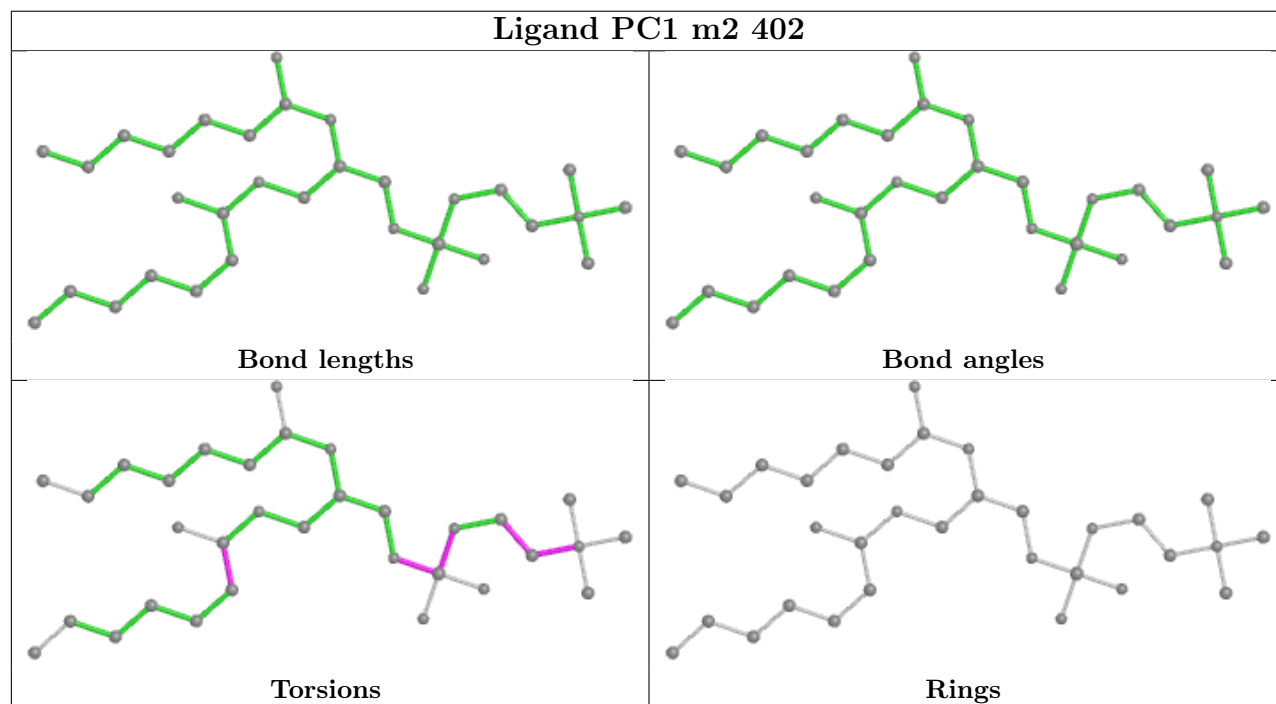
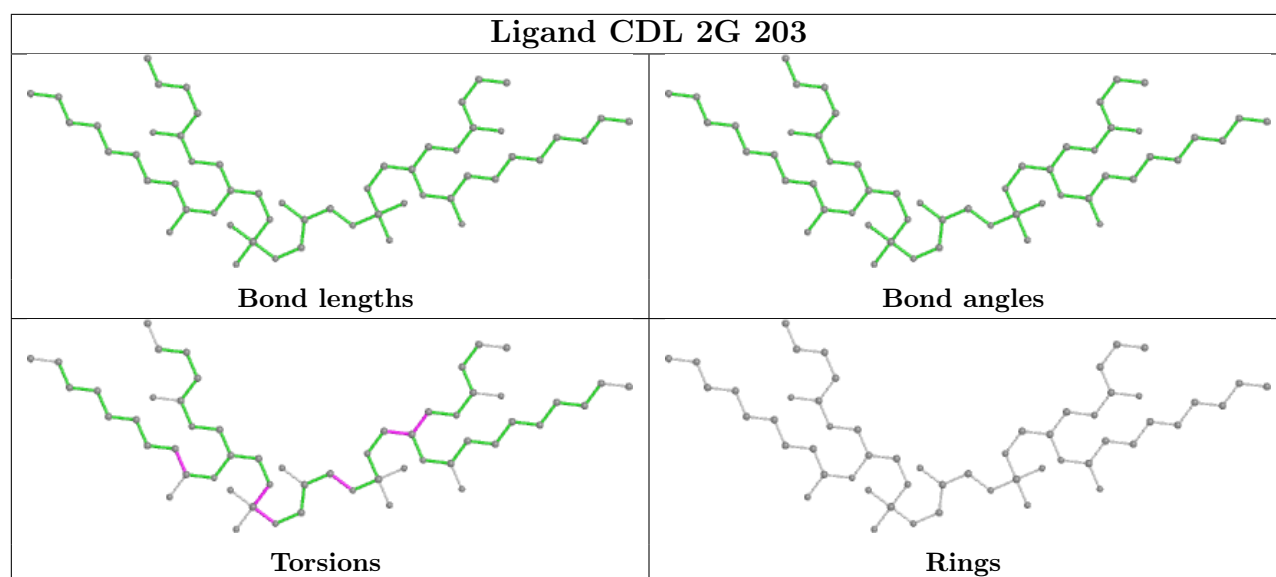


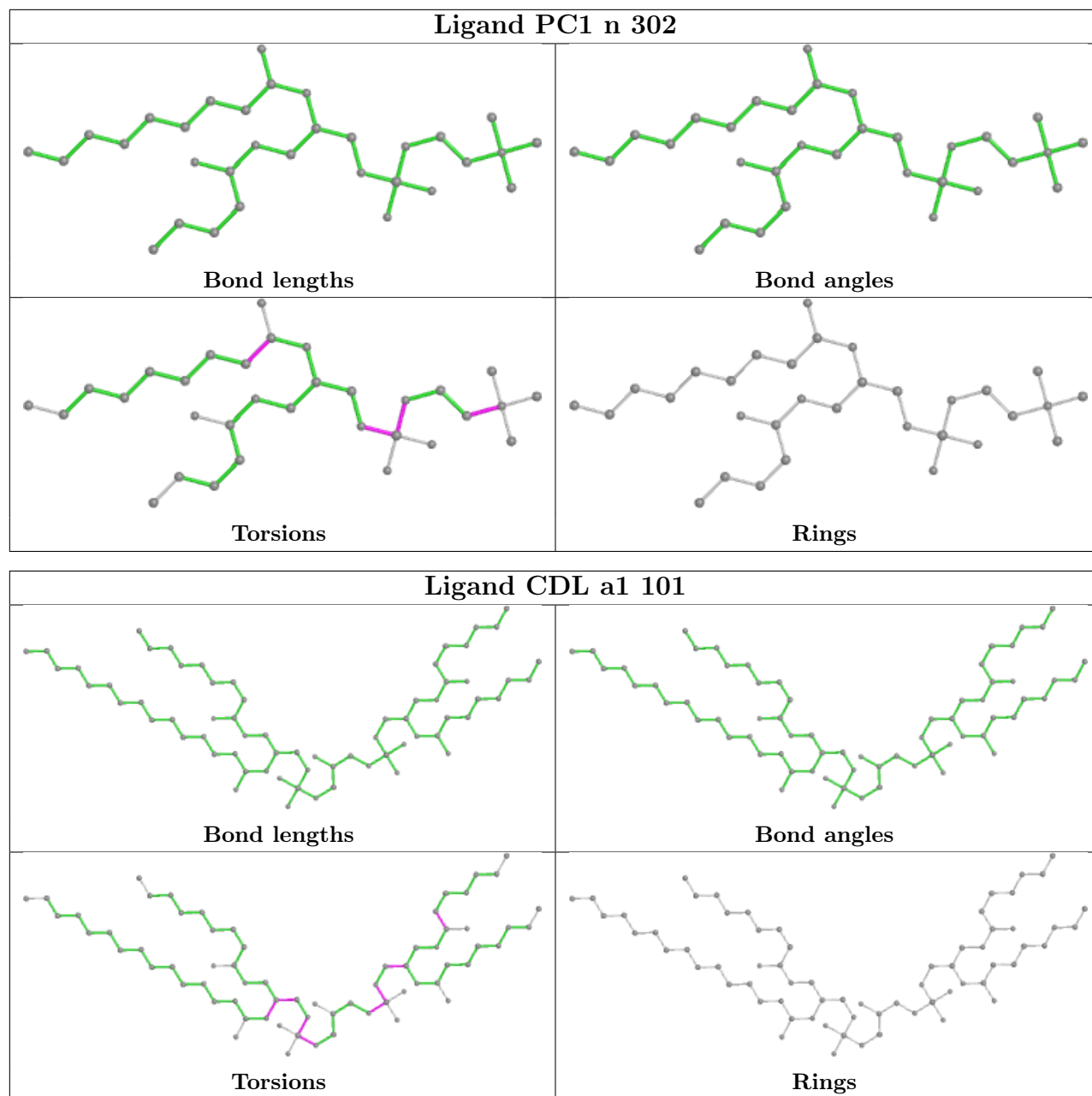


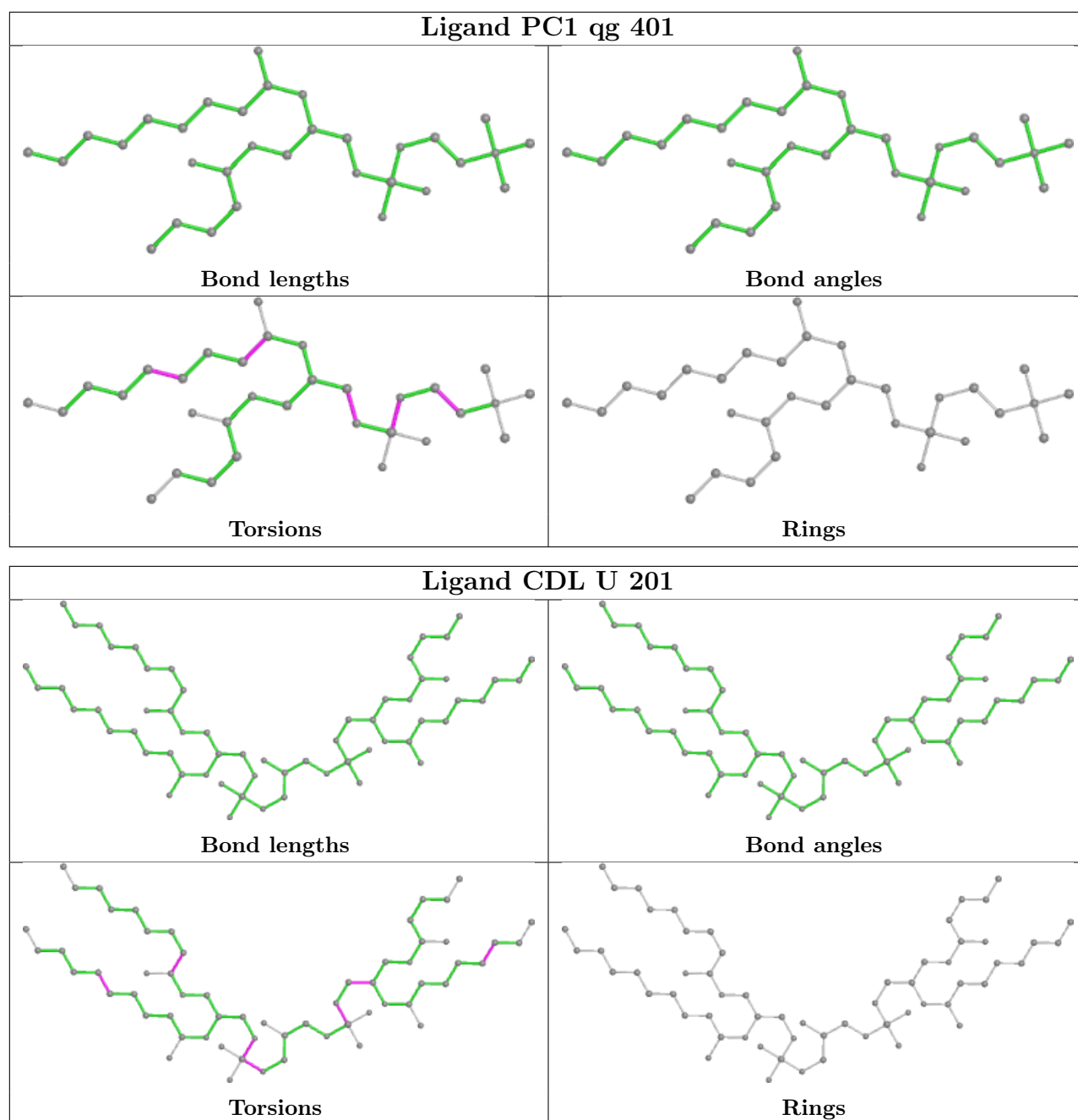
Ligand FMN V1 501

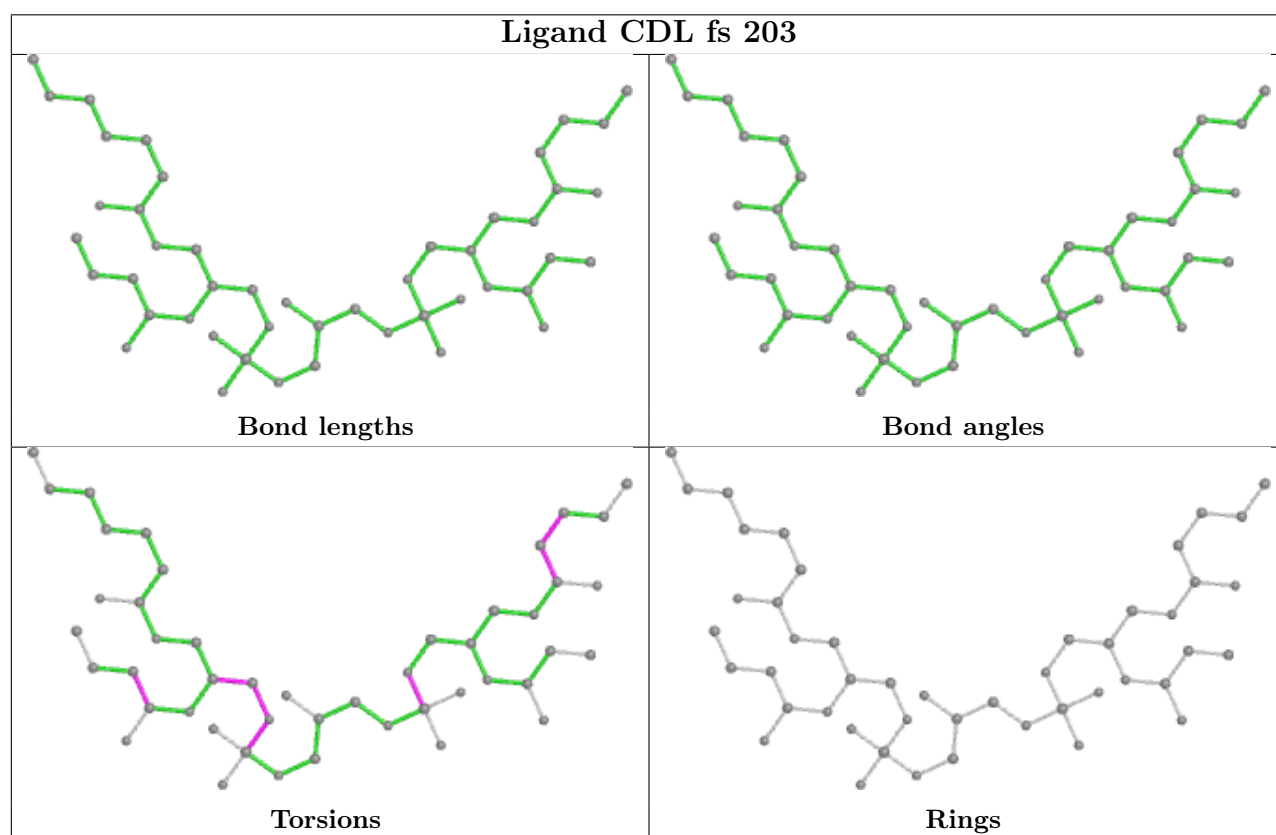
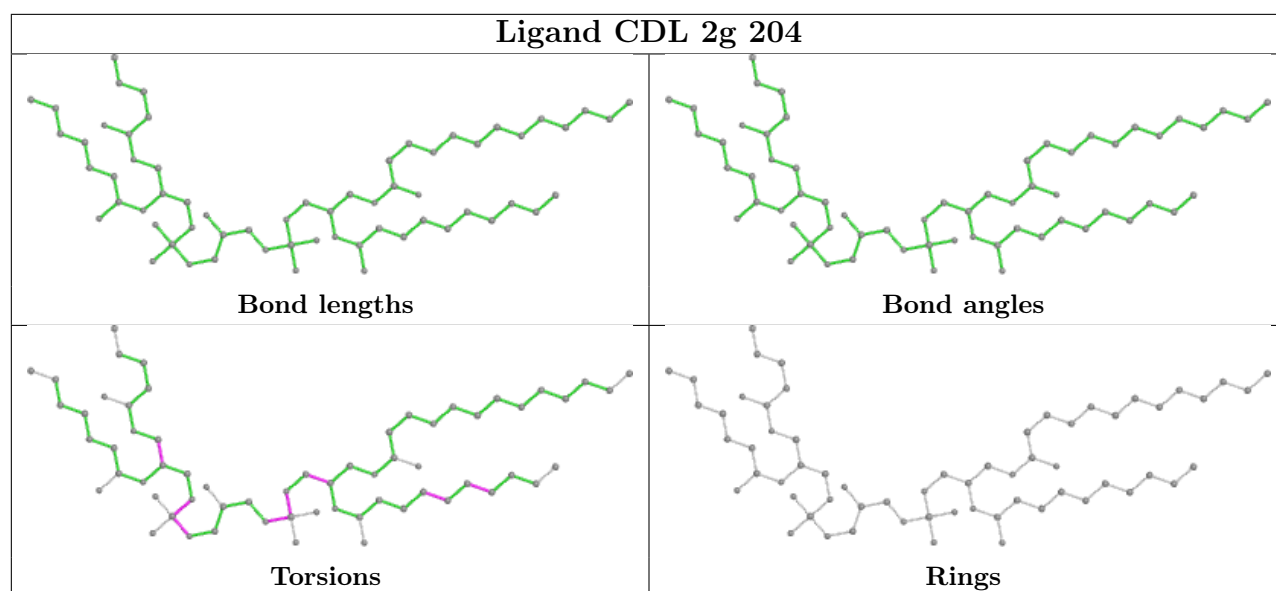


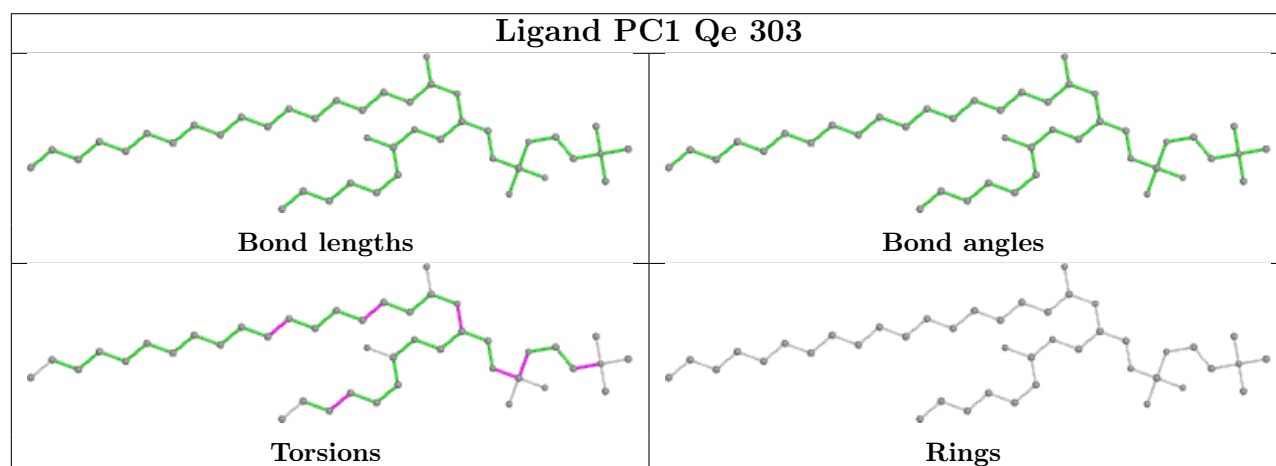
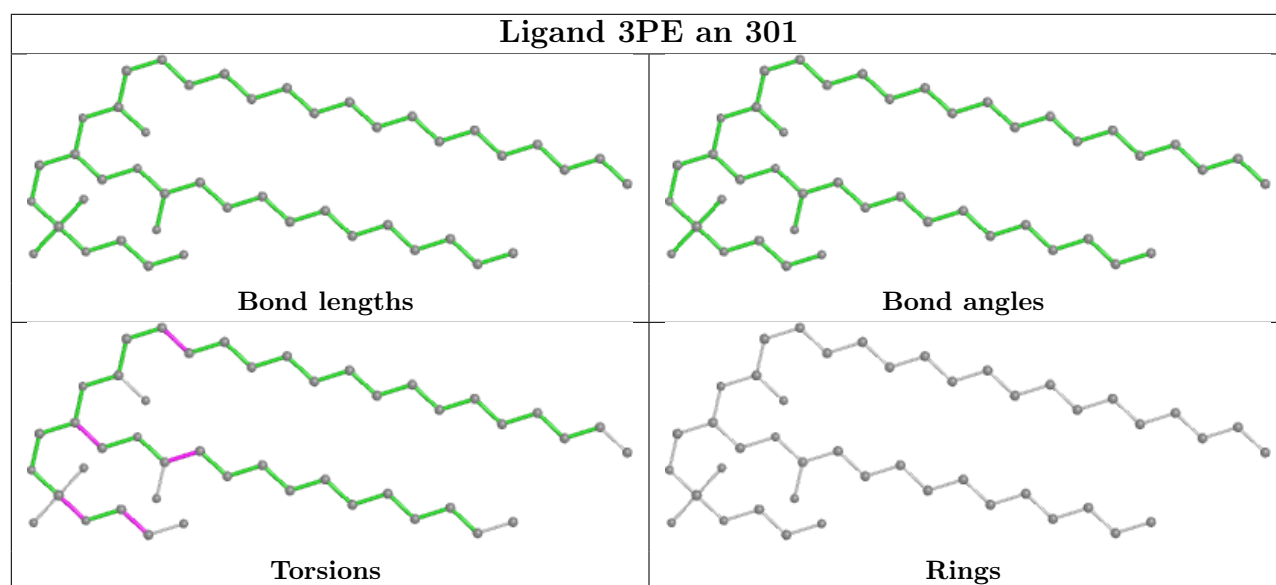
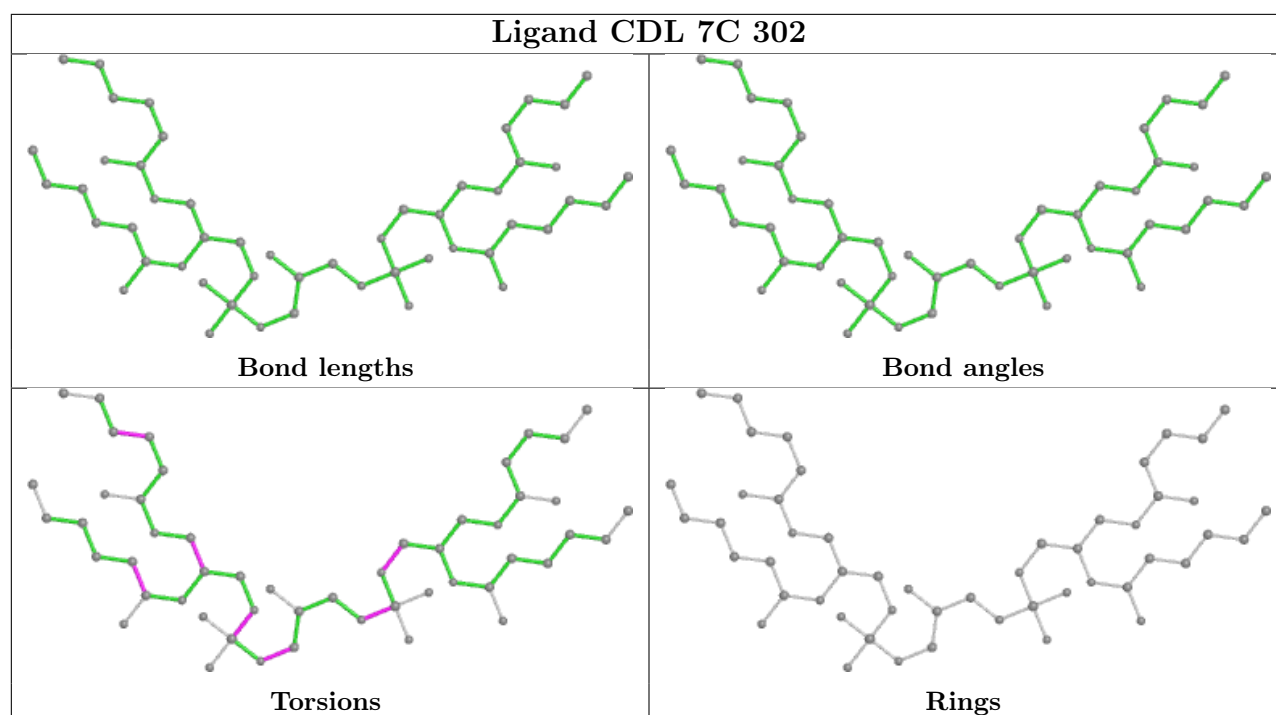


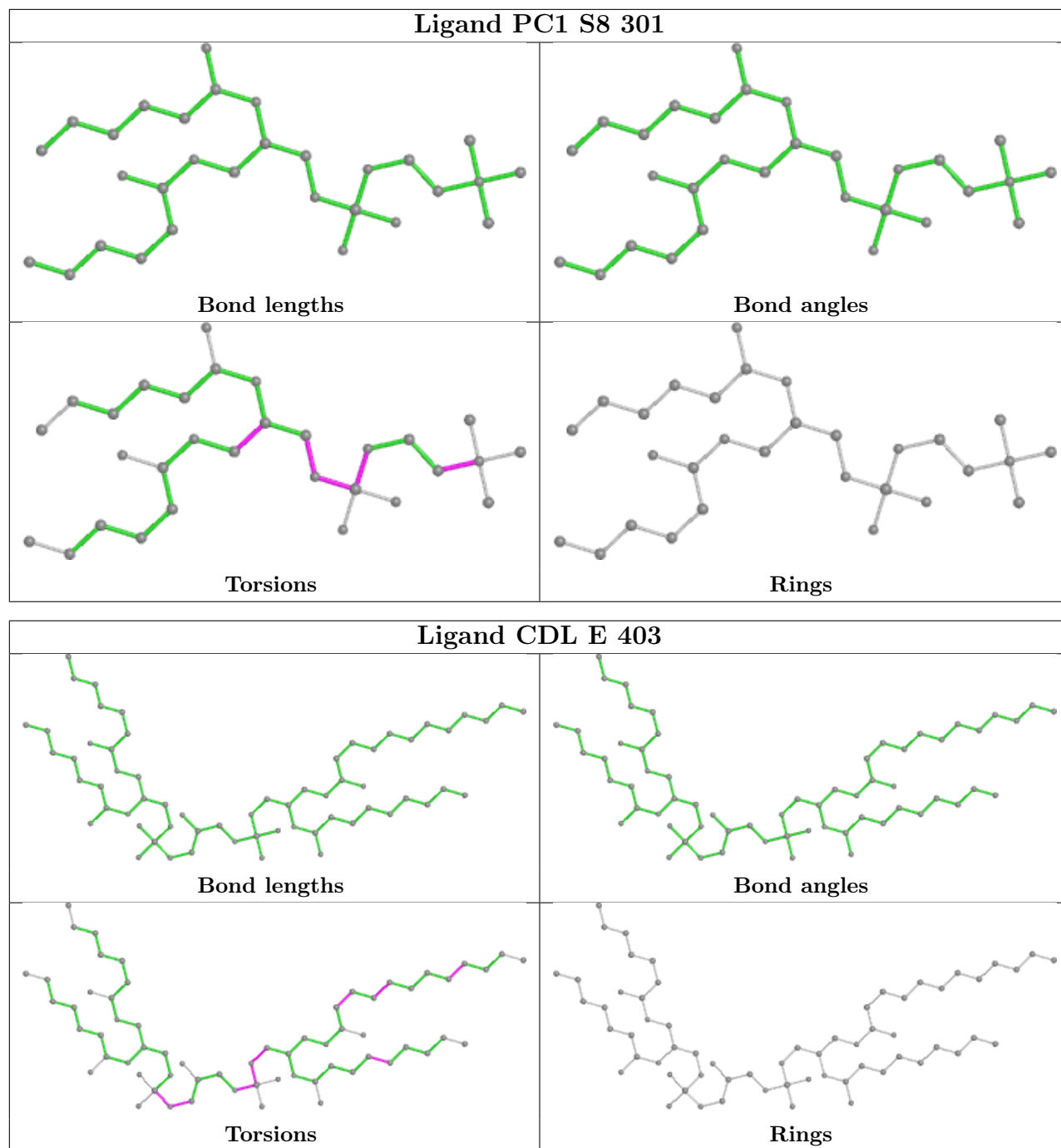


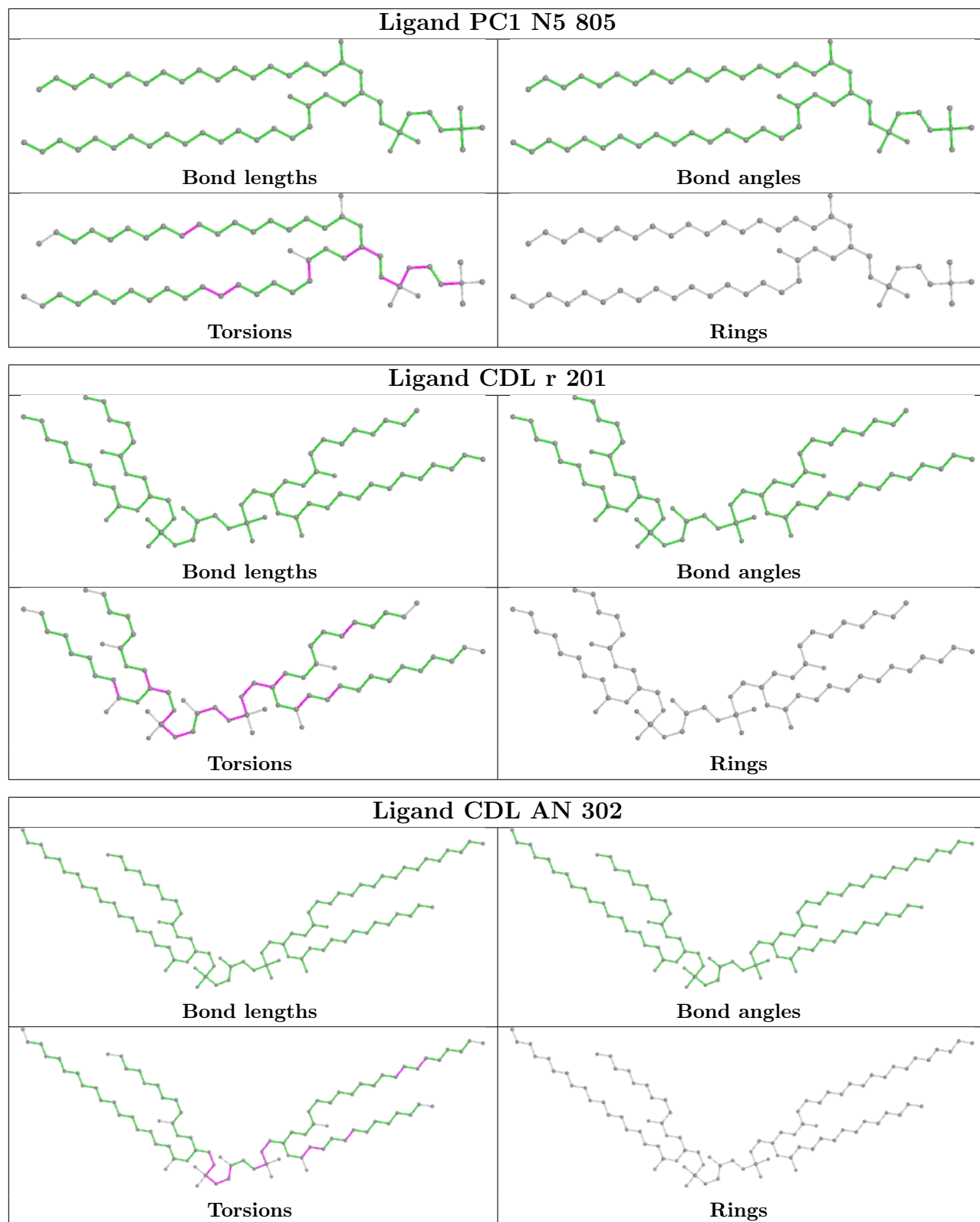


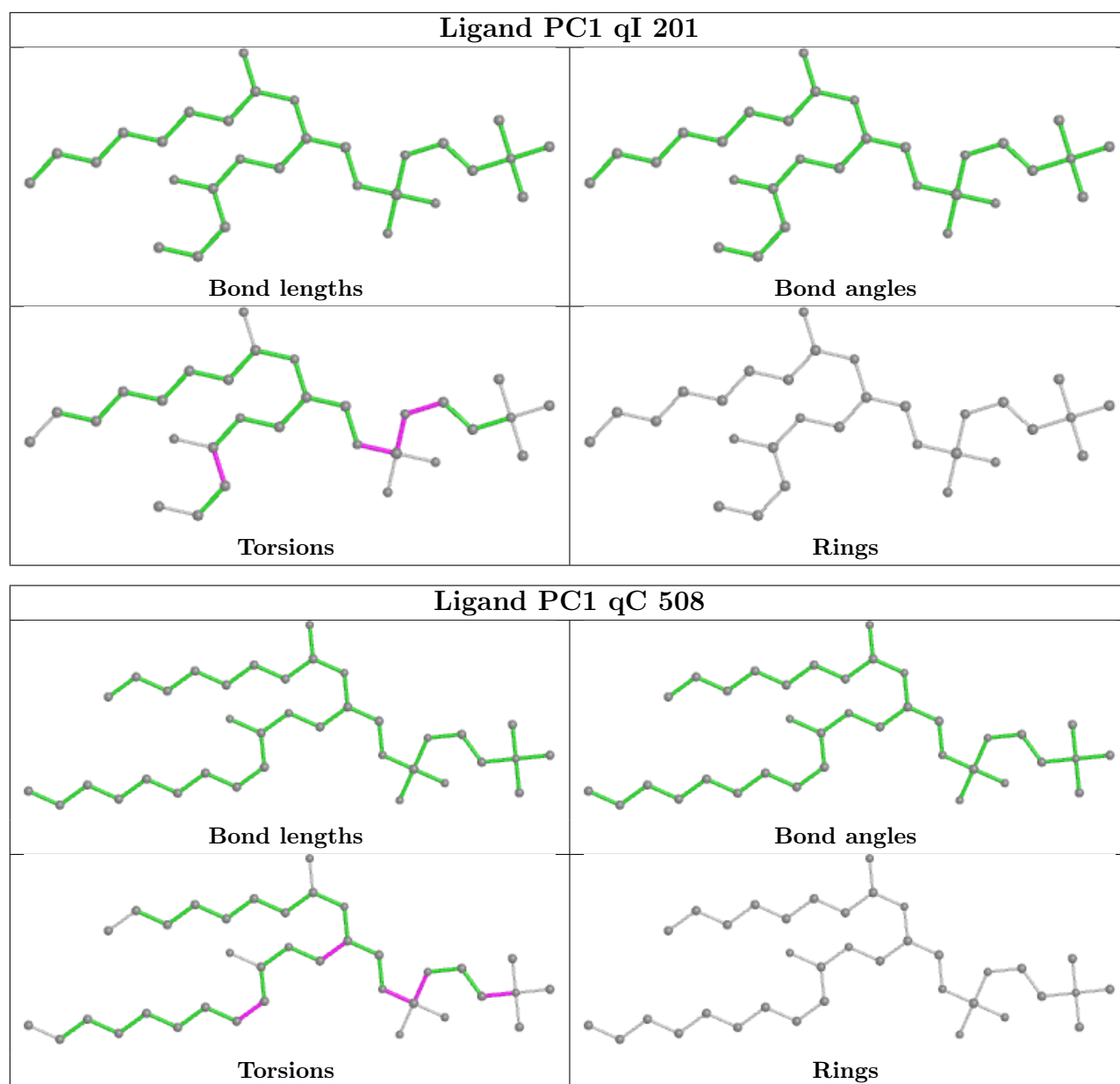


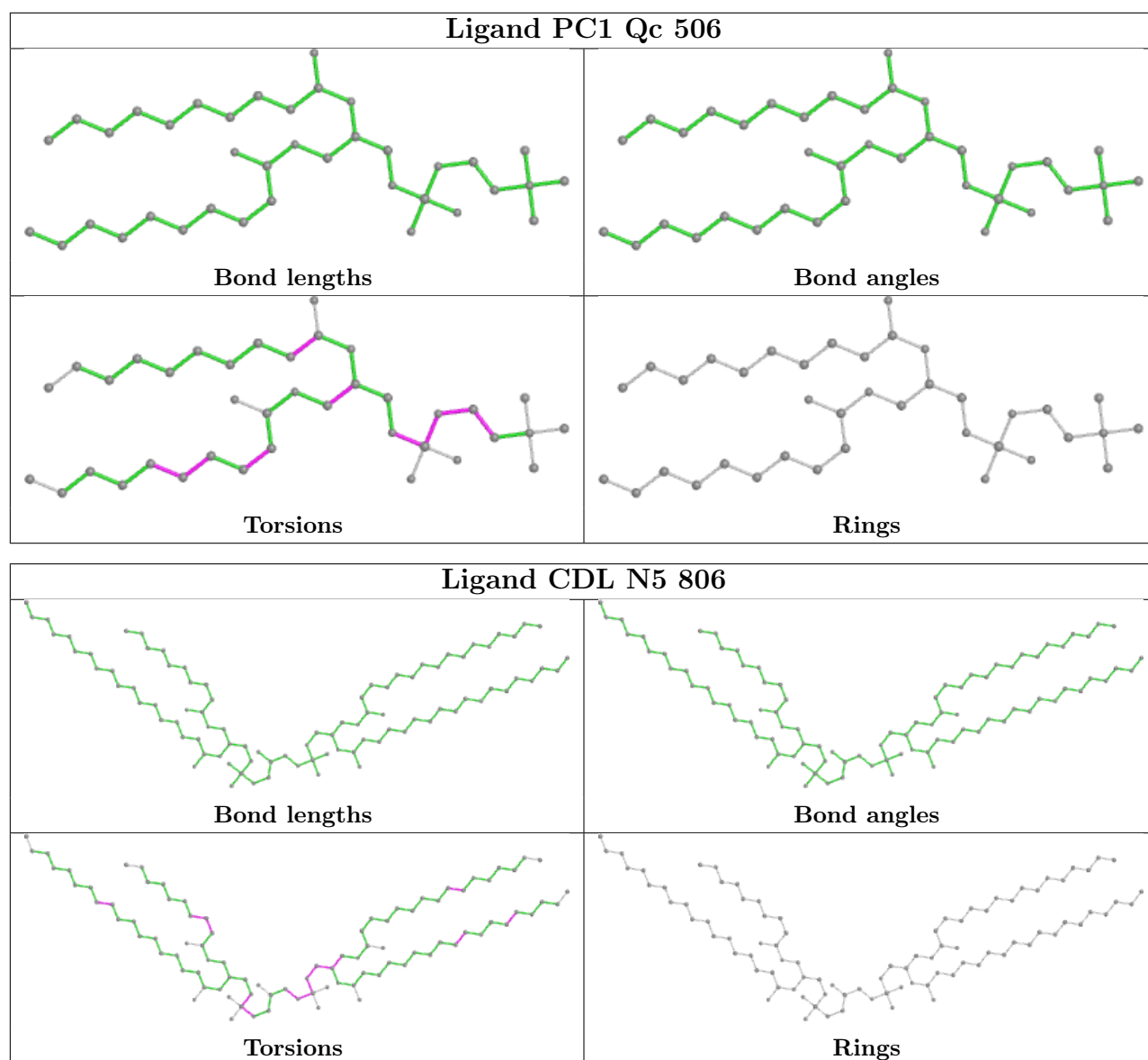


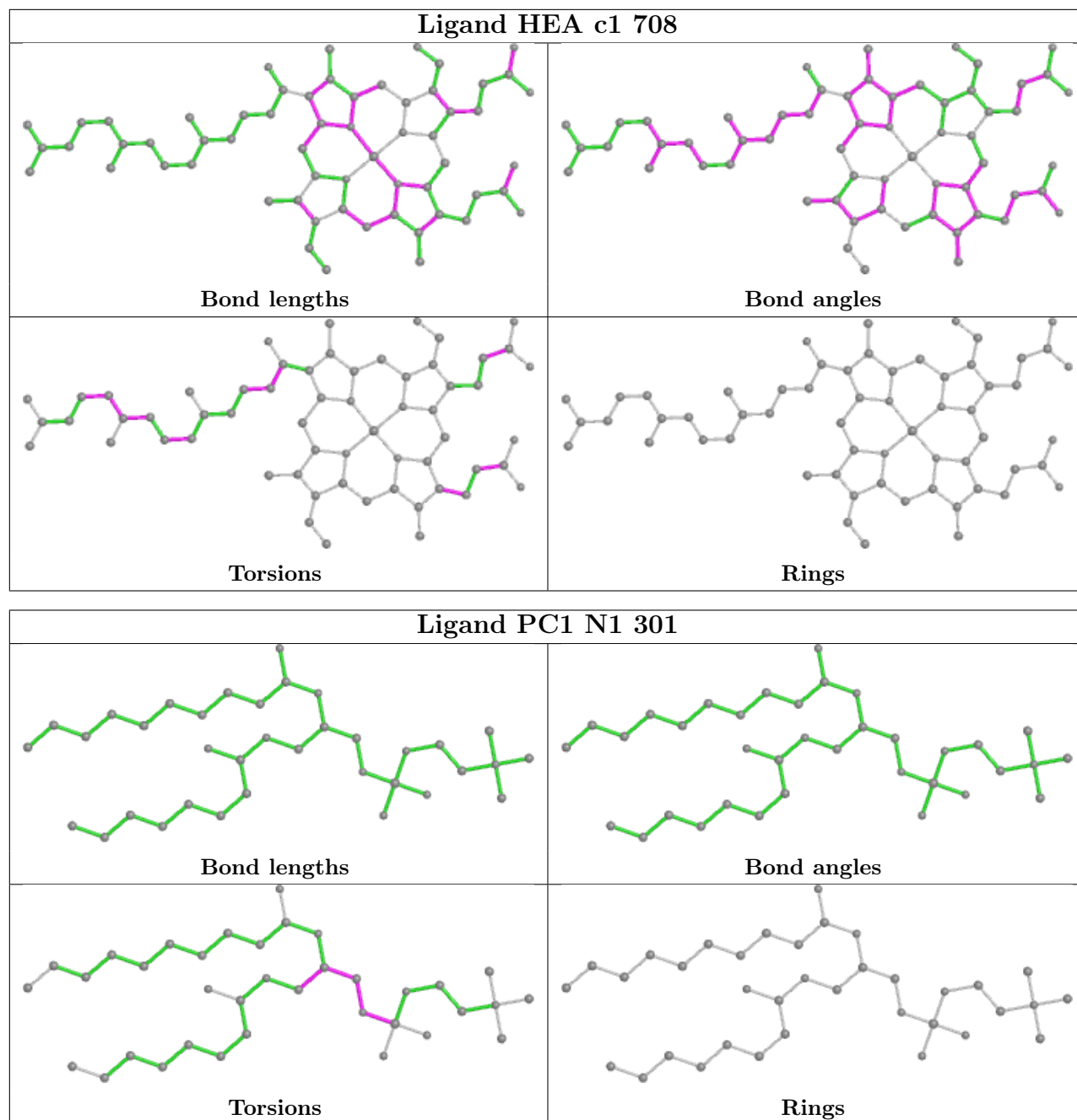


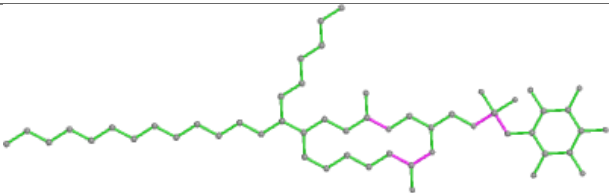
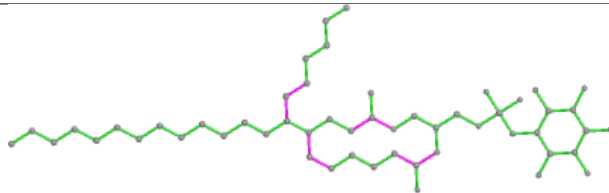
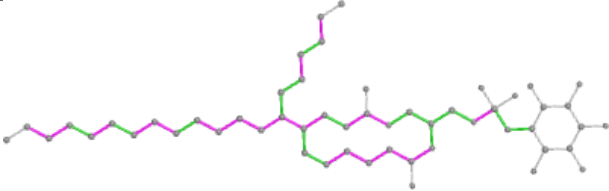
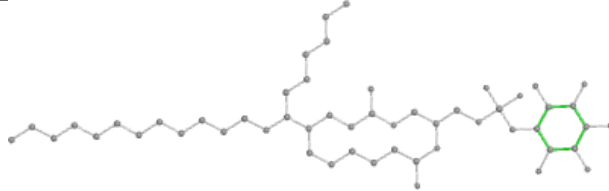


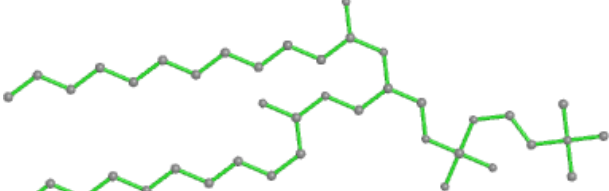
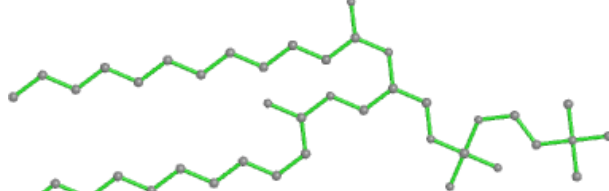
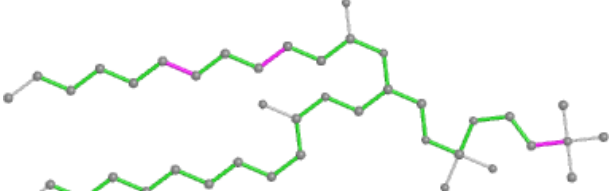
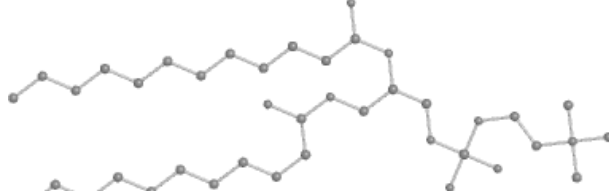


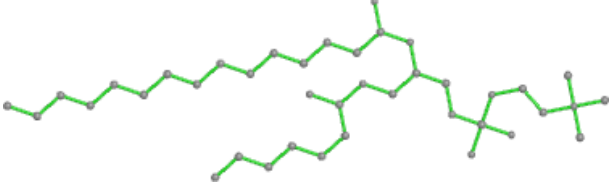
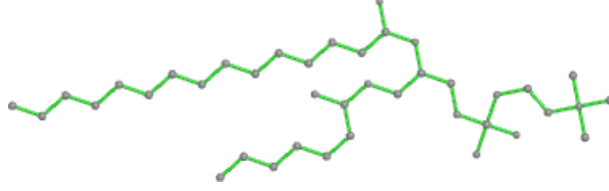
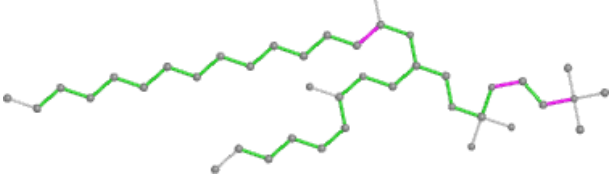
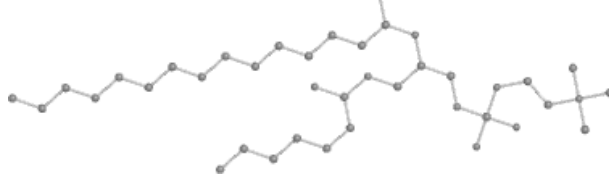


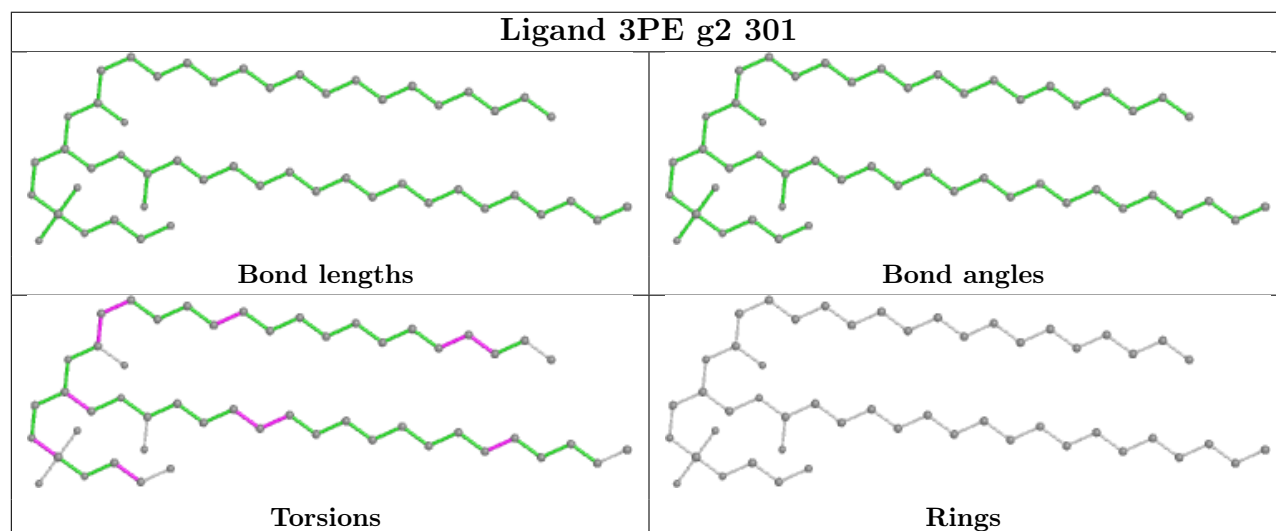
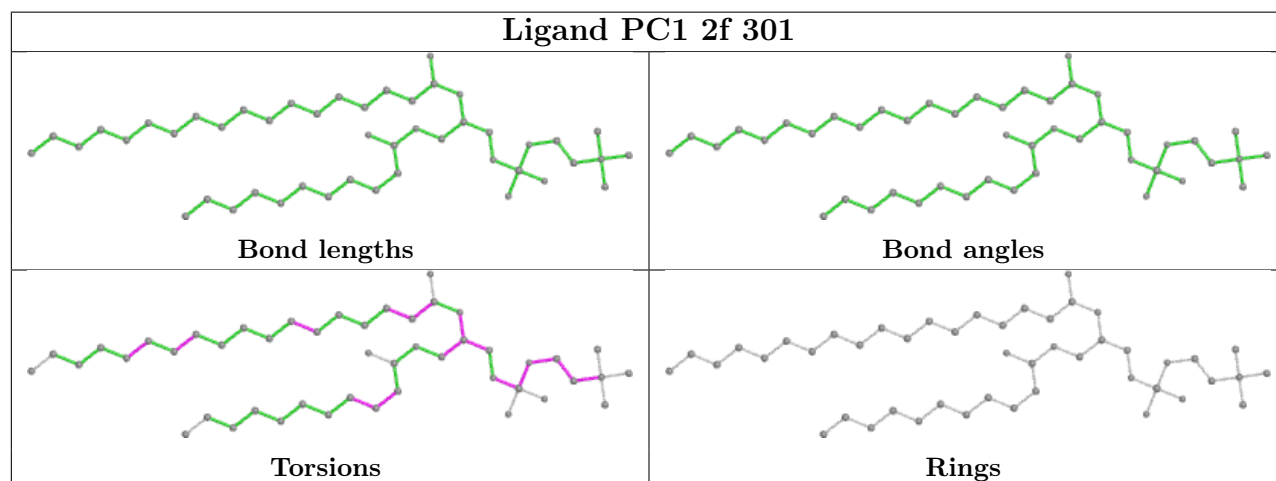
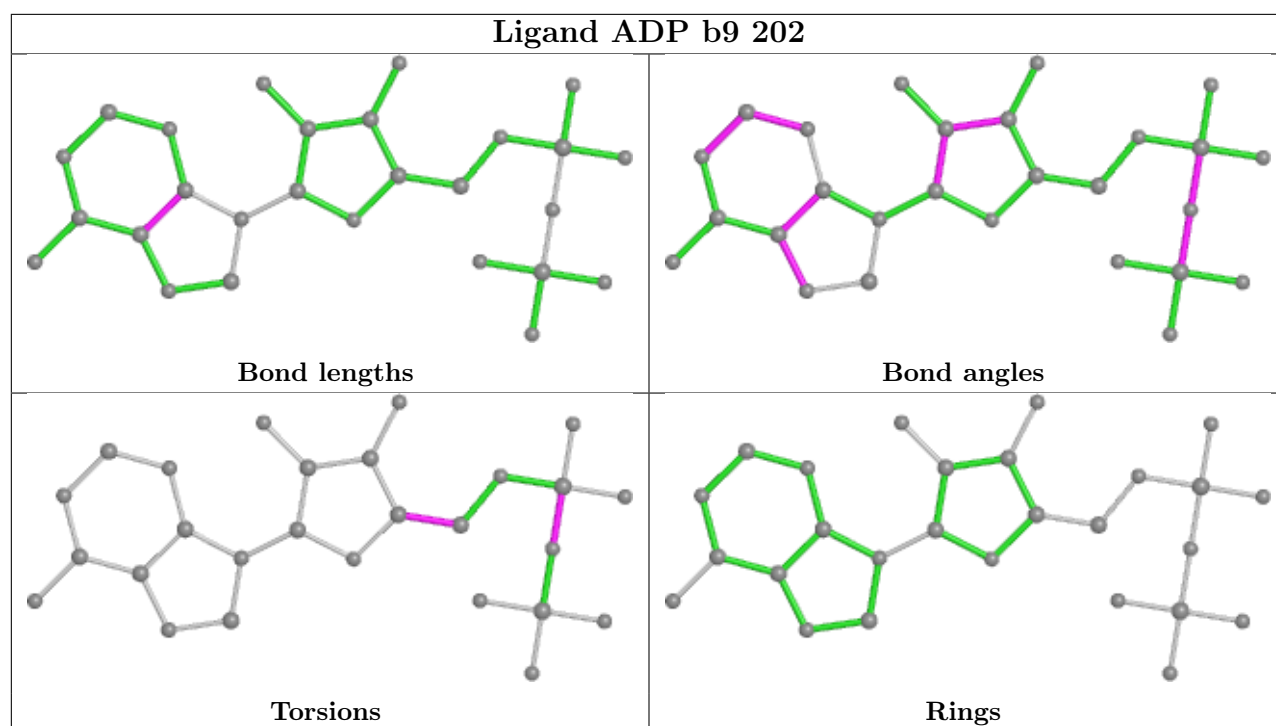


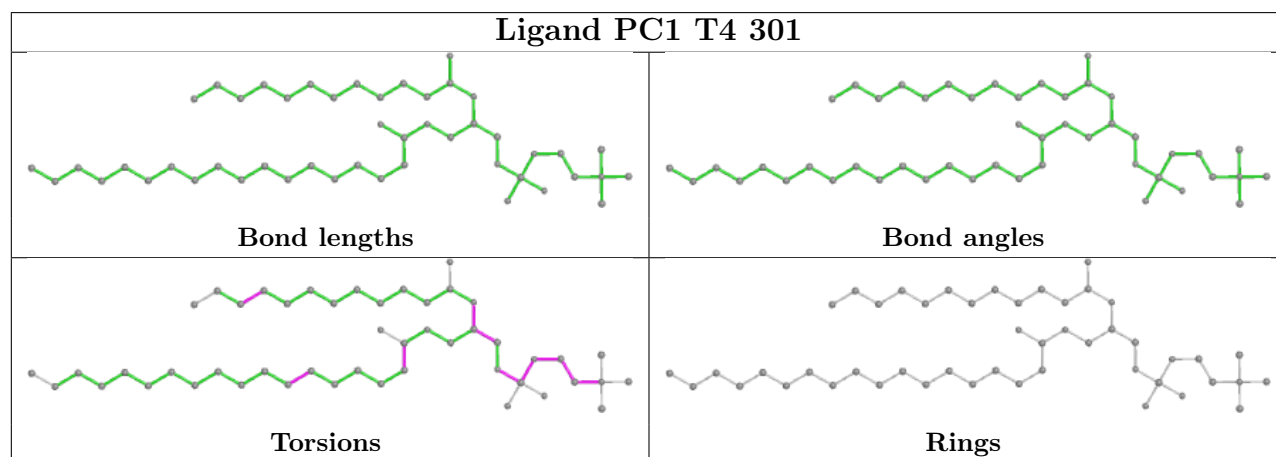
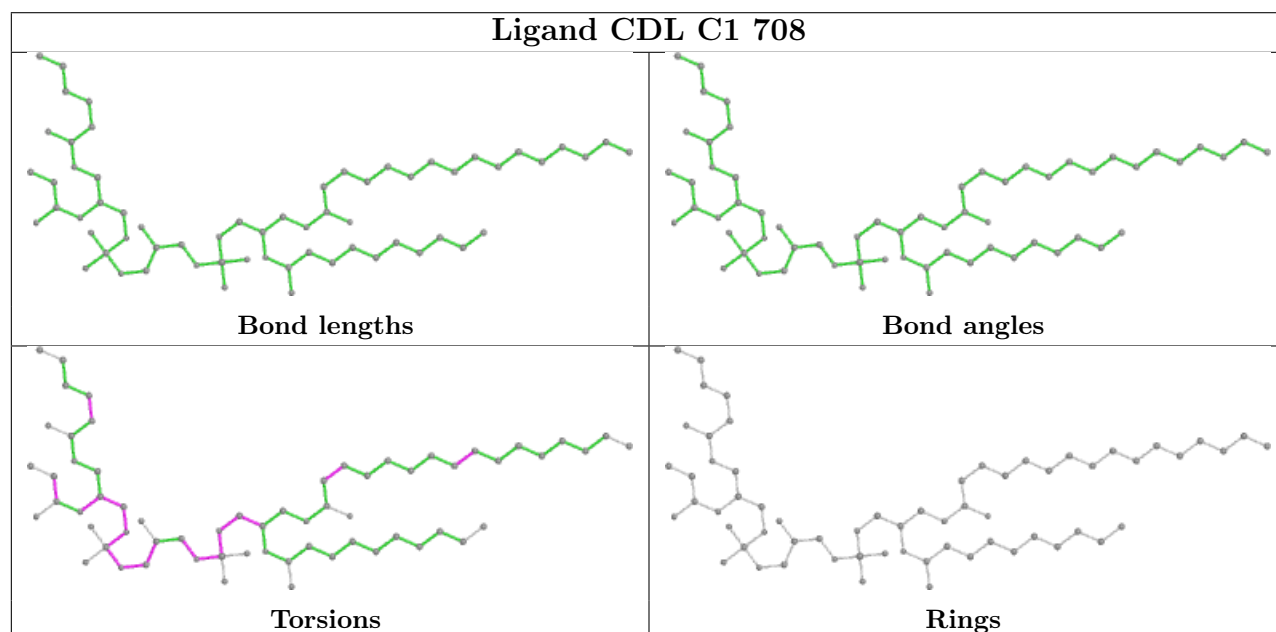
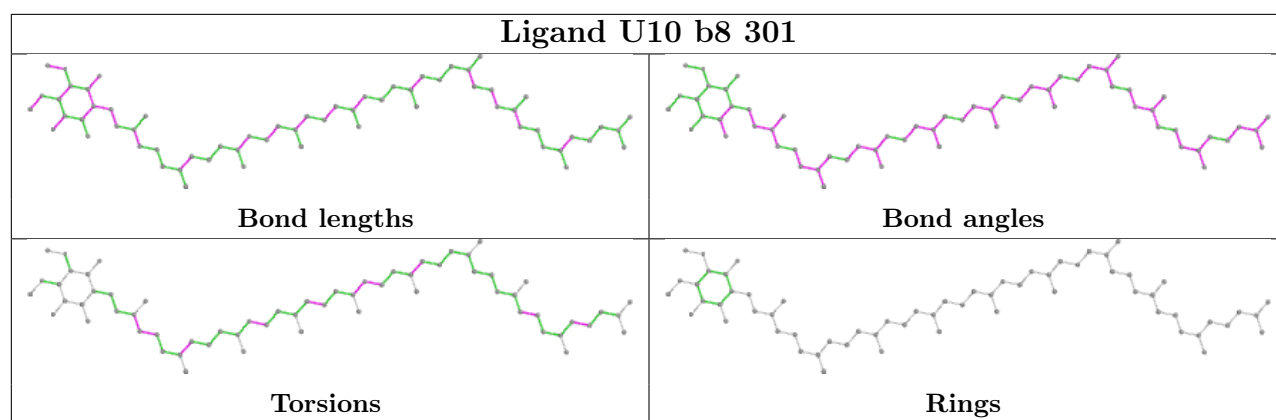


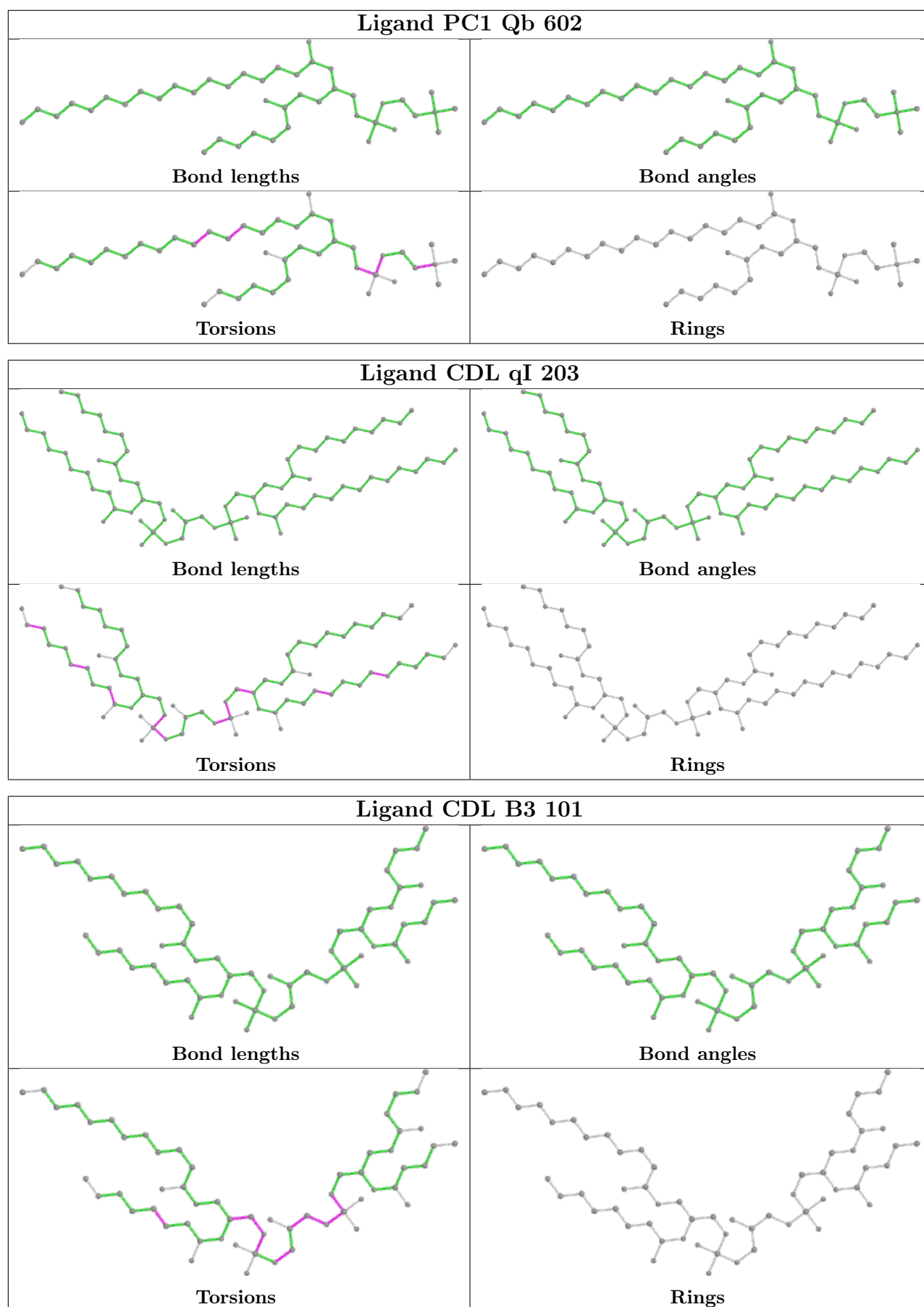
Ligand T7X b6 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

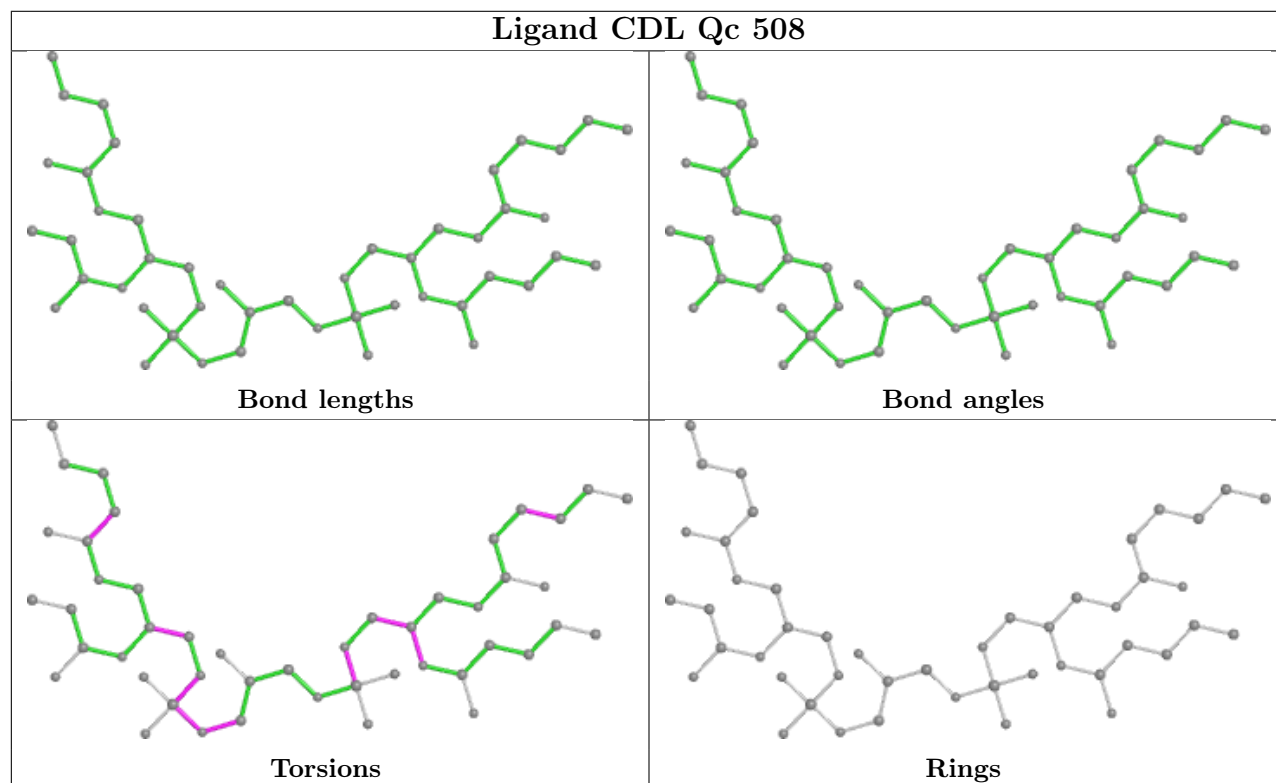
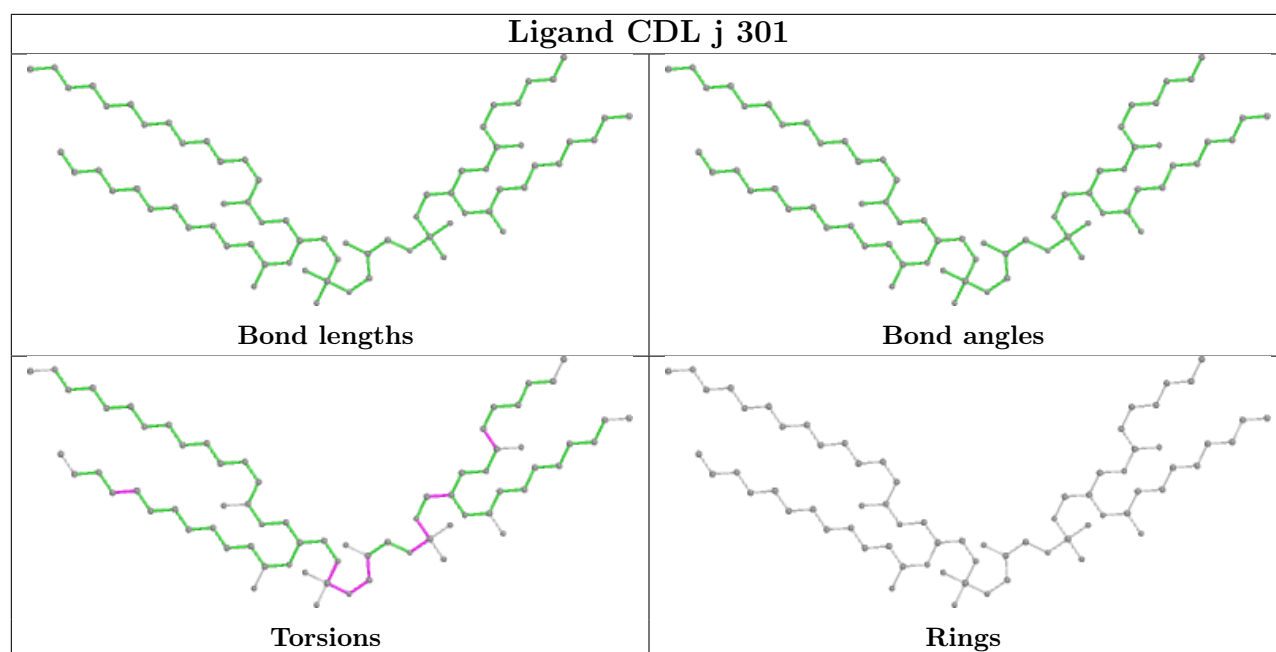
Ligand PC1 N 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

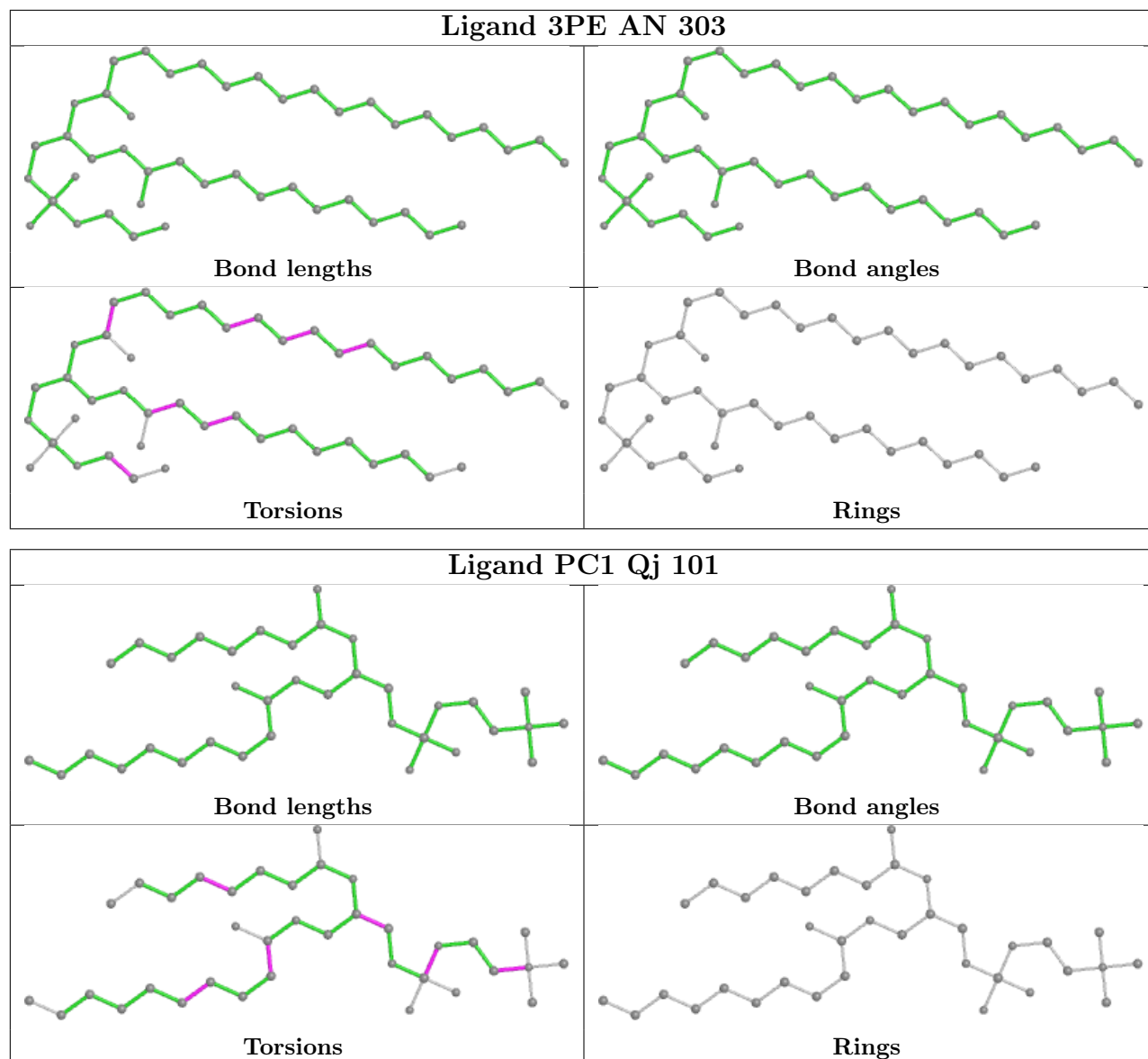
Ligand PC1 FS 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

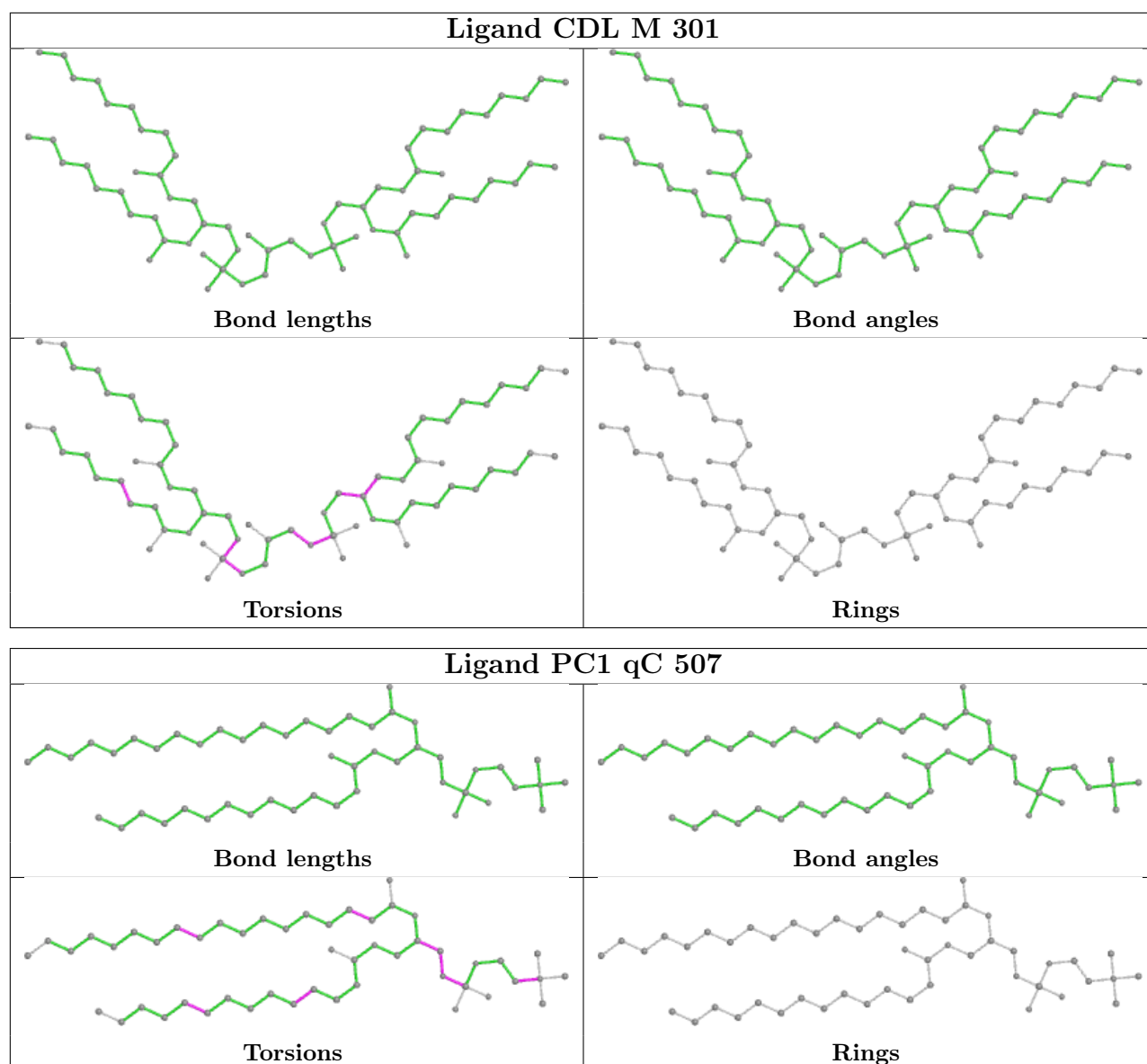


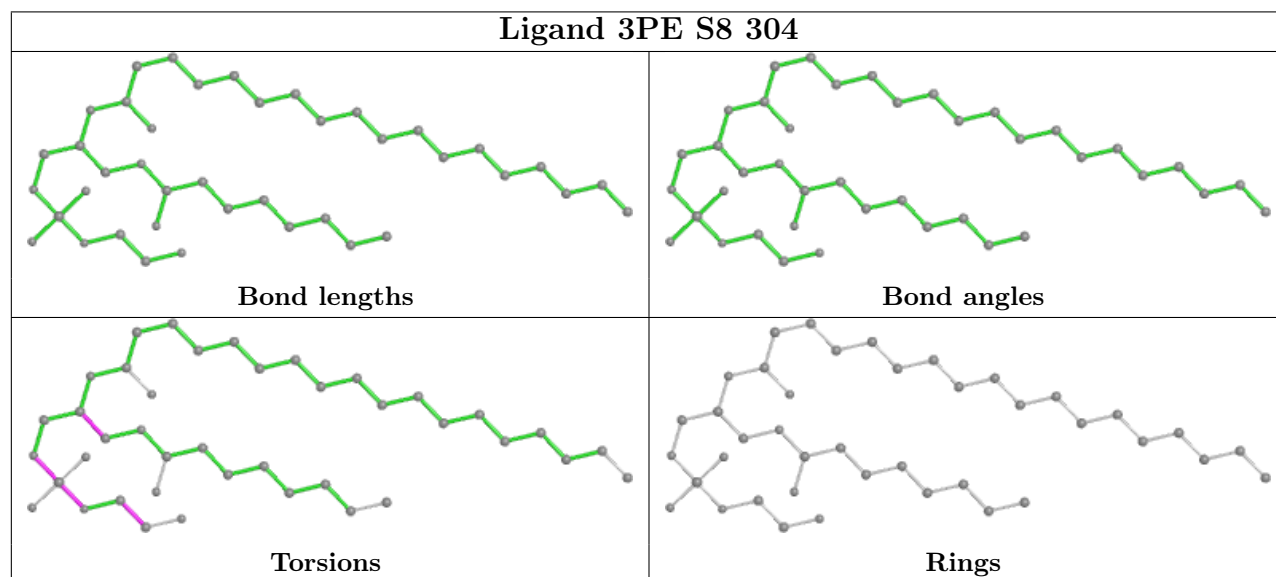
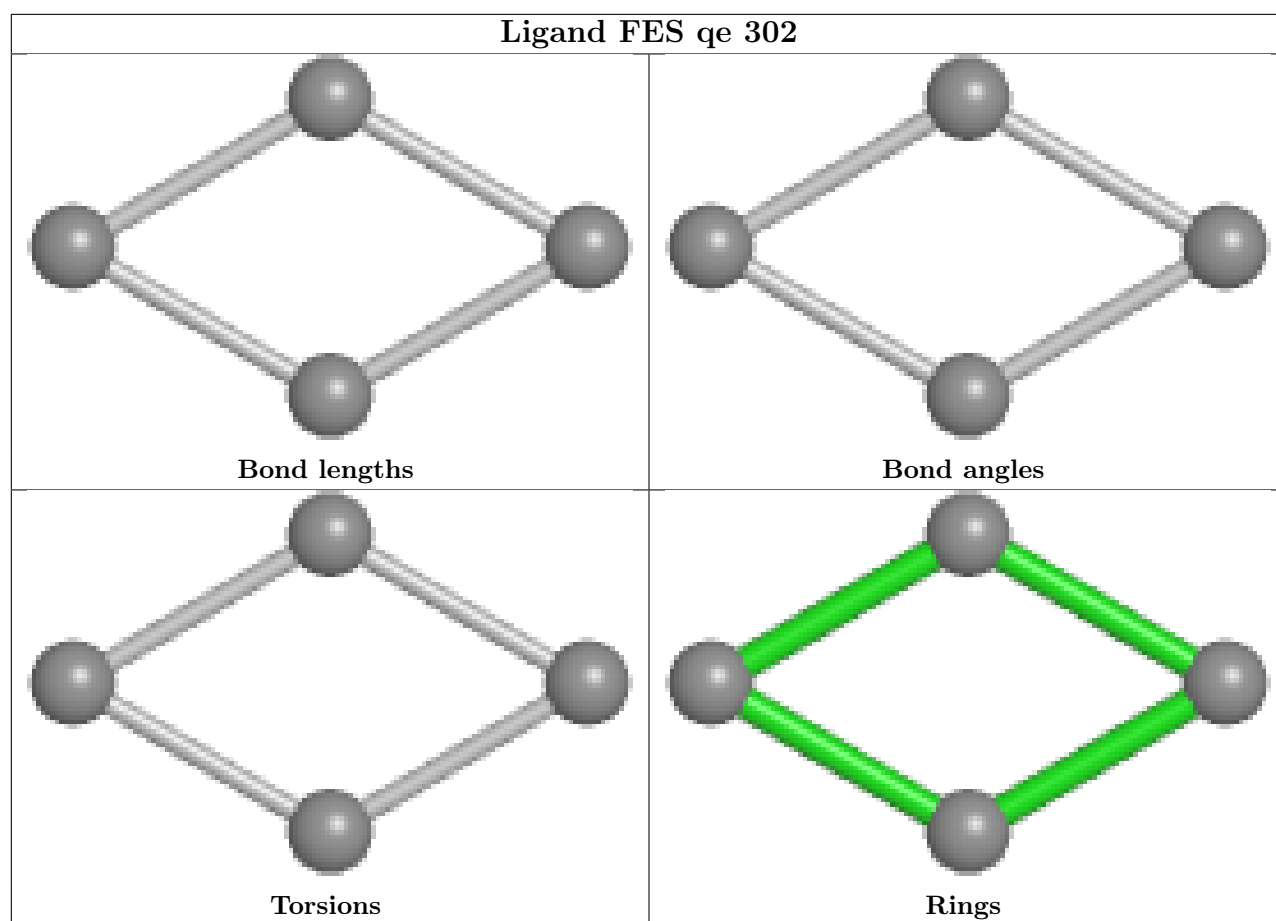


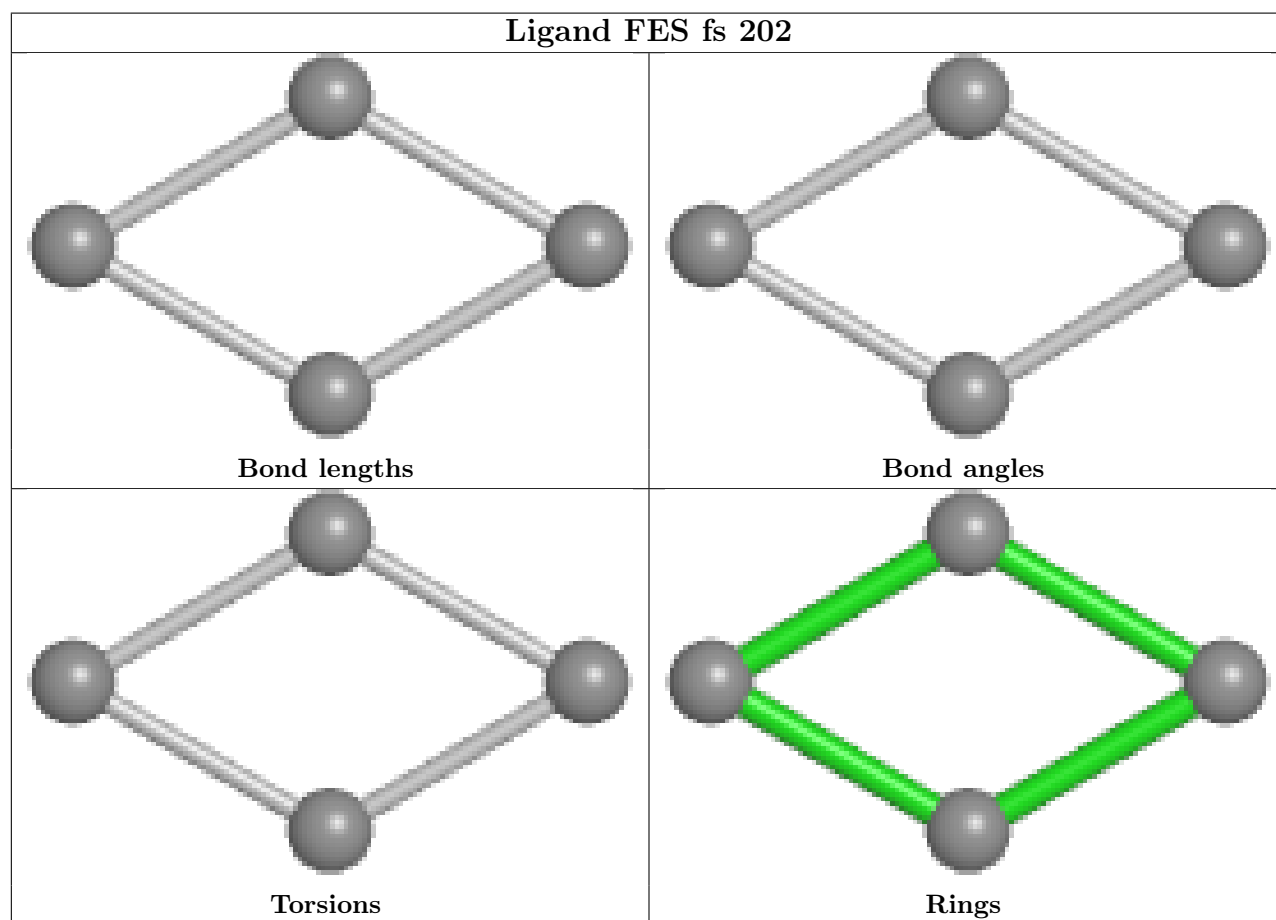
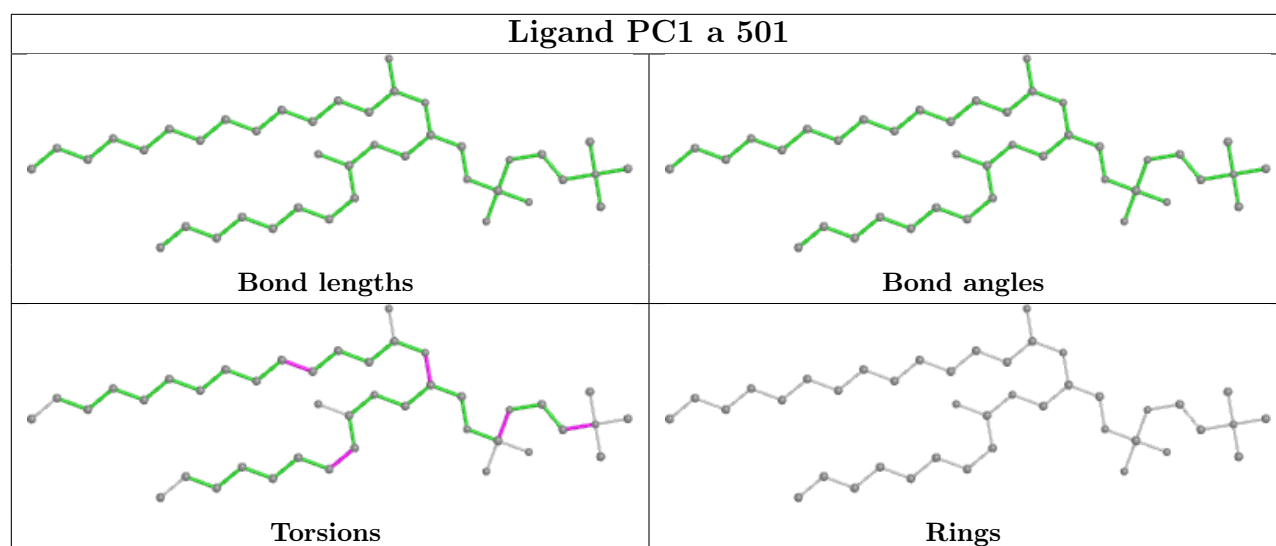


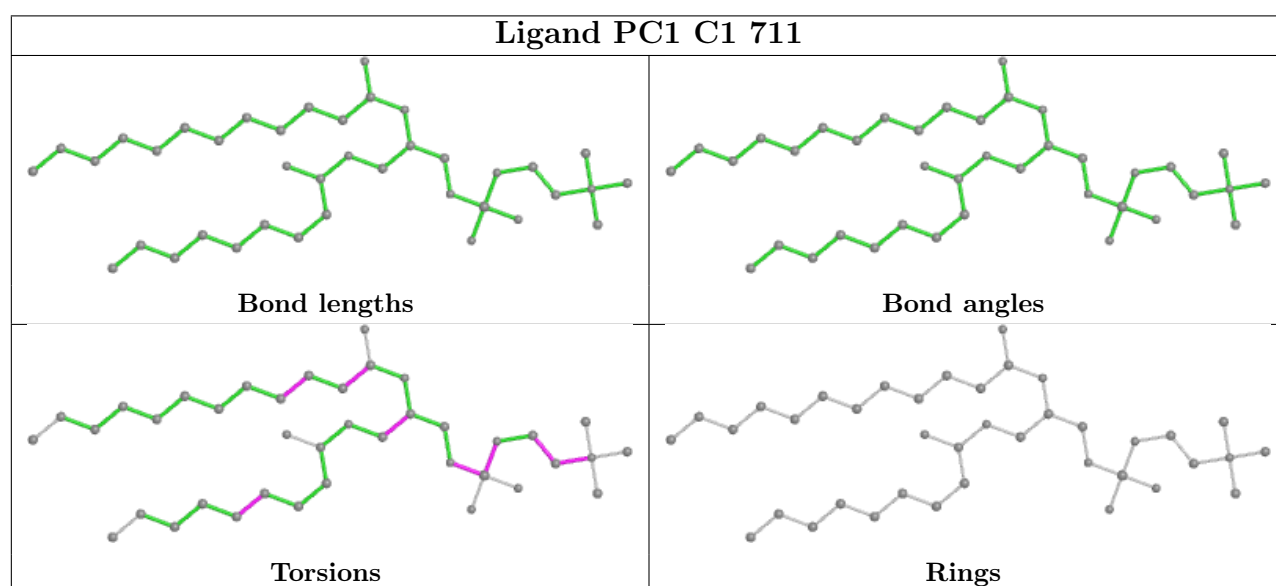
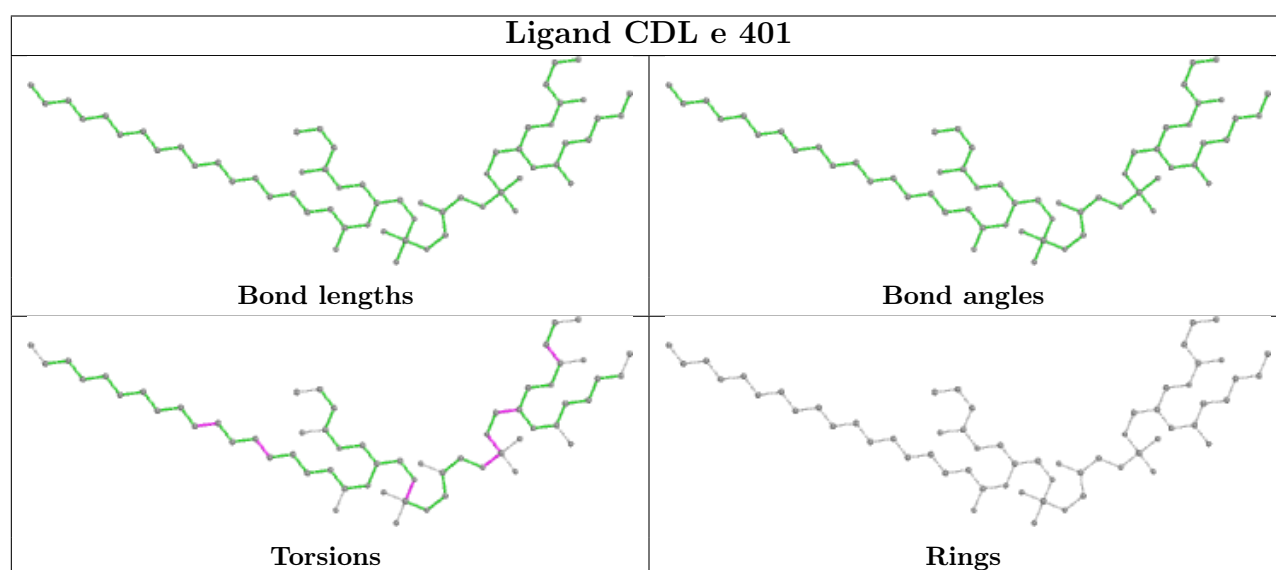
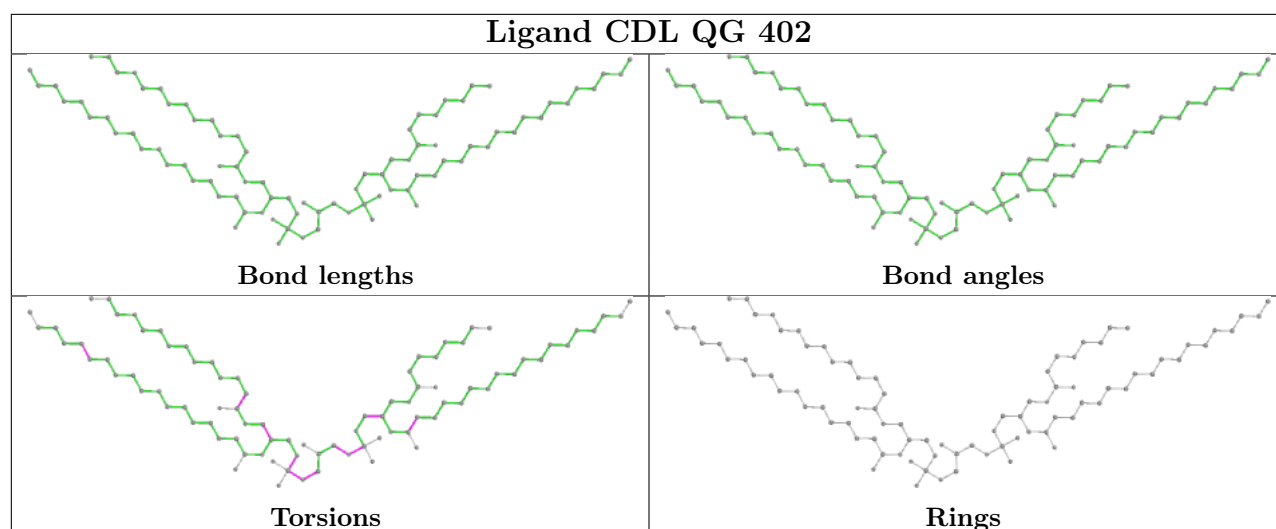


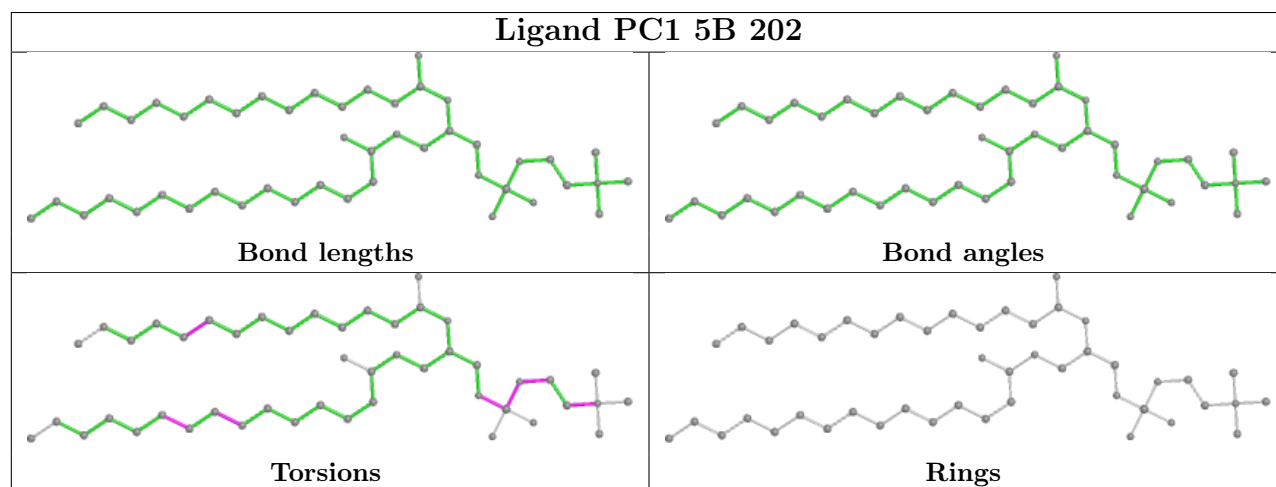
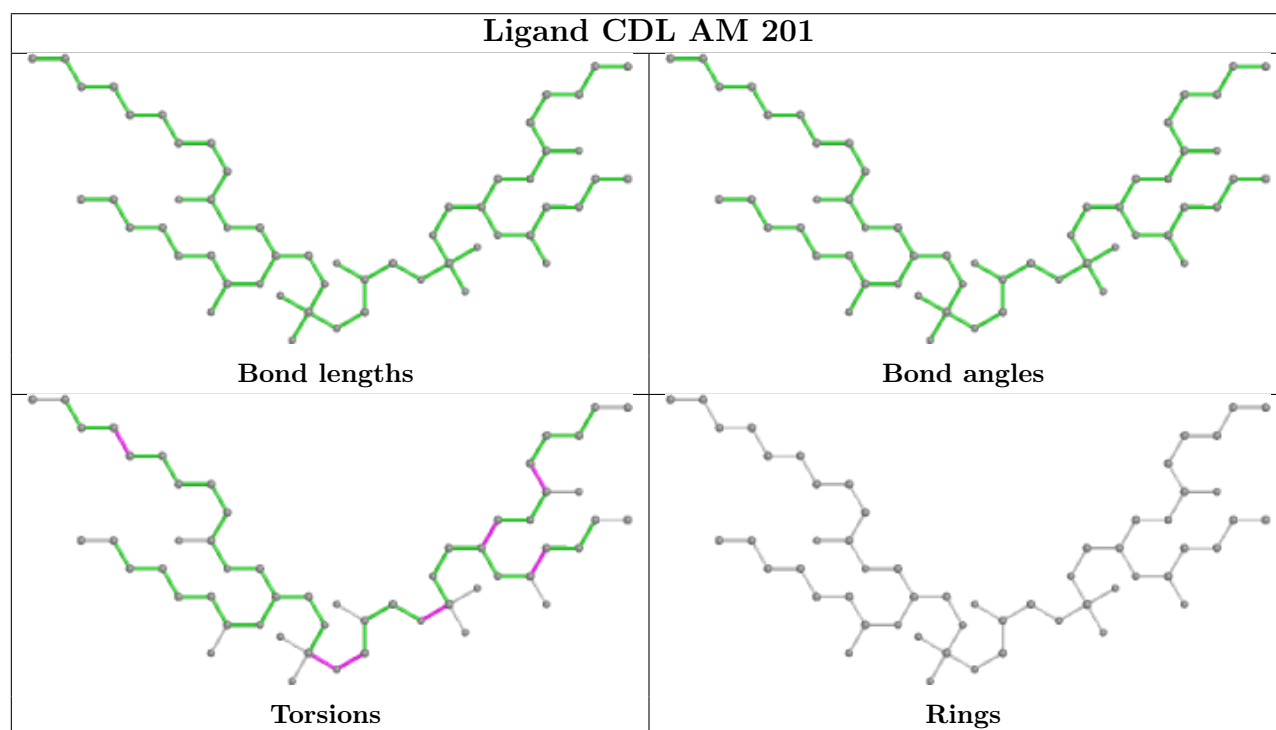
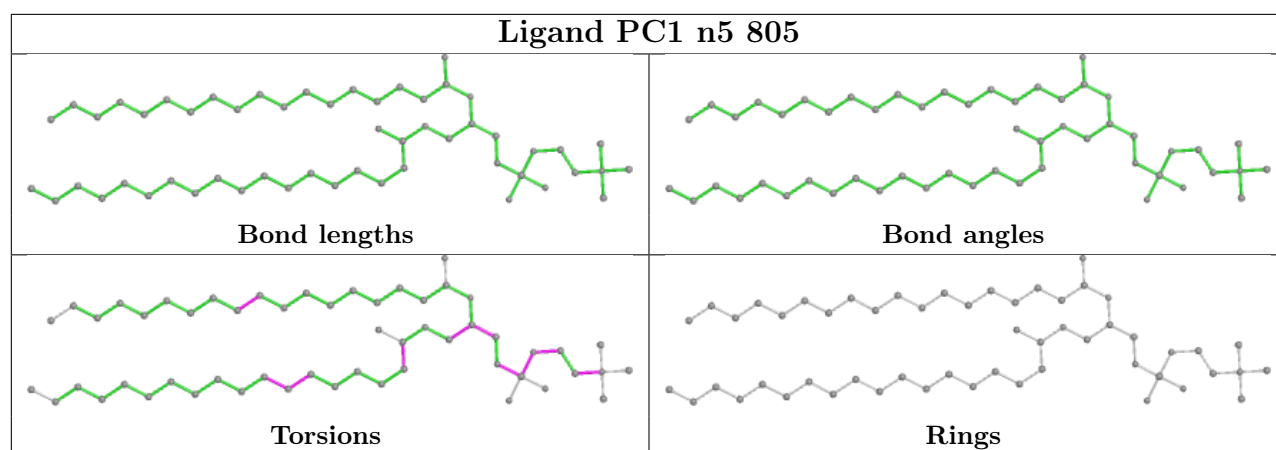


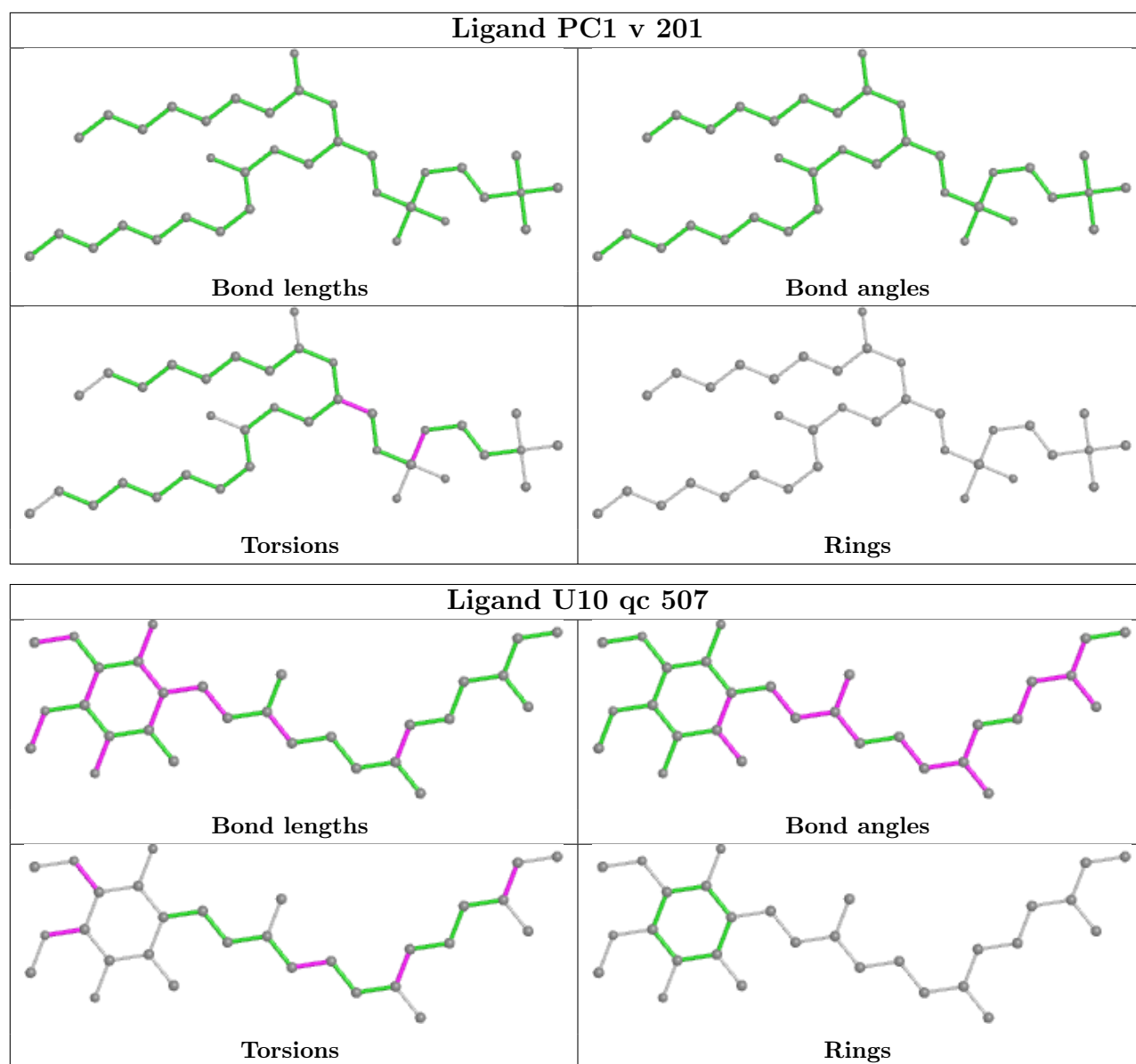


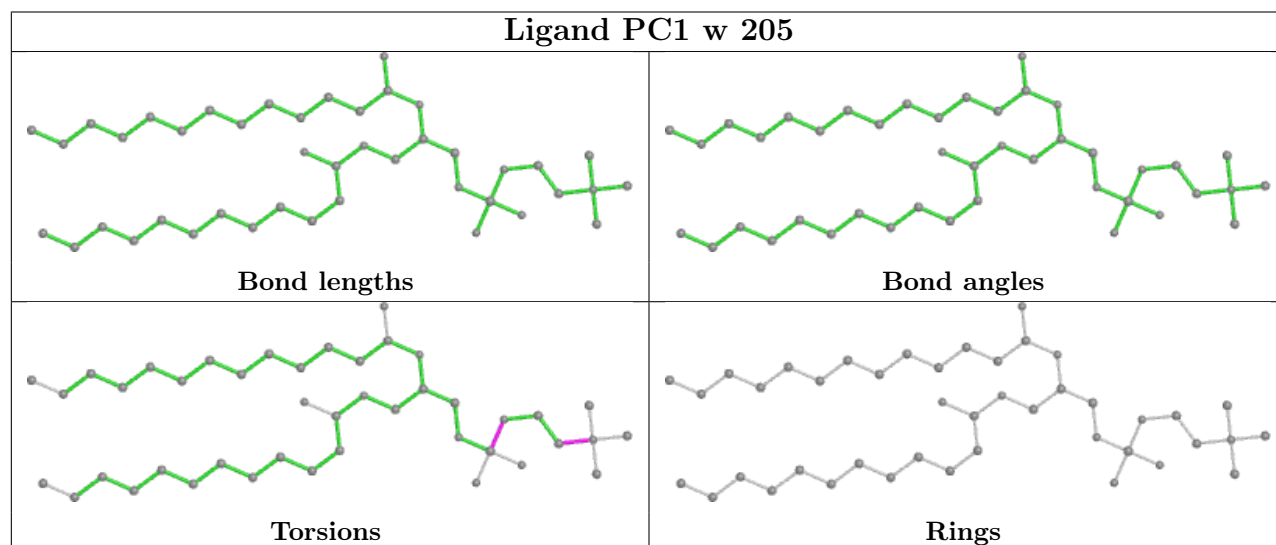
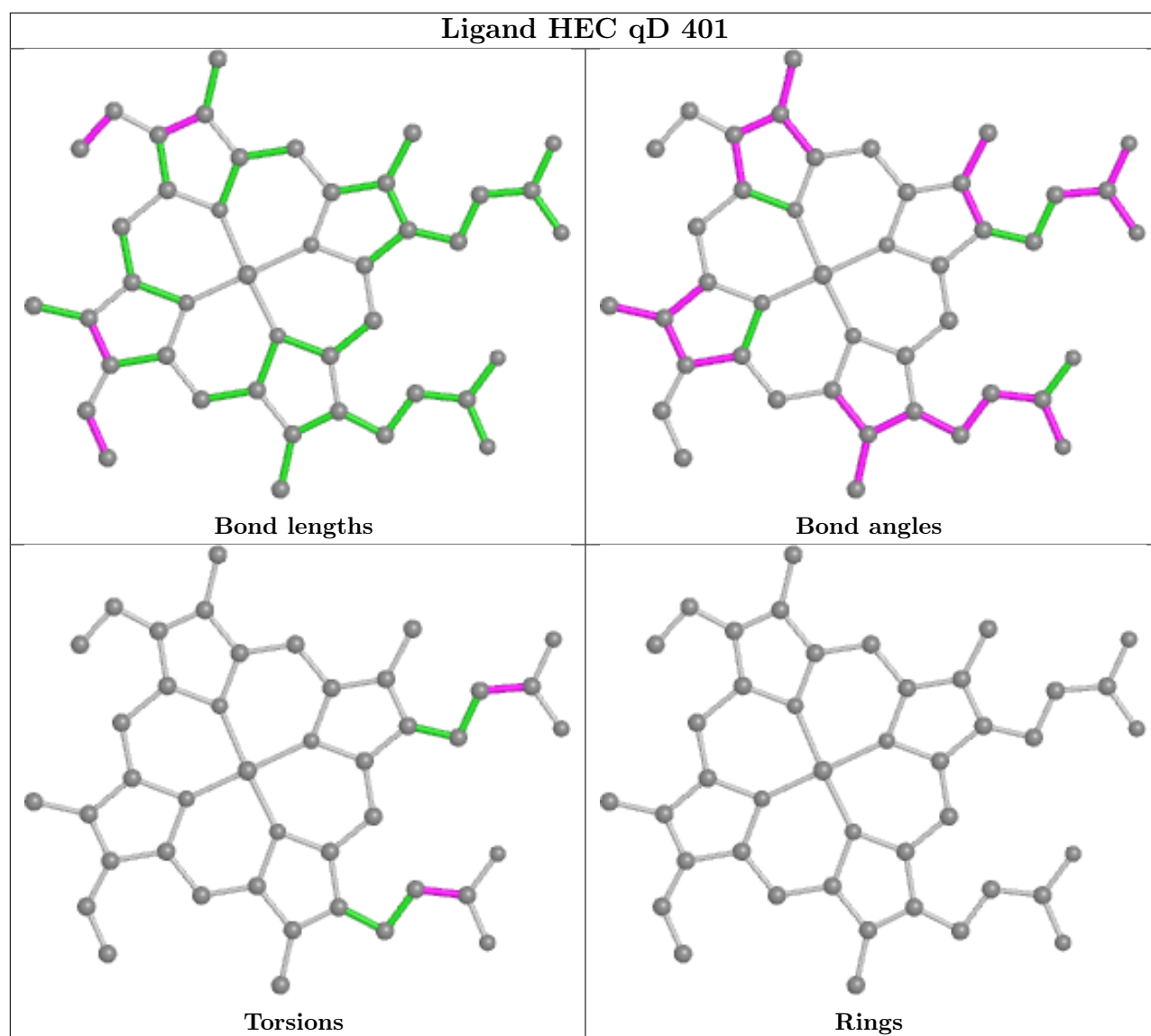


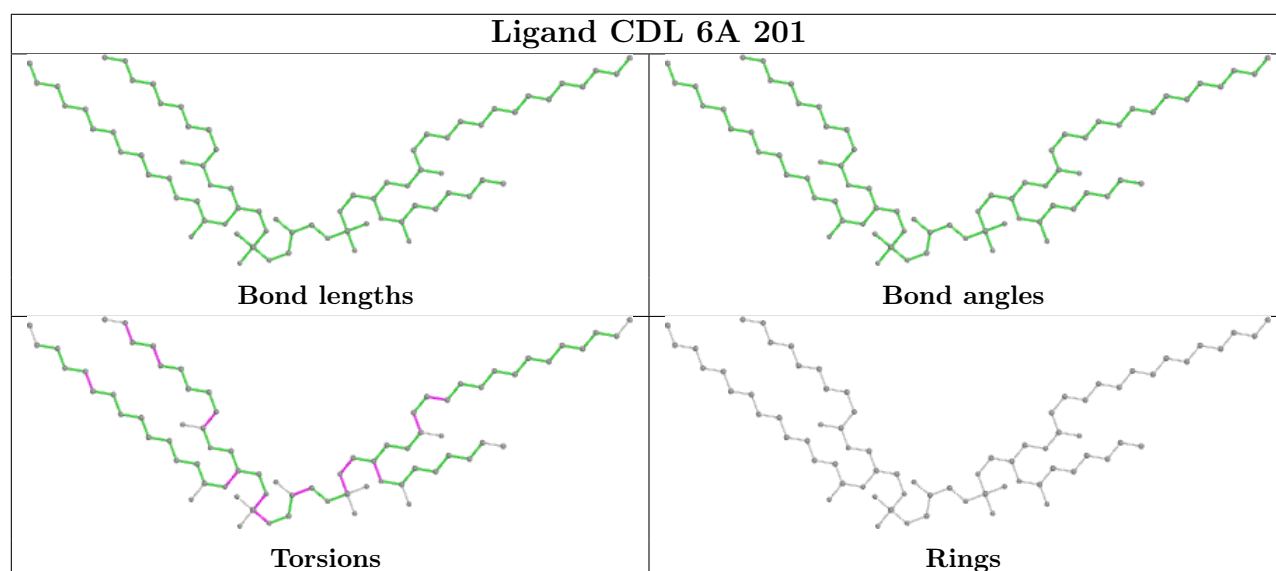
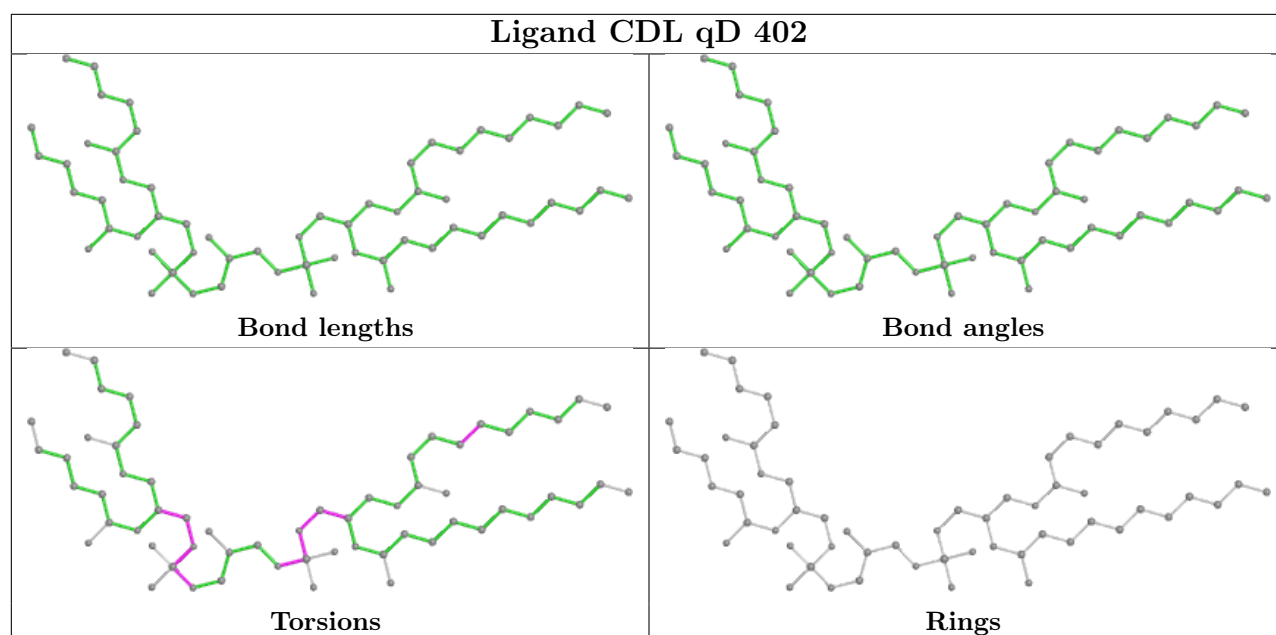


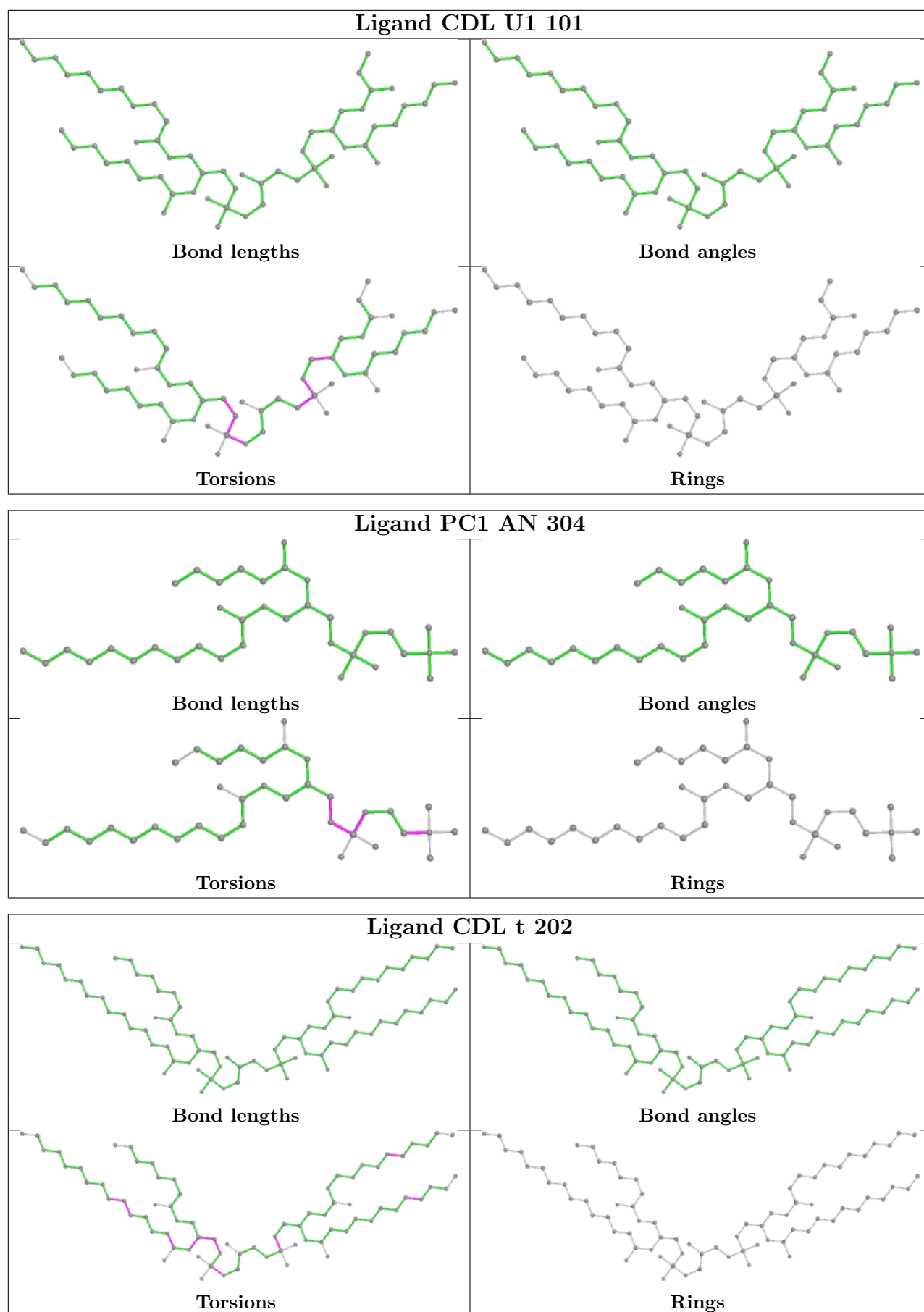


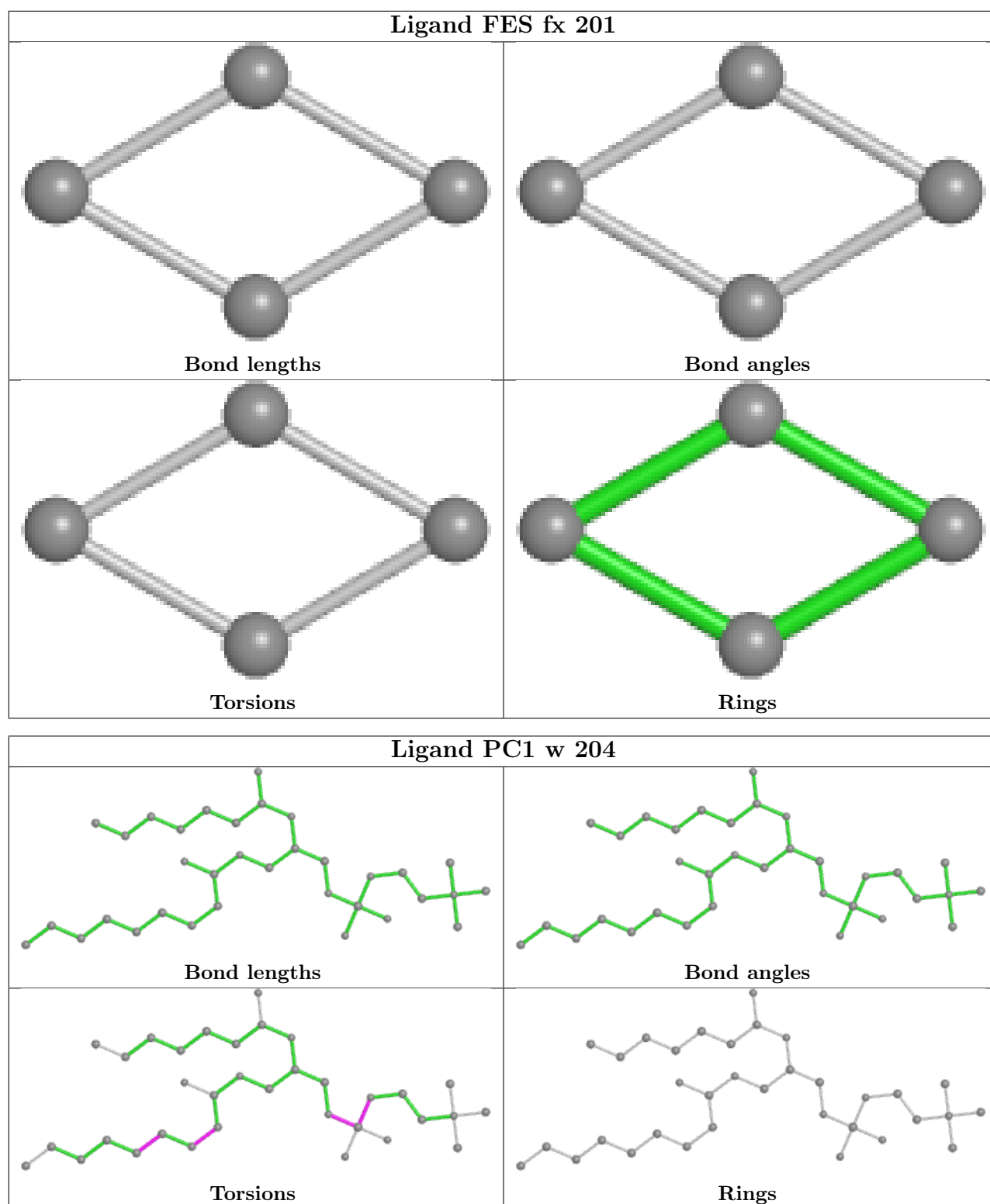


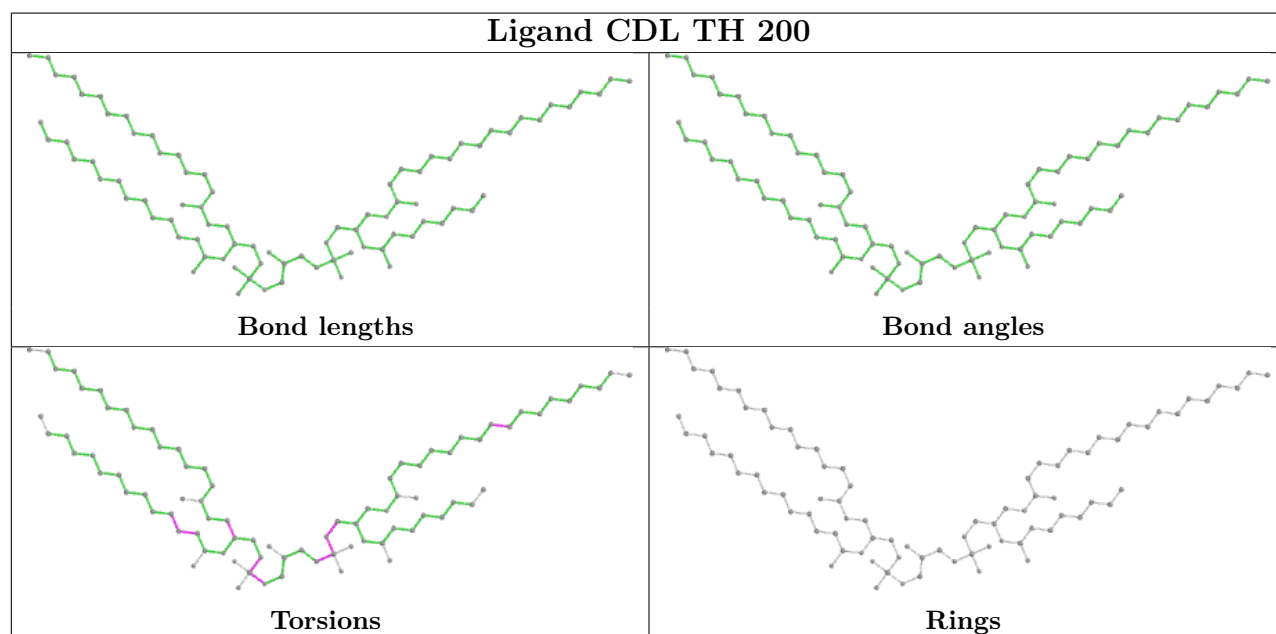
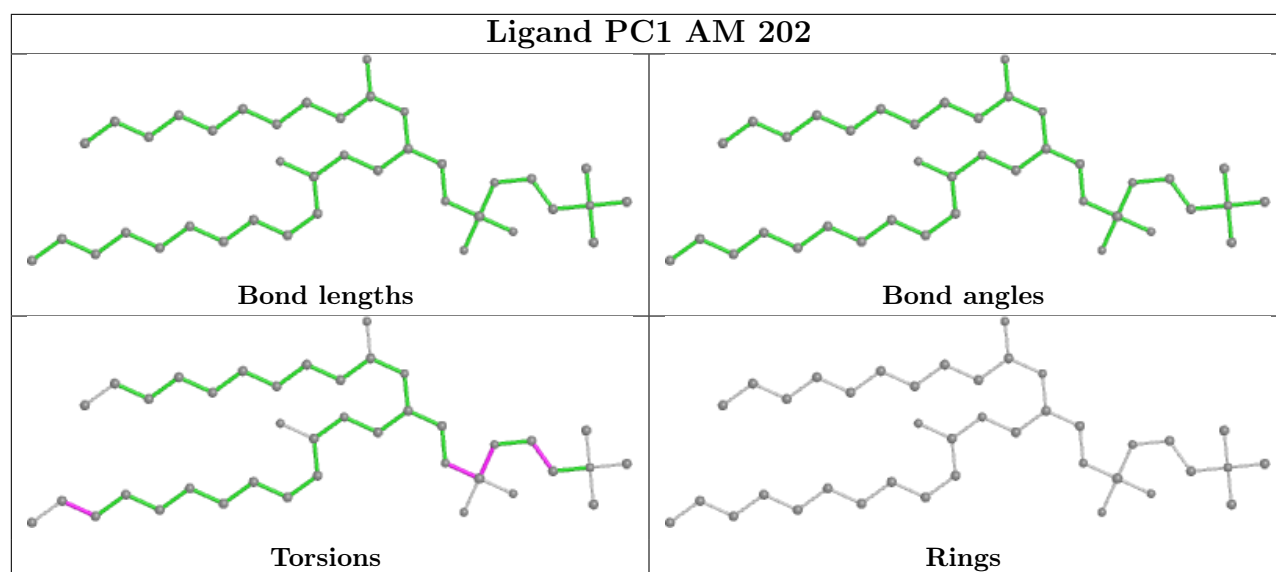


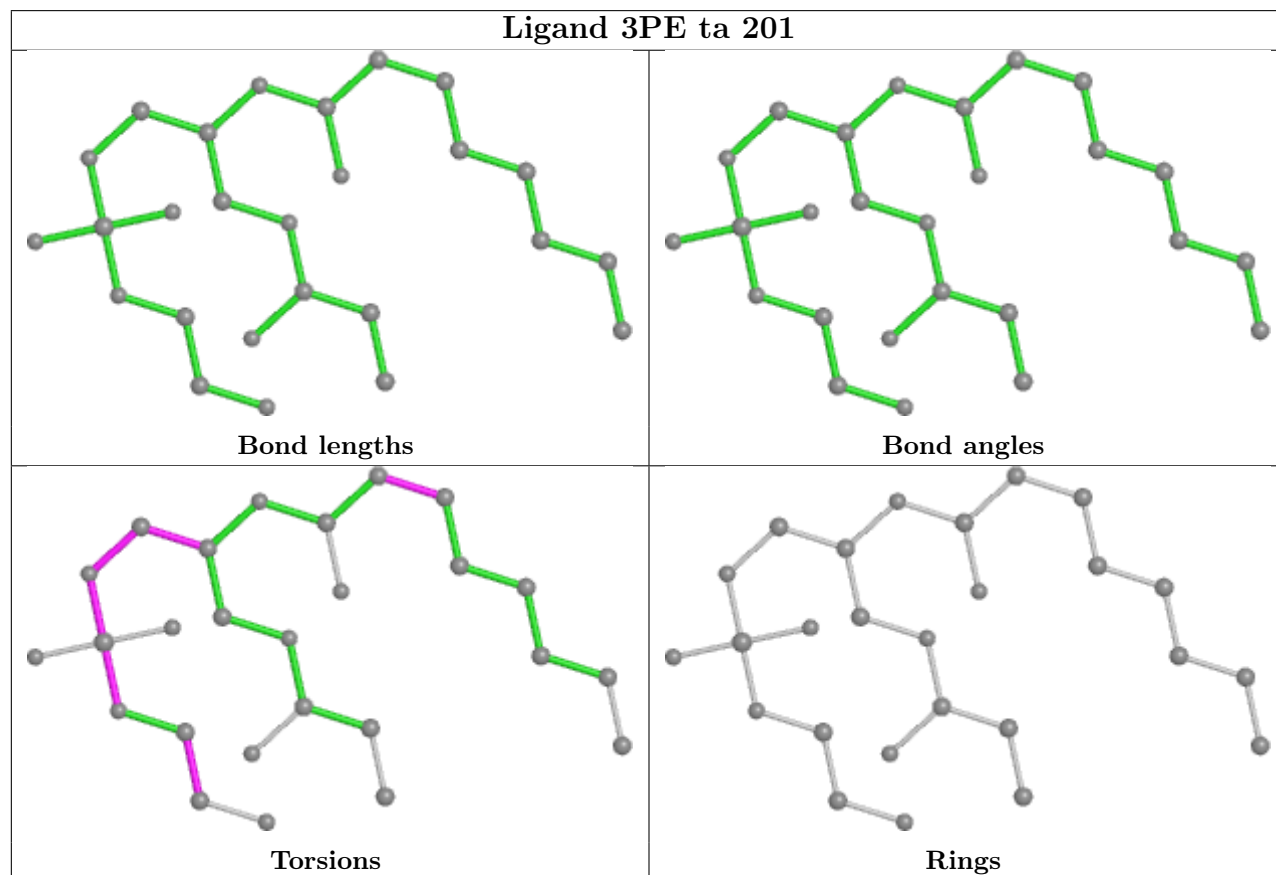
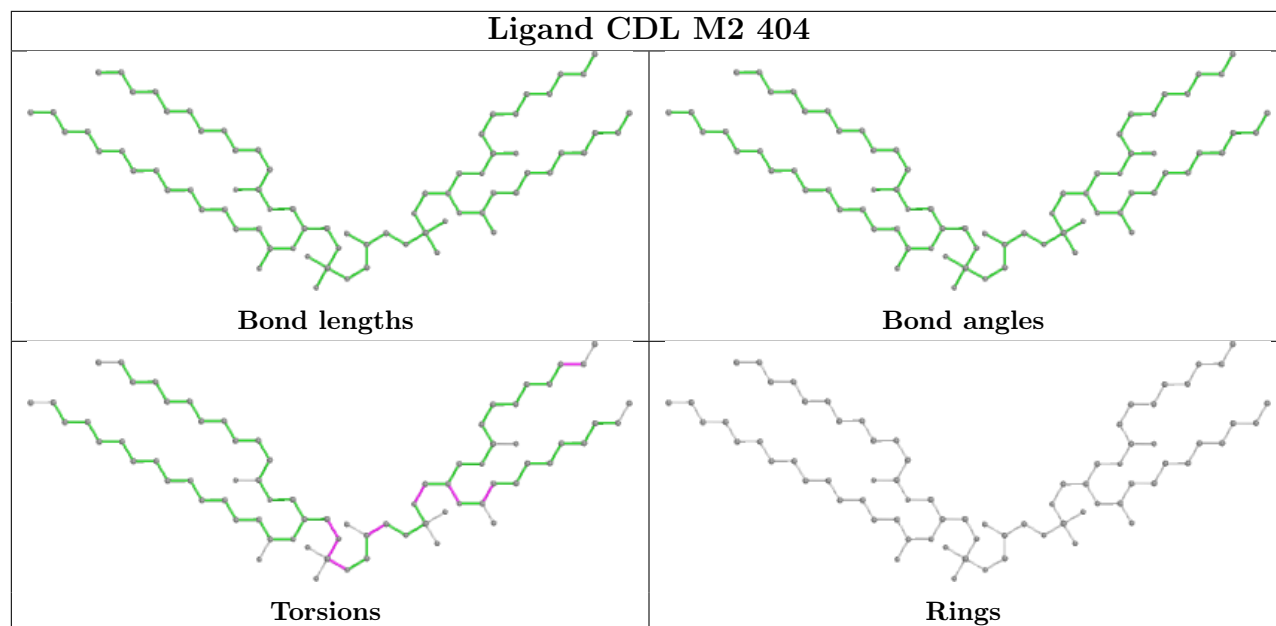


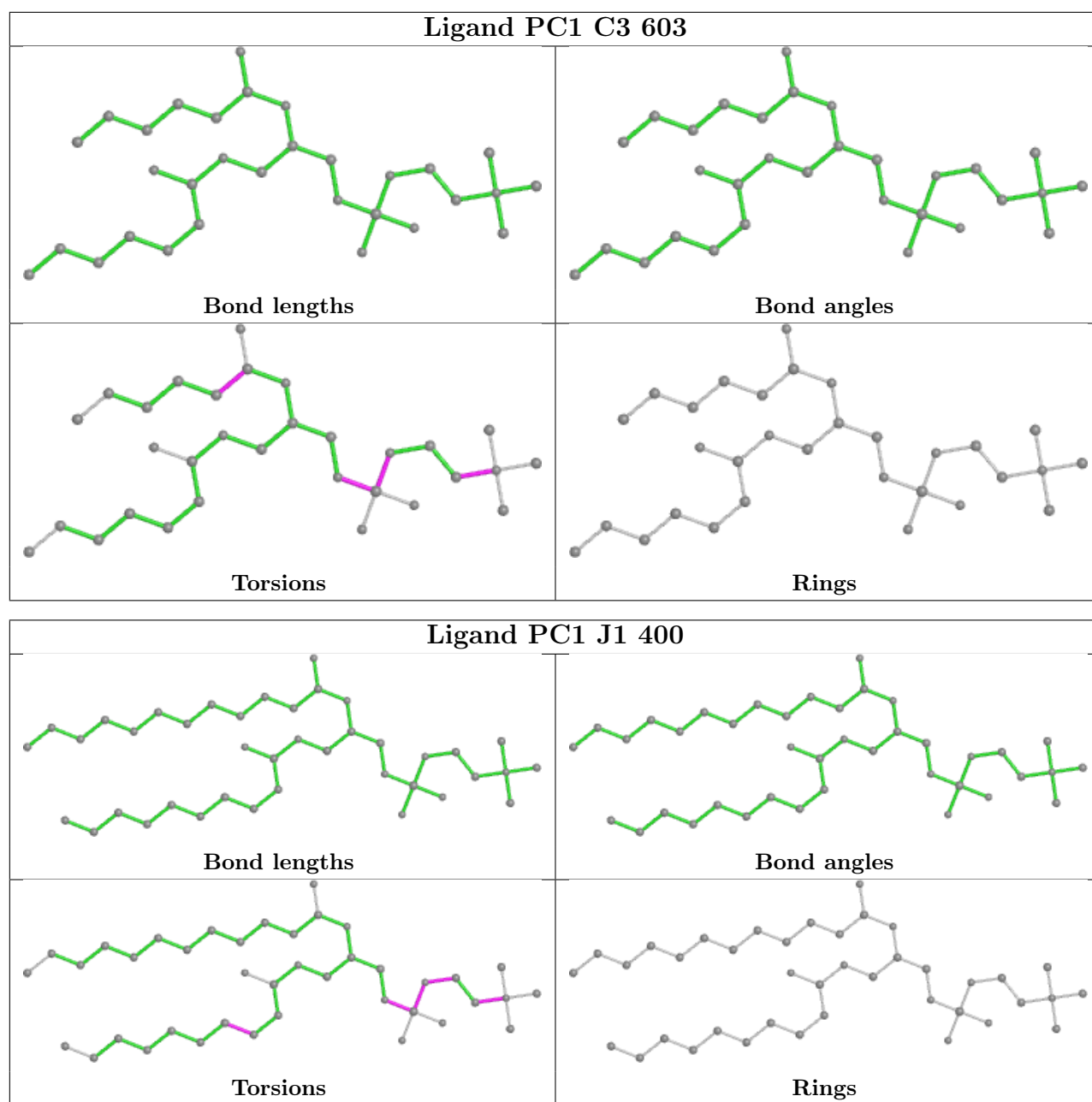


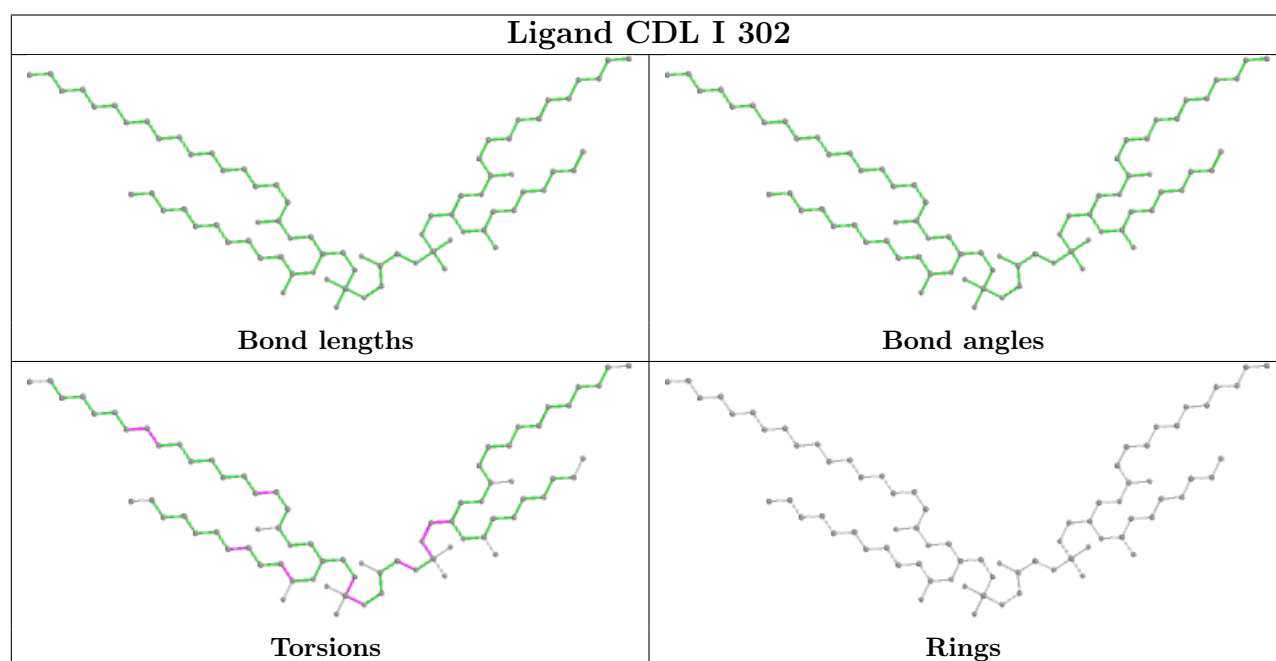
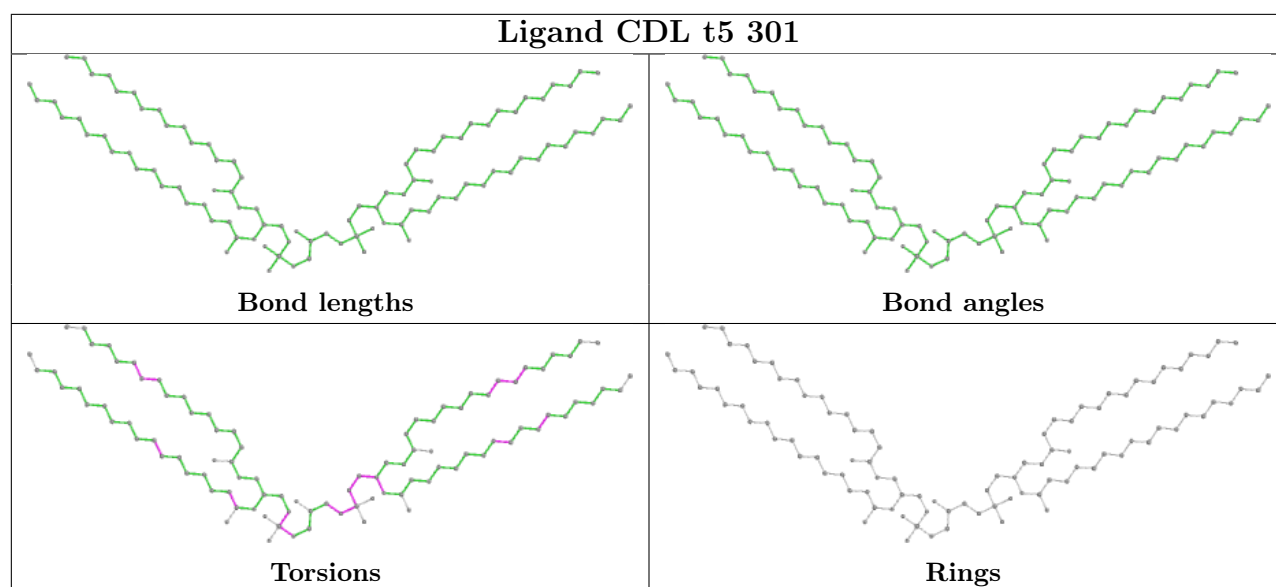




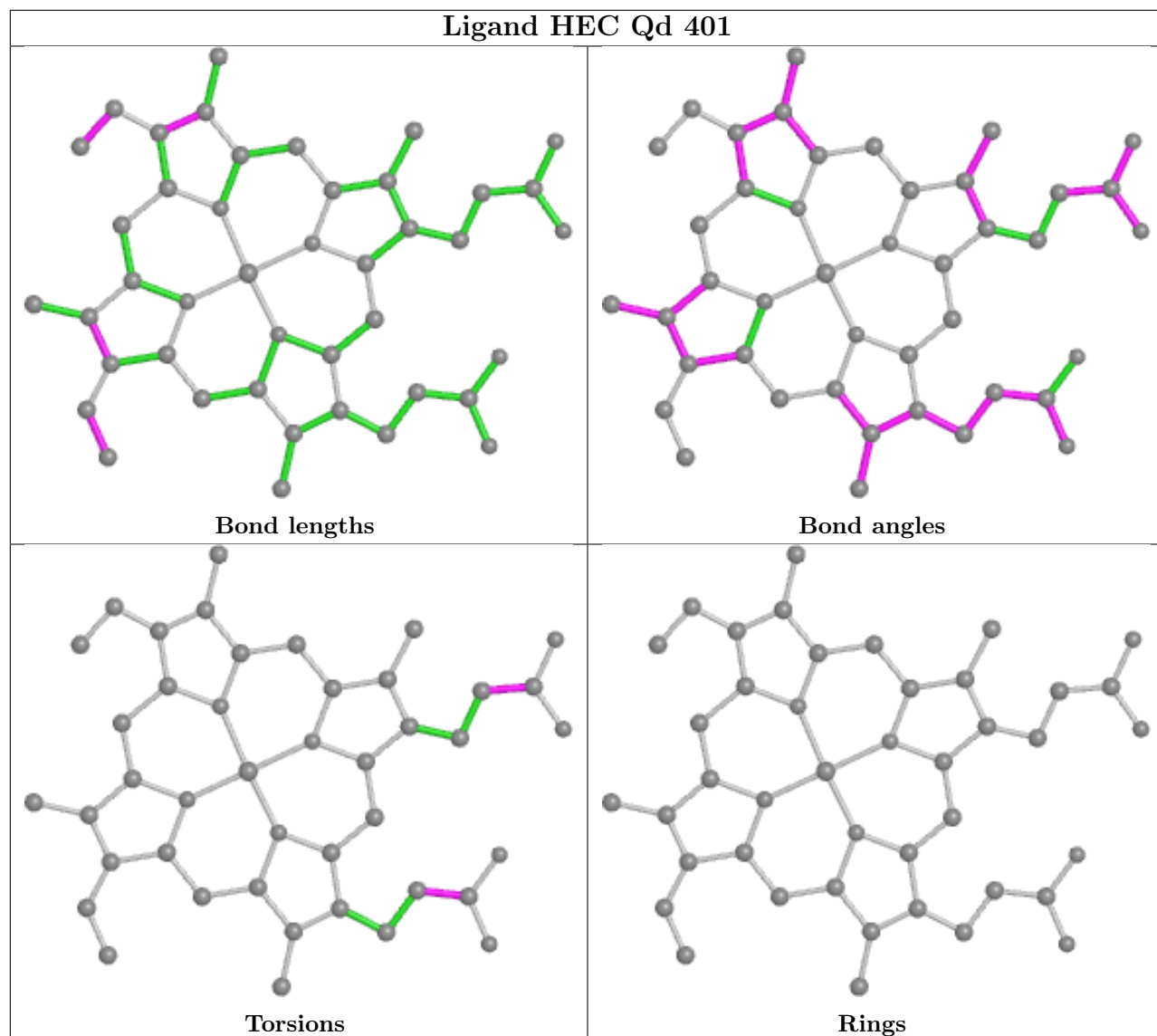


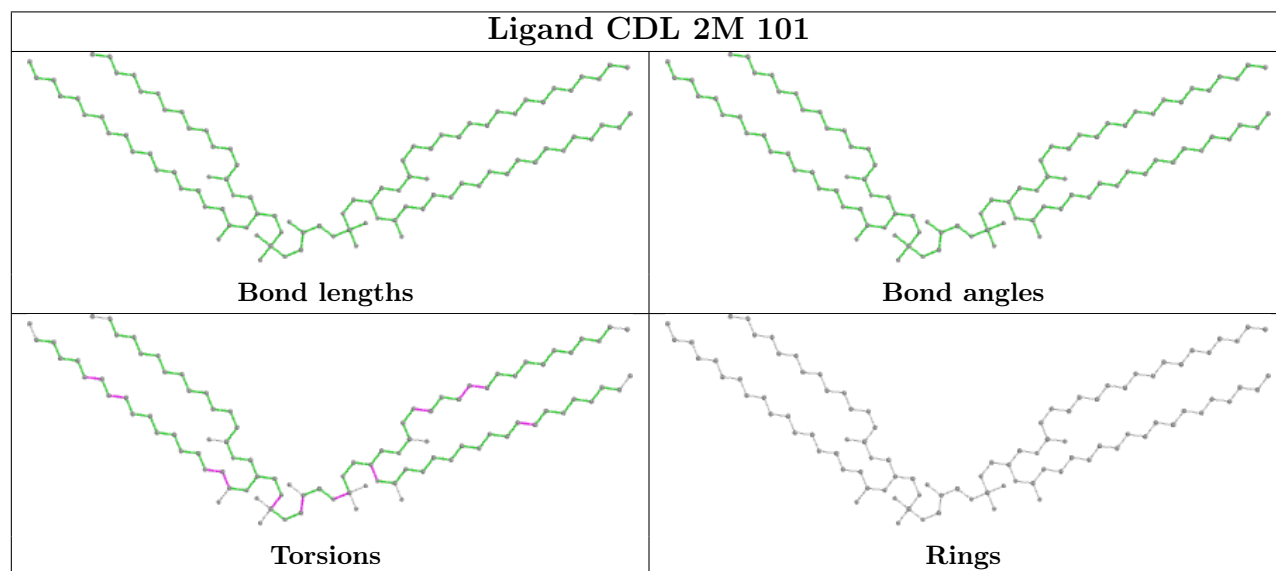
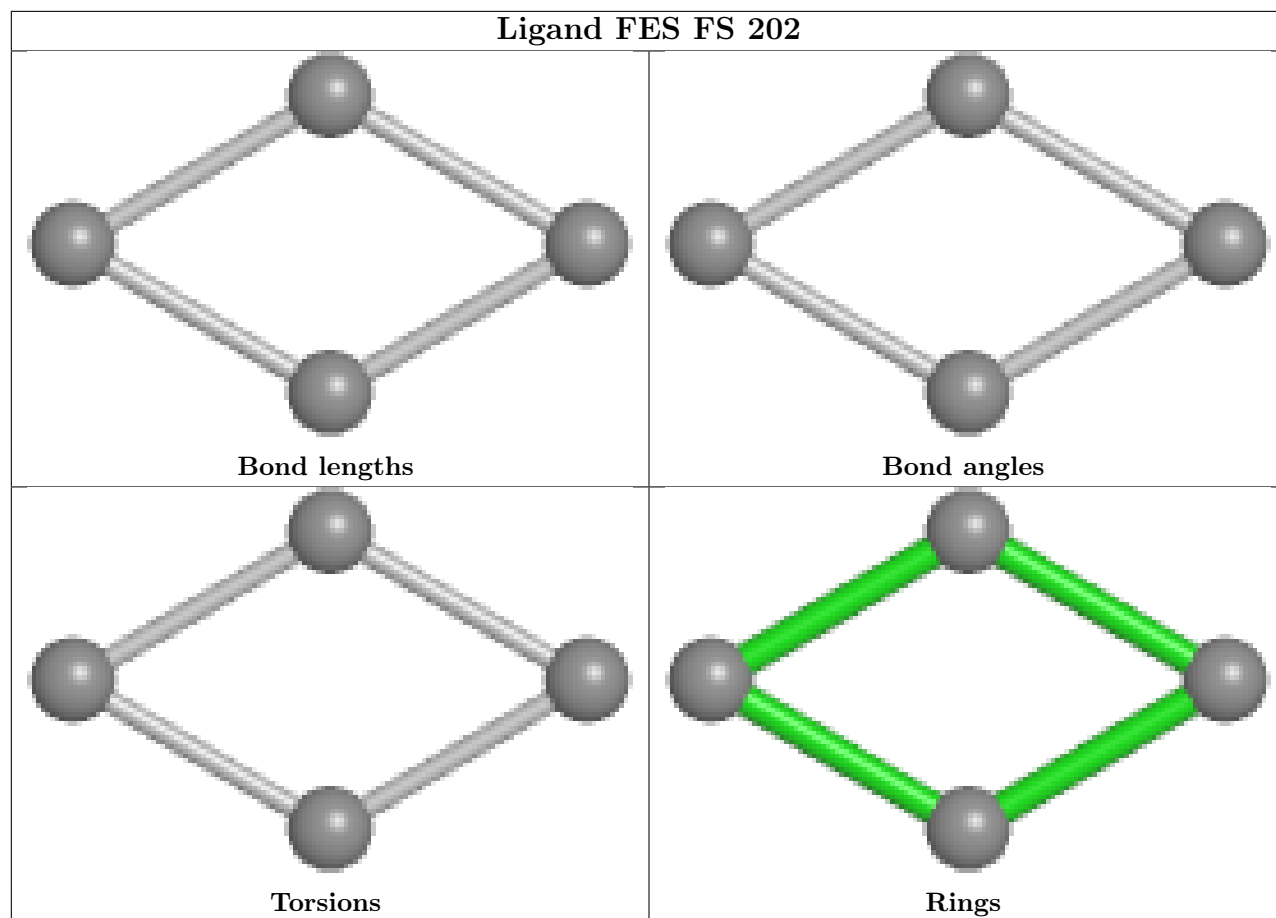


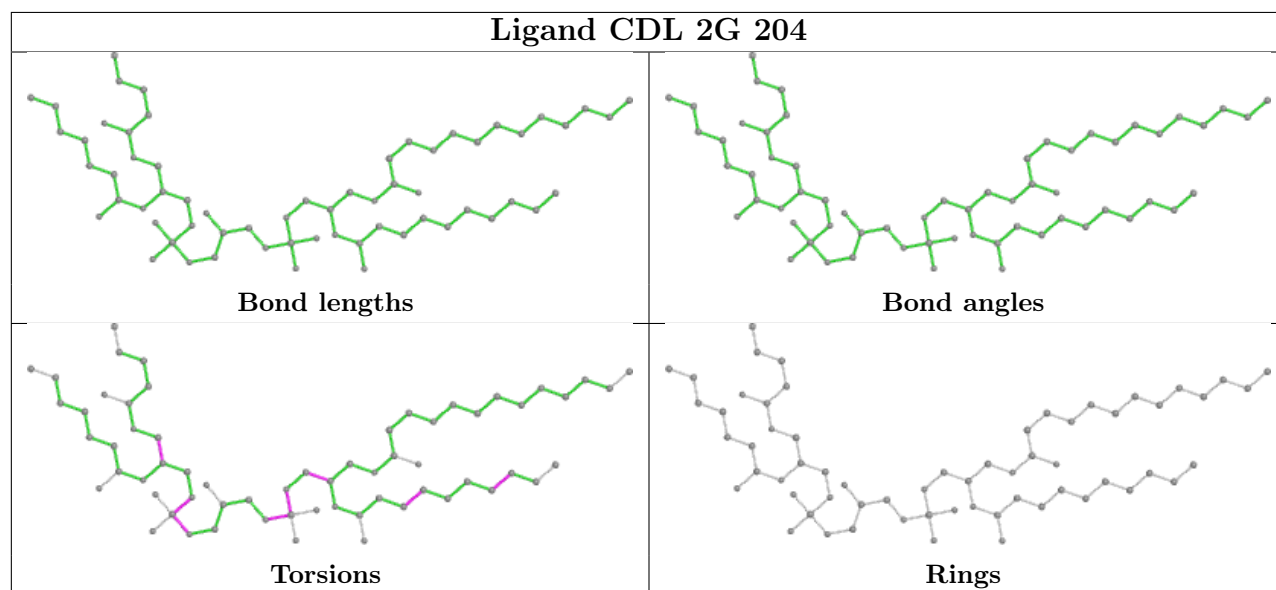
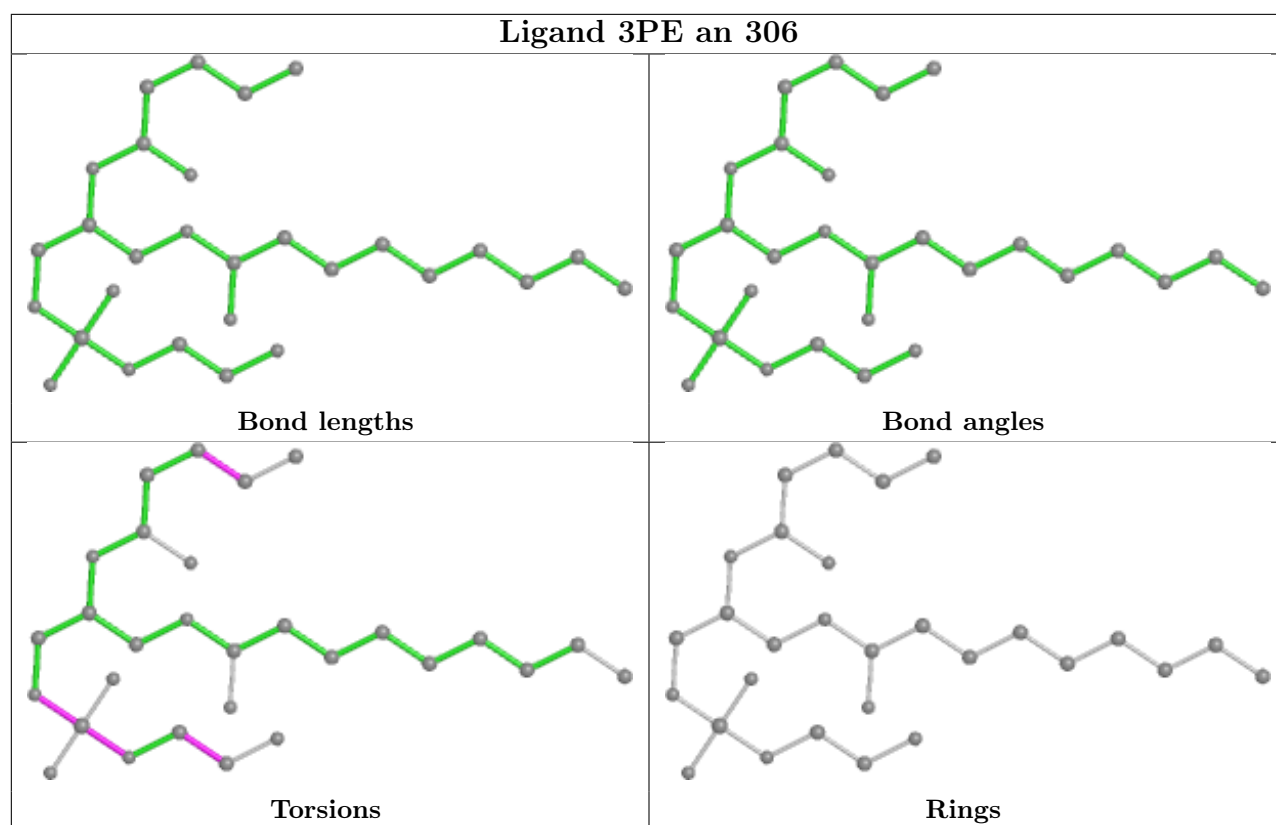


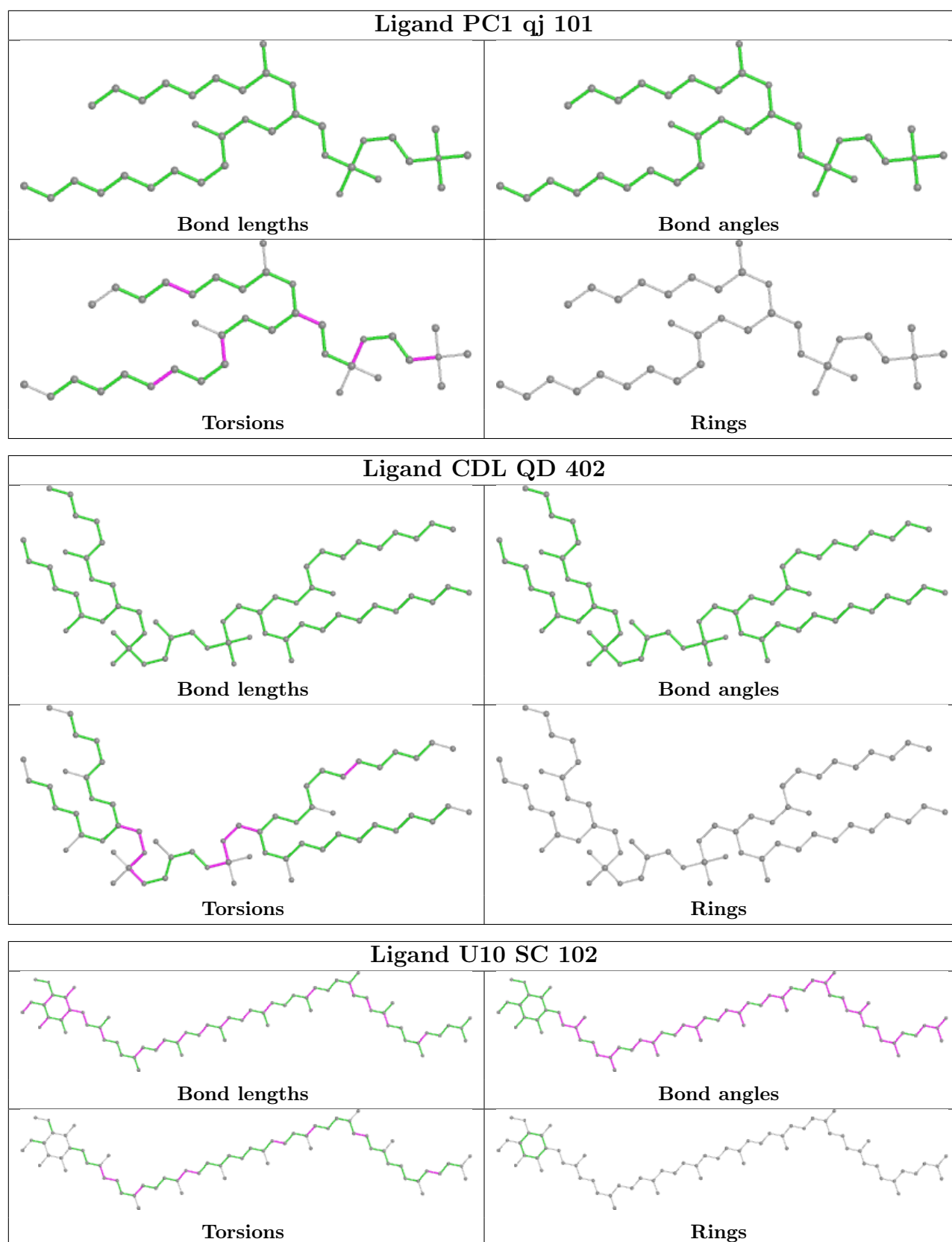


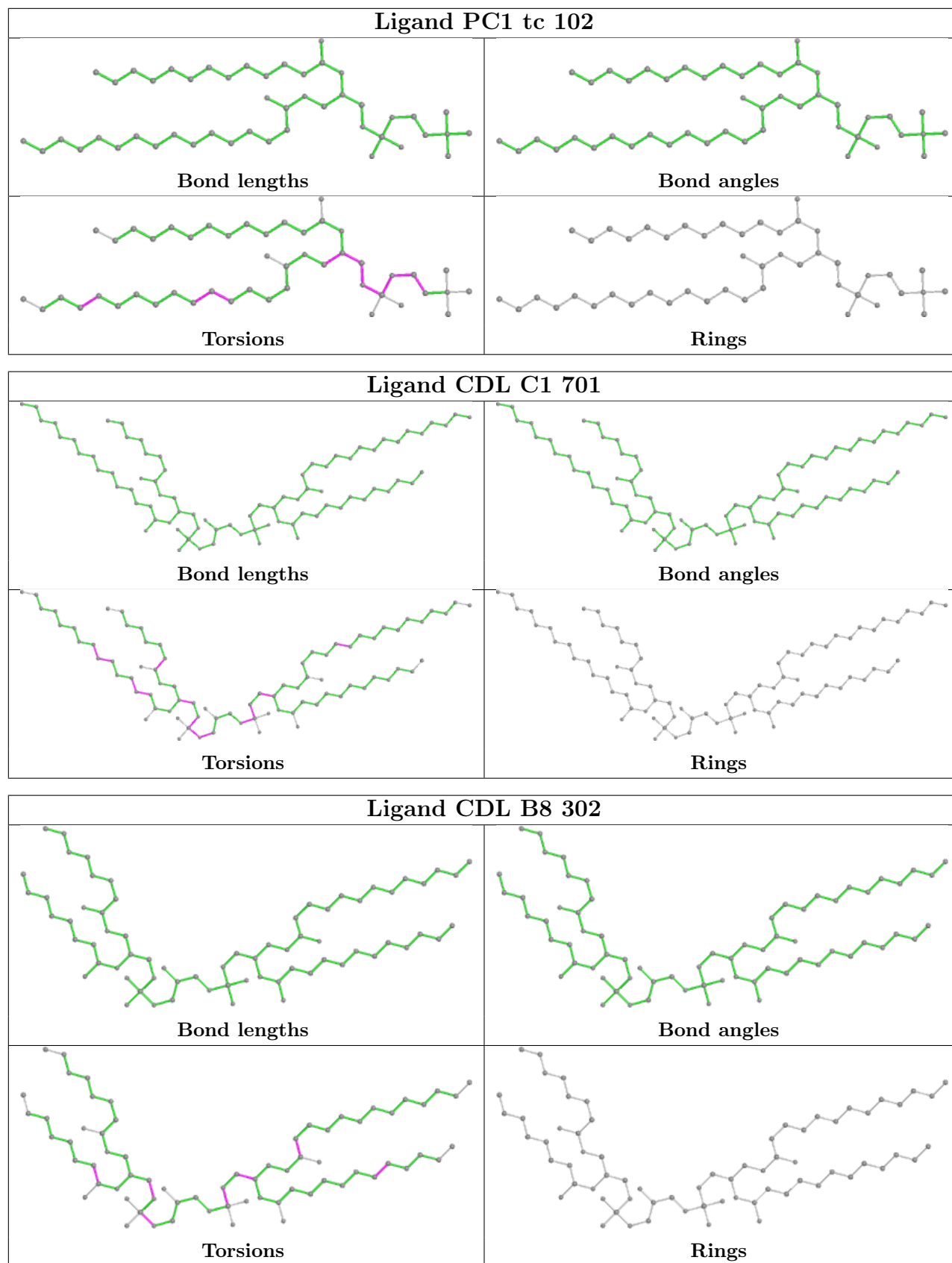
Ligand HEC Qd 401



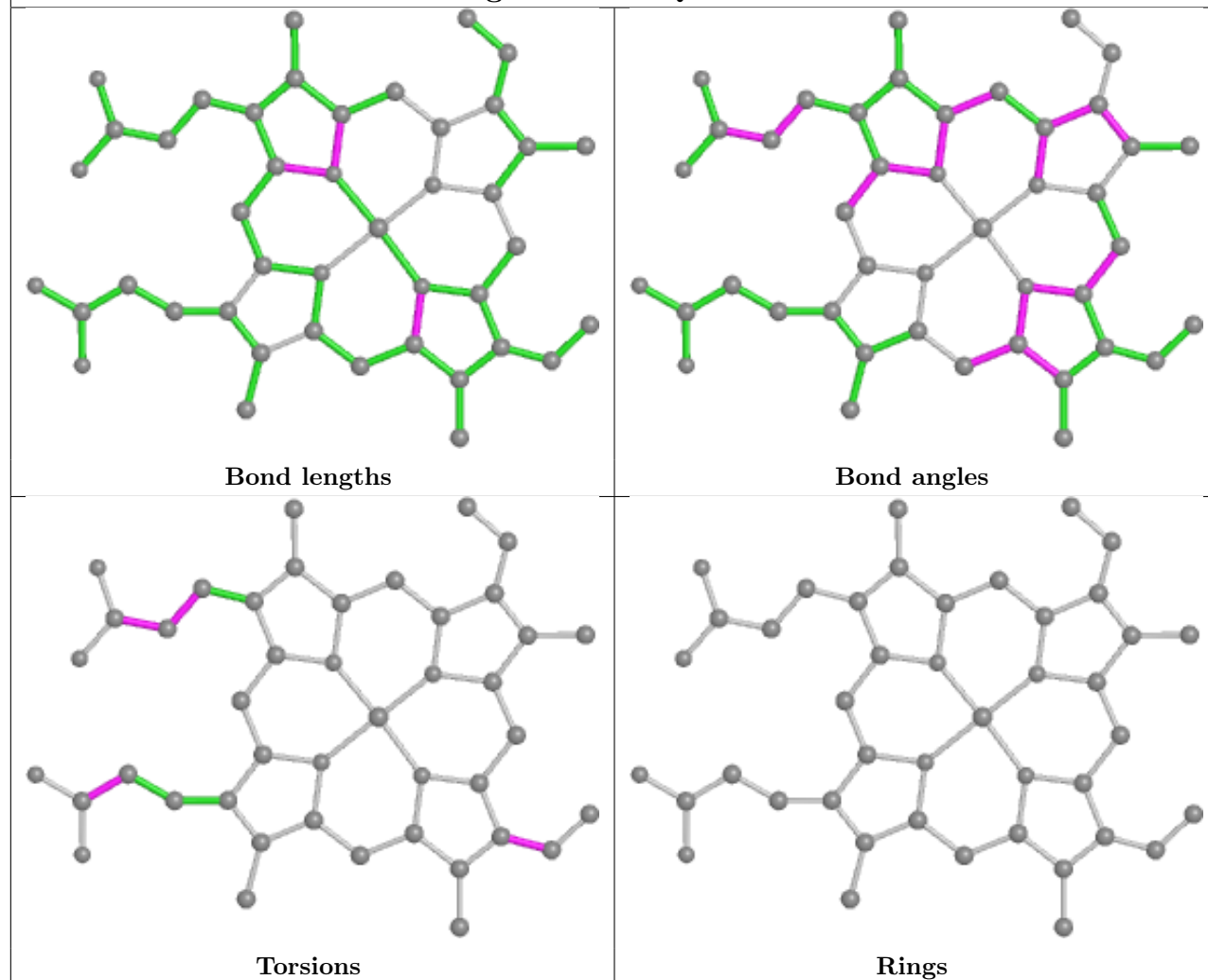




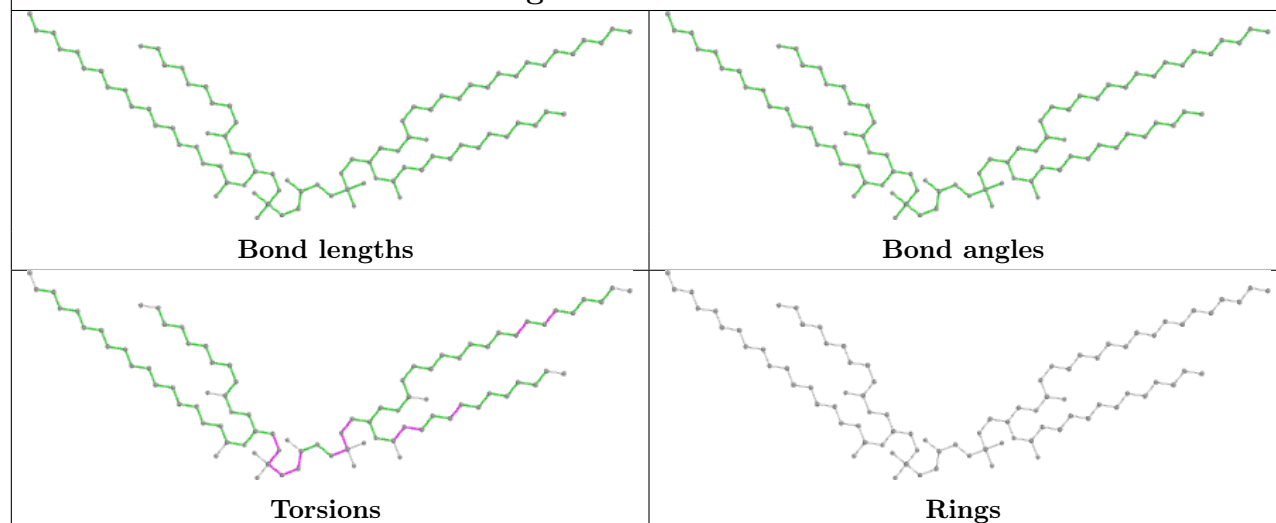


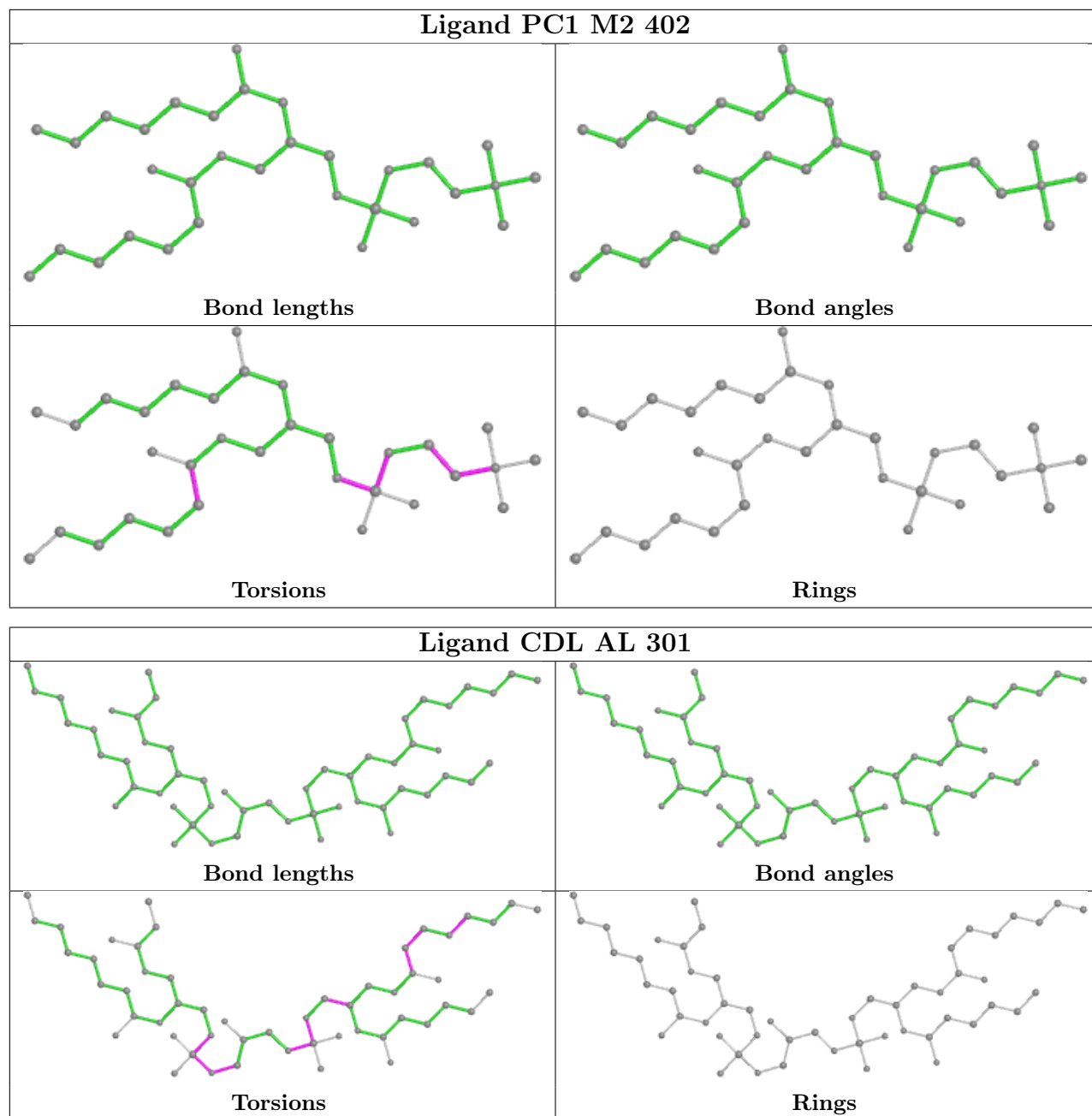


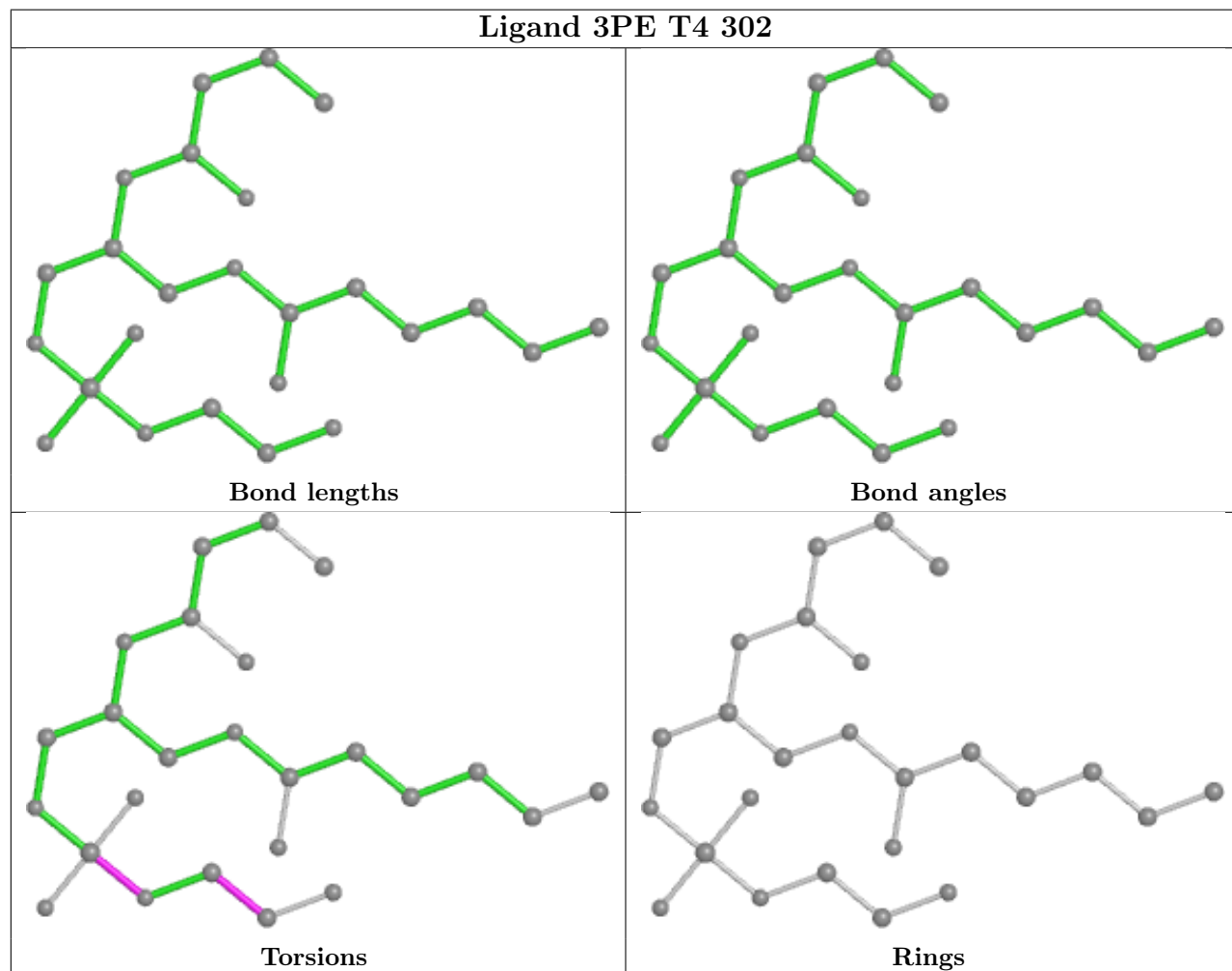
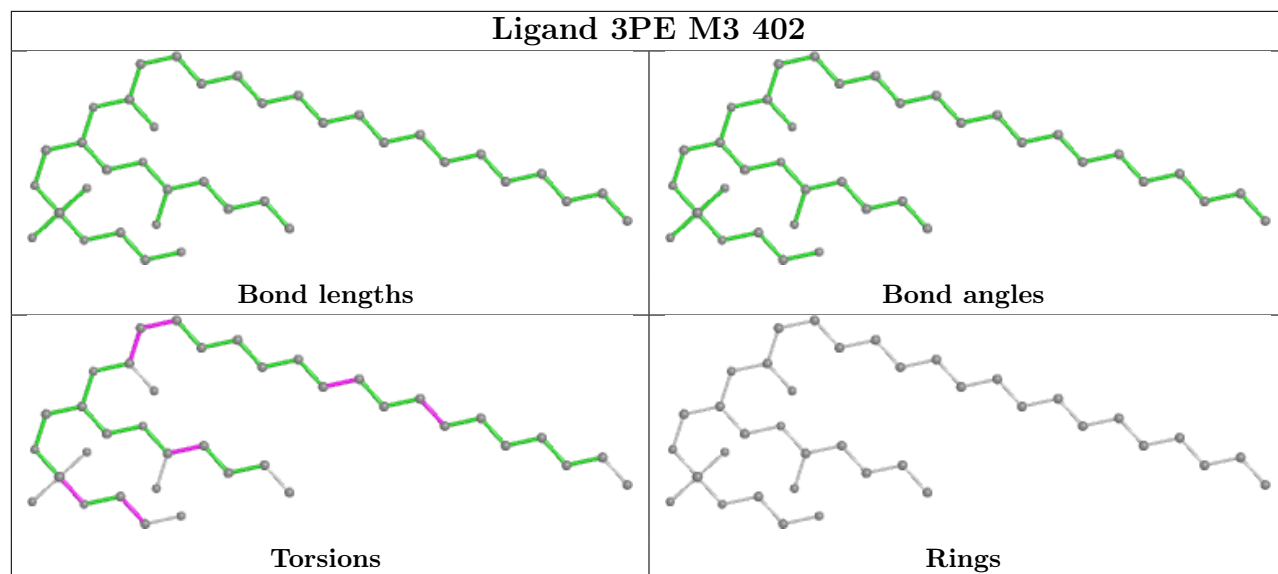
Ligand HEM QC 502

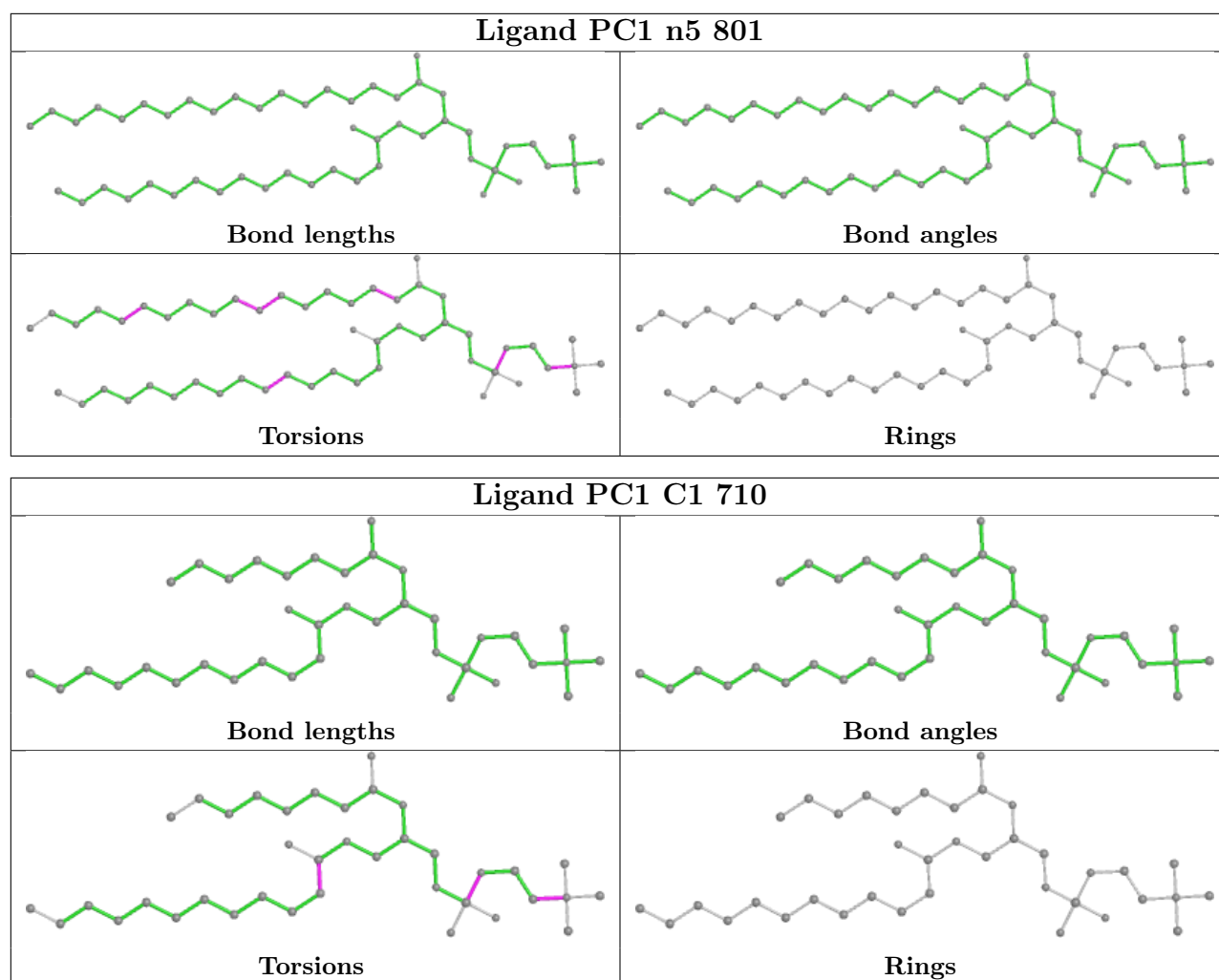


Ligand CDL an 302

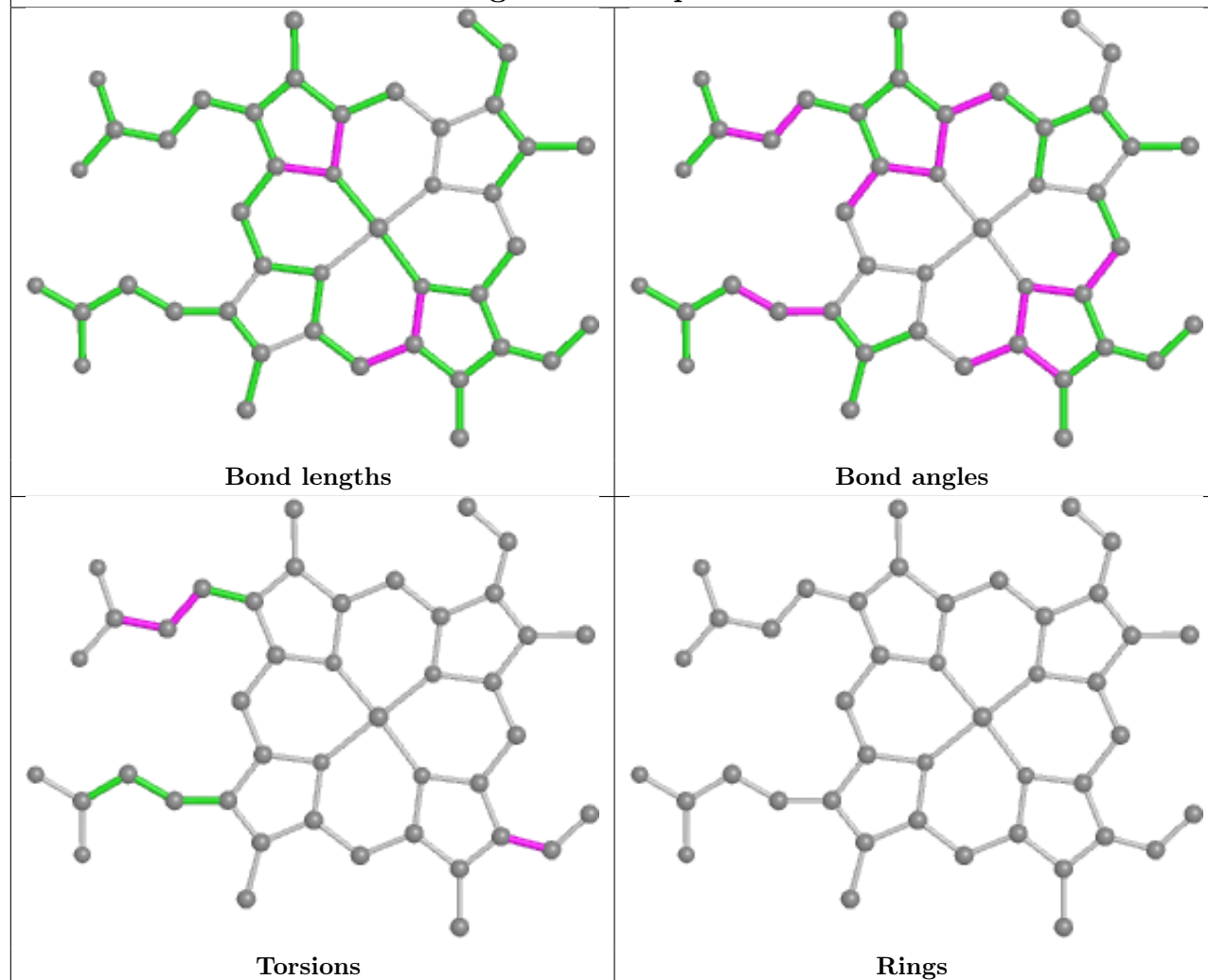




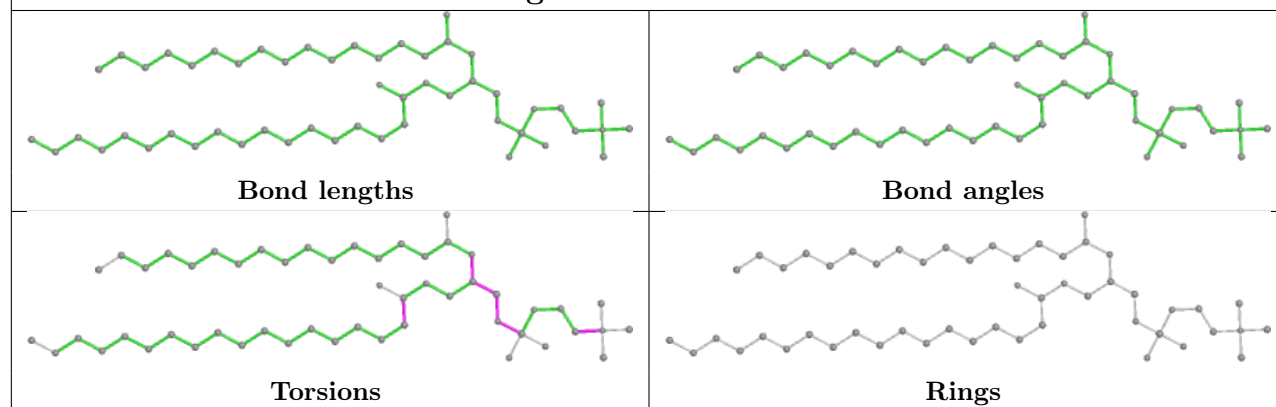


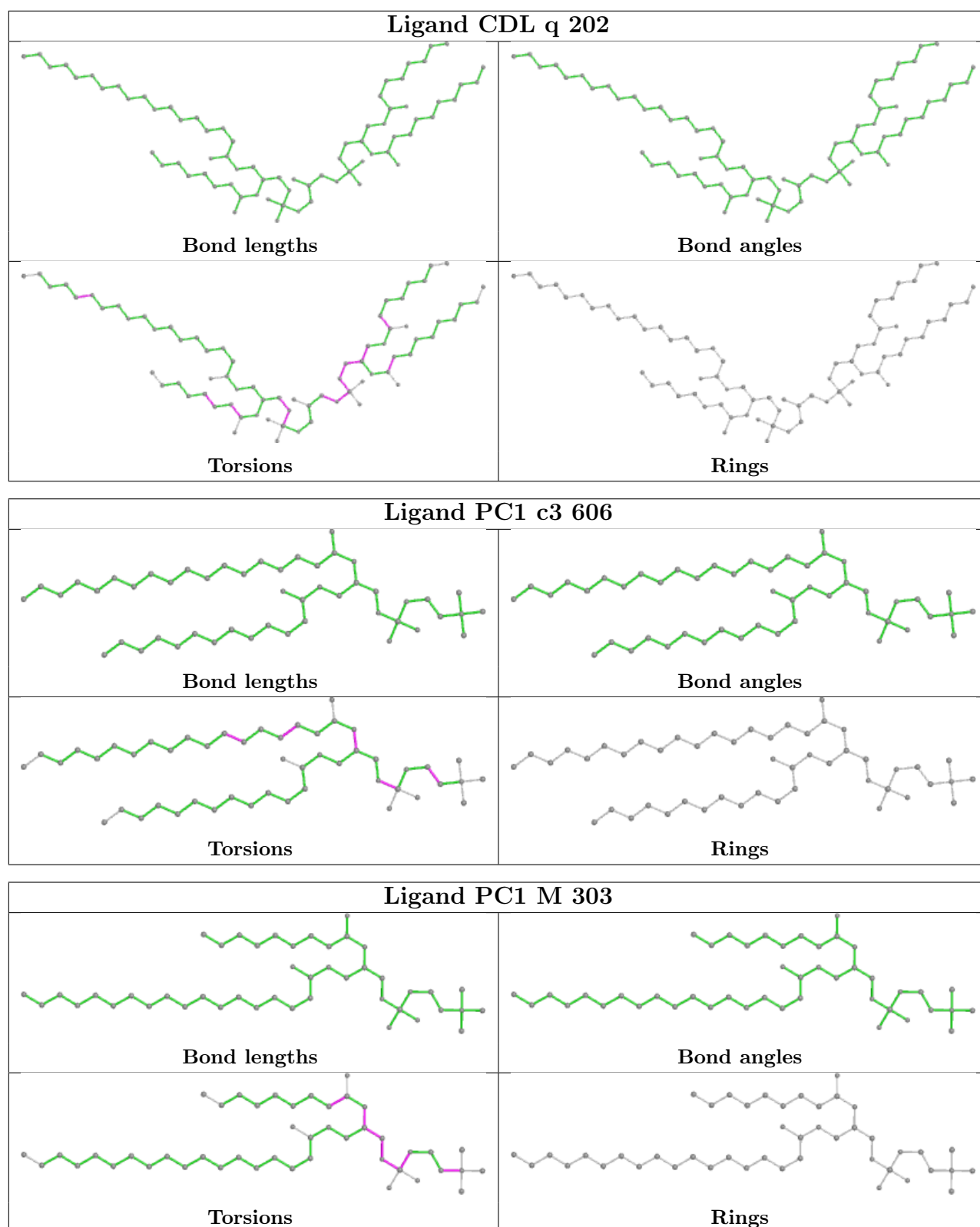


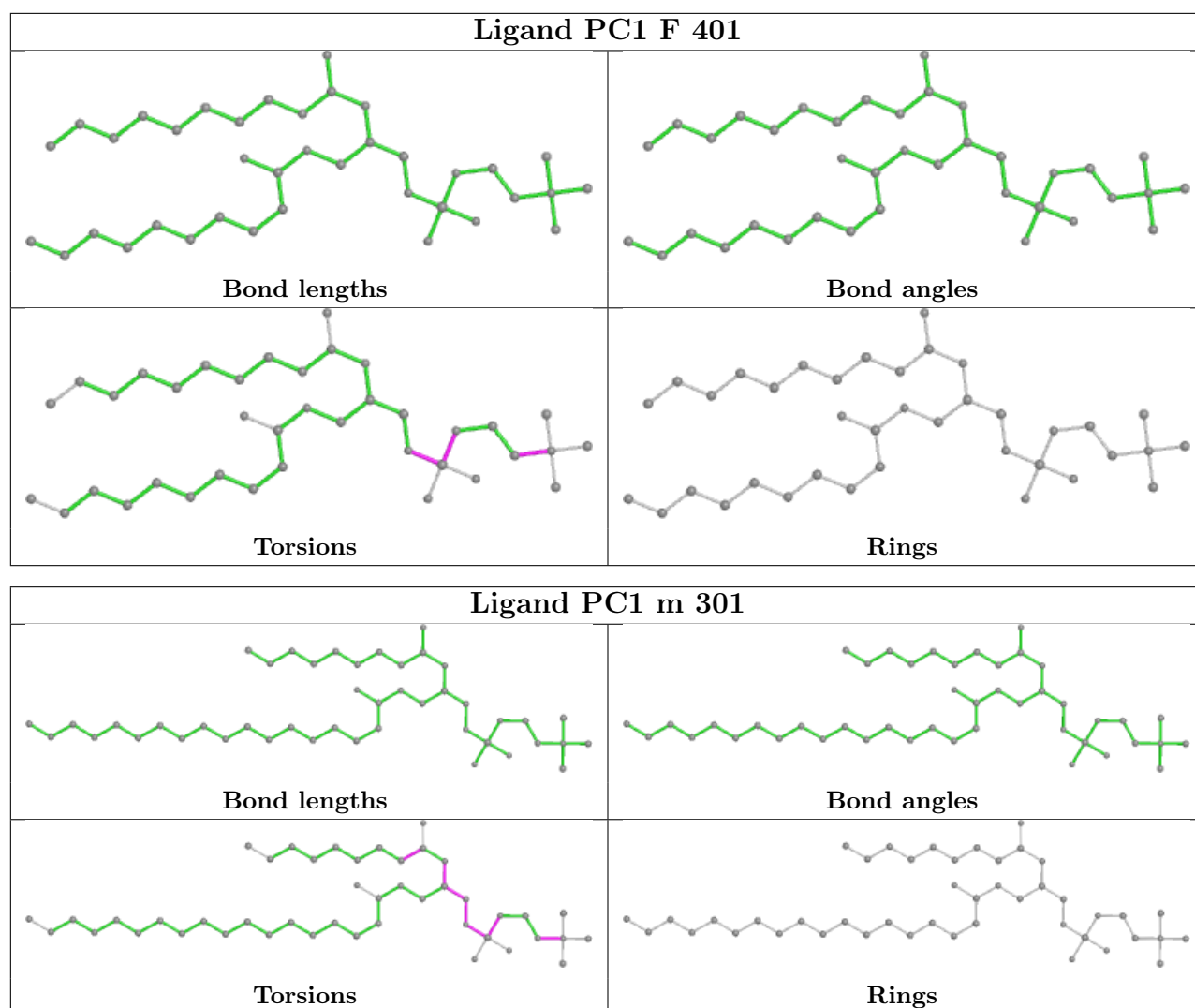
Ligand HEM qC 501

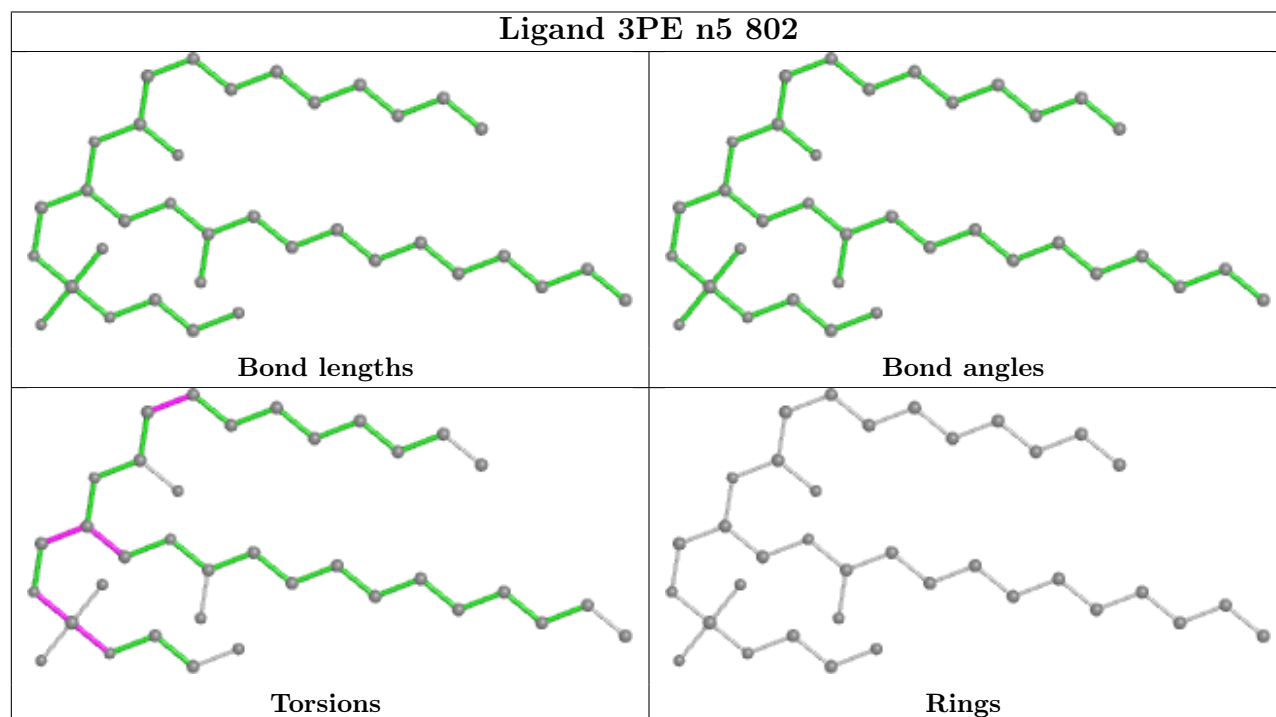
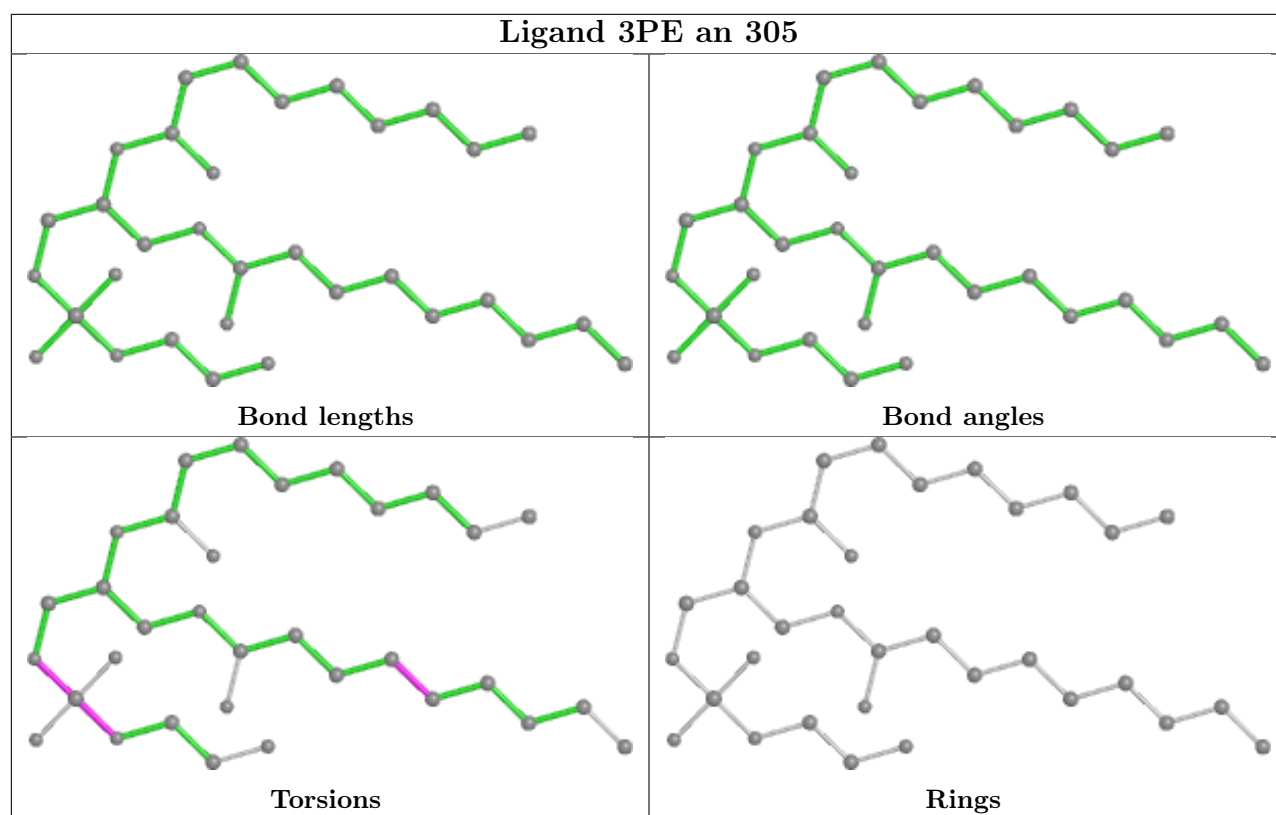


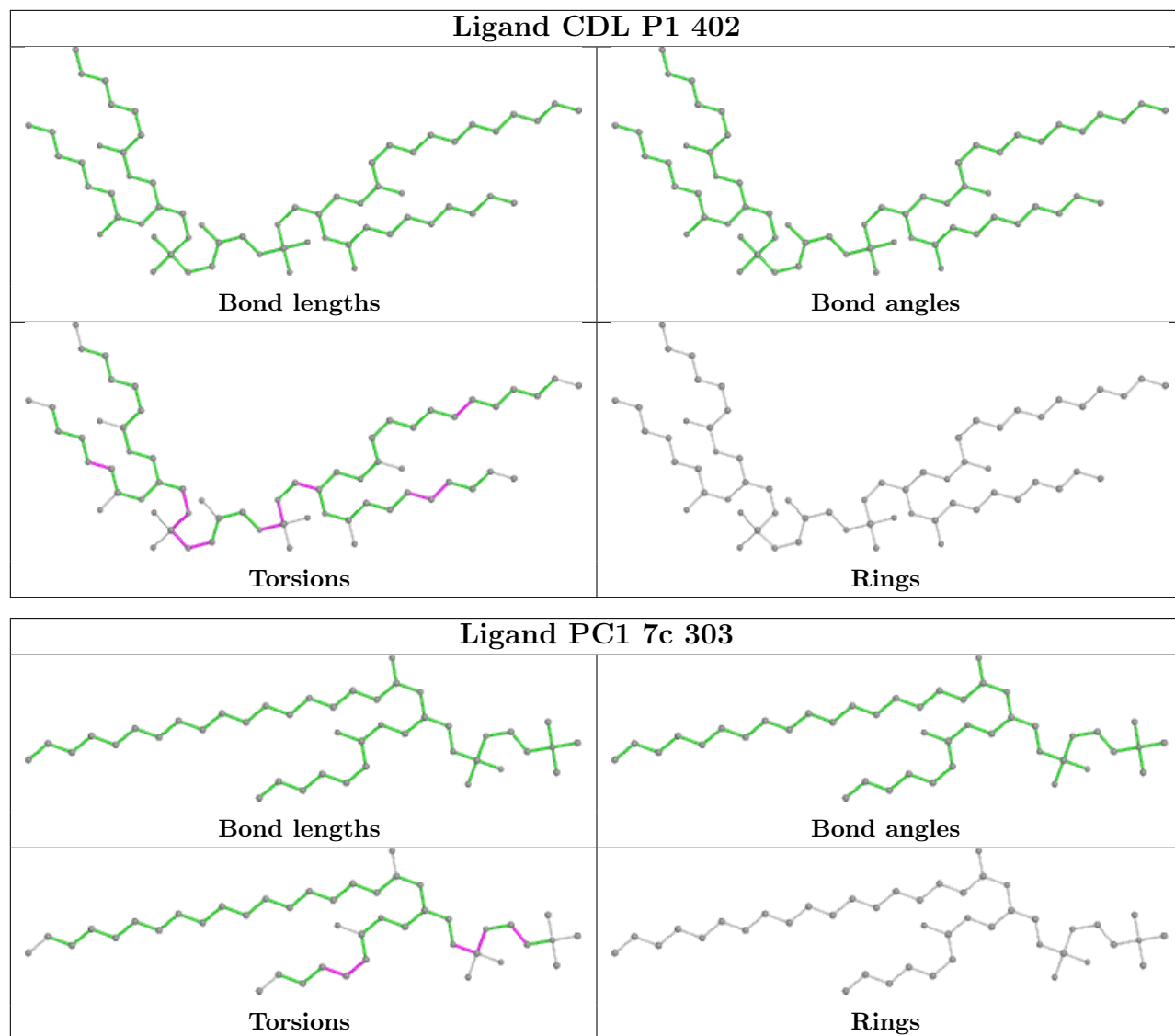
Ligand PC1 C3 601

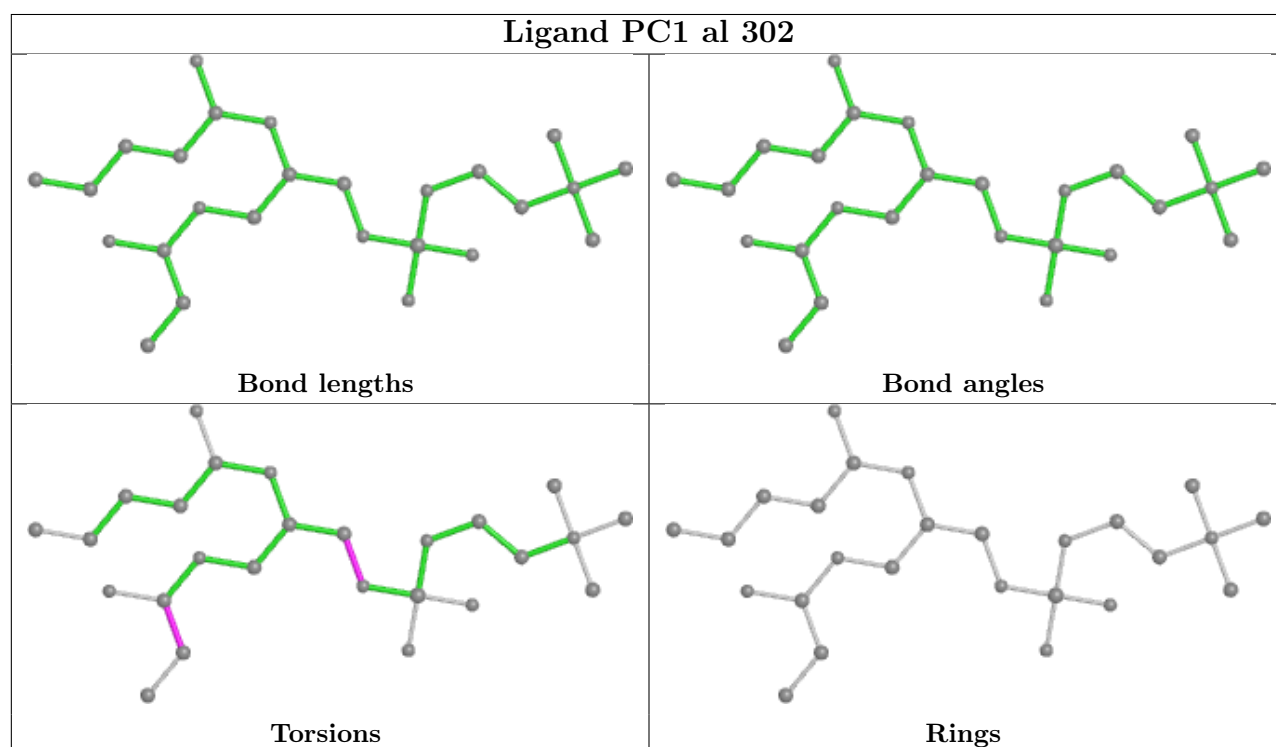
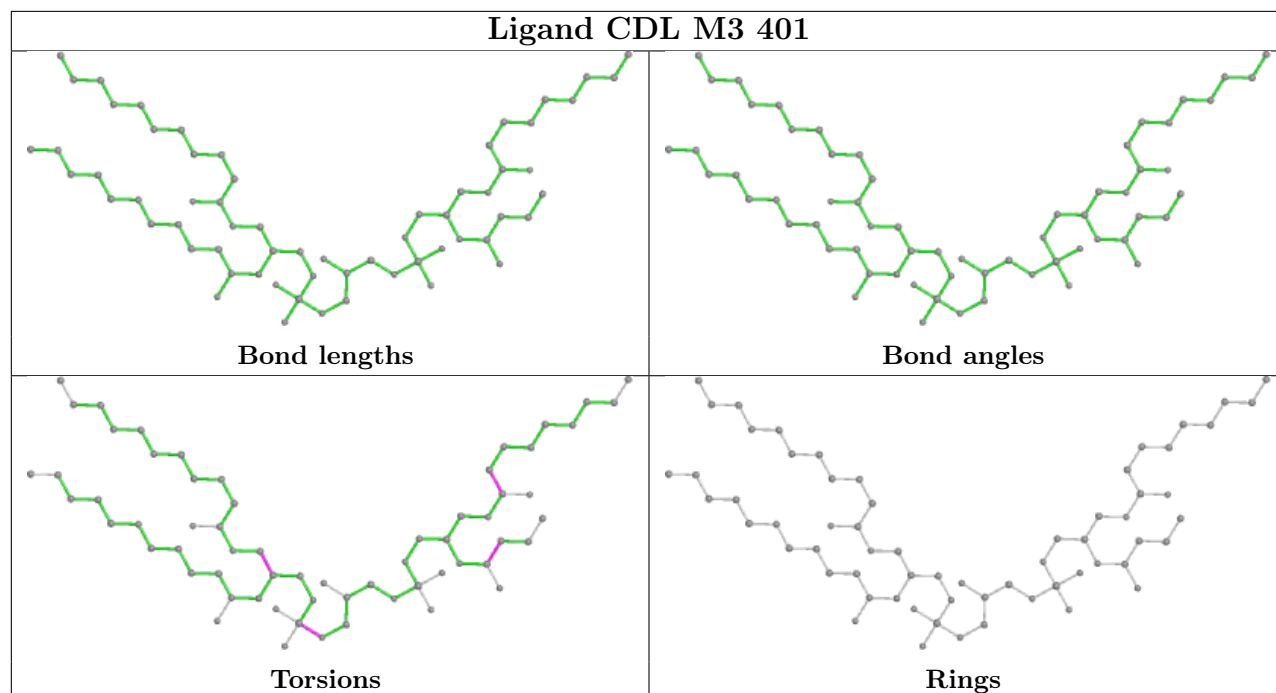


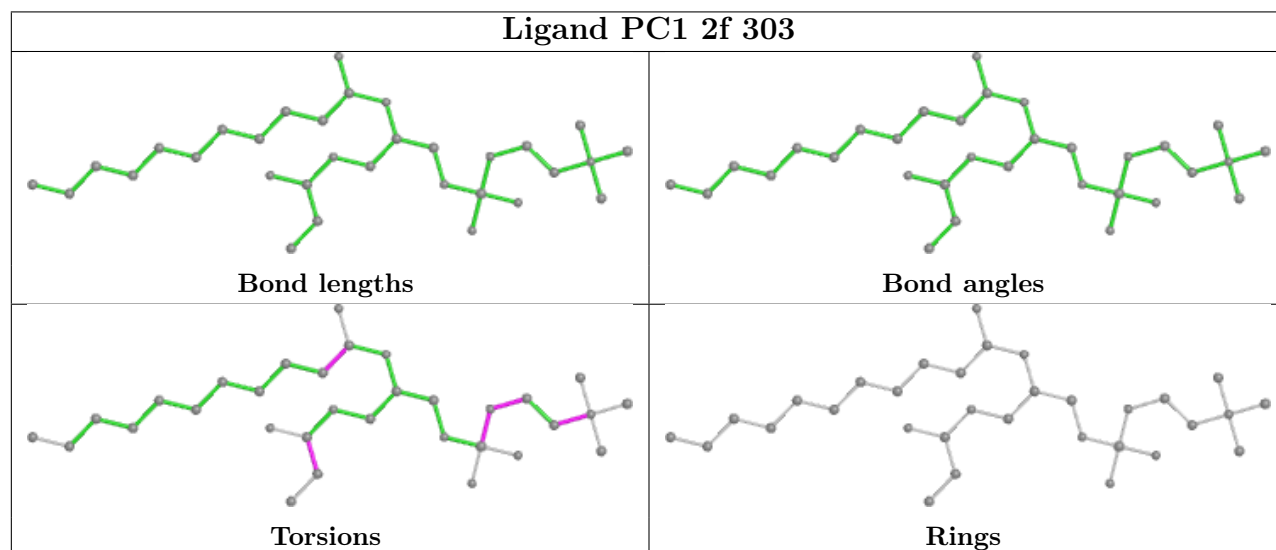
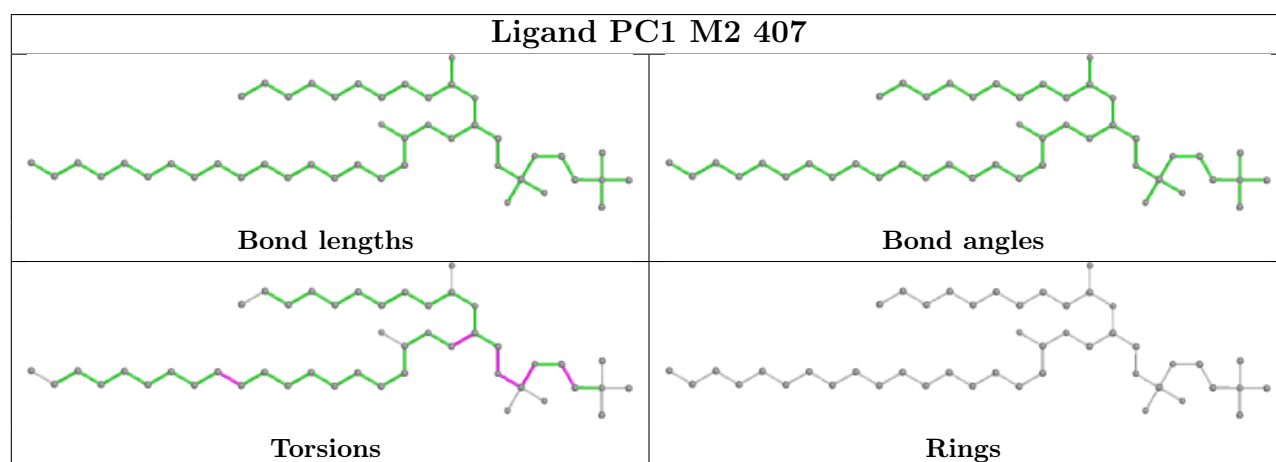
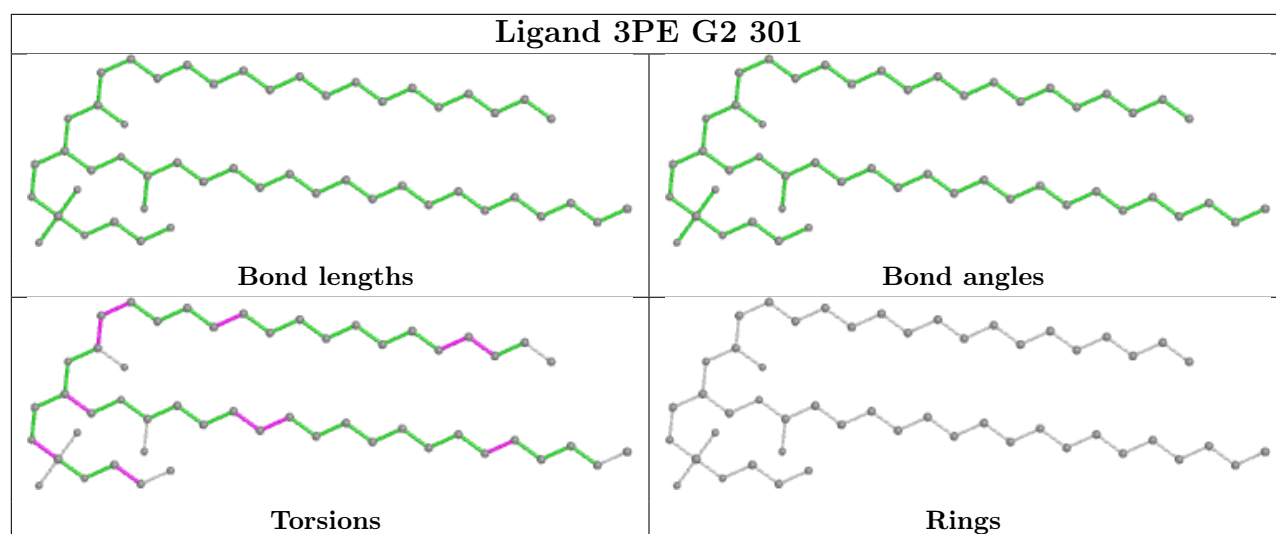


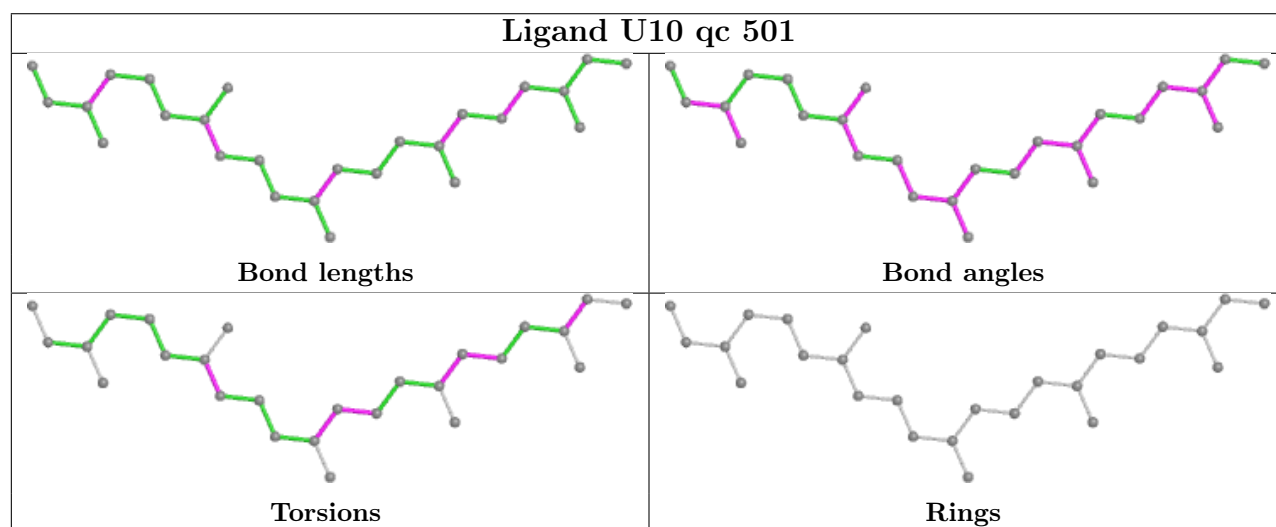
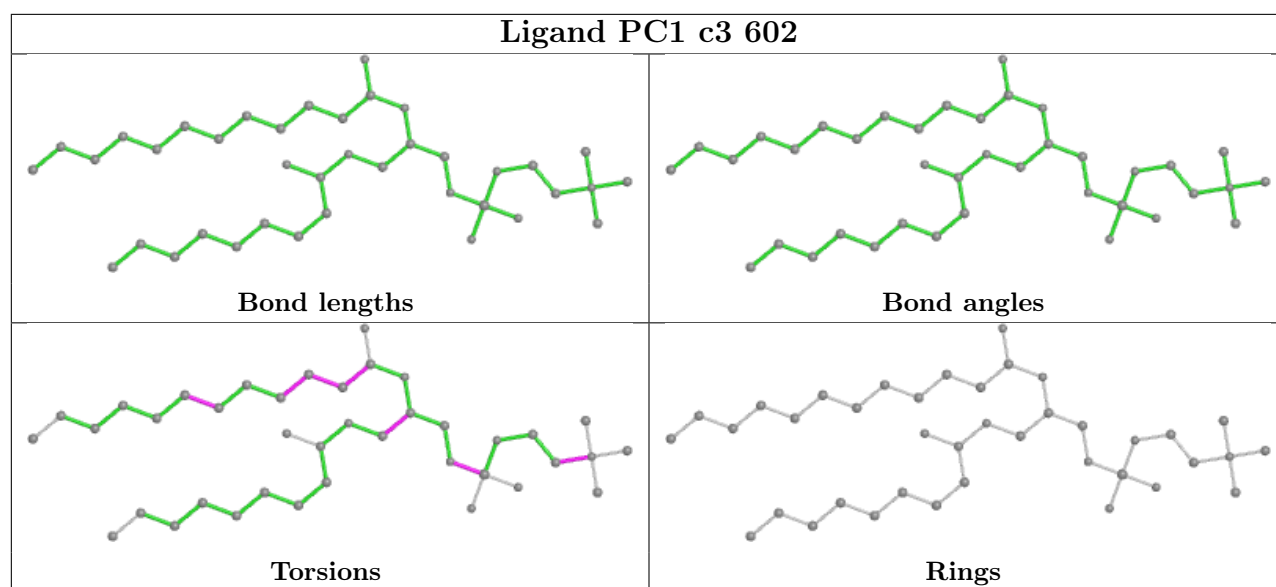




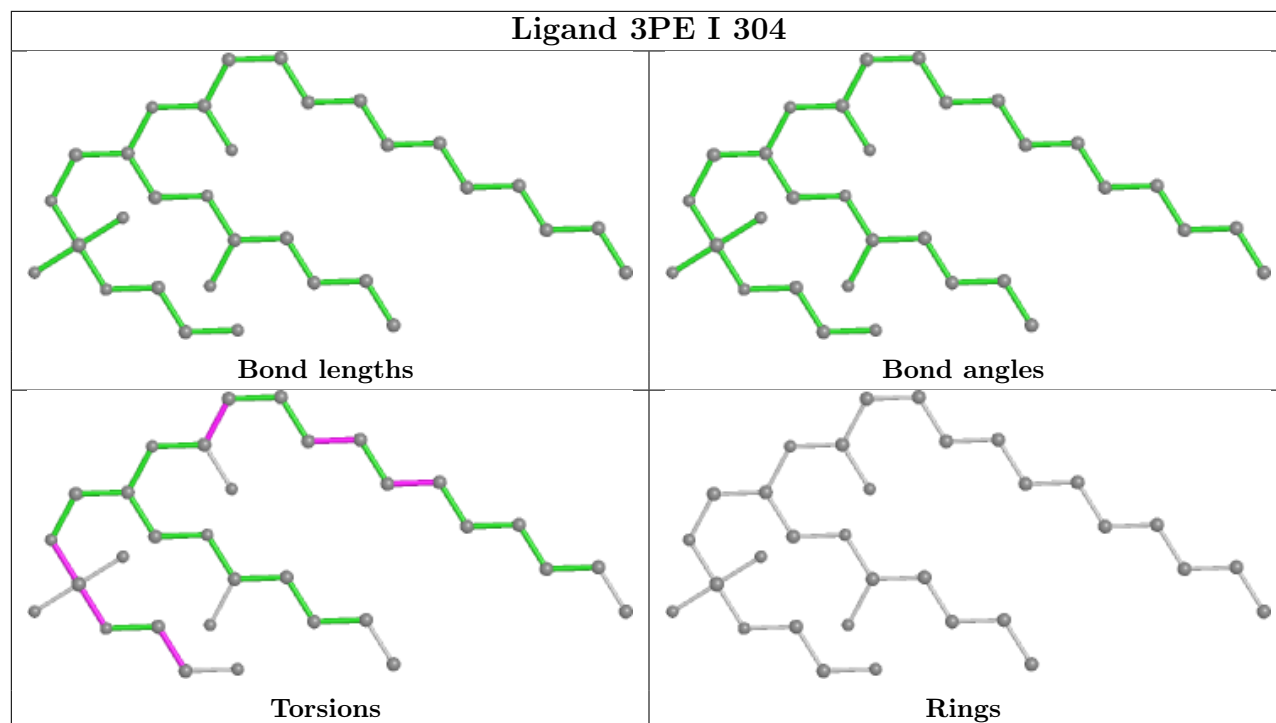




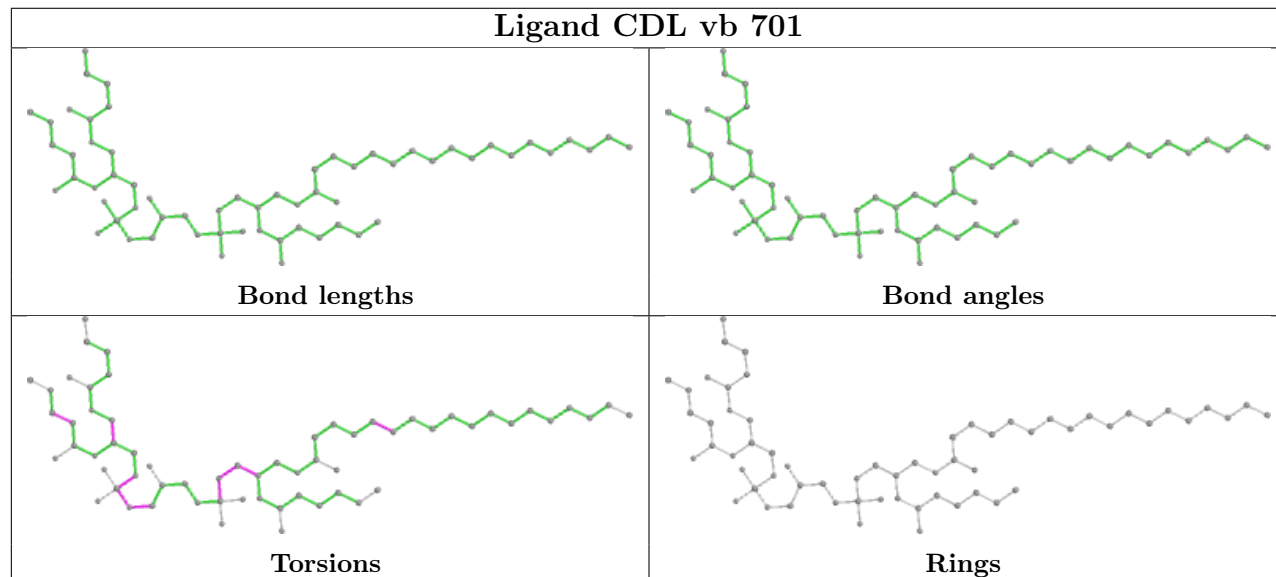


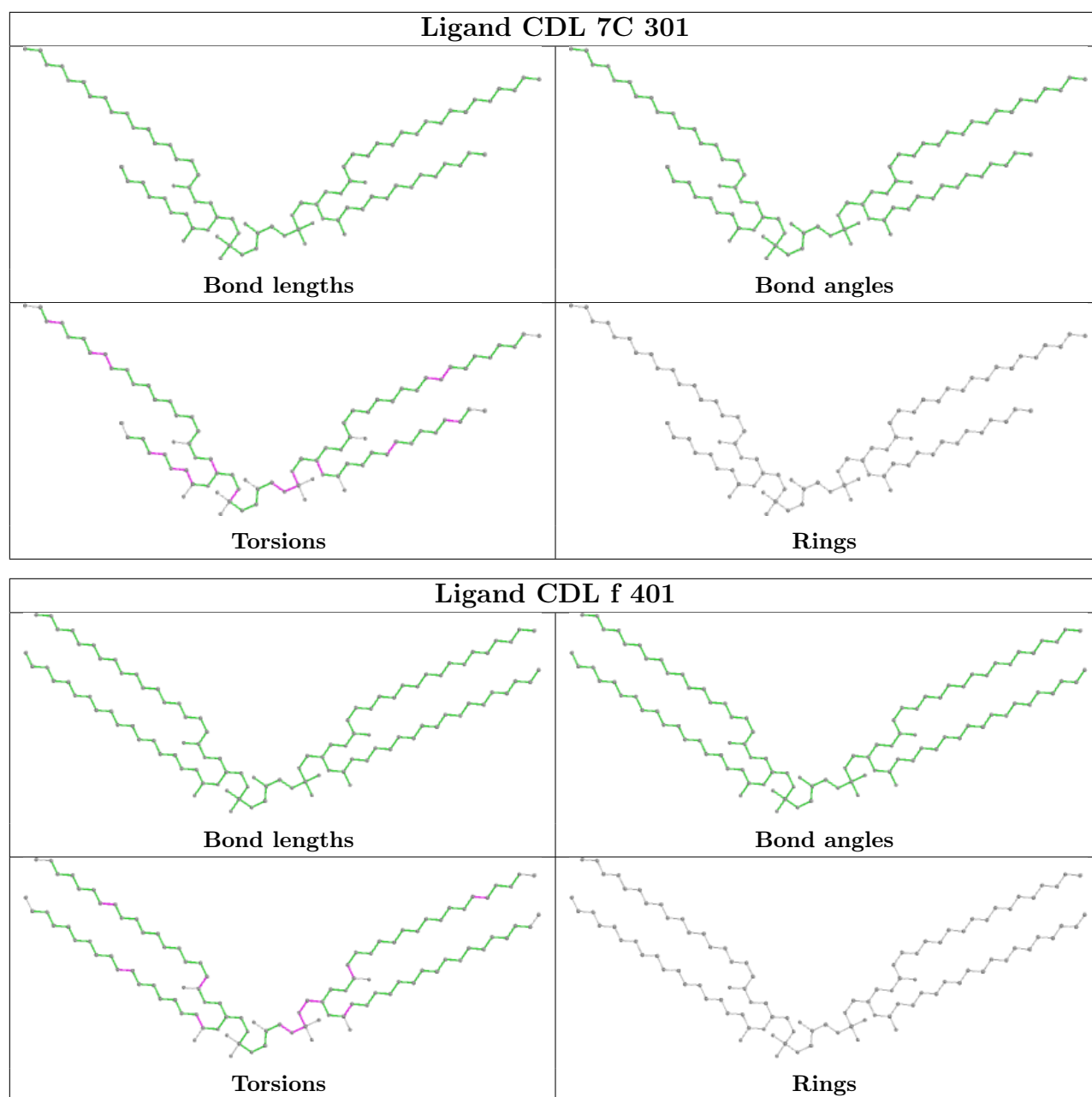


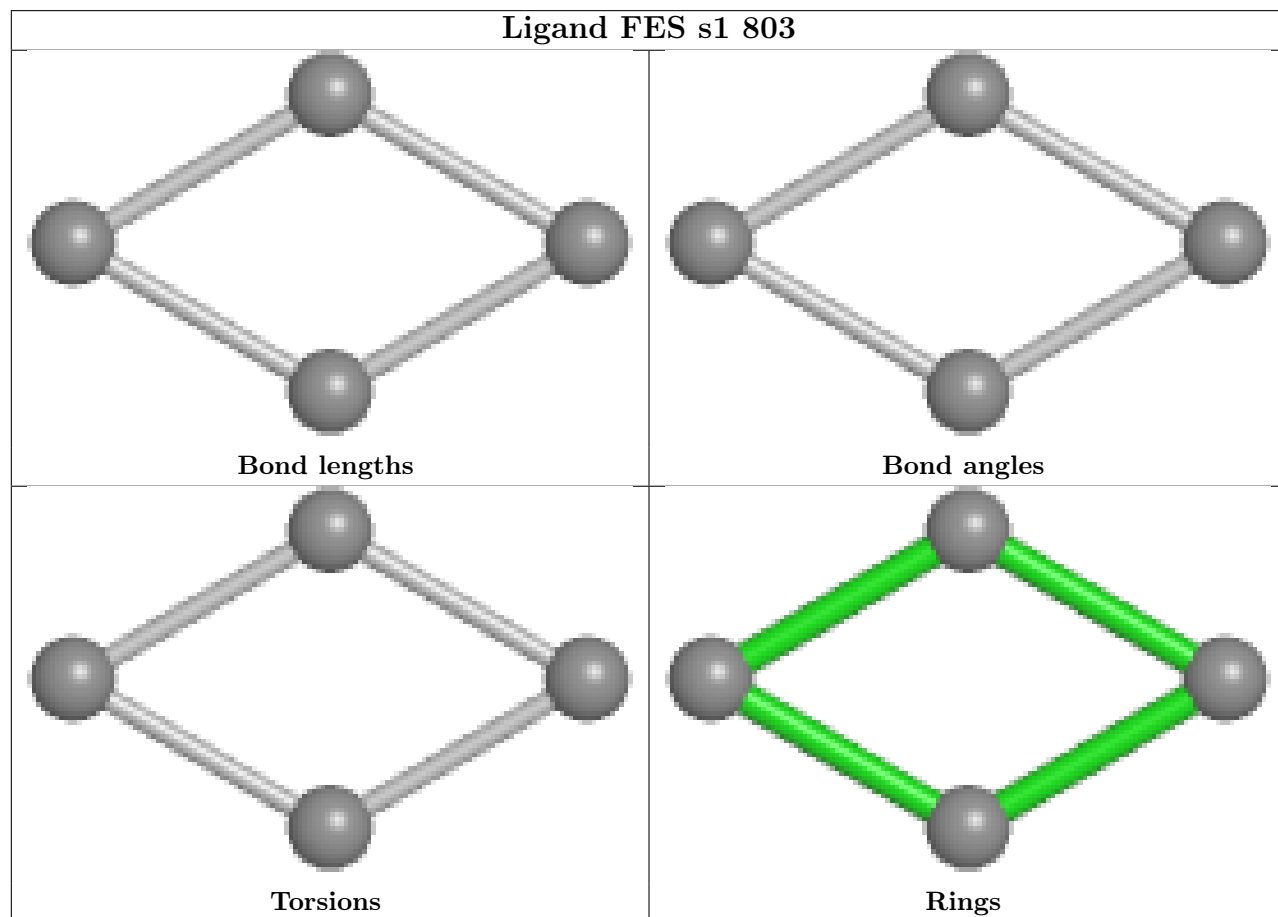
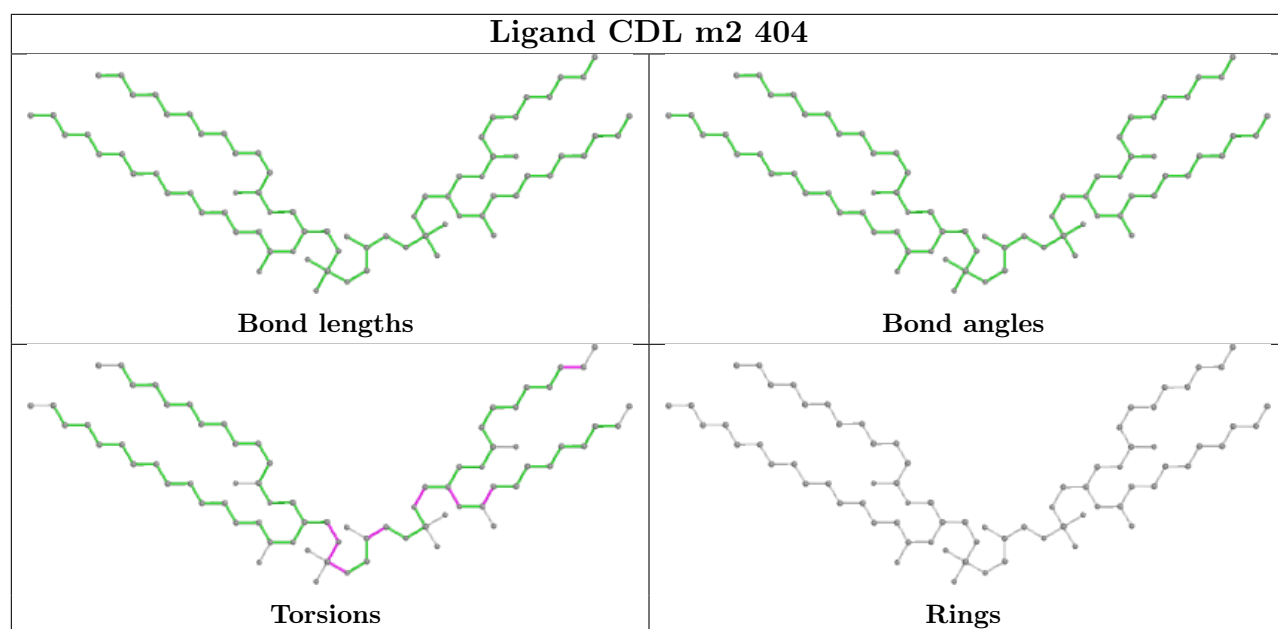
Ligand 3PE I 304

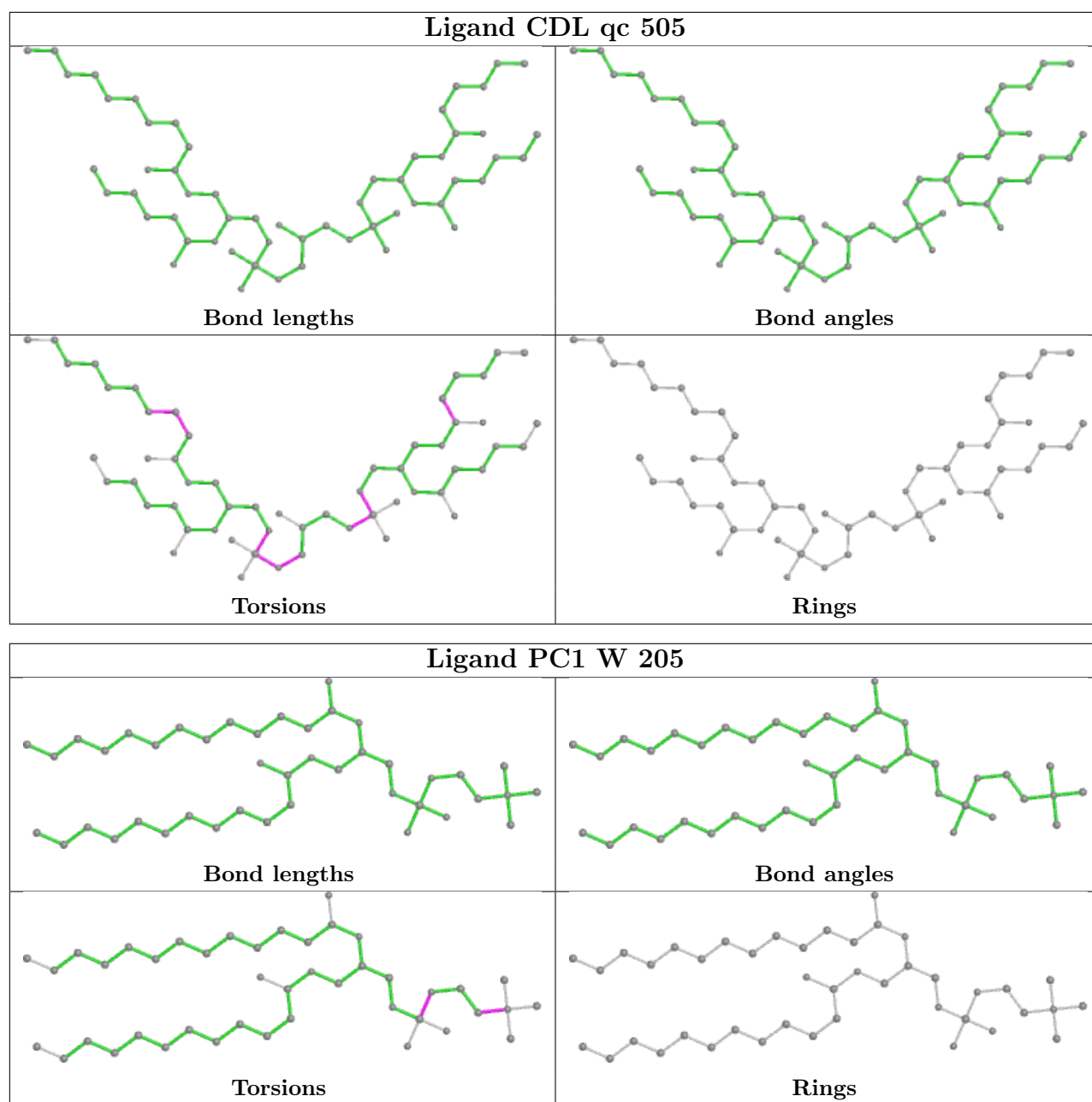


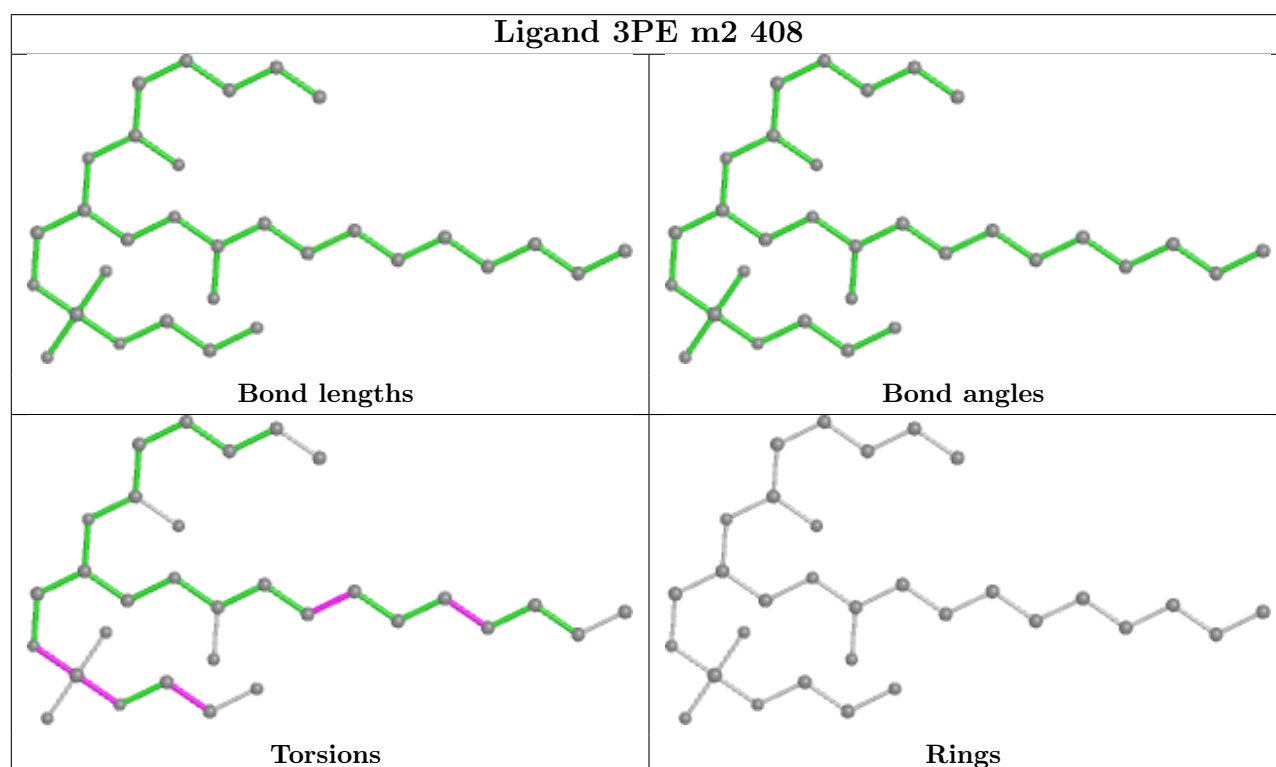
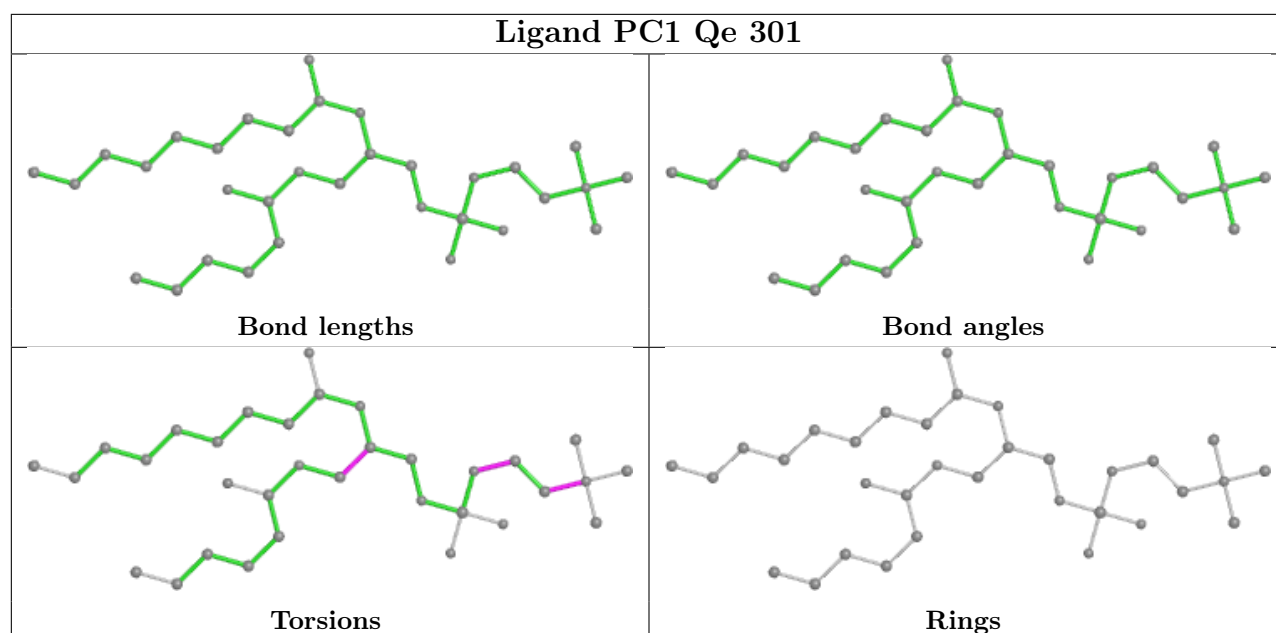
Ligand CDL vb 701

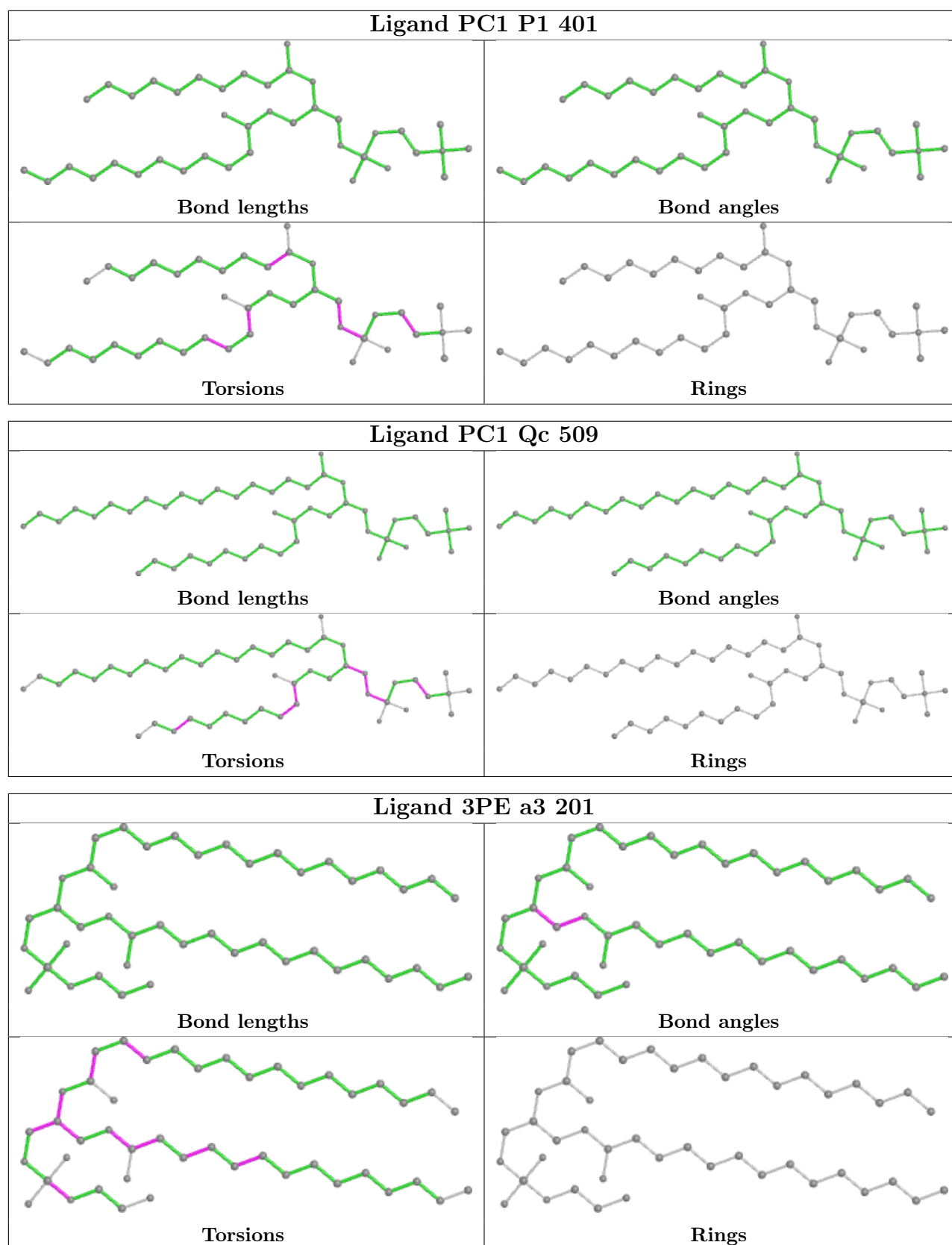


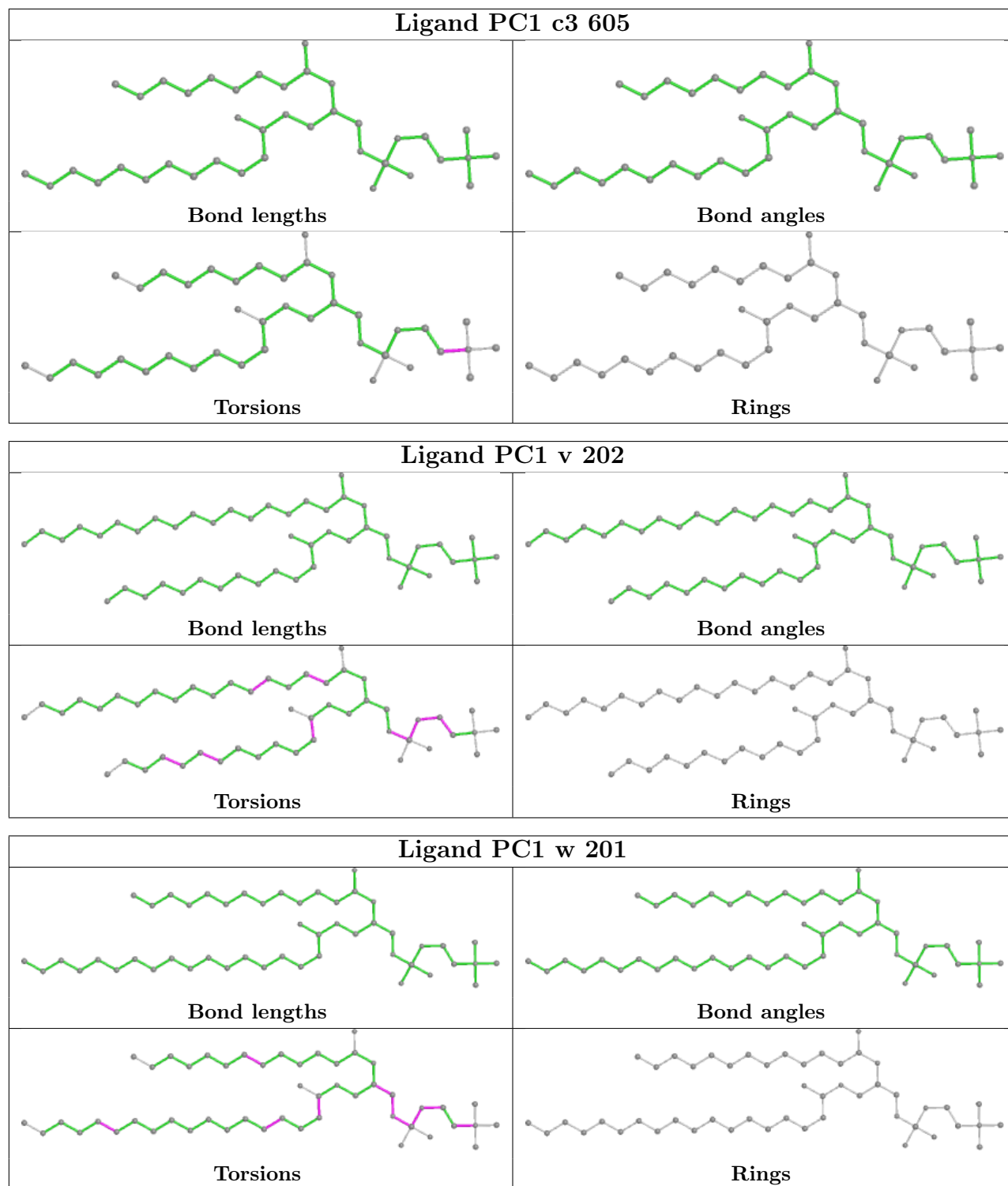


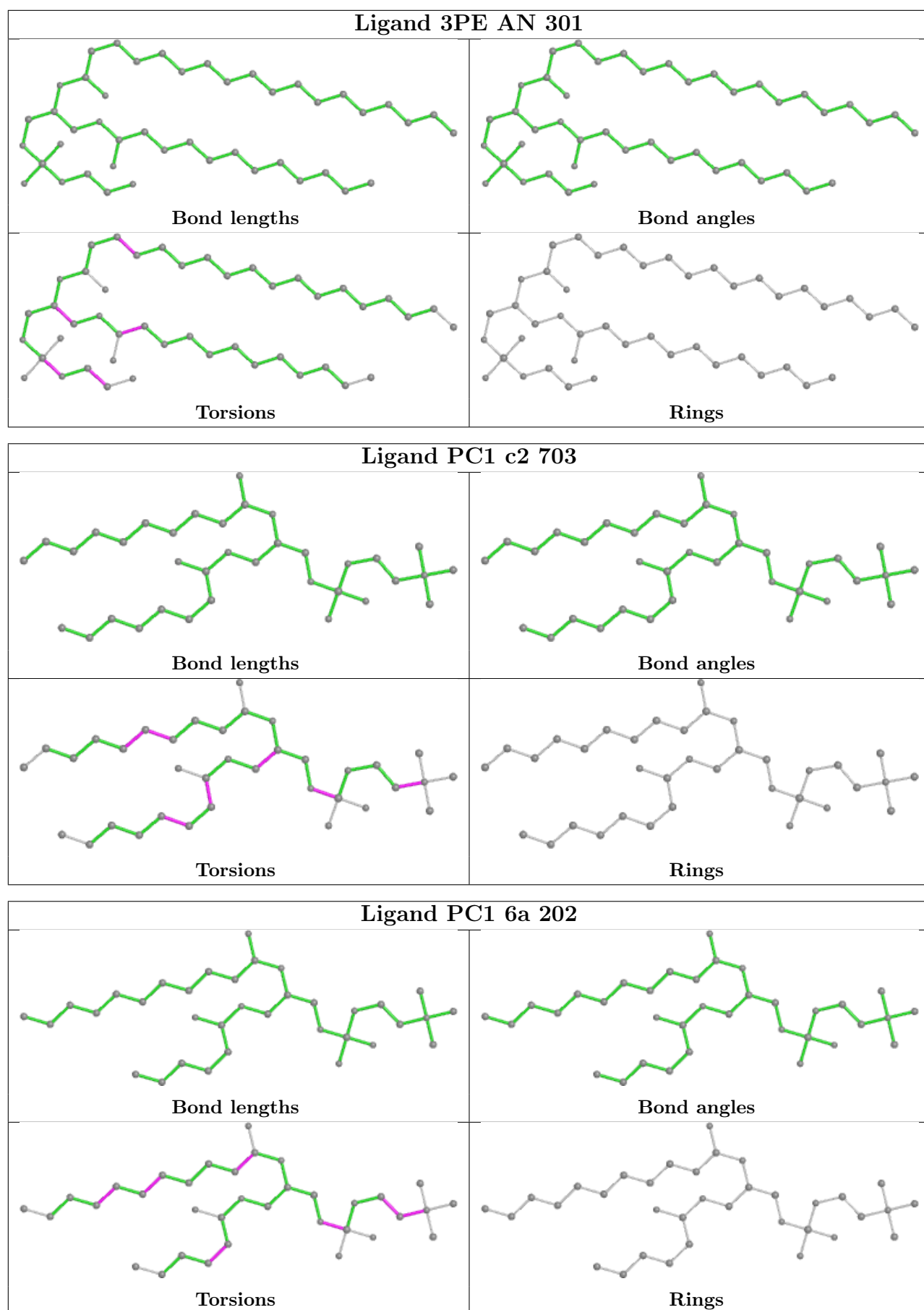


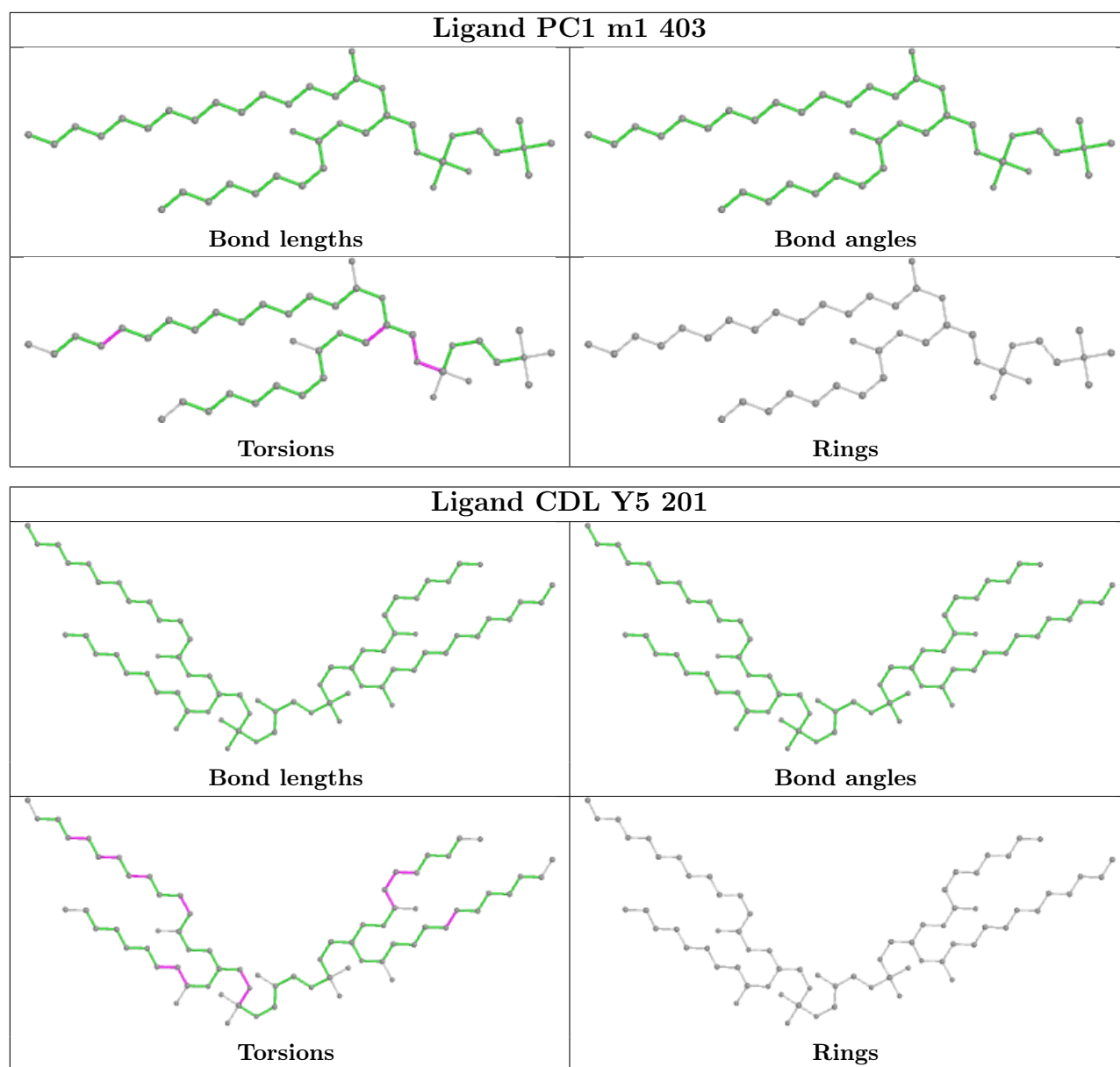


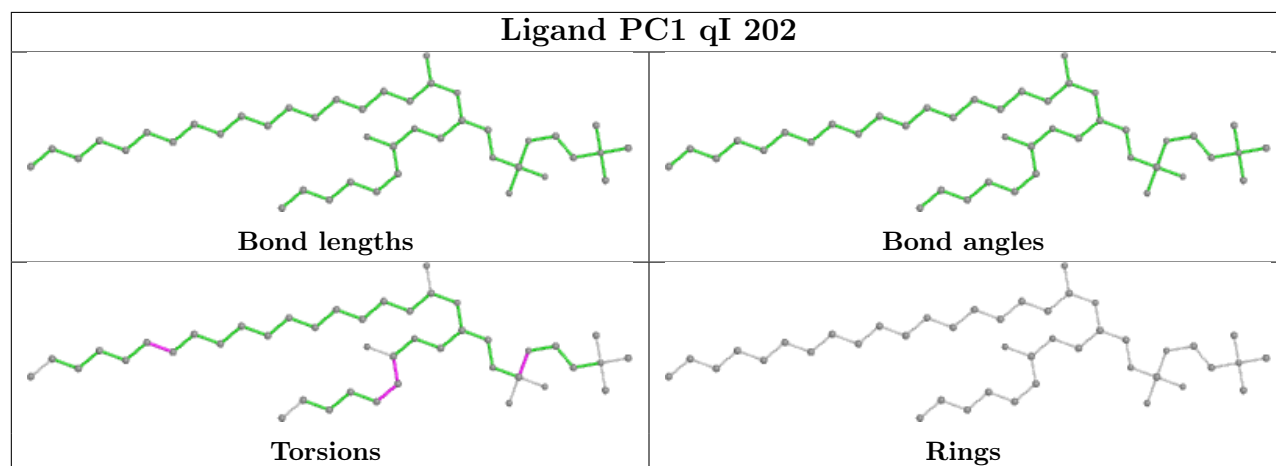
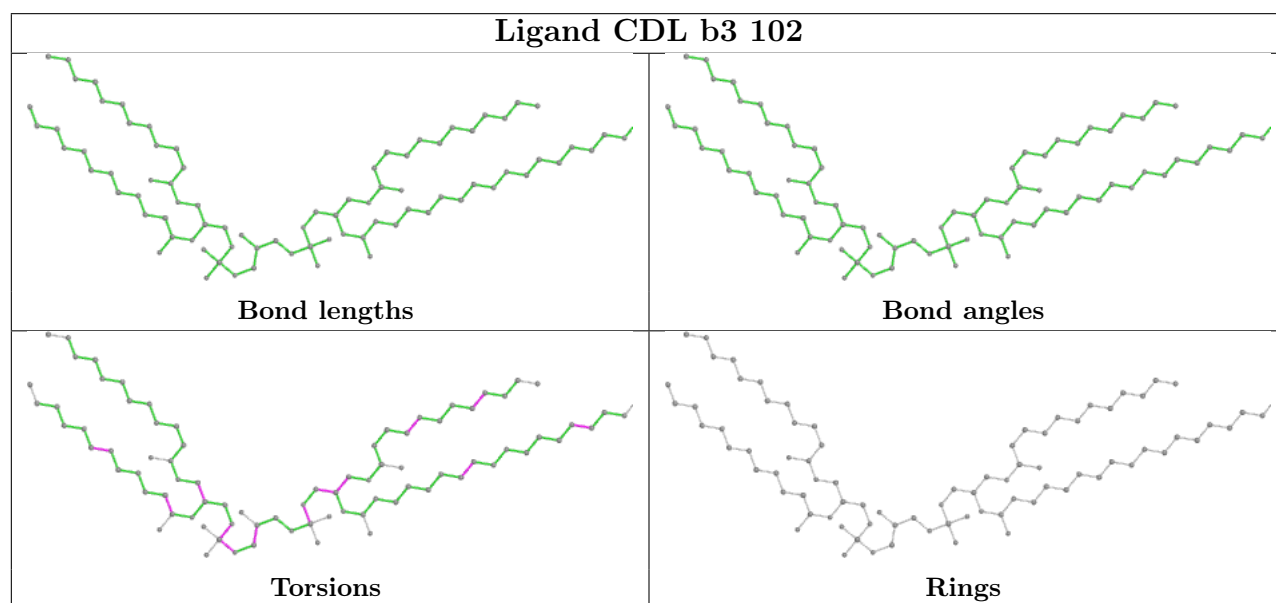
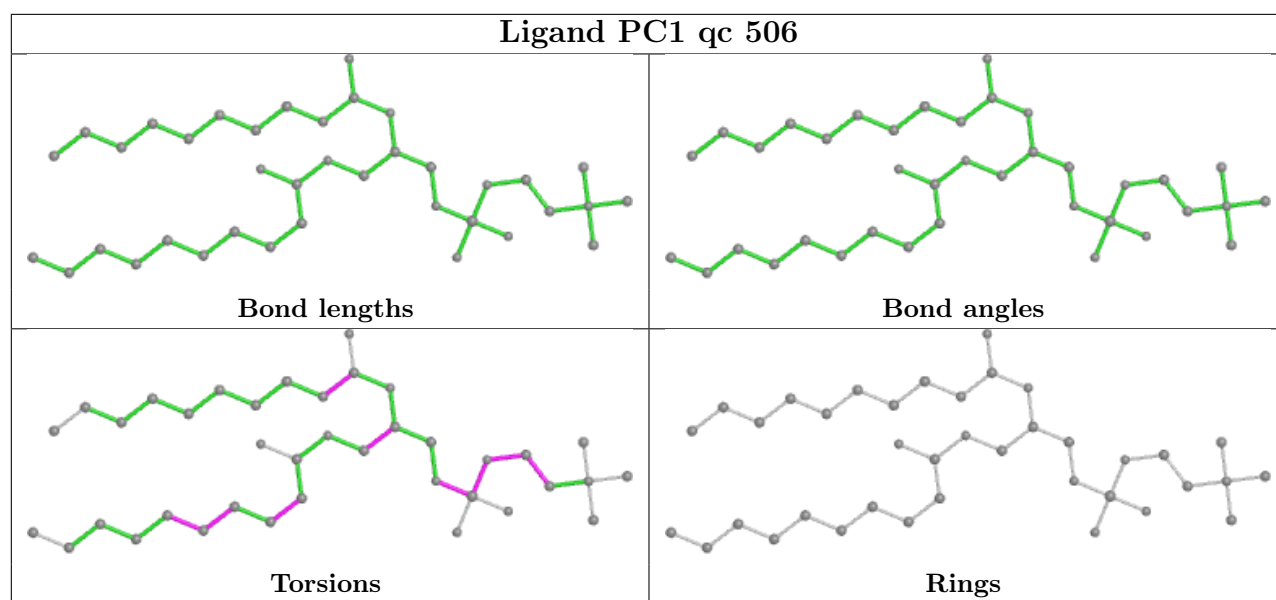


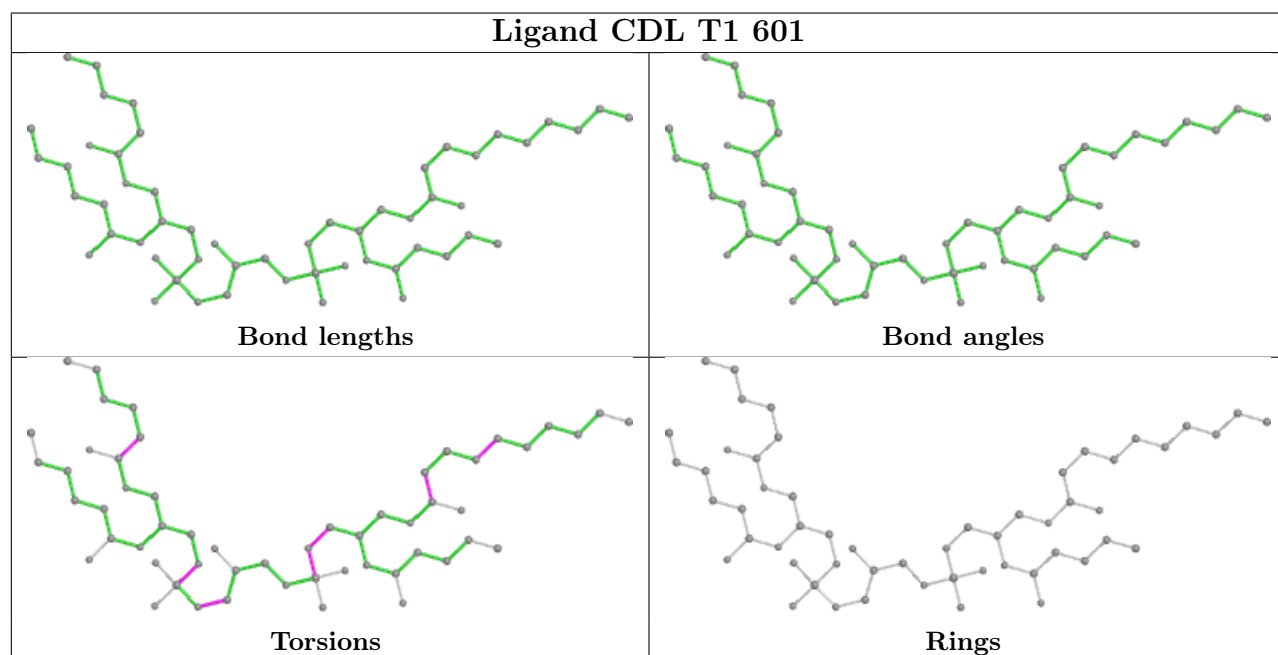
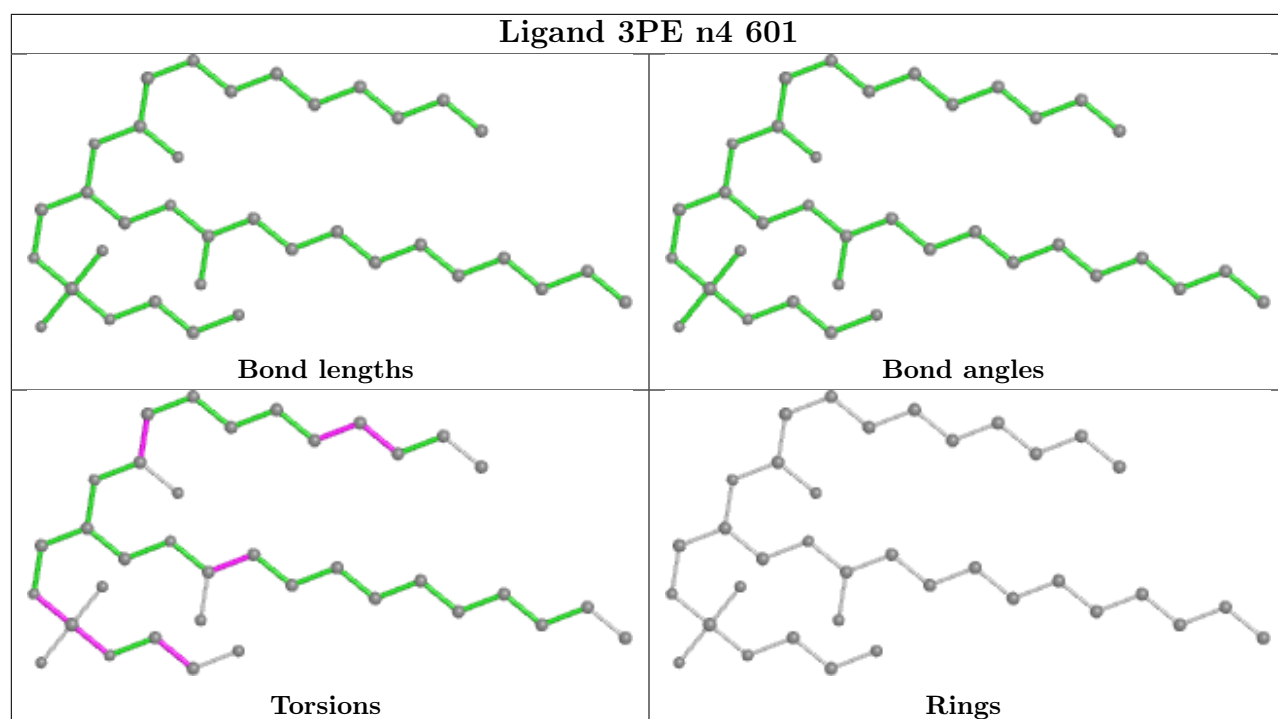


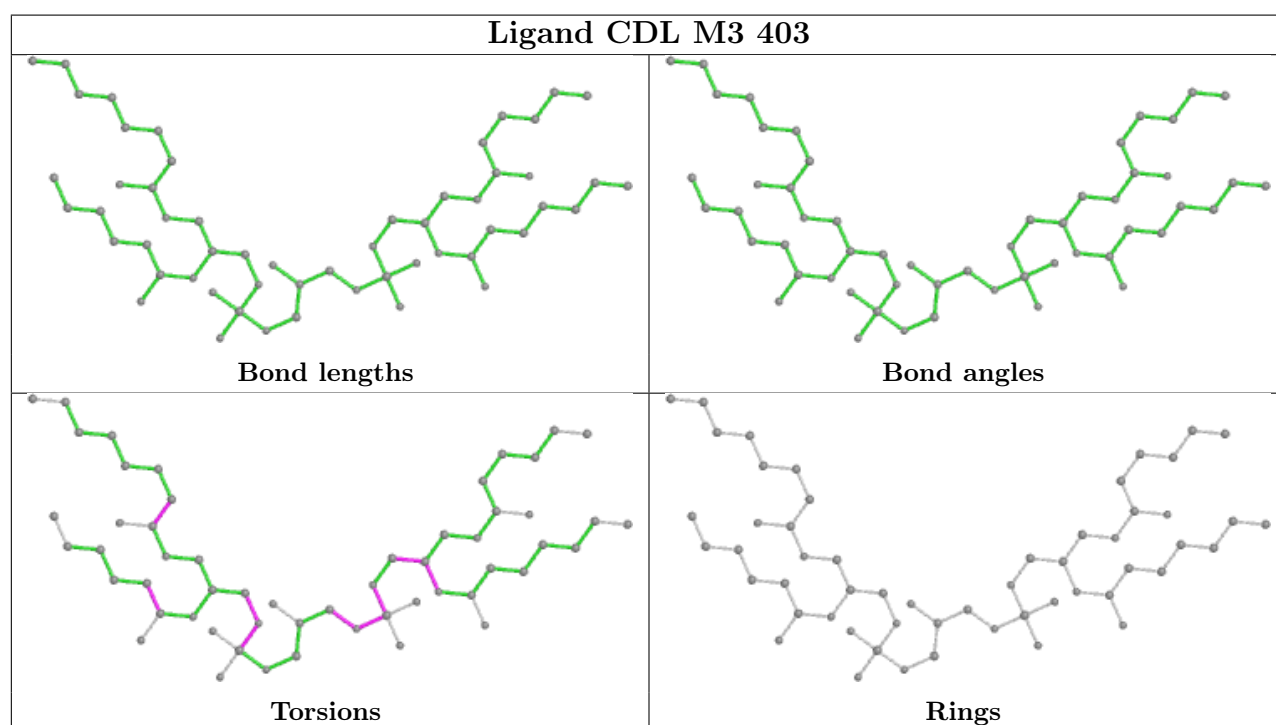
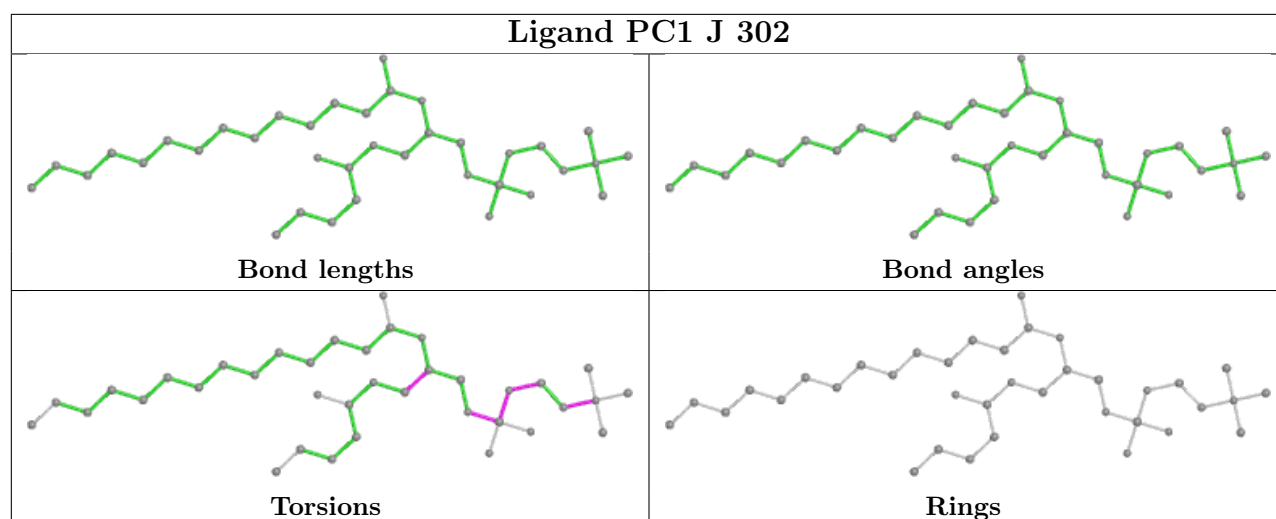


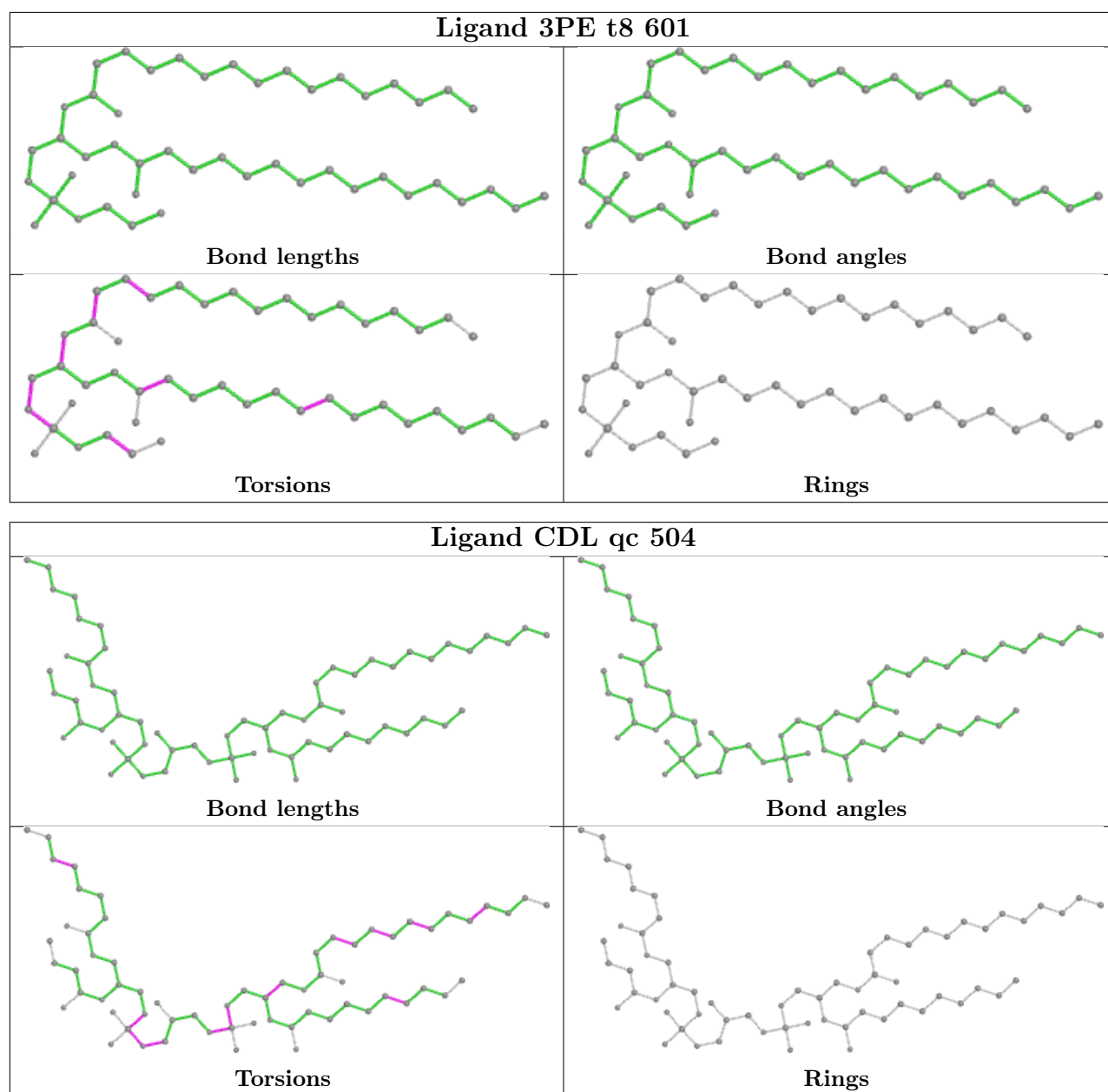




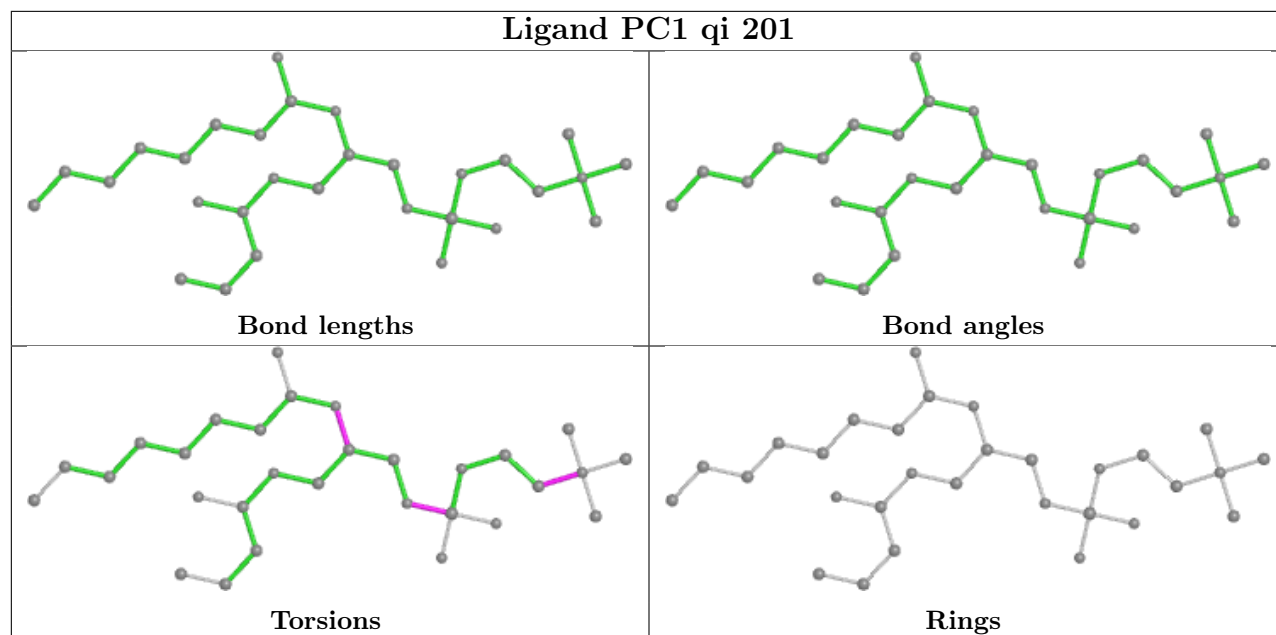




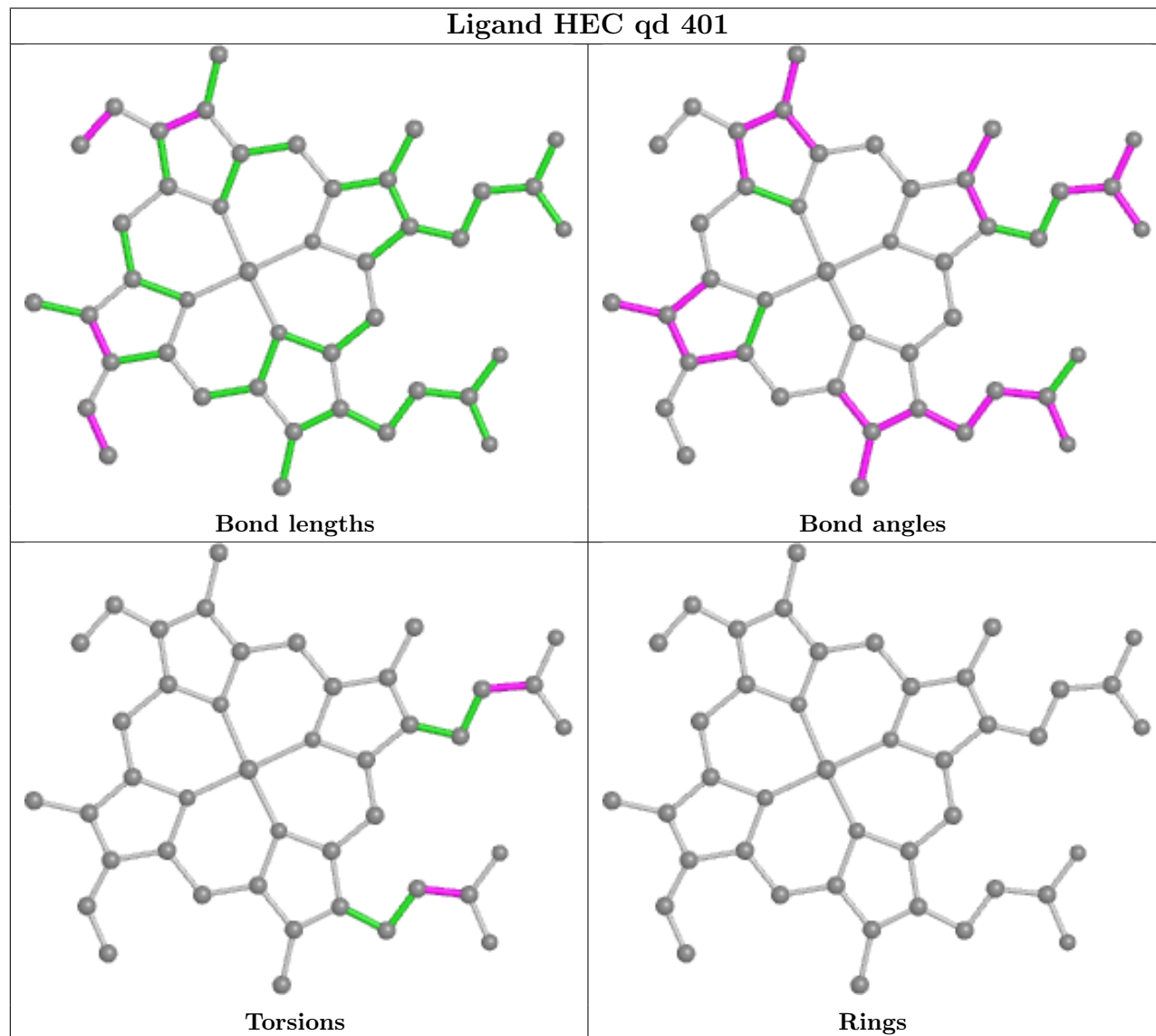


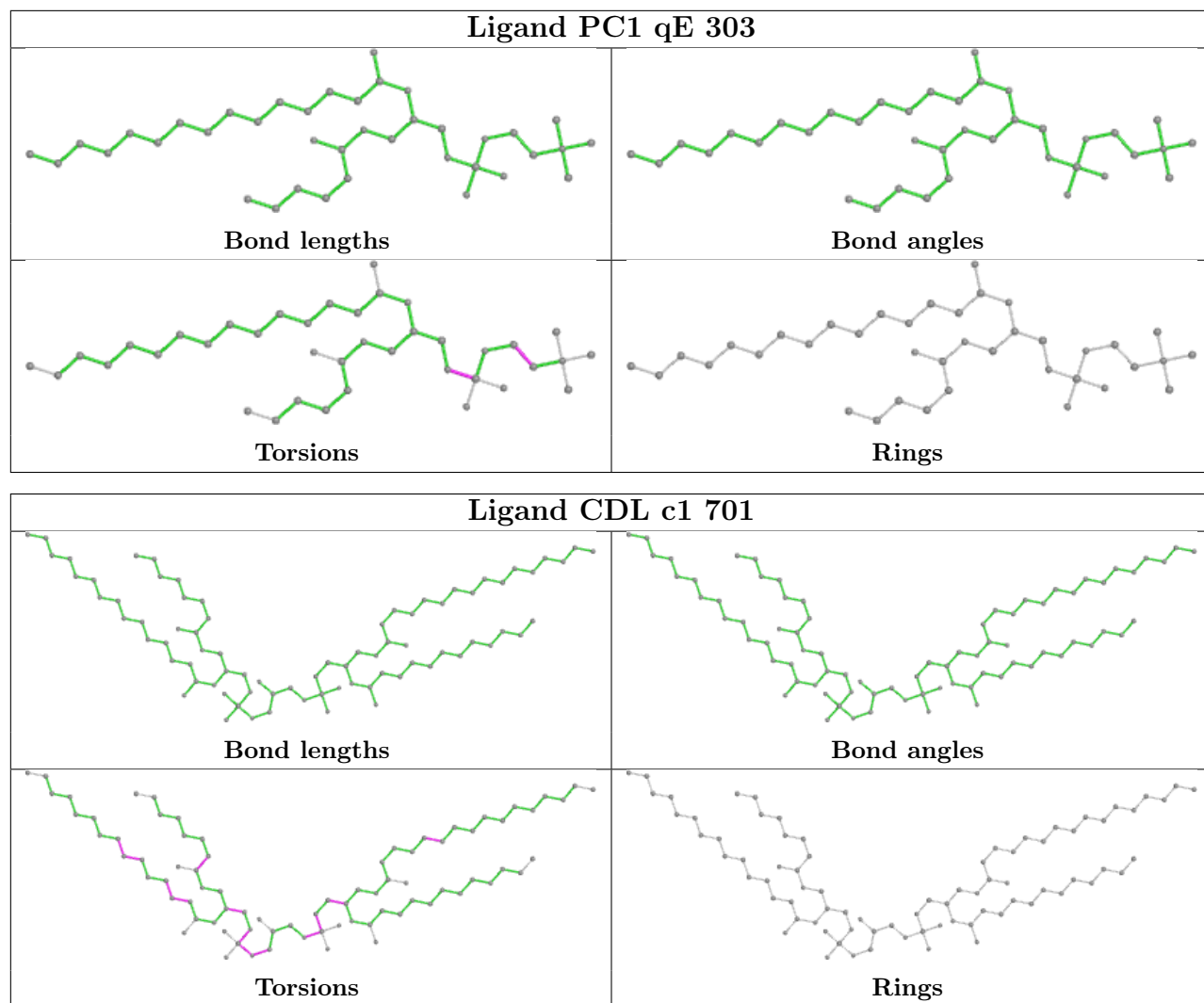


Ligand PC1 qi 201

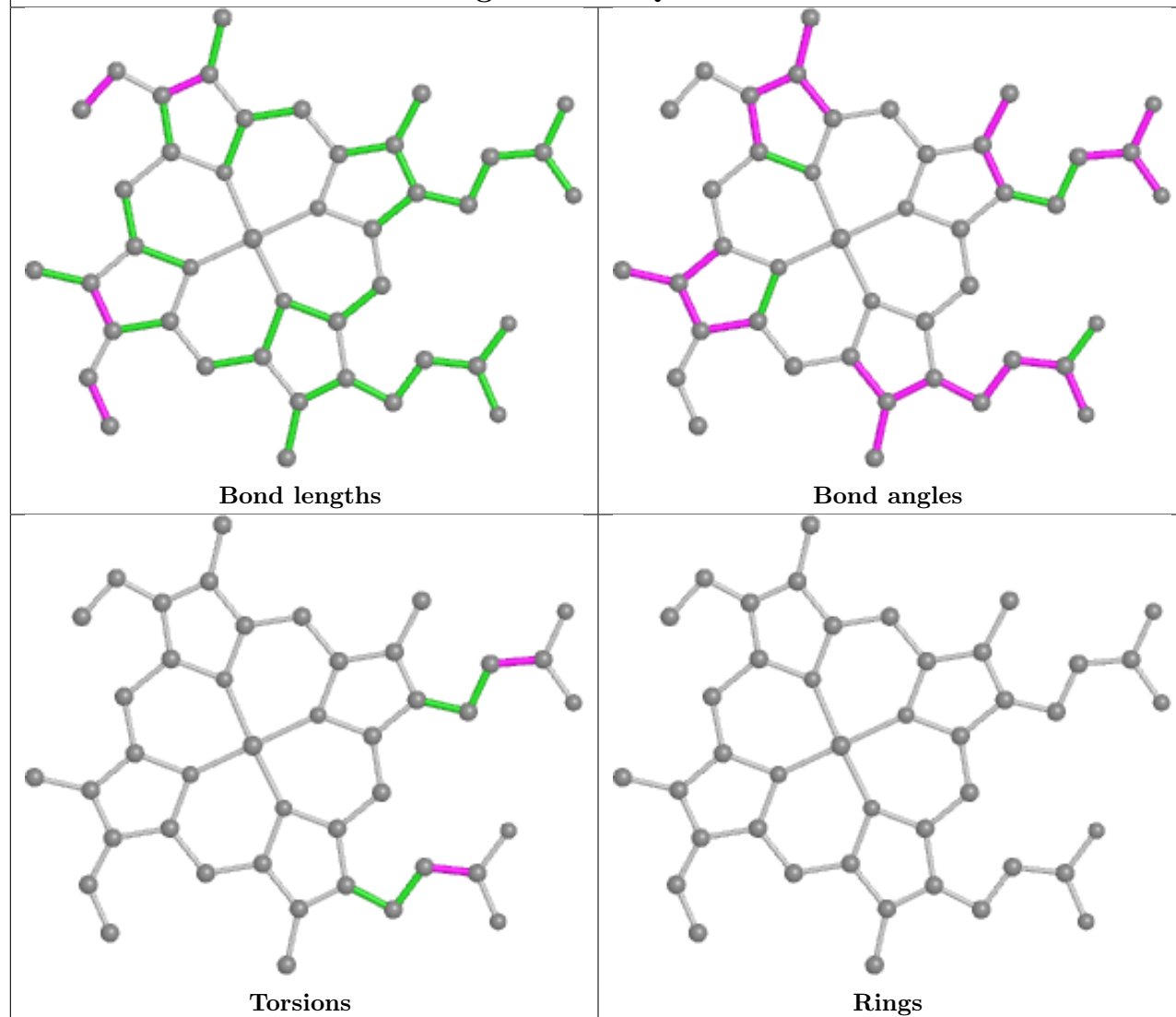


Ligand HEC qd 401

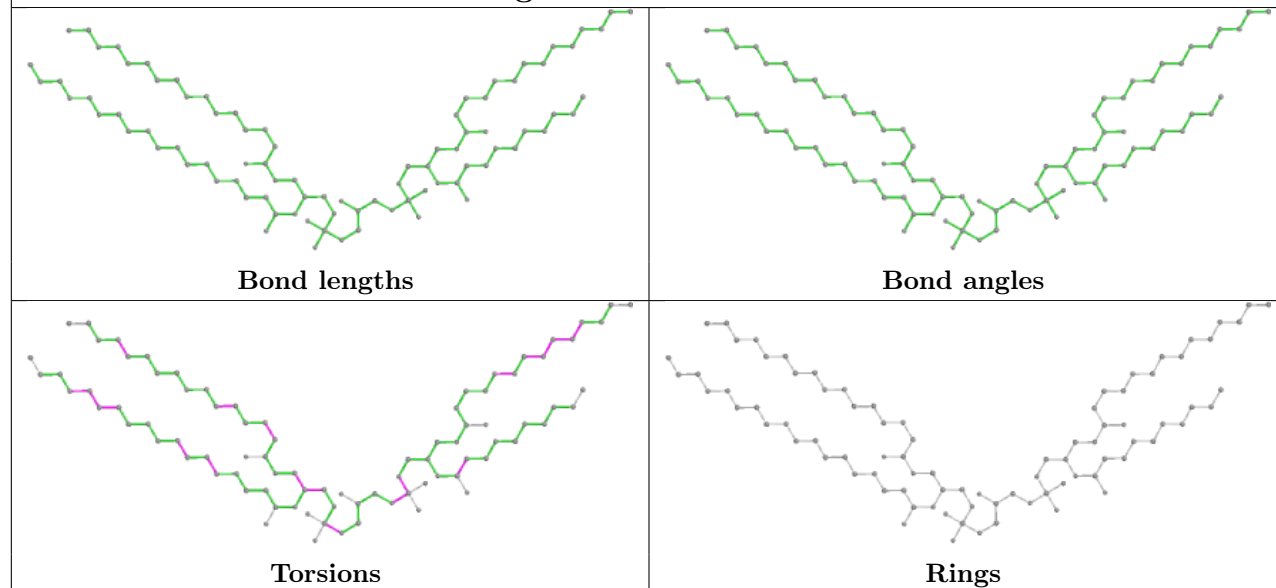


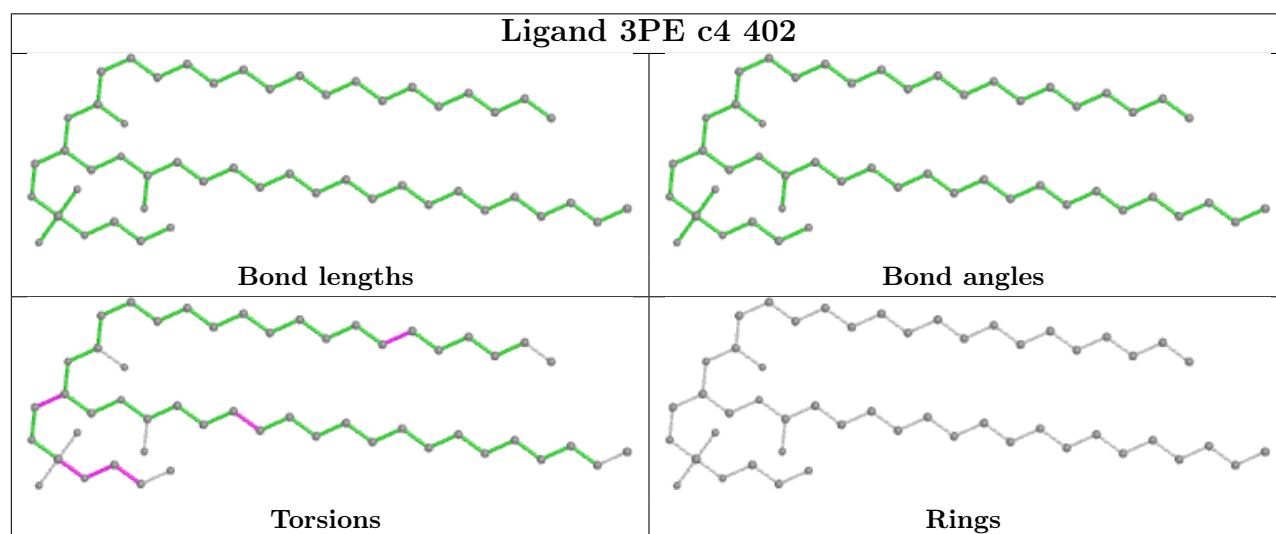
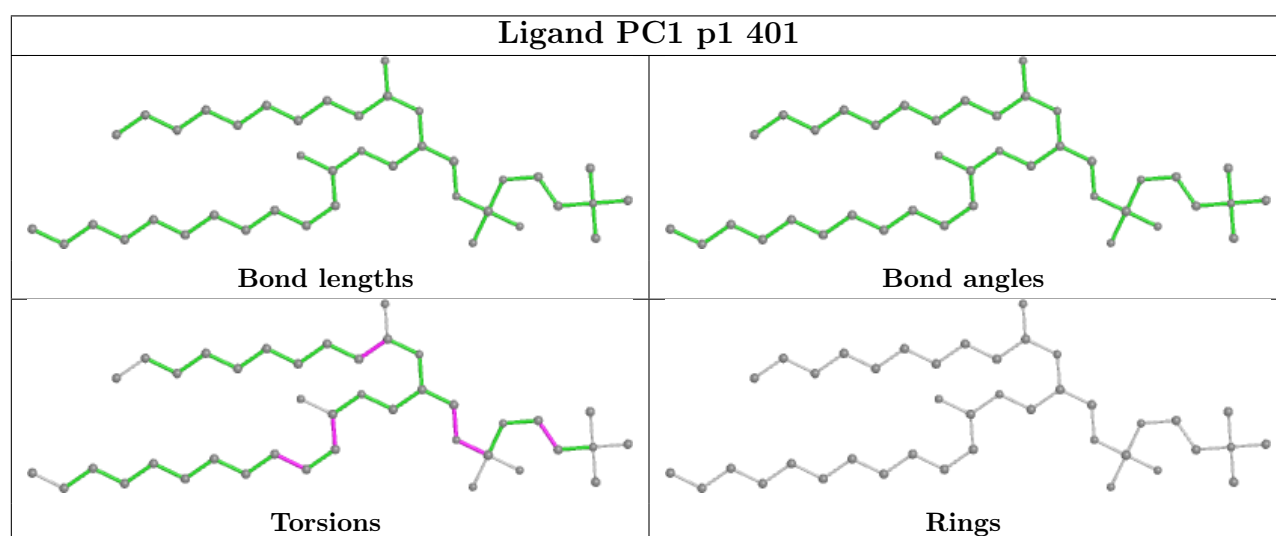
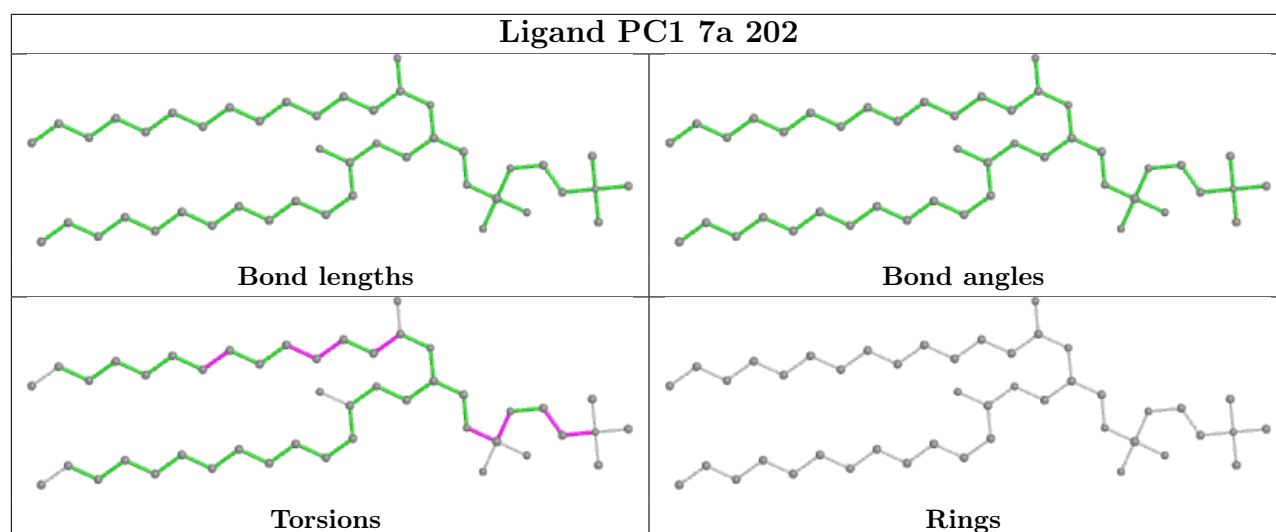


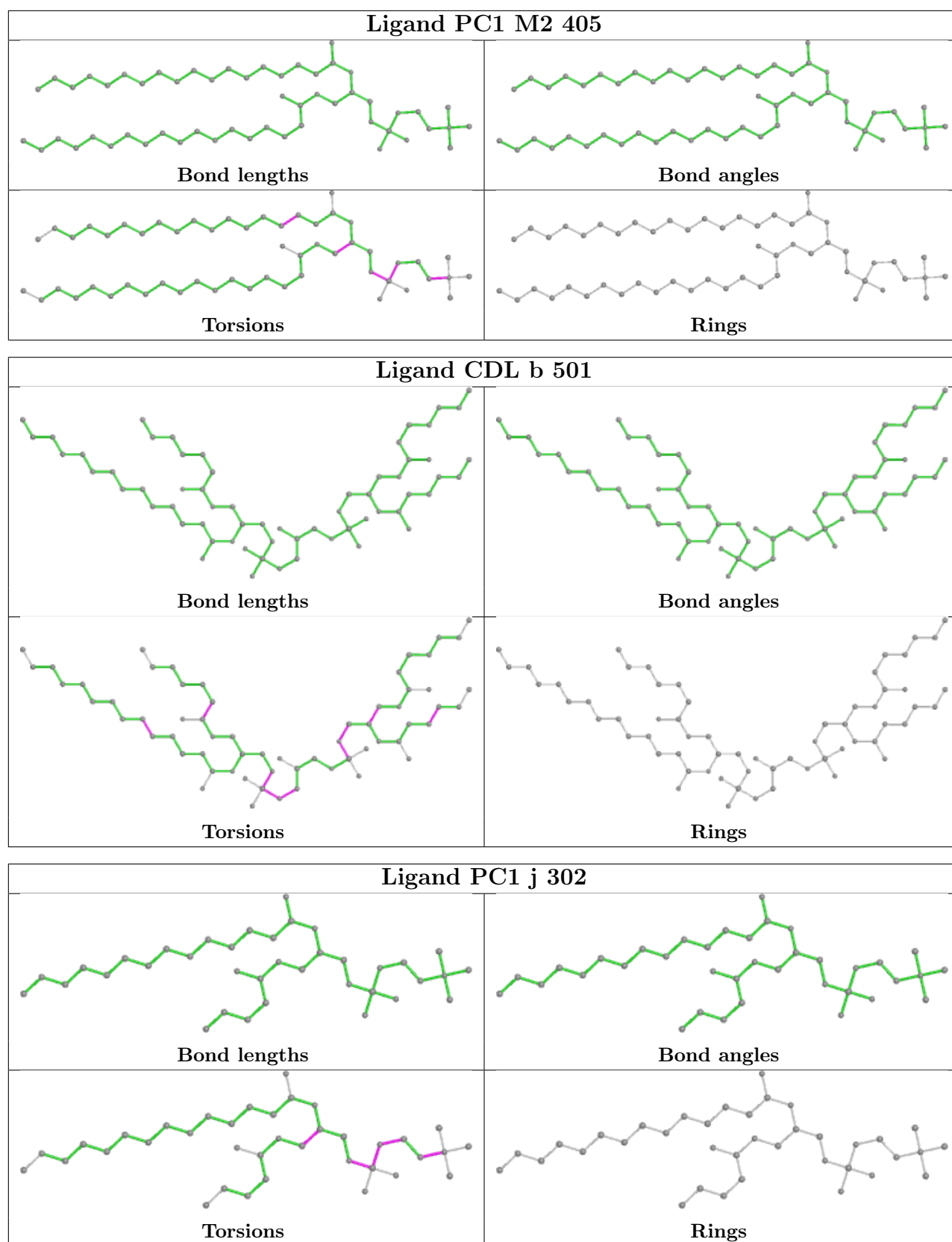
Ligand HEC QD 401

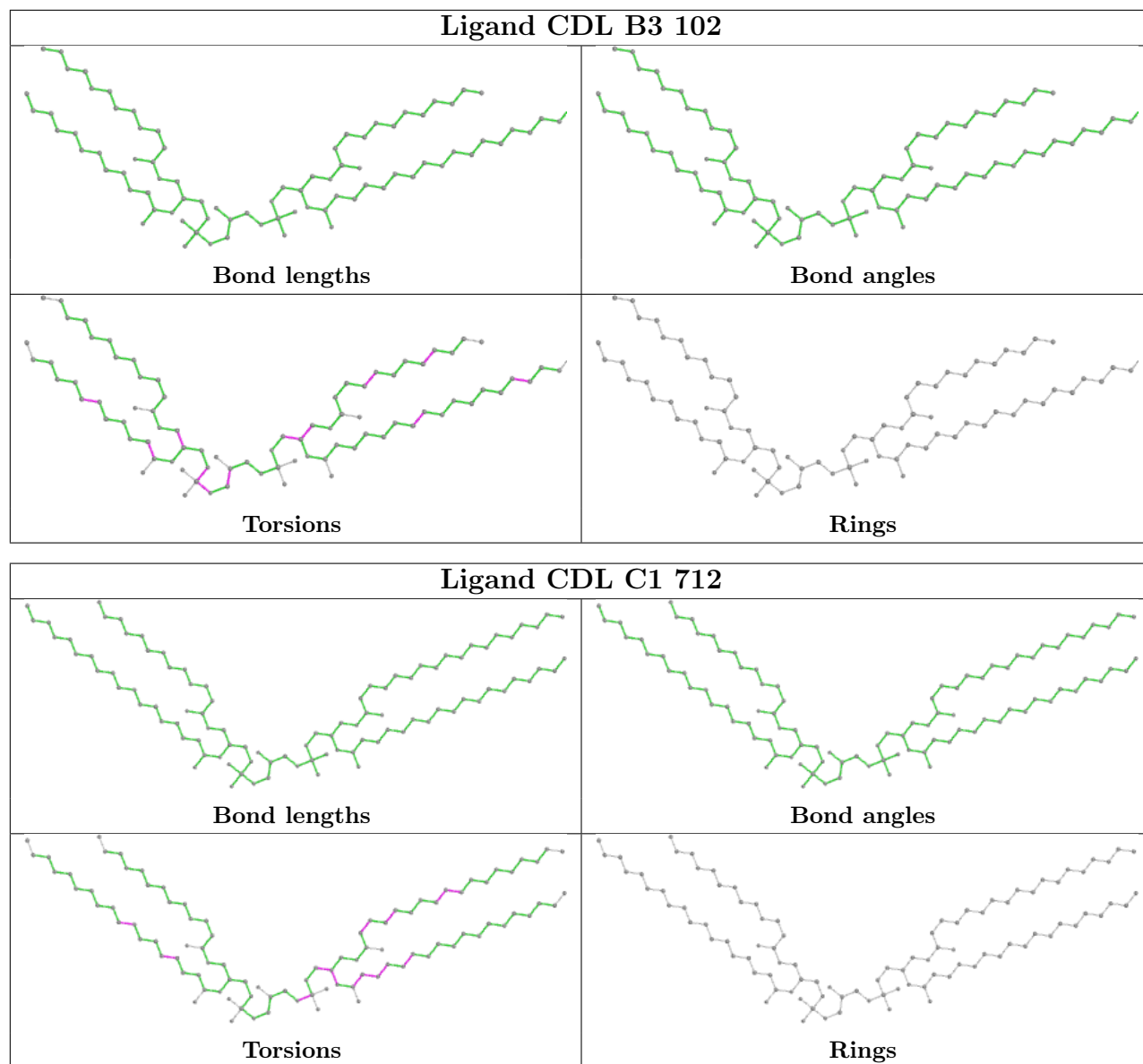


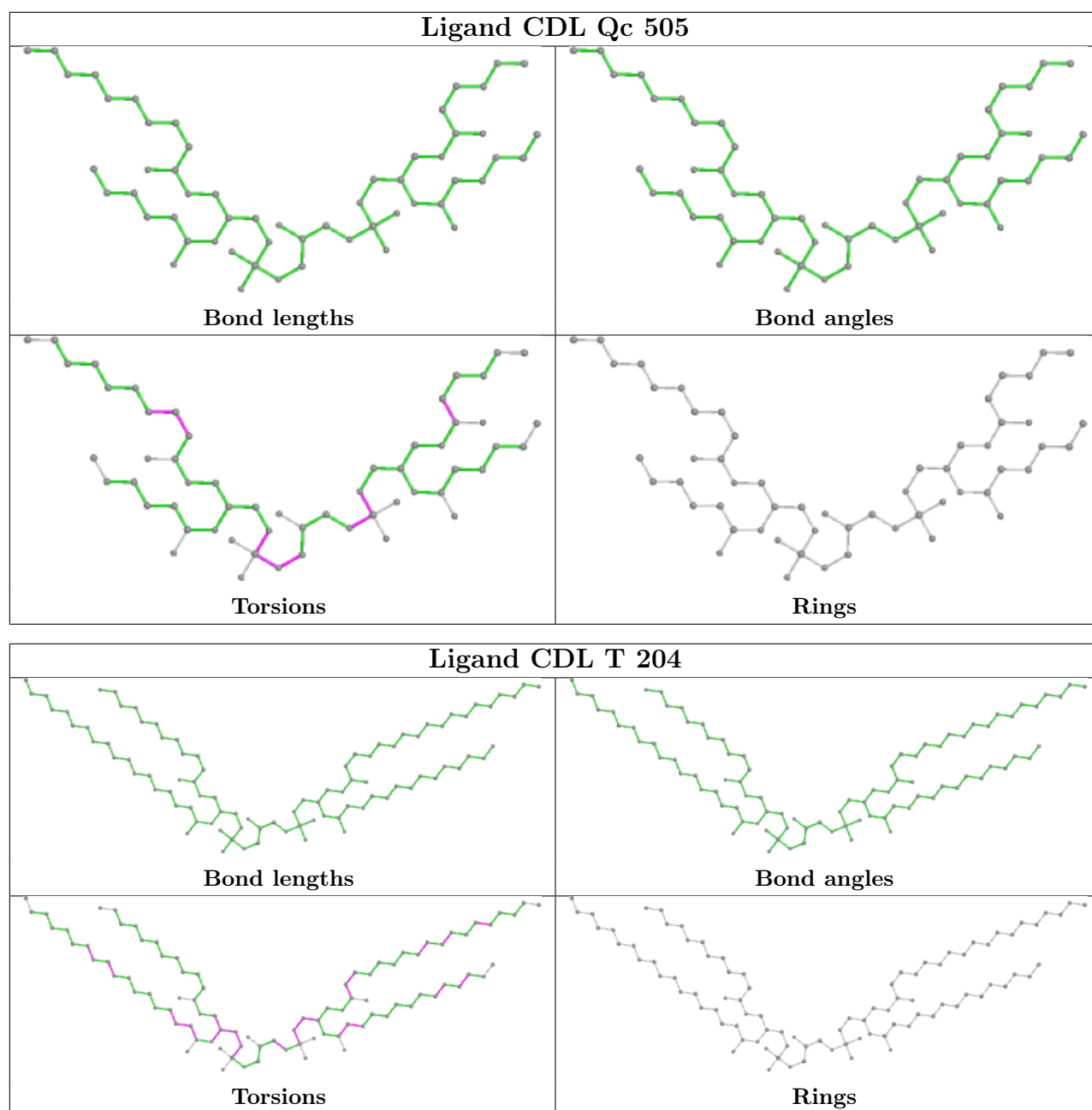
Ligand CDL BM 301

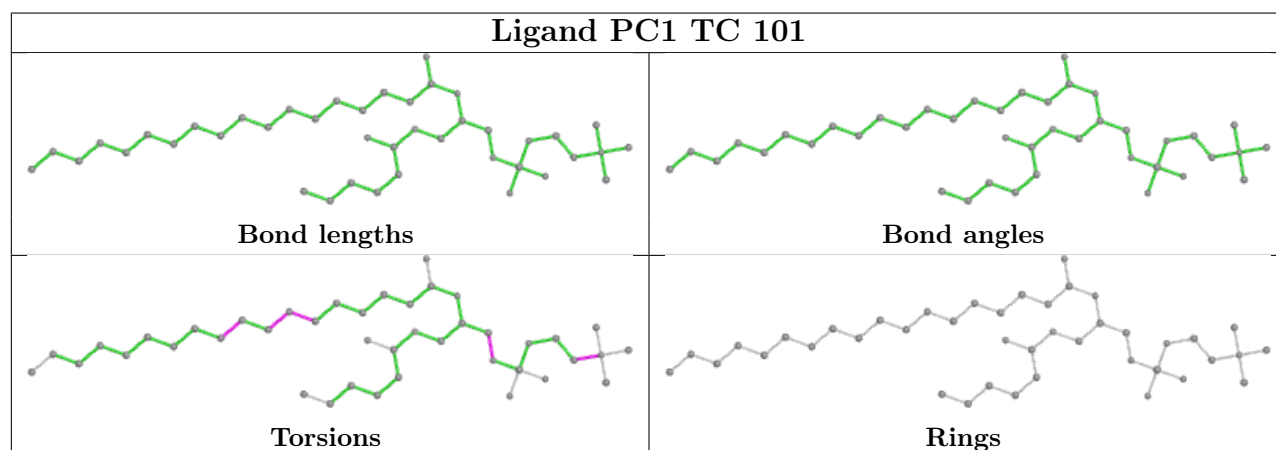
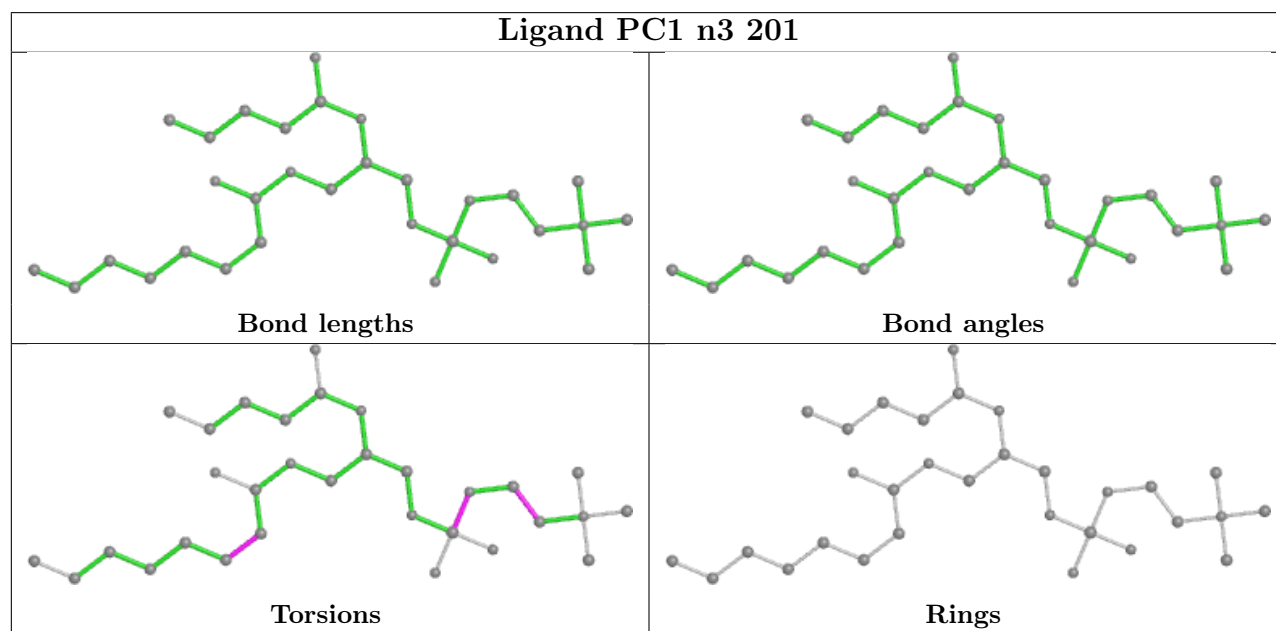
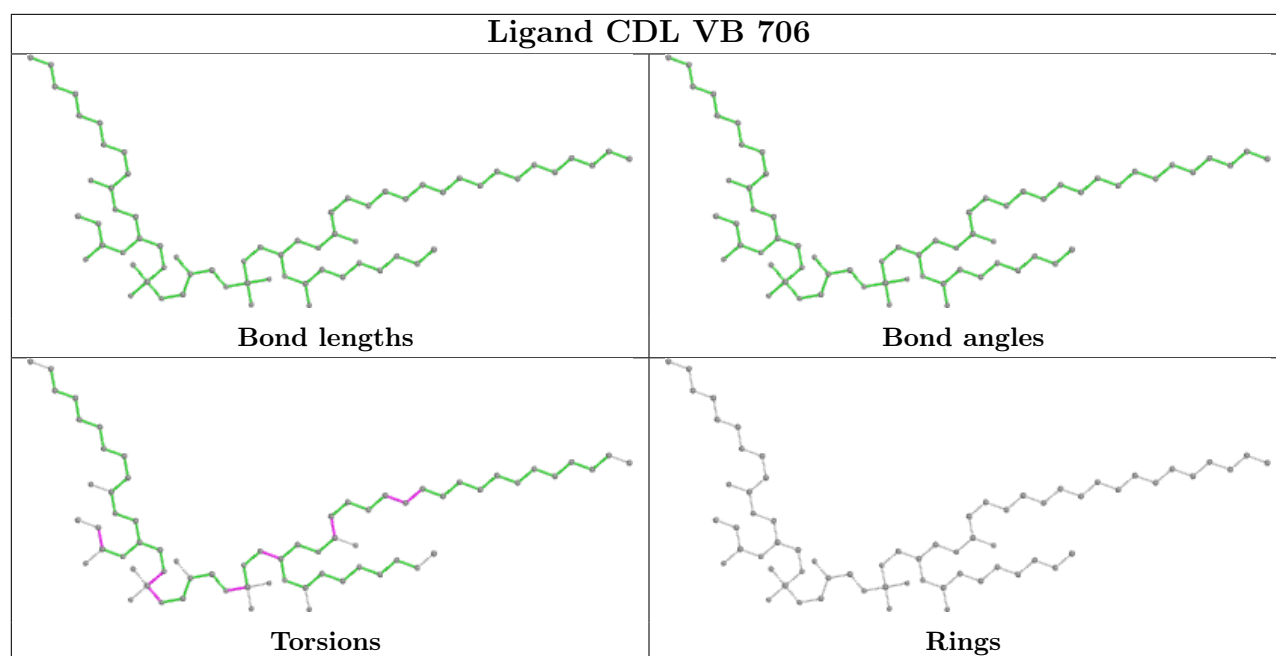


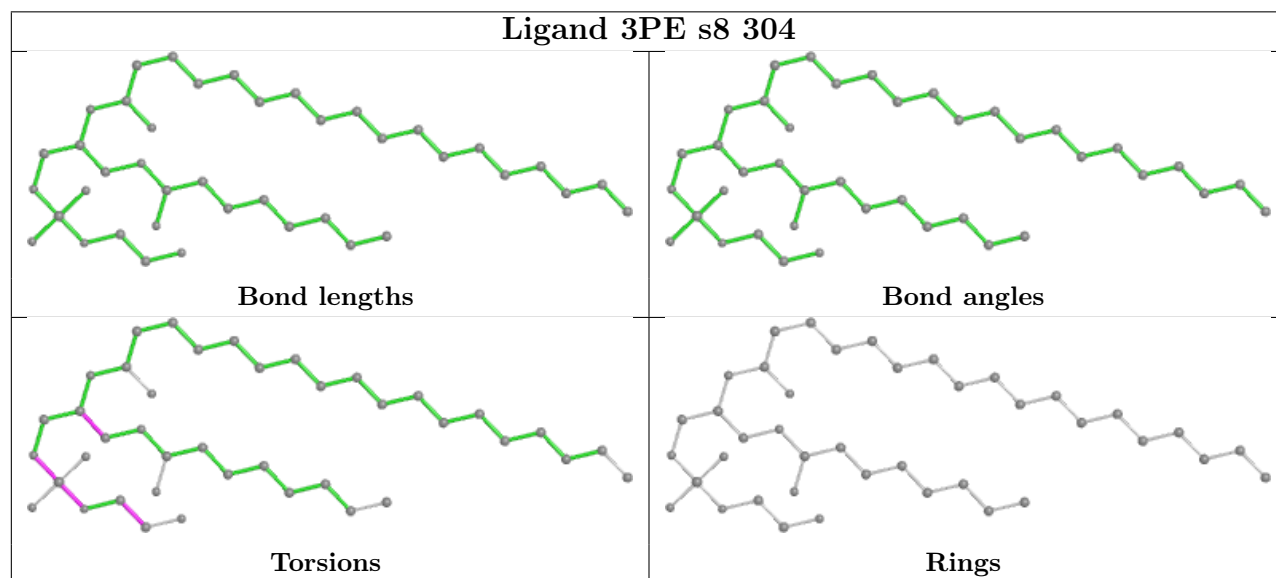
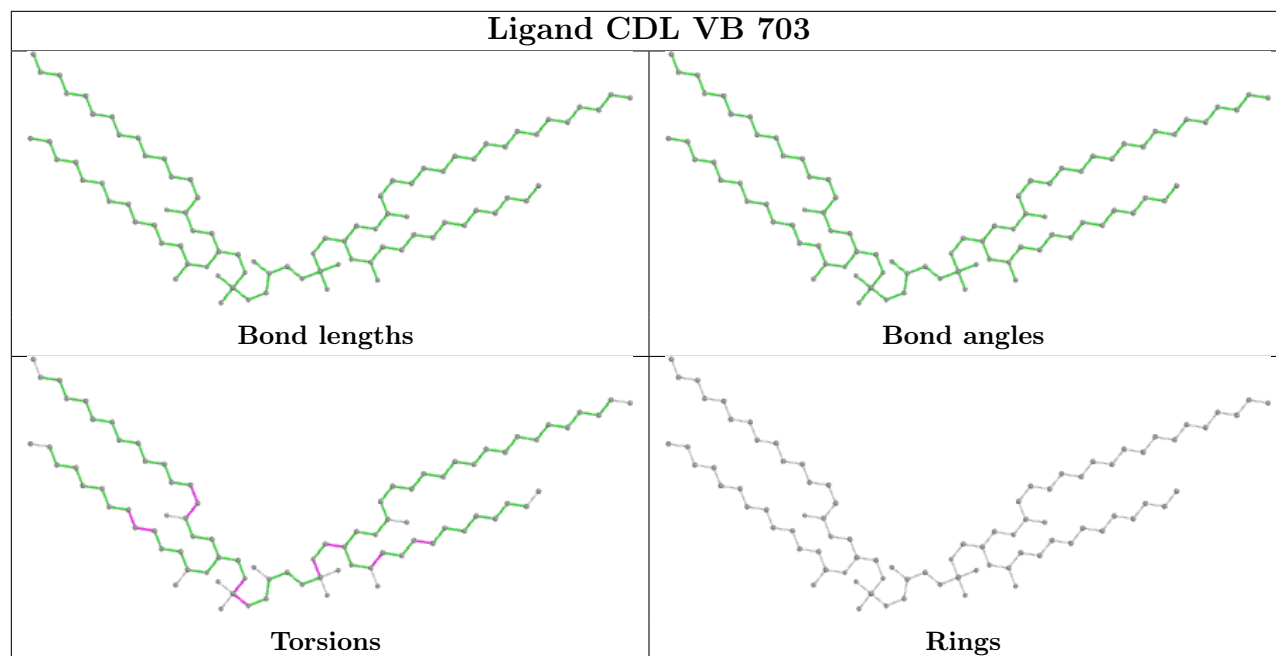


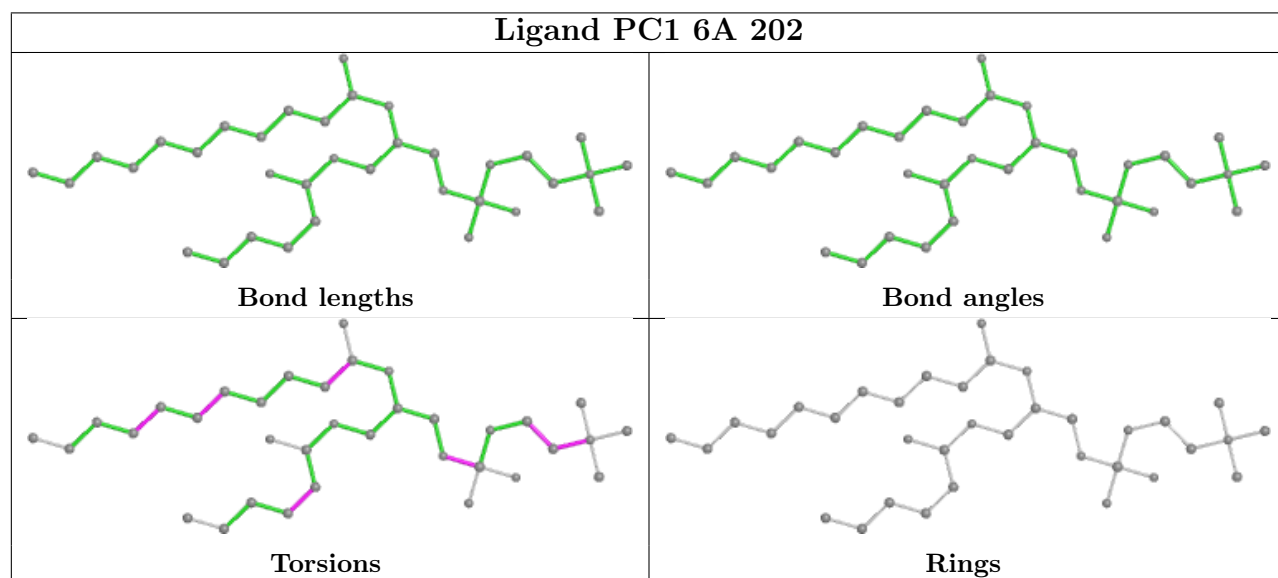
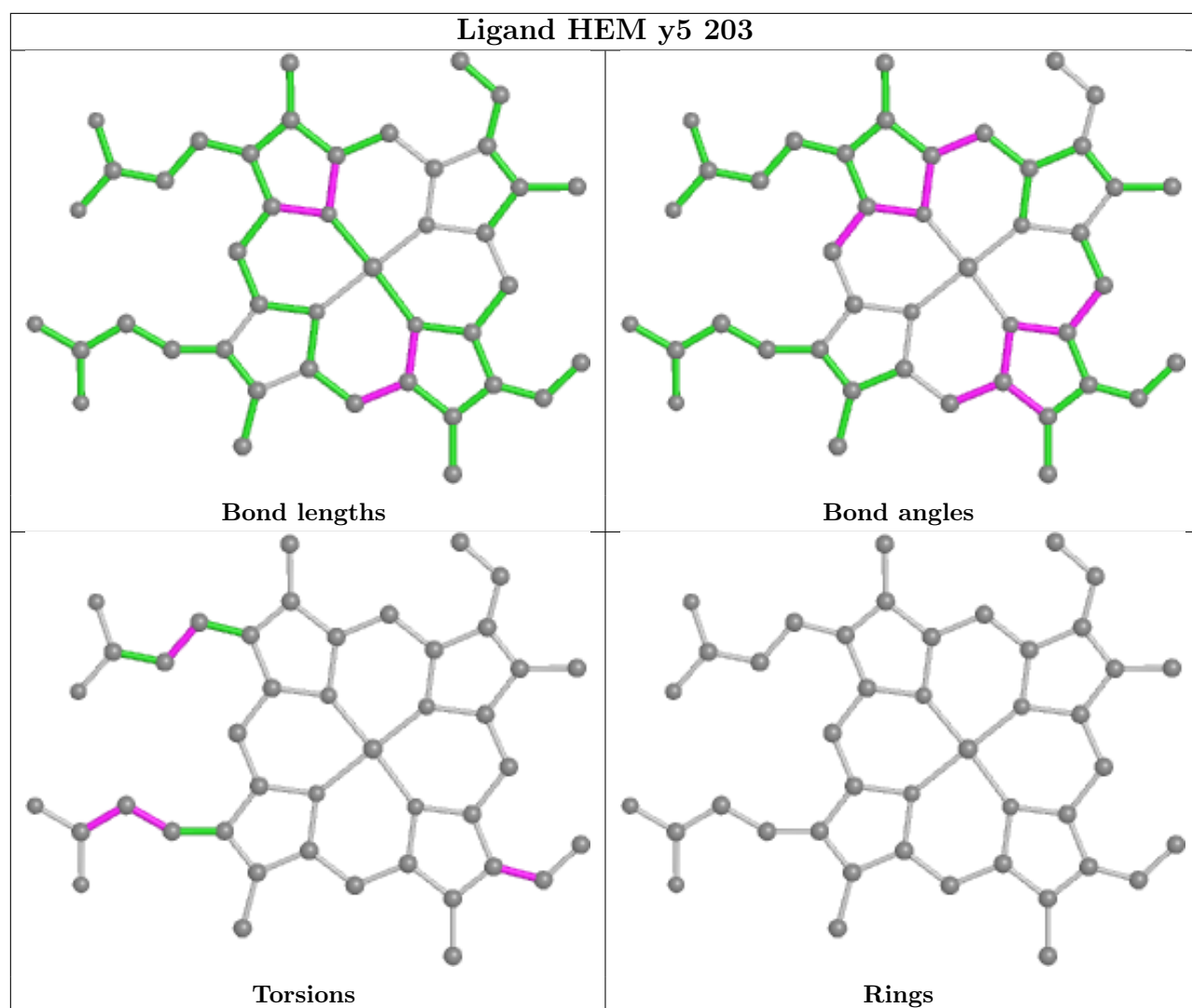


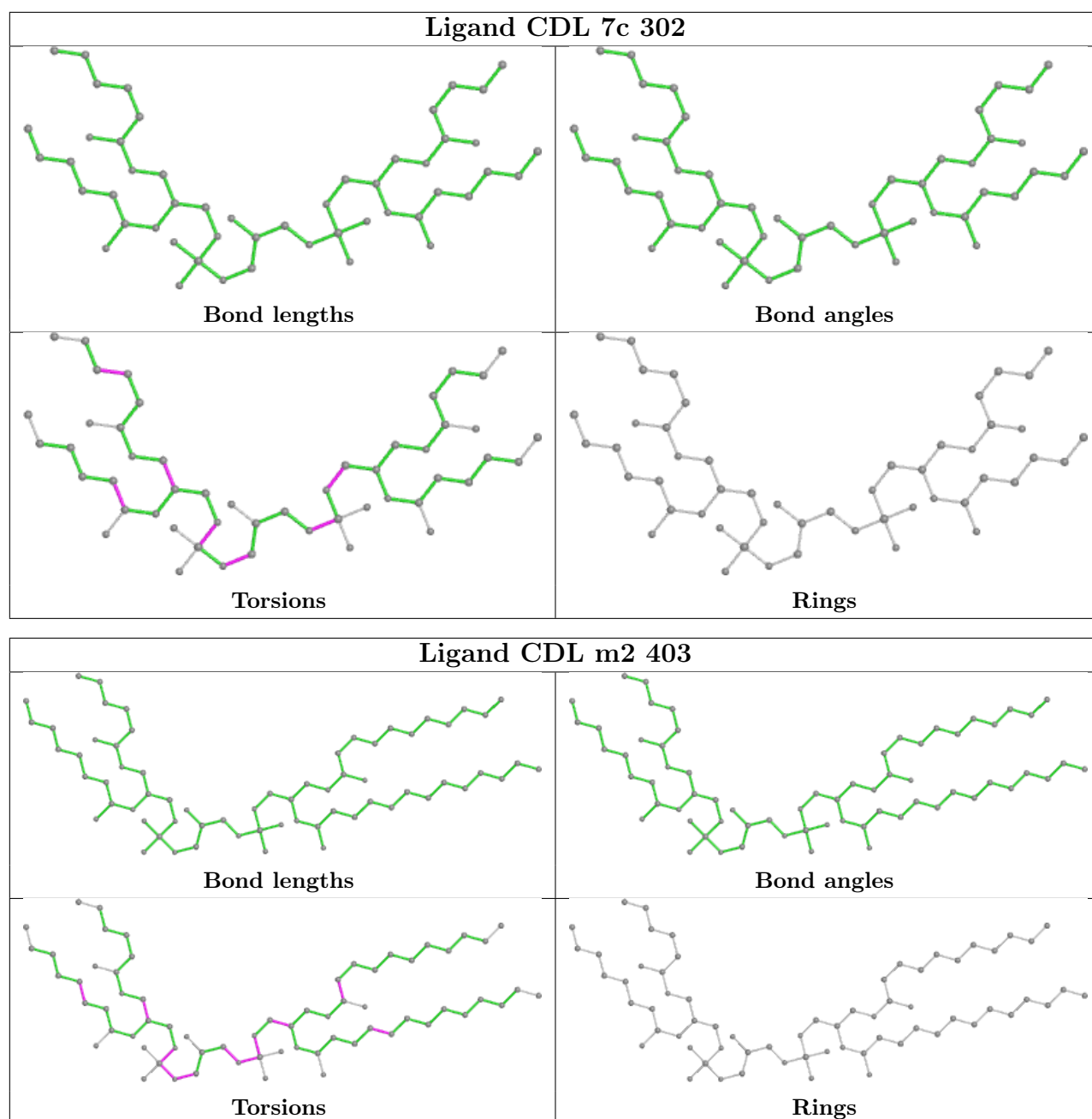


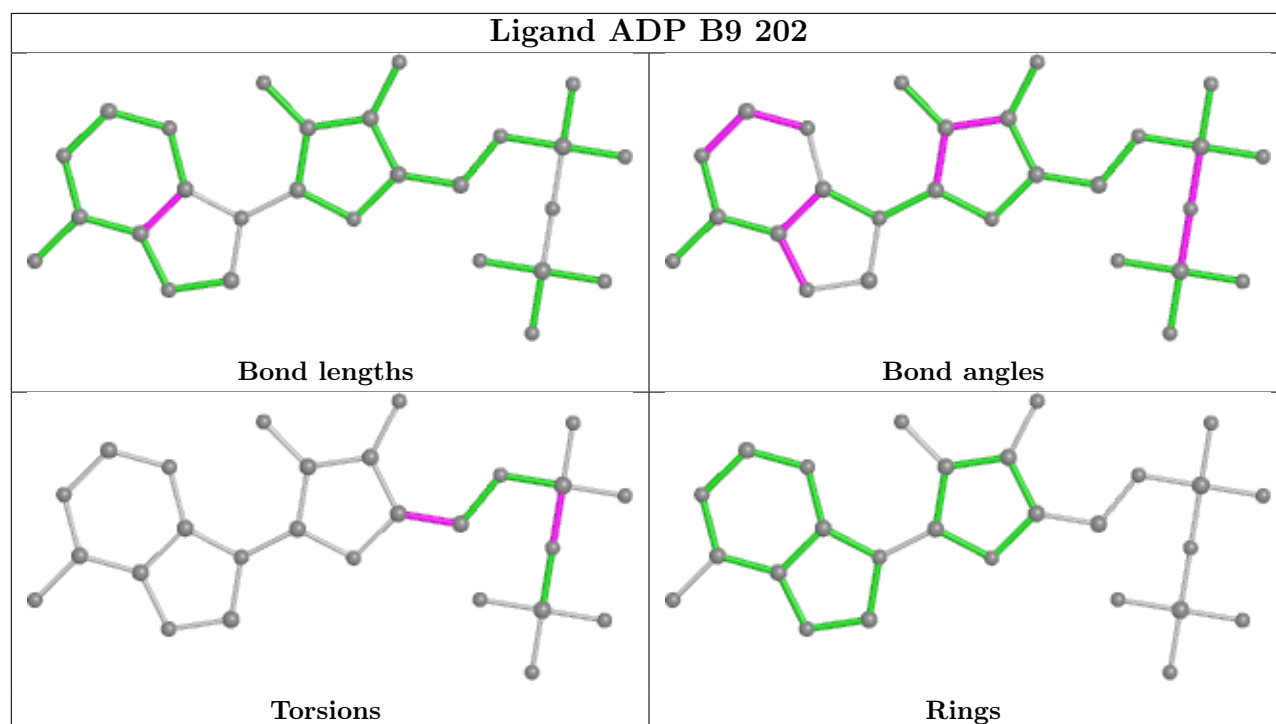
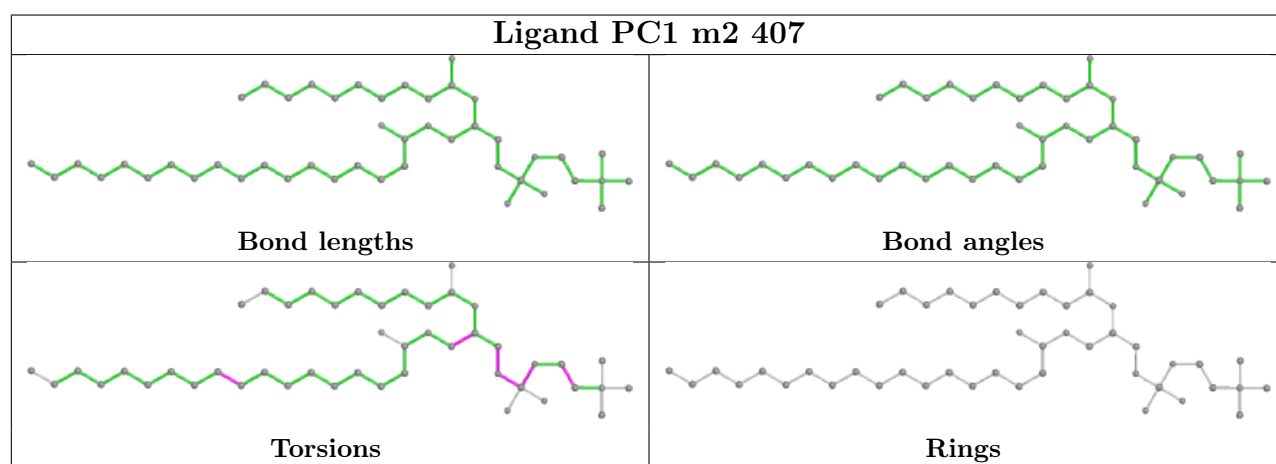
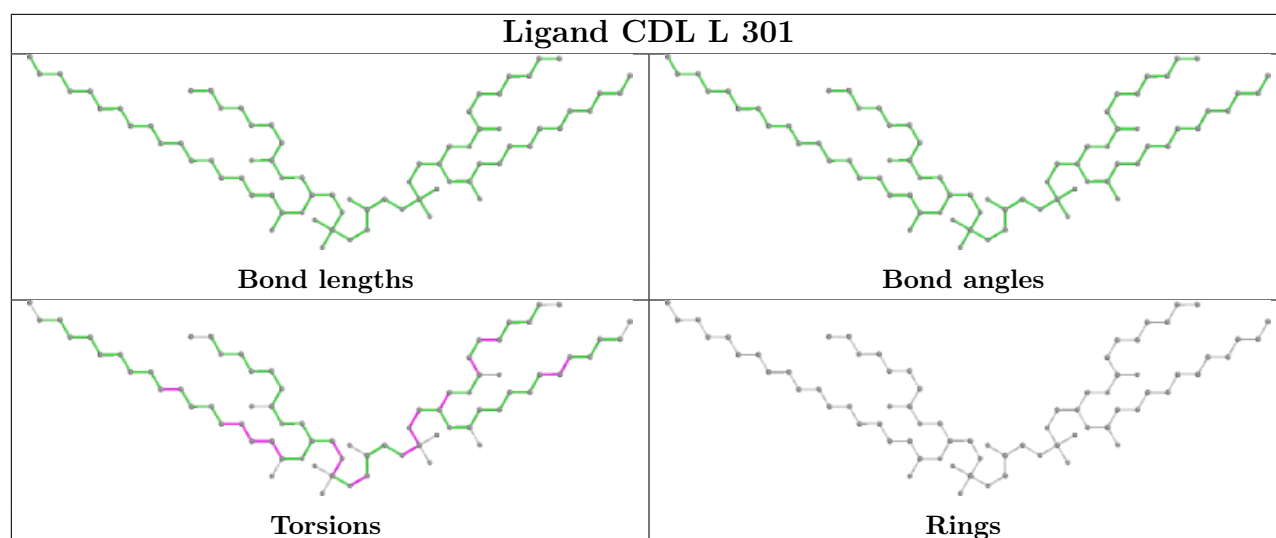


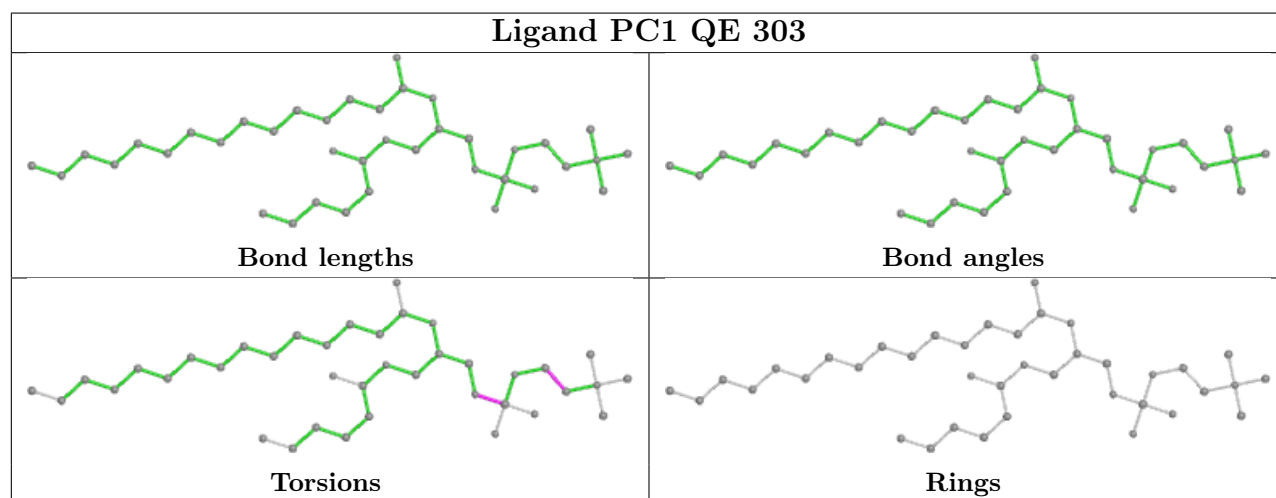
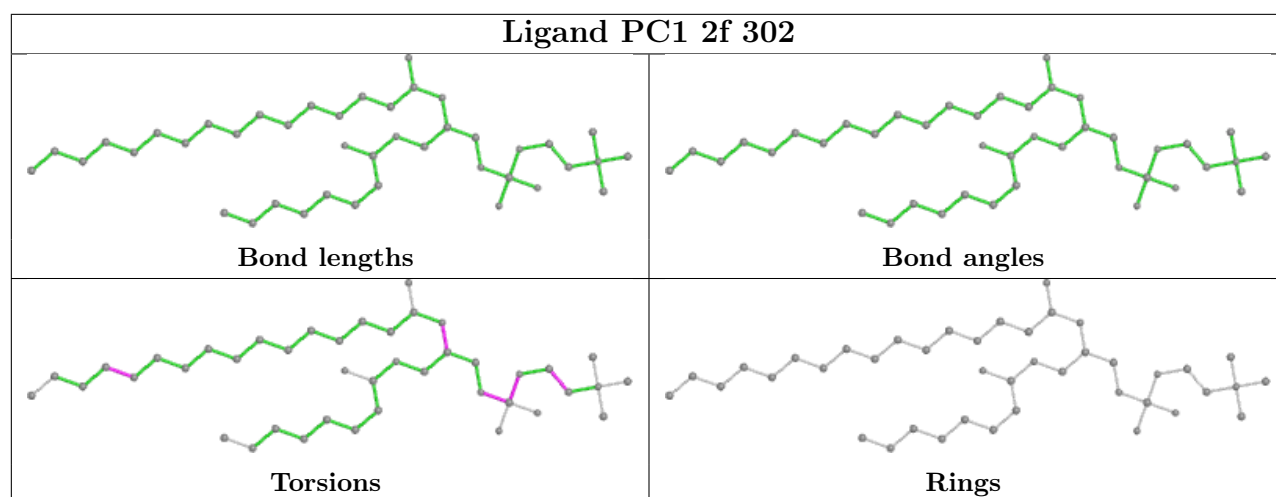
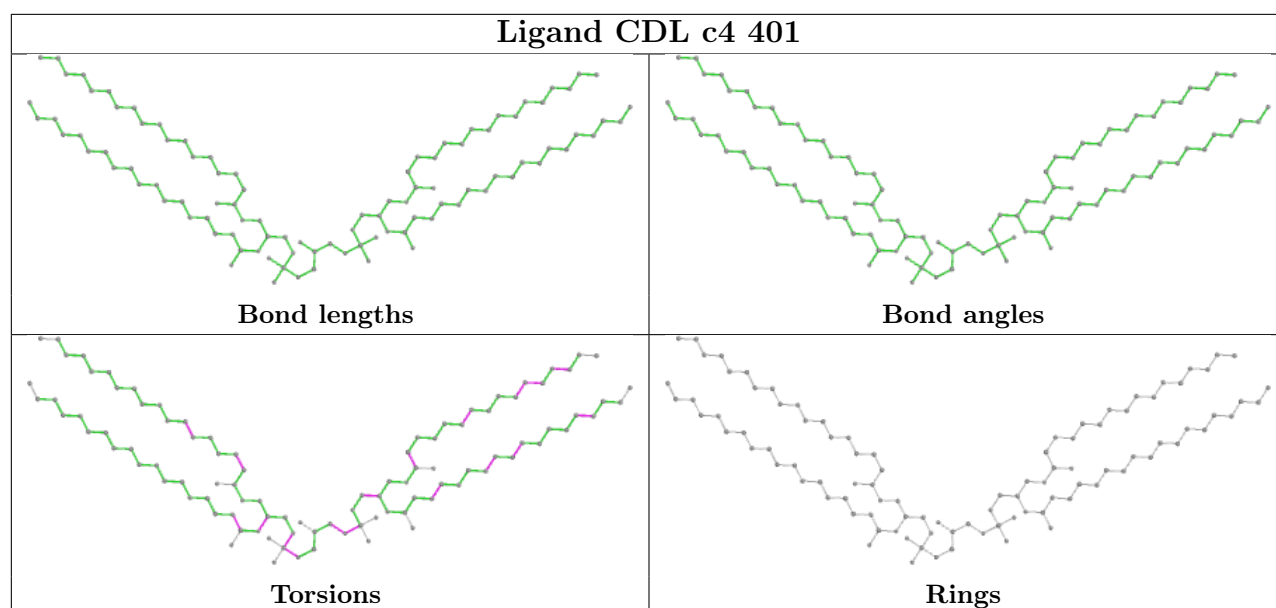


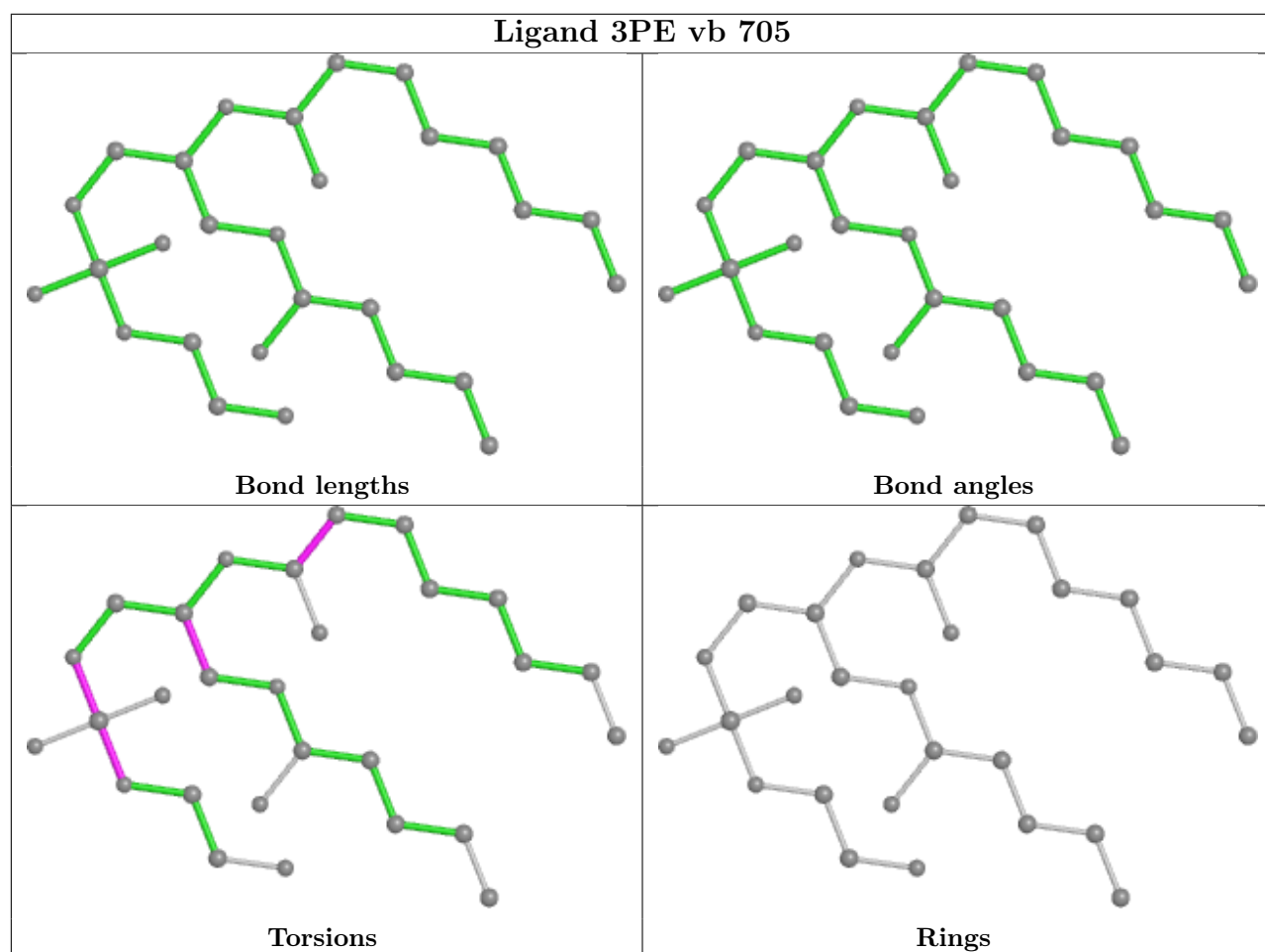
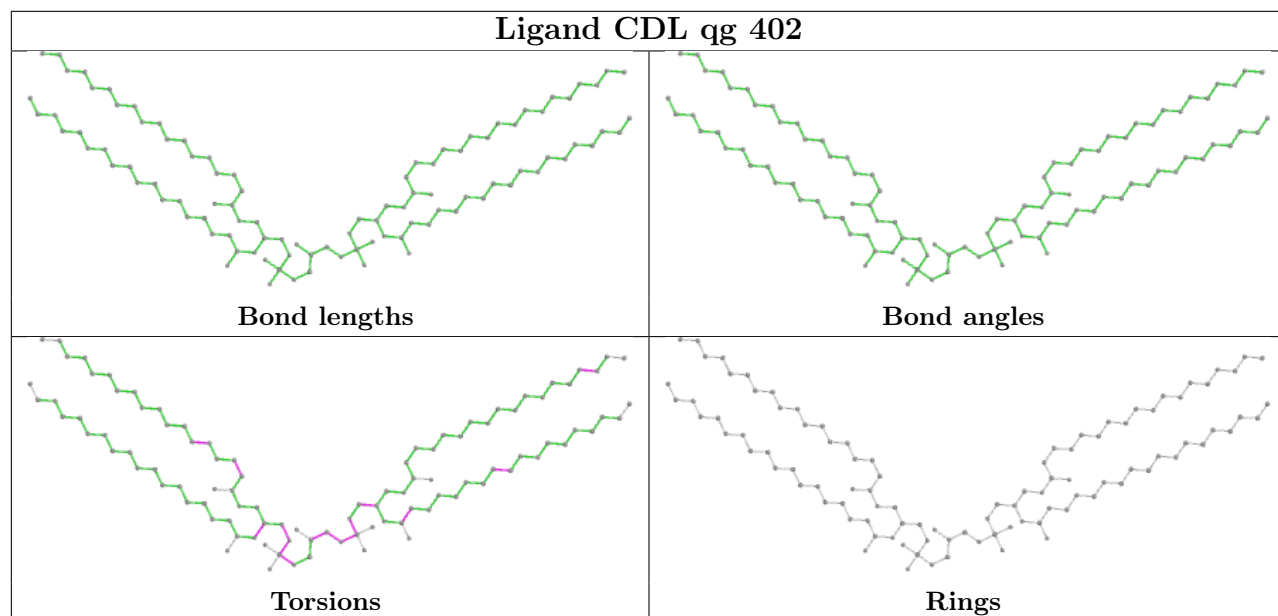


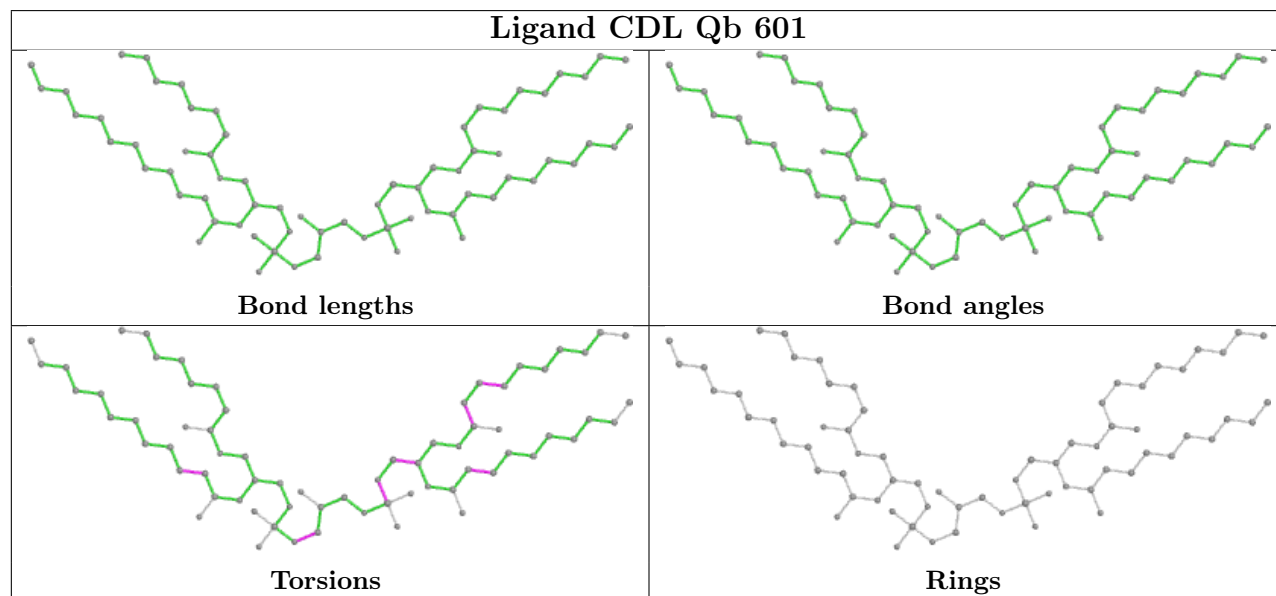
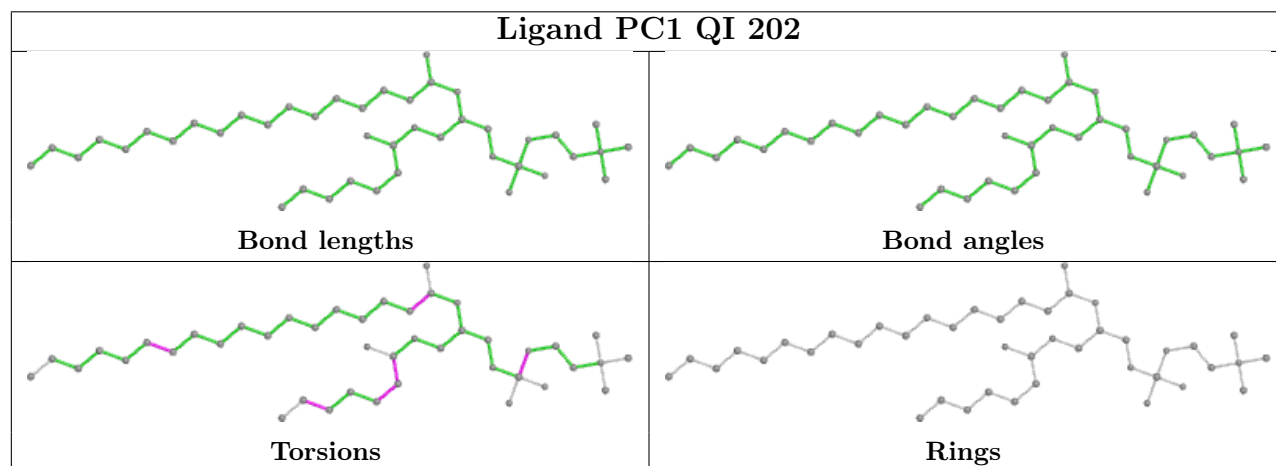
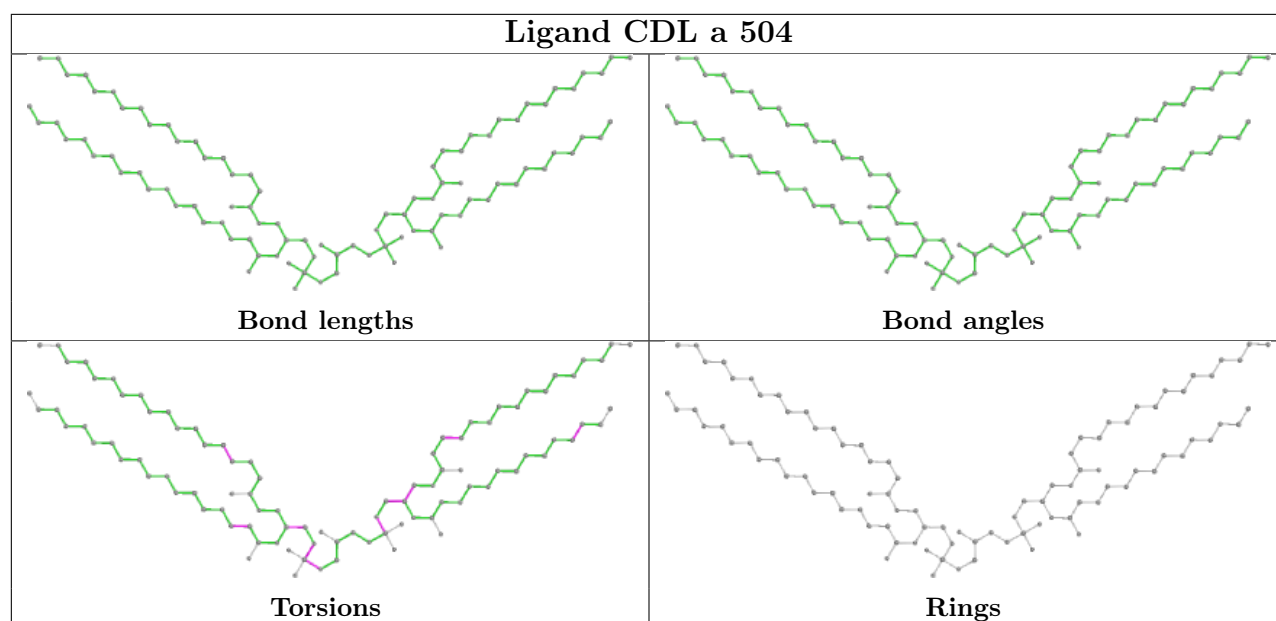


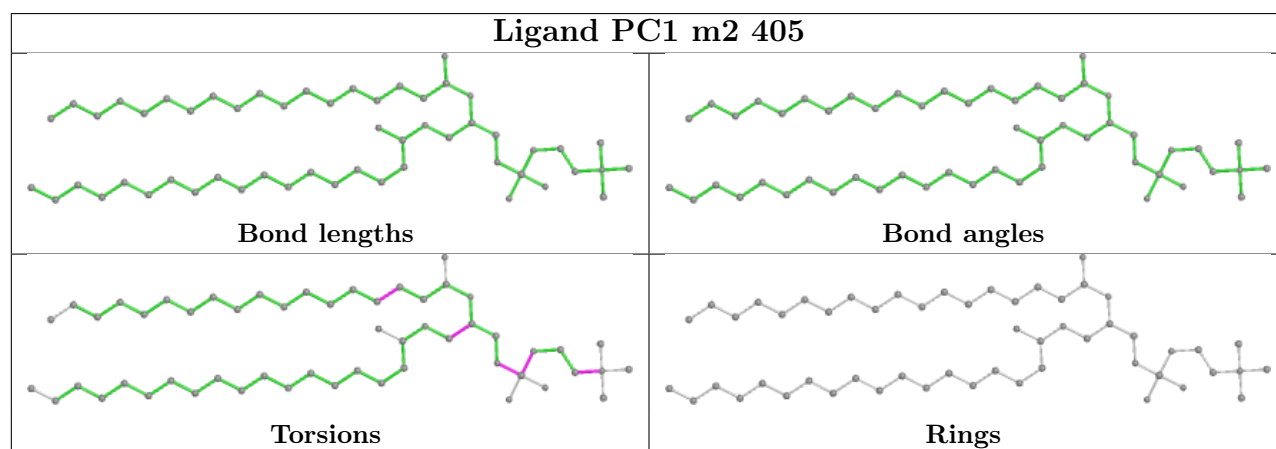
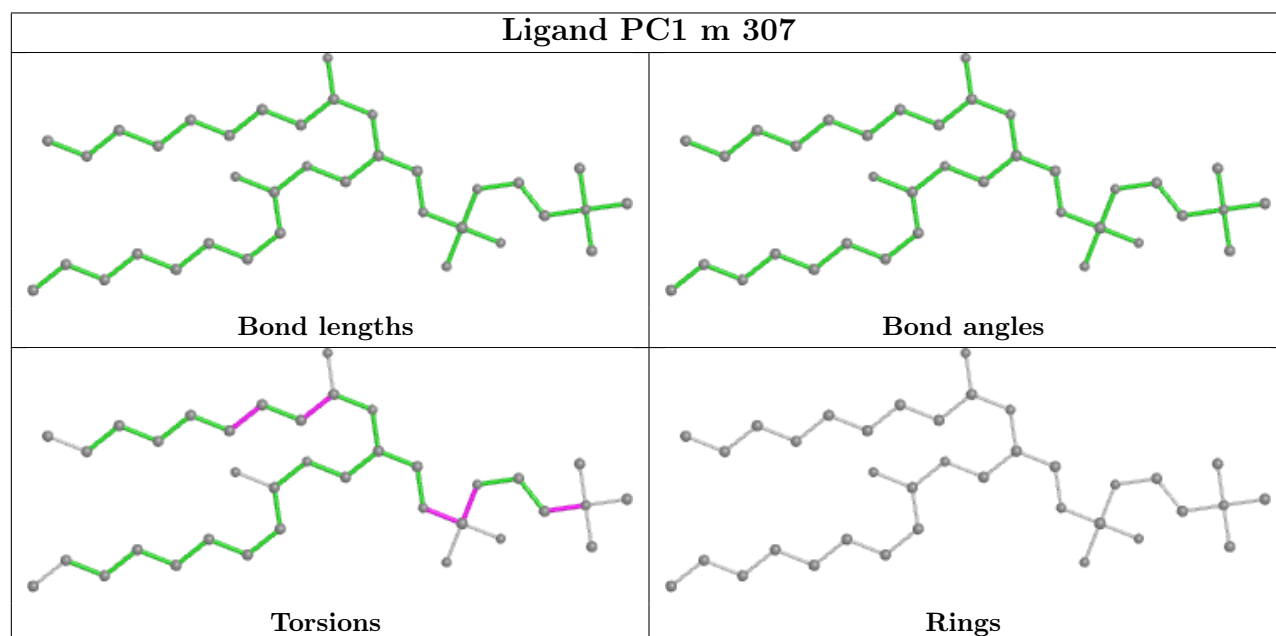
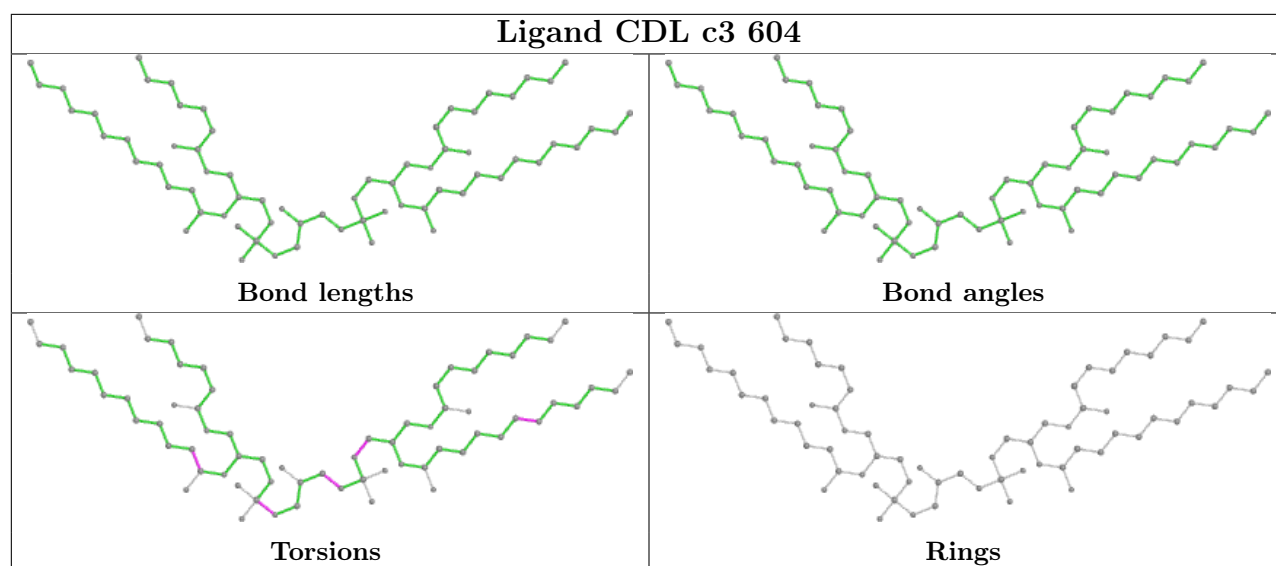


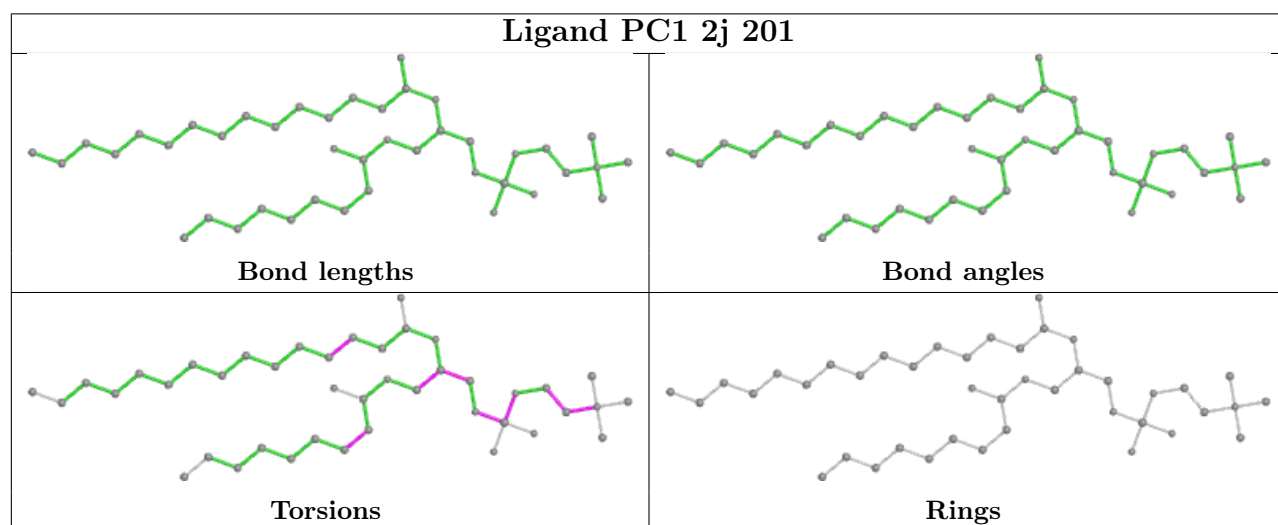
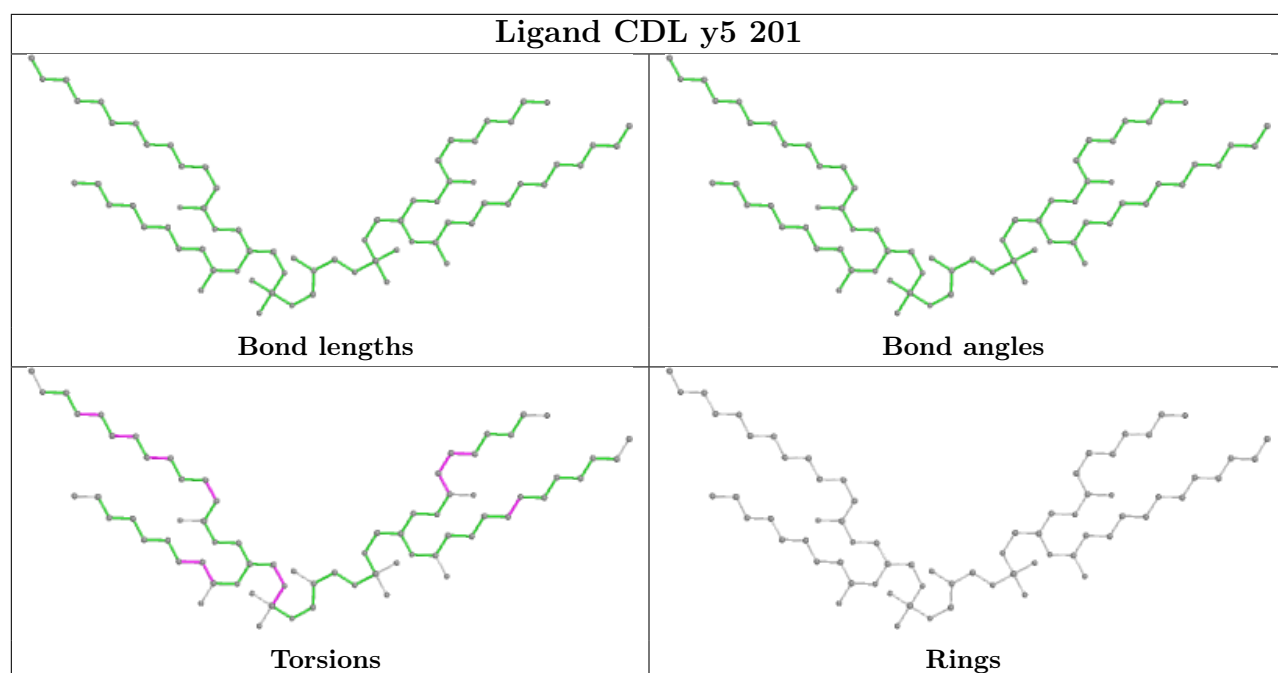


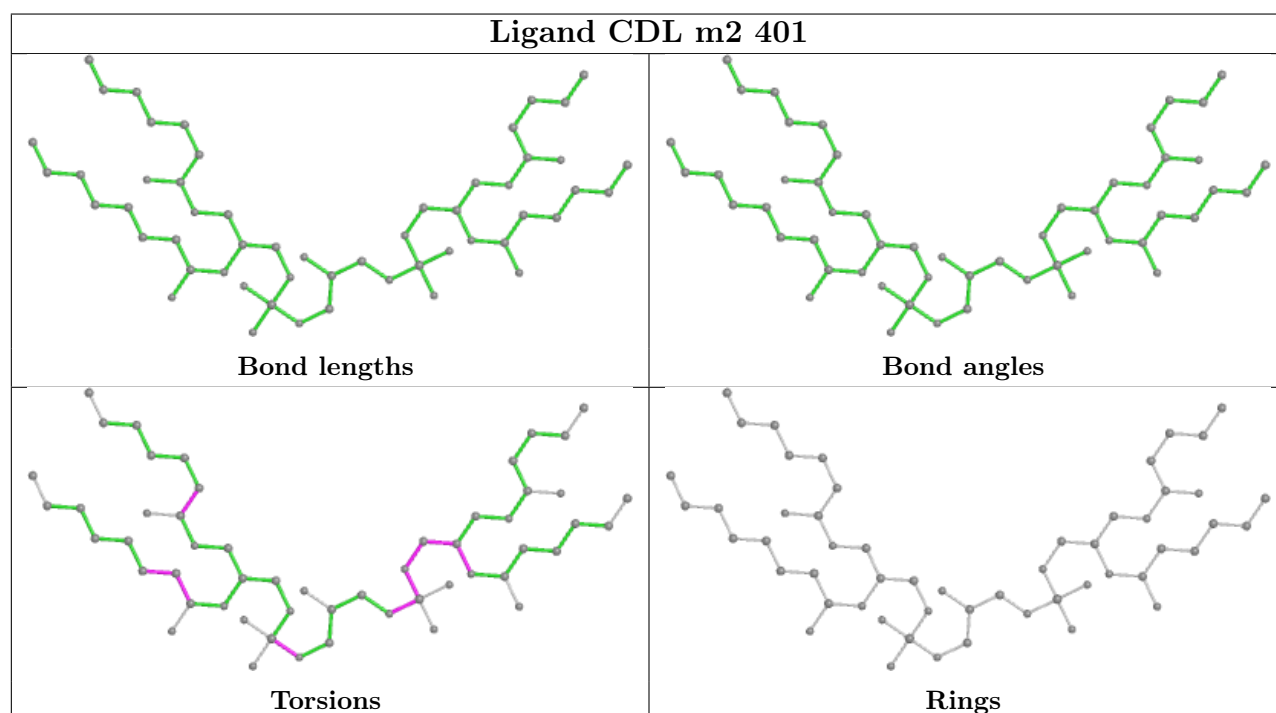
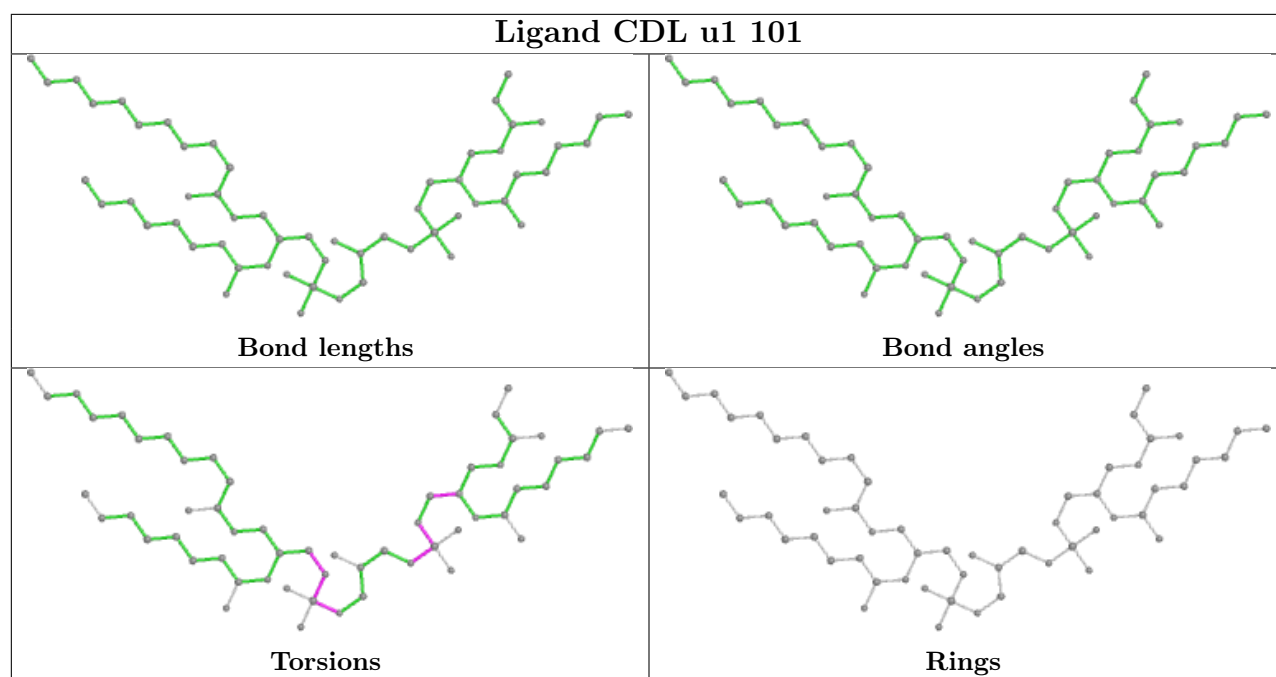


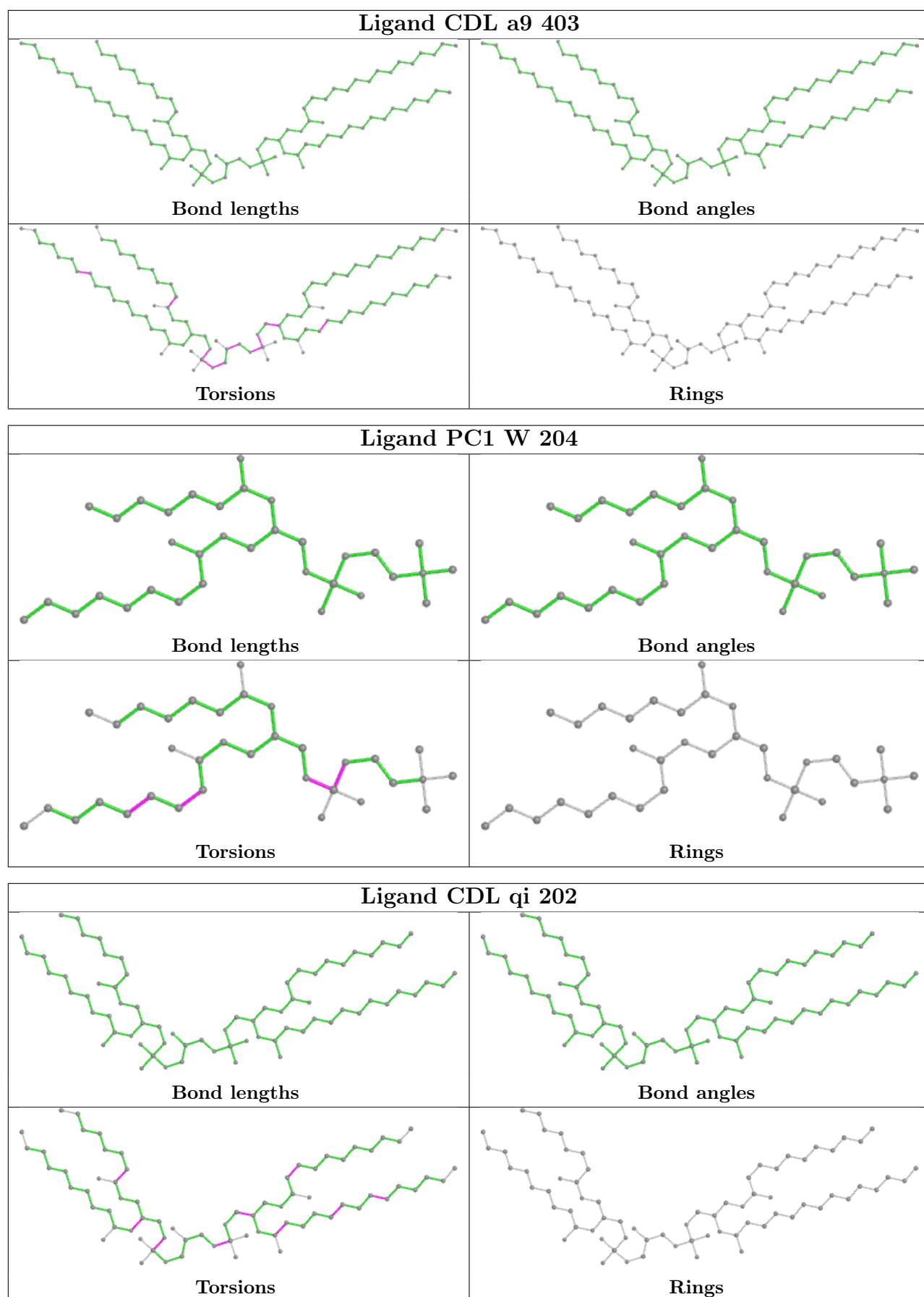


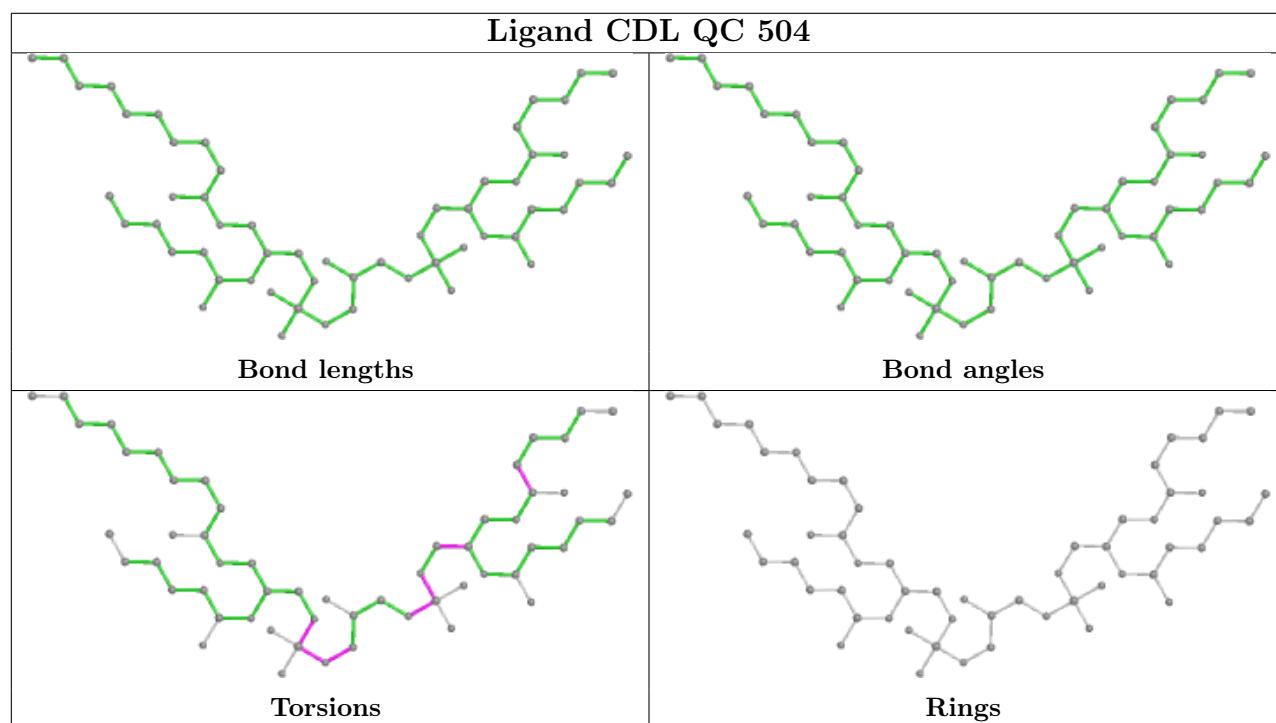
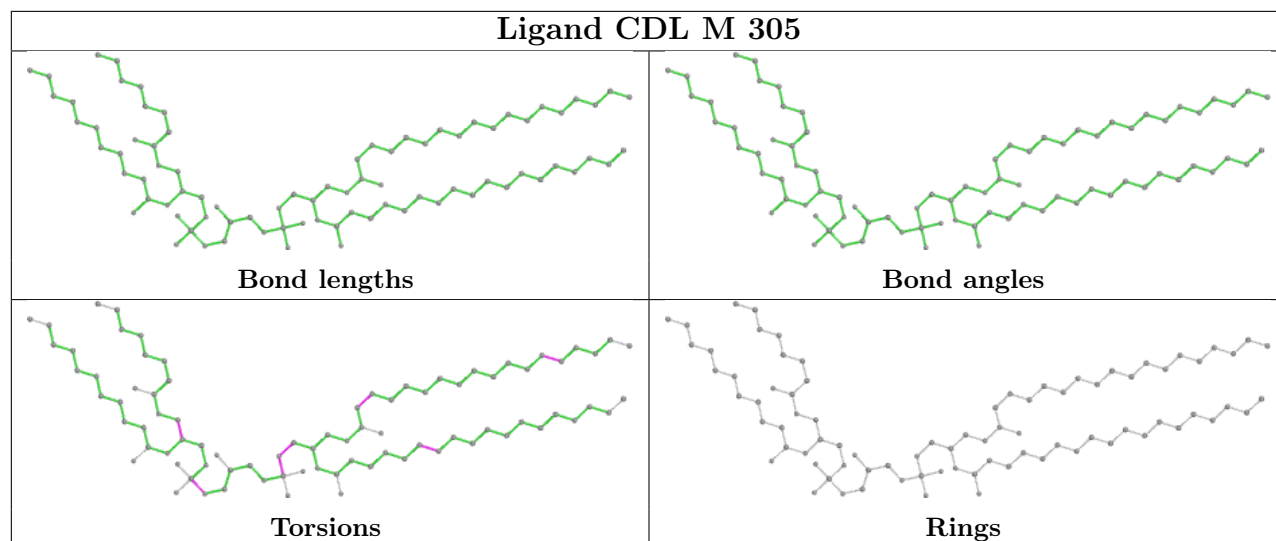


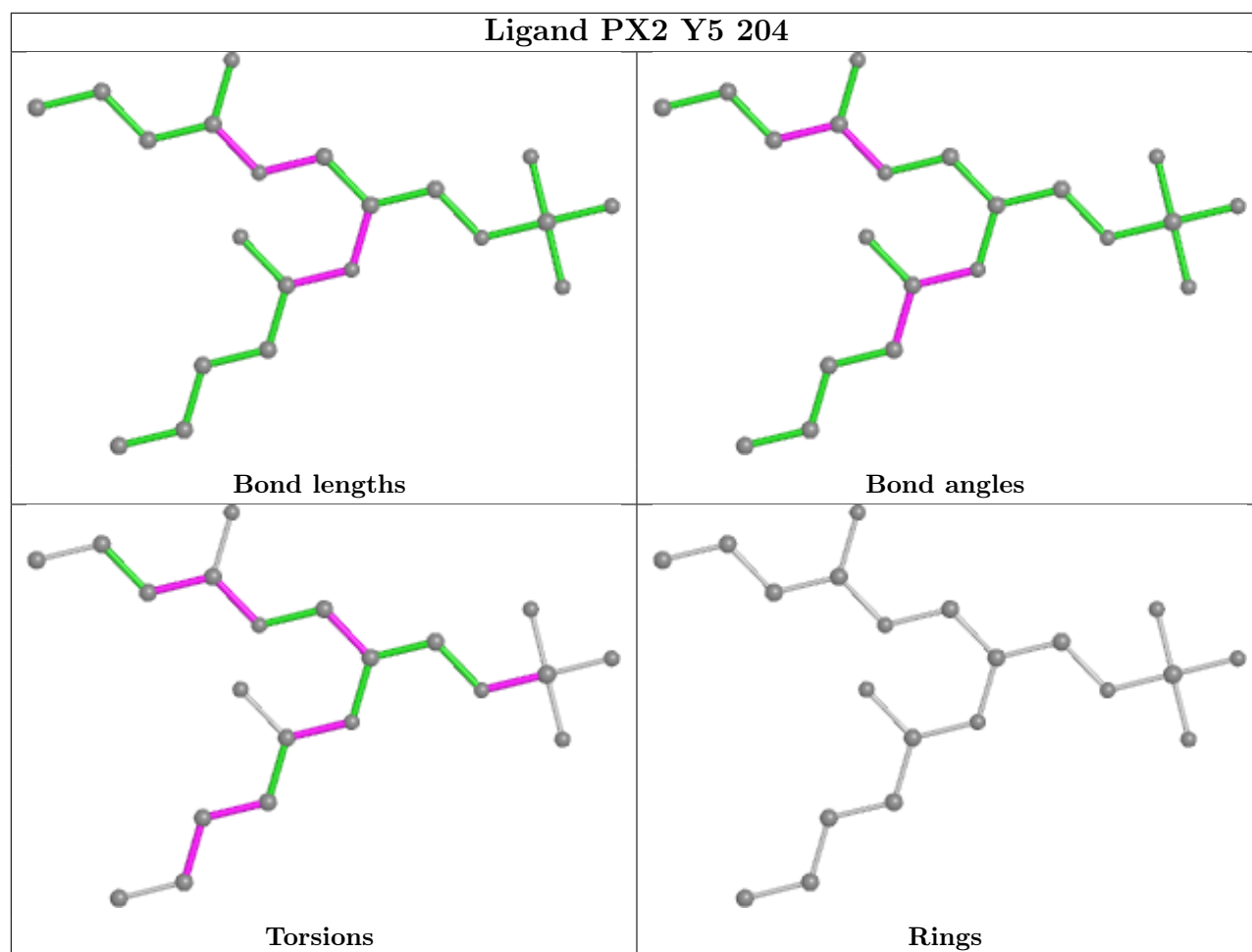
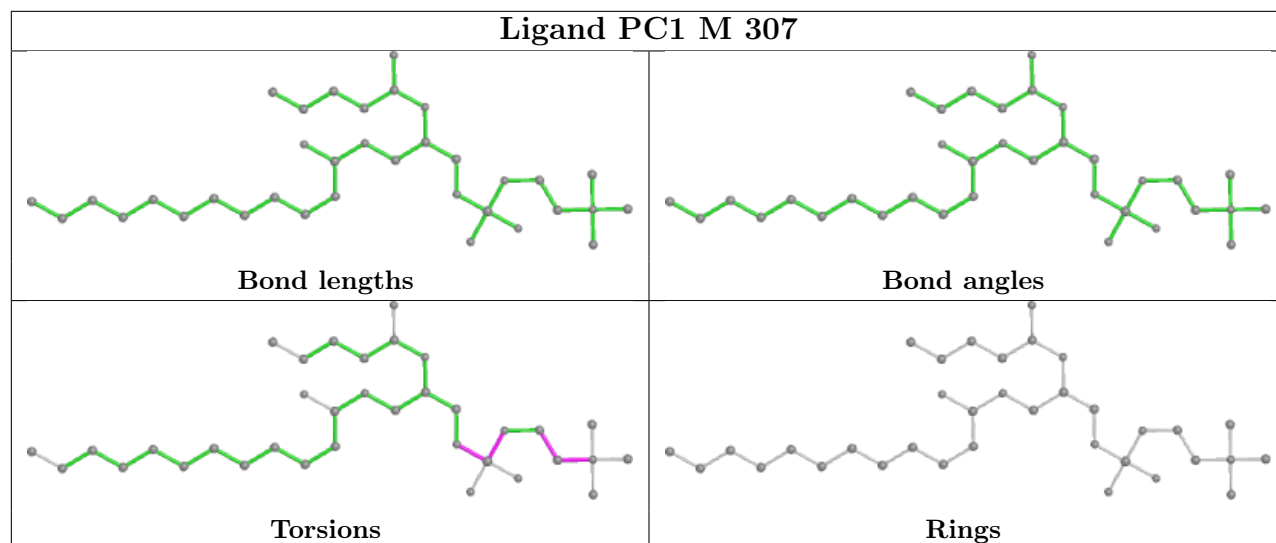


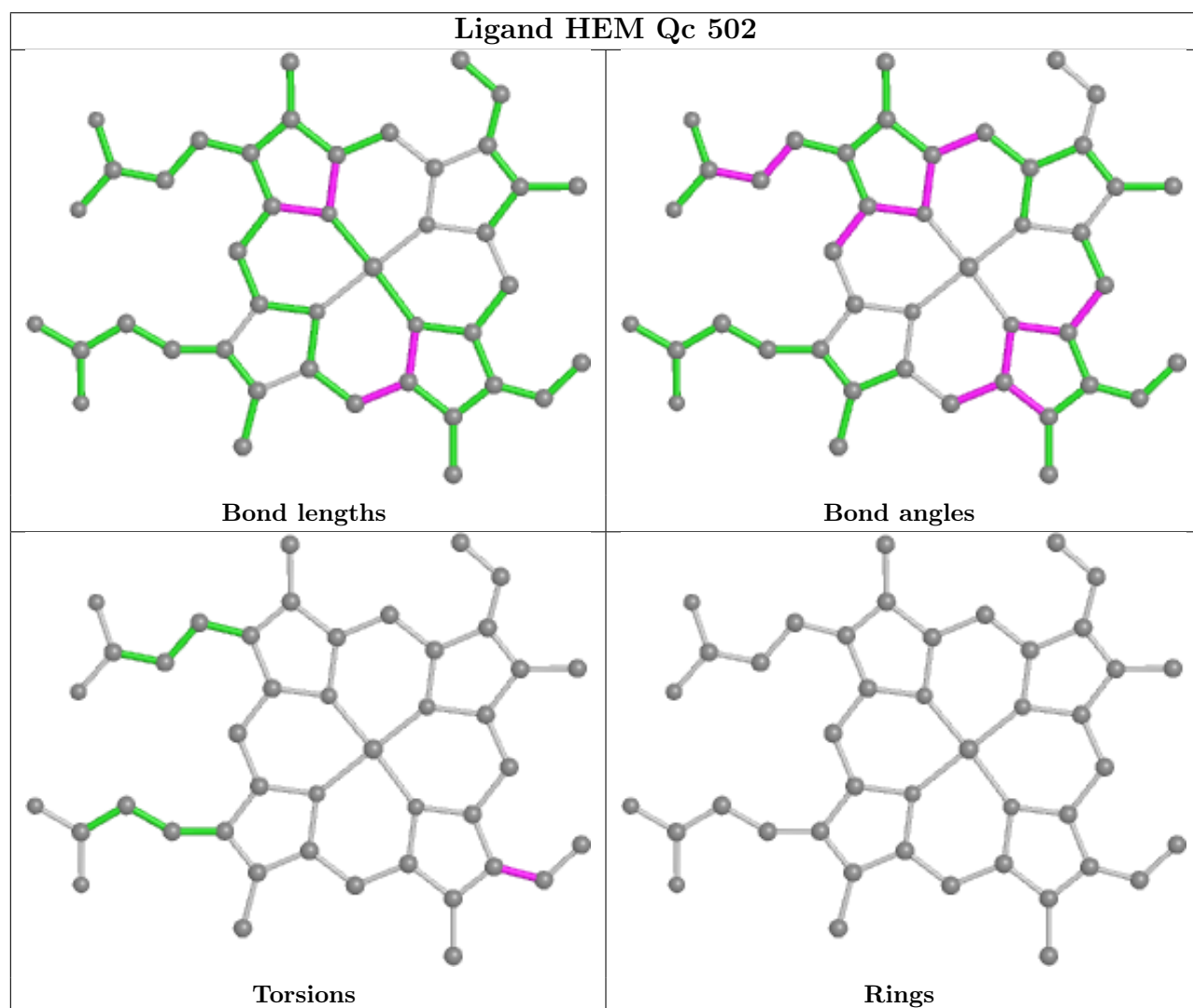
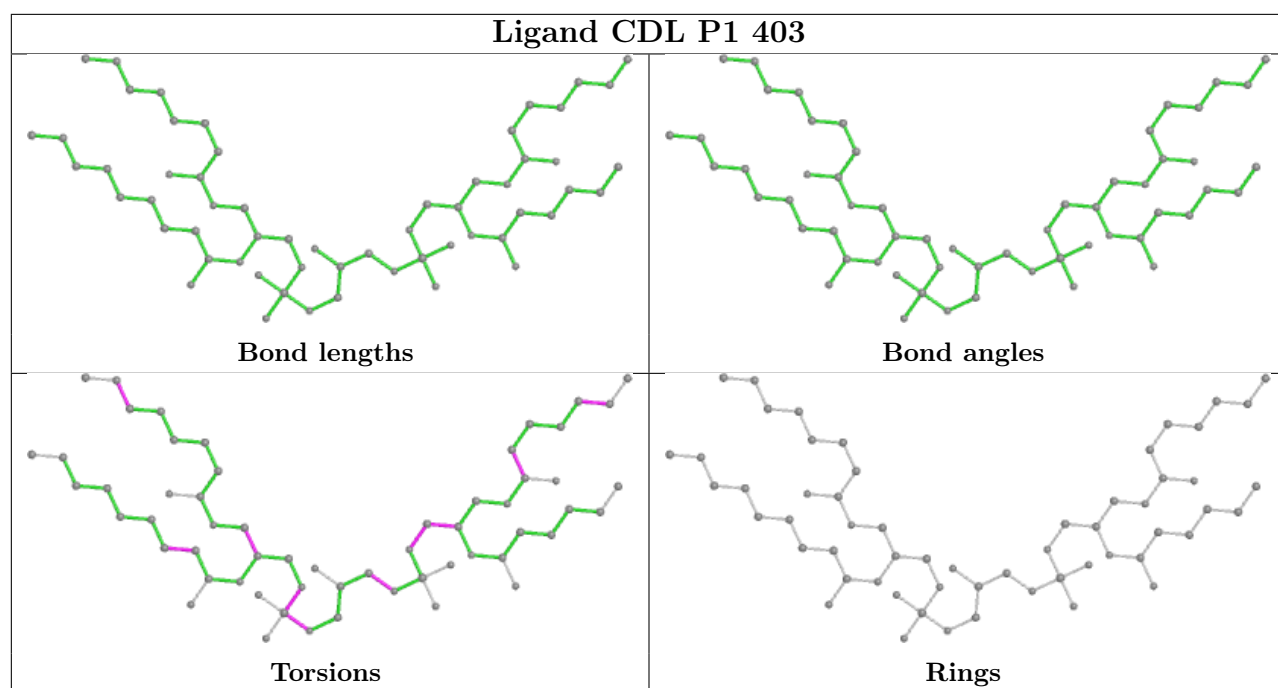


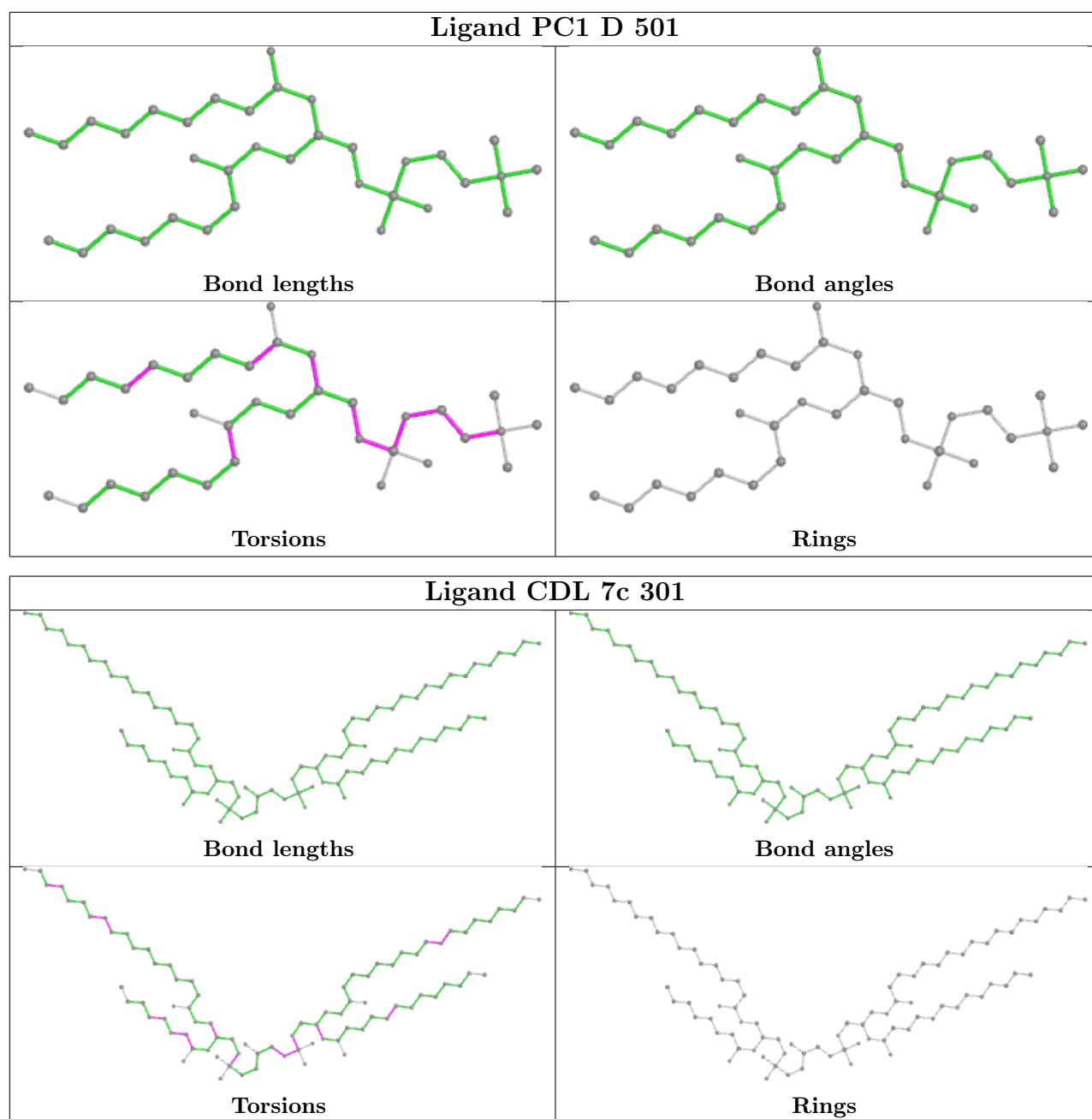


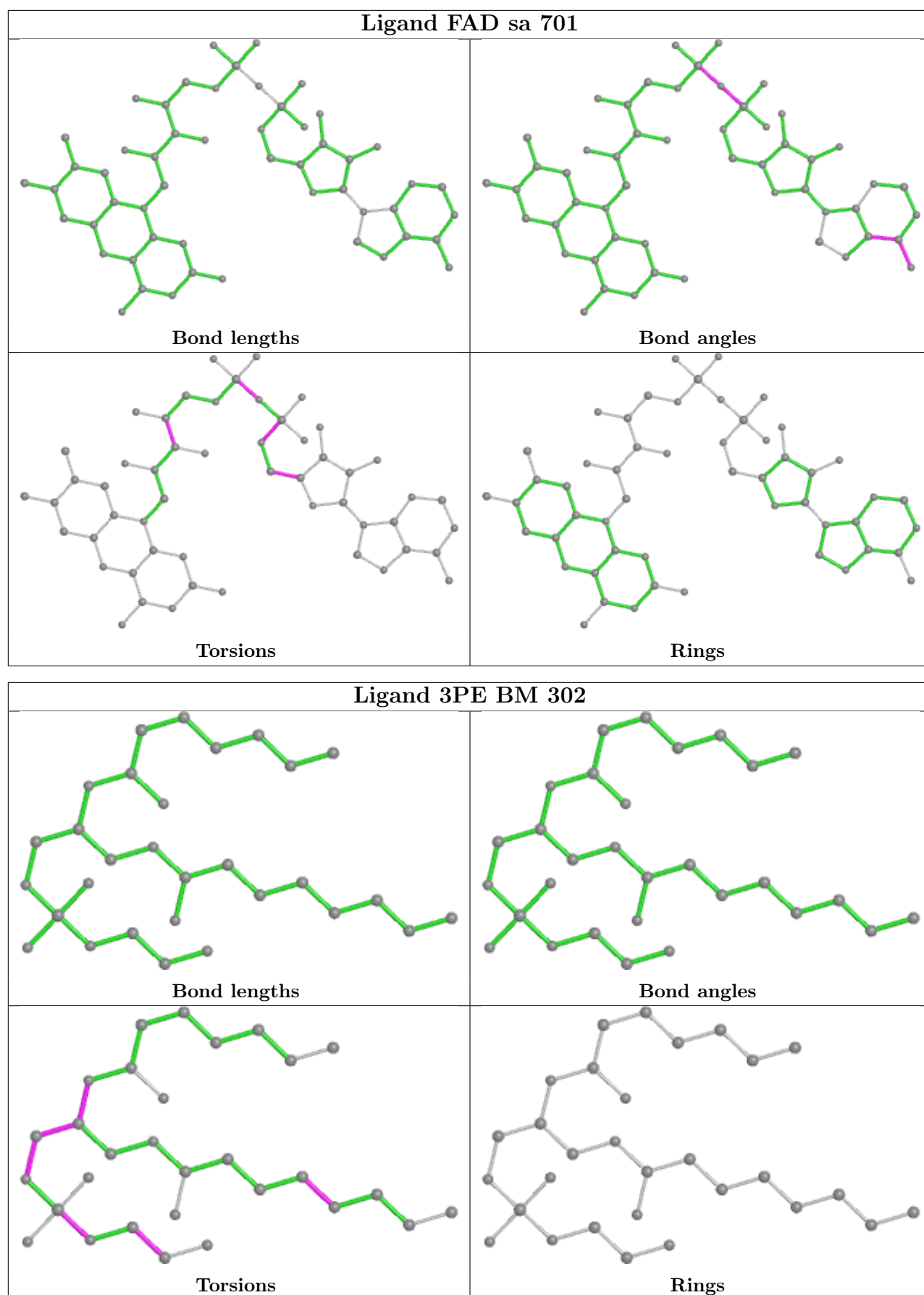


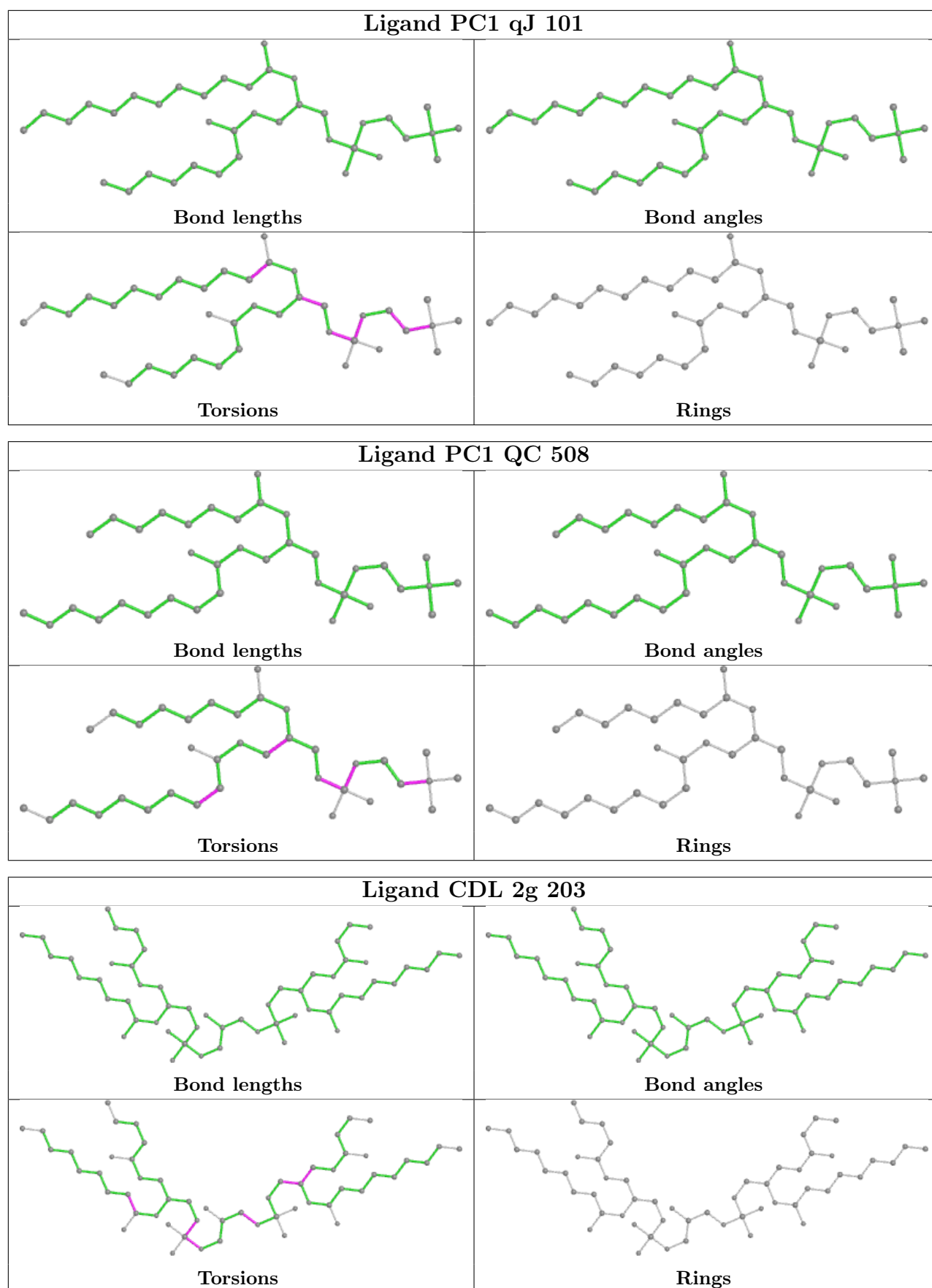


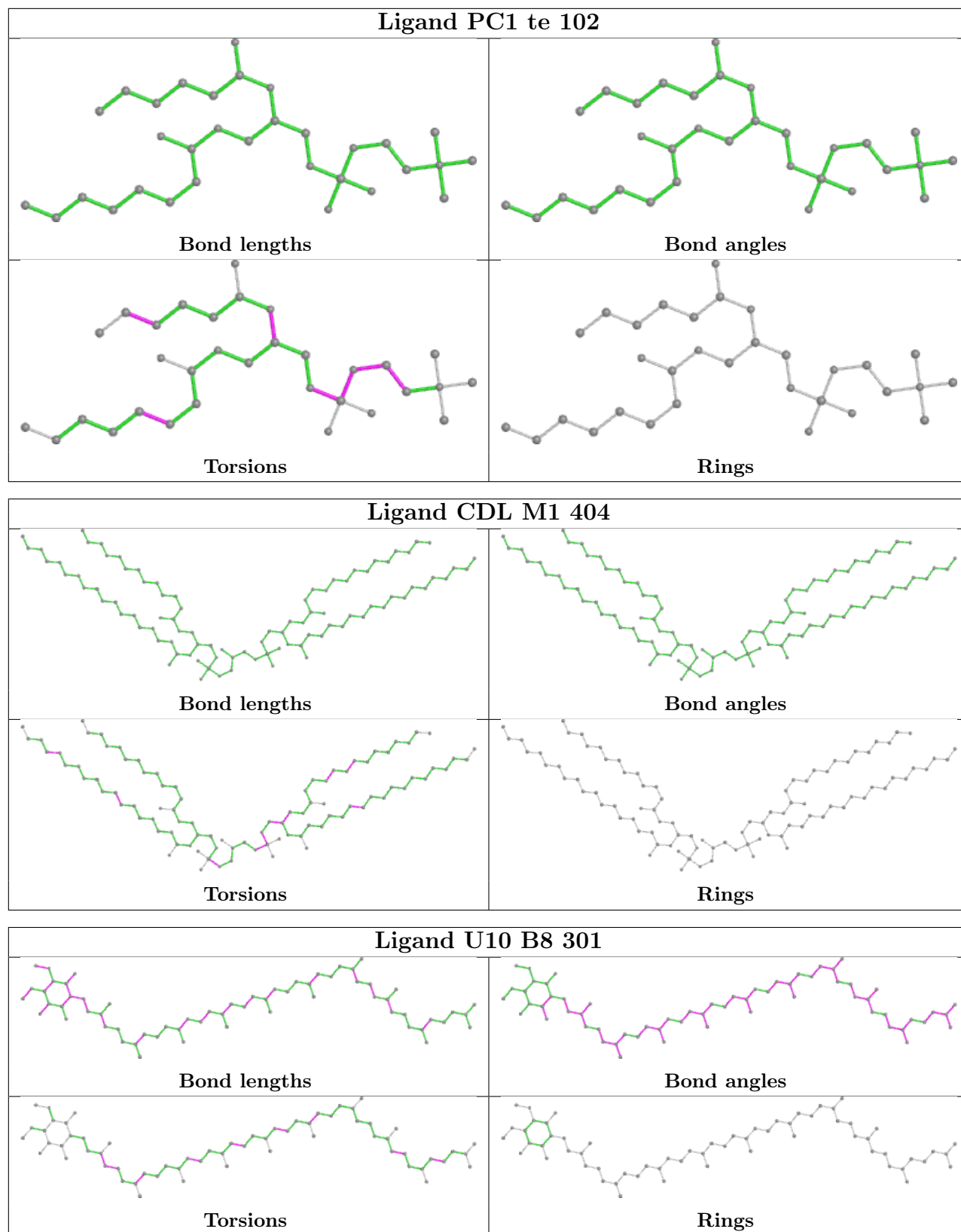


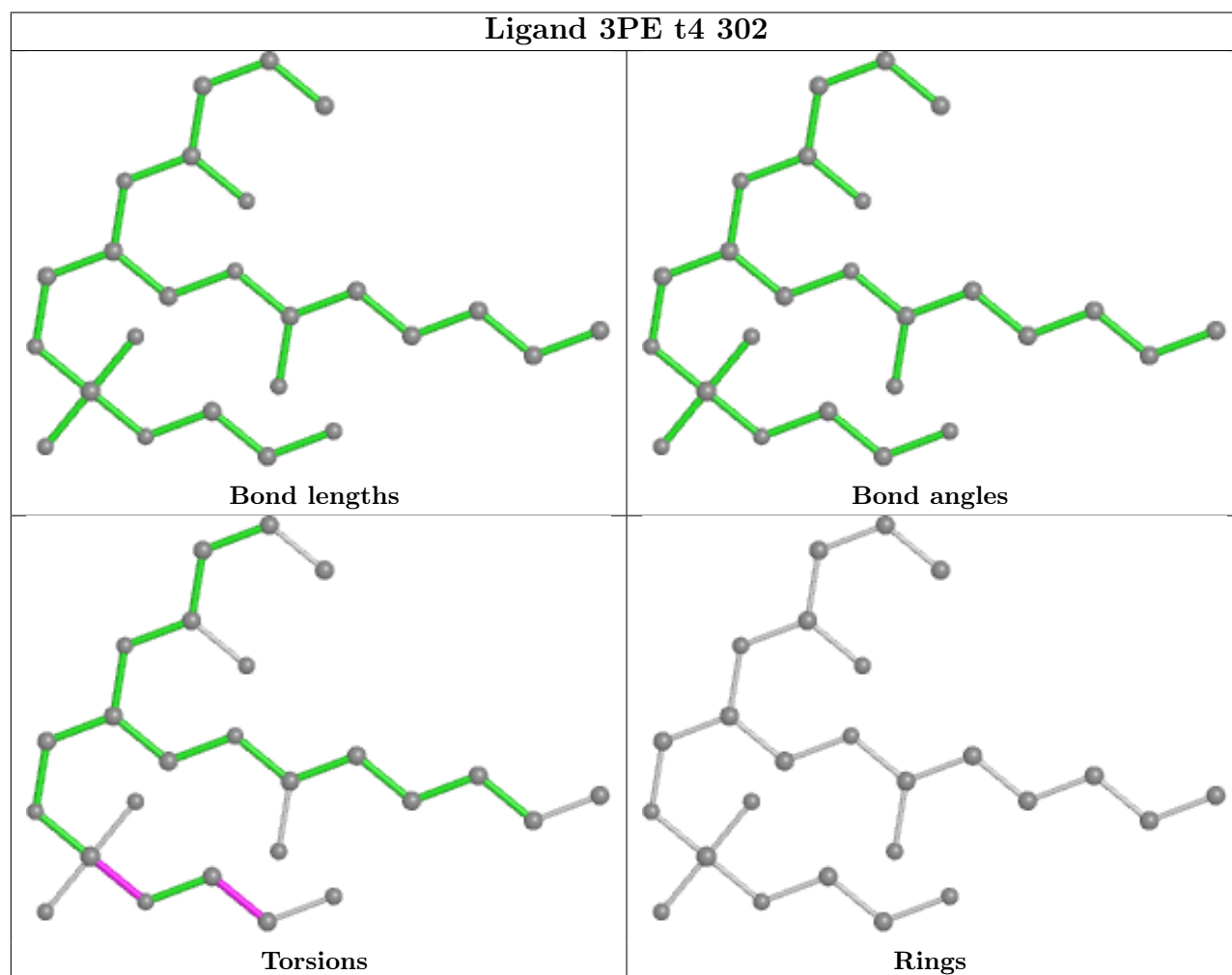
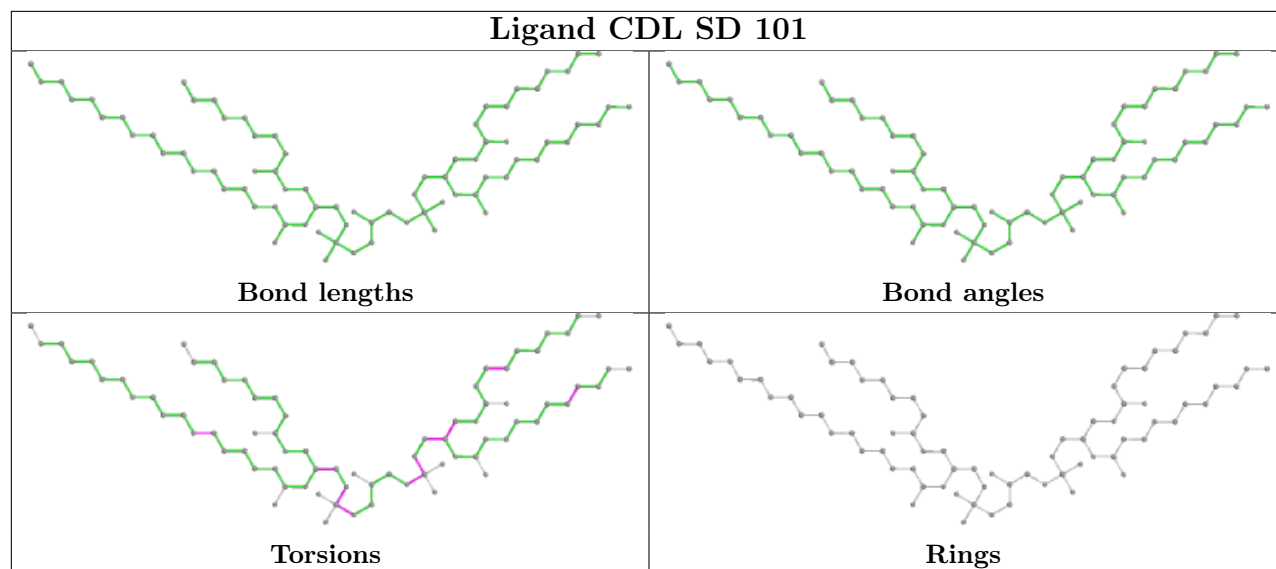


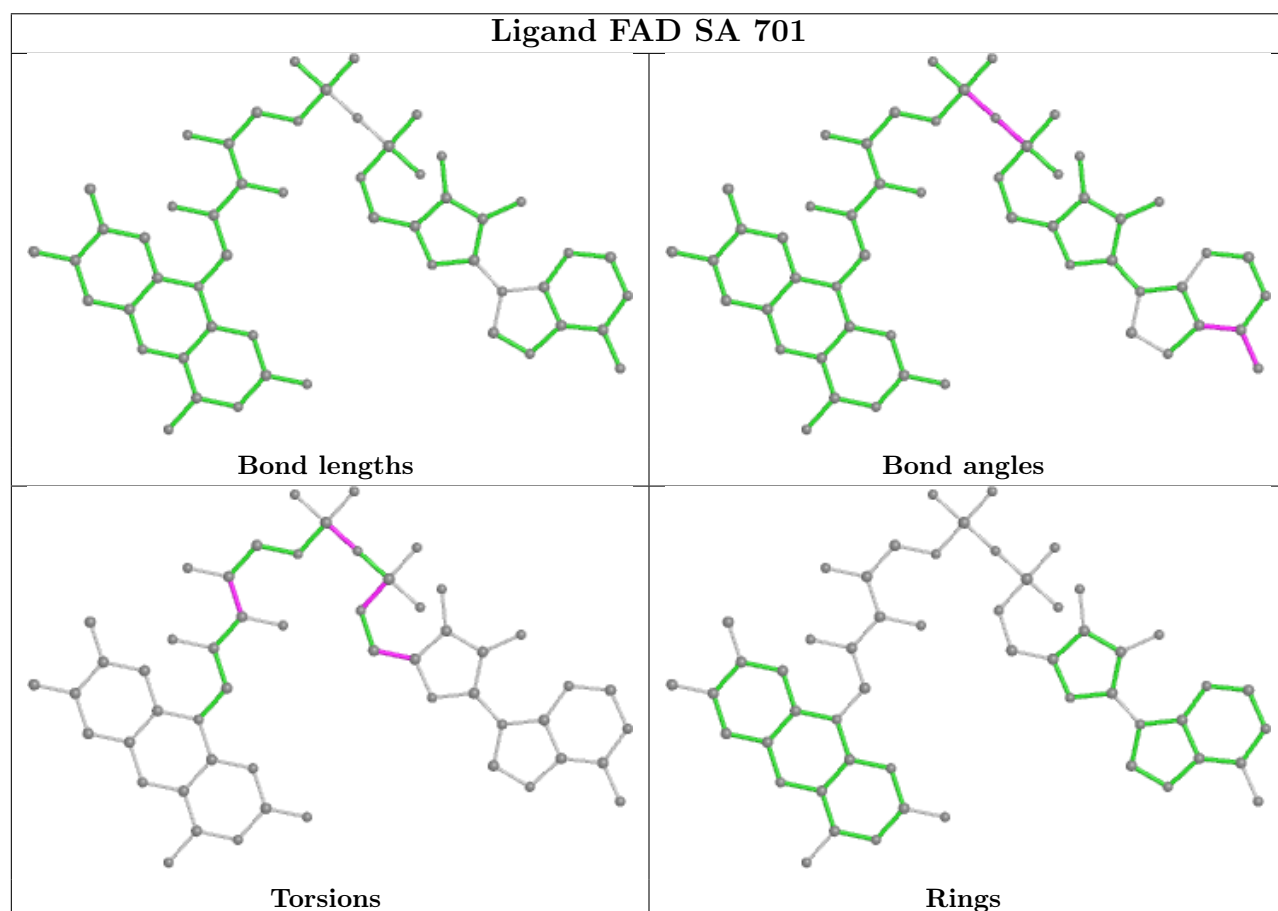
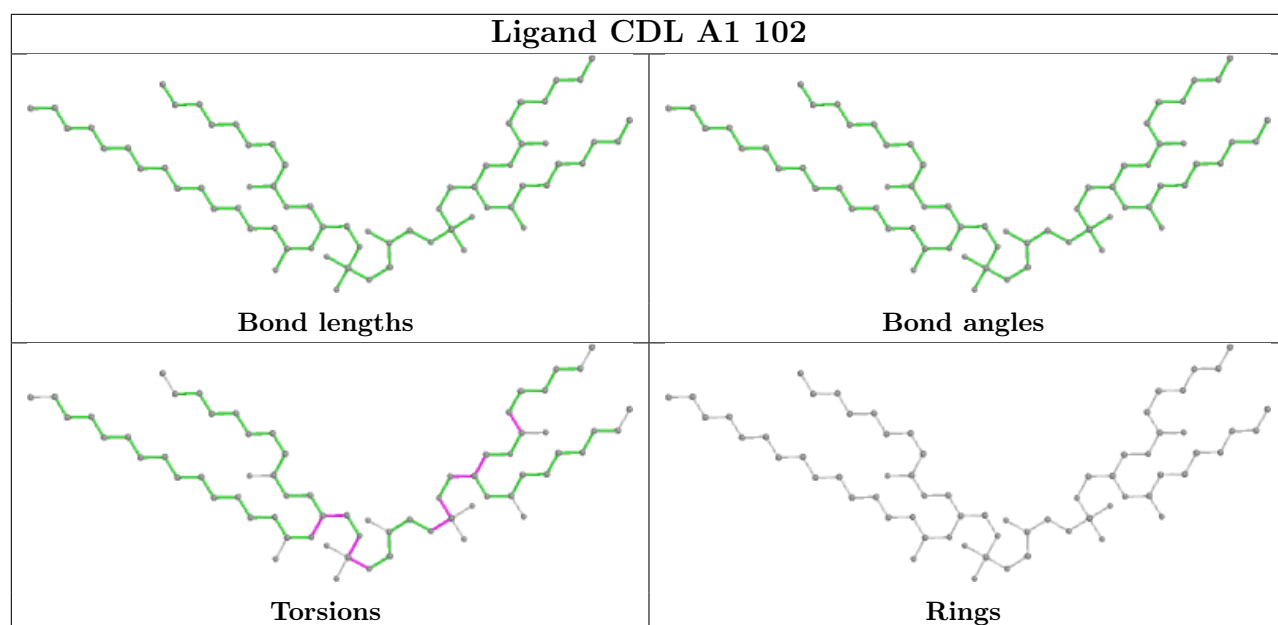


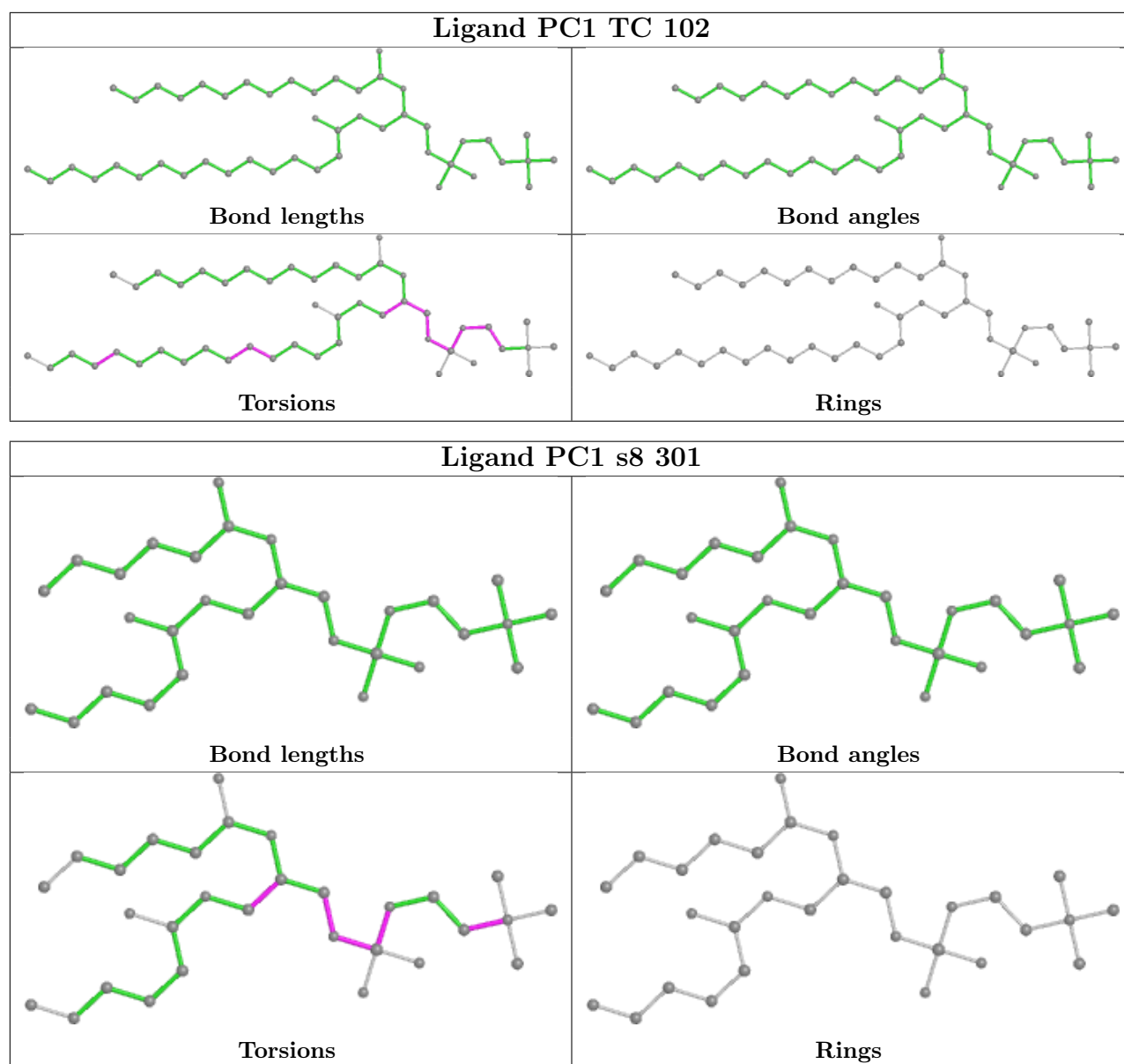


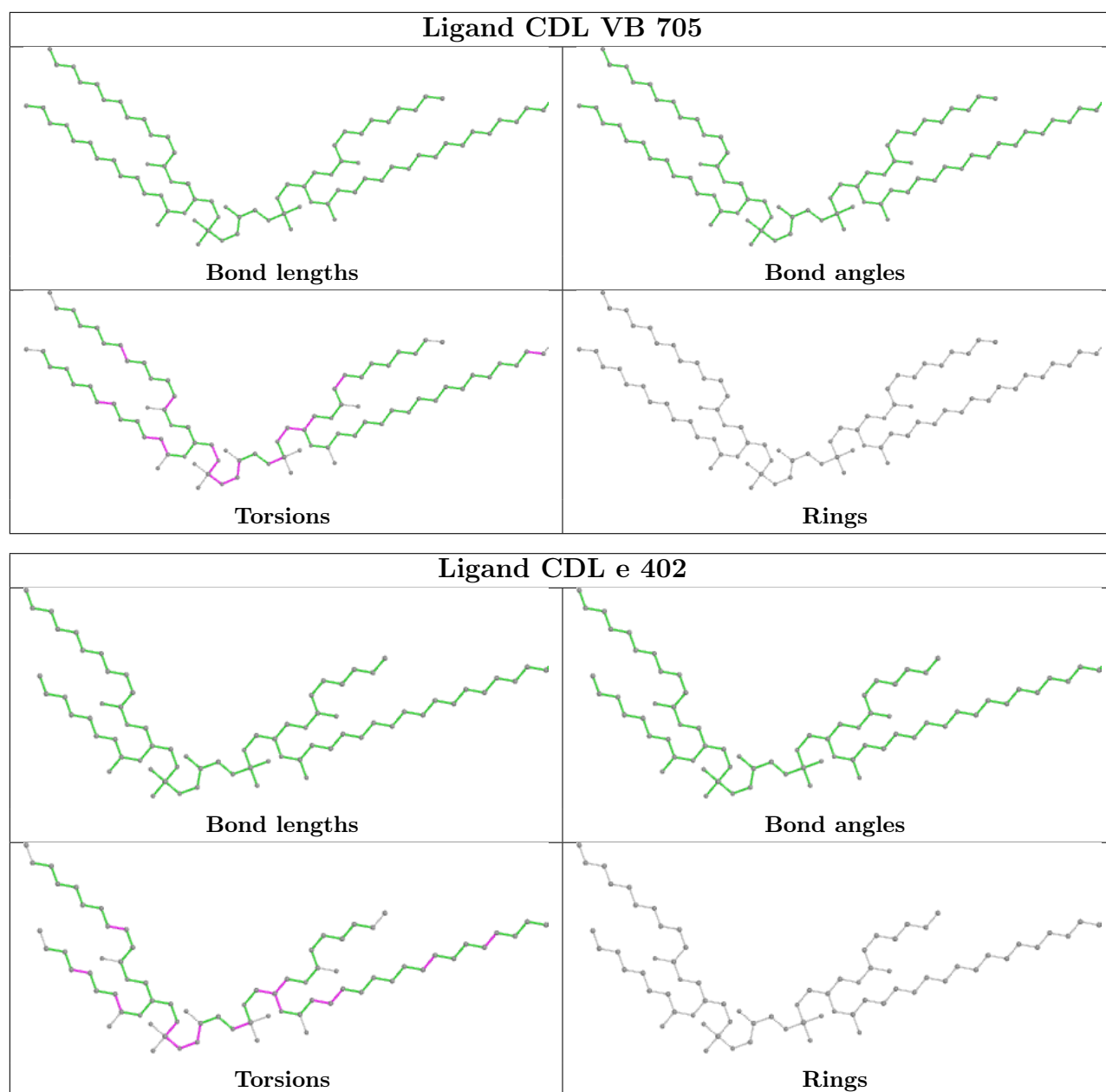


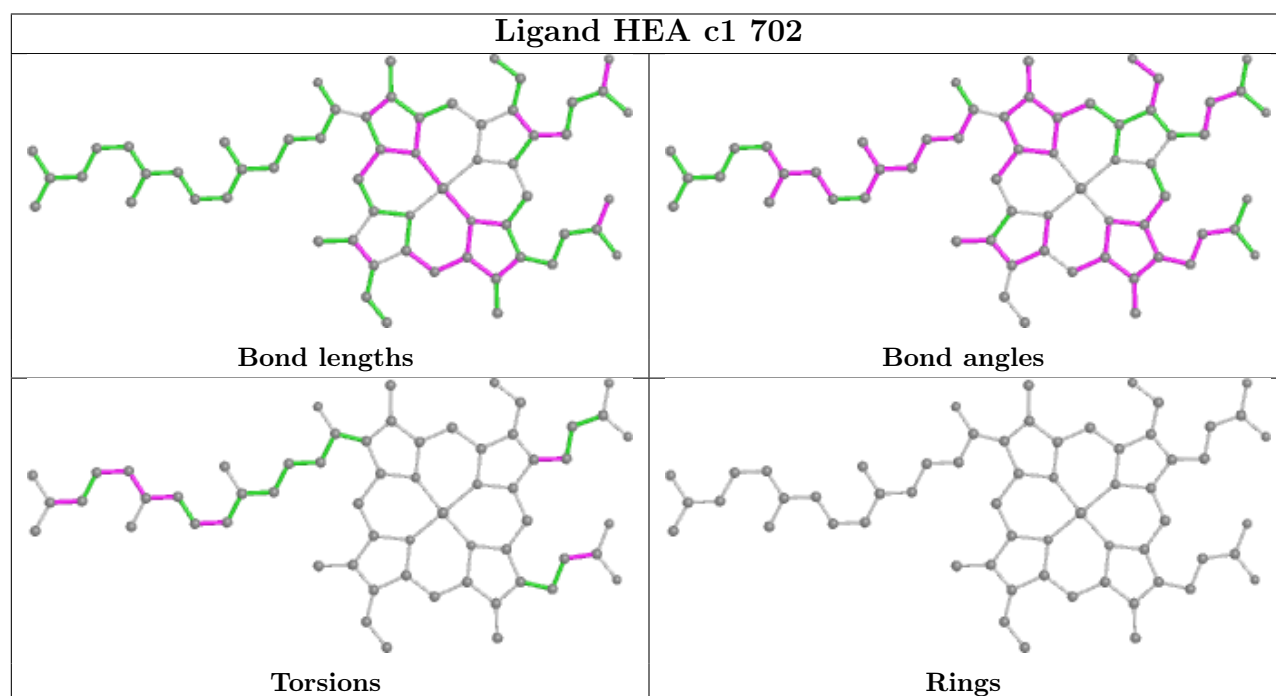
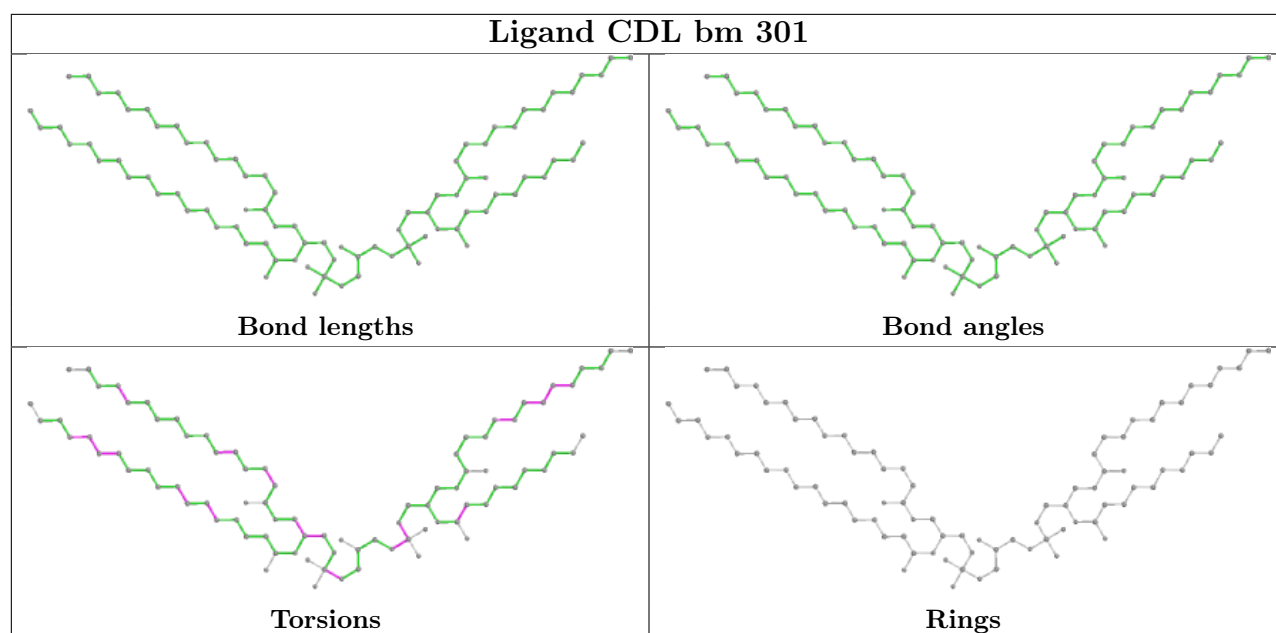


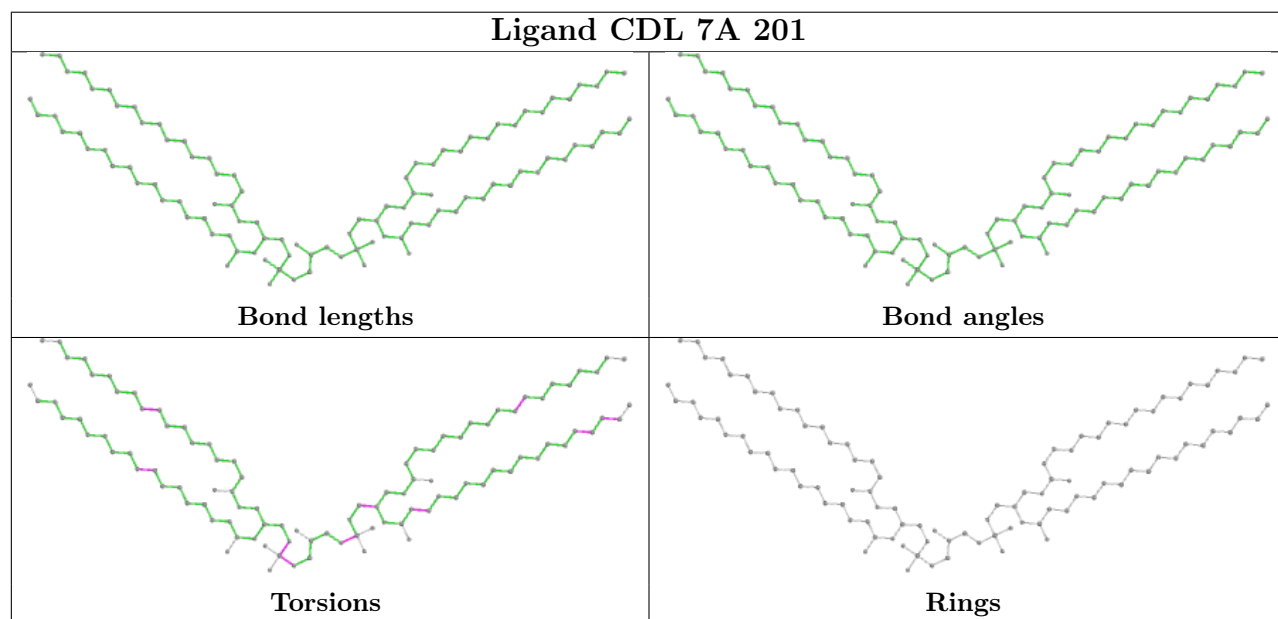
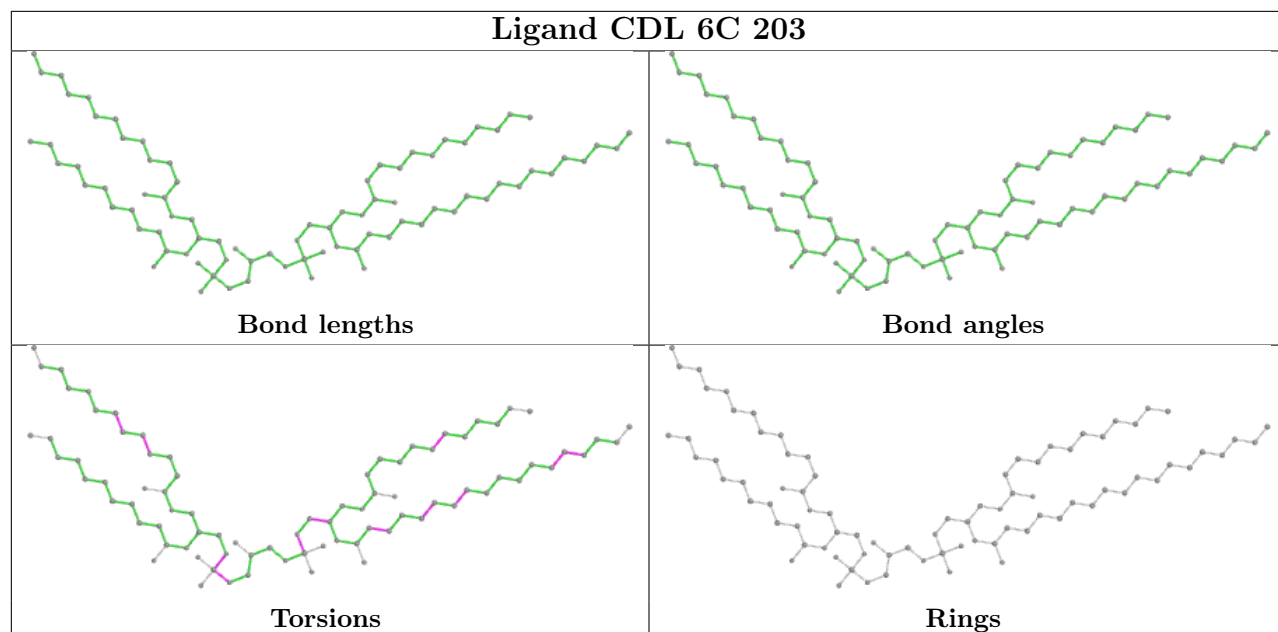


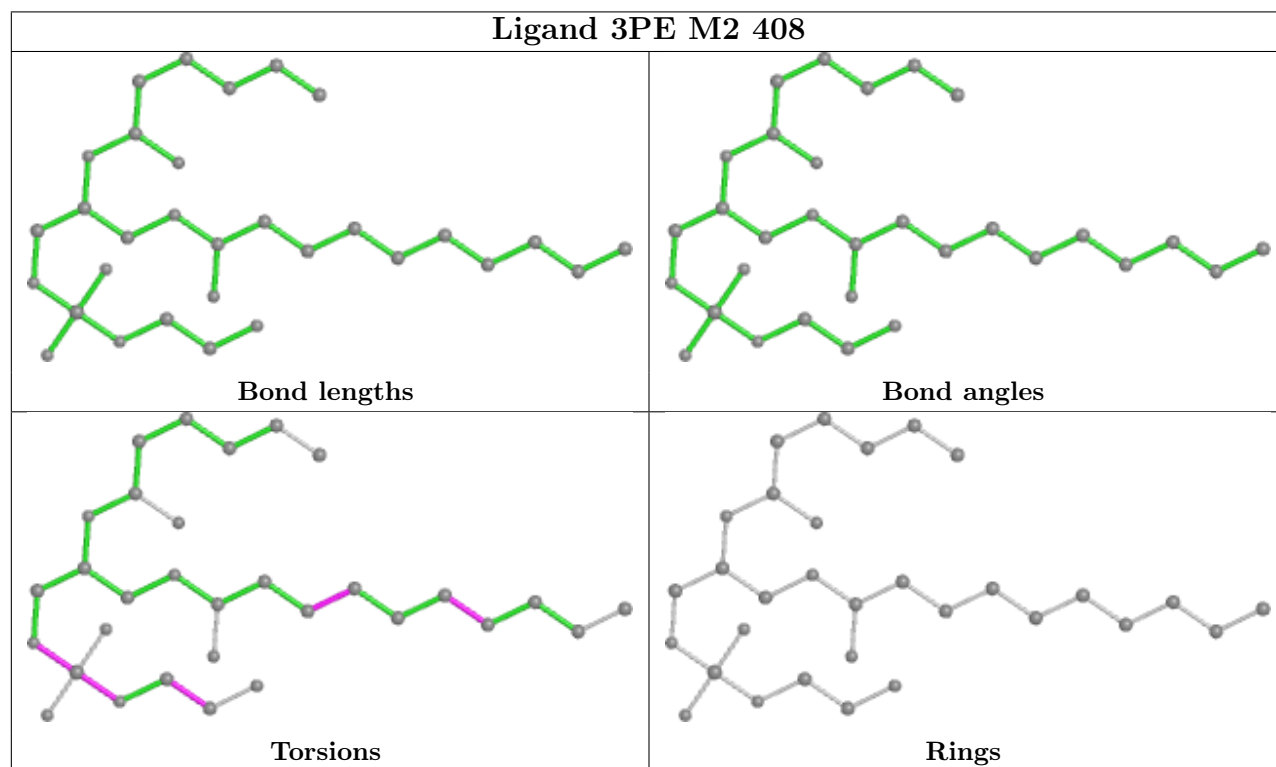
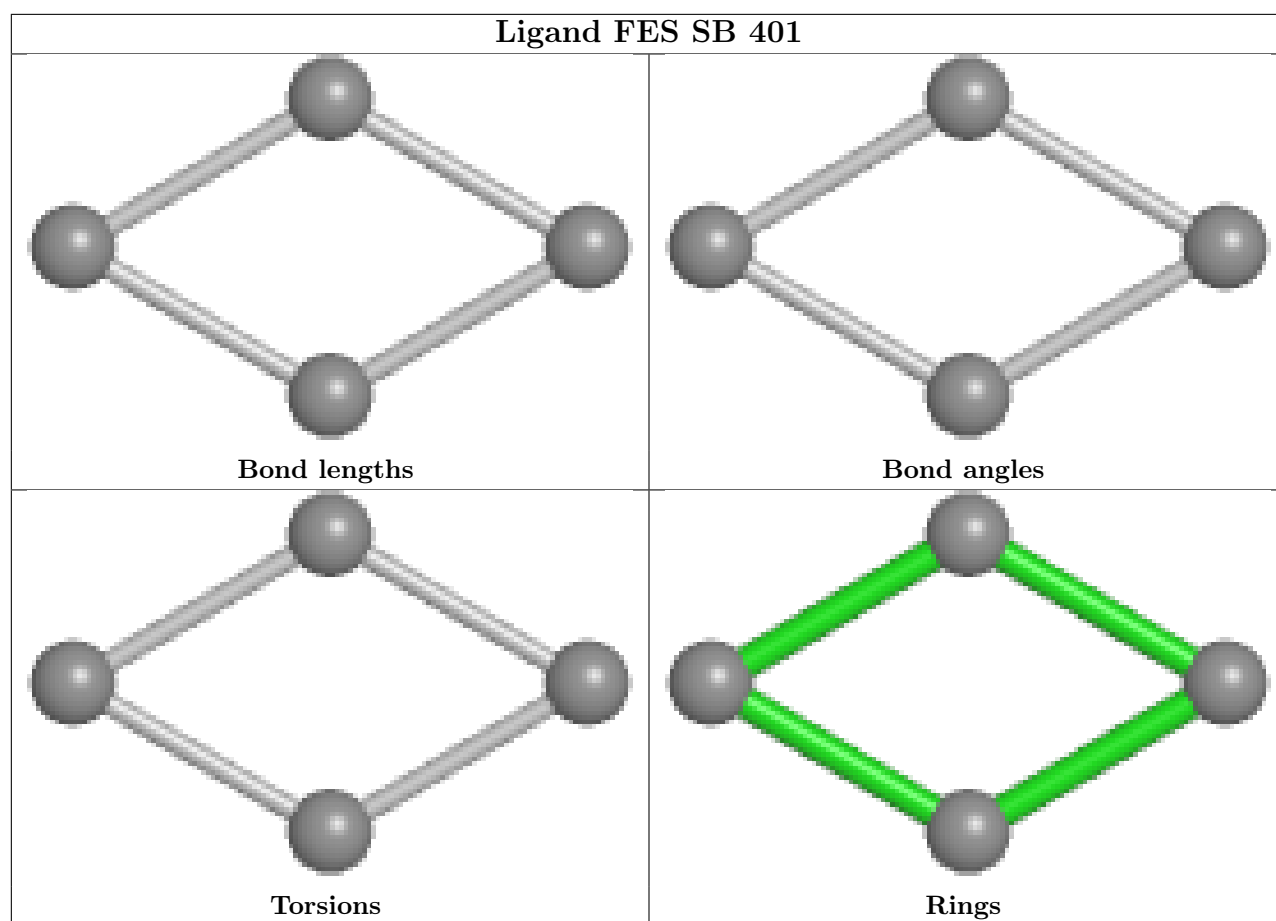


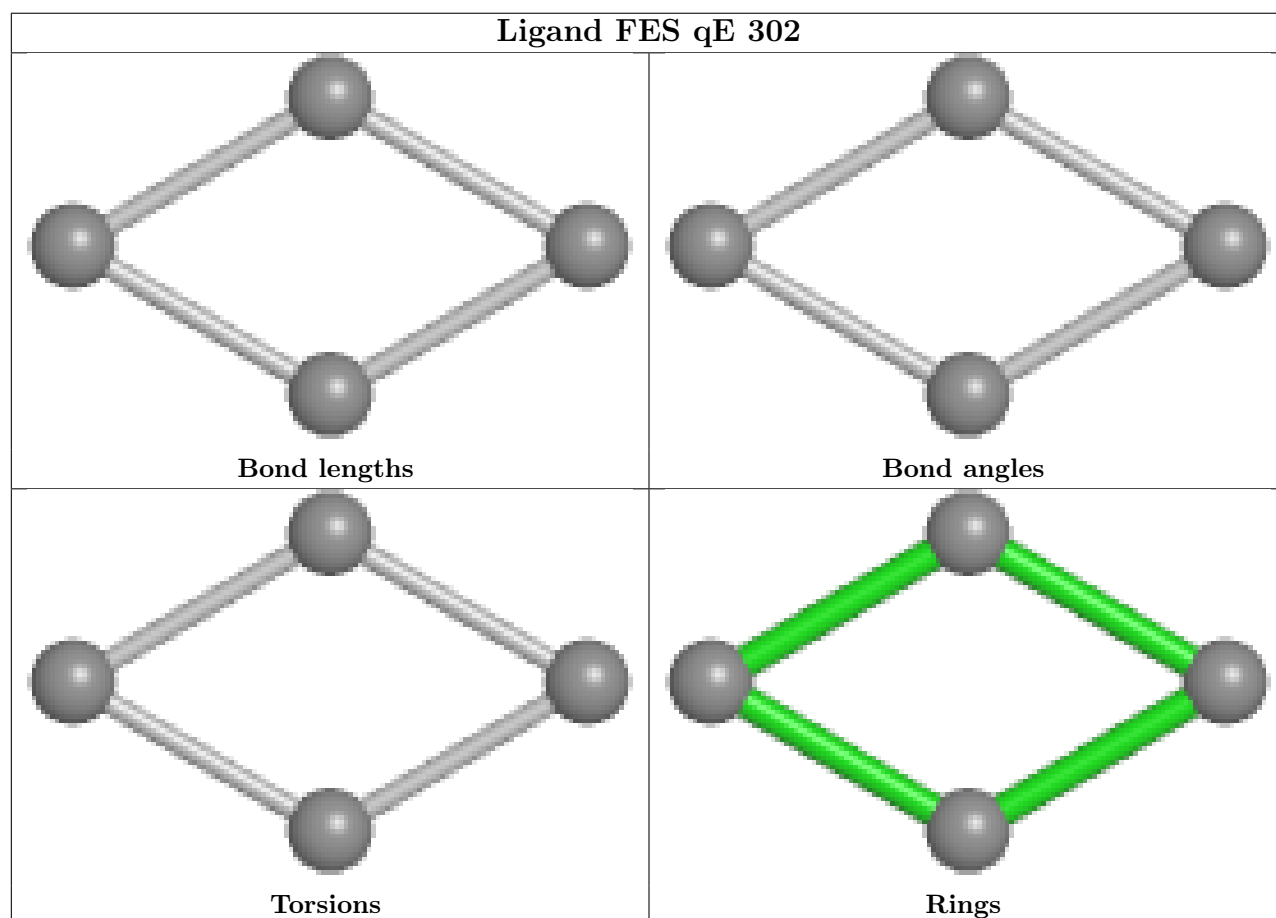
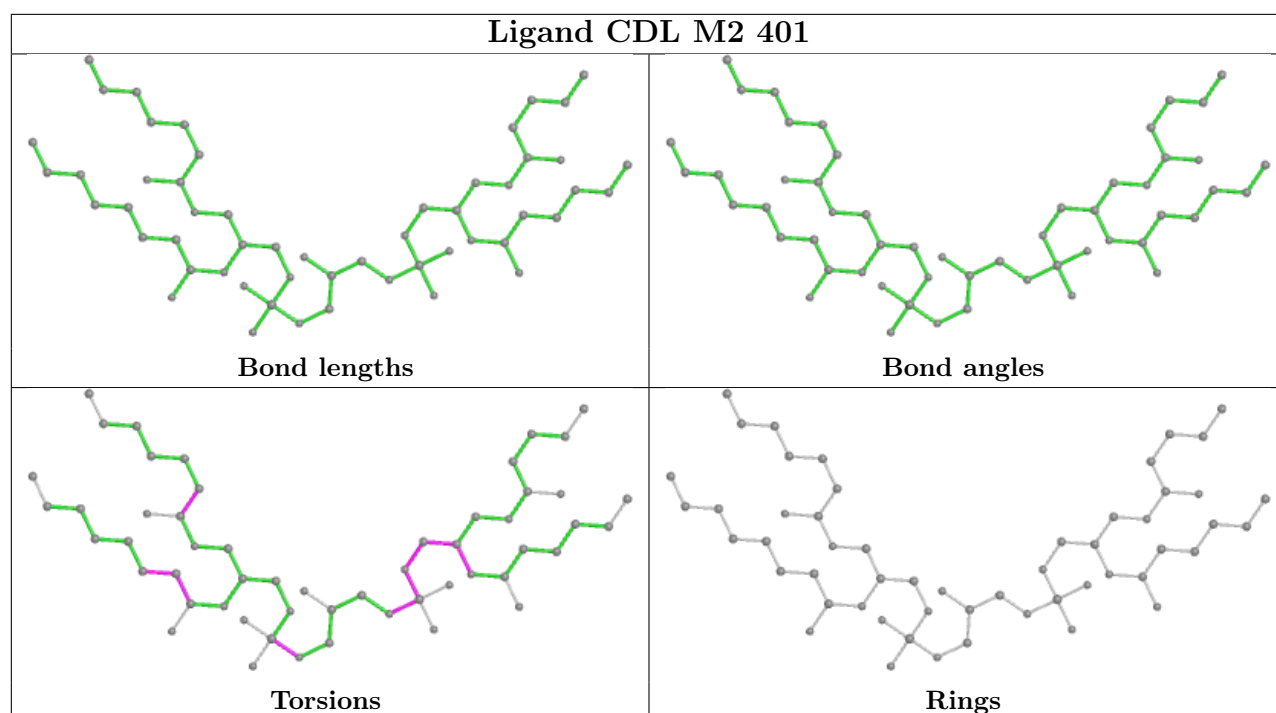


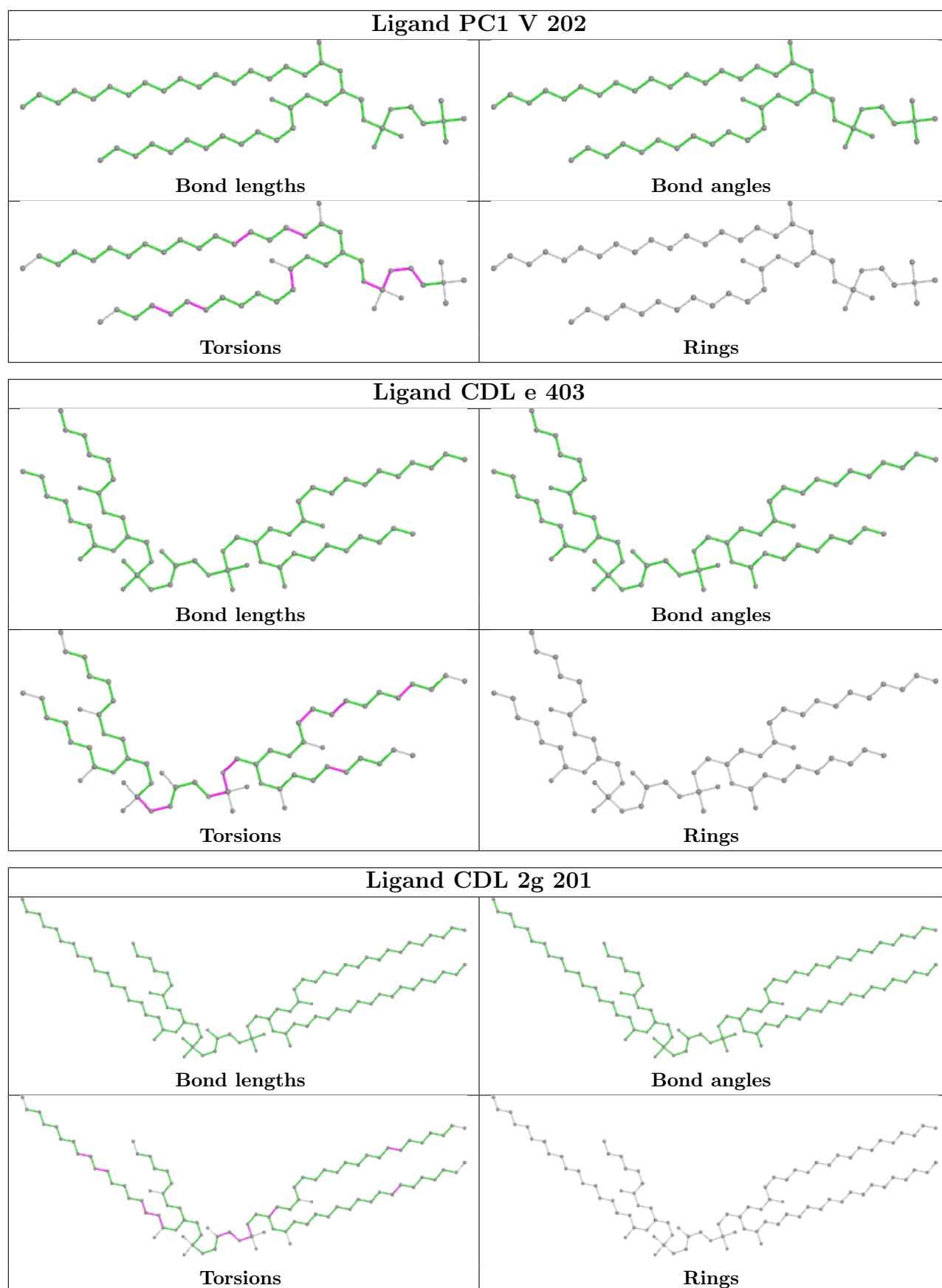


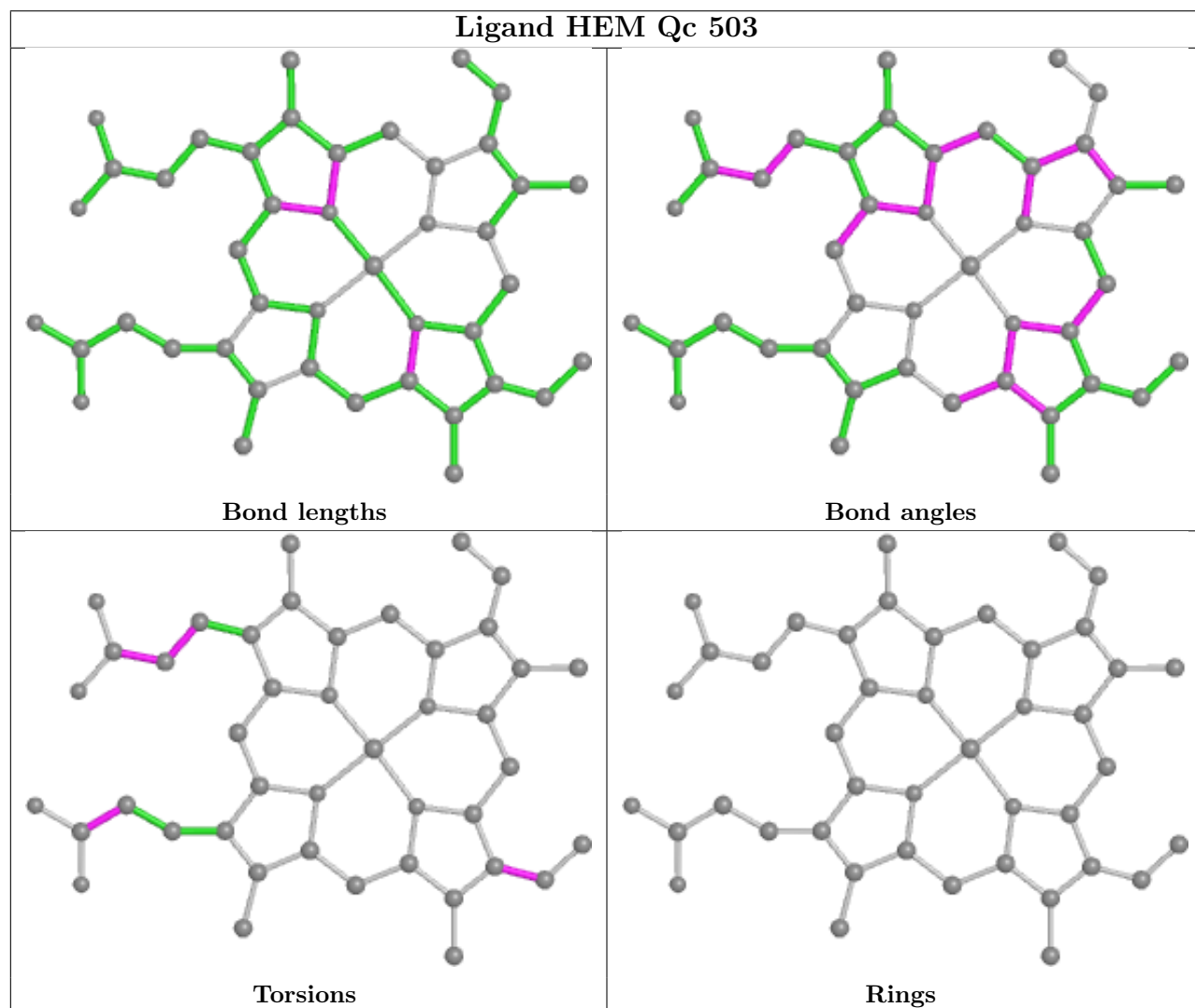
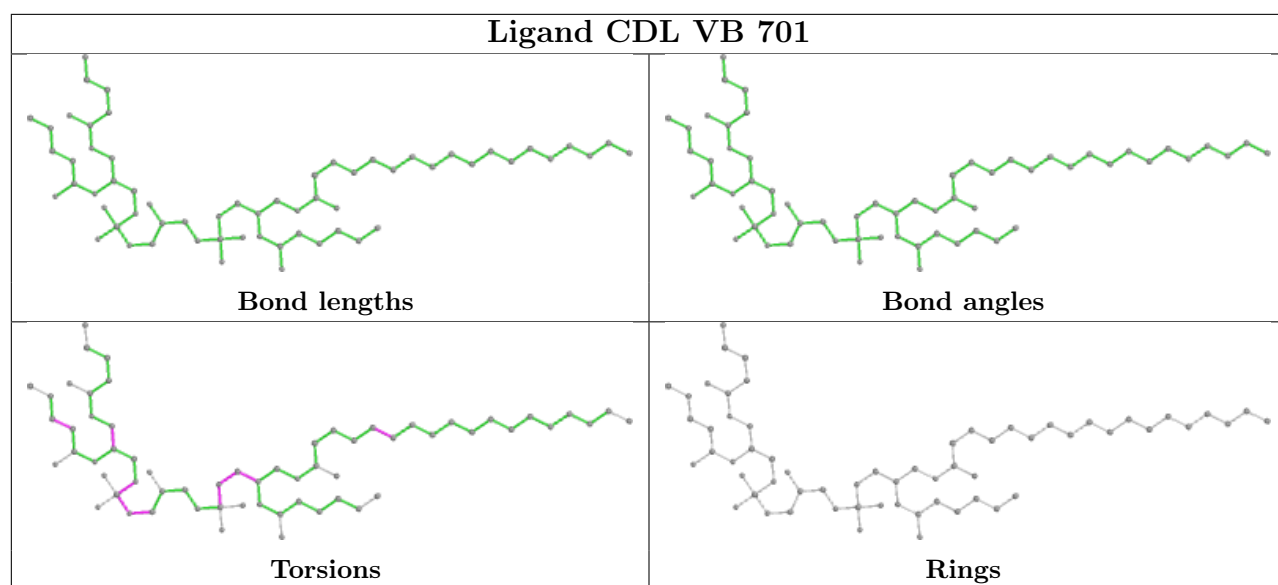


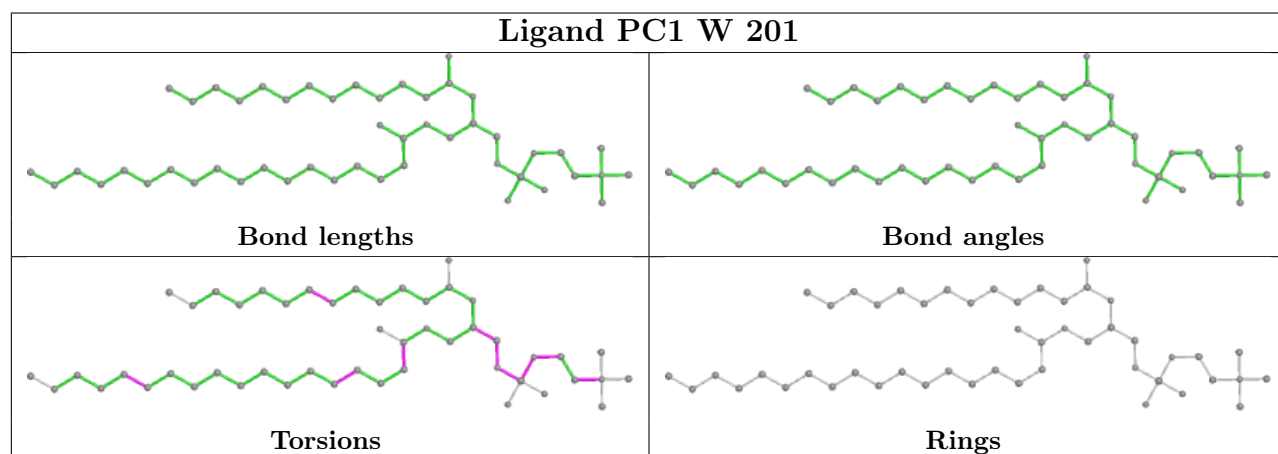
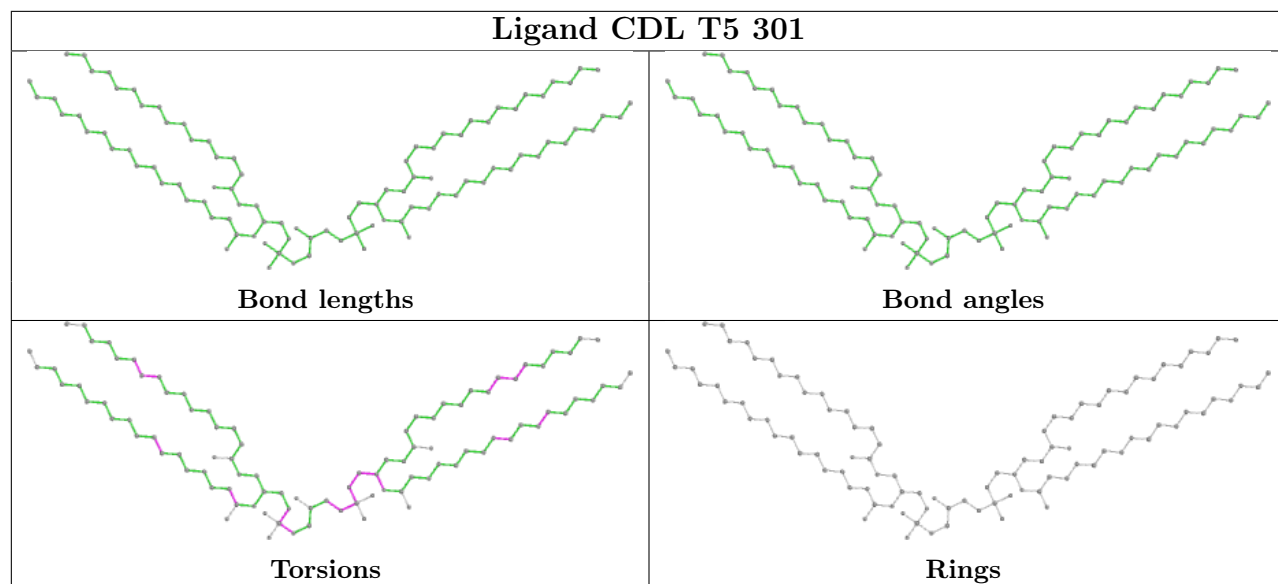


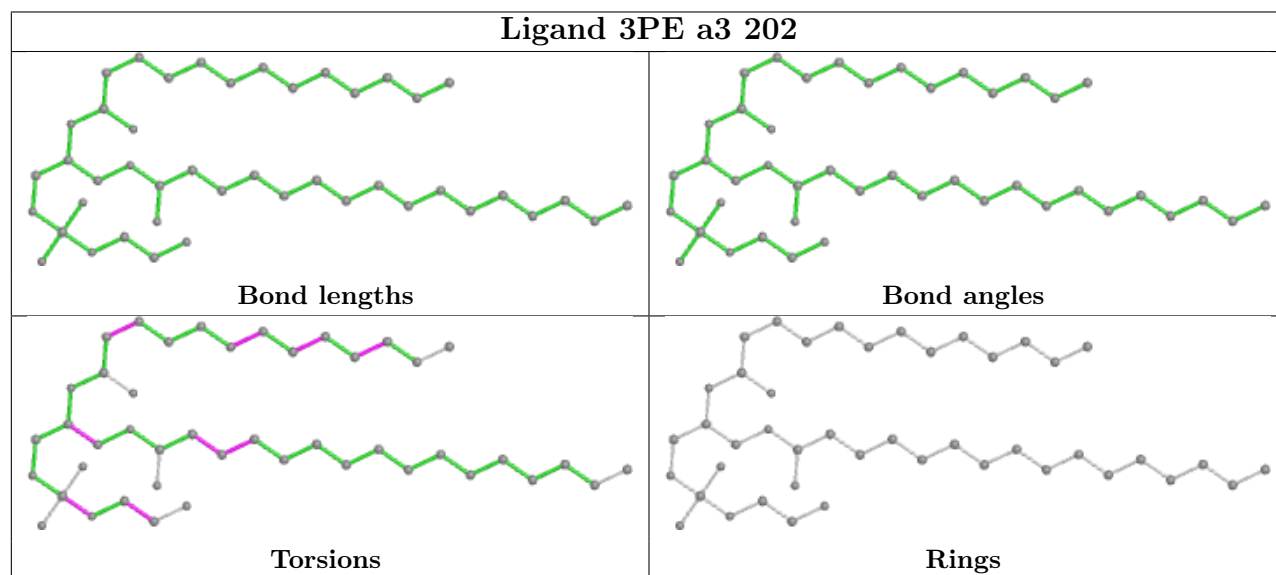
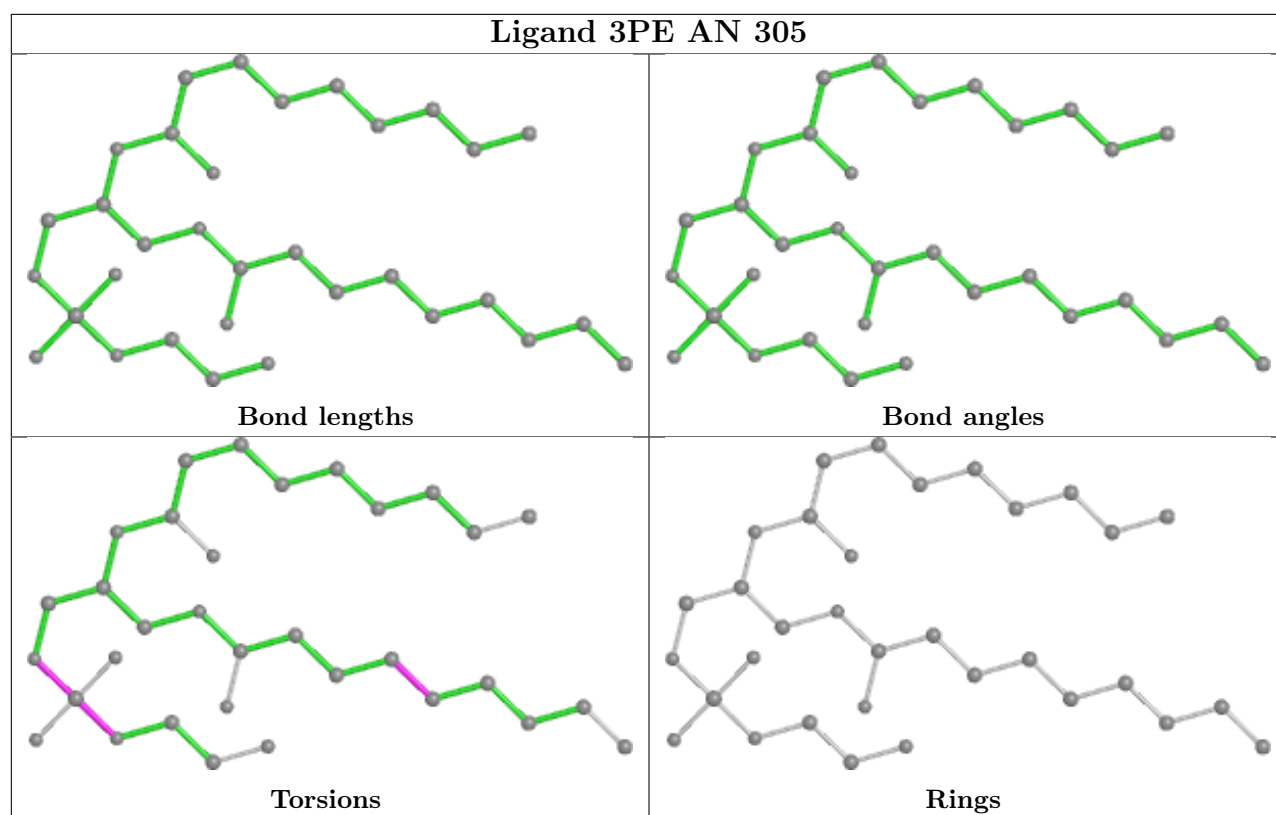


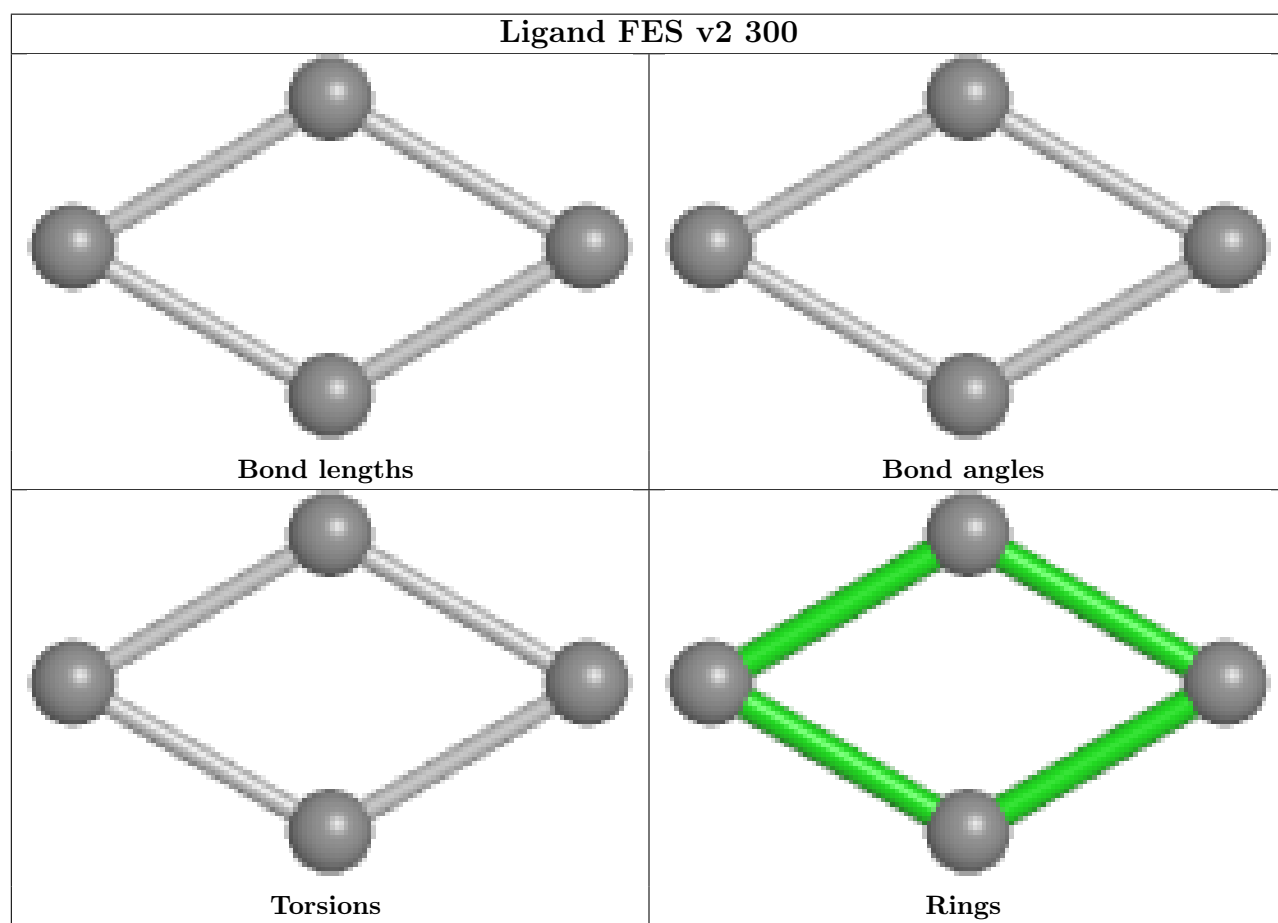
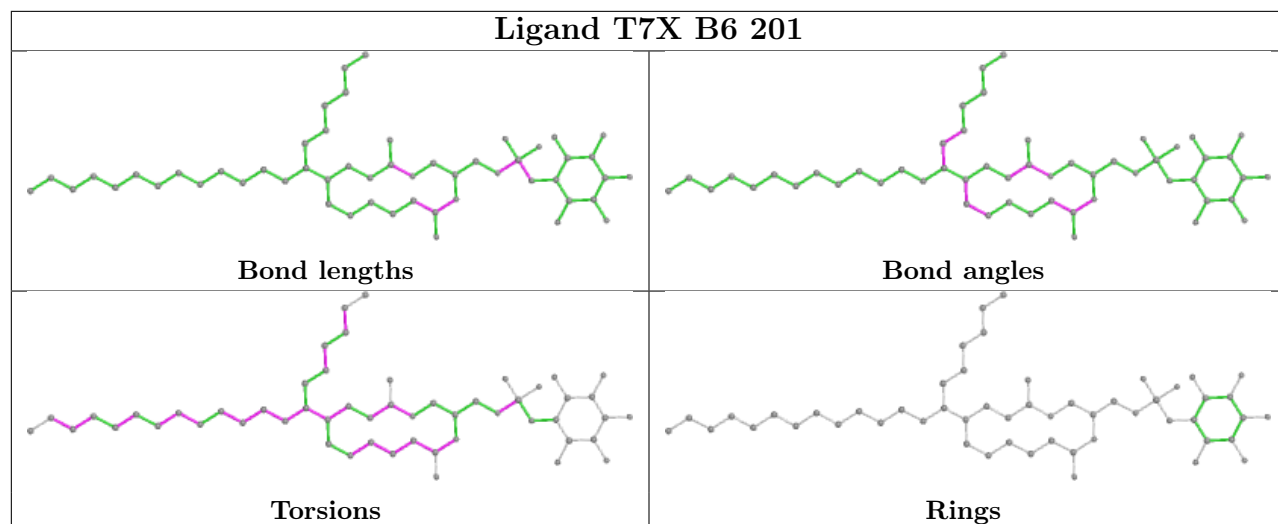


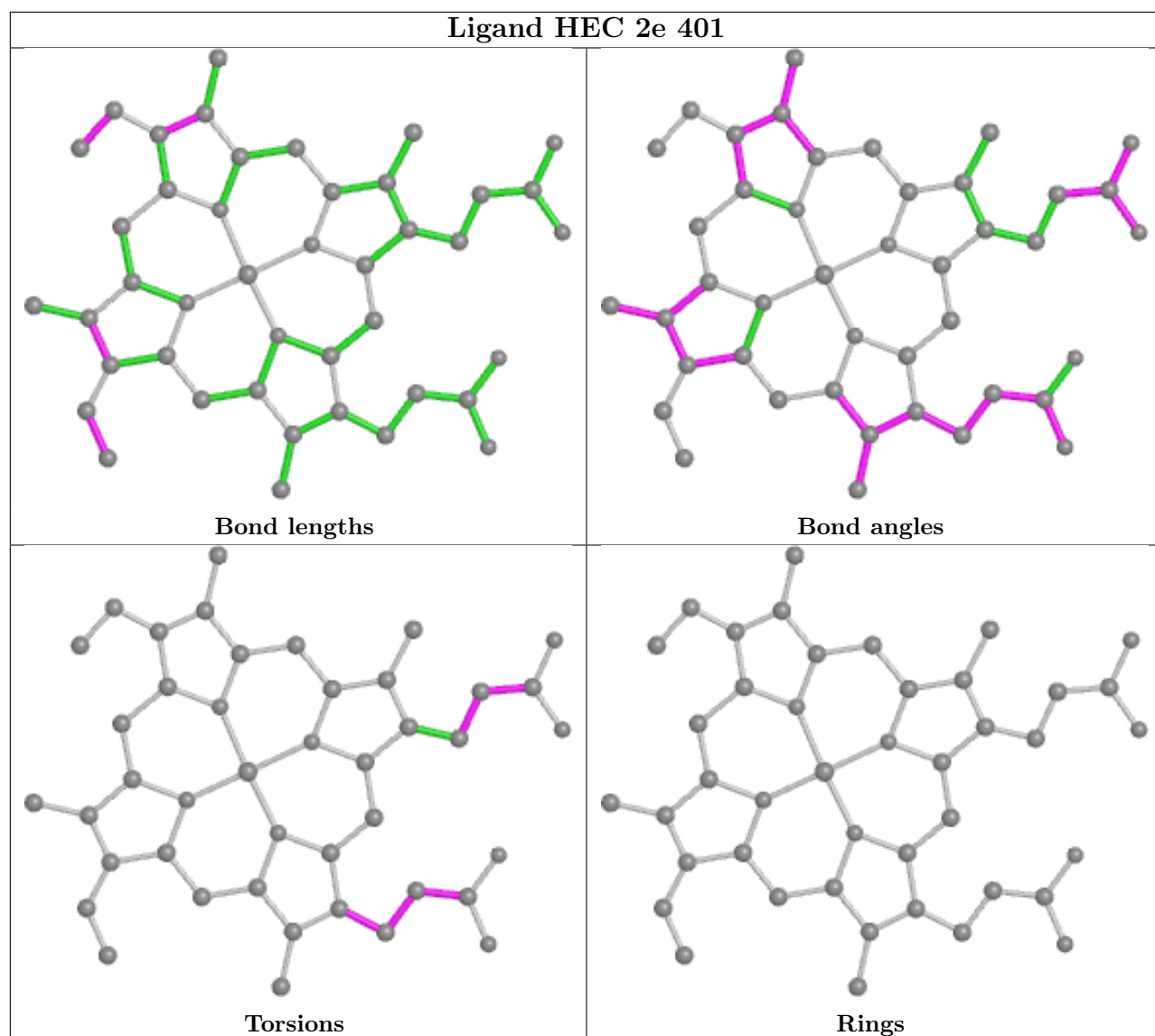
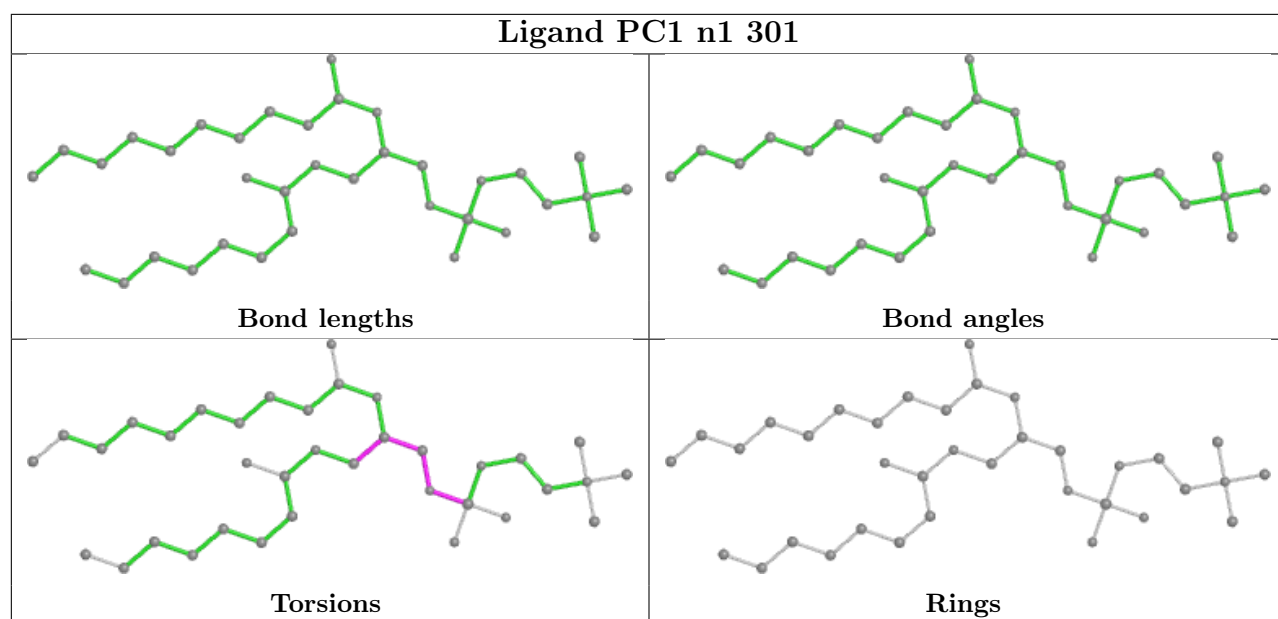


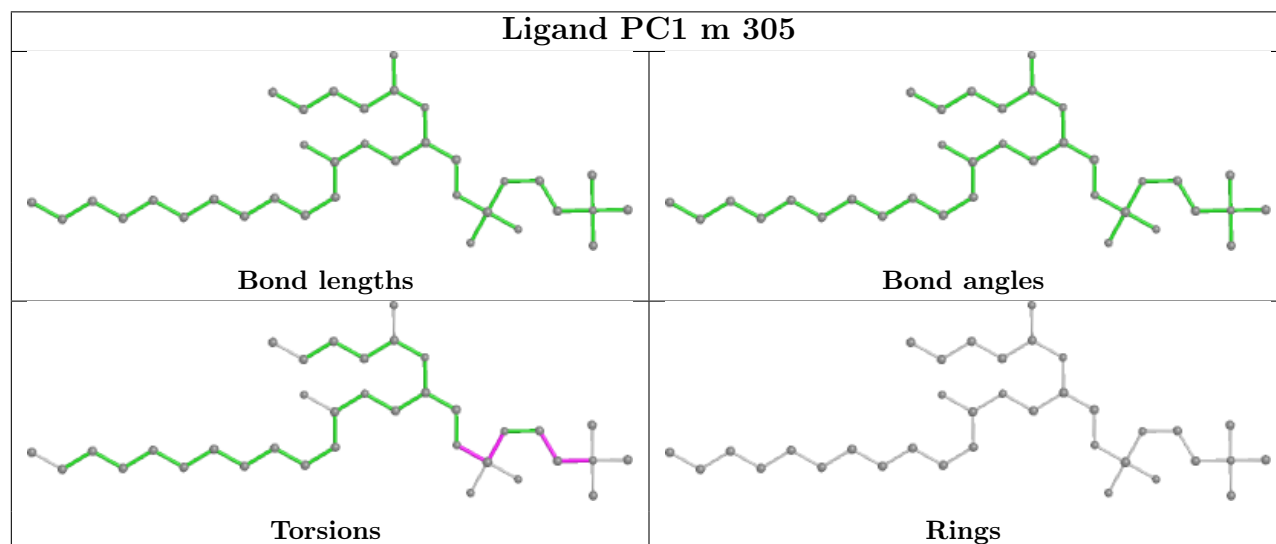
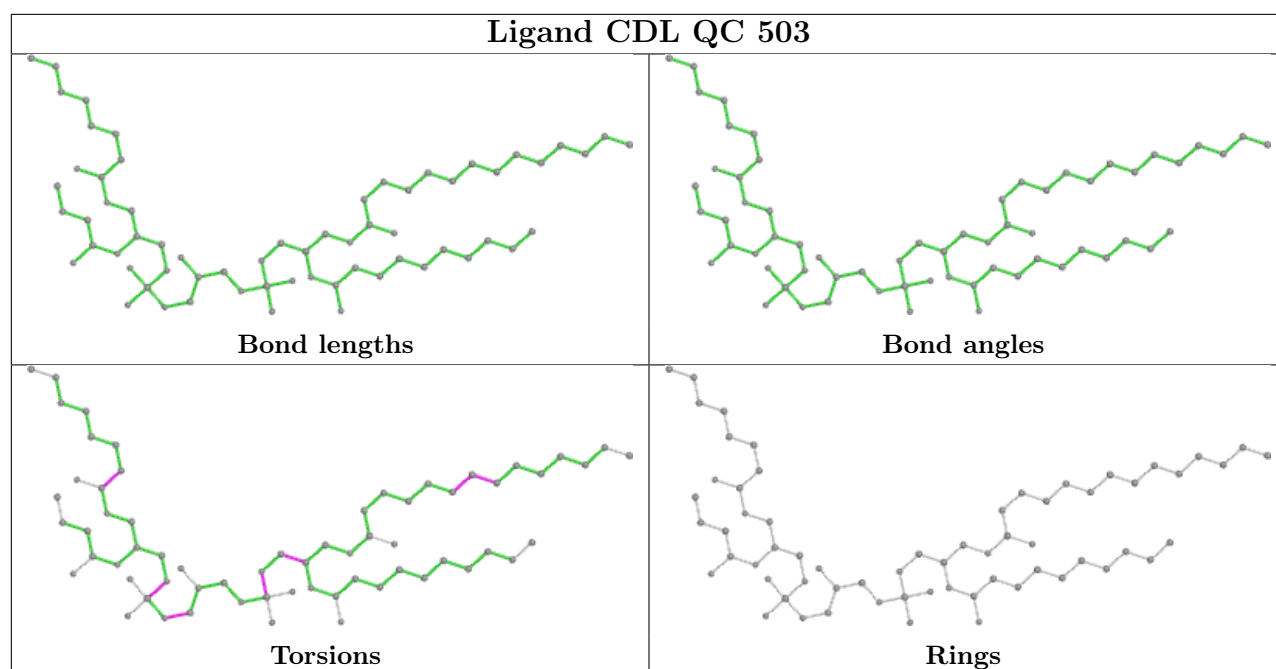


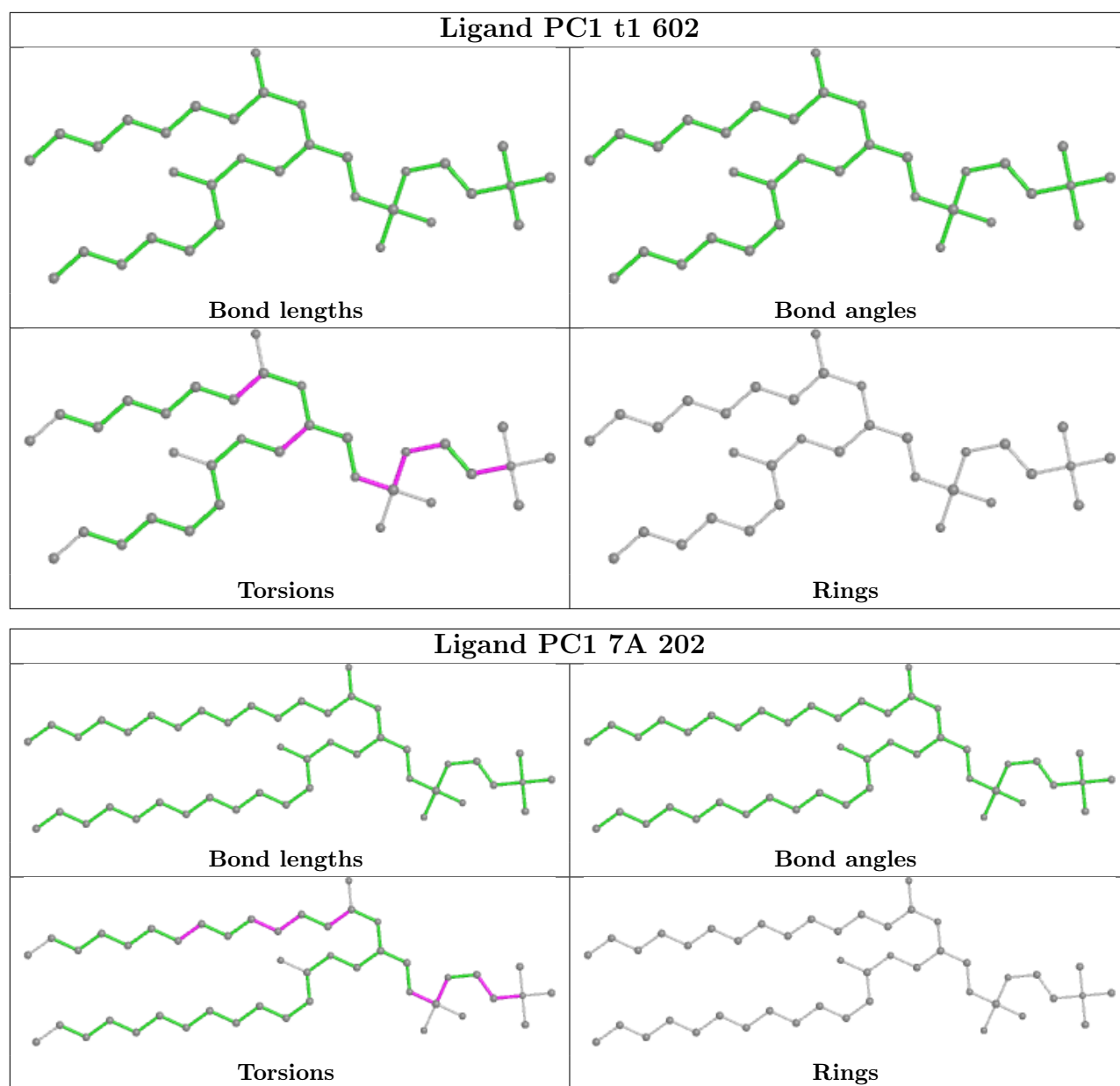


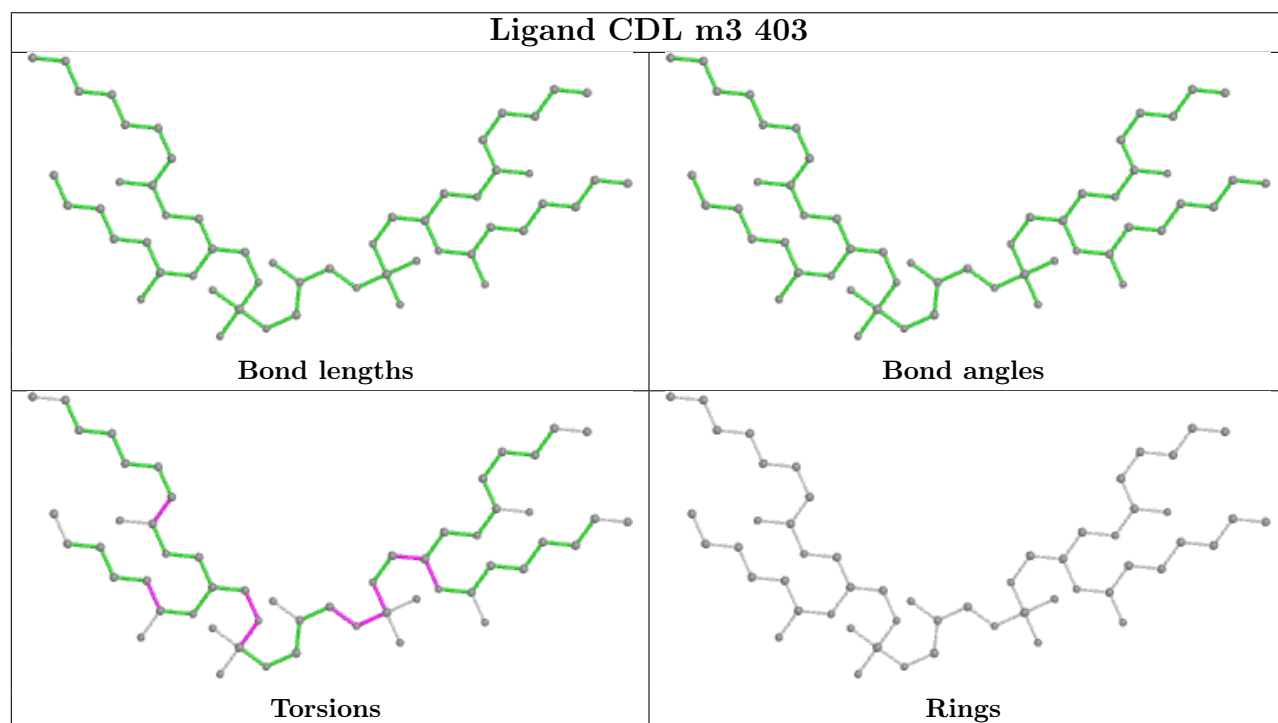
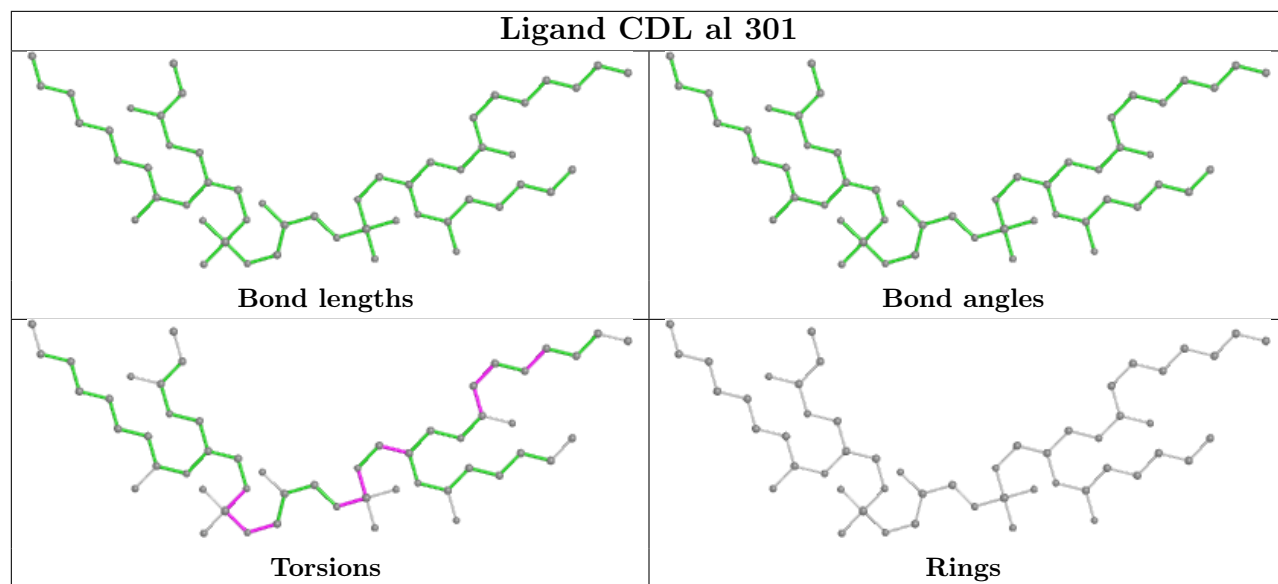


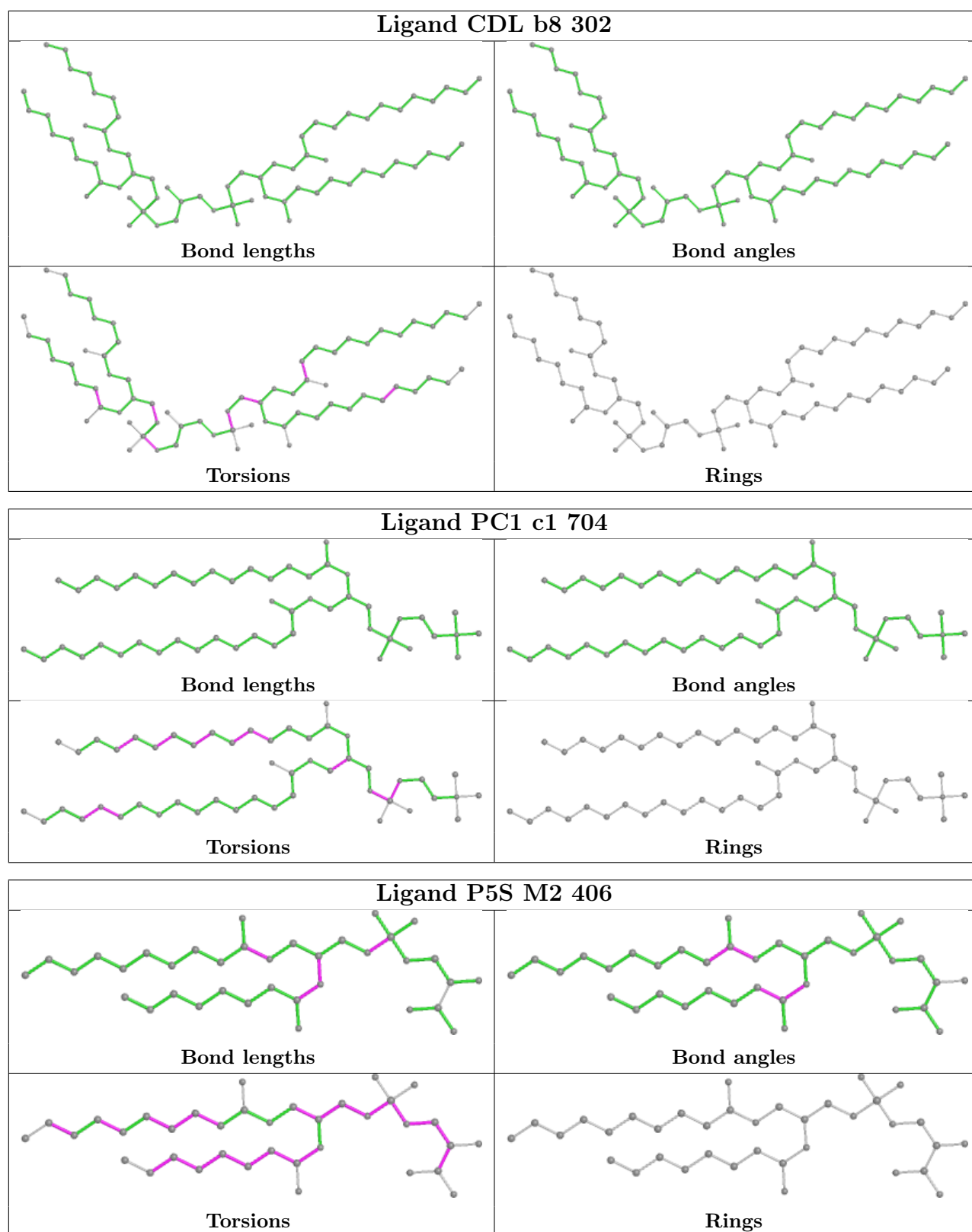


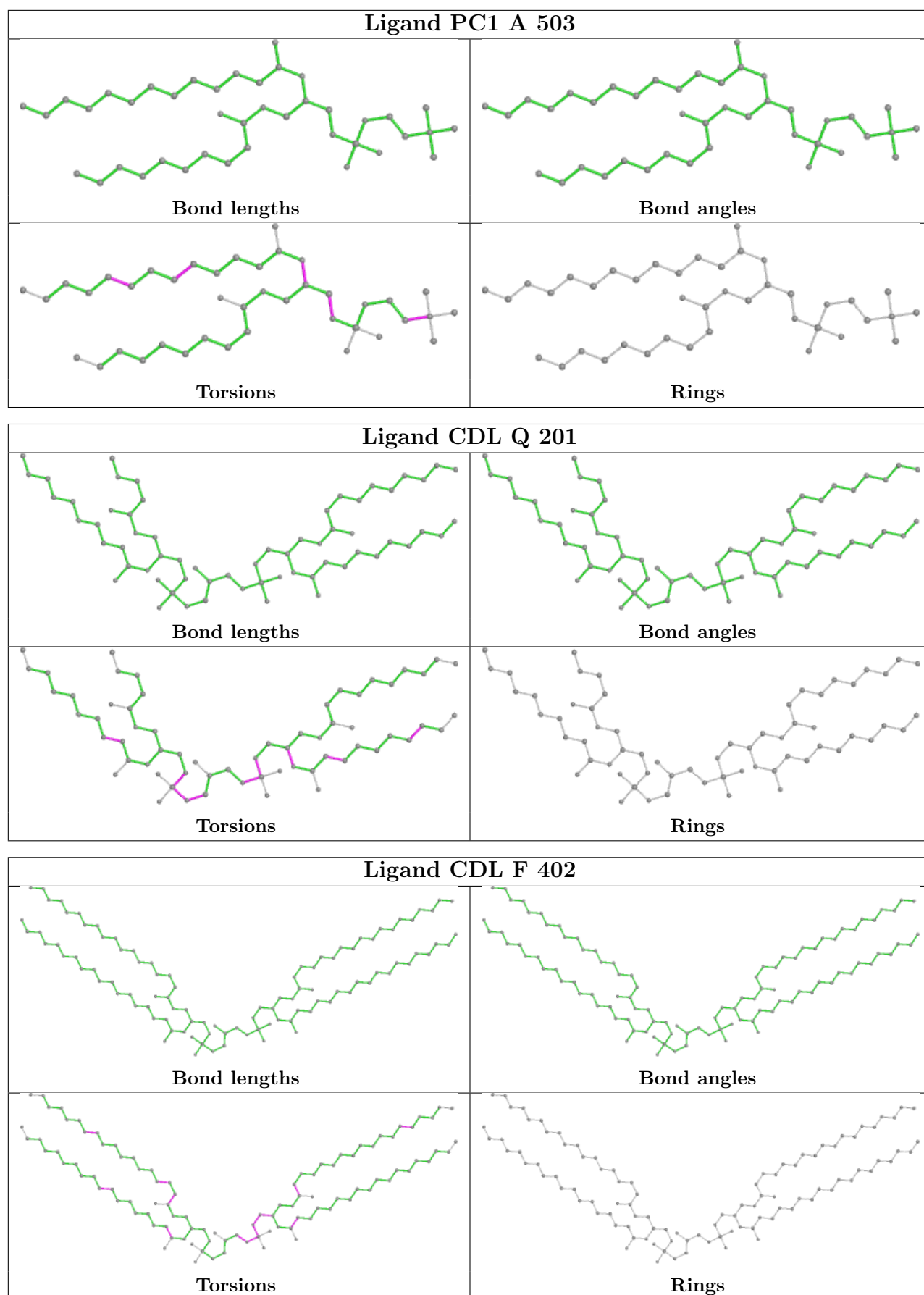


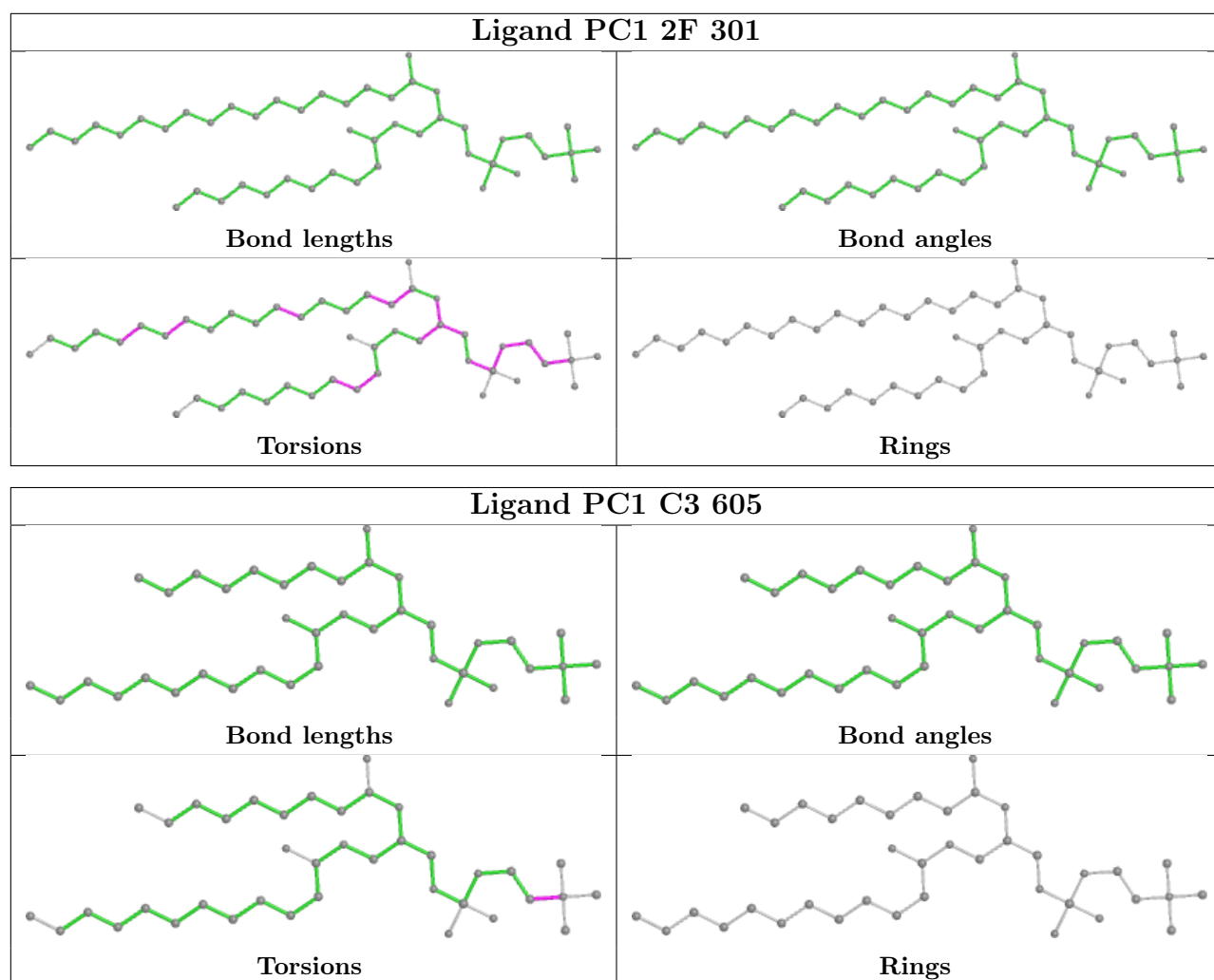


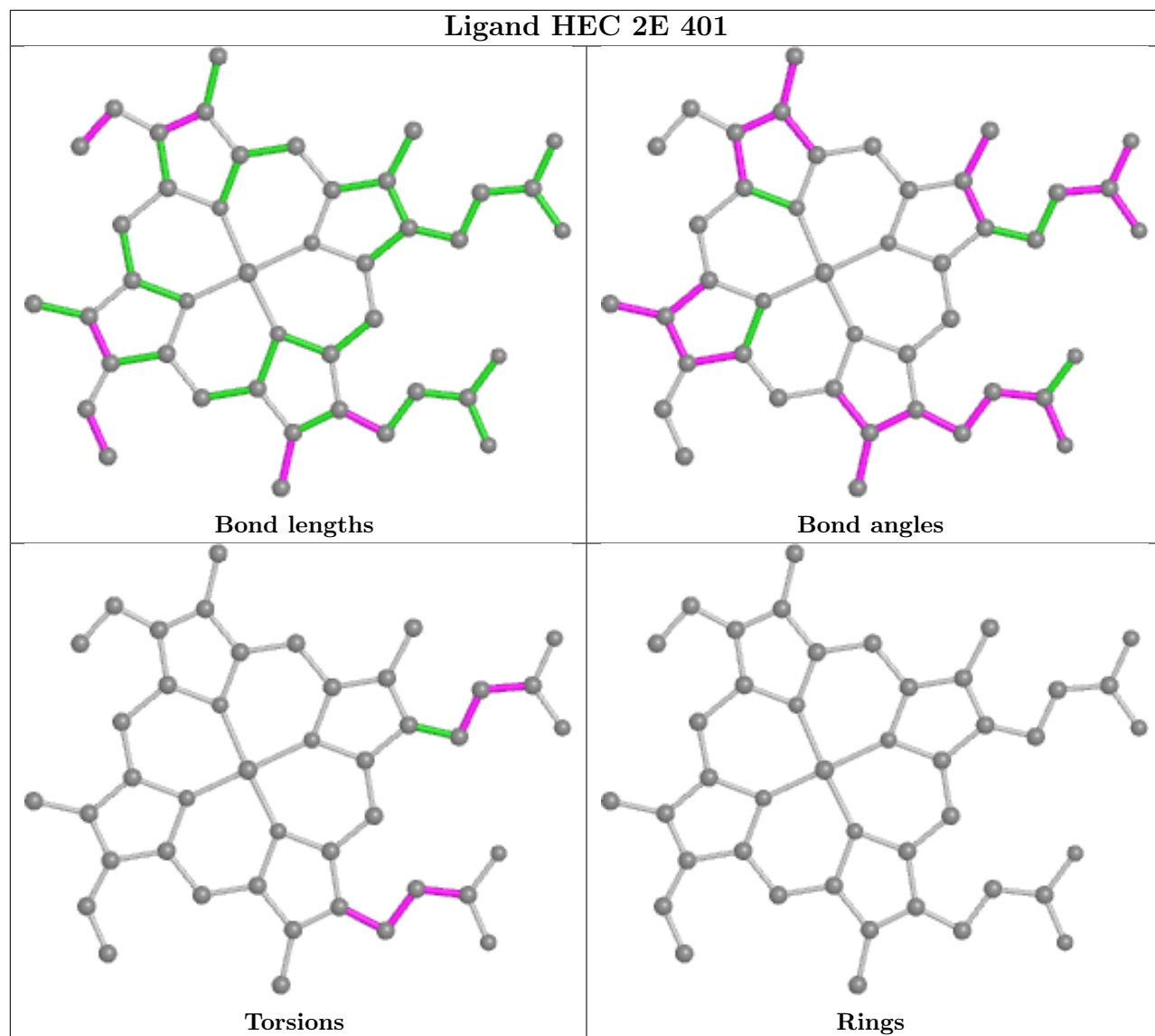




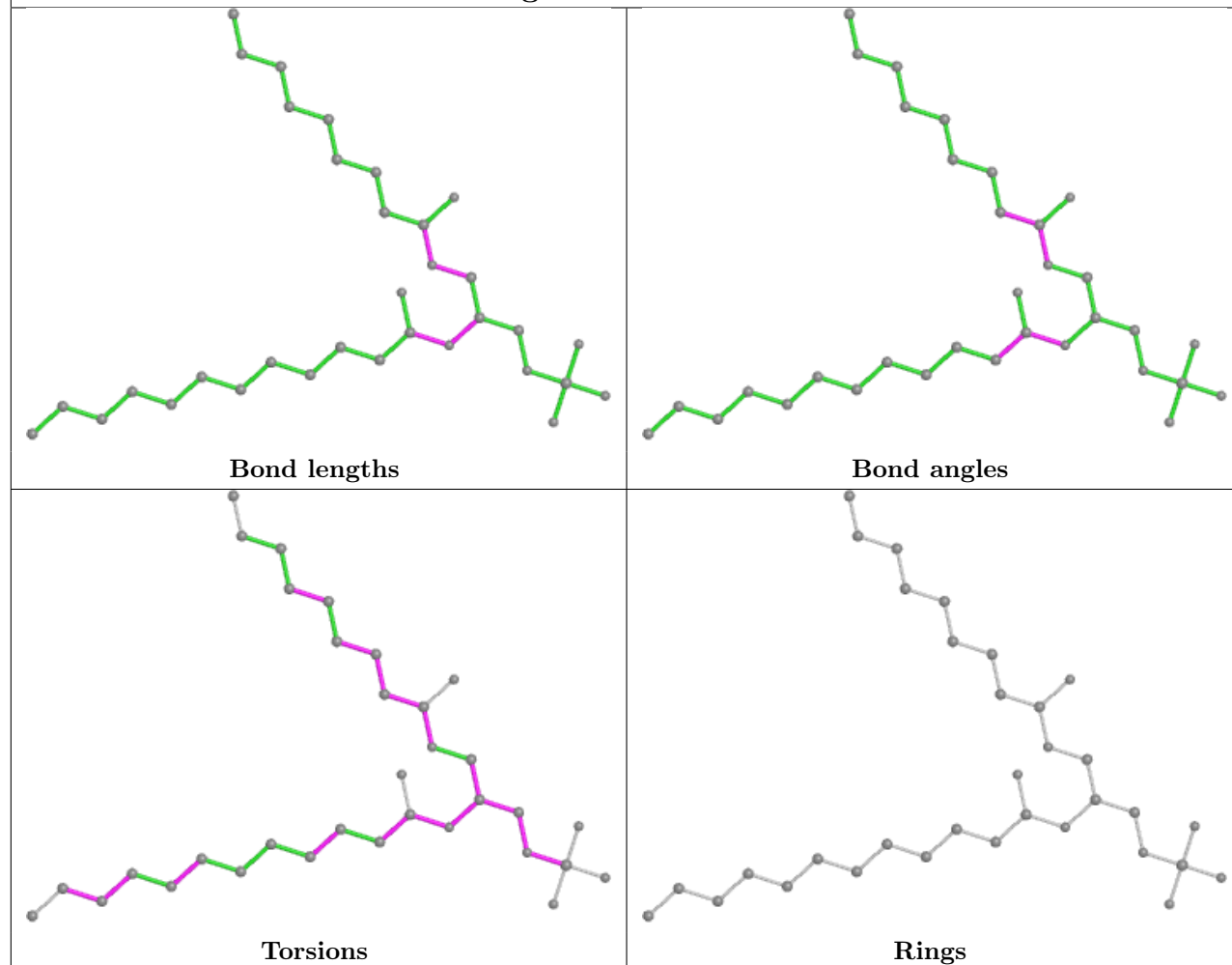




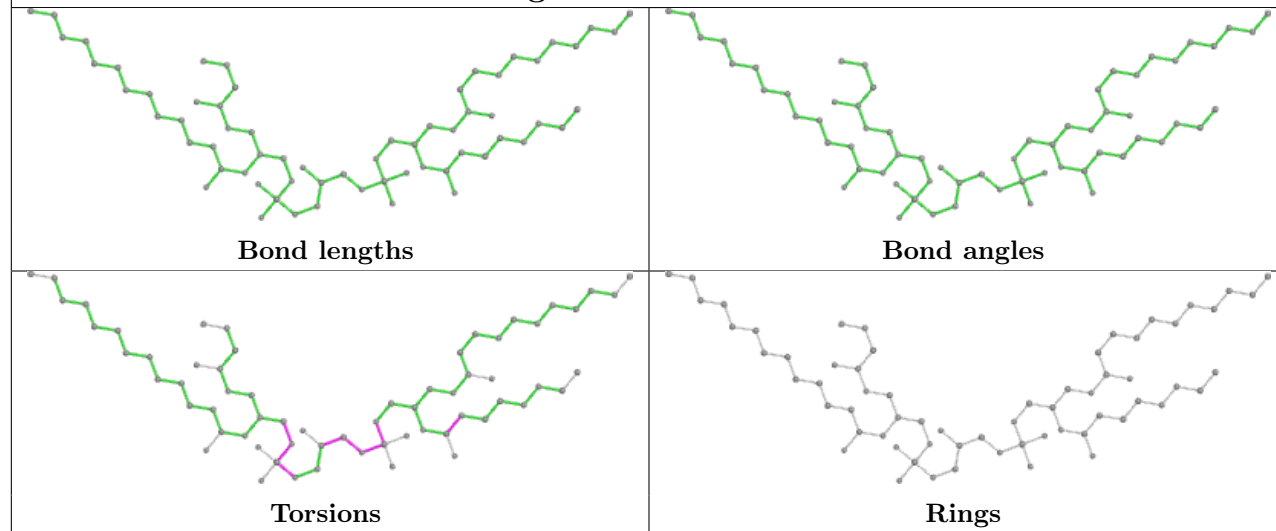


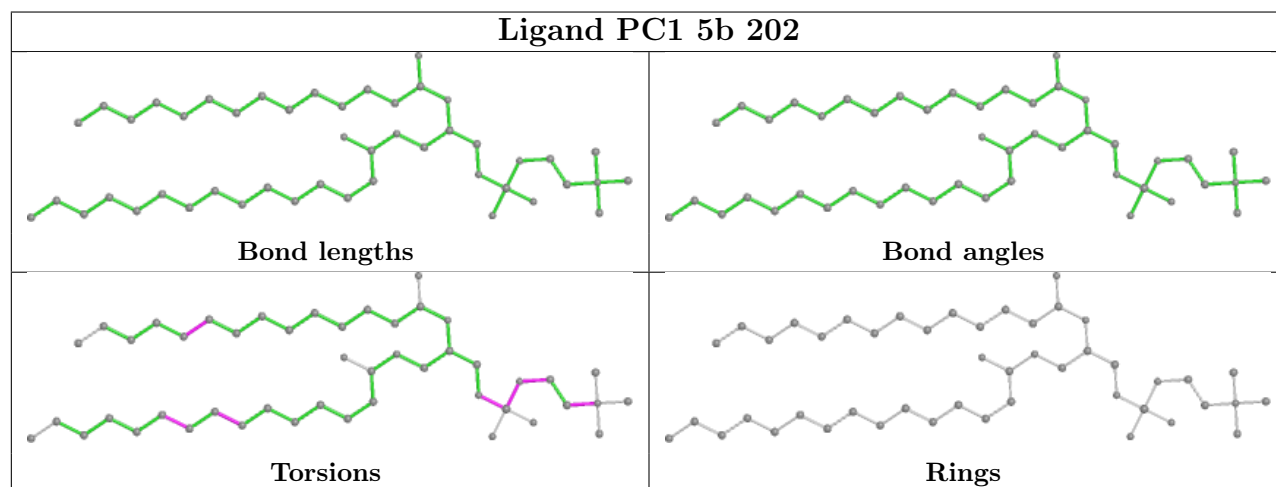
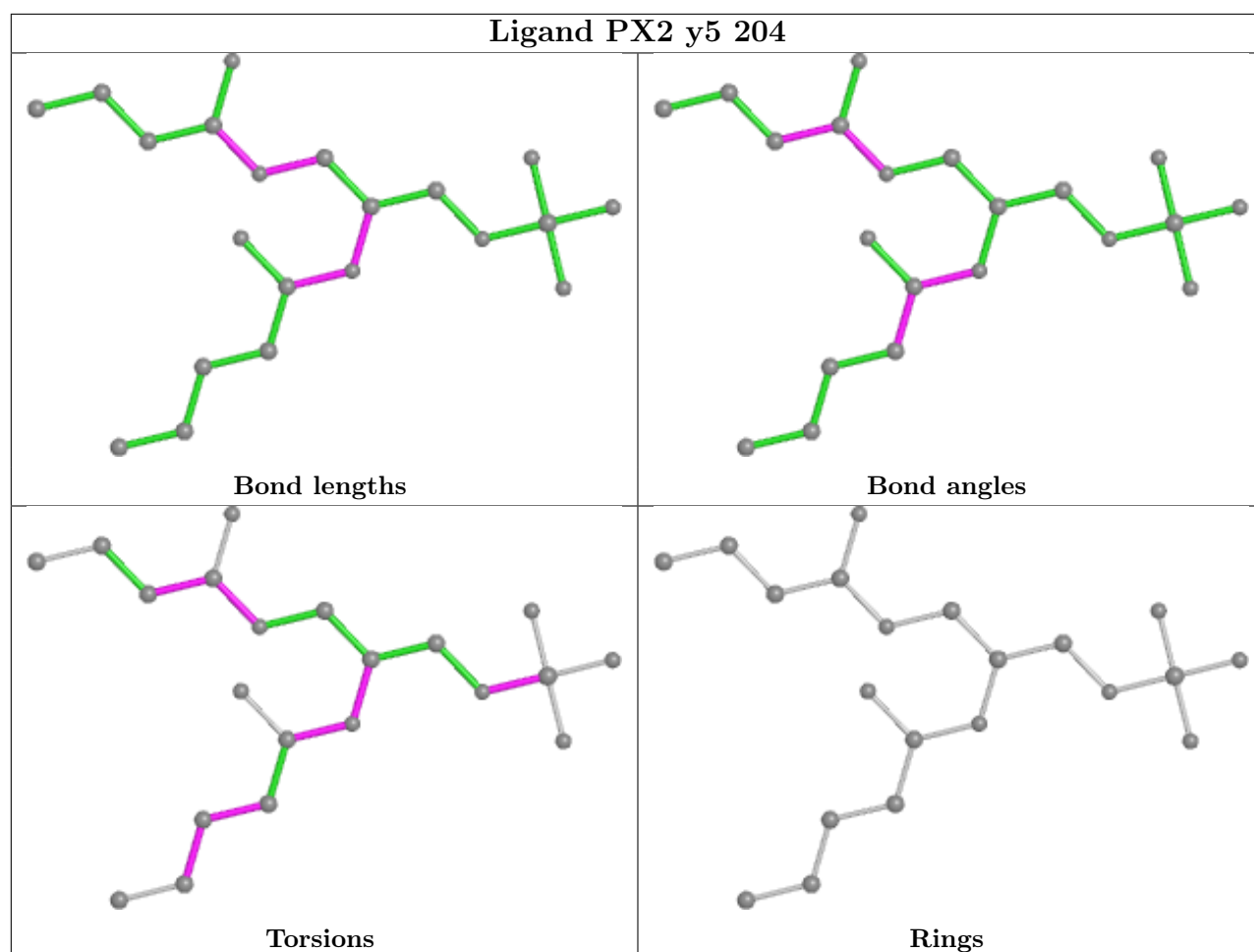


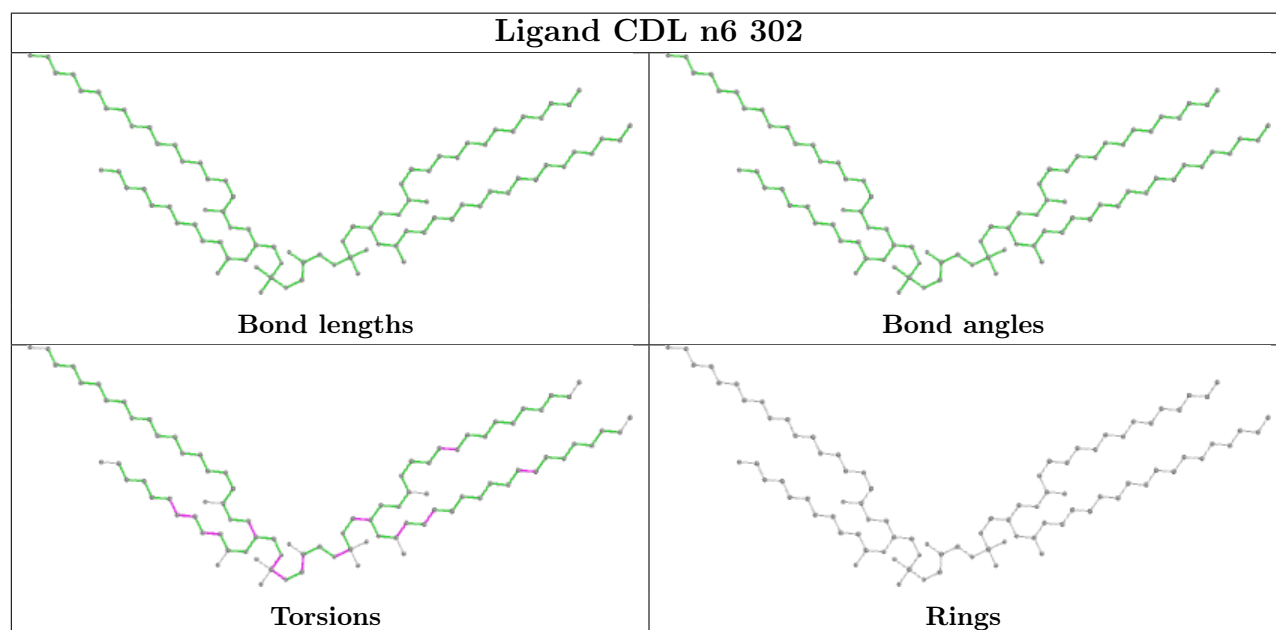
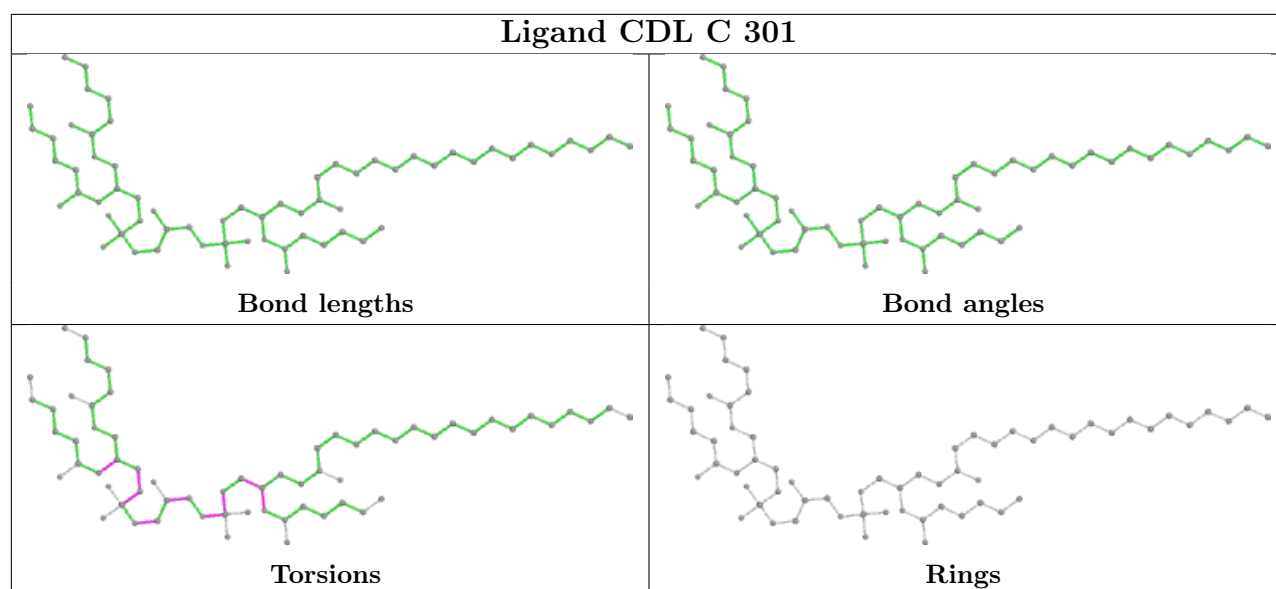
Ligand PX2 r 202

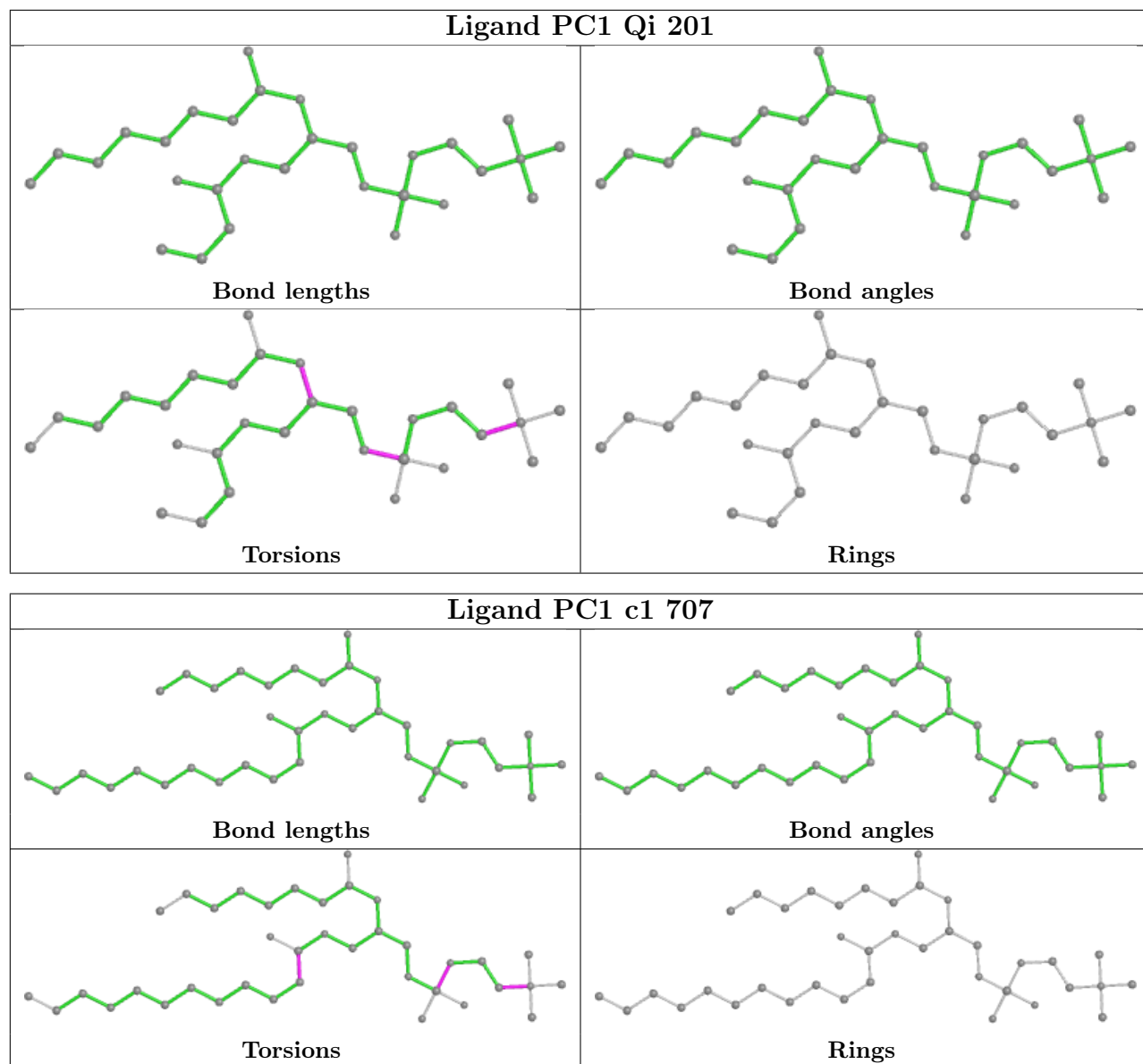


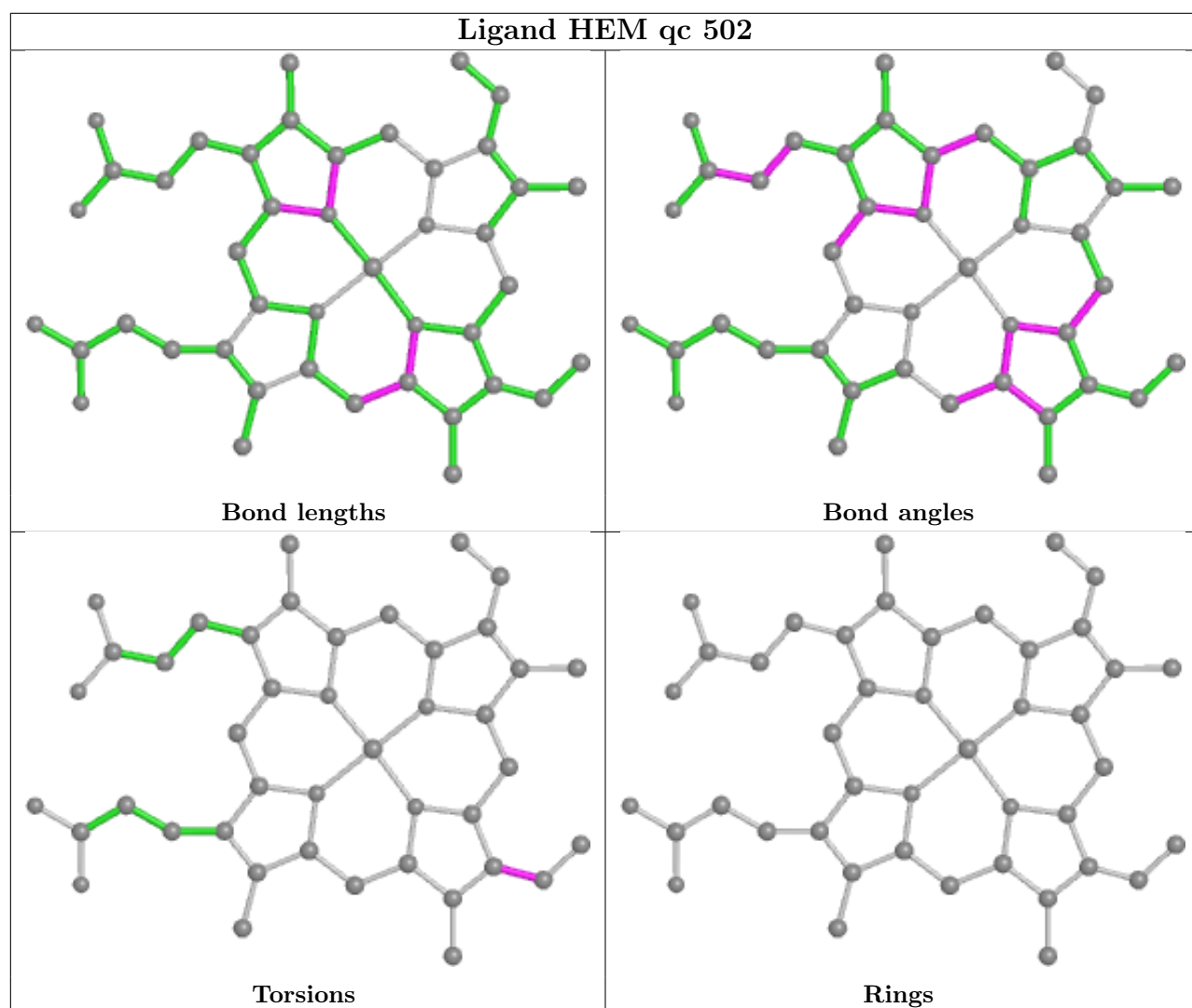
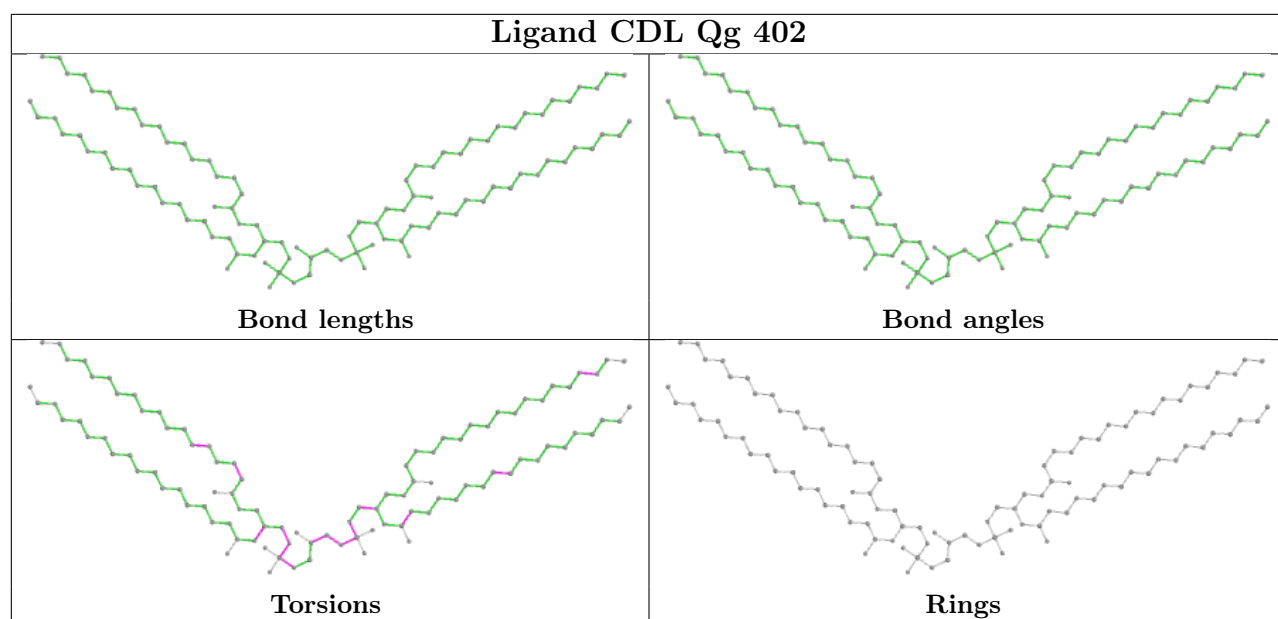
Ligand CDL M 306

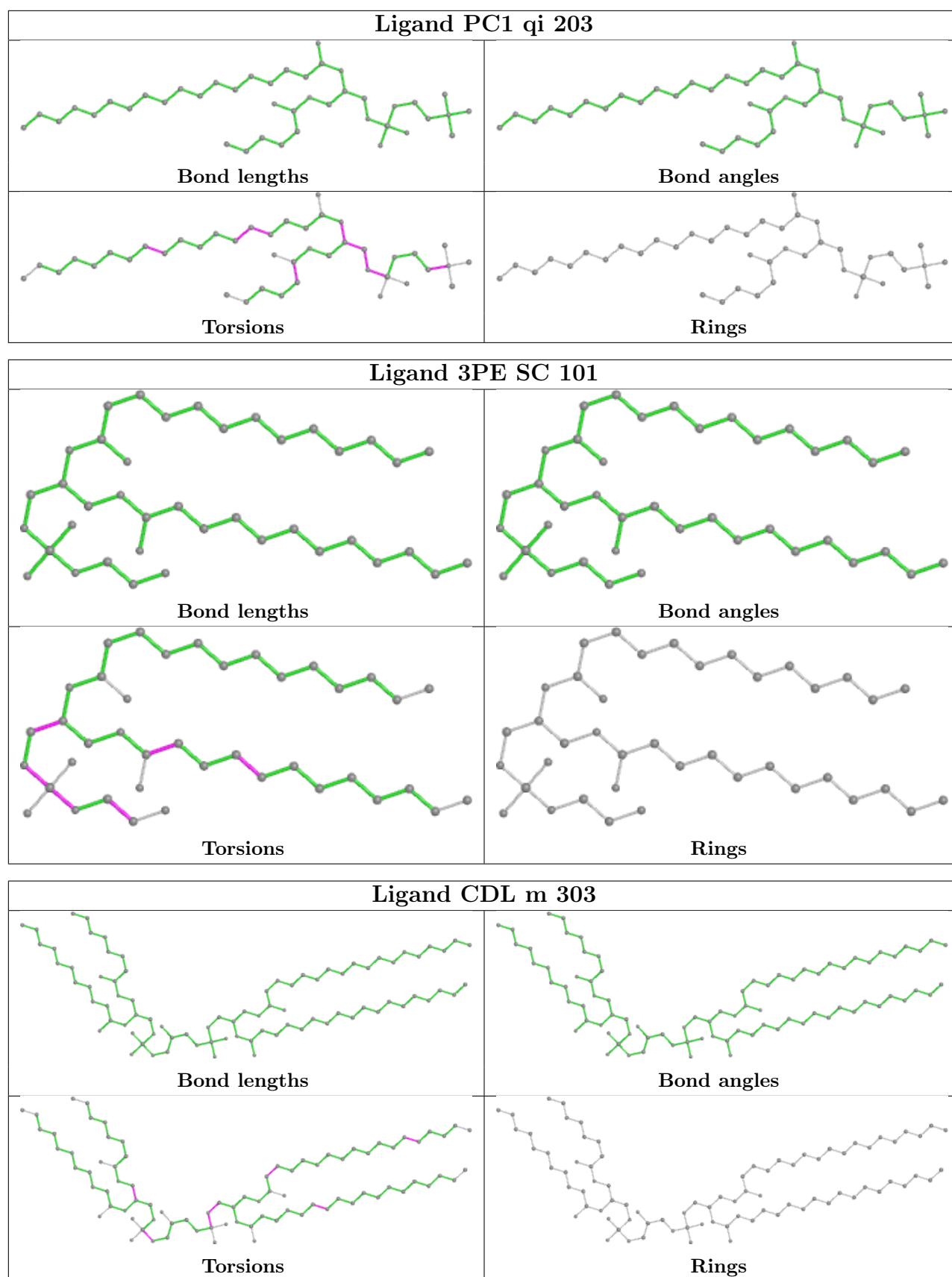


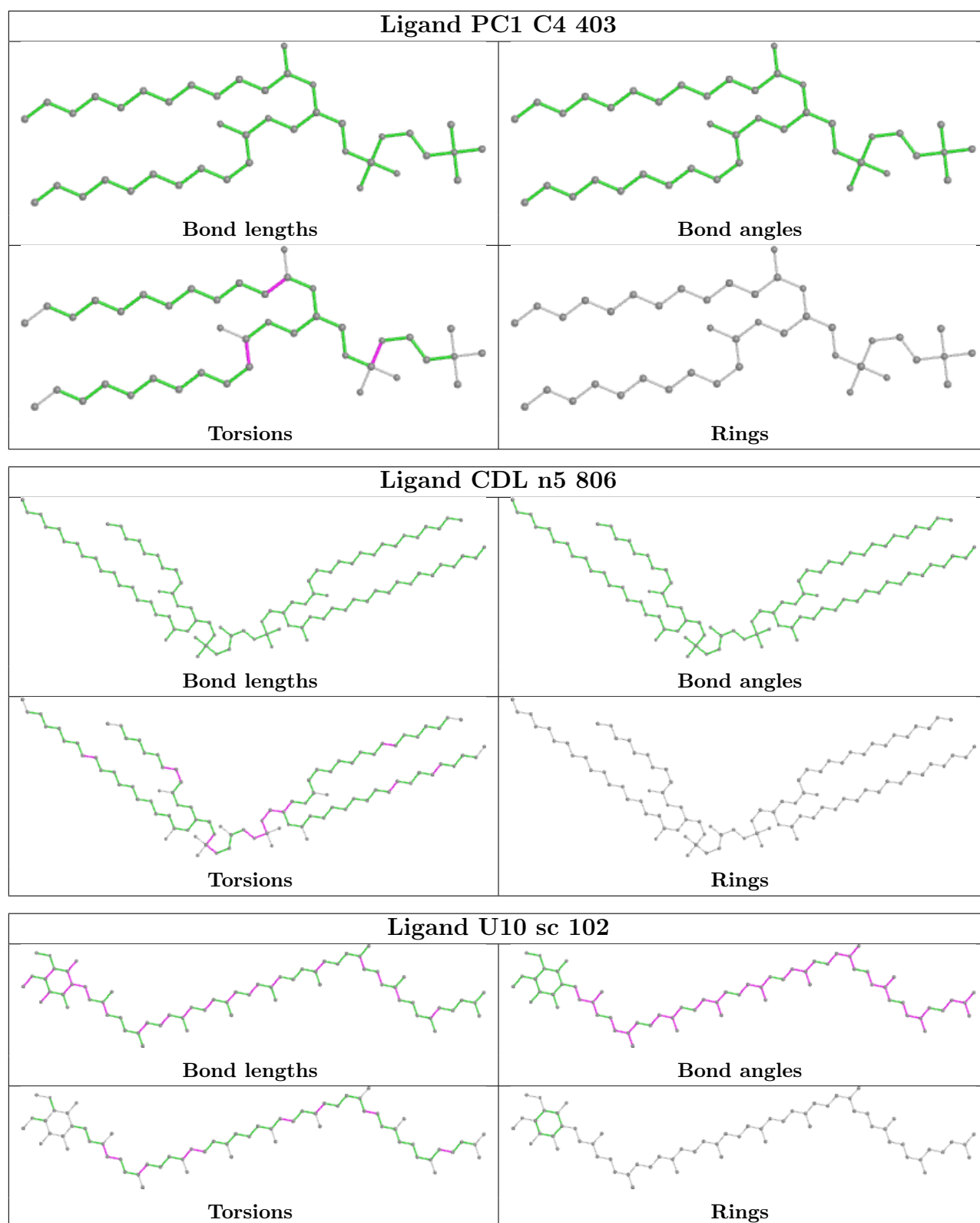


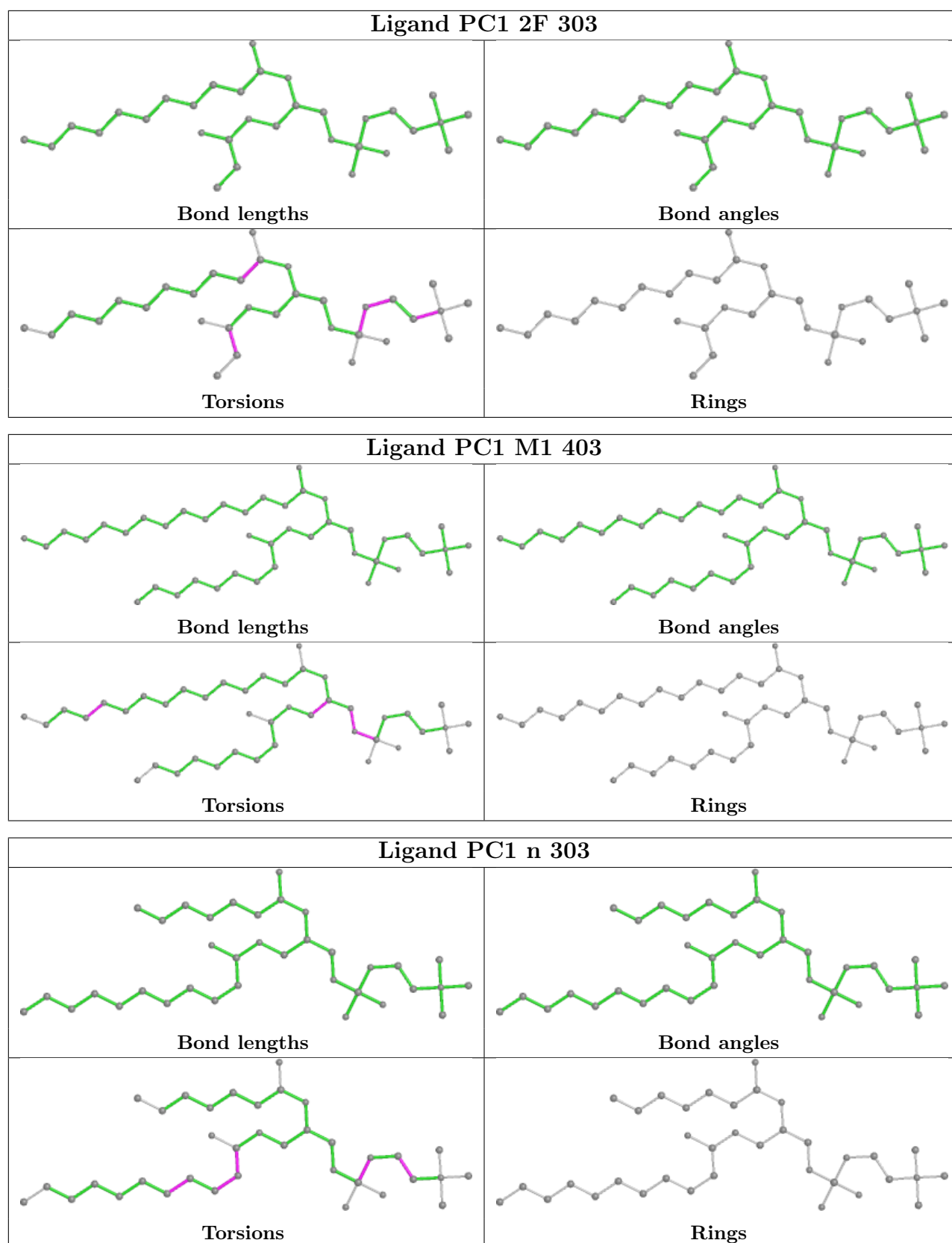


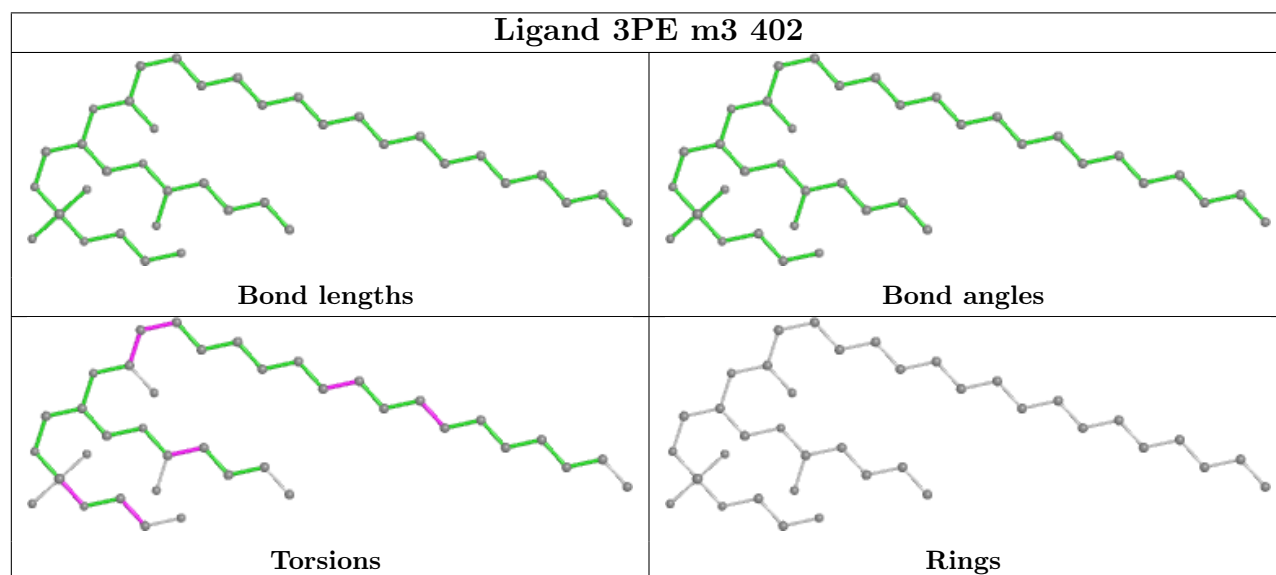
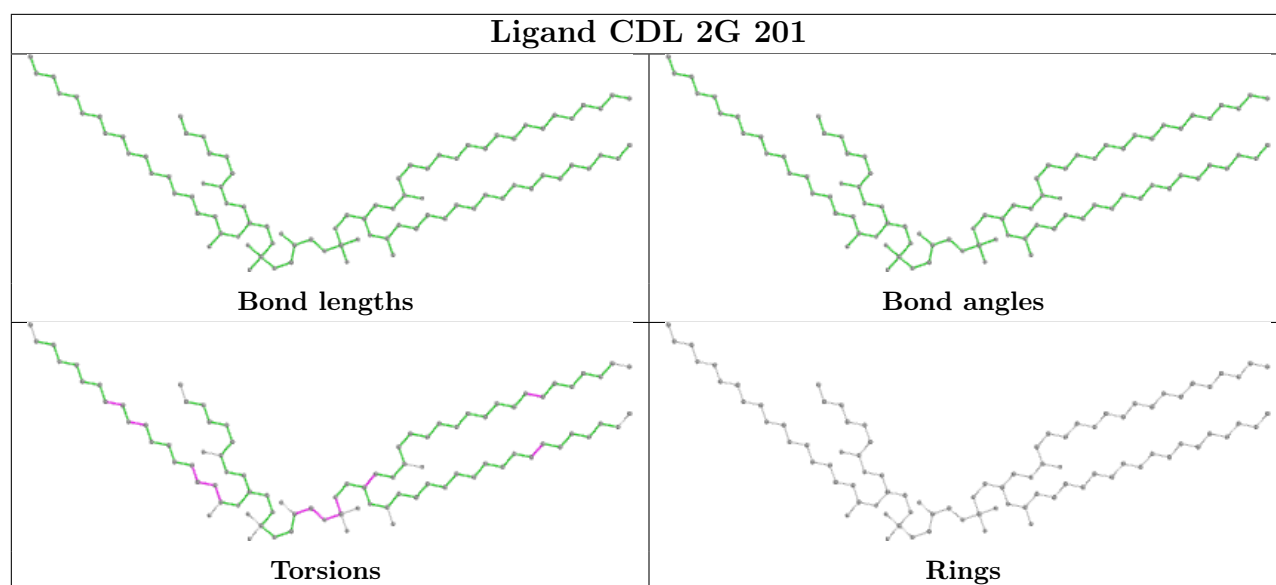


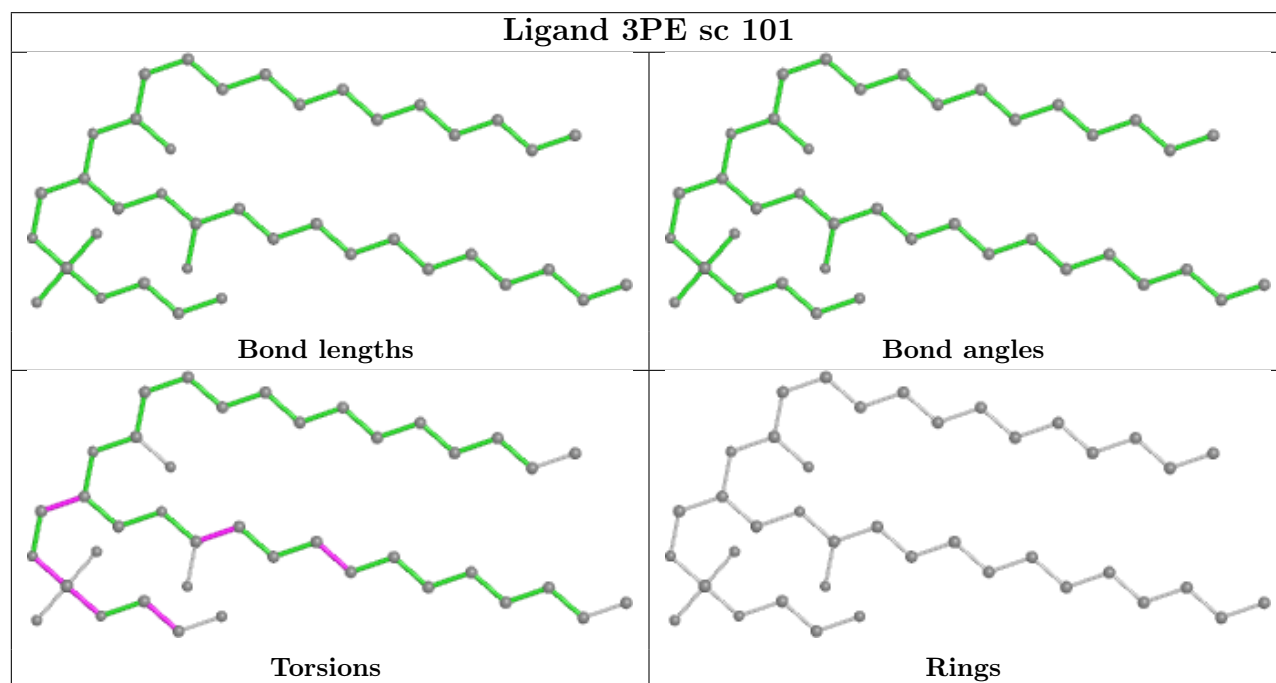
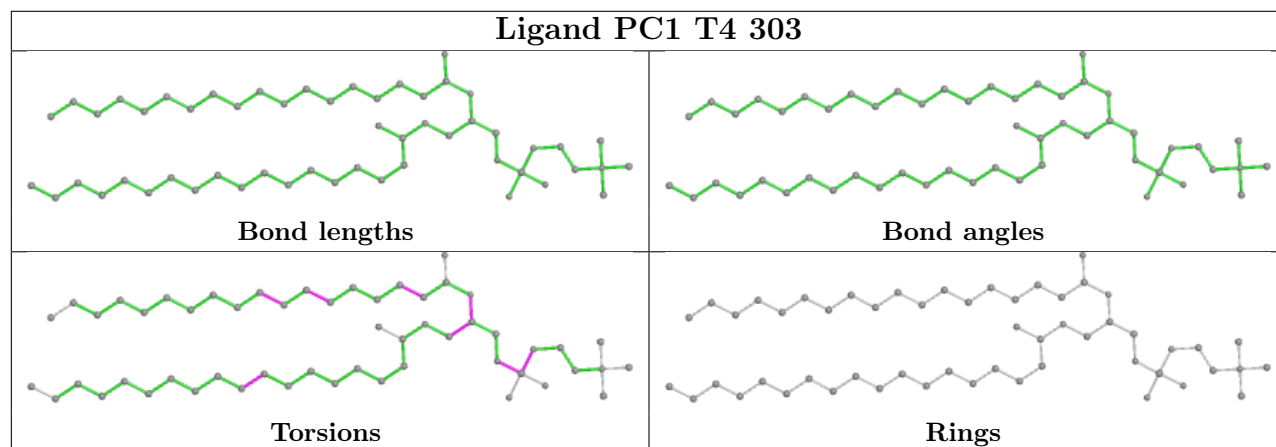
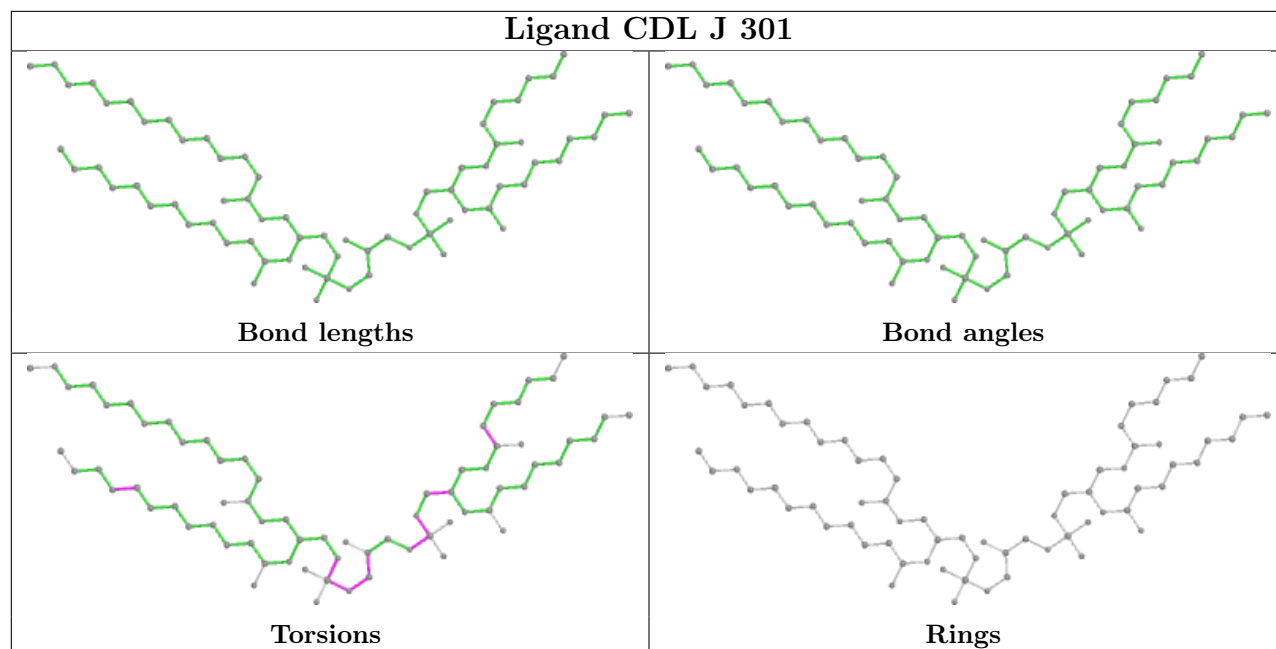


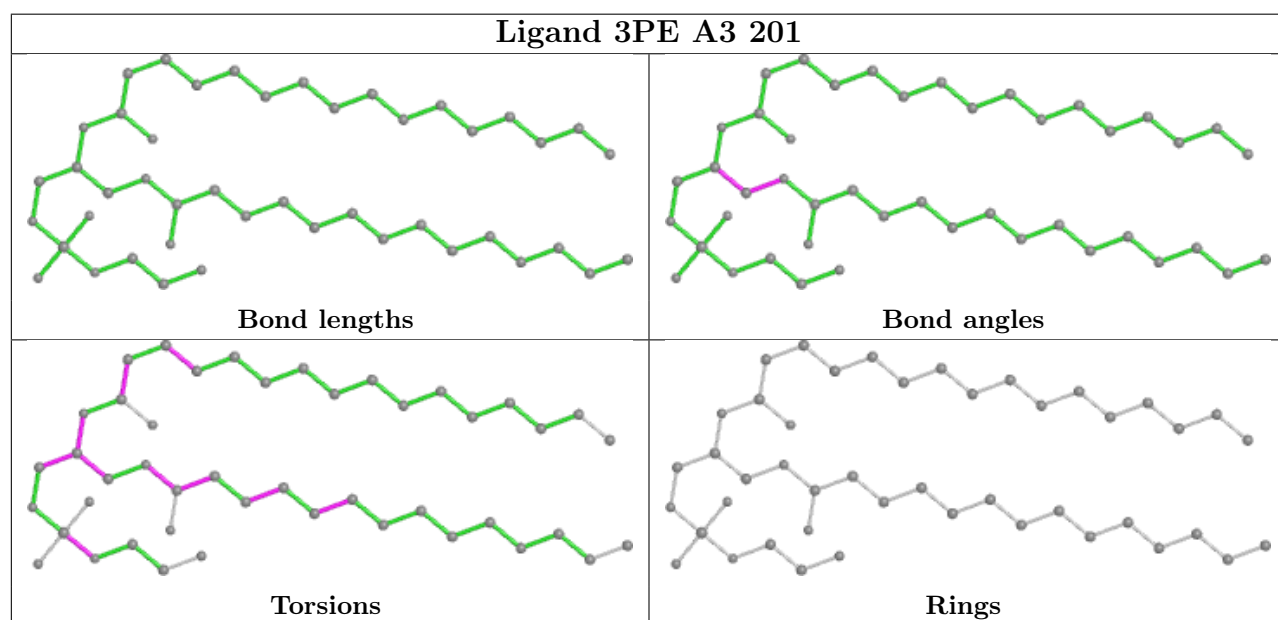
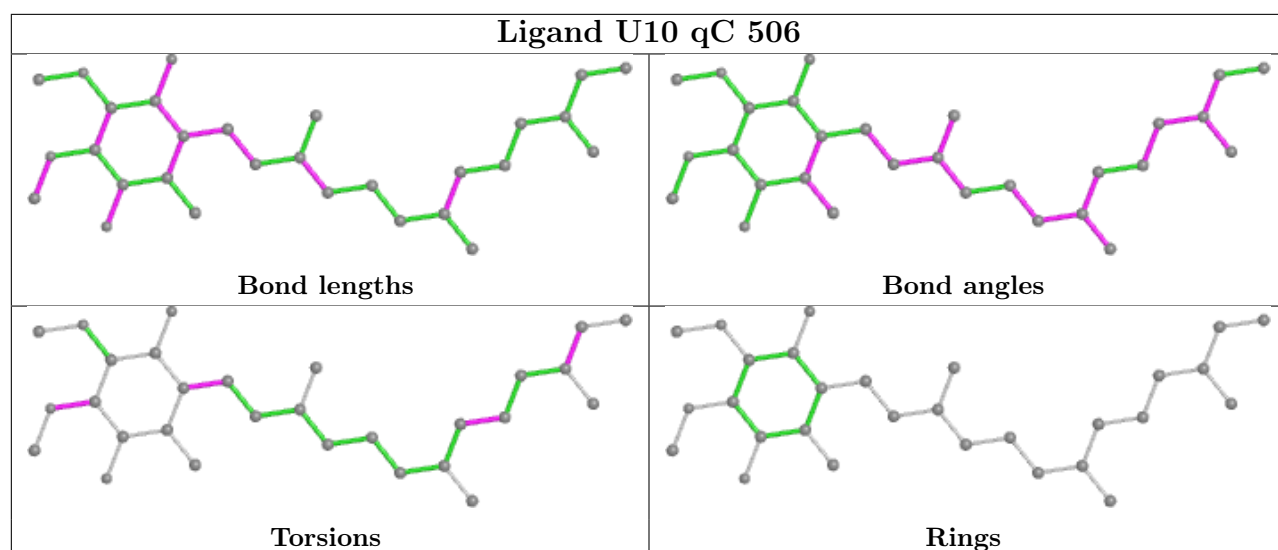


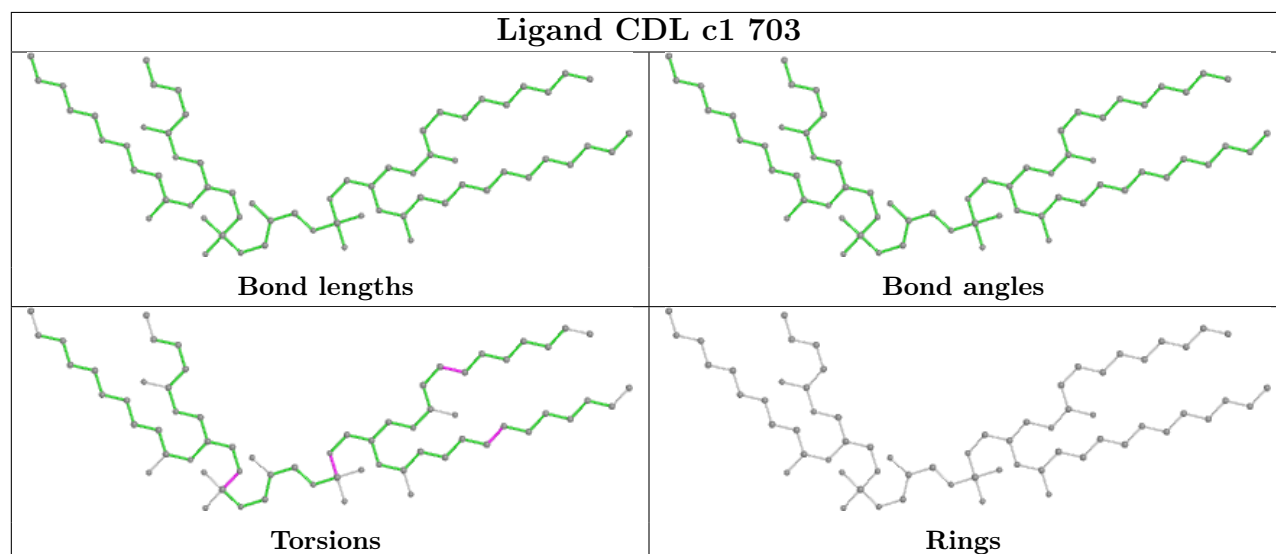
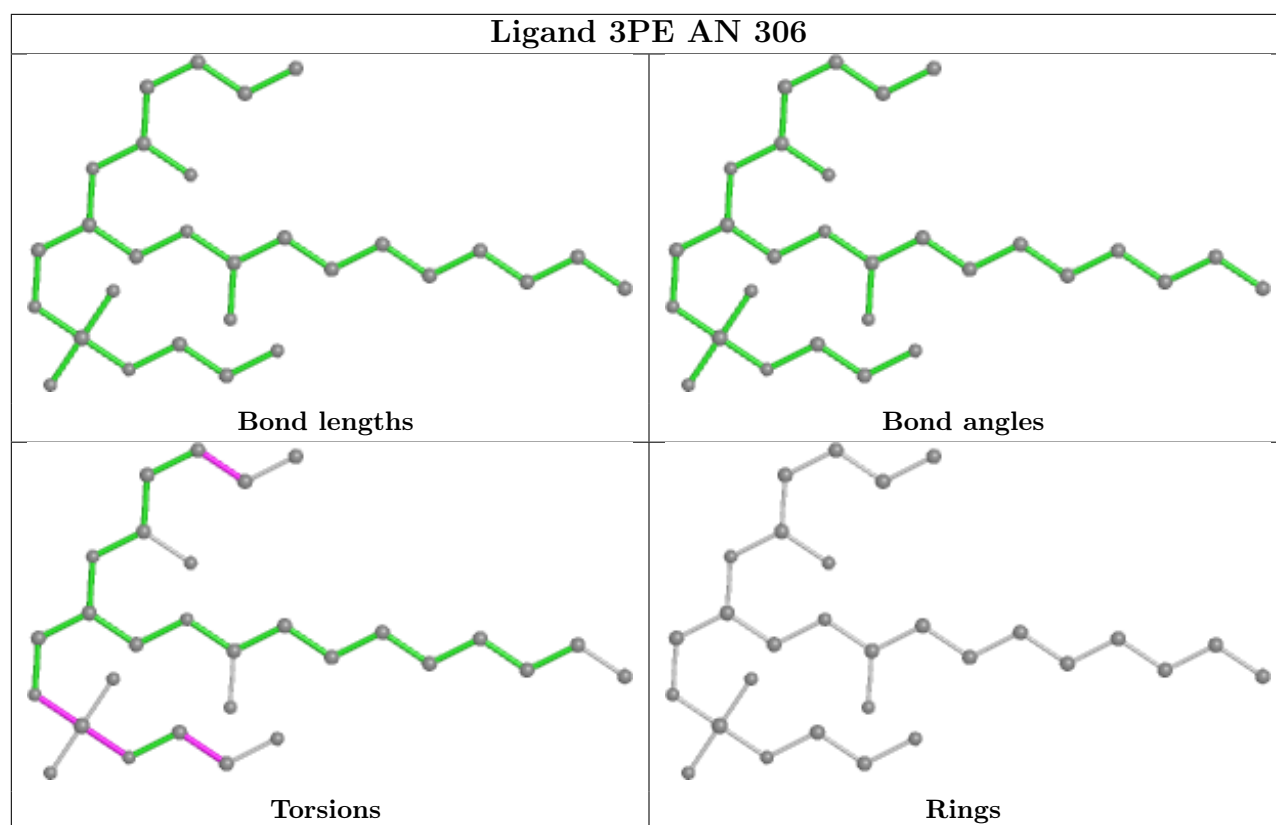


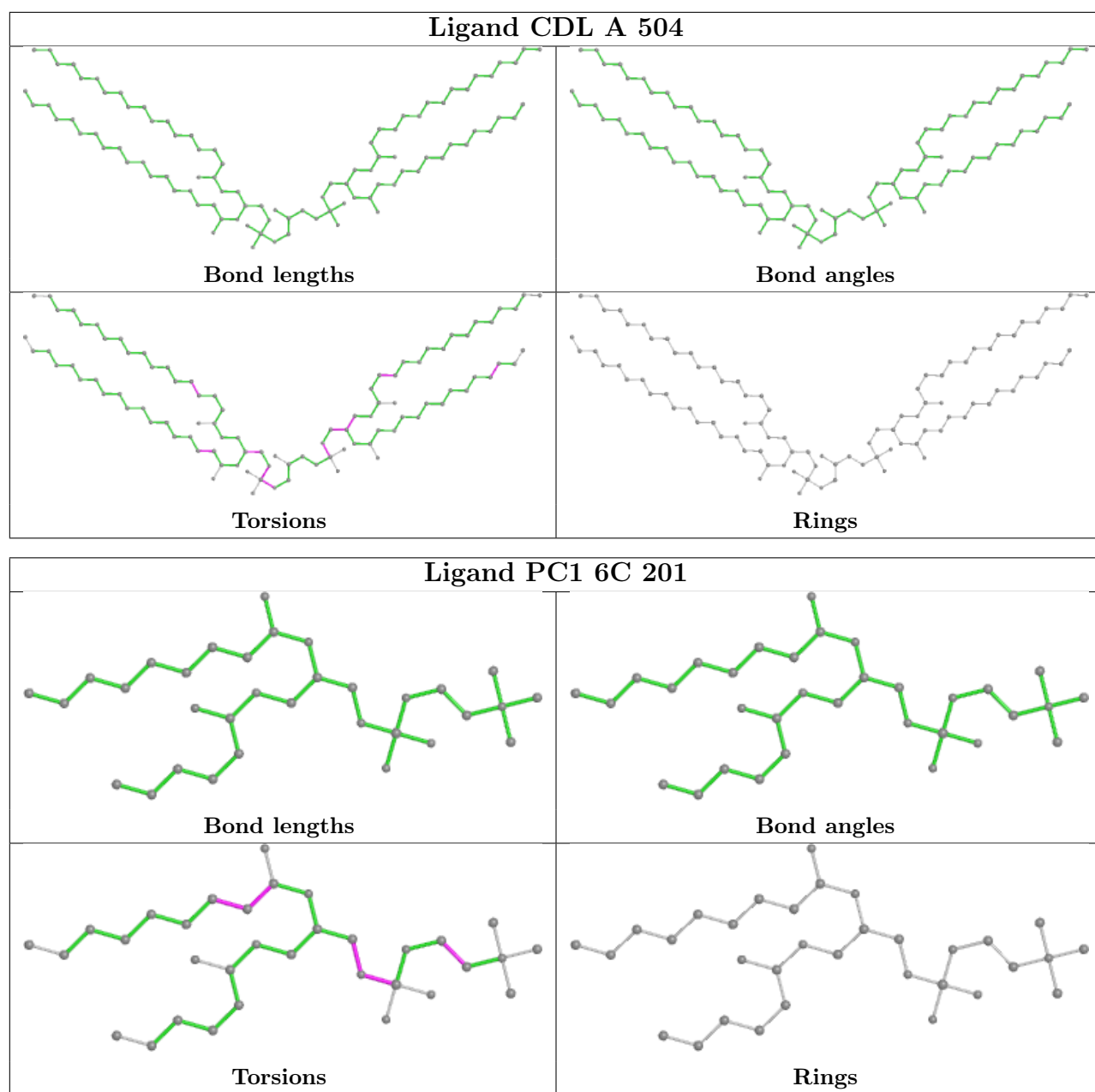


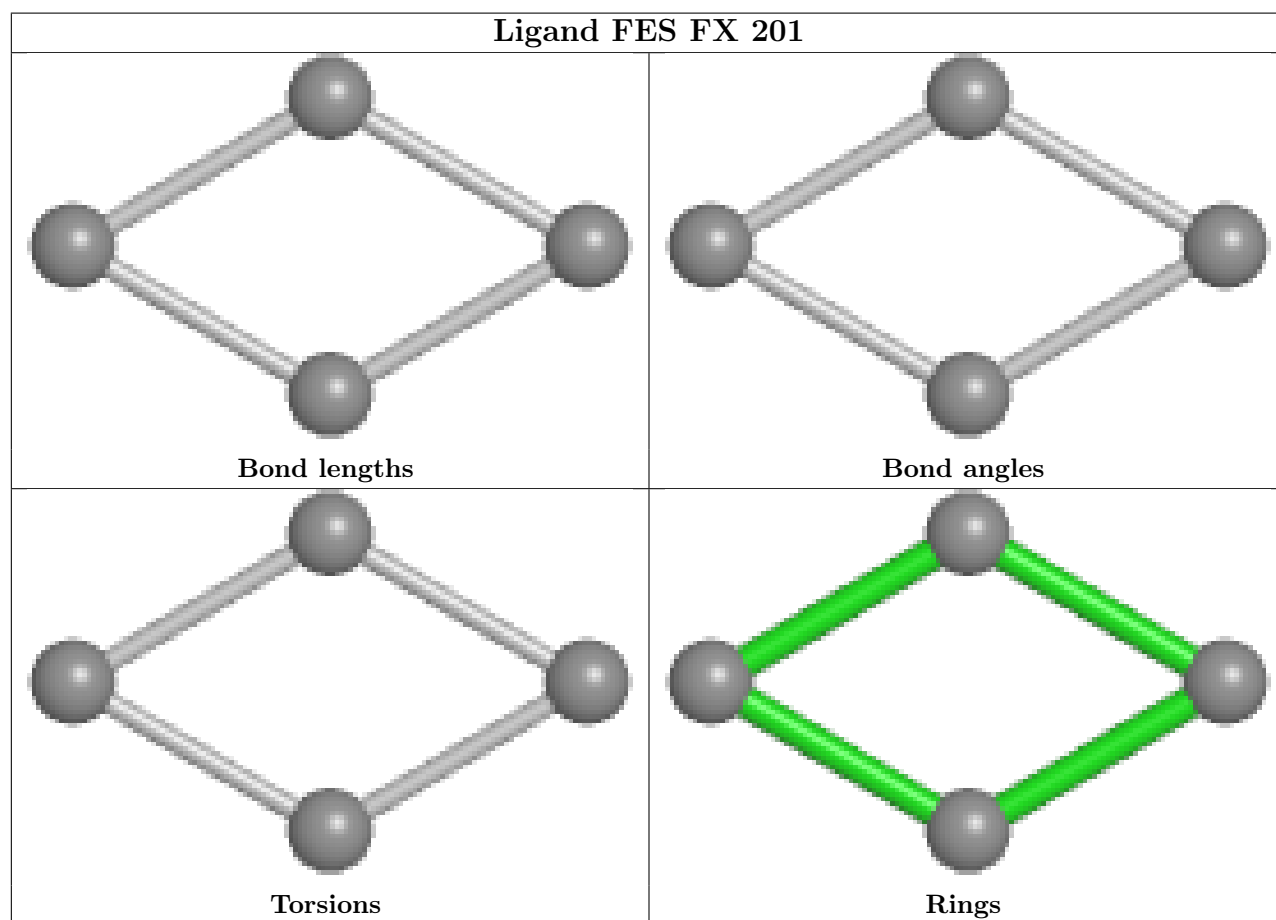
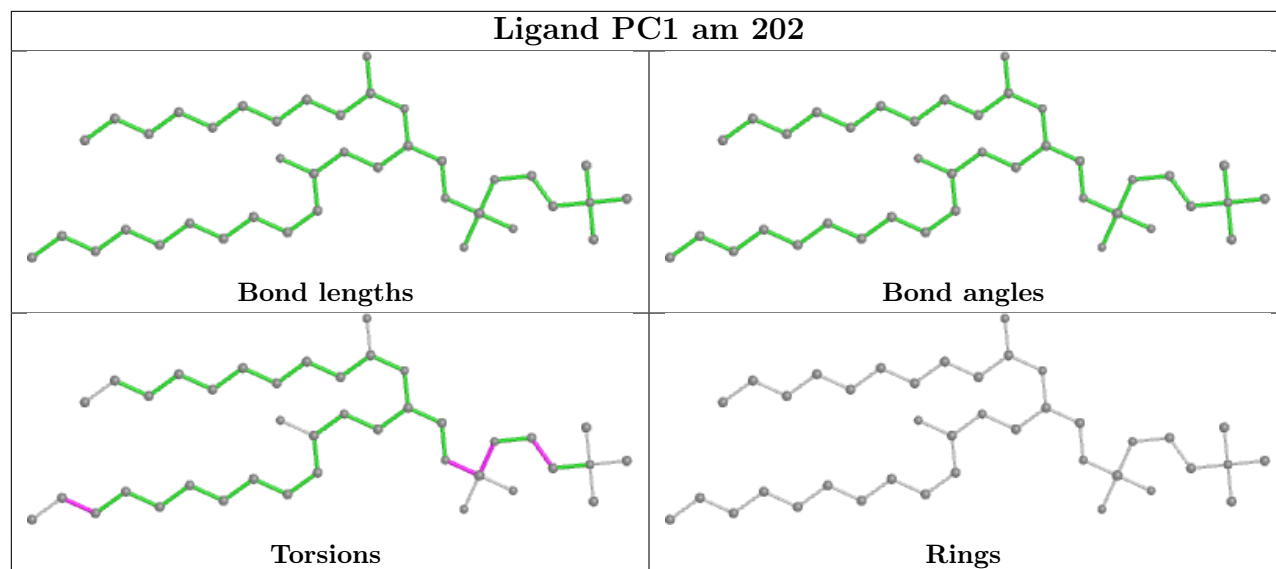


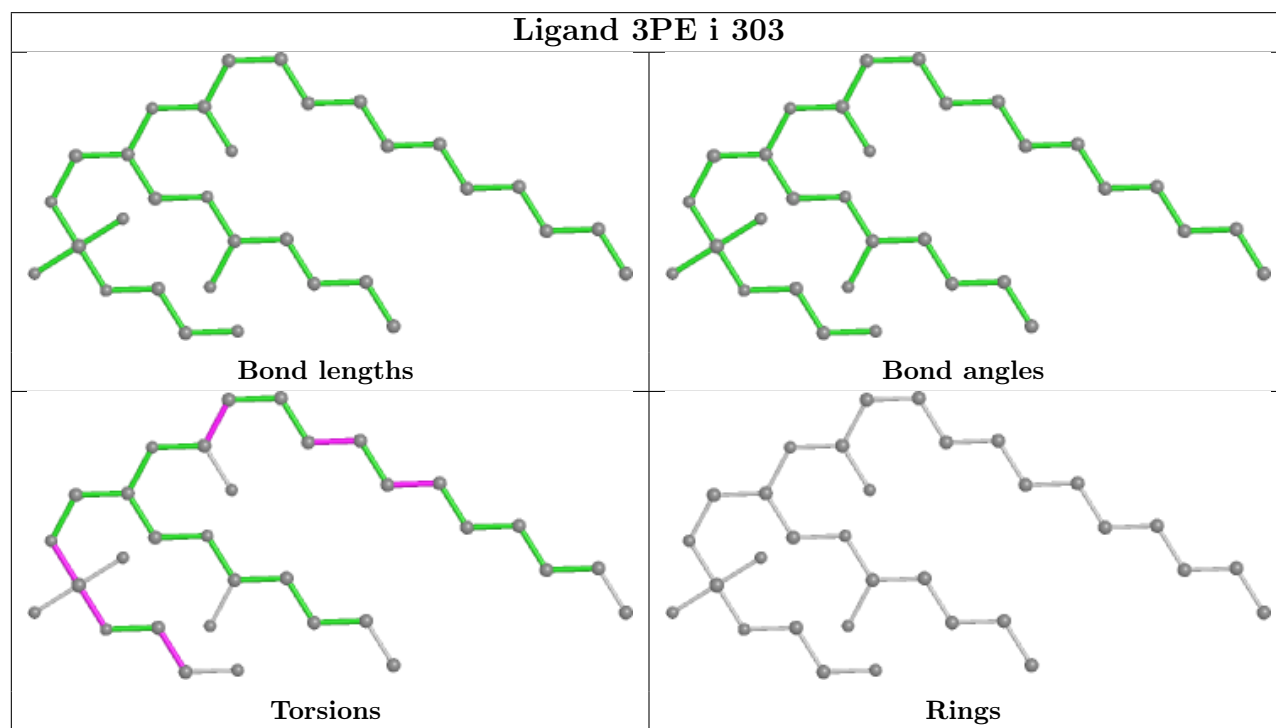
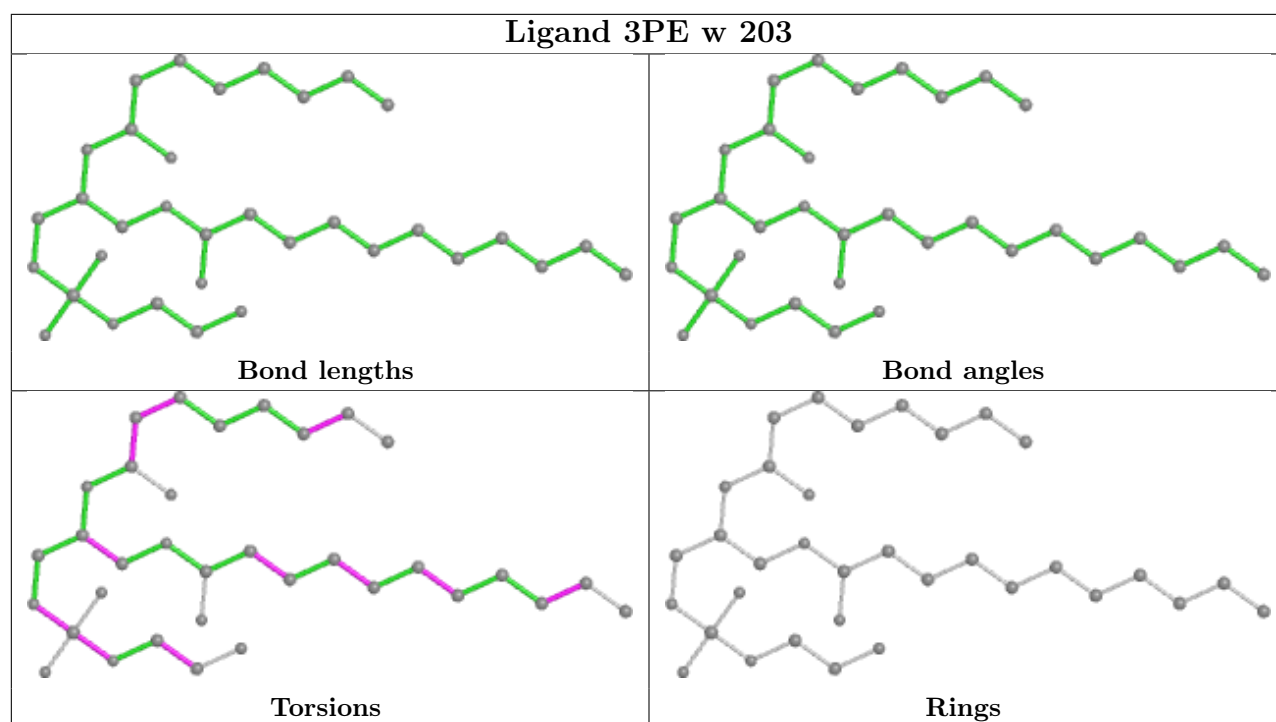


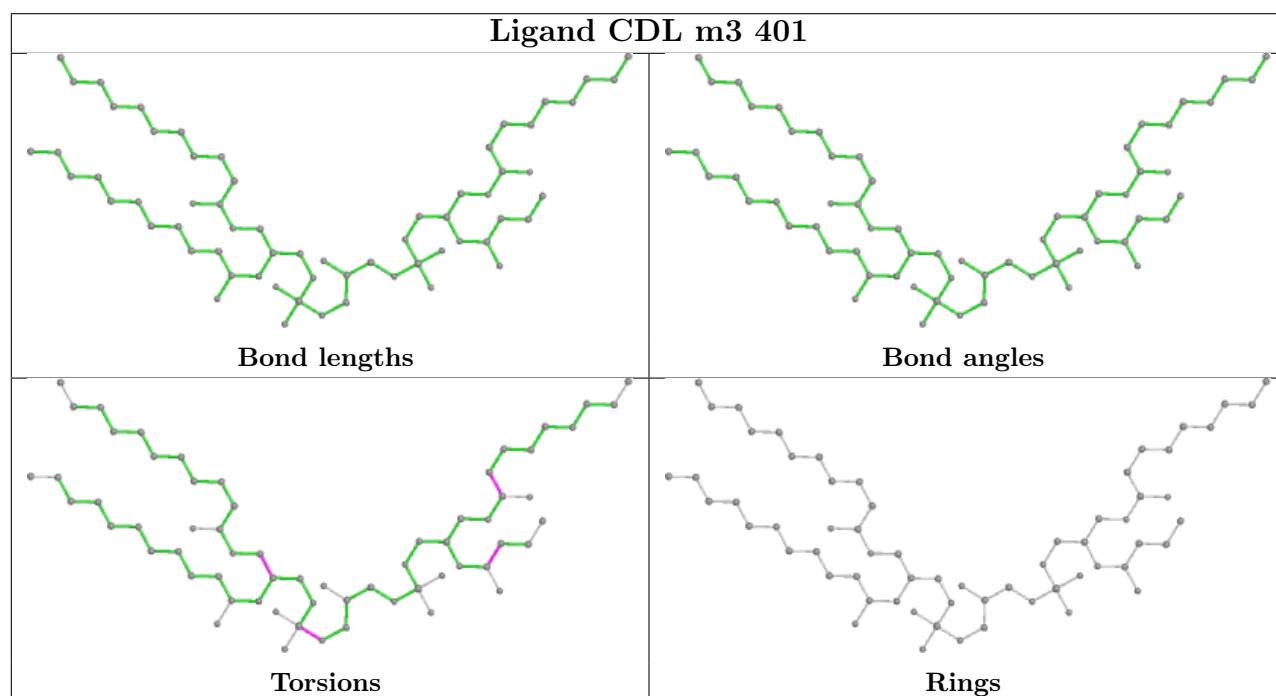
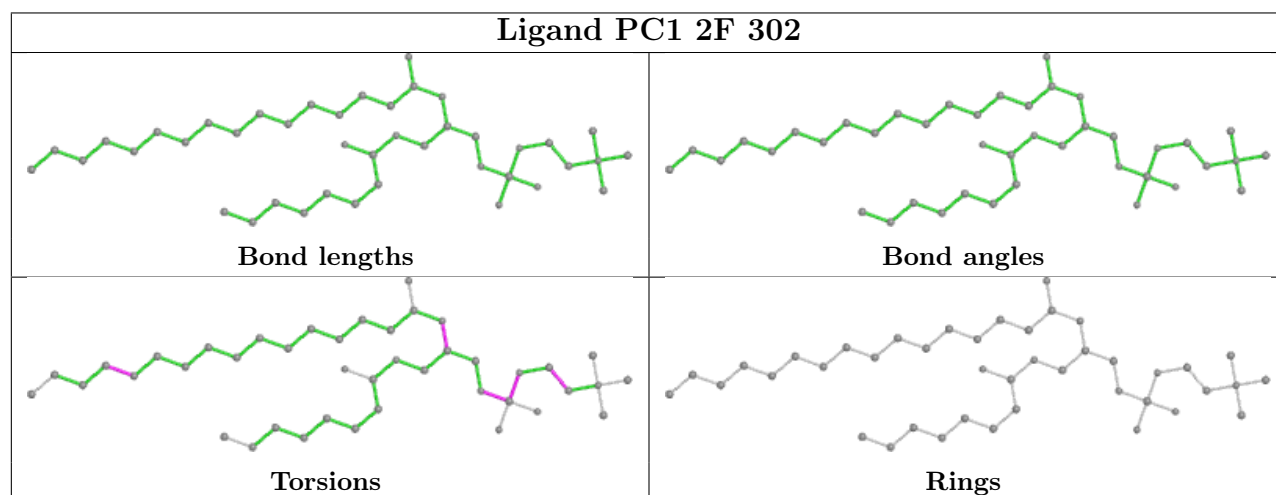
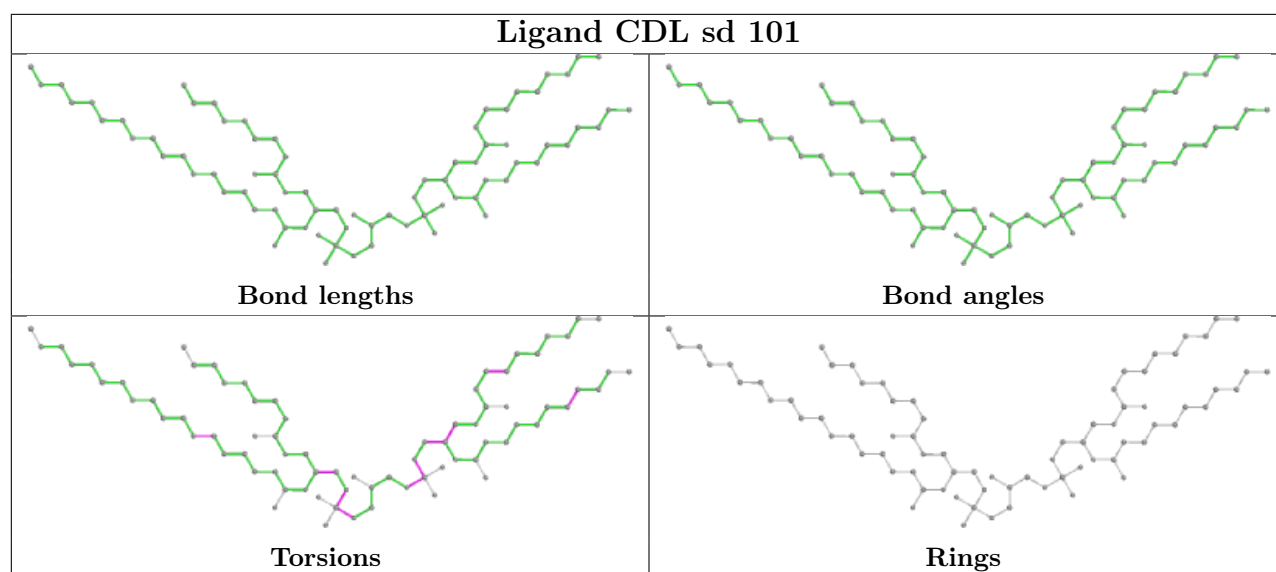


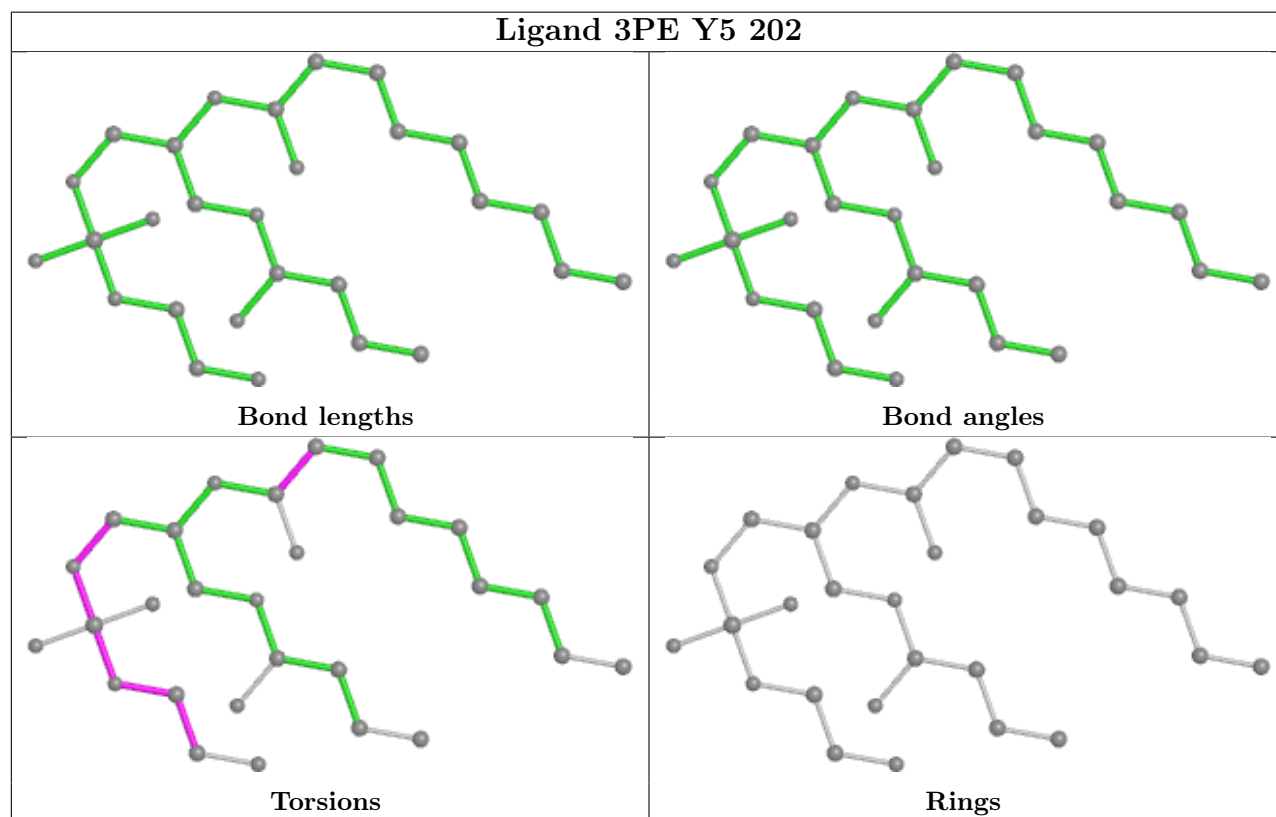
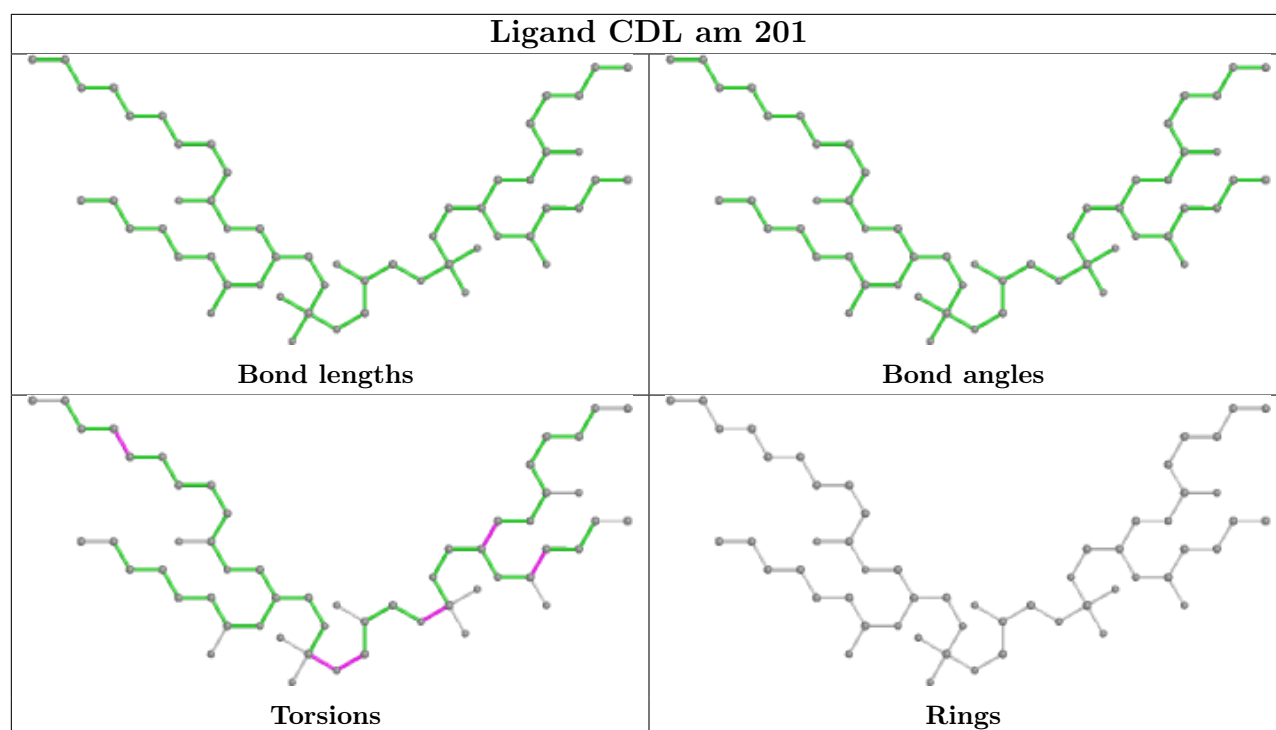


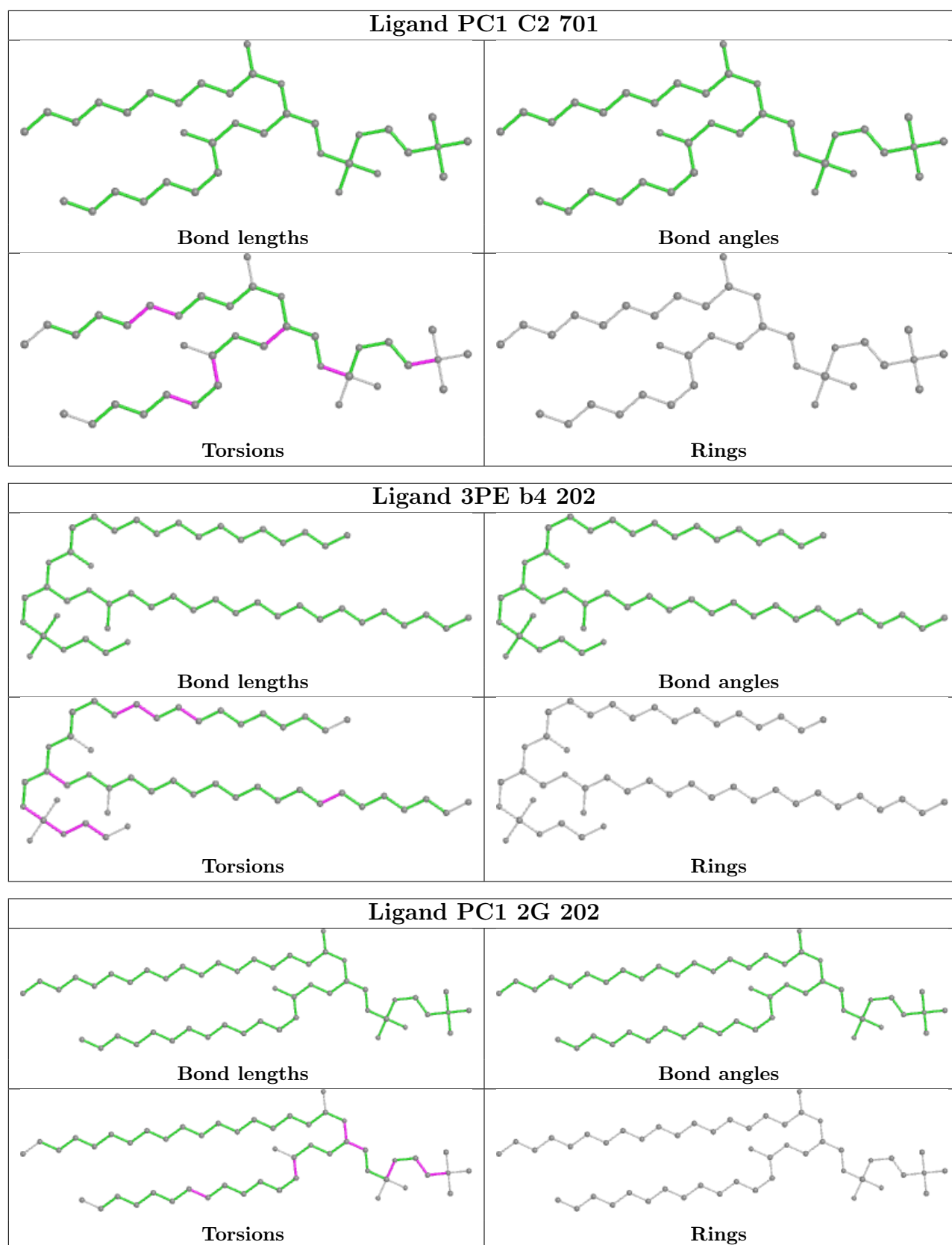


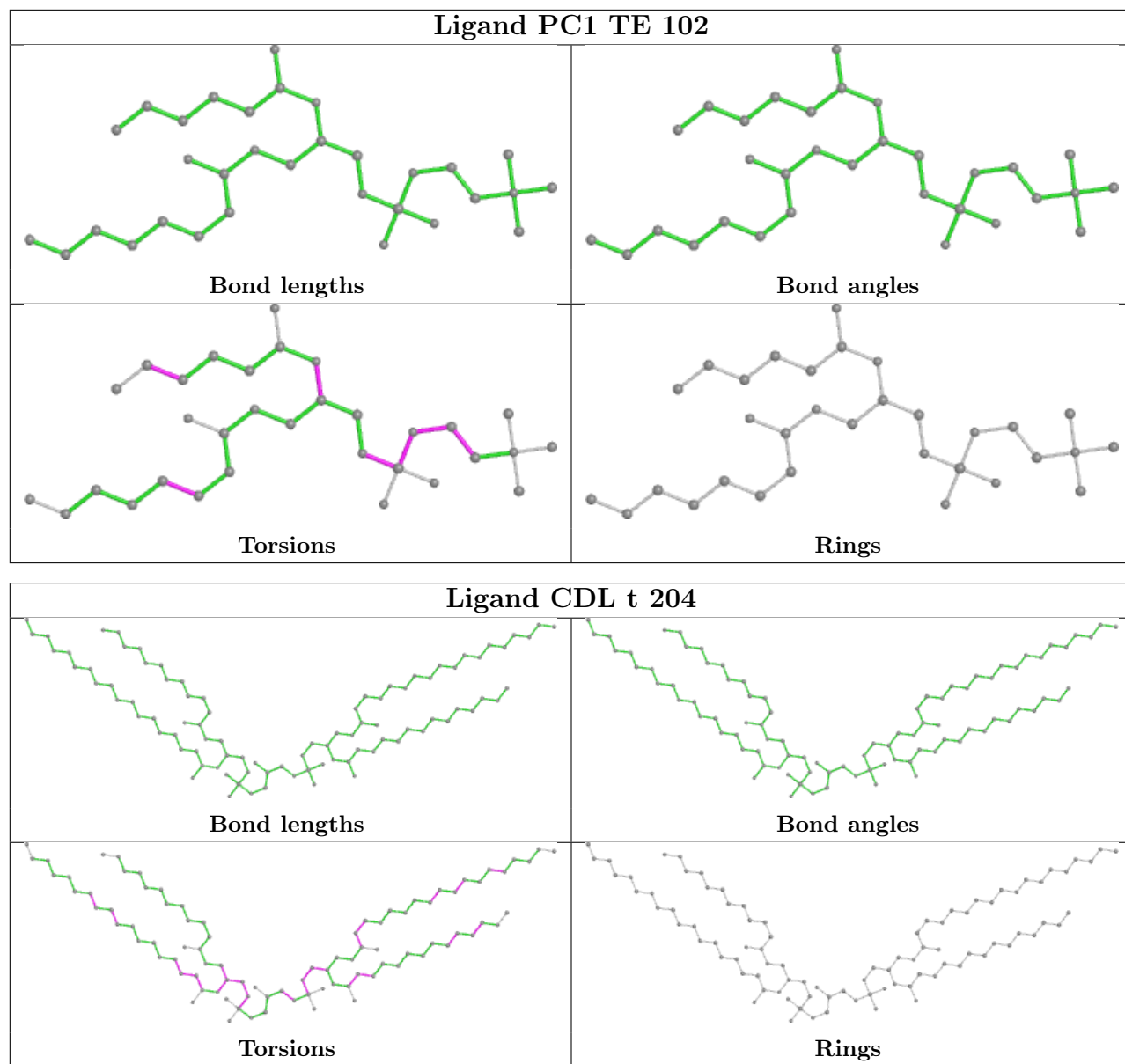




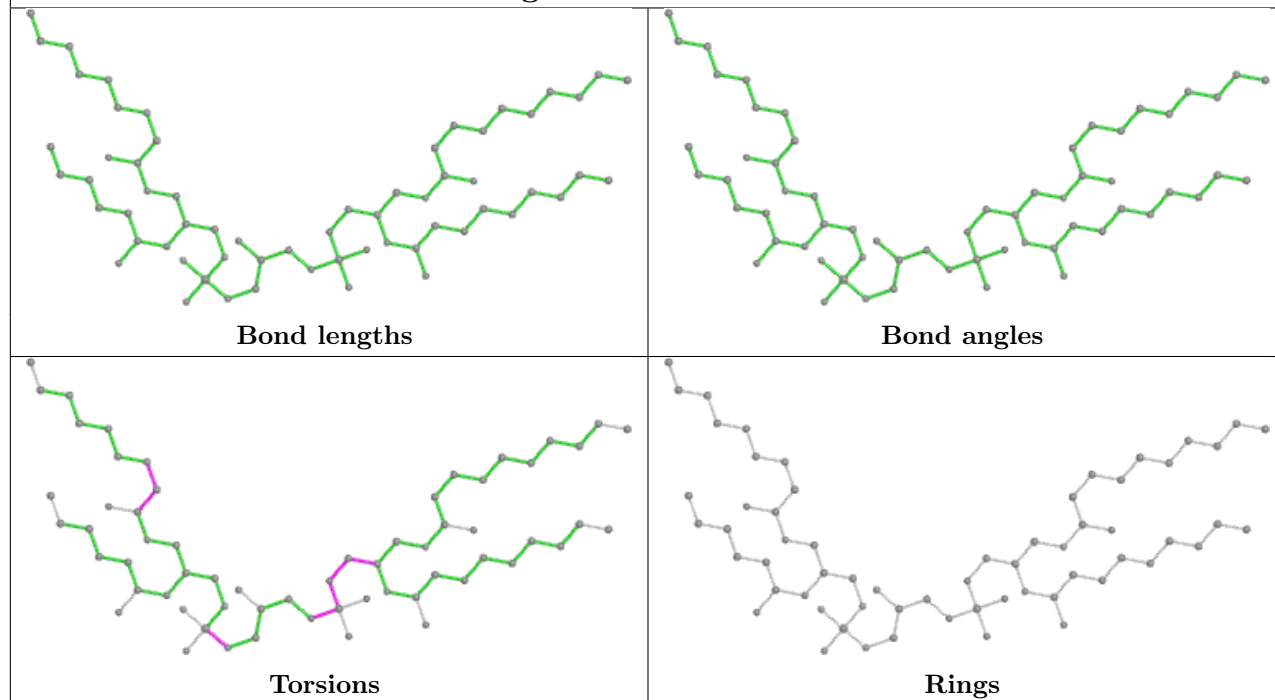




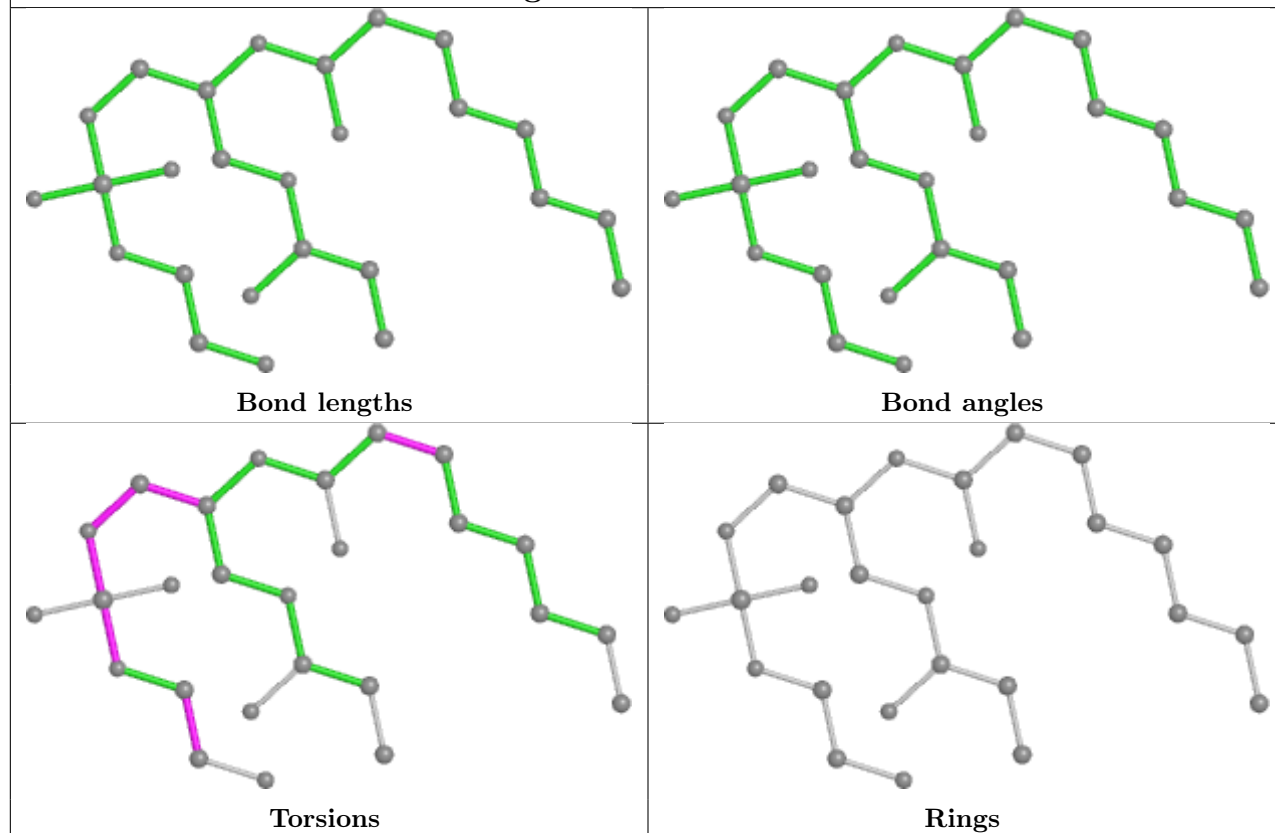


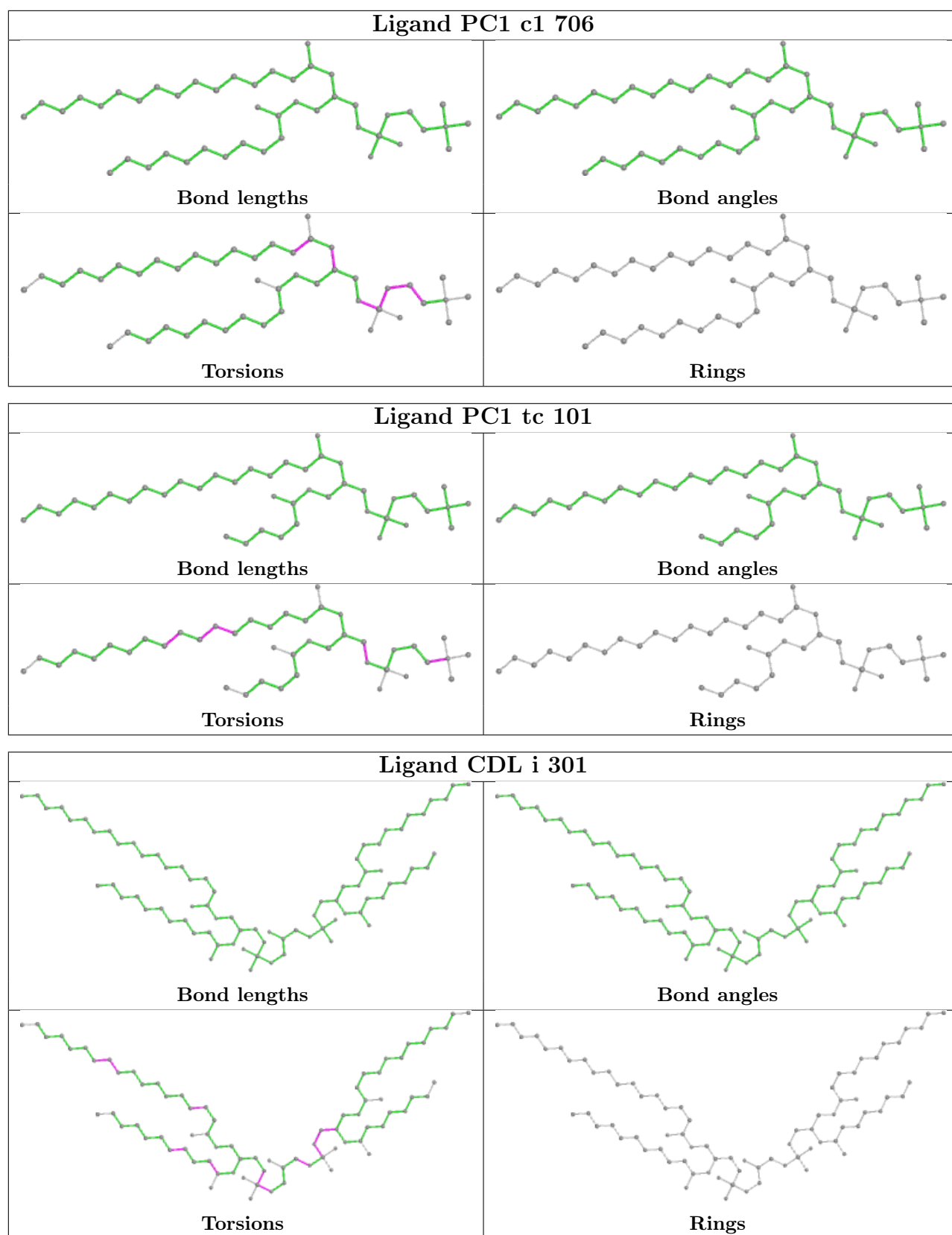


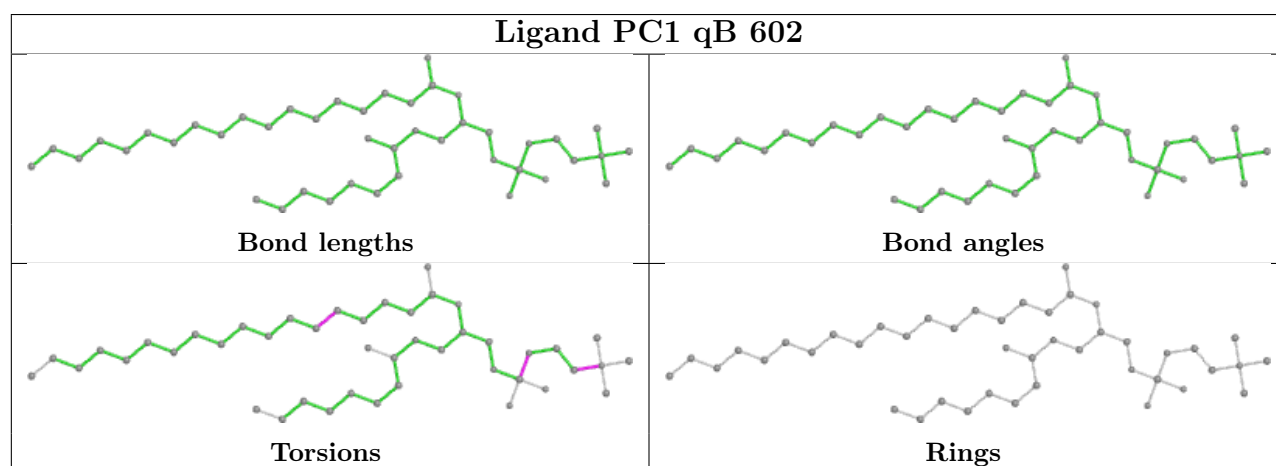
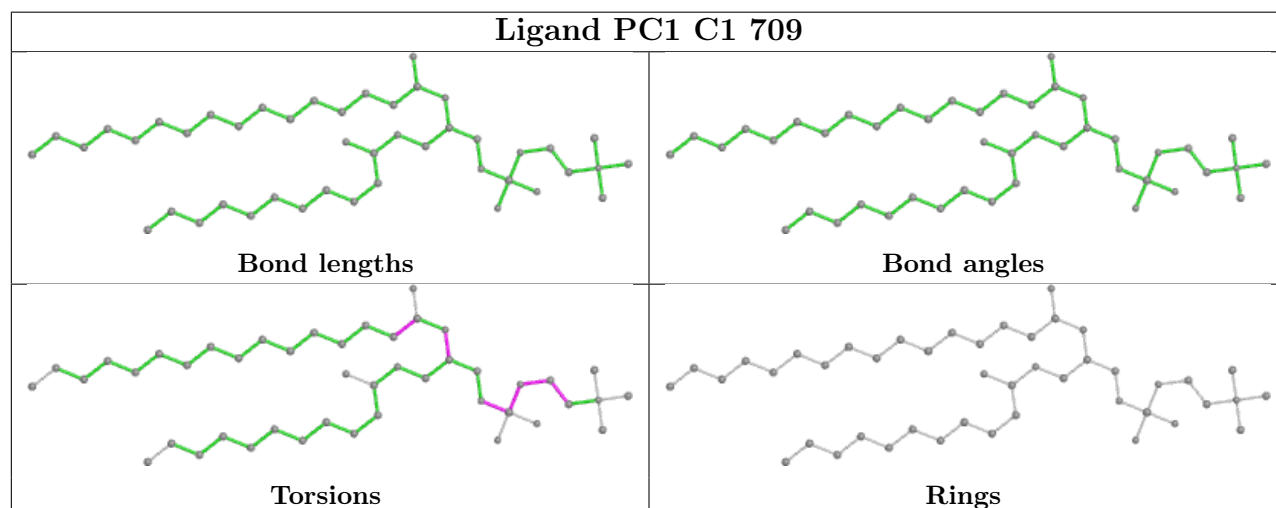
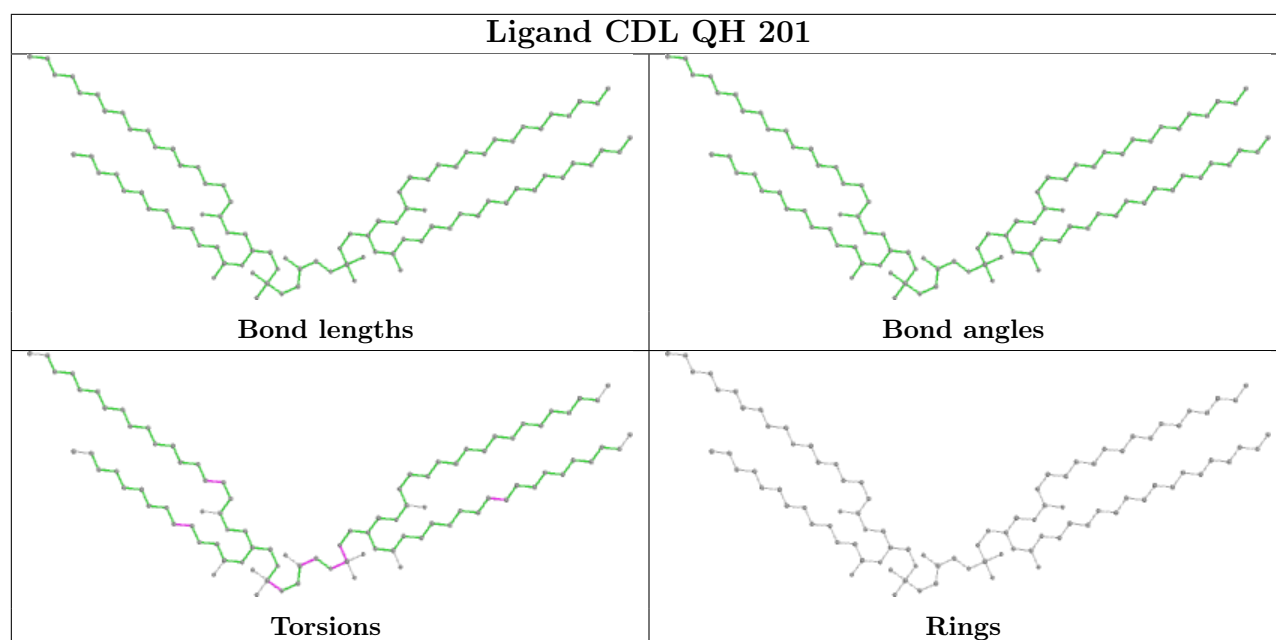
Ligand CDL 7A 203

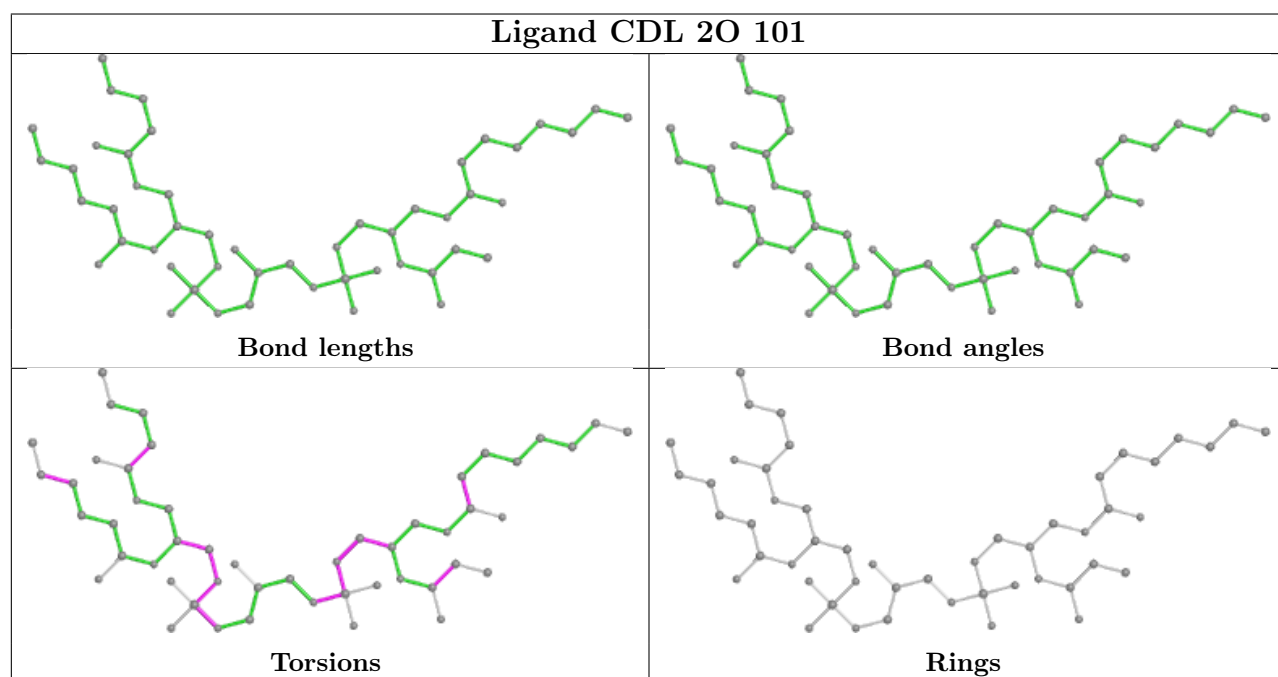
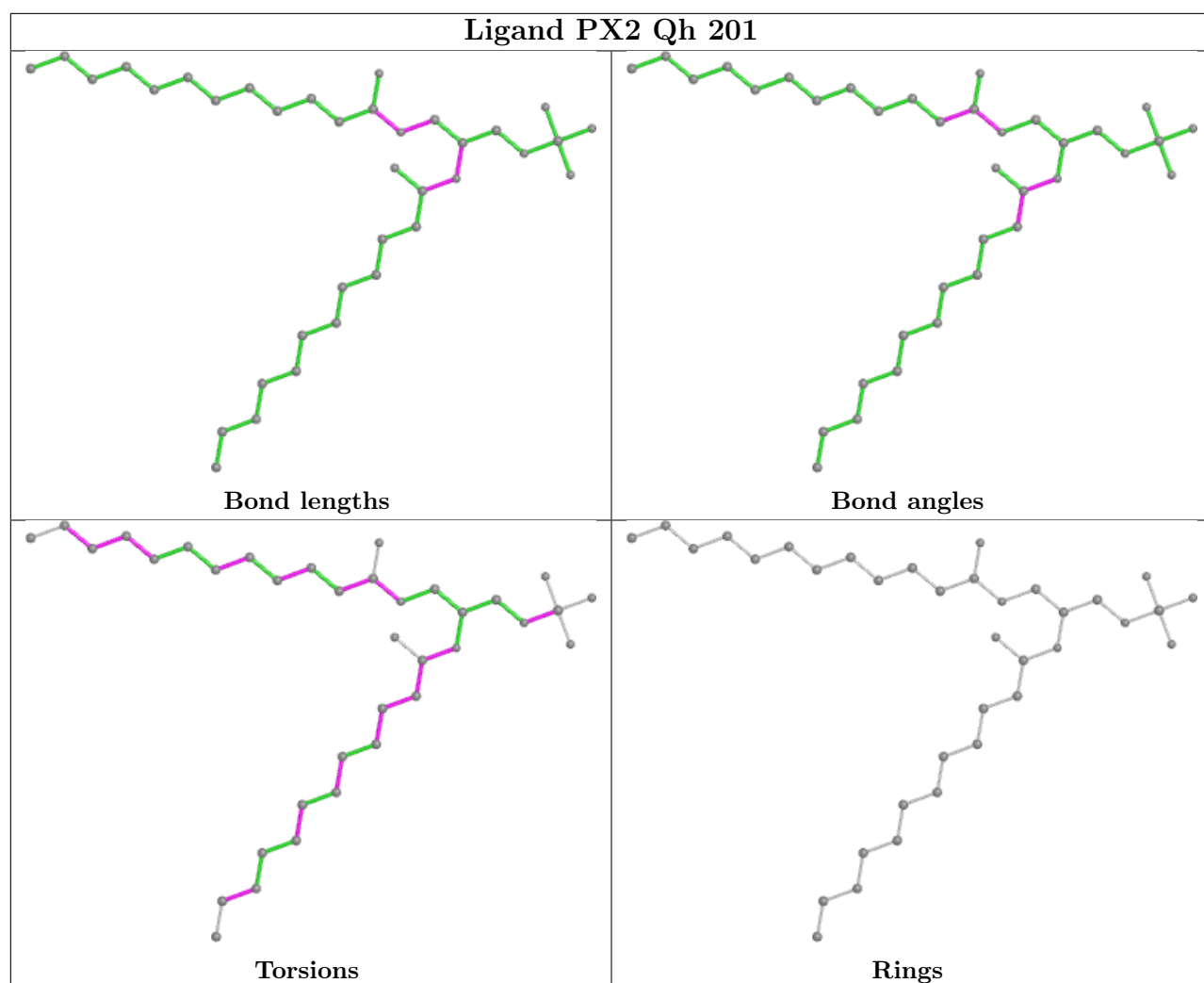


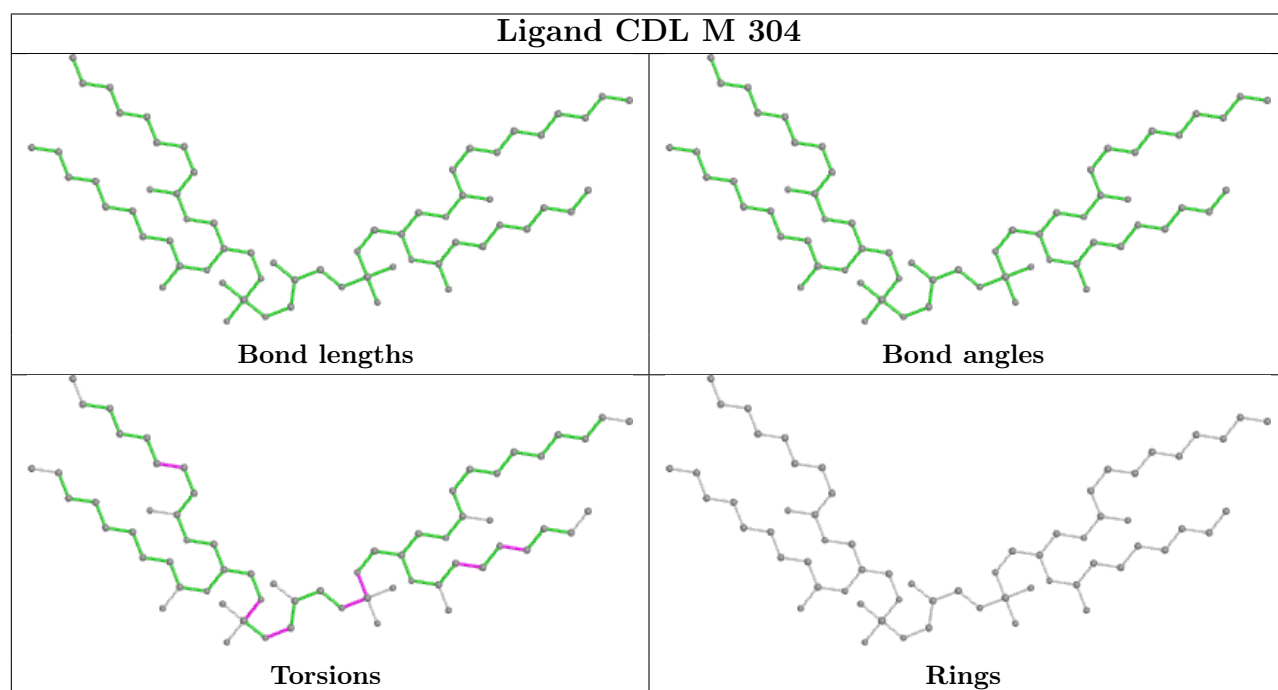
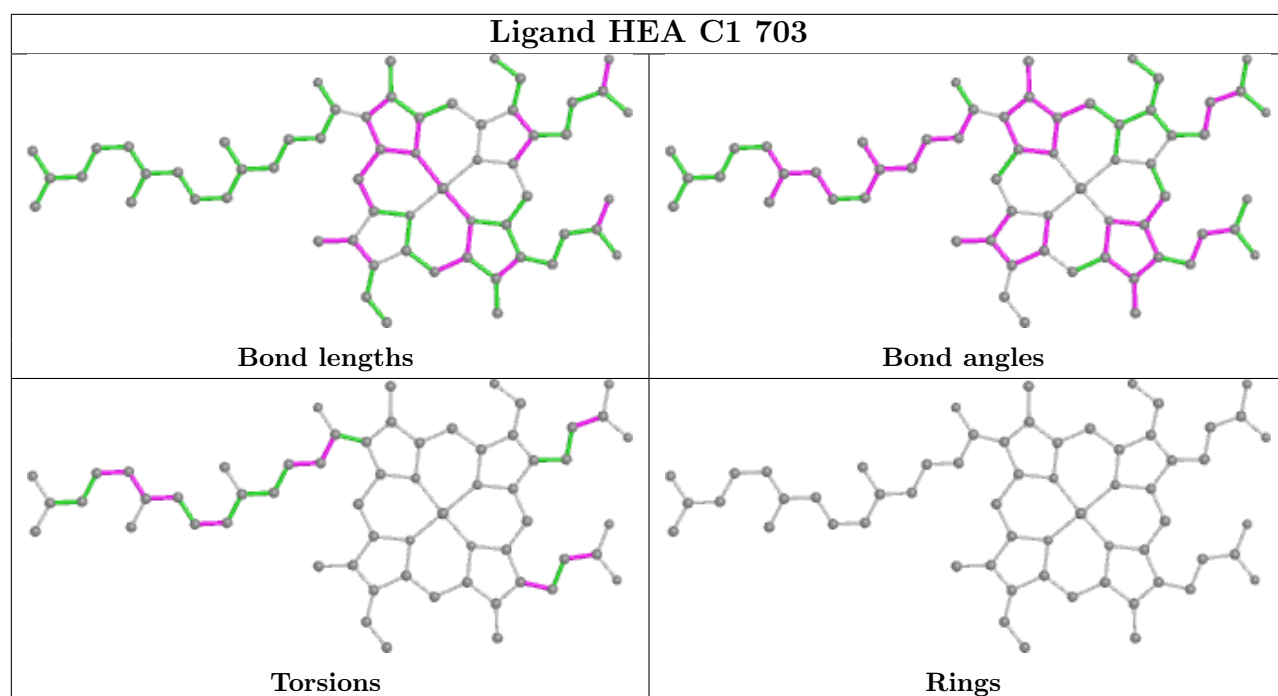
Ligand 3PE TA 201

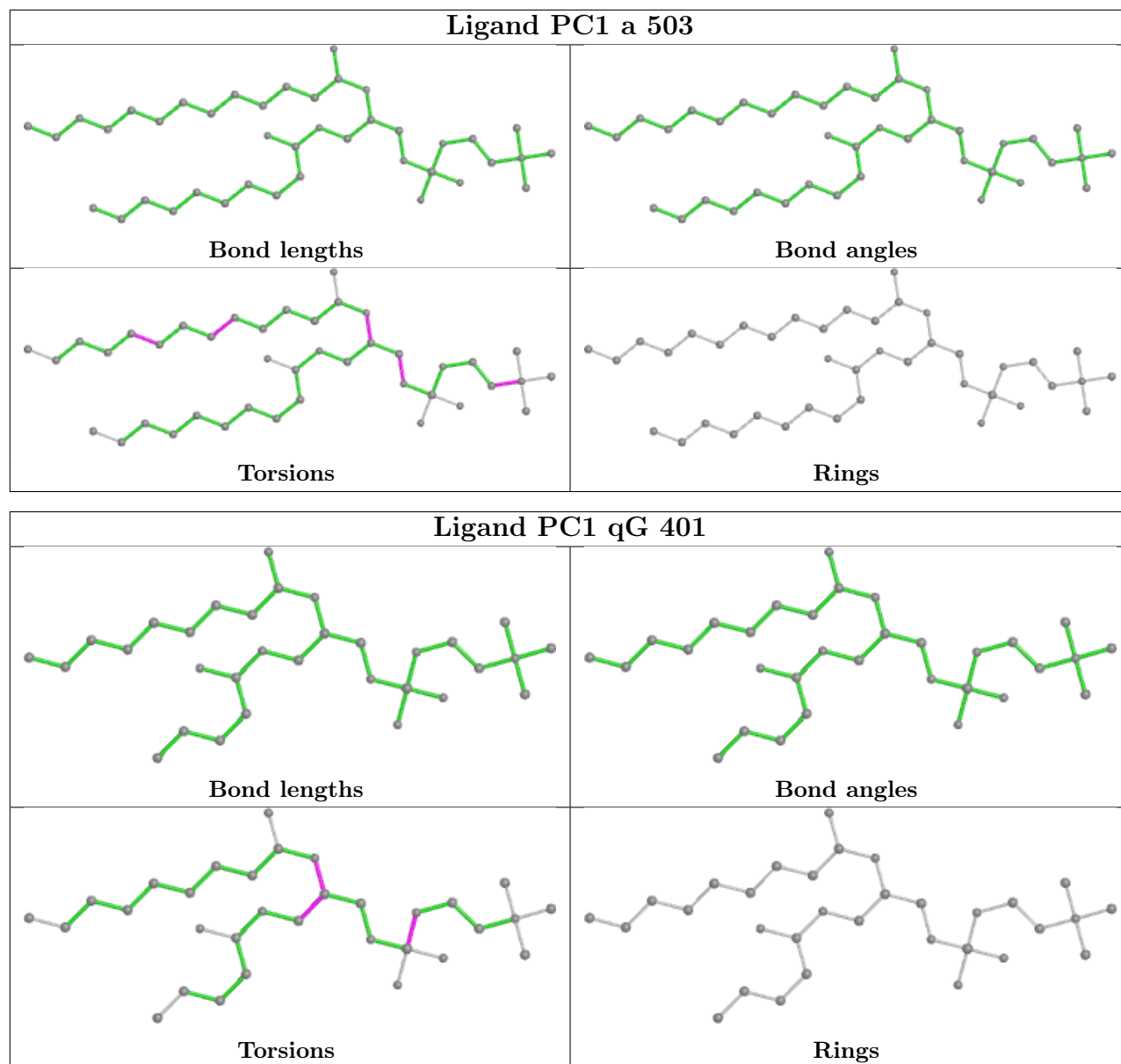


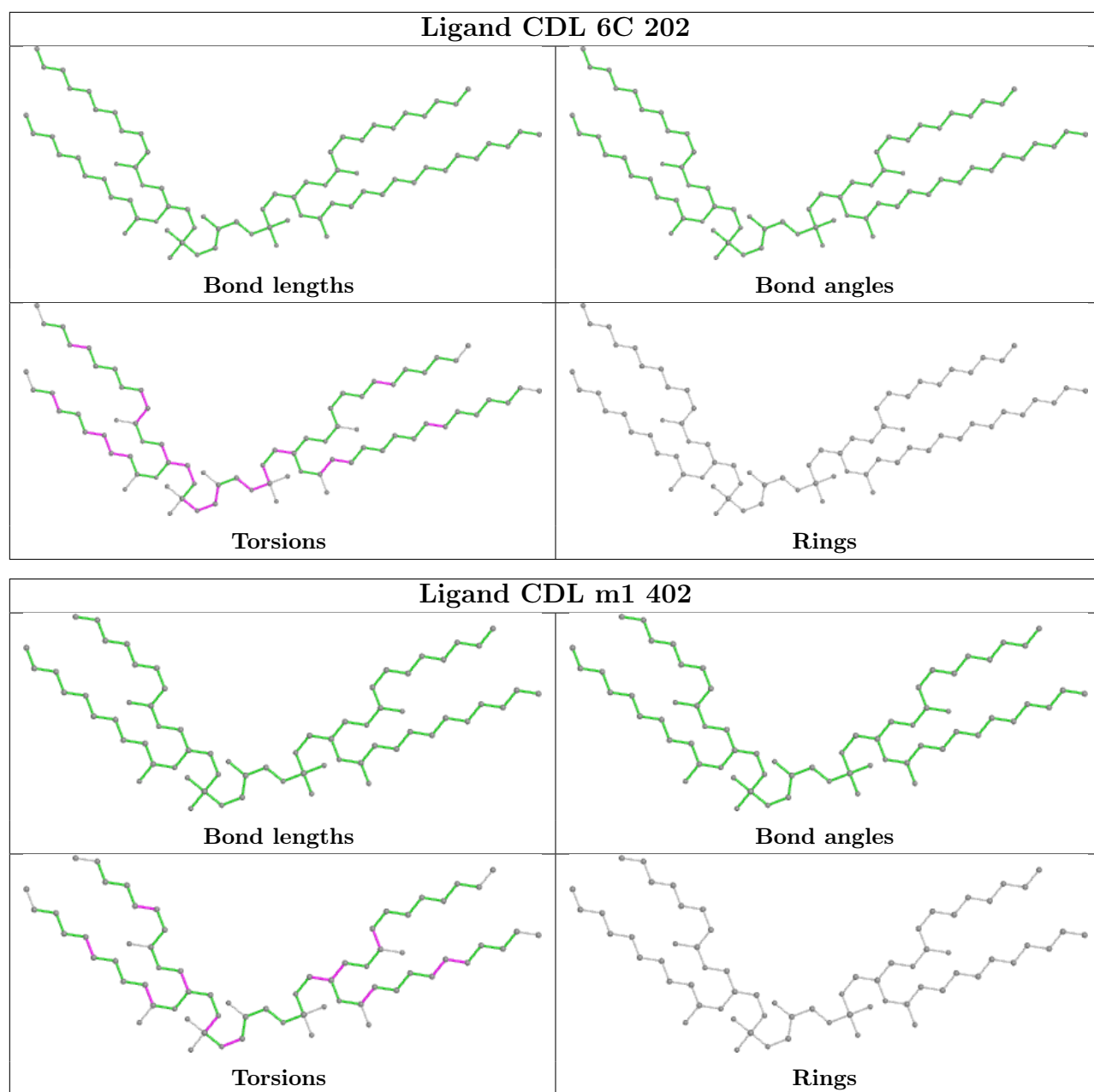


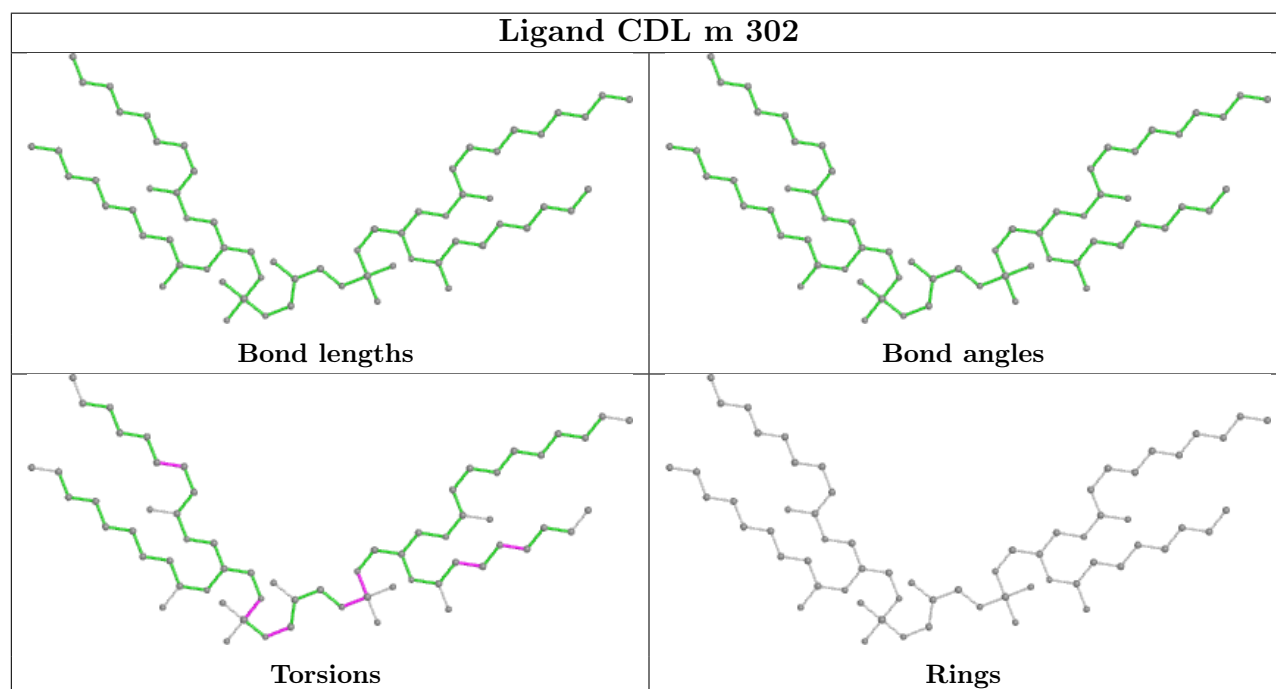
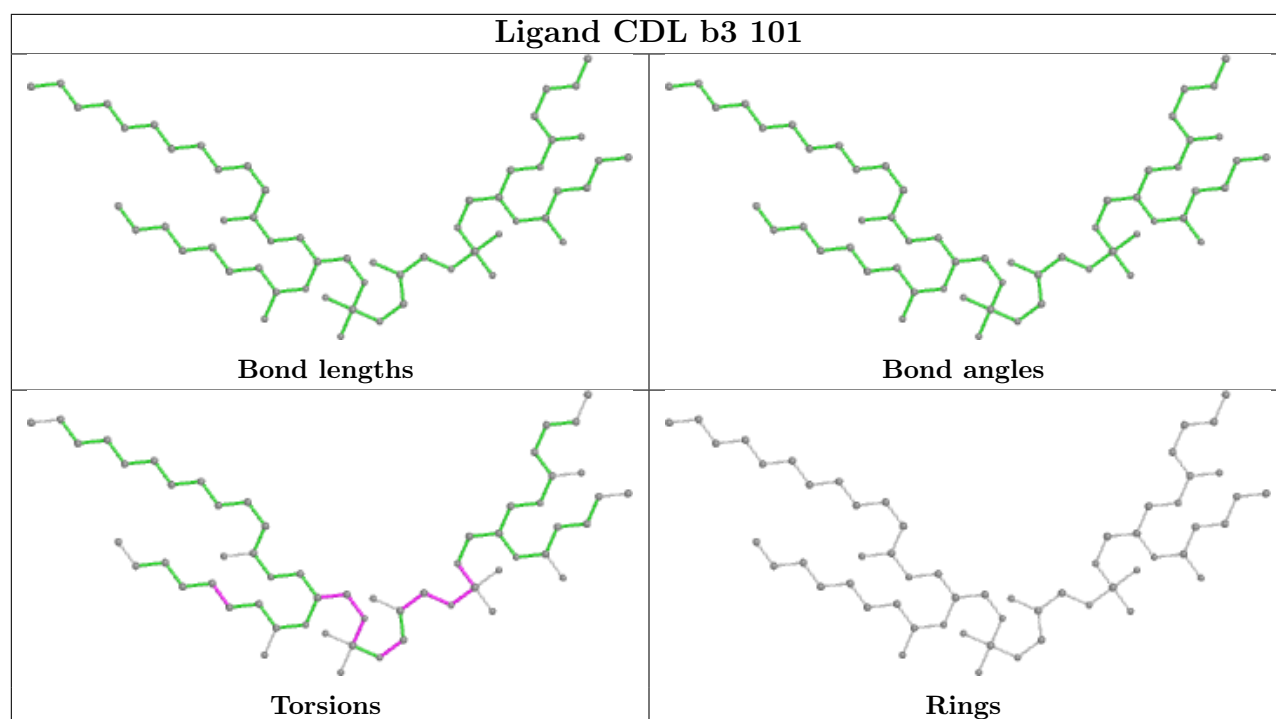


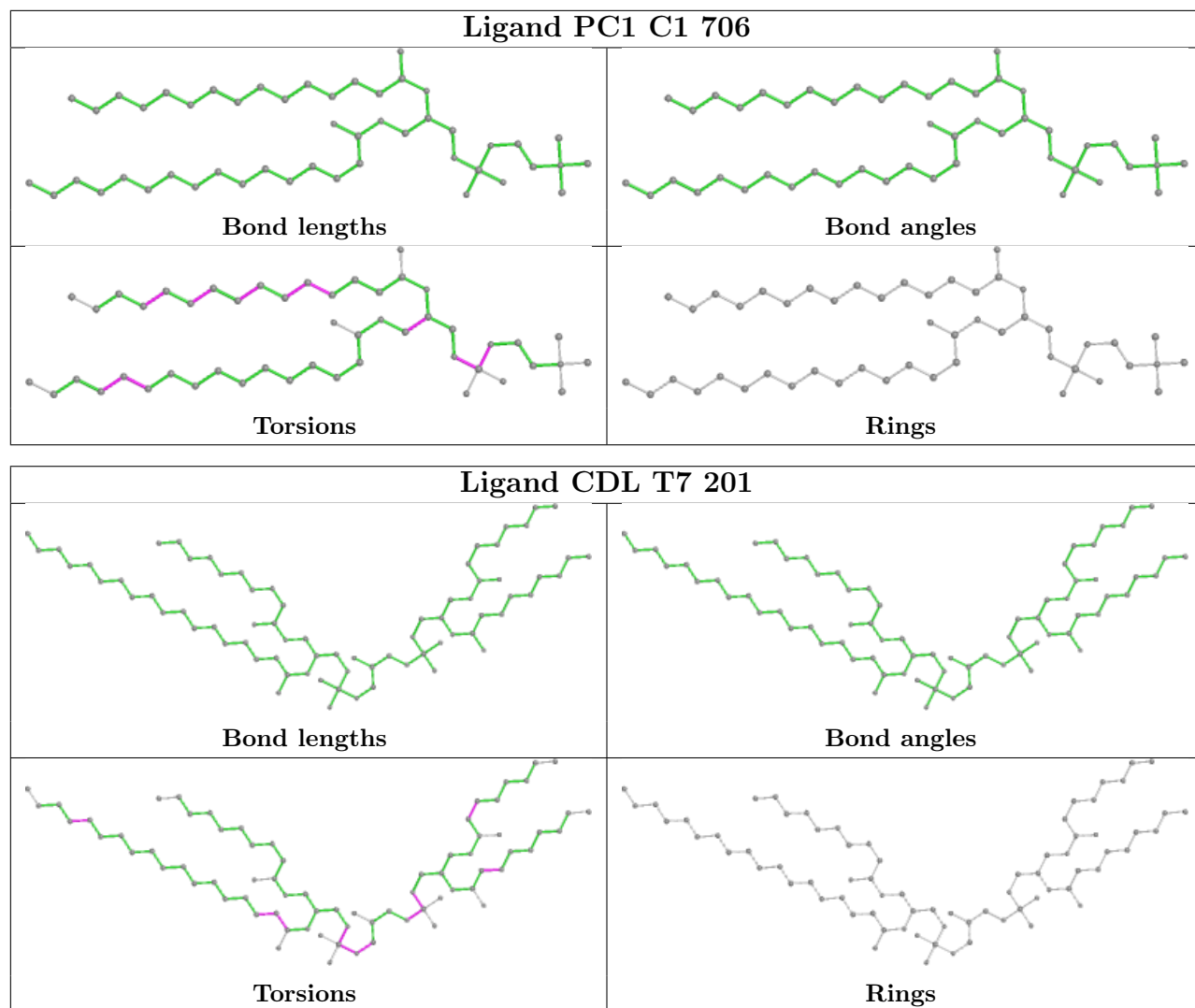




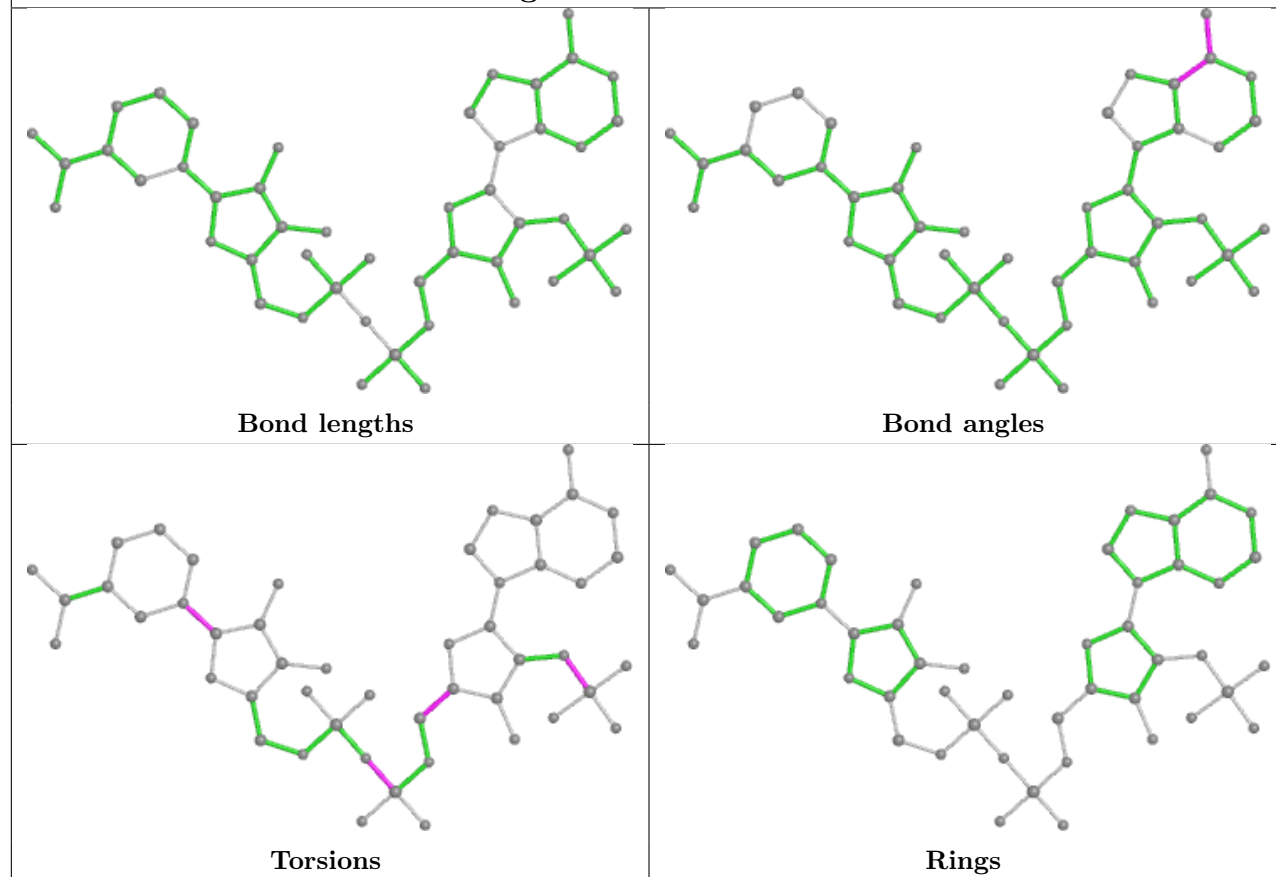




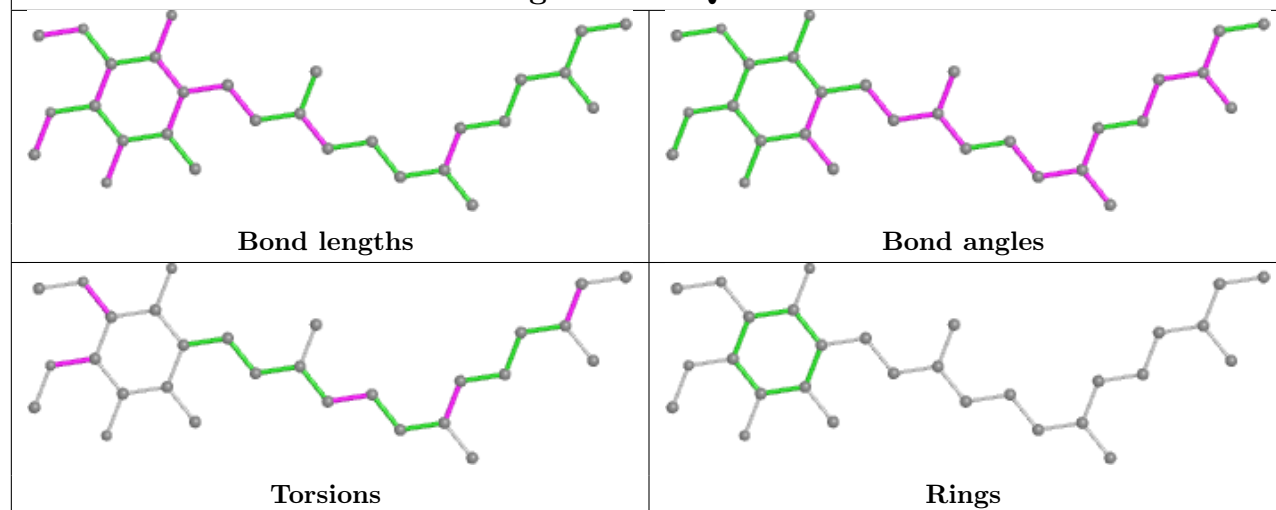


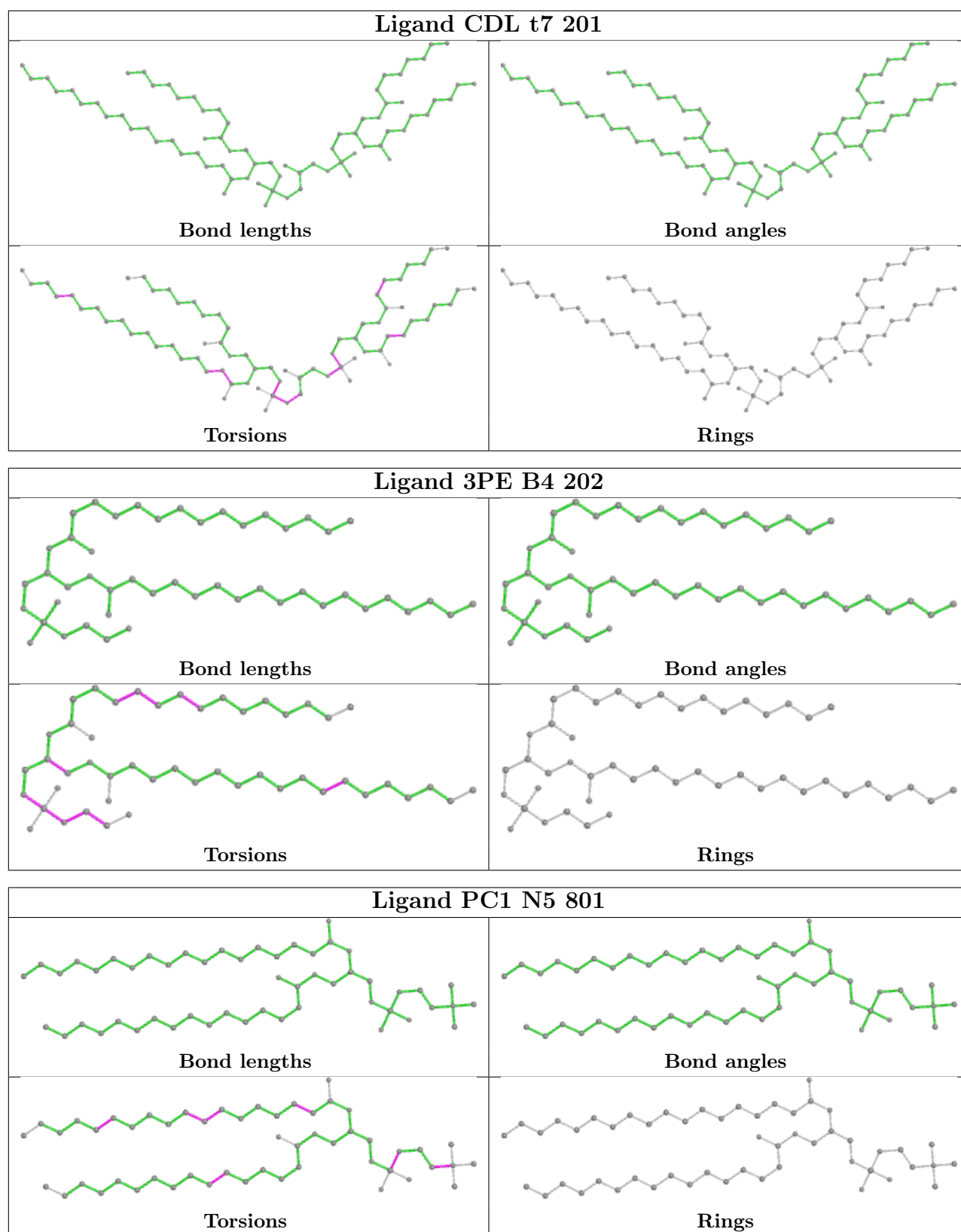


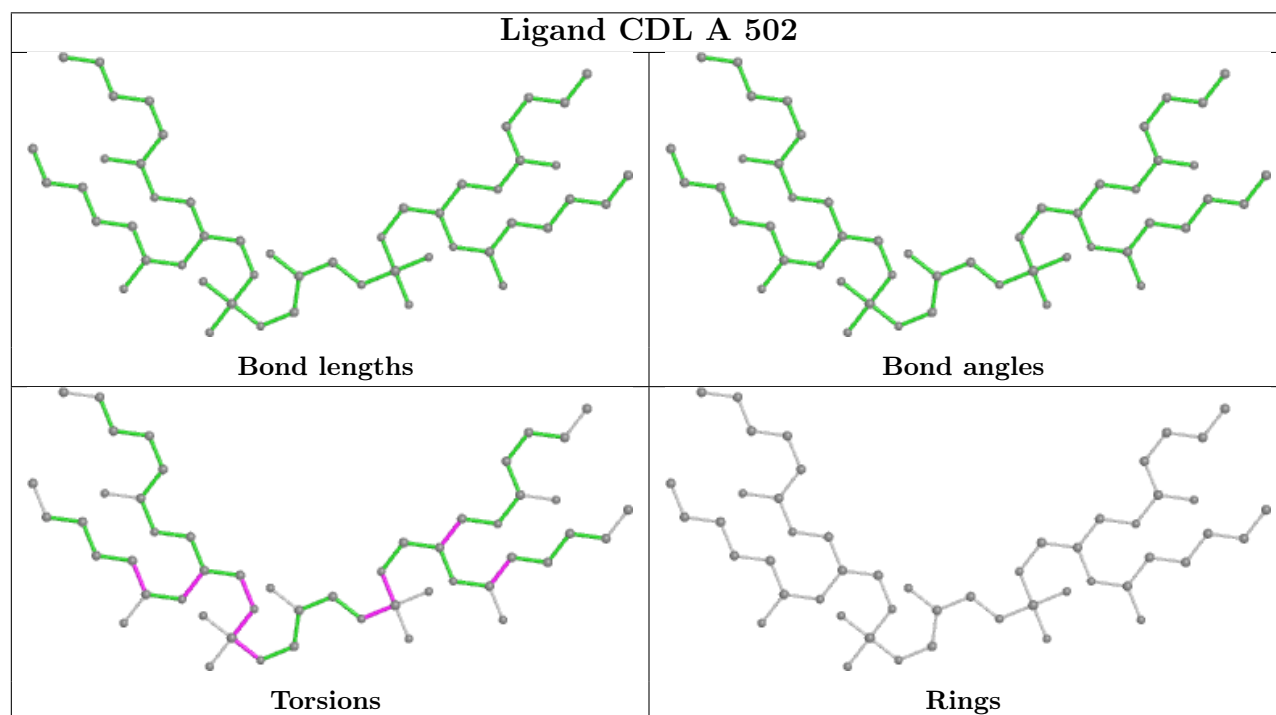
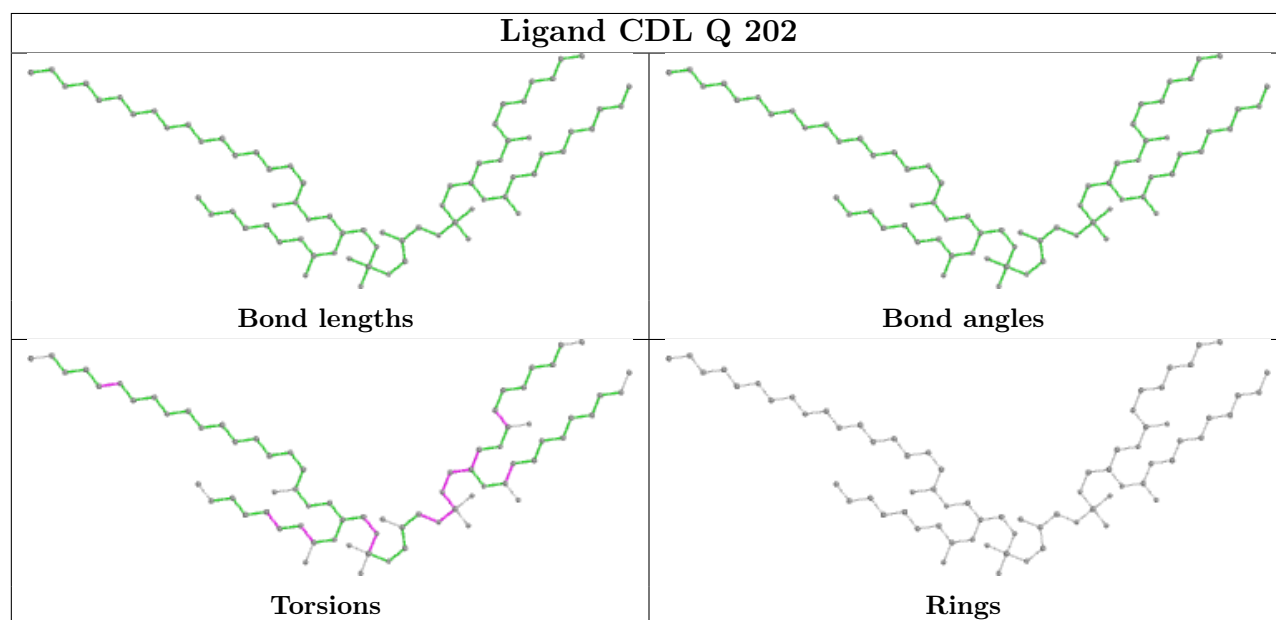
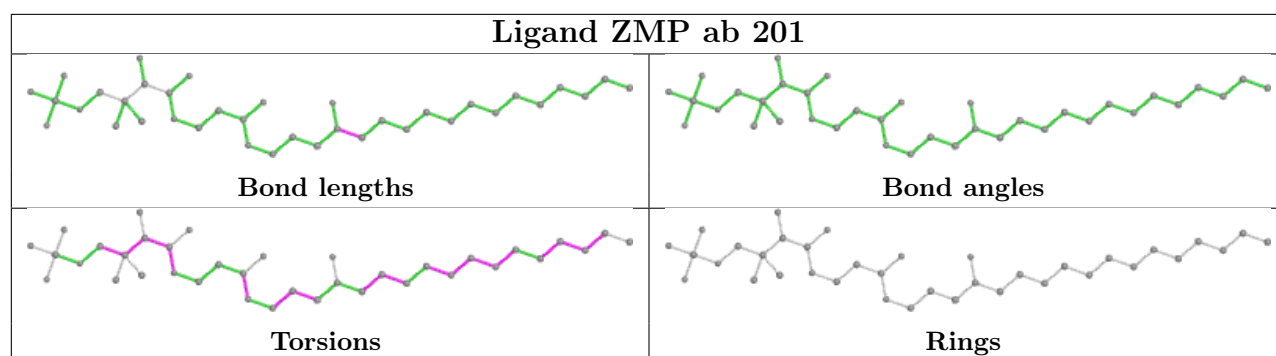
Ligand NDP A9 401

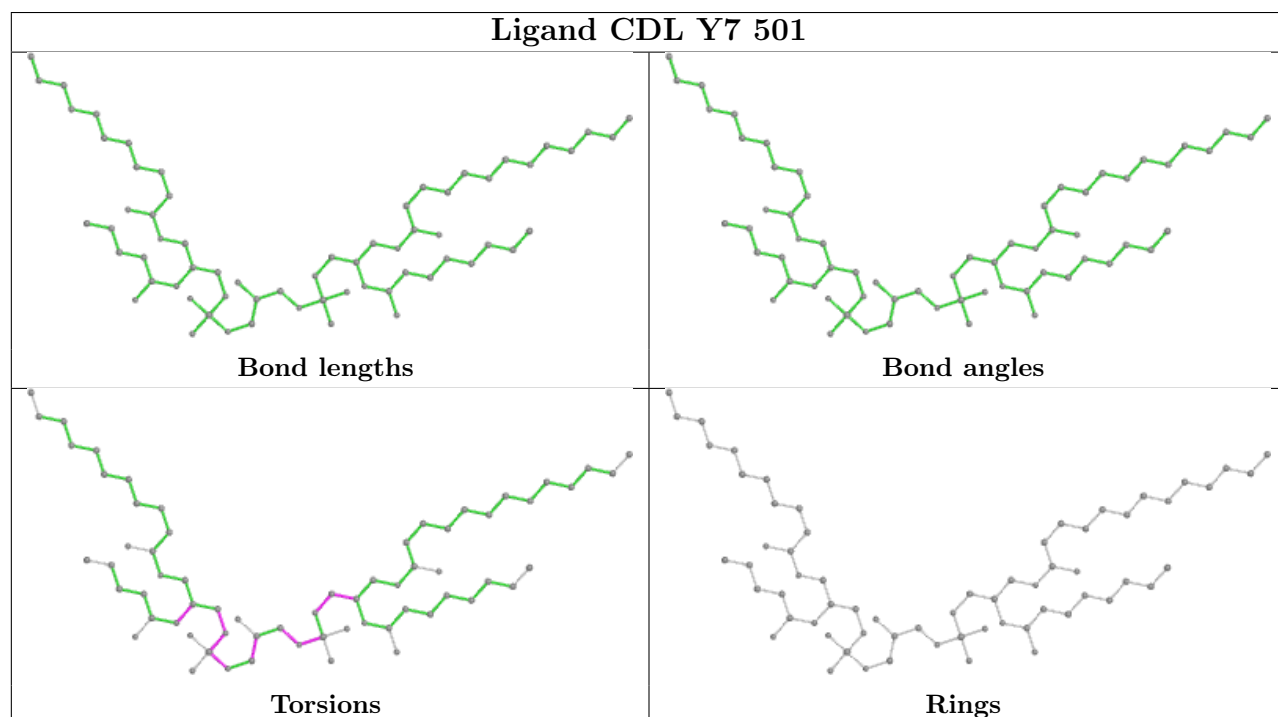
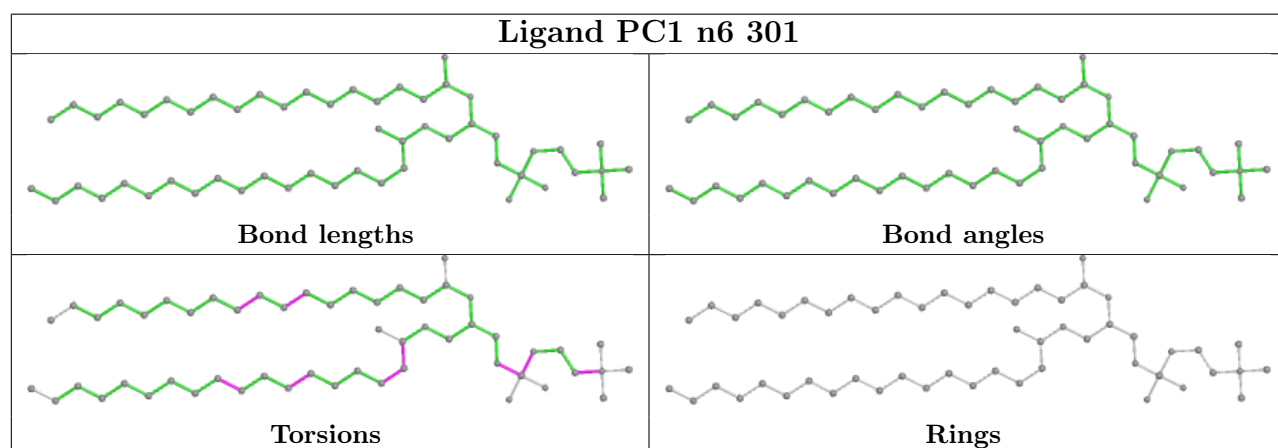
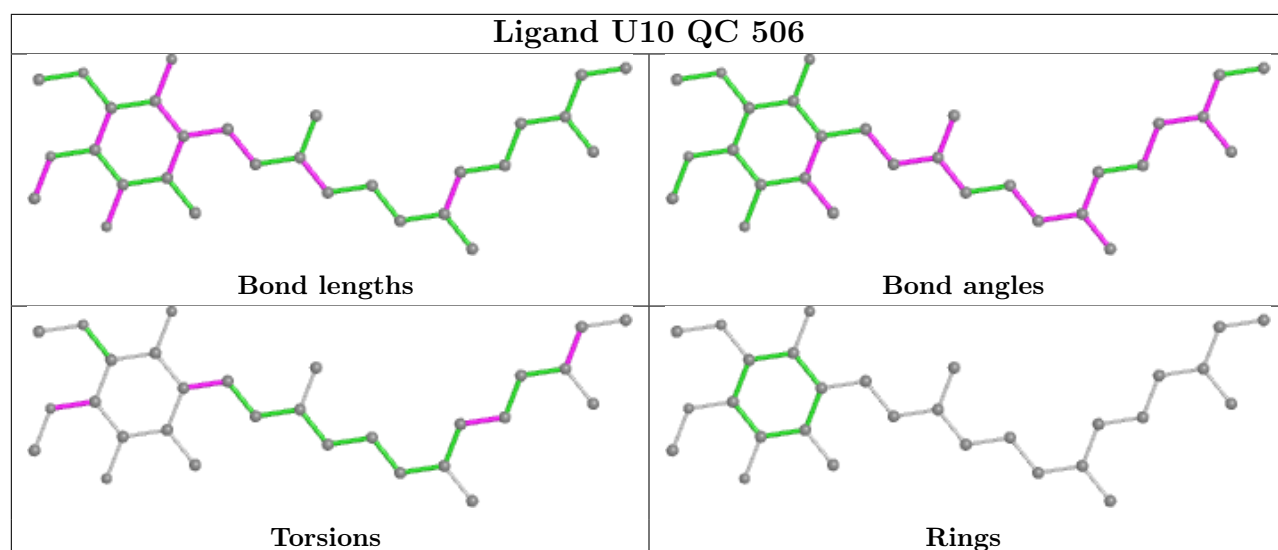


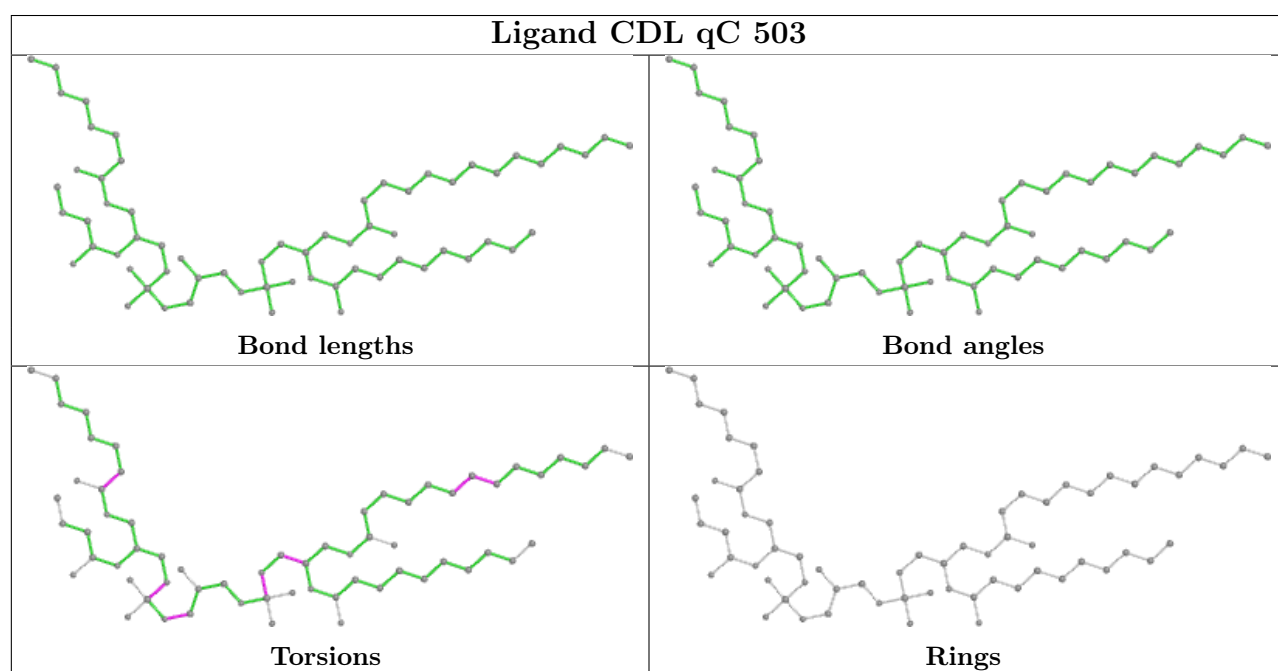
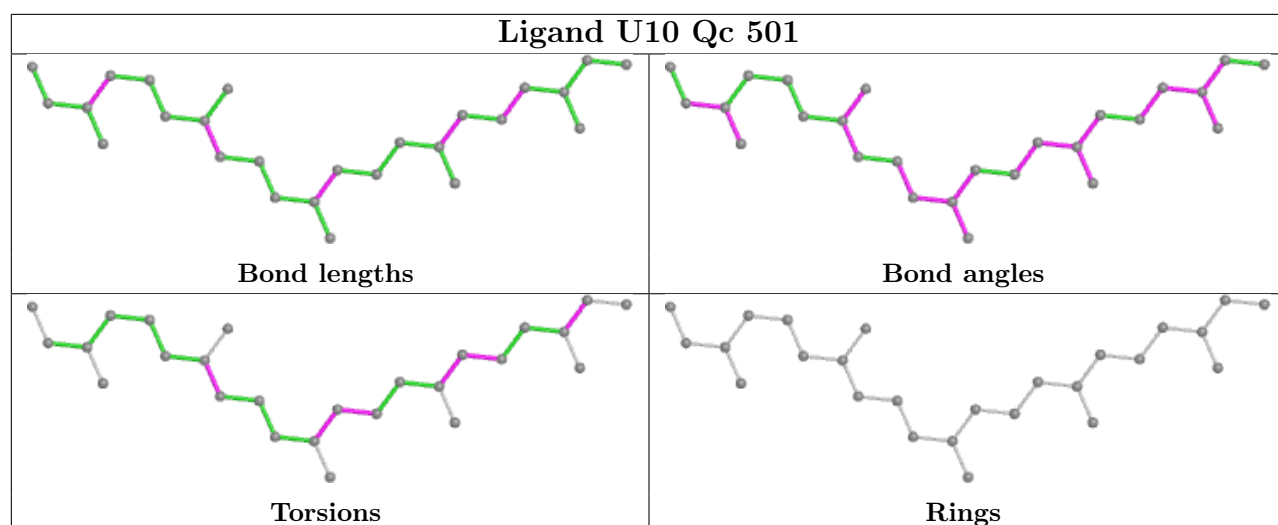
Ligand U10 Qc 507



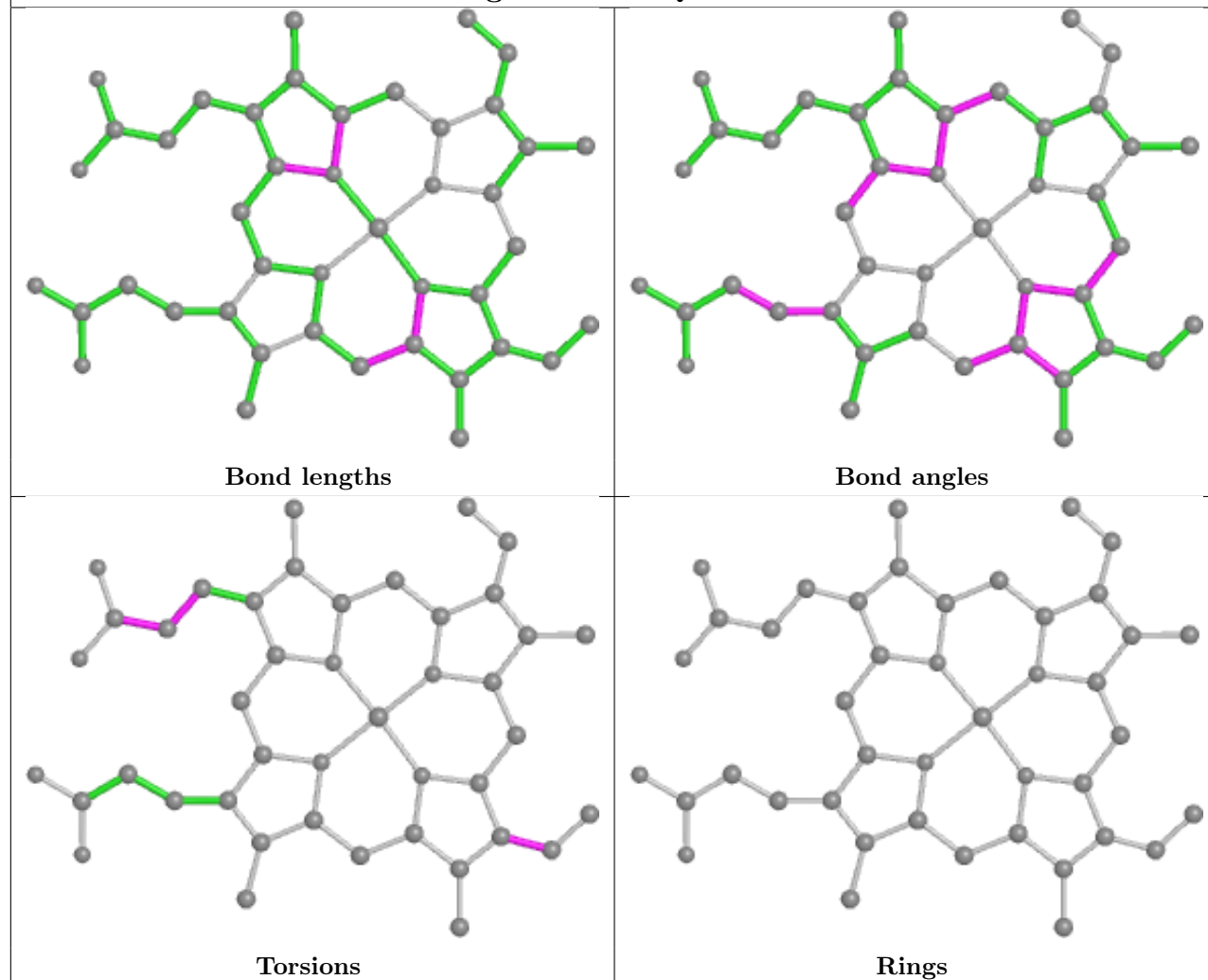




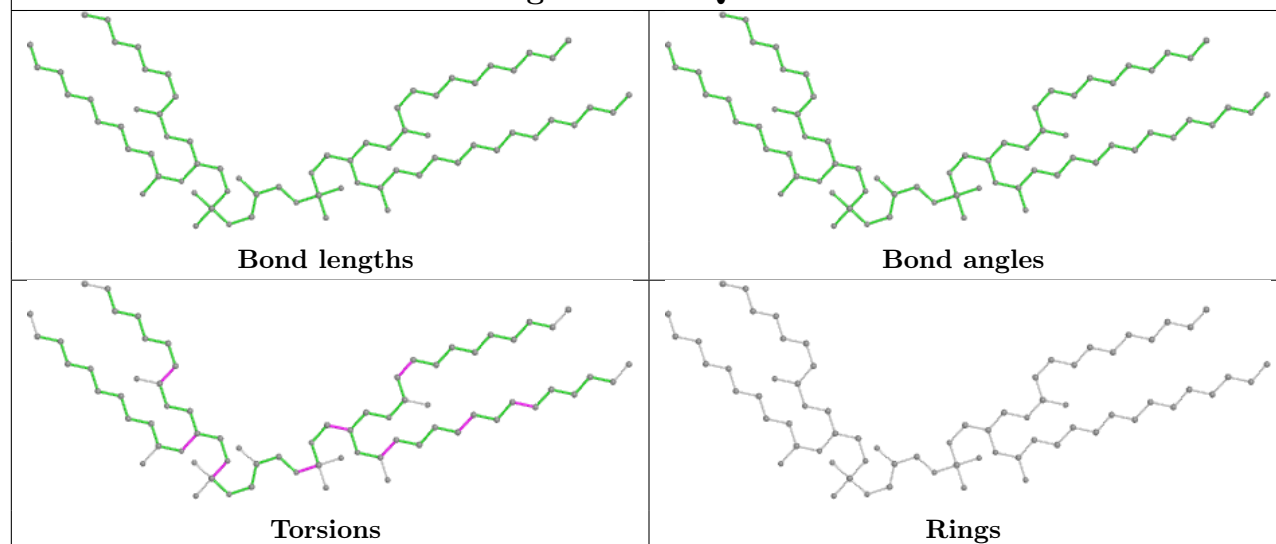


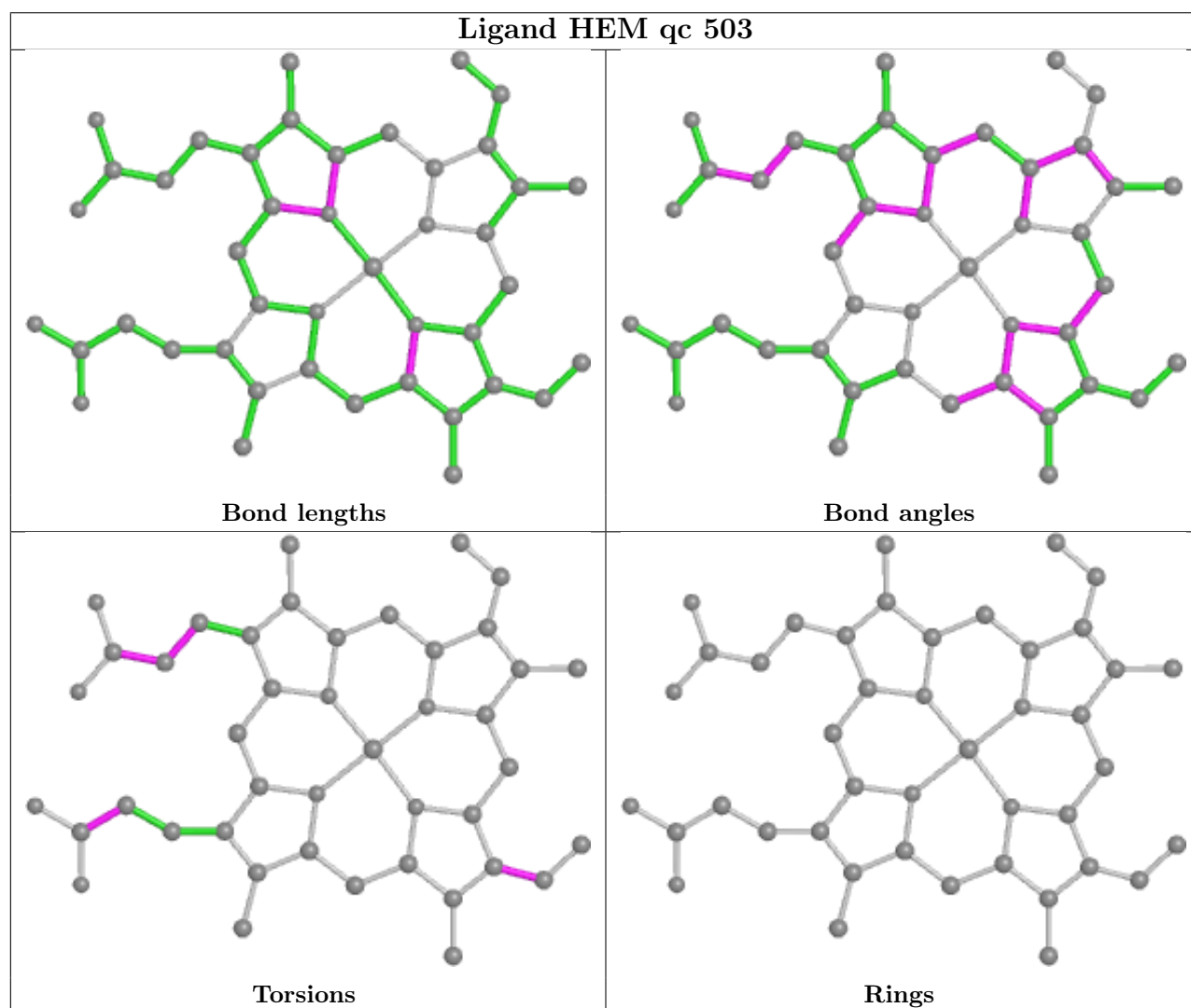
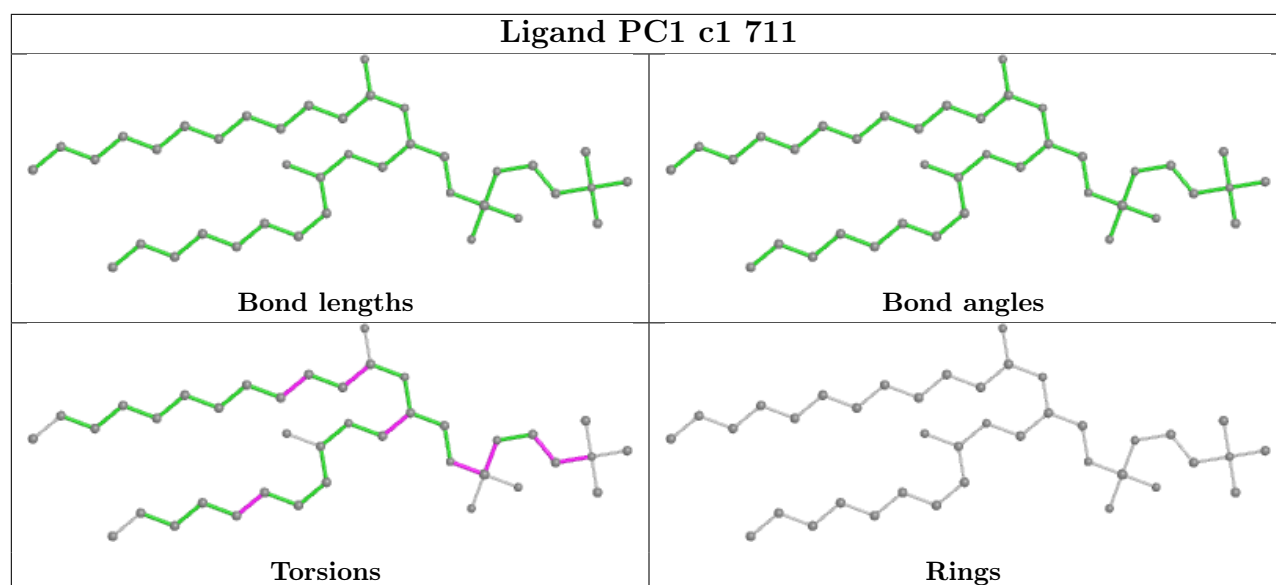


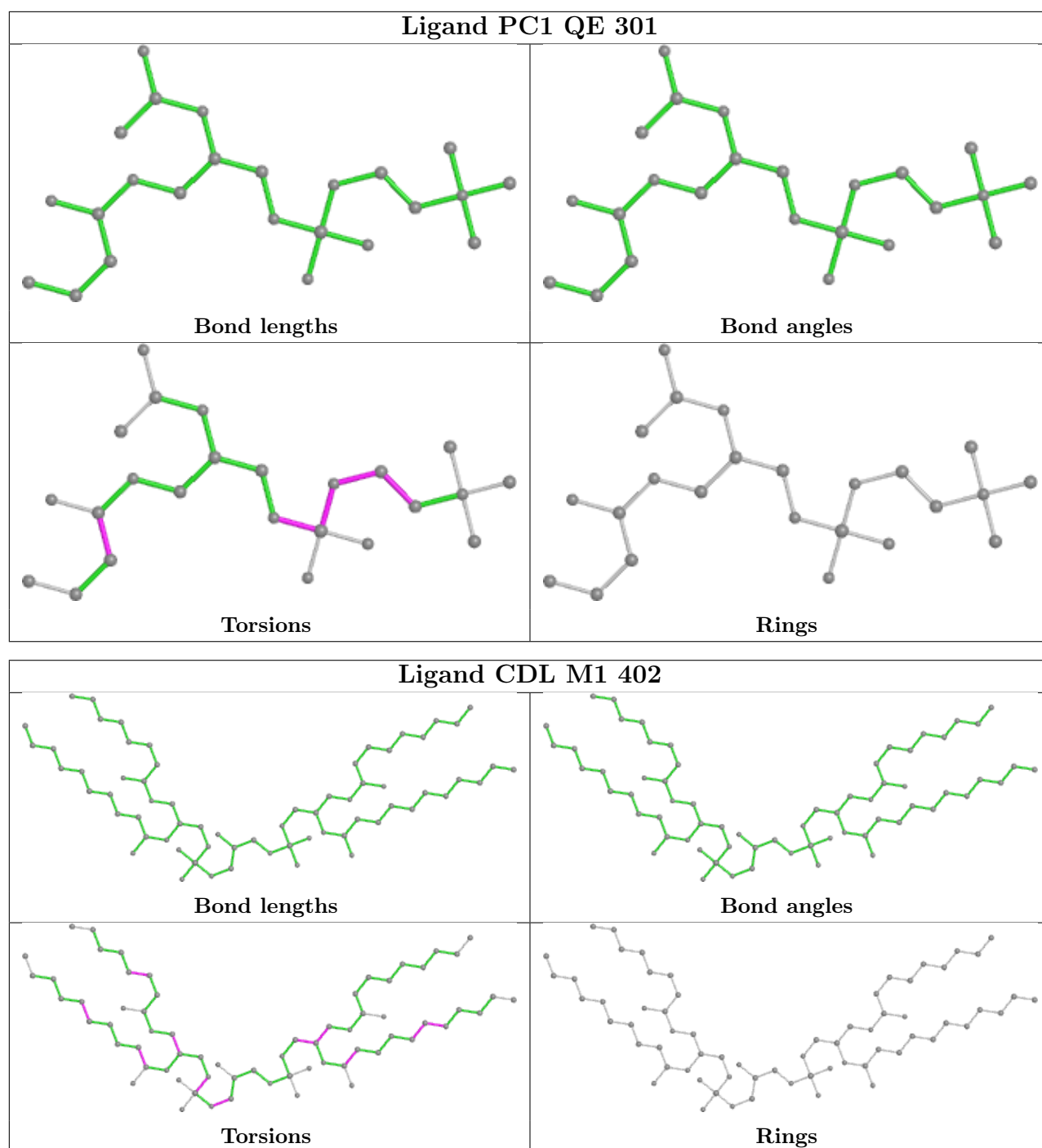
Ligand HEM QC 501

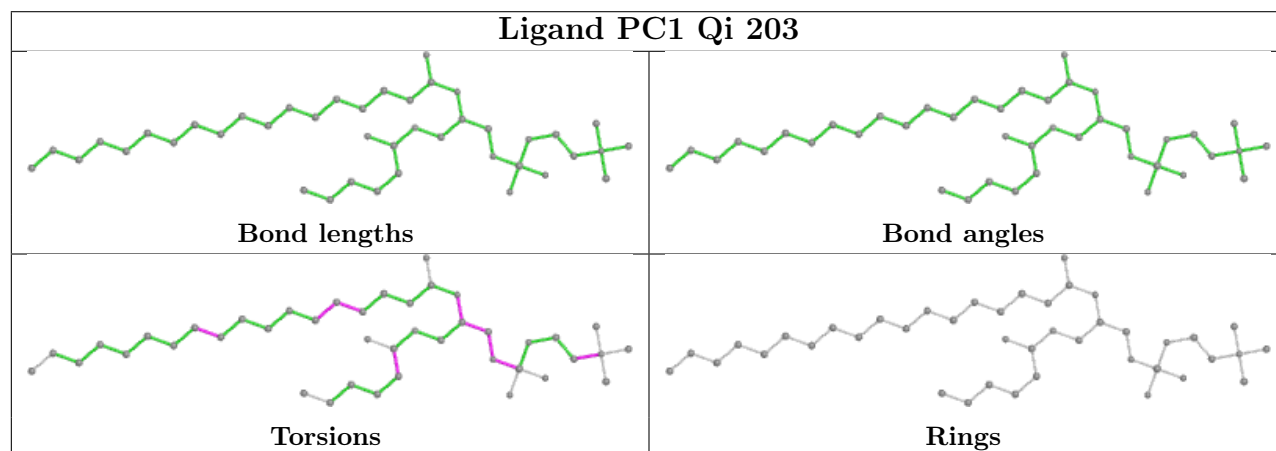
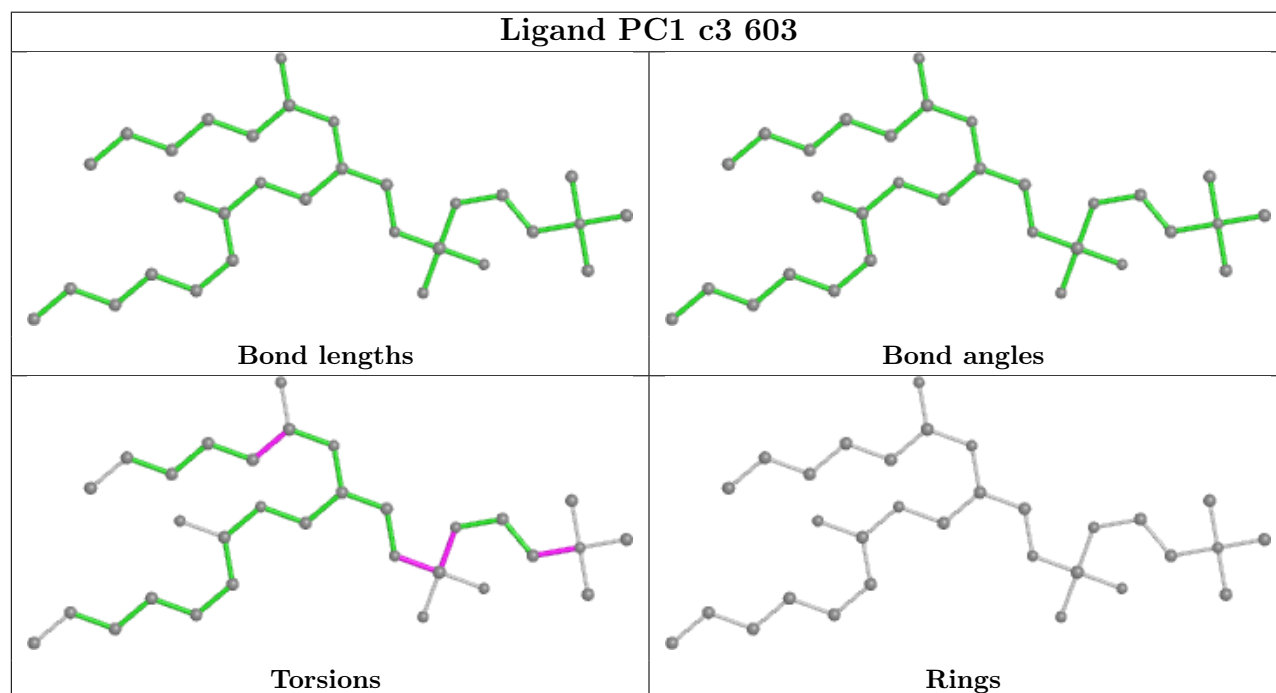
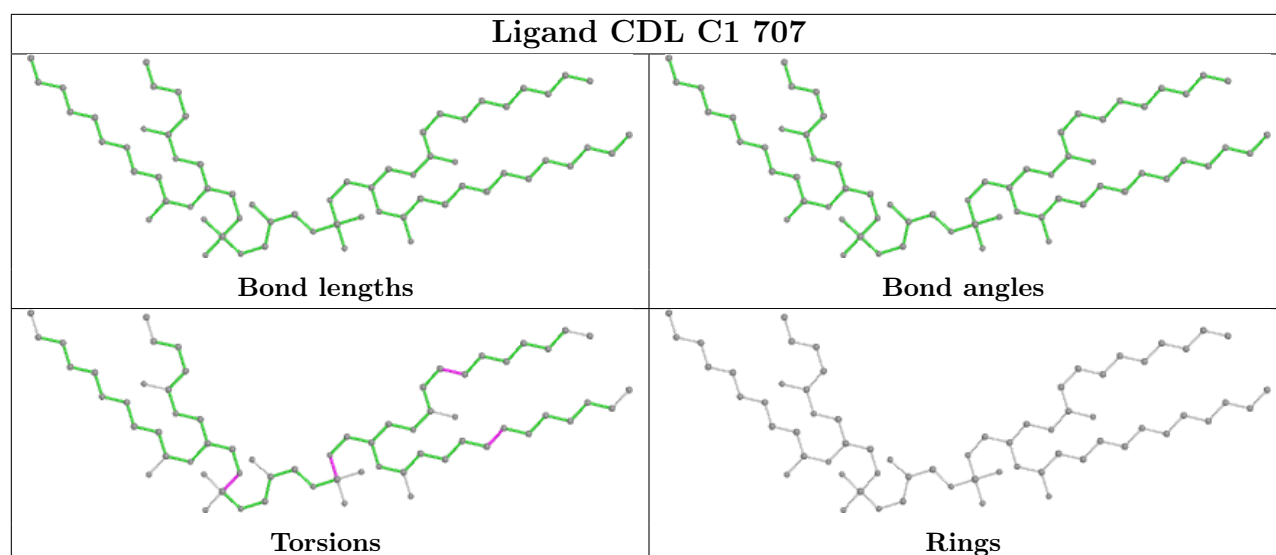


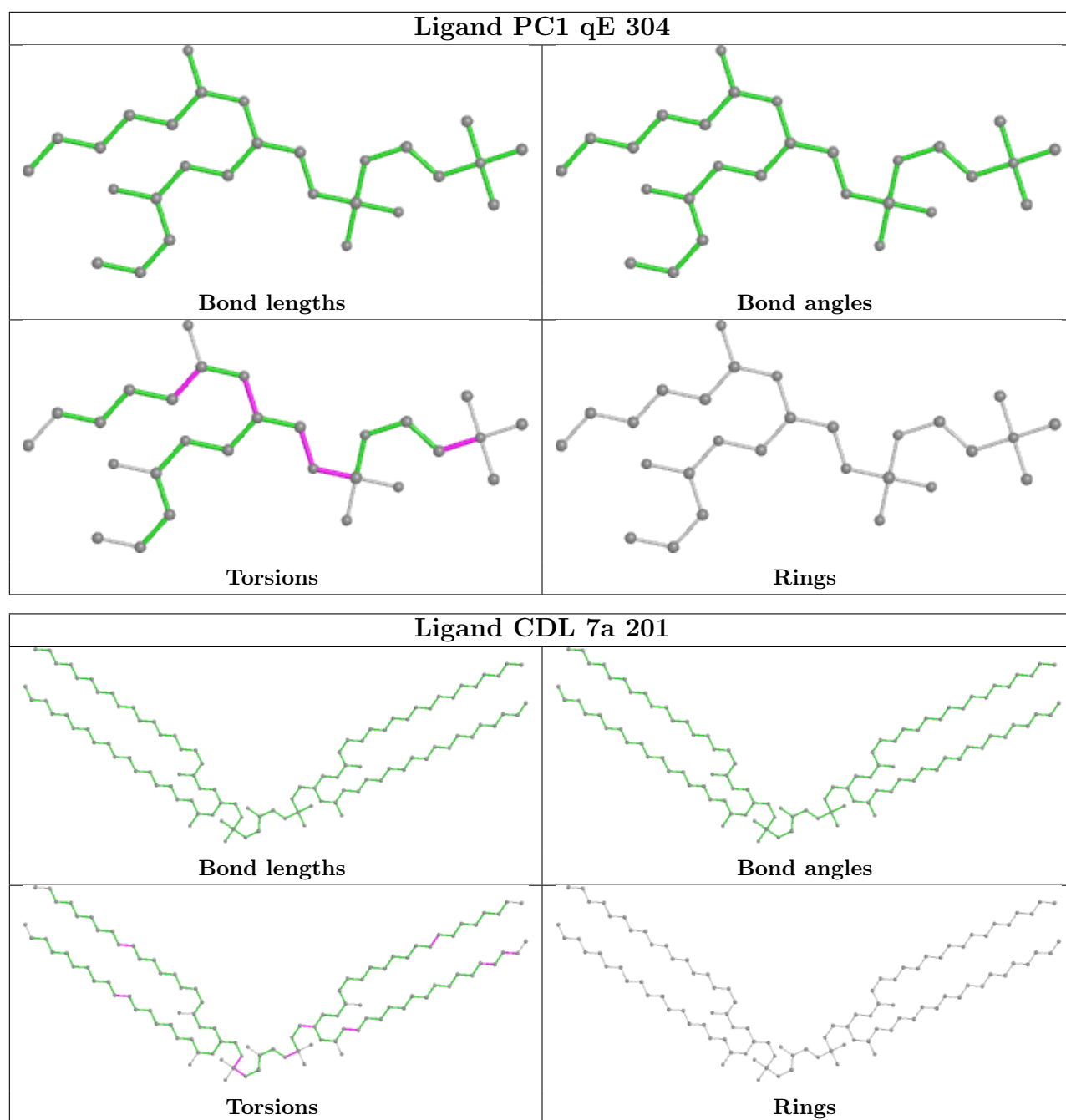
Ligand CDL Qi 202

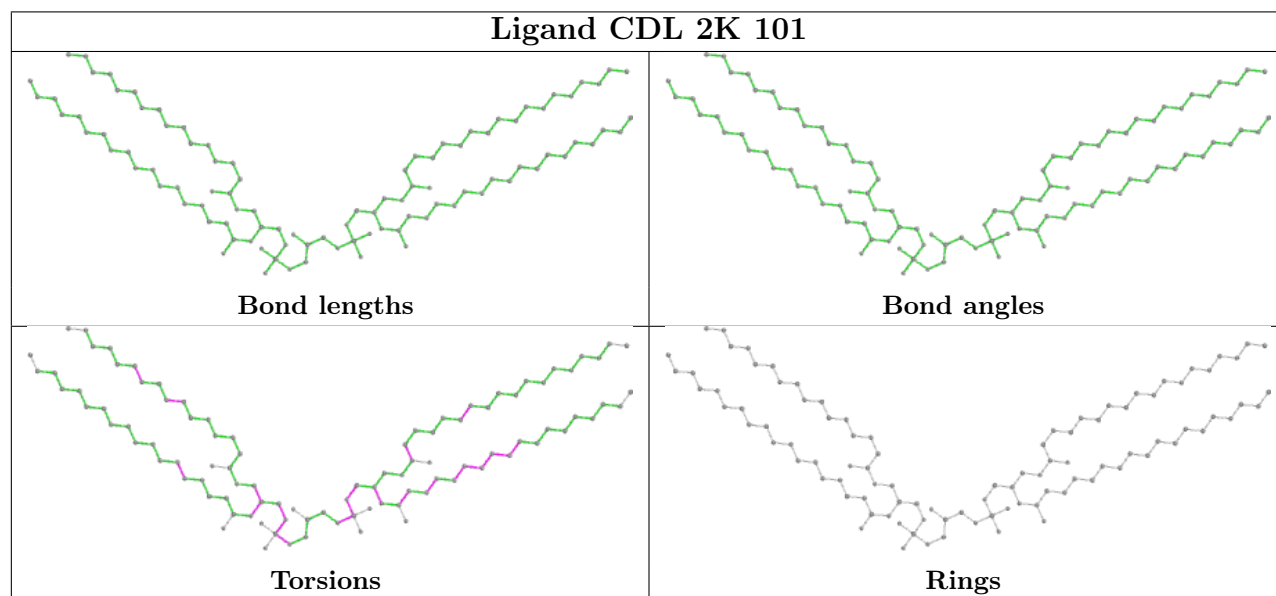
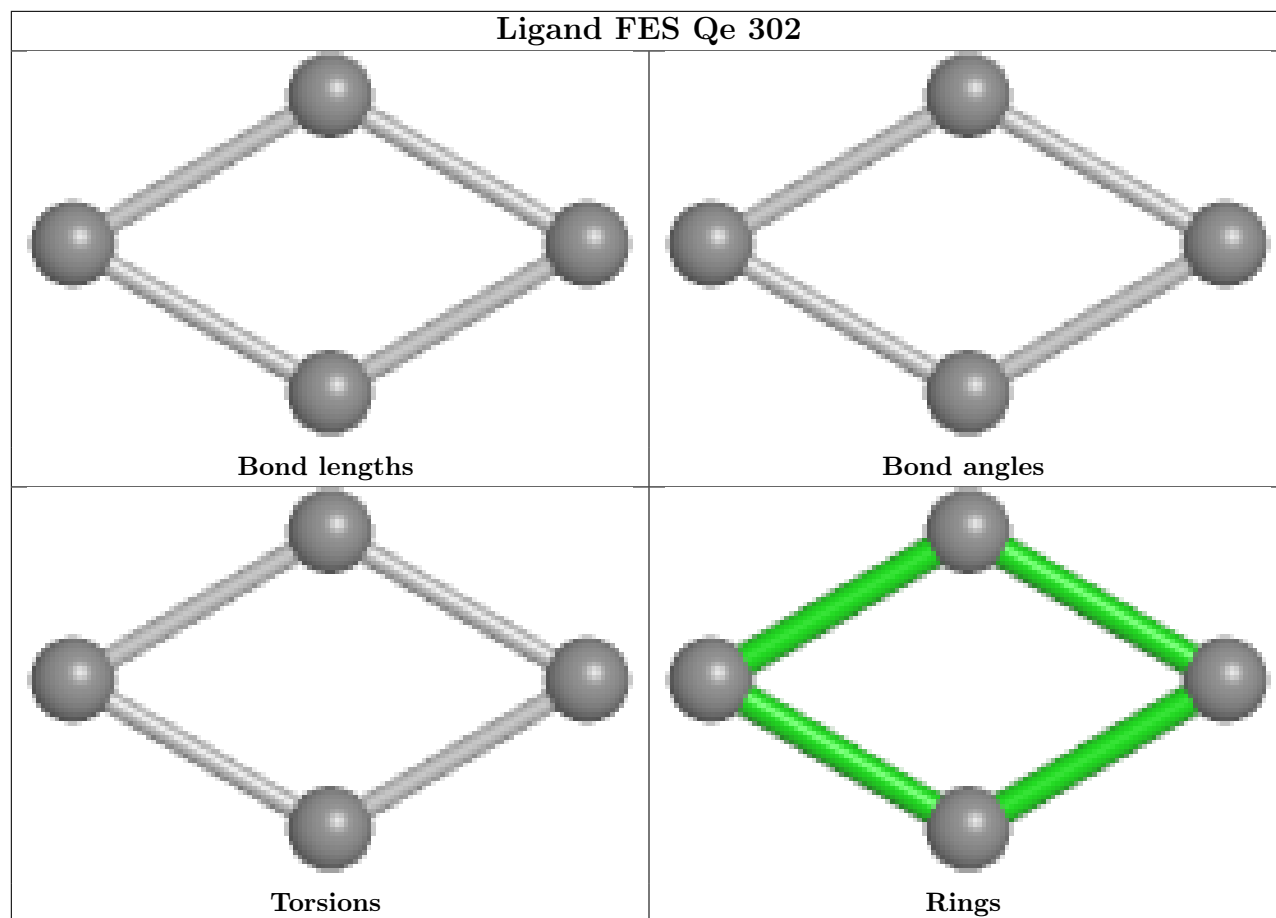


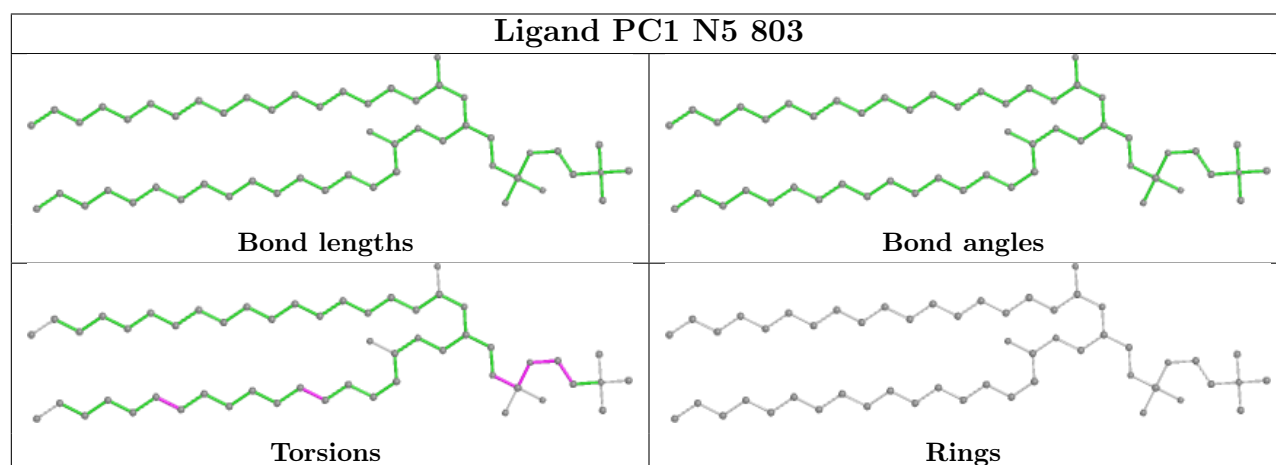
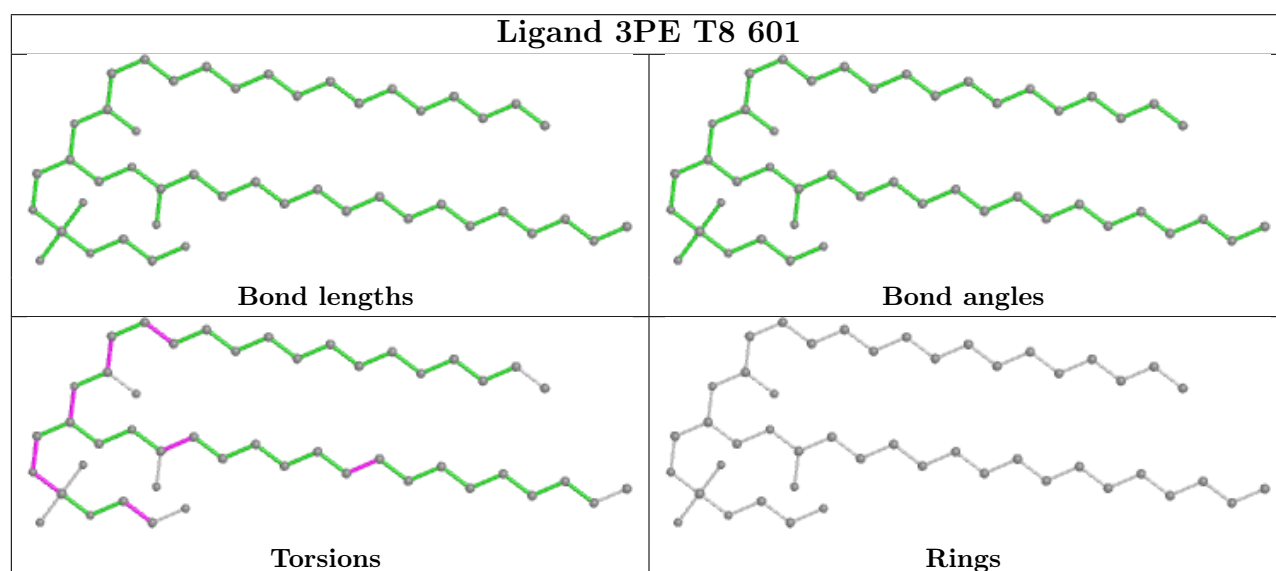
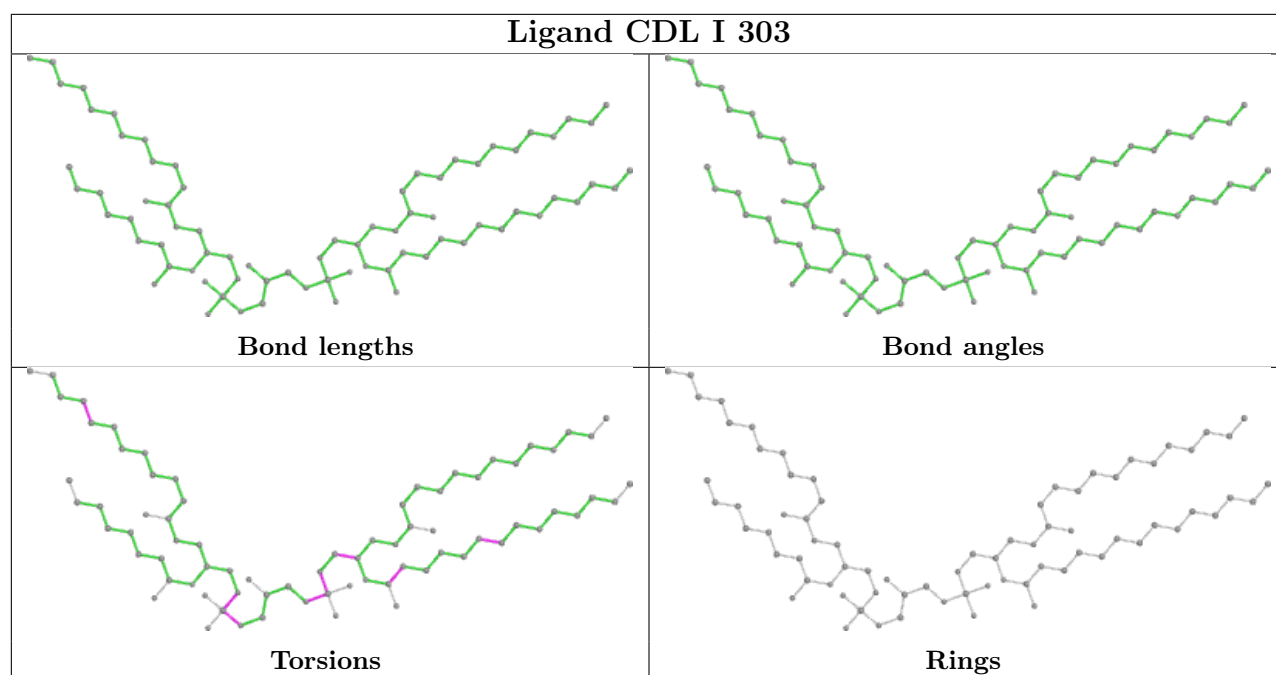


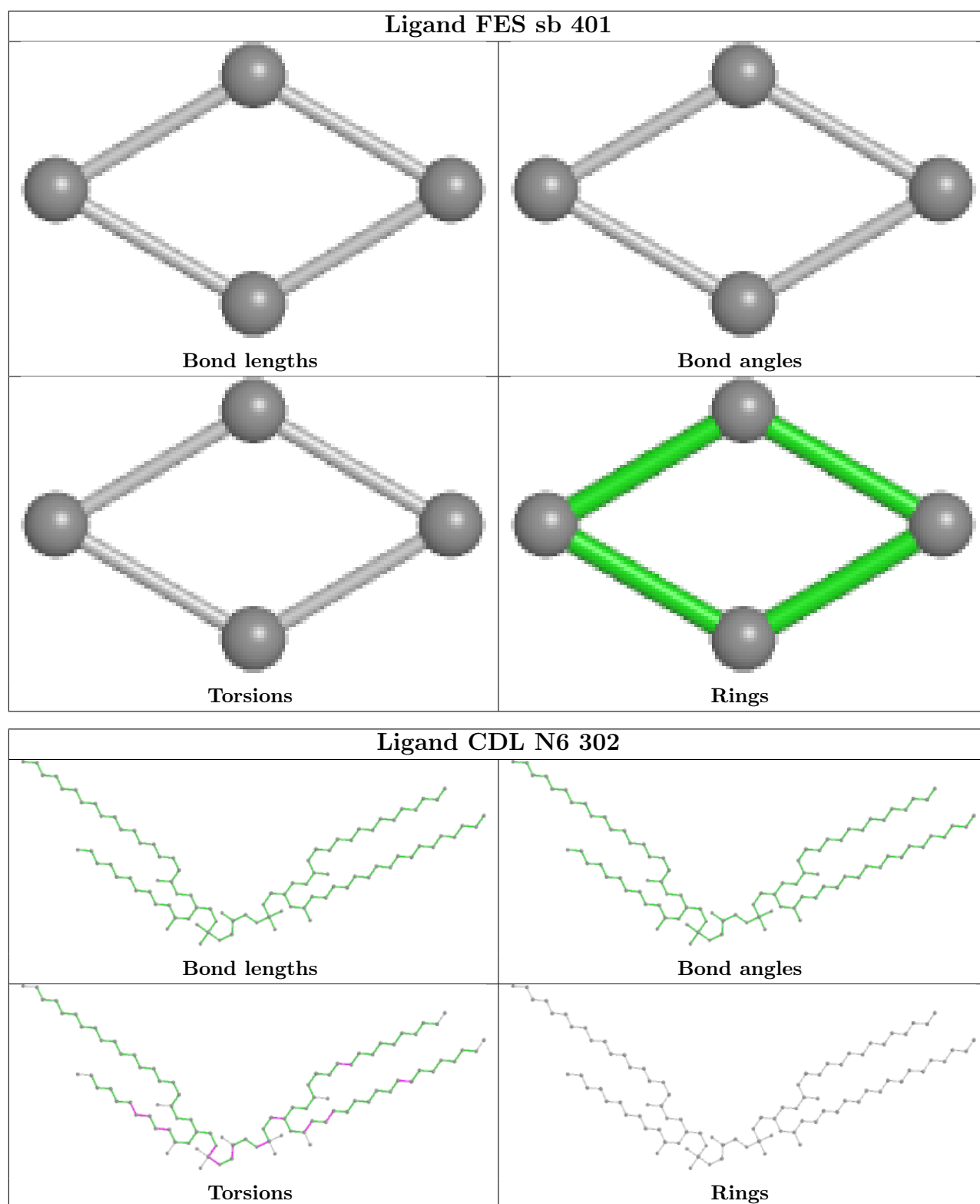


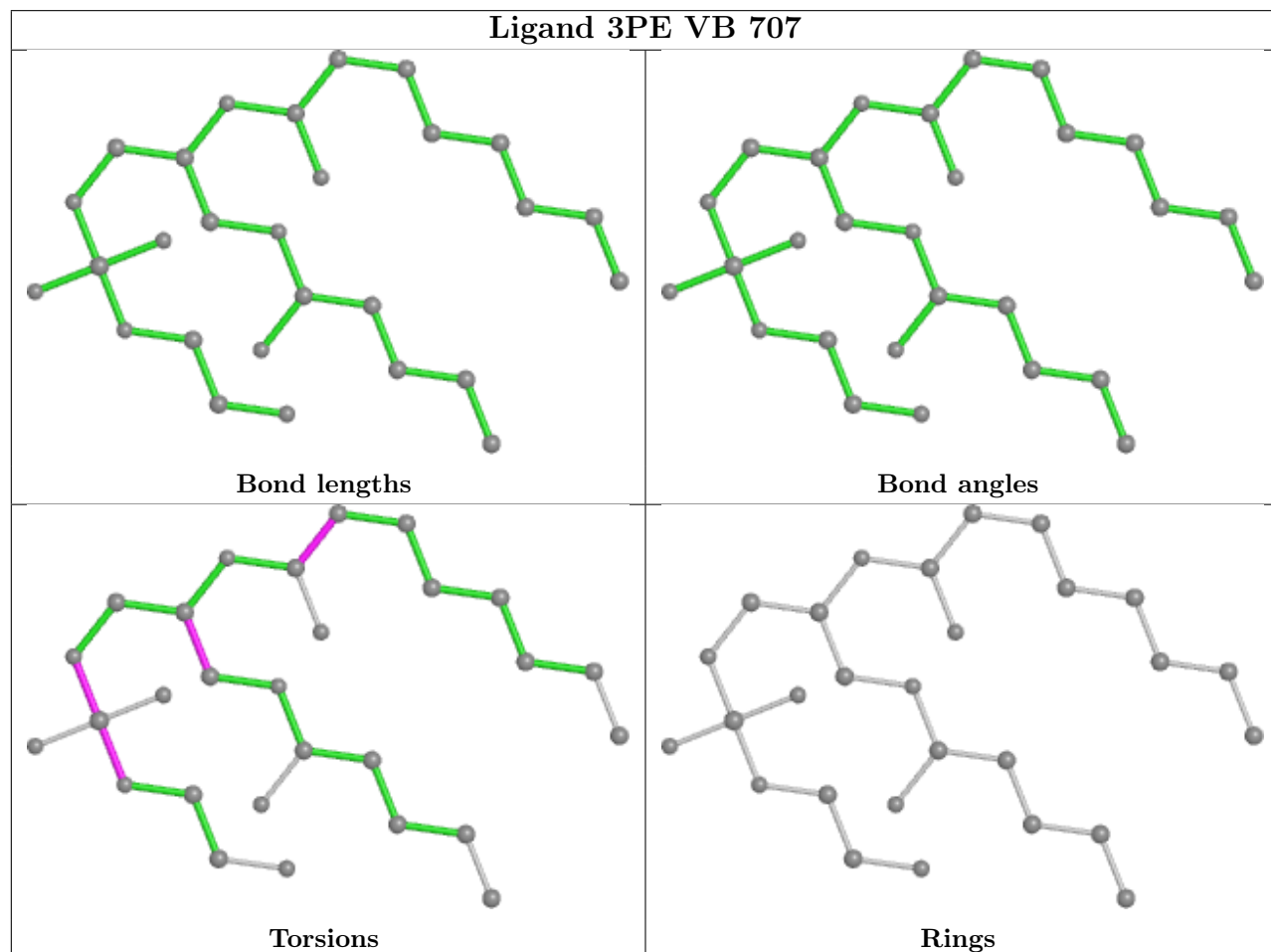
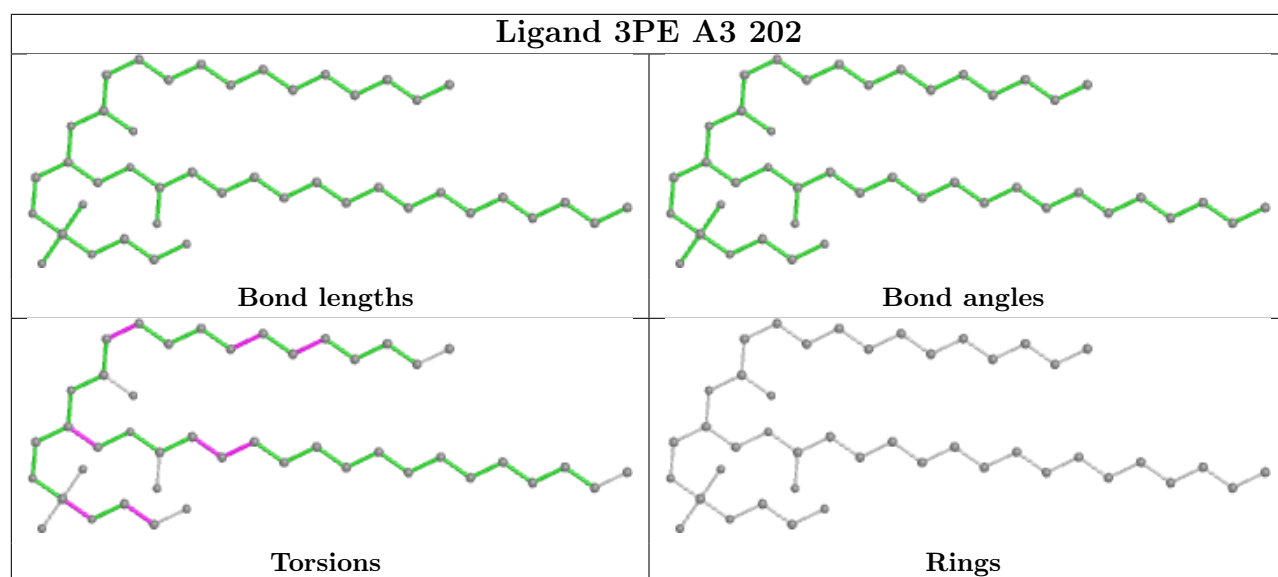


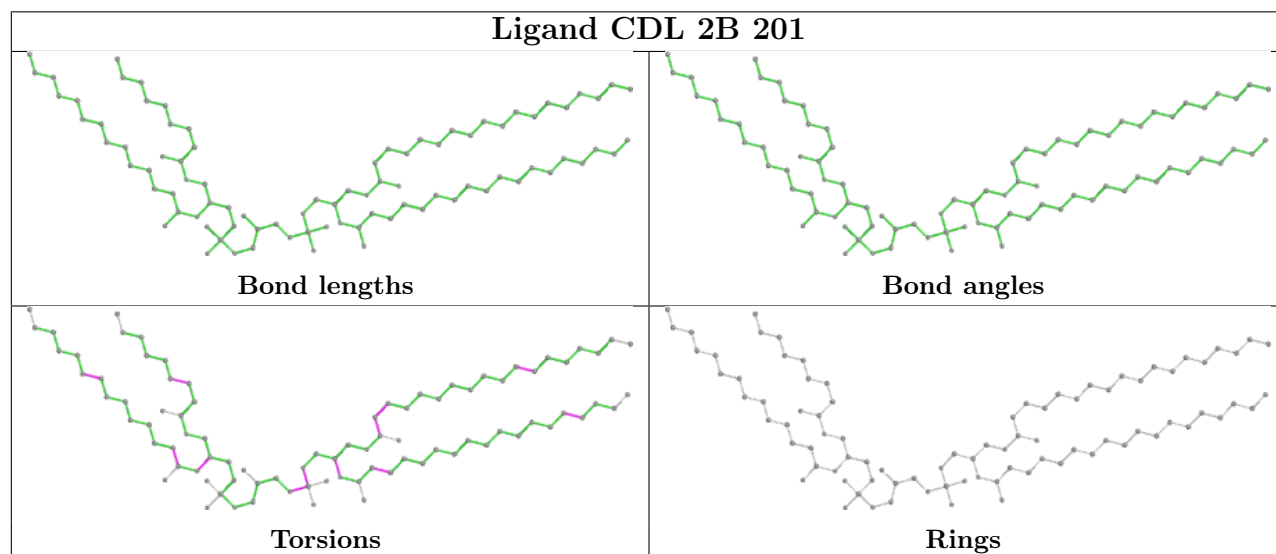
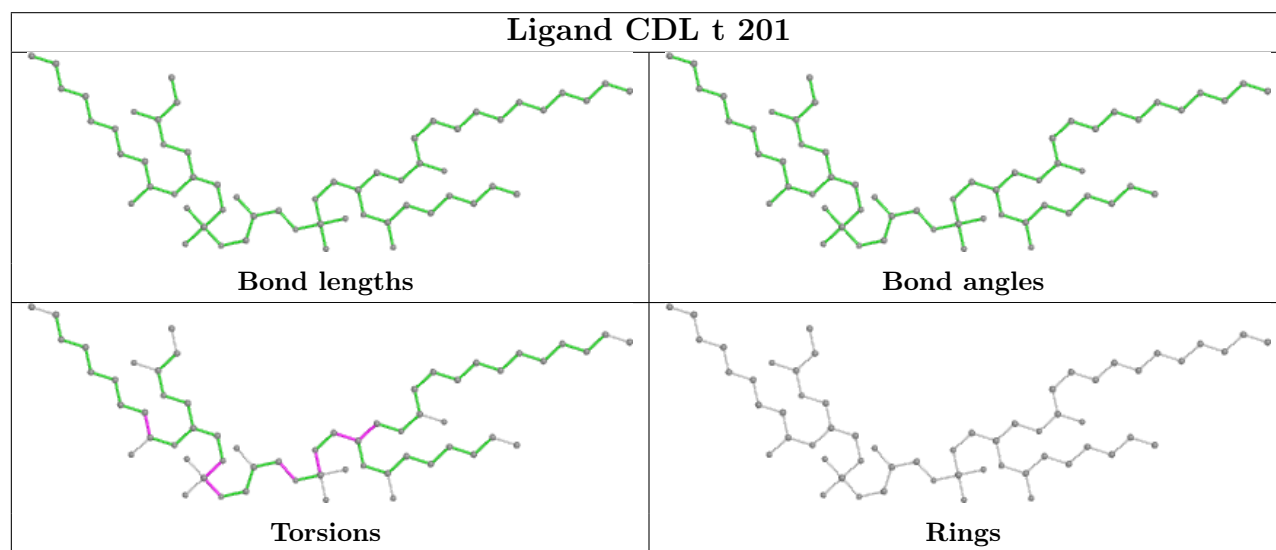
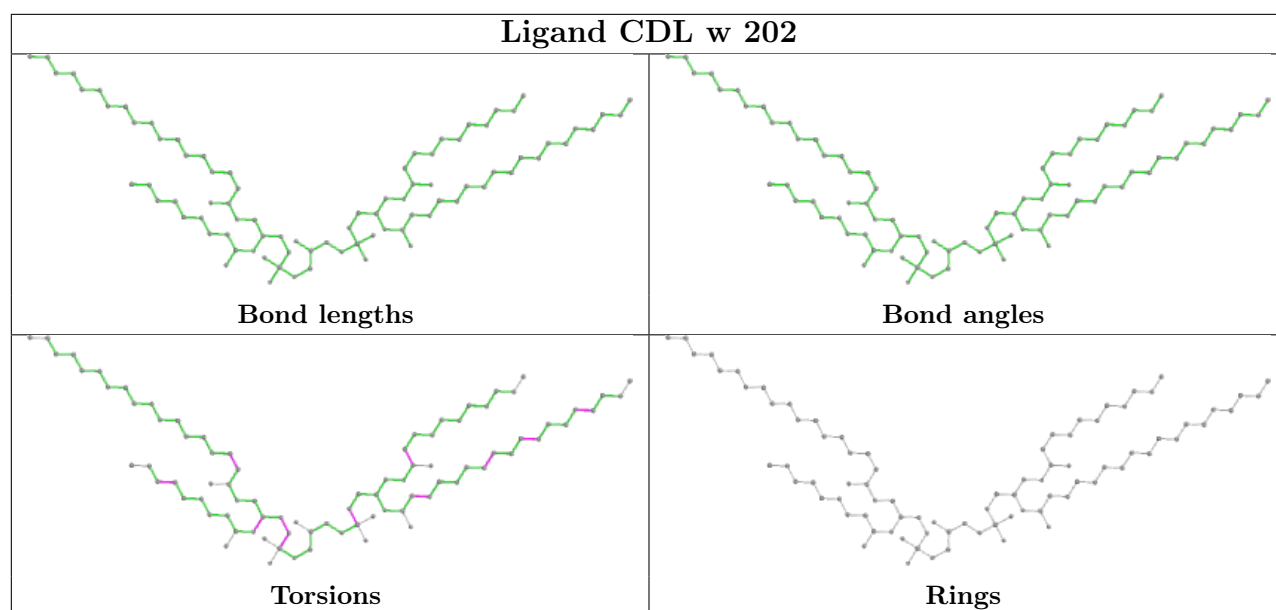


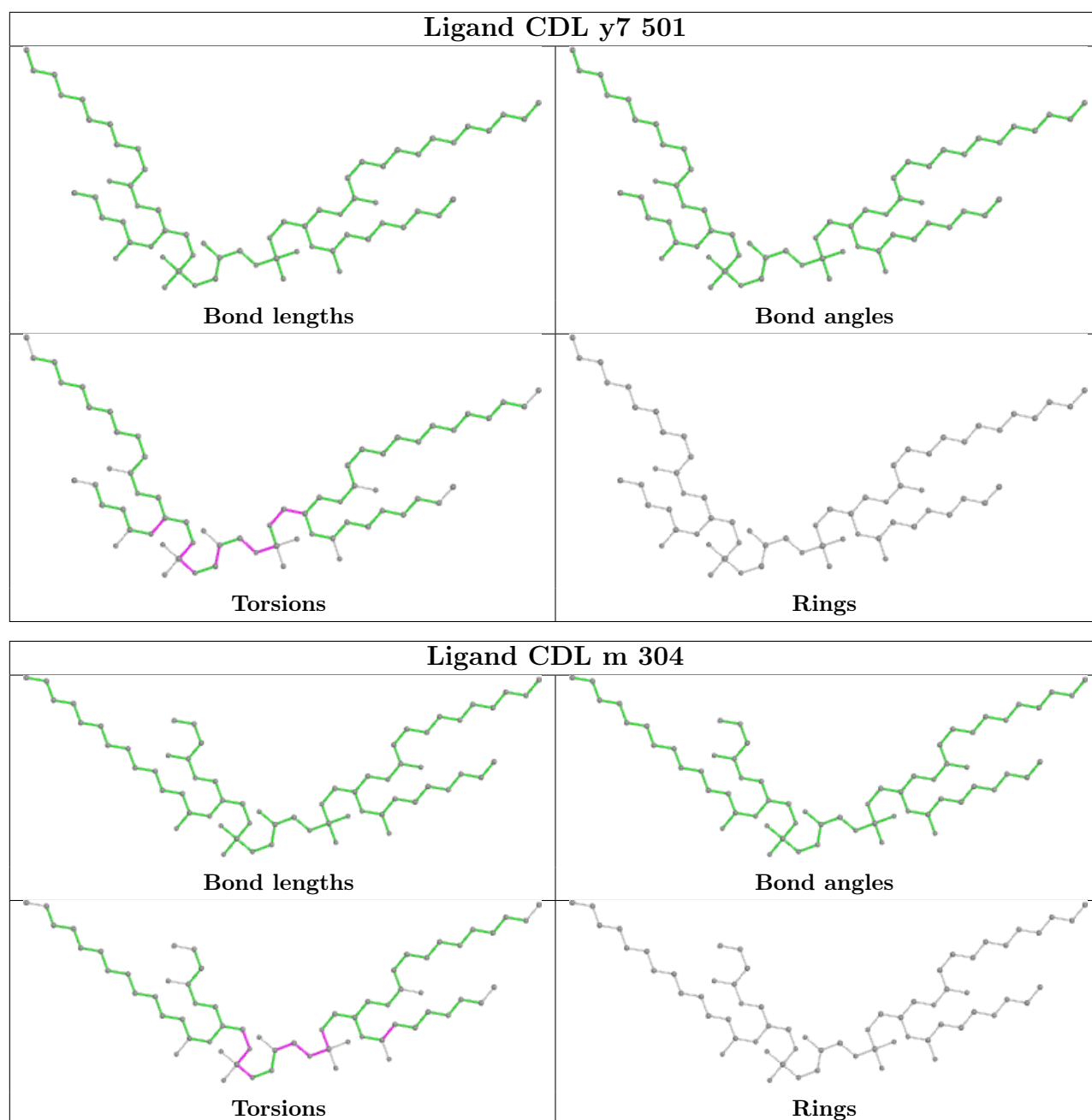


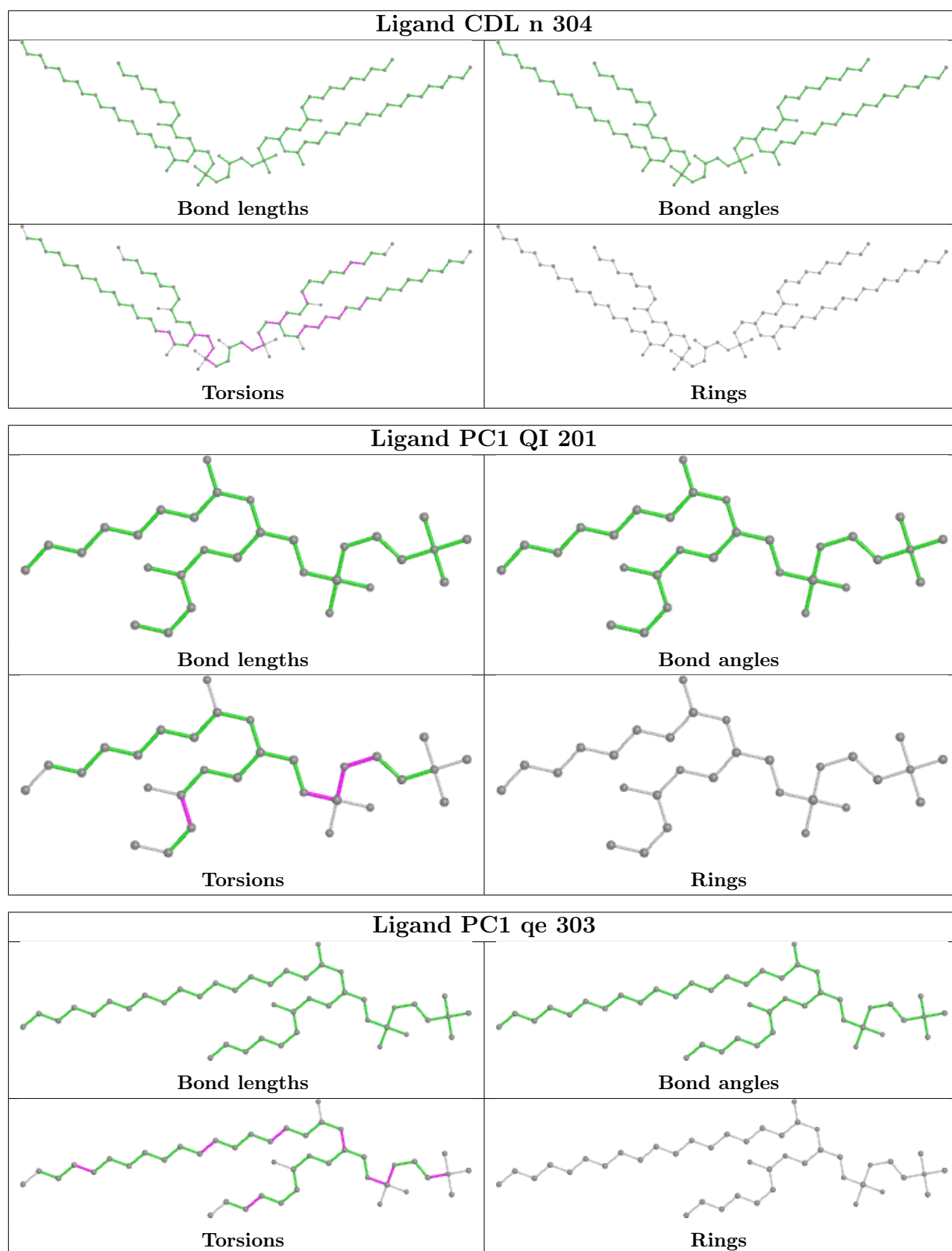


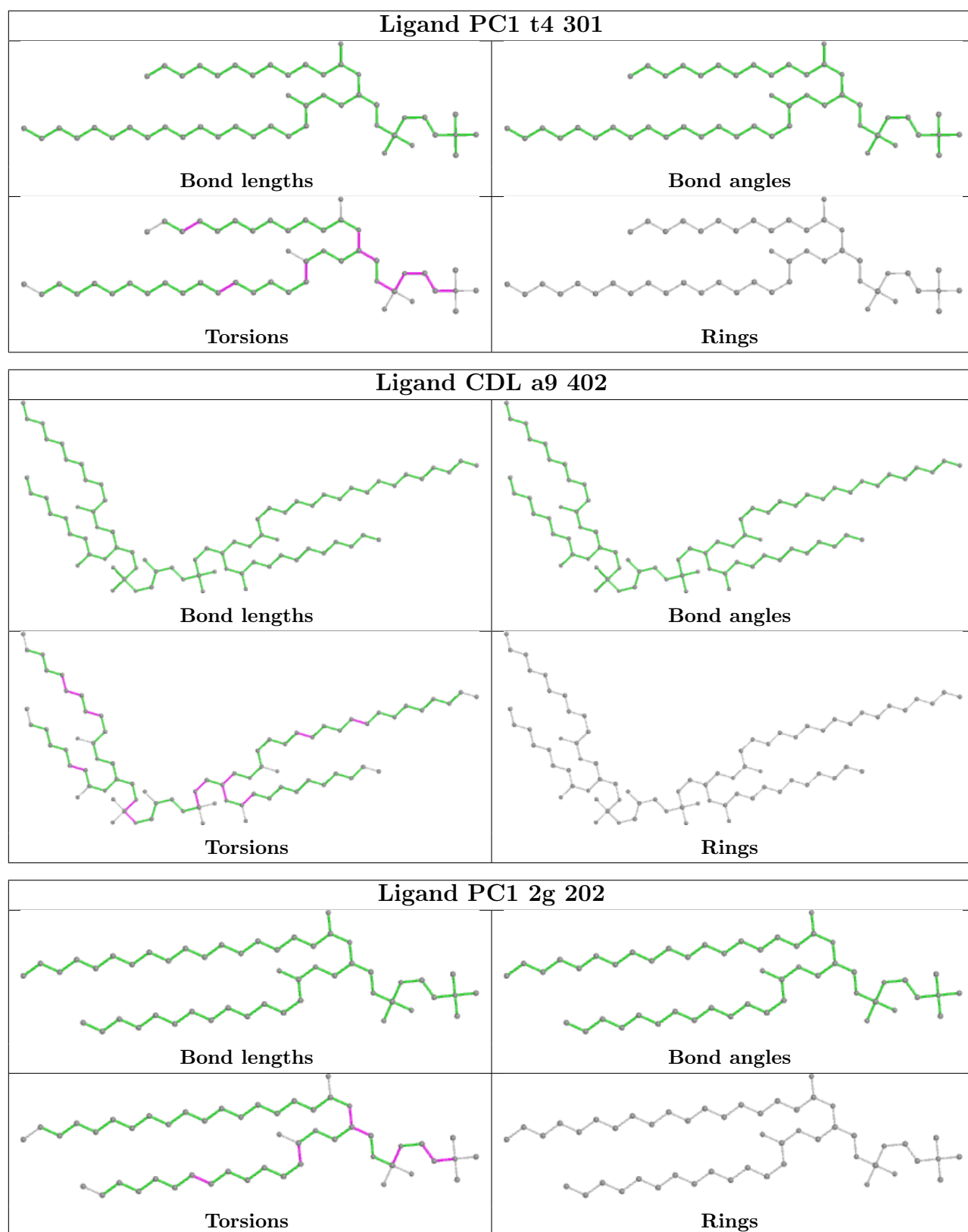


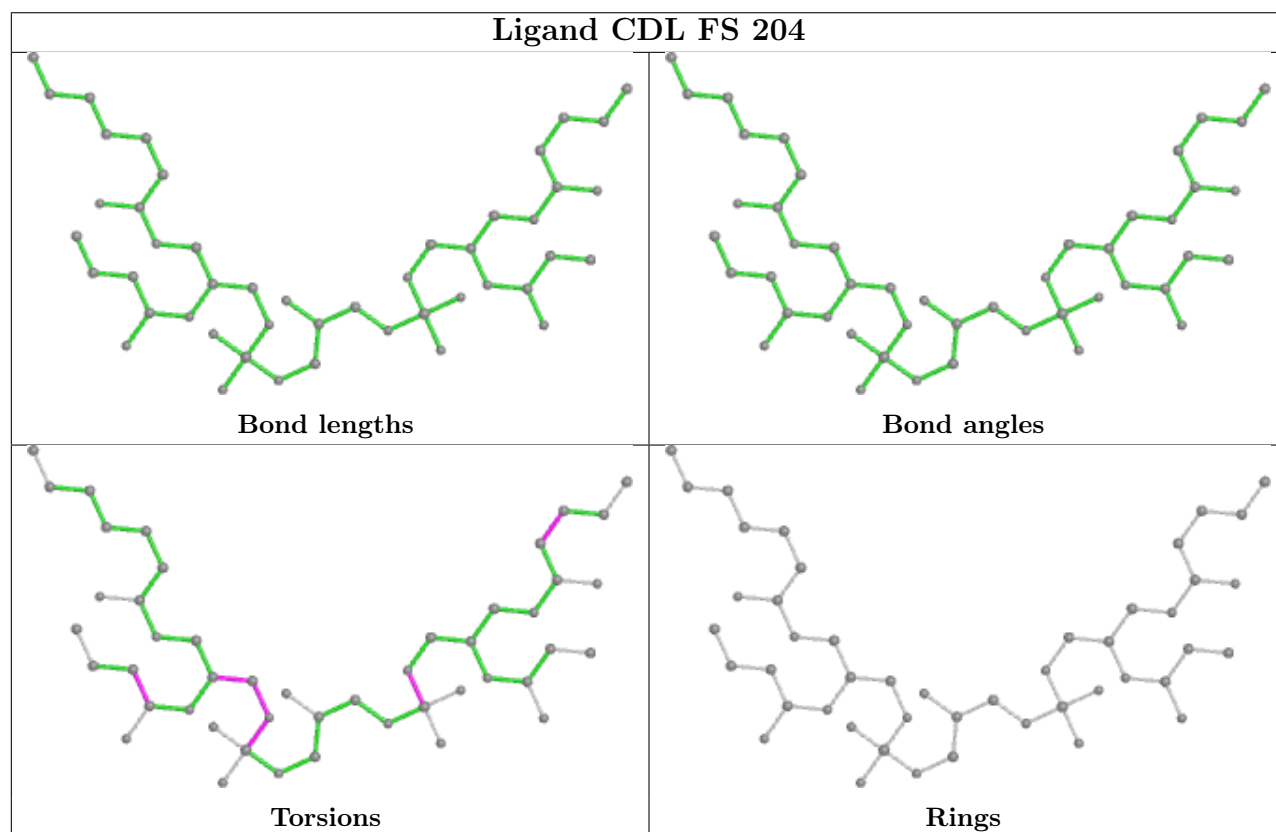
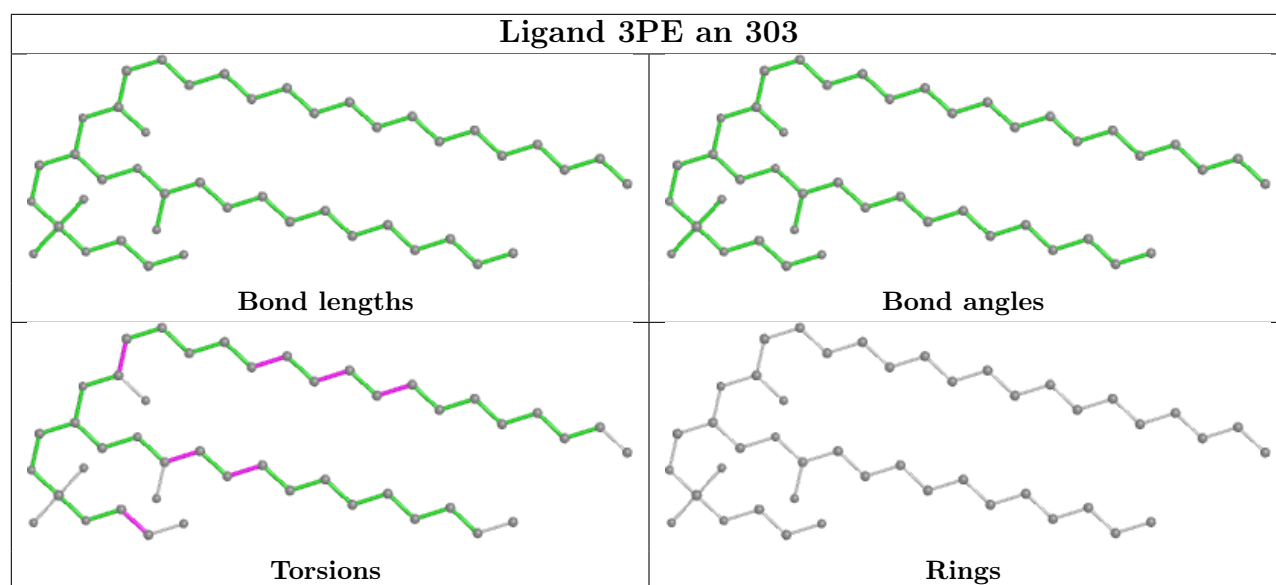


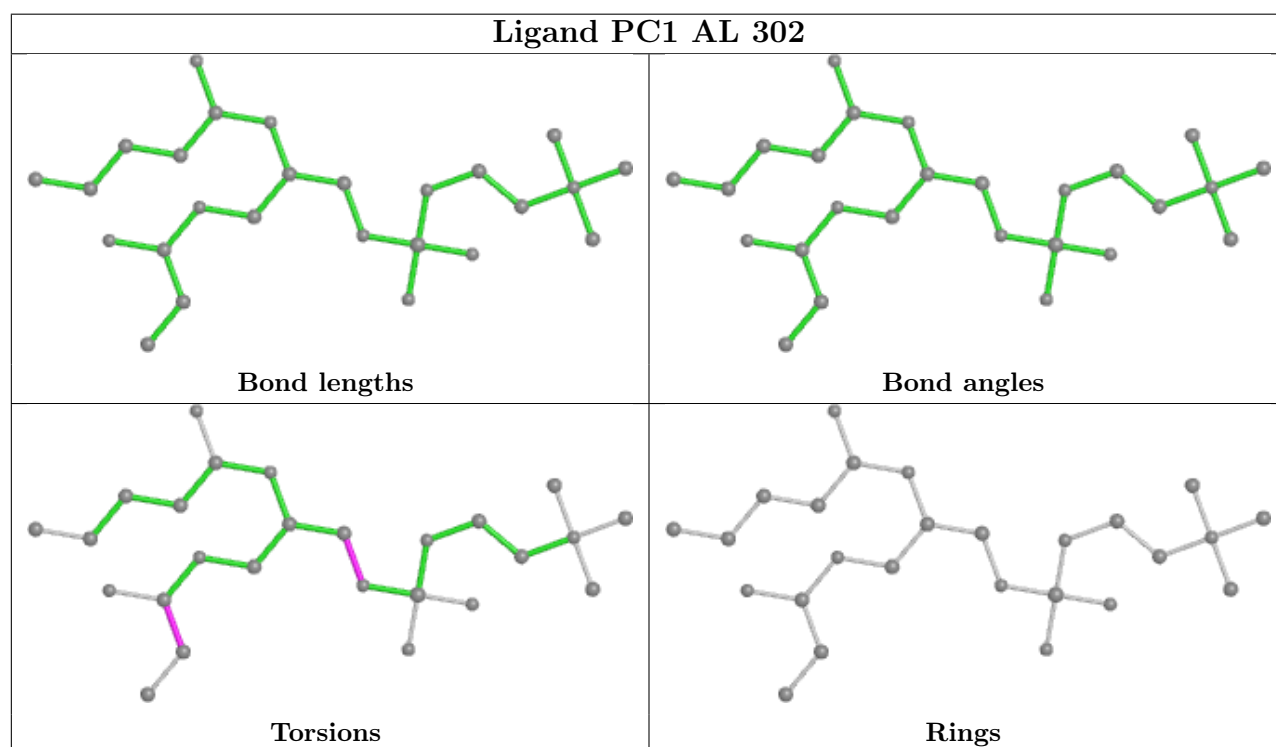
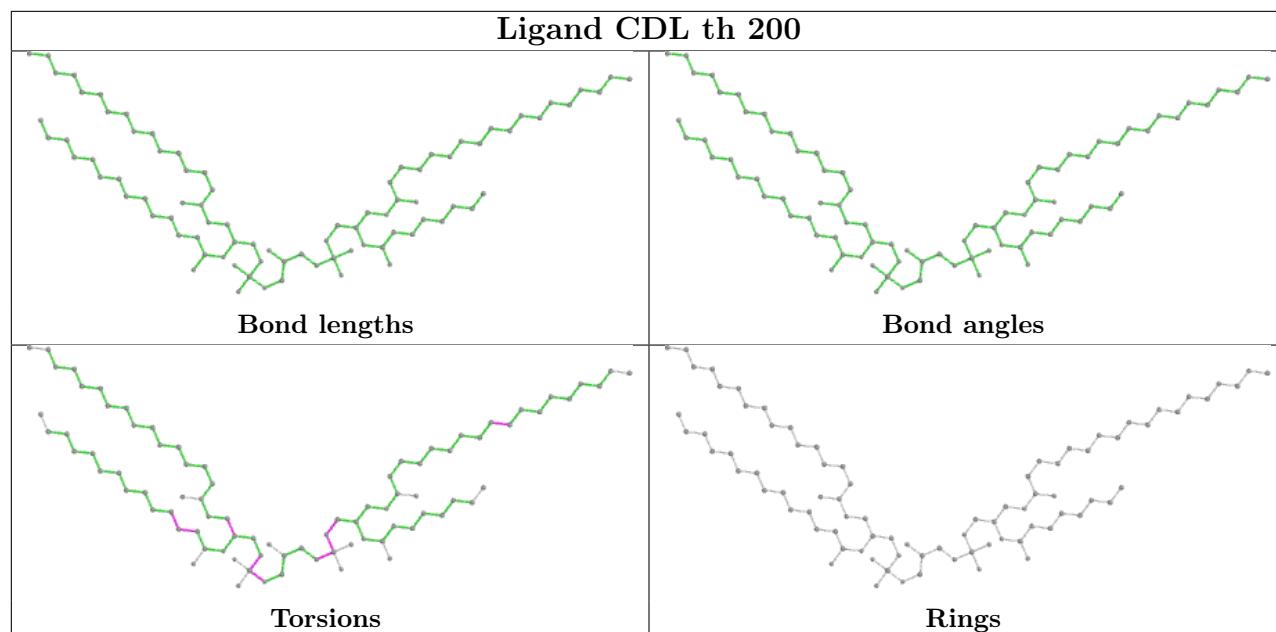


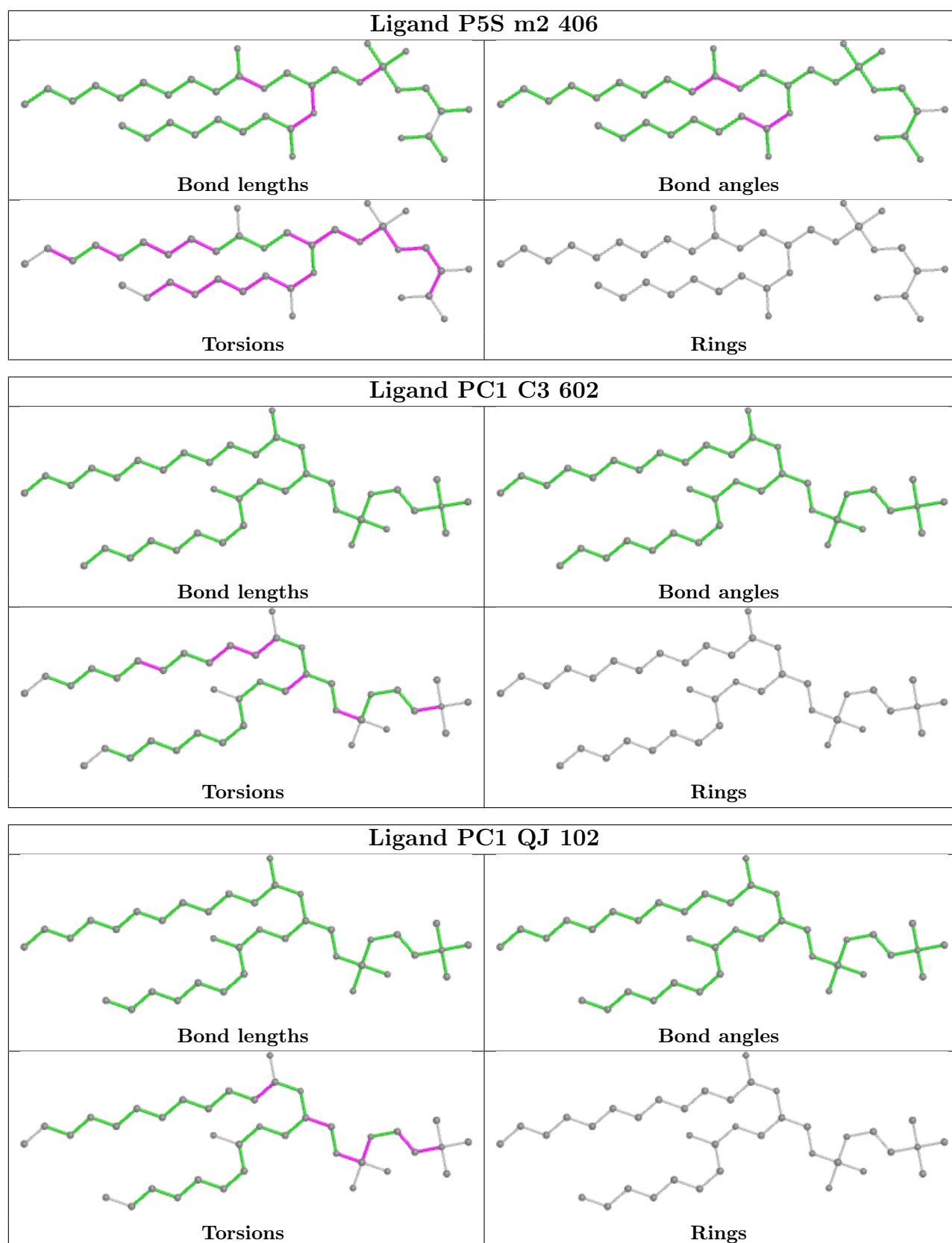


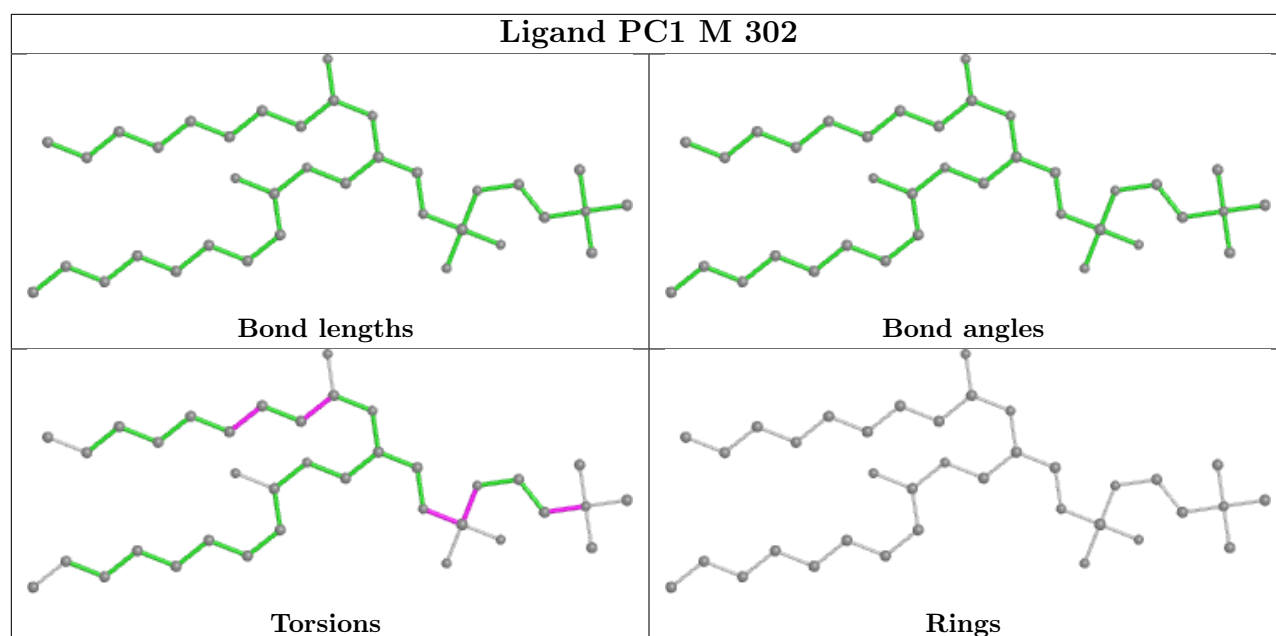
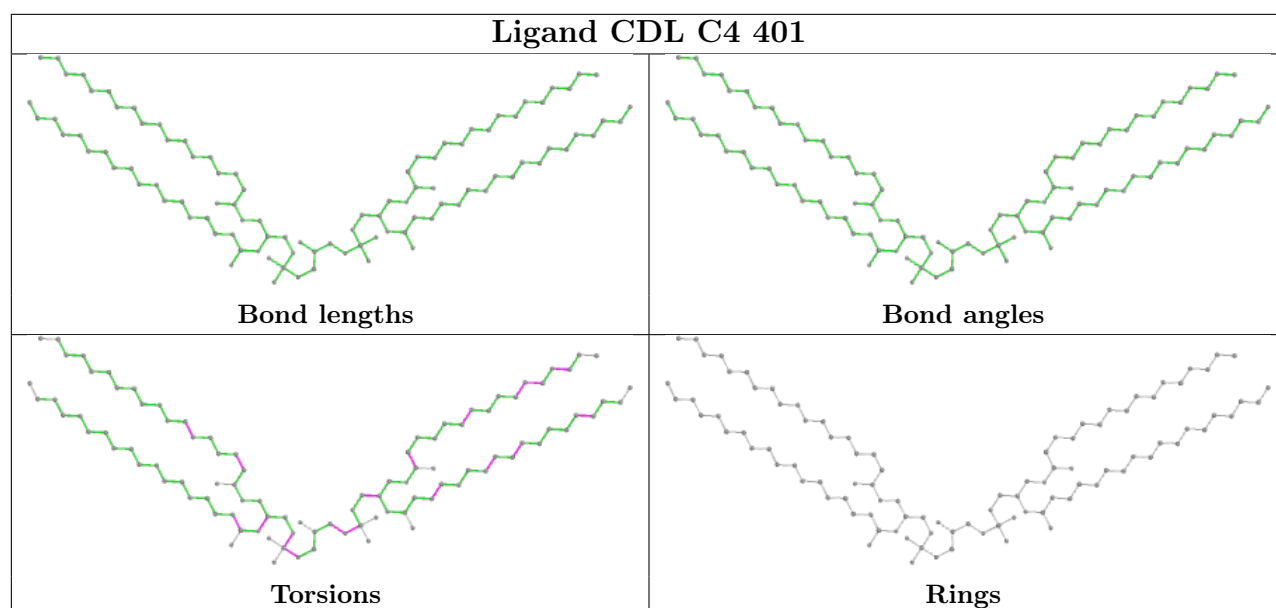


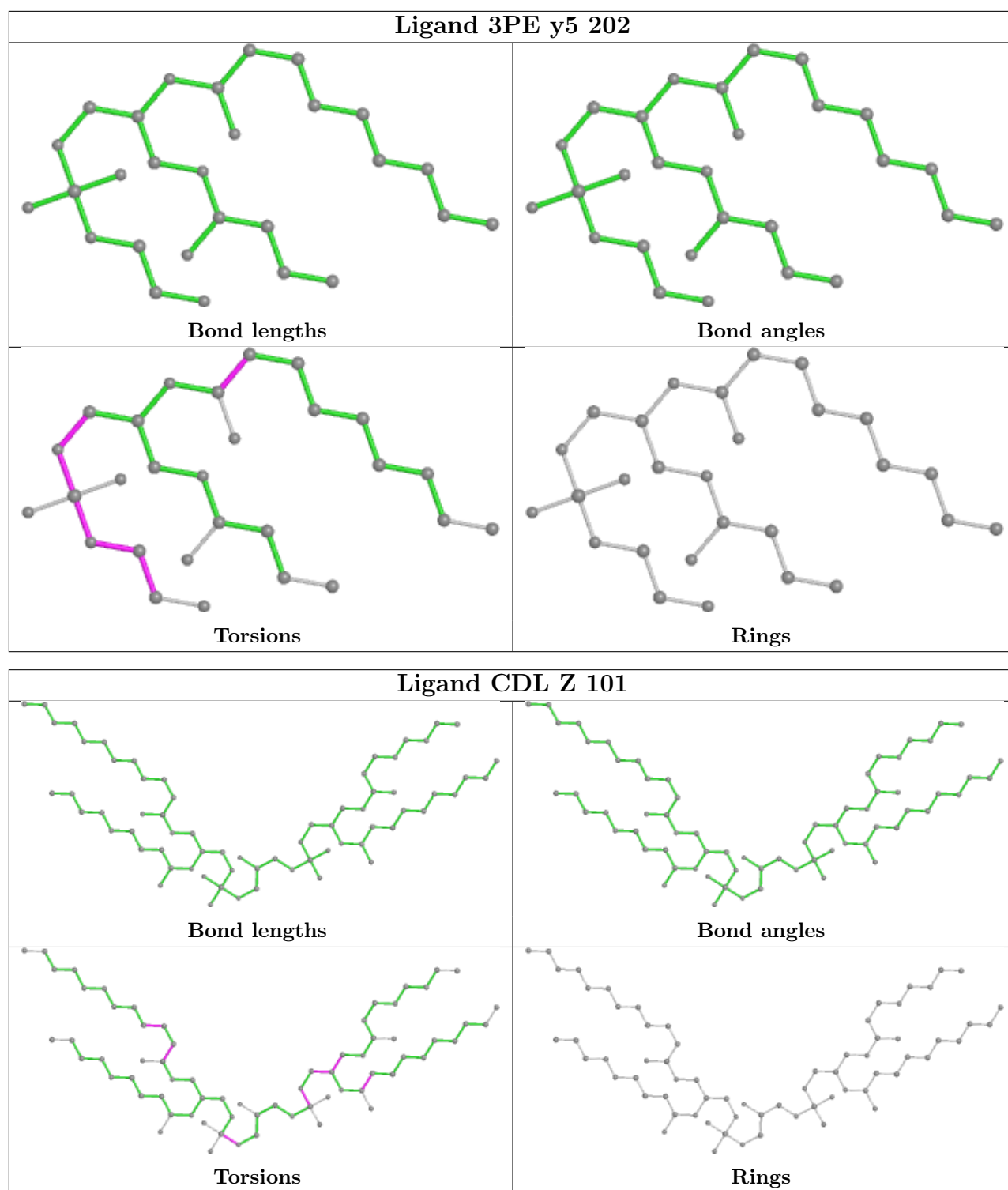


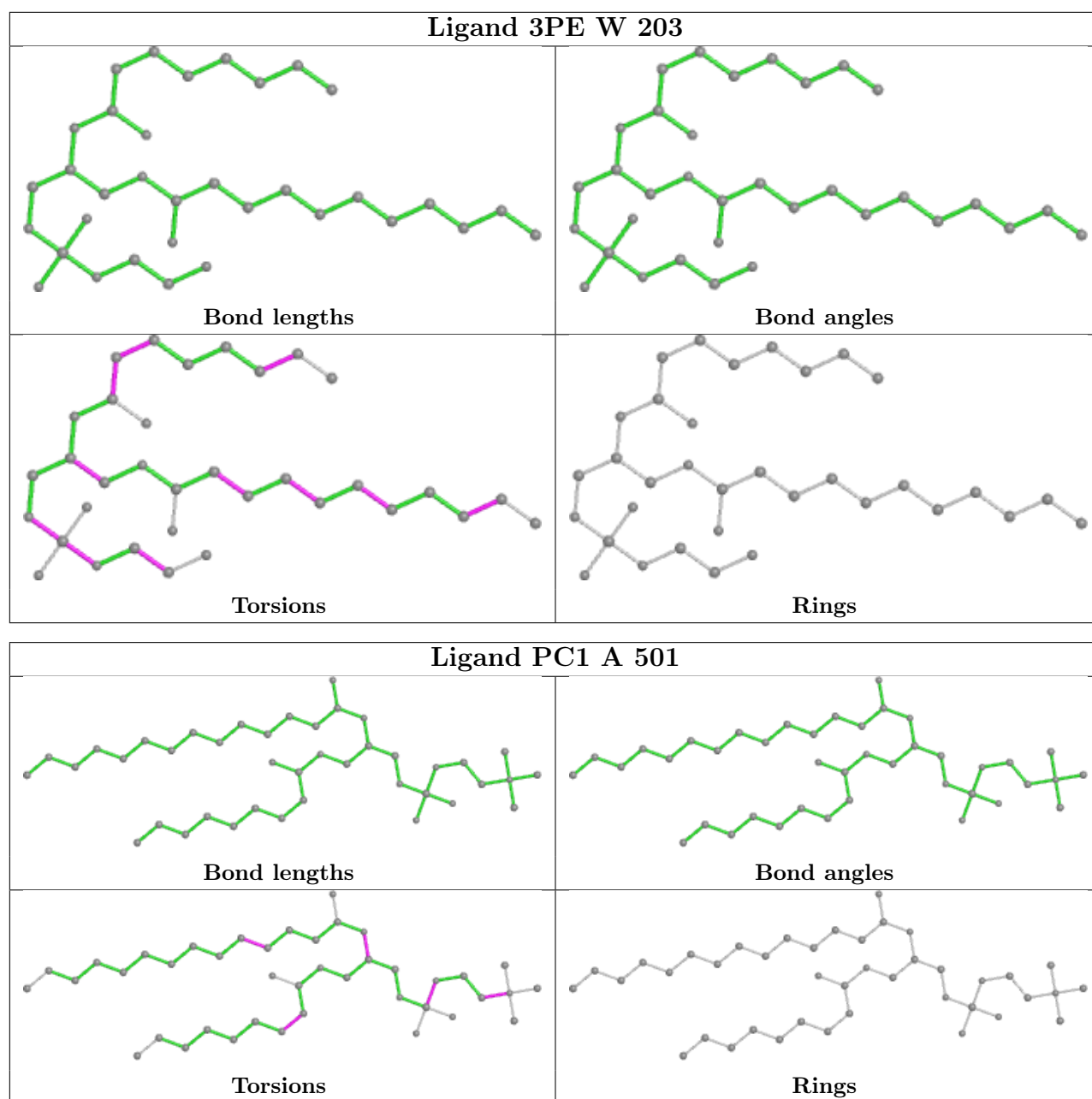


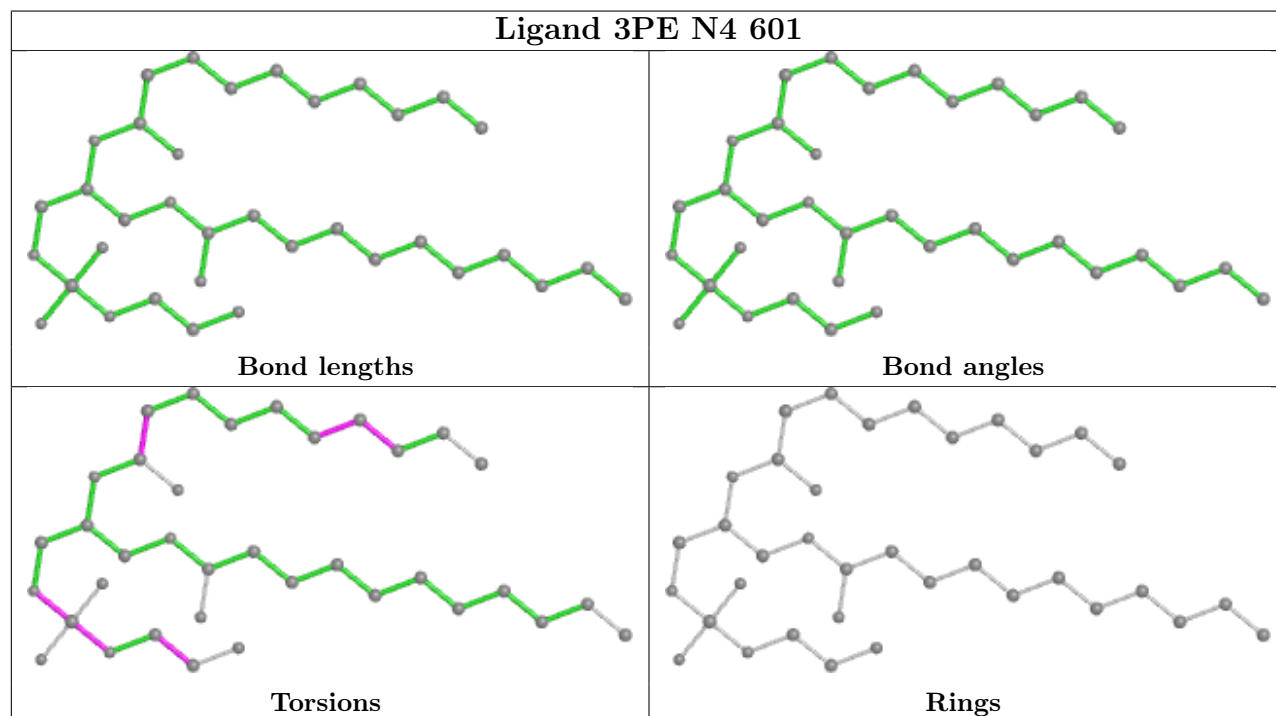
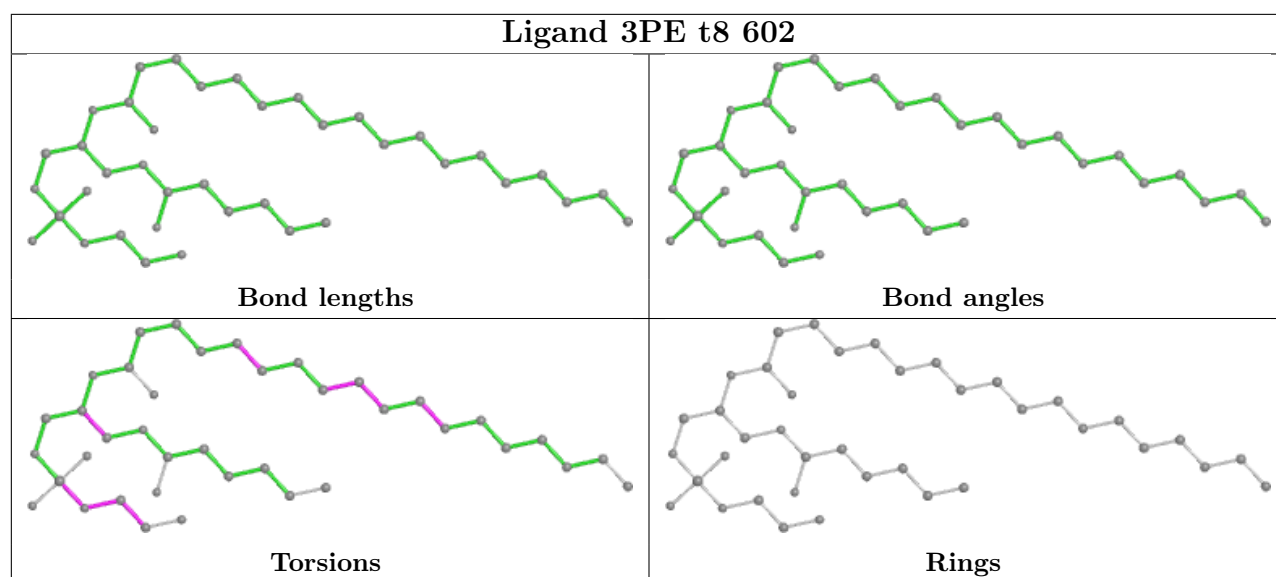


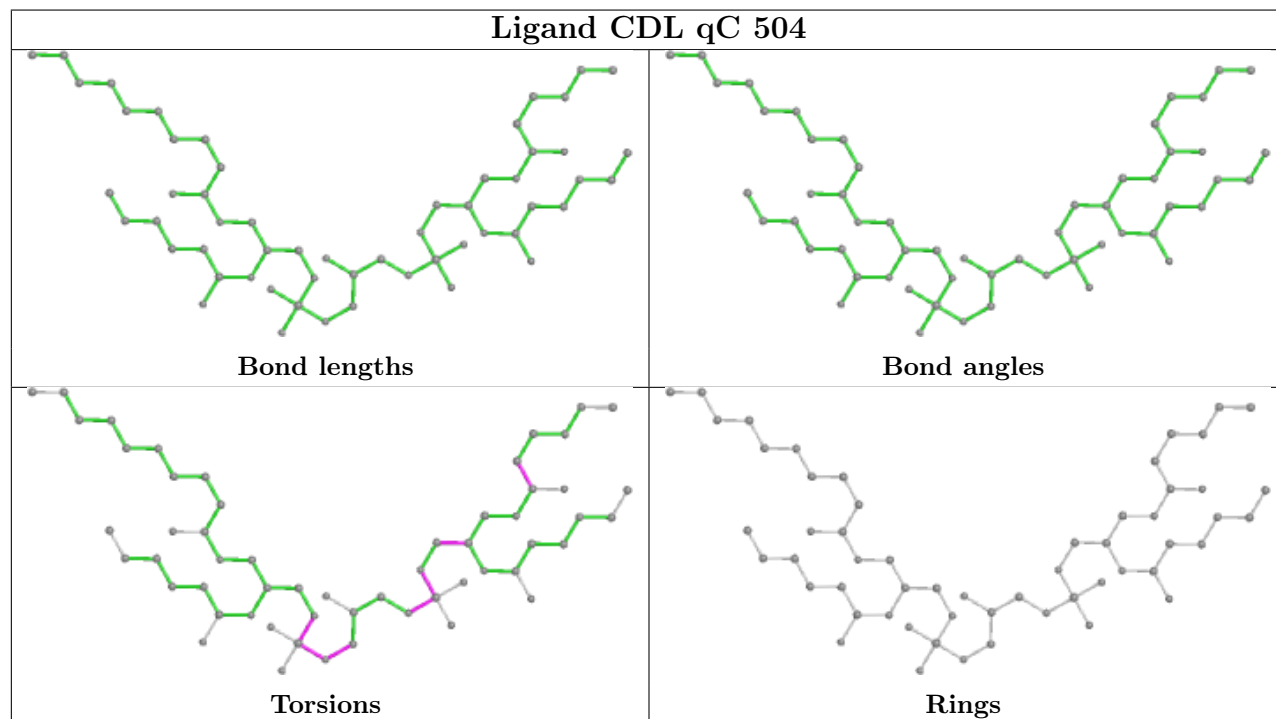
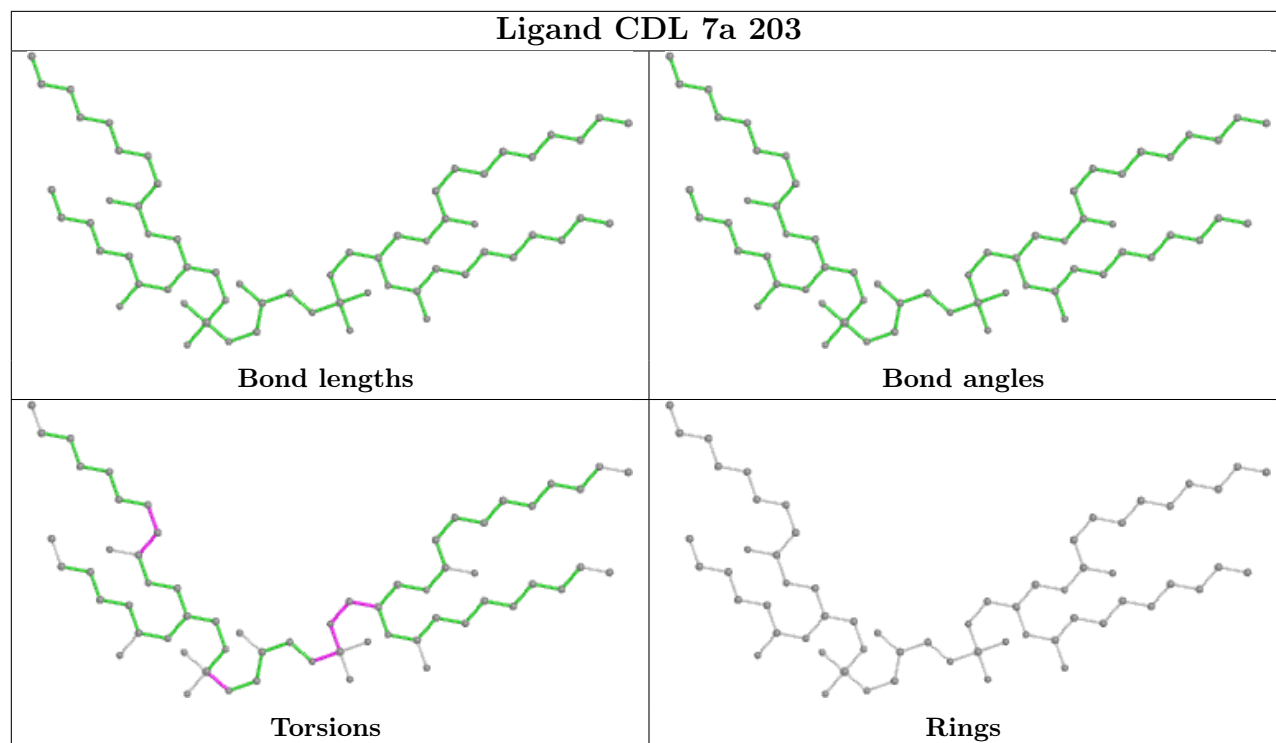


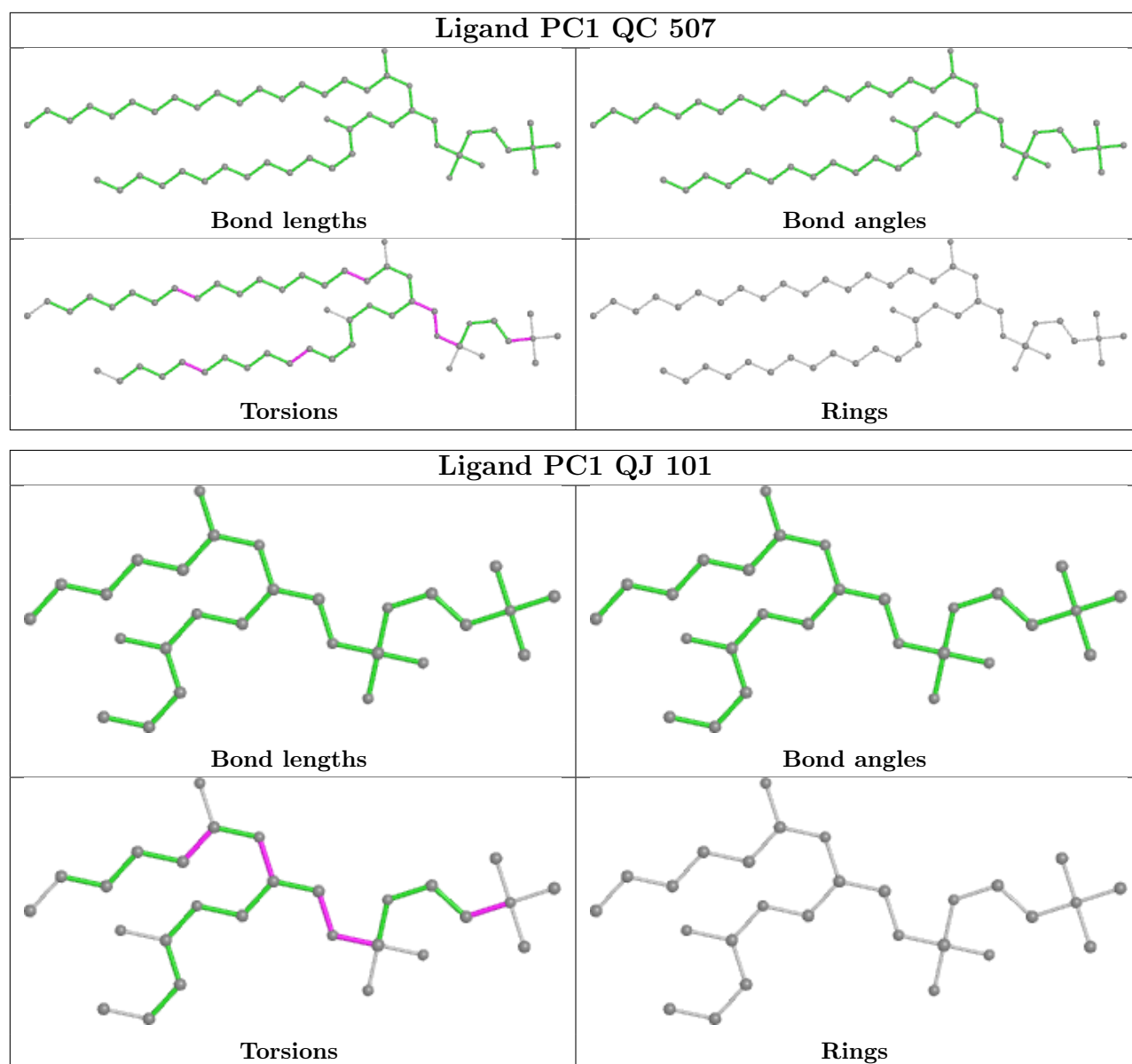




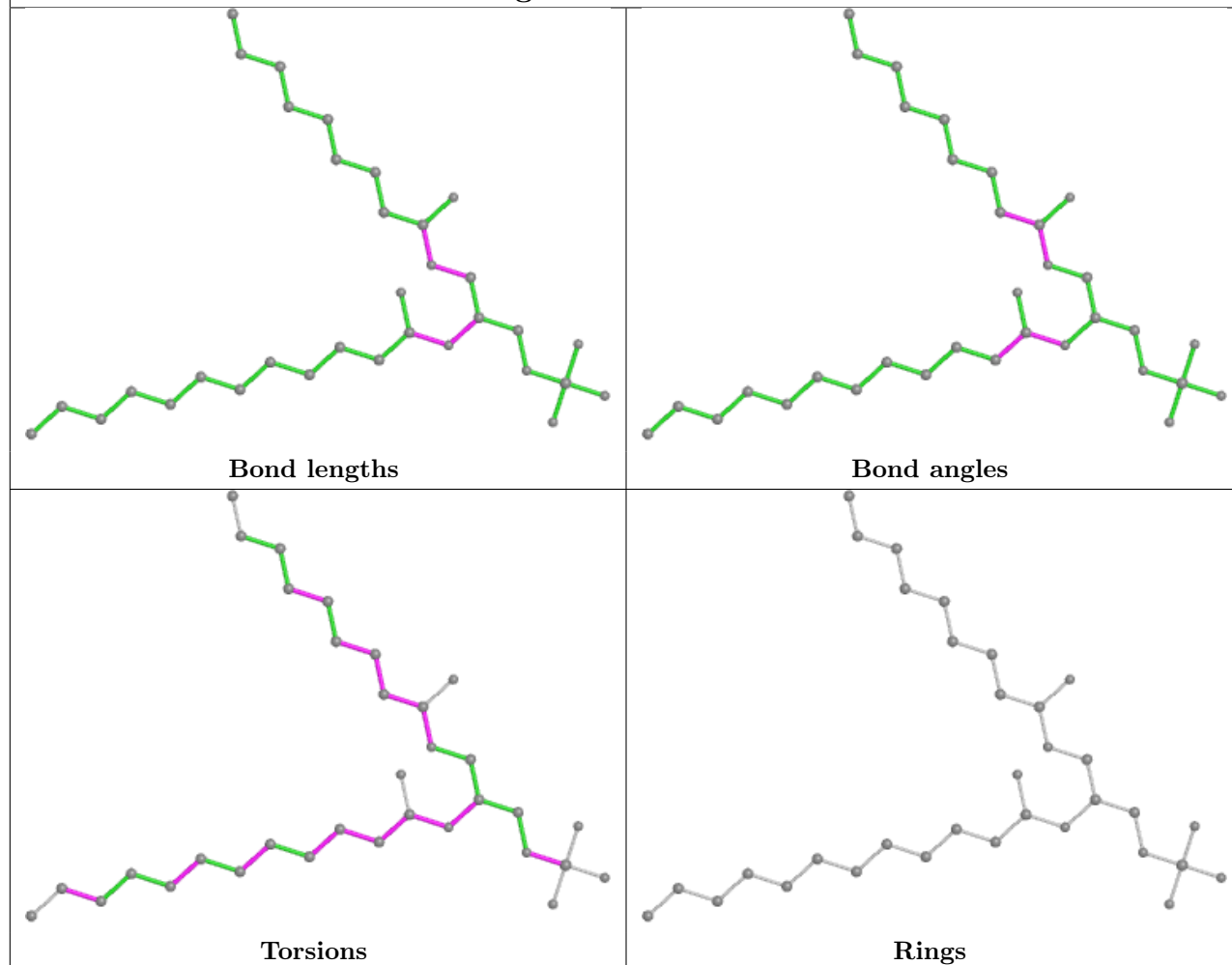




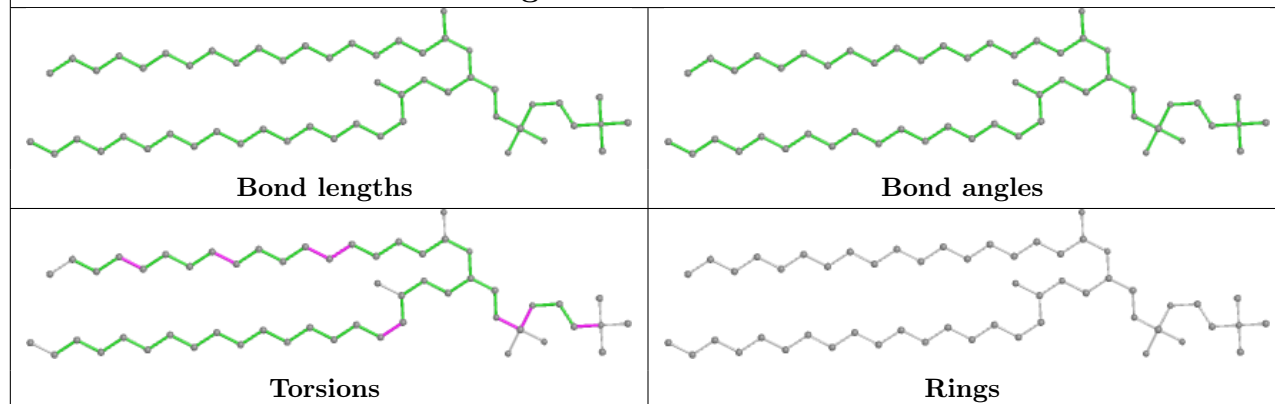




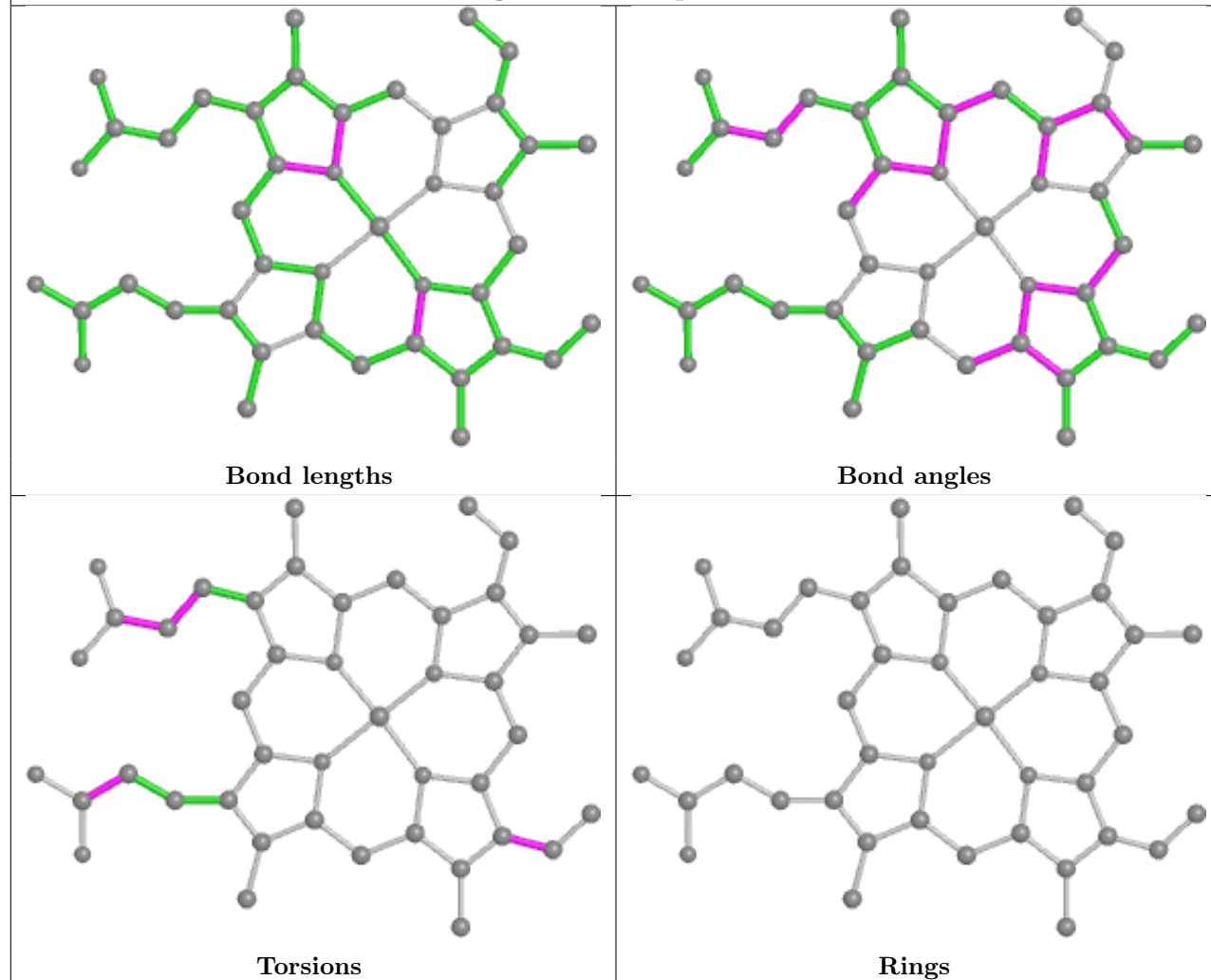
Ligand PX2 R 202



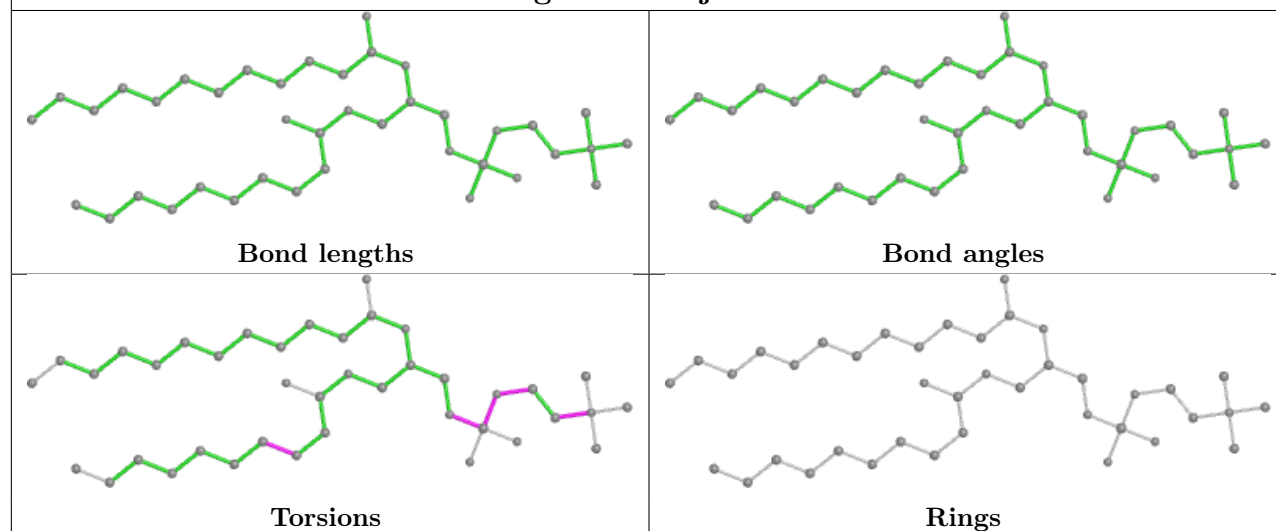
Ligand PC1 M1 401

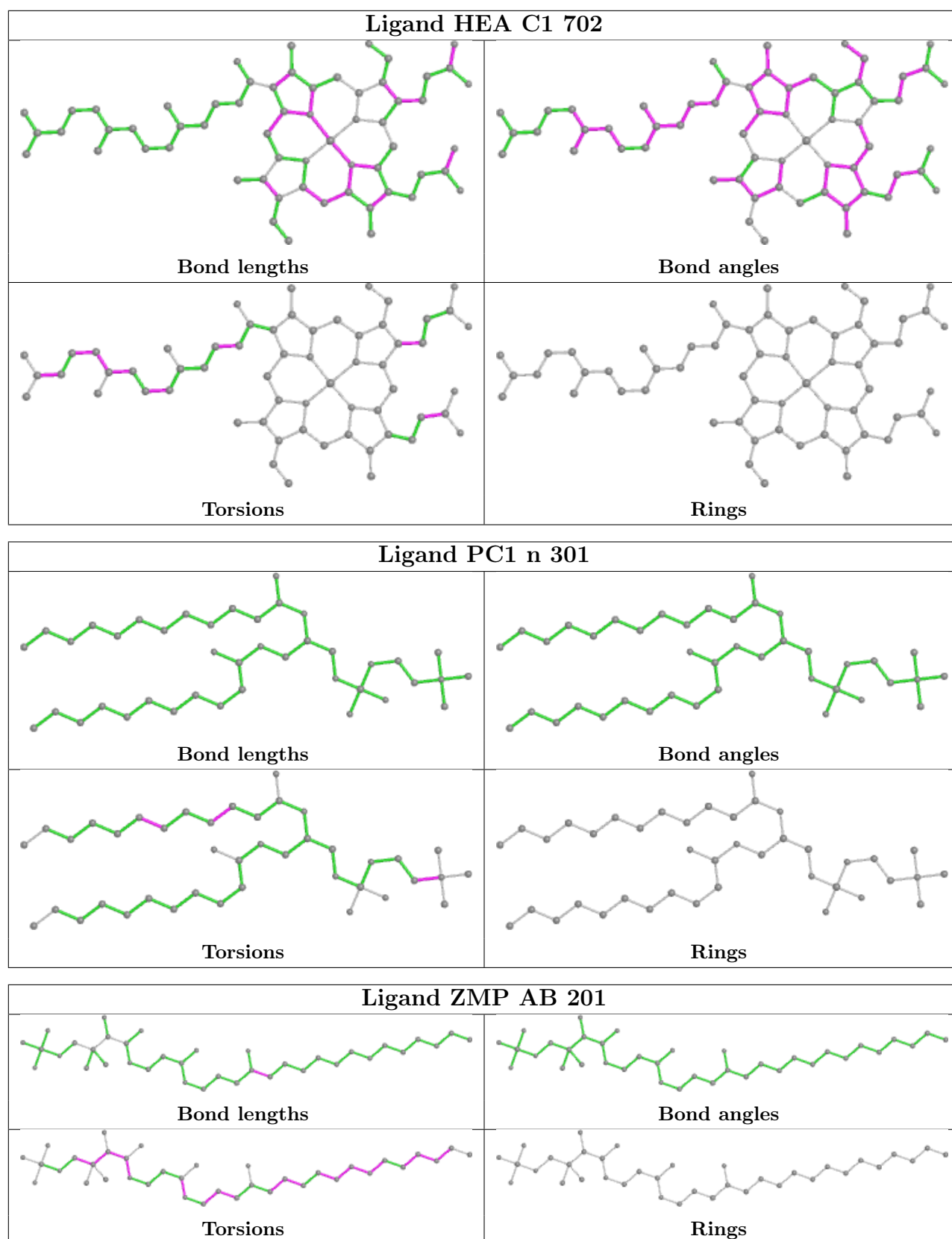


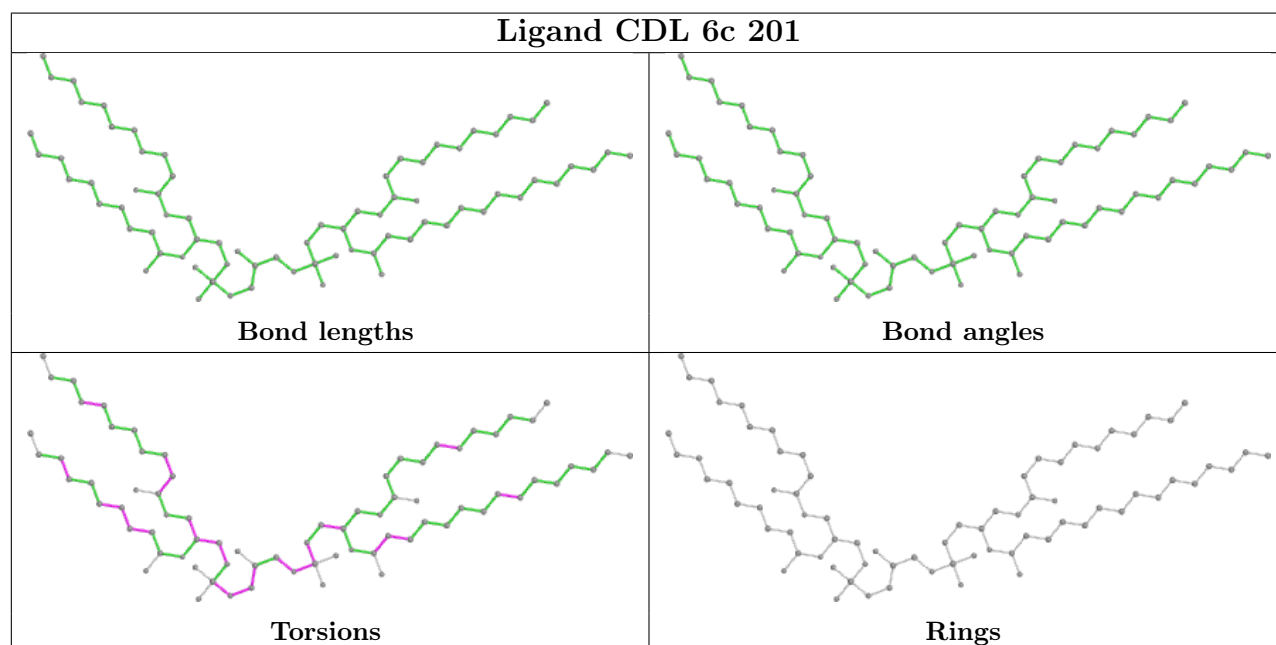
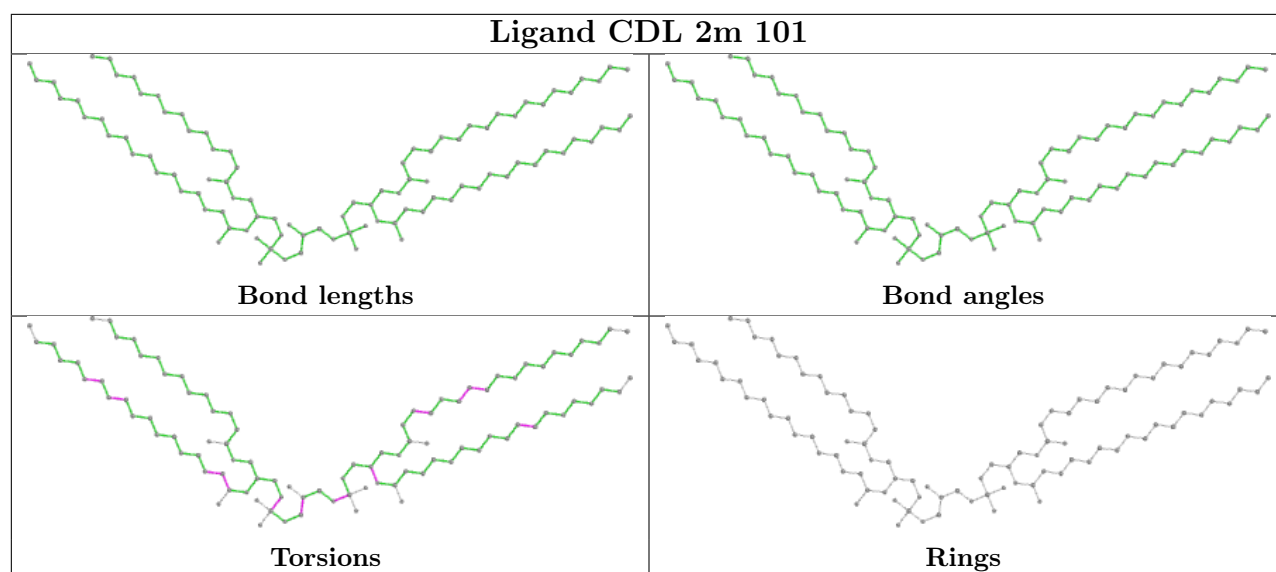
Ligand HEM qC 502

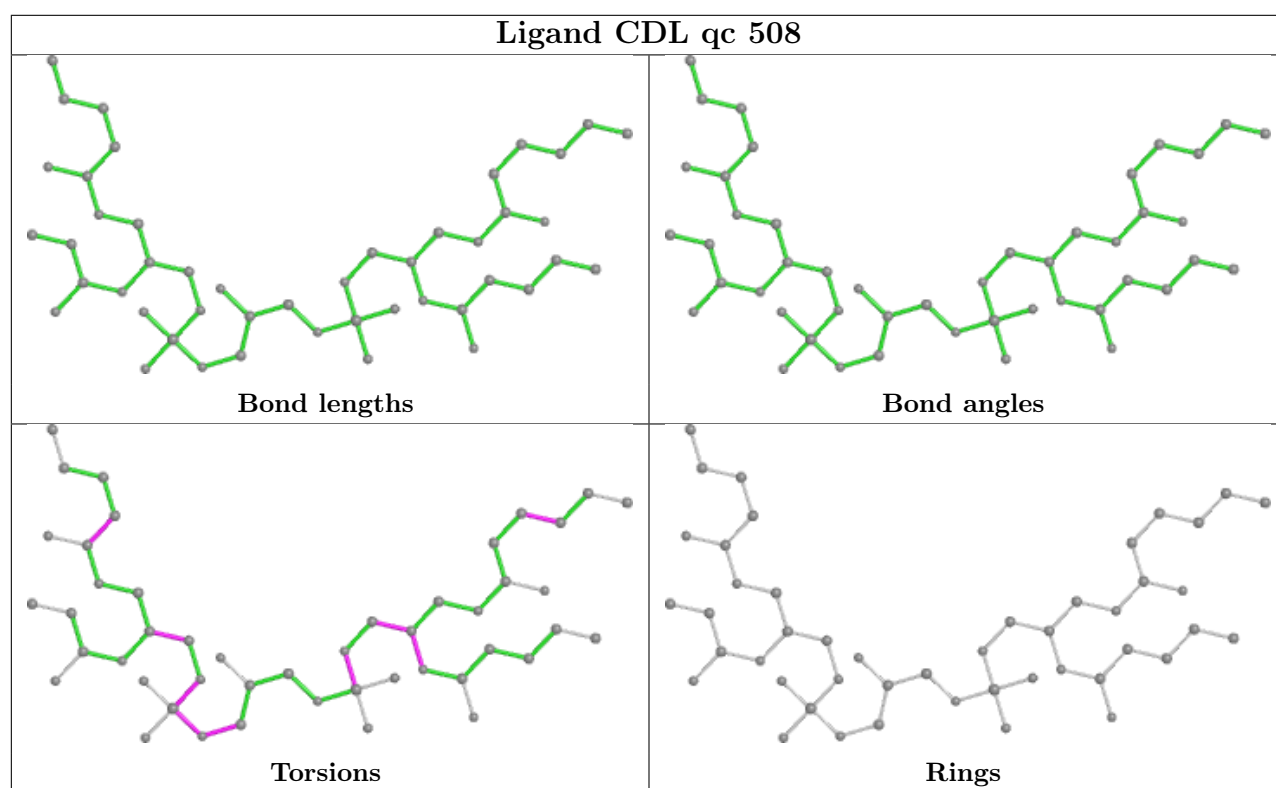
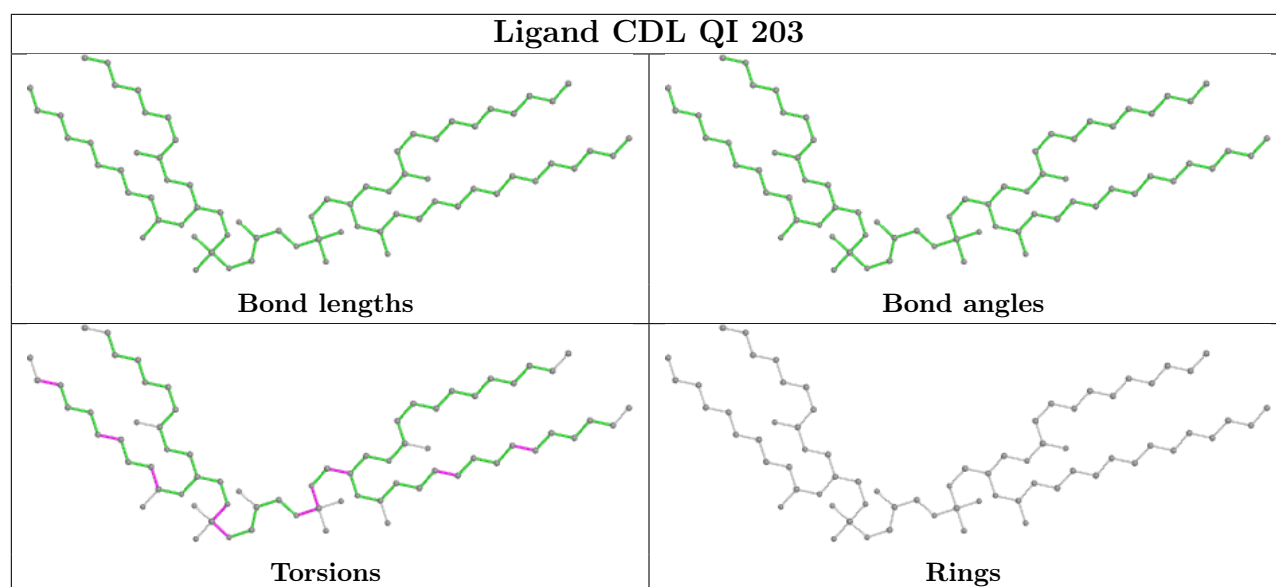


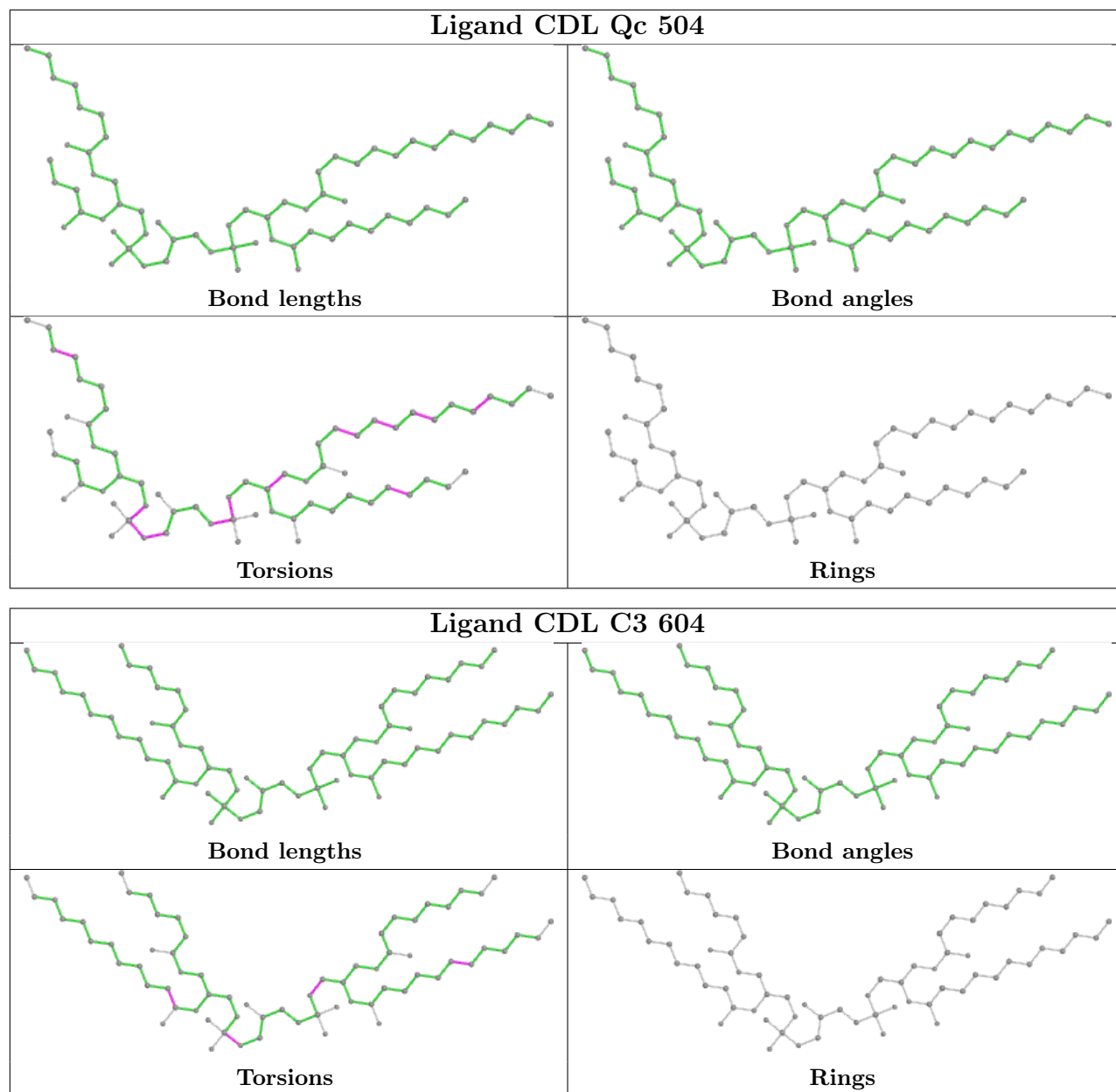
Ligand PC1 j1 400

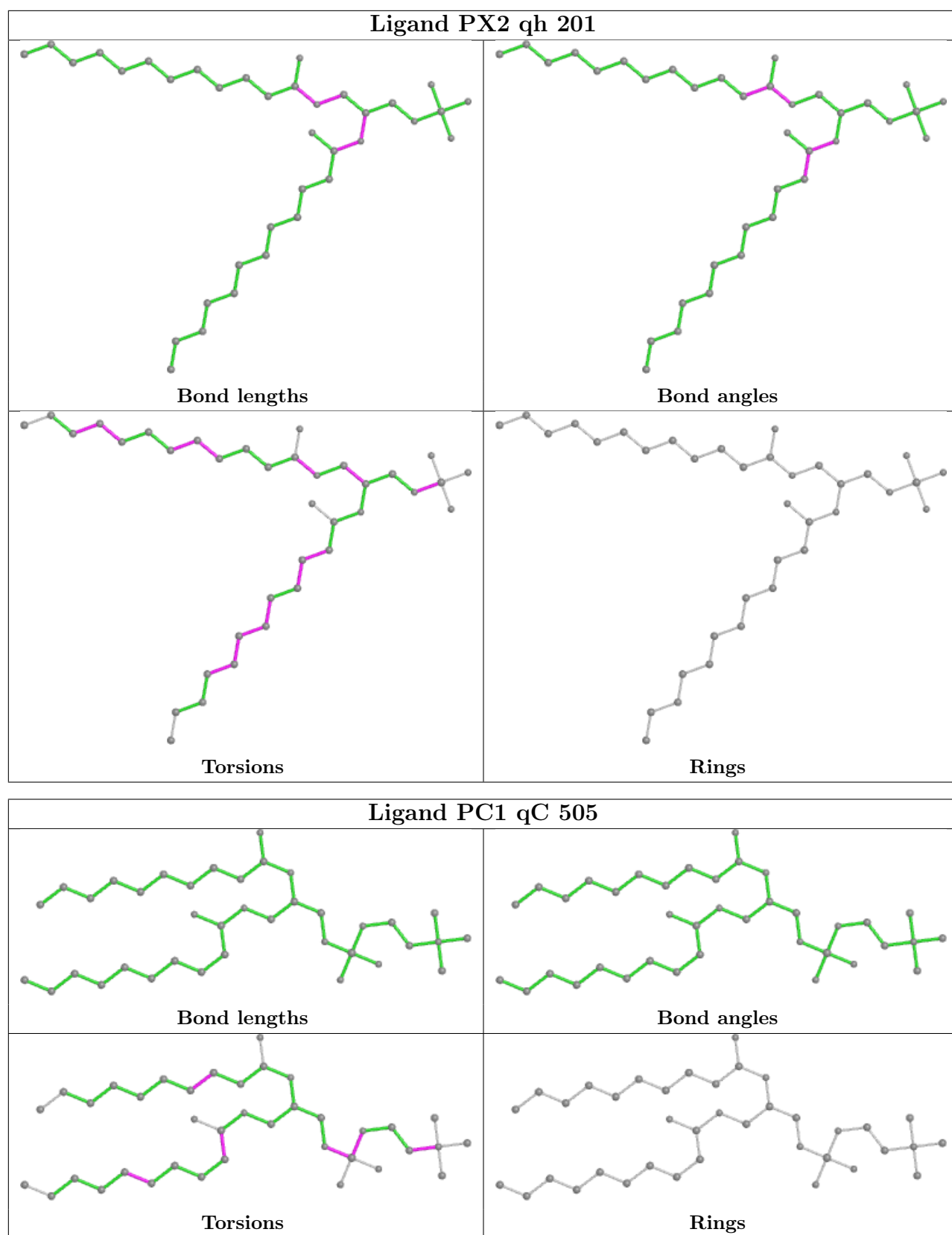


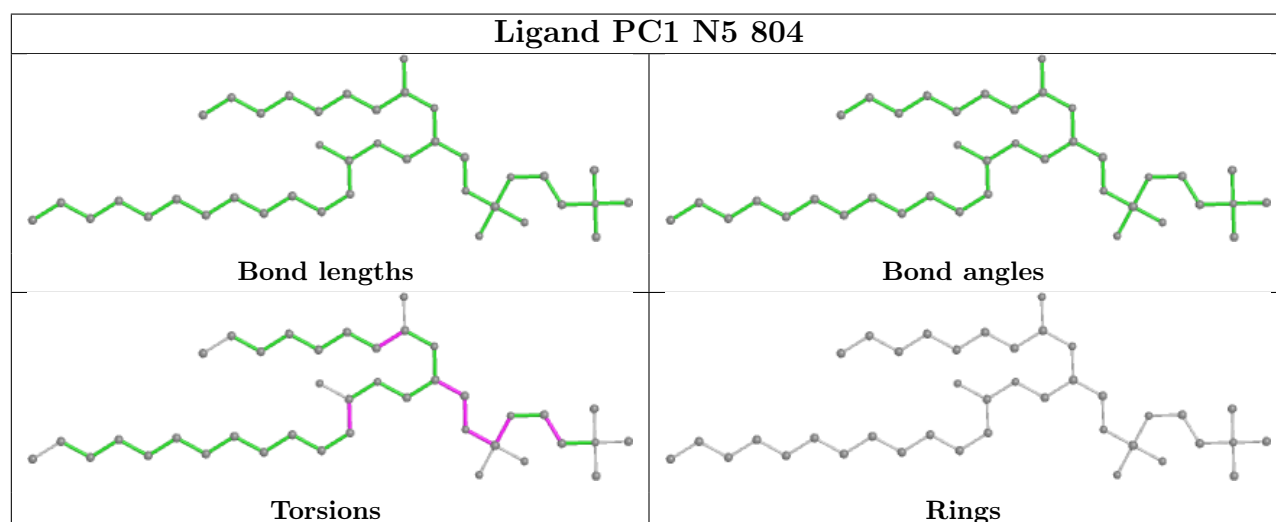
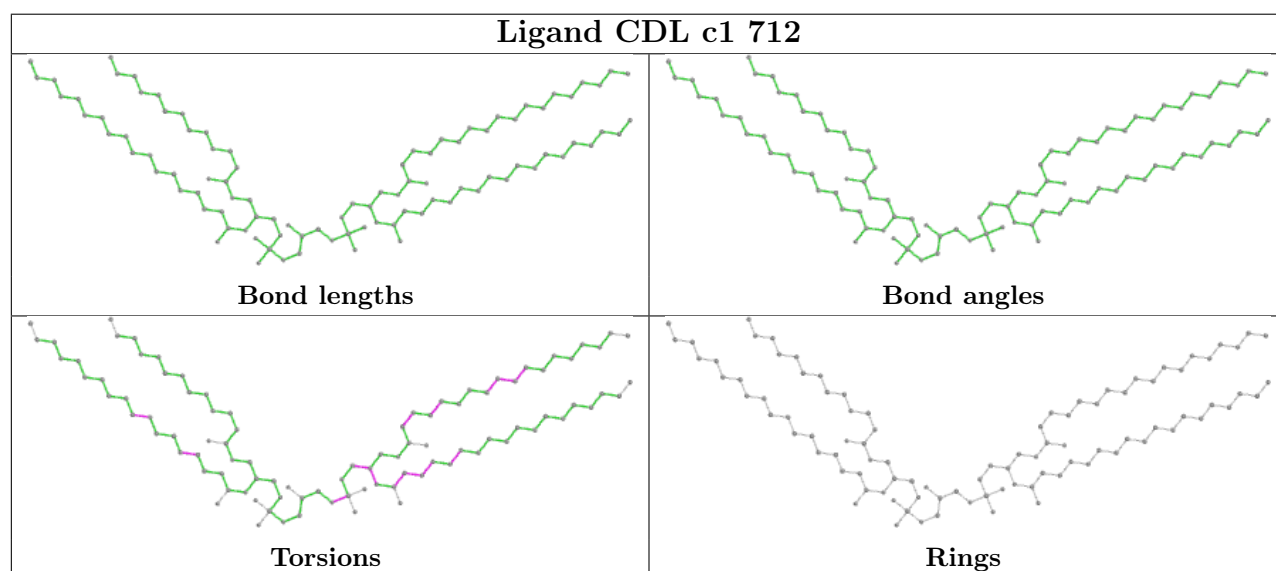
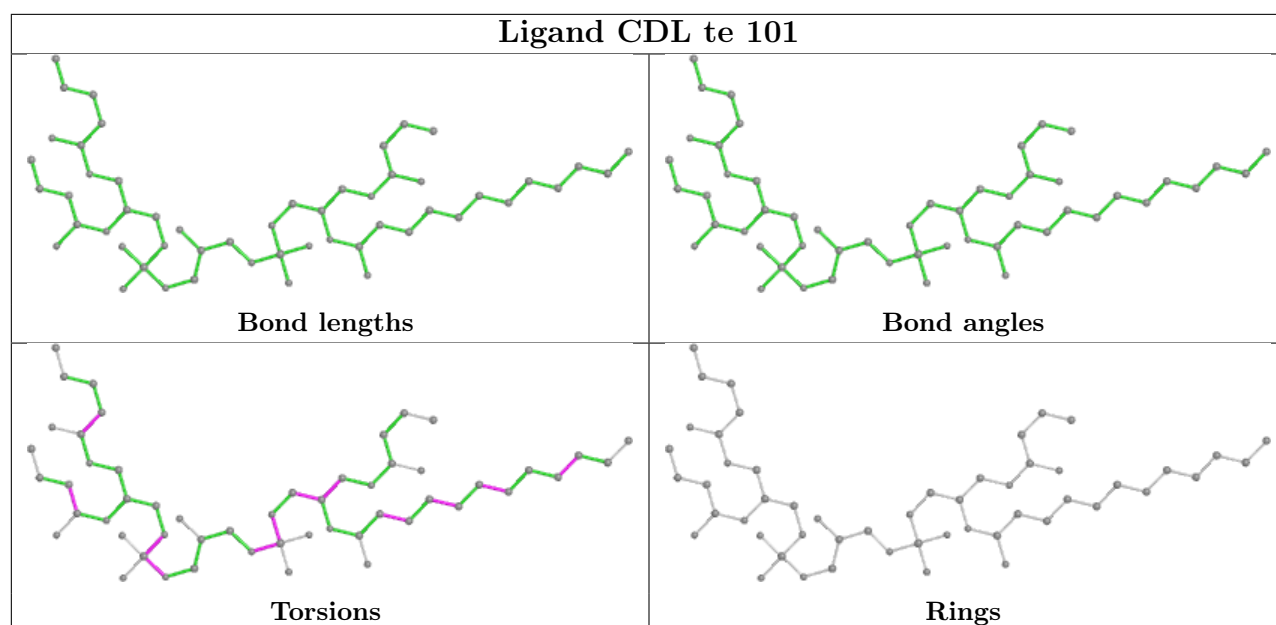


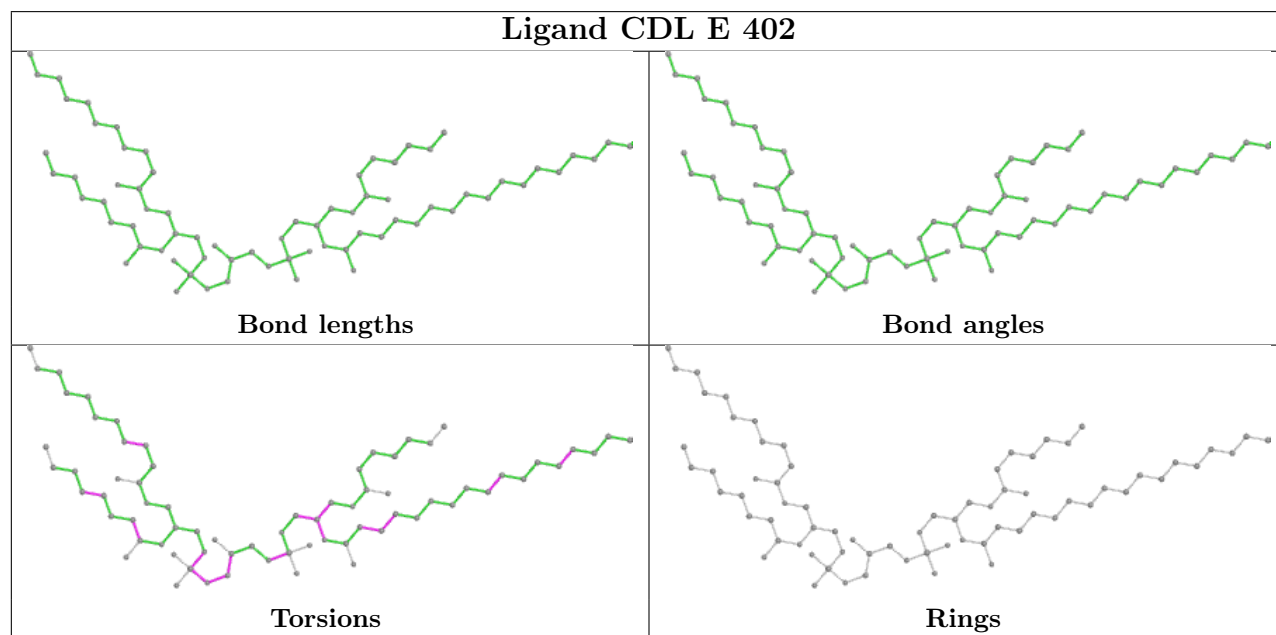
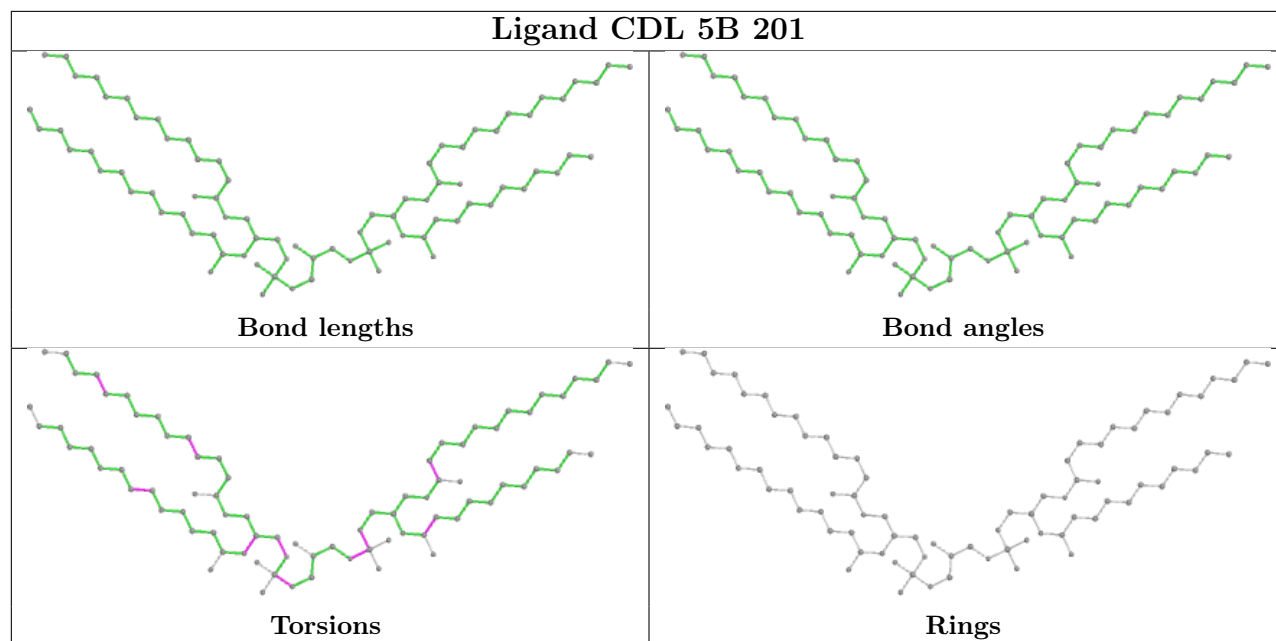


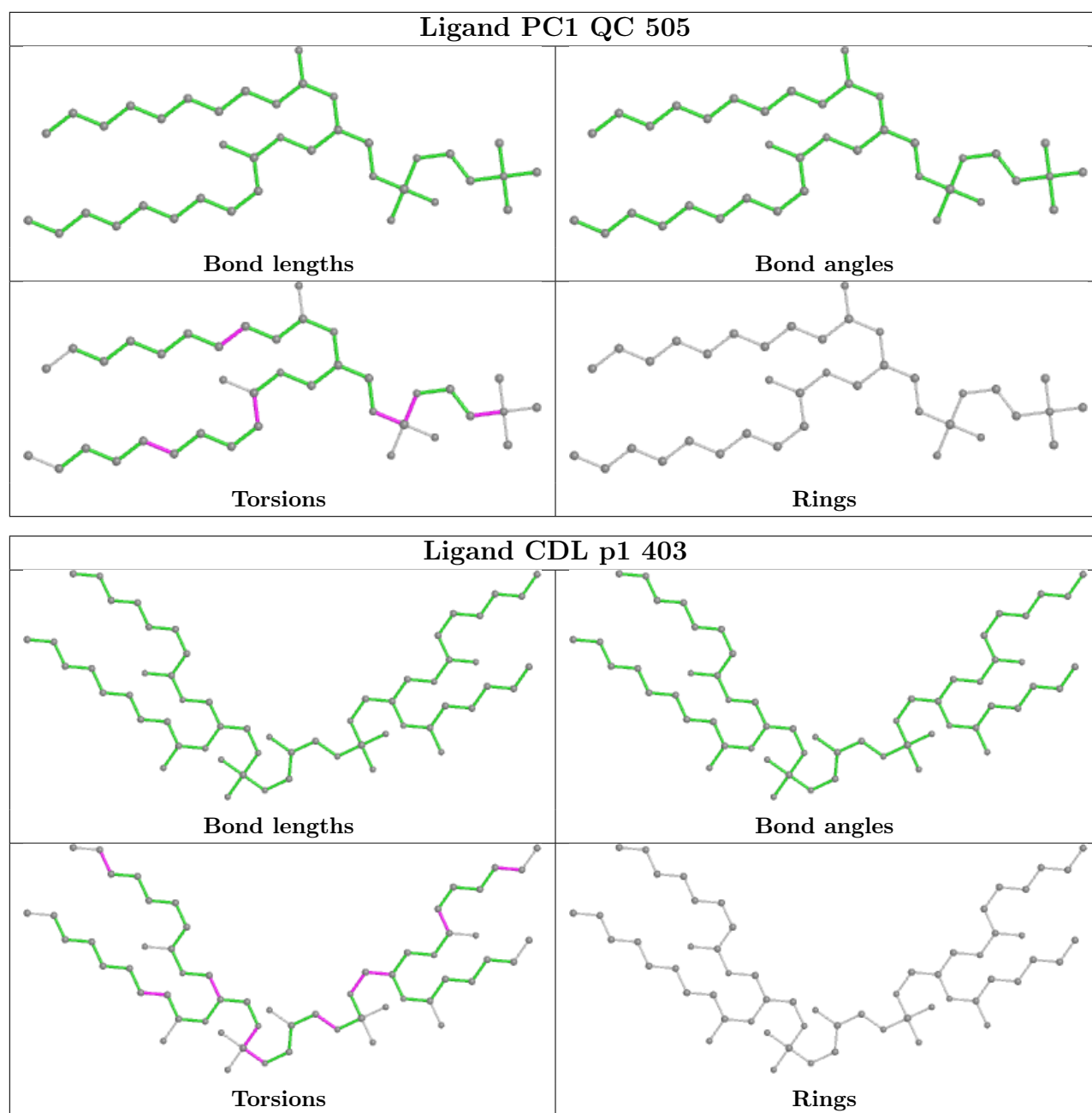


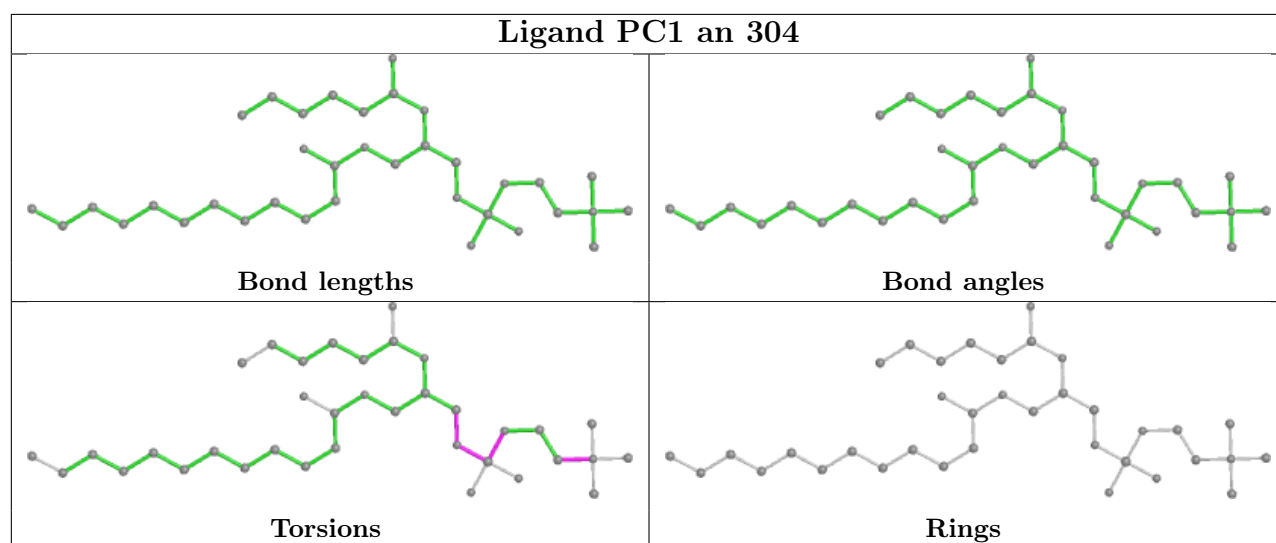
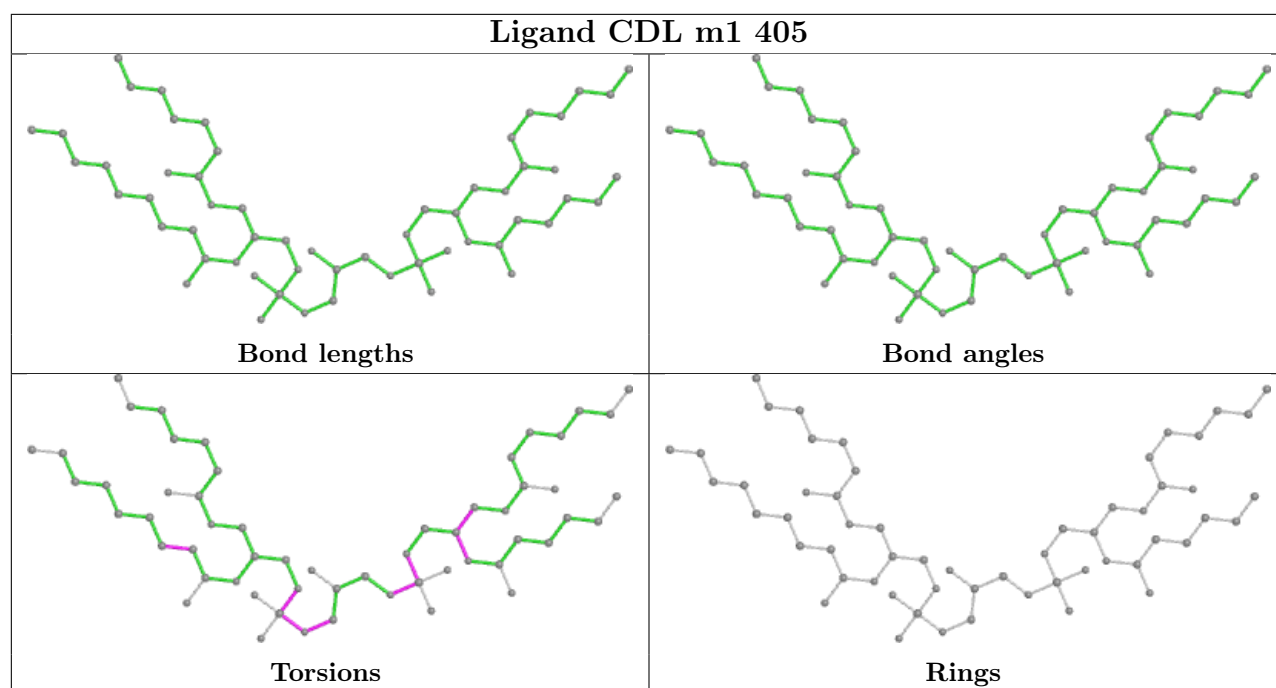


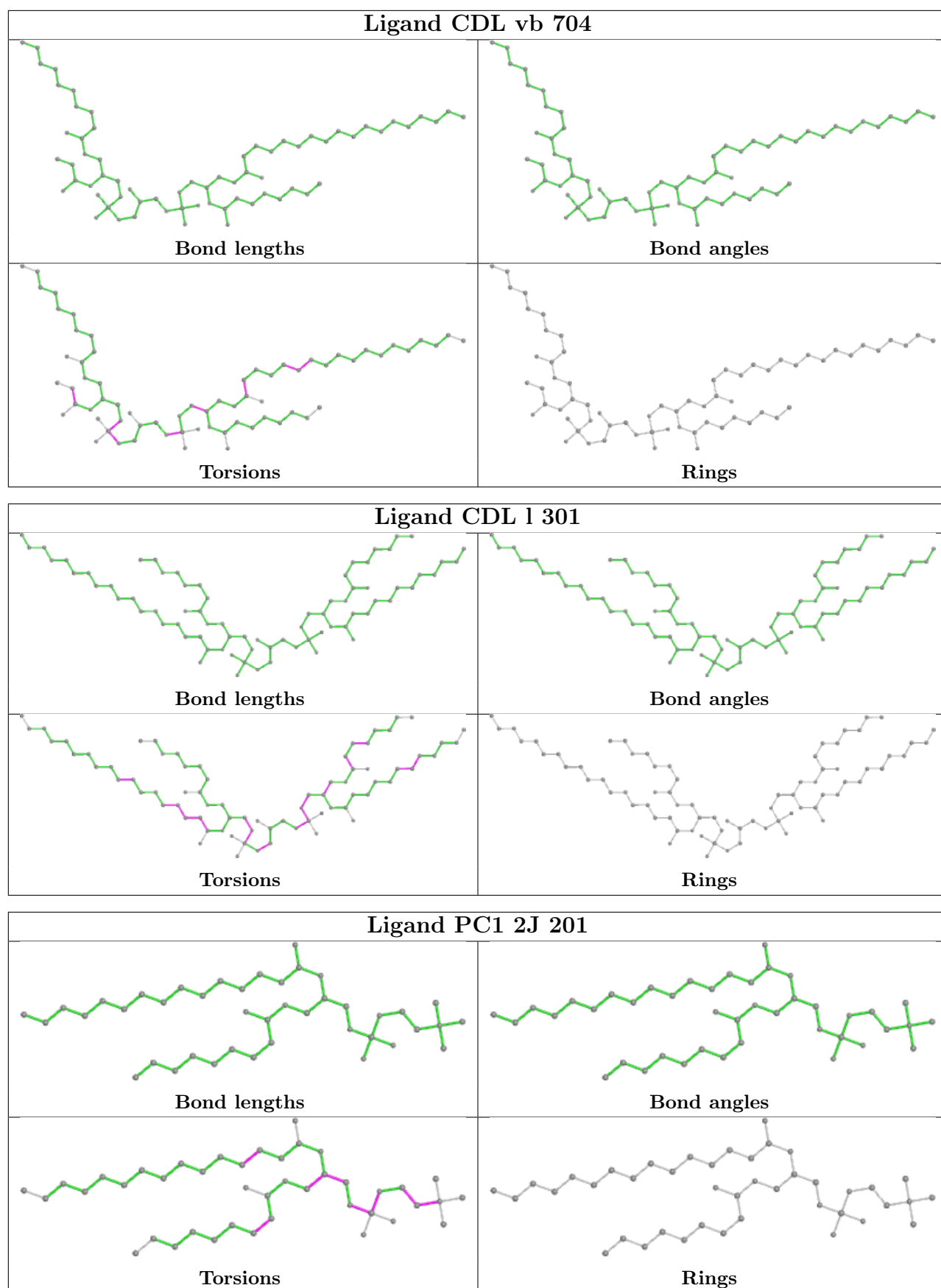


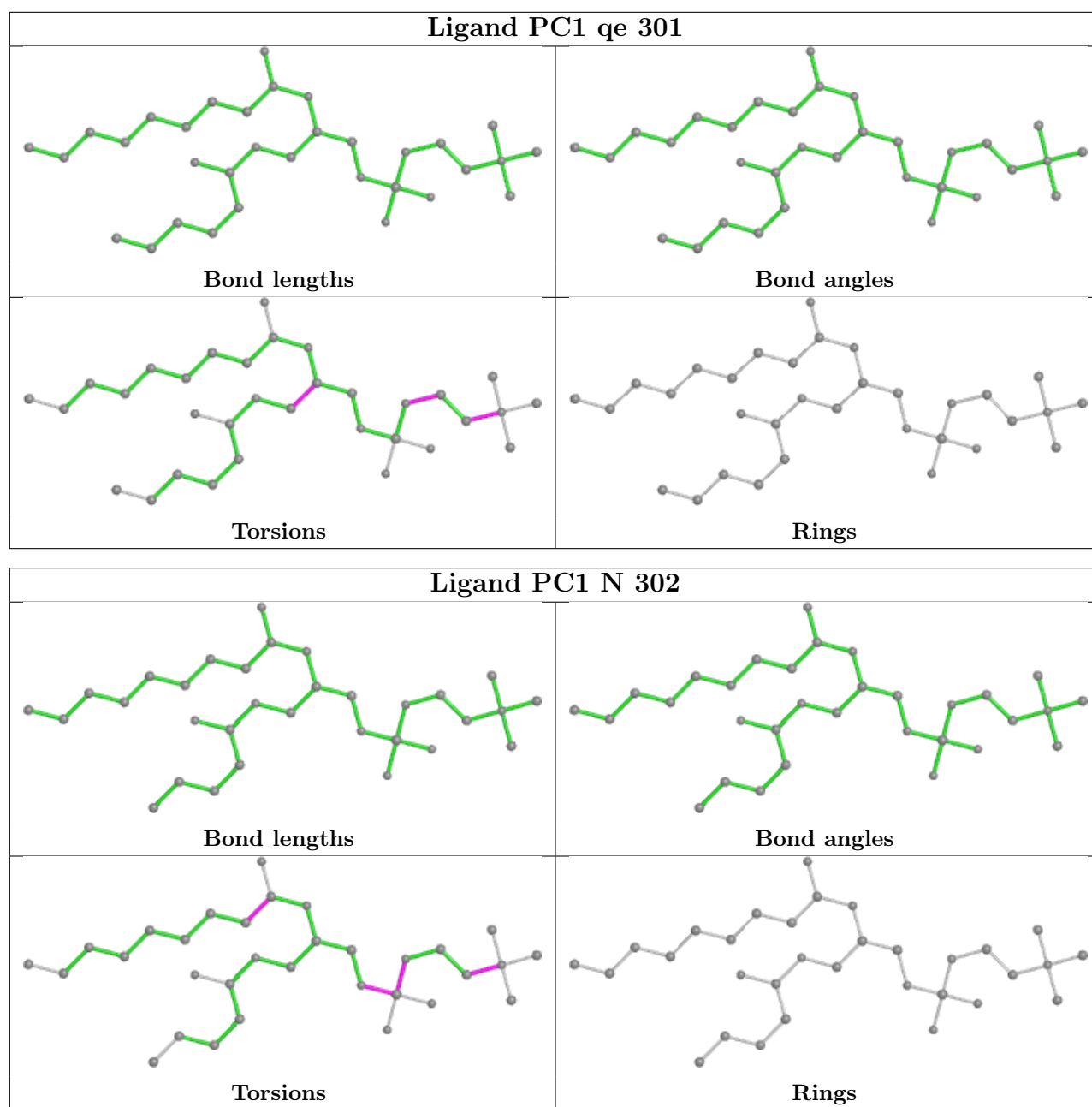


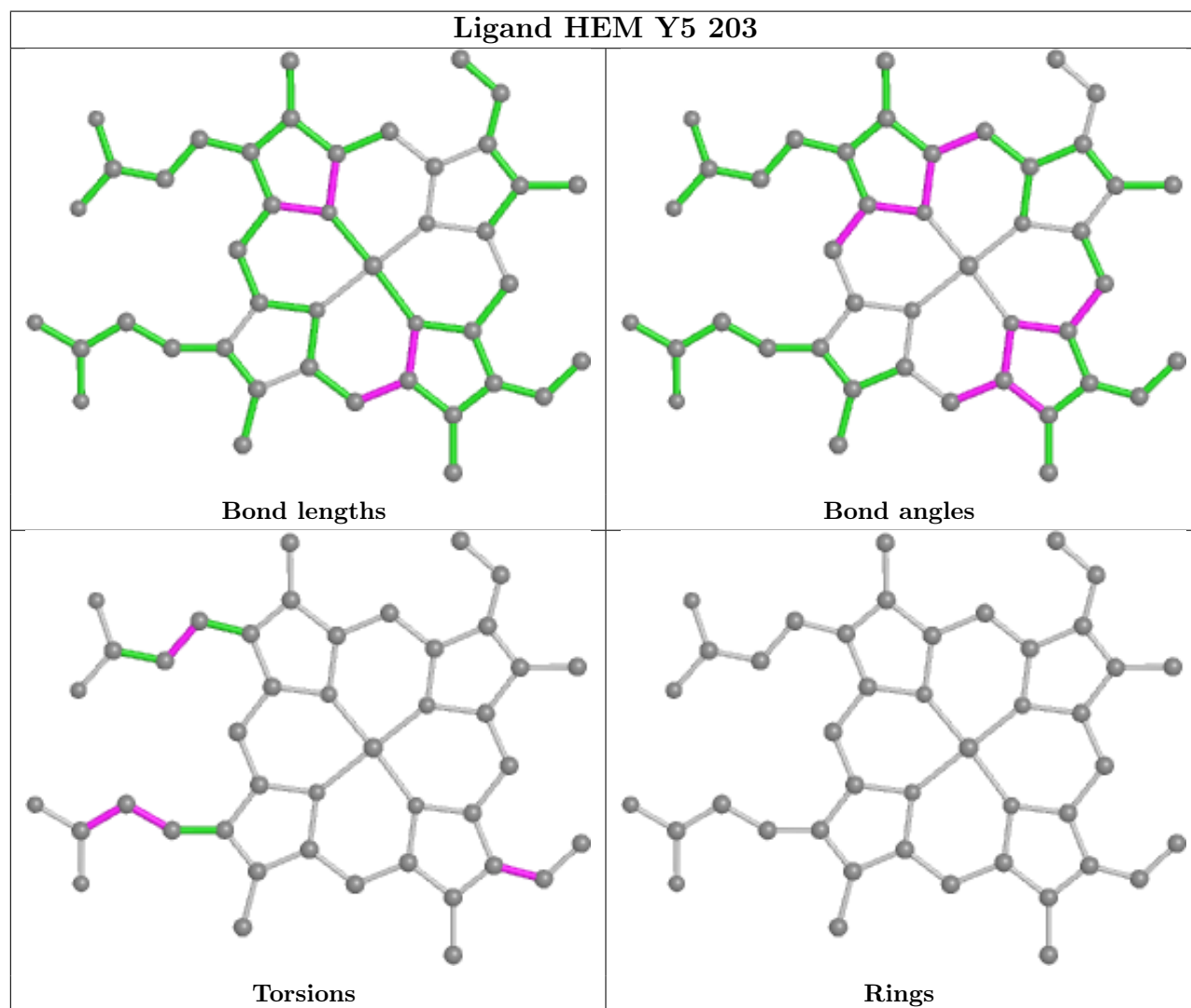
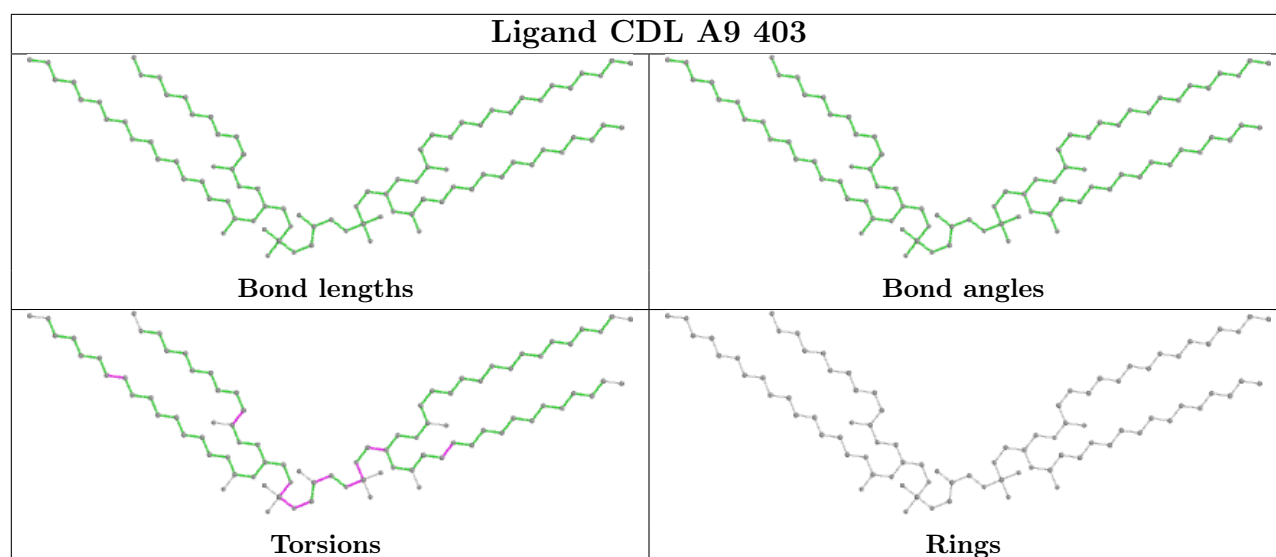


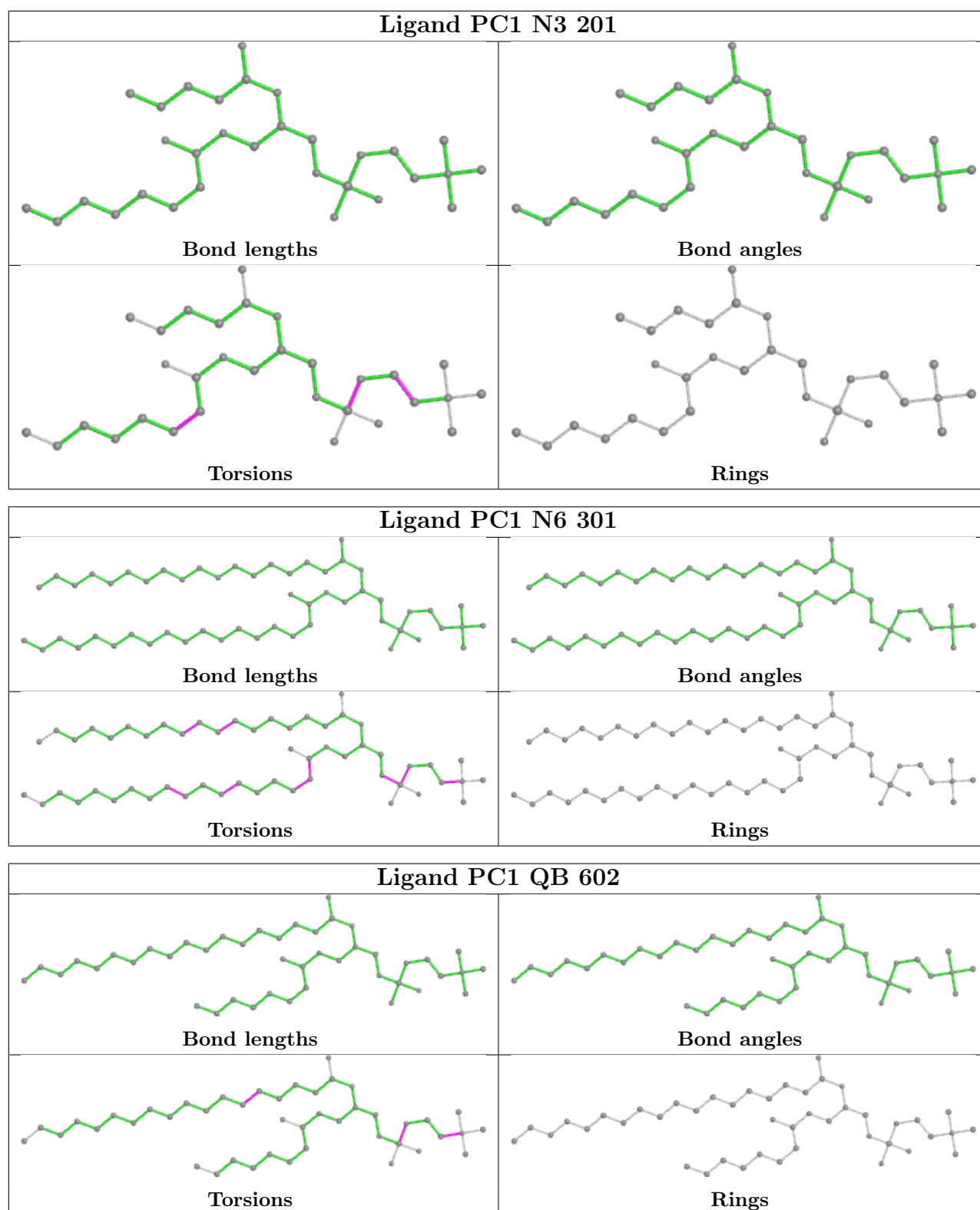


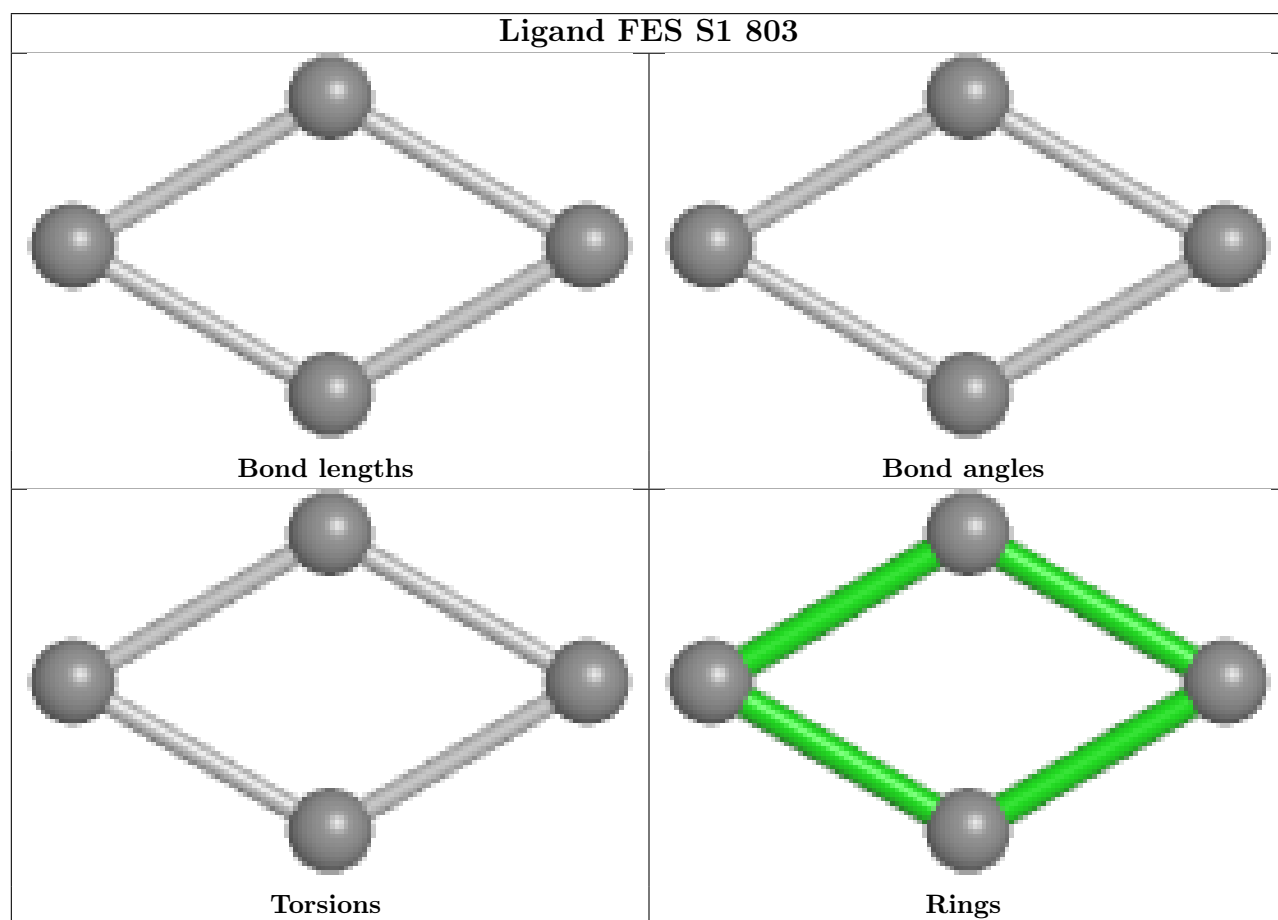
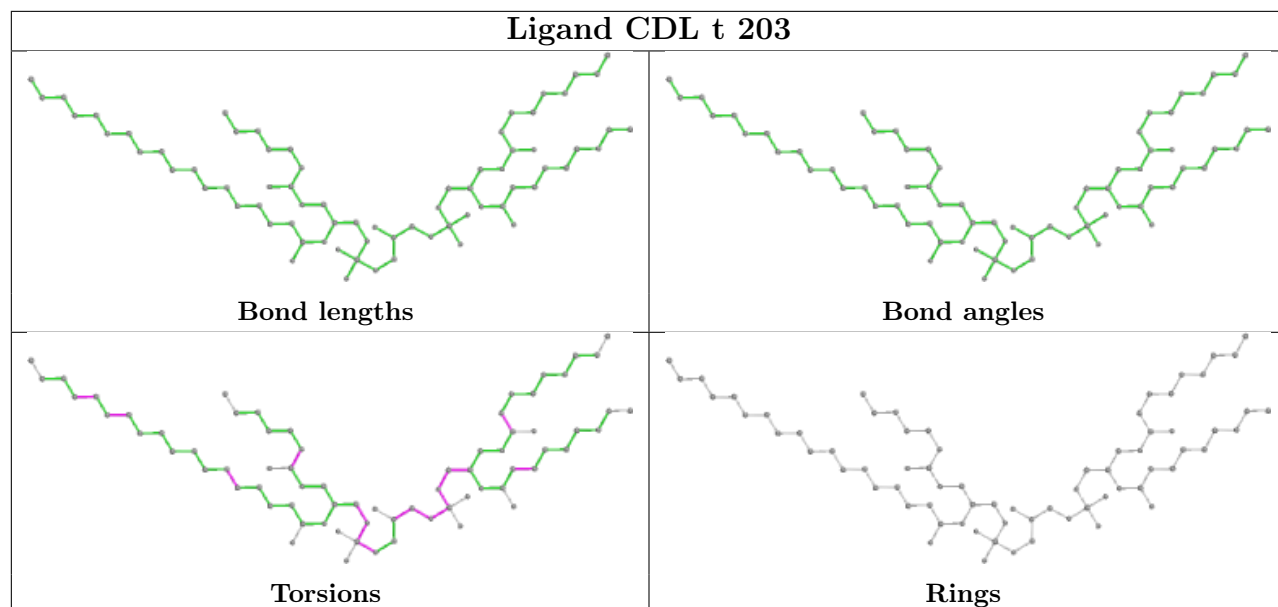


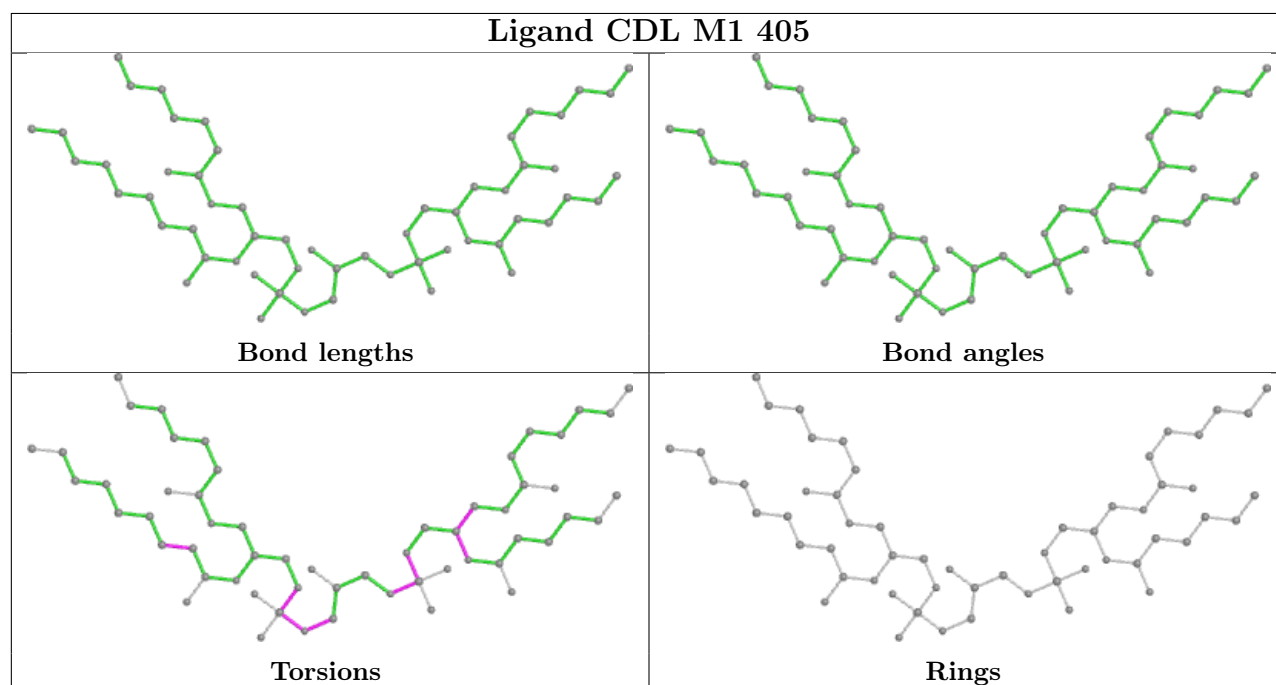
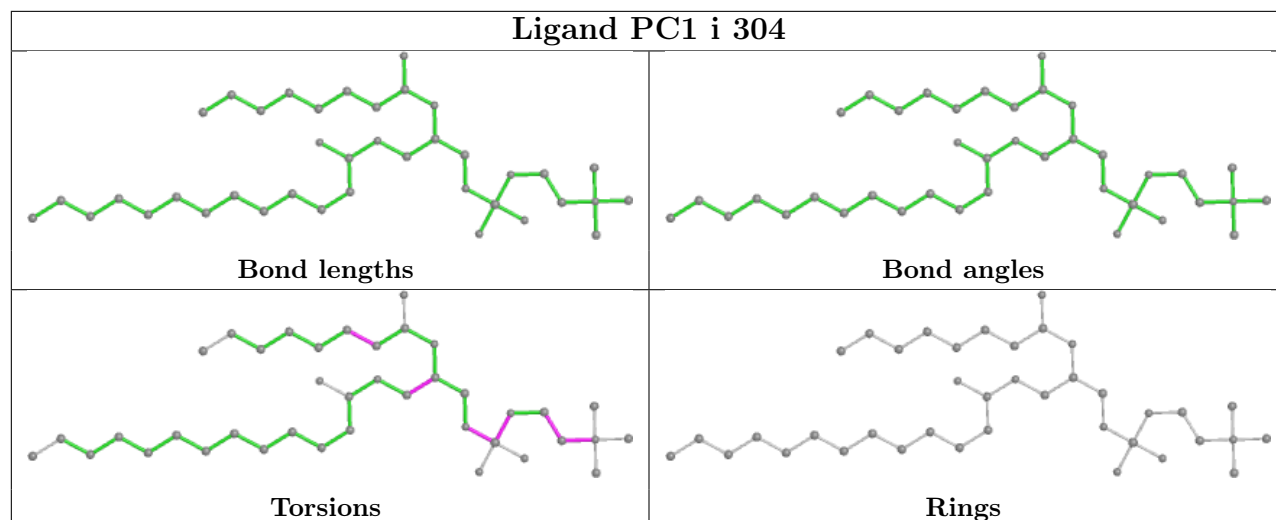


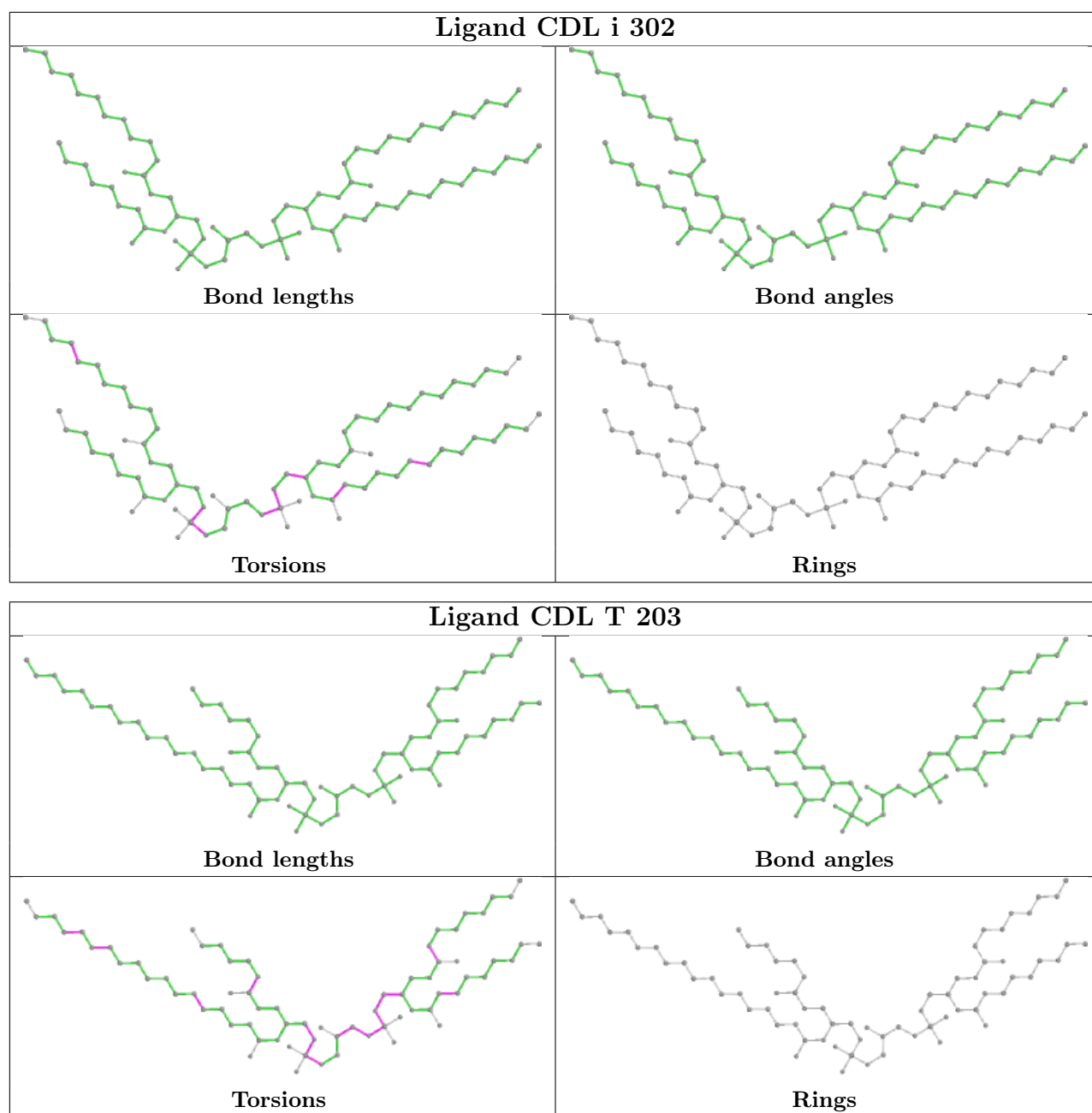


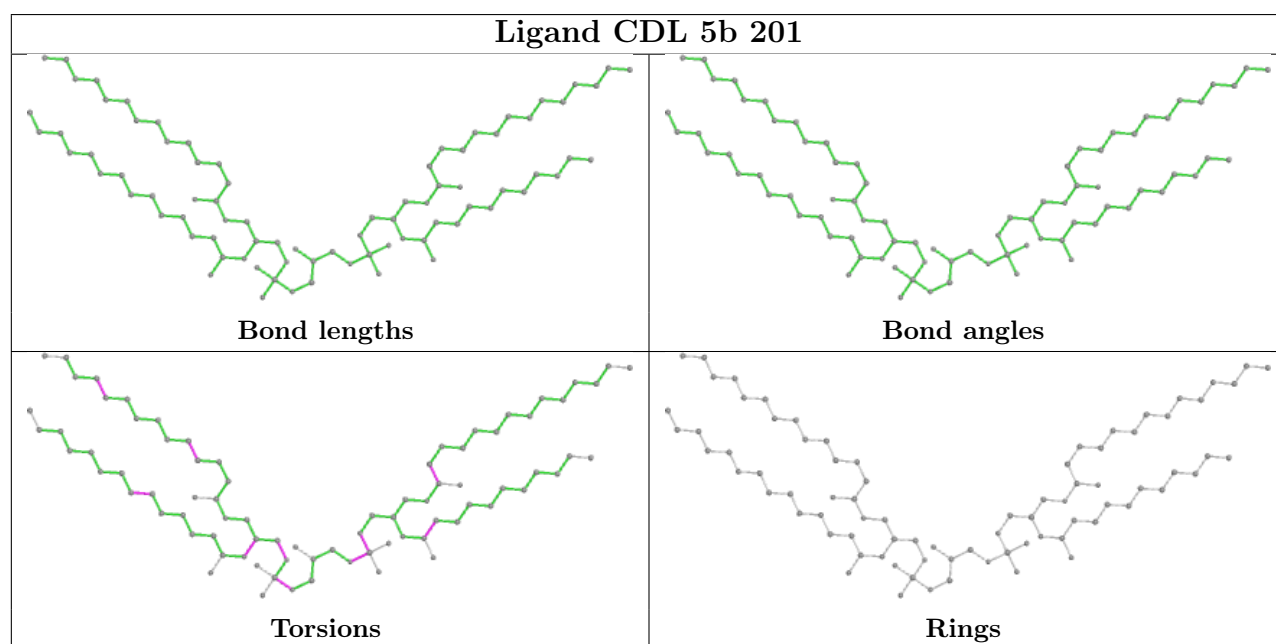
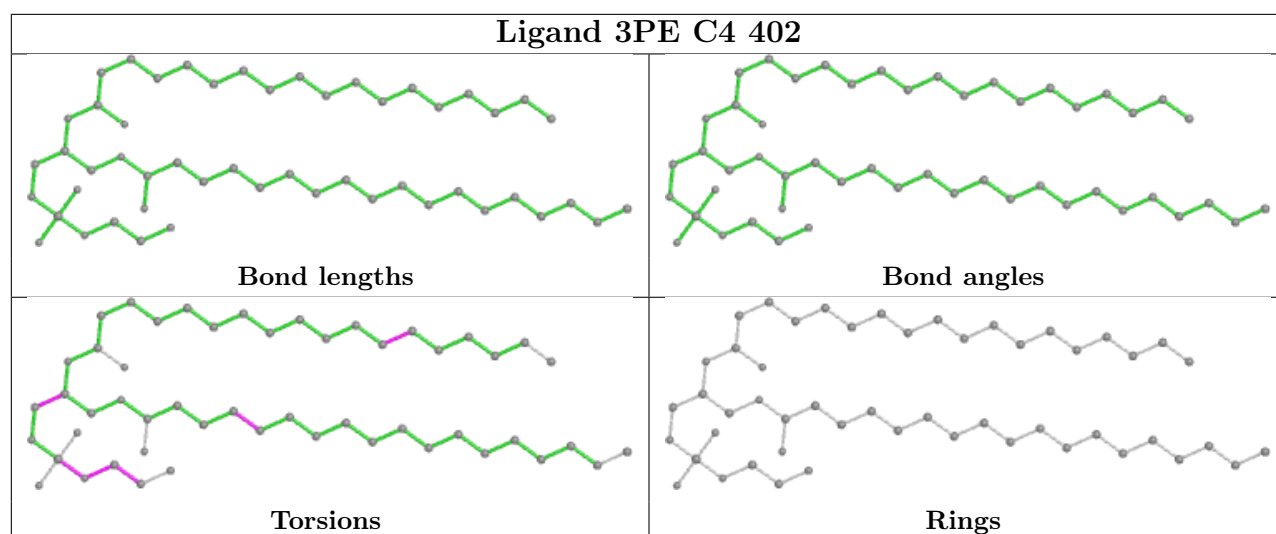


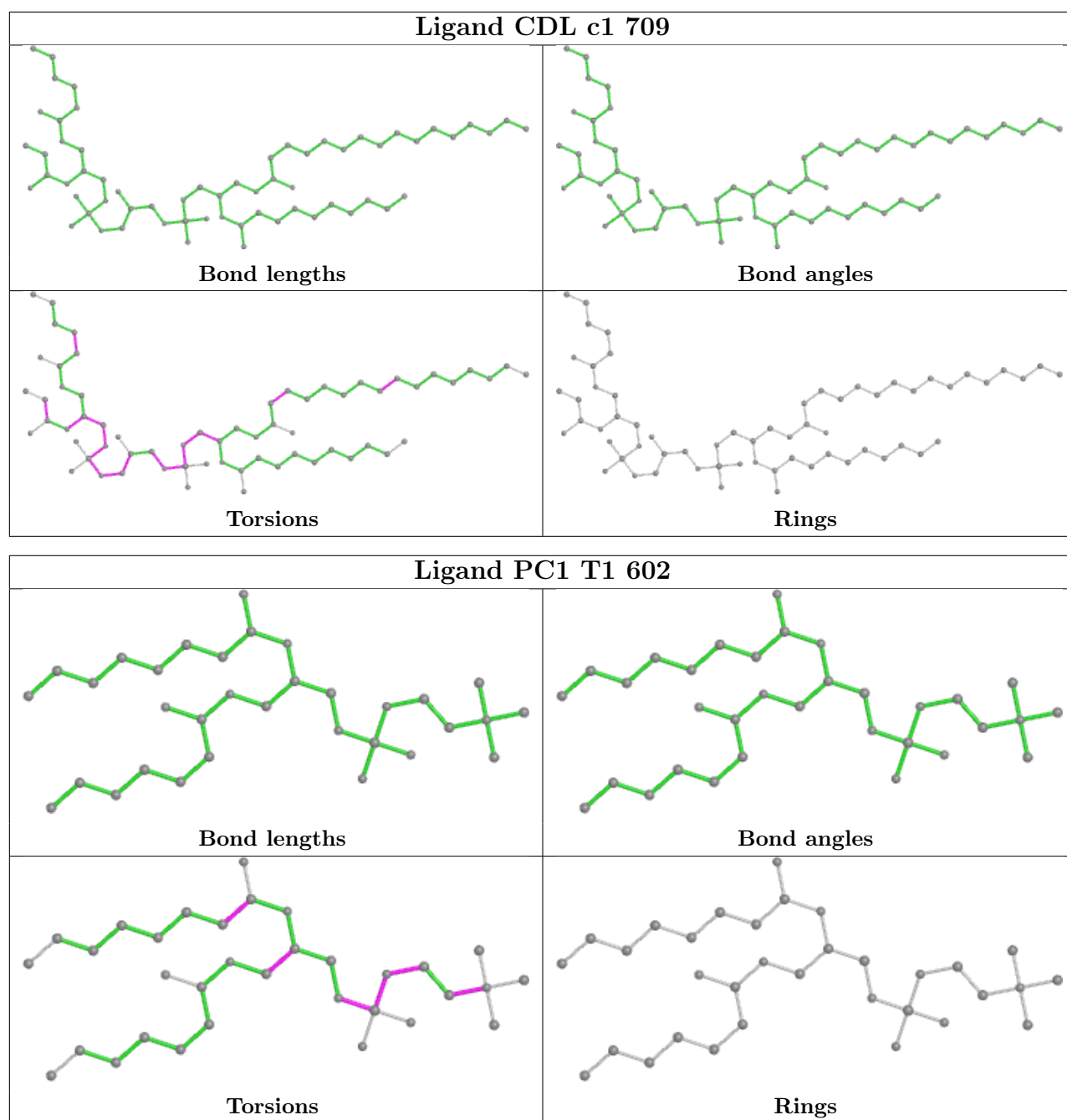












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

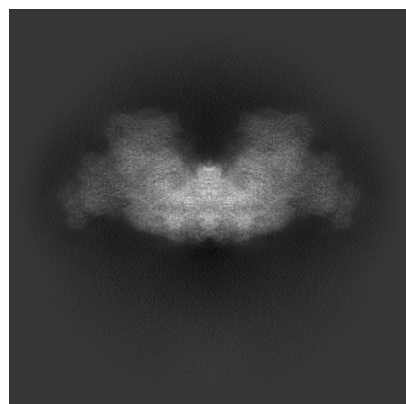
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34373. These allow visual inspection of the internal detail of the map and identification of artifacts.

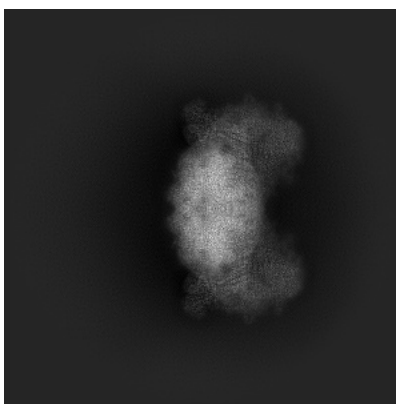
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

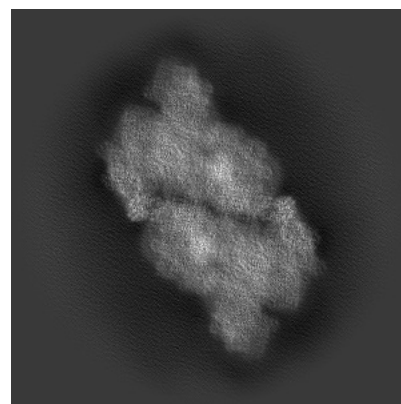
6.1.1 Primary map



X

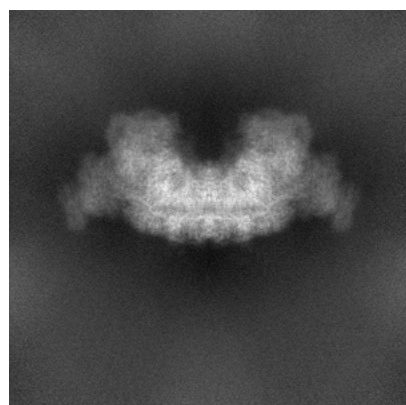


Y

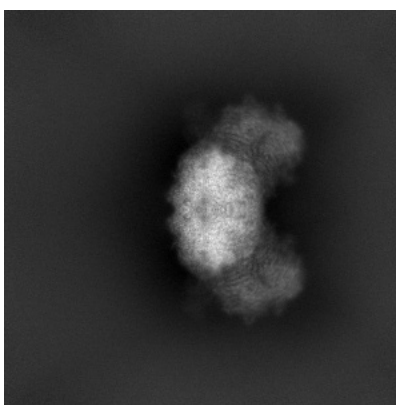


Z

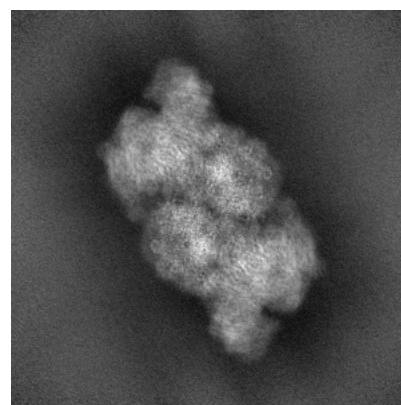
6.1.2 Raw map



X



Y

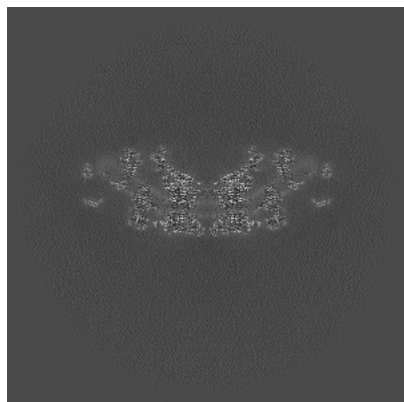


Z

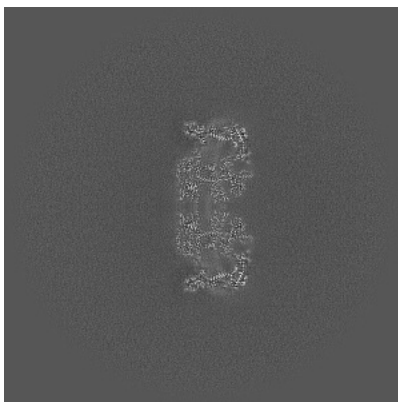
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

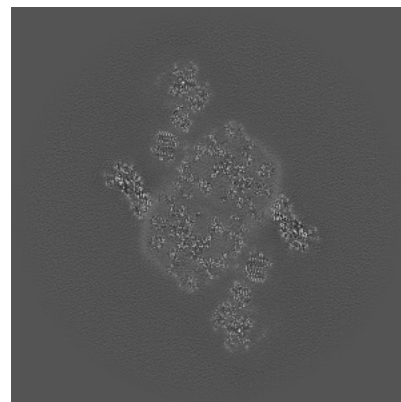
6.2.1 Primary map



X Index: 420

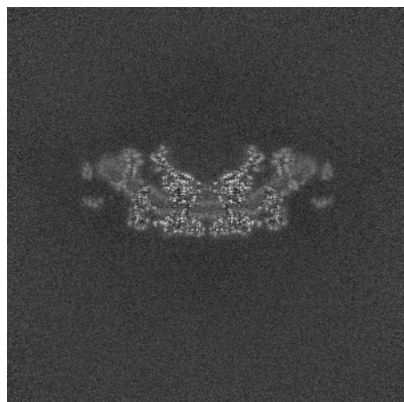


Y Index: 420

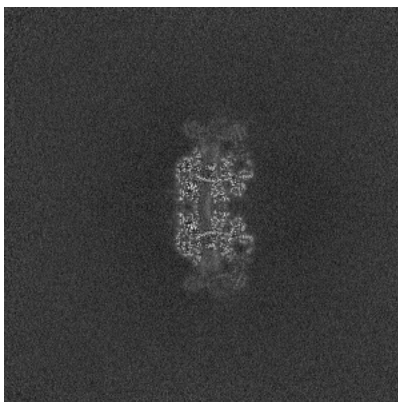


Z Index: 420

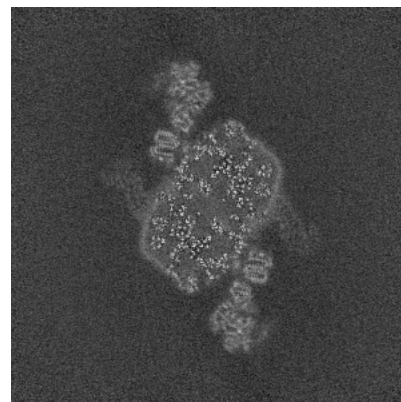
6.2.2 Raw map



X Index: 420



Y Index: 420

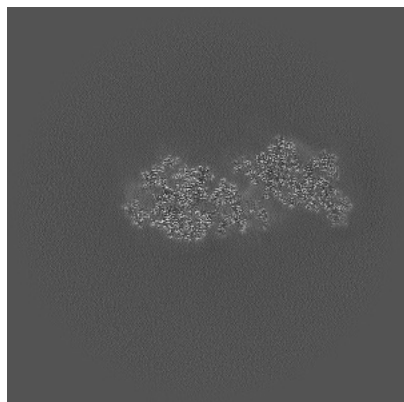


Z Index: 420

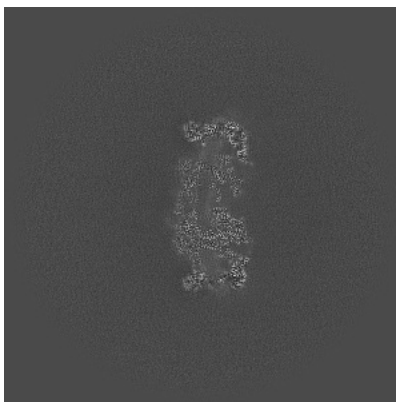
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

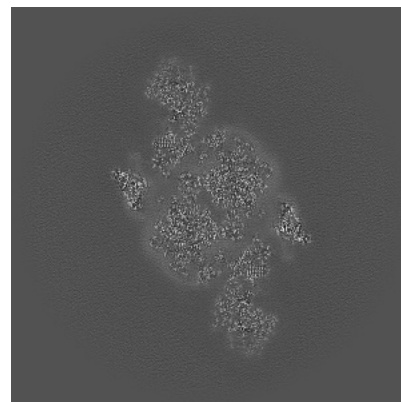
6.3.1 Primary map



X Index: 378

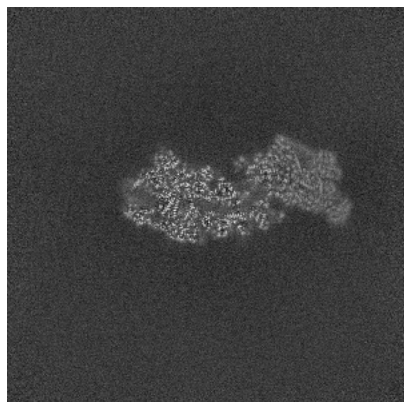


Y Index: 412

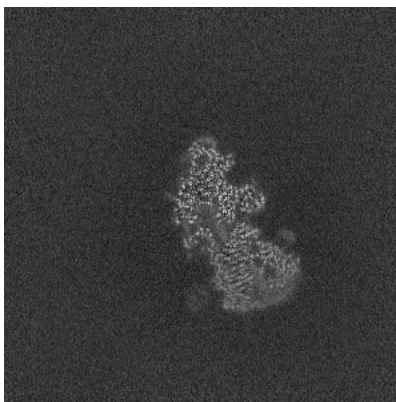


Z Index: 439

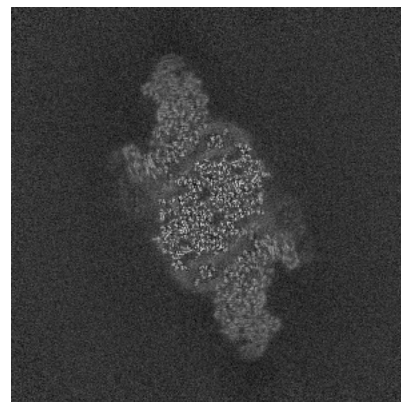
6.3.2 Raw map



X Index: 384



Y Index: 508

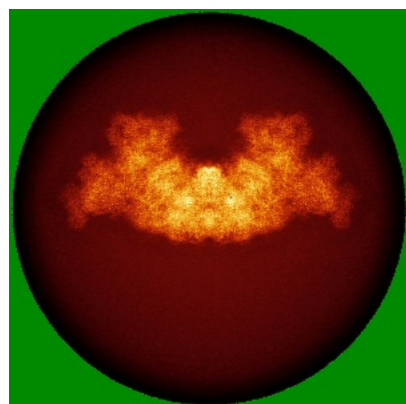


Z Index: 453

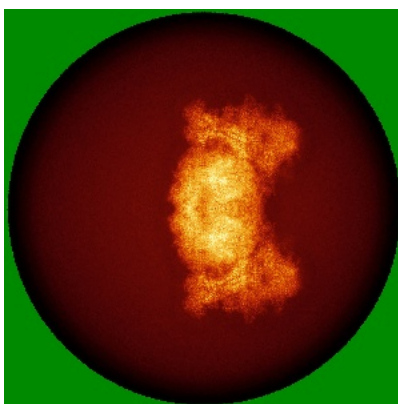
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

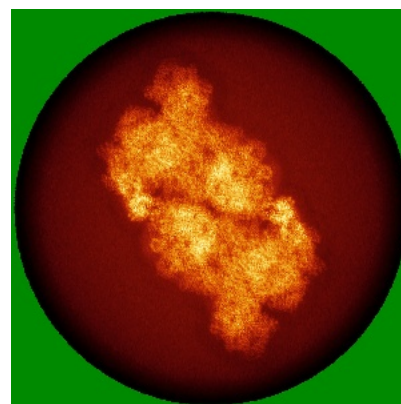
6.4.1 Primary map



X

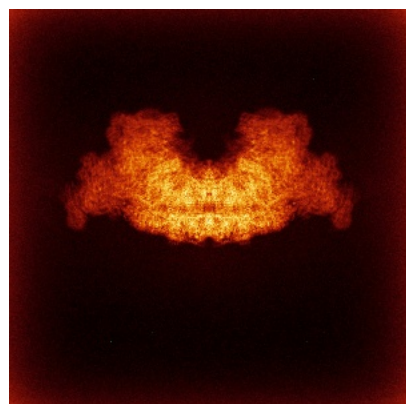


Y

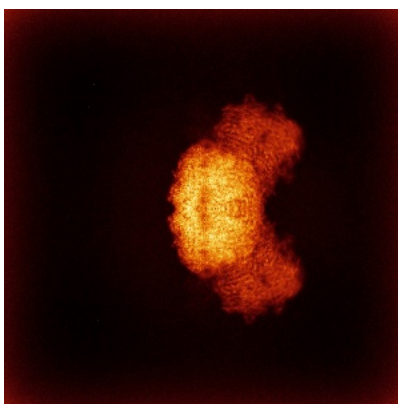


Z

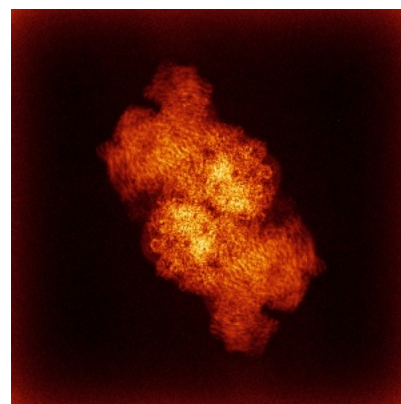
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

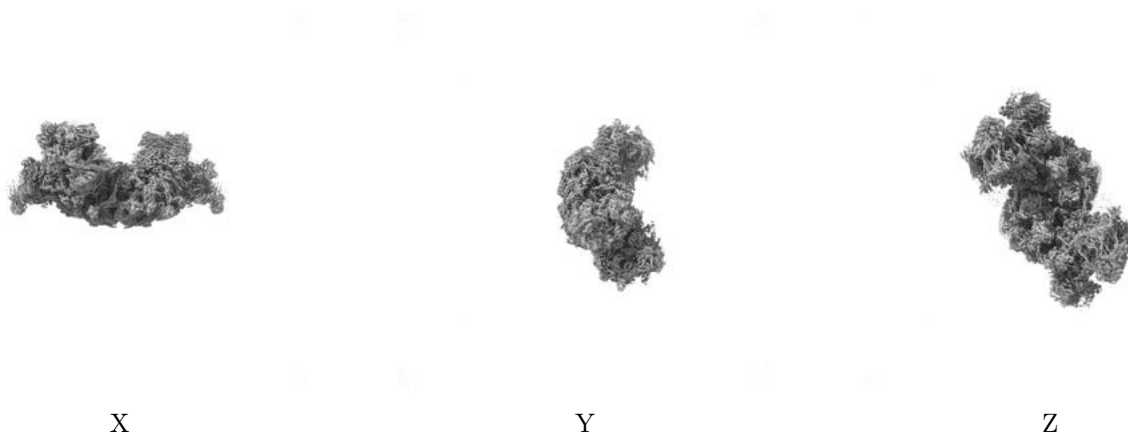
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

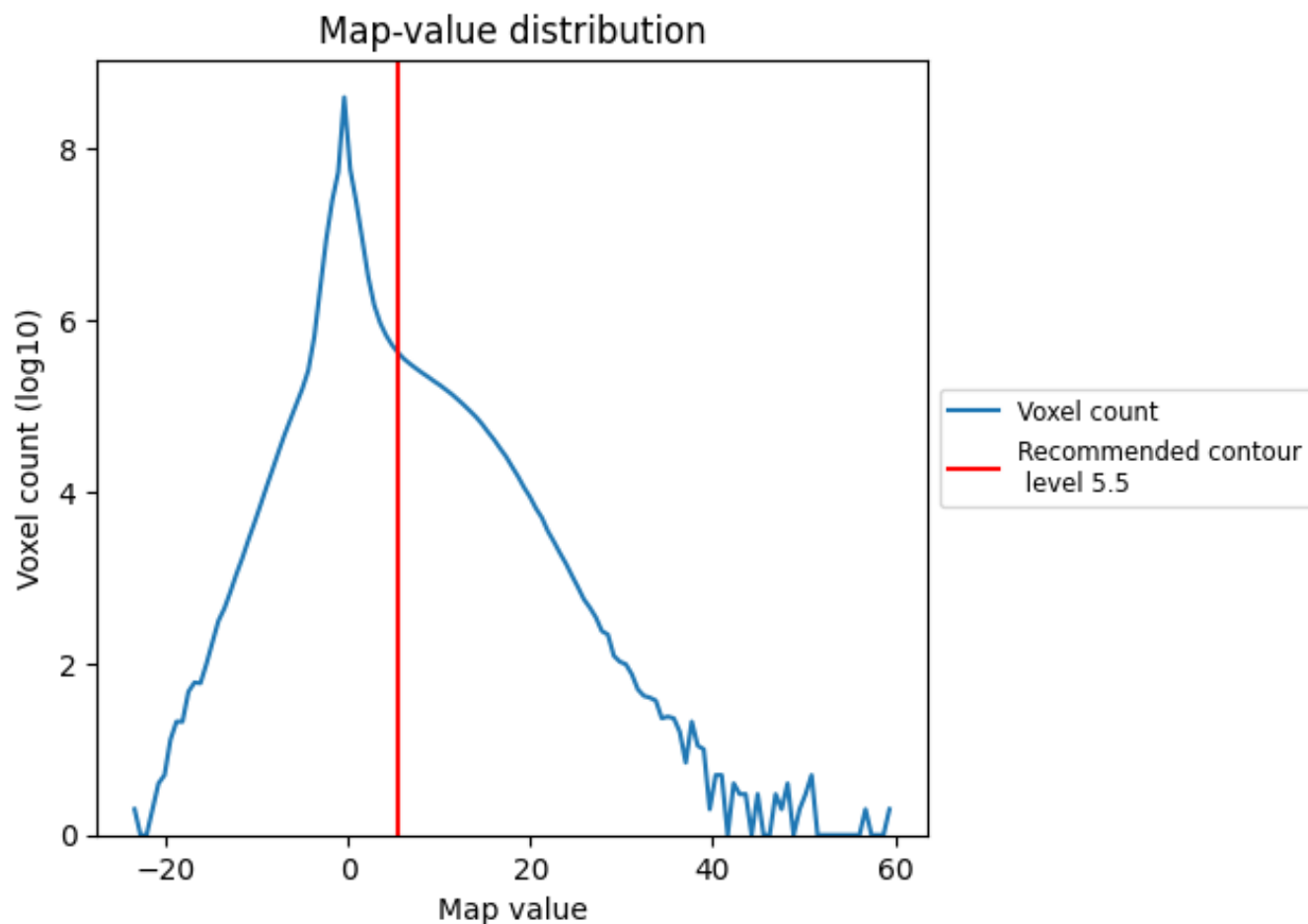
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

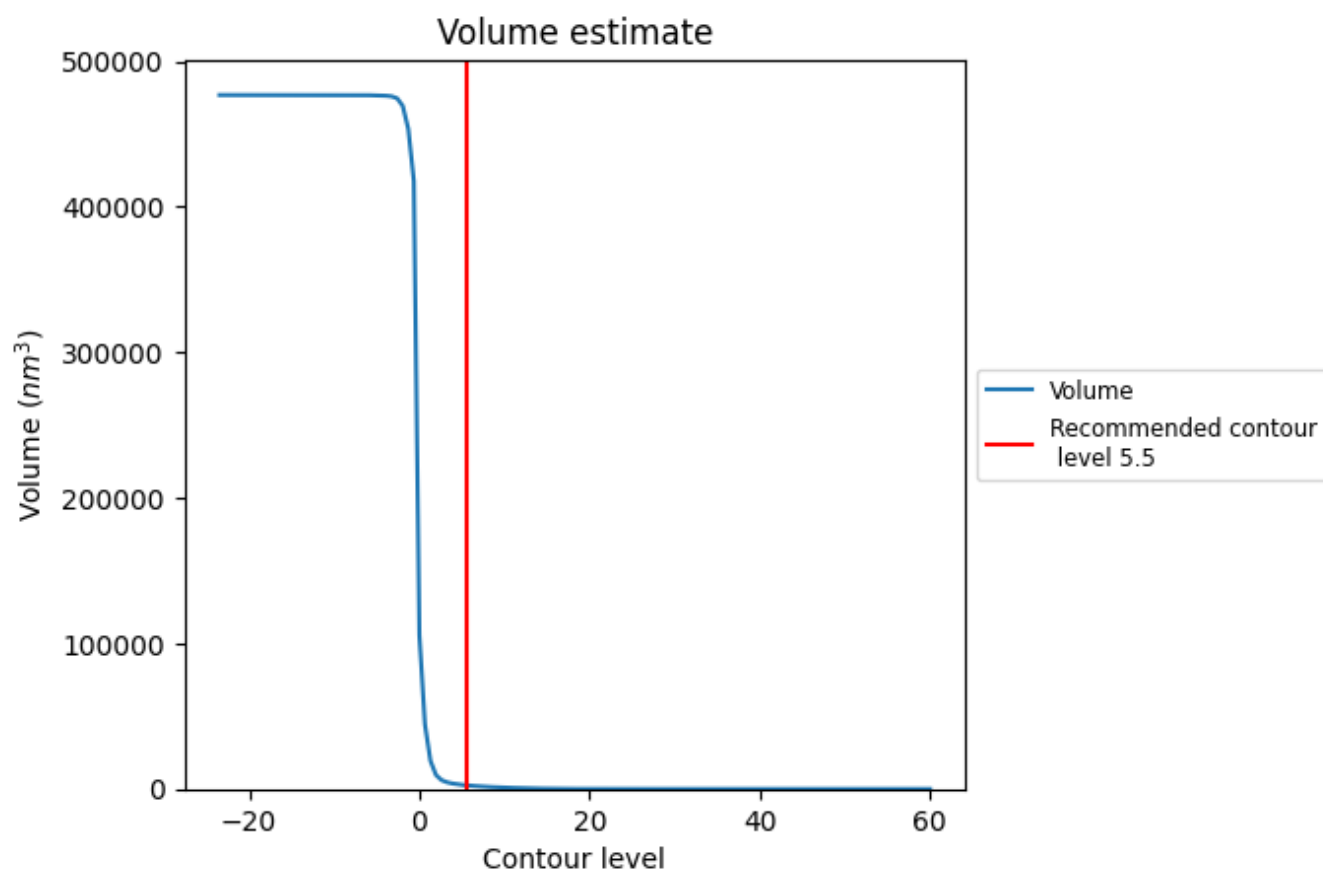
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

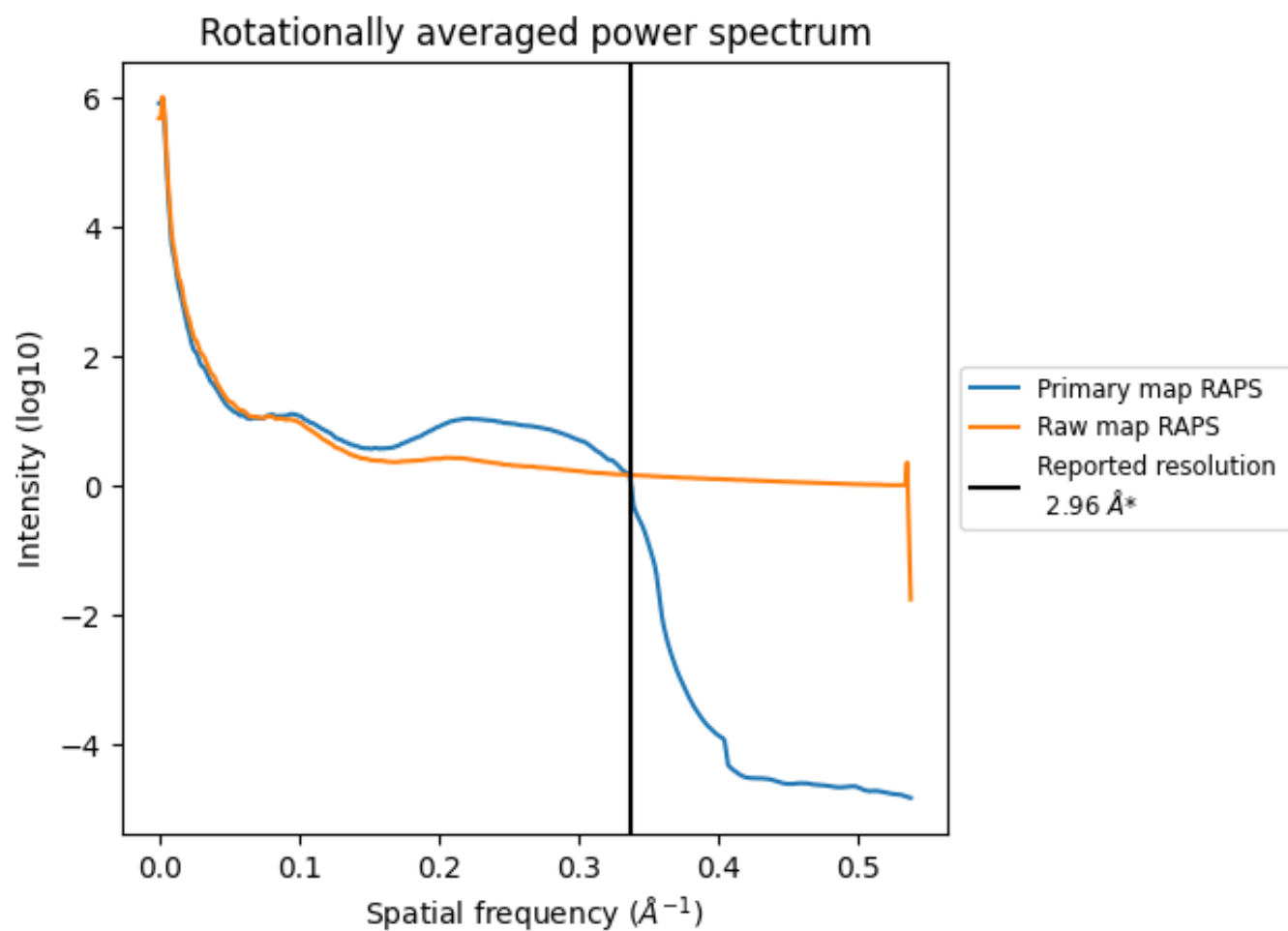
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2536 nm^3 ; this corresponds to an approximate mass of 2290 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

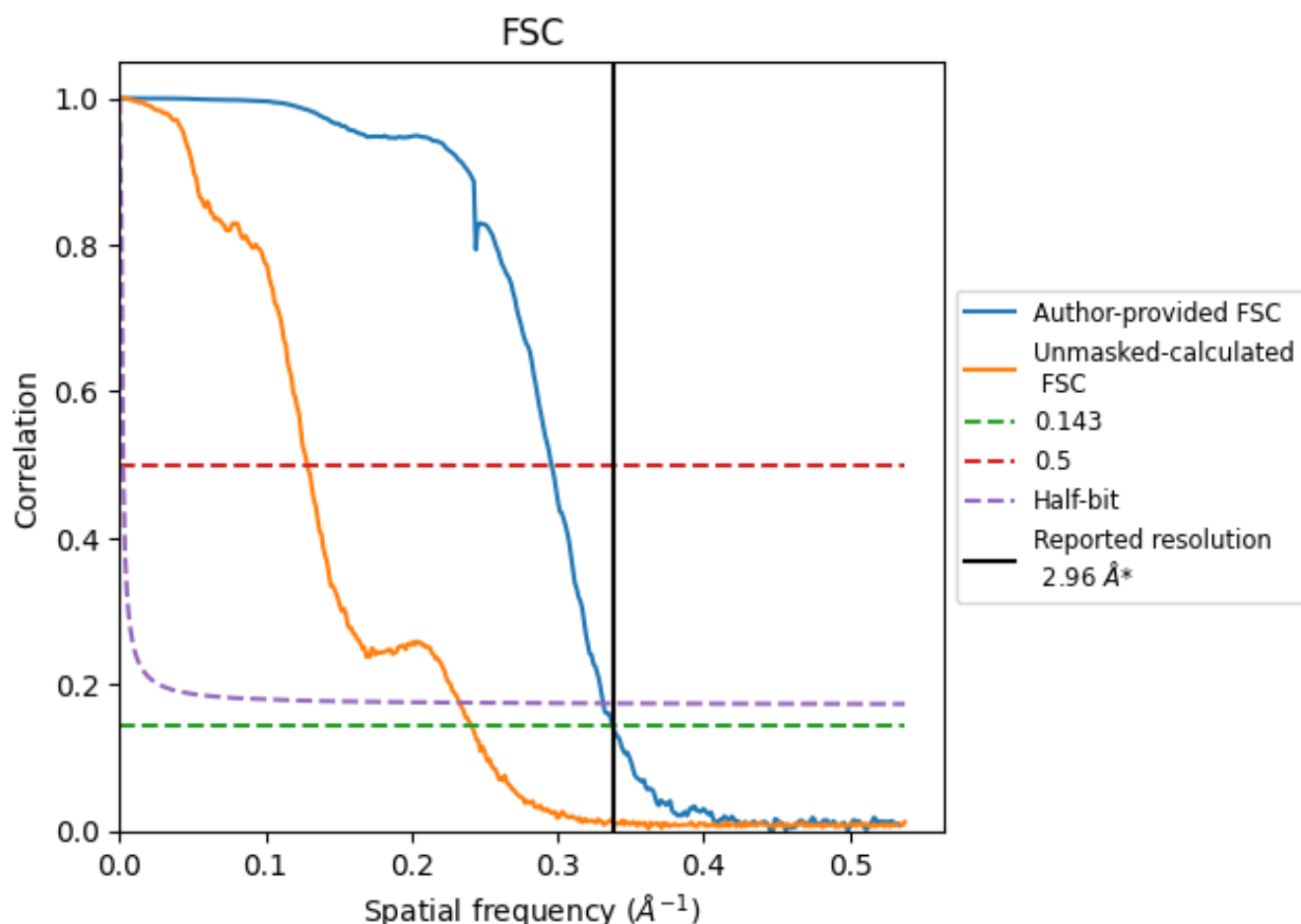


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

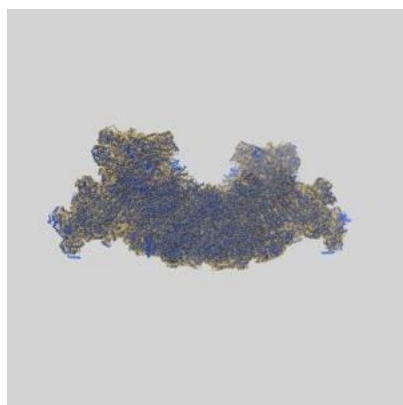
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.38	3.02
Unmasked-calculated*	4.15	7.78	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 2.96 by more than 10 %

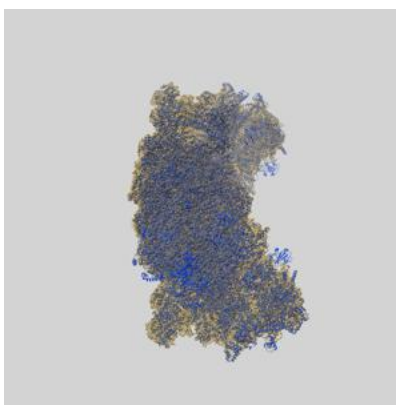
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34373 and PDB model 8GYM. Per-residue inclusion information can be found in [section 3](#) on [page 81](#).

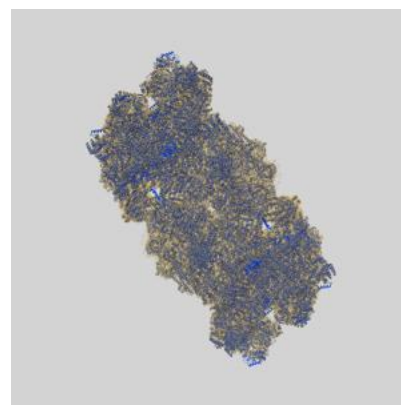
9.1 Map-model overlay [i](#)



X



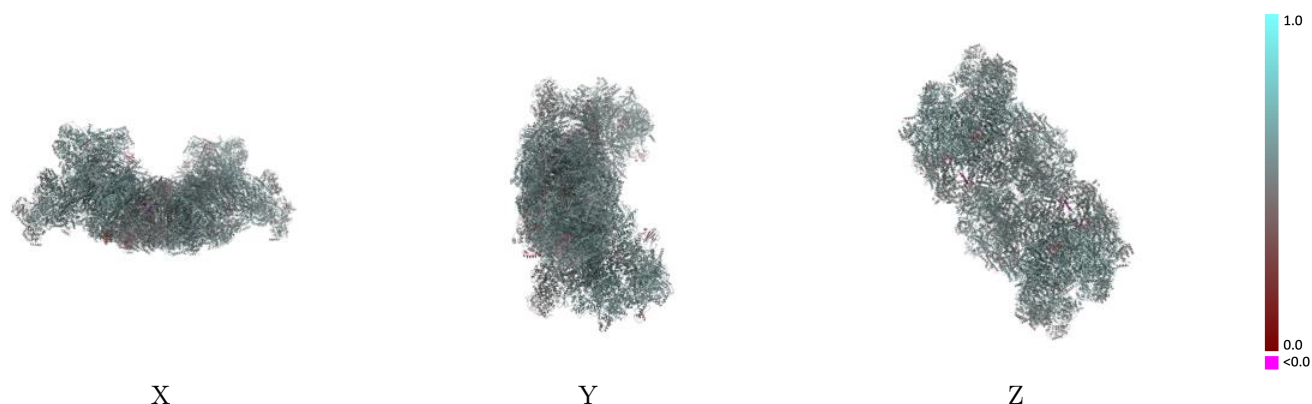
Y



Z

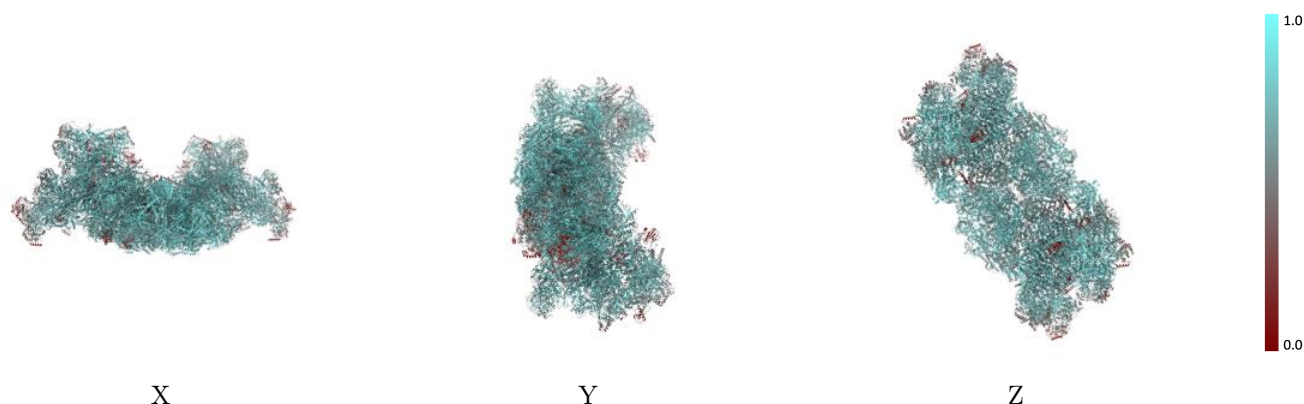
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



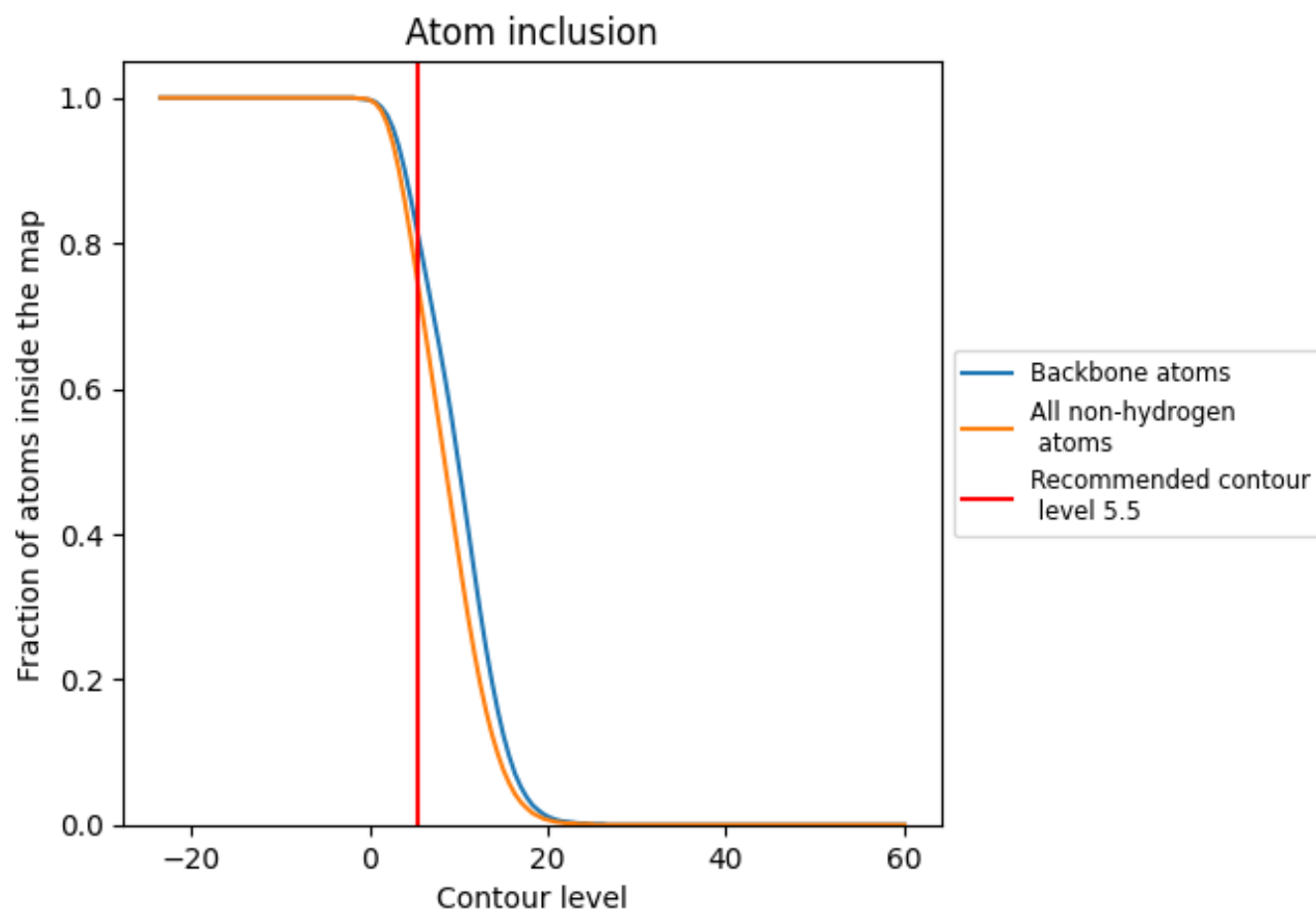
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.5560
1B	 0.8100	 0.6000
1T	 0.7970	 0.5540
1b	 0.8100	 0.6010
1t	 0.7970	 0.5530
2B	 0.8340	 0.6060
2E	 0.7130	 0.4660
2F	 0.8130	 0.5170
2G	 0.7650	 0.5060
2H	 0.8350	 0.4880
2I	 0.7720	 0.4860
2J	 0.7800	 0.4930
2K	 0.8000	 0.5180
2L	 0.8300	 0.4930
2M	 0.8460	 0.5290
2N	 0.8180	 0.5170
2O	 0.8480	 0.5140
2T	 0.6780	 0.5240
2b	 0.8340	 0.6030
2e	 0.7130	 0.4670
2f	 0.8130	 0.5150
2g	 0.7650	 0.5060
2h	 0.8350	 0.4860
2i	 0.7730	 0.4880
2j	 0.7870	 0.4970
2k	 0.8000	 0.5180
2l	 0.8300	 0.5010
2m	 0.8470	 0.5300
2n	 0.8120	 0.5150
2o	 0.8480	 0.5160
2t	 0.6780	 0.5220
3T	 0.6390	 0.5110
3t	 0.6410	 0.5070
4A	 0.8030	 0.5730
4L	 0.8160	 0.5960























































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
4T	 0.8030	 0.5430
4a	 0.8020	 0.5680
4l	 0.8170	 0.5960
4t	 0.8030	 0.5460
5B	 0.7820	 0.5970
5T	 0.6840	 0.5250
5b	 0.7810	 0.5960
5t	 0.6800	 0.5300
6A	 0.8000	 0.5630
6B	 0.8530	 0.5760
6C	 0.7880	 0.5460
6L	 0.7550	 0.5430
6T	 0.7230	 0.5270
6a	 0.8000	 0.5630
6b	 0.8530	 0.5740
6c	 0.7880	 0.5450
6l	 0.7550	 0.5450
6t	 0.7200	 0.5280
7A	 0.8230	 0.5770
7C	 0.8020	 0.5650
7L	 0.8110	 0.5670
7a	 0.8240	 0.5780
7c	 0.8040	 0.5640
7l	 0.8110	 0.5640
A	 0.8140	 0.5690
A1	 0.7460	 0.5910
A2	 0.6140	 0.5310
A3	 0.8070	 0.5960
A5	 0.7480	 0.5650
A6	 0.8350	 0.5950
A7	 0.6910	 0.5550
A8	 0.7900	 0.5900
A9	 0.7510	 0.5680
AB	 0.7580	 0.5870
AC	 0.7490	 0.5770
AL	 0.7400	 0.5780
AM	 0.7610	 0.5800
AN	 0.7360	 0.5850
B	 0.5360	 0.4790
B2	 0.6960	 0.5670
B3	 0.6410	 0.5610
B4	 0.7660	 0.5910





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B6	 0.7870	 0.5940
B7	 0.7590	 0.5710
B8	 0.7060	 0.5770
B9	 0.7830	 0.5890
BL	 0.8200	 0.5960
BM	 0.6820	 0.5620
BP	 0.7100	 0.5410
C	 0.4500	 0.4230
C1	 0.8230	 0.5670
C2	 0.8340	 0.5700
C3	 0.7730	 0.5490
C4	 0.7500	 0.5810
D	 0.7370	 0.5490
E	 0.7730	 0.5550
F	 0.7790	 0.5610
FS	 0.7890	 0.5670
FX	 0.8450	 0.5990
G	 0.8250	 0.5680
G1	 0.8580	 0.6060
G2	 0.8070	 0.5940
G3	 0.7790	 0.5810
H	 0.6900	 0.5160
I	 0.7220	 0.5430
J	 0.7560	 0.5670
J1	 0.7330	 0.5750
K	 0.7890	 0.5600
L	 0.7830	 0.5580
M	 0.7720	 0.5630
M1	 0.7860	 0.5530
M2	 0.7850	 0.5500
M3	 0.7710	 0.5560
N	 0.7960	 0.5660
N1	 0.7590	 0.5790
N2	 0.8230	 0.6010
N3	 0.7750	 0.5840
N4	 0.8290	 0.5950
N5	 0.6770	 0.5150
N6	 0.7900	 0.5960
O	 0.8560	 0.5710
P	 0.7370	 0.5430
P1	 0.7020	 0.5790
P2	 0.7180	 0.5760

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Q	 0.8470	 0.5690
QA	 0.6990	 0.5610
QB	 0.7790	 0.5830
QC	 0.7760	 0.5860
QD	 0.8320	 0.5990
QE	 0.5560	 0.4870
QF	 0.7010	 0.5690
QG	 0.6230	 0.5470
QH	 0.7790	 0.5940
QI	 0.7670	 0.5880
QJ	 0.7840	 0.5900
QL	 0.5640	 0.5540
QM	 0.8240	 0.5780
Qa	 0.6180	 0.5490
Qb	 0.6790	 0.5640
Qc	 0.7540	 0.5790
Qd	 0.7980	 0.5920
Qe	 0.4930	 0.4760
Qf	 0.5330	 0.5100
Qg	 0.6420	 0.5560
Qh	 0.7650	 0.5860
Qi	 0.6550	 0.5710
Qj	 0.7230	 0.5720
Ql	 0.6760	 0.5620
Qm	 0.8470	 0.5880
R	 0.7850	 0.5500
S	 0.7080	 0.5310
S1	 0.6940	 0.5540
S2	 0.7990	 0.5820
S3	 0.7890	 0.5780
S4	 0.7180	 0.5620
S5	 0.7760	 0.5920
S6	 0.6510	 0.5490
S7	 0.8210	 0.5870
S8	 0.8030	 0.5750
SA	 0.6350	 0.4790
SB	 0.7420	 0.5030
SC	 0.7570	 0.5080
SD	 0.8830	 0.5460
T	 0.7860	 0.5680
T1	 0.6060	 0.5210
T2	 0.2910	 0.4730





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T3	0.5540	0.5370
T4	0.5530	0.5240
T5	0.7240	0.5610
T6	0.7870	0.5900
T7	0.7060	0.5710
T8	0.7610	0.5850
T9	0.7880	0.5790
TA	0.7180	0.5600
TB	0.7710	0.5940
TC	0.7300	0.5840
TD	0.6320	0.5650
TE	0.6940	0.5760
TF	0.6720	0.5510
TG	0.5440	0.5120
TH	0.7770	0.5800
TX	0.7640	0.5840
U	0.7460	0.5510
U1	0.8220	0.5400
U2	0.8820	0.5480
V	0.7800	0.5590
V1	0.5920	0.5300
V2	0.4610	0.5070
VB	0.8000	0.5600
W	0.7380	0.5490
X	0.8620	0.5820
X1	0.7930	0.5900
Y	0.9100	0.5900
Y0	0.8650	0.5800
Y5	0.7220	0.5380
Y7	0.7200	0.5360
Z	0.7160	0.5390
Z1	0.8050	0.5550
a	0.8120	0.5700
a1	0.7720	0.5880
a2	0.6120	0.5300
a3	0.8090	0.6020
a5	0.7490	0.5670
a6	0.8370	0.5940
a7	0.6910	0.5550
a8	0.7900	0.5880
a9	0.7500	0.5670
ab	0.7580	0.5870





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ac	 0.7490	 0.5750
al	 0.7400	 0.5760
am	 0.7620	 0.5790
an	 0.7370	 0.5850
b	 0.5360	 0.4790
b2	 0.6950	 0.5670
b3	 0.6420	 0.5600
b4	 0.7660	 0.5880
b6	 0.7880	 0.5920
b7	 0.7600	 0.5750
b8	 0.7040	 0.5770
b9	 0.7820	 0.5860
bl	 0.8200	 0.5960
bm	 0.6820	 0.5610
bp	 0.7080	 0.5410
c	 0.4490	 0.4230
c1	 0.8230	 0.5670
c2	 0.8330	 0.5690
c3	 0.7740	 0.5480
c4	 0.7540	 0.5830
d	 0.7360	 0.5480
e	 0.7750	 0.5530
f	 0.7810	 0.5600
fs	 0.7870	 0.5670
fx	 0.8440	 0.5970
g	 0.8250	 0.5670
g1	 0.8570	 0.6070
g2	 0.8090	 0.5930
g3	 0.7790	 0.5790
h	 0.6890	 0.5160
i	 0.7200	 0.5430
j	 0.7560	 0.5640
j1	 0.7320	 0.5760
k	 0.7900	 0.5590
l	 0.7840	 0.5570
m	 0.7700	 0.5630
m1	 0.7870	 0.5530
m2	 0.7850	 0.5500
m3	 0.7710	 0.5570
n	 0.7940	 0.5640
n1	 0.7590	 0.5790
n2	 0.8240	 0.6010

















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n3	 0.7750	 0.5850
n4	 0.8280	 0.5930
n5	 0.6780	 0.5150
n6	 0.7890	 0.5940
o	 0.8550	 0.5720
p	 0.7360	 0.5410
p1	 0.7020	 0.5790
p2	 0.7160	 0.5760
q	 0.8240	 0.5630
qA	 0.6980	 0.5610
qB	 0.7800	 0.5820
qC	 0.7770	 0.5840
qD	 0.8340	 0.5980
qE	 0.5560	 0.4890
qF	 0.6960	 0.5650
qG	 0.6220	 0.5450
qH	 0.7790	 0.5920
qI	 0.7670	 0.5870
qJ	 0.7900	 0.5910
qL	 0.5640	 0.5510
qM	 0.8240	 0.5800
qa	 0.6180	 0.5470
qb	 0.6800	 0.5640
qc	 0.7530	 0.5790
qd	 0.7980	 0.5920
qe	 0.4950	 0.4750
qf	 0.5280	 0.5110
qg	 0.6410	 0.5570
qh	 0.7670	 0.5860
qi	 0.6550	 0.5690
qj	 0.7230	 0.5720
ql	 0.6680	 0.5630
qm	 0.8470	 0.5840
r	 0.7840	 0.5500
s	 0.7080	 0.5290
s1	 0.6950	 0.5540
s2	 0.7980	 0.5800
s3	 0.7890	 0.5770
s4	 0.7160	 0.5620
s5	 0.7770	 0.5870
s6	 0.6500	 0.5460
s7	 0.8220	 0.5870

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
s8	 0.8020	 0.5740
sa	 0.6340	 0.4790
sb	 0.7440	 0.5050
sc	 0.7550	 0.5110
sd	 0.8830	 0.5450
t	 0.7870	 0.5670
t1	 0.6050	 0.5210
t2	 0.2900	 0.4720
t3	 0.5550	 0.5360
t4	 0.5520	 0.5230
t5	 0.7220	 0.5620
t6	 0.7830	 0.5920
t7	 0.7010	 0.5710
t8	 0.7590	 0.5860
t9	 0.7880	 0.5770
ta	 0.7210	 0.5600
tb	 0.7710	 0.5970
tc	 0.7330	 0.5820
td	 0.6110	 0.5660
te	 0.6960	 0.5730
tf	 0.6720	 0.5500
tg	 0.5390	 0.5120
th	 0.7760	 0.5780
tx	 0.7640	 0.5840
u	 0.7460	 0.5510
u1	 0.8220	 0.5380
u2	 0.8820	 0.5380
v	 0.7790	 0.5600
v1	 0.5920	 0.5300
v2	 0.4630	 0.5090
vb	 0.8100	 0.5620
w	 0.7390	 0.5480
x	 0.8590	 0.5840
x1	 0.7950	 0.5880
y	 0.9100	 0.5900
y0	 0.8660	 0.5810
y5	 0.7220	 0.5370
y7	 0.7210	 0.5360
z	 0.7180	 0.5420
z1	 0.8030	 0.5530