



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:51 PM EDT

PDB ID : 8GYM / pdb_00008gym
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

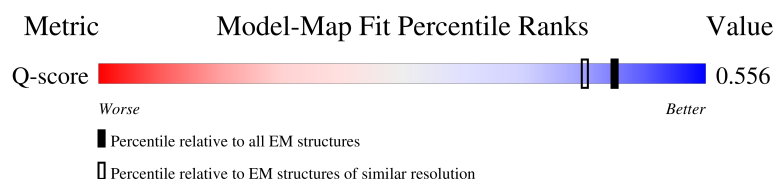
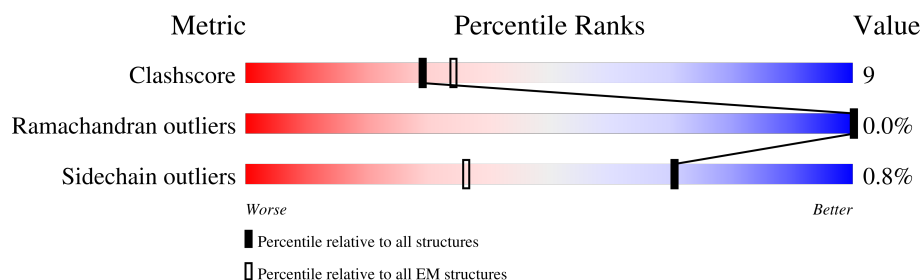
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



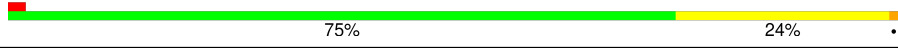
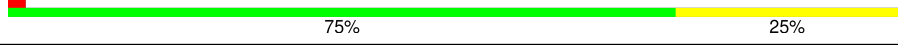
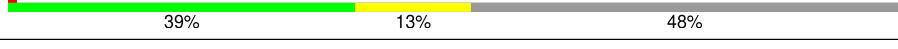
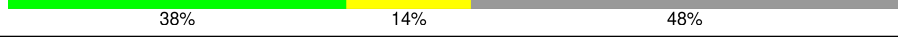
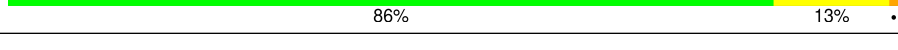
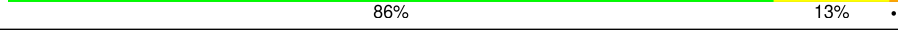
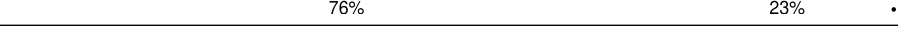
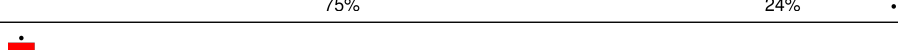
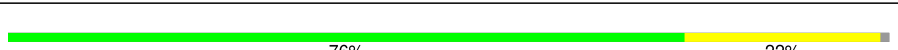
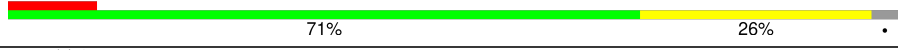
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	
1	1t	72	
2	2E	322	
2	2e	322	

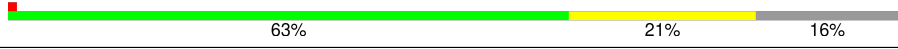
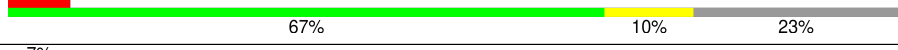
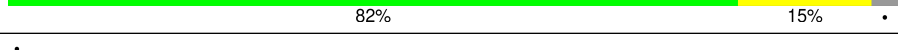
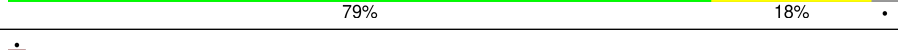
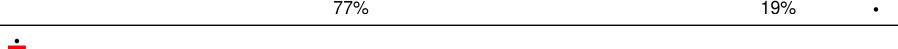
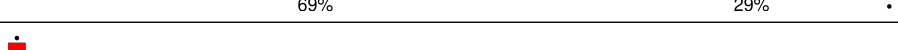
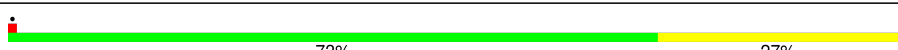
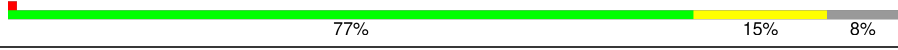
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	2F	296	
3	2f	296	
4	2G	198	
4	2g	198	
5	2H	195	
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	

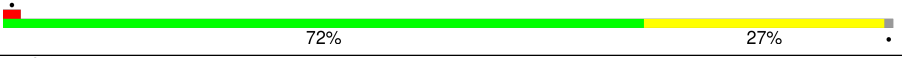
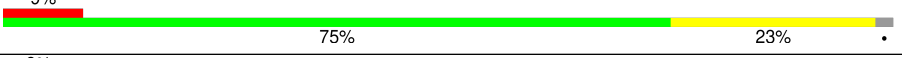
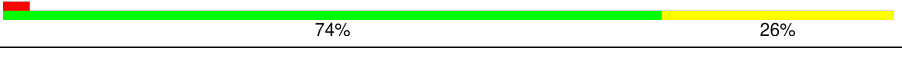
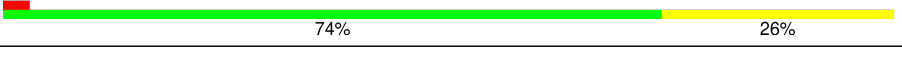
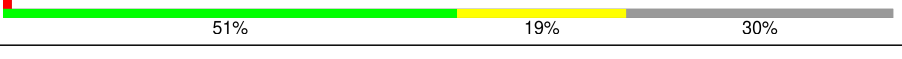
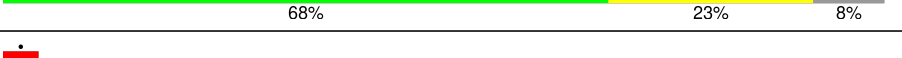
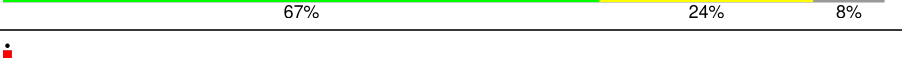
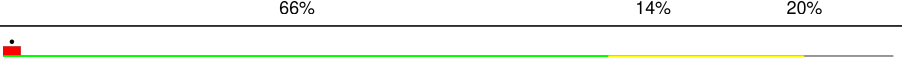
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	4a	127	
16	4T	68	
16	4t	68	
17	5T	81	
17	5t	81	
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	

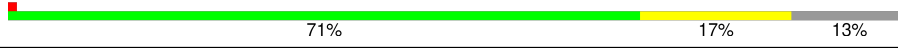
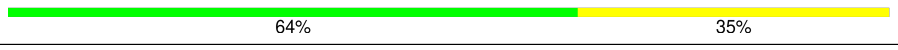
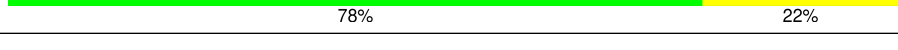
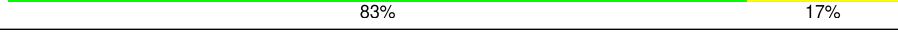
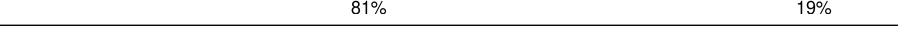
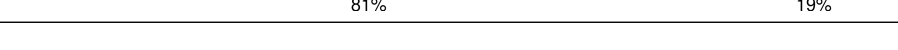
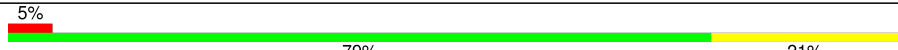
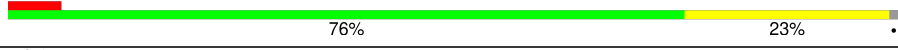
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BP	462	
28	bp	462	
29	C1	688	
29	c1	688	
30	C2	604	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	k	231	
41	L	222	
41	l	222	
42	M	220	
42	m	220	
43	M1	346	
43	m1	346	
44	M2	318	
44	m2	318	
45	M3	330	
45	m3	330	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	SA	636	
52	sa	636	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	SB	312	
53	sb	312	
54	SC	60	
54	sc	60	
55	SD	44	
55	sd	44	
56	T	158	
56	t	158	
57	U	154	
57	u	154	
58	V	149	
58	v	149	
59	VB	637	
59	vb	637	
60	W	124	
60	w	124	
61	X	122	
61	x	122	
62	Y	105	
62	y	105	
63	Y0	89	
63	y0	89	
64	Y5	190	
64	y5	190	
65	Y7	453	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
65	y7	453	
66	Z	90	
66	z	90	
67	Z1	100	
67	z1	100	
68	1B	59	
68	1b	59	
69	2B	178	
69	2b	178	
70	4L	116	
70	4l	116	
71	5B	100	
71	5b	100	
72	A1	94	
72	a1	94	
73	A2	103	
73	a2	103	
74	A3	135	
74	a3	135	
75	A5	206	
75	a5	206	
76	A6	172	
76	a6	172	
77	A7	282	
77	a7	282	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	A8	238	
78	a8	238	
79	A9	362	
79	a9	362	
80	AB	138	
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	

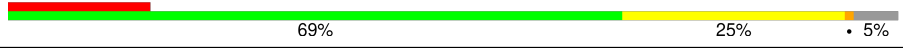
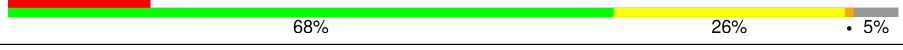
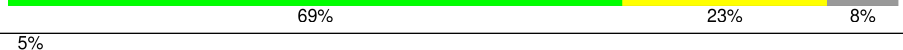
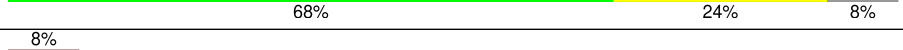
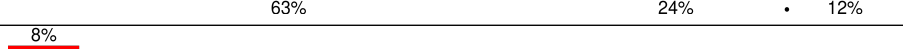
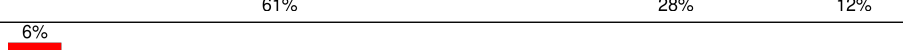
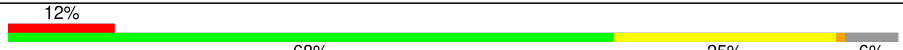
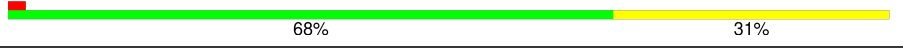
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
90	b8	207	
91	B9	189	
91	b9	189	
92	BL	188	
92	bl	188	
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	

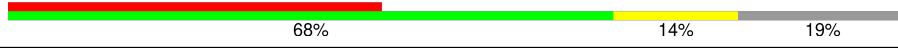
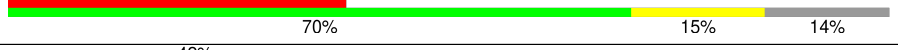
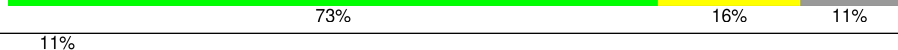
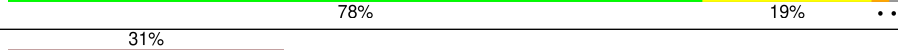
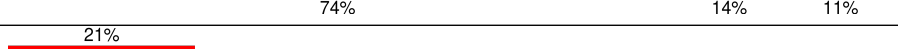
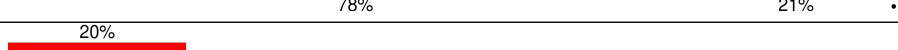
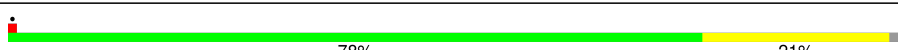
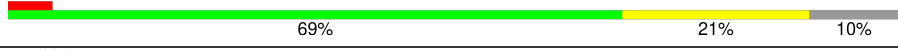
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
103	N4	505	
103	n4	505	
104	N5	750	
104	n5	750	
105	N6	255	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
111	qd	319	
112	QE	269	
112	Qe	269	
112	qE	269	
112	qe	269	
113	QF	90	
113	Qf	90	
113	qF	90	
113	qf	90	
114	QG	328	
114	Qg	328	
114	qG	328	
114	qg	328	
115	QH	130	
115	Qh	130	
115	qH	130	
115	qh	130	
116	QI	119	
116	Qi	119	
116	qI	119	
116	qi	119	
117	QJ	62	
117	Qj	62	
117	qJ	62	
117	qj	62	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
118	QL	41	
118	Ql	41	
118	qL	41	
118	ql	41	
119	QM	17	
119	Qm	17	
119	U2	17	
119	qM	17	
119	qm	17	
119	u2	17	
120	S1	718	
120	s1	718	
121	S2	442	
121	s2	442	
122	S3	198	
122	s3	198	
123	S4	185	
123	s4	185	
124	S5	94	
124	s5	94	
125	S6	132	
125	s6	132	
126	S7	162	
126	s7	162	
127	S8	236	

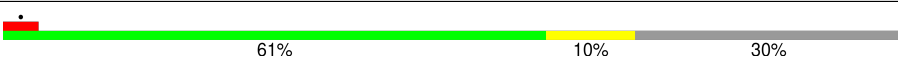
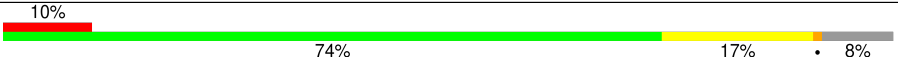
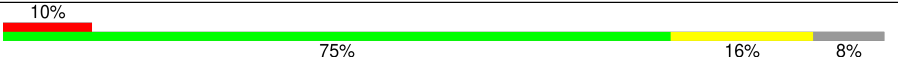
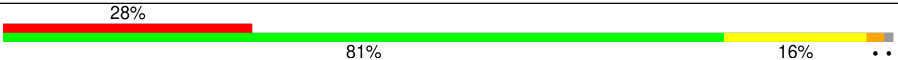
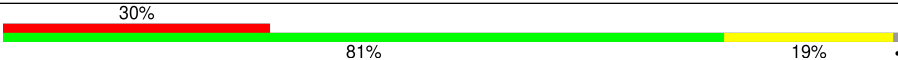
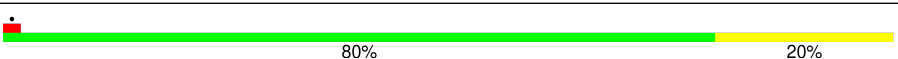
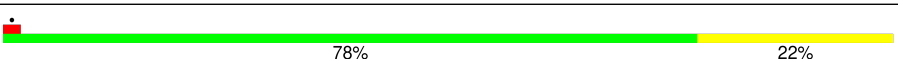
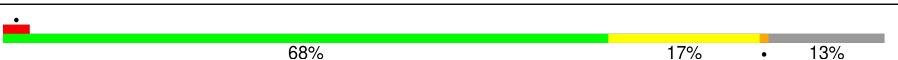
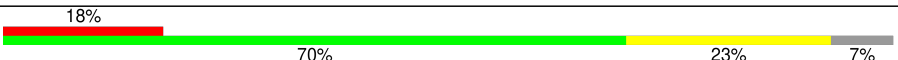
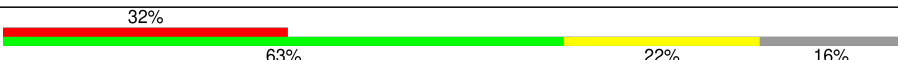
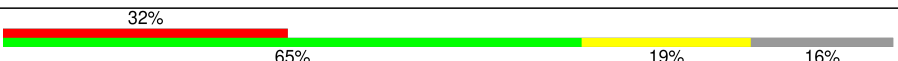
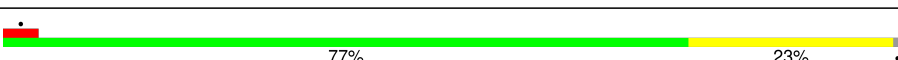
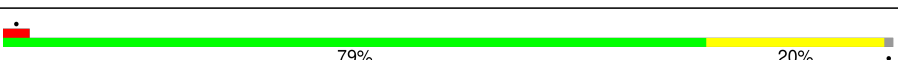
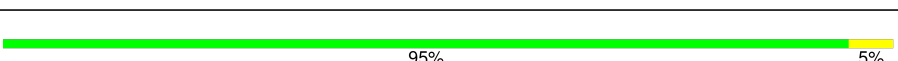
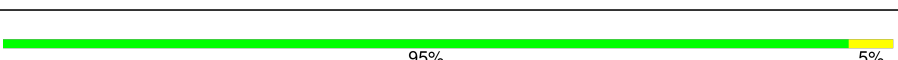
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
127	s8	236	
128	T1	516	
128	t1	516	
129	T2	333	
129	t2	333	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
140	TD	73	
140	td	73	
141	TE	71	
141	te	71	
142	TF	236	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
162	SF4	S1	801	-	-	X	-
162	SF4	S7	201	-	-	X	-
162	SF4	S8	302	-	-	X	-
162	SF4	s1	801	-	-	X	-
162	SF4	s7	201	-	-	X	-
162	SF4	s8	302	-	-	X	-

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 YftT 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		0	0
			481	314	85	82			
54	SC	58	Total	C	N	O		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		

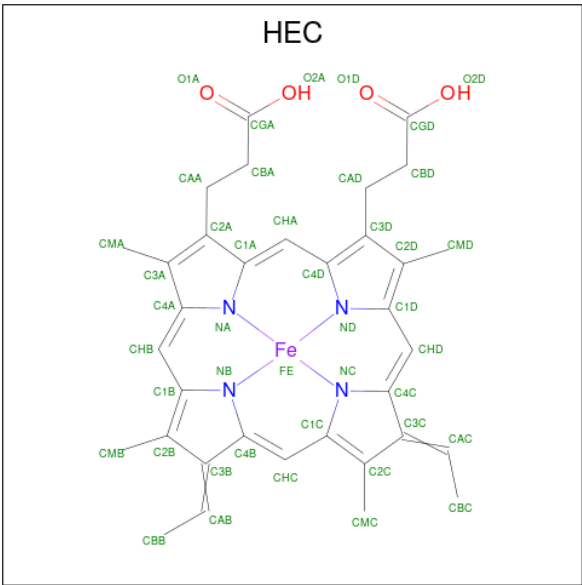
- Molecule 149 is a protein called COXTT3.

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.

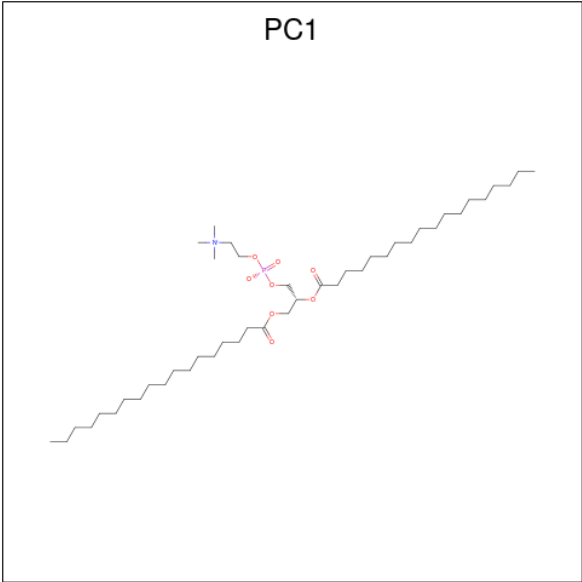
Mol	Chain	Residues	Atoms				AltConf	Trace
150	u1	92	Total	C	N	O	0	0
			460	276	92	92		
150	U1	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 151 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 152 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



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...

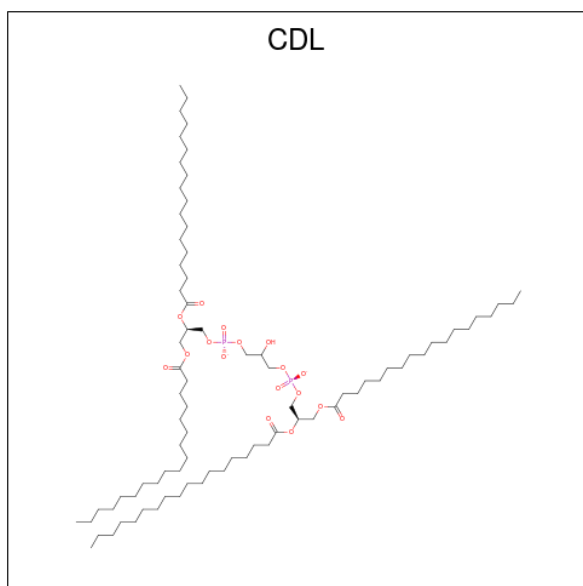
Mol	Chain	Residues	Atoms					AltConf
152	P1	1	Total 40	C 30	N 1	O 8	P 1	0
152	QB	1	Total 44	C 34	N 1	O 8	P 1	0
152	QC	1	Total 38	C 28	N 1	O 8	P 1	0
152	QC	1	Total 50	C 40	N 1	O 8	P 1	0
152	QC	1	Total 36	C 26	N 1	O 8	P 1	0
152	QE	1	Total 24	C 14	N 1	O 8	P 1	0
152	QE	1	Total 39	C 29	N 1	O 8	P 1	0
152	QG	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 28	C 18	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	

- Molecule 153 is CARDIOLIPIN (CCD ID: 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...

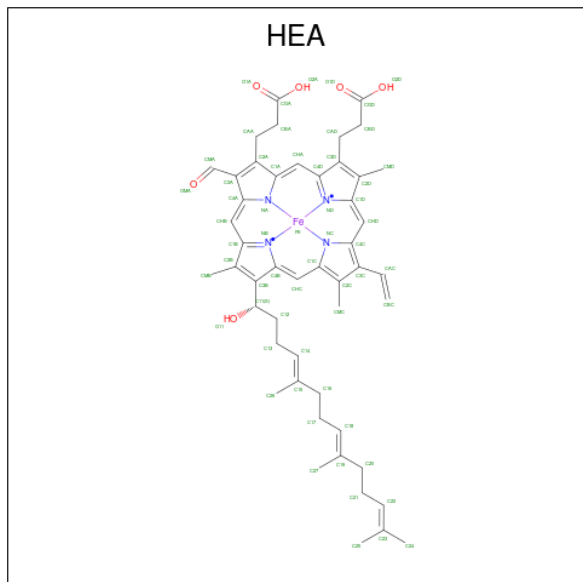
Mol	Chain	Residues	Atoms				AltConf
153	N5	1	Total	C	O	P	0
			90	71	17	2	
153	N6	1	Total	C	O	P	0
			90	71	17	2	
153	P1	1	Total	C	O	P	0
			63	44	17	2	
153	P1	1	Total	C	O	P	0
			58	39	17	2	
153	QB	1	Total	C	O	P	0
			68	49	17	2	
153	QC	1	Total	C	O	P	0
			64	45	17	2	
153	QC	1	Total	C	O	P	0
			56	37	17	2	
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 (CCD ID: 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	

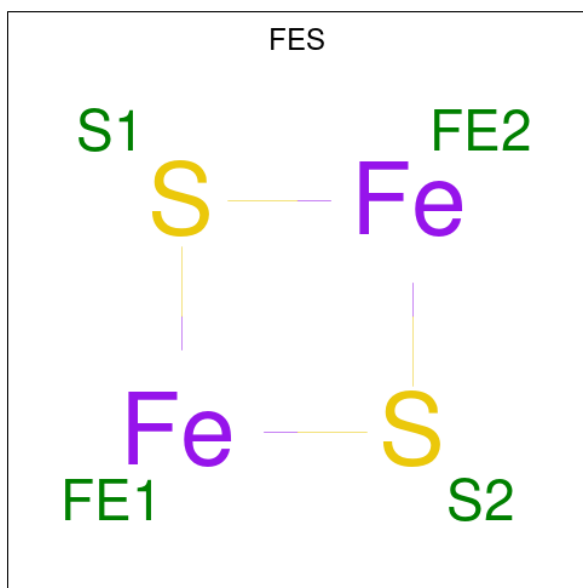
- Molecule 155 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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 (CCD ID: 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 (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



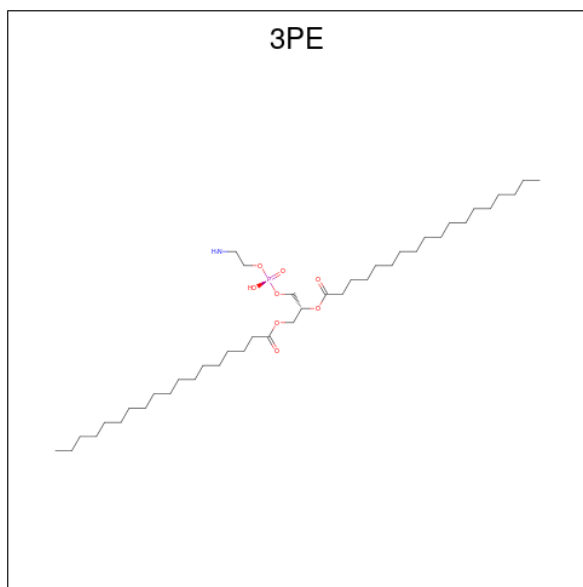
Mol	Chain	Residues	Atoms			AltConf
157	fs	1	Total 4	Fe 2	S 2	0
157	fs	1	Total 4	Fe 2	S 2	0
157	sb	1	Total 4	Fe 2	S 2	0

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 (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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...

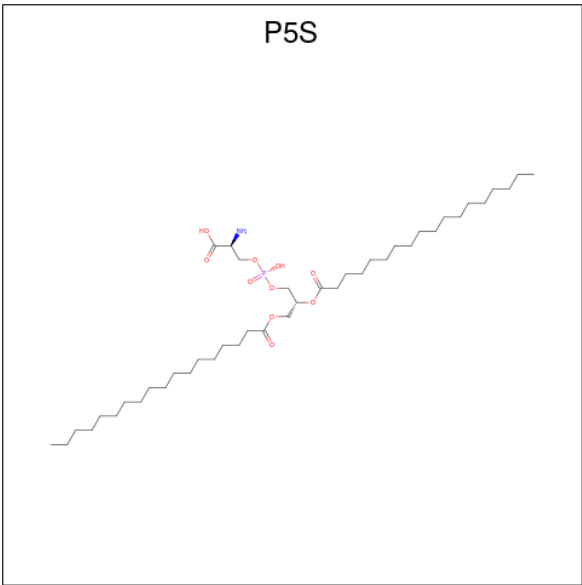
Mol	Chain	Residues	Atoms					AltConf
158	bm	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	c4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	g2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	n4	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	n5	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	s8	1	Total	C	N	O	P	0
			41	31	1	8	1	
158	t4	1	Total	C	N	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...

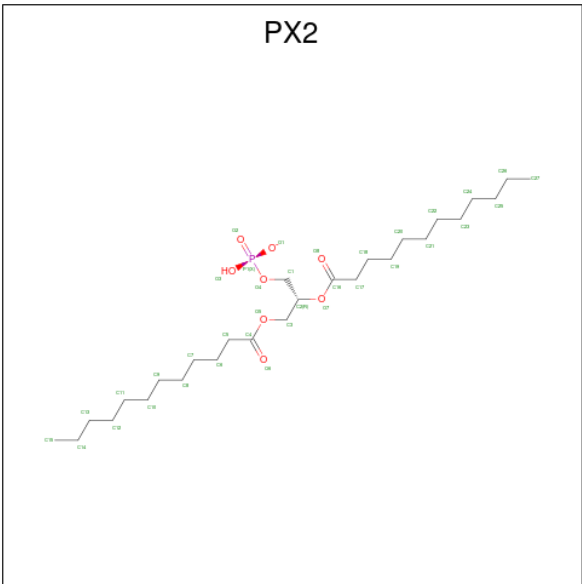
Mol	Chain	Residues	Atoms					AltConf
158	AN	1	Total	C	N	O	P	0
			33	23	1	8	1	
158	AN	1	Total	C	N	O	P	0
			29	19	1	8	1	
158	B4	1	Total	C	N	O	P	0
			48	38	1	8	1	
158	BM	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	C4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	G2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	N4	1	Total	C	N	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 (CCD ID: 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 (CCD ID: PX2) (formula: C₂₇H₅₂O₈P).



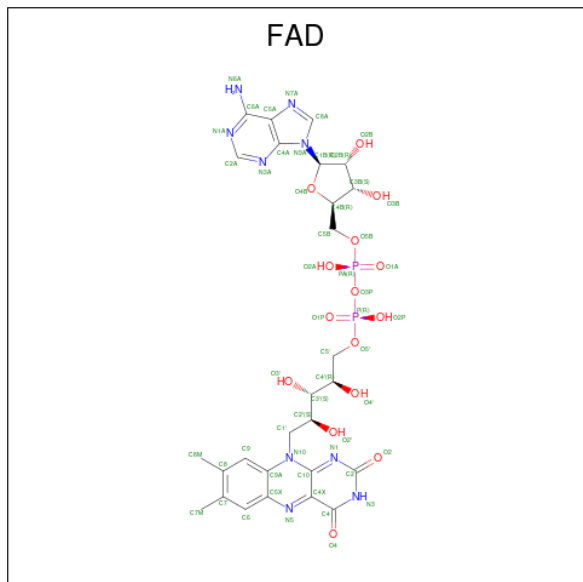
Mol	Chain	Residues	Atoms				AltConf
160	r	1	Total	C	O	P	0
			33	24	8	1	

Continued on next page...

Continued from previous page...

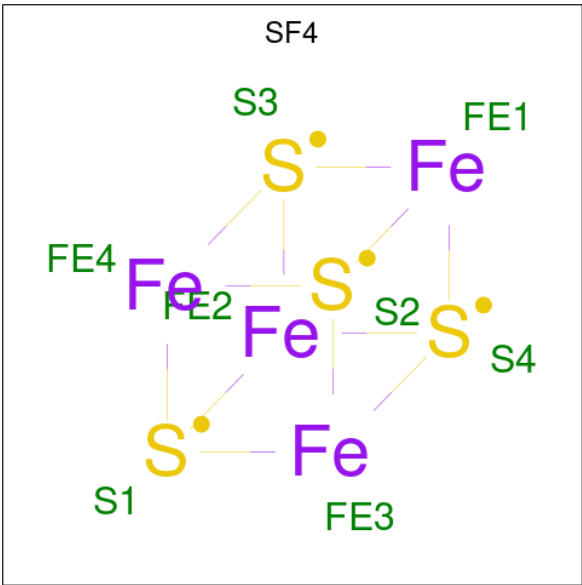
Mol	Chain	Residues	Atoms				AltConf
160	y5	1	Total	C	O	P	0
			21	12	8	1	
160	qh	1	Total	C	O	P	0
			36	27	8	1	
160	R	1	Total	C	O	P	0
			33	24	8	1	
160	Y5	1	Total	C	O	P	0
			21	12	8	1	
160	Qh	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 161 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



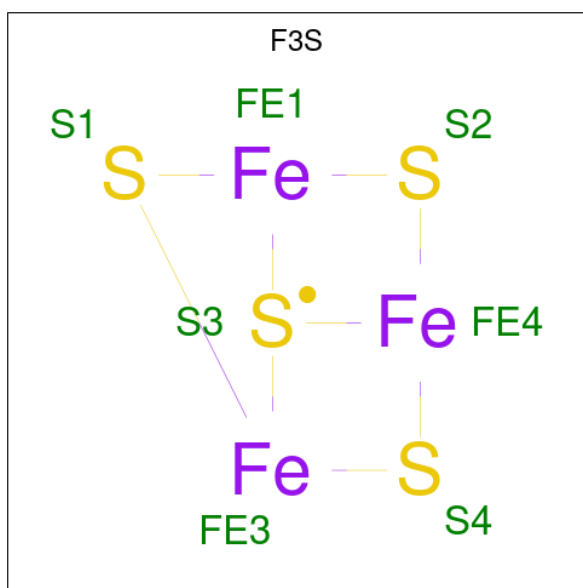
Mol	Chain	Residues	Atoms					AltConf
161	sa	1	Total	C	N	O	P	0
			53	27	9	15	2	
161	SA	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 162 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



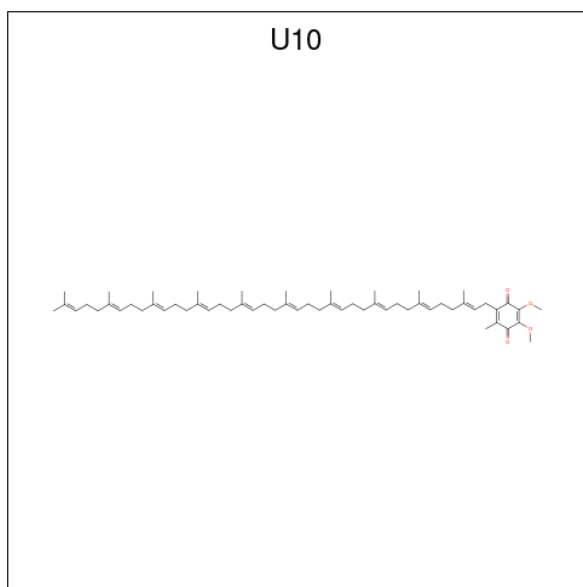
Mol	Chain	Residues	Atoms			AltConf
162	sb	1	Total	Fe	S	0
			8	4	4	
162	s1	1	Total	Fe	S	0
			8	4	4	
162	s1	1	Total	Fe	S	0
			8	4	4	
162	s7	1	Total	Fe	S	0
			8	4	4	
162	s8	1	Total	Fe	S	0
			8	4	4	
162	s8	1	Total	Fe	S	0
			8	4	4	
162	v1	1	Total	Fe	S	0
			8	4	4	
162	SB	1	Total	Fe	S	0
			8	4	4	
162	S1	1	Total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

- Molecule 163 is FE3-S4 CLUSTER (CCD ID: 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 (CCD ID: U10) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$) (labeled as "Ligand of Interest" by depositor).

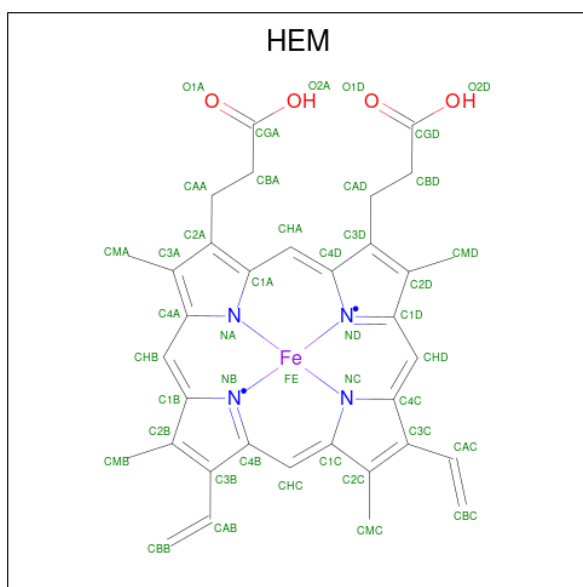


Mol	Chain	Residues	Atoms			AltConf
164	sc	1	Total	C	O	0
			63	59	4	
164	b8	1	Total	C	O	0
			63	59	4	
164	qC	1	Total	C	O	0
			29	25	4	
164	qc	1	Total	C		0
			26	26		
164	qc	1	Total	C	O	0
			29	25	4	
164	SC	1	Total	C	O	0
			63	59	4	
164	B8	1	Total	C	O	0
			63	59	4	
164	QC	1	Total	C	O	0
			29	25	4	
164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

- Molecule 165 is ZINC ION (CCD ID: 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 (CCD ID: 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	C	Fe	N	O	0
			43	34	1	4	4	
166	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Y5	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 167 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
167	a9	1	Total 48	C 21	N 7	O 17	P 3	0
167	A9	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 168 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl]-}\beta\text{-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



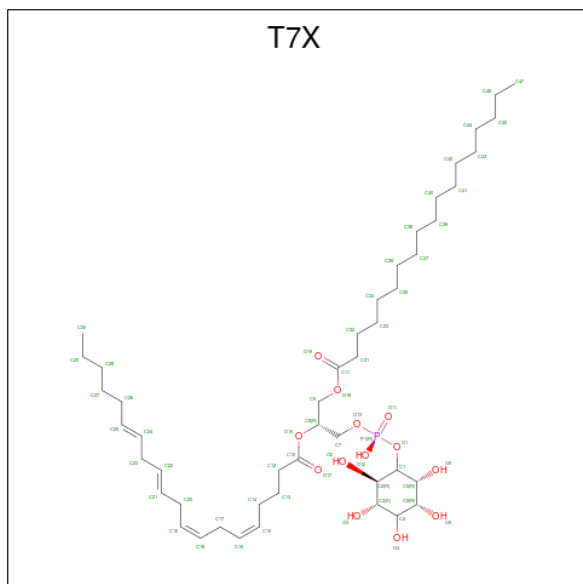
Mol	Chain	Residues	Atoms						AltConf
168	ab	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

Continued on next page...

Continued from previous page...

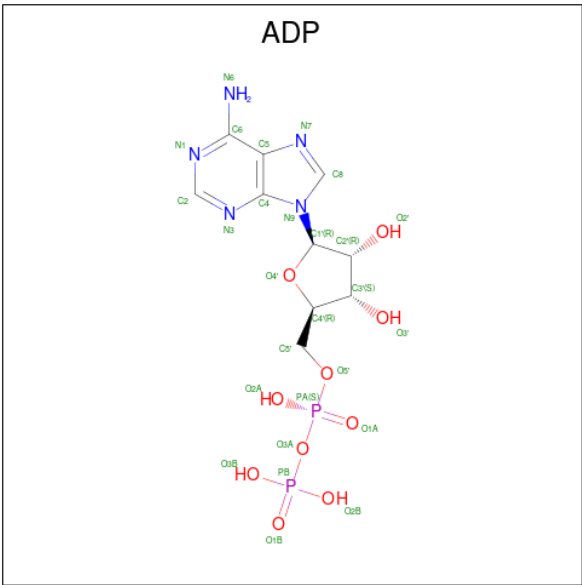
Mol	Chain	Residues	Atoms						AltConf
168	AB	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



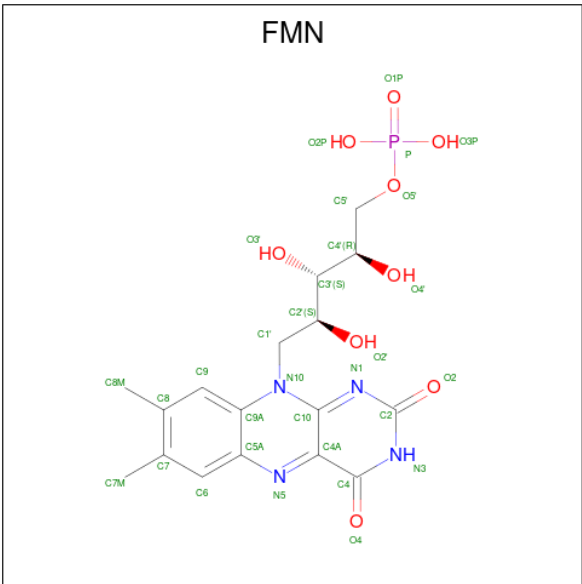
Mol	Chain	Residues	Atoms				AltConf
169	b6	1	Total	C	O	P	0
			55	41	13	1	
169	B6	1	Total	C	O	P	0
			55	41	13	1	

- Molecule 170 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: 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...

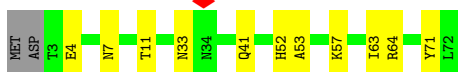
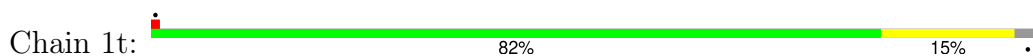
Continued from previous page...

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

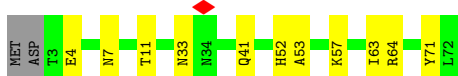
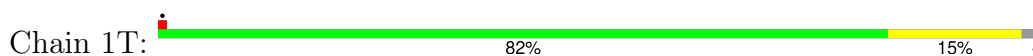
3 Residue-property plots

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.

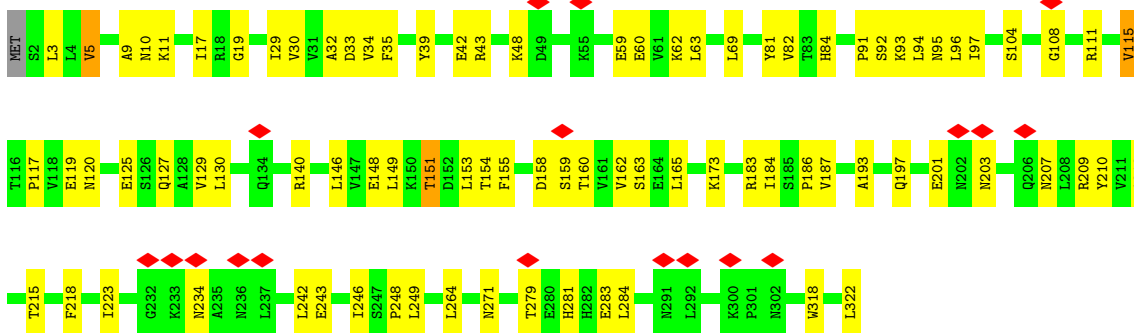
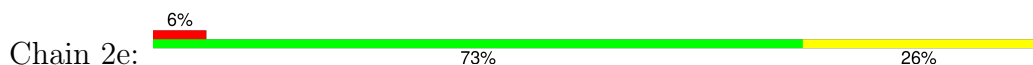
- Molecule 1: Tim10/DDP family zinc finger protein



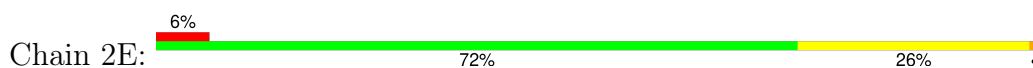
- Molecule 1: Tim10/DDP family zinc finger protein

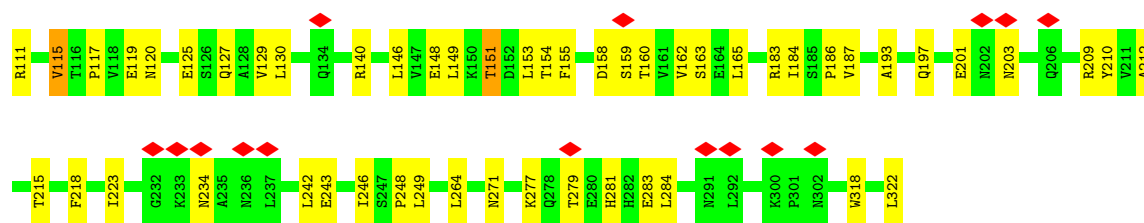


- Molecule 2: NmrA domain-containing protein

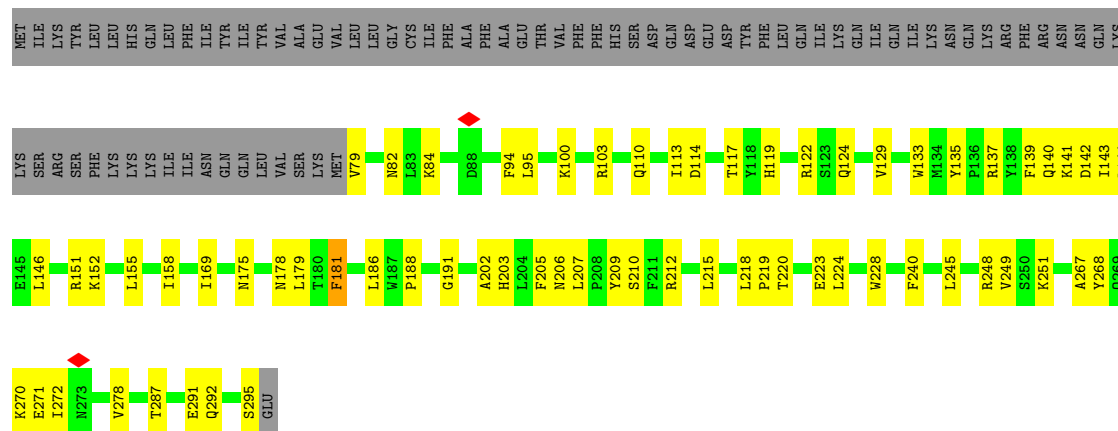


- Molecule 2: NmrA domain-containing protein

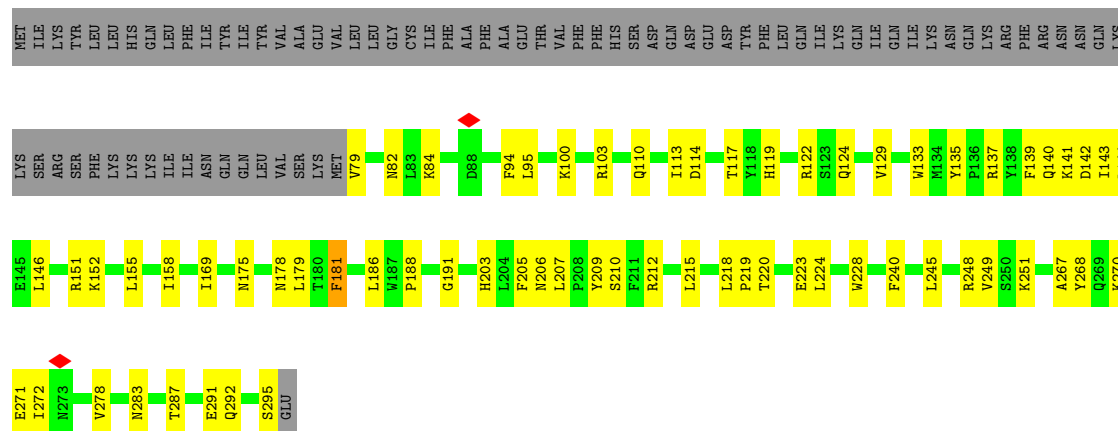




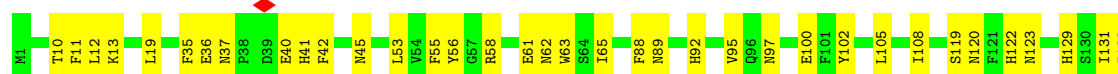
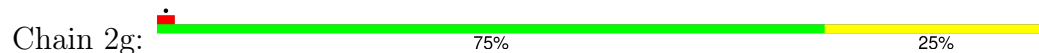
• Molecule 3: Transmembrane protein, putative



• Molecule 3: Transmembrane protein, putative

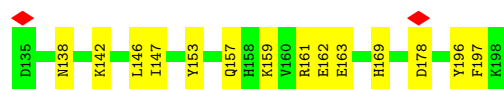
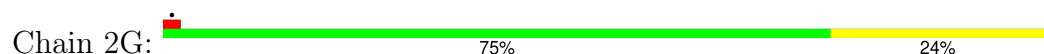


• Molecule 4: SDHTT3

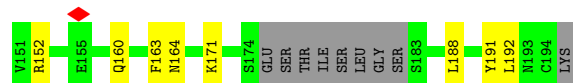
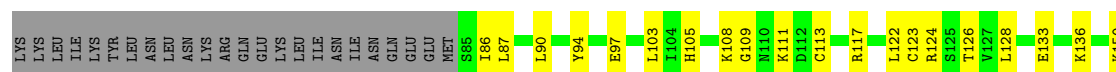
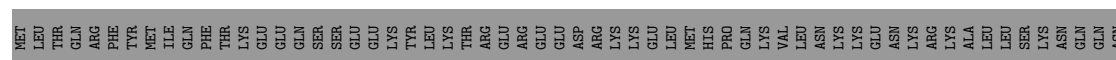




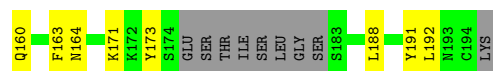
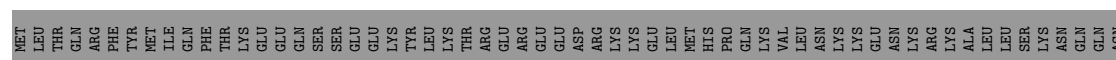
- Molecule 4: SDHTT3



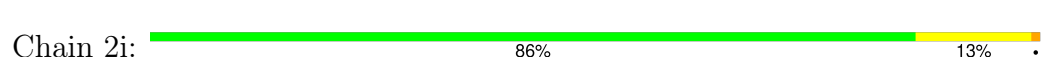
- Molecule 5: Dipthamide synthesis protein



- Molecule 5: Dipthamide synthesis protein



- Molecule 6: DUF4885 domain-containing protein



- Molecule 6: DUF4885 domain-containing protein

Chain 2I:  86% 13%



- Molecule 7: Transmembrane protein, putative

Chain 2j:  75% 24%



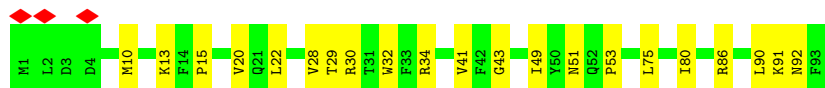
- Molecule 7: Transmembrane protein, putative

Chain 2J:  76% 23%



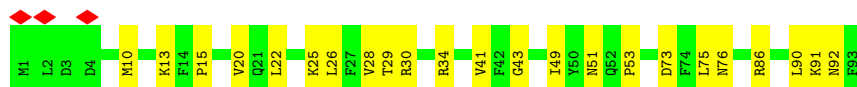
- Molecule 8: Transmembrane protein, putative

Chain 2k:  77% 23%



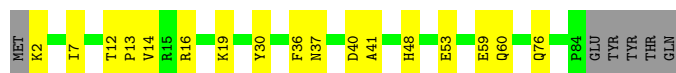
- Molecule 8: Transmembrane protein, putative

Chain 2K:  75% 25%



- Molecule 9: Transposase

Chain 2l:  74% 19% 7%



- Molecule 9: Transposase

Chain 2L:  71% 22% 7%



- Molecule 10: Transmembrane protein, putative

Chain 2m:  76% 22%



- Molecule 10: Transmembrane protein, putative

Chain 2M:  78% 21%



- Molecule 11: Transmembrane protein, putative

Chain 2n:  71% 27%



- Molecule 11: Transmembrane protein, putative

Chain 2N:  73% 24%



- Molecule 12: SDHTT11

Chain 2o:  76% 15% 9%



- Molecule 12: SDHTT11

Chain 2O:  72% 20% 9%

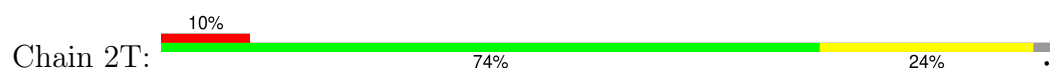


- Molecule 13: Zf-Tim10_DDP domain-containing protein

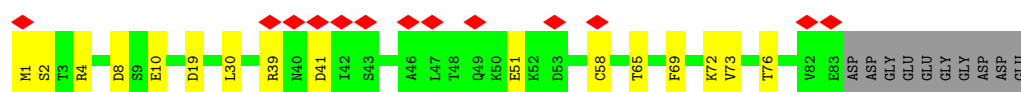
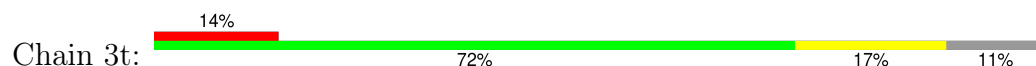
Chain 2t:  10% 71% 26%



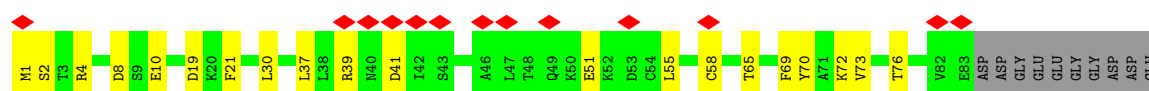
- Molecule 13: Zf-Tim10_DDP domain-containing protein



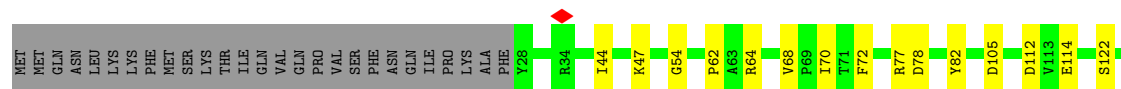
- Molecule 14: Zf-Tim10_DDP domain-containing protein



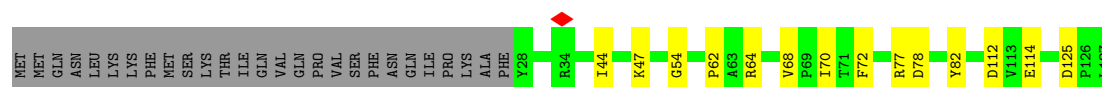
- Molecule 14: Zf-Tim10_DDP domain-containing protein



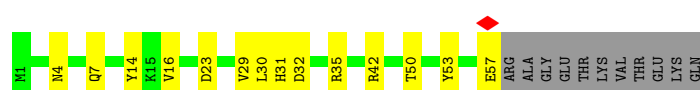
- Molecule 15: Phage protein



- Molecule 15: Phage protein



- Molecule 16: Transposase

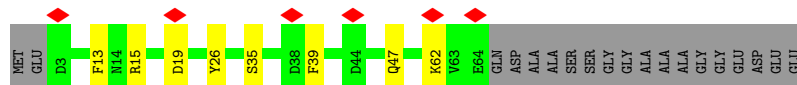


- Molecule 16: Transposase

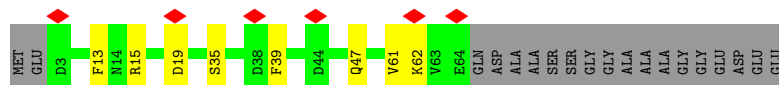




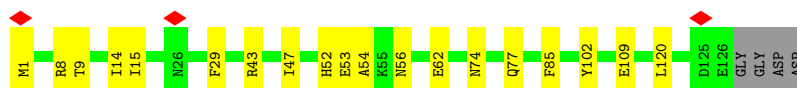
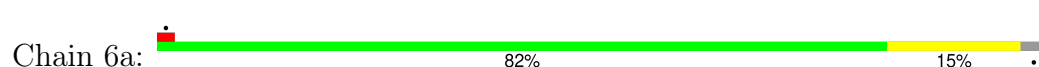
- Molecule 17: Cullin domain-containing protein



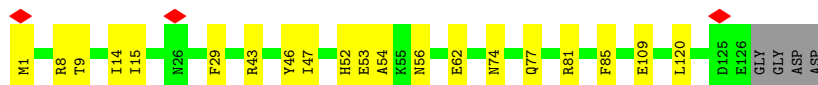
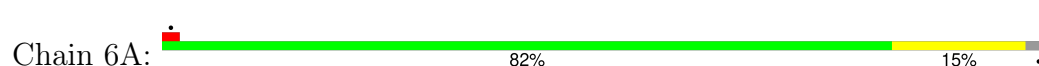
- Molecule 17: Cullin domain-containing protein



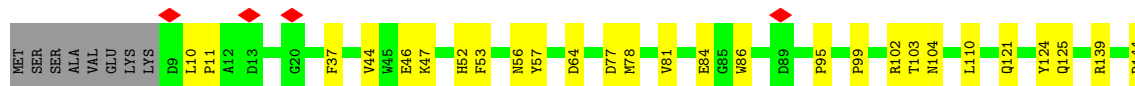
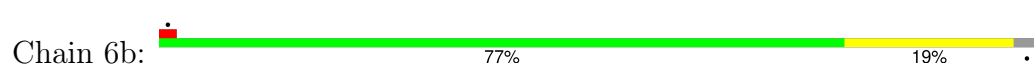
- Molecule 18: Transmembrane protein, putative



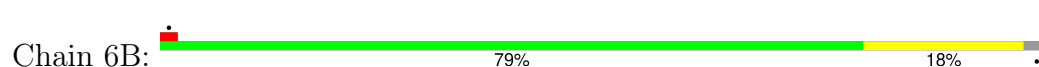
- Molecule 18: Transmembrane protein, putative



- Molecule 19: Structural protein

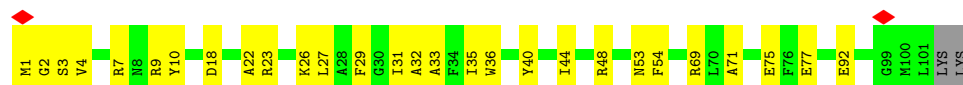


- Molecule 19: Structural protein

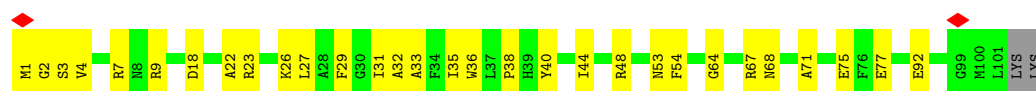




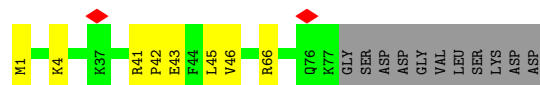
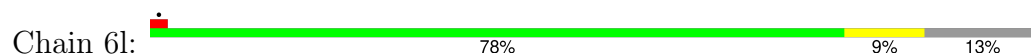
- Molecule 20: Transmembrane protein, putative



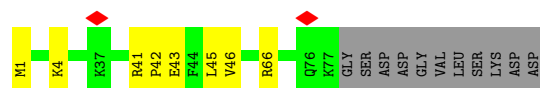
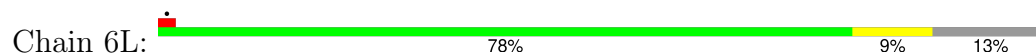
- Molecule 20: Transmembrane protein, putative



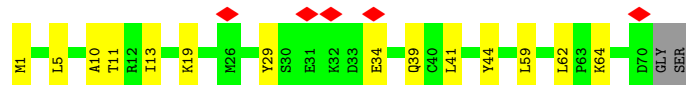
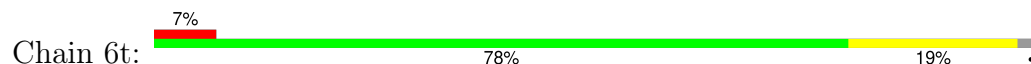
- Molecule 21: Decapping nuclease



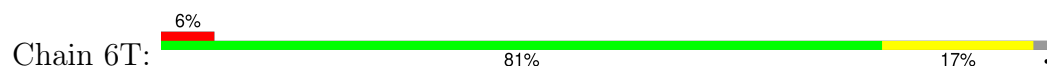
- Molecule 21: Decapping nuclease

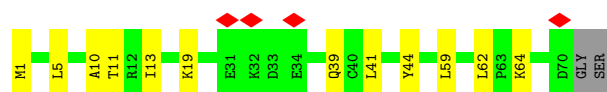


- Molecule 22: Annexin

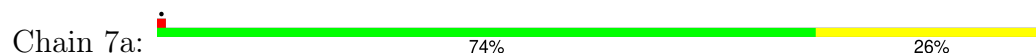


- Molecule 22: Annexin

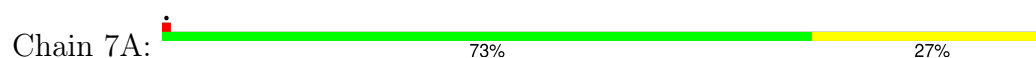




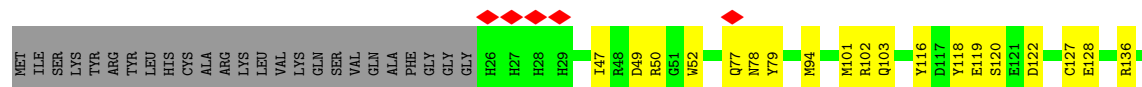
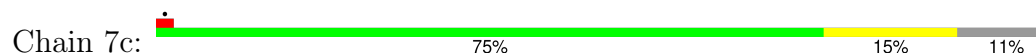
- Molecule 23: Transmembrane protein, putative



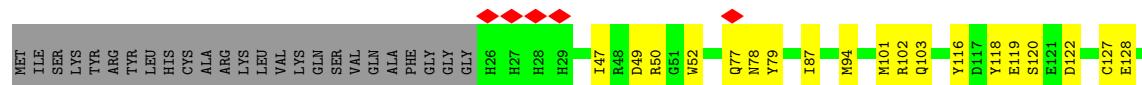
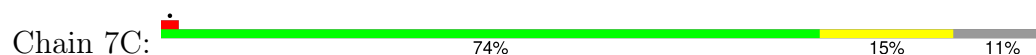
- Molecule 23: Transmembrane protein, putative



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 25: CTF/NF-I domain-containing protein

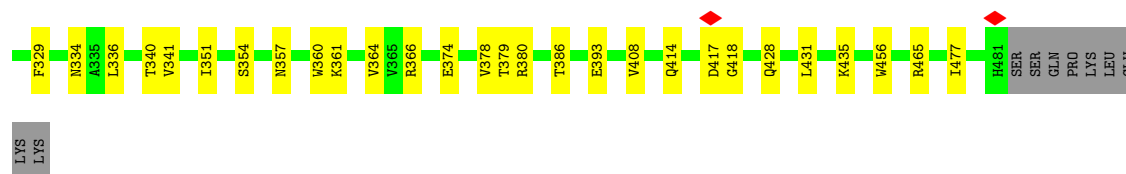
V926
I933
Y938
M939
R940
E952
C953
E954
R957
R965
K966
L970
T990

- | |
|-----|
| MET | ASN | LYS | LYS | SER | GLN | ASP | GLU | VAL | LYS | GLU | TYR | PHE | SER | ILE | LYS | LYS | LYS | LYS | TYR | ASN | SER | SER | LEU | ASP | CYS | VAL | LEU | SER | SER | PRO | ILE | VAL | THR | ARG | LYS | LYS | LYS | GLN | GLU | GLN | GLU | ASP | GLN | ASN | ASN | SER | SER | THR | ALA | ALA | VAL | PRO | GLU | GLU | SER | SER | PRO | PRO |
|-----|

V926	I933	Y938	M939	R940	E952	C953	E954	R957	R965	K966	L970	D980	T990
------	------	------	------	------	------	-------------	------	------	------	------	------	------	------

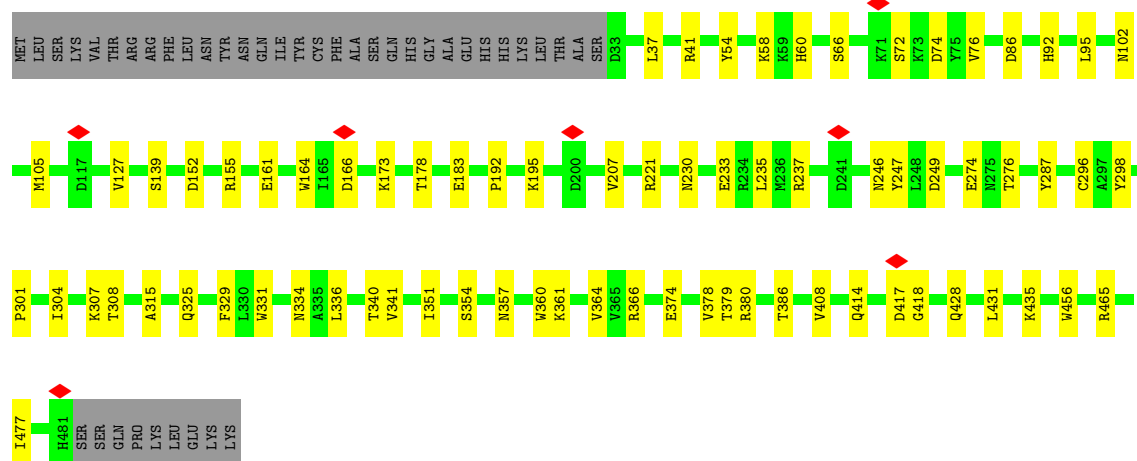
- Chain a: 78% 14% 8%

Protein	Score	Category
MET	0.00	Not Significant
LEU	0.00	Not Significant
SER	0.00	Not Significant
LYS	0.00	Not Significant
VAL	0.00	Not Significant
THR	0.00	Not Significant
ARG	0.00	Not Significant
ARG	0.00	Not Significant
PHE	0.00	Not Significant
LEU	0.00	Not Significant
ASN	0.00	Not Significant
TYR	0.00	Not Significant
ASN	0.00	Not Significant
GLN	0.00	Not Significant
ILE	0.00	Not Significant
TYR	0.00	Not Significant
CYS	0.00	Not Significant
PHE	0.00	Not Significant
ALA	0.00	Not Significant
SER	0.00	Not Significant
GLN	0.00	Not Significant
HIS	0.00	Not Significant
GLY	0.00	Not Significant
ALA	0.00	Not Significant
GLU	0.00	Not Significant
HIS	0.00	Not Significant
HIS	0.00	Not Significant
LEU	0.00	Not Significant
THR	0.00	Not Significant
ALA	0.00	Not Significant
SER	0.00	Not Significant
D33	0.00	Not Significant
L37	0.00	Not Significant
R41	0.00	Not Significant
Y54	0.00	Not Significant
K58	0.00	Not Significant
S66	0.00	Not Significant
K71	0.00	Not Significant
S72	0.00	Not Significant
K73	0.00	Not Significant
D74	0.00	Not Significant
Y75	0.00	Not Significant
W76	0.00	Not Significant
H92	0.00	Not Significant
L95	0.00	Not Significant
N102	0.00	Not Significant
M105	0.00	Not Significant
D117	0.00	Not Significant
V127	0.00	Not Significant
S139	0.00	Not Significant
D152	0.00	Not Significant
R155	0.00	Not Significant
E161	0.00	Not Significant
R162	0.00	Not Significant
R163	0.00	Not Significant
W164	0.00	Not Significant
I165	0.00	Not Significant
D166	0.00	Not Significant
K173	0.00	Not Significant
T178	0.00	Not Significant
E183	0.00	Not Significant
K195	0.00	Not Significant
D200	0.00	Not Significant
R221	0.00	Not Significant
N230	0.00	Not Significant
E233	0.00	Not Significant
R237	0.00	Not Significant
D241	0.00	Not Significant
N246	0.00	Not Significant
Y247	0.00	Not Significant
L248	0.00	Not Significant
D249	0.00	Not Significant
E274	0.00	Not Significant
N275	0.00	Not Significant
T276	0.00	Not Significant
Y287	0.00	Not Significant
C296	0.00	Not Significant
A297	0.00	Not Significant
Y298	0.00	Not Significant
P301	0.00	Not Significant
I304	0.00	Not Significant
K307	0.00	Not Significant
A315	0.00	Not Significant
P335	0.00	Not Significant



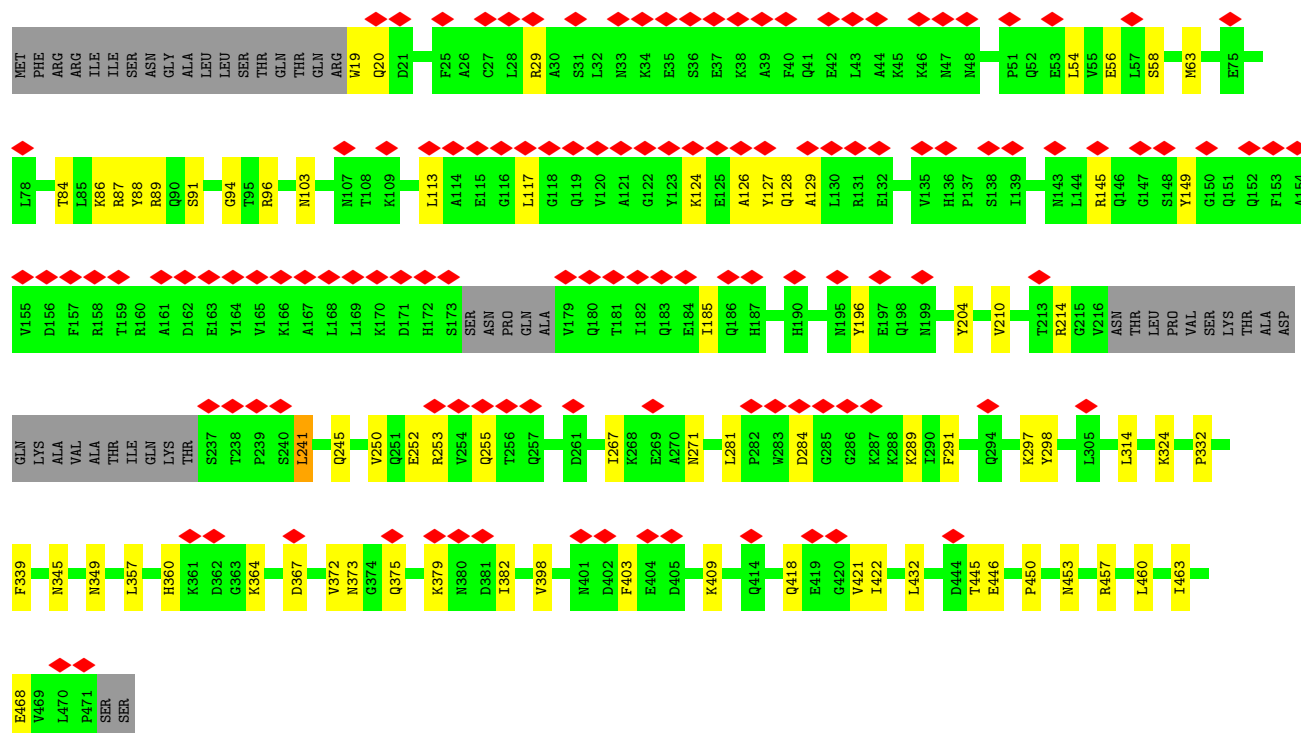
- Molecule 26: Transmembrane protein, putative

Chain A: 77% 15% 8%



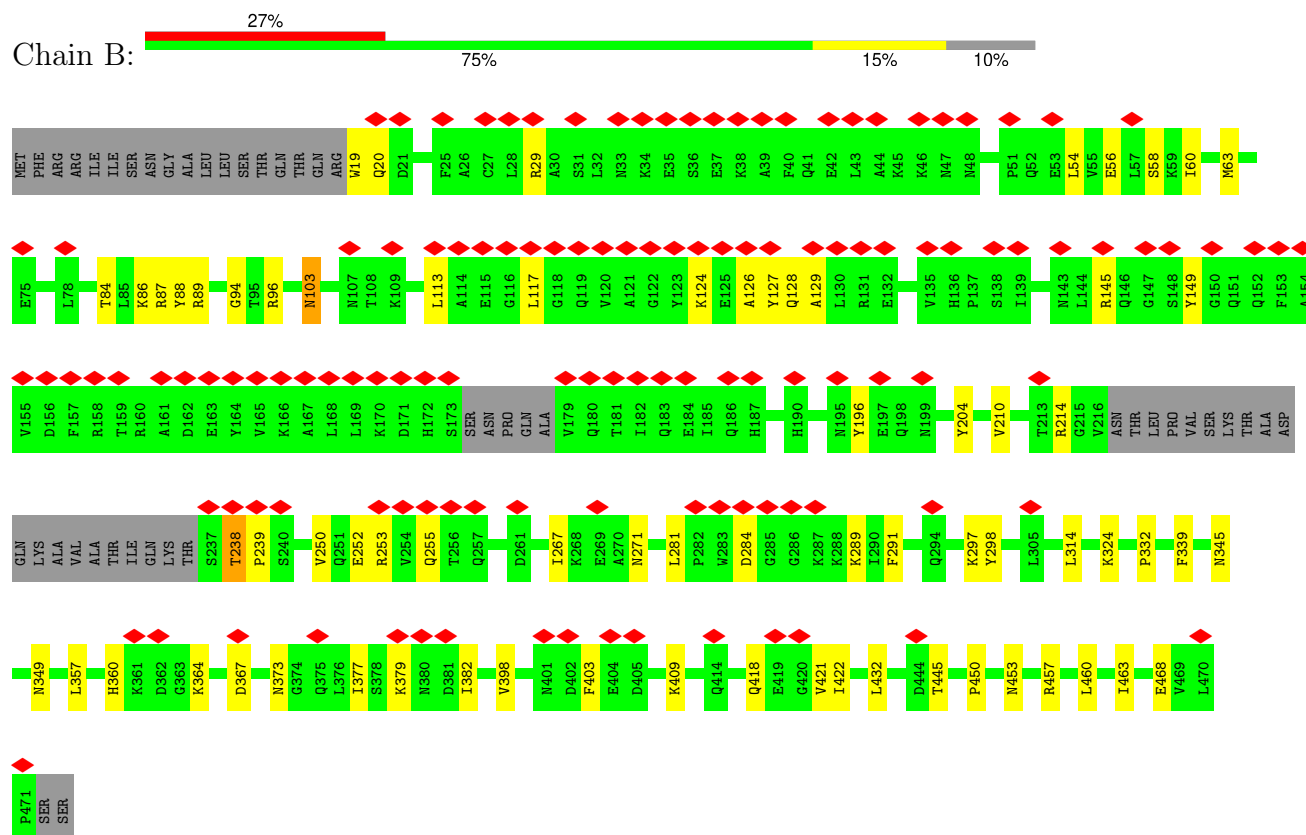
- Molecule 27: Protein phosphatase 2C, putative

Chain b: 27% 75% 15% 10%



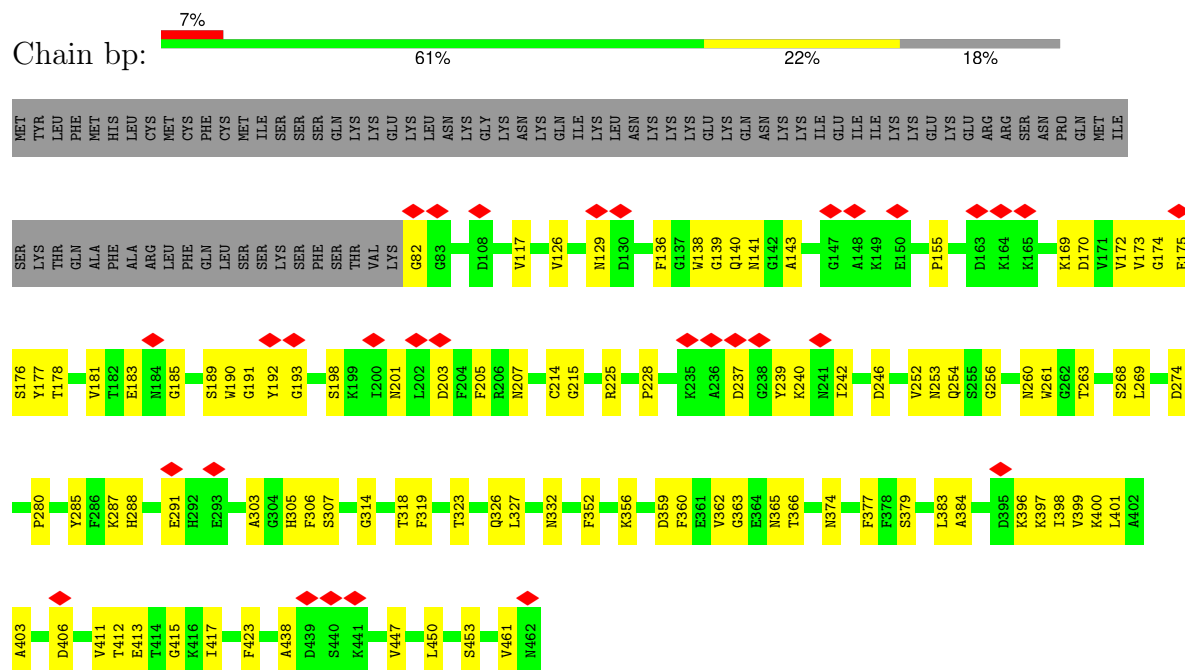
- Molecule 27: Protein phosphatase 2C, putative

Chain B:



- Molecule 28: Chromosome condensation regulator RCC1 repeat protein

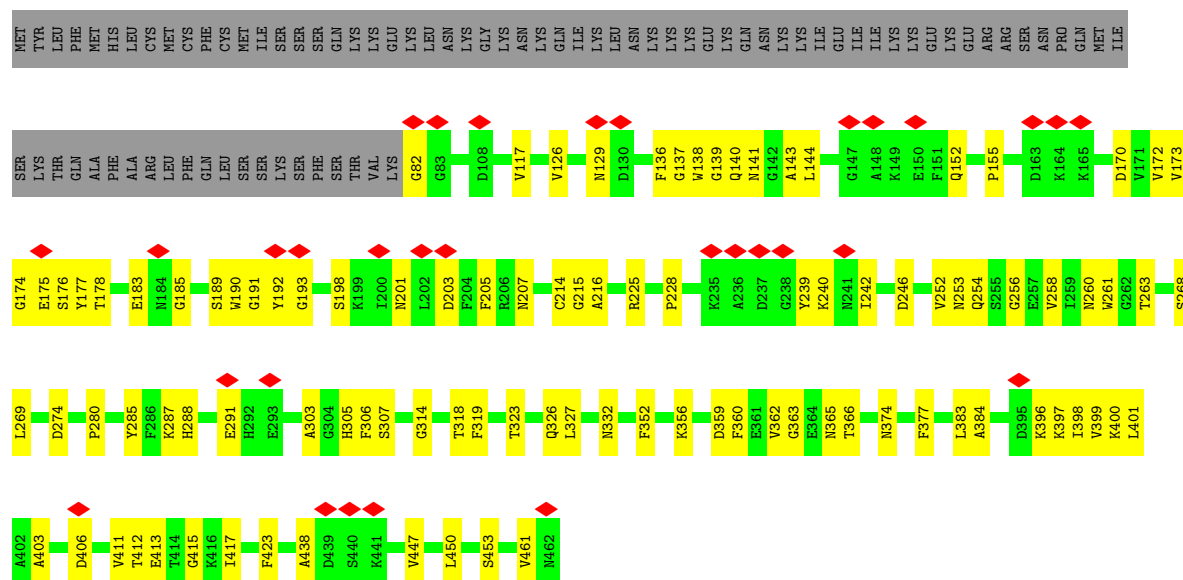
Chain bp:



- Molecule 28: Chromosome condensation regulator RCC1 repeat protein

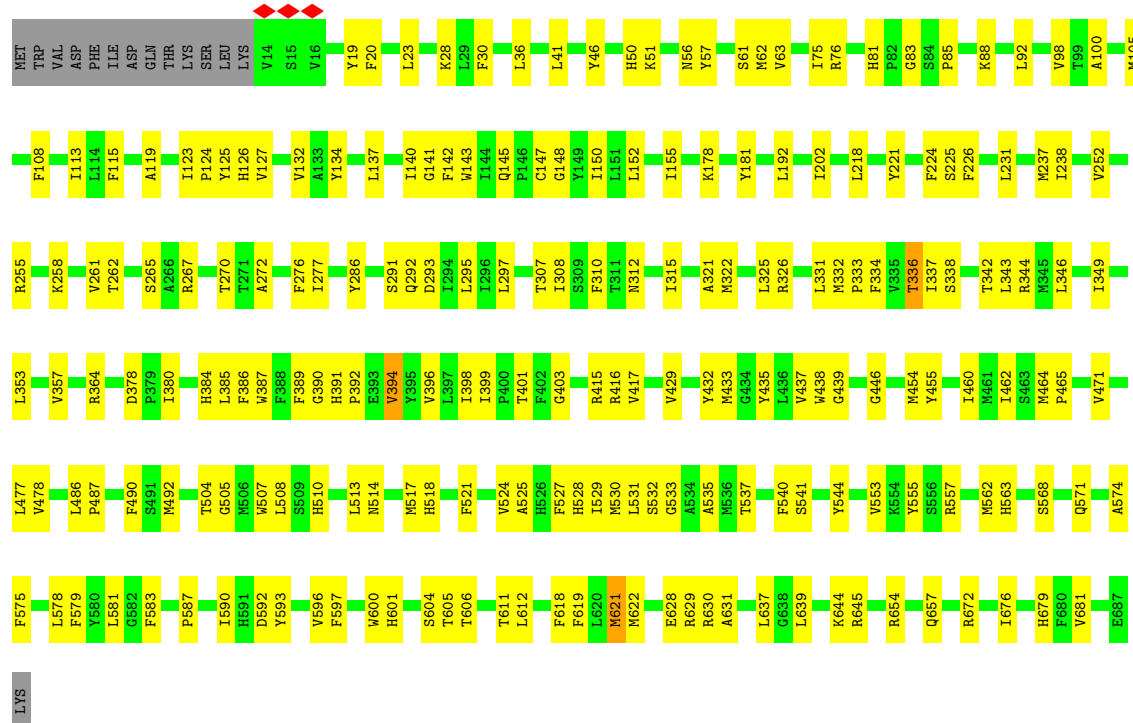
Chain BP:





• Molecule 29: Cytochrome c oxidase subunit 1

Chain c1: 68% 30%

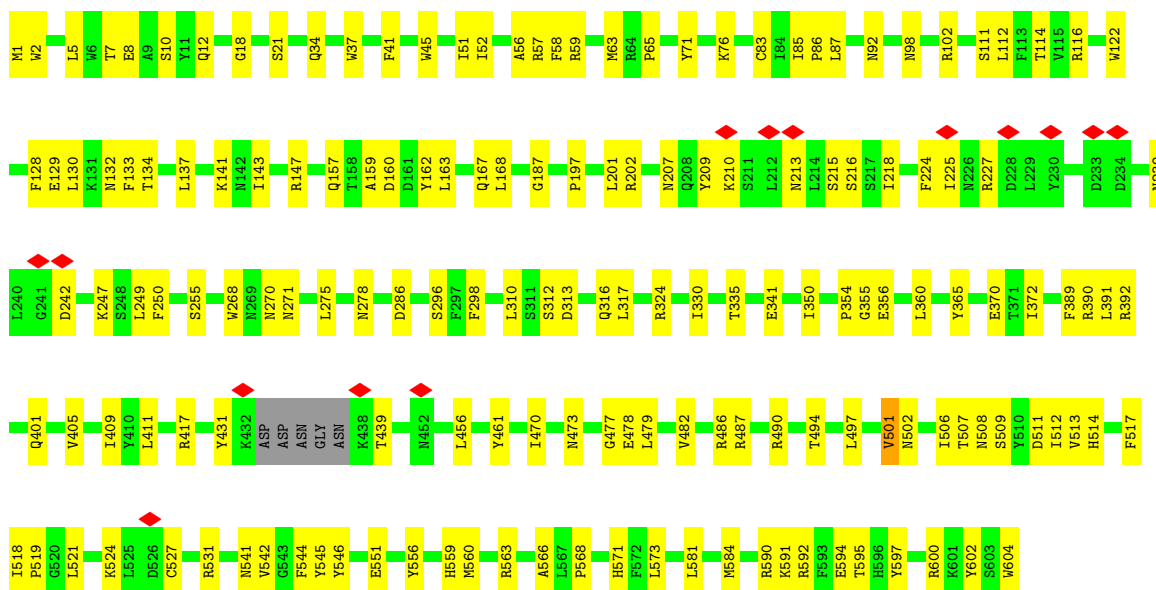


• Molecule 29: Cytochrome c oxidase subunit 1

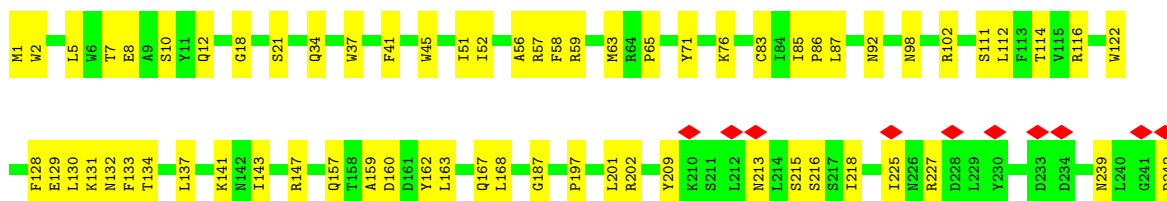
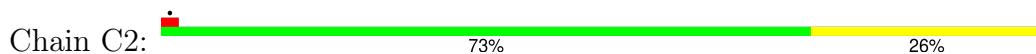
Chain C1: 69% 29%

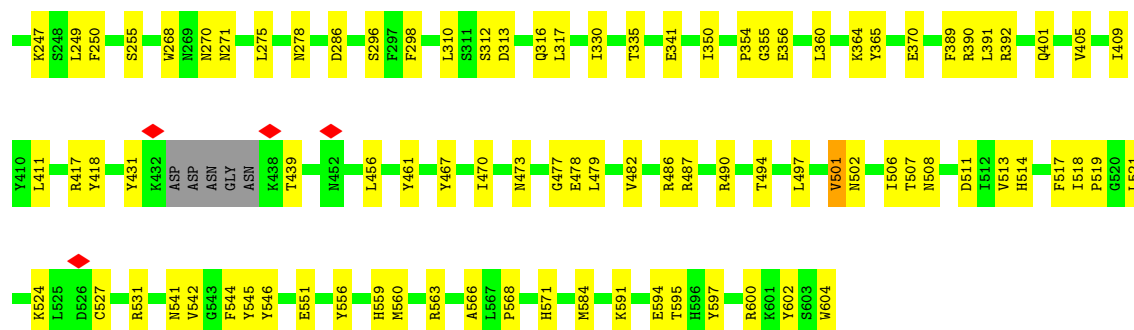


- Molecule 30: Cytochrome c oxidase subunit 2

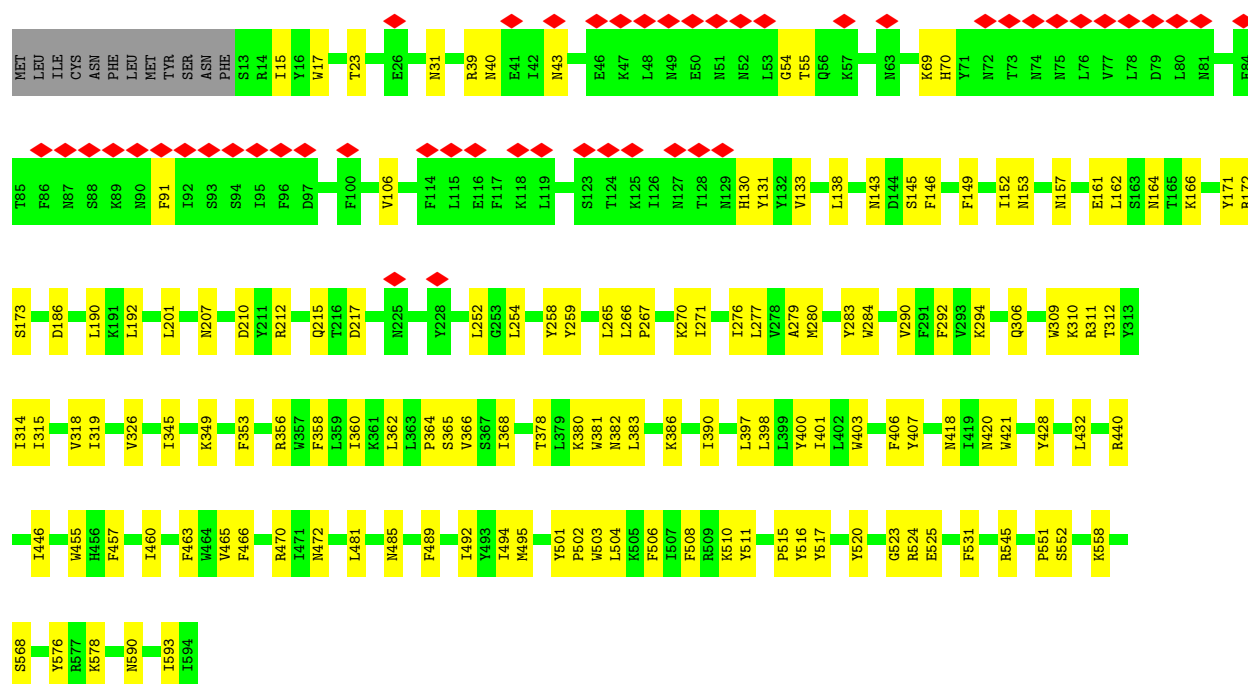
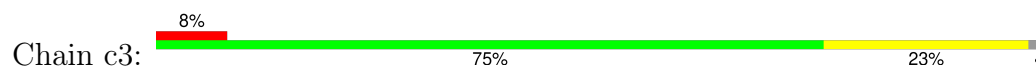


- Molecule 30: Cytochrome c oxidase subunit 2

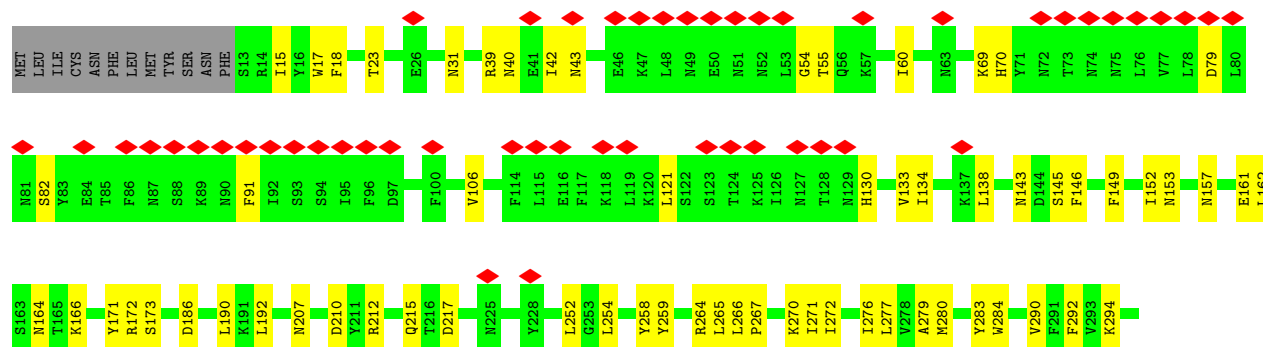
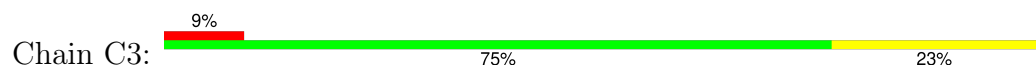


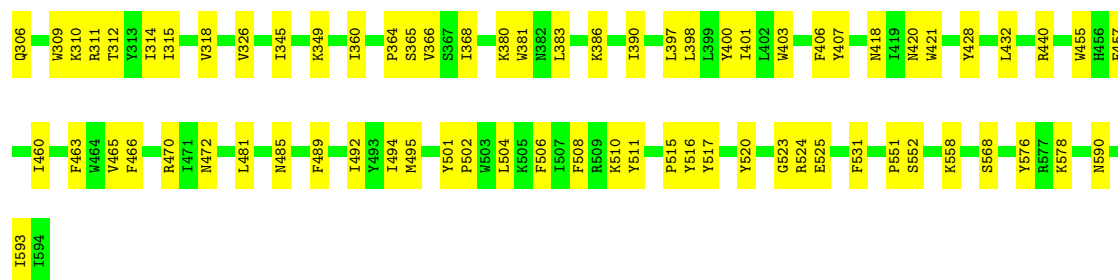


• Molecule 31: Ymf68

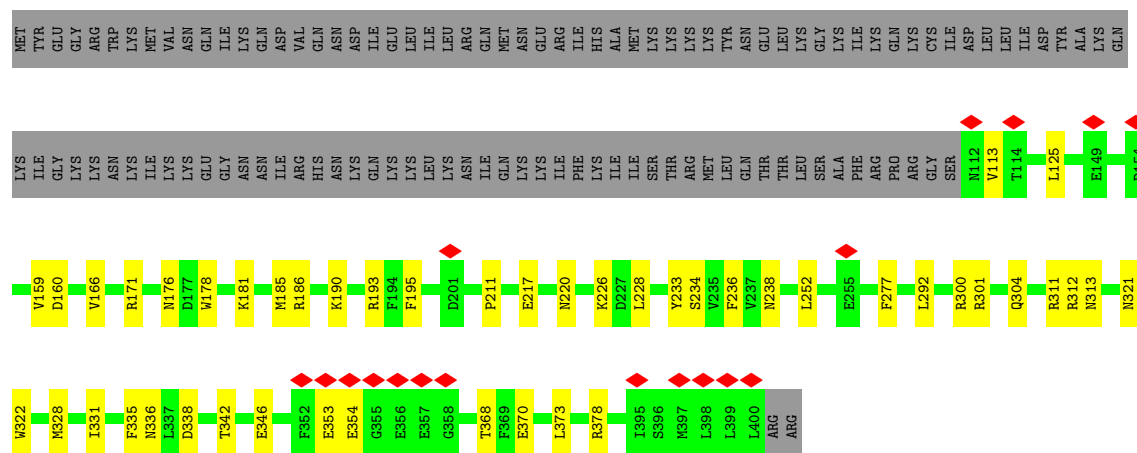


• Molecule 31: Ymf68

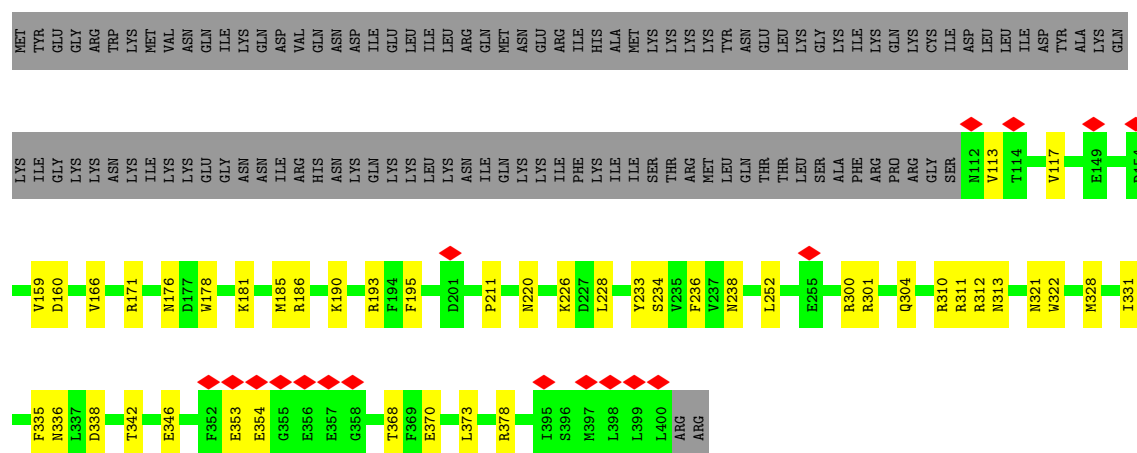




• Molecule 32: SURF1-like protein

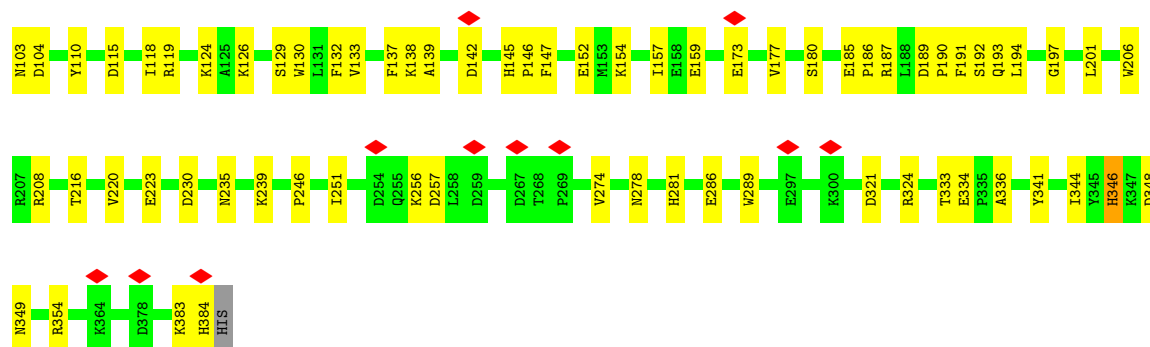


• Molecule 32: SURF1-like protein



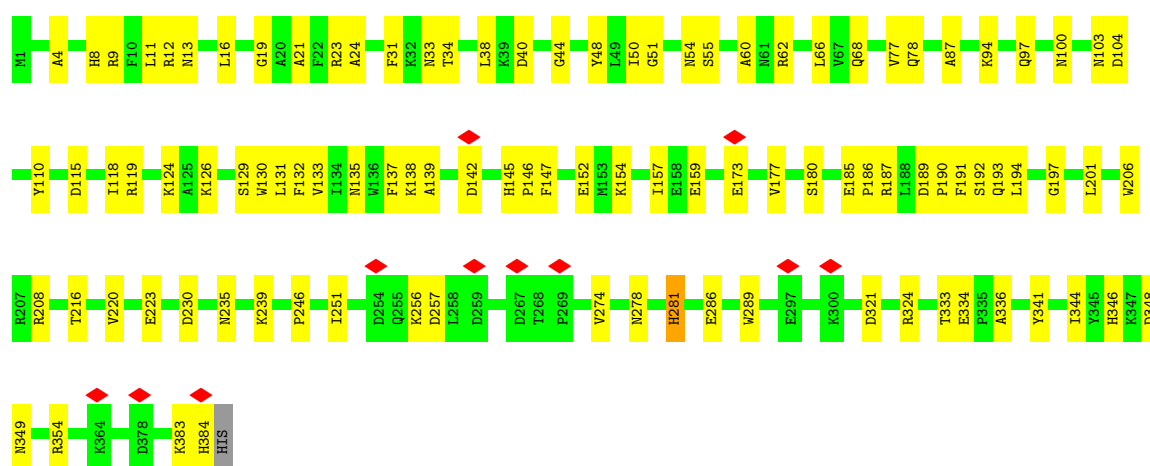
• Molecule 33: TraB family protein





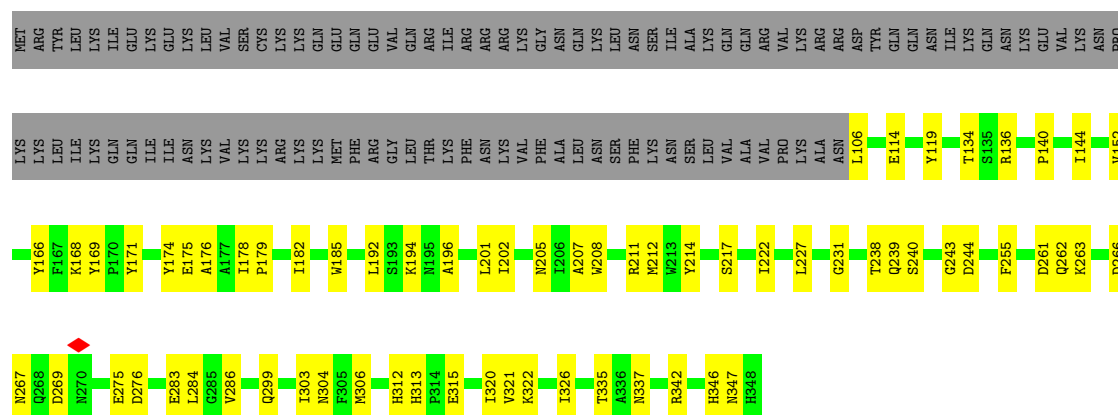
• Molecule 33: TraB family protein

Chain E: 74% 26%



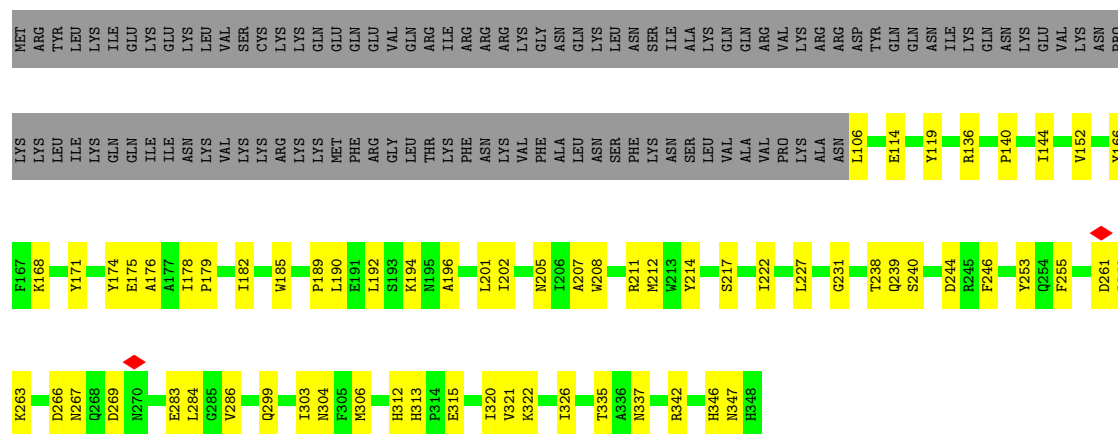
• Molecule 34: Transmembrane protein, putative

Chain f: 51% 19% 30%

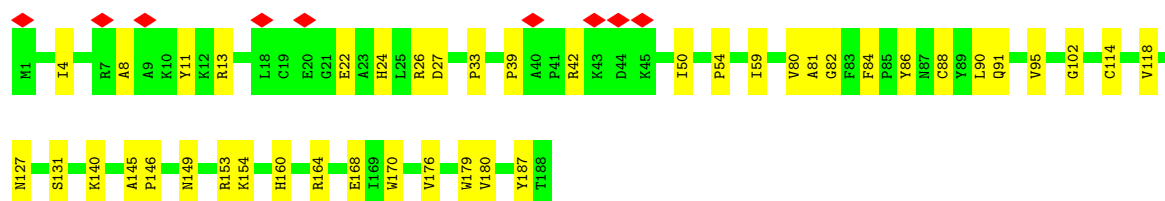
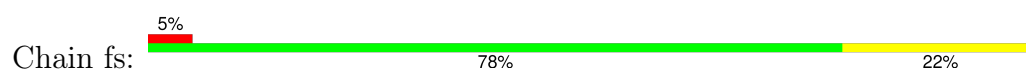


• Molecule 34: Transmembrane protein, putative

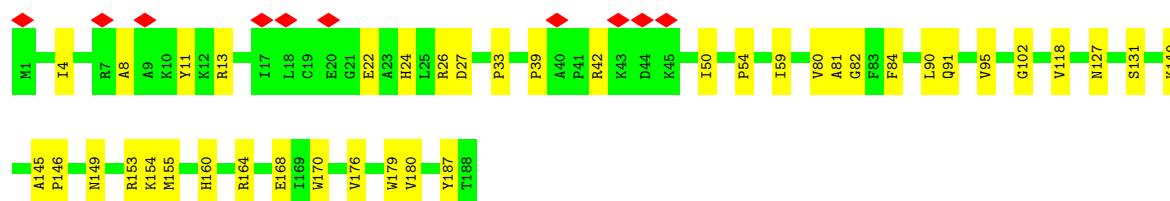
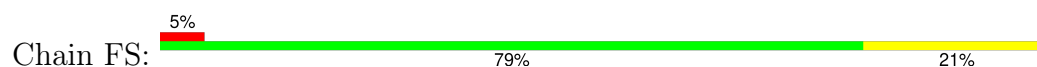
Chain F: 51% 19% 30%



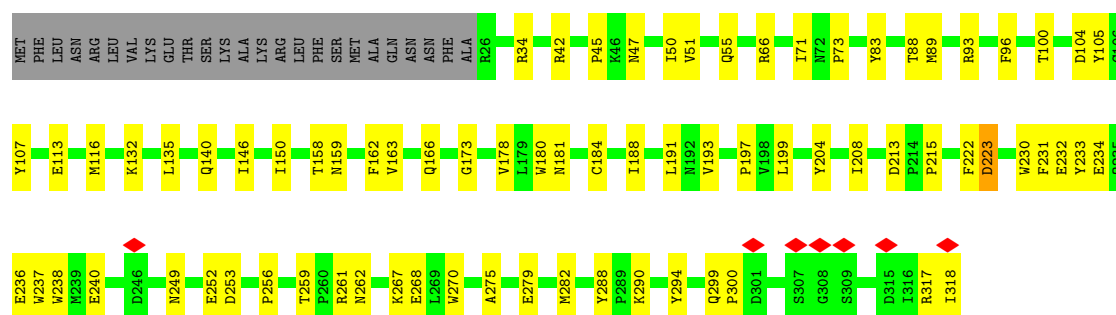
• Molecule 35: Iron-binding zinc finger CDGSH type protein



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

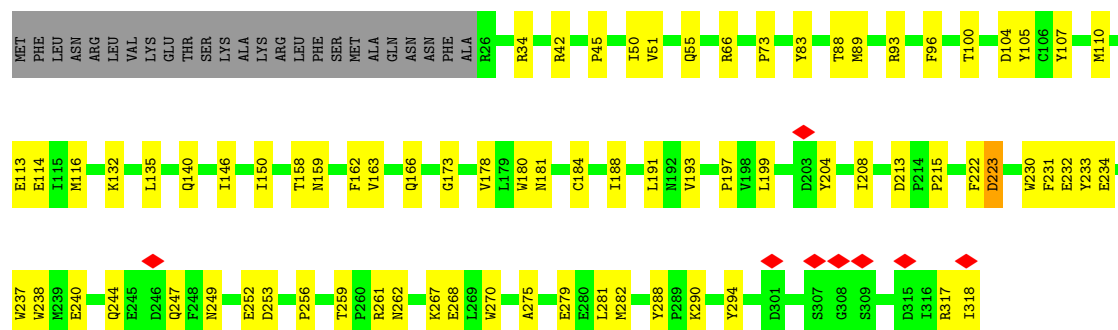


• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial



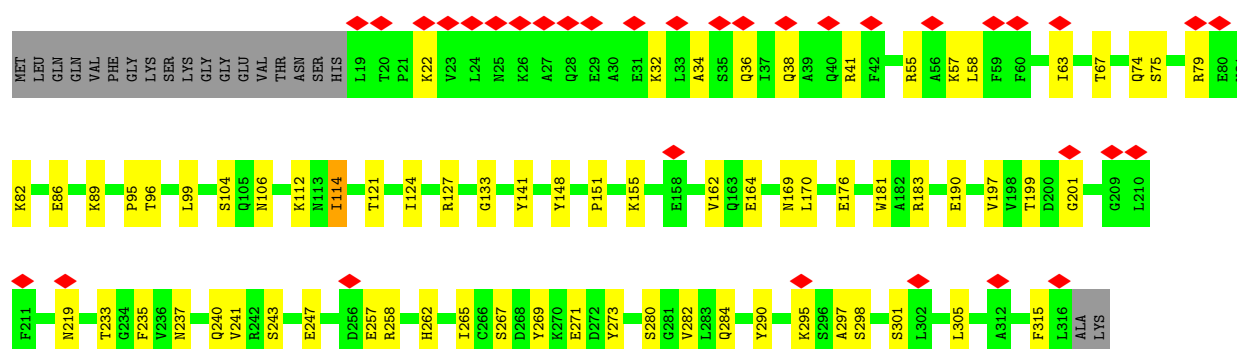
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain G: 



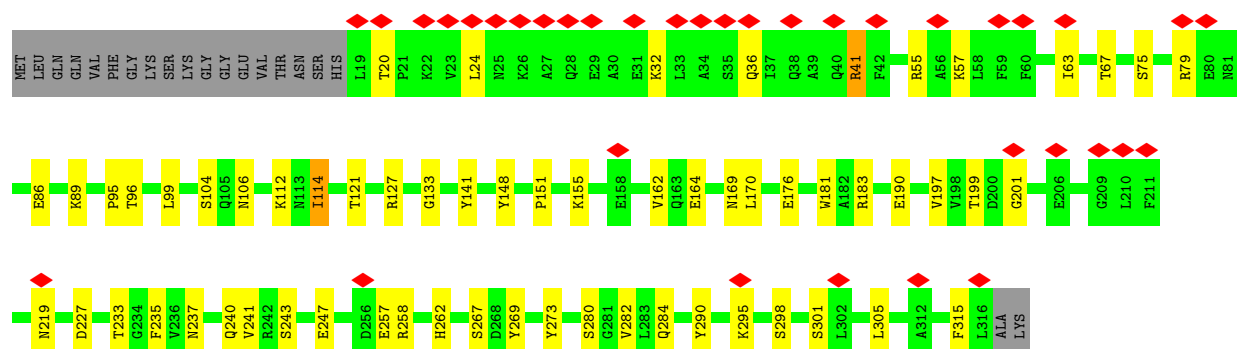
- Molecule 37: SURF1-like protein

Chain h: 



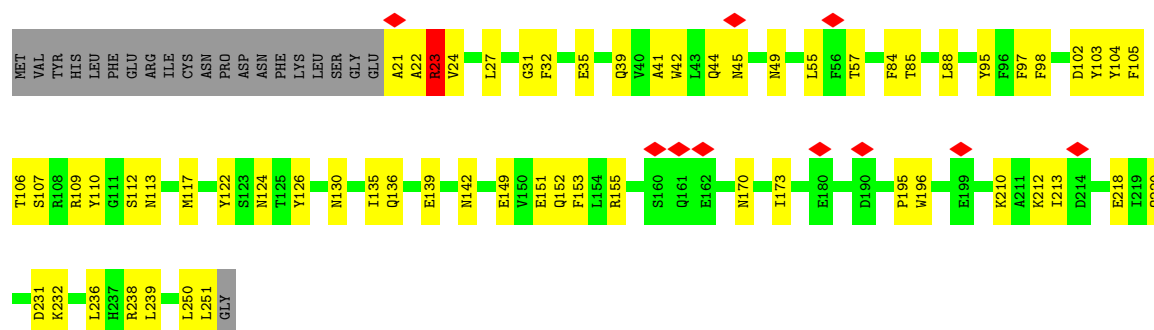
- Molecule 37: SURF1-like protein

Chain H: 

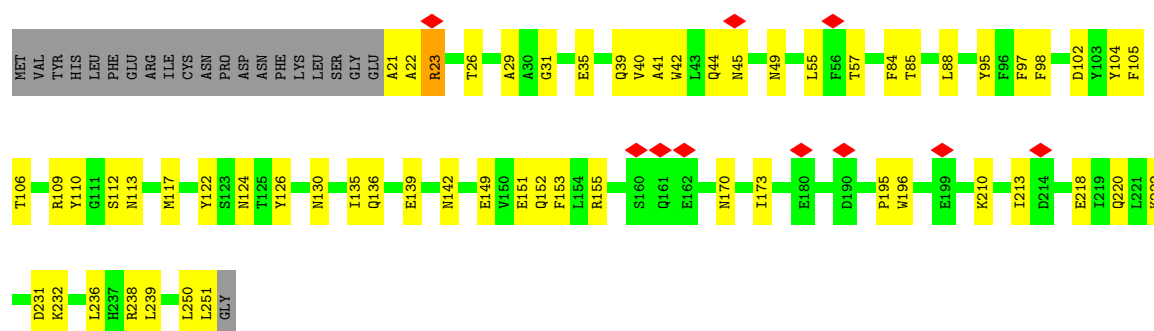


- Molecule 38: COXTT9

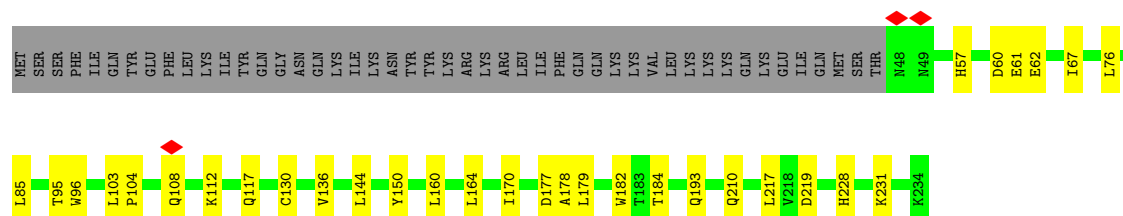
Chain i: 



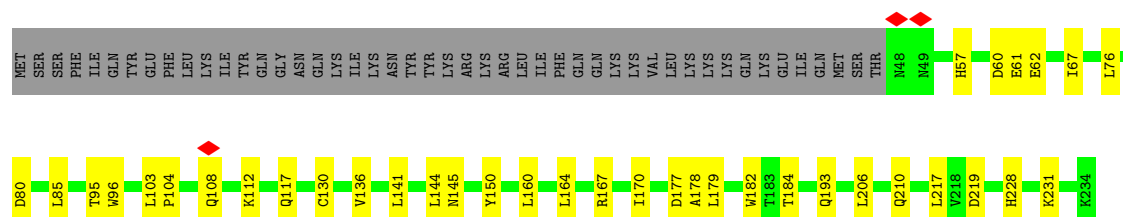
- Molecule 38: COXTT9



- Molecule 39: COXTT10



- Molecule 39: COXTT10

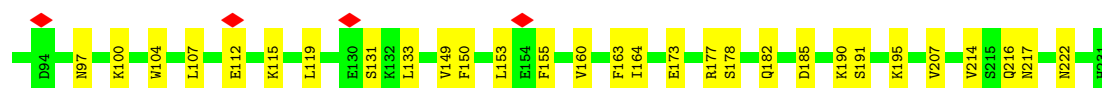
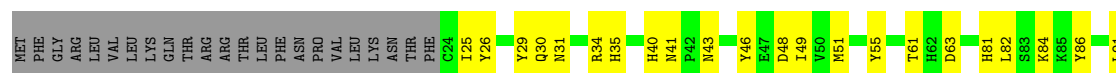


- Molecule 40: 39S ribosomal protein L9, mitochondrial

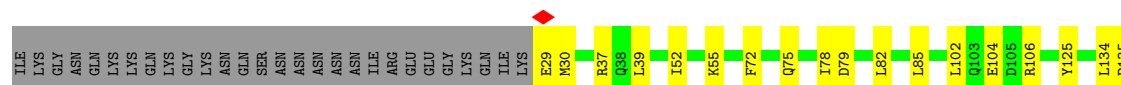




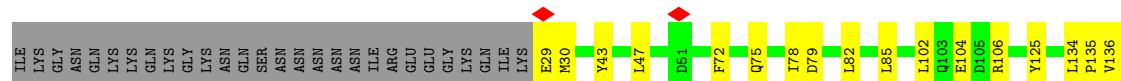
- Molecule 40: 39S ribosomal protein L9, mitochondrial



- 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

Chain M: 64% 35%



- Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain m1: 78% 22%



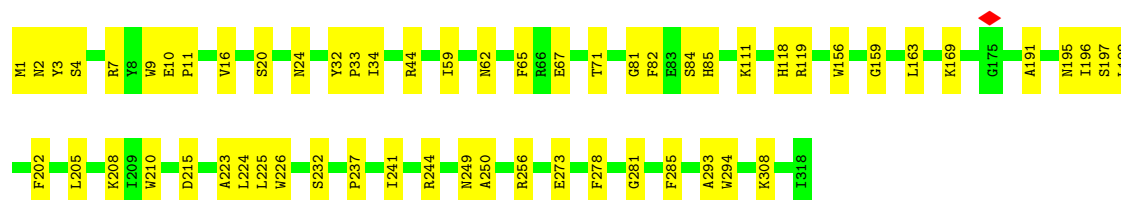
- Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain M1: 78% 22%

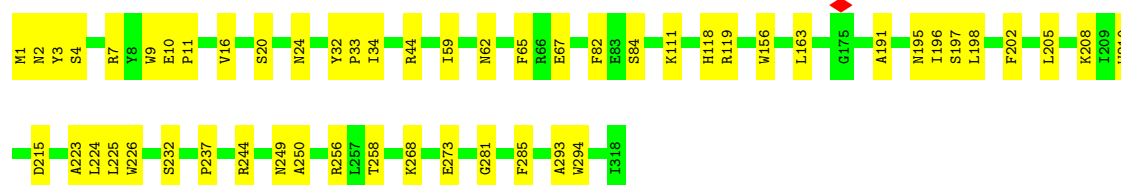
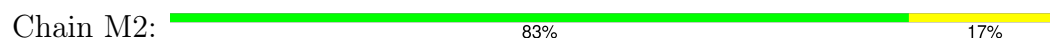


- Molecule 44: 2-oxoglutarate/malate carrier protein

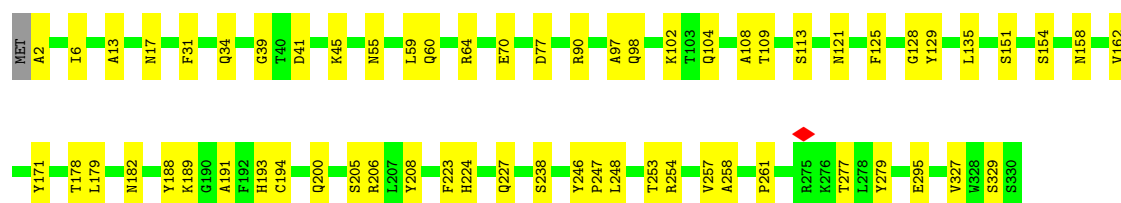
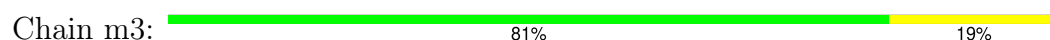
Chain m2: 81% 19%



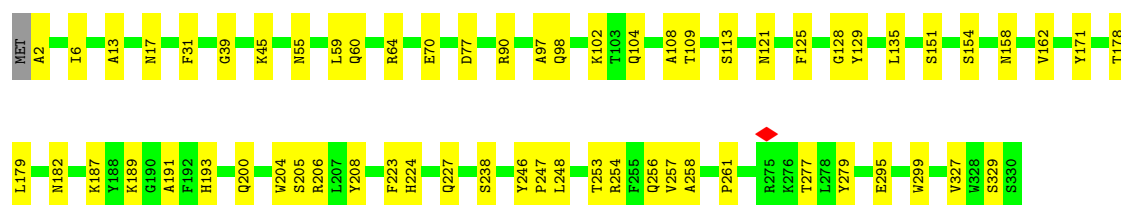
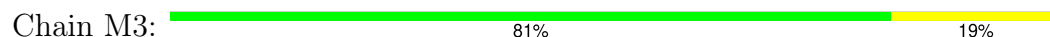
• Molecule 44: 2-oxoglutarate/malate carrier protein



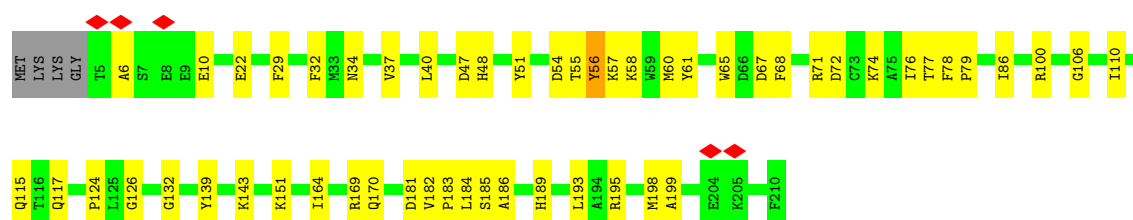
• Molecule 45: Carrier protein



• Molecule 45: Carrier protein

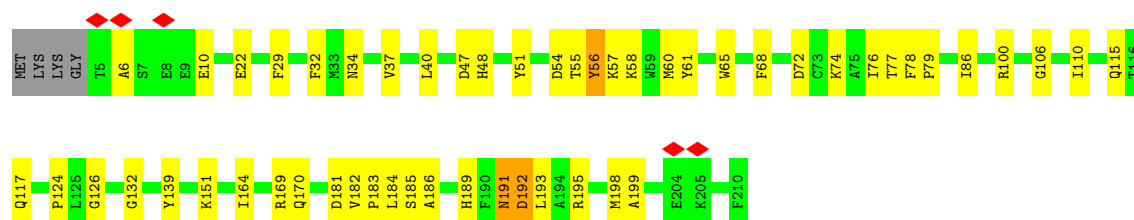


• Molecule 46: Transmembrane protein, putative



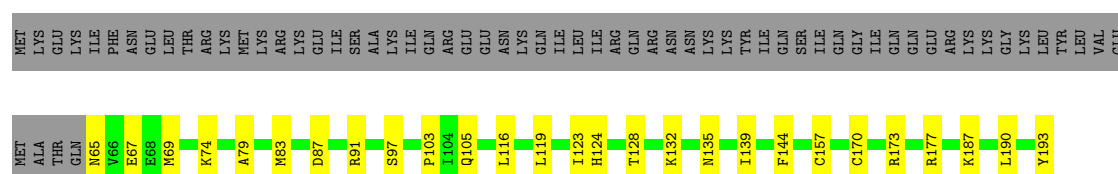
- Molecule 46: Transmembrane protein, putative

Chain N:  73% 24%



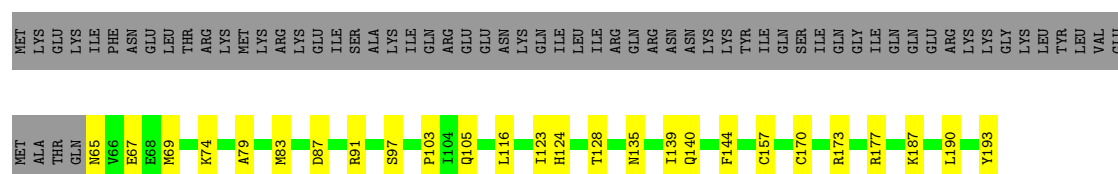
- Molecule 47: Mobilization protein

Chain o:  53% 14% 33%



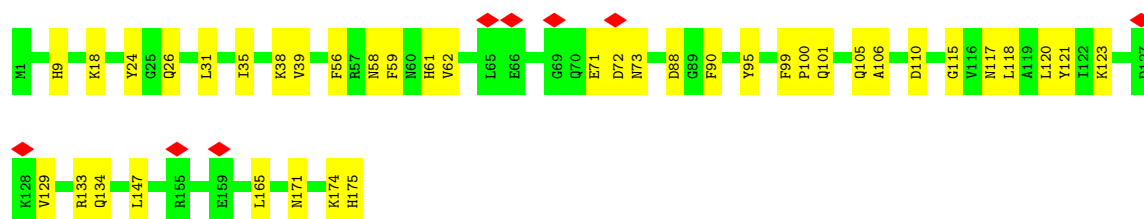
- Molecule 47: Mobilization protein

Chain O:  53% 13% 33%



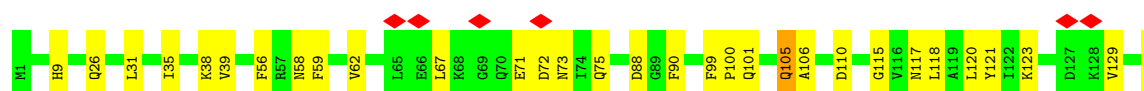
- Molecule 48: YffT domain-containing protein

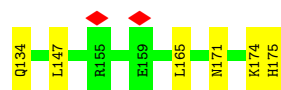
Chain p:  5% 78% 22%



- Molecule 48: YffT domain-containing protein

Chain P:  5% 79% 21%

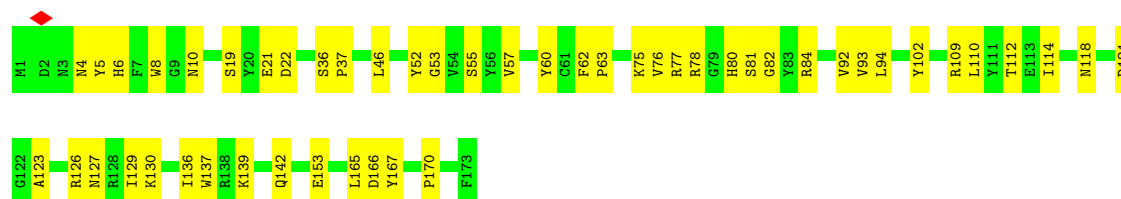




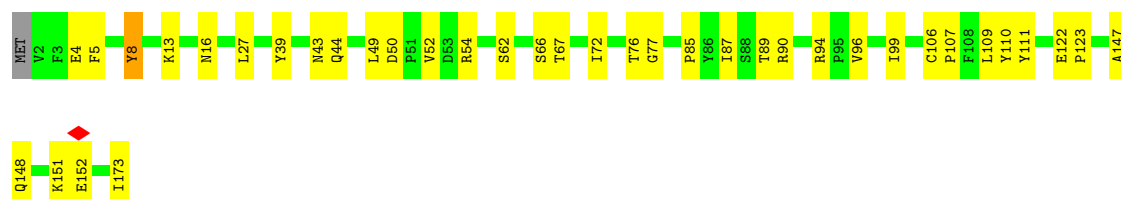
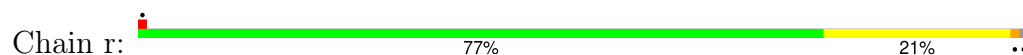
- Molecule 49: Transmembrane protein, putative



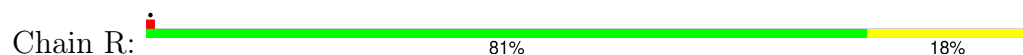
- Molecule 49: Transmembrane protein, putative



- Molecule 50: Transmembrane protein

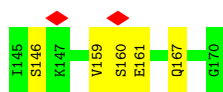


- Molecule 50: Transmembrane protein

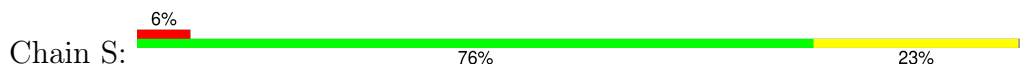


- Molecule 51: Complex III subunit VII

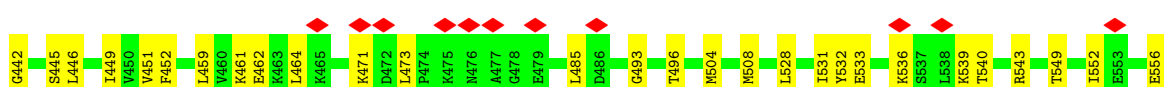
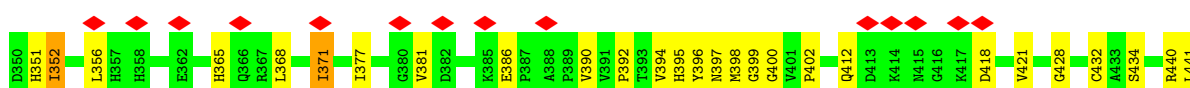
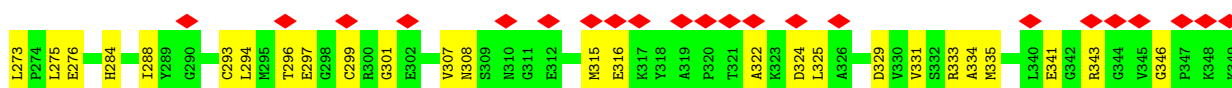
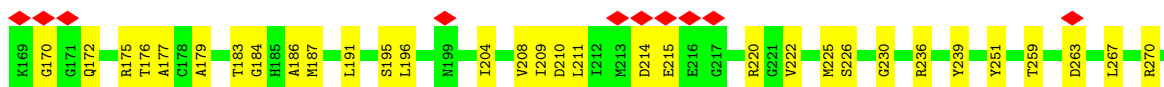
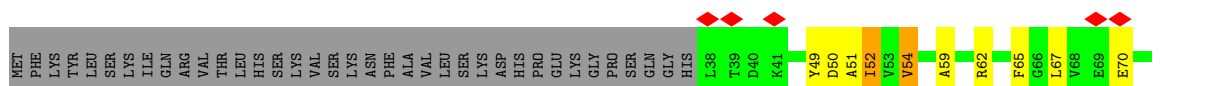




- Molecule 51: Complex III subunit VII

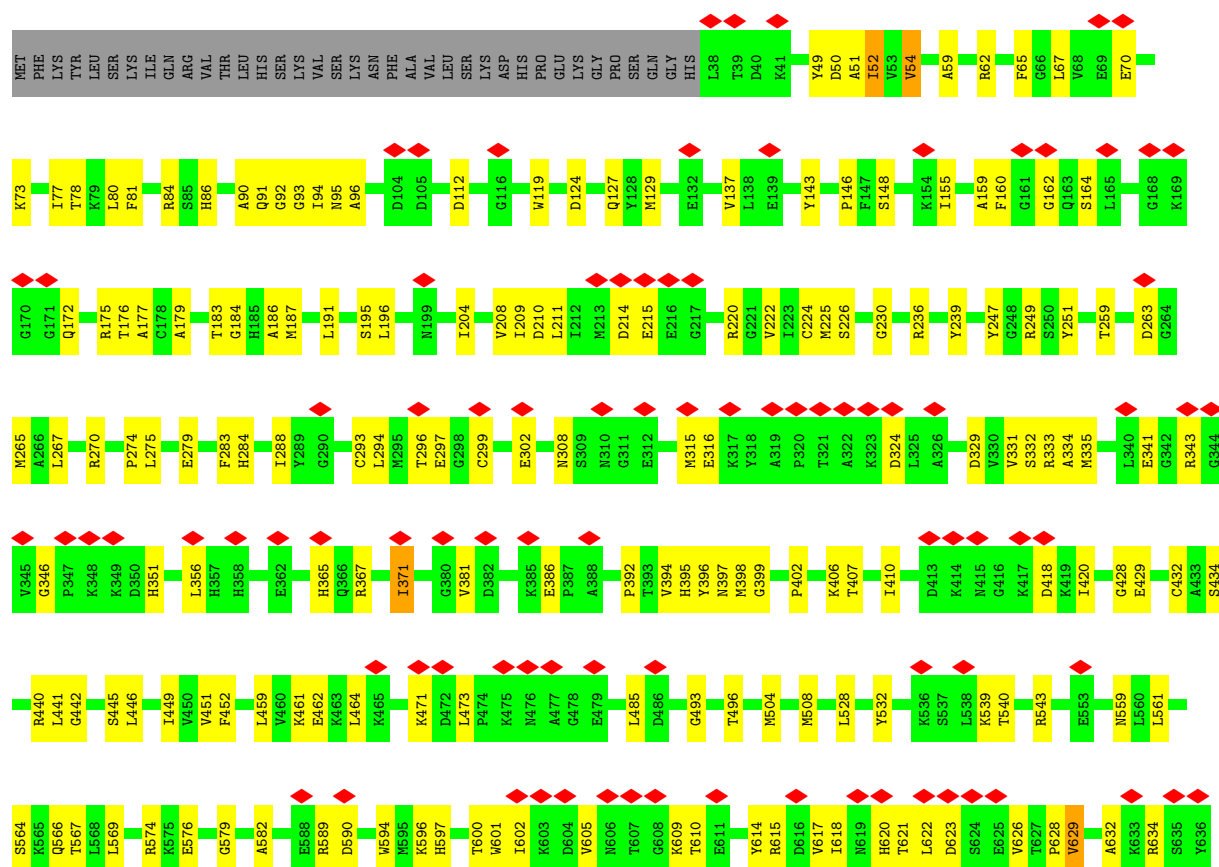


- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



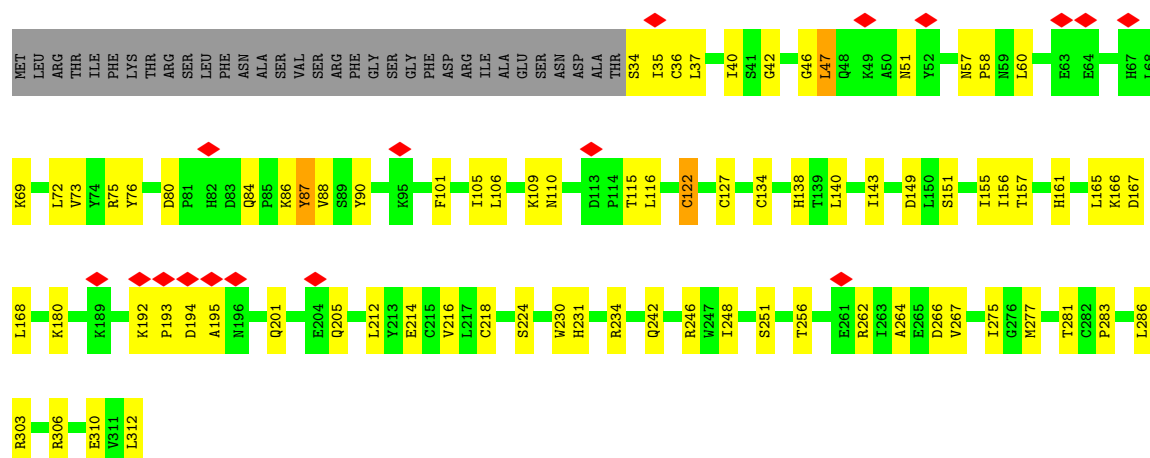
- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain SA: 



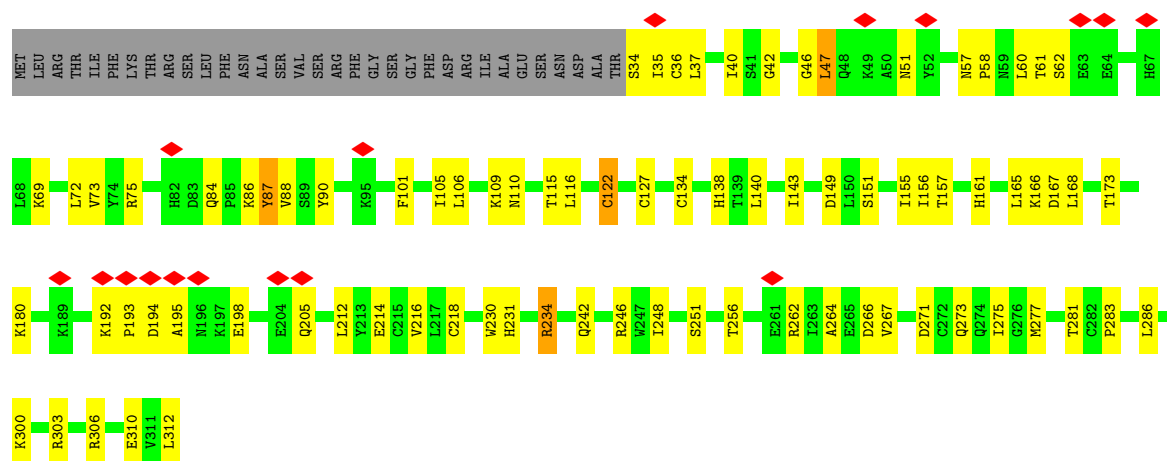
• Molecule 53: Succinate dehydrogenase (quinone)

Chain sb: 



• Molecule 53: Succinate dehydrogenase (quinone)

Chain SB: 



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain sc: 62% 35%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain SC: 62% 35%



- Molecule 55: SDHD

Chain sd: 68% 32%



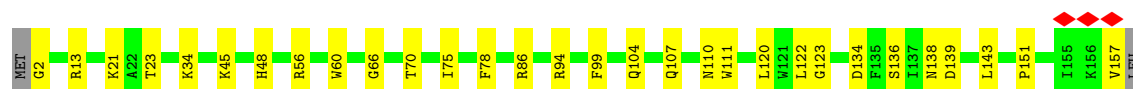
- Molecule 55: SDHD

Chain SD: 70% 30%



- Molecule 56: Transmembrane protein, putative

Chain t: 80% 19%



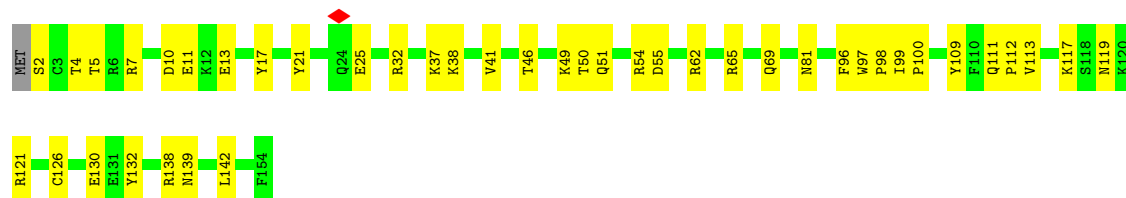
- Molecule 56: Transmembrane protein, putative

Chain T:  81% 18%



- Molecule 57: Transmembrane protein, putative

Chain u:  72% 27%



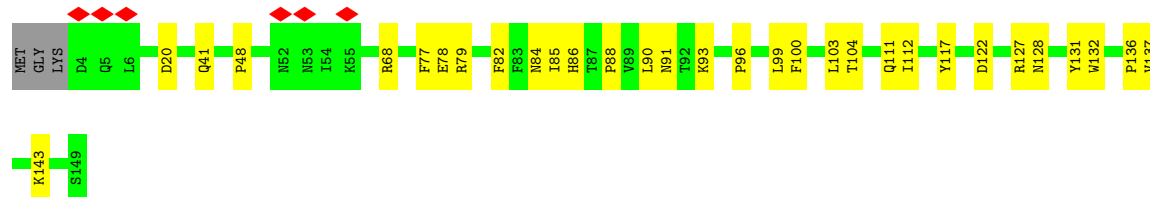
- Molecule 57: Transmembrane protein, putative

Chain U:  72% 27%



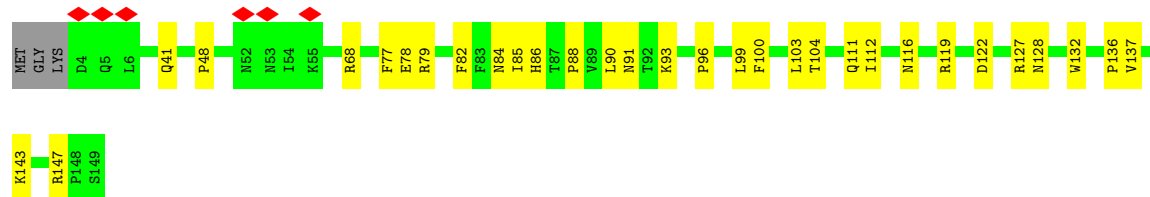
- Molecule 58: COXTT22

Chain v:  77% 21%



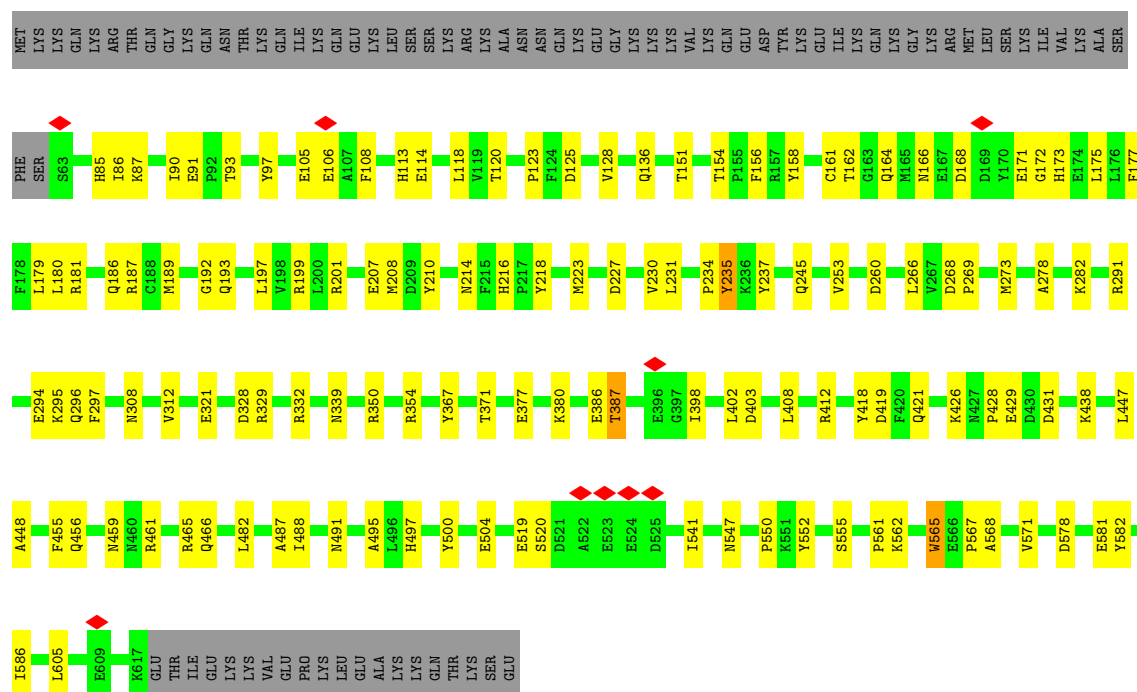
- Molecule 58: COXTT22

Chain V:  77% 21%



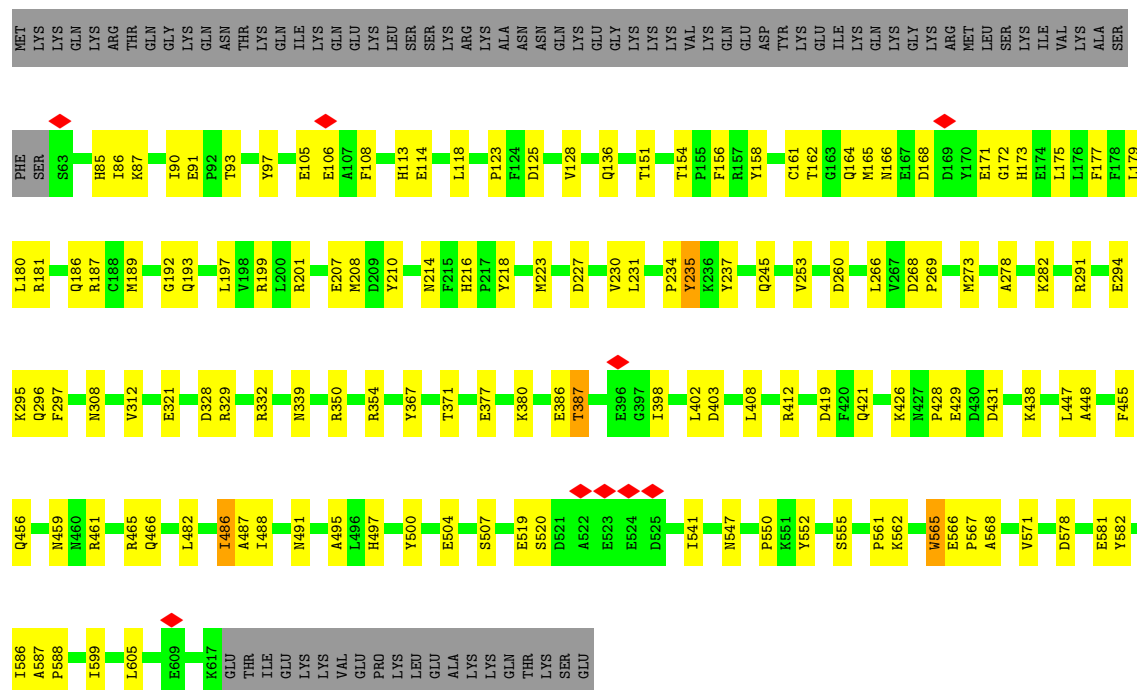
- Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain vb: 



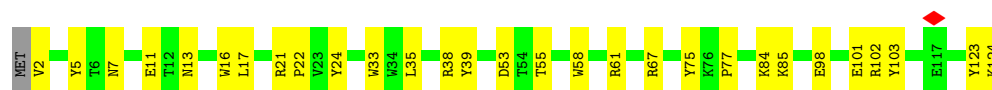
• Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain VB: 

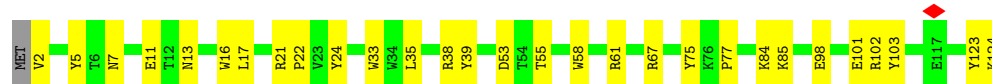
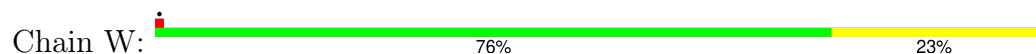


• Molecule 60: Transmembrane protein, putative

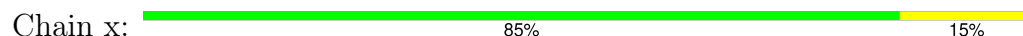
Chain w: 



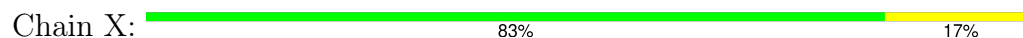
- Molecule 60: Transmembrane protein, putative



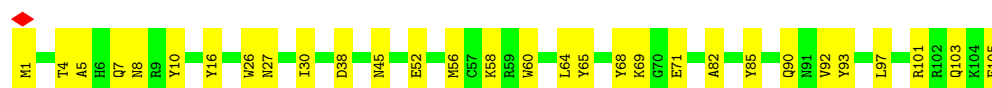
- Molecule 61: Transmembrane protein, putative



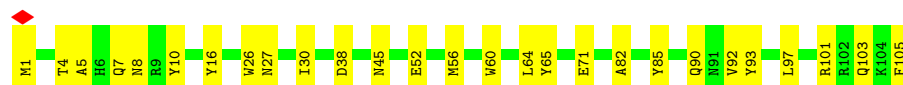
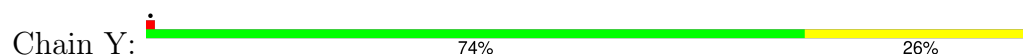
- Molecule 61: Transmembrane protein, putative



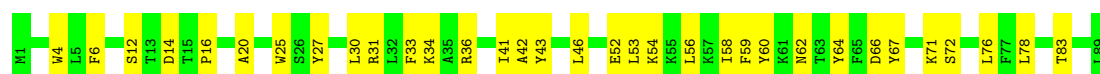
- Molecule 62: Lysozyme



- Molecule 62: Lysozyme



- Molecule 63: Ymf70



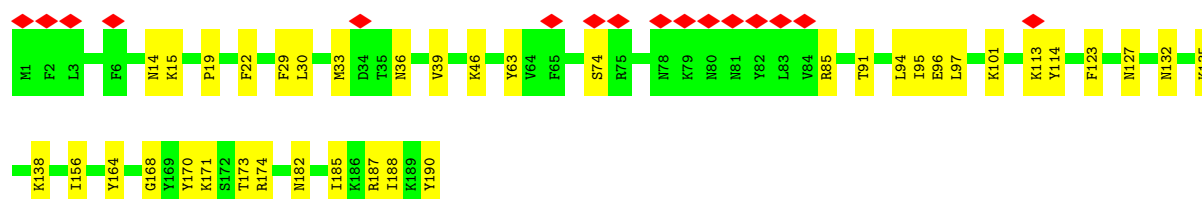
- Molecule 63: Ymf70

Chain Y0:  67% 33%



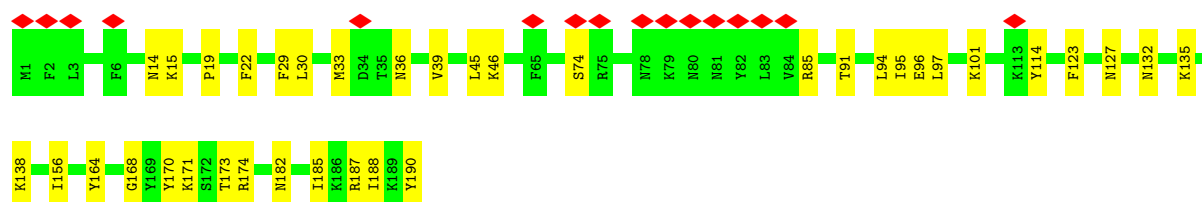
• Molecule 64: Ymf75

Chain y5:  8% 80% 20%



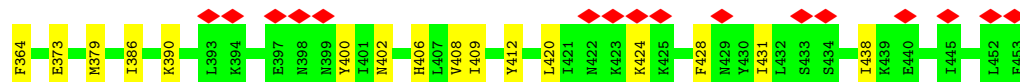
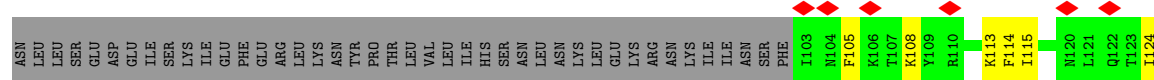
• Molecule 64: Ymf75

Chain Y5:  8% 81% 19%



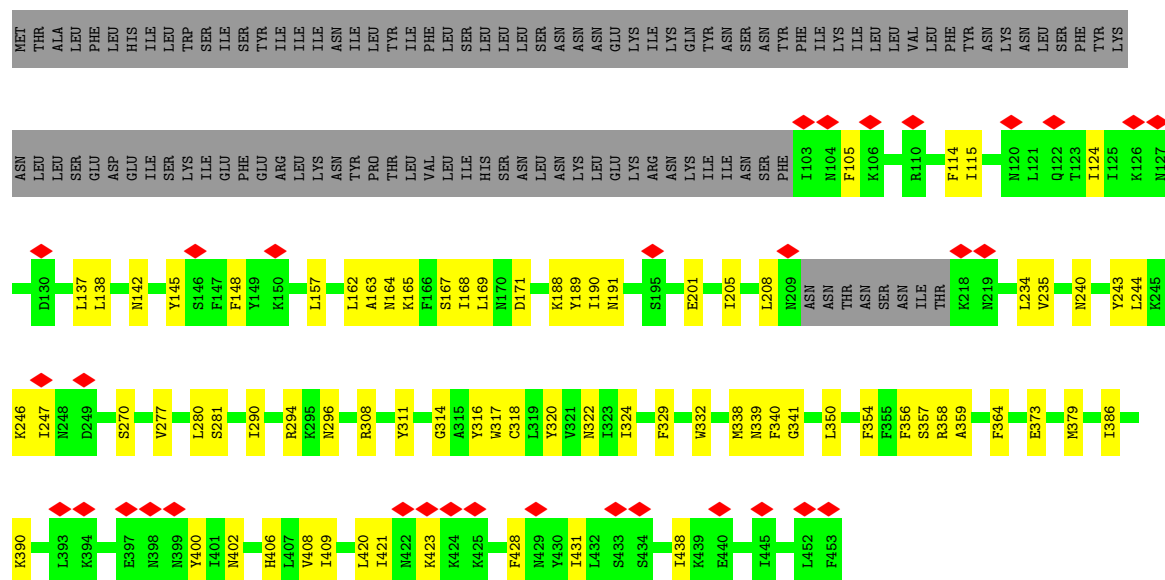
• Molecule 65: Ymf67

Chain y7:  7% 58% 18% 24%



• Molecule 65: Ymf67

Chain Y7:  7% 59% 17% 24%



• Molecule 66: ABC transporter



• Molecule 66: ABC transporter



• Molecule 67: COXTT28



• Molecule 67: COXTT28



• Molecule 68: NADH dehydrogenase subunit 1





- Molecule 68: NADH dehydrogenase subunit 1



- Molecule 69: NADH dehydrogenase subunit 2



- Molecule 69: NADH dehydrogenase subunit 2



- Molecule 70: Ymf58



- Molecule 70: Ymf58





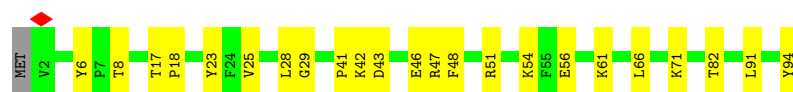
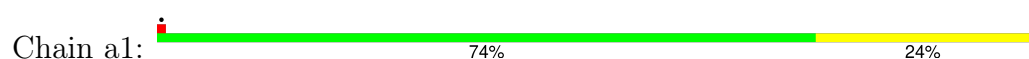
- Molecule 71: Ymf57



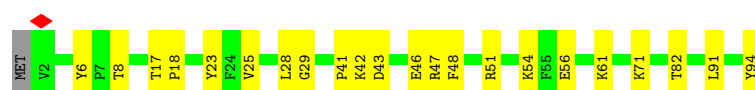
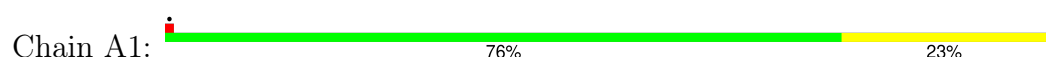
- Molecule 71: Ymf57



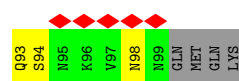
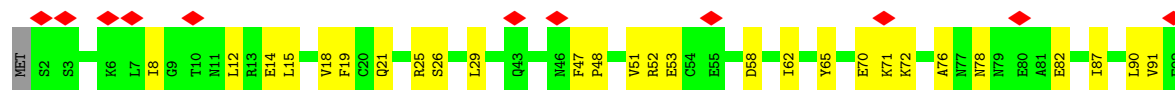
- Molecule 72: Transmembrane protein, putative



- Molecule 72: Transmembrane protein, putative

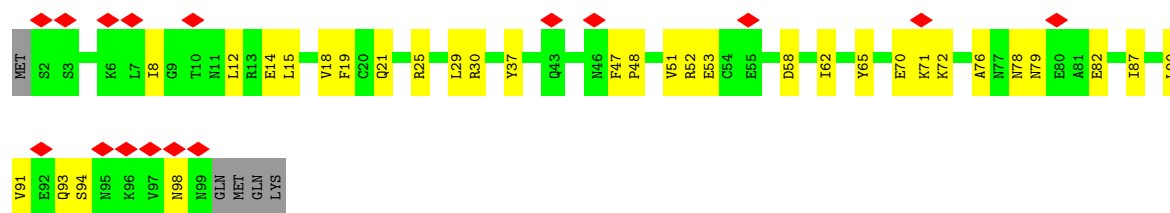


- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

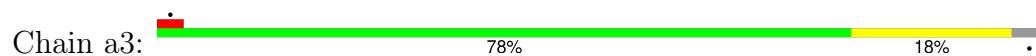


- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

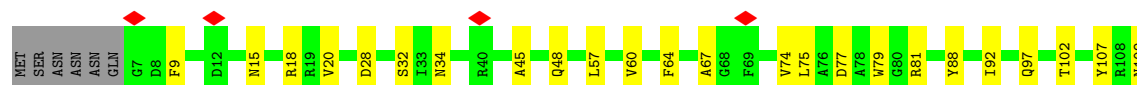
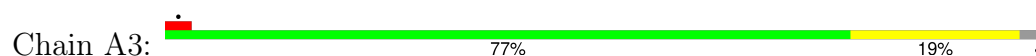




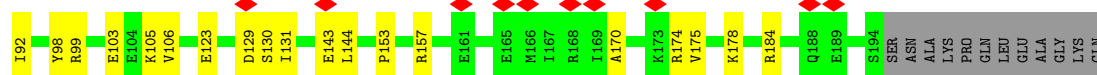
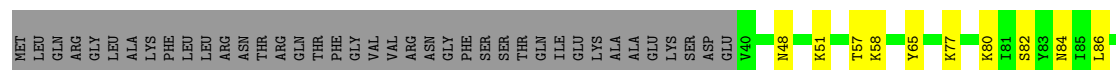
- Molecule 74: Transmembrane protein, putative



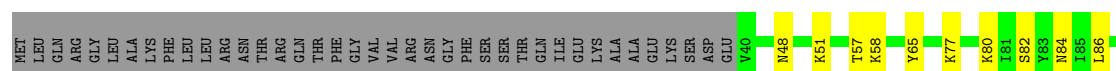
- Molecule 74: Transmembrane protein, putative



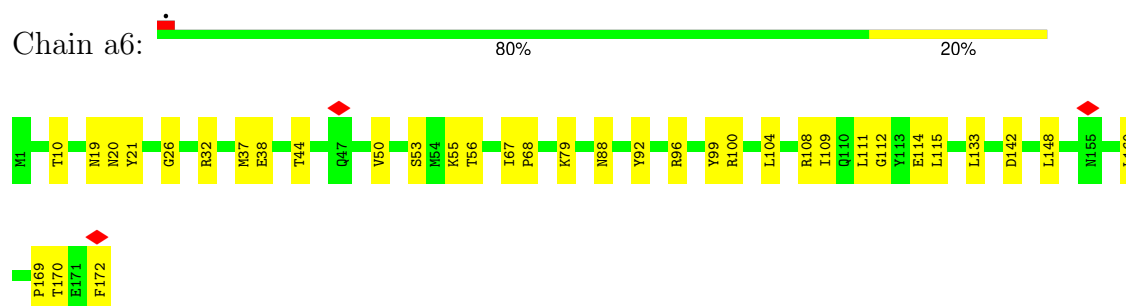
- Molecule 75: ETC complex I subunit motif protein



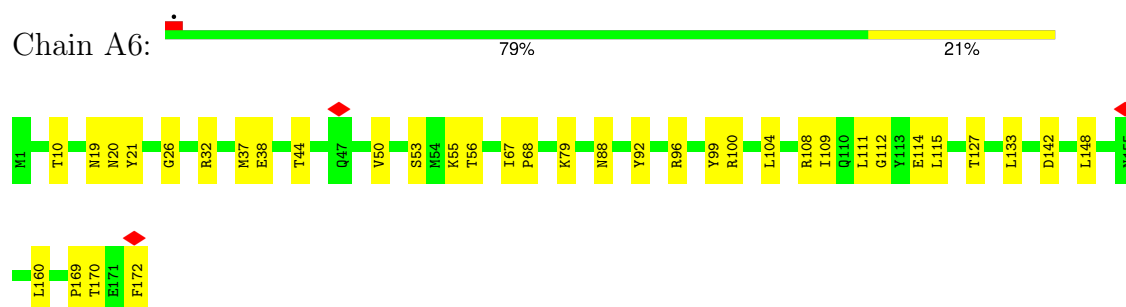
- Molecule 75: ETC complex I subunit motif protein



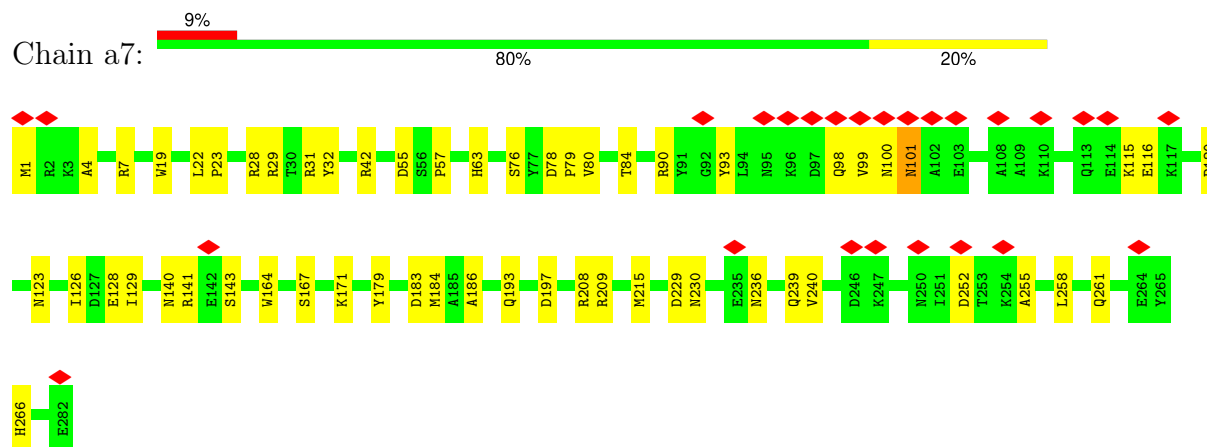
- Molecule 76: NADH dehydrogenase, putative



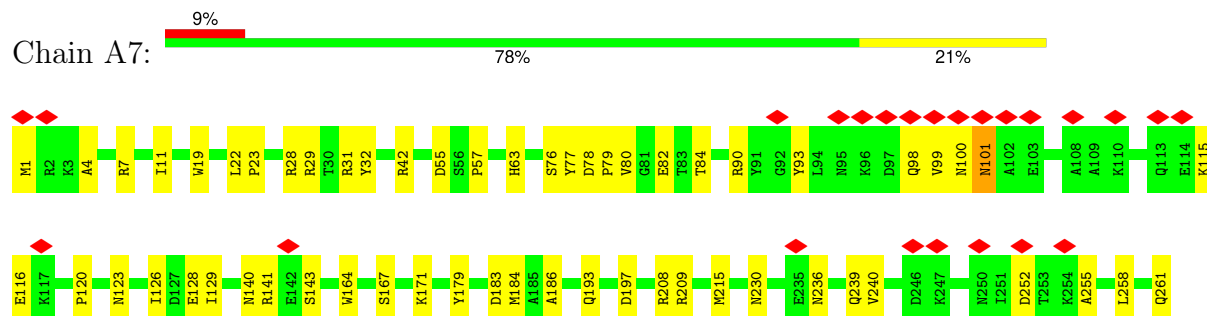
- Molecule 76: NADH dehydrogenase, putative

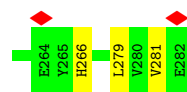


- Molecule 77: 37S ribosomal protein S25, mitochondrial



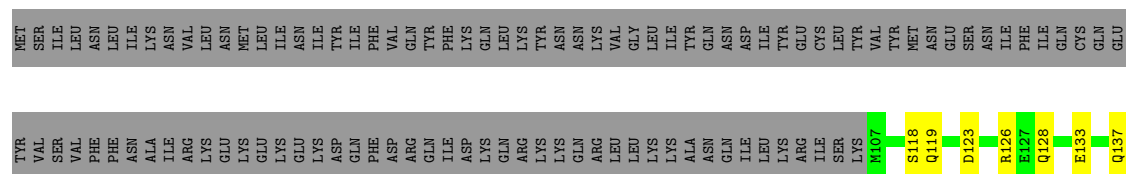
- Molecule 77: 37S ribosomal protein S25, mitochondrial





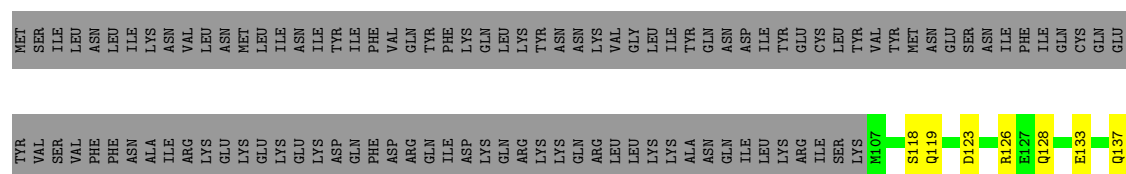
- Molecule 78: CX9C domain-containing protein

Chain a8:



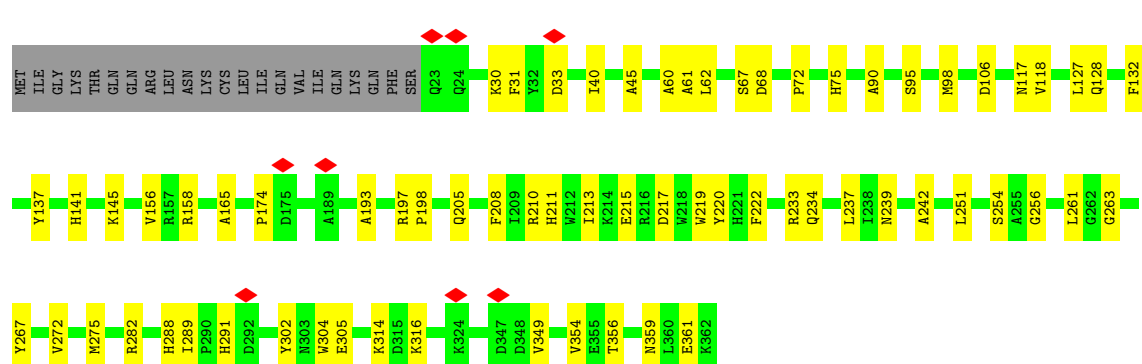
- Molecule 78: CX9C domain-containing protein

Chain A8:



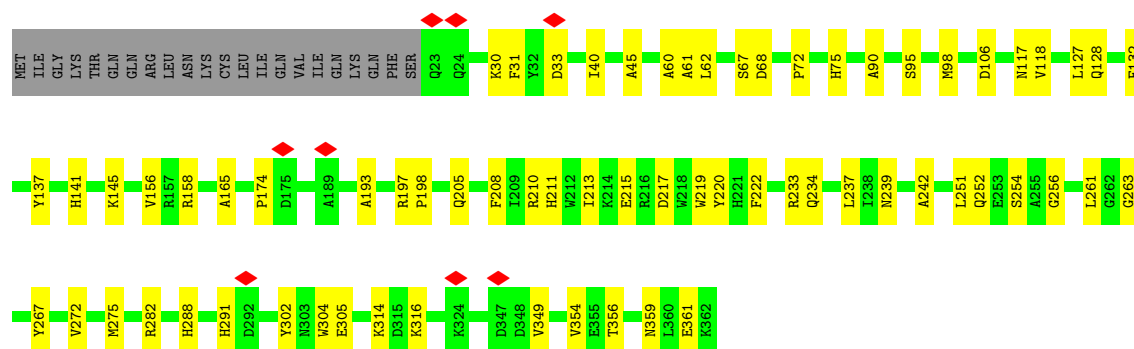
- Molecule 79: NAD-dependent epimerase/dehydratase family protein

Chain a9:

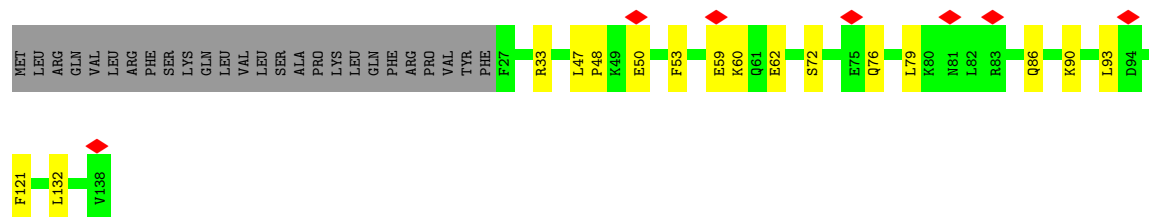


- Molecule 79: NAD-dependent epimerase/dehydratase family protein

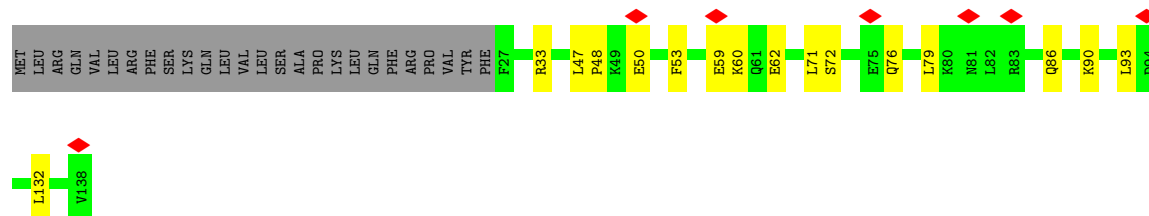
Chain A9:



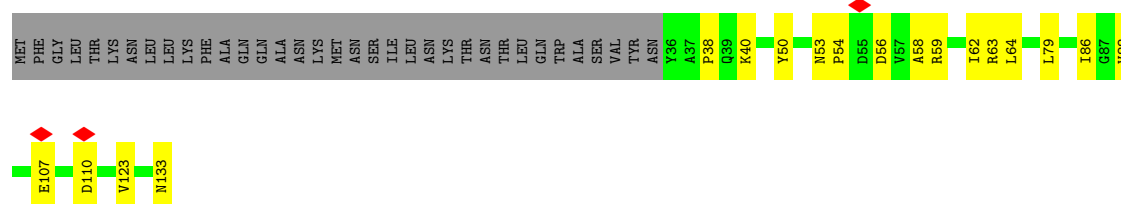
- Molecule 80: Acyl carrier protein



- Molecule 80: Acyl carrier protein

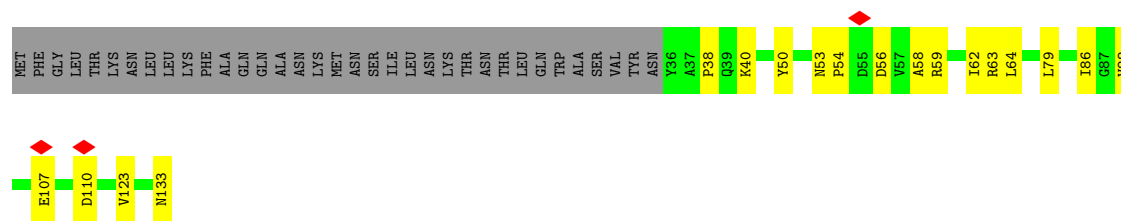


- Molecule 81: Acyl carrier protein

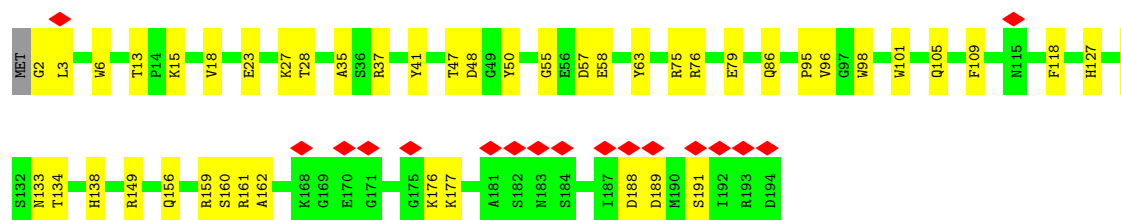
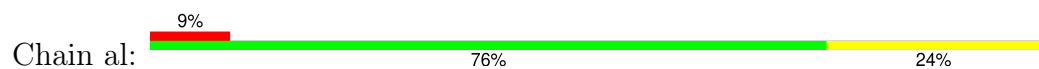


- Molecule 81: Acyl carrier protein

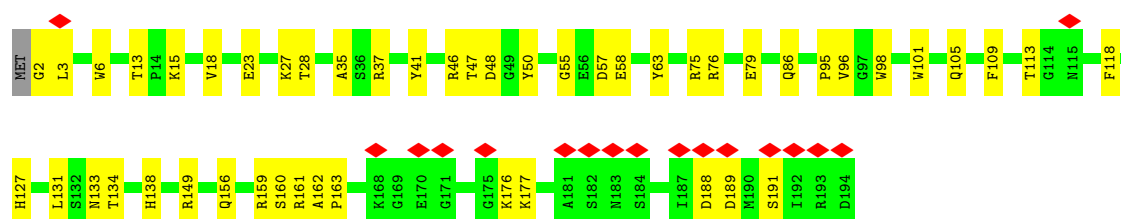
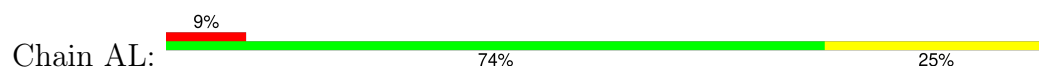




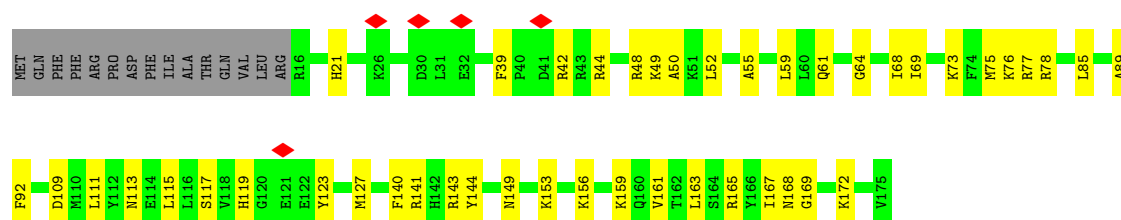
- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



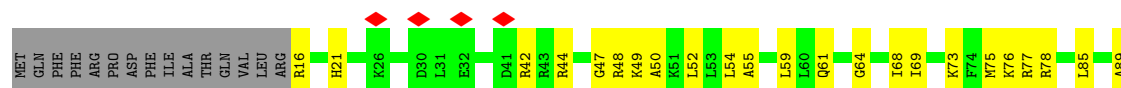
- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 83: NDUA13

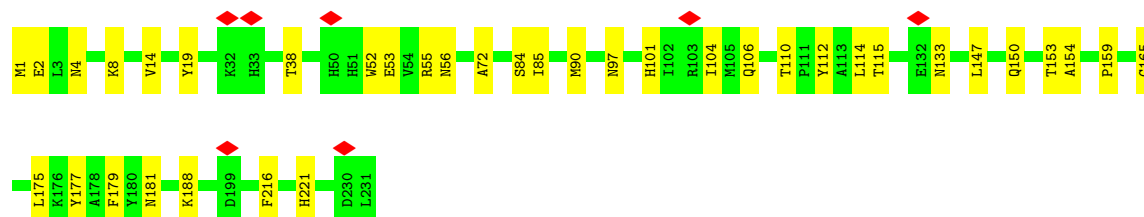
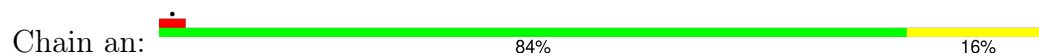


- Molecule 83: NDUA13

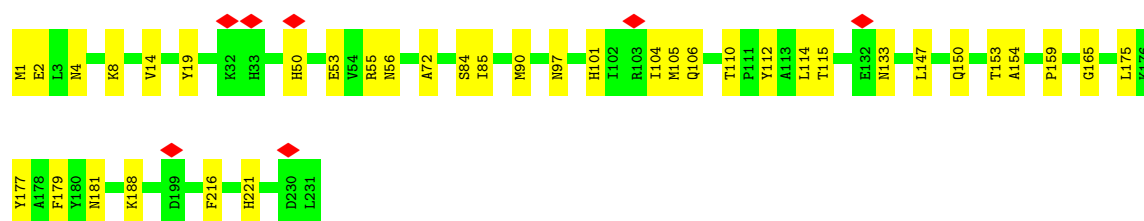
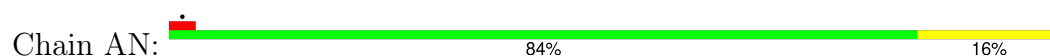




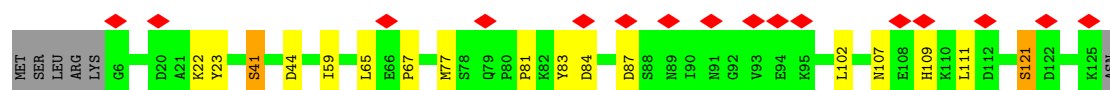
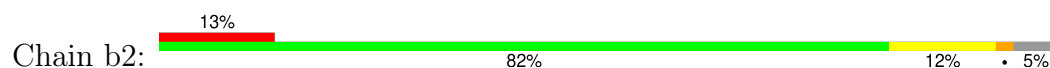
- Molecule 84: Transmembrane protein, putative



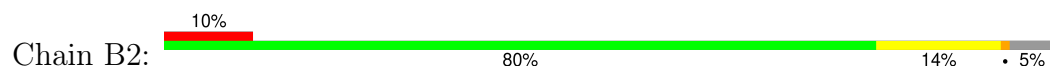
- Molecule 84: Transmembrane protein, putative



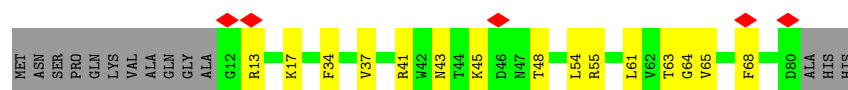
- Molecule 85: NDUB2



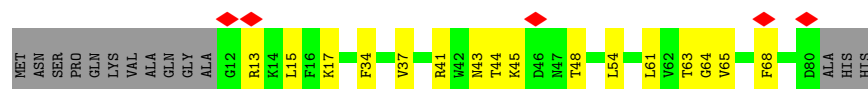
- Molecule 85: NDUB2



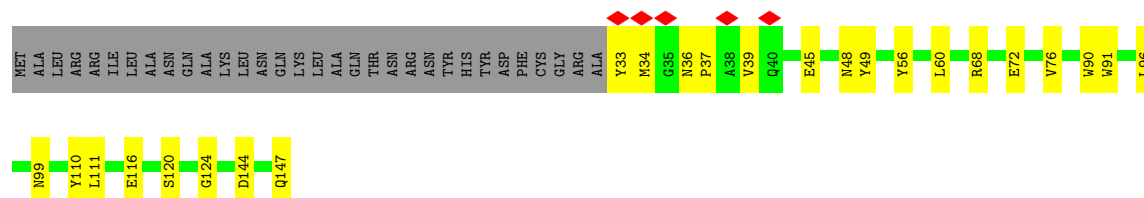
- Molecule 86: Transmembrane protein, putative



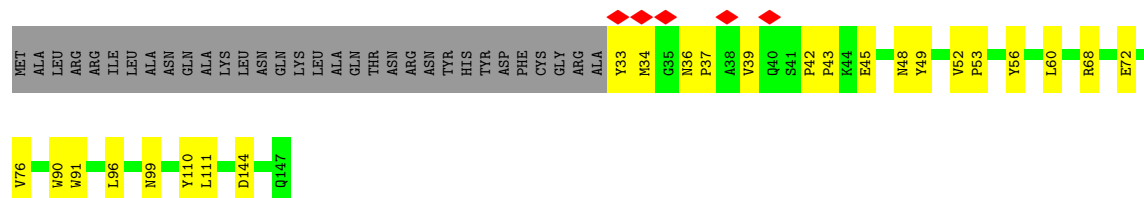
- Molecule 86: Transmembrane protein, putative



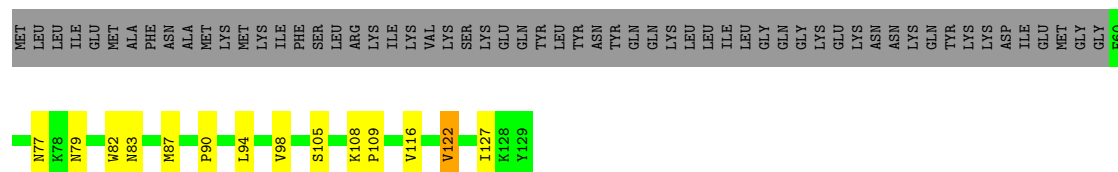
- Molecule 87: NDUB4



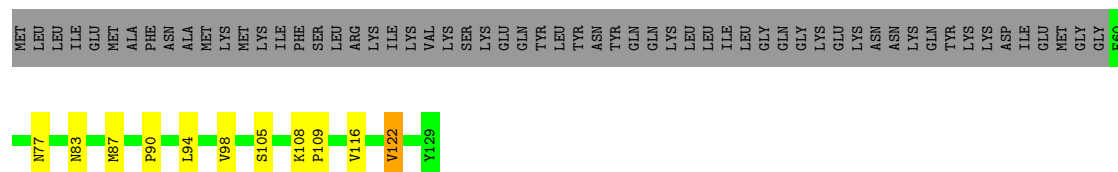
- Molecule 87: NDUB4



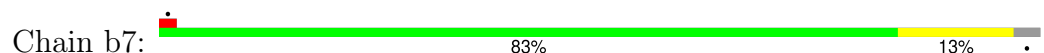
- Molecule 88: NDUB6



- Molecule 88: NDUB6

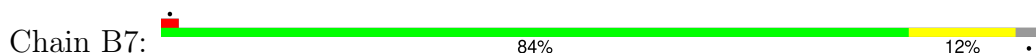


- Molecule 89: CHCH domain-containing protein

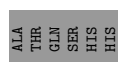
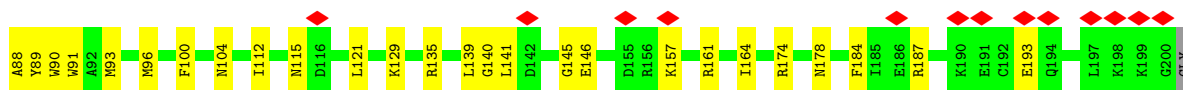
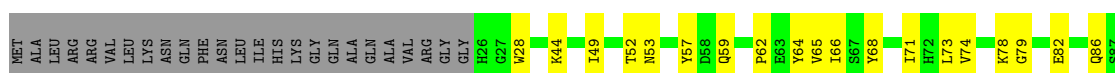




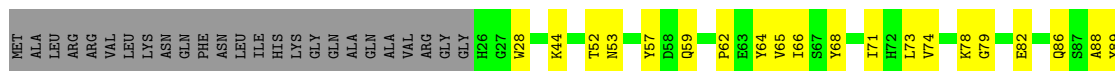
- Molecule 89: CHCH domain-containing protein



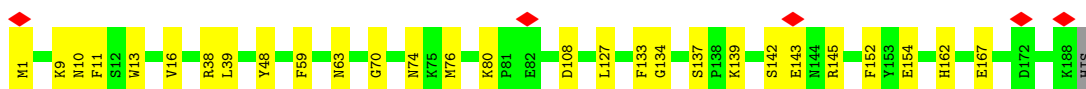
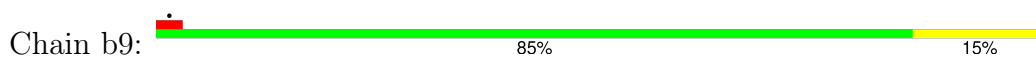
- Molecule 90: NDUB8



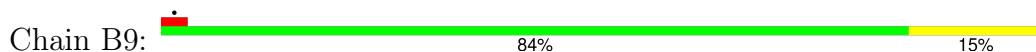
- Molecule 90: NDUB8

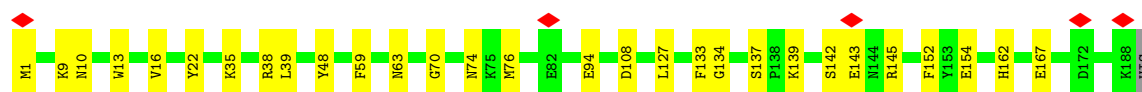


- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

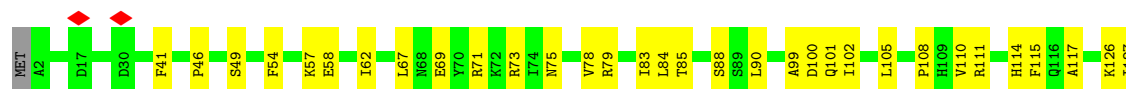


- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

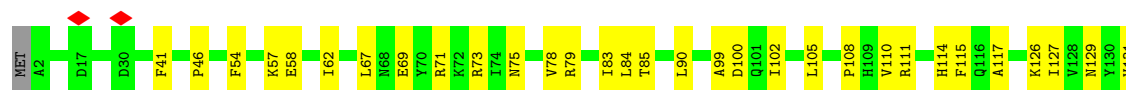




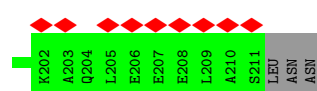
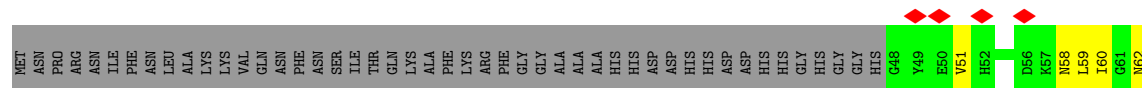
- Molecule 92: NDUB10



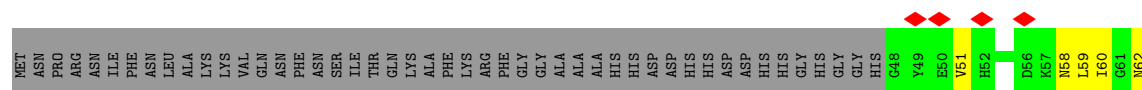
- Molecule 92: NDUB10

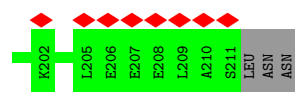


- Molecule 93: Transmembrane protein, putative

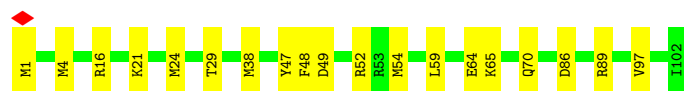
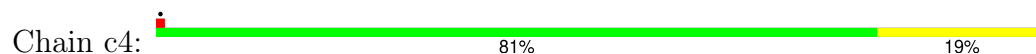


- Molecule 93: Transmembrane protein, putative

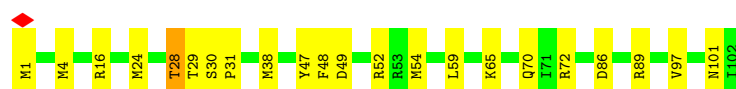
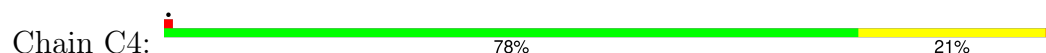




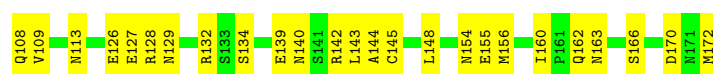
- Molecule 94: Complex I-MNLL



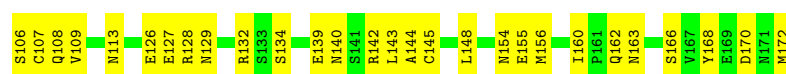
- Molecule 94: Complex I-MNLL



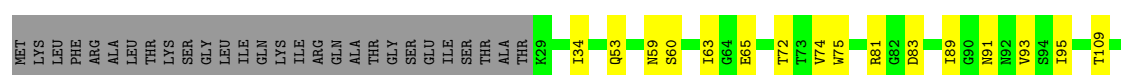
- Molecule 95: 2 iron, 2 sulfur cluster-binding protein



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



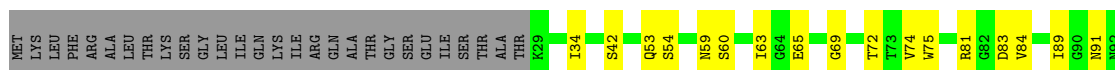
- Molecule 96: Gamma-carbonic anhydrase





- Molecule 96: Gamma-carbonic anhydrase

Chain G1: 69% 20% 11%



- Molecule 97: Gamma-carbonic anhydrase

Chain g2: 75% 24%



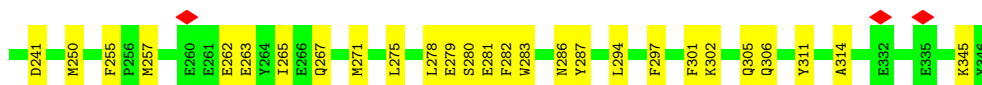
- Molecule 97: Gamma-carbonic anhydrase

Chain G2: 73% 25%



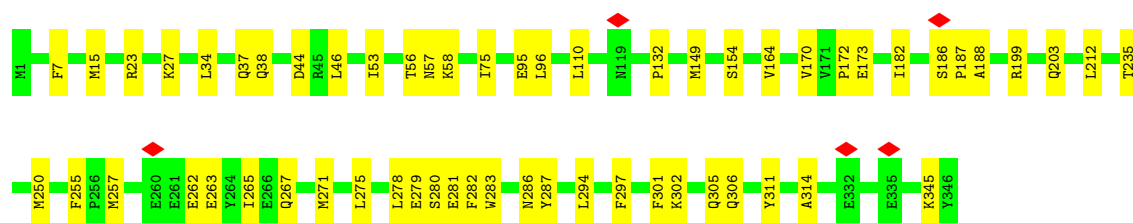
- Molecule 98: Transcription factor apf protein, putative

Chain g3: 83% 17%



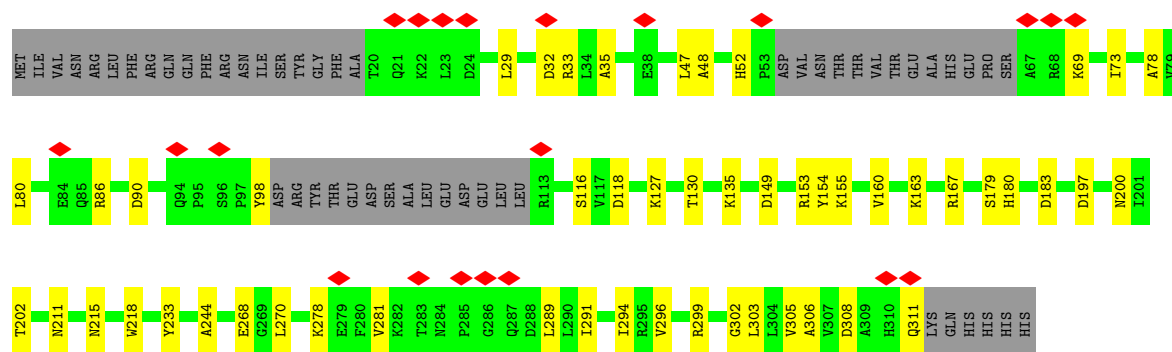
- Molecule 98: Transcription factor apf protein, putative

Chain G3:  83% 17%



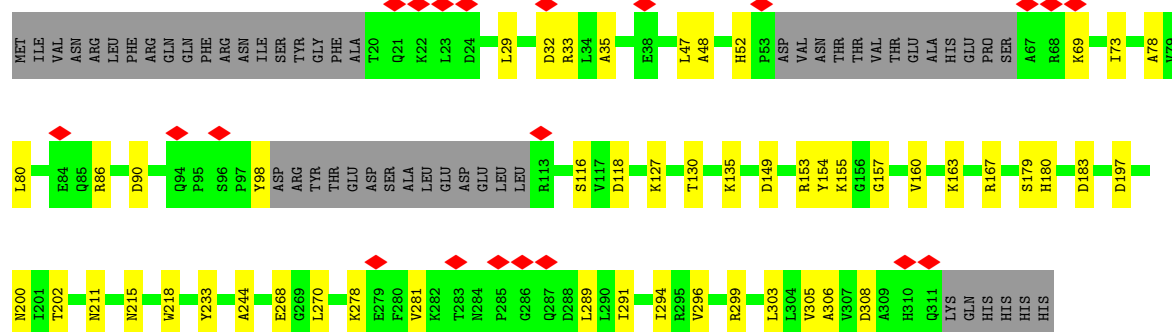
- Molecule 99: DnaJ domain protein

Chain j1:  7% 67% 16% 16%



- Molecule 99: DnaJ domain protein

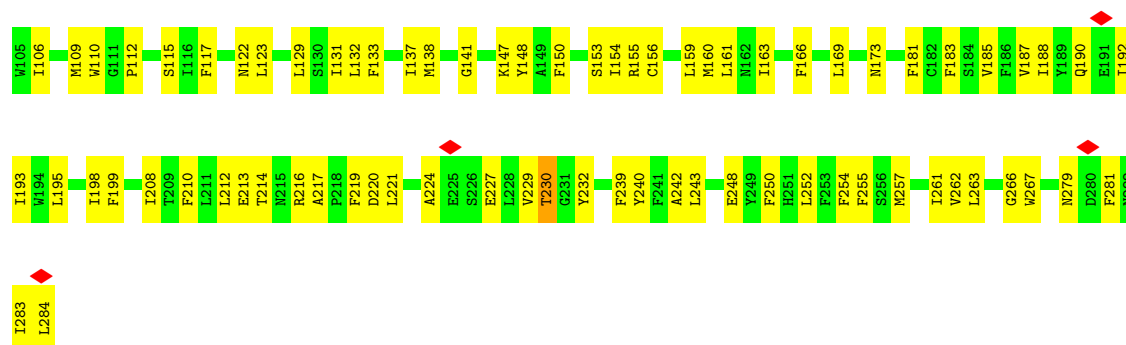
Chain J1:  7% 68% 16% 16%



- Molecule 100: NADH-ubiquinone oxidoreductase chain 1

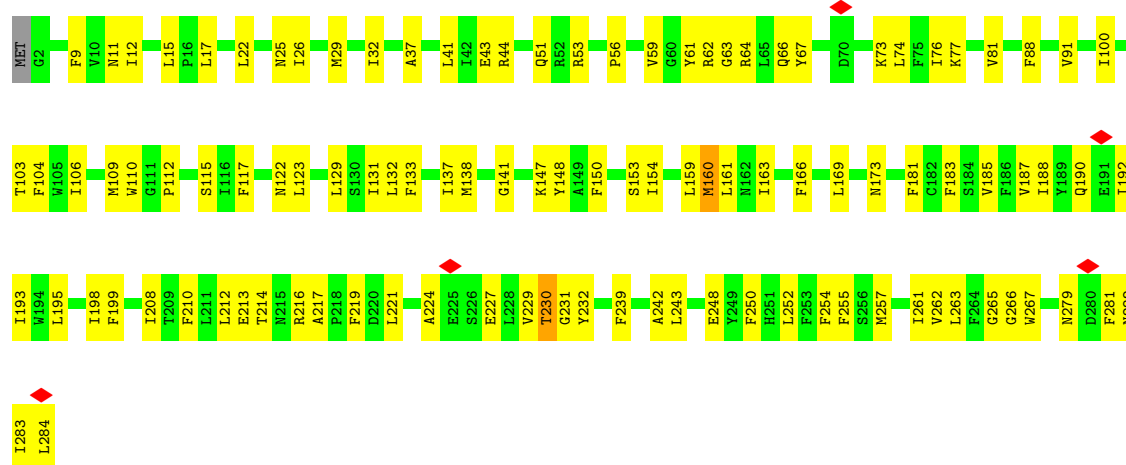
Chain n1:  62% 38%





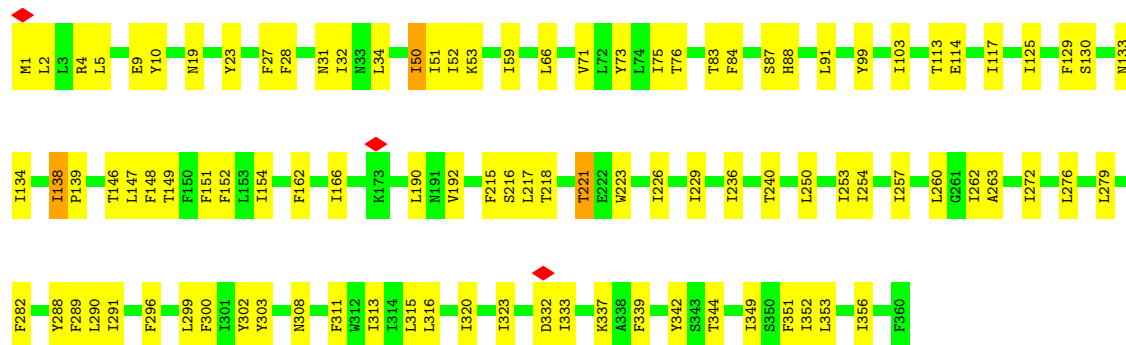
• Molecule 100: NADH-ubiquinone oxidoreductase chain 1

Chain N1: 62% 37% .



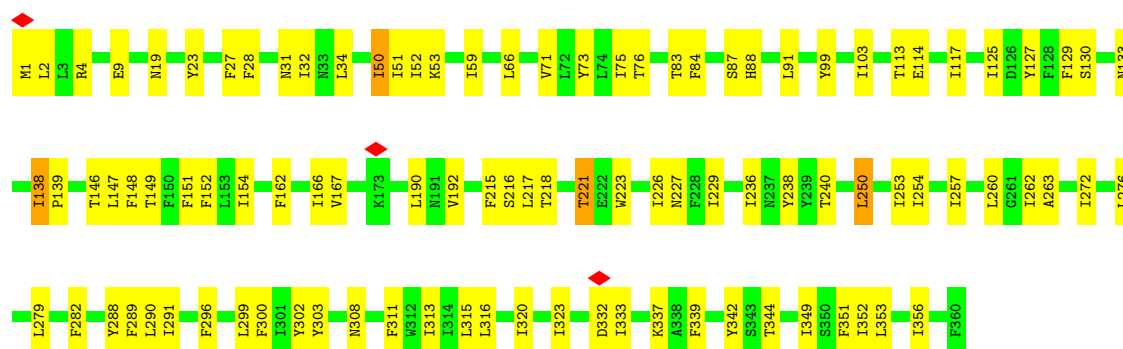
• Molecule 101: Ymf65

Chain n2: 72% 27% .

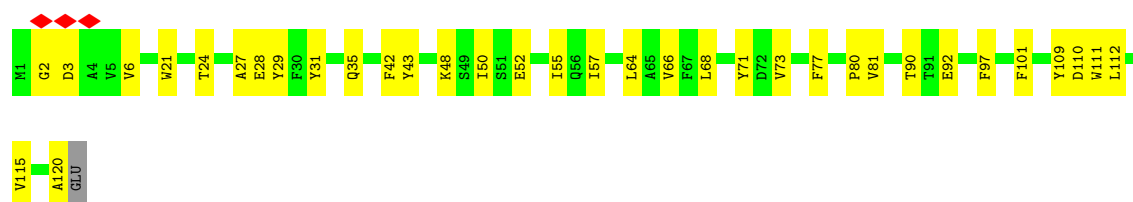


• Molecule 101: Ymf65

Chain N2: 72% 27% .



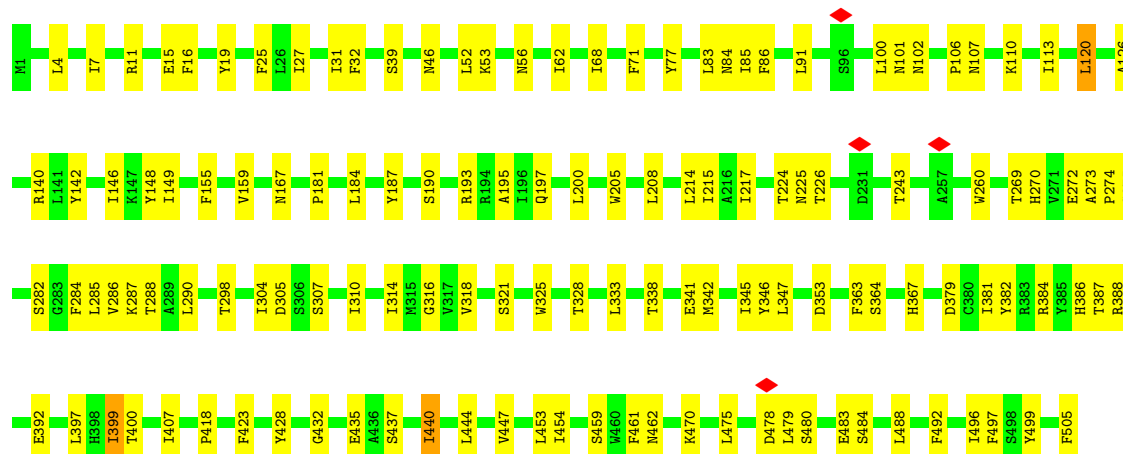
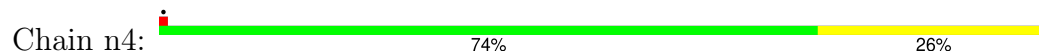
• Molecule 102: NADH-ubiquinone oxidoreductase chain 3



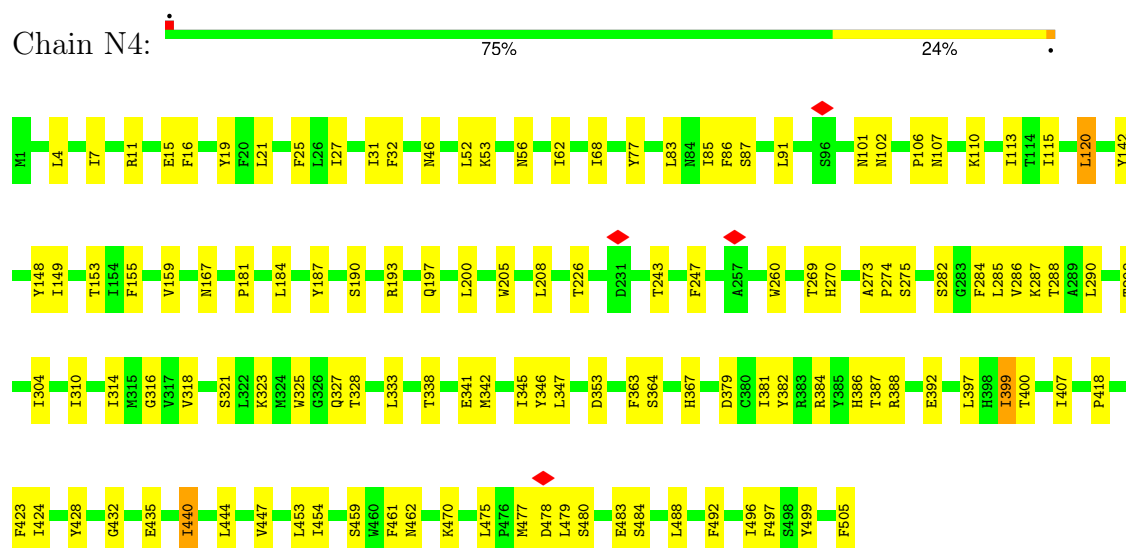
• Molecule 102: NADH-ubiquinone oxidoreductase chain 3



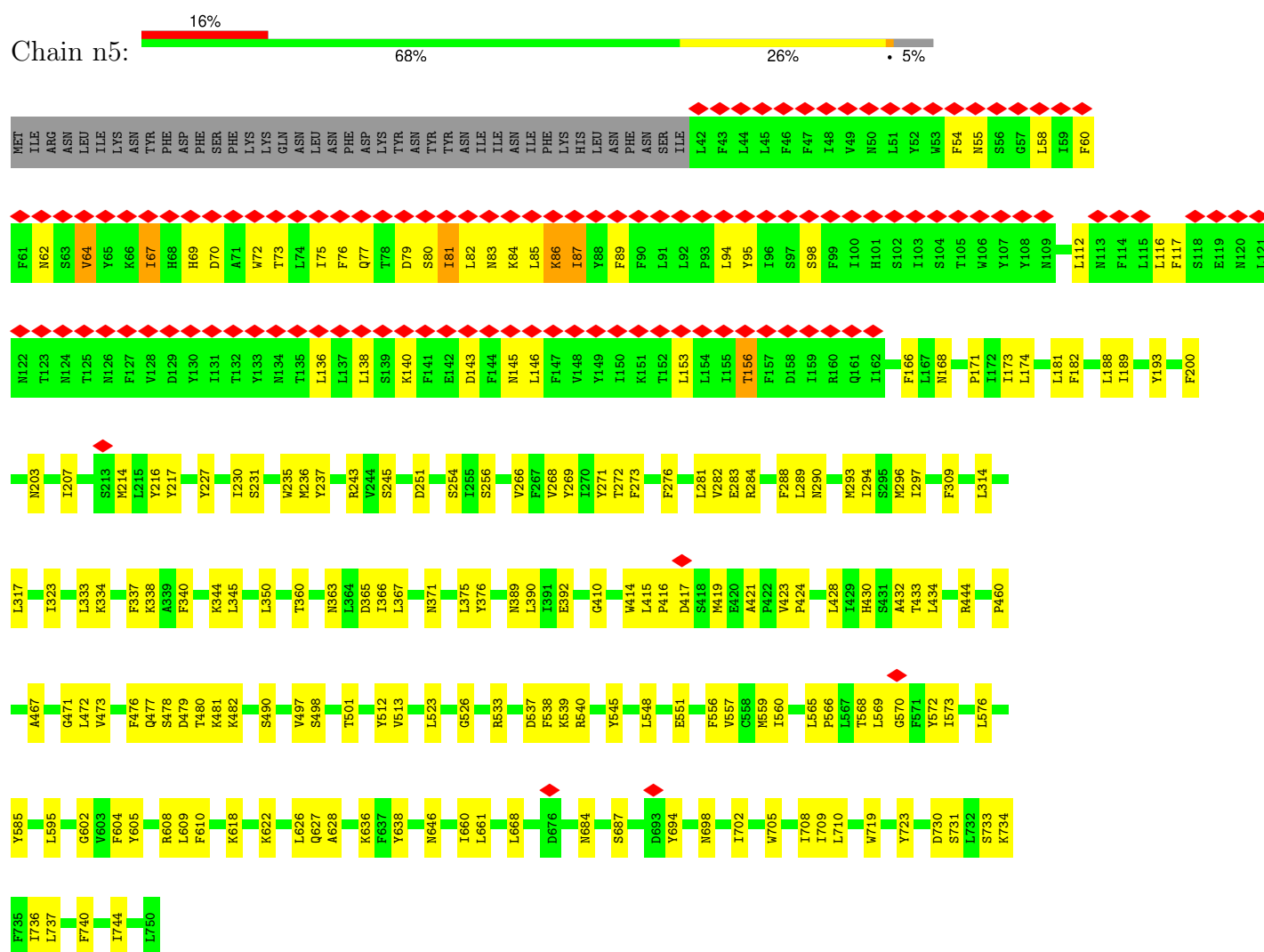
• Molecule 103: NADH-ubiquinone oxidoreductase chain 4



• Molecule 103: NADH-ubiquinone oxidoreductase chain 4

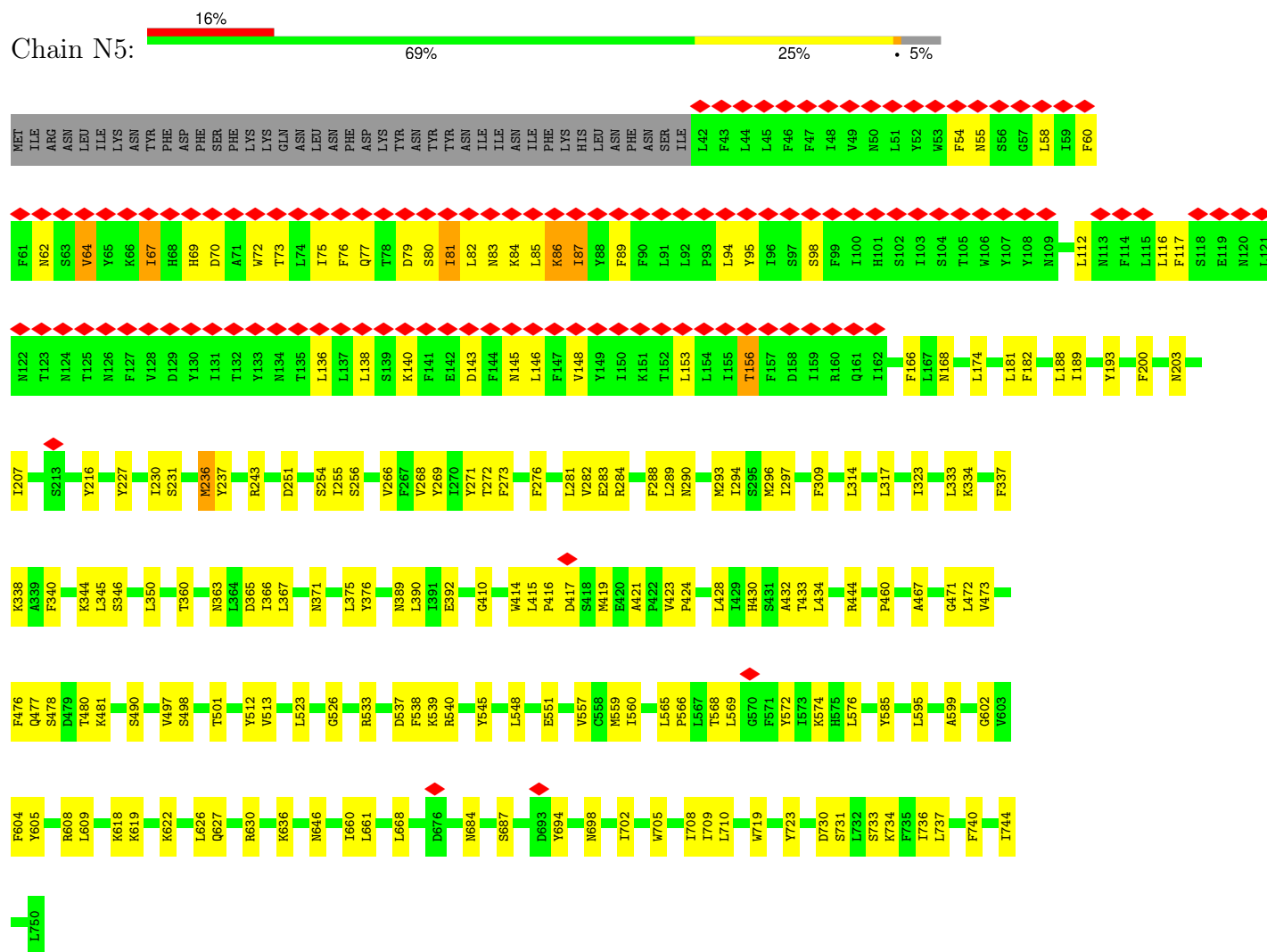


• Molecule 104: NADH dehydrogenase subunit 5



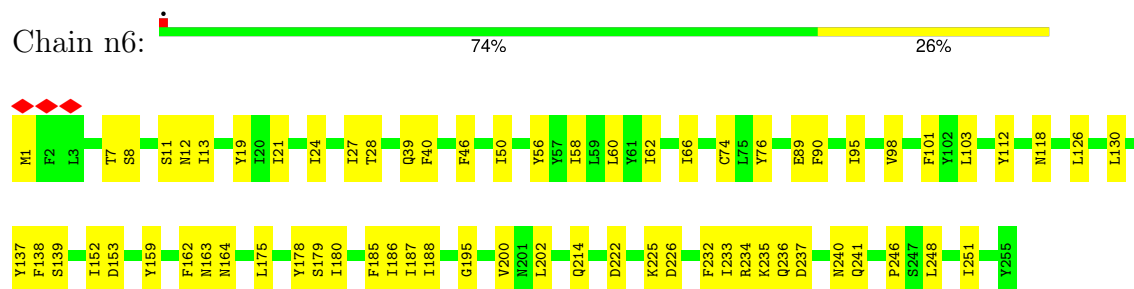
- Molecule 104: NADH dehydrogenase subunit 5

Chain N5:



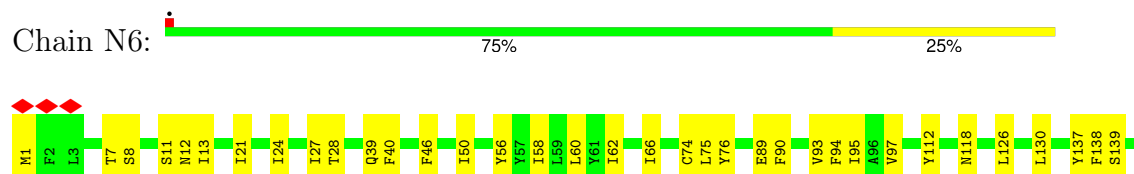
- Molecule 105: Ymf62

Chain n6:



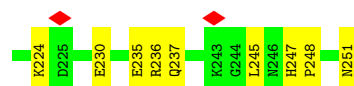
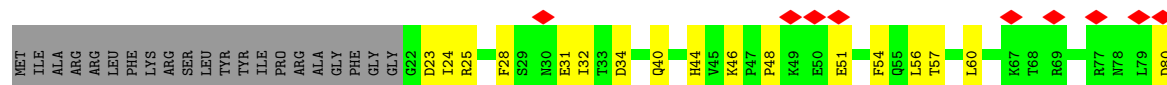
- Molecule 105: Ymf62

Chain N6:

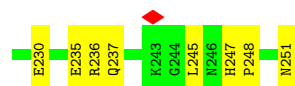
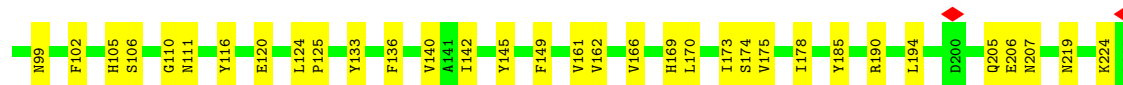




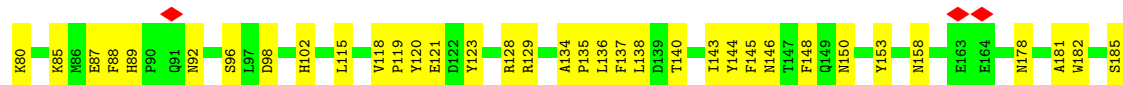
- Molecule 106: Transmembrane protein, putative



- Molecule 106: Transmembrane protein, putative

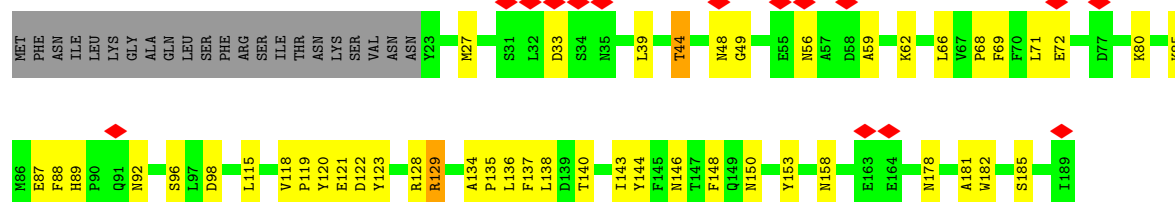


- Molecule 107: NDUPH2



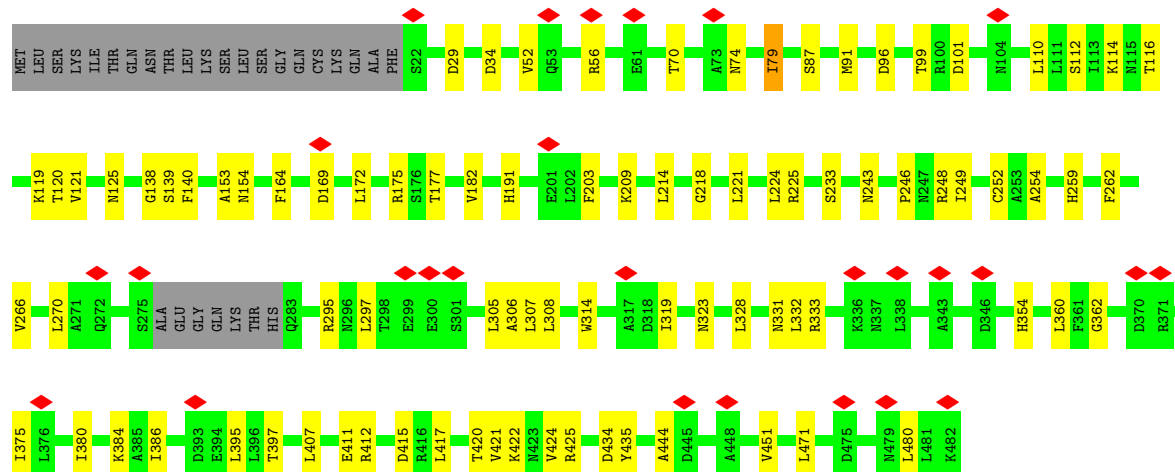
- Molecule 107: NDUPH2

Chain P2: 



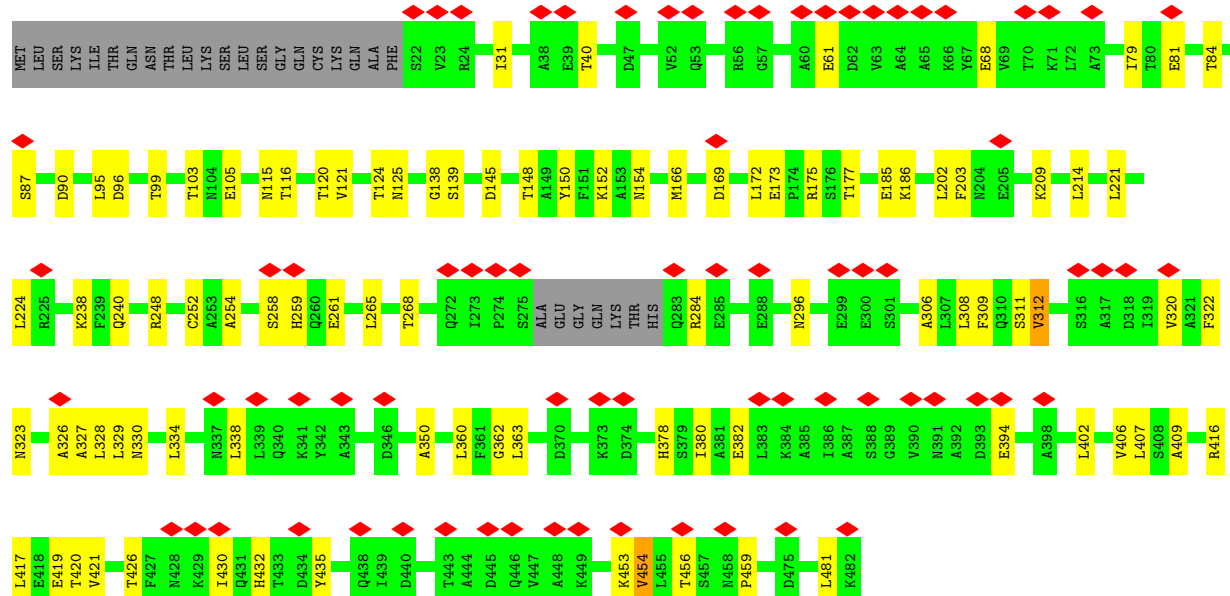
- Molecule 108: M16 family peptidase, putative

Chain qA: 

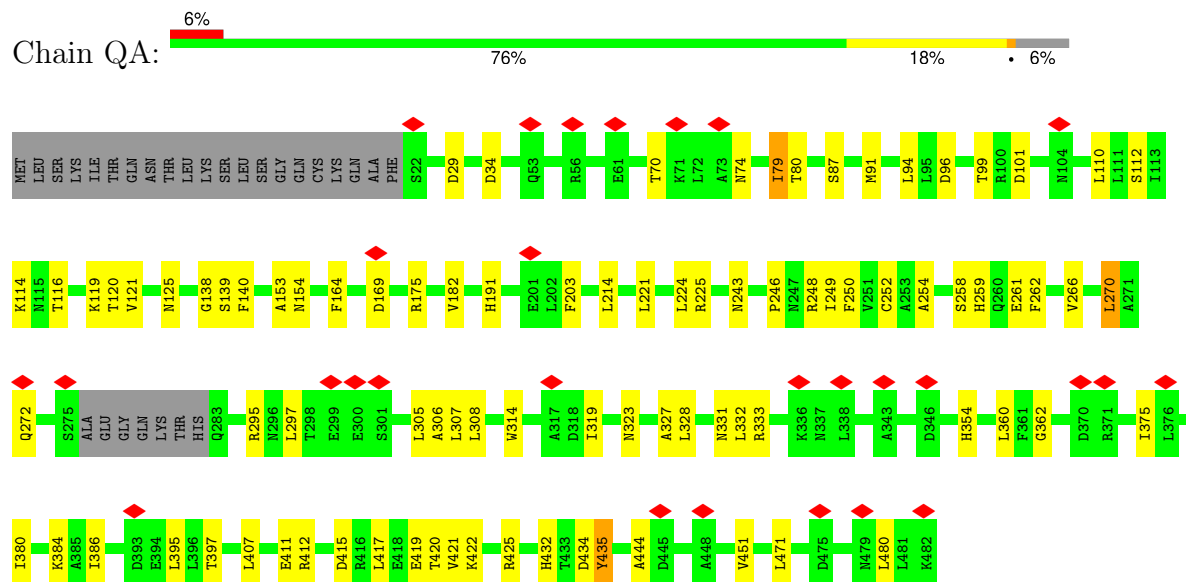


- Molecule 108: M16 family peptidase, putative

Chain qa: 



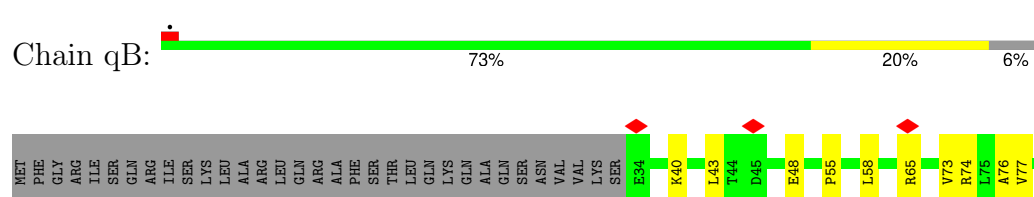
- Molecule 108: M16 family peptidase, putative

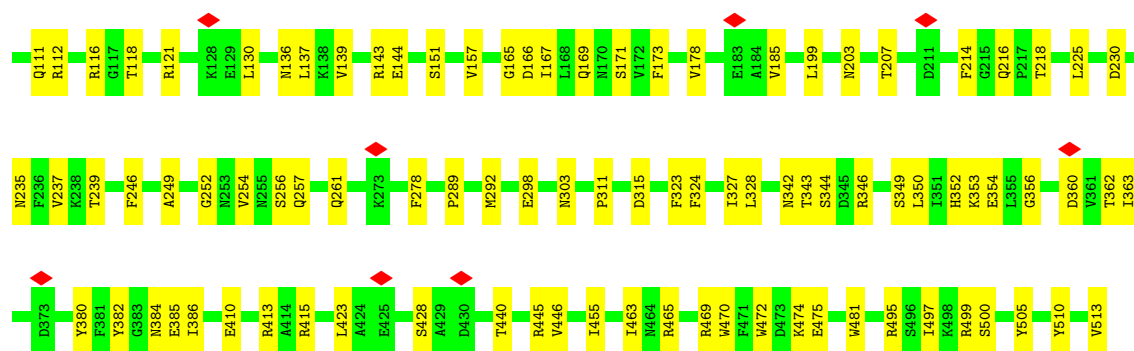


- Molecule 108: M16 family peptidase, putative

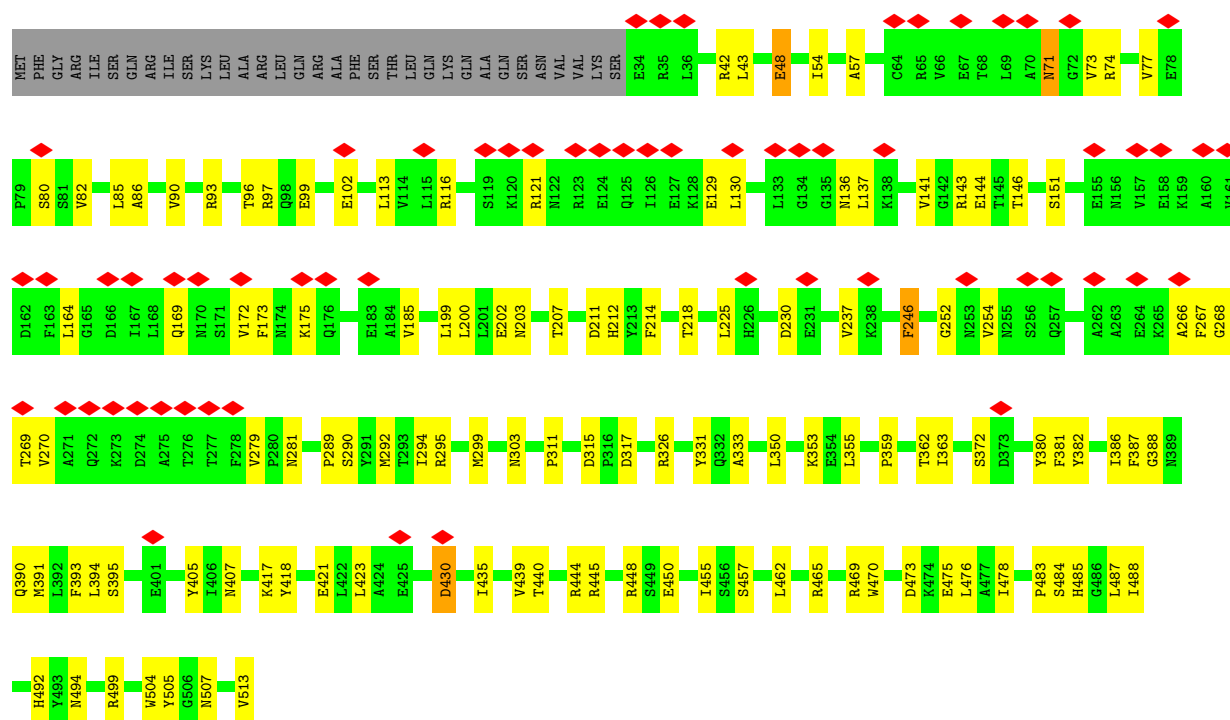


- Molecule 109: Peptidase M16 inactive domain protein

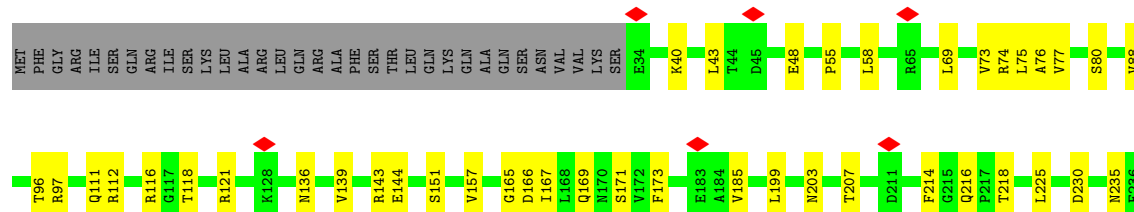
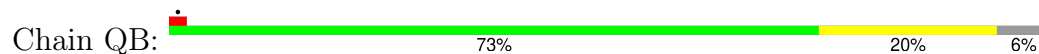


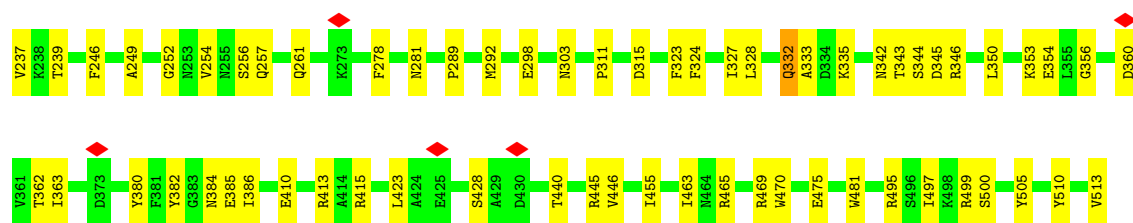


• Molecule 109: Peptidase M16 inactive domain protein

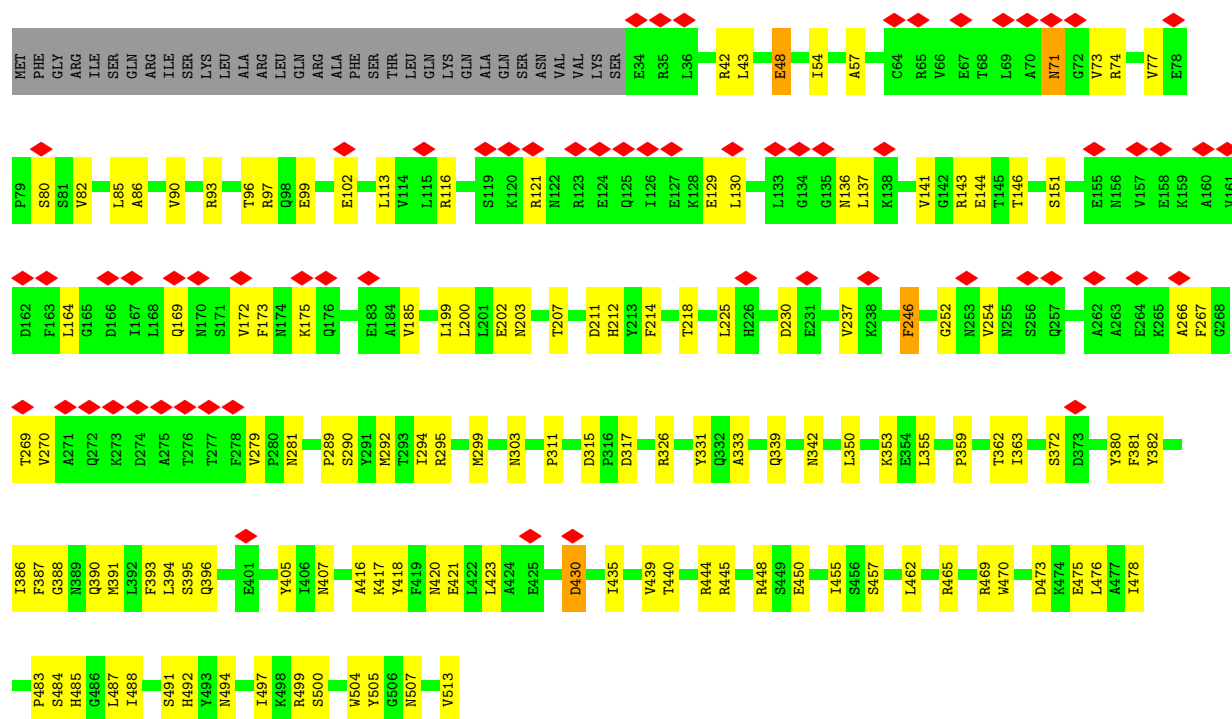


• Molecule 109: Peptidase M16 inactive domain protein

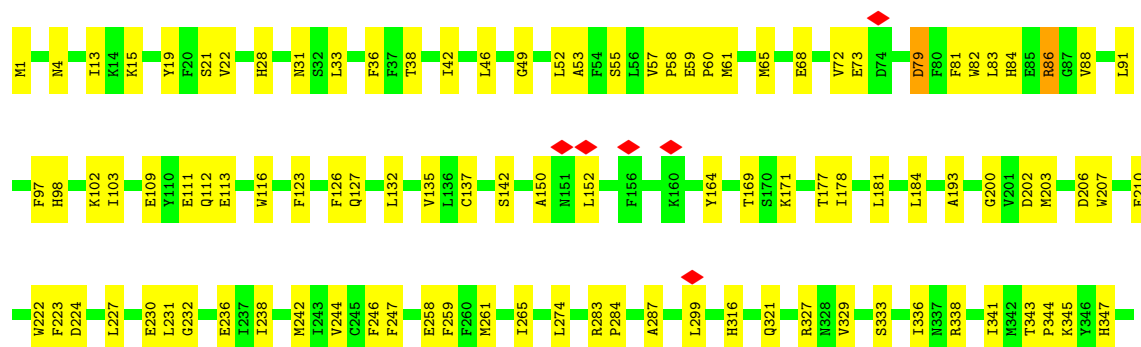
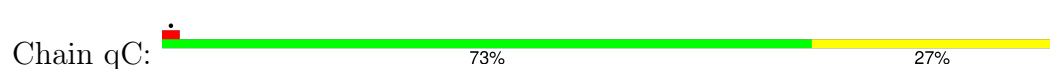




• Molecule 109: Peptidase M16 inactive domain protein

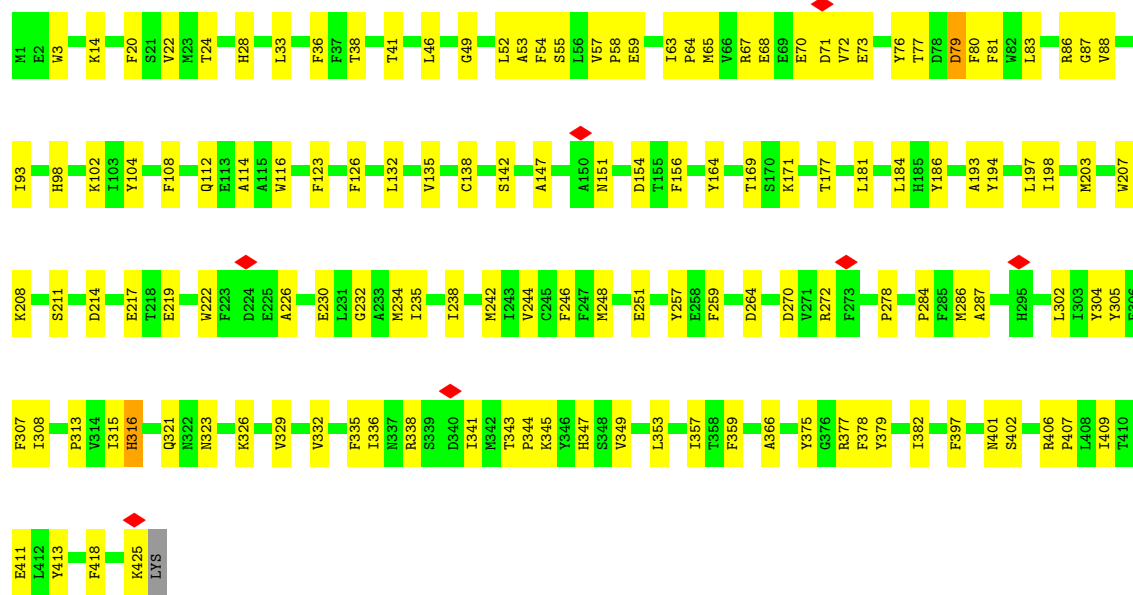


• Molecule 110: Apocytochrome b

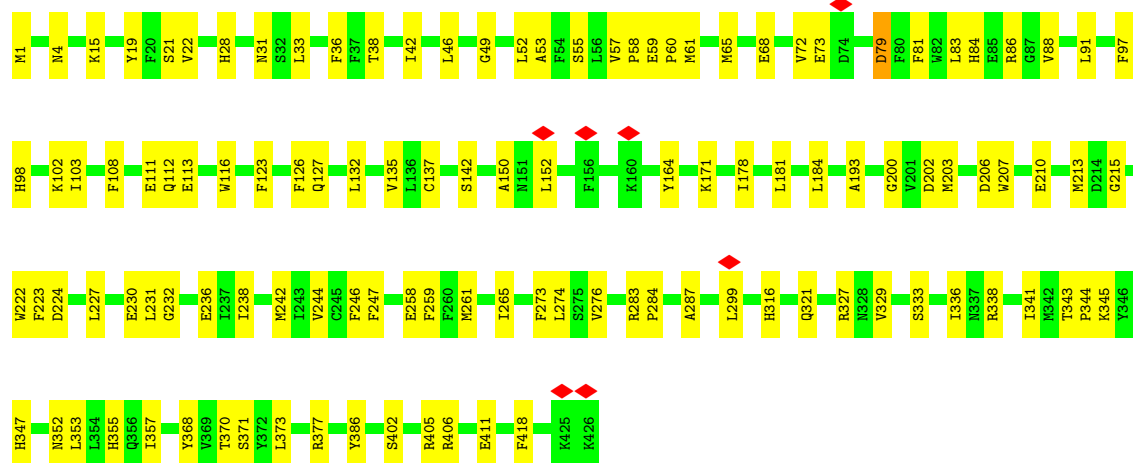
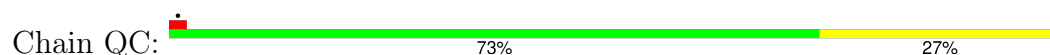




• Molecule 110: Apocytochrome b

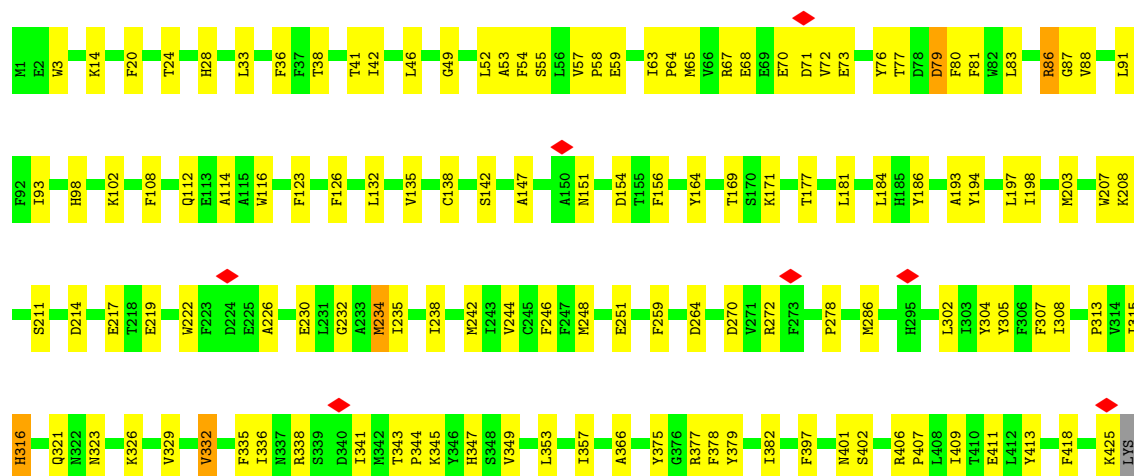


• Molecule 110: Apocytochrome b

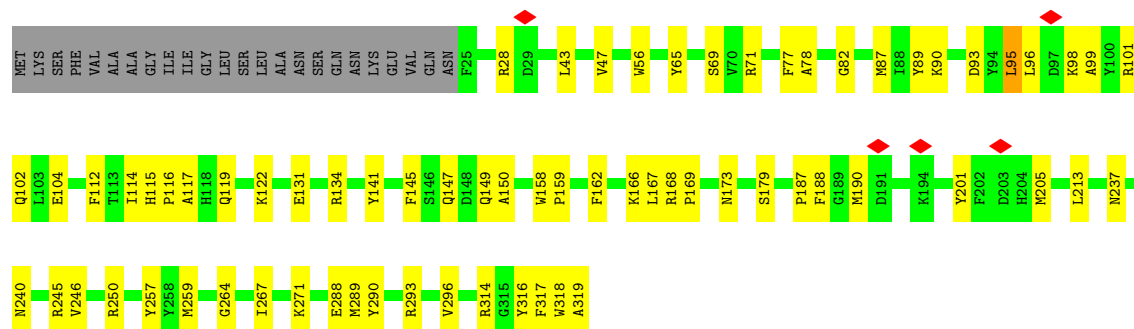


• Molecule 110: Apocytochrome b

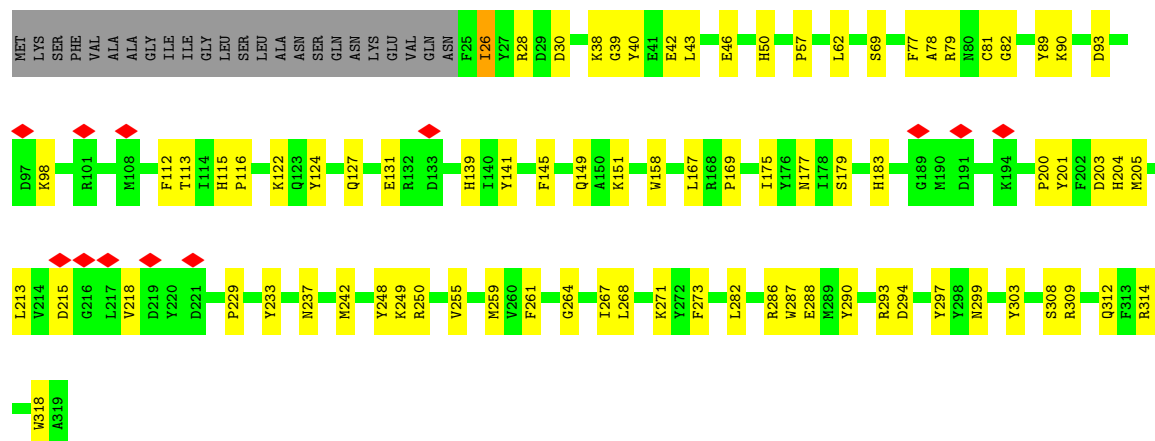




• Molecule 111: Cytochrome protein c1

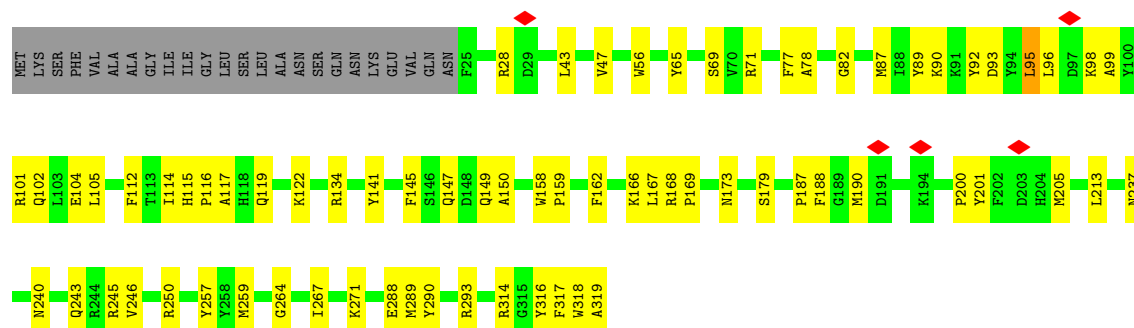


• Molecule 111: Cytochrome protein c1

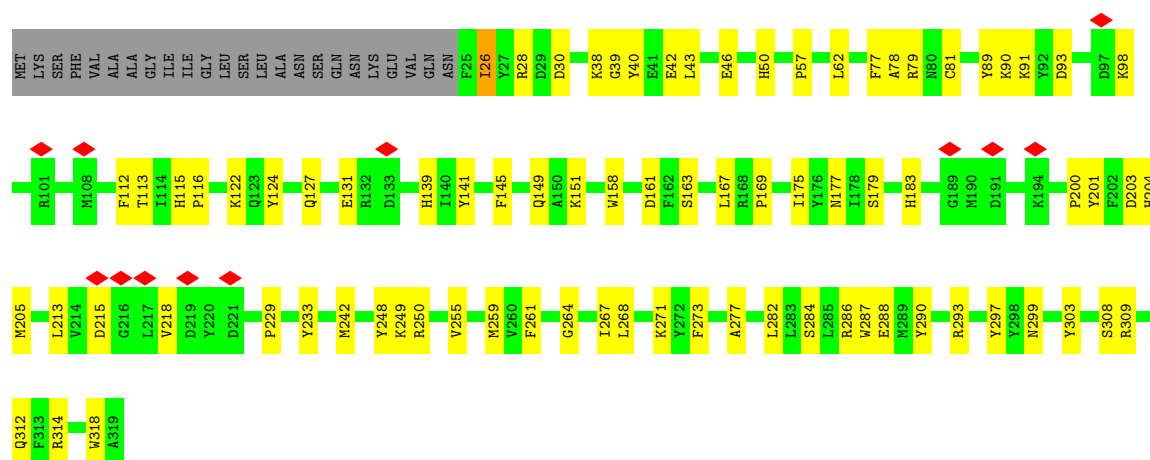


• Molecule 111: Cytochrome protein c1

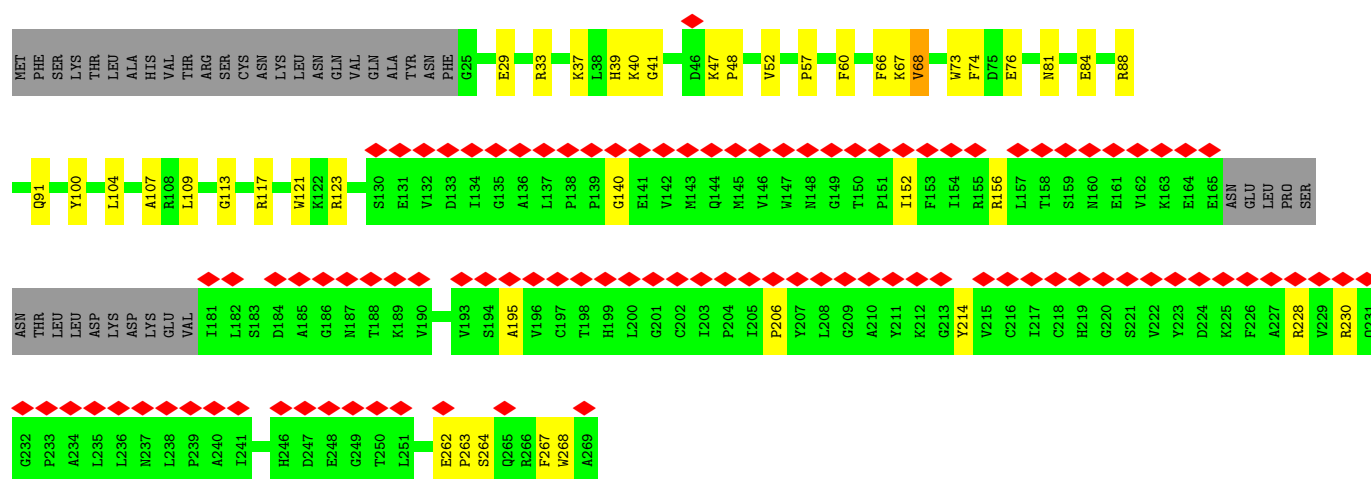
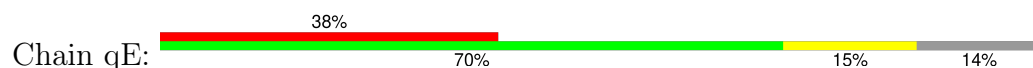




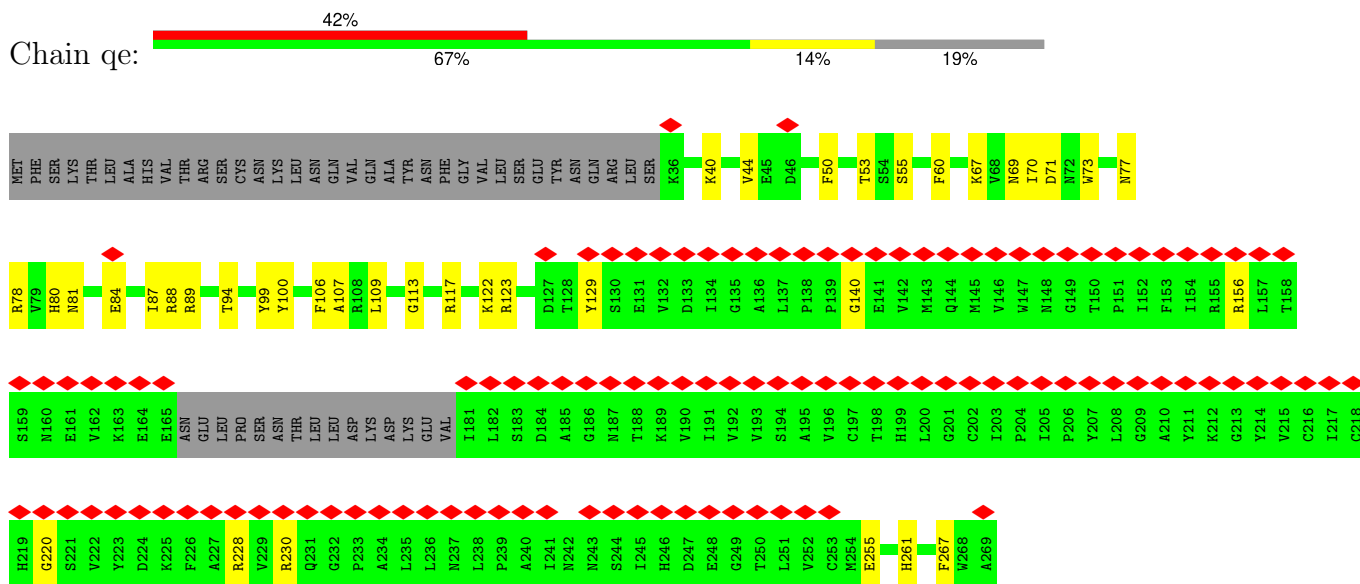
• Molecule 111: Cytochrome protein c1



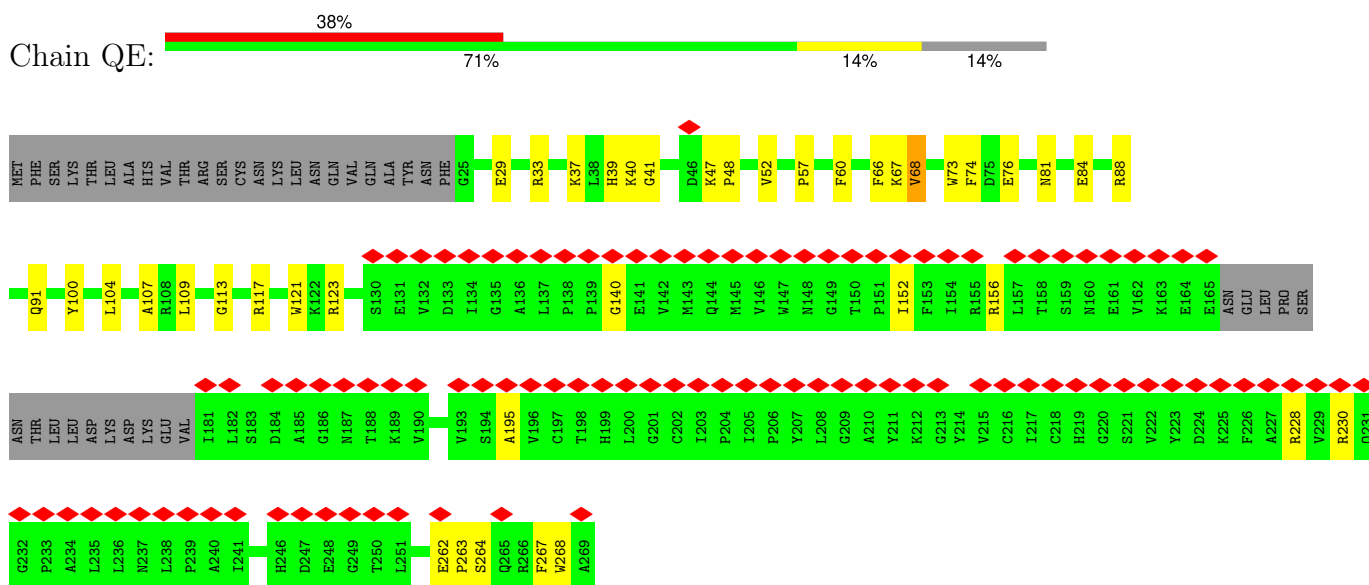
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



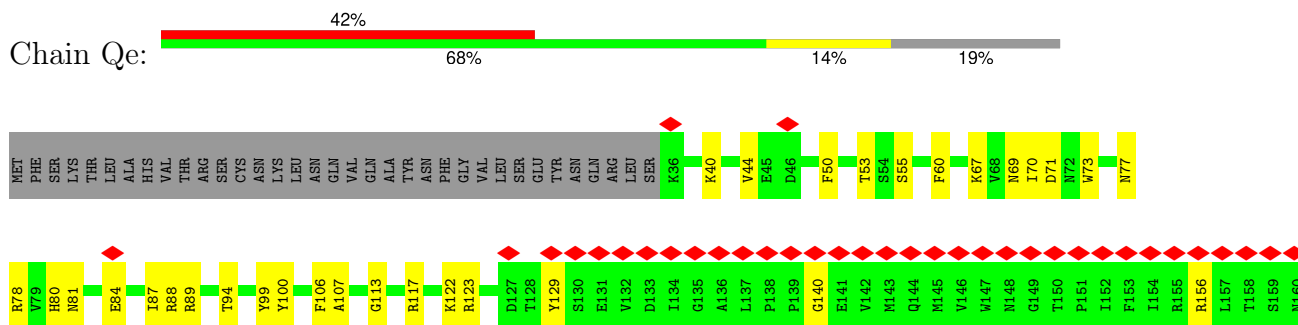
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit



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

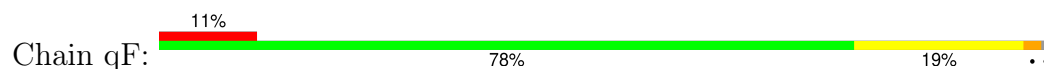


- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

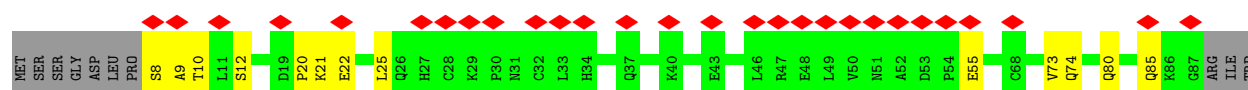
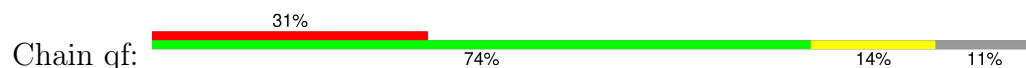




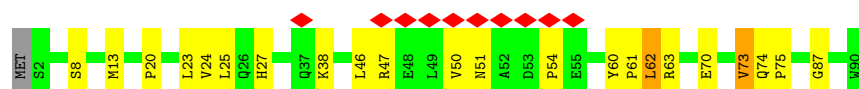
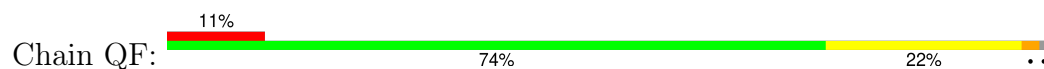
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein



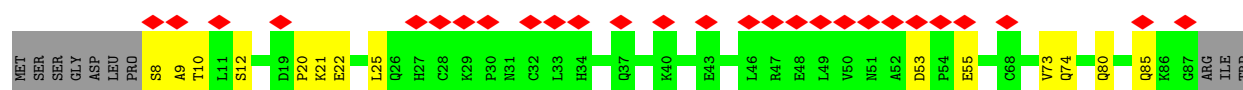
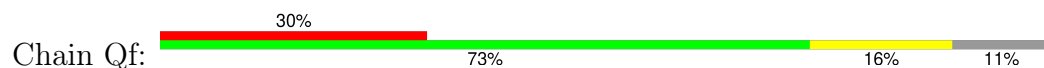
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein



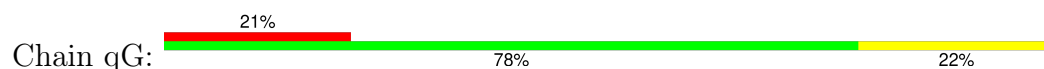
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

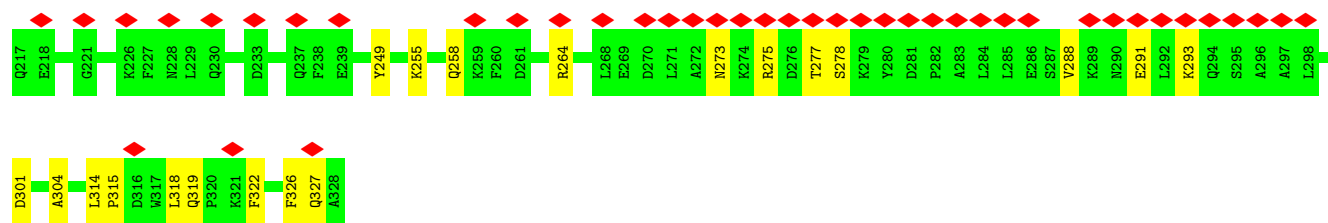


- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

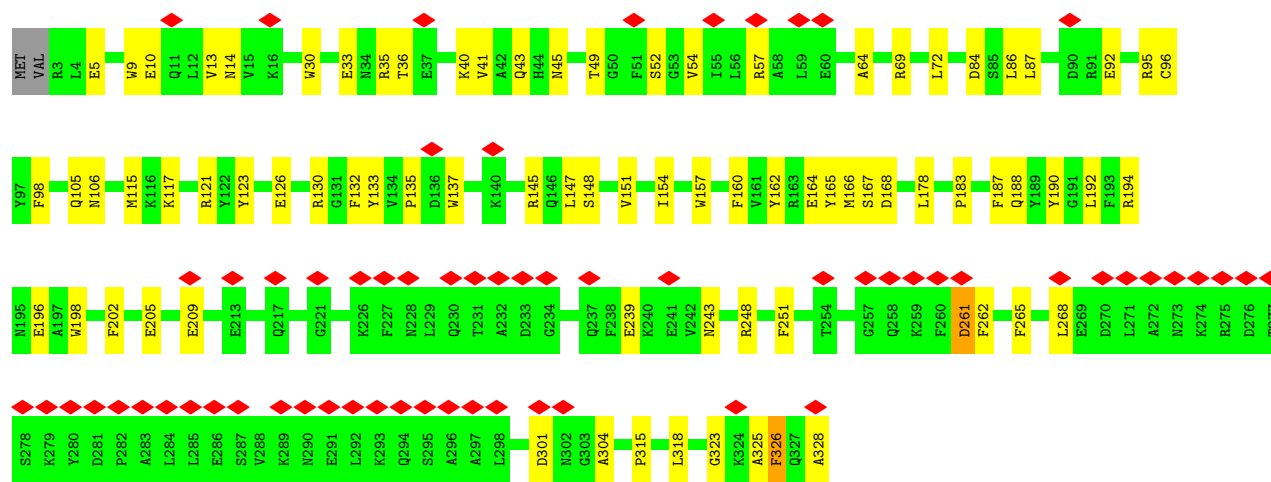
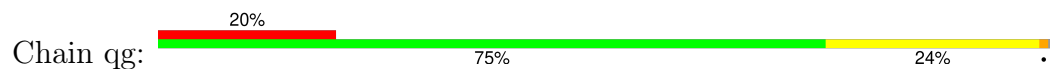


- Molecule 114: Sulphotransf domain-containing protein

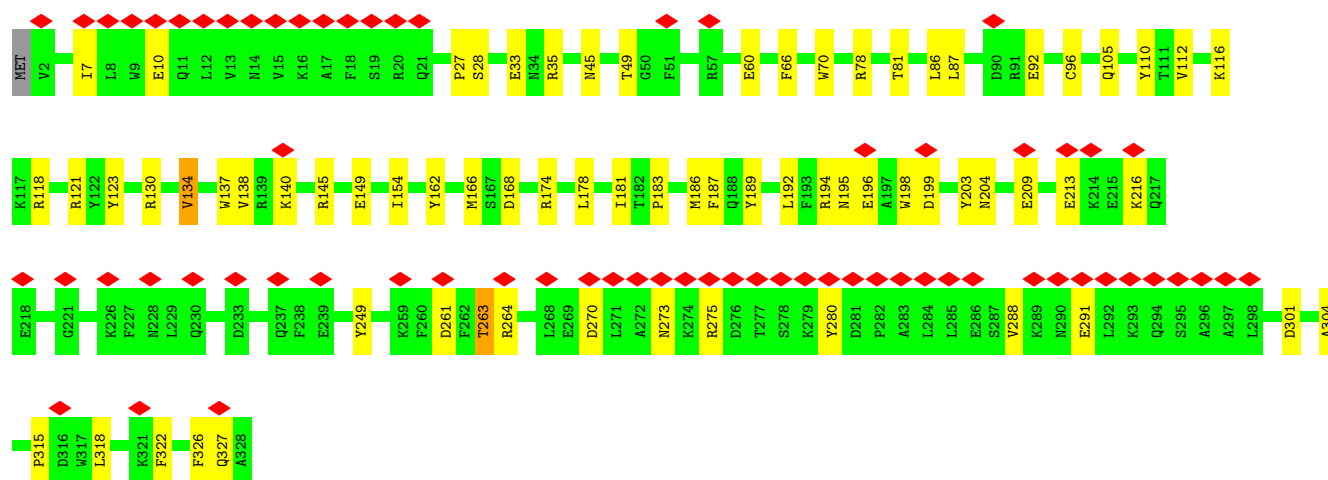
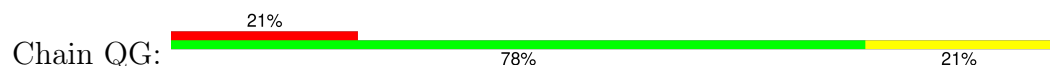




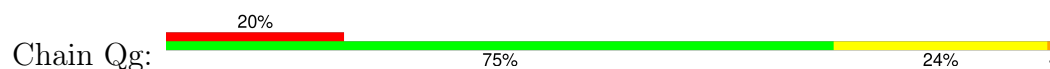
• Molecule 114: Sulphotransf domain-containing protein

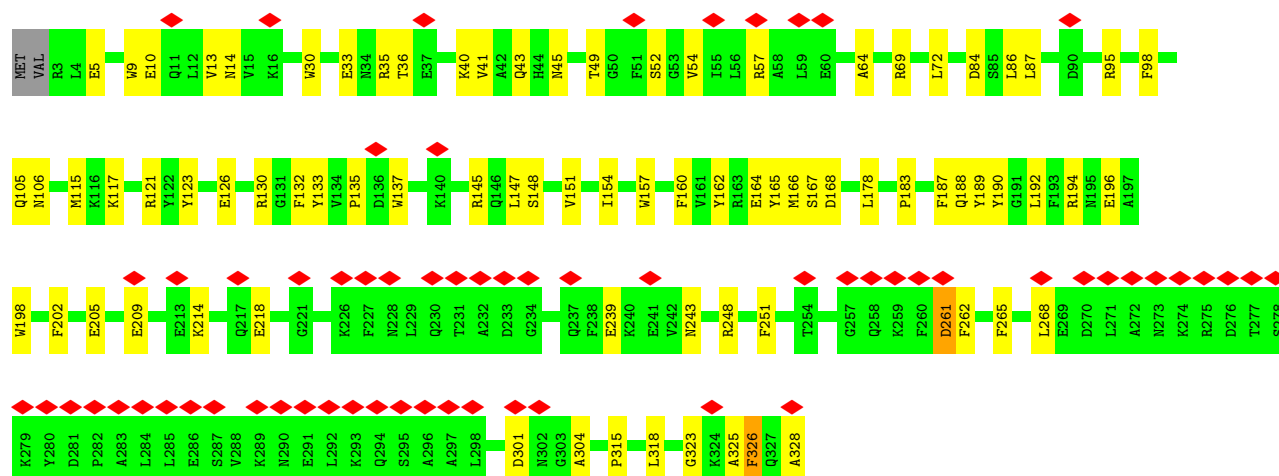


• Molecule 114: Sulphotransf domain-containing protein

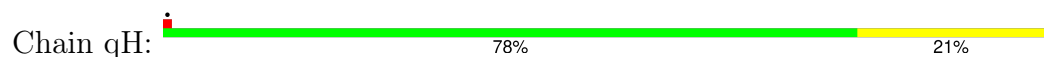


• Molecule 114: Sulphotransf domain-containing protein





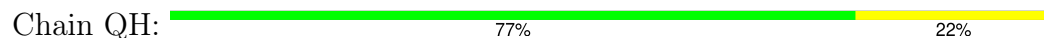
- Molecule 115: Transmembrane protein, putative



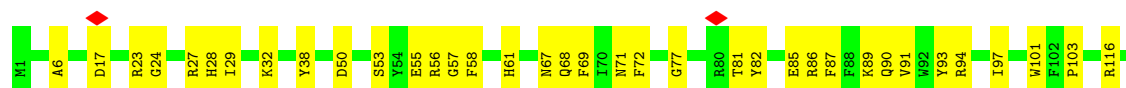
- Molecule 115: Transmembrane protein, putative



- Molecule 115: Transmembrane protein, putative



- Molecule 115: Transmembrane protein, putative



- Molecule 116: Transmembrane protein, putative

Chain qI: 



- Molecule 116: Transmembrane protein, putative

Chain qi: 



- Molecule 116: Transmembrane protein, putative

Chain QI: 



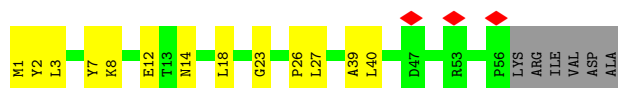
- Molecule 116: Transmembrane protein, putative

Chain Qi: 



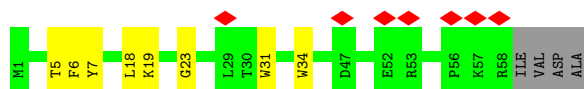
- Molecule 117: Transmembrane protein, putative

Chain qJ: 



- Molecule 117: Transmembrane protein, putative

Chain qj: 

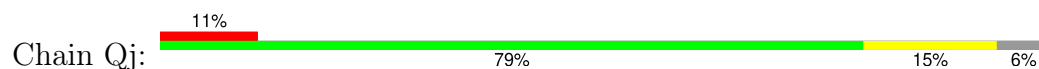


- Molecule 117: Transmembrane protein, putative

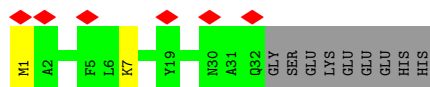
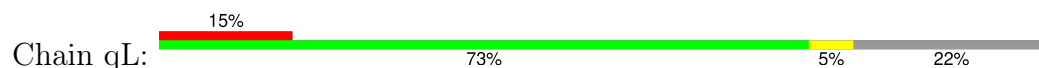
Chain QJ: 



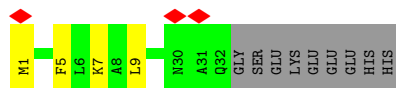
- Molecule 117: Transmembrane protein, putative



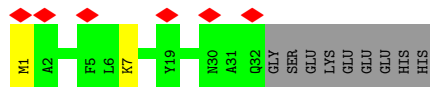
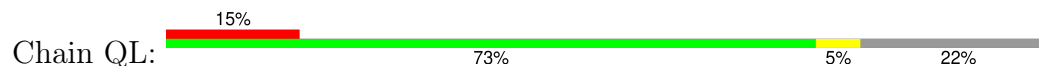
- Molecule 118: UQCRTT2



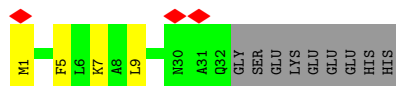
- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide

Chain qm:  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 119: Unknown peptide

Chain u2:  88%  12%



- Molecule 119: Unknown peptide

Chain U2:  88%  12%



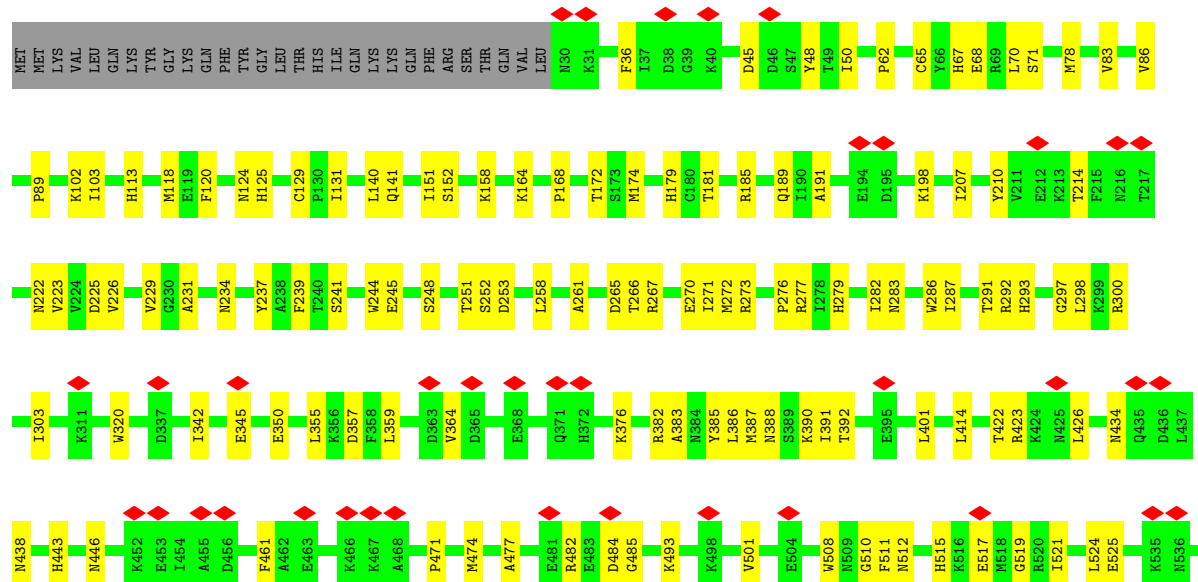
- Molecule 119: Unknown peptide

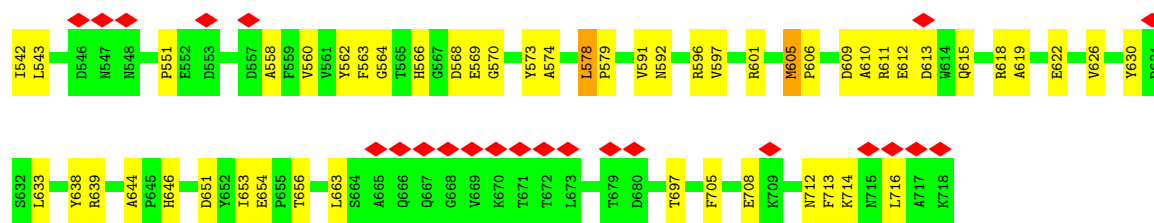
Chain QM:  100%

There are no outlier residues recorded for this chain.

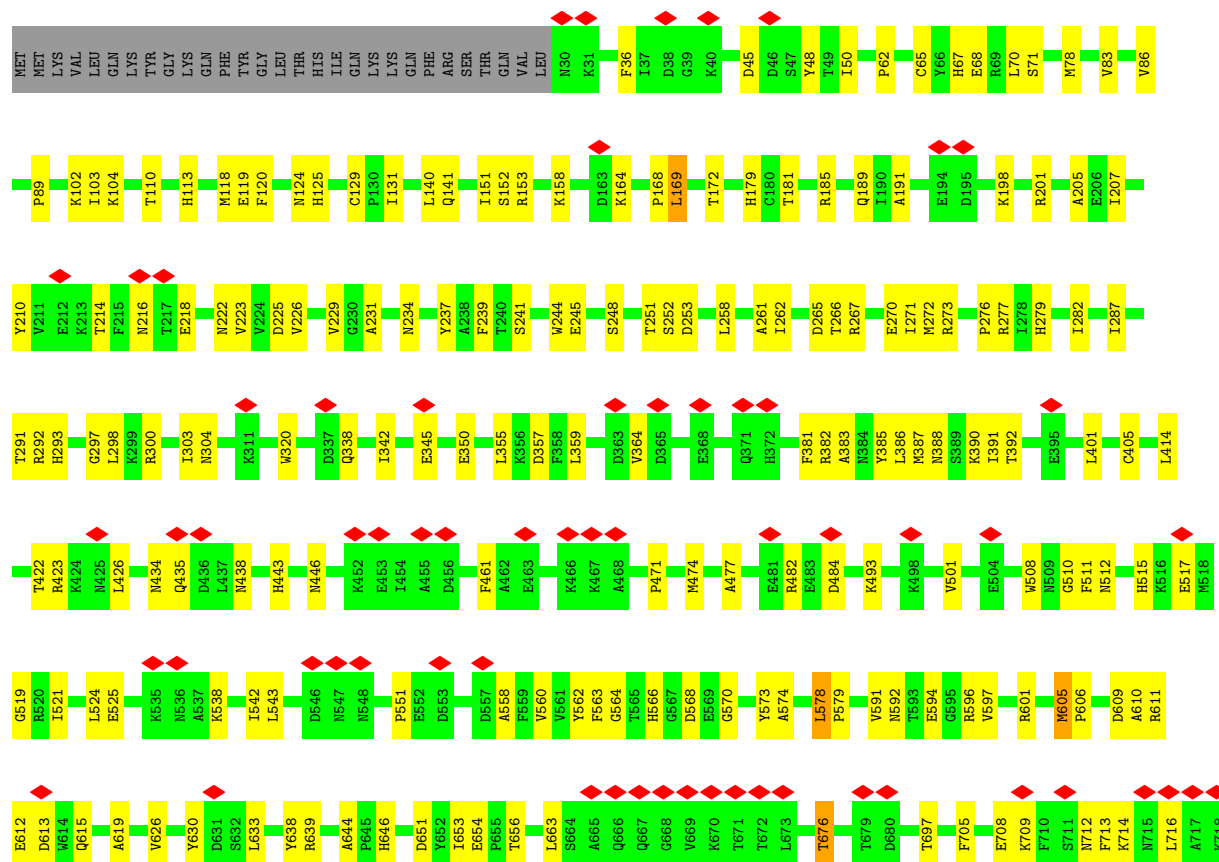
- Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain s1:  8%  71%  24%

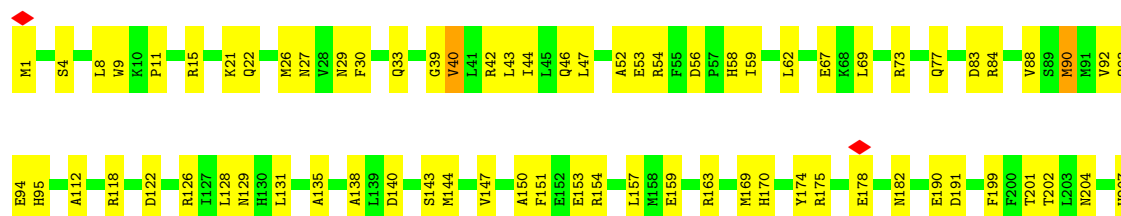


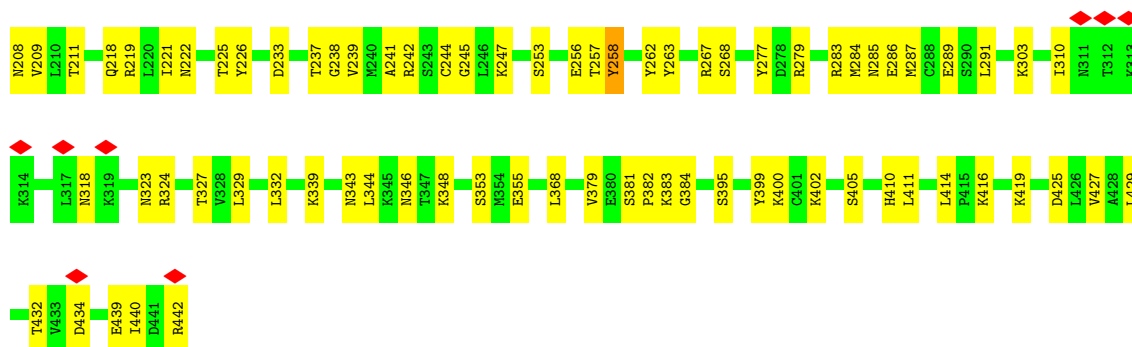


• Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

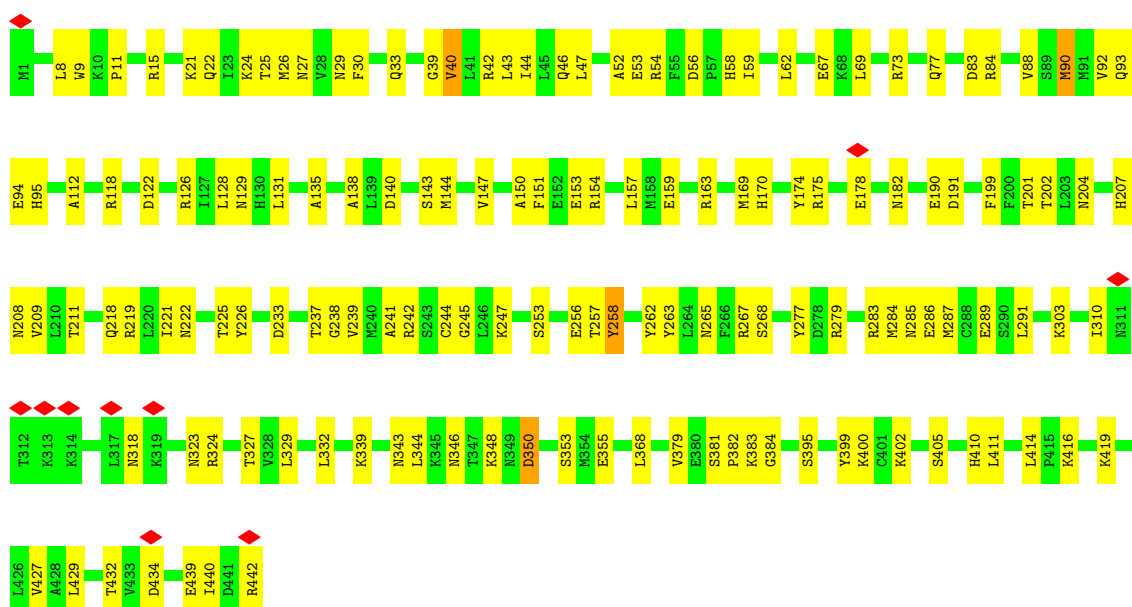


• Molecule 121: NADH dehydrogenase subunit 7

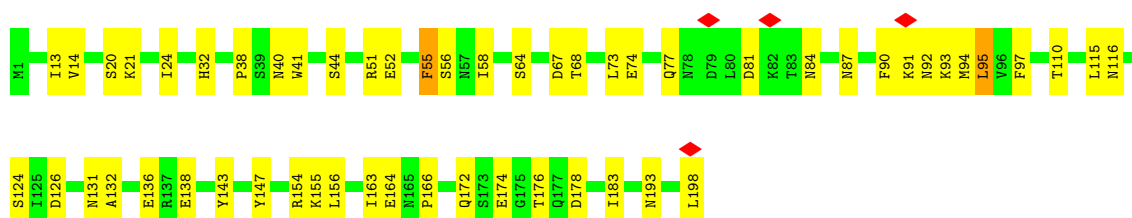




• Molecule 121: NADH dehydrogenase subunit 7

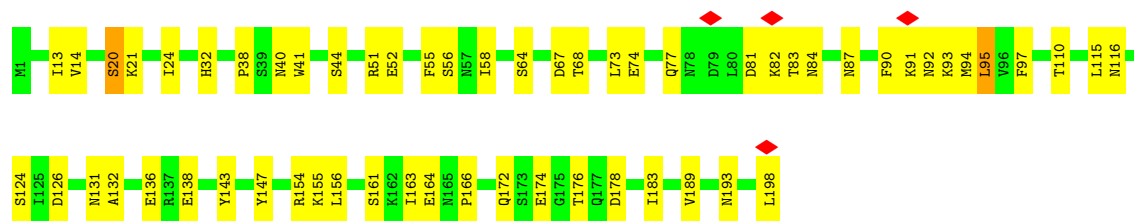


• Molecule 122: NADH dehydrogenase subunit 9

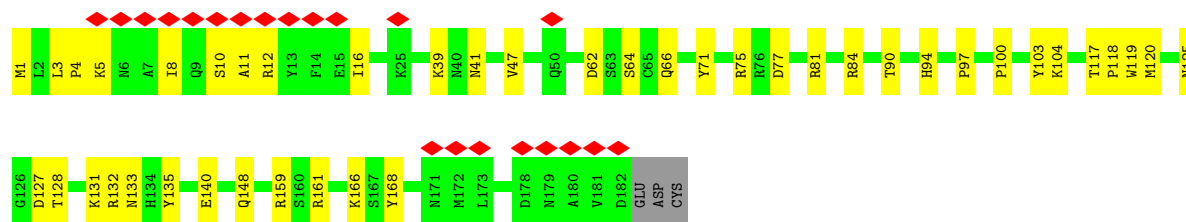
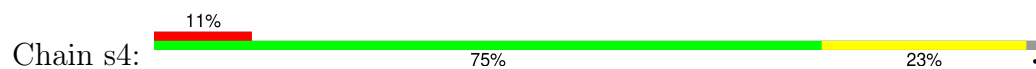


• Molecule 122: NADH dehydrogenase subunit 9

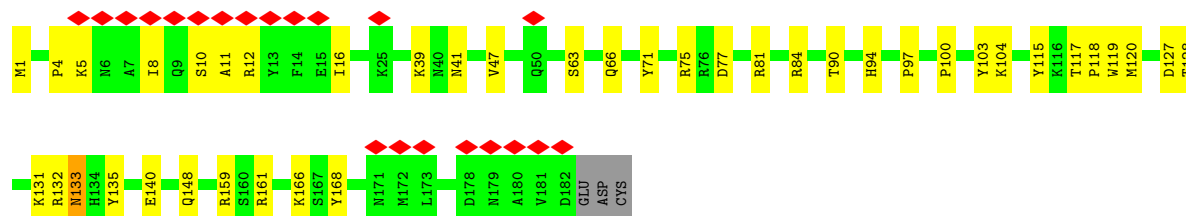
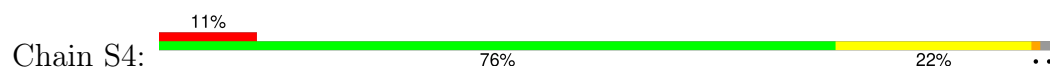




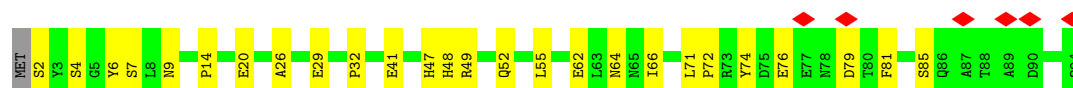
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



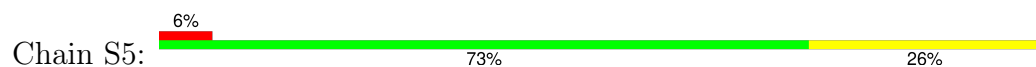
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 124: GRAM domain protein

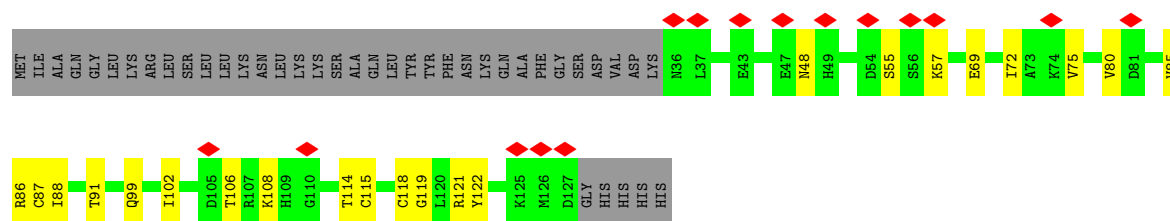


- Molecule 124: GRAM domain protein

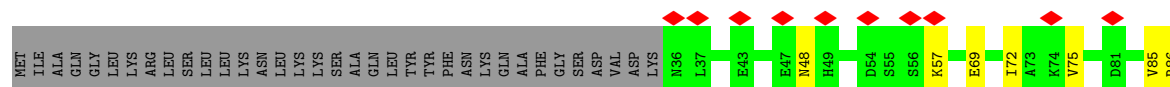


- Molecule 125: Zinc-finger protein

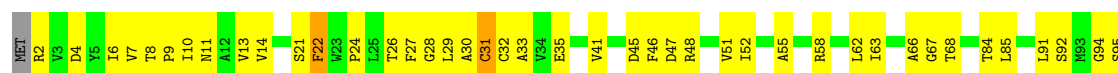




- Molecule 125: Zinc-finger protein



- Molecule 126: NADH dehydrogenase subunit 10



- Molecule 126: NADH dehydrogenase subunit 10

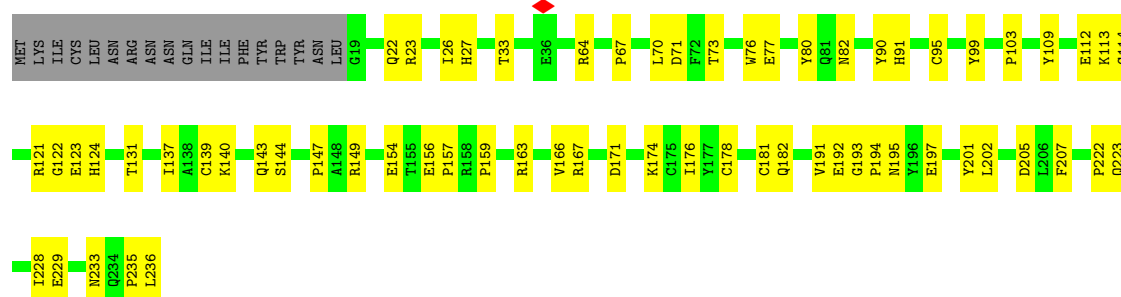


- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative

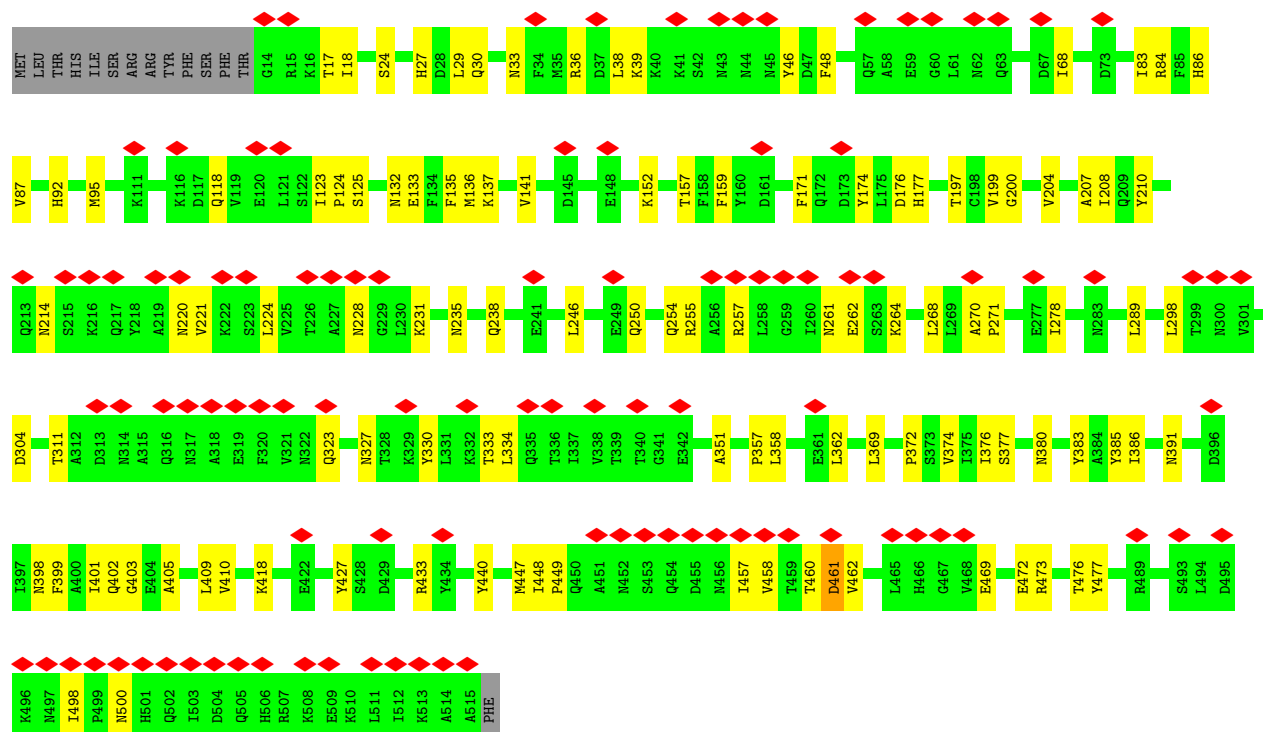


L236

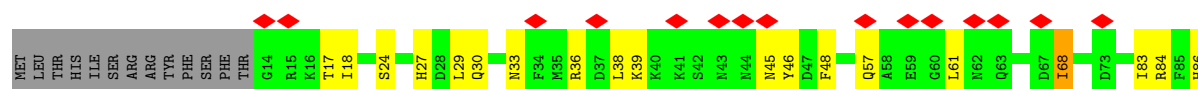
- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative

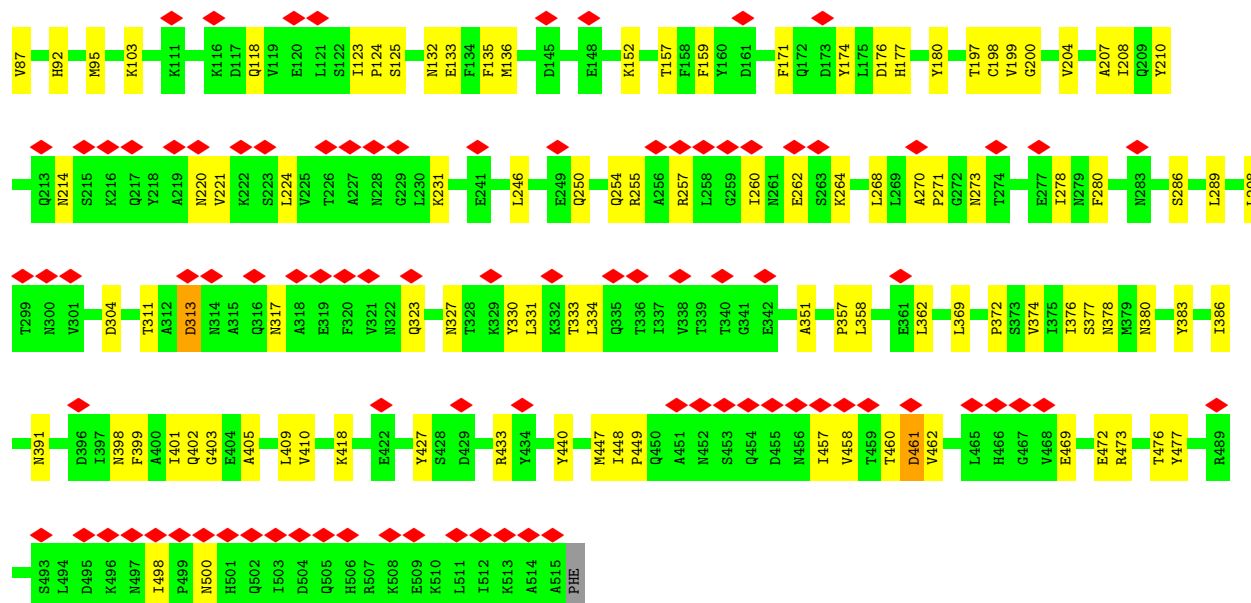
Chain S8: 

- Molecule 128: Lipid-A-disaccharide synthase

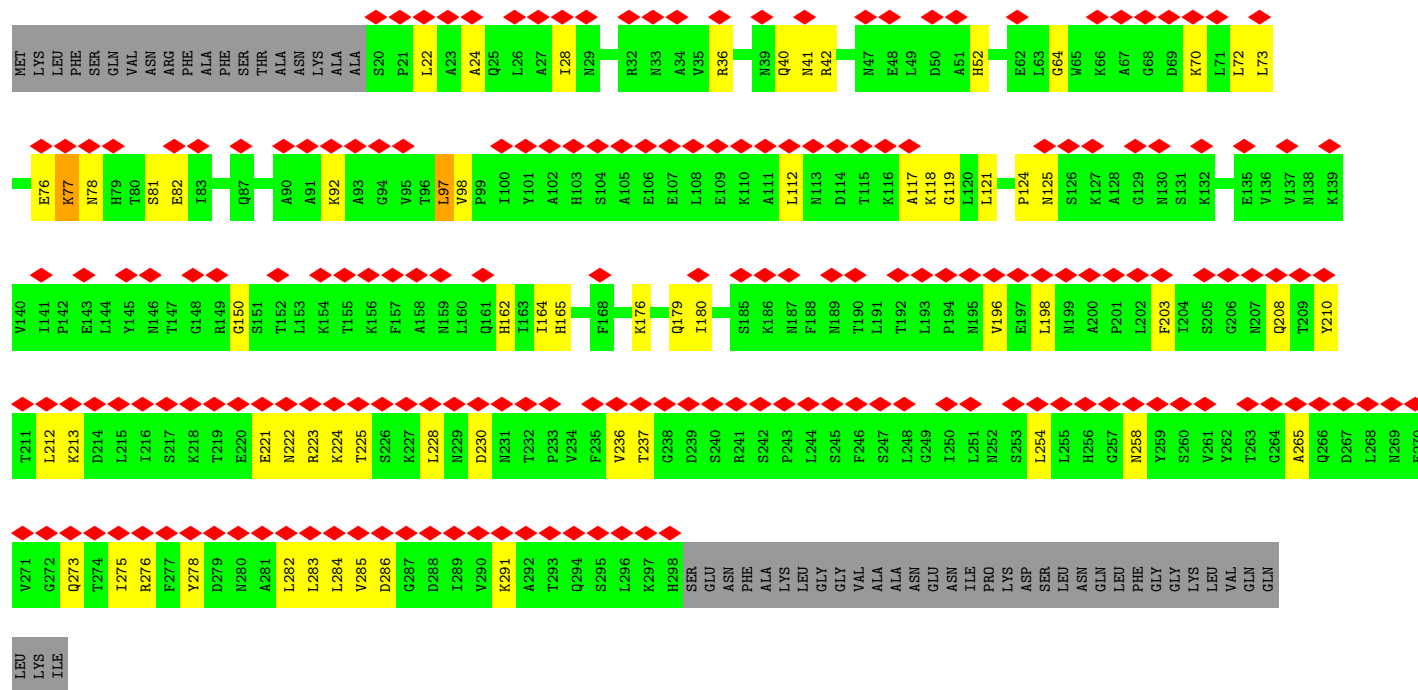
Chain t1: 

- Molecule 128: Lipid-A-disaccharide synthase

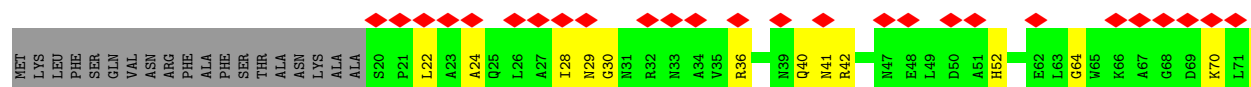
Chain T1: 

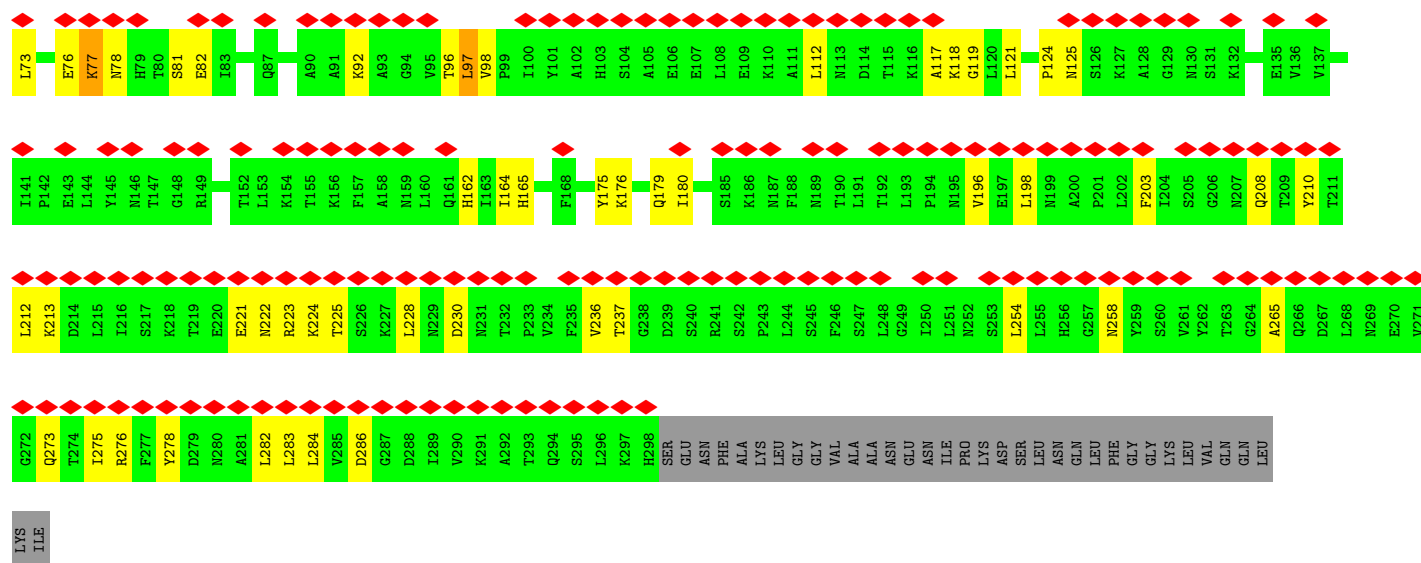


• Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

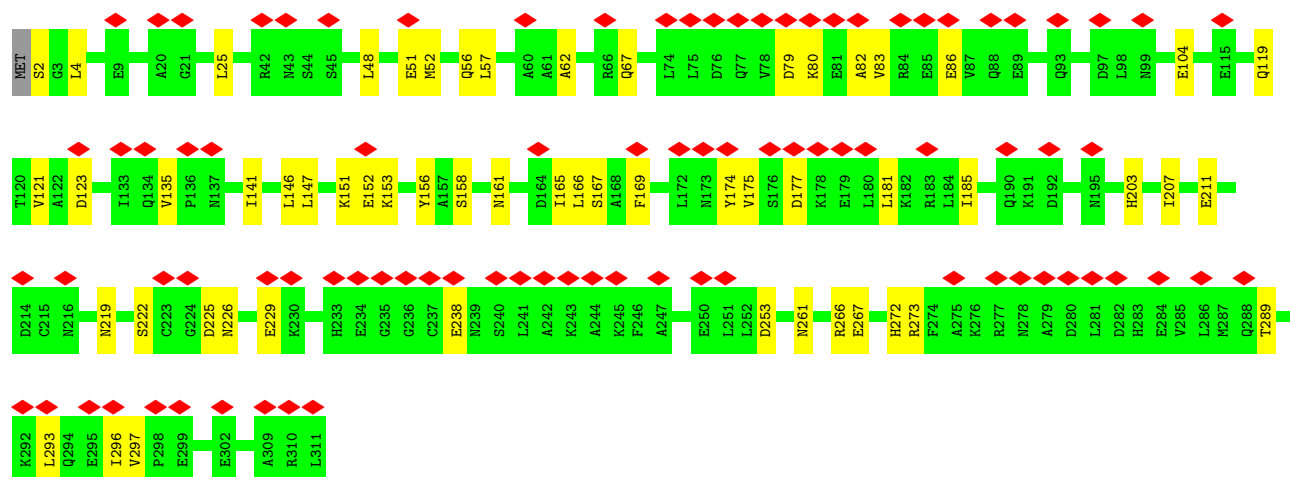
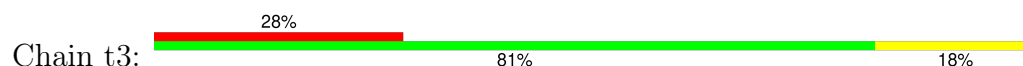


• Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

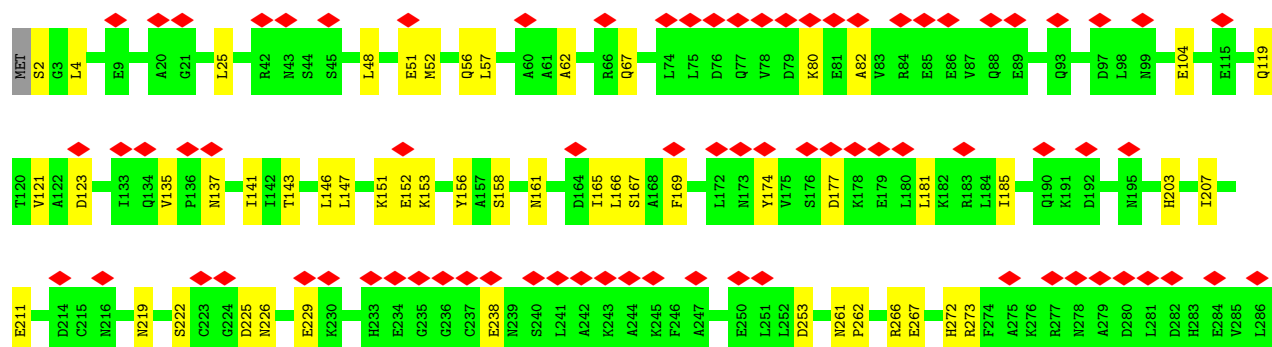
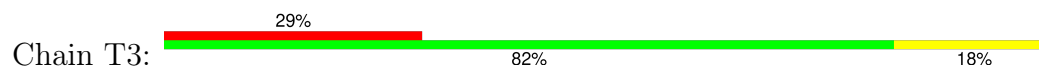




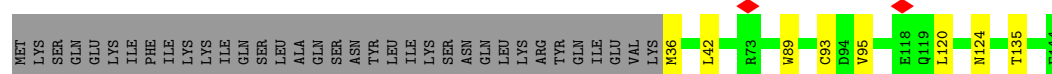
• Molecule 130: RNase III domain-containing protein



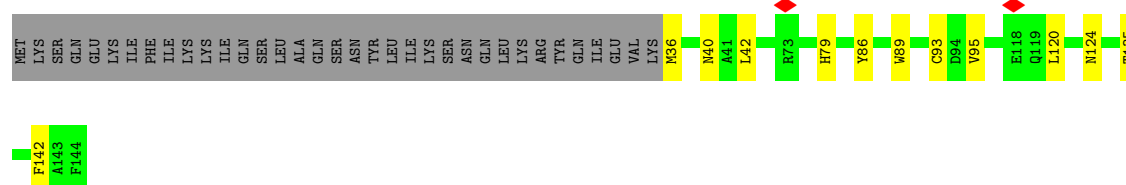
• Molecule 130: RNase III domain-containing protein



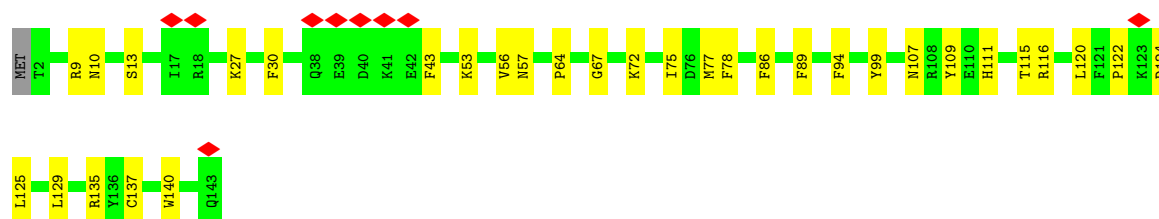
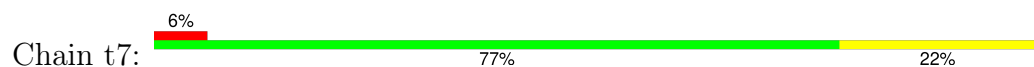
- Molecule 133: COX assembly mitochondrial protein



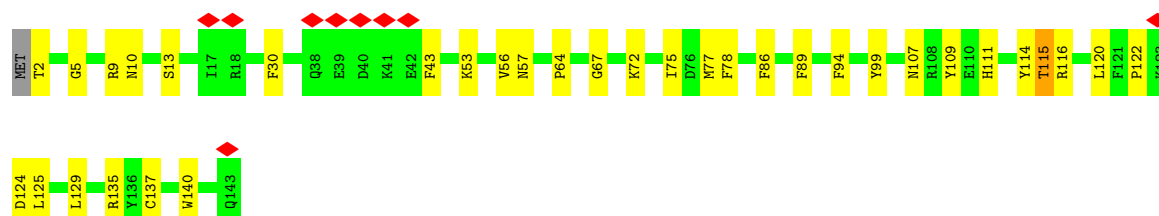
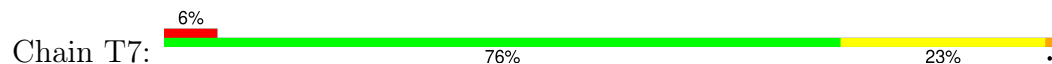
- Molecule 133: COX assembly mitochondrial protein



- Molecule 134: Transmembrane protein, putative



- Molecule 134: Transmembrane protein, putative



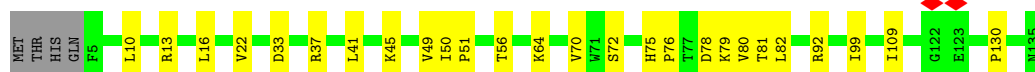
- Molecule 135: PH domain-containing protein

Chain t8: 



- Molecule 135: PH domain-containing protein

Chain T8: 



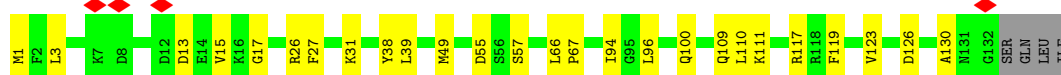
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain t9: 



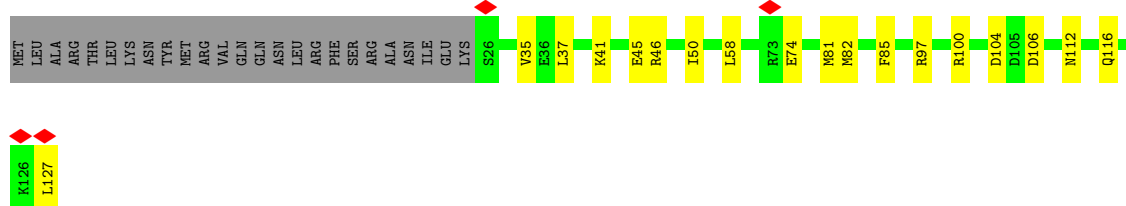
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain T9: 



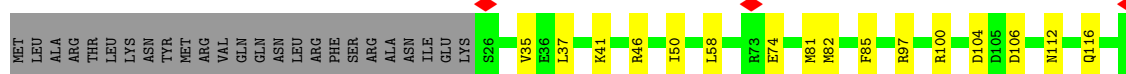
- Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain ta: 



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

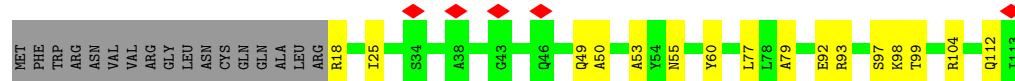
Chain TA: 



♦
L127

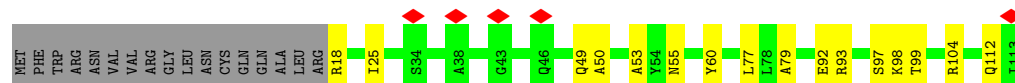
- Molecule 138: Transmembrane protein, putative

Chain tb:  71% 14% 15%



- Molecule 138: Transmembrane protein, putative

Chain TB:  71% 14% 15%



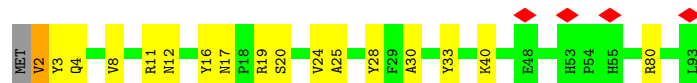
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain tc:  77% 20% ..



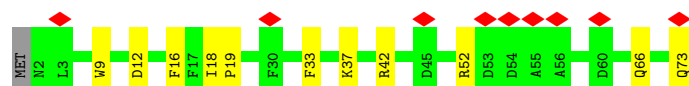
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain TC:  81% 17% ..



- Molecule 140: Transmembrane protein, putative

Chain td:  12% 84% 15% .

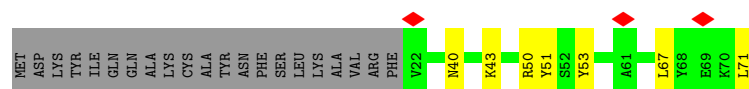


- Molecule 140: Transmembrane protein, putative

Chain TD:  12% 84% 15% .



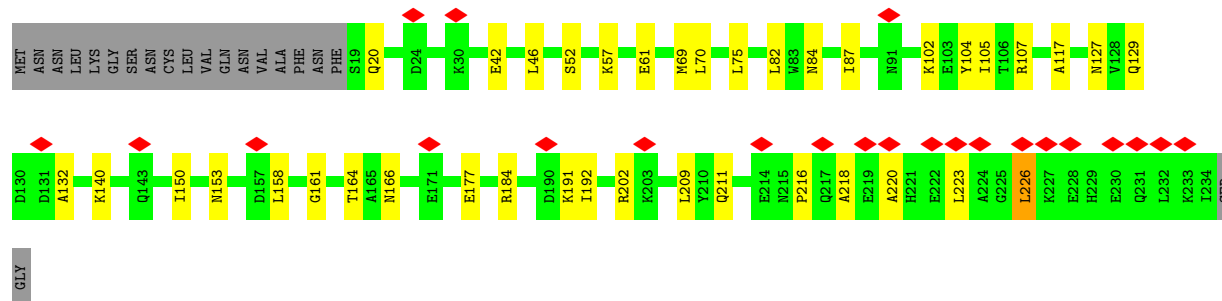
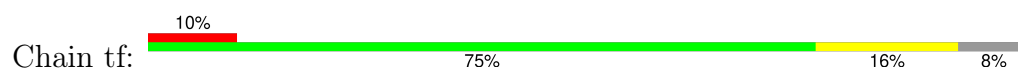
- Molecule 141: Transmembrane protein, putative



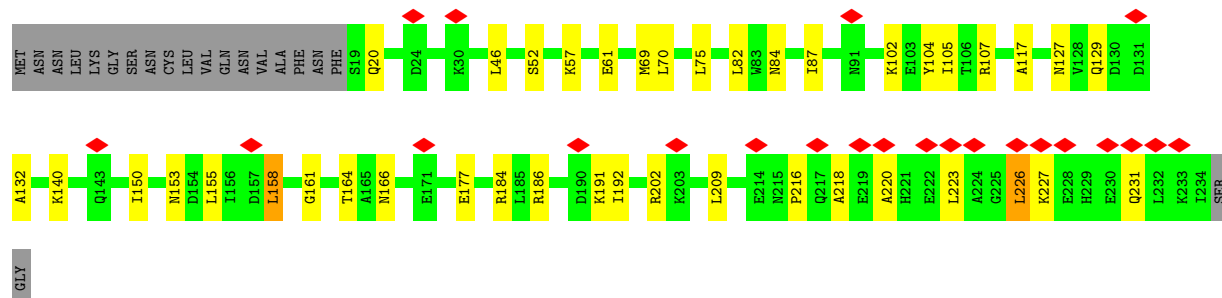
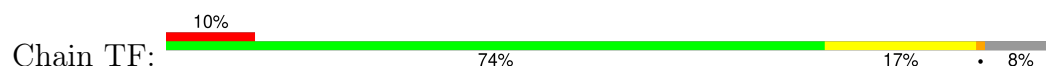
- Molecule 141: Transmembrane protein, putative



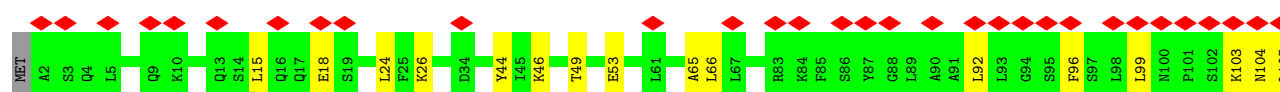
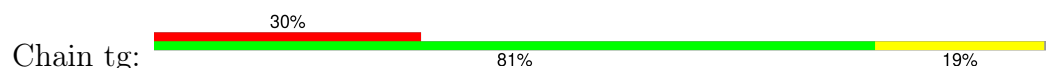
- Molecule 142: NDUTT15

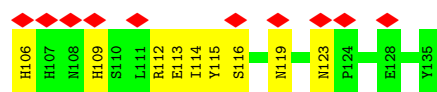


- Molecule 142: NDUTT15

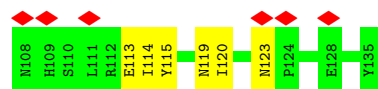
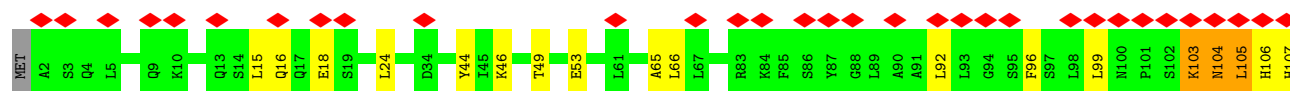
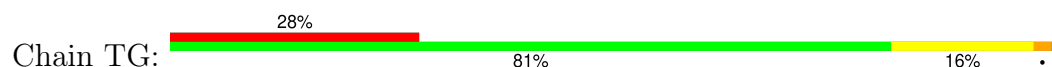


- Molecule 143: NDUTT16

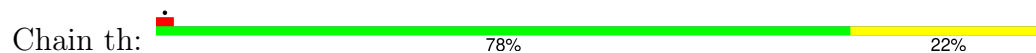




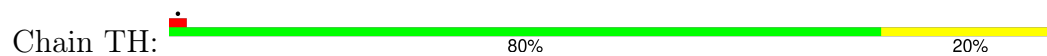
• Molecule 143: NDUTT16



• Molecule 144: NDUTT17



• Molecule 144: NDUTT17

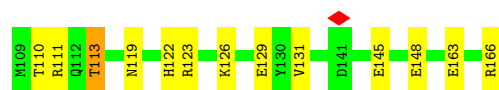


• Molecule 145: Thioredoxin

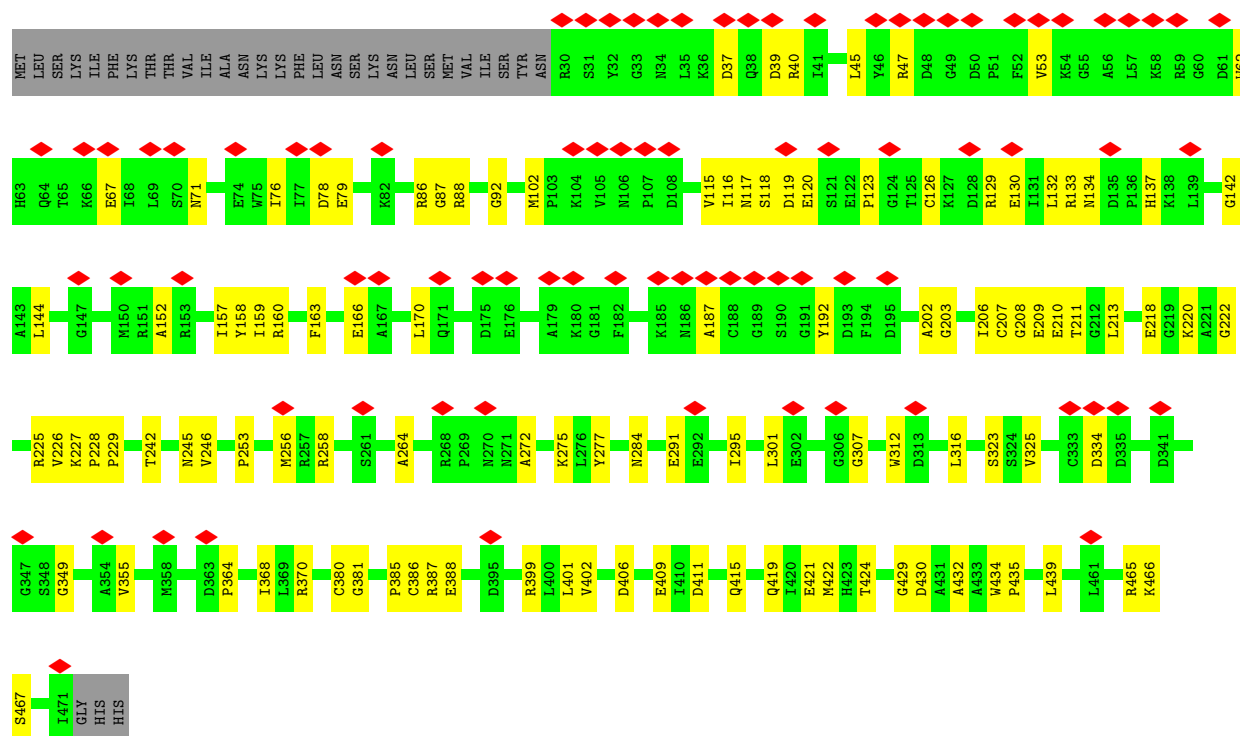


• Molecule 145: Thioredoxin

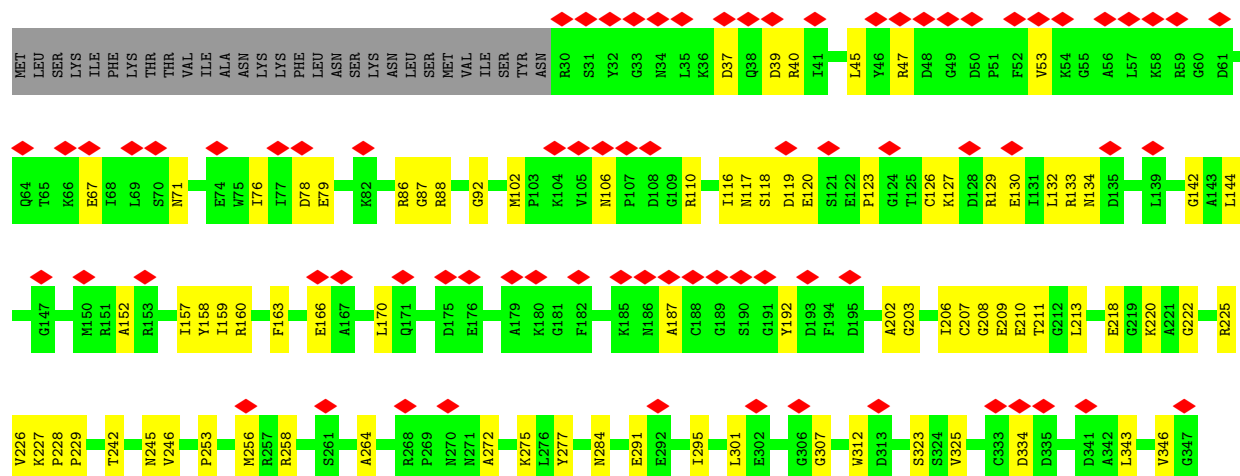




- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

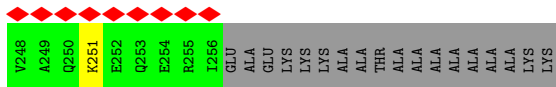


- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

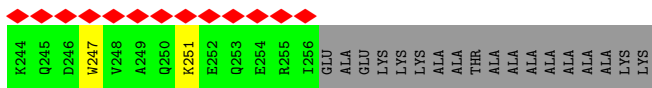




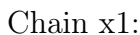
- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit



- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit

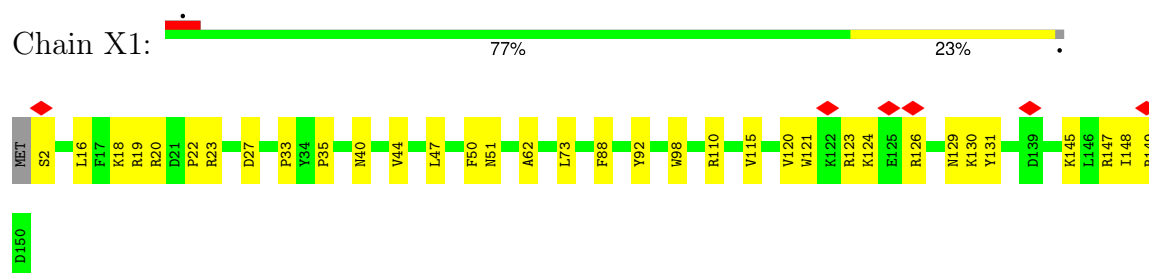


- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit



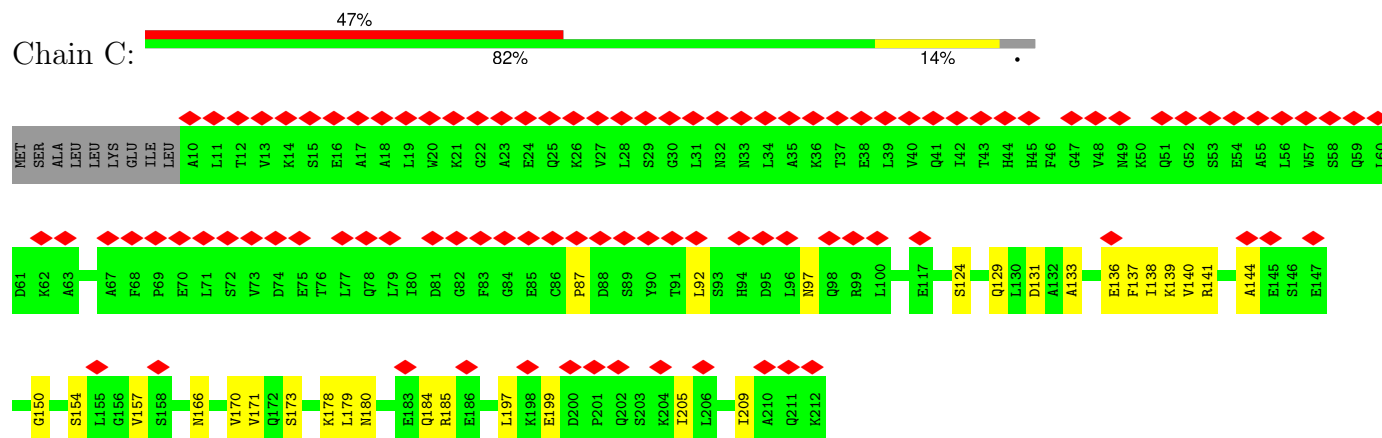
- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

Chain X1:



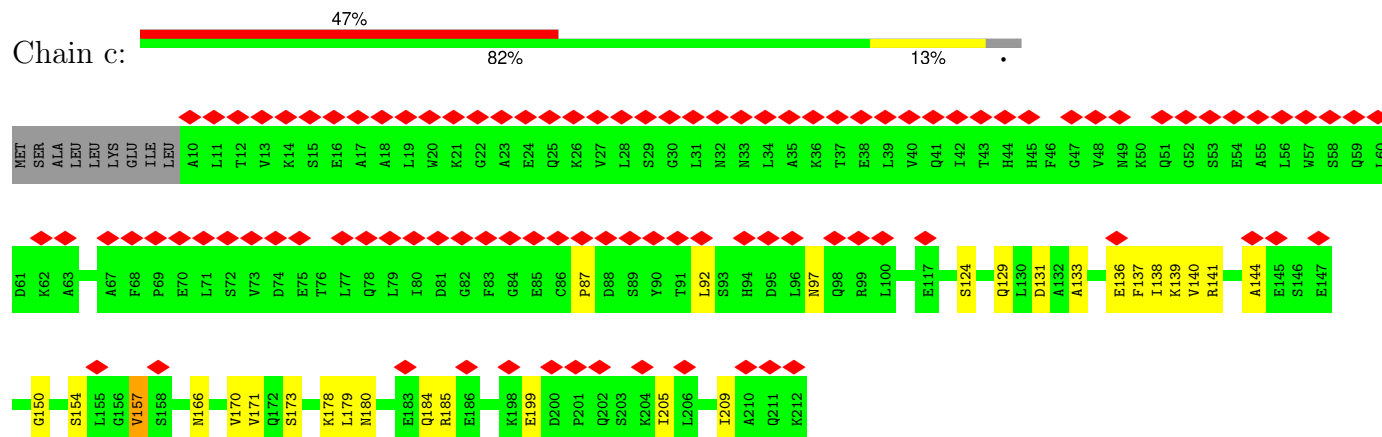
- Molecule 149: COXTT3

Chain C:



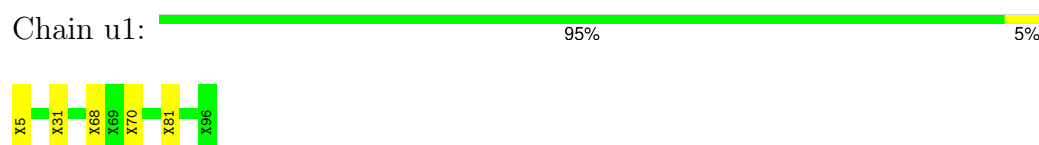
- Molecule 149: COXTT3

Chain c:



- Molecule 150: Unknown peptide

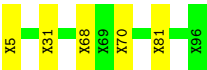
Chain u1:



- Molecule 150: Unknown peptide

Chain U1:





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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/546	0.19	0/735
1	1t	0.11	0/546	0.19	0/735
2	2E	0.10	0/2614	0.27	0/3553
2	2e	0.10	0/2614	0.27	0/3553
3	2F	0.12	0/1848	0.27	0/2500
3	2f	0.12	0/1848	0.27	0/2500
4	2G	0.12	0/1716	0.28	0/2317
4	2g	0.12	0/1716	0.28	0/2317
5	2H	0.11	0/812	0.24	0/1090
5	2h	0.11	0/812	0.24	0/1090
6	2I	0.12	0/930	0.24	0/1244
6	2i	0.12	0/930	0.25	0/1244
7	2J	0.12	0/866	0.24	0/1176
7	2j	0.12	0/866	0.24	0/1176
8	2K	0.15	0/821	0.30	0/1112
8	2k	0.15	0/821	0.30	0/1112
9	2L	0.12	0/738	0.25	0/990
9	2l	0.12	0/738	0.25	0/990
10	2M	0.11	0/660	0.25	0/895
10	2m	0.11	0/660	0.25	0/895
11	2N	0.12	0/521	0.33	0/708
11	2n	0.12	0/521	0.36	0/708
12	2O	0.12	0/367	0.23	0/496
12	2o	0.12	0/367	0.22	0/496
13	2T	0.09	0/574	0.22	0/772
13	2t	0.09	0/574	0.23	0/772
14	3T	0.10	0/662	0.21	0/888
14	3t	0.10	0/662	0.21	0/888
15	4A	0.09	0/836	0.22	0/1133
15	4a	0.09	0/836	0.21	0/1133
16	4T	0.10	0/491	0.21	0/662

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	4t	0.10	0/491	0.20	0/662
17	5T	0.10	0/514	0.23	0/693
17	5t	0.10	0/514	0.23	0/693
18	6A	0.13	0/1116	0.25	0/1512
18	6a	0.13	0/1116	0.25	0/1512
19	6B	0.11	0/1976	0.24	0/2673
19	6b	0.11	0/1976	0.24	0/2673
20	6C	0.20	0/926	0.33	0/1256
20	6c	0.20	0/926	0.33	0/1256
21	6L	0.10	0/649	0.26	0/871
21	6l	0.10	0/649	0.26	0/871
22	6T	0.09	0/573	0.22	0/770
22	6t	0.09	0/573	0.21	0/770
23	7A	0.10	0/1206	0.25	0/1631
23	7a	0.10	0/1206	0.24	0/1631
24	7C	0.09	0/1881	0.24	0/2558
24	7c	0.09	0/1881	0.24	0/2558
25	7L	0.11	0/1107	0.24	0/1505
25	7l	0.11	0/1107	0.24	0/1505
26	A	0.10	0/3874	0.25	0/5273
26	a	0.10	0/3874	0.26	0/5273
27	B	0.09	0/3453	0.24	0/4671
27	b	0.09	0/3453	0.24	0/4671
28	BP	0.11	0/2988	0.33	0/4052
28	bp	0.11	0/2988	0.33	0/4052
29	C1	0.12	0/5765	0.28	0/7819
29	c1	0.12	0/5765	0.28	0/7819
30	C2	0.12	0/5244	0.28	0/7107
30	c2	0.12	0/5244	0.28	0/7107
31	C3	0.12	0/5256	0.27	0/7142
31	c3	0.12	0/5256	0.27	0/7142
32	D	0.10	0/2430	0.26	0/3303
32	d	0.10	0/2430	0.26	0/3303
33	E	0.11	0/3266	0.30	2/4435 (0.0%)
33	e	0.10	0/3266	0.25	0/4435
34	F	0.10	0/2077	0.26	0/2824
34	f	0.10	0/2077	0.26	0/2824
35	FS	0.12	0/1562	0.28	0/2123
35	fs	0.12	0/1562	0.28	0/2123
36	G	0.10	0/2517	0.26	0/3433
36	g	0.10	0/2517	0.25	0/3433
37	H	0.11	0/2423	0.25	0/3279
37	h	0.11	0/2423	0.25	0/3279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	I	0.10	0/2001	0.25	0/2702
38	i	0.10	0/2001	0.25	0/2702
39	J	0.11	0/1621	0.25	0/2201
39	j	0.11	0/1621	0.26	0/2201
40	K	0.10	0/1755	0.25	0/2376
40	k	0.10	0/1755	0.24	0/2376
41	L	0.12	0/1718	0.24	0/2333
41	l	0.12	0/1718	0.24	0/2333
42	M	0.12	0/1941	0.26	0/2637
42	m	0.12	0/1941	0.26	0/2637
43	M1	0.12	0/2958	0.29	0/4013
43	m1	0.12	0/2958	0.29	0/4013
44	M2	0.11	0/2629	0.25	0/3564
44	m2	0.11	0/2629	0.25	0/3564
45	M3	0.10	0/2689	0.26	0/3657
45	m3	0.10	0/2689	0.25	0/3657
46	N	0.09	0/1770	0.24	0/2391
46	n	0.09	0/1770	0.23	0/2391
47	O	0.12	0/1098	0.23	0/1477
47	o	0.12	0/1098	0.23	0/1477
48	P	0.09	0/1436	0.23	0/1941
48	p	0.09	0/1436	0.23	0/1941
49	Q	0.12	0/1478	0.29	0/2005
49	q	0.12	0/1478	0.27	0/2005
50	R	0.10	0/1441	0.25	0/1952
50	r	0.10	0/1441	0.25	0/1952
51	S	0.12	0/1409	0.26	0/1900
51	s	0.12	0/1409	0.26	0/1900
52	SA	0.11	0/4722	0.28	0/6385
52	sa	0.11	0/4722	0.29	0/6385
53	SB	0.12	0/2315	0.28	0/3136
53	sb	0.12	0/2315	0.28	0/3136
54	SC	0.14	0/493	0.27	0/664
54	sc	0.14	0/493	0.27	0/664
55	SD	0.11	0/404	0.23	0/542
55	sd	0.11	0/404	0.22	0/542
56	T	0.11	0/1359	0.23	0/1842
56	t	0.11	0/1359	0.23	0/1842
57	U	0.12	0/1335	0.24	0/1794
57	u	0.12	0/1335	0.24	0/1794
58	V	0.10	0/1277	0.25	0/1735
58	v	0.11	0/1277	0.24	0/1735
59	VB	0.10	0/4712	0.24	0/6357

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
59	vb	0.10	0/4712	0.24	0/6357
60	W	0.10	0/1136	0.25	0/1545
60	w	0.10	0/1136	0.25	0/1545
61	X	0.12	0/1043	0.24	0/1413
61	x	0.11	0/1043	0.24	0/1413
62	Y	0.12	0/882	0.26	0/1192
62	y	0.12	0/882	0.27	0/1192
63	Y0	0.10	0/801	0.28	0/1087
63	y0	0.10	0/801	0.28	0/1087
64	Y5	0.10	0/1708	0.22	0/2306
64	y5	0.10	0/1708	0.22	0/2306
65	Y7	0.10	0/3012	0.22	0/4072
65	y7	0.10	0/3012	0.22	0/4072
66	Z	0.11	0/737	0.26	0/995
66	z	0.11	0/737	0.27	0/995
67	Z1	0.13	0/781	0.23	0/1053
67	z1	0.13	0/781	0.23	0/1053
68	1B	0.11	0/536	0.25	0/727
68	1b	0.11	0/536	0.24	0/727
69	2B	0.11	0/1520	0.26	0/2058
69	2b	0.11	0/1520	0.26	0/2058
70	4L	0.13	0/982	0.29	0/1335
70	4l	0.12	0/982	0.29	0/1335
71	5B	0.11	0/915	0.29	0/1224
71	5b	0.11	0/915	0.30	0/1224
72	A1	0.12	0/834	0.34	0/1132
72	a1	0.12	0/834	0.34	0/1132
73	A2	0.09	0/826	0.27	0/1116
73	a2	0.09	0/826	0.27	0/1116
74	A3	0.10	0/1115	0.23	0/1507
74	a3	0.09	0/1115	0.23	0/1507
75	A5	0.08	0/1336	0.20	0/1797
75	a5	0.08	0/1336	0.20	0/1797
76	A6	0.10	0/1459	0.24	0/1965
76	a6	0.10	0/1459	0.24	0/1965
77	A7	0.08	0/2408	0.23	0/3269
77	a7	0.08	0/2408	0.23	0/3269
78	A8	0.09	0/1099	0.23	0/1477
78	a8	0.09	0/1099	0.23	0/1477
79	A9	0.11	0/2807	0.26	0/3801
79	a9	0.11	0/2807	0.26	0/3801
80	AB	0.10	0/942	0.23	0/1272
80	ab	0.10	0/942	0.23	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
81	AC	0.10	0/822	0.23	0/1114
81	ac	0.10	0/822	0.23	0/1114
82	AL	0.08	0/1667	0.23	0/2256
82	al	0.09	0/1667	0.23	0/2256
83	AM	0.11	0/1379	0.26	0/1841
83	am	0.11	0/1379	0.26	0/1841
84	AN	0.09	0/1935	0.24	0/2616
84	an	0.09	0/1935	0.24	0/2616
85	B2	0.10	0/991	0.25	0/1333
85	b2	0.10	0/991	0.23	0/1333
86	B3	0.10	0/621	0.27	0/840
86	b3	0.10	0/621	0.26	0/840
87	B4	0.09	0/1015	0.21	0/1381
87	b4	0.09	0/1015	0.21	0/1381
88	B6	0.12	0/623	0.23	0/850
88	b6	0.12	0/623	0.23	0/850
89	B7	0.10	0/968	0.24	0/1307
89	b7	0.10	0/968	0.23	0/1307
90	B8	0.09	0/1494	0.25	0/2016
90	b8	0.09	0/1494	0.26	0/2016
91	B9	0.09	0/1644	0.24	0/2224
91	b9	0.09	0/1644	0.23	0/2224
92	BL	0.11	0/1489	0.24	0/2000
92	bl	0.11	0/1489	0.24	0/2000
93	BM	0.09	0/1351	0.23	0/1829
93	bm	0.09	0/1351	0.23	0/1829
94	C4	0.13	0/873	0.26	0/1175
94	c4	0.13	0/873	0.25	0/1175
95	FX	0.12	0/1186	0.33	0/1607
95	fx	0.12	0/1186	0.33	0/1607
96	G1	0.10	0/1810	0.26	0/2465
96	g1	0.10	0/1810	0.26	0/2465
97	G2	0.11	0/1793	0.27	0/2438
97	g2	0.10	0/1793	0.26	0/2438
98	G3	0.11	0/2865	0.25	0/3877
98	g3	0.10	0/2865	0.25	0/3877
99	J1	0.09	0/2219	0.21	0/2988
99	j1	0.09	0/2219	0.21	0/2988
100	N1	0.11	0/2376	0.27	0/3234
100	n1	0.11	0/2376	0.27	0/3234
101	N2	0.12	0/3173	0.27	0/4312
101	n2	0.12	0/3173	0.27	0/4312
102	N3	0.12	0/1051	0.24	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
102	n3	0.12	0/1051	0.24	0/1429
103	N4	0.13	0/4303	0.27	0/5844
103	n4	0.13	0/4303	0.27	0/5844
104	N5	0.12	0/6098	0.27	0/8297
104	n5	0.12	0/6098	0.27	0/8297
105	N6	0.11	0/2232	0.24	0/3035
105	n6	0.11	0/2232	0.24	0/3035
106	P1	0.10	0/1963	0.28	0/2658
106	p1	0.10	0/1963	0.28	0/2658
107	P2	0.10	0/1454	0.28	0/1970
107	p2	0.11	0/1454	0.28	0/1970
108	QA	0.10	0/3569	0.25	0/4835
108	Qa	0.09	0/3569	0.25	0/4835
108	qA	0.10	0/3569	0.25	0/4835
108	qa	0.09	0/3569	0.25	0/4835
109	QB	0.10	0/3921	0.26	0/5325
109	Qb	0.12	0/3921	0.28	0/5325
109	qB	0.11	0/3921	0.26	0/5325
109	qb	0.11	0/3921	0.28	0/5325
110	QC	0.12	0/3715	0.28	0/5046
110	Qc	0.12	0/3706	0.26	0/5035
110	qC	0.12	0/3715	0.27	0/5046
110	qc	0.12	0/3706	0.27	0/5035
111	QD	0.11	0/2580	0.27	0/3491
111	Qd	0.10	0/2580	0.25	0/3491
111	qD	0.11	0/2580	0.26	0/3491
111	qd	0.10	0/2580	0.25	0/3491
112	QE	0.11	0/1588	0.25	0/2162
112	Qe	0.11	0/1499	0.26	0/2042
112	qE	0.11	0/1588	0.25	0/2162
112	qe	0.11	0/1499	0.25	0/2042
113	QF	0.12	0/716	0.28	0/969
113	Qf	0.10	0/641	0.26	0/866
113	qF	0.11	0/716	0.29	0/969
113	qf	0.10	0/641	0.26	0/866
114	QG	0.10	0/2845	0.26	0/3839
114	Qg	0.09	0/2838	0.24	0/3829
114	qG	0.11	0/2845	0.26	0/3839
114	qg	0.09	0/2838	0.24	0/3829
115	QH	0.10	0/1133	0.28	0/1524
115	Qh	0.10	0/1133	0.27	0/1524
115	qH	0.10	0/1133	0.28	0/1524
115	qh	0.10	0/1133	0.27	0/1524

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
116	QI	0.09	0/1005	0.22	0/1365
116	Qi	0.11	0/1005	0.25	0/1365
116	qI	0.09	0/1005	0.22	0/1365
116	qi	0.10	0/1005	0.25	0/1365
117	QJ	0.10	0/502	0.22	0/687
117	Qj	0.09	0/522	0.22	0/712
117	qJ	0.10	0/502	0.22	0/687
117	qj	0.10	0/522	0.22	0/712
118	QL	0.07	0/273	0.19	0/371
118	Ql	0.09	0/273	0.20	0/371
118	qL	0.08	0/273	0.20	0/371
118	ql	0.09	0/273	0.19	0/371
120	S1	0.09	0/5518	0.25	0/7476
120	s1	0.09	0/5518	0.25	0/7476
121	S2	0.12	0/3680	0.27	0/4969
121	s2	0.12	0/3680	0.27	0/4969
122	S3	0.11	0/1718	0.29	0/2319
122	s3	0.11	0/1718	0.29	0/2319
123	S4	0.10	0/1543	0.27	0/2088
123	s4	0.10	0/1543	0.27	0/2088
124	S5	0.10	0/775	0.25	0/1048
124	s5	0.10	0/775	0.25	0/1048
125	S6	0.10	0/755	0.27	0/1022
125	s6	0.10	0/755	0.27	0/1022
126	S7	0.12	0/1311	0.29	0/1779
126	s7	0.11	0/1311	0.29	0/1779
127	S8	0.11	0/1867	0.27	0/2538
127	s8	0.11	0/1867	0.27	0/2538
128	T1	0.10	0/4153	0.25	0/5618
128	t1	0.10	0/4153	0.25	0/5618
129	T2	0.08	0/2224	0.23	0/3022
129	t2	0.08	0/2224	0.23	0/3022
130	T3	0.08	0/2527	0.22	0/3423
130	t3	0.08	0/2527	0.22	0/3423
131	T4	0.09	0/1689	0.23	0/2284
131	t4	0.09	0/1689	0.22	0/2284
132	T5	0.11	0/1163	0.25	0/1574
132	t5	0.11	0/1163	0.25	0/1574
133	T6	0.10	0/923	0.22	0/1239
133	t6	0.10	0/923	0.23	0/1239
134	T7	0.09	0/1223	0.21	0/1648
134	t7	0.09	0/1223	0.21	0/1648
135	T8	0.10	0/1112	0.23	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
135	t8	0.10	0/1112	0.23	0/1507
136	T9	0.10	0/1088	0.25	0/1458
136	t9	0.10	0/1088	0.26	0/1458
137	TA	0.10	0/877	0.23	0/1181
137	ta	0.10	0/877	0.24	0/1181
138	TB	0.09	0/825	0.19	0/1115
138	tb	0.09	0/825	0.19	0/1115
139	TC	0.09	0/811	0.21	0/1093
139	tc	0.09	0/811	0.21	0/1093
140	TD	0.08	0/634	0.20	0/855
140	td	0.08	0/634	0.20	0/855
141	TE	0.10	0/432	0.25	0/583
141	te	0.10	0/432	0.25	0/583
142	TF	0.08	0/1828	0.22	0/2472
142	tf	0.08	0/1828	0.22	0/2472
143	TG	0.09	0/1101	0.22	0/1486
143	tg	0.08	0/1101	0.22	0/1486
144	TH	0.10	0/1015	0.22	0/1366
144	th	0.09	0/1015	0.22	0/1366
145	TX	0.10	0/1235	0.23	0/1662
145	tx	0.10	0/1235	0.23	0/1662
146	V1	0.11	0/3485	0.27	0/4713
146	v1	0.10	0/3485	0.27	0/4713
147	V2	0.09	0/1895	0.26	0/2559
147	v2	0.09	0/1895	0.26	0/2559
148	X1	0.10	0/1261	0.24	0/1698
148	x1	0.10	0/1261	0.24	0/1698
149	C	0.09	0/1383	0.22	0/1880
149	c	0.09	0/1383	0.22	0/1880
All	All	0.11	0/556450	0.26	2/753536 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	281	HIS	CA-C-N	7.24	126.12	120.33
33	E	281	HIS	C-N-CA	7.24	126.12	120.33

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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1T	540	0	532	11	0
1	1t	540	0	532	11	0
2	2E	2560	0	2553	61	0
2	2e	2560	0	2553	60	0
3	2F	1803	0	1779	65	0
3	2f	1803	0	1779	63	0
4	2G	1671	0	1617	47	0
4	2g	1671	0	1617	49	0
5	2H	801	0	788	20	0
5	2h	801	0	788	23	0
6	2I	915	0	890	14	0
6	2i	915	0	890	13	0
7	2J	839	0	803	24	0
7	2j	839	0	803	24	0
8	2K	795	0	782	28	0
8	2k	795	0	782	30	0
9	2L	722	0	709	19	0
9	2l	722	0	709	18	0
10	2M	640	0	611	14	0
10	2m	640	0	611	16	0
11	2N	505	0	509	15	0
11	2n	505	0	509	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	2O	356	0	365	9	0
12	2o	356	0	365	7	0
13	2T	567	0	569	18	0
13	2t	567	0	569	20	0
14	3T	655	0	669	16	0
14	3t	655	0	669	13	0
15	4A	816	0	795	10	0
15	4a	816	0	795	13	0
16	4T	481	0	465	12	0
16	4t	481	0	465	12	0
17	5T	506	0	506	8	0
17	5t	506	0	506	8	0
18	6A	1083	0	1020	24	0
18	6a	1083	0	1020	21	0
19	6B	1912	0	1768	38	0
19	6b	1912	0	1768	41	0
20	6C	891	0	811	30	0
20	6c	891	0	811	29	0
21	6L	636	0	639	6	0
21	6l	636	0	639	6	0
22	6T	561	0	564	14	0
22	6t	561	0	564	13	0
23	7A	1166	0	1129	35	0
23	7a	1166	0	1129	33	0
24	7C	1825	0	1636	31	0
24	7c	1825	0	1636	30	0
25	7L	1078	0	1071	33	0
25	7l	1078	0	1071	33	0
26	A	3756	0	3557	62	0
26	a	3756	0	3557	59	0
27	B	3398	0	3463	50	0
27	b	3398	0	3463	52	0
28	BP	2920	0	2817	65	0
28	bp	2920	0	2817	65	0
29	C1	5576	0	5621	166	0
29	c1	5576	0	5621	173	0
30	C2	5094	0	5078	135	0
30	c2	5094	0	5078	142	0
31	C3	5084	0	5067	125	0
31	c3	5084	0	5067	130	0
32	D	2366	0	2290	34	0
32	d	2366	0	2290	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	E	3176	0	3108	76	0
33	e	3176	0	3108	75	0
34	F	2024	0	1958	55	0
34	f	2024	0	1958	56	0
35	FS	1509	0	1477	37	0
35	fs	1509	0	1477	38	0
36	G	2442	0	2290	70	0
36	g	2442	0	2290	72	0
37	H	2369	0	2319	49	0
37	h	2369	0	2319	54	0
38	I	1943	0	1865	48	0
38	i	1943	0	1865	45	0
39	J	1575	0	1567	26	0
39	j	1575	0	1567	25	0
40	K	1714	0	1678	37	0
40	k	1714	0	1678	34	0
41	L	1668	0	1643	34	0
41	l	1668	0	1643	33	0
42	M	1872	0	1760	74	0
42	m	1872	0	1760	74	0
43	M1	2863	0	2781	63	0
43	m1	2863	0	2781	65	0
44	M2	2558	0	2552	41	0
44	m2	2558	0	2552	45	0
45	M3	2620	0	2584	45	0
45	m3	2620	0	2584	43	0
46	N	1716	0	1648	45	0
46	n	1716	0	1648	44	0
47	O	1081	0	1053	17	0
47	o	1081	0	1053	18	0
48	P	1410	0	1391	27	0
48	p	1410	0	1391	27	0
49	Q	1434	0	1393	42	0
49	q	1434	0	1393	38	0
50	R	1407	0	1419	28	0
50	r	1407	0	1419	33	0
51	S	1388	0	1407	39	0
51	s	1388	0	1407	32	0
52	SA	4624	0	4573	124	0
52	sa	4624	0	4573	121	0
53	SB	2260	0	2233	60	0
53	sb	2260	0	2233	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	SC	481	0	475	18	0
54	sc	481	0	475	17	0
55	SD	393	0	413	13	0
55	sd	393	0	413	14	0
56	T	1315	0	1286	28	0
56	t	1315	0	1286	29	0
57	U	1304	0	1299	34	0
57	u	1304	0	1299	34	0
58	V	1234	0	1194	33	0
58	v	1234	0	1194	34	0
59	VB	4630	0	4406	120	0
59	vb	4630	0	4406	115	0
60	W	1096	0	1031	29	0
60	w	1096	0	1031	29	0
61	X	1012	0	1000	14	0
61	x	1012	0	1000	13	0
62	Y	859	0	812	23	0
62	y	859	0	812	26	0
63	Y0	775	0	798	23	0
63	y0	775	0	798	25	0
64	Y5	1659	0	1726	35	0
64	y5	1659	0	1726	35	0
65	Y7	2938	0	3010	69	0
65	y7	2938	0	3010	70	0
66	Z	717	0	694	19	0
66	z	717	0	694	21	0
67	Z1	766	0	747	9	0
67	z1	766	0	747	9	0
68	1B	516	0	528	24	0
68	1b	516	0	528	25	0
69	2B	1483	0	1554	43	0
69	2b	1483	0	1554	40	0
70	4L	957	0	987	34	0
70	4l	957	0	987	35	0
71	5B	888	0	917	30	0
71	5b	888	0	917	34	0
72	A1	806	0	801	22	0
72	a1	806	0	801	23	0
73	A2	811	0	800	26	0
73	a2	811	0	800	24	0
74	A3	1077	0	1004	27	0
74	a3	1077	0	1004	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	A5	1307	0	1317	25	0
75	a5	1307	0	1317	25	0
76	A6	1421	0	1382	39	0
76	a6	1421	0	1382	36	0
77	A7	2347	0	2249	50	0
77	a7	2347	0	2249	48	0
78	A8	1075	0	1024	22	0
78	a8	1075	0	1024	23	0
79	A9	2736	0	2665	49	0
79	a9	2736	0	2665	49	0
80	AB	926	0	902	12	0
80	ab	926	0	902	12	0
81	AC	806	0	784	15	0
81	ac	806	0	784	15	0
82	AL	1612	0	1511	40	0
82	al	1612	0	1511	39	0
83	AM	1349	0	1375	52	0
83	am	1349	0	1375	52	0
84	AN	1879	0	1818	27	0
84	an	1879	0	1818	28	0
85	B2	966	0	940	22	0
85	b2	966	0	940	20	0
86	B3	602	0	593	17	0
86	b3	602	0	593	16	0
87	B4	976	0	880	20	0
87	b4	976	0	880	21	0
88	B6	596	0	583	12	0
88	b6	596	0	583	15	0
89	B7	941	0	884	16	0
89	b7	941	0	884	17	0
90	B8	1456	0	1415	43	0
90	b8	1456	0	1415	44	0
91	B9	1596	0	1507	25	0
91	b9	1596	0	1507	25	0
92	BL	1461	0	1467	30	0
92	bl	1461	0	1467	36	0
93	BM	1321	0	1256	26	0
93	bm	1321	0	1256	27	0
94	C4	850	0	840	22	0
94	c4	850	0	840	18	0
95	FX	1162	0	1120	35	0
95	fx	1162	0	1120	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
96	G1	1773	0	1732	39	0
96	g1	1773	0	1732	39	0
97	G2	1762	0	1775	51	0
97	g2	1762	0	1775	45	0
98	G3	2804	0	2727	46	0
98	g3	2804	0	2727	47	0
99	J1	2170	0	2130	39	0
99	j1	2170	0	2130	40	0
100	N1	2305	0	2349	91	0
100	n1	2305	0	2349	93	0
101	N2	3073	0	3153	81	0
101	n2	3073	0	3153	77	0
102	N3	1017	0	1014	34	0
102	n3	1017	0	1014	34	0
103	N4	4170	0	4223	97	0
103	n4	4170	0	4223	104	0
104	N5	5908	0	5946	165	0
104	n5	5908	0	5946	165	0
105	N6	2168	0	2167	57	0
105	n6	2168	0	2167	63	0
106	P1	1908	0	1861	52	0
106	p1	1908	0	1861	51	0
107	P2	1414	0	1378	38	0
107	p2	1414	0	1378	40	0
108	QA	3517	0	3512	56	0
108	Qa	3517	0	3512	65	0
108	qA	3517	0	3512	57	0
108	qa	3517	0	3512	65	0
109	QB	3835	0	3734	63	0
109	Qb	3835	0	3734	89	0
109	qB	3835	0	3734	62	0
109	qb	3835	0	3734	84	0
110	QC	3589	0	3483	94	0
110	Qc	3580	0	3470	110	0
110	qC	3589	0	3483	99	0
110	qc	3580	0	3470	110	0
111	QD	2489	0	2343	54	0
111	Qd	2489	0	2343	65	0
111	qD	2489	0	2343	53	0
111	qd	2489	0	2343	63	0
112	QE	1559	0	1222	35	0
112	Qe	1471	0	1136	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
112	qE	1559	0	1222	36	0
112	qe	1471	0	1136	40	0
113	QF	702	0	700	21	0
113	Qf	630	0	633	12	0
113	qF	702	0	700	19	0
113	qf	630	0	633	11	0
114	QG	2767	0	2706	49	0
114	Qg	2760	0	2697	67	0
114	qG	2767	0	2706	54	0
114	qg	2760	0	2697	68	0
115	QH	1098	0	1040	28	0
115	Qh	1098	0	1040	36	0
115	qH	1098	0	1040	28	0
115	qh	1098	0	1040	35	0
116	QI	971	0	986	14	0
116	Qi	971	0	986	19	0
116	qI	971	0	986	13	0
116	qi	971	0	986	20	0
117	QJ	481	0	477	14	0
117	Qj	501	0	503	8	0
117	qJ	481	0	477	14	0
117	qj	501	0	503	9	0
118	QL	266	0	282	2	0
118	Ql	266	0	282	4	0
118	qL	266	0	282	2	0
118	ql	266	0	282	4	0
119	QM	85	0	19	0	0
119	Qm	85	0	19	0	0
119	U2	85	0	20	1	0
119	qM	85	0	19	0	0
119	qm	85	0	19	0	0
119	u2	85	0	20	1	0
120	S1	5410	0	5364	134	0
120	s1	5410	0	5364	125	0
121	S2	3598	0	3552	112	0
121	s2	3598	0	3552	110	0
122	S3	1681	0	1679	55	0
122	s3	1681	0	1679	51	0
123	S4	1500	0	1449	42	0
123	s4	1500	0	1449	39	0
124	S5	756	0	725	25	0
124	s5	756	0	725	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
125	S6	738	0	724	12	0
125	s6	738	0	724	16	0
126	S7	1278	0	1271	43	0
126	s7	1278	0	1271	42	0
127	S8	1812	0	1688	62	0
127	s8	1812	0	1688	59	0
128	T1	4059	0	4009	71	0
128	t1	4059	0	4009	67	0
129	T2	2180	0	2178	42	0
129	t2	2180	0	2178	40	0
130	T3	2479	0	2473	42	0
130	t3	2479	0	2473	42	0
131	T4	1644	0	1632	35	0
131	t4	1644	0	1632	33	0
132	T5	1138	0	1160	29	0
132	t5	1138	0	1160	28	0
133	T6	903	0	853	7	0
133	t6	903	0	853	4	0
134	T7	1187	0	1137	24	0
134	t7	1187	0	1137	22	0
135	T8	1084	0	1110	28	0
135	t8	1084	0	1110	28	0
136	T9	1066	0	1023	19	0
136	t9	1066	0	1023	20	0
137	TA	854	0	839	16	0
137	ta	854	0	839	18	0
138	TB	801	0	763	17	0
138	tb	801	0	763	17	0
139	TC	789	0	745	19	0
139	tc	789	0	745	21	0
140	TD	616	0	611	8	0
140	td	616	0	611	8	0
141	TE	420	0	427	8	0
141	te	420	0	427	7	0
142	TF	1789	0	1795	26	0
142	tf	1789	0	1795	25	0
143	TG	1081	0	1091	12	0
143	tg	1081	0	1091	12	0
144	TH	996	0	1023	20	0
144	th	996	0	1023	22	0
145	TX	1206	0	1155	24	0
145	tx	1206	0	1155	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
146	V1	3410	0	3357	71	0
146	v1	3410	0	3357	71	0
147	V2	1858	0	1842	43	0
147	v2	1858	0	1842	37	0
148	X1	1227	0	1208	26	0
148	x1	1227	0	1208	25	0
149	C	1368	0	1172	21	0
149	c	1368	0	1172	22	0
150	U1	460	0	95	4	0
150	u1	460	0	95	4	0
151	2E	43	0	31	1	0
151	2e	43	0	31	1	0
151	QD	43	0	30	1	0
151	Qd	43	0	30	0	0
151	qD	43	0	30	1	0
151	qd	43	0	30	0	0
152	2F	121	0	167	10	0
152	2G	50	0	77	3	0
152	2J	42	0	58	0	0
152	2f	121	0	167	10	0
152	2g	50	0	77	3	0
152	2j	42	0	58	0	0
152	5B	47	0	68	3	0
152	5b	47	0	68	3	0
152	6A	35	0	44	1	0
152	6C	33	0	40	0	0
152	6a	35	0	44	1	0
152	6c	33	0	40	0	0
152	7A	45	0	64	3	0
152	7C	43	0	63	5	0
152	7a	45	0	64	3	0
152	7c	43	0	63	5	0
152	A	82	0	112	6	0
152	AL	26	0	26	1	0
152	AM	39	0	52	4	0
152	AN	36	0	46	3	0
152	B9	34	0	42	3	0
152	C1	171	0	238	19	0
152	C2	36	0	46	1	0
152	C3	210	0	296	12	0
152	C4	41	0	56	4	0
152	D	35	0	44	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
152	F	38	0	50	2	0
152	FS	40	0	54	5	0
152	I	39	0	52	7	0
152	J	37	0	48	1	0
152	J1	40	0	54	3	0
152	M	116	0	157	6	0
152	M1	96	0	146	10	0
152	M2	132	0	195	6	0
152	N	109	0	140	11	0
152	N1	36	0	46	2	0
152	N3	31	0	36	1	0
152	N5	198	0	304	21	0
152	N6	54	0	88	7	0
152	P1	40	0	54	1	0
152	QB	44	0	65	4	0
152	QC	124	0	173	6	0
152	QE	63	0	74	6	0
152	QG	32	0	38	0	0
152	QI	73	0	97	11	0
152	QJ	66	0	80	6	0
152	Qb	43	0	63	4	0
152	Qc	85	0	121	6	0
152	Qe	76	0	103	3	0
152	Qg	32	0	38	3	0
152	Qi	72	0	95	5	0
152	Qj	36	0	46	2	0
152	S8	30	0	34	2	0
152	T1	33	0	40	0	0
152	T4	102	0	161	5	0
152	TC	89	0	129	6	0
152	TE	32	0	38	1	0
152	V	84	0	119	3	0
152	W	126	0	177	11	0
152	a	82	0	112	6	0
152	al	26	0	26	1	0
152	am	39	0	52	4	0
152	an	36	0	46	3	0
152	b9	34	0	42	3	0
152	c1	171	0	238	17	0
152	c2	36	0	46	1	0
152	c3	210	0	296	13	0
152	c4	41	0	56	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
152	d	35	0	44	5	0
152	f	38	0	50	2	0
152	fs	40	0	54	5	0
152	i	39	0	52	7	0
152	j	37	0	48	1	0
152	j1	40	0	54	3	0
152	m	116	0	157	6	0
152	m1	96	0	146	10	0
152	m2	132	0	195	7	0
152	n	109	0	140	12	0
152	n1	36	0	46	2	0
152	n3	31	0	36	2	0
152	n5	198	0	304	21	0
152	n6	54	0	88	6	0
152	p1	40	0	54	1	0
152	qB	44	0	65	5	0
152	qC	124	0	173	7	0
152	qE	91	0	104	8	0
152	qG	32	0	38	0	0
152	qI	73	0	97	10	0
152	qJ	38	0	50	4	0
152	qb	43	0	63	2	0
152	qc	85	0	121	6	0
152	qe	76	0	103	4	0
152	qg	32	0	38	3	0
152	qi	72	0	95	5	0
152	qj	36	0	46	2	0
152	s8	30	0	34	2	0
152	t1	33	0	40	0	0
152	t4	102	0	161	4	0
152	tc	89	0	129	9	0
152	te	32	0	38	1	0
152	v	84	0	119	4	0
152	w	126	0	177	11	0
153	2B	87	0	124	11	0
153	2G	207	0	255	13	0
153	2K	98	0	149	8	0
153	2M	96	0	145	8	0
153	2O	50	0	44	1	0
153	2b	87	0	124	10	0
153	2g	207	0	255	11	0
153	2k	98	0	149	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	2m	96	0	145	6	0
153	2o	50	0	44	1	0
153	5B	81	0	106	8	0
153	5b	81	0	106	7	0
153	6A	74	0	92	2	0
153	6C	157	0	205	16	0
153	6a	74	0	92	3	0
153	6c	157	0	205	15	0
153	7A	162	0	224	15	0
153	7C	136	0	166	8	0
153	7a	162	0	224	16	0
153	7c	136	0	166	8	0
153	A	145	0	184	11	0
153	A1	133	0	154	11	0
153	A9	163	0	217	10	0
153	AL	53	0	50	3	0
153	AM	56	0	56	6	0
153	AN	87	0	124	6	0
153	B	62	0	68	1	0
153	B3	140	0	171	6	0
153	B4	37	0	18	2	0
153	B8	69	0	82	5	0
153	BM	86	0	119	12	0
153	C	64	0	75	3	0
153	C1	302	0	389	34	0
153	C3	68	0	80	4	0
153	C4	98	0	149	4	0
153	E	195	0	228	17	0
153	F	100	0	156	10	0
153	FS	47	0	38	6	0
153	I	152	0	195	11	0
153	J	70	0	84	2	0
153	L	74	0	95	2	0
153	M	277	0	336	19	0
153	M1	214	0	266	16	0
153	M2	194	0	220	11	0
153	M3	118	0	124	5	0
153	N	84	0	118	7	0
153	N5	90	0	130	7	0
153	N6	90	0	130	7	0
153	P1	121	0	130	7	0
153	Q	135	0	161	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	QB	68	0	80	6	0
153	QC	120	0	128	9	0
153	QD	61	0	66	1	0
153	QG	86	0	122	1	0
153	QH	94	0	138	8	0
153	QI	71	0	86	5	0
153	Qb	68	0	80	3	0
153	Qc	167	0	166	3	0
153	Qg	100	0	156	9	0
153	Qi	71	0	86	5	0
153	R	65	0	74	4	0
153	SD	76	0	99	5	0
153	T	295	0	375	30	0
153	T1	55	0	54	4	0
153	T5	96	0	142	13	0
153	T7	73	0	93	8	0
153	TE	53	0	50	5	0
153	TH	84	0	115	5	0
153	U	60	0	64	4	0
153	U1	57	0	58	2	0
153	VB	297	0	382	26	0
153	W	84	0	118	7	0
153	Y5	70	0	84	1	0
153	Y7	65	0	74	2	0
153	Z	67	0	78	1	0
153	a	227	0	295	16	0
153	a1	67	0	78	9	0
153	a9	163	0	217	10	0
153	al	53	0	50	3	0
153	am	56	0	56	6	0
153	an	87	0	124	5	0
153	b	62	0	68	1	0
153	b3	140	0	171	5	0
153	b4	37	0	18	2	0
153	b8	69	0	82	5	0
153	bm	86	0	119	12	0
153	c	64	0	75	4	0
153	c1	302	0	389	32	0
153	c3	68	0	80	4	0
153	c4	98	0	149	5	0
153	e	195	0	228	17	0
153	f	100	0	156	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	fs	47	0	38	5	0
153	i	152	0	195	14	0
153	j	70	0	84	3	0
153	l	74	0	95	2	0
153	m	277	0	336	19	0
153	m1	214	0	266	15	0
153	m2	194	0	220	11	0
153	m3	118	0	124	5	0
153	n	84	0	118	7	0
153	n5	90	0	130	10	0
153	n6	90	0	130	7	0
153	p1	121	0	130	8	0
153	q	221	0	280	21	0
153	qB	68	0	80	6	0
153	qC	120	0	128	9	0
153	qD	61	0	66	1	0
153	qG	86	0	122	1	0
153	qH	94	0	138	8	0
153	qI	71	0	86	4	0
153	qb	68	0	80	3	0
153	qc	167	0	166	4	0
153	qg	100	0	156	8	0
153	qi	71	0	86	5	0
153	r	65	0	74	4	0
153	sd	76	0	99	5	0
153	t	295	0	375	31	0
153	t1	55	0	54	4	0
153	t5	96	0	142	12	0
153	t7	73	0	93	7	0
153	td	66	0	76	2	0
153	te	53	0	50	5	0
153	th	84	0	115	5	0
153	u	60	0	64	4	0
153	u1	57	0	58	2	0
153	vb	129	0	152	11	0
153	w	84	0	118	7	0
153	y5	70	0	84	1	0
153	y7	65	0	74	2	0
153	z	67	0	78	1	0
154	C1	120	0	108	19	0
154	c1	120	0	108	22	0
155	C1	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
155	C2	2	0	0	0	0
155	c1	1	0	0	0	0
155	c2	2	0	0	0	0
156	C1	1	0	0	0	0
156	c1	1	0	0	0	0
157	FS	8	0	0	0	0
157	FX	4	0	0	0	0
157	QE	4	0	0	0	0
157	Qe	4	0	0	0	0
157	S1	4	0	0	0	0
157	SB	4	0	0	0	0
157	V2	4	0	0	0	0
157	fs	8	0	0	1	0
157	fx	4	0	0	0	0
157	qE	4	0	0	0	0
157	qe	4	0	0	0	0
157	s1	4	0	0	0	0
157	sb	4	0	0	0	0
157	v2	4	0	0	0	0
158	A3	89	0	126	10	0
158	AN	152	0	206	7	0
158	B4	48	0	73	6	0
158	BM	30	0	34	1	0
158	C4	51	0	82	3	0
158	G2	51	0	82	2	0
158	I	32	0	38	1	0
158	M2	31	0	36	2	0
158	M3	38	0	53	2	0
158	N4	36	0	46	0	0
158	N5	36	0	46	5	0
158	S8	41	0	59	0	0
158	SC	40	0	54	2	0
158	T4	25	0	24	1	0
158	T8	86	0	123	9	0
158	TA	26	0	26	1	0
158	VB	28	0	30	0	0
158	W	34	0	42	4	0
158	Y5	28	0	30	1	0
158	a3	89	0	126	10	0
158	an	152	0	206	7	0
158	b4	48	0	73	5	0
158	bm	30	0	34	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
158	c4	51	0	82	3	0
158	g2	51	0	82	1	0
158	i	32	0	38	1	0
158	m2	31	0	36	2	0
158	m3	38	0	53	2	0
158	n4	36	0	46	1	0
158	n5	36	0	46	4	0
158	s8	41	0	59	0	0
158	sc	40	0	54	2	0
158	t4	25	0	24	0	0
158	t8	86	0	123	9	0
158	ta	26	0	26	1	0
158	vb	28	0	30	0	0
158	w	34	0	42	4	0
158	y5	28	0	30	1	0
159	M2	36	0	38	1	0
159	m2	36	0	38	1	0
160	Qh	36	0	52	4	0
160	R	33	0	43	2	0
160	Y5	21	0	16	1	0
160	qh	36	0	52	4	0
160	r	33	0	43	2	0
160	y5	21	0	16	1	0
161	SA	53	0	29	5	0
161	sa	53	0	29	5	0
162	S1	16	0	0	3	0
162	S7	8	0	0	2	0
162	S8	16	0	0	2	0
162	SB	8	0	0	0	0
162	V1	8	0	0	1	0
162	s1	16	0	0	3	0
162	s7	8	0	0	2	0
162	s8	16	0	0	3	0
162	sb	8	0	0	0	0
162	v1	8	0	0	1	0
163	SB	7	0	0	1	0
163	sb	7	0	0	1	0
164	B8	63	0	90	8	0
164	QC	29	0	33	2	0
164	Qc	55	0	68	6	0
164	SC	63	0	90	6	0
164	b8	63	0	90	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
164	qC	29	0	33	1	0
164	qc	55	0	68	5	0
164	sc	63	0	90	7	0
165	S6	1	0	0	0	0
165	VB	2	0	0	0	0
165	s6	1	0	0	0	0
165	vb	2	0	0	0	0
166	QC	86	0	60	9	0
166	Qc	86	0	60	12	0
166	Y5	43	0	30	0	0
166	qC	86	0	60	10	0
166	qc	86	0	60	13	0
166	y5	43	0	30	0	0
167	A9	48	0	26	1	0
167	a9	48	0	26	1	0
168	AB	37	0	47	12	0
168	ab	37	0	47	12	0
169	B6	55	0	0	0	0
169	b6	55	0	0	0	0
170	B9	27	0	12	0	0
170	b9	27	0	12	1	0
171	V1	31	0	19	2	0
171	v1	31	0	19	1	0
All	All	568568	0	562502	10494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 10494 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:192:SER:HG	42:M:2:SER:N	1.56	1.02
31:c3:258:TYR:HH	45:m3:2:ALA:N	1.70	0.89
28:bp:176:SER:HB2	28:bp:192:TYR:O	1.72	0.88
28:BP:176:SER:HB2	28:BP:192:TYR:O	1.75	0.87
42:m:2:SER:N	33:E:192:SER:HG	1.74	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	43	66
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	53
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	53
100	n1	281/284 (99%)	268 (95%)	12 (4%)	1 (0%)	30	53
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	53
129	t2	277/333 (83%)	267 (96%)	9 (3%)	1 (0%)	30	53
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	49
149	c	201/212 (95%)	192 (96%)	8 (4%)	1 (0%)	24	49
All	All	65386/73196 (89%)	63252 (97%)	2126 (3%)	8 (0%)	100	100

5 of 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

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%)	61 (100%)	0	100	100
1	1t	61/63 (97%)	61 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2E	286/287 (100%)	279 (98%)	7 (2%)	43	67
2	2e	286/287 (100%)	278 (97%)	8 (3%)	38	62
3	2F	193/268 (72%)	190 (98%)	3 (2%)	55	75
3	2f	193/268 (72%)	190 (98%)	3 (2%)	55	75
4	2G	181/181 (100%)	178 (98%)	3 (2%)	53	73
4	2g	181/181 (100%)	179 (99%)	2 (1%)	65	80
5	2H	93/184 (50%)	93 (100%)	0	100	100
5	2h	93/184 (50%)	93 (100%)	0	100	100
6	2I	97/97 (100%)	95 (98%)	2 (2%)	47	69
6	2i	97/97 (100%)	94 (97%)	3 (3%)	35	59
7	2J	85/86 (99%)	85 (100%)	0	100	100
7	2j	85/86 (99%)	85 (100%)	0	100	100
8	2K	85/85 (100%)	85 (100%)	0	100	100
8	2k	85/85 (100%)	85 (100%)	0	100	100
9	2L	77/83 (93%)	75 (97%)	2 (3%)	40	65
9	2l	77/83 (93%)	76 (99%)	1 (1%)	61	78
10	2M	66/67 (98%)	65 (98%)	1 (2%)	57	76
10	2m	66/67 (98%)	65 (98%)	1 (2%)	57	76
11	2N	55/56 (98%)	53 (96%)	2 (4%)	31	56
11	2n	55/56 (98%)	54 (98%)	1 (2%)	51	72
12	2O	37/40 (92%)	37 (100%)	0	100	100
12	2o	37/40 (92%)	37 (100%)	0	100	100
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%)	40	65
14	3t	76/83 (92%)	74 (97%)	2 (3%)	40	65
15	4A	87/113 (77%)	87 (100%)	0	100	100
15	4a	87/113 (77%)	87 (100%)	0	100	100
16	4T	54/63 (86%)	54 (100%)	0	100	100
16	4t	54/63 (86%)	54 (100%)	0	100	100
17	5T	56/66 (85%)	56 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	5t	56/66 (85%)	56 (100%)	0	100	100
18	6A	114/116 (98%)	114 (100%)	0	100	100
18	6a	114/116 (98%)	114 (100%)	0	100	100
19	6B	200/207 (97%)	200 (100%)	0	100	100
19	6b	200/207 (97%)	200 (100%)	0	100	100
20	6C	86/88 (98%)	86 (100%)	0	100	100
20	6c	86/88 (98%)	86 (100%)	0	100	100
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%)	120 (100%)	0	100	100
23	7a	120/120 (100%)	120 (100%)	0	100	100
24	7C	198/218 (91%)	198 (100%)	0	100	100
24	7c	198/218 (91%)	198 (100%)	0	100	100
25	7L	122/943 (13%)	119 (98%)	3 (2%)	42	66
25	7l	122/943 (13%)	120 (98%)	2 (2%)	55	75
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%)	371 (99%)	3 (1%)	73	85
27	b	374/413 (91%)	371 (99%)	3 (1%)	73	85
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%)	68	82
29	c1	599/613 (98%)	593 (99%)	6 (1%)	68	82
30	C2	565/569 (99%)	561 (99%)	4 (1%)	76	87
30	c2	565/569 (99%)	561 (99%)	4 (1%)	76	87
31	C3	553/565 (98%)	548 (99%)	5 (1%)	70	83
31	c3	553/565 (98%)	550 (100%)	3 (0%)	81	90
32	D	253/358 (71%)	251 (99%)	2 (1%)	73	85
32	d	253/358 (71%)	251 (99%)	2 (1%)	73	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	E	342/343 (100%)	341 (100%)	1 (0%)	86	92
33	e	342/343 (100%)	341 (100%)	1 (0%)	86	92
34	F	219/318 (69%)	217 (99%)	2 (1%)	70	83
34	f	219/318 (69%)	217 (99%)	2 (1%)	70	83
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%)	76	87
36	g	267/289 (92%)	266 (100%)	1 (0%)	84	92
37	H	256/272 (94%)	248 (97%)	8 (3%)	35	59
37	h	256/272 (94%)	249 (97%)	7 (3%)	39	64
38	I	200/219 (91%)	199 (100%)	1 (0%)	81	90
38	i	200/219 (91%)	198 (99%)	2 (1%)	68	82
39	J	170/216 (79%)	169 (99%)	1 (1%)	78	89
39	j	170/216 (79%)	170 (100%)	0	100	100
40	K	191/213 (90%)	191 (100%)	0	100	100
40	k	191/213 (90%)	191 (100%)	0	100	100
41	L	181/206 (88%)	180 (99%)	1 (1%)	78	89
41	l	181/206 (88%)	180 (99%)	1 (1%)	78	89
42	M	198/199 (100%)	198 (100%)	0	100	100
42	m	198/199 (100%)	198 (100%)	0	100	100
43	M1	294/294 (100%)	294 (100%)	0	100	100
43	m1	294/294 (100%)	294 (100%)	0	100	100
44	M2	260/260 (100%)	260 (100%)	0	100	100
44	m2	260/260 (100%)	260 (100%)	0	100	100
45	M3	275/276 (100%)	275 (100%)	0	100	100
45	m3	275/276 (100%)	274 (100%)	1 (0%)	84	92
46	N	178/181 (98%)	174 (98%)	4 (2%)	45	69
46	n	178/181 (98%)	176 (99%)	2 (1%)	65	80
47	O	120/180 (67%)	120 (100%)	0	100	100
47	o	120/180 (67%)	120 (100%)	0	100	100
48	P	157/157 (100%)	156 (99%)	1 (1%)	78	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	p	157/157 (100%)	157 (100%)	0	100	100
49	Q	157/157 (100%)	157 (100%)	0	100	100
49	q	157/157 (100%)	156 (99%)	1 (1%)	78	89
50	R	156/157 (99%)	154 (99%)	2 (1%)	61	78
50	r	156/157 (99%)	154 (99%)	2 (1%)	61	78
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%)	44	67
52	sa	481/515 (93%)	471 (98%)	10 (2%)	47	69
53	SB	255/283 (90%)	245 (96%)	10 (4%)	28	54
53	sb	255/283 (90%)	247 (97%)	8 (3%)	35	59
54	SC	49/51 (96%)	46 (94%)	3 (6%)	17	40
54	sc	49/51 (96%)	46 (94%)	3 (6%)	17	40
55	SD	43/43 (100%)	43 (100%)	0	100	100
55	sd	43/43 (100%)	43 (100%)	0	100	100
56	T	137/139 (99%)	137 (100%)	0	100	100
56	t	137/139 (99%)	137 (100%)	0	100	100
57	U	137/138 (99%)	137 (100%)	0	100	100
57	u	137/138 (99%)	137 (100%)	0	100	100
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%)	498 (99%)	5 (1%)	68	82
59	vb	503/579 (87%)	500 (99%)	3 (1%)	78	89
60	W	112/113 (99%)	111 (99%)	1 (1%)	70	83
60	w	112/113 (99%)	111 (99%)	1 (1%)	70	83
61	X	105/105 (100%)	103 (98%)	2 (2%)	50	71
61	x	105/105 (100%)	104 (99%)	1 (1%)	68	82
62	Y	88/88 (100%)	88 (100%)	0	100	100
62	y	88/88 (100%)	88 (100%)	0	100	100
63	Y0	84/84 (100%)	84 (100%)	0	100	100
63	y0	84/84 (100%)	84 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86	92
65	y7	333/442 (75%)	332 (100%)	1 (0%)	86	92
66	Z	77/80 (96%)	76 (99%)	1 (1%)	61	78
66	z	77/80 (96%)	76 (99%)	1 (1%)	61	78
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%)	78	89
69	2b	170/170 (100%)	169 (99%)	1 (1%)	78	89
70	4L	108/108 (100%)	106 (98%)	2 (2%)	50	71
70	4l	108/108 (100%)	106 (98%)	2 (2%)	50	71
71	5B	98/98 (100%)	98 (100%)	0	100	100
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%)	88 (100%)	0	100	100
73	a2	88/93 (95%)	88 (100%)	0	100	100
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%)	144 (100%)	0	100	100
75	a5	144/186 (77%)	144 (100%)	0	100	100
76	A6	154/154 (100%)	154 (100%)	0	100	100
76	a6	154/154 (100%)	154 (100%)	0	100	100
77	A7	257/257 (100%)	255 (99%)	2 (1%)	73	85
77	a7	257/257 (100%)	256 (100%)	1 (0%)	84	92
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	a9	290/311 (93%)	290 (100%)	0	100	100
80	AB	104/129 (81%)	103 (99%)	1 (1%)	68	82
80	ab	104/129 (81%)	103 (99%)	1 (1%)	68	82
81	AC	88/119 (74%)	87 (99%)	1 (1%)	65	80
81	ac	88/119 (74%)	87 (99%)	1 (1%)	65	80
82	AL	169/170 (99%)	167 (99%)	2 (1%)	63	79
82	al	169/170 (99%)	168 (99%)	1 (1%)	78	89
83	AM	142/156 (91%)	142 (100%)	0	100	100
83	am	142/156 (91%)	142 (100%)	0	100	100
84	AN	199/199 (100%)	199 (100%)	0	100	100
84	an	199/199 (100%)	199 (100%)	0	100	100
85	B2	103/109 (94%)	101 (98%)	2 (2%)	50	71
85	b2	103/109 (94%)	101 (98%)	2 (2%)	50	71
86	B3	64/74 (86%)	63 (98%)	1 (2%)	55	75
86	b3	64/74 (86%)	63 (98%)	1 (2%)	55	75
87	B4	102/128 (80%)	102 (100%)	0	100	100
87	b4	102/128 (80%)	102 (100%)	0	100	100
88	B6	64/117 (55%)	63 (98%)	1 (2%)	55	75
88	b6	64/117 (55%)	63 (98%)	1 (2%)	55	75
89	B7	97/99 (98%)	97 (100%)	0	100	100
89	b7	97/99 (98%)	97 (100%)	0	100	100
90	B8	156/180 (87%)	155 (99%)	1 (1%)	78	89
90	b8	156/180 (87%)	156 (100%)	0	100	100
91	B9	171/172 (99%)	171 (100%)	0	100	100
91	b9	171/172 (99%)	171 (100%)	0	100	100
92	BL	160/172 (93%)	160 (100%)	0	100	100
92	bl	160/172 (93%)	160 (100%)	0	100	100
93	BM	142/182 (78%)	141 (99%)	1 (1%)	76	87
93	bm	142/182 (78%)	141 (99%)	1 (1%)	76	87
94	C4	89/89 (100%)	88 (99%)	1 (1%)	65	80
94	c4	89/89 (100%)	89 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
95	FX	130/152 (86%)	130 (100%)	0	100	100
95	fx	130/152 (86%)	130 (100%)	0	100	100
96	G1	195/218 (89%)	194 (100%)	1 (0%)	81	90
96	g1	195/218 (89%)	194 (100%)	1 (0%)	81	90
97	G2	195/197 (99%)	191 (98%)	4 (2%)	47	69
97	g2	195/197 (99%)	193 (99%)	2 (1%)	68	82
98	G3	309/309 (100%)	309 (100%)	0	100	100
98	g3	309/309 (100%)	309 (100%)	0	100	100
99	J1	222/270 (82%)	222 (100%)	0	100	100
99	j1	222/270 (82%)	222 (100%)	0	100	100
100	N1	249/250 (100%)	241 (97%)	8 (3%)	34	59
100	n1	249/250 (100%)	244 (98%)	5 (2%)	48	71
101	N2	346/346 (100%)	340 (98%)	6 (2%)	53	73
101	n2	346/346 (100%)	342 (99%)	4 (1%)	63	79
102	N3	111/112 (99%)	110 (99%)	1 (1%)	70	83
102	n3	111/112 (99%)	110 (99%)	1 (1%)	70	83
103	N4	463/463 (100%)	457 (99%)	6 (1%)	61	78
103	n4	463/463 (100%)	456 (98%)	7 (2%)	57	76
104	N5	653/694 (94%)	644 (99%)	9 (1%)	59	77
104	n5	653/694 (94%)	646 (99%)	7 (1%)	65	80
105	N6	244/244 (100%)	243 (100%)	1 (0%)	84	92
105	n6	244/244 (100%)	244 (100%)	0	100	100
106	P1	207/223 (93%)	206 (100%)	1 (0%)	81	90
106	p1	207/223 (93%)	206 (100%)	1 (0%)	81	90
107	P2	158/178 (89%)	156 (99%)	2 (1%)	61	78
107	p2	158/178 (89%)	158 (100%)	0	100	100
108	QA	385/409 (94%)	381 (99%)	4 (1%)	68	82
108	Qa	385/409 (94%)	380 (99%)	5 (1%)	61	78
108	qA	385/409 (94%)	383 (100%)	2 (0%)	81	90
108	qa	385/409 (94%)	380 (99%)	5 (1%)	61	78
109	QB	411/440 (93%)	406 (99%)	5 (1%)	63	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
109	Qb	411/440 (93%)	403 (98%)	8 (2%)	50	71
109	qB	411/440 (93%)	407 (99%)	4 (1%)	68	82
109	qb	411/440 (93%)	403 (98%)	8 (2%)	50	71
110	QC	386/386 (100%)	380 (98%)	6 (2%)	55	75
110	Qc	385/386 (100%)	376 (98%)	9 (2%)	44	67
110	qC	386/386 (100%)	381 (99%)	5 (1%)	61	78
110	qc	385/386 (100%)	378 (98%)	7 (2%)	51	72
111	QD	255/274 (93%)	254 (100%)	1 (0%)	84	92
111	Qd	255/274 (93%)	254 (100%)	1 (0%)	84	92
111	qD	255/274 (93%)	254 (100%)	1 (0%)	84	92
111	qd	255/274 (93%)	254 (100%)	1 (0%)	84	92
112	QE	109/237 (46%)	108 (99%)	1 (1%)	70	83
112	Qe	99/237 (42%)	99 (100%)	0	100	100
112	qE	109/237 (46%)	108 (99%)	1 (1%)	70	83
112	qe	99/237 (42%)	99 (100%)	0	100	100
113	QF	80/81 (99%)	78 (98%)	2 (2%)	42	66
113	Qf	72/81 (89%)	72 (100%)	0	100	100
113	qF	80/81 (99%)	78 (98%)	2 (2%)	42	66
113	qf	72/81 (89%)	72 (100%)	0	100	100
114	QG	288/289 (100%)	284 (99%)	4 (1%)	59	77
114	Qg	287/289 (99%)	285 (99%)	2 (1%)	76	87
114	qG	288/289 (100%)	285 (99%)	3 (1%)	68	82
114	qg	287/289 (99%)	285 (99%)	2 (1%)	76	87
115	QH	117/118 (99%)	117 (100%)	0	100	100
115	Qh	117/118 (99%)	117 (100%)	0	100	100
115	qH	117/118 (99%)	117 (100%)	0	100	100
115	qh	117/118 (99%)	117 (100%)	0	100	100
116	QI	104/109 (95%)	103 (99%)	1 (1%)	68	82
116	Qi	104/109 (95%)	104 (100%)	0	100	100
116	qI	104/109 (95%)	102 (98%)	2 (2%)	50	71
116	qi	104/109 (95%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
117	QJ	51/56 (91%)	51 (100%)	0	100	100
117	Qj	53/56 (95%)	53 (100%)	0	100	100
117	qJ	51/56 (91%)	51 (100%)	0	100	100
117	qj	53/56 (95%)	53 (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
118	ql	28/36 (78%)	28 (100%)	0	100	100
120	S1	590/617 (96%)	585 (99%)	5 (1%)	73	85
120	s1	590/617 (96%)	587 (100%)	3 (0%)	81	90
121	S2	399/399 (100%)	390 (98%)	9 (2%)	44	67
121	s2	399/399 (100%)	391 (98%)	8 (2%)	48	71
122	S3	191/191 (100%)	188 (98%)	3 (2%)	55	75
122	s3	191/191 (100%)	187 (98%)	4 (2%)	47	69
123	S4	160/163 (98%)	158 (99%)	2 (1%)	61	78
123	s4	160/163 (98%)	158 (99%)	2 (1%)	61	78
124	S5	82/83 (99%)	81 (99%)	1 (1%)	63	79
124	s5	82/83 (99%)	82 (100%)	0	100	100
125	S6	82/116 (71%)	81 (99%)	1 (1%)	63	79
125	s6	82/116 (71%)	82 (100%)	0	100	100
126	S7	136/137 (99%)	132 (97%)	4 (3%)	37	61
126	s7	136/137 (99%)	132 (97%)	4 (3%)	37	61
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%)	430 (98%)	10 (2%)	44	67
128	t1	440/454 (97%)	432 (98%)	8 (2%)	51	72
129	T2	237/280 (85%)	234 (99%)	3 (1%)	61	78
129	t2	237/280 (85%)	234 (99%)	3 (1%)	61	78
130	T3	272/275 (99%)	270 (99%)	2 (1%)	76	87
130	t3	272/275 (99%)	270 (99%)	2 (1%)	76	87
131	T4	178/190 (94%)	178 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
131	t4	178/190 (94%)	178 (100%)	0	100	100
132	T5	119/179 (66%)	118 (99%)	1 (1%)	73	85
132	t5	119/179 (66%)	118 (99%)	1 (1%)	73	85
133	T6	97/131 (74%)	96 (99%)	1 (1%)	68	82
133	t6	97/131 (74%)	96 (99%)	1 (1%)	68	82
134	T7	124/125 (99%)	122 (98%)	2 (2%)	55	75
134	t7	124/125 (99%)	123 (99%)	1 (1%)	73	85
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%)	118 (100%)	0	100	100
136	t9	118/122 (97%)	118 (100%)	0	100	100
137	TA	94/117 (80%)	93 (99%)	1 (1%)	65	80
137	ta	94/117 (80%)	93 (99%)	1 (1%)	65	80
138	TB	82/97 (84%)	82 (100%)	0	100	100
138	tb	82/97 (84%)	82 (100%)	0	100	100
139	TC	83/84 (99%)	82 (99%)	1 (1%)	63	79
139	tc	83/84 (99%)	82 (99%)	1 (1%)	63	79
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%)	44 (98%)	1 (2%)	45	69
141	te	45/63 (71%)	45 (100%)	0	100	100
142	TF	195/212 (92%)	193 (99%)	2 (1%)	68	82
142	tf	195/212 (92%)	193 (99%)	2 (1%)	68	82
143	TG	121/122 (99%)	114 (94%)	7 (6%)	18	41
143	tg	121/122 (99%)	116 (96%)	5 (4%)	27	53
144	TH	108/108 (100%)	108 (100%)	0	100	100
144	th	108/108 (100%)	108 (100%)	0	100	100
145	TX	128/147 (87%)	126 (98%)	2 (2%)	55	75
145	tx	128/147 (87%)	127 (99%)	1 (1%)	73	85
146	V1	362/392 (92%)	359 (99%)	3 (1%)	73	85
146	v1	362/392 (92%)	359 (99%)	3 (1%)	73	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
147	V2	205/236 (87%)	204 (100%)	1 (0%)	81	90
147	v2	205/236 (87%)	204 (100%)	1 (0%)	81	90
148	X1	132/133 (99%)	132 (100%)	0	100	100
148	x1	132/133 (99%)	132 (100%)	0	100	100
149	C	106/178 (60%)	105 (99%)	1 (1%)	70	83
149	c	106/178 (60%)	105 (99%)	1 (1%)	70	83
All	All	58230/65244 (89%)	57737 (99%)	493 (1%)	70	85

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2F	181	PHE
122	S3	20	SER
46	N	191	ASN
121	S2	207	HIS
137	TA	35	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1355 such sidechains are listed below:

Mol	Chain	Res	Type
59	VB	214	ASN
110	QC	209	ASN
65	Y7	339	ASN
58	V	31	GLN
93	BM	166	ASN

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	$\# Z > 2$
24	SEP	7c	120	24	8,9,10	0.87	0	7,12,14	0.75	0
59	SEP	vb	520	59	8,9,10	0.89	0	7,12,14	0.84	0
59	TPO	vb	387	59	8,10,11	1.25	1 (12%)	10,14,16	1.13	0
24	SEP	7C	120	24	8,9,10	0.88	0	7,12,14	0.75	0
59	SEP	VB	520	59	8,9,10	0.89	0	7,12,14	0.83	0
59	TPO	VB	387	59	8,10,11	1.25	1 (12%)	10,14,16	1.13	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
24	SEP	7c	120	24	-	3/6/8/10	-
59	SEP	vb	520	59	-	3/6/8/10	-
59	TPO	vb	387	59	-	1/9/11/13	-
24	SEP	7C	120	24	-	3/6/8/10	-
59	SEP	VB	520	59	-	3/6/8/10	-
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	3.13	1.65	1.59
59	vb	387	TPO	P-OG1	3.12	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 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
24	7c	120	SEP	CB-OG-P-O3P
59	vb	387	TPO	O-C-CA-CB
59	vb	520	SEP	CB-OG-P-O1P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7c	120	SEP	1	0
59	vb	520	SEP	1	0
59	vb	387	TPO	1	0
24	7C	120	SEP	1	0
59	VB	520	SEP	1	0
59	VB	387	TPO	1	0

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	$\# Z > 2$
153	CDL	p1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	E	402	-	71,71,99	0.34	0	77,83,111	0.35	0
151	HEC	Qd	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.85	8 (13%)
152	PC1	qc	506	-	37,37,53	0.34	0	43,45,61	0.33	0
153	CDL	C	301	-	63,63,99	0.37	0	69,75,111	0.44	0
158	3PE	AN	301	-	44,44,50	0.32	0	47,49,55	0.28	0
152	PC1	P1	401	-	39,39,53	0.33	0	45,47,61	0.33	0
153	CDL	qI	203	-	70,70,99	0.35	0	76,82,111	0.31	0
158	3PE	A3	201	-	44,44,50	0.33	0	47,49,55	0.56	1 (2%)
153	CDL	N5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
153	CDL	N6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
153	CDL	R	201	-	64,64,99	0.36	0	70,76,111	0.32	0
168	ZMP	ab	201	80	34,36,36	0.69	1 (2%)	41,45,45	0.75	0
152	PC1	qc	509	-	46,46,53	0.30	0	52,54,61	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	TE	101	-	52,52,99	0.39	0	58,64,111	0.33	0
153	CDL	2O	101	-	49,49,99	0.41	0	55,61,111	0.35	0
152	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.33	0
157	FES	FS	203	35	0,4,4	-	-	-		
160	PX2	y5	204	-	20,20,35	1.30	4 (20%)	23,25,40	1.31	2 (8%)
152	PC1	I	301	-	38,38,53	0.34	0	44,46,61	0.34	0
153	CDL	Qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
152	PC1	M1	401	-	53,53,53	0.29	0	59,61,61	0.30	0
160	PX2	r	202	-	32,32,35	1.03	4 (12%)	35,37,40	1.00	2 (5%)
152	PC1	qj	101	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	b3	101	-	57,57,99	0.37	0	63,69,111	0.32	0
153	CDL	u1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
164	U10	qc	501	-	25,25,63	2.30	7 (28%)	24,29,79	1.92	8 (33%)
158	3PE	G2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
158	3PE	S8	304	-	40,40,50	0.33	0	43,45,55	0.32	0
153	CDL	2b	201	-	86,86,99	0.31	0	92,98,111	0.36	0
158	3PE	g2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
153	CDL	U1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
158	3PE	y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
153	CDL	c1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
152	PC1	B9	201	-	33,33,53	0.37	0	39,41,61	0.54	0
152	PC1	n5	805	-	53,53,53	0.28	0	59,61,61	0.33	0
152	PC1	M	303	-	44,44,53	0.31	0	50,52,61	0.39	0
152	PC1	TE	102	-	31,31,53	0.37	0	37,39,61	0.42	0
152	PC1	T4	301	-	47,47,53	0.31	0	53,55,61	0.38	0
157	FES	SB	401	53	0,4,4	-	-	-		
152	PC1	6a	202	-	34,34,53	0.36	0	40,42,61	0.36	0
153	CDL	7A	201	-	99,99,99	0.30	0	105,111,111	0.28	0
152	PC1	2F	302	-	41,41,53	0.33	0	47,49,61	0.43	0
153	CDL	qB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
158	3PE	T8	602	-	38,38,50	0.33	0	41,43,55	0.36	0
152	PC1	M2	405	-	53,53,53	0.29	0	59,61,61	0.28	0
153	CDL	6C	203	-	81,81,99	0.32	0	87,93,111	0.30	0
152	PC1	qb	602	-	42,42,53	0.31	0	48,50,61	0.32	0
153	CDL	t5	301	-	95,95,99	0.30	0	101,107,111	0.32	0
160	PX2	R	202	-	32,32,35	1.02	4 (12%)	35,37,40	0.94	2 (5%)
152	PC1	t1	602	-	32,32,53	0.36	0	38,40,61	0.35	0
153	CDL	AL	301	-	52,52,99	0.39	0	58,64,111	0.33	0
152	PC1	c3	605	-	38,38,53	0.33	0	44,46,61	0.33	0
157	FES	FS	202	35	0,4,4	-	-	-		
158	3PE	I	304	-	31,31,50	0.37	0	34,36,55	0.33	0
157	FES	sb	401	53	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
164	U10	b8	301	-	63,63,63	2.20	25 (39%)	78,79,79	1.70	23 (29%)
153	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
166	HEM	QC	502	110	50,50,50	1.30	7 (14%)	67,82,82	1.60	12 (17%)
153	CDL	n6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
152	PC1	W	201	-	48,48,53	0.30	0	54,56,61	0.30	0
152	PC1	N	303	-	35,35,53	0.34	0	41,43,61	0.35	0
152	PC1	N5	804	-	38,38,53	0.33	0	44,46,61	0.34	0
153	CDL	m	306	-	65,65,99	0.36	0	71,77,111	0.31	0
158	3PE	A3	202	-	43,43,50	0.32	0	46,48,55	0.30	0
169	T7X	B6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.10	4 (6%)
152	PC1	qG	401	-	31,31,53	0.37	0	37,39,61	0.42	0
153	CDL	Y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
158	3PE	vb	705	-	27,27,50	0.39	0	30,32,55	0.35	0
153	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
153	CDL	T5	301	-	95,95,99	0.30	0	101,107,111	0.32	0
153	CDL	qH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
151	HEC	qd	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.85	8 (13%)
152	PC1	qi	201	-	29,29,53	0.39	0	35,37,61	0.43	0
153	CDL	qC	503	-	63,63,99	0.36	0	69,75,111	0.31	0
152	PC1	C3	605	-	38,38,53	0.33	0	44,46,61	0.33	0
161	FAD	SA	701	-	58,58,58	0.32	0	85,89,89	0.27	0
152	PC1	QE	303	-	38,38,53	0.34	0	44,46,61	0.34	0
153	CDL	Q	202	-	71,71,99	0.34	0	77,83,111	0.30	0
153	CDL	TH	200	-	83,83,99	0.32	0	89,95,111	0.28	0
158	3PE	a3	202	-	43,43,50	0.32	0	46,48,55	0.30	0
158	3PE	a3	201	-	44,44,50	0.33	0	47,49,55	0.56	1 (2%)
153	CDL	sd	101	-	75,75,99	0.34	0	81,87,111	0.31	0
158	3PE	c4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
153	CDL	t	203	-	70,70,99	0.35	0	76,82,111	0.32	0
158	3PE	t8	602	-	38,38,50	0.33	0	41,43,55	0.36	0
153	CDL	i	302	-	74,74,99	0.34	0	80,86,111	0.29	0
152	PC1	N3	201	-	30,30,53	0.37	0	36,38,61	0.38	0
153	CDL	VB	705	-	81,81,99	0.32	0	87,93,111	0.29	0
153	CDL	B8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
153	CDL	t	204	-	89,89,99	0.33	0	95,101,111	0.33	0
153	CDL	qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
162	SF4	v1	500	146	0,12,12	-	-	-	-	-
157	FES	fs	202	35	0,4,4	-	-	-	-	-
152	PC1	QC	507	-	49,49,53	0.30	0	55,57,61	0.31	0
153	CDL	q	203	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	m	305	-	34,34,53	0.35	0	40,42,61	0.35	0
170	ADP	B9	202	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
152	PC1	W	205	-	42,42,53	0.32	0	48,50,61	0.31	0
152	PC1	FS	201	-	39,39,53	0.33	0	45,47,61	0.28	0
152	PC1	Qi	203	-	41,41,53	0.33	0	47,49,61	0.37	0
153	CDL	6a	201	-	73,73,99	0.35	0	79,85,111	0.41	0
152	PC1	qE	304	-	27,27,53	0.39	0	33,35,61	0.46	0
153	CDL	A9	403	-	86,86,99	0.32	0	92,98,111	0.27	0
153	CDL	b4	201	-	36,36,99	0.43	0	42,48,111	0.40	0
153	CDL	E	401	-	59,59,99	0.37	0	65,71,111	0.34	0
157	FES	fx	201	95	0,4,4	-	-	-	-	-
153	CDL	F	402	-	99,99,99	0.29	0	105,111,111	0.29	0
162	SF4	s8	302	127	0,12,12	-	-	-	-	-
153	CDL	p1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
169	T7X	b6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.10	4 (6%)
154	HEA	C1	703	29	67,67,67	2.29	26 (38%)	81,103,103	2.45	25 (30%)
152	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.33	0
153	CDL	VB	706	-	66,66,99	0.35	0	72,78,111	0.31	0
152	PC1	m1	403	-	41,41,53	0.33	0	47,49,61	0.39	0
152	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.34	0
158	3PE	M2	408	-	30,30,50	0.38	0	33,35,55	0.37	0
153	CDL	7a	201	-	99,99,99	0.30	0	105,111,111	0.28	0
153	CDL	I	303	-	74,74,99	0.34	0	80,86,111	0.29	0
158	3PE	w	203	-	33,33,50	0.36	0	36,38,55	0.32	0
158	3PE	N4	601	-	35,35,50	0.35	0	38,40,55	0.37	0
153	CDL	qb	601	-	67,67,99	0.35	0	73,79,111	0.30	0
158	3PE	N5	802	-	35,35,50	0.36	0	38,40,55	0.32	0
153	CDL	m2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
153	CDL	y5	201	-	69,69,99	0.35	0	75,81,111	0.31	0
153	CDL	VB	703	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	7A	202	-	44,44,53	0.31	0	50,52,61	0.33	0
153	CDL	e	401	-	59,59,99	0.37	0	65,71,111	0.34	0
170	ADP	b9	202	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
153	CDL	r	201	-	64,64,99	0.36	0	70,76,111	0.32	0
160	PX2	qh	201	-	35,35,35	1.00	4 (11%)	38,40,40	1.02	2 (5%)
153	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.35	0
153	CDL	QB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
152	PC1	c1	704	-	48,48,53	0.30	0	54,56,61	0.28	0
152	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.36	0
152	PC1	C1	706	-	48,48,53	0.30	0	54,56,61	0.28	0
153	CDL	C1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
164	U10	SC	102	-	63,63,63	2.22	24 (38%)	78,79,79	1.65	20 (25%)
152	PC1	2f	302	-	41,41,53	0.33	0	47,49,61	0.43	0
152	PC1	b9	201	-	33,33,53	0.37	0	39,41,61	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
164	U10	B8	301	-	63,63,63	2.20	25 (39%)	78,79,79	1.70	23 (29%)
152	PC1	N5	805	-	53,53,53	0.28	0	59,61,61	0.33	0
162	SF4	s1	801	120	0,12,12	-	-	-	-	-
152	PC1	p1	401	-	39,39,53	0.33	0	45,47,61	0.33	0
153	CDL	a	502	-	50,50,99	0.41	0	56,62,111	0.48	0
153	CDL	a9	403	-	86,86,99	0.32	0	92,98,111	0.27	0
153	CDL	c	301	-	63,63,99	0.37	0	69,75,111	0.44	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
153	CDL	i	301	-	76,76,99	0.33	0	82,88,111	0.31	0
152	PC1	m2	405	-	53,53,53	0.29	0	59,61,61	0.28	0
153	CDL	qG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
152	PC1	7C	303	-	42,42,53	0.32	0	48,50,61	0.34	0
153	CDL	U	201	-	59,59,99	0.38	0	65,71,111	0.33	0
152	PC1	qC	505	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	W	202	-	83,83,99	0.32	0	89,95,111	0.33	0
153	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.32	0
162	SF4	S8	302	127	0,12,12	-	-	-	-	-
153	CDL	c1	709	-	62,62,99	0.37	0	68,74,111	0.39	0
153	CDL	5b	201	-	80,80,99	0.33	0	86,92,111	0.33	0
153	CDL	2G	203	-	54,54,99	0.39	0	60,66,111	0.36	0
153	CDL	M	305	-	82,82,99	0.32	0	88,94,111	0.31	0
153	CDL	T	201	-	58,58,99	0.38	0	64,70,111	0.32	0
152	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.35	0
152	PC1	Qe	301	-	32,32,53	0.36	0	38,40,61	0.36	0
153	CDL	t7	201	-	72,72,99	0.34	0	78,84,111	0.29	0
152	PC1	N1	301	-	35,35,53	0.35	0	41,43,61	0.35	0
153	CDL	2M	101	-	95,95,99	0.30	0	101,107,111	0.31	0
158	3PE	i	303	-	31,31,50	0.37	0	34,36,55	0.33	0
157	FES	Qe	302	-	0,4,4	-	-	-	-	-
152	PC1	D	501	-	34,34,53	0.36	0	40,42,61	0.40	0
153	CDL	td	101	-	65,65,99	0.36	0	71,77,111	0.33	0
152	PC1	v	201	-	34,34,53	0.35	0	40,42,61	0.33	0
152	PC1	c3	606	-	48,48,53	0.31	0	54,56,61	0.37	0
166	HEM	Qc	502	110	50,50,50	1.29	7 (14%)	67,82,82	1.59	10 (14%)
153	CDL	m3	401	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	fs	204	-	39,39,53	0.33	0	45,47,61	0.28	0
153	CDL	C1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
152	PC1	C1	710	-	37,37,53	0.34	0	43,45,61	0.33	0
161	FAD	sa	701	-	58,58,58	0.32	0	85,89,89	0.27	0
153	CDL	qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
153	CDL	QD	402	-	60,60,99	0.37	0	66,72,111	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	T4	303	-	53,53,53	0.30	0	59,61,61	0.37	0
153	CDL	m	303	-	82,82,99	0.32	0	88,94,111	0.31	0
158	3PE	n4	601	-	35,35,50	0.35	0	38,40,55	0.36	0
162	SF4	s7	201	126	0,12,12	-	-	-		
152	PC1	AL	302	-	25,25,53	0.40	0	31,33,61	0.39	0
152	PC1	QB	602	-	43,43,53	0.31	0	49,51,61	0.30	0
158	3PE	T8	601	-	46,46,50	0.33	0	49,51,55	0.40	0
158	3PE	t8	601	-	46,46,50	0.33	0	49,51,55	0.40	0
153	CDL	C3	604	-	67,67,99	0.35	0	73,79,111	0.31	0
152	PC1	Qe	303	-	42,42,53	0.32	0	48,50,61	0.45	0
152	PC1	6c	203	-	32,32,53	0.36	0	38,40,61	0.37	0
152	PC1	F	401	-	37,37,53	0.34	0	43,45,61	0.30	0
153	CDL	vb	701	-	61,61,99	0.36	0	67,73,111	0.32	0
152	PC1	c1	711	-	38,38,53	0.33	0	44,46,61	0.35	0
163	F3S	SB	403	53	0,9,9	-	-	-		
152	PC1	N5	803	-	52,52,53	0.29	0	58,60,61	0.31	0
153	CDL	VB	701	-	61,61,99	0.36	0	67,73,111	0.32	0
153	CDL	QH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
153	CDL	c3	604	-	67,67,99	0.35	0	73,79,111	0.31	0
157	FES	fs	201	35	0,4,4	-	-	-		
162	SF4	S8	303	127	0,12,12	-	-	-		
158	3PE	ta	201	-	25,25,50	0.41	0	28,30,55	0.41	0
153	CDL	M	306	-	63,63,99	0.36	0	69,75,111	0.32	0
162	SF4	S1	801	120	0,12,12	-	-	-		
152	PC1	al	302	-	25,25,53	0.40	0	31,33,61	0.39	0
152	PC1	c4	403	-	40,40,53	0.32	0	46,48,61	0.31	0
158	3PE	BM	302	-	29,29,50	0.39	0	32,34,55	0.47	0
153	CDL	C1	708	-	62,62,99	0.37	0	68,74,111	0.39	0
166	HEM	qC	501	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	10 (14%)
153	CDL	th	200	-	83,83,99	0.32	0	89,95,111	0.28	0
158	3PE	Y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
153	CDL	m1	405	-	56,56,99	0.38	0	62,68,111	0.38	0
152	PC1	a	503	-	40,40,53	0.34	0	46,48,61	0.37	0
162	SF4	s1	802	120	0,12,12	-	-	-		
152	PC1	qg	401	-	31,31,53	0.36	0	37,39,61	0.35	0
153	CDL	Y5	201	-	69,69,99	0.35	0	75,81,111	0.31	0
158	3PE	m3	402	-	37,37,50	0.34	0	40,42,55	0.31	0
153	CDL	7c	302	-	50,50,99	0.40	0	56,62,111	0.35	0
152	PC1	f	402	-	37,37,53	0.34	0	43,45,61	0.30	0
153	CDL	bm	301	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	c2	703	-	35,35,53	0.35	0	41,43,61	0.32	0
153	CDL	2o	101	-	49,49,99	0.41	0	55,61,111	0.35	0
152	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	m1	401	-	53,53,53	0.29	0	59,61,61	0.30	0
152	PC1	N	302	-	31,31,53	0.36	0	37,39,61	0.33	0
153	CDL	qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
164	U10	QC	506	-	29,29,63	2.74	12 (41%)	36,38,79	1.62	8 (22%)
158	3PE	sc	101	-	39,39,50	0.33	0	42,44,55	0.31	0
152	PC1	v	202	-	48,48,53	0.31	0	54,56,61	0.34	0
153	CDL	A1	102	-	66,66,99	0.36	0	72,78,111	0.37	0
153	CDL	FS	204	-	46,46,99	0.42	0	52,58,111	0.35	0
152	PC1	an	304	-	35,35,53	0.35	0	41,43,61	0.34	0
158	3PE	VB	707	-	27,27,50	0.39	0	30,32,55	0.35	0
153	CDL	q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
153	CDL	a	504	-	93,93,99	0.30	0	99,105,111	0.27	0
153	CDL	AM	201	-	55,55,99	0.39	0	61,67,111	0.33	0
153	CDL	a9	402	-	75,75,99	0.34	0	81,87,111	0.35	0
152	PC1	C3	606	-	48,48,53	0.31	0	54,56,61	0.37	0
152	PC1	QJ	101	-	27,27,53	0.39	0	33,35,61	0.45	0
152	PC1	Qi	201	-	29,29,53	0.39	0	35,37,61	0.43	0
158	3PE	C4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
153	CDL	2G	204	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	qI	202	-	42,42,53	0.31	0	48,50,61	0.32	0
153	CDL	u	201	-	59,59,99	0.38	0	65,71,111	0.33	0
152	PC1	C3	602	-	38,38,53	0.33	0	44,46,61	0.32	0
153	CDL	M3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
152	PC1	qE	303	-	38,38,53	0.33	0	44,46,61	0.34	0
153	CDL	Qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
153	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.32	0
153	CDL	Qb	601	-	67,67,99	0.35	0	73,79,111	0.30	0
152	PC1	7a	202	-	44,44,53	0.31	0	50,52,61	0.33	0
153	CDL	QG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
162	SF4	sb	402	53	0,12,12	-	-	-	-	-
153	CDL	am	201	-	55,55,99	0.39	0	61,67,111	0.33	0
167	NDP	a9	401	-	51,52,52	0.32	0	71,80,80	0.36	0
171	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.36	0
153	CDL	m3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
152	PC1	qB	602	-	43,43,53	0.32	0	49,51,61	0.30	0
152	PC1	2J	201	-	41,41,53	0.33	0	47,49,61	0.38	0
163	F3S	sb	403	53	0,9,9	-	-	-	-	-
166	HEM	qC	502	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	12 (17%)
153	CDL	2m	101	-	95,95,99	0.30	0	101,107,111	0.31	0
152	PC1	t4	303	-	53,53,53	0.30	0	59,61,61	0.37	0
152	PC1	C2	701	-	35,35,53	0.35	0	41,43,61	0.32	0
152	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	Qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
153	CDL	a	505	-	81,81,99	0.32	0	87,93,111	0.29	0
162	SF4	S7	201	126	0,12,12	-	-	-		
153	CDL	Z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	T7	201	-	72,72,99	0.34	0	78,84,111	0.29	0
153	CDL	b8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
153	CDL	B4	201	-	36,36,99	0.43	0	42,48,111	0.40	0
153	CDL	f	401	-	99,99,99	0.29	0	105,111,111	0.29	0
153	CDL	B3	102	-	81,81,99	0.33	0	87,93,111	0.29	0
153	CDL	c1	703	-	64,64,99	0.36	0	70,76,111	0.31	0
152	PC1	qC	507	-	49,49,53	0.30	0	55,57,61	0.31	0
158	3PE	B4	202	-	47,47,50	0.31	0	50,52,55	0.29	0
152	PC1	m2	402	-	31,31,53	0.36	0	37,39,61	0.41	0
166	HEM	qc	503	110	50,50,50	1.30	7 (14%)	67,82,82	1.62	12 (17%)
153	CDL	m1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
158	3PE	m2	408	-	30,30,50	0.38	0	33,35,55	0.37	0
164	U10	qC	506	-	29,29,63	2.74	12 (41%)	36,38,79	1.62	8 (22%)
152	PC1	N5	801	-	51,51,53	0.30	0	57,59,61	0.30	0
153	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.33	0
152	PC1	qe	301	-	32,32,53	0.36	0	38,40,61	0.36	0
153	CDL	A	504	-	93,93,99	0.30	0	99,105,111	0.27	0
152	PC1	w	204	-	33,33,53	0.36	0	39,41,61	0.36	0
152	PC1	a	501	-	40,40,53	0.33	0	46,48,61	0.36	0
152	PC1	s8	301	-	29,29,53	0.38	0	35,37,61	0.36	0
153	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
162	SF4	V1	500	146	0,12,12	-	-	-		
152	PC1	te	102	-	31,31,53	0.37	0	37,39,61	0.42	0
152	PC1	M2	402	-	31,31,53	0.36	0	37,39,61	0.41	0
153	CDL	I	302	-	76,76,99	0.33	0	82,88,111	0.31	0
157	FES	QE	302	-	0,4,4	-	-	-		
153	CDL	y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
160	PX2	Qh	201	-	35,35,35	1.00	4 (11%)	38,40,40	1.05	2 (5%)
154	HEA	c1	708	29	67,67,67	2.32	26 (38%)	81,103,103	2.64	34 (41%)
153	CDL	q	202	-	71,71,99	0.34	0	77,83,111	0.30	0
168	ZMP	AB	201	80	34,36,36	0.69	1 (2%)	41,45,45	0.76	0
152	PC1	2f	301	-	46,46,53	0.32	0	52,54,61	0.52	0
152	PC1	M2	407	-	45,45,53	0.31	0	51,53,61	0.39	0
152	PC1	S8	301	-	29,29,53	0.38	0	35,37,61	0.36	0
158	3PE	an	306	-	28,28,50	0.40	0	31,33,55	0.43	0
158	3PE	W	203	-	33,33,50	0.36	0	36,38,55	0.32	0
152	PC1	2g	202	-	49,49,53	0.31	0	55,57,61	0.41	0
153	CDL	vb	704	-	66,66,99	0.35	0	72,78,111	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	al	301	-	52,52,99	0.39	0	58,64,111	0.33	0
152	PC1	c1	706	-	44,44,53	0.32	0	50,52,61	0.44	0
152	PC1	QI	202	-	42,42,53	0.31	0	48,50,61	0.32	0
158	3PE	TA	201	-	25,25,50	0.41	0	28,30,55	0.41	0
158	3PE	bm	302	-	29,29,50	0.39	0	32,34,55	0.47	0
152	PC1	C4	403	-	40,40,53	0.33	0	46,48,61	0.32	0
152	PC1	Qb	602	-	42,42,53	0.31	0	48,50,61	0.32	0
157	FES	FX	201	95	0,4,4	-	-	-	-	-
166	HEM	y5	203	-	50,50,50	1.28	6 (12%)	67,82,82	1.61	10 (14%)
153	CDL	n5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
166	HEM	QC	501	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	10 (14%)
152	PC1	A	503	-	40,40,53	0.34	0	46,48,61	0.37	0
152	PC1	qi	203	-	41,41,53	0.33	0	47,49,61	0.37	0
153	CDL	c4	401	-	97,97,99	0.30	0	103,109,111	0.31	0
153	CDL	t1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
153	CDL	AN	302	-	86,86,99	0.32	0	92,98,111	0.29	0
152	PC1	Qc	509	-	46,46,53	0.30	0	52,54,61	0.36	0
153	CDL	Qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
152	PC1	J1	400	-	39,39,53	0.33	0	45,47,61	0.34	0
153	CDL	E	403	-	62,62,99	0.37	0	68,74,111	0.31	0
159	P5S	m2	406	-	34,35,53	1.38	4 (11%)	36,42,60	1.02	2 (5%)
153	CDL	m	304	-	63,63,99	0.36	0	69,75,111	0.32	0
153	CDL	T1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
166	HEM	qc	502	110	50,50,50	1.29	7 (14%)	67,82,82	1.59	10 (14%)
164	U10	Qc	507	-	29,29,63	2.75	13 (44%)	36,38,79	1.57	8 (22%)
152	PC1	TC	101	-	41,41,53	0.32	0	47,49,61	0.30	0
153	CDL	7a	203	-	61,61,99	0.37	0	67,73,111	0.34	0
152	PC1	C3	601	-	51,51,53	0.30	0	57,59,61	0.36	0
152	PC1	n5	801	-	51,51,53	0.30	0	57,59,61	0.31	0
164	U10	Qc	501	-	25,25,63	2.29	7 (28%)	24,29,79	1.92	8 (33%)
152	PC1	qE	301	-	23,23,53	0.40	0	29,31,61	0.39	0
153	CDL	6A	201	-	73,73,99	0.35	0	79,85,111	0.41	0
157	FES	qE	302	-	0,4,4	-	-	-	-	-
158	3PE	an	305	-	32,32,50	0.37	0	35,37,55	0.35	0
153	CDL	5B	201	-	80,80,99	0.33	0	86,92,111	0.33	0
153	CDL	2K	101	-	97,97,99	0.30	0	103,109,111	0.35	0
157	FES	V2	300	147	0,4,4	-	-	-	-	-
153	CDL	m	302	-	63,63,99	0.36	0	69,75,111	0.32	0
158	3PE	n5	802	-	35,35,50	0.36	0	38,40,55	0.32	0
152	PC1	t4	301	-	47,47,53	0.31	0	53,55,61	0.38	0
159	P5S	M2	406	-	34,35,53	1.38	4 (11%)	36,42,60	1.02	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	m2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
157	FES	s1	803	120	0,4,4	-	-	-		
153	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.35	0
153	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
158	3PE	AN	303	-	44,44,50	0.32	0	47,49,55	0.29	0
152	PC1	6A	202	-	34,34,53	0.36	0	40,42,61	0.36	0
158	3PE	AN	305	-	32,32,50	0.37	0	35,37,55	0.35	0
152	PC1	AM	202	-	38,38,53	0.33	0	44,46,61	0.33	0
158	3PE	SC	101	-	39,39,50	0.33	0	42,44,55	0.31	0
153	CDL	T	203	-	70,70,99	0.35	0	76,82,111	0.32	0
152	PC1	T1	602	-	32,32,53	0.36	0	38,40,61	0.35	0
162	SF4	S1	802	120	0,12,12	-	-	-		
167	NDP	A9	401	-	51,52,52	0.32	0	71,80,80	0.36	0
162	SF4	SB	402	53	0,12,12	-	-	-		
152	PC1	qI	201	-	29,29,53	0.38	0	35,37,61	0.34	0
152	PC1	2f	303	-	31,31,53	0.37	0	37,39,61	0.33	0
152	PC1	tc	101	-	41,41,53	0.32	0	47,49,61	0.30	0
152	PC1	am	202	-	38,38,53	0.33	0	44,46,61	0.33	0
152	PC1	V	202	-	48,48,53	0.31	0	54,56,61	0.34	0
153	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.35	0
153	CDL	t	201	-	58,58,99	0.38	0	64,70,111	0.32	0
153	CDL	c1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
158	3PE	t4	302	-	24,24,50	0.42	0	27,29,55	0.36	0
152	PC1	m	307	-	35,35,53	0.35	0	41,43,61	0.34	0
158	3PE	M3	402	-	37,37,50	0.34	0	40,42,55	0.31	0
152	PC1	N	301	-	40,40,53	0.33	0	46,48,61	0.30	0
157	FES	qe	302	-	0,4,4	-	-	-		
153	CDL	M1	404	-	90,90,99	0.31	0	96,102,111	0.28	0
152	PC1	m	301	-	44,44,53	0.31	0	50,52,61	0.39	0
152	PC1	n5	804	-	38,38,53	0.33	0	44,46,61	0.34	0
152	PC1	C1	709	-	44,44,53	0.32	0	50,52,61	0.44	0
152	PC1	2G	202	-	49,49,53	0.31	0	55,57,61	0.41	0
153	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
153	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.29	0
153	CDL	w	202	-	83,83,99	0.32	0	89,95,111	0.33	0
152	PC1	5B	202	-	46,46,53	0.31	0	52,54,61	0.29	0
153	CDL	SD	101	-	75,75,99	0.34	0	81,87,111	0.31	0
152	PC1	2F	301	-	46,46,53	0.32	0	52,54,61	0.52	0
153	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.29	0
152	PC1	QC	508	-	35,35,53	0.35	0	41,43,61	0.35	0
152	PC1	c1	707	-	37,37,53	0.34	0	43,45,61	0.33	0
152	PC1	2F	303	-	31,31,53	0.37	0	37,39,61	0.33	0
152	PC1	Qc	506	-	37,37,53	0.34	0	43,45,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
152	PC1	AN	304	-	35,35,53	0.35	0	41,43,61	0.34	0
153	CDL	Qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
152	PC1	QJ	102	-	37,37,53	0.34	0	43,45,61	0.38	0
152	PC1	N6	301	-	53,53,53	0.28	0	59,61,61	0.31	0
158	3PE	AN	306	-	28,28,50	0.40	0	31,33,55	0.43	0
152	PC1	w	201	-	48,48,53	0.30	0	54,56,61	0.30	0
152	PC1	M1	403	-	41,41,53	0.33	0	47,49,61	0.39	0
152	PC1	Qj	101	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	P1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	b3	102	-	81,81,99	0.33	0	87,93,111	0.30	0
158	3PE	an	303	-	44,44,50	0.32	0	47,49,55	0.29	0
152	PC1	6C	201	-	32,32,53	0.36	0	38,40,61	0.37	0
154	HEA	c1	702	29	67,67,67	2.32	25 (37%)	81,103,103	2.58	32 (39%)
152	PC1	n6	301	-	53,53,53	0.28	0	59,61,61	0.31	0
152	PC1	QE	301	-	23,23,53	0.40	0	29,31,61	0.39	0
153	CDL	an	302	-	86,86,99	0.32	0	92,98,111	0.29	0
153	CDL	M3	401	-	62,62,99	0.36	0	68,74,111	0.32	0
153	CDL	2B	201	-	86,86,99	0.31	0	92,98,111	0.36	0
166	HEM	Y5	203	-	50,50,50	1.28	6 (12%)	67,82,82	1.61	10 (14%)
152	PC1	n	301	-	40,40,53	0.33	0	46,48,61	0.30	0
152	PC1	d	501	-	34,34,53	0.36	0	40,42,61	0.40	0
153	CDL	2k	101	-	97,97,99	0.30	0	103,109,111	0.35	0
153	CDL	qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
153	CDL	6C	202	-	74,74,99	0.34	0	80,86,111	0.33	0
152	PC1	tc	102	-	46,46,53	0.31	0	52,54,61	0.32	0
153	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
153	CDL	7A	203	-	61,61,99	0.37	0	67,73,111	0.34	0
153	CDL	A1	101	-	65,65,99	0.36	0	71,77,111	0.33	0
152	PC1	qC	508	-	35,35,53	0.35	0	41,43,61	0.35	0
164	U10	qc	507	-	29,29,63	2.75	13 (44%)	36,38,79	1.57	8 (22%)
153	CDL	qD	402	-	60,60,99	0.37	0	66,72,111	0.31	0
153	CDL	qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
152	PC1	QI	201	-	29,29,53	0.38	0	35,37,61	0.34	0
152	PC1	A	501	-	40,40,53	0.33	0	46,48,61	0.37	0
152	PC1	n	303	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.33	0
152	PC1	m2	407	-	45,45,53	0.31	0	51,53,61	0.39	0
152	PC1	QC	505	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	C4	401	-	97,97,99	0.30	0	103,109,111	0.31	0
153	CDL	A	502	-	50,50,99	0.41	0	56,62,111	0.48	0
158	3PE	T4	302	-	24,24,50	0.42	0	27,29,55	0.37	0
157	FES	S1	803	120	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	6c	202	-	81,81,99	0.32	0	87,93,111	0.30	0
153	CDL	te	101	-	52,52,99	0.39	0	58,64,111	0.33	0
162	SF4	s8	303	127	0,12,12	-	-	-		
158	3PE	b4	202	-	47,47,50	0.31	0	50,52,55	0.29	0
152	PC1	M	307	-	34,34,53	0.35	0	40,42,61	0.35	0
153	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
152	PC1	TC	102	-	46,46,53	0.31	0	52,54,61	0.32	0
166	HEM	Qc	503	110	50,50,50	1.30	7 (14%)	67,82,82	1.62	12 (17%)
152	PC1	V	201	-	34,34,53	0.35	0	40,42,61	0.33	0
153	CDL	2g	204	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	Qg	401	-	31,31,53	0.36	0	37,39,61	0.35	0
152	PC1	qJ	101	-	37,37,53	0.34	0	43,45,61	0.38	0
152	PC1	n1	301	-	35,35,53	0.35	0	41,43,61	0.35	0
153	CDL	z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	2g	203	-	54,54,99	0.39	0	60,66,111	0.36	0
164	U10	sc	102	-	63,63,63	2.22	24 (38%)	78,79,79	1.64	20 (25%)
171	FMN	v1	501	-	33,33,33	0.20	0	48,50,50	0.36	0
153	CDL	n	304	-	83,83,99	0.32	0	89,95,111	0.32	0
153	CDL	QC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
152	PC1	W	204	-	33,33,53	0.36	0	39,41,61	0.36	0
153	CDL	BM	301	-	85,85,99	0.32	0	91,97,111	0.31	0
153	CDL	a1	101	-	66,66,99	0.36	0	72,78,111	0.37	0
153	CDL	qC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
152	PC1	i	304	-	38,38,53	0.34	0	44,46,61	0.34	0
153	CDL	6c	201	-	74,74,99	0.34	0	80,86,111	0.33	0
151	HEC	qD	401	111	46,50,50	1.92	9 (19%)	58,82,82	1.85	8 (13%)
157	FES	v2	300	147	0,4,4	-	-	-		
152	PC1	n5	803	-	52,52,53	0.29	0	58,60,61	0.31	0
152	PC1	5b	202	-	46,46,53	0.31	0	52,54,61	0.29	0
152	PC1	n3	201	-	30,30,53	0.37	0	36,38,61	0.38	0
152	PC1	2j	201	-	41,41,53	0.33	0	47,49,61	0.38	0
153	CDL	P1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
153	CDL	M2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
152	PC1	qe	303	-	42,42,53	0.32	0	48,50,61	0.45	0
152	PC1	w	205	-	42,42,53	0.32	0	48,50,61	0.31	0
153	CDL	M	304	-	63,63,99	0.36	0	69,75,111	0.32	0
153	CDL	A9	402	-	75,75,99	0.34	0	81,87,111	0.35	0
153	CDL	M	301	-	65,65,99	0.36	0	71,77,111	0.31	0
153	CDL	2G	201	-	88,88,99	0.31	0	94,100,111	0.28	0
154	HEA	C1	702	29	67,67,67	2.28	26 (38%)	81,103,103	2.48	29 (35%)
158	3PE	s8	304	-	40,40,50	0.33	0	43,45,55	0.32	0
153	CDL	e	403	-	62,62,99	0.37	0	68,74,111	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
153	CDL	M1	405	-	56,56,99	0.38	0	62,68,111	0.38	0
152	PC1	QG	401	-	31,31,53	0.37	0	37,39,61	0.42	0
153	CDL	T	204	-	89,89,99	0.33	0	95,101,111	0.33	0
153	CDL	Q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
153	CDL	m1	404	-	90,90,99	0.31	0	96,102,111	0.28	0
160	PX2	Y5	204	-	20,20,35	1.30	4 (20%)	23,25,40	1.30	2 (8%)
152	PC1	j1	400	-	39,39,53	0.33	0	45,47,61	0.34	0
153	CDL	N	304	-	83,83,99	0.32	0	89,95,111	0.32	0
153	CDL	QC	503	-	63,63,99	0.36	0	69,75,111	0.31	0
151	HEC	QD	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.84	8 (13%)
151	HEC	2e	401	2	46,50,50	1.92	9 (19%)	58,82,82	1.93	8 (13%)
152	PC1	M	302	-	35,35,53	0.35	0	41,43,61	0.34	0
153	CDL	QI	203	-	70,70,99	0.35	0	76,82,111	0.31	0
153	CDL	B3	101	-	57,57,99	0.37	0	63,69,111	0.32	0
153	CDL	2g	201	-	88,88,99	0.31	0	94,100,111	0.28	0
152	PC1	C1	711	-	38,38,53	0.33	0	44,46,61	0.35	0
152	PC1	n	302	-	31,31,53	0.36	0	37,39,61	0.33	0
151	HEC	2E	401	2	46,50,50	1.92	7 (15%)	58,82,82	1.85	8 (13%)
158	3PE	an	301	-	44,44,50	0.32	0	47,49,55	0.28	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
153	CDL	p1	402	-	-	19/73/73/110	-
153	CDL	E	402	-	-	20/82/82/110	-
151	HEC	Qd	401	111	-	8/14/54/54	-
152	PC1	qc	506	-	-	16/41/41/57	-
153	CDL	C	301	-	-	12/74/74/110	-
158	3PE	AN	301	-	-	4/48/48/54	-
152	PC1	P1	401	-	-	9/43/43/57	-
153	CDL	qI	203	-	-	17/81/81/110	-
158	3PE	A3	201	-	-	12/48/48/54	-
153	CDL	N5	806	-	-	20/100/100/110	-
153	CDL	N6	302	-	-	18/100/100/110	-
153	CDL	R	201	-	-	24/75/75/110	-
168	ZMP	ab	201	80	-	22/43/43/43	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	qc	509	-	-	11/50/50/57	-
153	CDL	TE	101	-	-	19/63/63/110	-
153	CDL	2O	101	-	-	18/60/60/110	-
152	PC1	j	302	-	-	4/40/40/57	-
157	FES	FS	203	35	-	-	0/1/1/1
160	PX2	y5	204	-	-	13/22/22/37	-
152	PC1	I	301	-	-	11/42/42/57	-
153	CDL	Qg	402	-	-	23/110/110/110	-
152	PC1	M1	401	-	-	14/57/57/57	-
160	PX2	r	202	-	-	23/34/34/37	-
152	PC1	qj	101	-	-	11/39/39/57	-
153	CDL	b3	101	-	-	13/68/68/110	-
153	CDL	u1	101	-	-	13/67/67/110	-
164	U10	qc	501	-	-	10/28/28/87	-
158	3PE	G2	301	-	-	13/54/54/54	-
158	3PE	S8	304	-	-	8/44/44/54	-
153	CDL	2b	201	-	-	16/97/97/110	-
158	3PE	g2	301	-	-	13/54/54/54	-
153	CDL	U1	101	-	-	13/67/67/110	-
158	3PE	y5	202	-	-	8/31/31/54	-
153	CDL	c1	712	-	-	16/105/105/110	-
152	PC1	B9	201	-	-	13/37/37/57	-
152	PC1	n5	805	-	-	15/57/57/57	-
152	PC1	M	303	-	-	15/48/48/57	-
152	PC1	TE	102	-	-	9/35/35/57	-
152	PC1	T4	301	-	-	18/51/51/57	-
157	FES	SB	401	53	-	-	0/1/1/1
152	PC1	6a	202	-	-	13/38/38/57	-
153	CDL	7A	201	-	-	14/110/110/110	-
152	PC1	2F	302	-	-	8/45/45/57	-
153	CDL	qB	601	-	-	10/78/78/110	-
158	3PE	T8	602	-	-	10/42/42/54	-
152	PC1	M2	405	-	-	8/57/57/57	-
153	CDL	6C	203	-	-	16/92/92/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	qb	602	-	-	6/46/46/57	-
153	CDL	t5	301	-	-	24/106/106/110	-
160	PX2	R	202	-	-	19/34/34/37	-
152	PC1	t1	602	-	-	12/36/36/57	-
153	CDL	AL	301	-	-	16/63/63/110	-
152	PC1	c3	605	-	-	3/42/42/57	-
157	FES	FS	202	35	-	-	0/1/1/1
158	3PE	I	304	-	-	8/35/35/54	-
157	FES	sb	401	53	-	-	0/1/1/1
164	U10	b8	301	-	-	13/63/87/87	0/1/1/1
153	CDL	M2	403	-	-	18/76/76/110	-
166	HEM	QC	502	110	-	8/14/54/54	-
153	CDL	n6	302	-	-	19/100/100/110	-
152	PC1	W	201	-	-	13/52/52/57	-
152	PC1	N	303	-	-	5/39/39/57	-
152	PC1	N5	804	-	-	11/42/42/57	-
153	CDL	m	306	-	-	15/76/76/110	-
158	3PE	A3	202	-	-	12/47/47/54	-
169	T7X	B6	201	-	-	24/50/74/80	0/1/1/1
152	PC1	qG	401	-	-	6/35/35/57	-
153	CDL	Y7	501	-	-	13/75/75/110	-
158	3PE	vb	705	-	-	10/31/31/54	-
153	CDL	m2	403	-	-	18/76/76/110	-
153	CDL	T5	301	-	-	24/106/106/110	-
153	CDL	qH	201	-	-	13/104/104/110	-
151	HEC	qd	401	111	-	8/14/54/54	-
152	PC1	qi	201	-	-	8/33/33/57	-
153	CDL	qC	503	-	-	7/74/74/110	-
152	PC1	C3	605	-	-	3/42/42/57	-
161	FAD	SA	701	-	-	10/34/50/50	0/6/6/6
152	PC1	QE	303	-	-	2/42/42/57	-
153	CDL	Q	202	-	-	19/82/82/110	-
153	CDL	TH	200	-	-	17/94/94/110	-
158	3PE	a3	202	-	-	12/47/47/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	a3	201	-	-	12/48/48/54	-
153	CDL	sd	101	-	-	16/86/86/110	-
158	3PE	c4	402	-	-	7/54/54/54	-
153	CDL	t	203	-	-	22/81/81/110	-
158	3PE	t8	602	-	-	10/42/42/54	-
153	CDL	i	302	-	-	13/85/85/110	-
152	PC1	N3	201	-	-	3/34/34/57	-
153	CDL	VB	705	-	-	17/92/92/110	-
153	CDL	B8	302	-	-	10/79/79/110	-
153	CDL	t	204	-	-	30/100/100/110	-
153	CDL	qc	504	-	-	21/74/74/110	-
162	SF4	v1	500	146	-	-	0/6/5/5
157	FES	fs	202	35	-	-	0/1/1/1
152	PC1	QC	507	-	-	12/53/53/57	-
153	CDL	q	203	-	-	15/96/96/110	-
152	PC1	m	305	-	-	10/38/38/57	-
170	ADP	B9	202	-	-	4/16/32/32	0/3/3/3
152	PC1	W	205	-	-	6/46/46/57	-
152	PC1	FS	201	-	-	5/43/43/57	-
152	PC1	Qi	203	-	-	14/45/45/57	-
153	CDL	6a	201	-	-	21/84/84/110	-
152	PC1	qE	304	-	-	10/31/31/57	-
153	CDL	A9	403	-	-	19/97/97/110	-
153	CDL	b4	201	-	-	9/44/44/110	-
153	CDL	E	401	-	-	15/70/70/110	-
157	FES	fx	201	95	-	-	0/1/1/1
153	CDL	F	402	-	-	17/110/110/110	-
162	SF4	s8	302	127	-	-	0/6/5/5
153	CDL	p1	403	-	-	14/68/68/110	-
169	T7X	b6	201	-	-	23/50/74/80	0/1/1/1
154	HEA	C1	703	29	-	15/36/76/76	-
152	PC1	J	302	-	-	4/40/40/57	-
153	CDL	VB	706	-	-	16/77/77/110	-
152	PC1	m1	403	-	-	7/45/45/57	-
152	PC1	7c	303	-	-	7/46/46/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	M2	408	-	-	9/34/34/54	-
153	CDL	7a	201	-	-	15/110/110/110	-
153	CDL	I	303	-	-	13/85/85/110	-
158	3PE	w	203	-	-	14/37/37/54	-
158	3PE	N4	601	-	-	7/39/39/54	-
153	CDL	qb	601	-	-	9/78/78/110	-
158	3PE	N5	802	-	-	8/39/39/54	-
153	CDL	m2	404	-	-	10/84/84/110	-
153	CDL	y5	201	-	-	12/80/80/110	-
153	CDL	VB	703	-	-	14/96/96/110	-
152	PC1	7A	202	-	-	12/48/48/57	-
153	CDL	e	401	-	-	15/70/70/110	-
170	ADP	b9	202	-	-	4/16/32/32	0/3/3/3
153	CDL	r	201	-	-	24/75/75/110	-
160	PX2	qh	201	-	-	17/37/37/37	-
153	CDL	T	202	-	-	12/85/85/110	-
153	CDL	QB	601	-	-	10/78/78/110	-
152	PC1	c1	704	-	-	14/52/52/57	-
152	PC1	c3	601	-	-	10/55/55/57	-
152	PC1	C1	706	-	-	14/52/52/57	-
153	CDL	C1	712	-	-	16/105/105/110	-
164	U10	SC	102	-	-	12/63/87/87	0/1/1/1
152	PC1	2f	302	-	-	8/45/45/57	-
152	PC1	b9	201	-	-	13/37/37/57	-
164	U10	B8	301	-	-	13/63/87/87	0/1/1/1
152	PC1	N5	805	-	-	16/57/57/57	-
162	SF4	s1	801	120	-	-	0/6/5/5
152	PC1	p1	401	-	-	9/43/43/57	-
153	CDL	a	502	-	-	13/61/61/110	-
153	CDL	a9	403	-	-	19/97/97/110	-
153	CDL	c	301	-	-	11/74/74/110	-
153	CDL	fs	203	-	-	10/57/57/110	-
153	CDL	7C	302	-	-	10/61/61/110	-
153	CDL	i	301	-	-	16/87/87/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	m2	405	-	-	8/57/57/57	-
153	CDL	qG	402	-	-	16/96/96/110	-
152	PC1	7C	303	-	-	7/46/46/57	-
153	CDL	U	201	-	-	11/70/70/110	-
152	PC1	qC	505	-	-	12/41/41/57	-
153	CDL	W	202	-	-	16/94/94/110	-
153	CDL	b	501	-	-	15/72/72/110	-
162	SF4	S8	302	127	-	-	0/6/5/5
153	CDL	c1	709	-	-	23/73/73/110	-
153	CDL	5b	201	-	-	16/91/91/110	-
153	CDL	2G	203	-	-	10/65/65/110	-
153	CDL	M	305	-	-	9/93/93/110	-
153	CDL	T	201	-	-	11/69/69/110	-
152	PC1	C3	603	-	-	6/34/34/57	-
152	PC1	Qe	301	-	-	5/36/36/57	-
153	CDL	t7	201	-	-	15/83/83/110	-
152	PC1	N1	301	-	-	9/39/39/57	-
153	CDL	2M	101	-	-	18/106/106/110	-
158	3PE	i	303	-	-	8/35/35/54	-
157	FES	Qe	302	-	-	-	0/1/1/1
152	PC1	D	501	-	-	15/38/38/57	-
153	CDL	td	101	-	-	17/76/76/110	-
152	PC1	v	201	-	-	4/38/38/57	-
152	PC1	c3	606	-	-	7/52/52/57	-
166	HEM	Qc	502	110	-	4/14/54/54	-
153	CDL	m3	401	-	-	7/73/73/110	-
152	PC1	fs	204	-	-	5/43/43/57	-
153	CDL	C1	701	-	-	22/89/89/110	-
152	PC1	C1	710	-	-	6/41/41/57	-
161	FAD	sa	701	-	-	10/34/50/50	0/6/6/6
153	CDL	qc	508	-	-	9/57/57/110	-
153	CDL	QD	402	-	-	16/71/71/110	-
152	PC1	T4	303	-	-	12/57/57/57	-
153	CDL	m	303	-	-	9/93/93/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	n4	601	-	-	8/39/39/54	-
162	SF4	s7	201	126	-	-	0/6/5/5
152	PC1	AL	302	-	-	2/29/29/57	-
152	PC1	QB	602	-	-	6/47/47/57	-
158	3PE	T8	601	-	-	12/50/50/54	-
158	3PE	t8	601	-	-	12/50/50/54	-
153	CDL	C3	604	-	-	5/78/78/110	-
152	PC1	Qe	303	-	-	13/46/46/57	-
152	PC1	6c	203	-	-	8/36/36/57	-
152	PC1	F	401	-	-	8/41/41/57	-
153	CDL	vb	701	-	-	14/72/72/110	-
152	PC1	c1	711	-	-	10/42/42/57	-
163	F3S	SB	403	53	-	-	0/3/3/3
152	PC1	N5	803	-	-	8/56/56/57	-
153	CDL	VB	701	-	-	13/72/72/110	-
153	CDL	QH	201	-	-	13/104/104/110	-
153	CDL	c3	604	-	-	6/78/78/110	-
157	FES	fs	201	35	-	-	0/1/1/1
162	SF4	S8	303	127	-	-	0/6/5/5
158	3PE	ta	201	-	-	10/29/29/54	-
153	CDL	M	306	-	-	11/74/74/110	-
162	SF4	S1	801	120	-	-	0/6/5/5
152	PC1	al	302	-	-	2/29/29/57	-
152	PC1	c4	403	-	-	5/44/44/57	-
158	3PE	BM	302	-	-	8/33/33/54	-
153	CDL	C1	708	-	-	24/73/73/110	-
166	HEM	qC	501	110	-	7/14/54/54	-
153	CDL	th	200	-	-	17/94/94/110	-
158	3PE	Y5	202	-	-	8/31/31/54	-
153	CDL	m1	405	-	-	14/67/67/110	-
152	PC1	a	503	-	-	8/44/44/57	-
162	SF4	s1	802	120	-	-	0/6/5/5
152	PC1	qg	401	-	-	6/35/35/57	-
153	CDL	Y5	201	-	-	14/80/80/110	-
158	3PE	m3	402	-	-	7/41/41/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	7c	302	-	-	10/61/61/110	-
152	PC1	f	402	-	-	8/41/41/57	-
153	CDL	bm	301	-	-	22/96/96/110	-
152	PC1	c2	703	-	-	10/39/39/57	-
153	CDL	2o	101	-	-	17/60/60/110	-
152	PC1	c3	602	-	-	13/42/42/57	-
152	PC1	m1	401	-	-	14/57/57/57	-
152	PC1	N	302	-	-	8/35/35/57	-
153	CDL	qg	402	-	-	23/110/110/110	-
164	U10	QC	506	-	-	4/23/47/87	0/1/1/1
158	3PE	sc	101	-	-	10/43/43/54	-
152	PC1	v	202	-	-	13/52/52/57	-
153	CDL	A1	102	-	-	14/77/77/110	-
153	CDL	FS	204	-	-	9/57/57/110	-
152	PC1	an	304	-	-	9/39/39/57	-
158	3PE	VB	707	-	-	10/31/31/54	-
153	CDL	q	201	-	-	11/73/73/110	-
153	CDL	a	504	-	-	15/104/104/110	-
153	CDL	AM	201	-	-	11/66/66/110	-
153	CDL	a9	402	-	-	14/86/86/110	-
152	PC1	C3	606	-	-	7/52/52/57	-
152	PC1	QJ	101	-	-	10/31/31/57	-
152	PC1	Qi	201	-	-	8/33/33/57	-
158	3PE	C4	402	-	-	7/54/54/54	-
153	CDL	2G	204	-	-	15/73/73/110	-
152	PC1	qI	202	-	-	6/46/46/57	-
153	CDL	u	201	-	-	11/70/70/110	-
152	PC1	C3	602	-	-	13/42/42/57	-
153	CDL	M3	403	-	-	12/65/65/110	-
152	PC1	qE	303	-	-	2/42/42/57	-
153	CDL	Qi	202	-	-	14/81/81/110	-
153	CDL	B	501	-	-	15/72/72/110	-
153	CDL	Qb	601	-	-	9/78/78/110	-
152	PC1	7a	202	-	-	12/48/48/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	QG	402	-	-	16/96/96/110	-
167	NDP	a9	401	-	-	7/34/77/77	0/5/5/5
153	CDL	am	201	-	-	11/66/66/110	-
171	FMN	V1	501	-	-	2/18/18/18	0/3/3/3
162	SF4	sb	402	53	-	-	0/6/5/5
153	CDL	m3	403	-	-	12/65/65/110	-
152	PC1	qB	602	-	-	6/47/47/57	-
152	PC1	2J	201	-	-	14/45/45/57	-
163	F3S	sb	403	53	-	-	0/3/3/3
166	HEM	qC	502	110	-	8/14/54/54	-
153	CDL	2m	101	-	-	18/106/106/110	-
152	PC1	t4	303	-	-	12/57/57/57	-
152	PC1	C2	701	-	-	10/39/39/57	-
152	PC1	c3	603	-	-	7/34/34/57	-
153	CDL	Qc	508	-	-	9/57/57/110	-
153	CDL	a	505	-	-	17/92/92/110	-
162	SF4	S7	201	126	-	-	0/6/5/5
153	CDL	Z	101	-	-	12/77/77/110	-
153	CDL	T7	201	-	-	15/83/83/110	-
153	CDL	b8	302	-	-	10/79/79/110	-
153	CDL	B4	201	-	-	9/44/44/110	-
153	CDL	f	401	-	-	16/110/110/110	-
153	CDL	B3	102	-	-	18/92/92/110	-
153	CDL	c1	703	-	-	8/75/75/110	-
152	PC1	qC	507	-	-	12/53/53/57	-
158	3PE	B4	202	-	-	10/51/51/54	-
152	PC1	m2	402	-	-	12/35/35/57	-
166	HEM	qc	503	110	-	9/14/54/54	-
153	CDL	m1	402	-	-	13/76/76/110	-
158	3PE	m2	408	-	-	9/34/34/54	-
164	U10	qC	506	-	-	4/23/47/87	0/1/1/1
152	PC1	N5	801	-	-	11/55/55/57	-
153	CDL	7c	301	-	-	23/95/95/110	-
152	PC1	qe	301	-	-	5/36/36/57	-
153	CDL	A	504	-	-	15/104/104/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	w	204	-	-	6/37/37/57	-
152	PC1	a	501	-	-	10/44/44/57	-
152	PC1	s8	301	-	-	9/33/33/57	-
153	CDL	M2	404	-	-	10/84/84/110	-
162	SF4	V1	500	146	-	-	0/6/5/5
152	PC1	te	102	-	-	10/35/35/57	-
152	PC1	M2	402	-	-	12/35/35/57	-
153	CDL	I	302	-	-	16/87/87/110	-
157	FES	QE	302	-	-	-	0/1/1/1
153	CDL	y7	501	-	-	12/75/75/110	-
160	PX2	Qh	201	-	-	20/37/37/37	-
154	HEA	c1	708	29	-	16/36/76/76	-
153	CDL	q	202	-	-	19/82/82/110	-
168	ZMP	AB	201	80	-	22/43/43/43	-
152	PC1	2f	301	-	-	21/50/50/57	-
152	PC1	M2	407	-	-	9/49/49/57	-
152	PC1	S8	301	-	-	9/33/33/57	-
158	3PE	an	306	-	-	5/32/32/54	-
158	3PE	W	203	-	-	12/37/37/54	-
152	PC1	2g	202	-	-	13/53/53/57	-
153	CDL	vb	704	-	-	16/77/77/110	-
153	CDL	al	301	-	-	15/63/63/110	-
152	PC1	c1	706	-	-	8/48/48/57	-
152	PC1	QI	202	-	-	6/46/46/57	-
158	3PE	TA	201	-	-	11/29/29/54	-
158	3PE	bm	302	-	-	8/33/33/54	-
152	PC1	C4	403	-	-	5/44/44/57	-
152	PC1	Qb	602	-	-	6/46/46/57	-
157	FES	FX	201	95	-	-	0/1/1/1
166	HEM	y5	203	-	-	8/14/54/54	-
153	CDL	n5	806	-	-	20/100/100/110	-
166	HEM	QC	501	110	-	7/14/54/54	-
152	PC1	A	503	-	-	8/44/44/57	-
152	PC1	qi	203	-	-	14/45/45/57	-
153	CDL	c4	401	-	-	22/108/108/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	t1	601	-	-	10/65/65/110	-
153	CDL	AN	302	-	-	15/97/97/110	-
152	PC1	Qc	509	-	-	11/50/50/57	-
153	CDL	Qc	505	-	-	16/66/66/110	-
152	PC1	J1	400	-	-	9/43/43/57	-
153	CDL	E	403	-	-	12/73/73/110	-
159	P5S	m2	406	-	-	30/41/41/59	-
153	CDL	m	304	-	-	11/74/74/110	-
153	CDL	T1	601	-	-	10/65/65/110	-
166	HEM	qc	502	110	-	4/14/54/54	-
164	U10	Qc	507	-	-	7/23/47/87	0/1/1/1
152	PC1	TC	101	-	-	7/45/45/57	-
153	CDL	7a	203	-	-	11/72/72/110	-
152	PC1	C3	601	-	-	10/55/55/57	-
152	PC1	n5	801	-	-	11/55/55/57	-
164	U10	Qc	501	-	-	10/28/28/87	-
152	PC1	qE	301	-	-	7/26/26/57	-
153	CDL	6A	201	-	-	20/84/84/110	-
157	FES	qE	302	-	-	-	0/1/1/1
158	3PE	an	305	-	-	4/36/36/54	-
153	CDL	5B	201	-	-	15/91/91/110	-
153	CDL	2K	101	-	-	32/108/108/110	-
157	FES	V2	300	147	-	-	0/1/1/1
153	CDL	m	302	-	-	11/74/74/110	-
158	3PE	n5	802	-	-	8/39/39/54	-
152	PC1	t4	301	-	-	18/51/51/57	-
159	P5S	M2	406	-	-	29/41/41/59	-
153	CDL	m2	401	-	-	15/64/64/110	-
157	FES	s1	803	120	-	-	0/1/1/1
153	CDL	e	402	-	-	20/82/82/110	-
153	CDL	L	301	-	-	22/84/84/110	-
158	3PE	AN	303	-	-	8/48/48/54	-
152	PC1	6A	202	-	-	13/38/38/57	-
158	3PE	AN	305	-	-	4/36/36/54	-
152	PC1	AM	202	-	-	8/42/42/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	SC	101	-	-	10/43/43/54	-
153	CDL	T	203	-	-	22/81/81/110	-
152	PC1	T1	602	-	-	12/36/36/57	-
162	SF4	S1	802	120	-	-	0/6/5/5
167	NDP	A9	401	-	-	7/34/77/77	0/5/5/5
162	SF4	SB	402	53	-	-	0/6/5/5
152	PC1	qI	201	-	-	5/33/33/57	-
152	PC1	2f	303	-	-	9/35/35/57	-
152	PC1	tc	101	-	-	7/45/45/57	-
152	PC1	am	202	-	-	8/42/42/57	-
152	PC1	V	202	-	-	13/52/52/57	-
153	CDL	t	202	-	-	12/85/85/110	-
153	CDL	t	201	-	-	12/69/69/110	-
153	CDL	c1	701	-	-	22/89/89/110	-
158	3PE	t4	302	-	-	4/28/28/54	-
152	PC1	m	307	-	-	11/39/39/57	-
158	3PE	M3	402	-	-	7/41/41/54	-
152	PC1	N	301	-	-	5/44/44/57	-
157	FES	qe	302	-	-	-	0/1/1/1
153	CDL	M1	404	-	-	17/101/101/110	-
152	PC1	m	301	-	-	15/48/48/57	-
152	PC1	n5	804	-	-	11/42/42/57	-
152	PC1	C1	709	-	-	8/48/48/57	-
152	PC1	2G	202	-	-	13/53/53/57	-
153	CDL	C1	707	-	-	8/75/75/110	-
153	CDL	j	301	-	-	15/80/80/110	-
153	CDL	w	202	-	-	16/94/94/110	-
152	PC1	5B	202	-	-	10/50/50/57	-
153	CDL	SD	101	-	-	16/86/86/110	-
152	PC1	2F	301	-	-	21/50/50/57	-
153	CDL	J	301	-	-	15/80/80/110	-
152	PC1	QC	508	-	-	9/39/39/57	-
152	PC1	c1	707	-	-	6/41/41/57	-
152	PC1	2F	303	-	-	9/35/35/57	-
152	PC1	Qc	506	-	-	16/41/41/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	AN	304	-	-	9/39/39/57	-
153	CDL	Qc	504	-	-	21/74/74/110	-
152	PC1	QJ	102	-	-	12/41/41/57	-
152	PC1	N6	301	-	-	12/57/57/57	-
158	3PE	AN	306	-	-	5/32/32/54	-
152	PC1	w	201	-	-	13/52/52/57	-
152	PC1	M1	403	-	-	7/45/45/57	-
152	PC1	Qj	101	-	-	11/39/39/57	-
153	CDL	P1	402	-	-	19/73/73/110	-
153	CDL	b3	102	-	-	20/92/92/110	-
158	3PE	an	303	-	-	7/48/48/54	-
152	PC1	6C	201	-	-	8/36/36/57	-
154	HEA	c1	702	29	-	12/36/76/76	-
152	PC1	n6	301	-	-	12/57/57/57	-
152	PC1	QE	301	-	-	7/26/26/57	-
153	CDL	an	302	-	-	15/97/97/110	-
153	CDL	M3	401	-	-	7/73/73/110	-
153	CDL	2B	201	-	-	16/97/97/110	-
166	HEM	Y5	203	-	-	8/14/54/54	-
152	PC1	n	301	-	-	5/44/44/57	-
152	PC1	d	501	-	-	15/38/38/57	-
153	CDL	2k	101	-	-	32/108/108/110	-
153	CDL	qc	505	-	-	16/66/66/110	-
153	CDL	6C	202	-	-	27/85/85/110	-
152	PC1	tc	102	-	-	14/50/50/57	-
153	CDL	l	301	-	-	22/84/84/110	-
153	CDL	7A	203	-	-	11/72/72/110	-
153	CDL	A1	101	-	-	17/76/76/110	-
152	PC1	qC	508	-	-	9/39/39/57	-
164	U10	qc	507	-	-	7/23/47/87	0/1/1/1
153	CDL	qD	402	-	-	16/71/71/110	-
153	CDL	qi	202	-	-	14/81/81/110	-
152	PC1	QI	201	-	-	4/33/33/57	-
152	PC1	A	501	-	-	10/44/44/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	n	303	-	-	6/39/39/57	-
153	CDL	7C	301	-	-	23/95/95/110	-
152	PC1	m2	407	-	-	9/49/49/57	-
152	PC1	QC	505	-	-	12/41/41/57	-
153	CDL	C4	401	-	-	22/108/108/110	-
153	CDL	A	502	-	-	13/61/61/110	-
158	3PE	T4	302	-	-	4/28/28/54	-
157	FES	S1	803	120	-	-	0/1/1/1
153	CDL	6c	202	-	-	16/92/92/110	-
153	CDL	te	101	-	-	20/63/63/110	-
162	SF4	s8	303	127	-	-	0/6/5/5
158	3PE	b4	202	-	-	11/51/51/54	-
152	PC1	M	307	-	-	10/38/38/57	-
153	CDL	M1	402	-	-	13/76/76/110	-
152	PC1	TC	102	-	-	14/50/50/57	-
166	HEM	Qc	503	110	-	9/14/54/54	-
152	PC1	V	201	-	-	4/38/38/57	-
153	CDL	2g	204	-	-	16/73/73/110	-
152	PC1	Qg	401	-	-	7/35/35/57	-
152	PC1	qJ	101	-	-	12/41/41/57	-
152	PC1	n1	301	-	-	9/39/39/57	-
153	CDL	z	101	-	-	12/77/77/110	-
153	CDL	2g	203	-	-	10/65/65/110	-
164	U10	sc	102	-	-	12/63/87/87	0/1/1/1
171	FMN	v1	501	-	-	2/18/18/18	0/3/3/3
153	CDL	n	304	-	-	33/94/94/110	-
153	CDL	QC	504	-	-	11/66/66/110	-
152	PC1	W	204	-	-	6/37/37/57	-
153	CDL	BM	301	-	-	22/96/96/110	-
153	CDL	a1	101	-	-	13/77/77/110	-
153	CDL	qC	504	-	-	11/66/66/110	-
152	PC1	i	304	-	-	11/42/42/57	-
153	CDL	6c	201	-	-	27/85/85/110	-
151	HEC	qD	401	111	-	6/14/54/54	-
157	FES	v2	300	147	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	n5	803	-	-	8/56/56/57	-
152	PC1	5b	202	-	-	10/50/50/57	-
152	PC1	n3	201	-	-	3/34/34/57	-
152	PC1	2j	201	-	-	14/45/45/57	-
153	CDL	P1	403	-	-	14/68/68/110	-
153	CDL	M2	401	-	-	15/64/64/110	-
152	PC1	qe	303	-	-	13/46/46/57	-
152	PC1	w	205	-	-	6/46/46/57	-
153	CDL	M	304	-	-	11/74/74/110	-
153	CDL	A9	402	-	-	15/86/86/110	-
153	CDL	M	301	-	-	15/76/76/110	-
153	CDL	2G	201	-	-	19/99/99/110	-
154	HEA	C1	702	29	-	12/36/76/76	-
158	3PE	s8	304	-	-	8/44/44/54	-
153	CDL	e	403	-	-	12/73/73/110	-
153	CDL	M1	405	-	-	15/67/67/110	-
152	PC1	QG	401	-	-	6/35/35/57	-
153	CDL	T	204	-	-	30/100/100/110	-
153	CDL	Q	201	-	-	11/73/73/110	-
153	CDL	m1	404	-	-	17/101/101/110	-
160	PX2	Y5	204	-	-	13/22/22/37	-
152	PC1	j1	400	-	-	9/43/43/57	-
153	CDL	N	304	-	-	33/94/94/110	-
153	CDL	QC	503	-	-	7/74/74/110	-
151	HEC	QD	401	111	-	6/14/54/54	-
151	HEC	2e	401	2	-	9/14/54/54	-
152	PC1	M	302	-	-	11/39/39/57	-
153	CDL	QI	203	-	-	17/81/81/110	-
153	CDL	B3	101	-	-	13/68/68/110	-
153	CDL	2g	201	-	-	19/99/99/110	-
152	PC1	C1	711	-	-	10/42/42/57	-
152	PC1	n	302	-	-	8/35/35/57	-
151	HEC	2E	401	2	-	9/14/54/54	-
158	3PE	an	301	-	-	3/48/48/54	-

The worst 5 of 440 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	sc	102	U10	C6-C1	10.50	1.54	1.35
164	SC	102	U10	C6-C1	10.49	1.54	1.35
164	qc	507	U10	C6-C1	10.36	1.53	1.35
164	Qc	507	U10	C6-C1	10.36	1.53	1.35
164	qC	506	U10	C6-C1	10.30	1.53	1.35

The worst 5 of 452 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
151	2e	401	HEC	CBB-CAB-C3B	-9.14	109.17	127.43
151	2E	401	HEC	CBB-CAB-C3B	-8.91	109.62	127.43
151	qd	401	HEC	CBB-CAB-C3B	-8.86	109.72	127.43
151	Qd	401	HEC	CBB-CAB-C3B	-8.84	109.76	127.43
151	qD	401	HEC	CBB-CAB-C3B	-8.73	109.98	127.43

There are no chirality outliers.

5 of 5653 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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-O12

There are no ring outliers.

445 monomers are involved in 1712 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	p1	402	CDL	4	0
153	E	402	CDL	5	0
152	qc	506	PC1	2	0
153	C	301	CDL	3	0
158	AN	301	3PE	3	0
152	P1	401	PC1	1	0
153	qI	203	CDL	4	0
158	A3	201	3PE	6	0
153	N5	806	CDL	7	0
153	N6	302	CDL	7	0
153	R	201	CDL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
168	ab	201	ZMP	12	0
152	qc	509	PC1	4	0
153	TE	101	CDL	5	0
153	2O	101	CDL	1	0
152	j	302	PC1	1	0
160	y5	204	PX2	1	0
152	I	301	PC1	7	0
153	Qg	402	CDL	9	0
152	M1	401	PC1	6	0
160	r	202	PX2	2	0
152	qj	101	PC1	2	0
153	u1	101	CDL	2	0
164	qc	501	U10	4	0
158	G2	301	3PE	2	0
153	2b	201	CDL	10	0
158	g2	301	3PE	1	0
153	U1	101	CDL	2	0
158	y5	202	3PE	1	0
153	c1	712	CDL	15	0
152	B9	201	PC1	3	0
152	n5	805	PC1	5	0
152	M	303	PC1	2	0
152	TE	102	PC1	1	0
152	T4	301	PC1	2	0
152	6a	202	PC1	1	0
153	7A	201	CDL	11	0
152	2F	302	PC1	3	0
153	qB	601	CDL	6	0
158	T8	602	3PE	5	0
152	M2	405	PC1	3	0
153	6C	203	CDL	9	0
152	qb	602	PC1	2	0
153	t5	301	CDL	12	0
160	R	202	PX2	2	0
153	AL	301	CDL	3	0
152	c3	605	PC1	5	0
158	I	304	3PE	1	0
164	b8	301	U10	6	0
153	M2	403	CDL	3	0
166	QC	502	HEM	7	0
153	n6	302	CDL	7	0
152	W	201	PC1	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	N	303	PC1	4	0
152	N5	804	PC1	4	0
153	m	306	CDL	2	0
158	A3	202	3PE	4	0
153	Y7	501	CDL	2	0
153	m2	403	CDL	3	0
153	T5	301	CDL	13	0
153	qH	201	CDL	8	0
152	qi	201	PC1	3	0
153	qC	503	CDL	3	0
152	C3	605	PC1	5	0
161	SA	701	FAD	5	0
152	QE	303	PC1	5	0
153	Q	202	CDL	6	0
153	TH	200	CDL	5	0
158	a3	202	3PE	4	0
158	a3	201	3PE	6	0
153	sd	101	CDL	5	0
158	c4	402	3PE	3	0
153	t	203	CDL	6	0
158	t8	602	3PE	5	0
153	i	302	CDL	6	0
152	N3	201	PC1	1	0
153	VB	705	CDL	5	0
153	B8	302	CDL	5	0
153	t	204	CDL	14	0
153	qc	504	CDL	2	0
162	v1	500	SF4	1	0
152	QC	507	PC1	2	0
153	q	203	CDL	11	0
152	m	305	PC1	2	0
152	FS	201	PC1	5	0
152	Qi	203	PC1	2	0
153	6a	201	CDL	3	0
152	qE	304	PC1	2	0
153	A9	403	CDL	4	0
153	b4	201	CDL	2	0
153	E	401	CDL	3	0
153	F	402	CDL	10	0
162	s8	302	SF4	3	0
153	p1	403	CDL	4	0
154	C1	703	HEA	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	J	302	PC1	1	0
153	VB	706	CDL	9	0
152	m1	403	PC1	4	0
152	7c	303	PC1	5	0
158	M2	408	3PE	2	0
153	7a	201	CDL	11	0
153	I	303	CDL	5	0
158	w	203	3PE	4	0
153	qb	601	CDL	3	0
158	N5	802	3PE	5	0
153	m2	404	CDL	5	0
153	y5	201	CDL	1	0
153	VB	703	CDL	12	0
152	7A	202	PC1	3	0
153	e	401	CDL	3	0
170	b9	202	ADP	1	0
153	r	201	CDL	4	0
160	qh	201	PX2	4	0
153	T	202	CDL	9	0
153	QB	601	CDL	6	0
152	c1	704	PC1	3	0
152	c3	601	PC1	4	0
152	C1	706	PC1	3	0
153	C1	712	CDL	16	0
164	SC	102	U10	6	0
152	2f	302	PC1	3	0
152	b9	201	PC1	3	0
164	B8	301	U10	8	0
152	N5	805	PC1	5	0
162	s1	801	SF4	2	0
152	p1	401	PC1	1	0
153	a	502	CDL	2	0
153	a9	403	CDL	4	0
153	c	301	CDL	4	0
153	fs	203	CDL	5	0
153	7C	302	CDL	2	0
153	i	301	CDL	8	0
152	m2	405	PC1	4	0
153	qG	402	CDL	1	0
152	7C	303	PC1	5	0
153	U	201	CDL	4	0
152	qC	505	PC1	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	W	202	CDL	7	0
153	b	501	CDL	1	0
162	S8	302	SF4	2	0
153	c1	709	CDL	7	0
153	5b	201	CDL	7	0
153	2G	203	CDL	1	0
153	M	305	CDL	8	0
153	T	201	CDL	2	0
152	C3	603	PC1	1	0
153	t7	201	CDL	7	0
152	N1	301	PC1	2	0
153	2M	101	CDL	8	0
158	i	303	3PE	1	0
152	D	501	PC1	4	0
153	td	101	CDL	2	0
152	v	201	PC1	1	0
152	c3	606	PC1	1	0
166	Qc	502	HEM	3	0
153	m3	401	CDL	2	0
152	fs	204	PC1	5	0
153	C1	701	CDL	8	0
152	C1	710	PC1	2	0
161	sa	701	FAD	5	0
153	QD	402	CDL	1	0
152	T4	303	PC1	3	0
153	m	303	CDL	8	0
158	n4	601	3PE	1	0
162	s7	201	SF4	2	0
152	AL	302	PC1	1	0
152	QB	602	PC1	4	0
158	T8	601	3PE	5	0
158	t8	601	3PE	5	0
153	C3	604	CDL	4	0
152	Qe	303	PC1	3	0
152	F	401	PC1	2	0
153	vb	701	CDL	3	0
152	c1	711	PC1	8	0
163	SB	403	F3S	1	0
152	N5	803	PC1	8	0
153	VB	701	CDL	3	0
153	QH	201	CDL	8	0
153	c3	604	CDL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
157	fs	201	FES	1	0
158	ta	201	3PE	1	0
153	M	306	CDL	5	0
162	S1	801	SF4	2	0
152	al	302	PC1	1	0
152	c4	403	PC1	5	0
158	BM	302	3PE	1	0
153	C1	708	CDL	7	0
166	qC	501	HEM	2	0
153	th	200	CDL	5	0
158	Y5	202	3PE	1	0
153	m1	405	CDL	3	0
152	a	503	PC1	2	0
162	s1	802	SF4	1	0
152	qg	401	PC1	3	0
153	Y5	201	CDL	1	0
158	m3	402	3PE	2	0
153	7c	302	CDL	2	0
152	f	402	PC1	2	0
153	bm	301	CDL	12	0
152	c2	703	PC1	1	0
153	2o	101	CDL	1	0
152	c3	602	PC1	2	0
152	m1	401	PC1	6	0
153	qg	402	CDL	8	0
164	QC	506	U10	2	0
158	sc	101	3PE	2	0
152	v	202	PC1	3	0
153	A1	102	CDL	9	0
153	FS	204	CDL	6	0
152	an	304	PC1	3	0
153	q	201	CDL	5	0
153	a	504	CDL	9	0
153	AM	201	CDL	6	0
153	a9	402	CDL	6	0
152	C3	606	PC1	1	0
152	QJ	101	PC1	2	0
152	Qi	201	PC1	3	0
158	C4	402	3PE	3	0
153	2G	204	CDL	7	0
152	qI	202	PC1	7	0
153	u	201	CDL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	C3	602	PC1	2	0
153	M3	403	CDL	3	0
152	qE	303	PC1	5	0
153	Qi	202	CDL	5	0
153	B	501	CDL	1	0
153	Qb	601	CDL	3	0
152	7a	202	PC1	3	0
153	QG	402	CDL	1	0
153	am	201	CDL	6	0
167	a9	401	NDP	1	0
171	V1	501	FMN	2	0
153	m3	403	CDL	3	0
152	qB	602	PC1	5	0
163	sb	403	F3S	1	0
166	qC	502	HEM	8	0
153	2m	101	CDL	6	0
152	t4	303	PC1	2	0
152	C2	701	PC1	1	0
152	c3	603	PC1	1	0
153	a	505	CDL	5	0
162	S7	201	SF4	2	0
153	Z	101	CDL	1	0
153	T7	201	CDL	8	0
153	b8	302	CDL	5	0
153	B4	201	CDL	2	0
153	f	401	CDL	11	0
153	B3	102	CDL	6	0
153	c1	703	CDL	3	0
152	qC	507	PC1	2	0
158	B4	202	3PE	6	0
152	m2	402	PC1	2	0
166	qc	503	HEM	10	0
153	m1	402	CDL	6	0
158	m2	408	3PE	2	0
164	qC	506	U10	1	0
152	N5	801	PC1	4	0
153	7c	301	CDL	6	0
153	A	504	CDL	9	0
152	w	204	PC1	5	0
152	a	501	PC1	4	0
152	s8	301	PC1	2	0
153	M2	404	CDL	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
162	V1	500	SF4	1	0
152	te	102	PC1	1	0
152	M2	402	PC1	2	0
153	I	302	CDL	6	0
153	y7	501	CDL	2	0
160	Qh	201	PX2	4	0
154	c1	708	HEA	11	0
153	q	202	CDL	6	0
168	AB	201	ZMP	12	0
152	2f	301	PC1	4	0
152	M2	407	PC1	1	0
152	S8	301	PC1	2	0
158	an	306	3PE	2	0
158	W	203	3PE	4	0
152	2g	202	PC1	3	0
153	vb	704	CDL	8	0
153	al	301	CDL	3	0
152	c1	706	PC1	4	0
152	QI	202	PC1	9	0
158	TA	201	3PE	1	0
158	bm	302	3PE	1	0
152	C4	403	PC1	4	0
152	Qb	602	PC1	4	0
153	n5	806	CDL	10	0
166	QC	501	HEM	2	0
152	A	503	PC1	2	0
152	qi	203	PC1	2	0
153	c4	401	CDL	5	0
153	t1	601	CDL	4	0
153	AN	302	CDL	6	0
152	Qc	509	PC1	3	0
153	Qc	505	CDL	2	0
152	J1	400	PC1	3	0
153	E	403	CDL	9	0
159	m2	406	P5S	1	0
153	m	304	CDL	5	0
153	T1	601	CDL	4	0
166	qc	502	HEM	3	0
164	Qc	507	U10	3	0
152	TC	101	PC1	4	0
153	7a	203	CDL	5	0
152	C3	601	PC1	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	n5	801	PC1	4	0
164	Qc	501	U10	3	0
152	qE	301	PC1	1	0
153	6A	201	CDL	2	0
158	an	305	3PE	1	0
153	5B	201	CDL	8	0
153	2K	101	CDL	8	0
153	m	302	CDL	4	0
158	n5	802	3PE	4	0
152	t4	301	PC1	2	0
159	M2	406	P5S	1	0
153	m2	401	CDL	3	0
153	e	402	CDL	5	0
153	L	301	CDL	2	0
158	AN	303	3PE	1	0
152	6A	202	PC1	1	0
158	AN	305	3PE	1	0
152	AM	202	PC1	4	0
158	SC	101	3PE	2	0
153	T	203	CDL	6	0
162	S1	802	SF4	1	0
167	A9	401	NDP	1	0
152	qI	201	PC1	3	0
152	2f	303	PC1	3	0
152	tc	101	PC1	5	0
152	am	202	PC1	4	0
152	V	202	PC1	2	0
153	t	202	CDL	9	0
153	t	201	CDL	2	0
153	c1	701	CDL	7	0
152	m	307	PC1	2	0
158	M3	402	3PE	2	0
152	N	301	PC1	7	0
153	M1	404	CDL	7	0
152	m	301	PC1	2	0
152	n5	804	PC1	4	0
152	C1	709	PC1	4	0
152	2G	202	PC1	3	0
153	C1	707	CDL	3	0
153	j	301	CDL	3	0
153	w	202	CDL	7	0
152	5B	202	PC1	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	SD	101	CDL	5	0
152	2F	301	PC1	4	0
153	J	301	CDL	2	0
152	c1	707	PC1	2	0
152	2F	303	PC1	3	0
152	Qc	506	PC1	3	0
152	AN	304	PC1	3	0
153	Qc	504	CDL	1	0
152	QJ	102	PC1	4	0
152	N6	301	PC1	7	0
158	AN	306	3PE	2	0
152	w	201	PC1	6	0
152	M1	403	PC1	4	0
152	Qj	101	PC1	2	0
153	P1	402	CDL	3	0
153	b3	102	CDL	5	0
158	an	303	3PE	1	0
154	c1	702	HEA	11	0
152	n6	301	PC1	6	0
152	QE	301	PC1	1	0
153	an	302	CDL	5	0
153	M3	401	CDL	2	0
153	2B	201	CDL	11	0
152	n	301	PC1	7	0
152	d	501	PC1	5	0
153	2k	101	CDL	9	0
153	qc	505	CDL	2	0
153	6C	202	CDL	7	0
152	tc	102	PC1	4	0
153	l	301	CDL	2	0
153	7A	203	CDL	4	0
153	A1	101	CDL	2	0
164	qc	507	U10	1	0
153	qD	402	CDL	1	0
153	qi	202	CDL	5	0
152	QI	201	PC1	2	0
152	A	501	PC1	4	0
152	n	303	PC1	4	0
153	7C	301	CDL	6	0
152	m2	407	PC1	1	0
152	QC	505	PC1	4	0
153	C4	401	CDL	4	0

Continued on next page...

Continued from previous page...

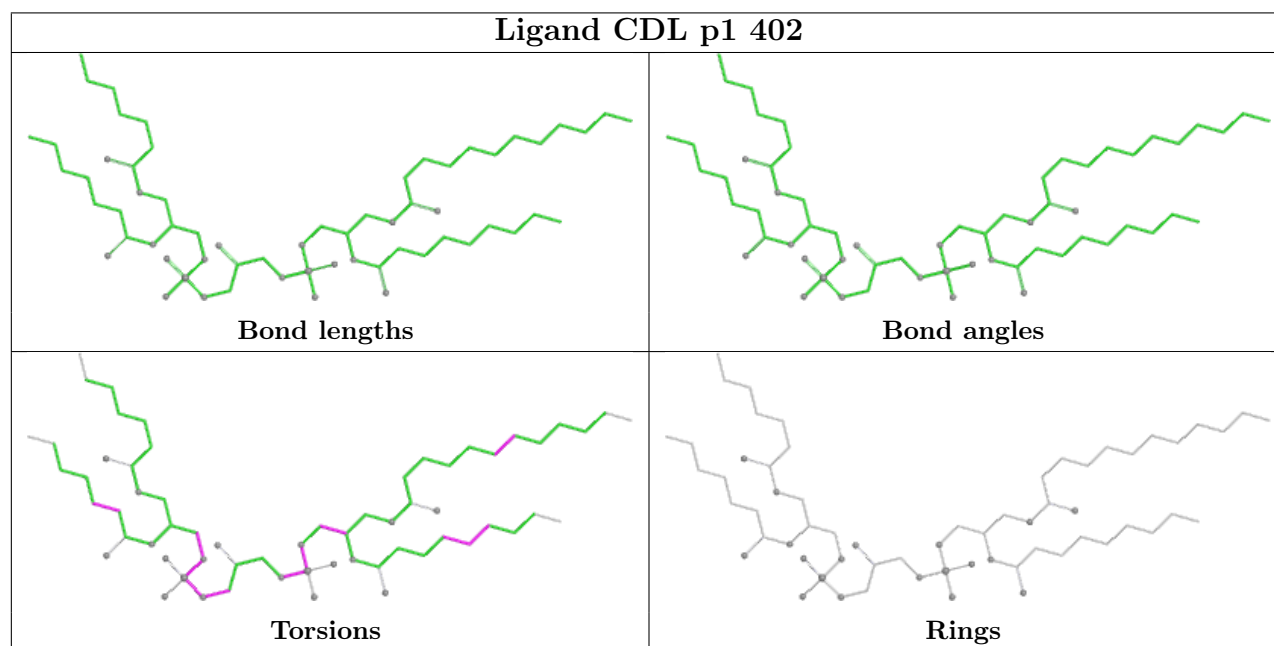
Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	A	502	CDL	2	0
158	T4	302	3PE	1	0
153	6c	202	CDL	8	0
153	te	101	CDL	5	0
158	b4	202	3PE	5	0
152	M	307	PC1	2	0
153	M1	402	CDL	6	0
152	TC	102	PC1	2	0
166	Qc	503	HEM	9	0
152	V	201	PC1	1	0
153	2g	204	CDL	4	0
152	Qg	401	PC1	3	0
152	qJ	101	PC1	4	0
152	n1	301	PC1	2	0
153	z	101	CDL	1	0
153	2g	203	CDL	2	0
164	sc	102	U10	7	0
171	v1	501	FMN	1	0
153	n	304	CDL	7	0
153	QC	504	CDL	6	0
152	W	204	PC1	5	0
153	BM	301	CDL	12	0
153	a1	101	CDL	9	0
153	qC	504	CDL	6	0
152	i	304	PC1	7	0
153	6c	201	CDL	7	0
151	qD	401	HEC	1	0
152	n5	803	PC1	8	0
152	5b	202	PC1	3	0
152	n3	201	PC1	2	0
153	P1	403	CDL	4	0
153	M2	401	CDL	3	0
152	qe	303	PC1	4	0
153	M	304	CDL	4	0
153	A9	402	CDL	6	0
153	M	301	CDL	2	0
153	2G	201	CDL	5	0
154	C1	702	HEA	8	0
153	e	403	CDL	9	0
153	M1	405	CDL	3	0
153	T	204	CDL	13	0
153	Q	201	CDL	6	0

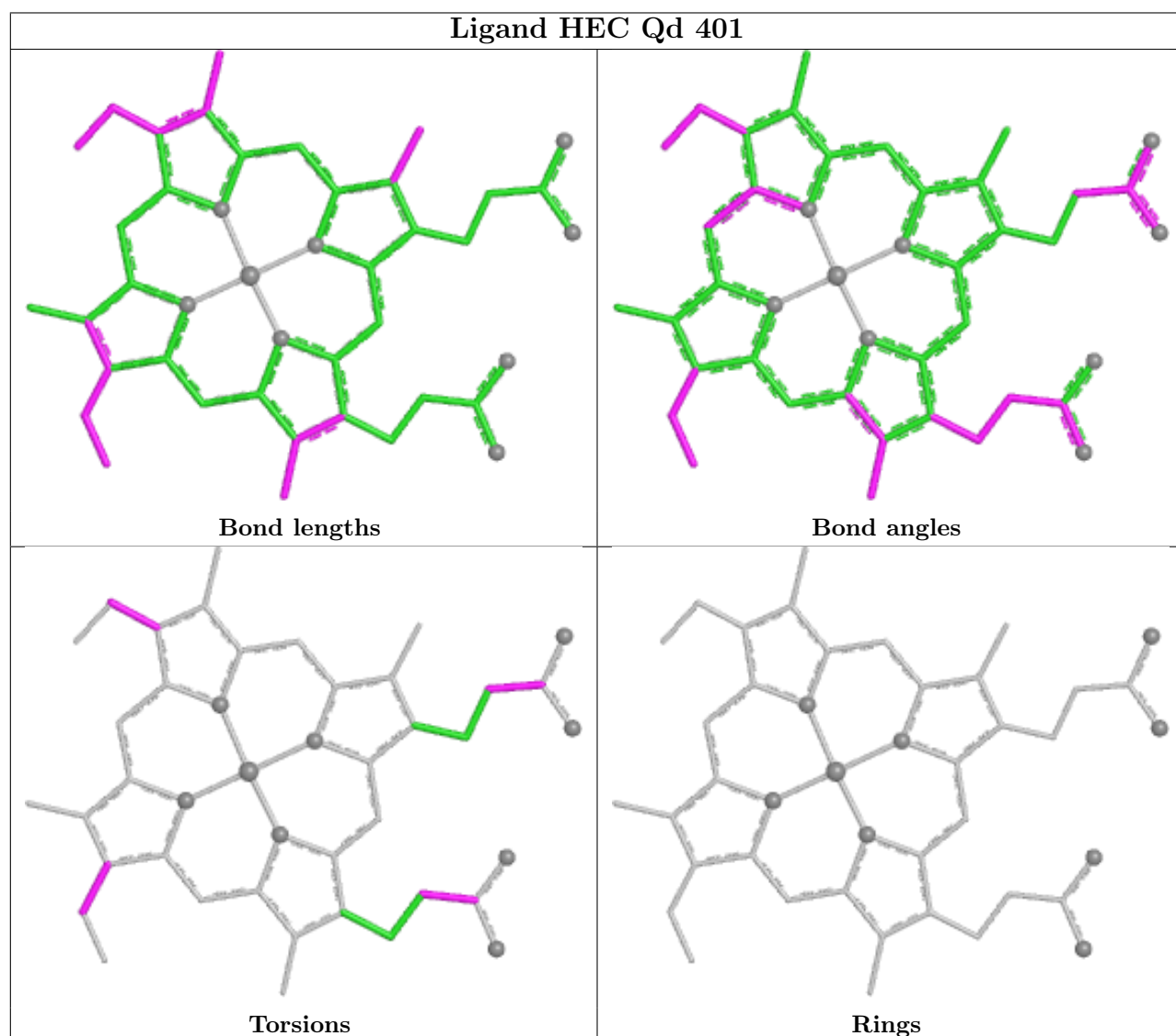
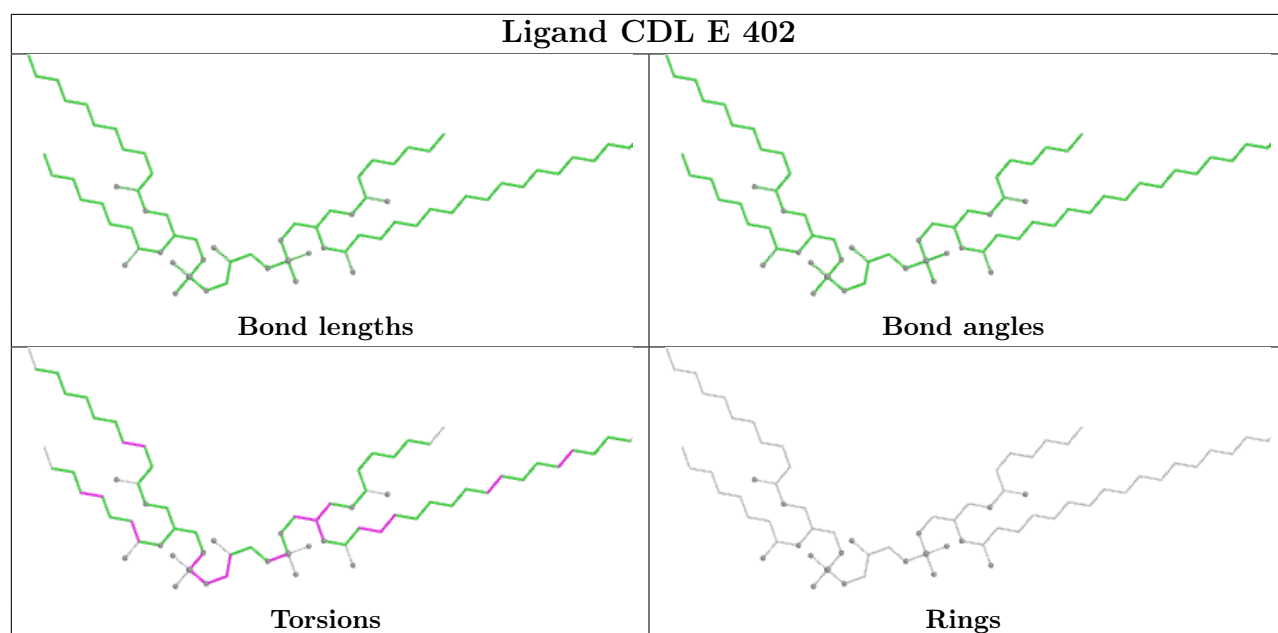
Continued on next page...

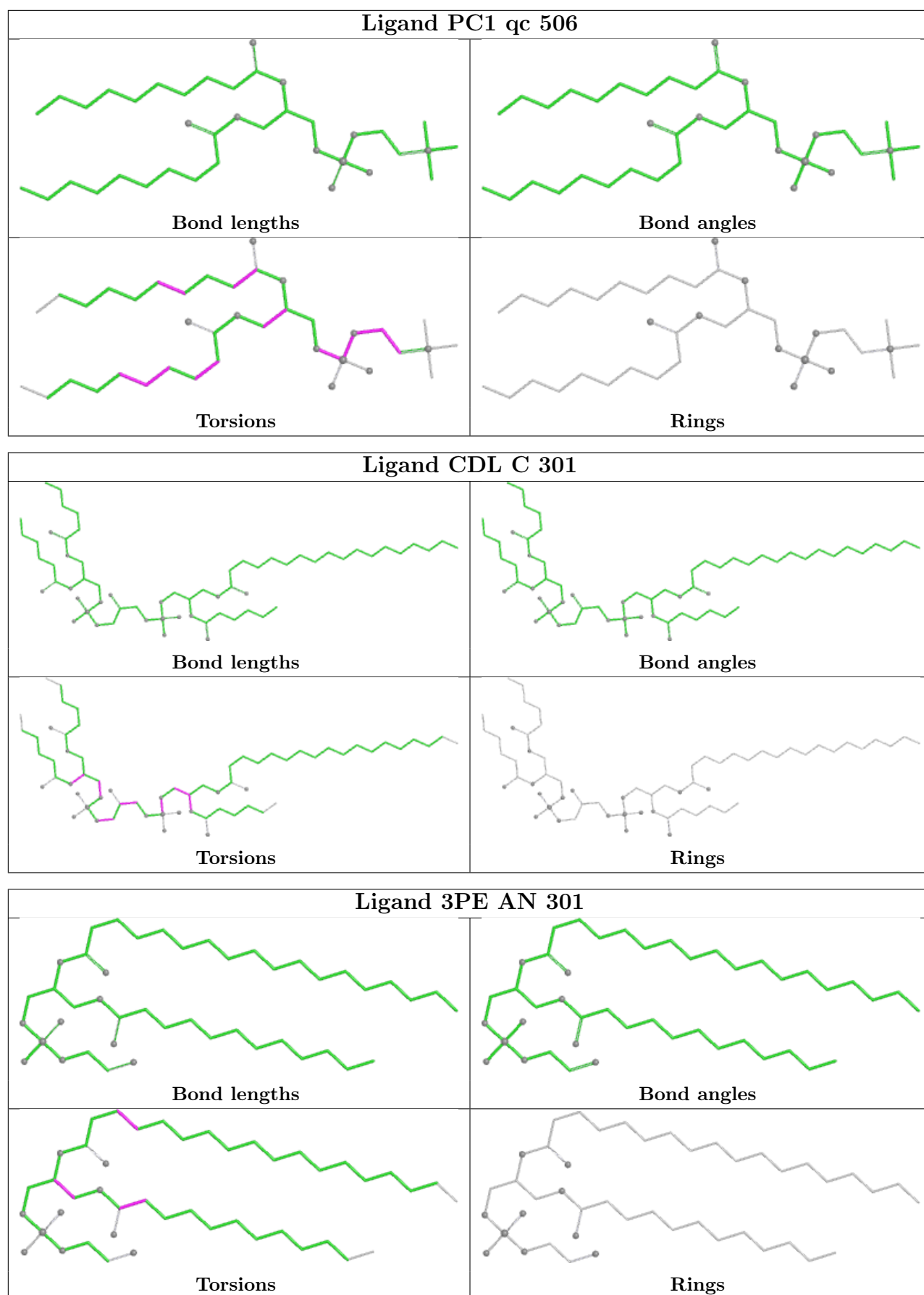
Continued from previous page...

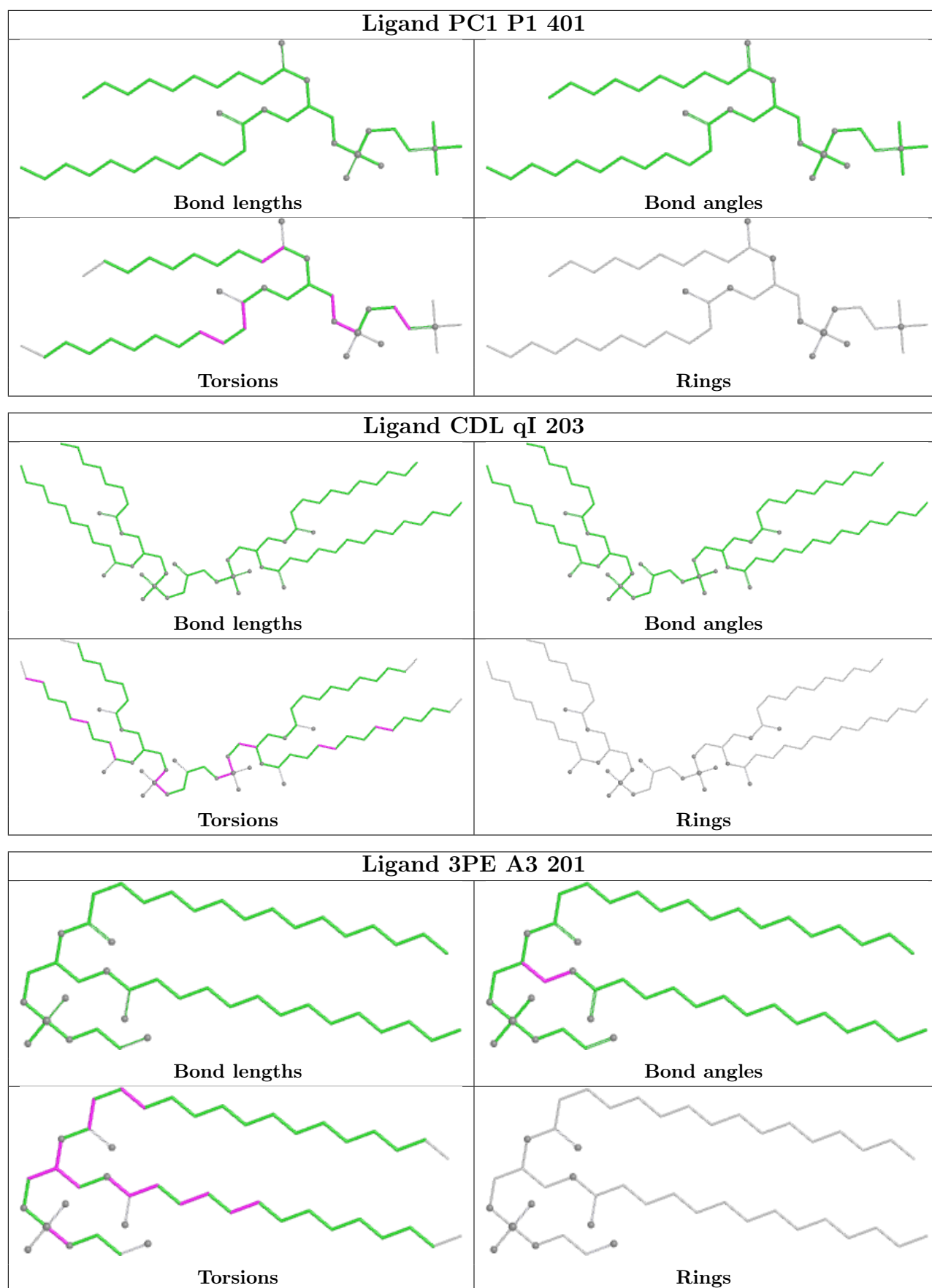
Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	m1	404	CDL	6	0
160	Y5	204	PX2	1	0
152	j1	400	PC1	3	0
153	N	304	CDL	7	0
153	QC	503	CDL	3	0
151	QD	401	HEC	1	0
151	2e	401	HEC	1	0
152	M	302	PC1	2	0
153	QI	203	CDL	5	0
153	2g	201	CDL	5	0
152	C1	711	PC1	10	0
152	n	302	PC1	1	0
151	2E	401	HEC	1	0
158	an	301	3PE	3	0

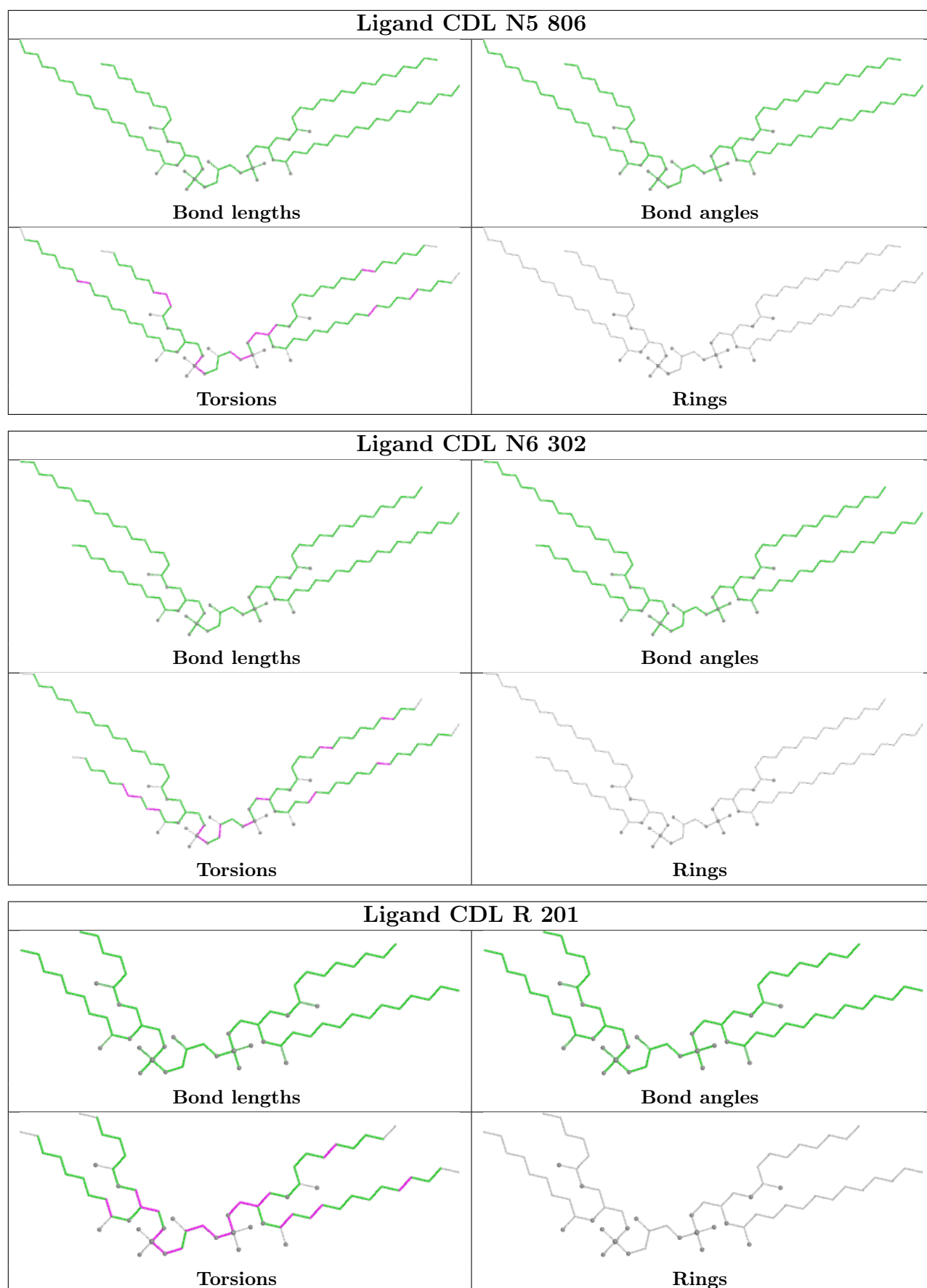
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

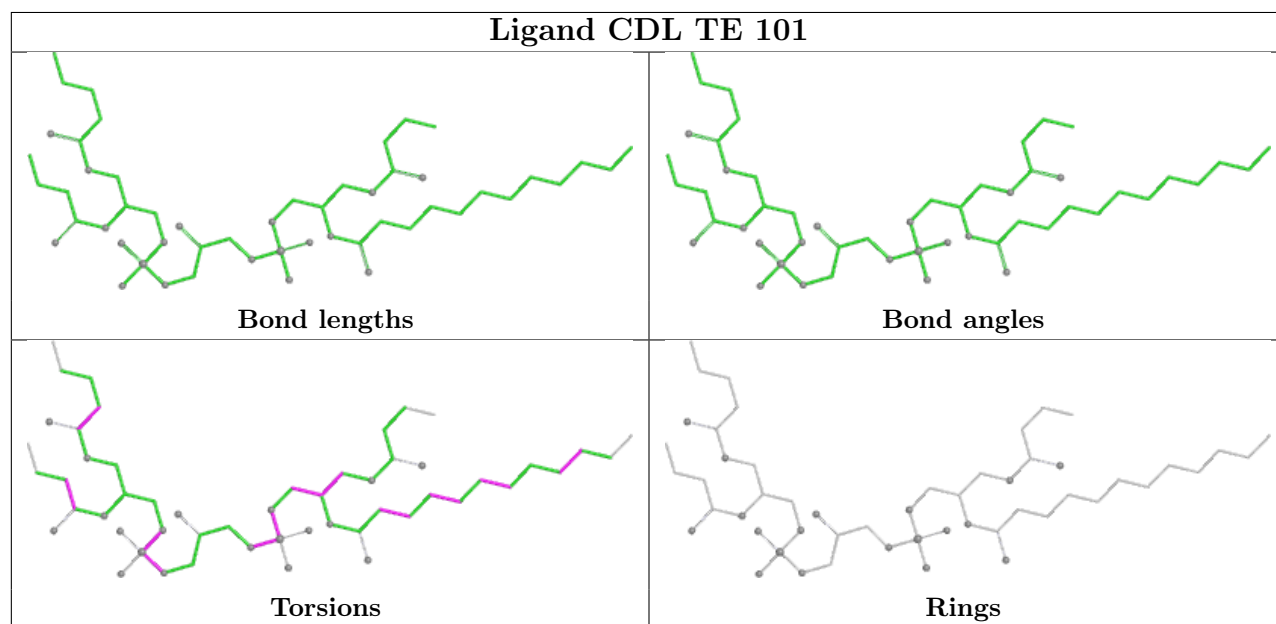
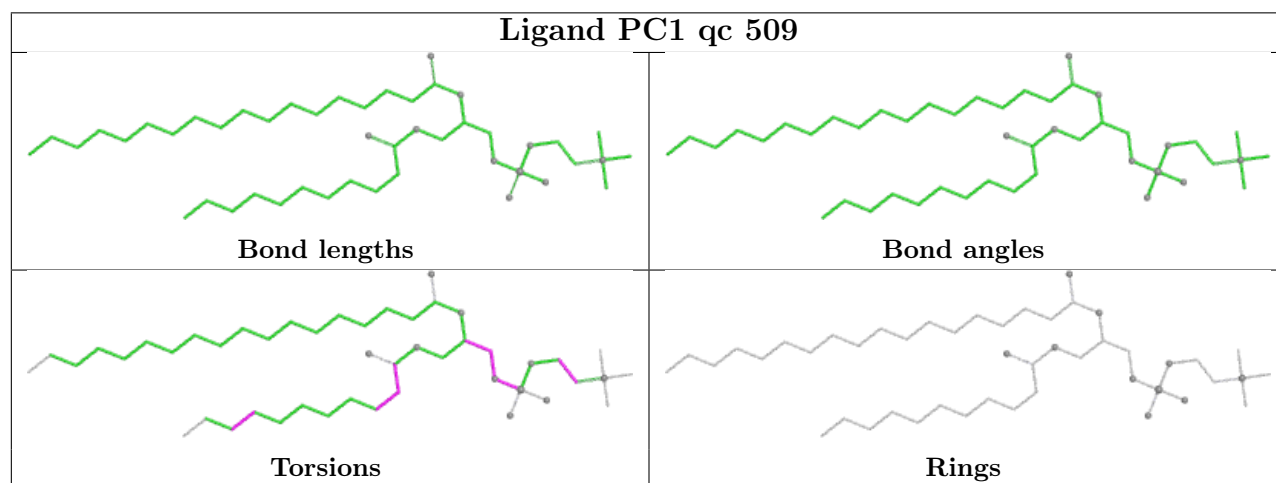
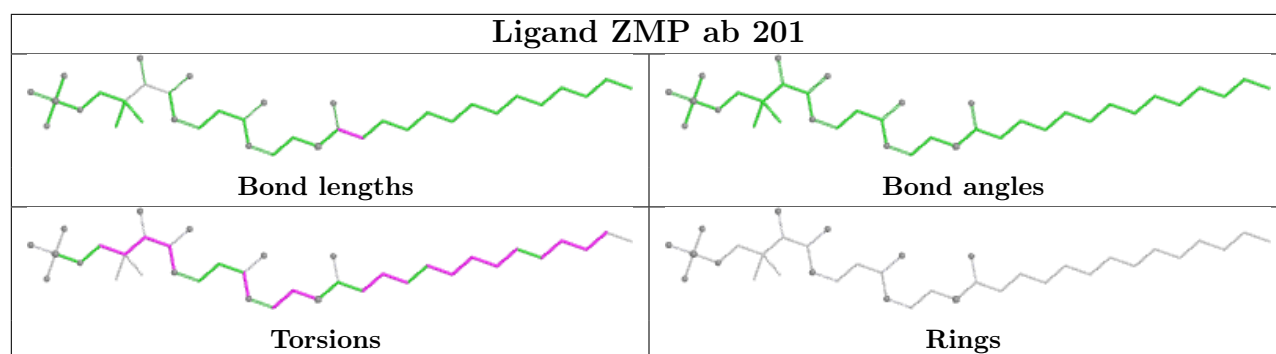


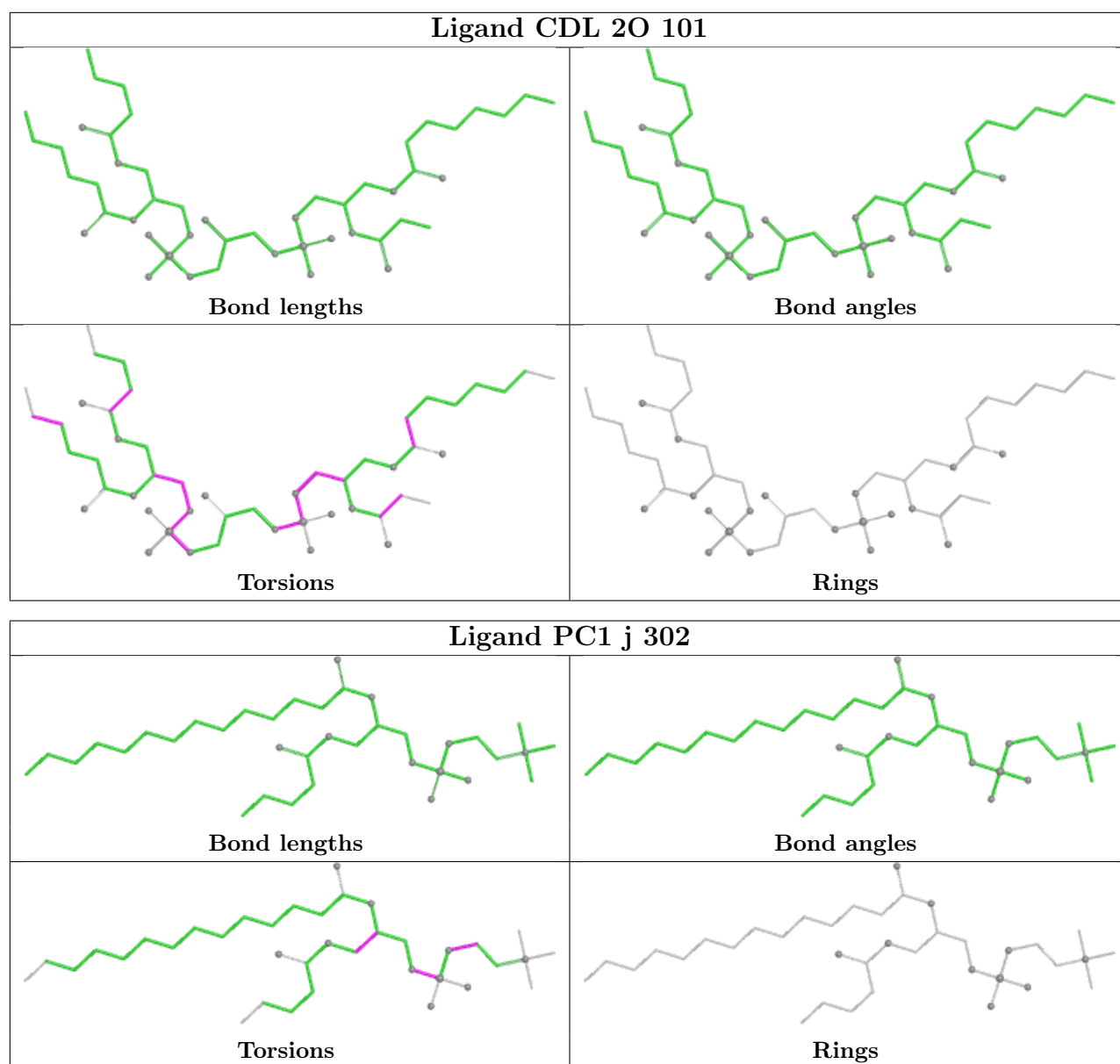


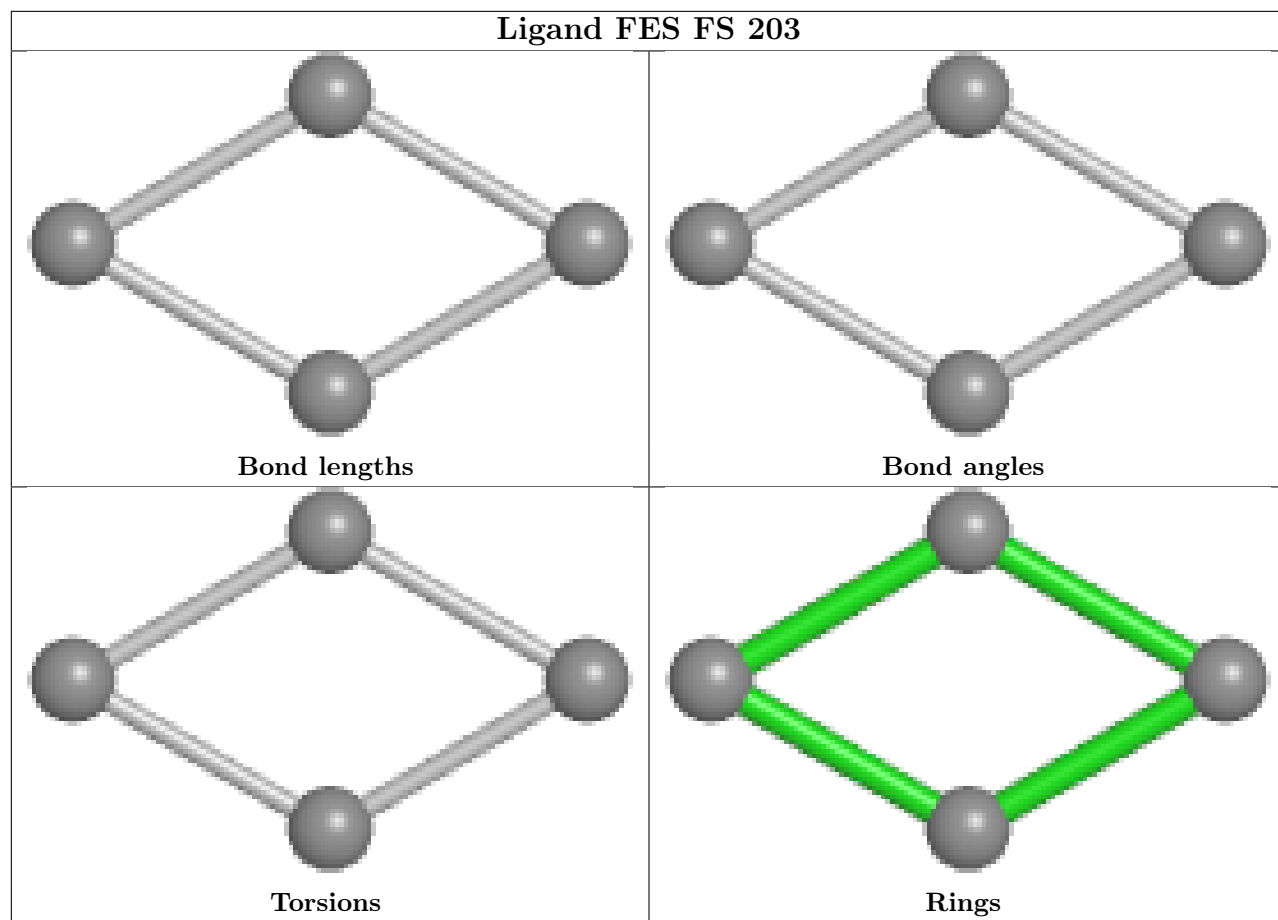


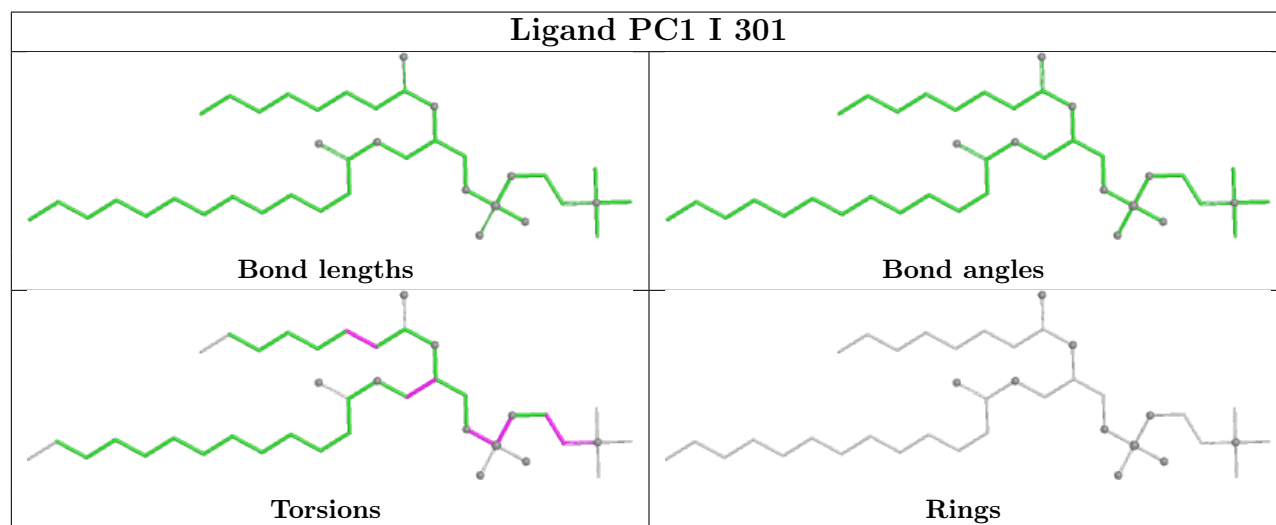
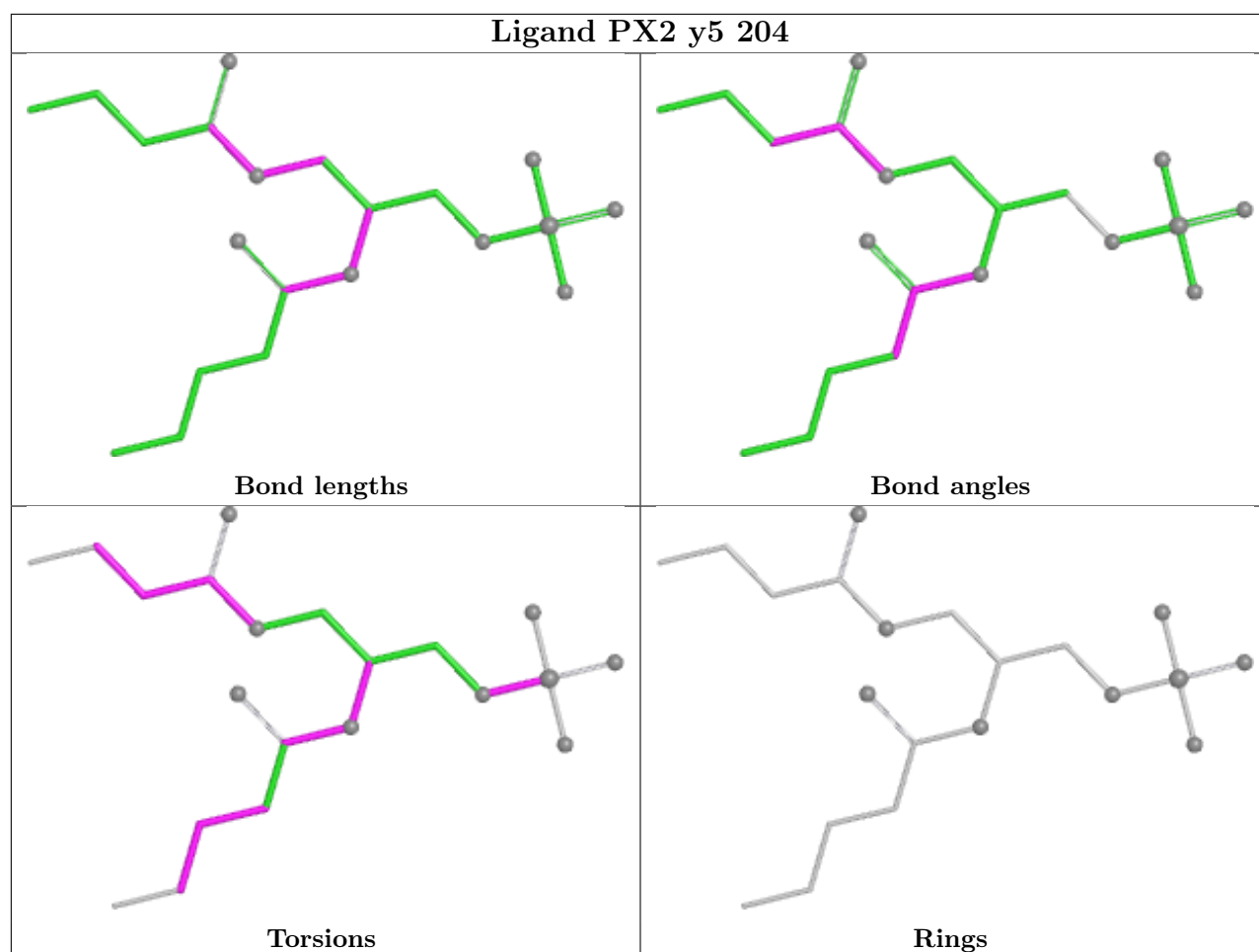


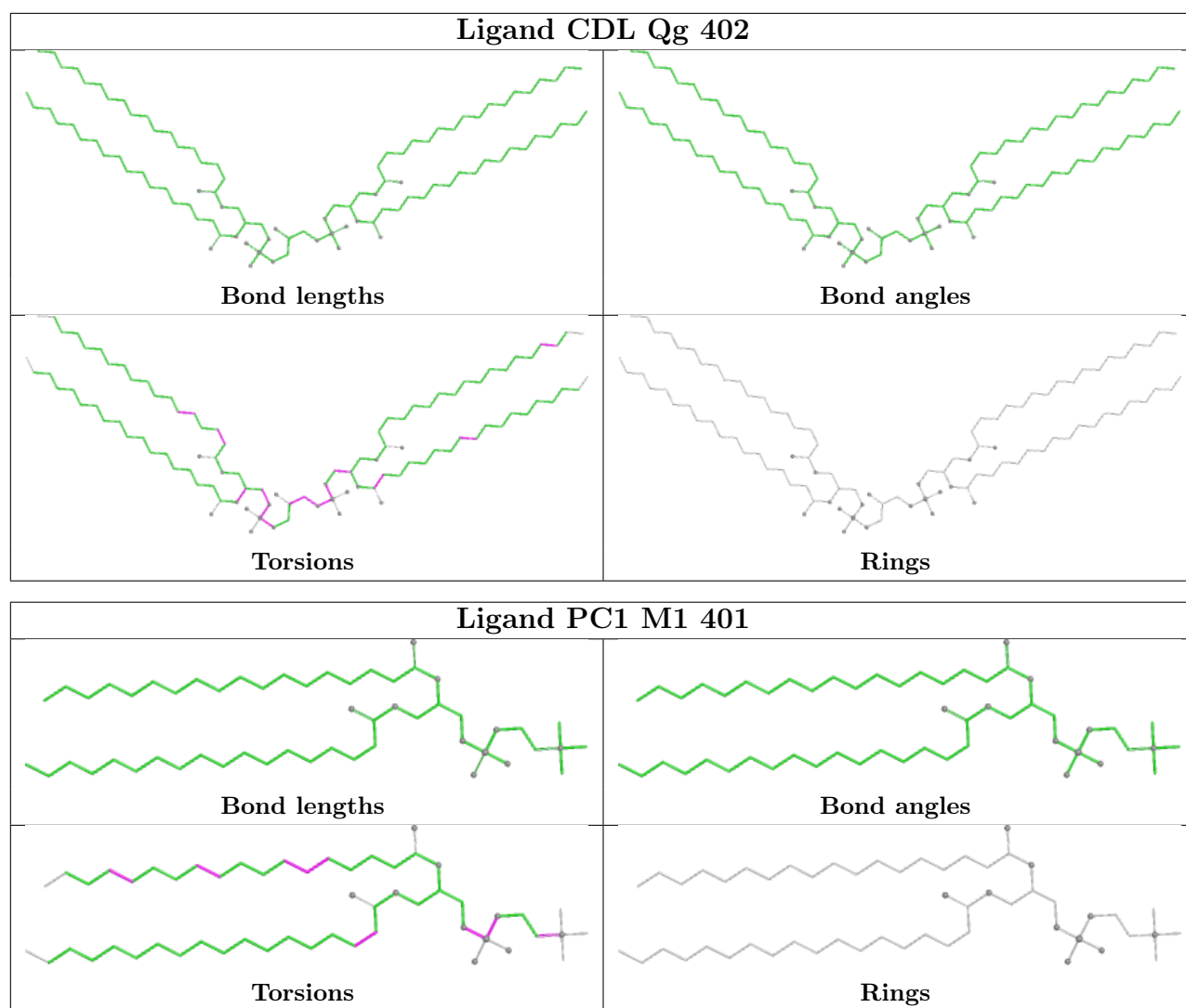


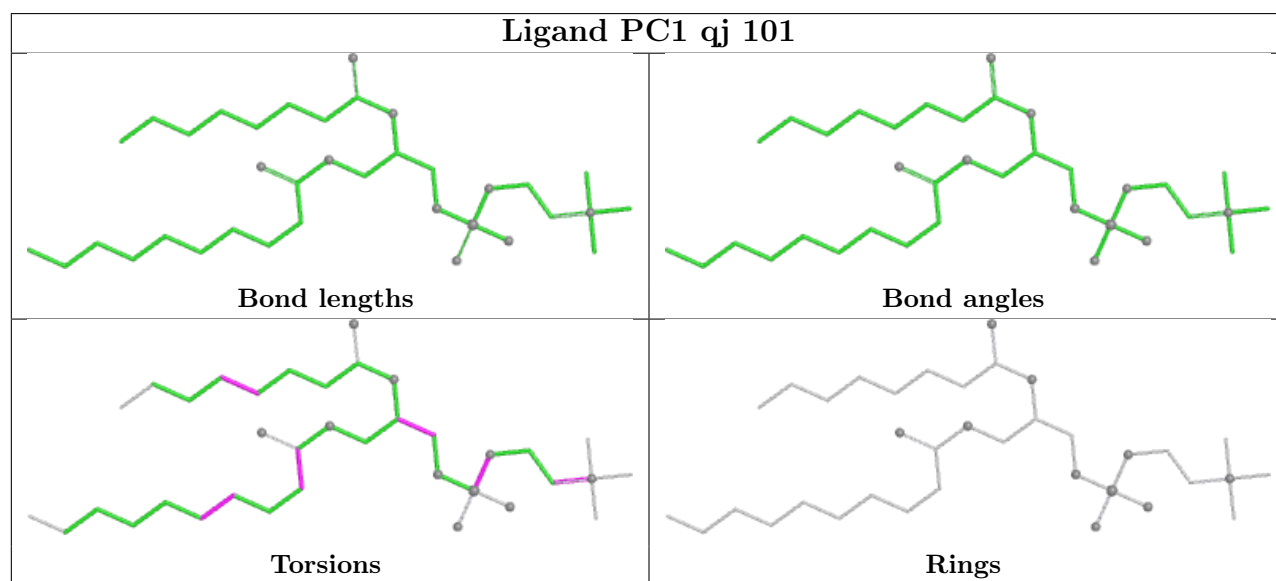
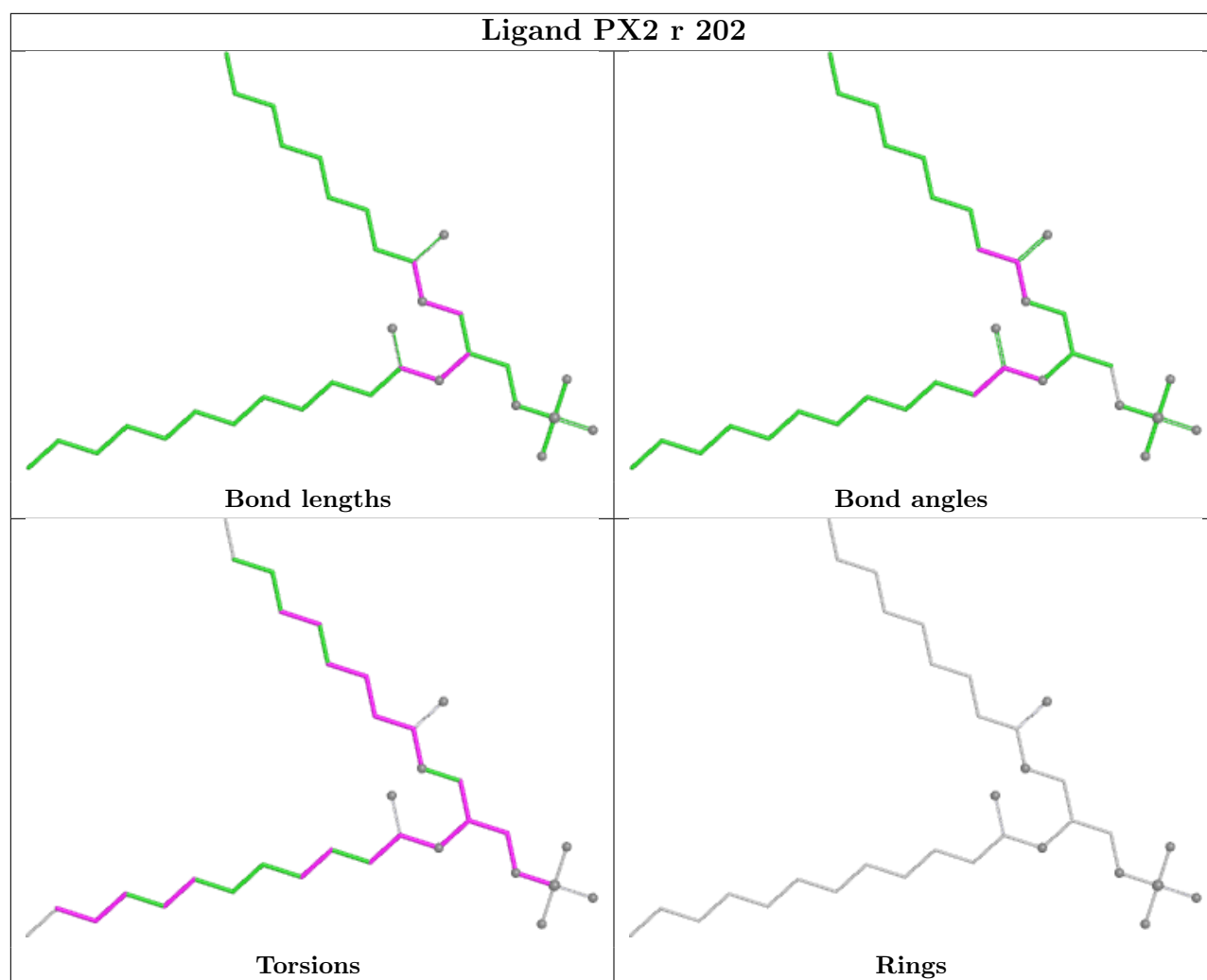


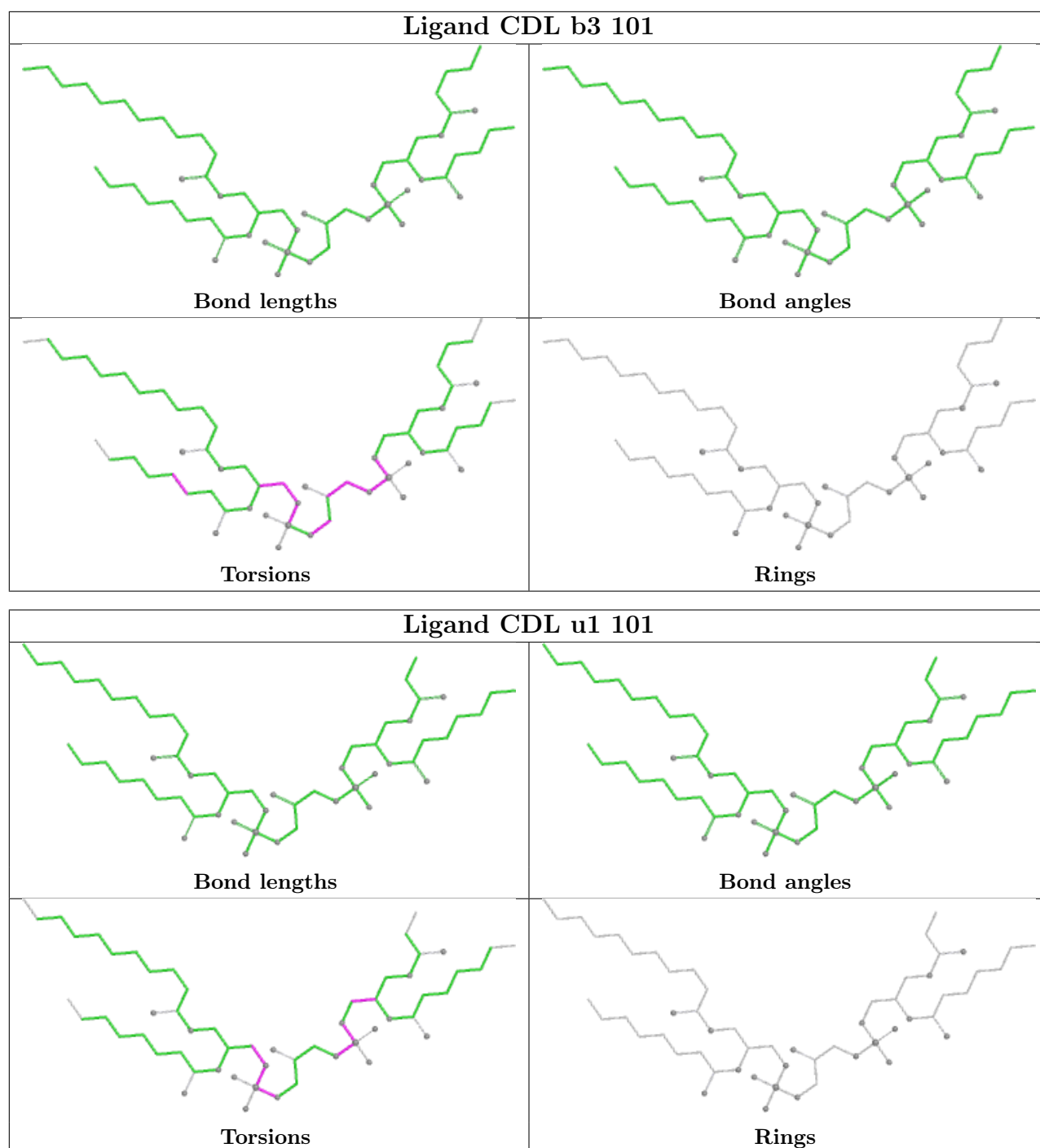


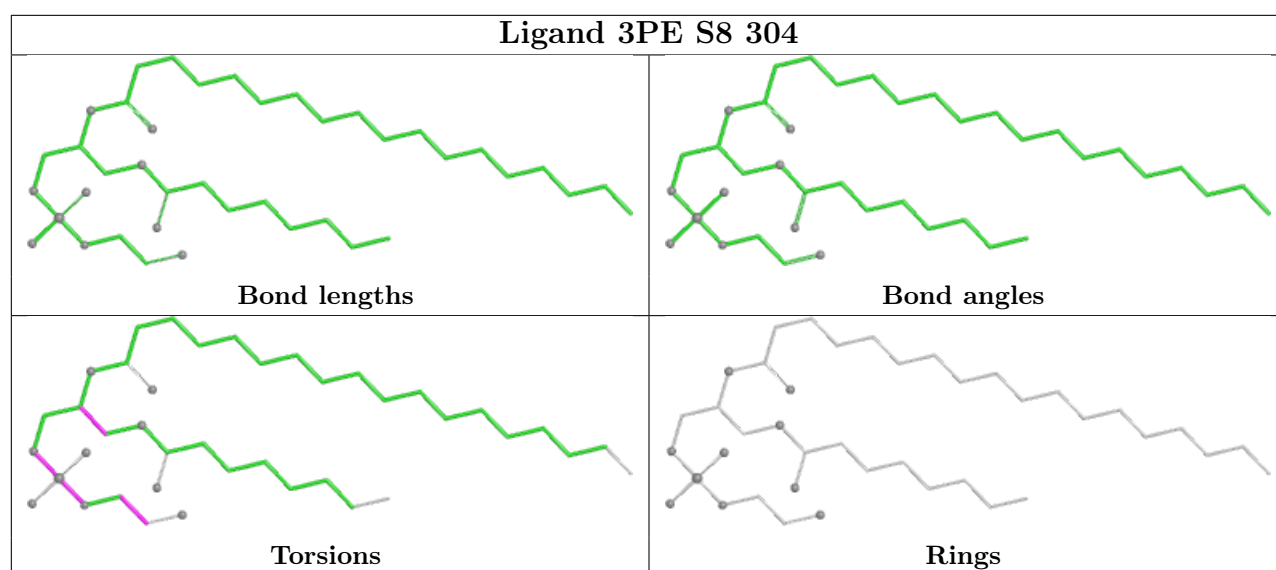
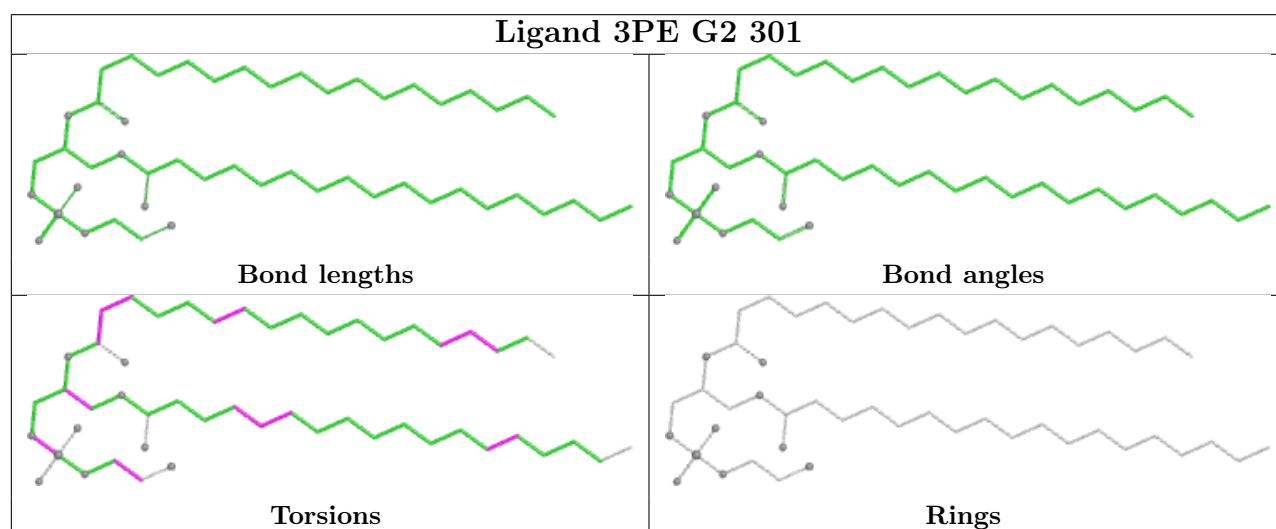
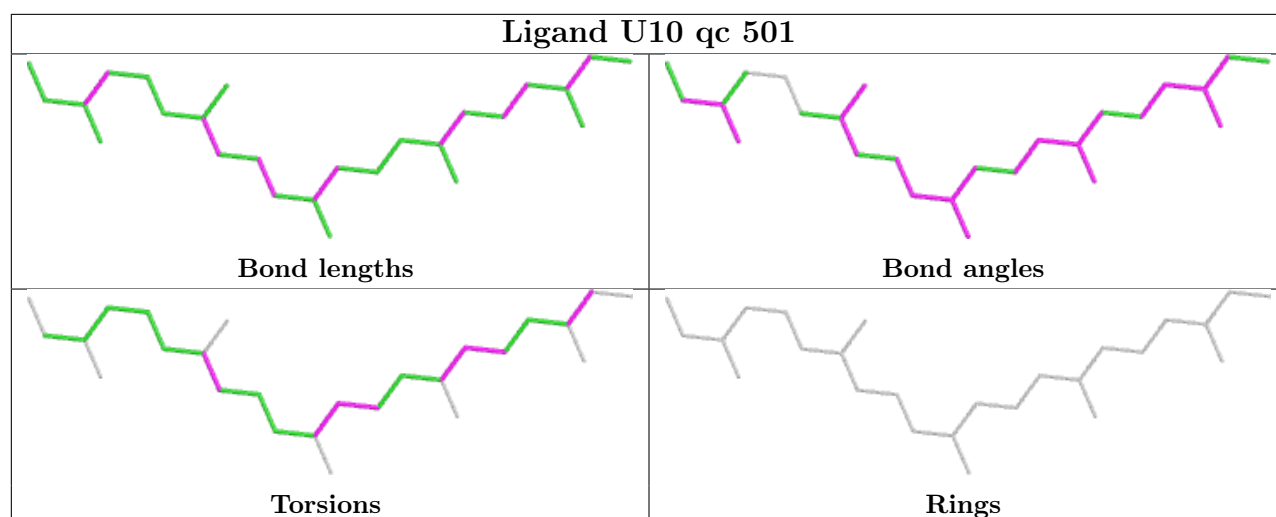


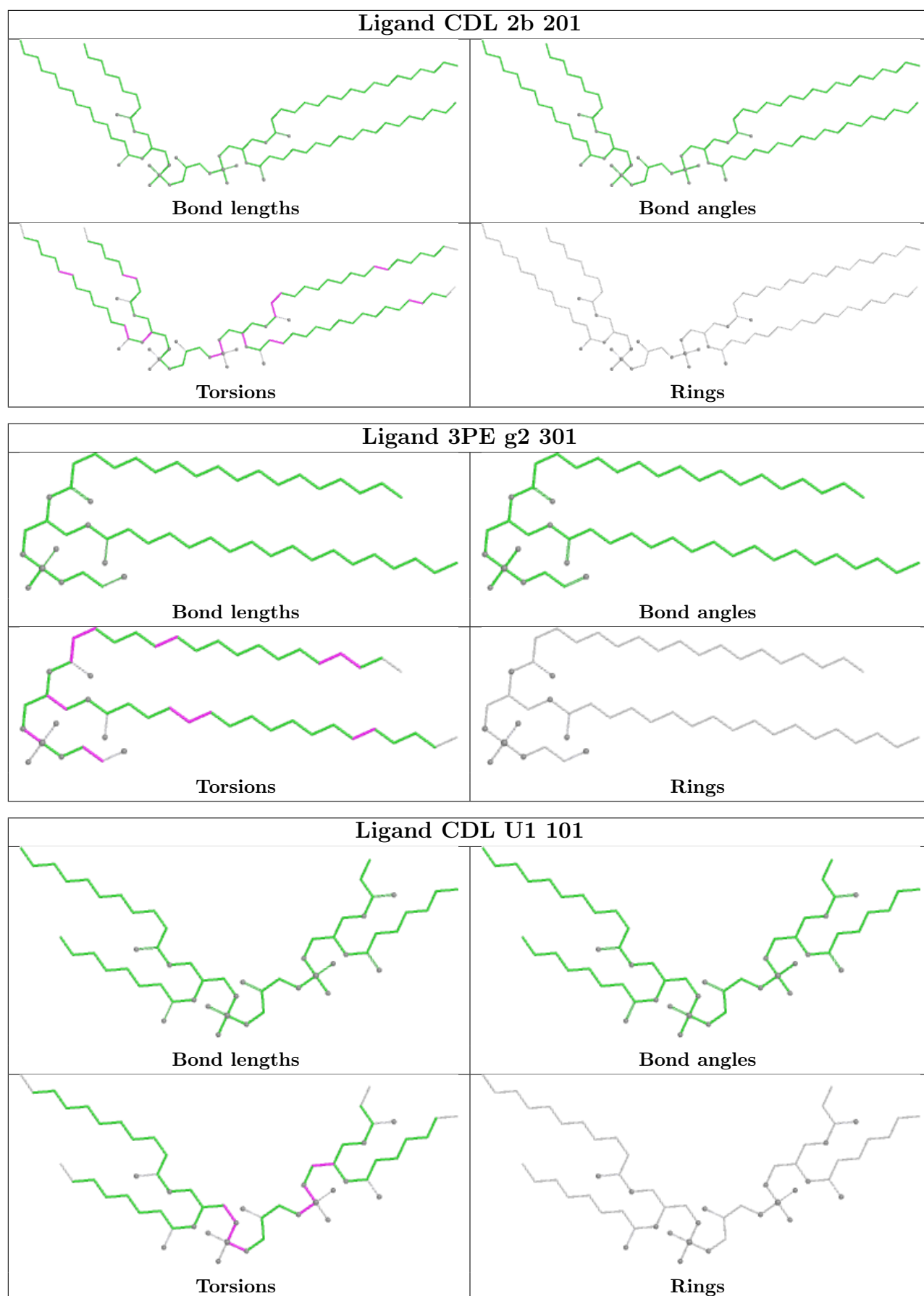


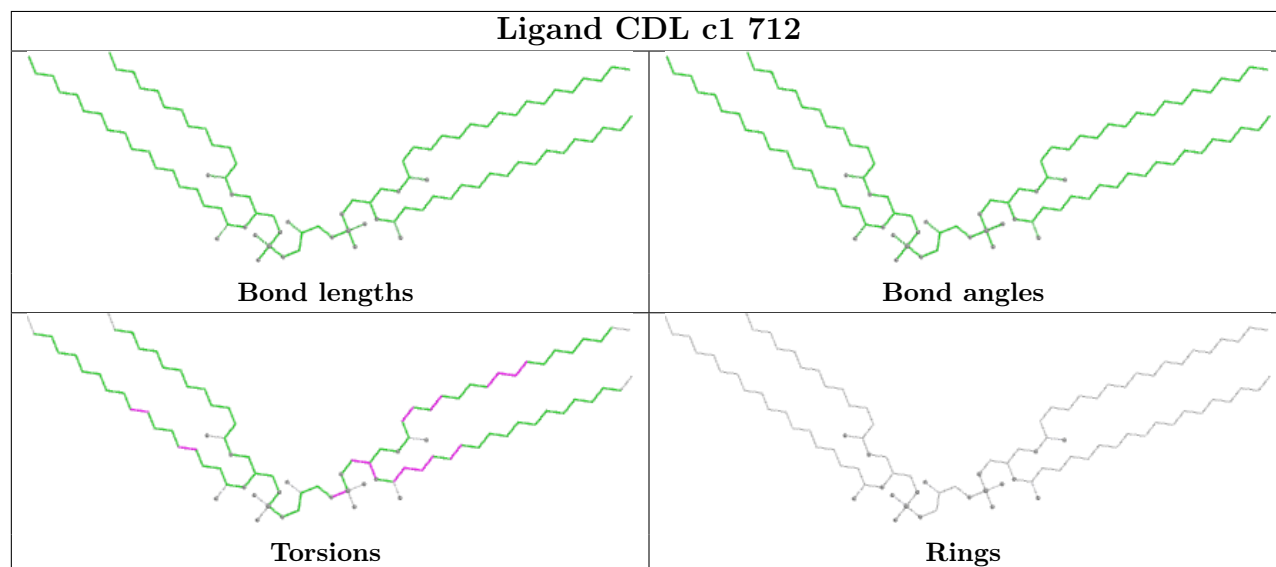
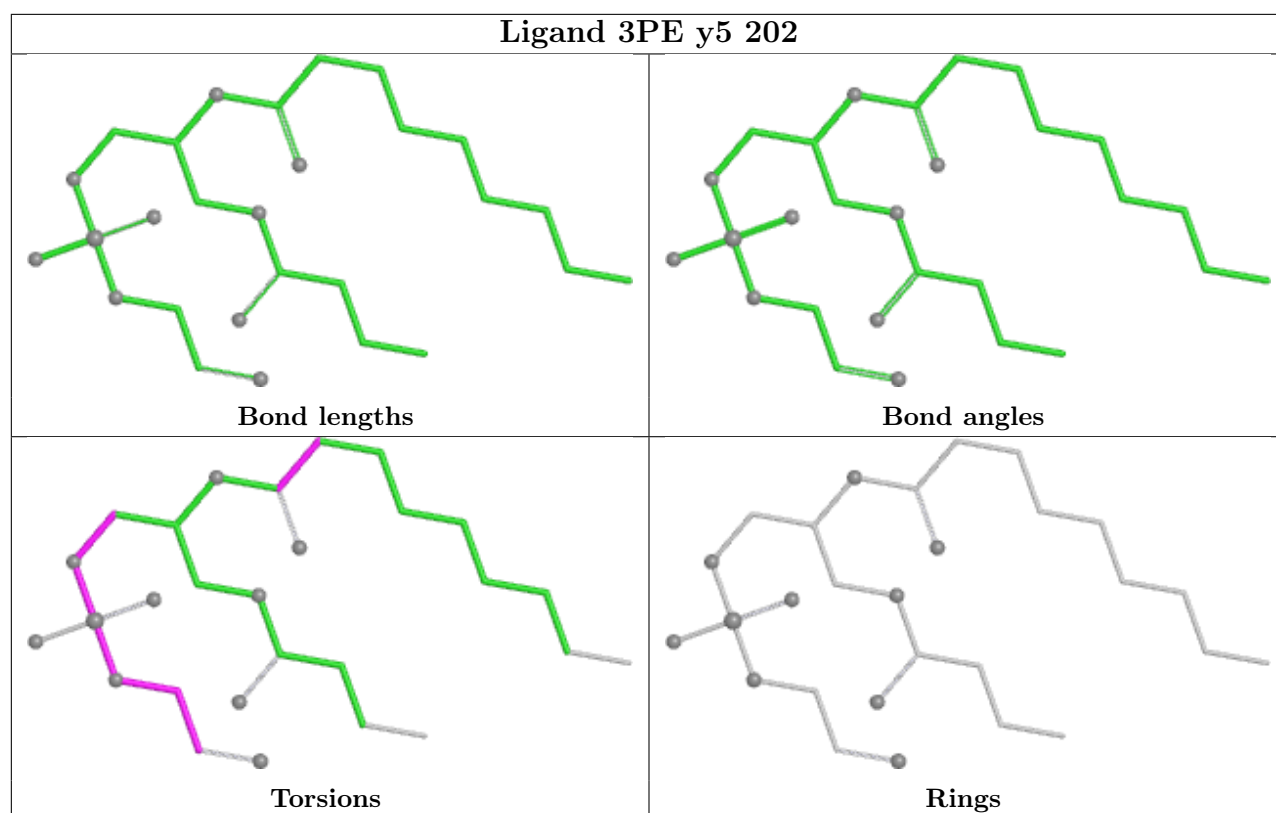


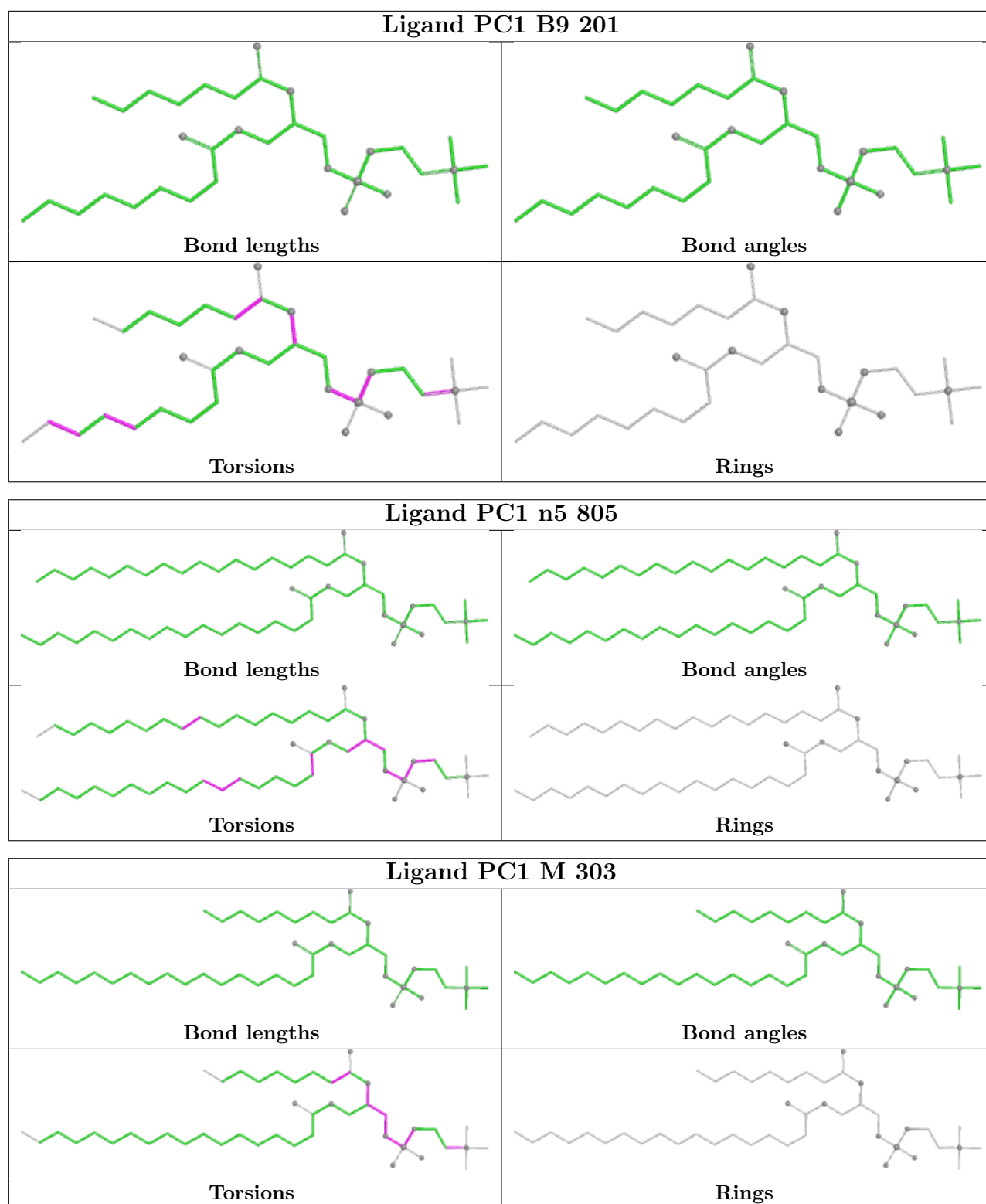


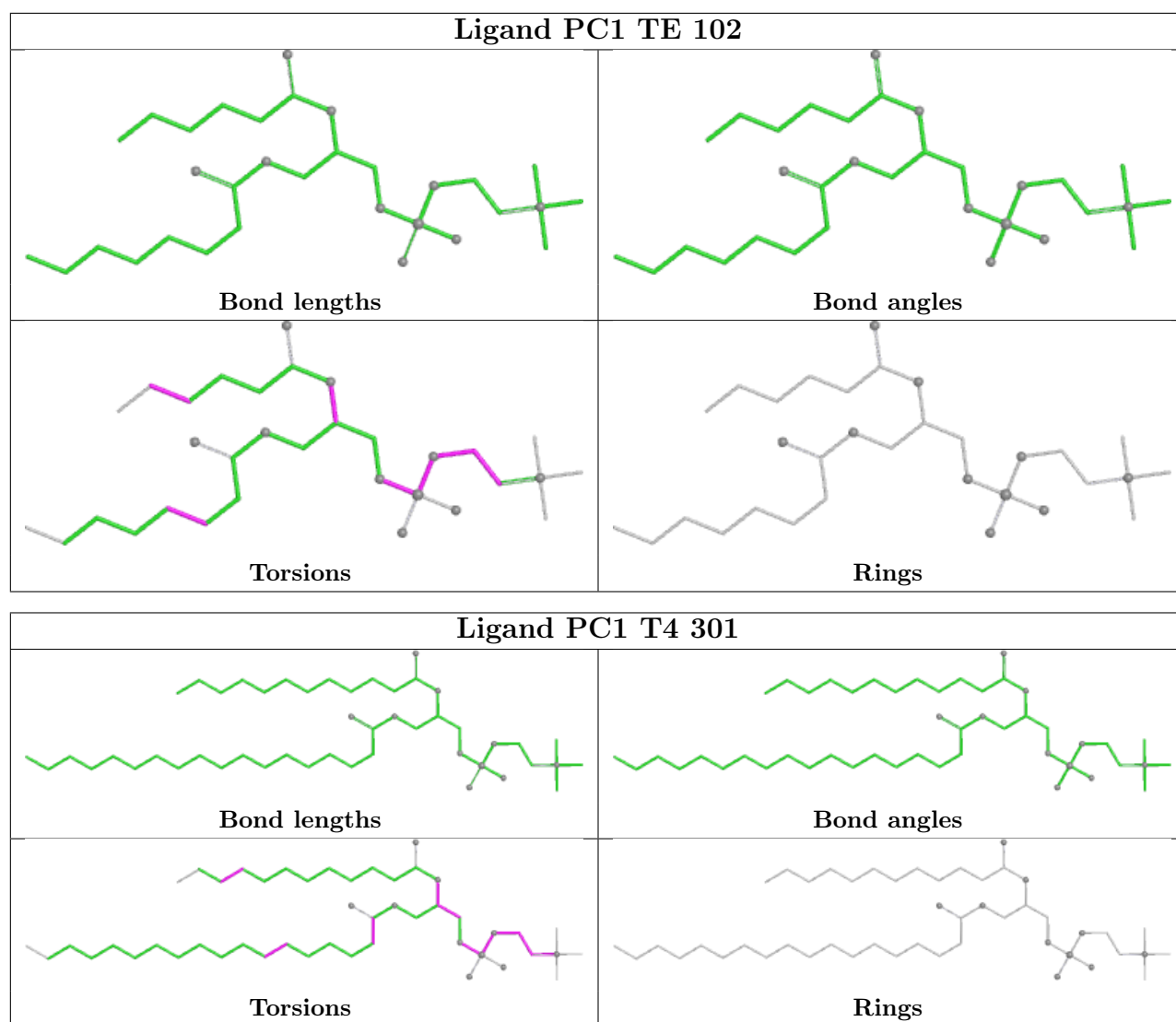


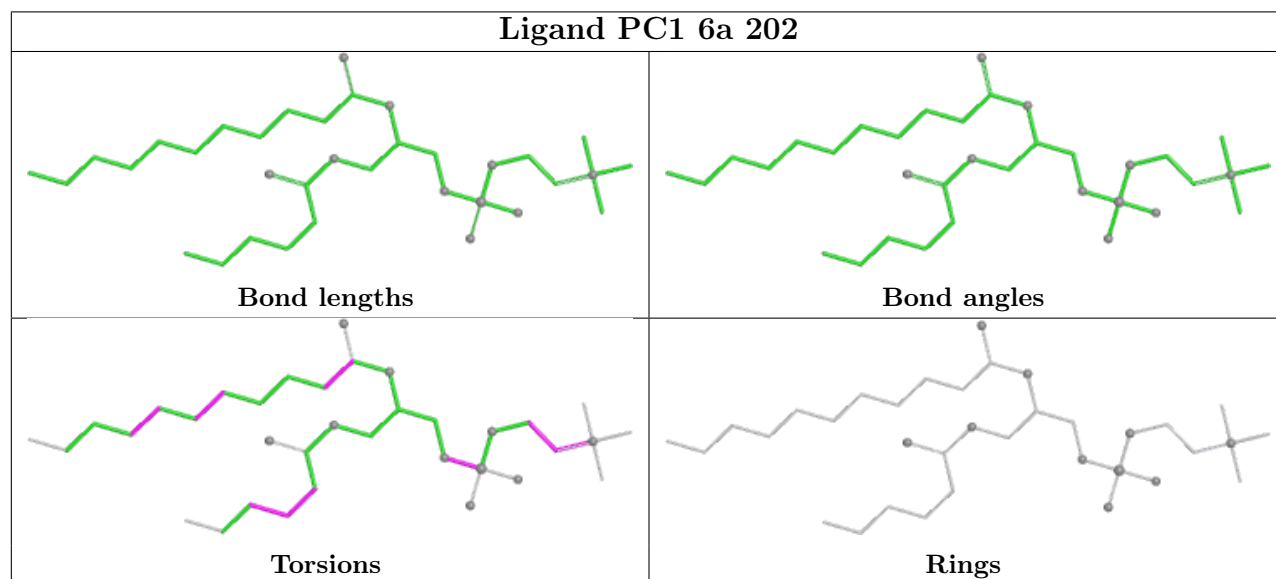
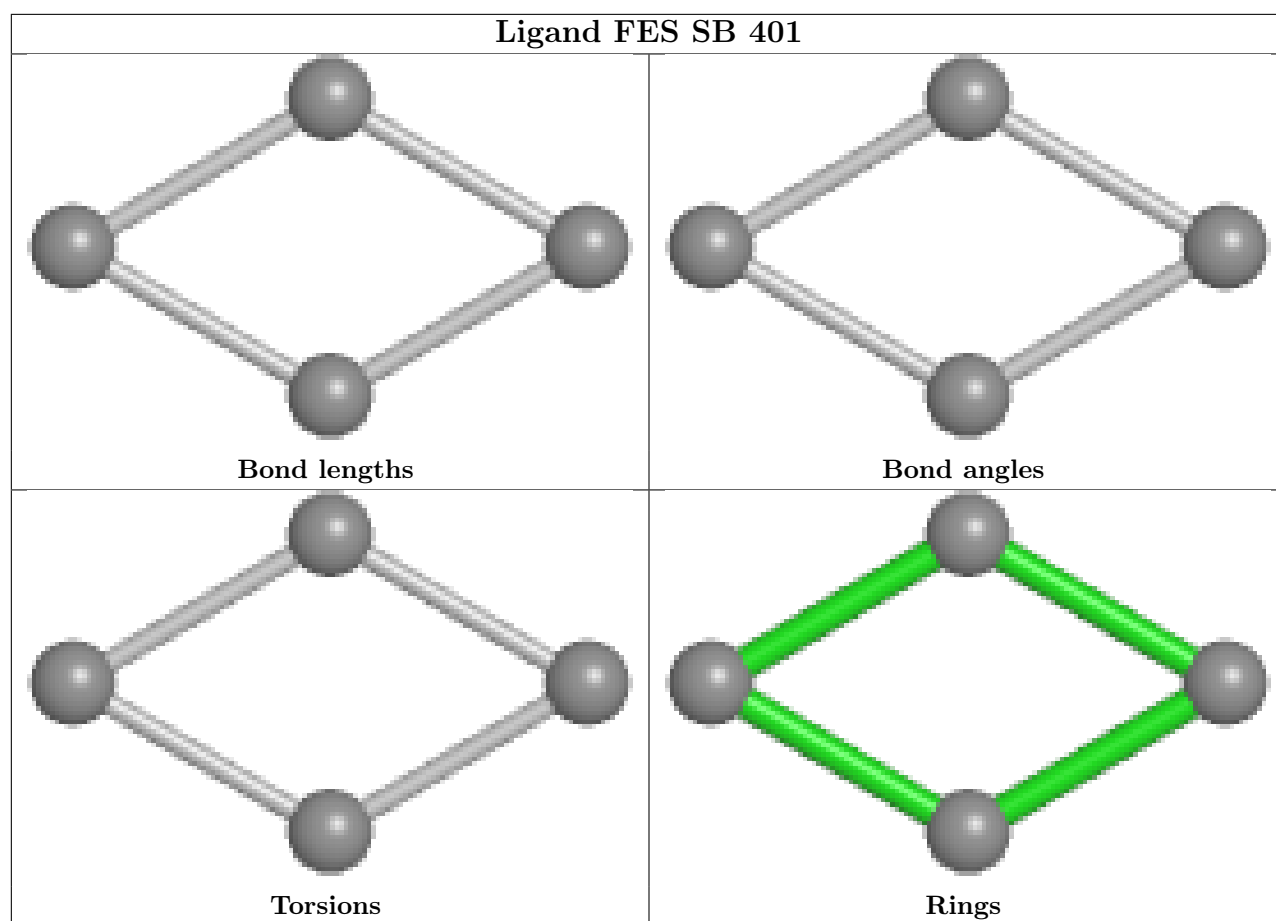


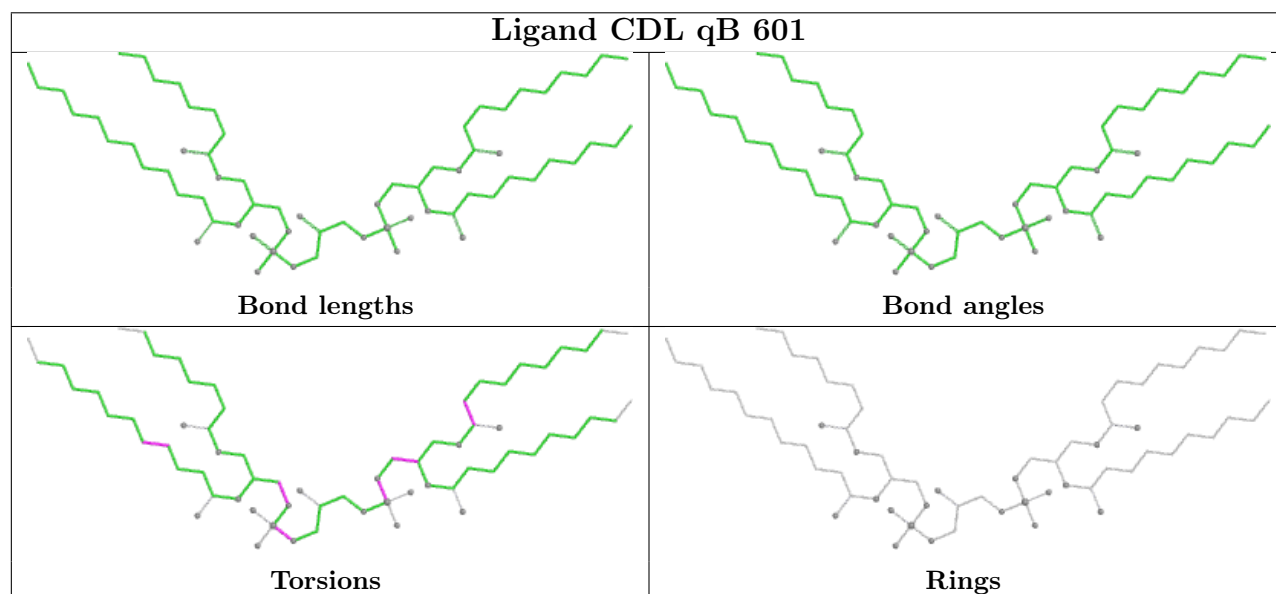
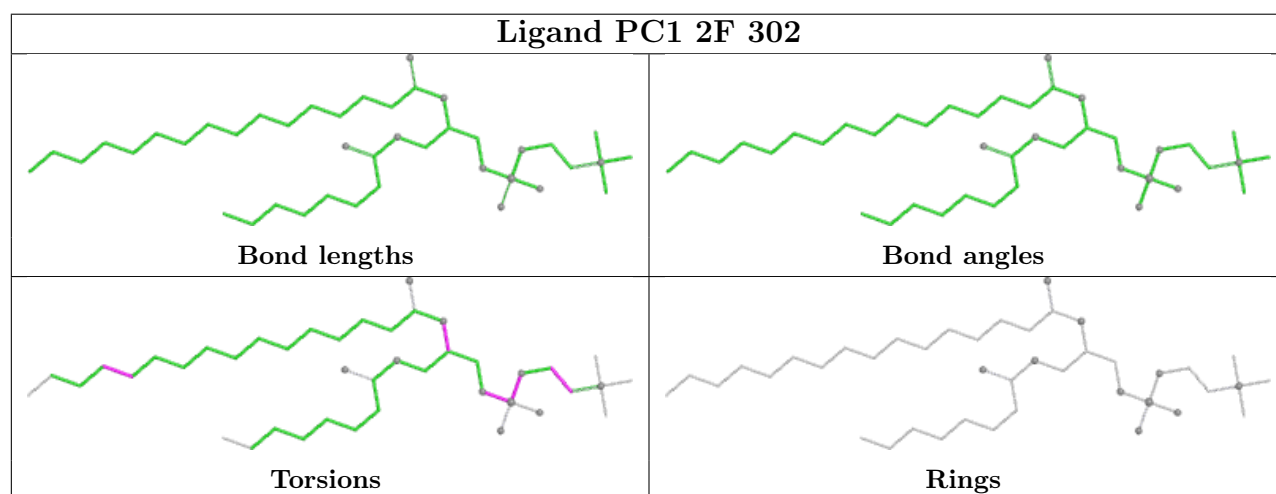
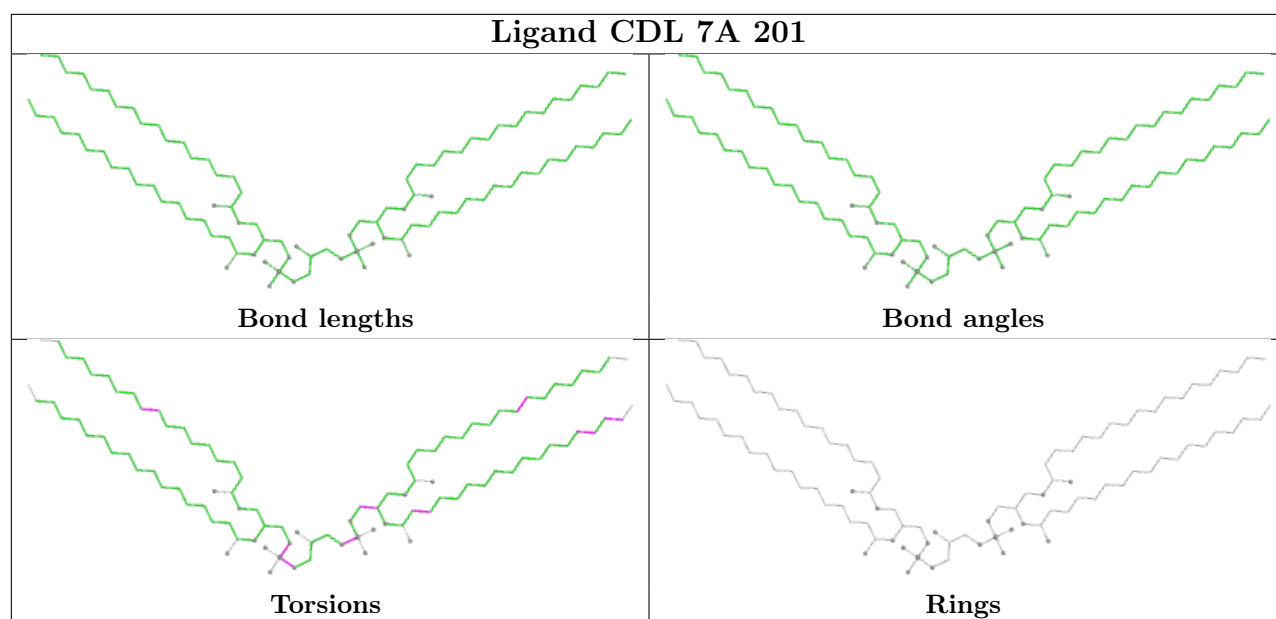


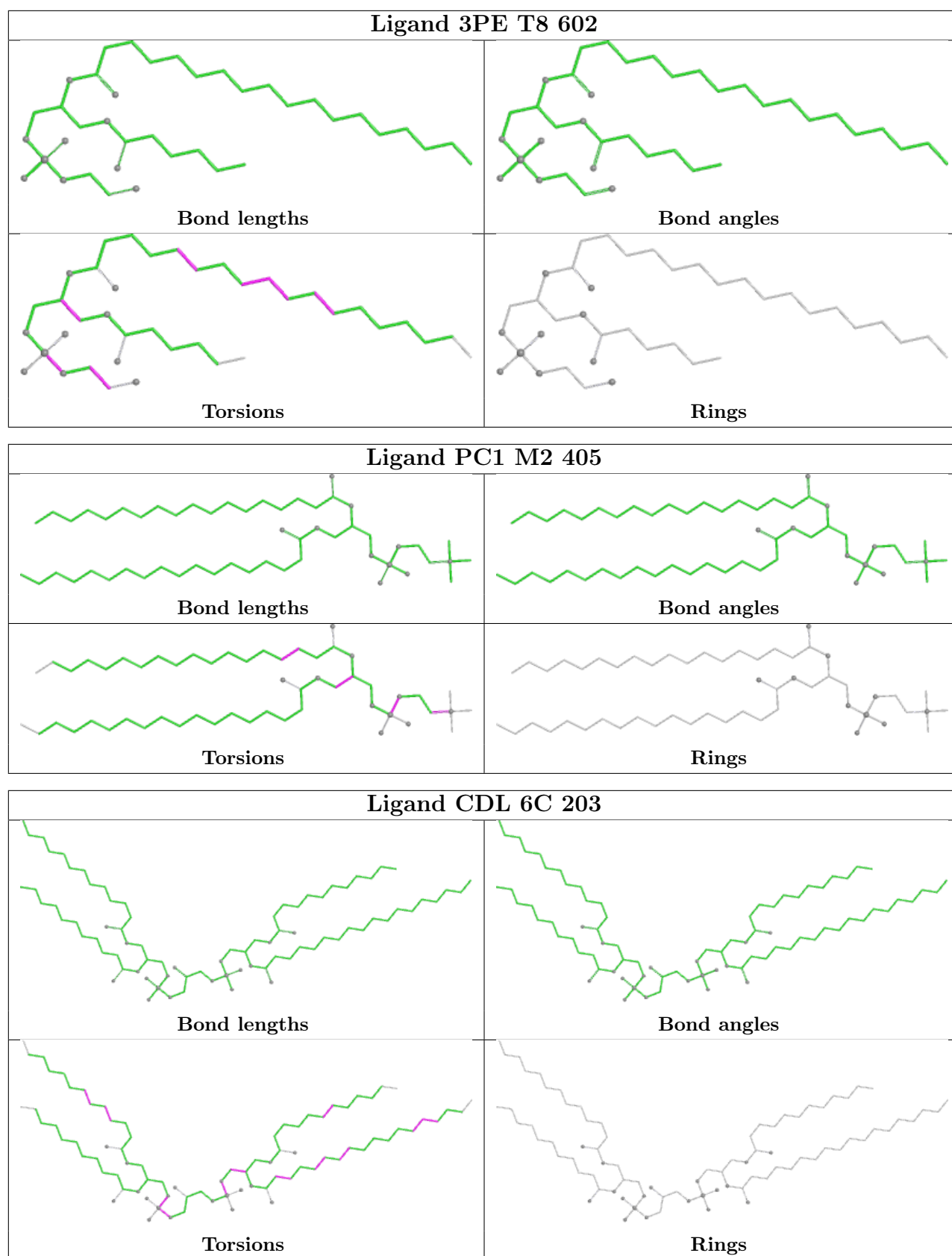


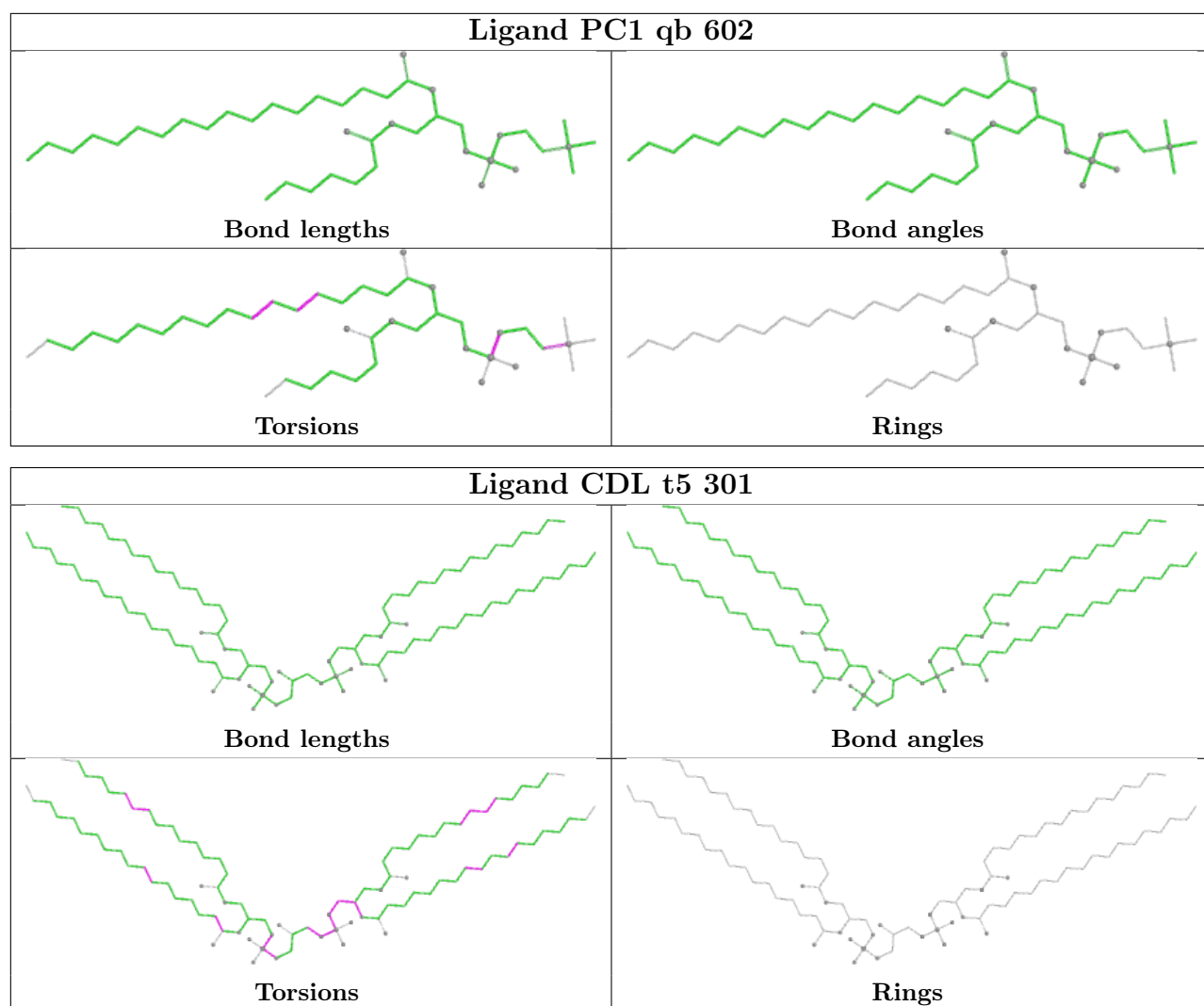


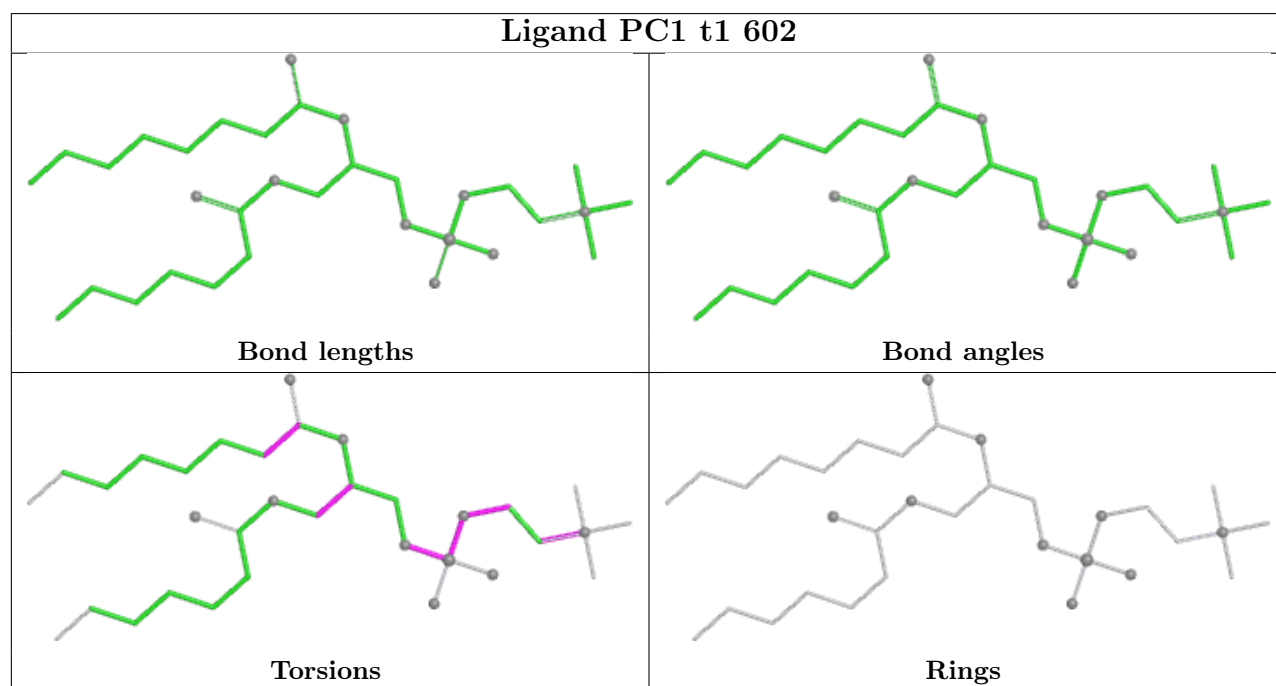
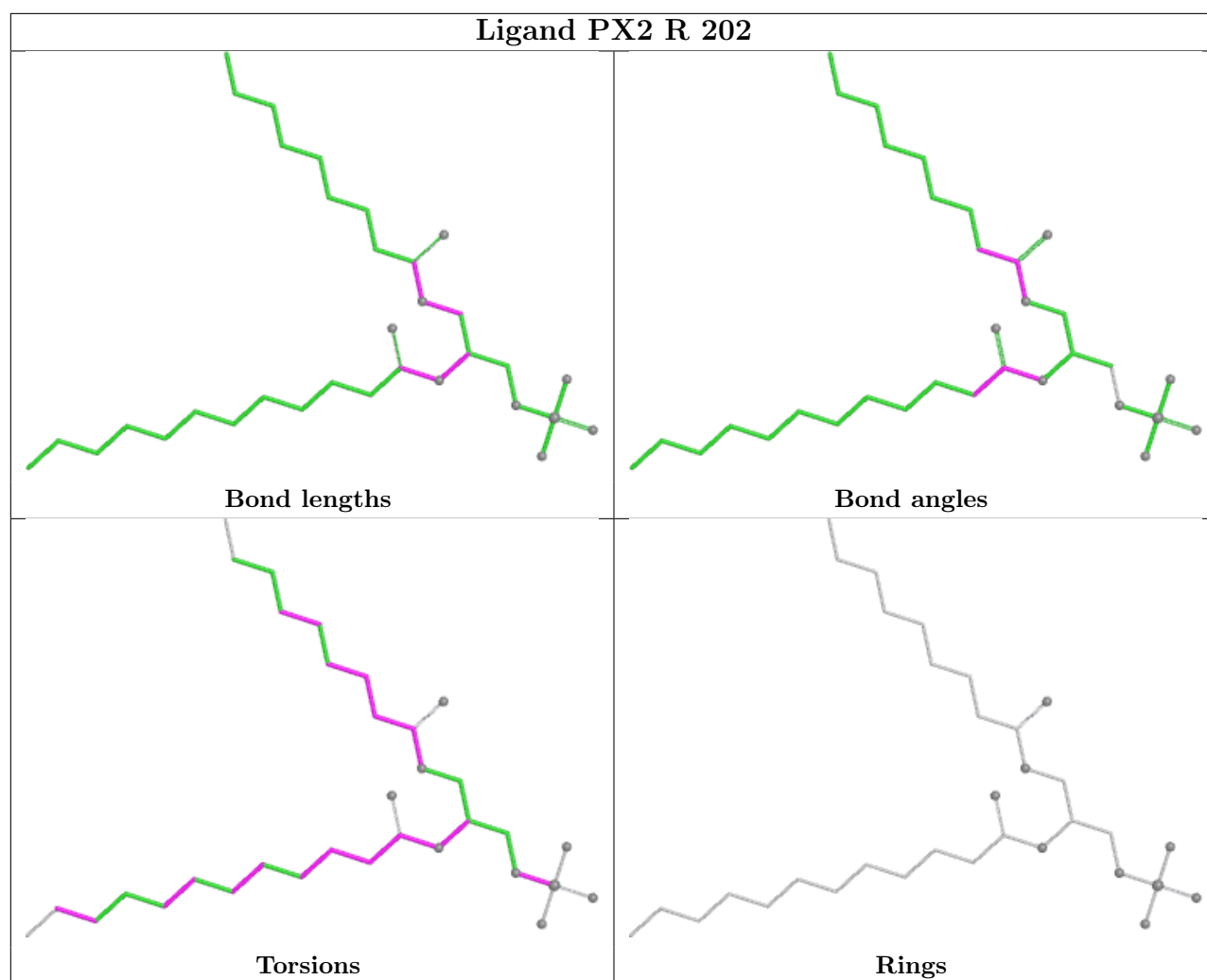


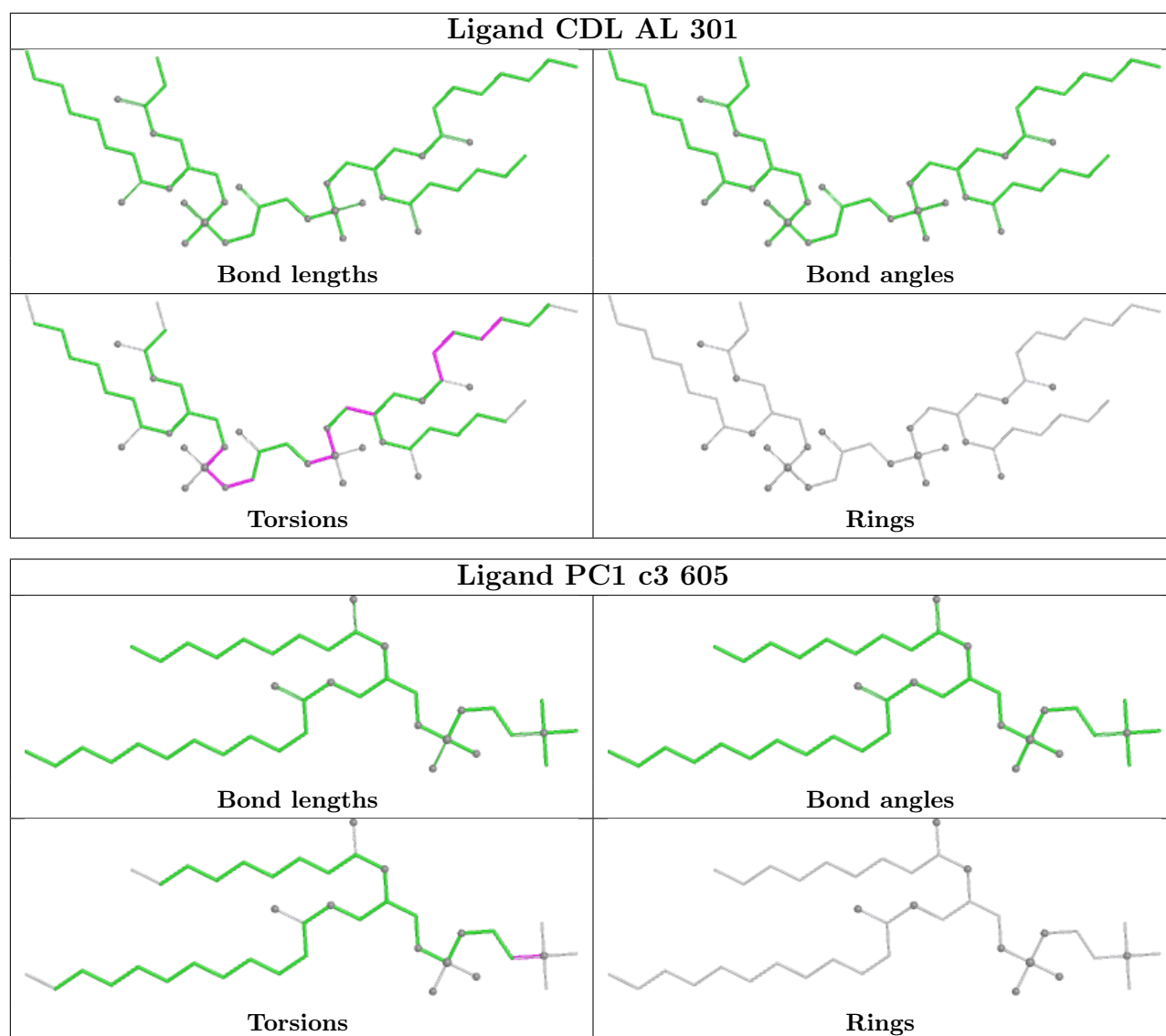


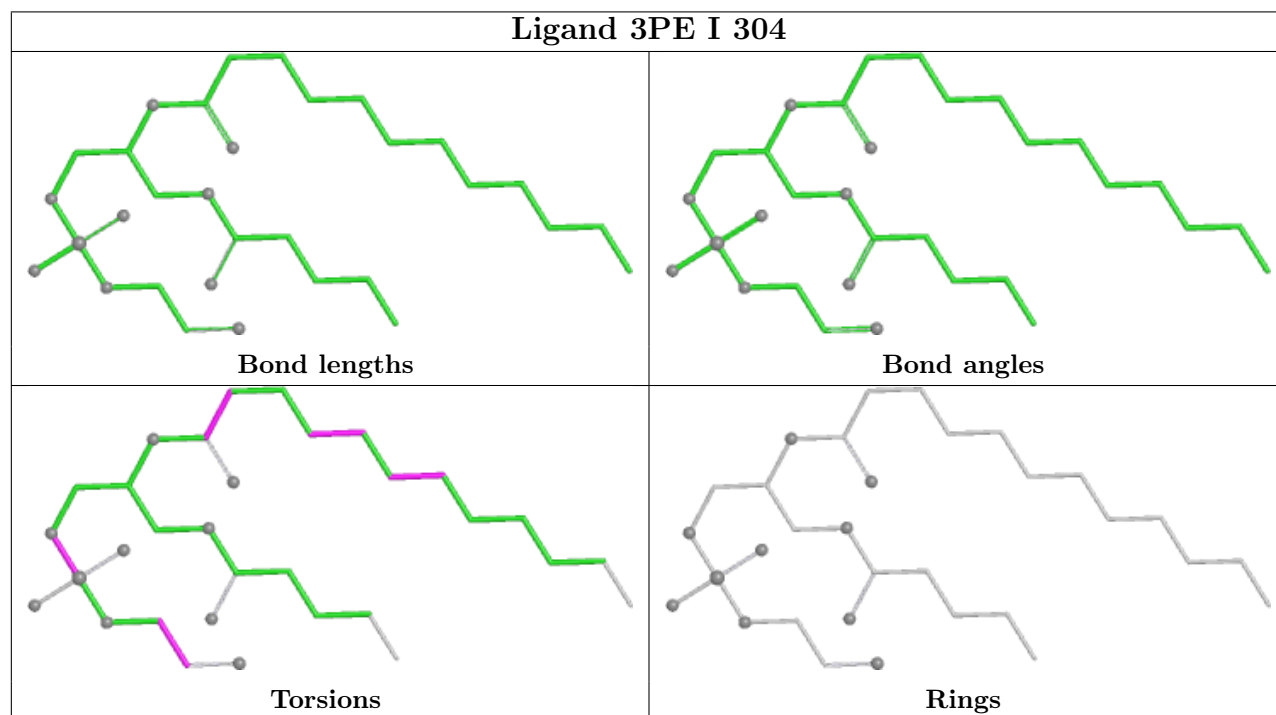
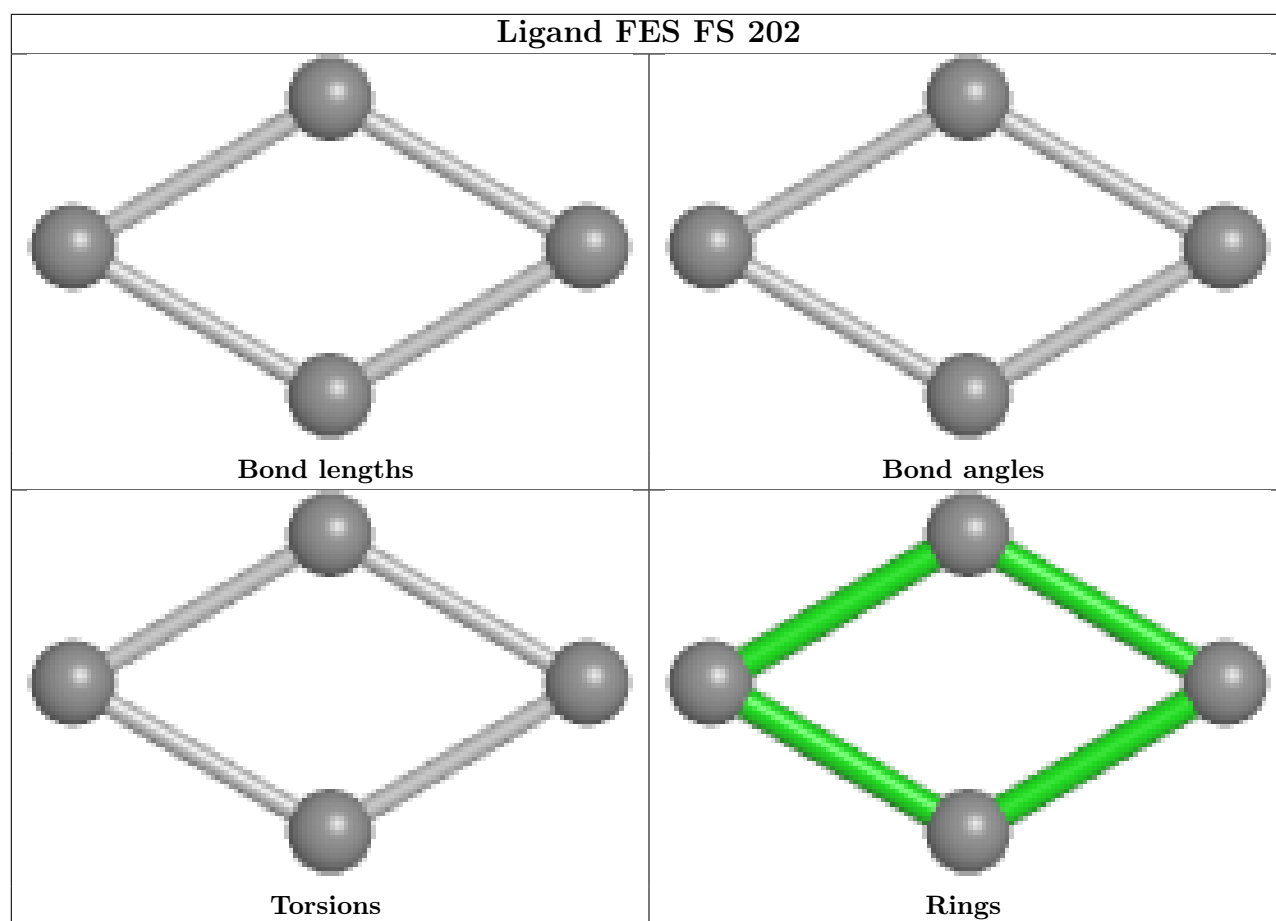


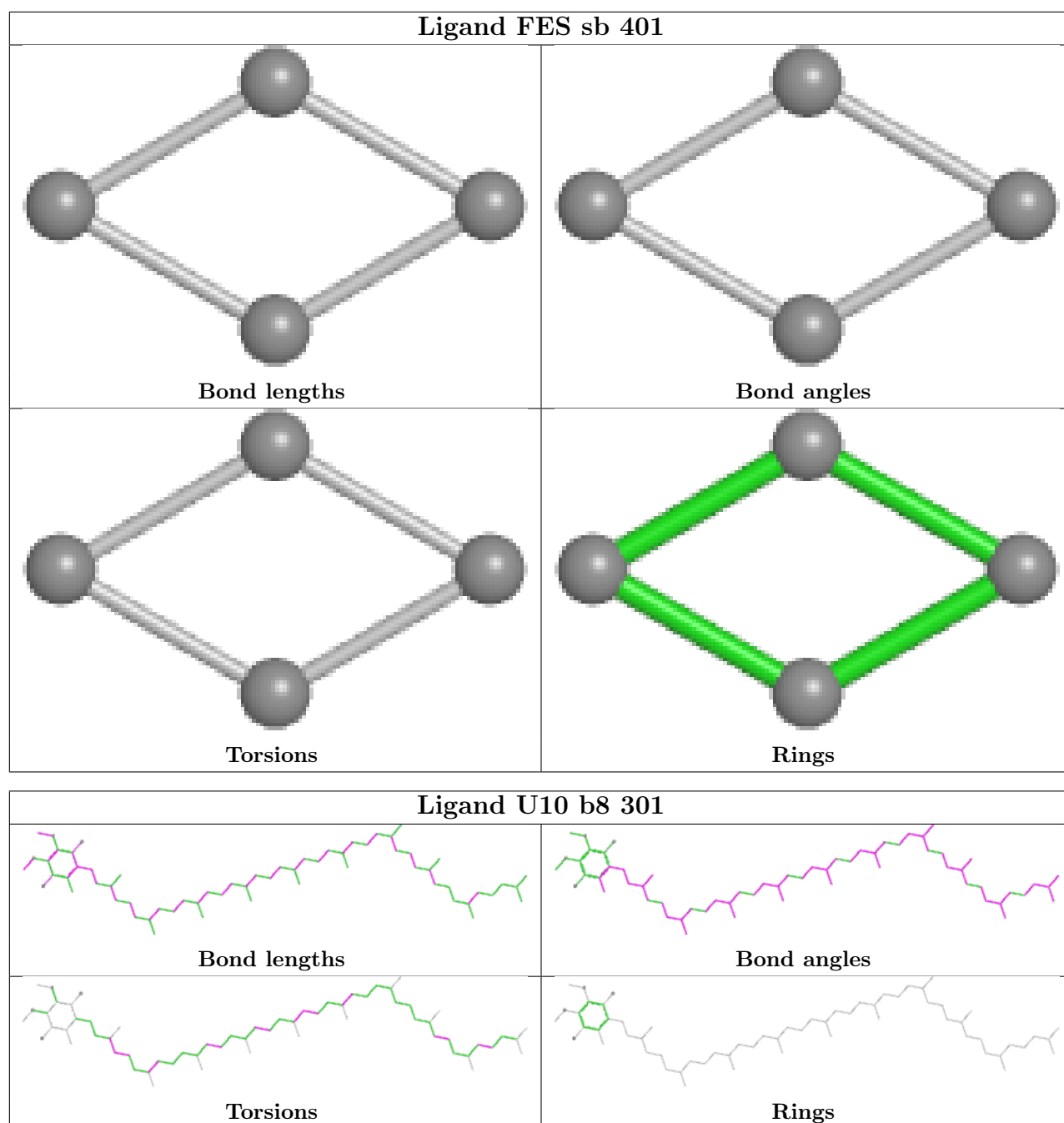


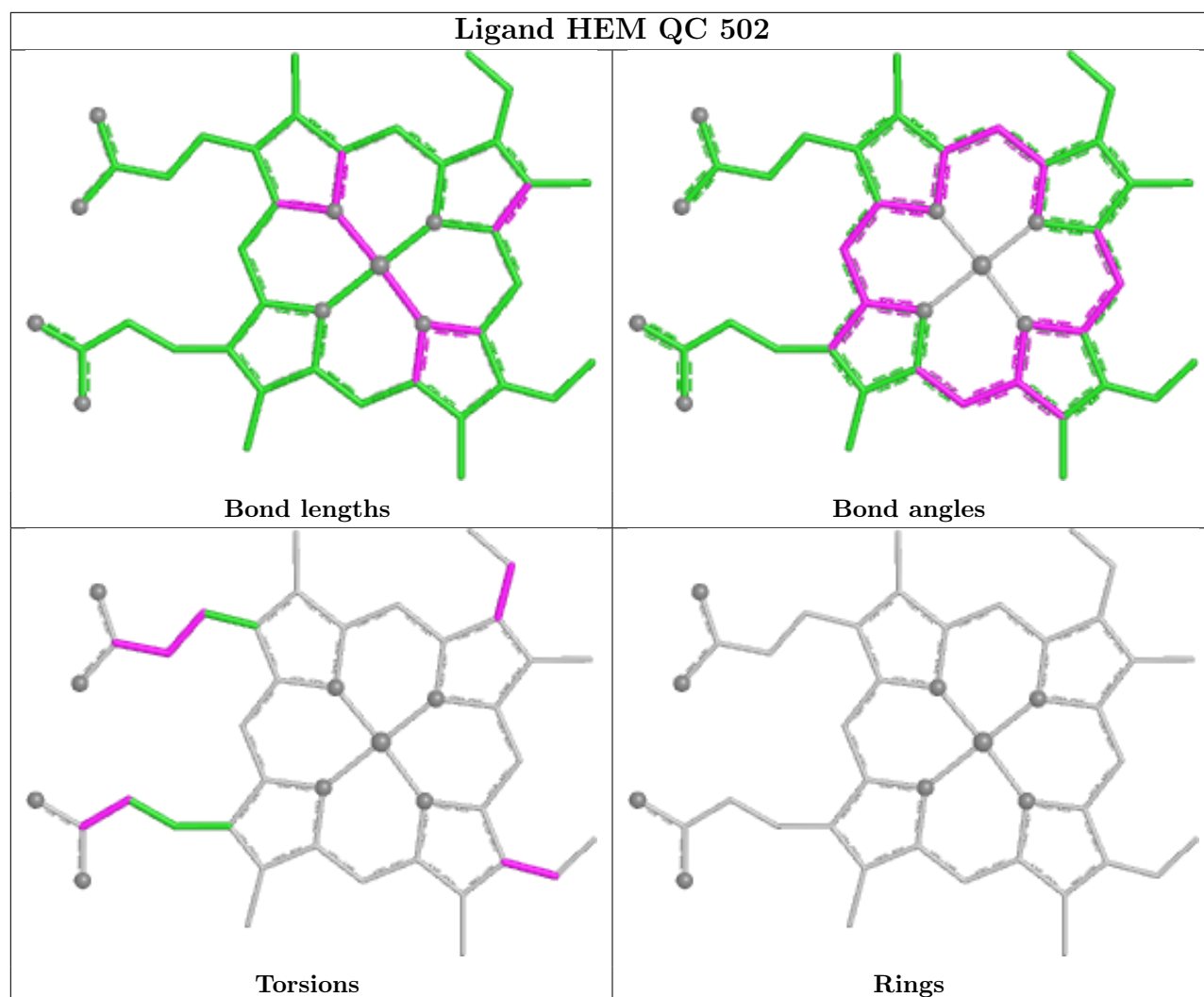
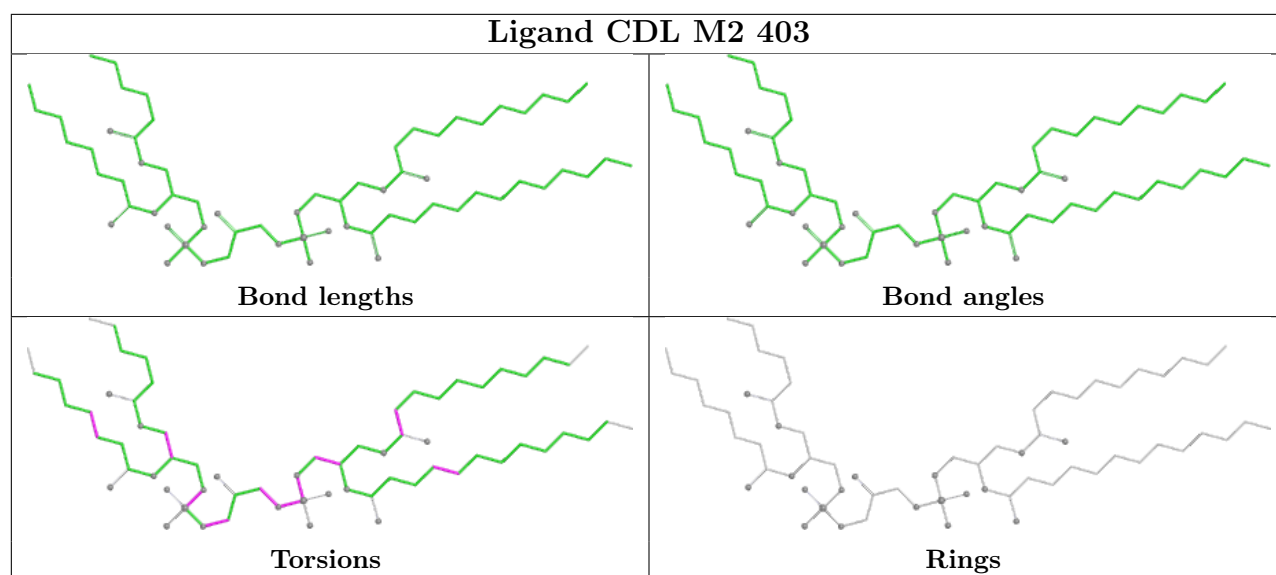


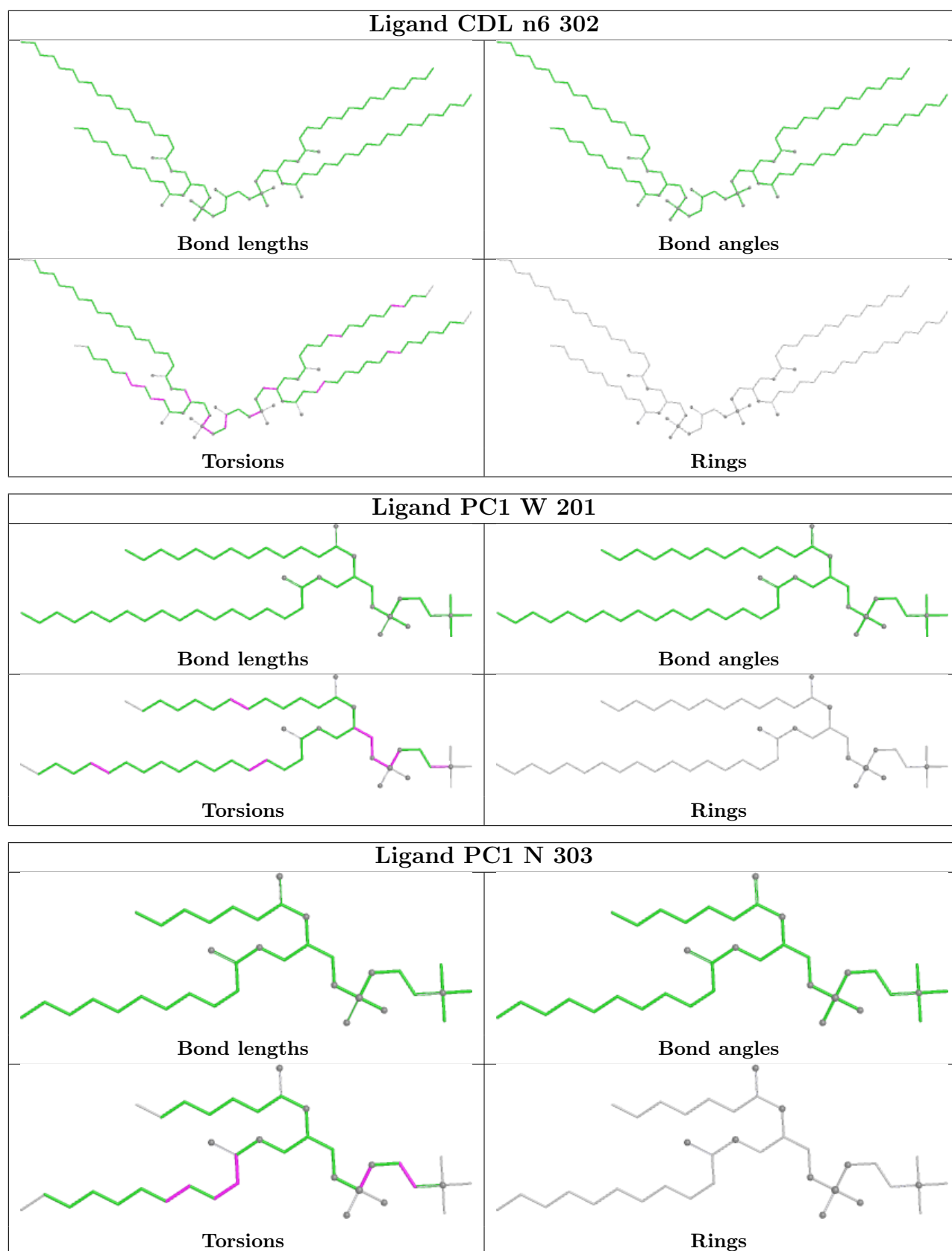


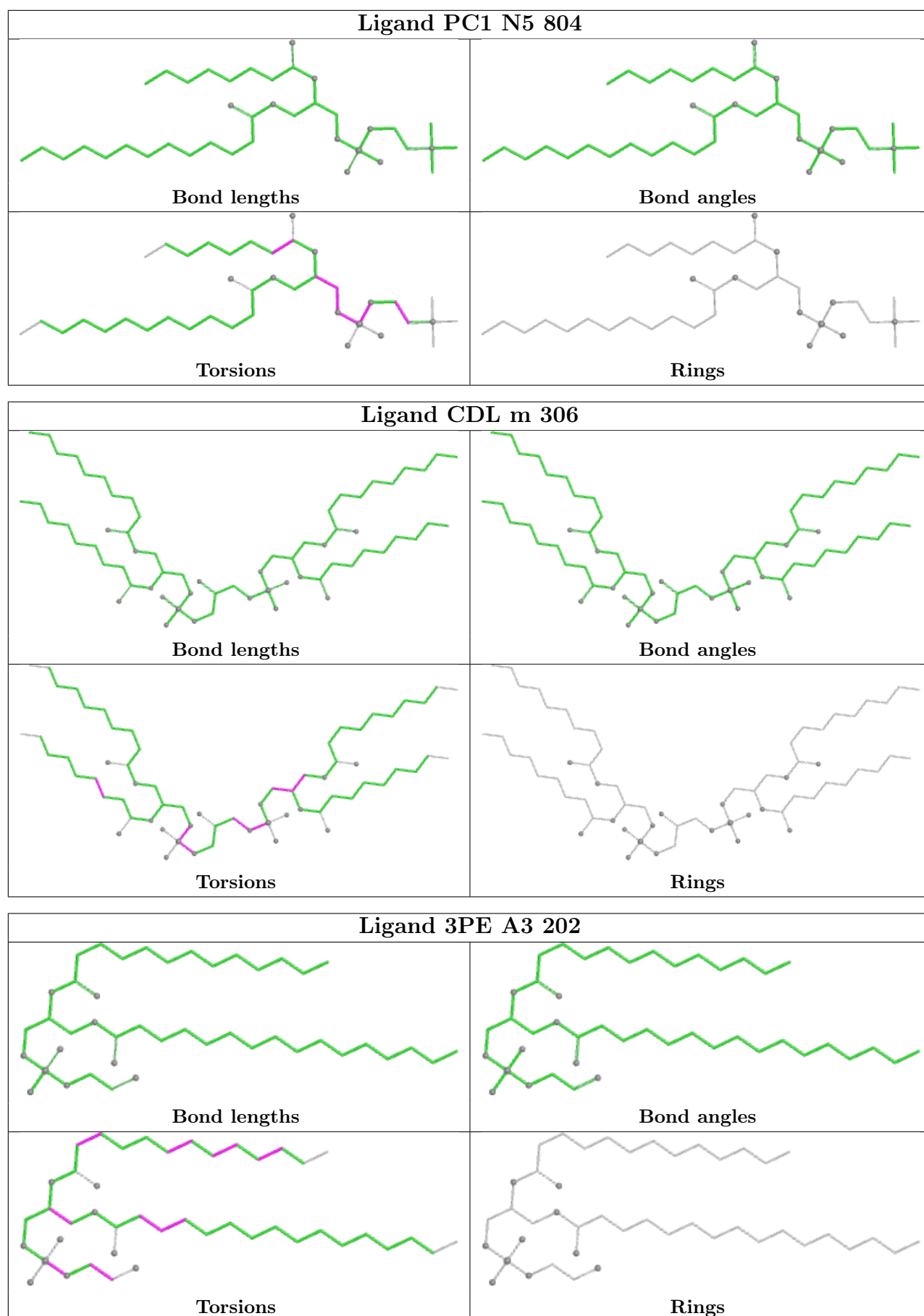


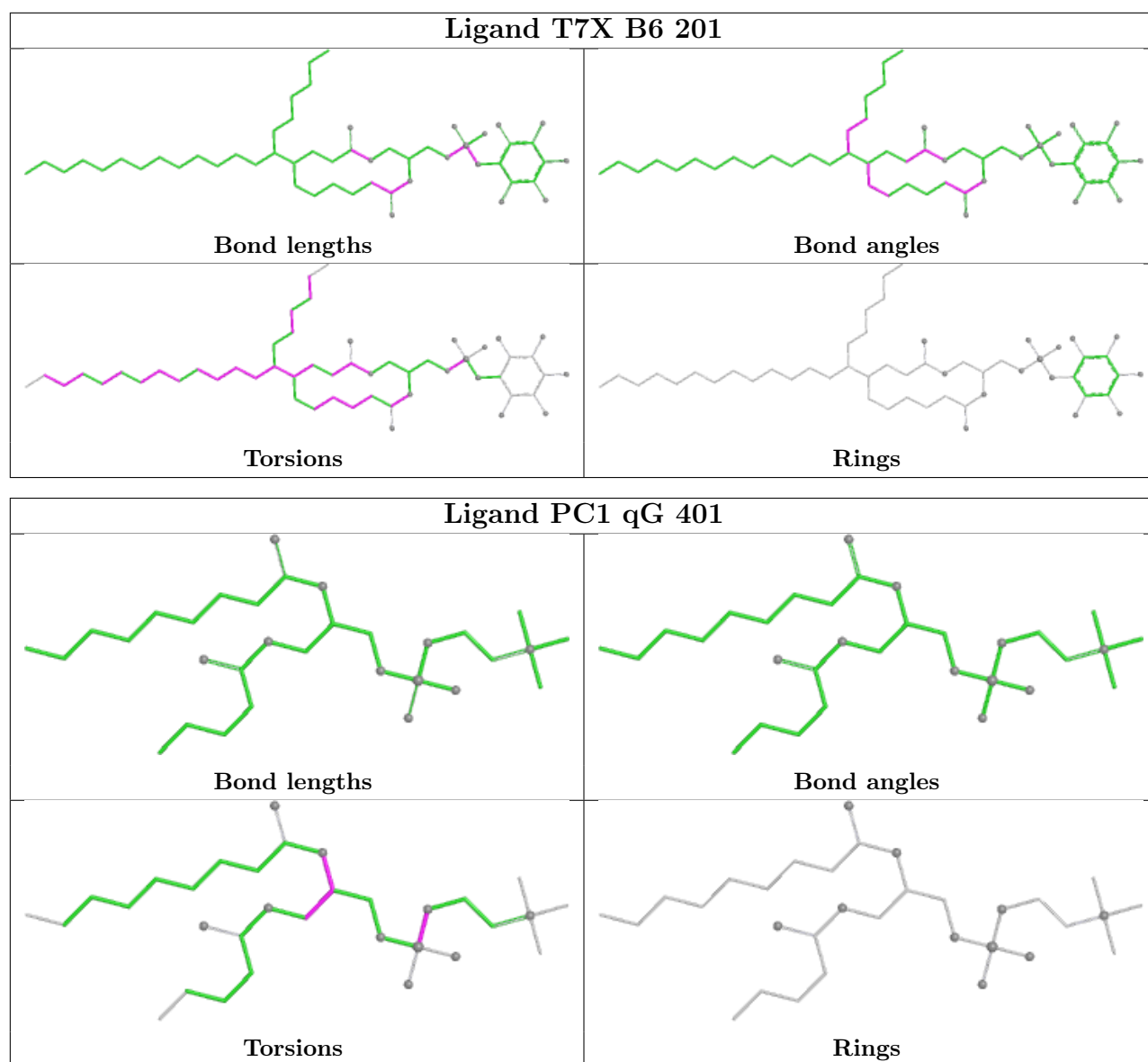


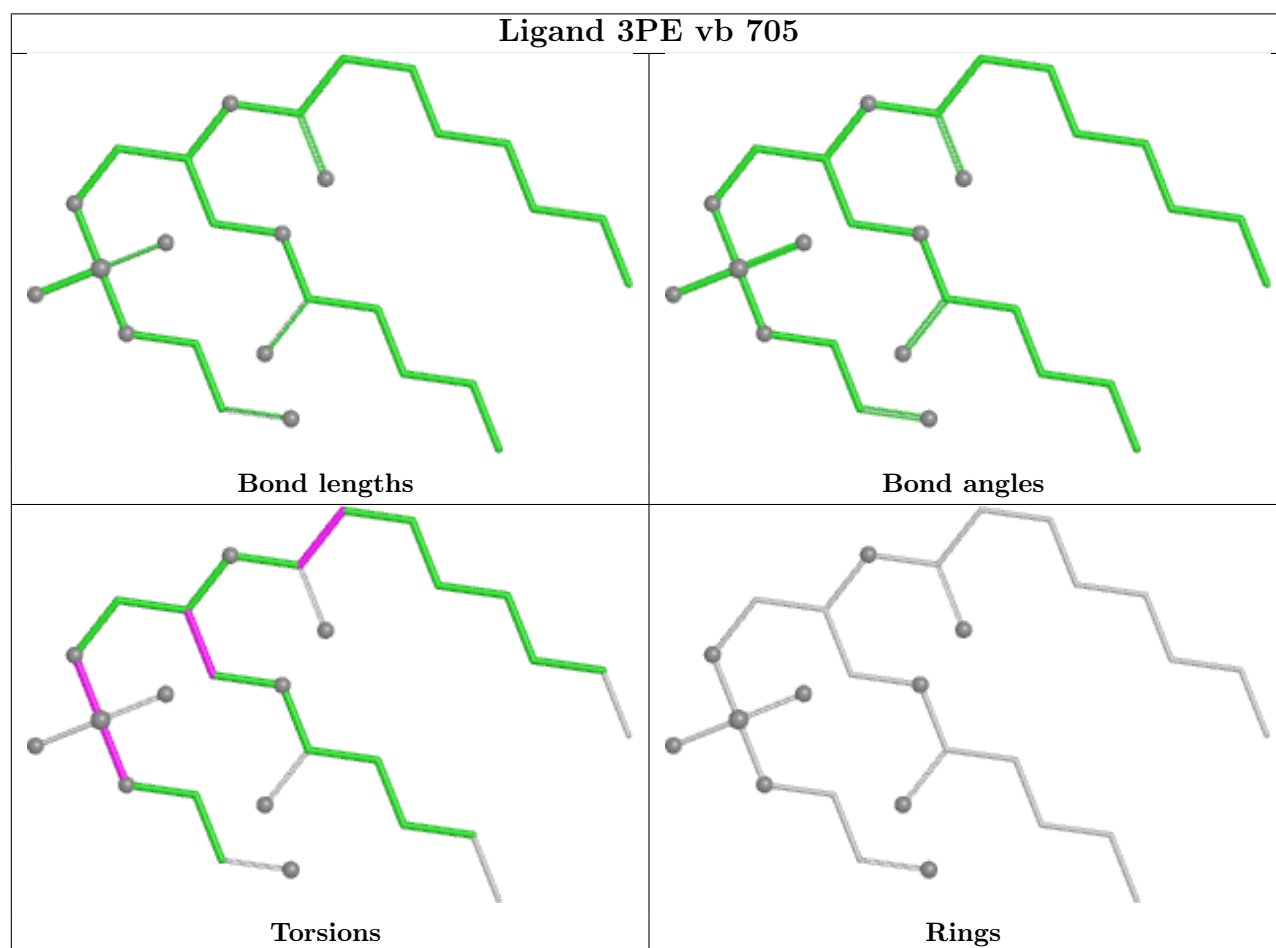
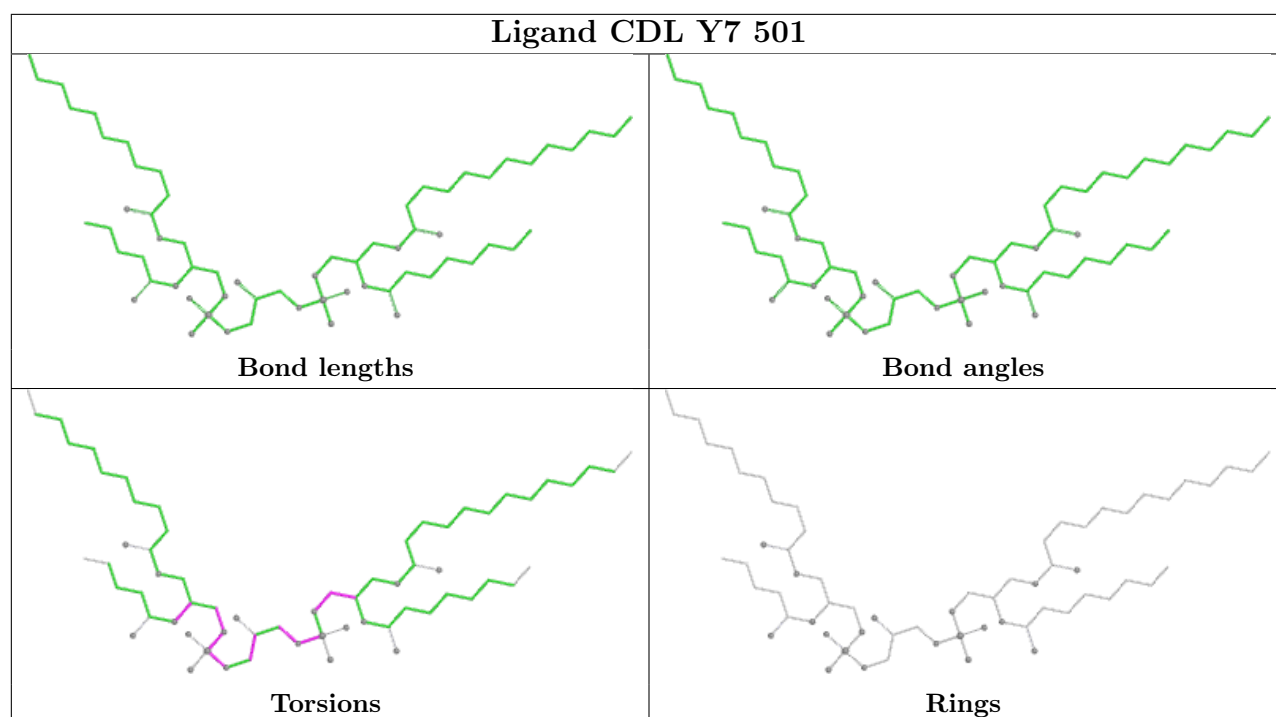


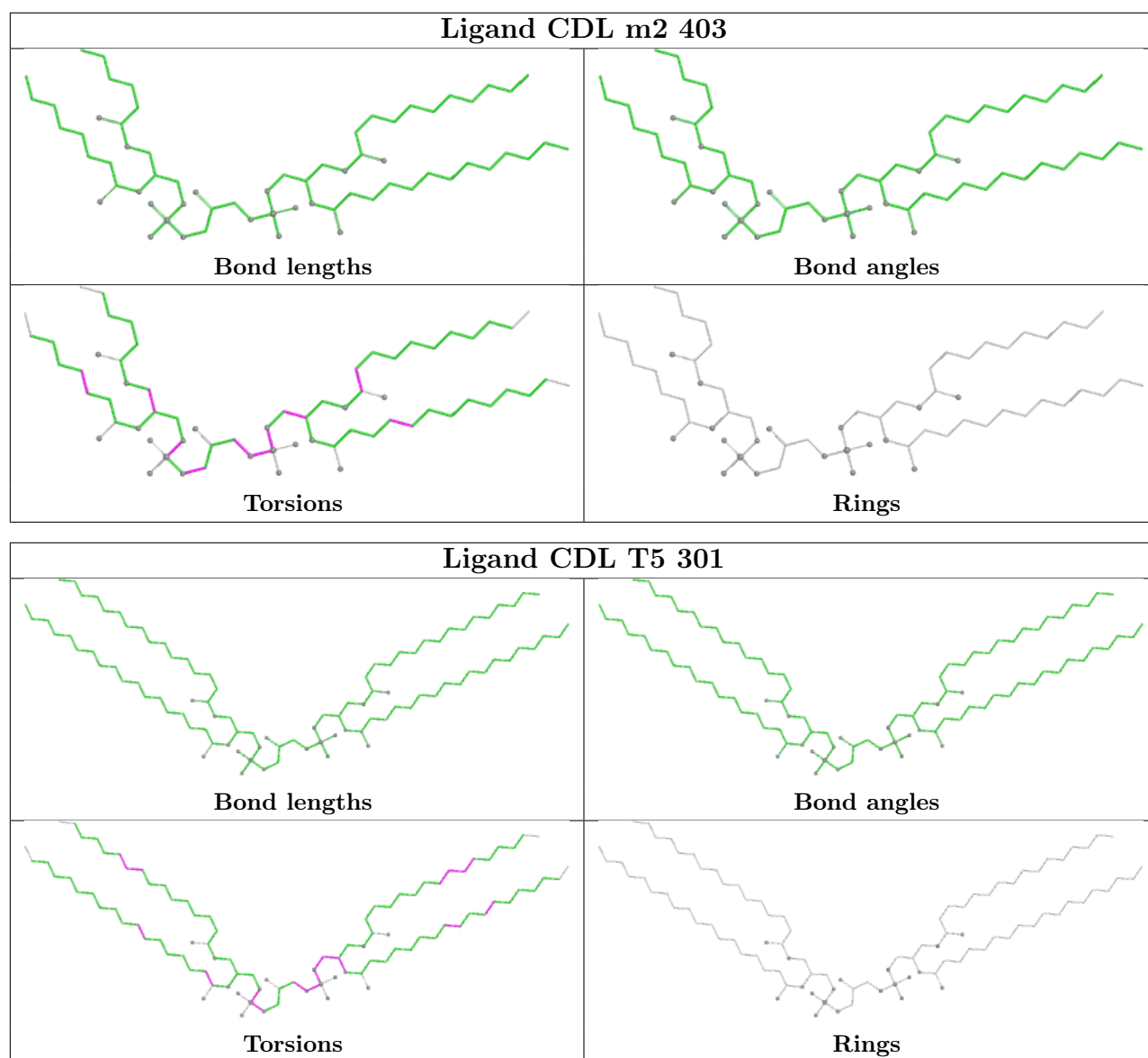


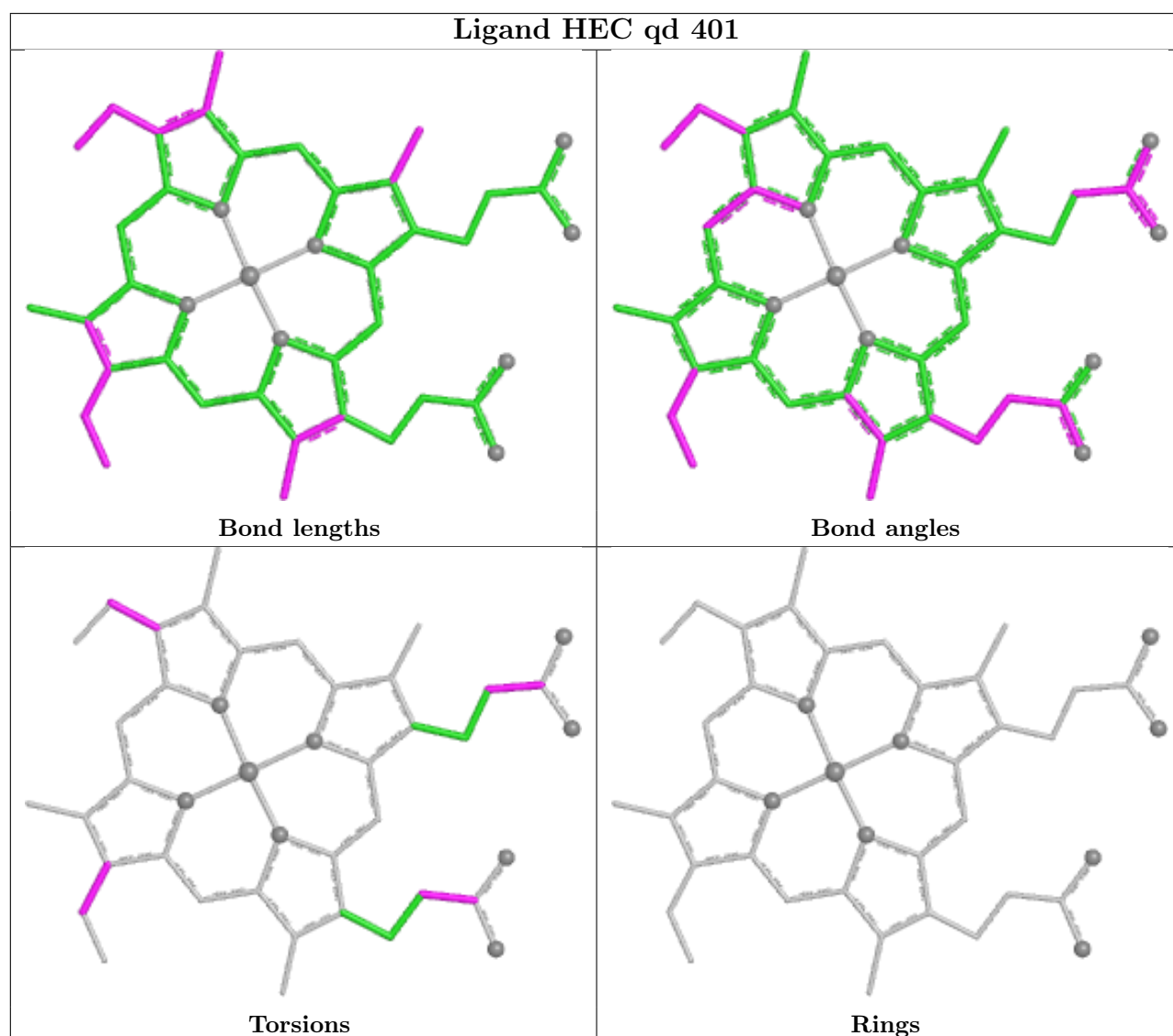
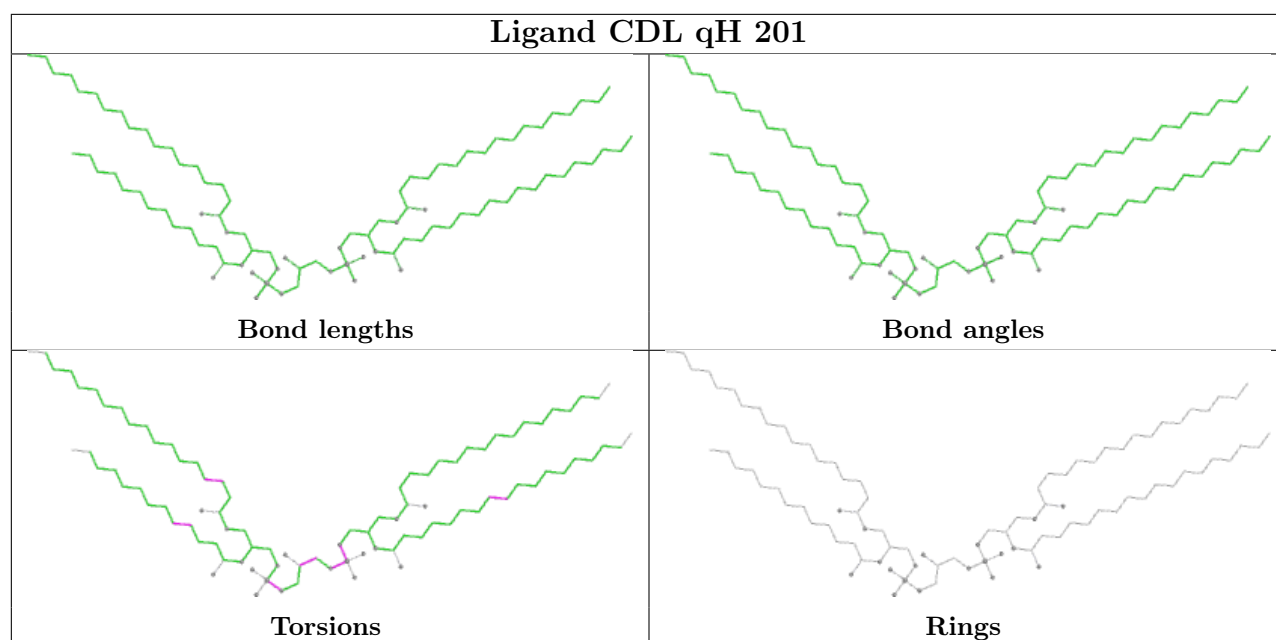


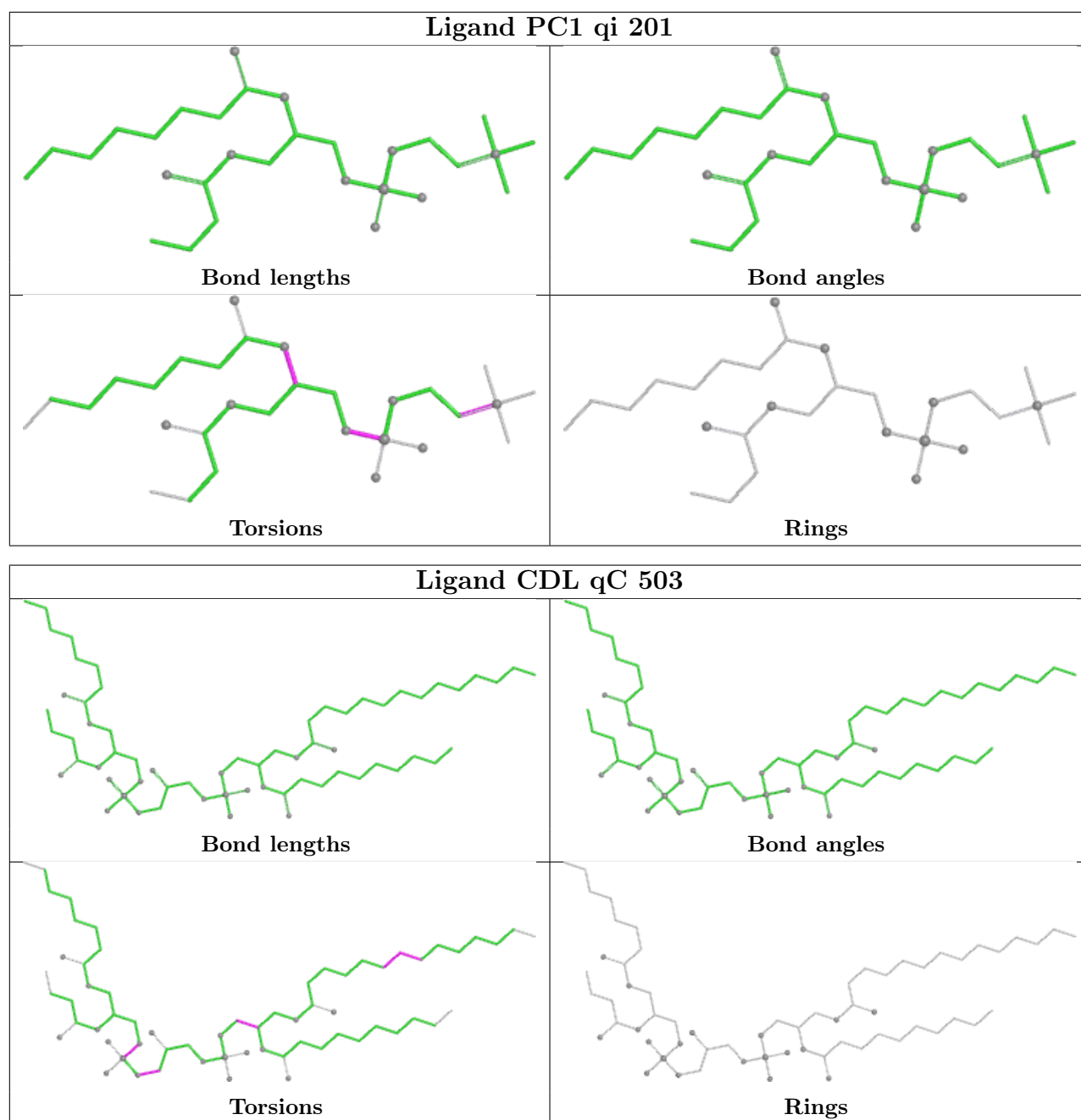


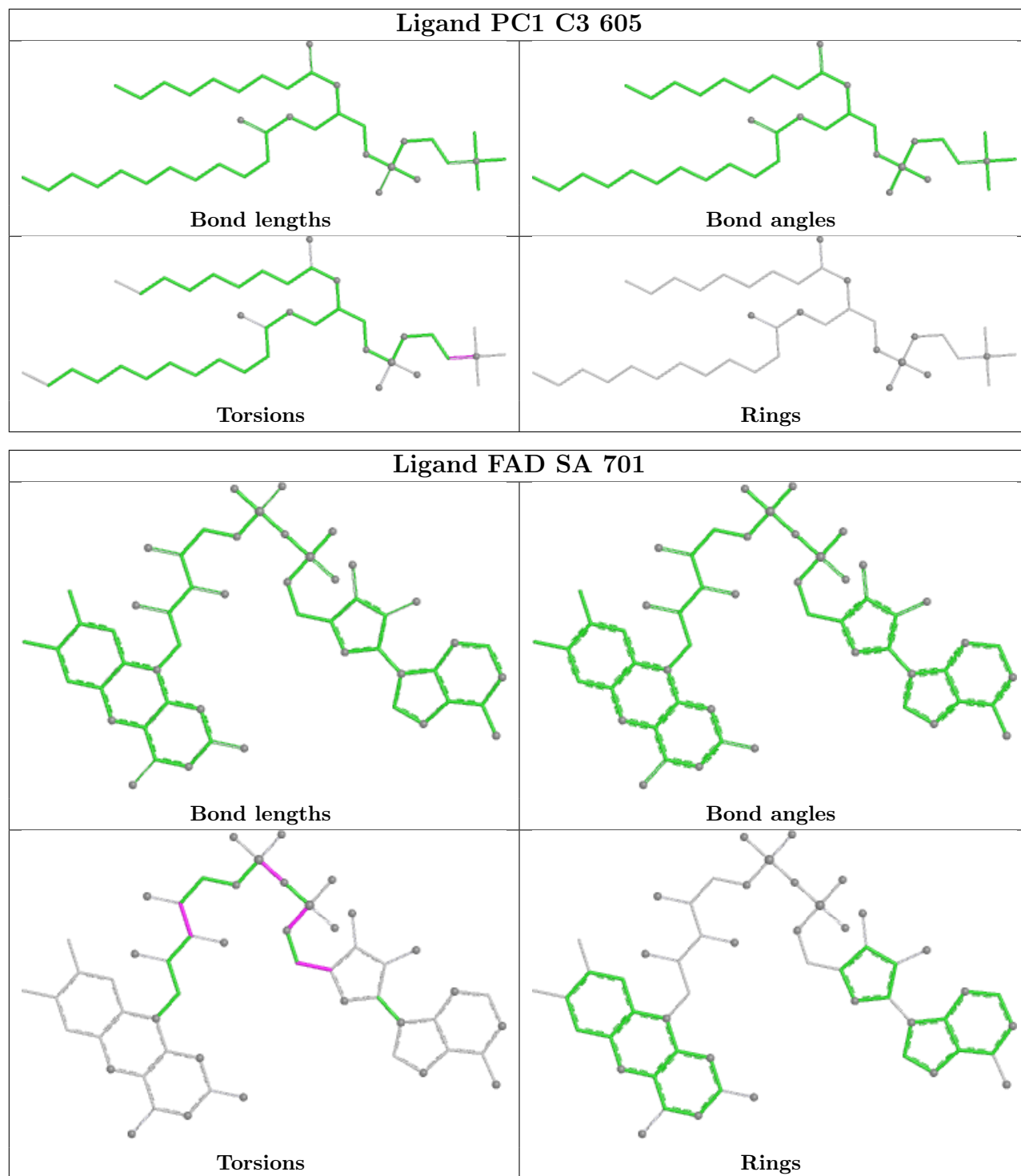


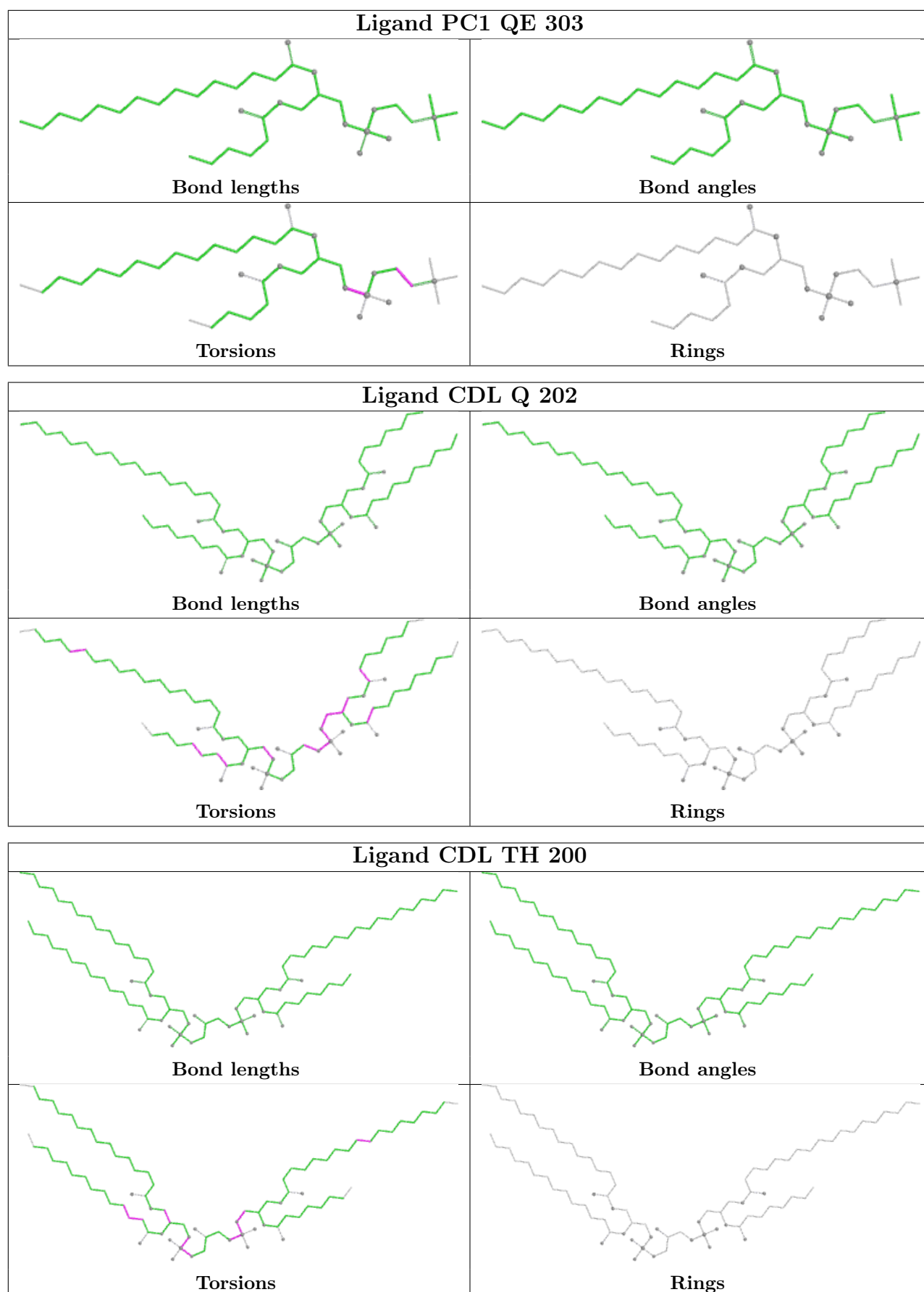


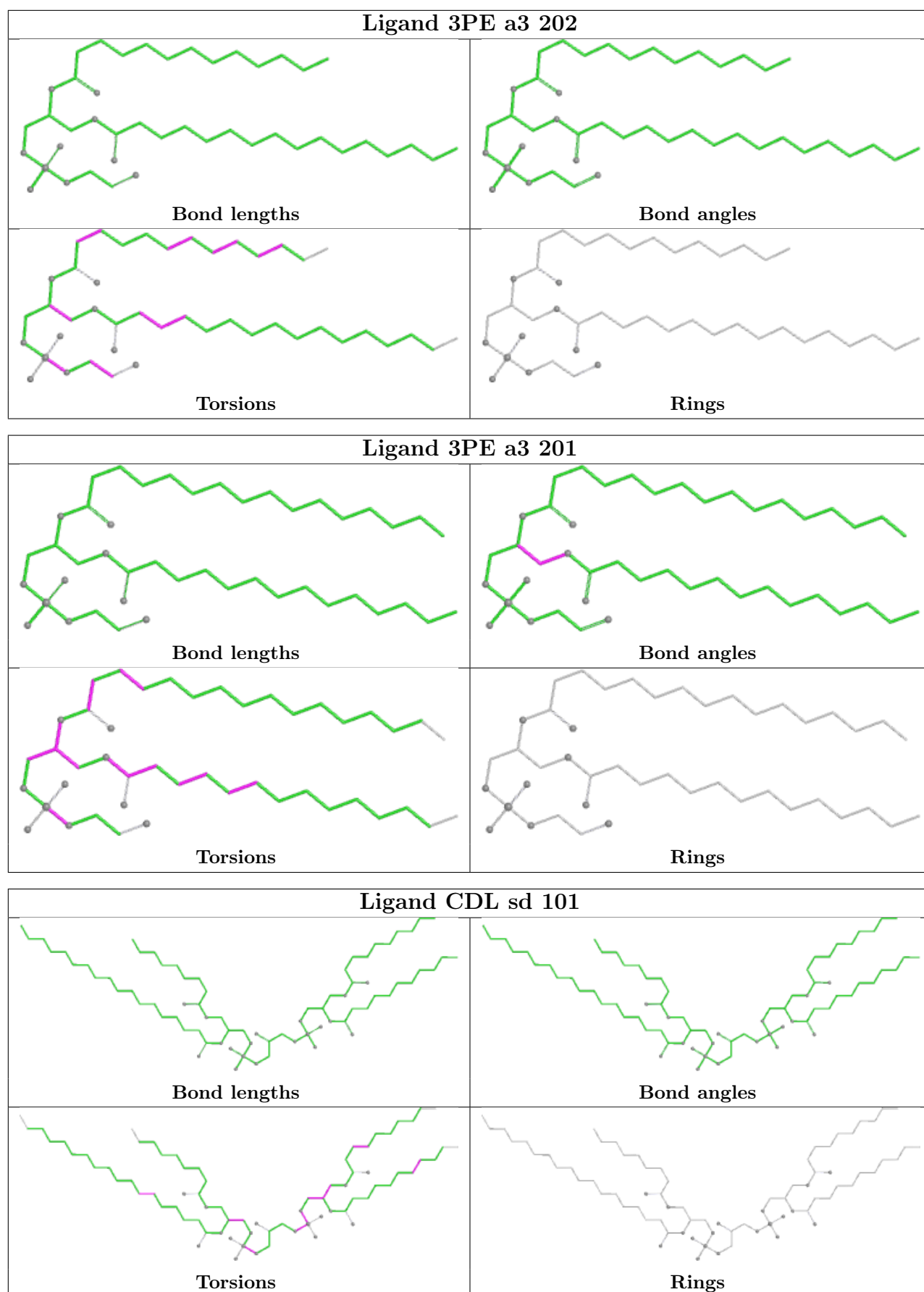


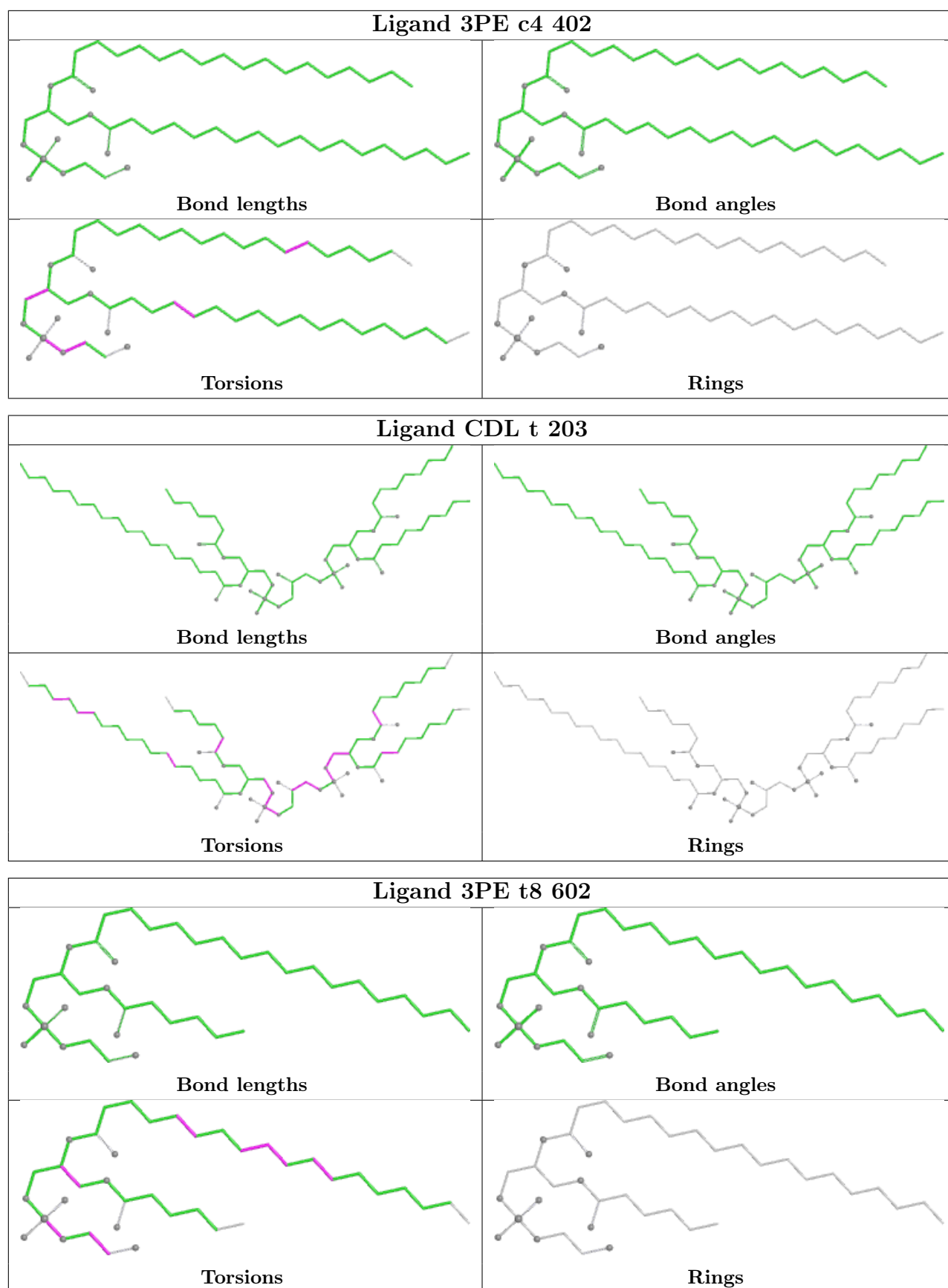


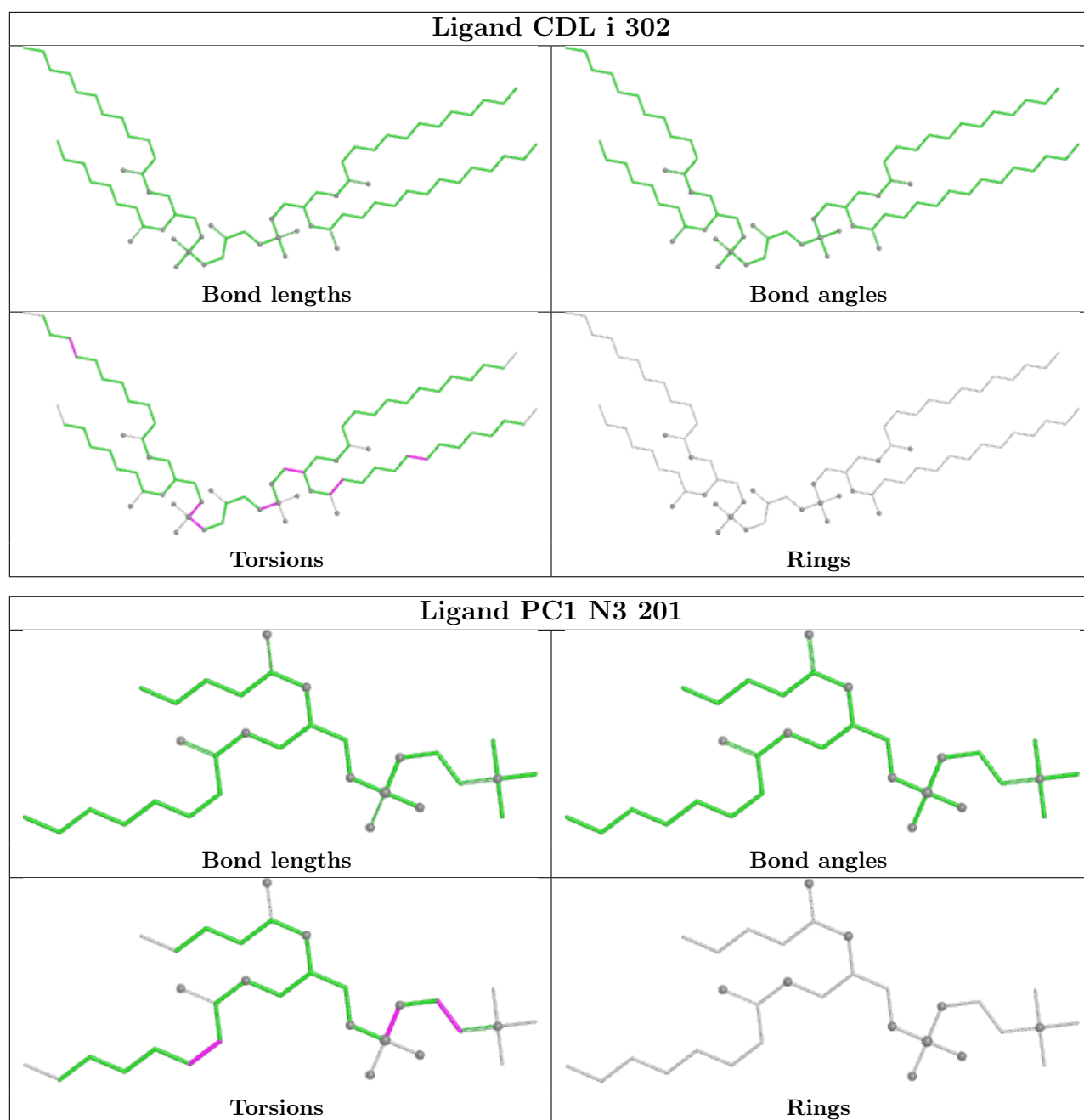


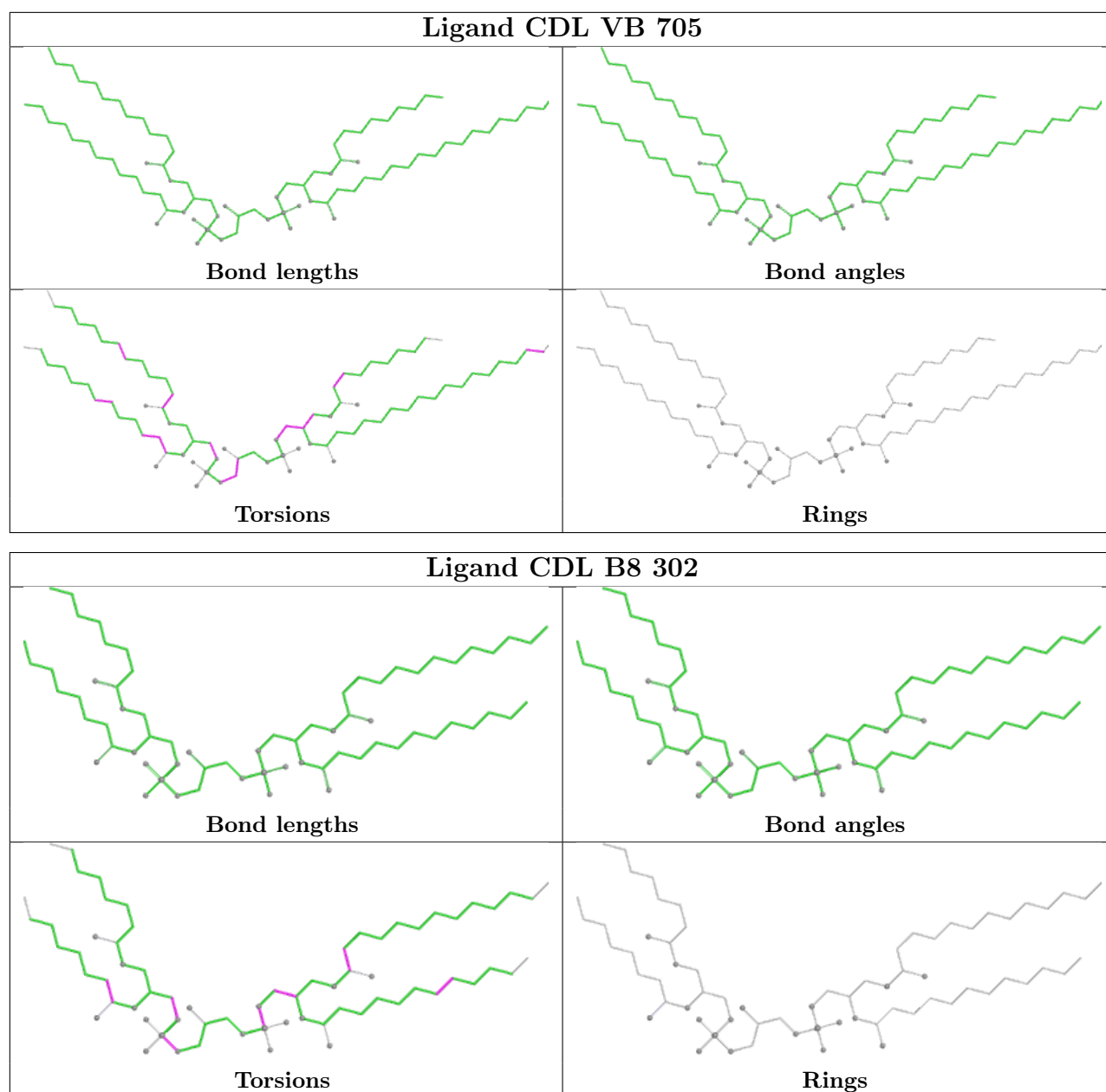


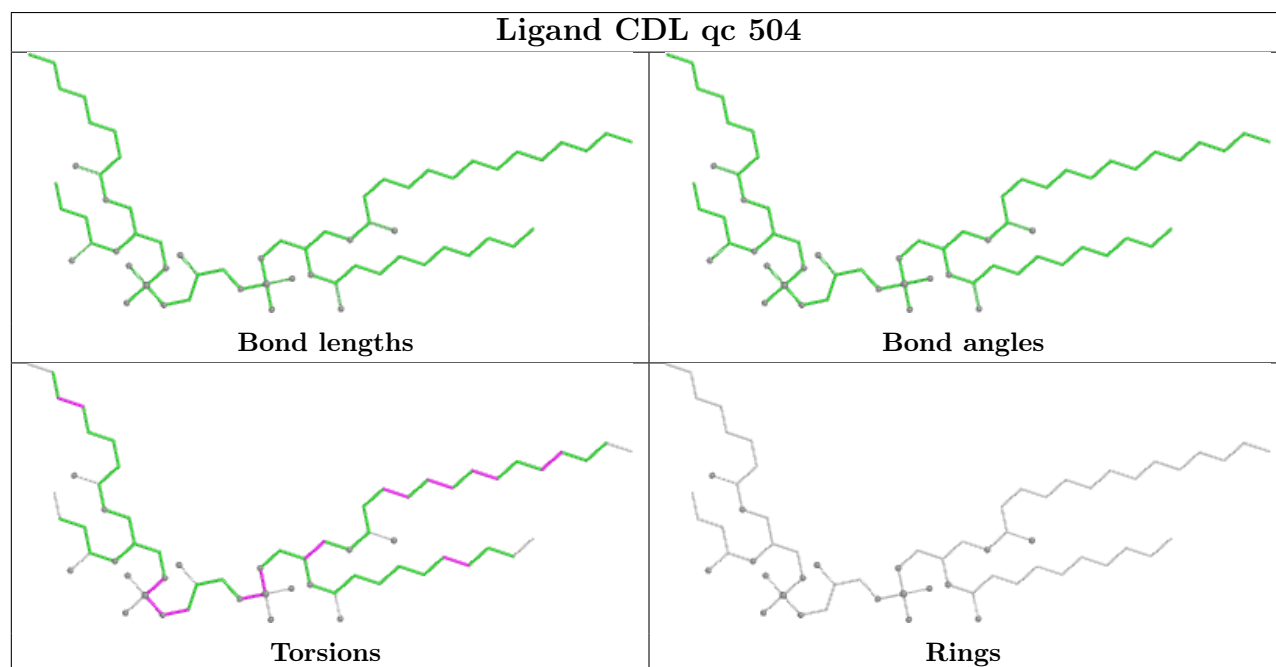
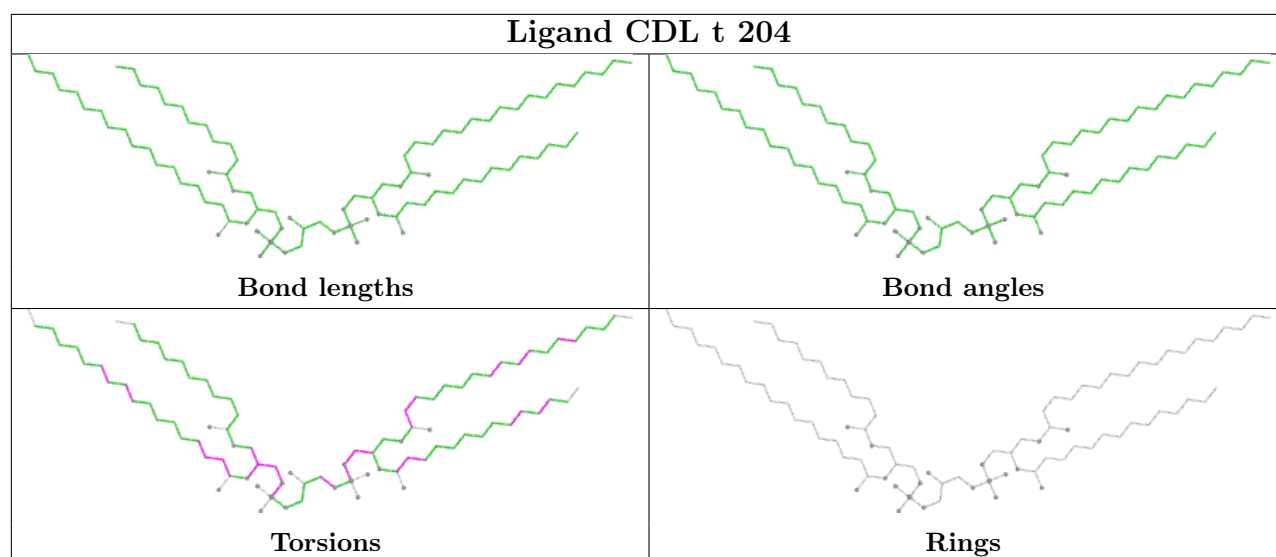


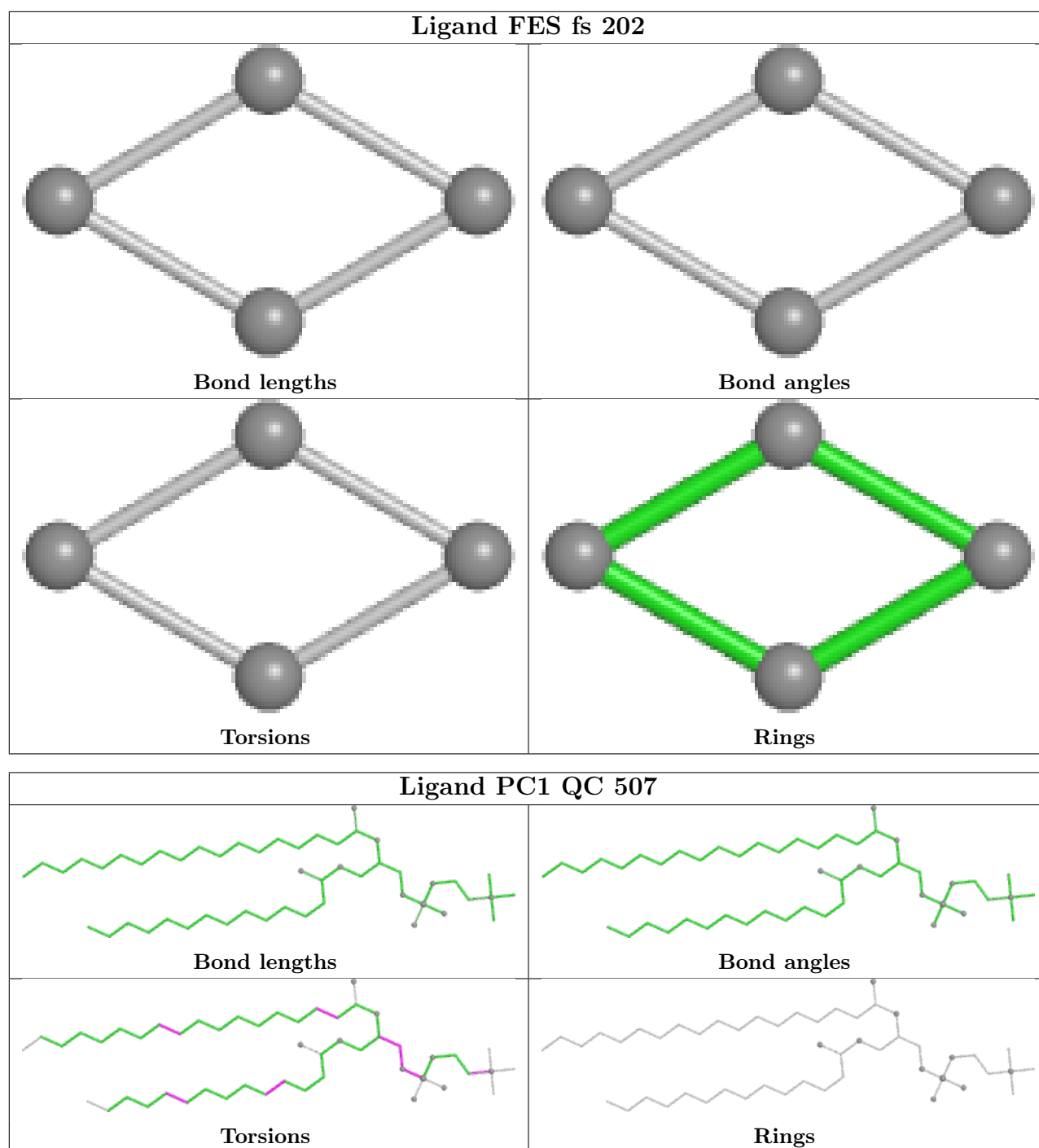


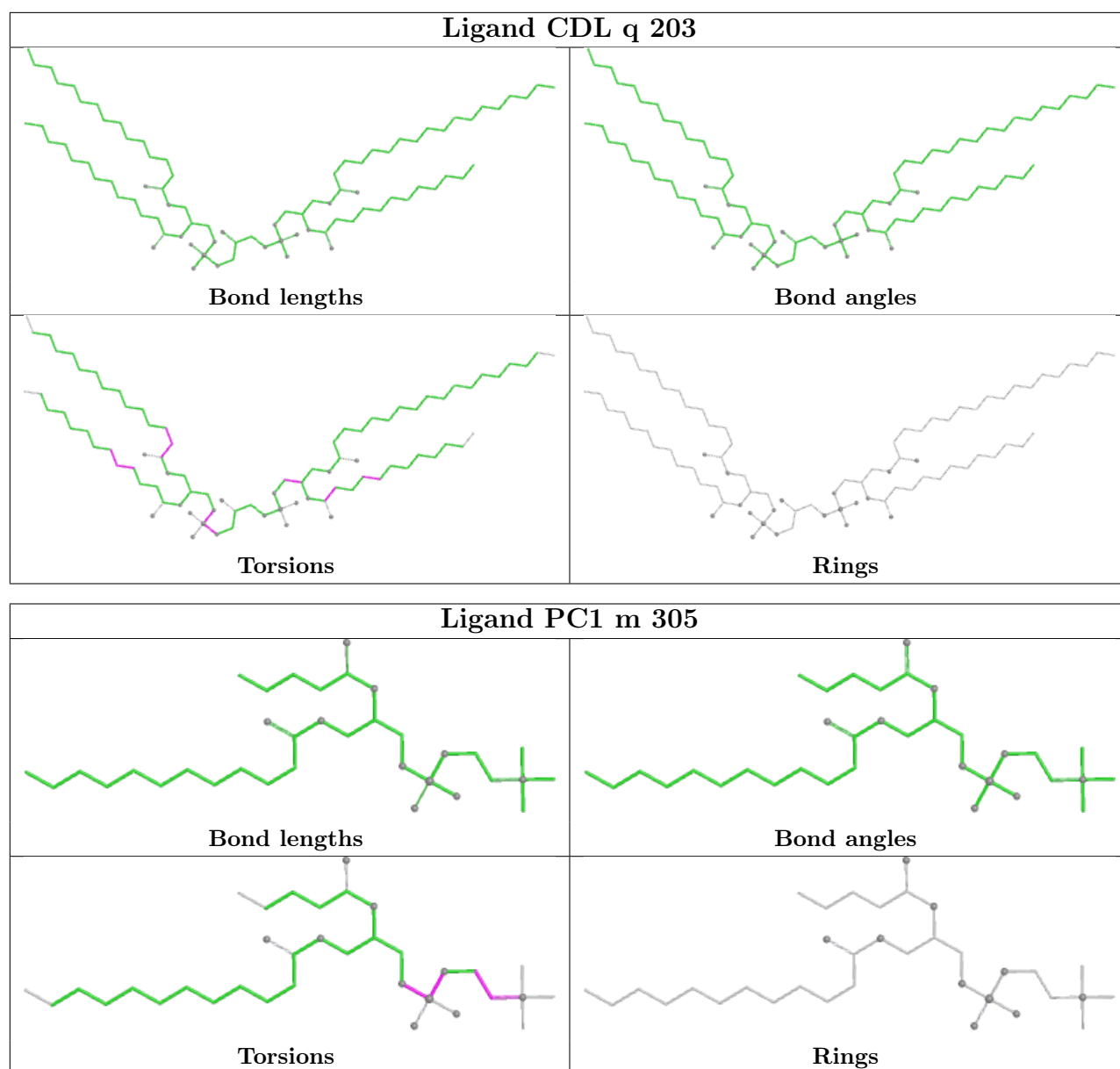


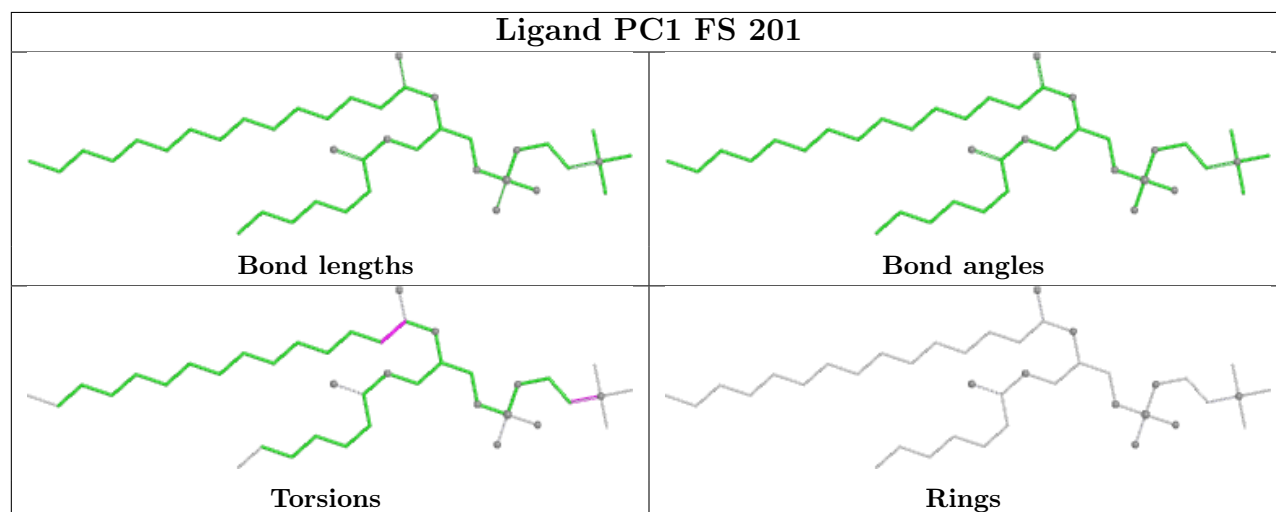
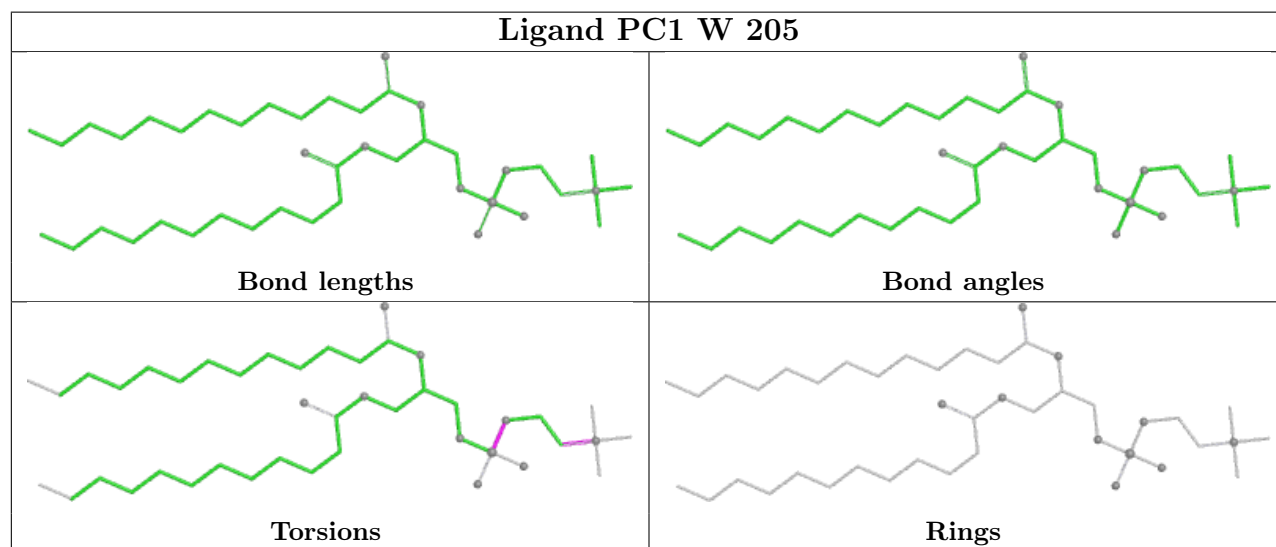
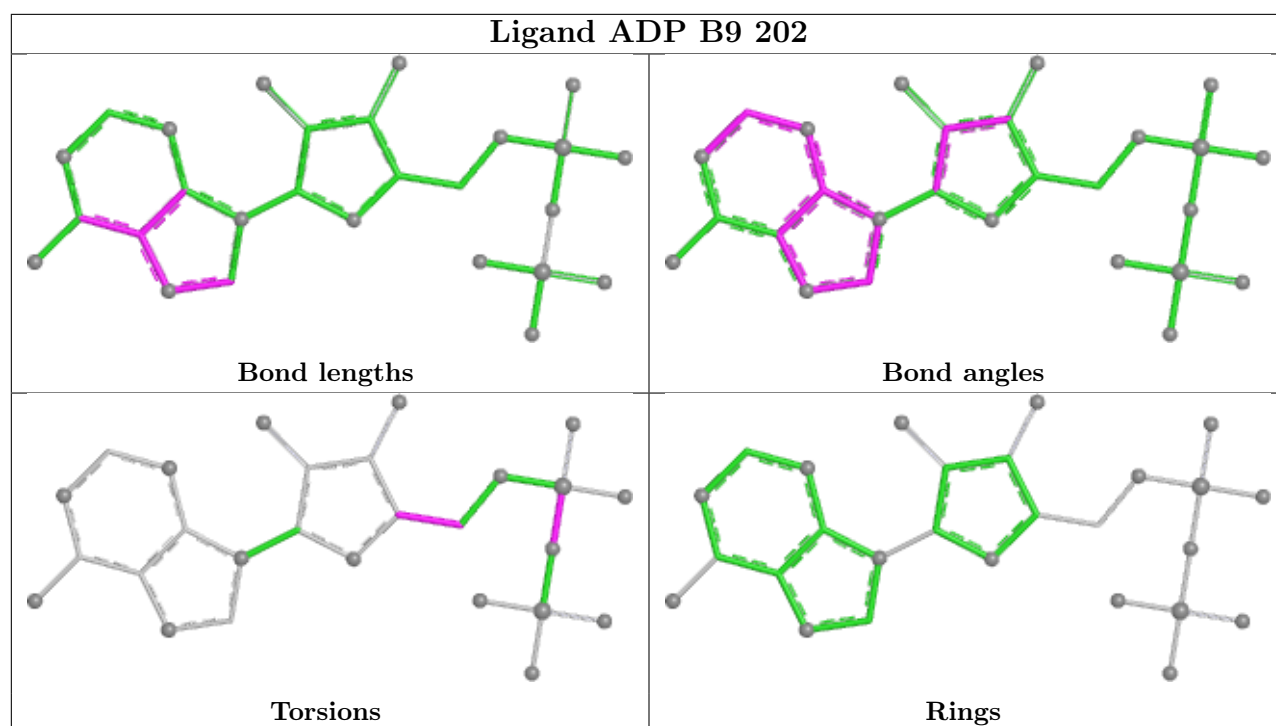


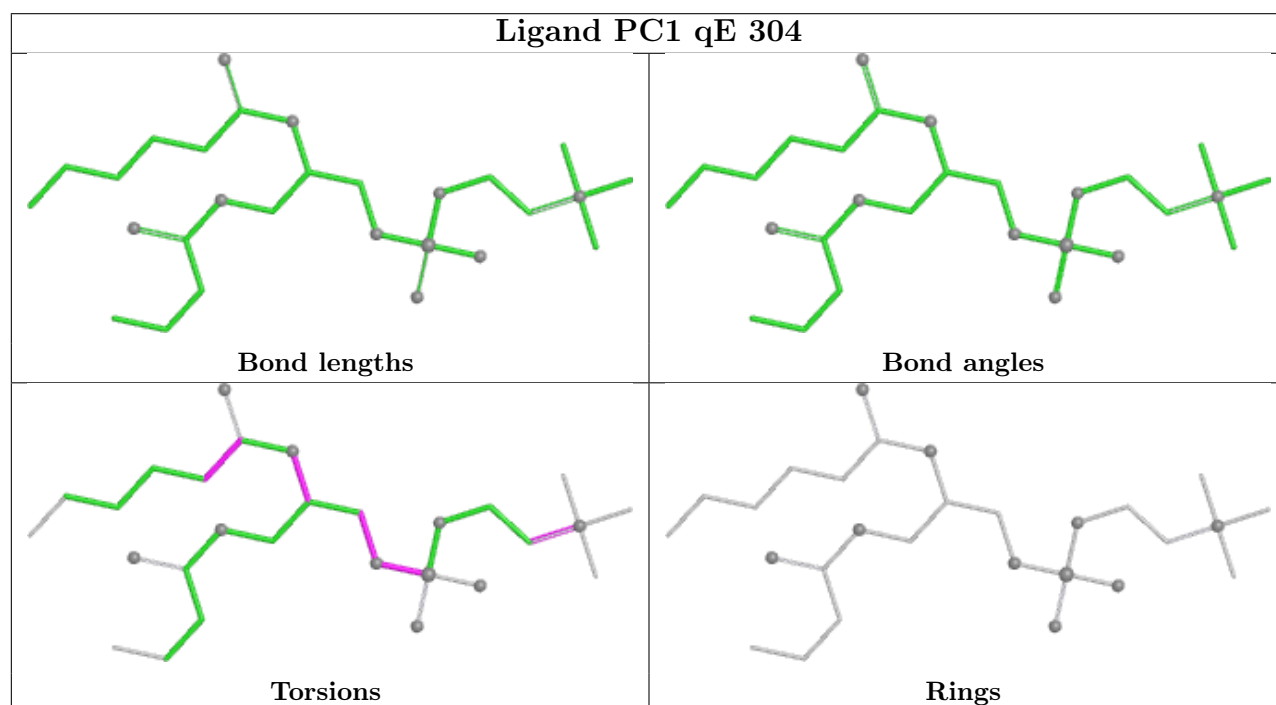
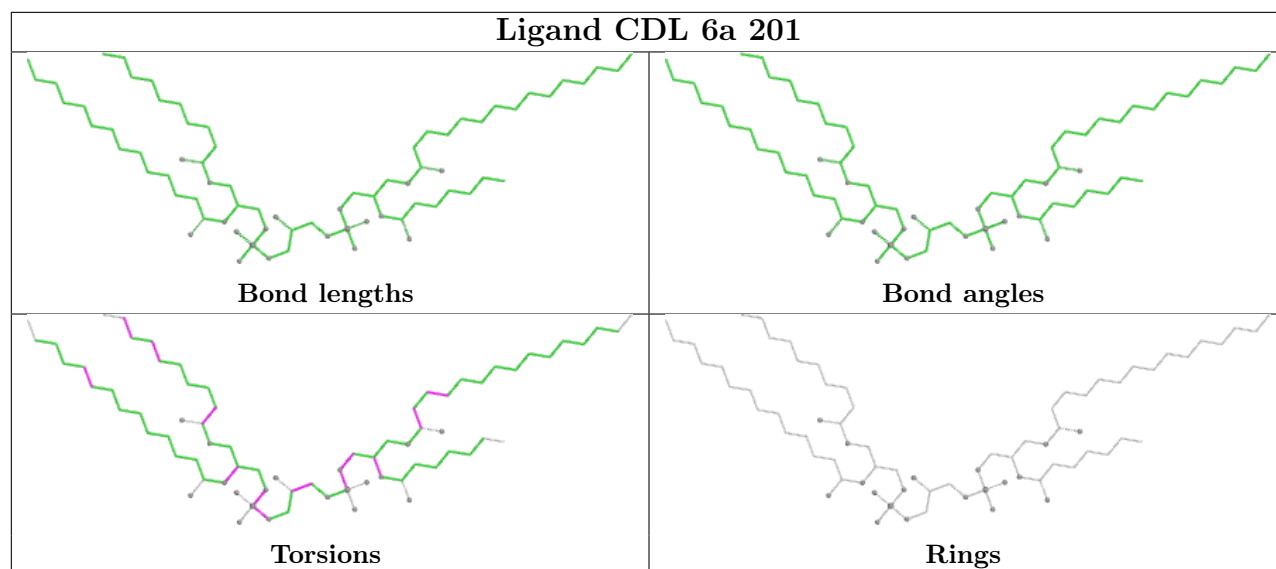
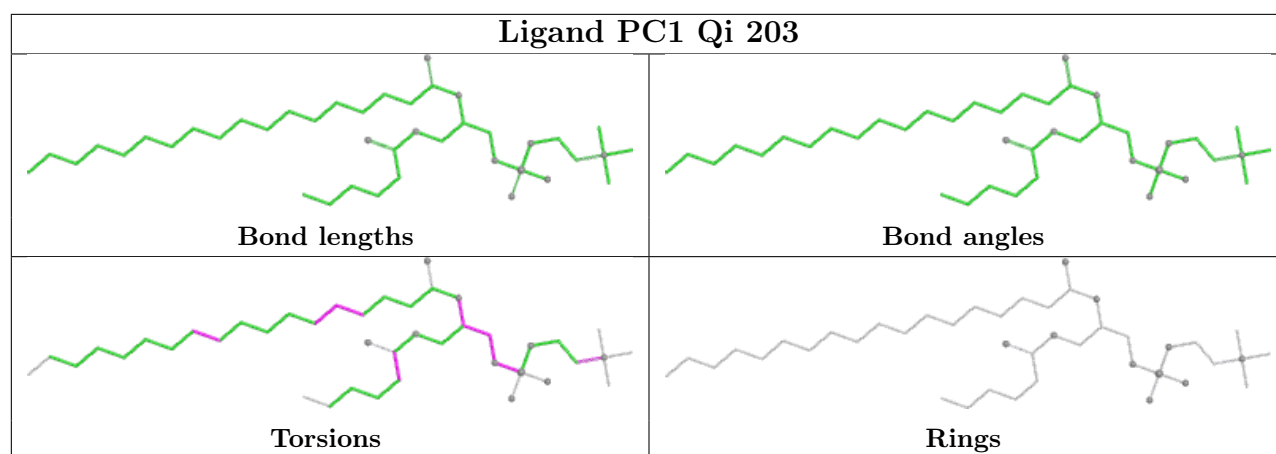


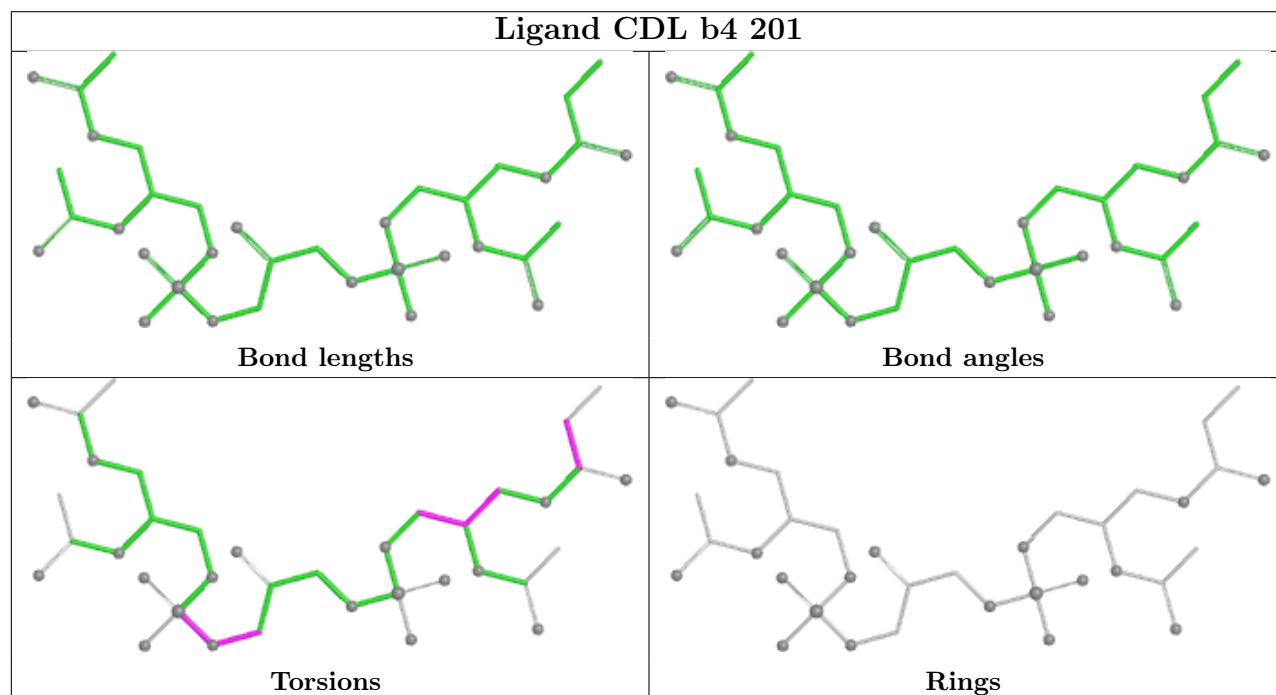
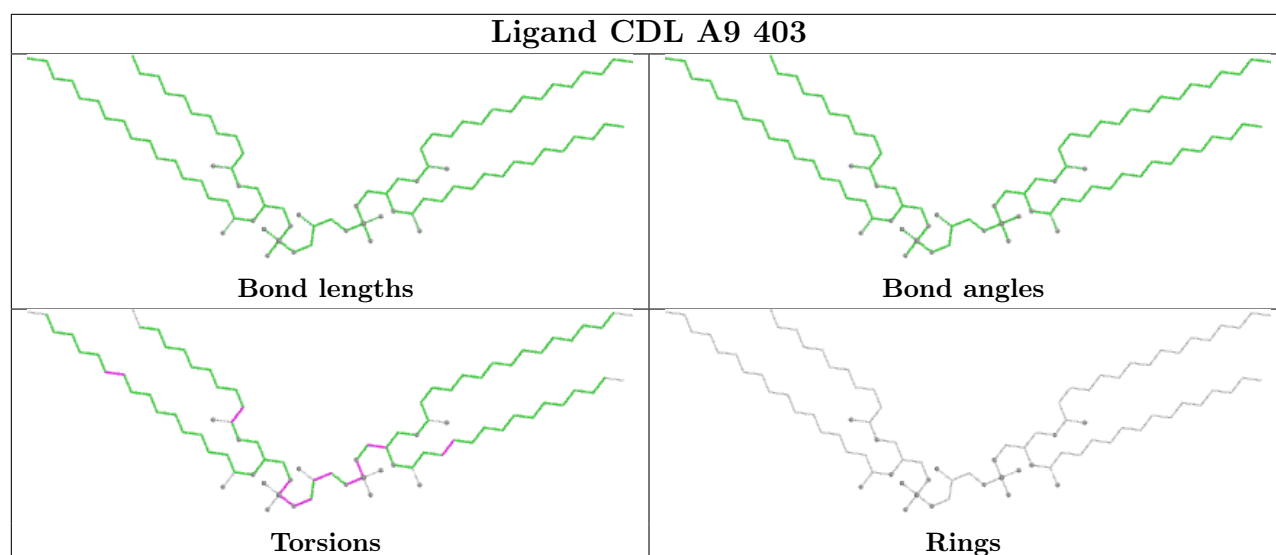


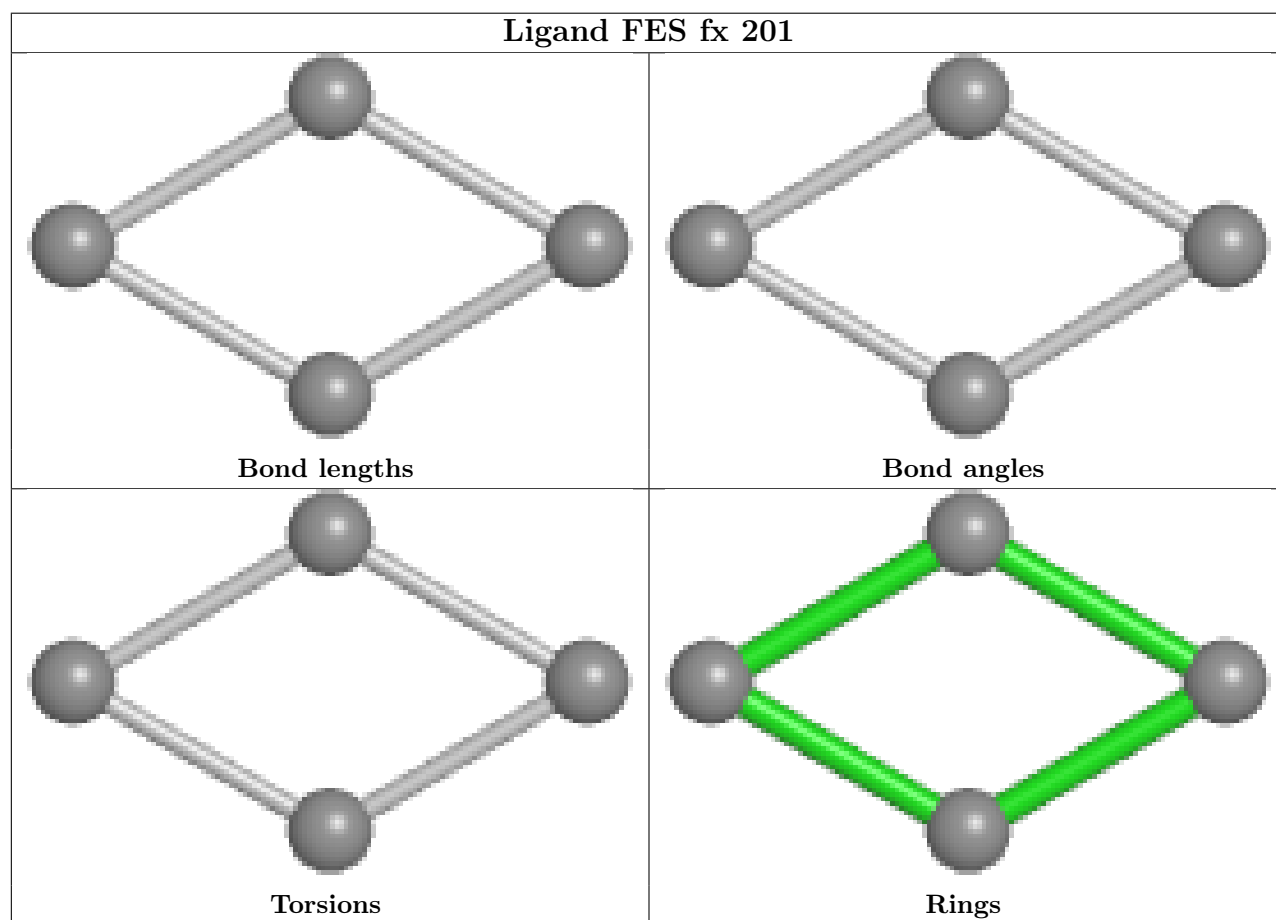
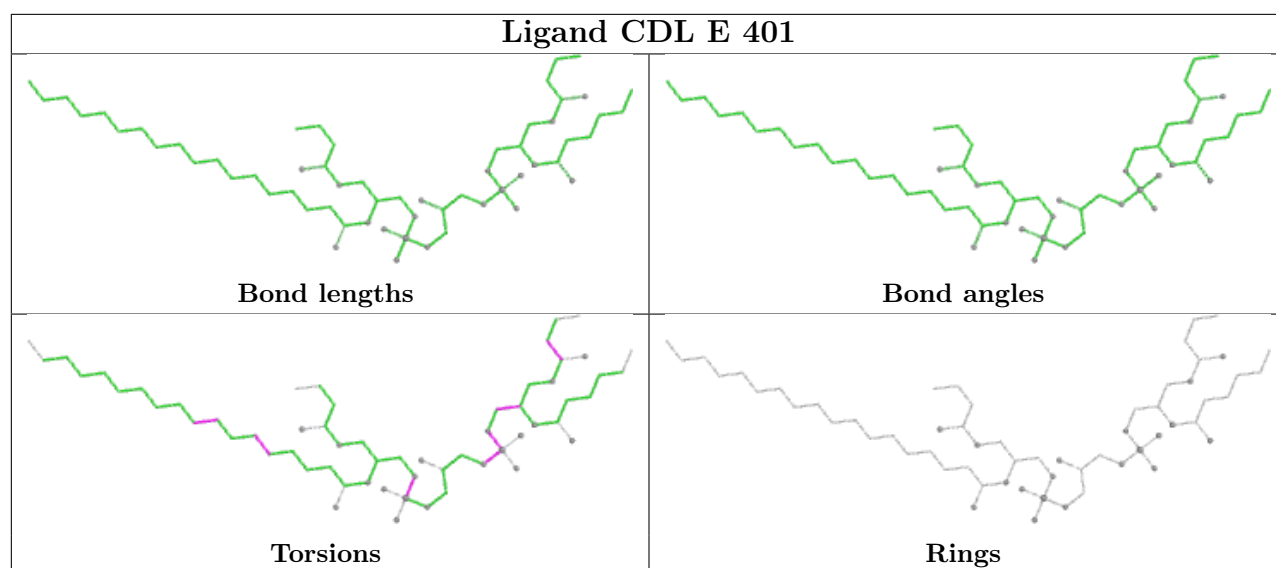


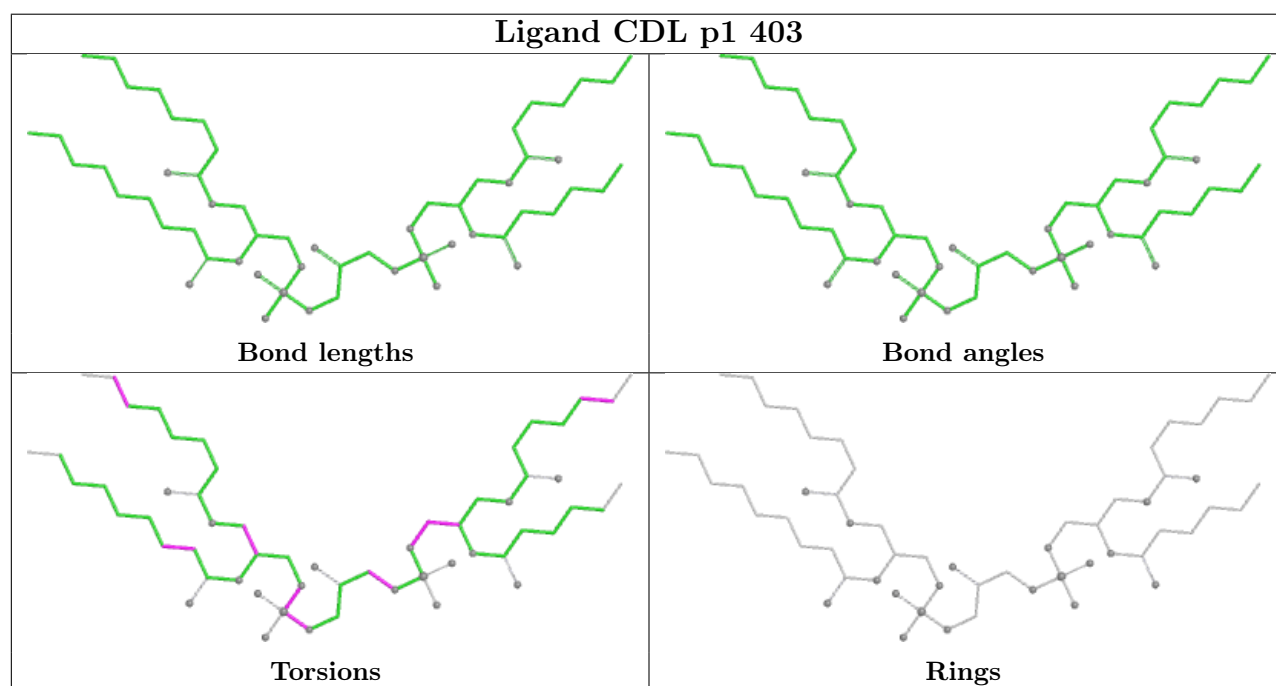
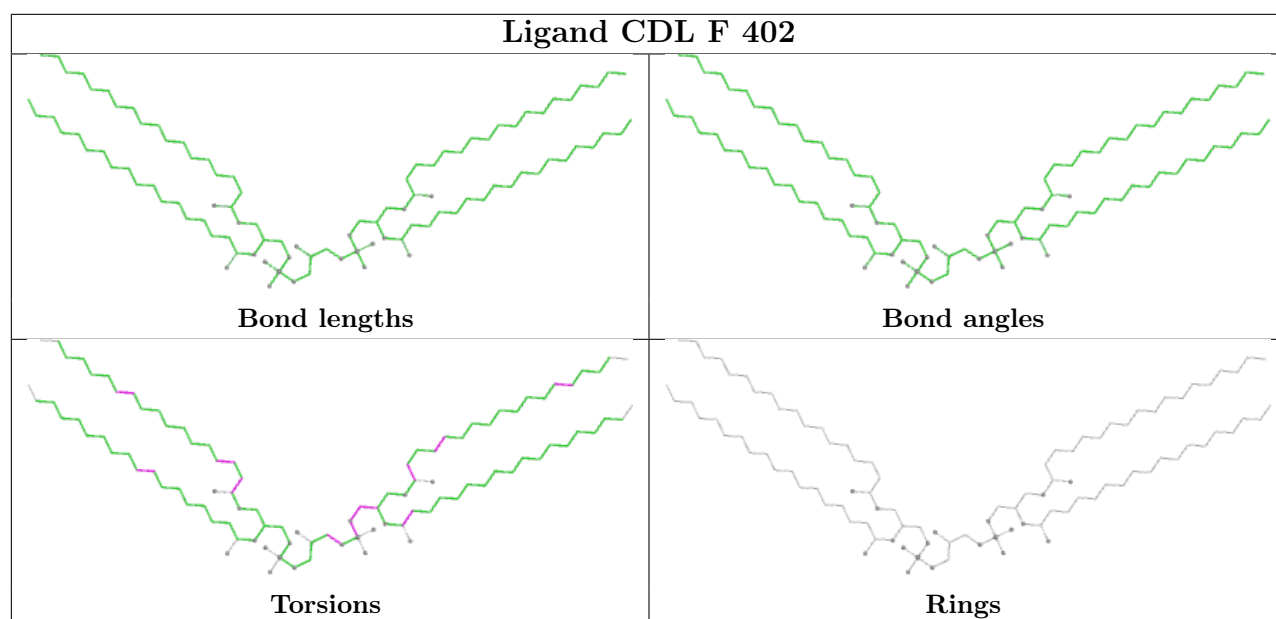


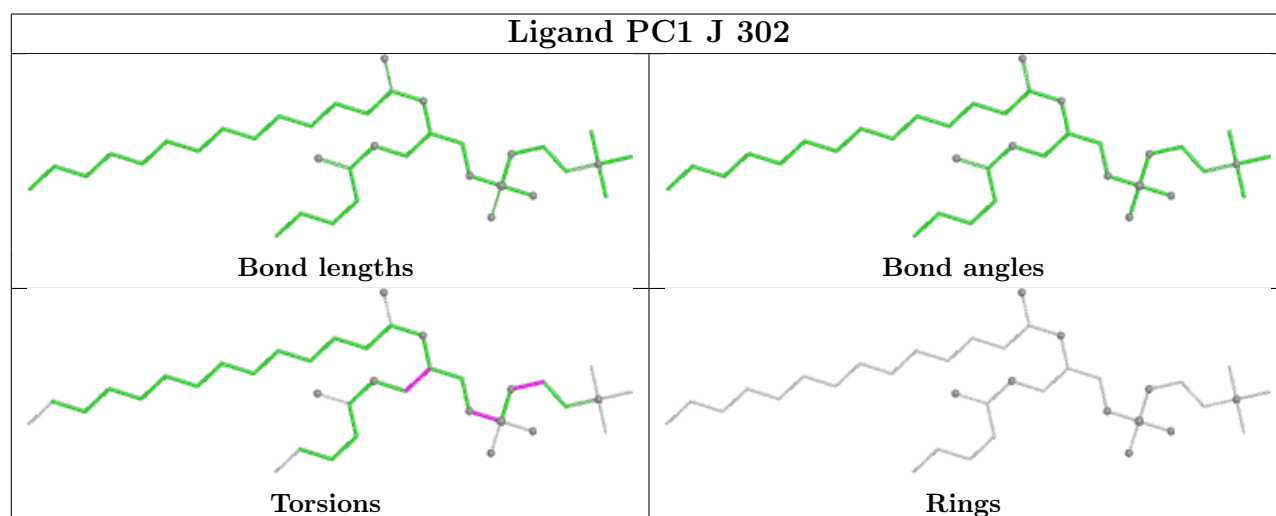
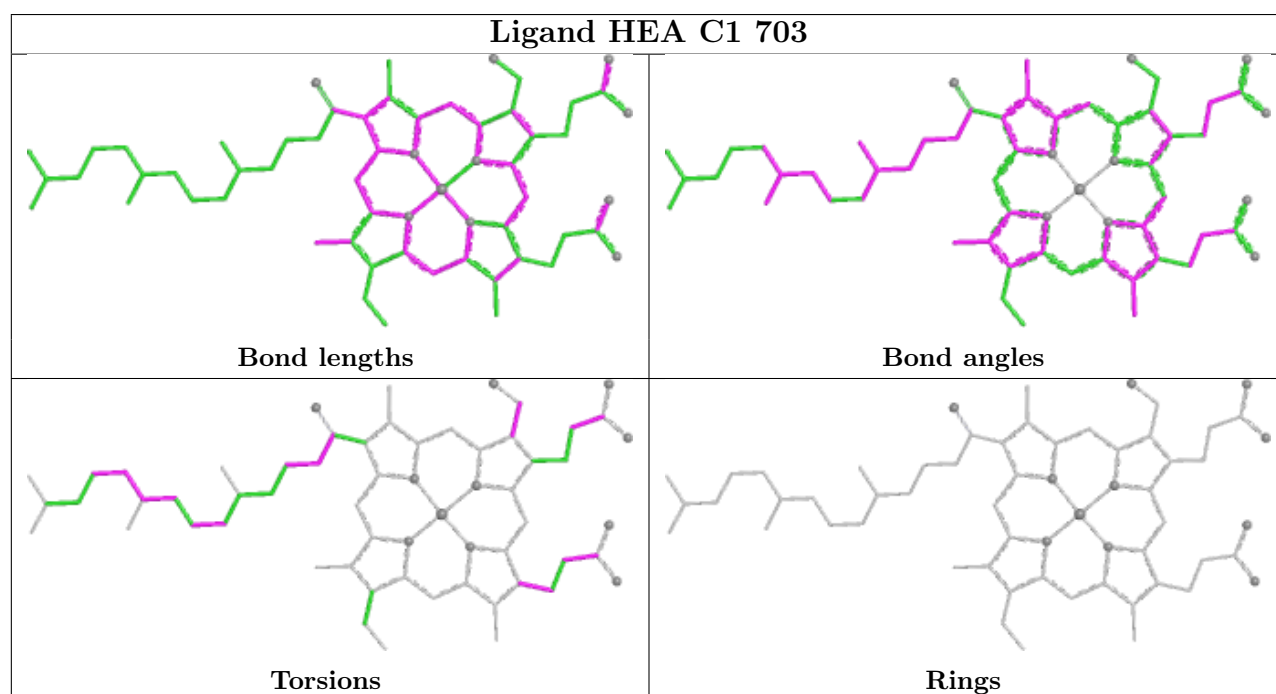
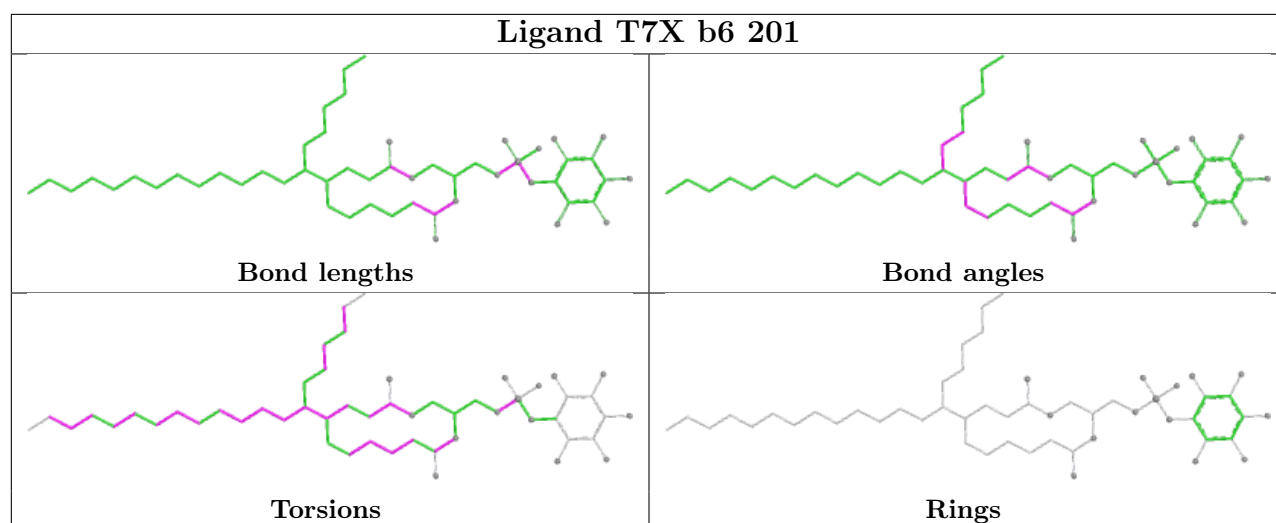


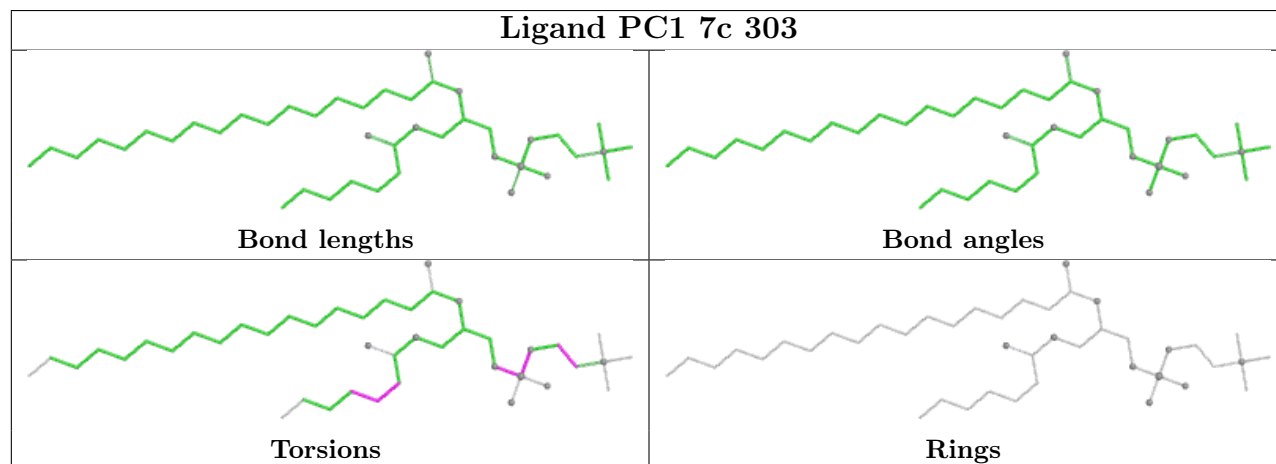
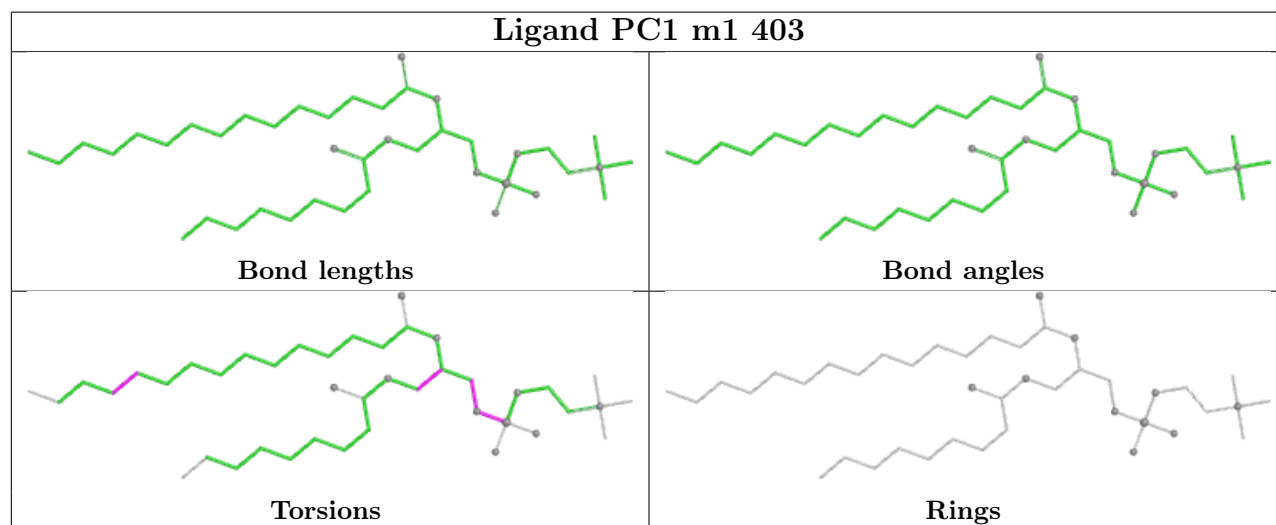
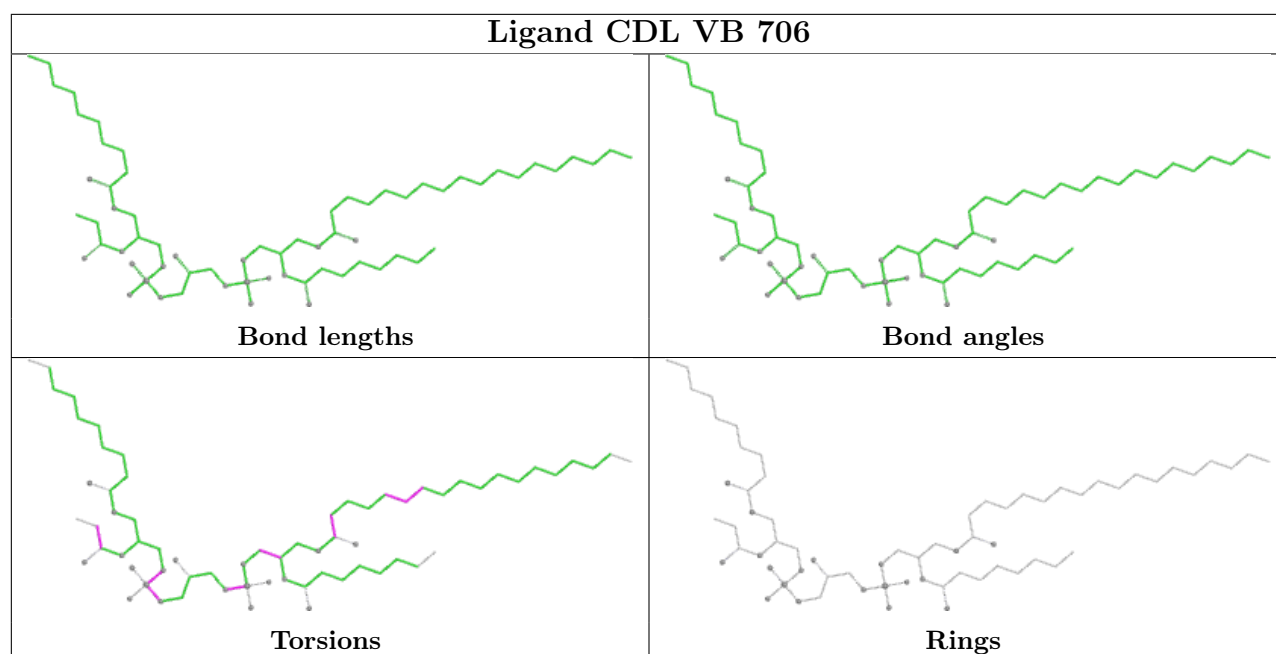


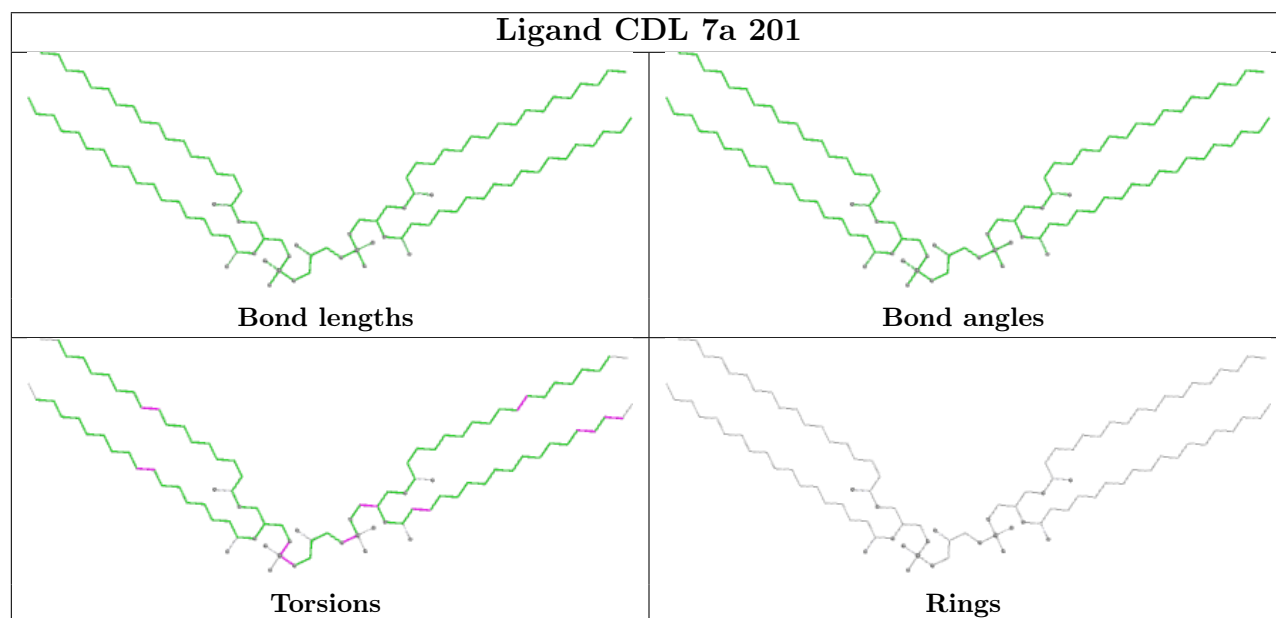
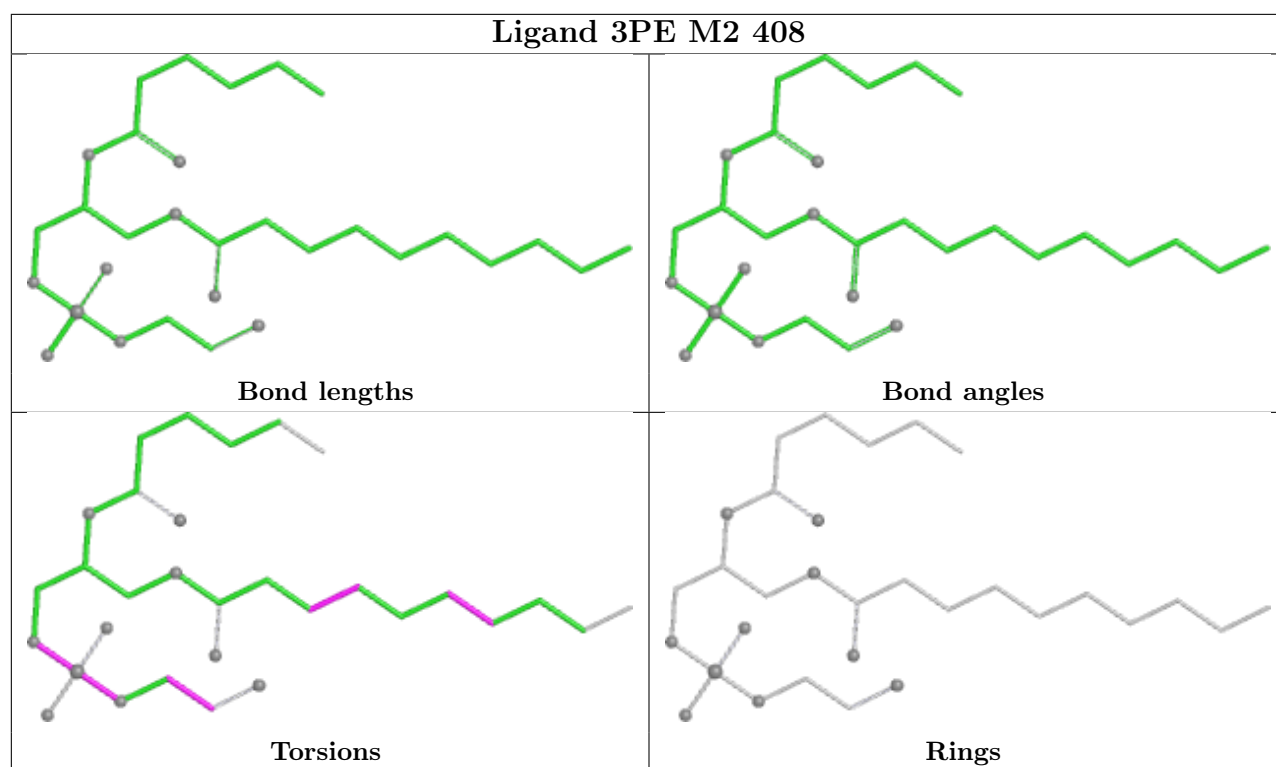


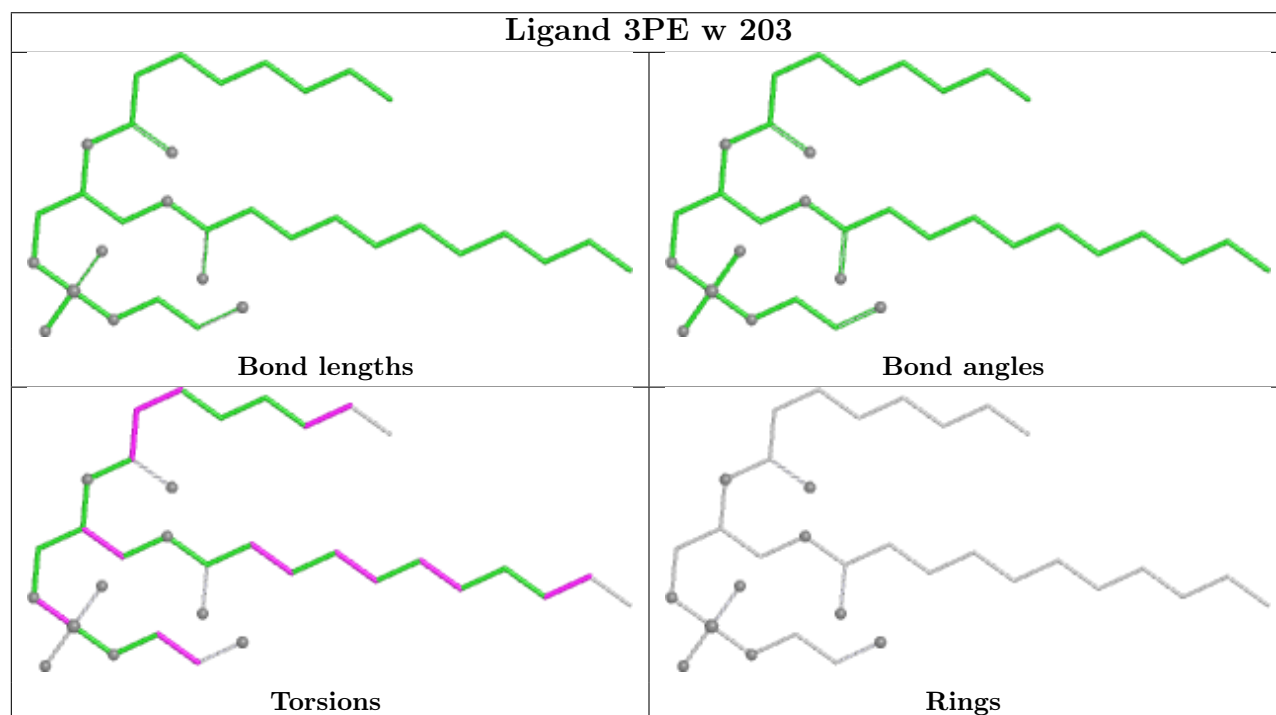
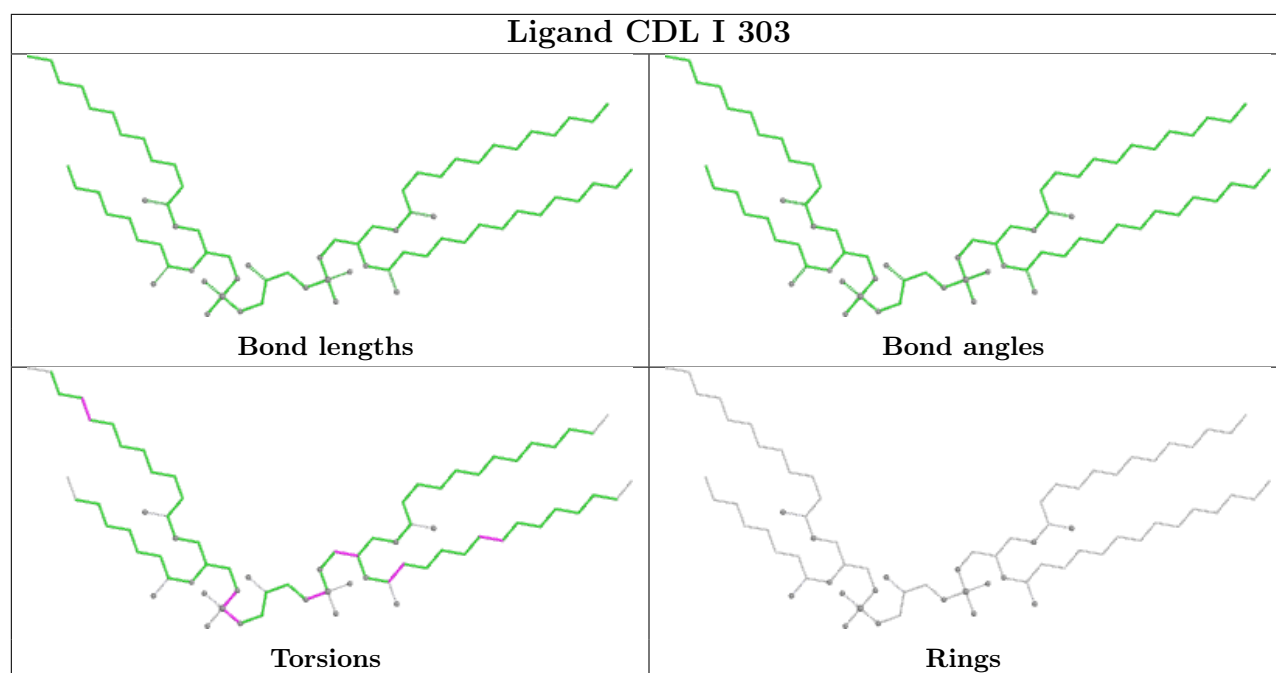


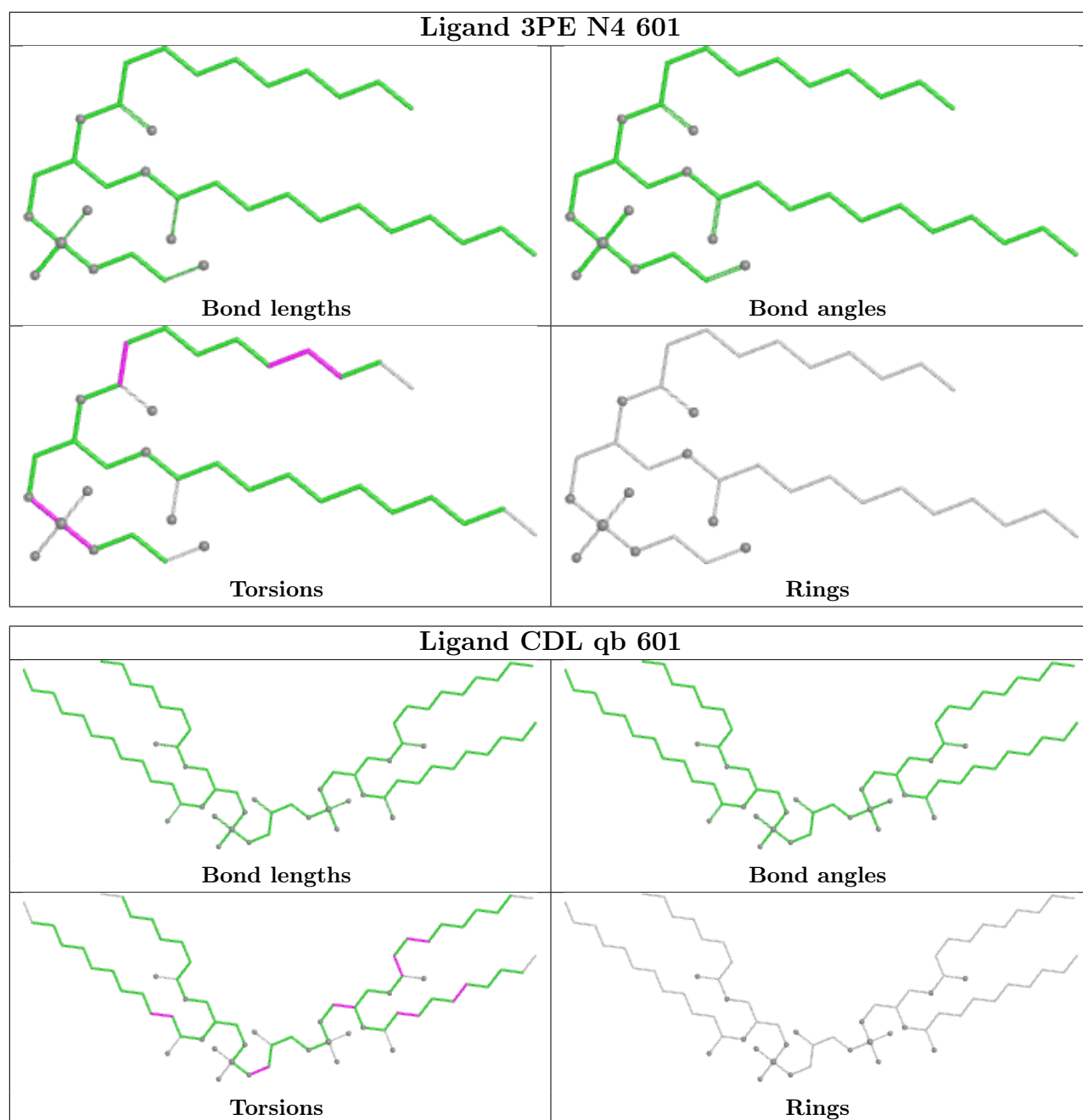


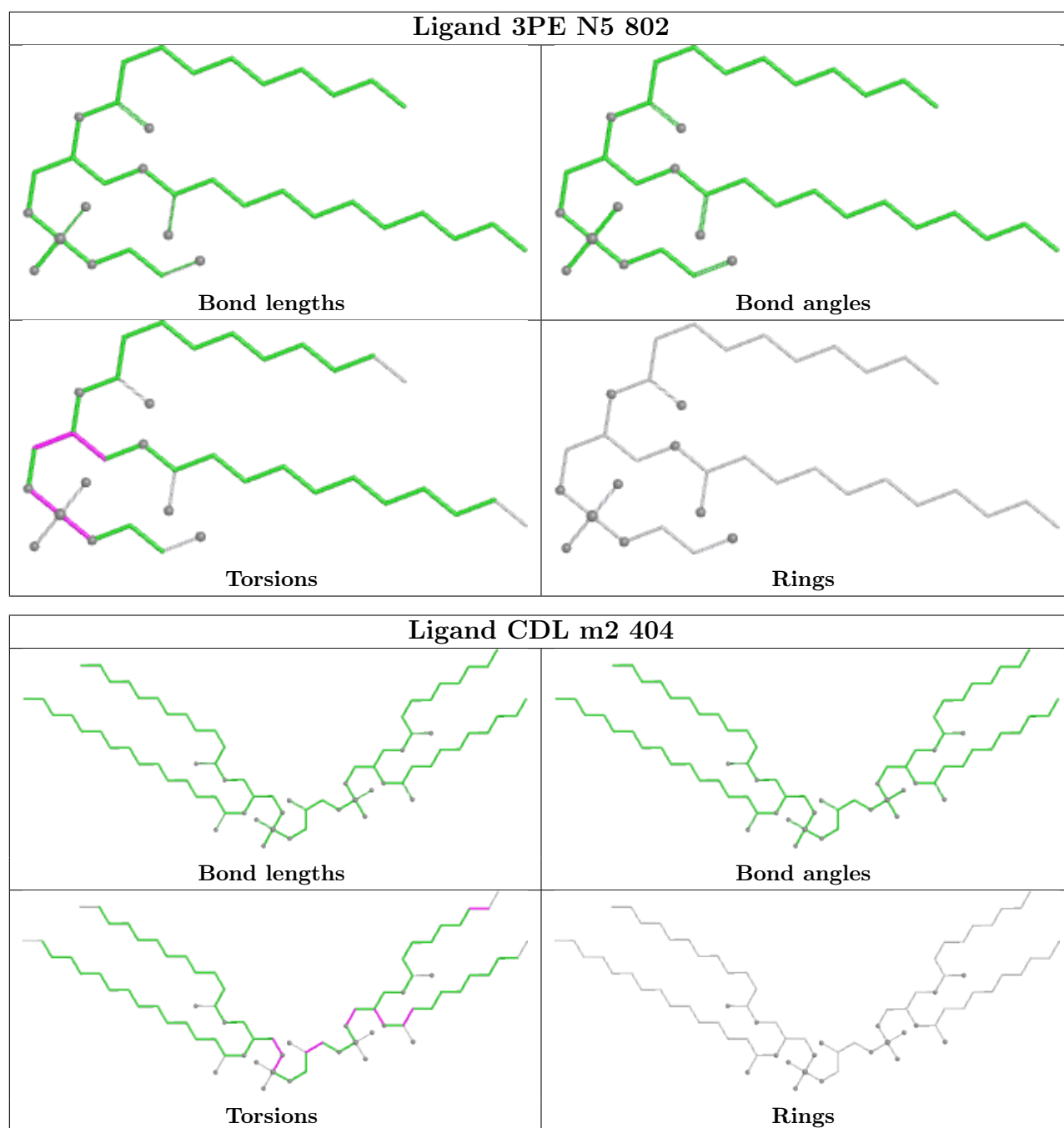


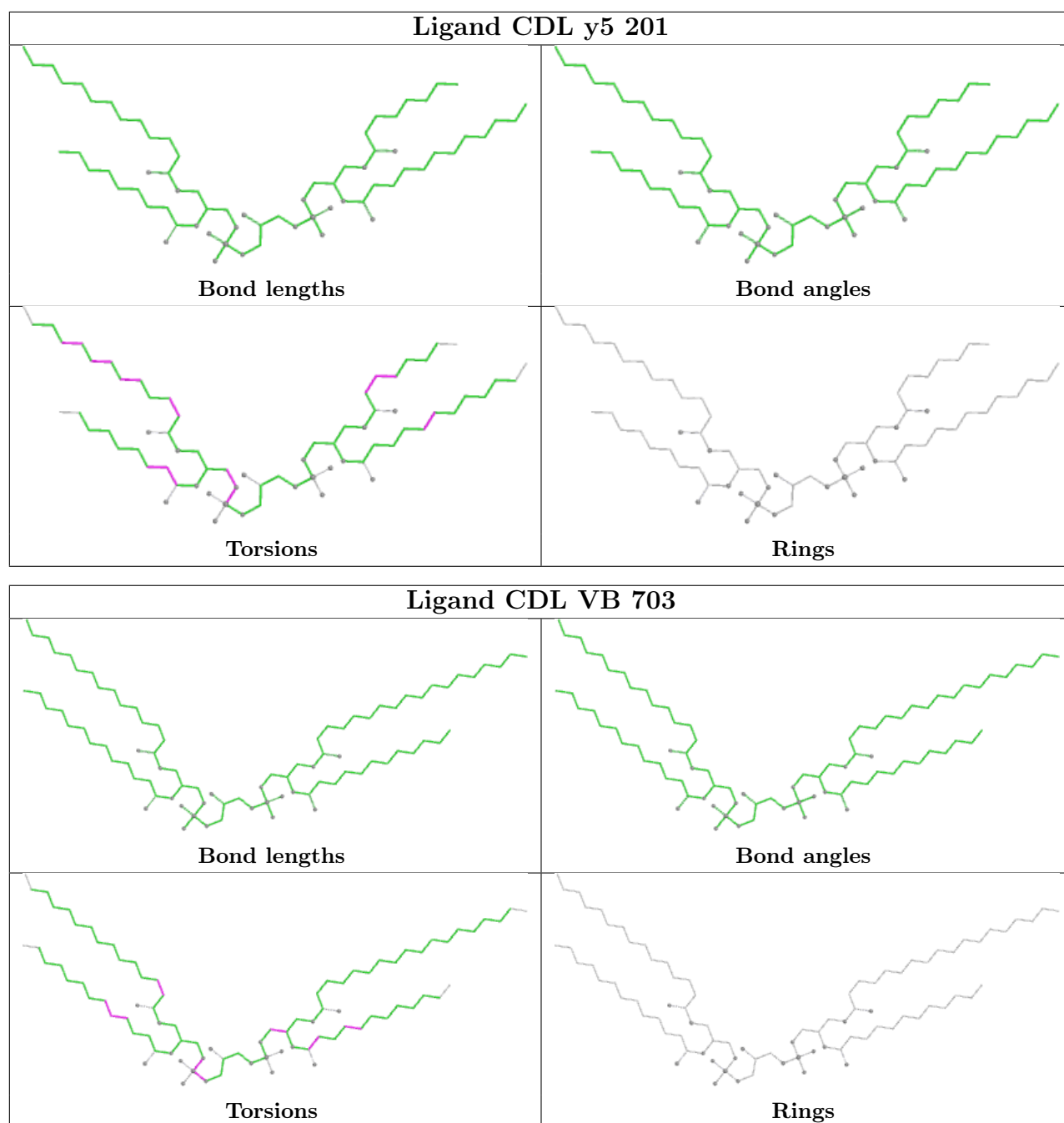


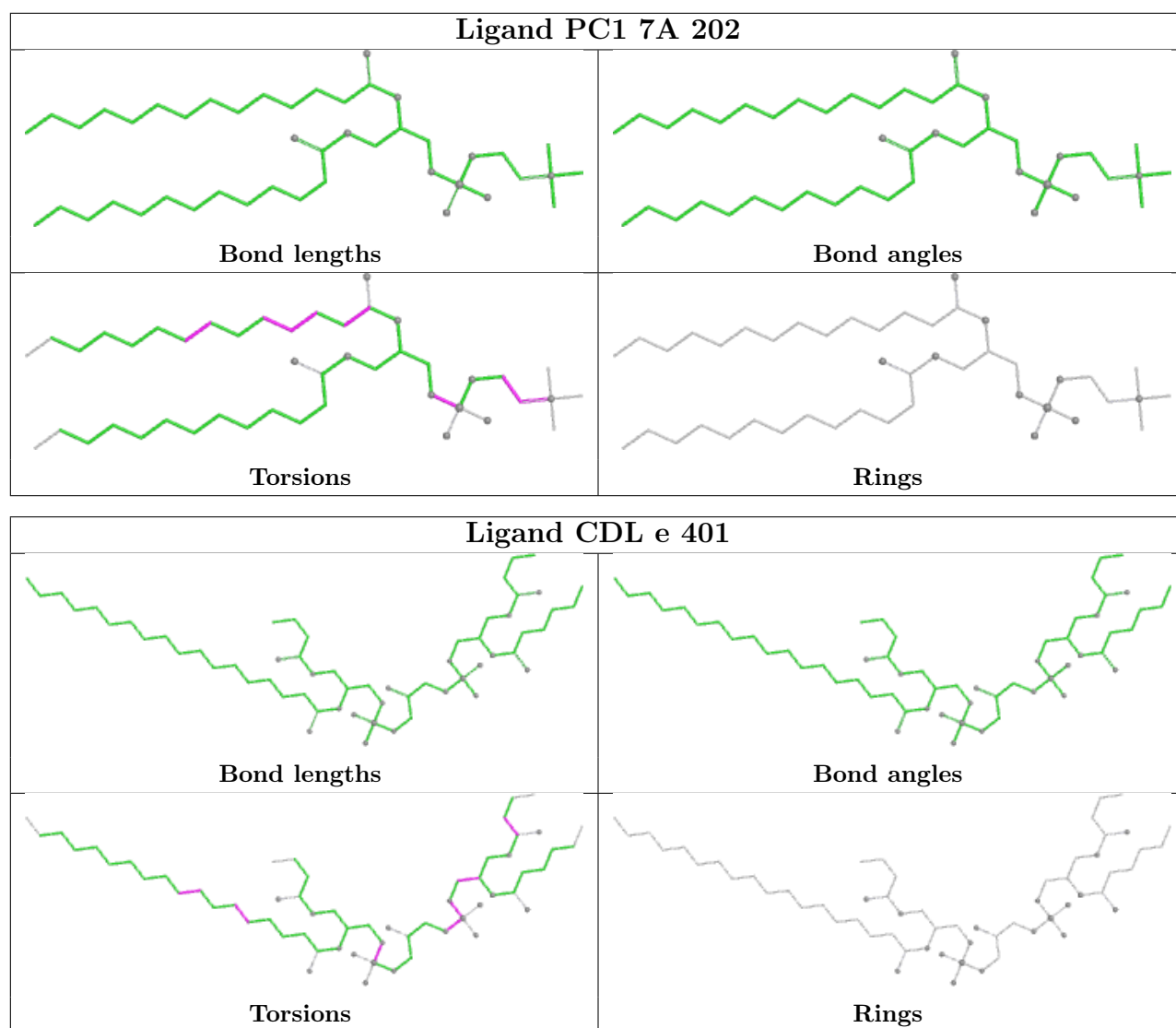


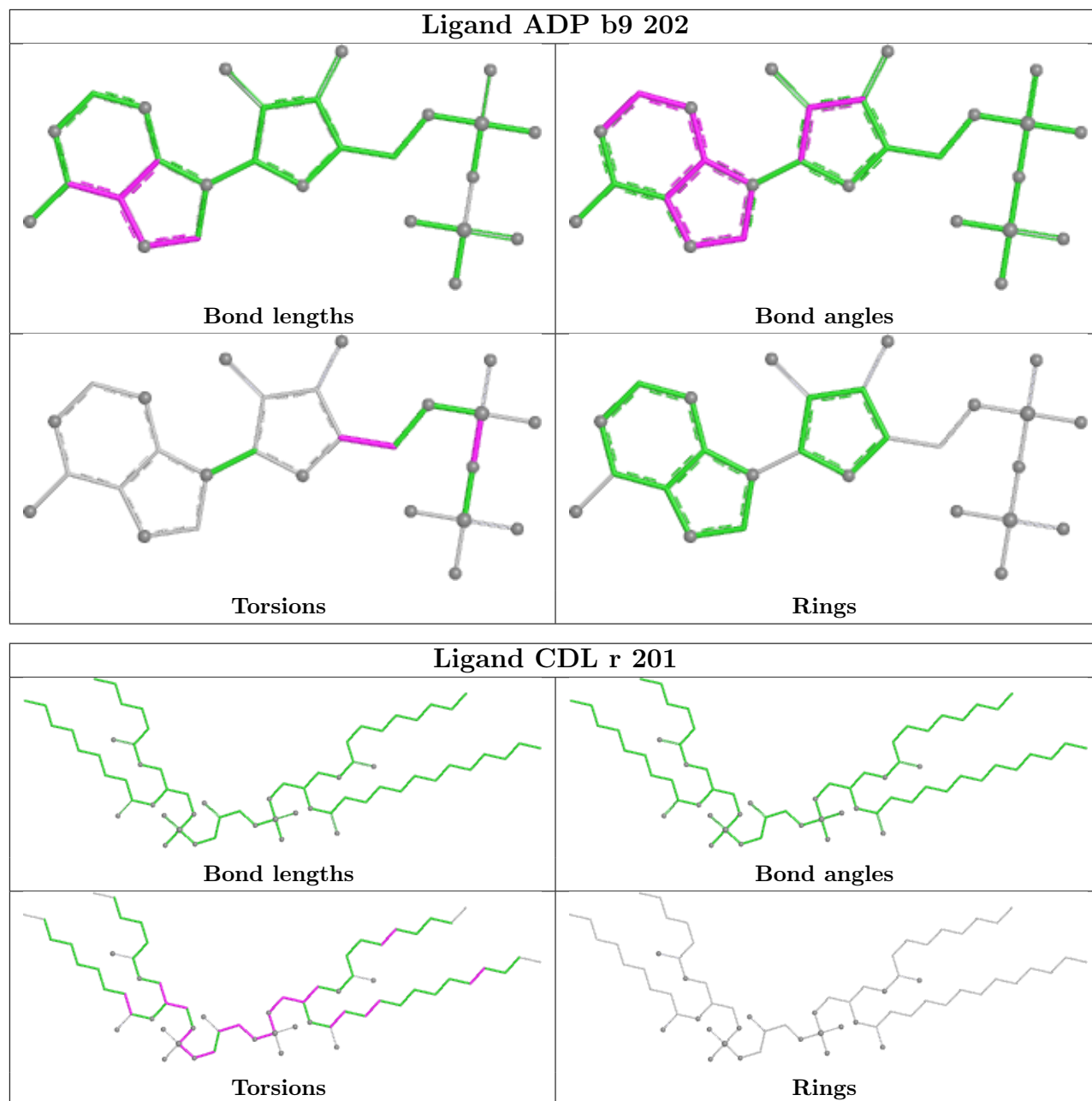


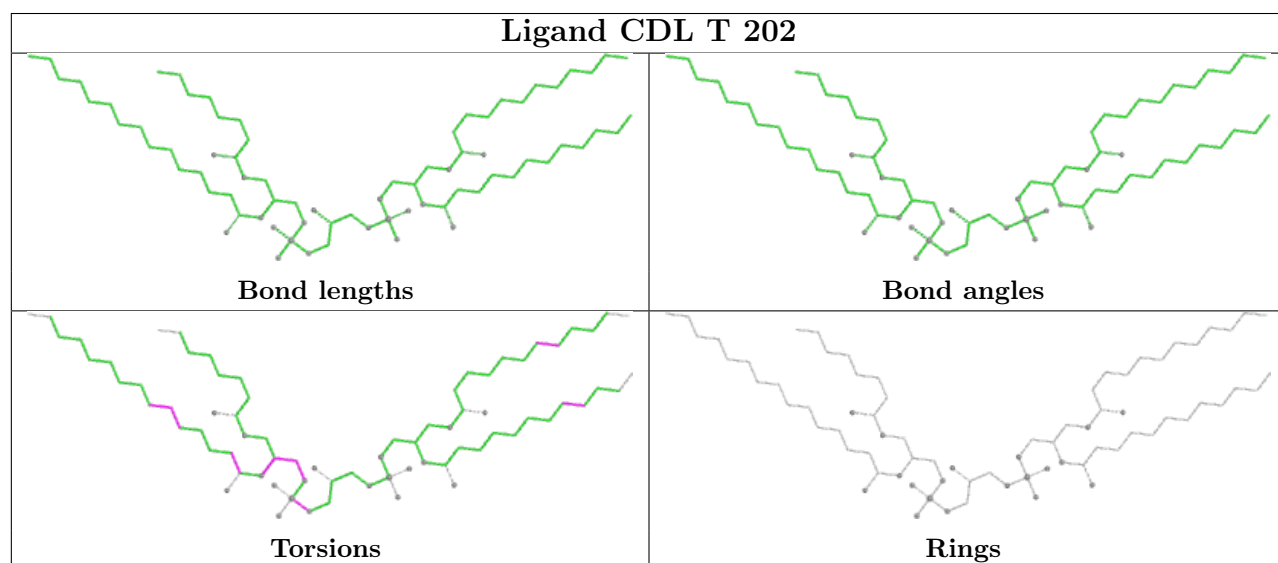
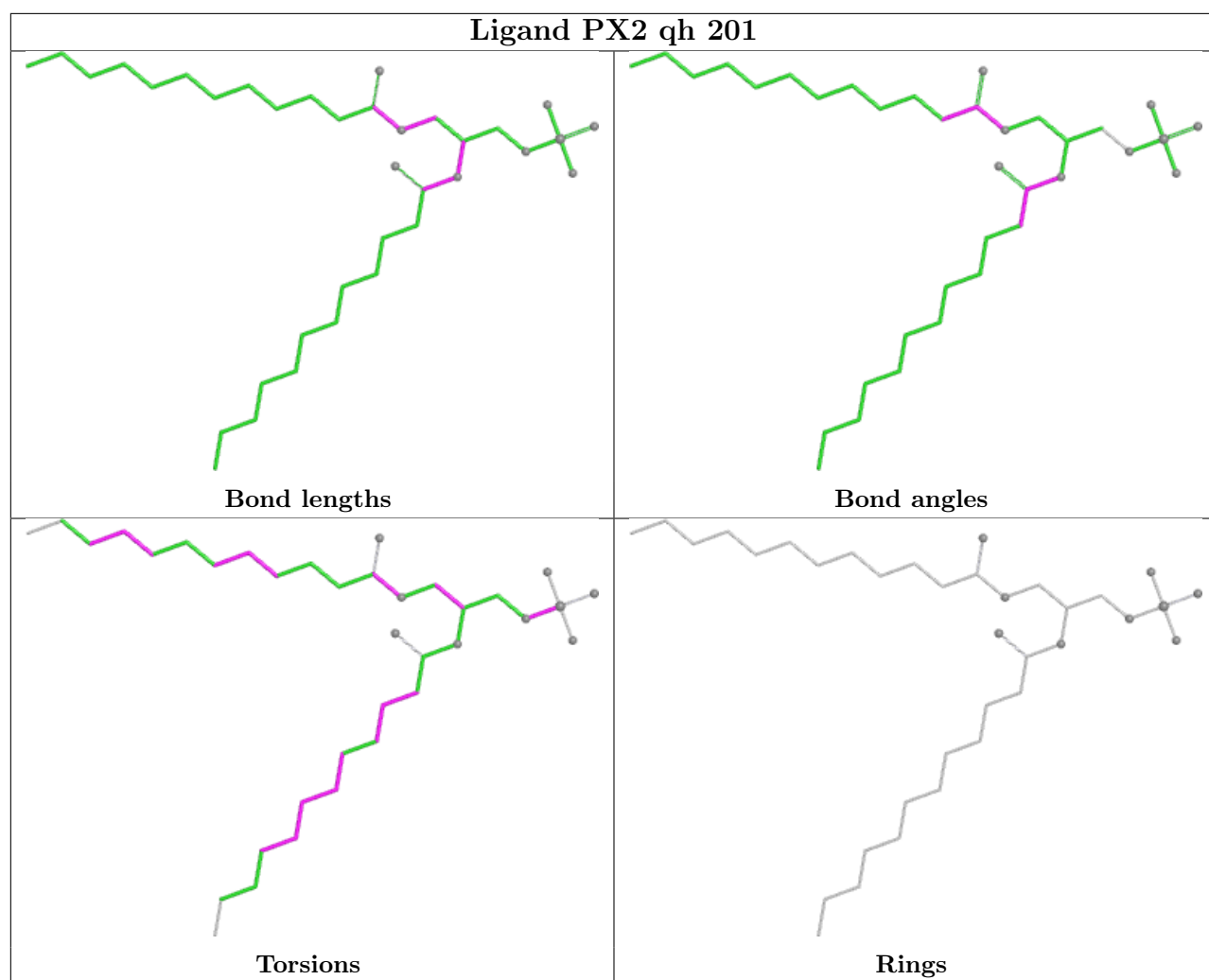


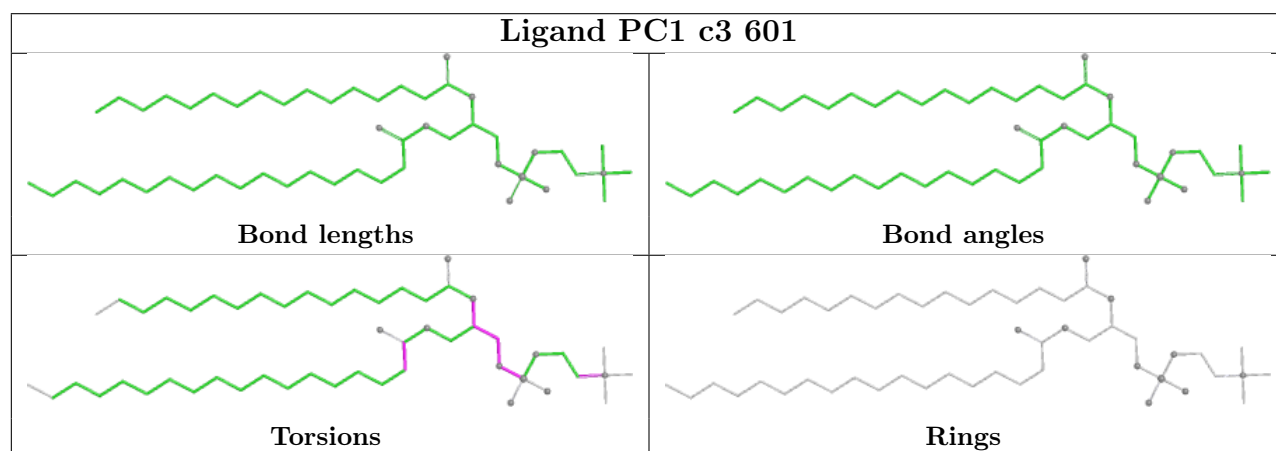
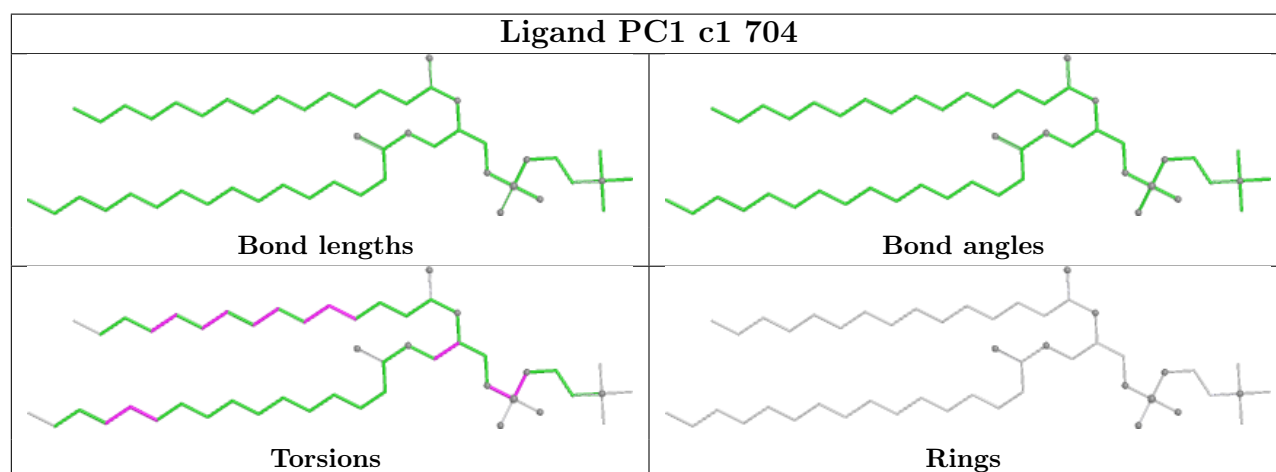
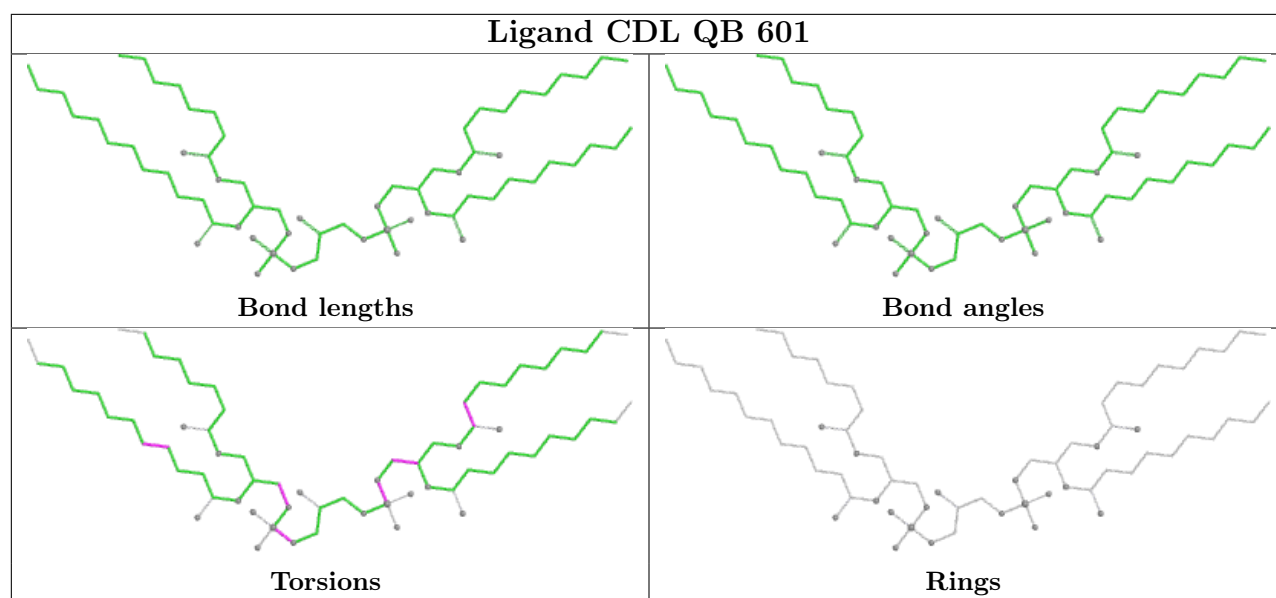


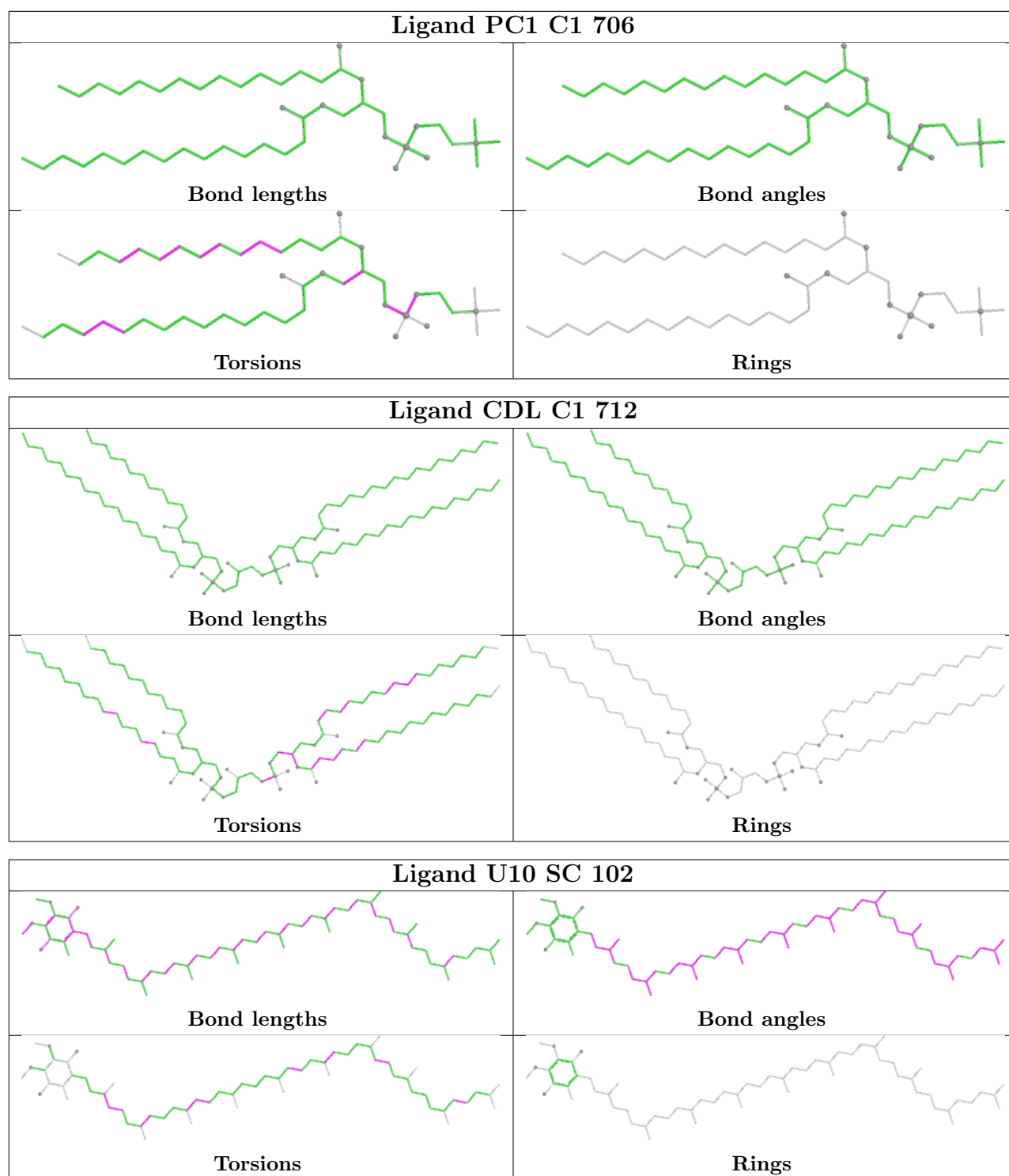


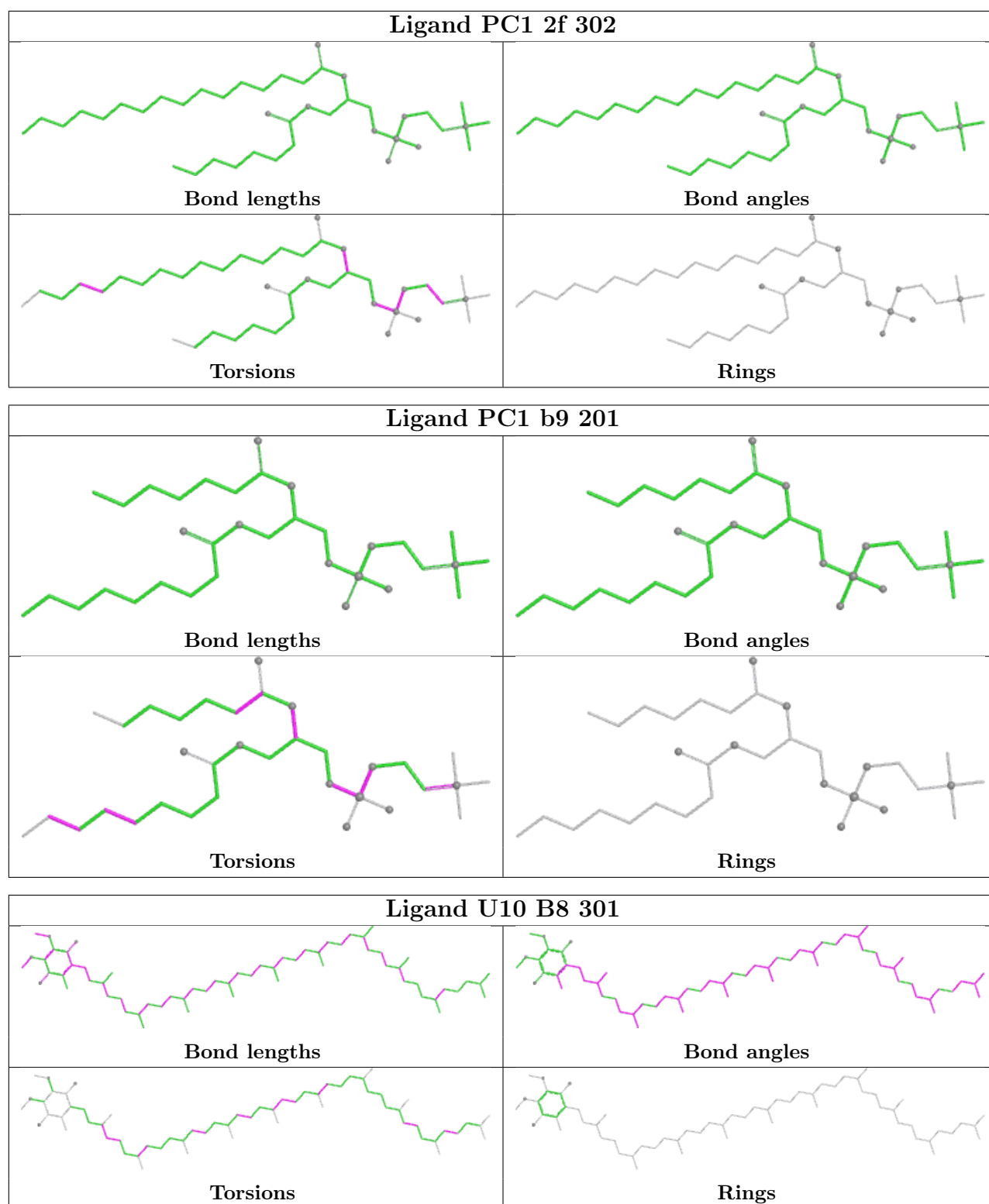


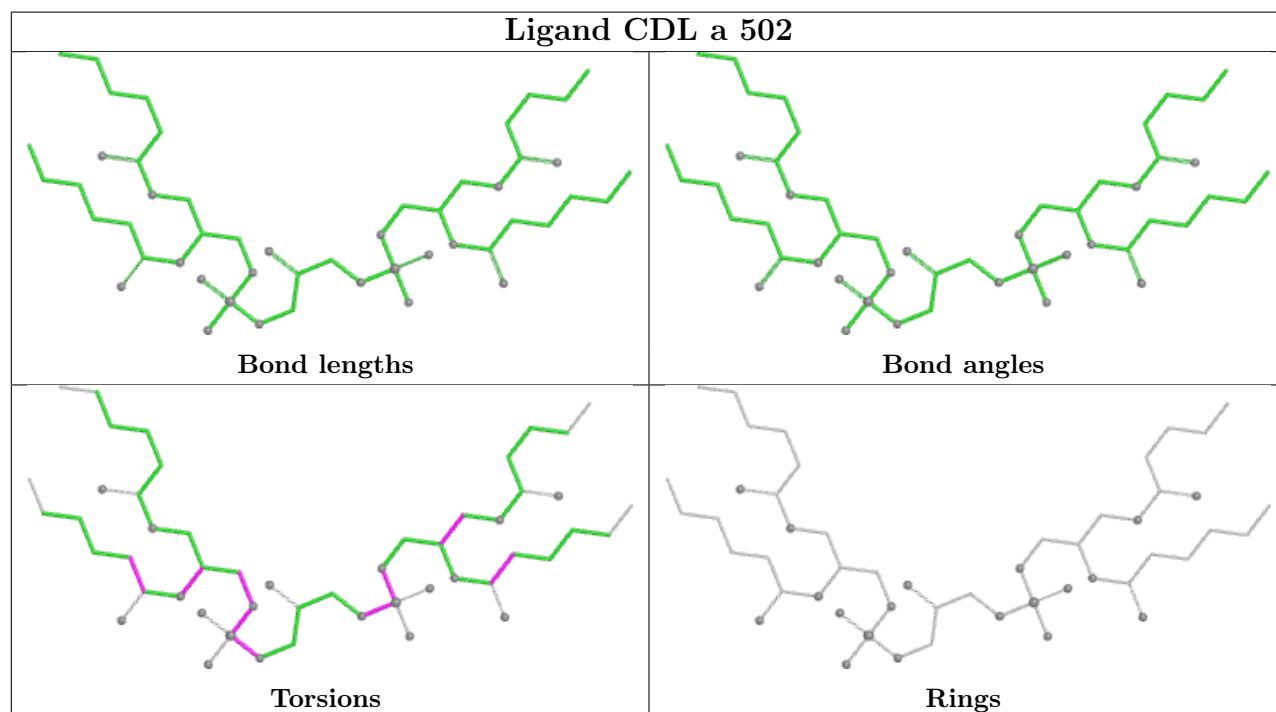
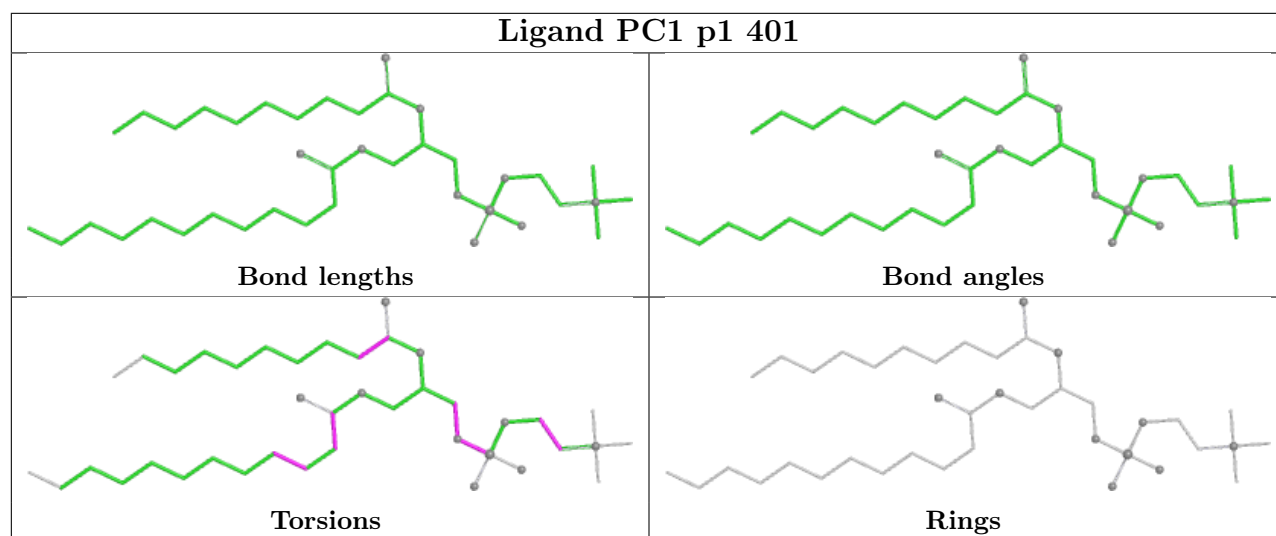
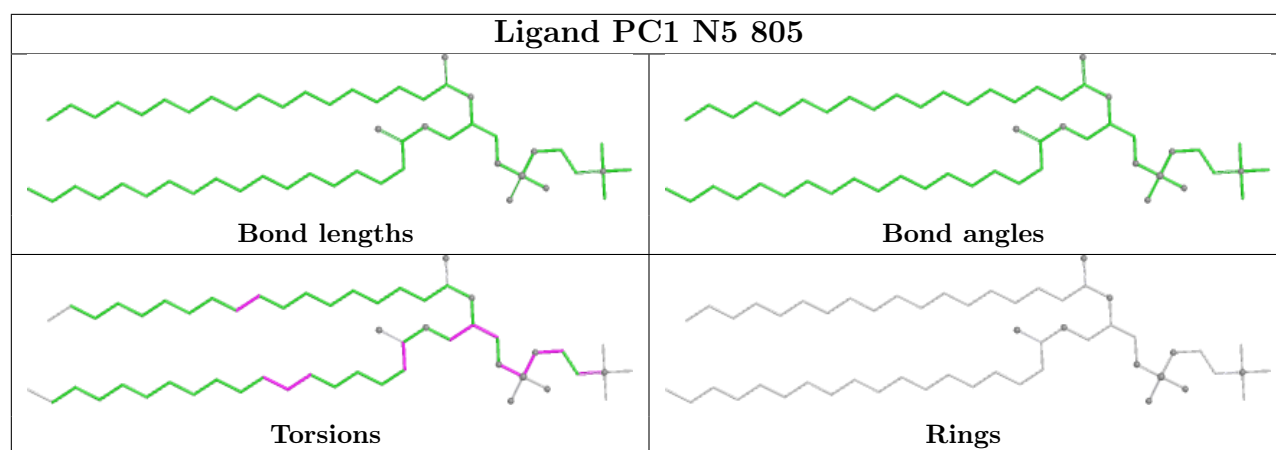


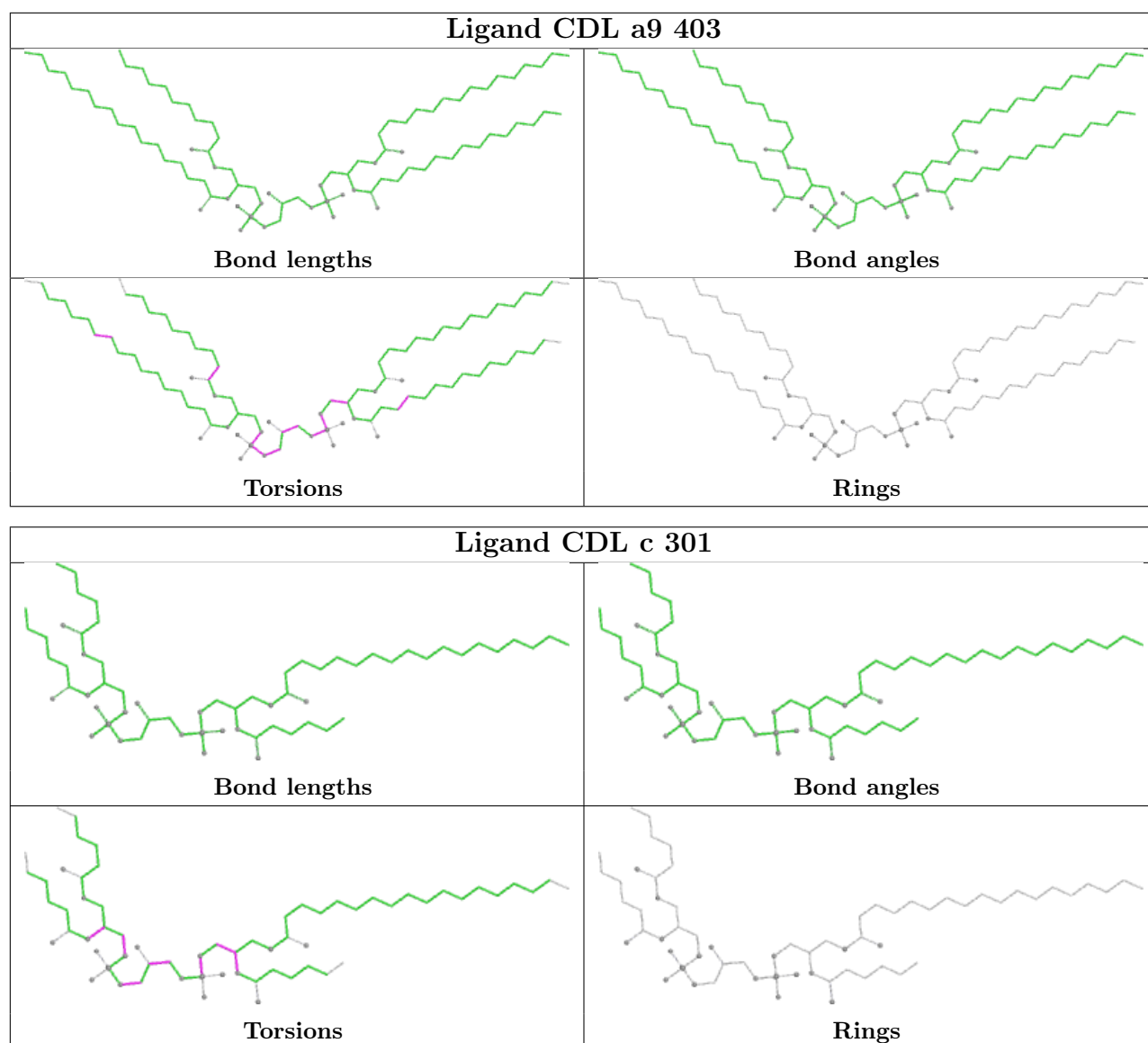


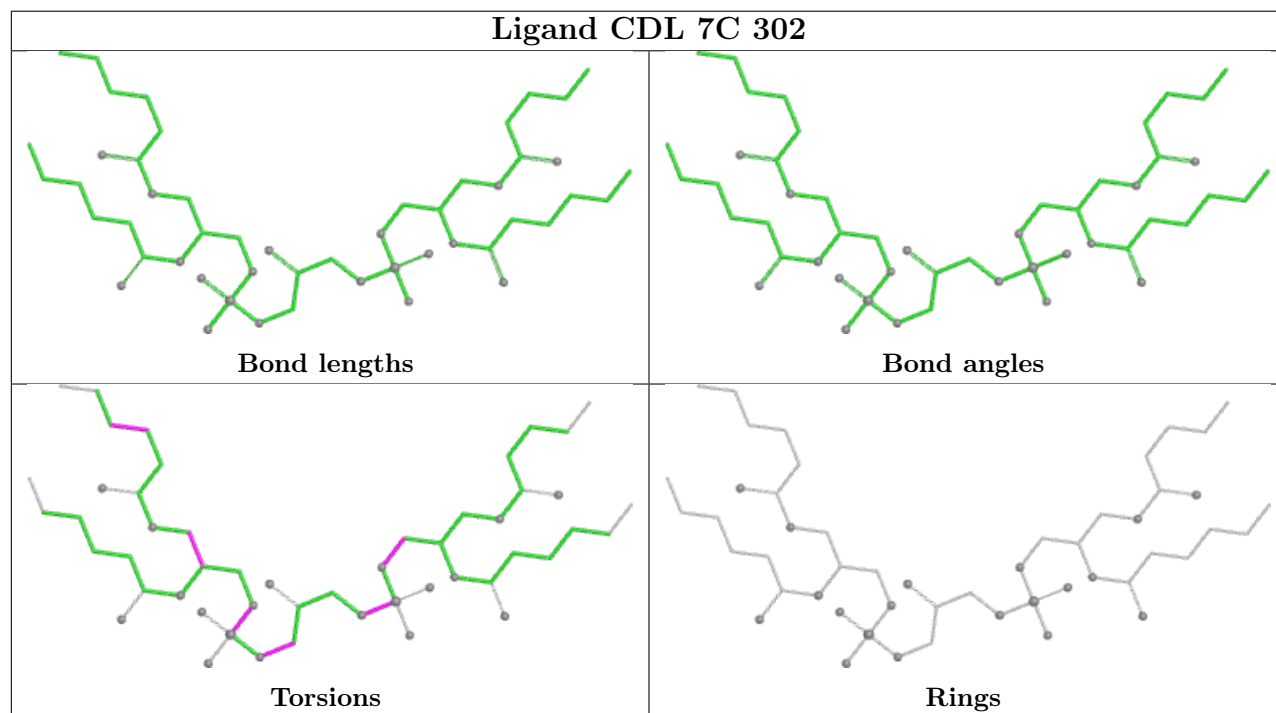
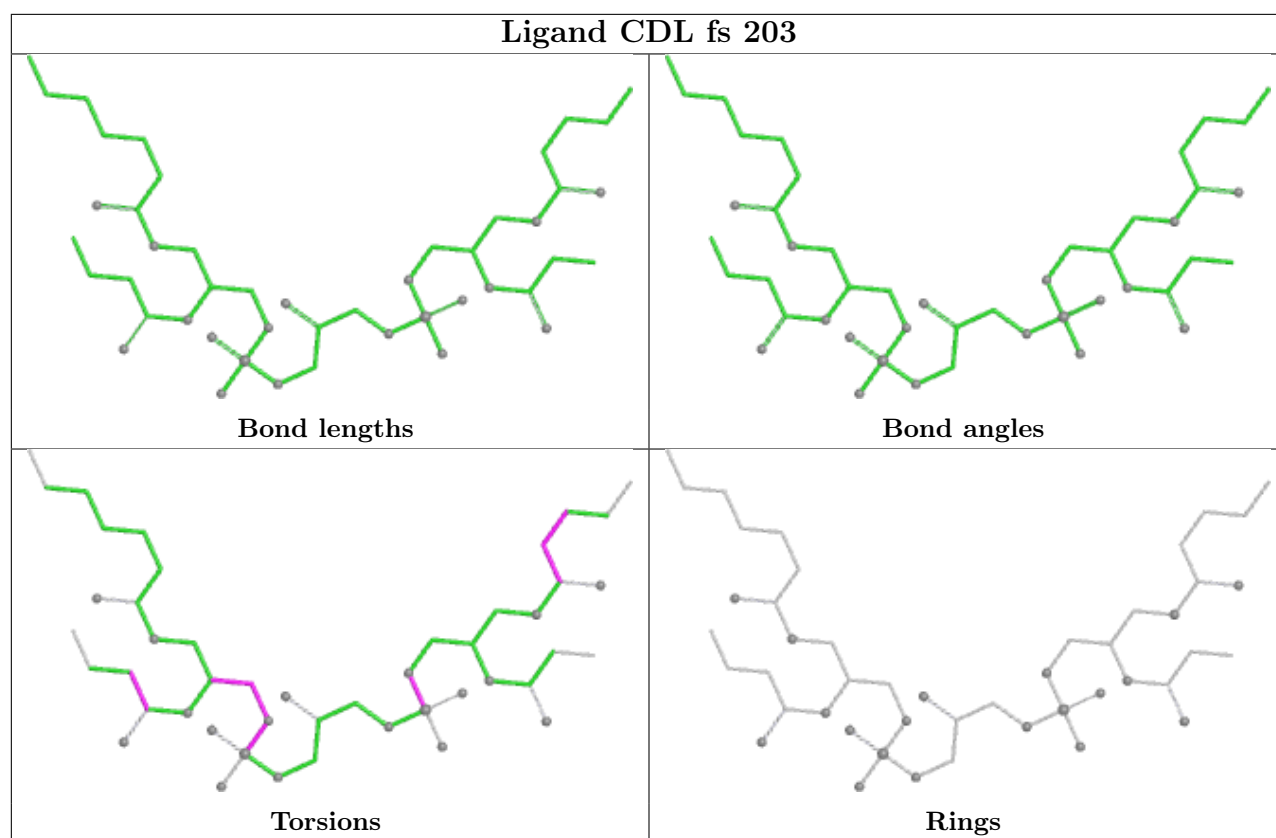


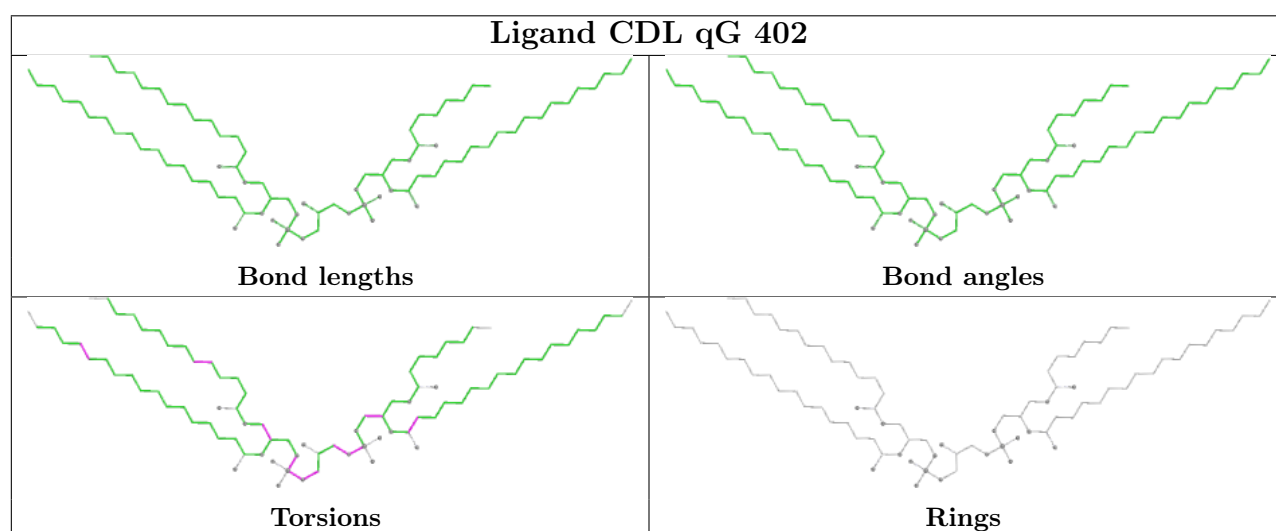
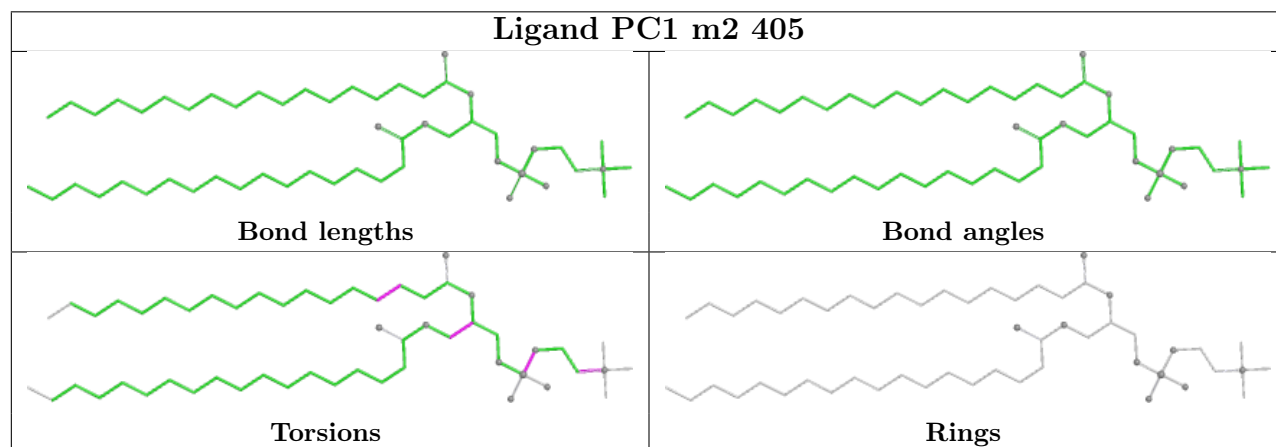
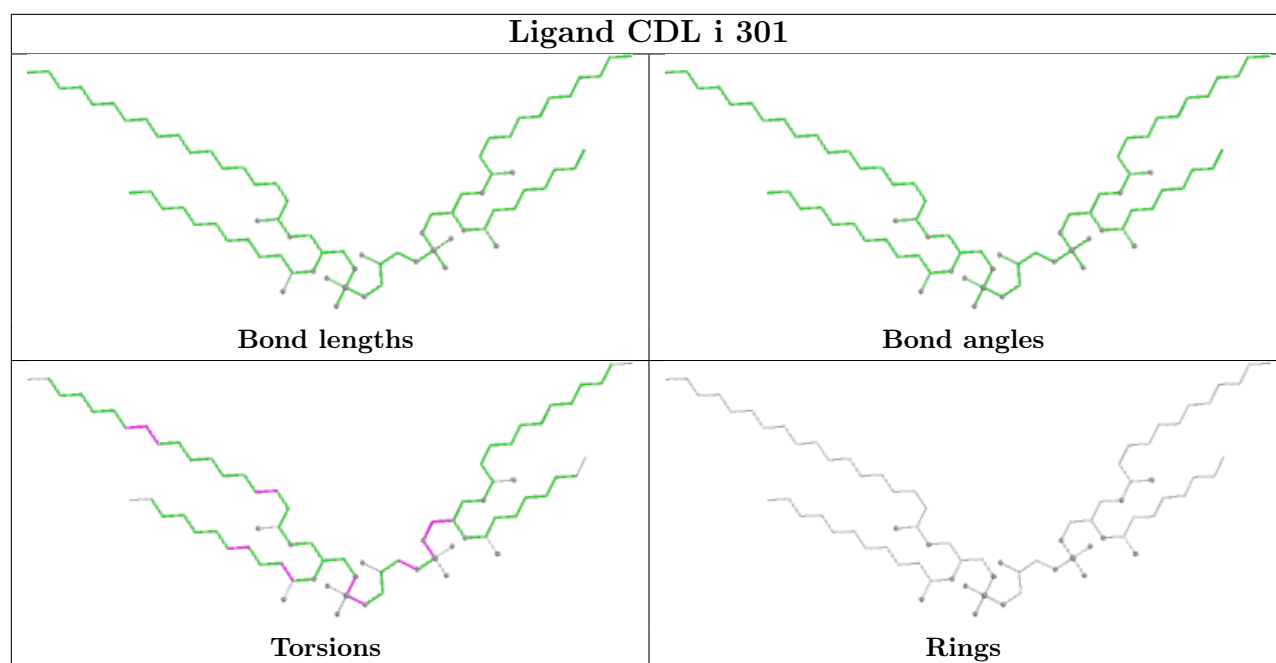


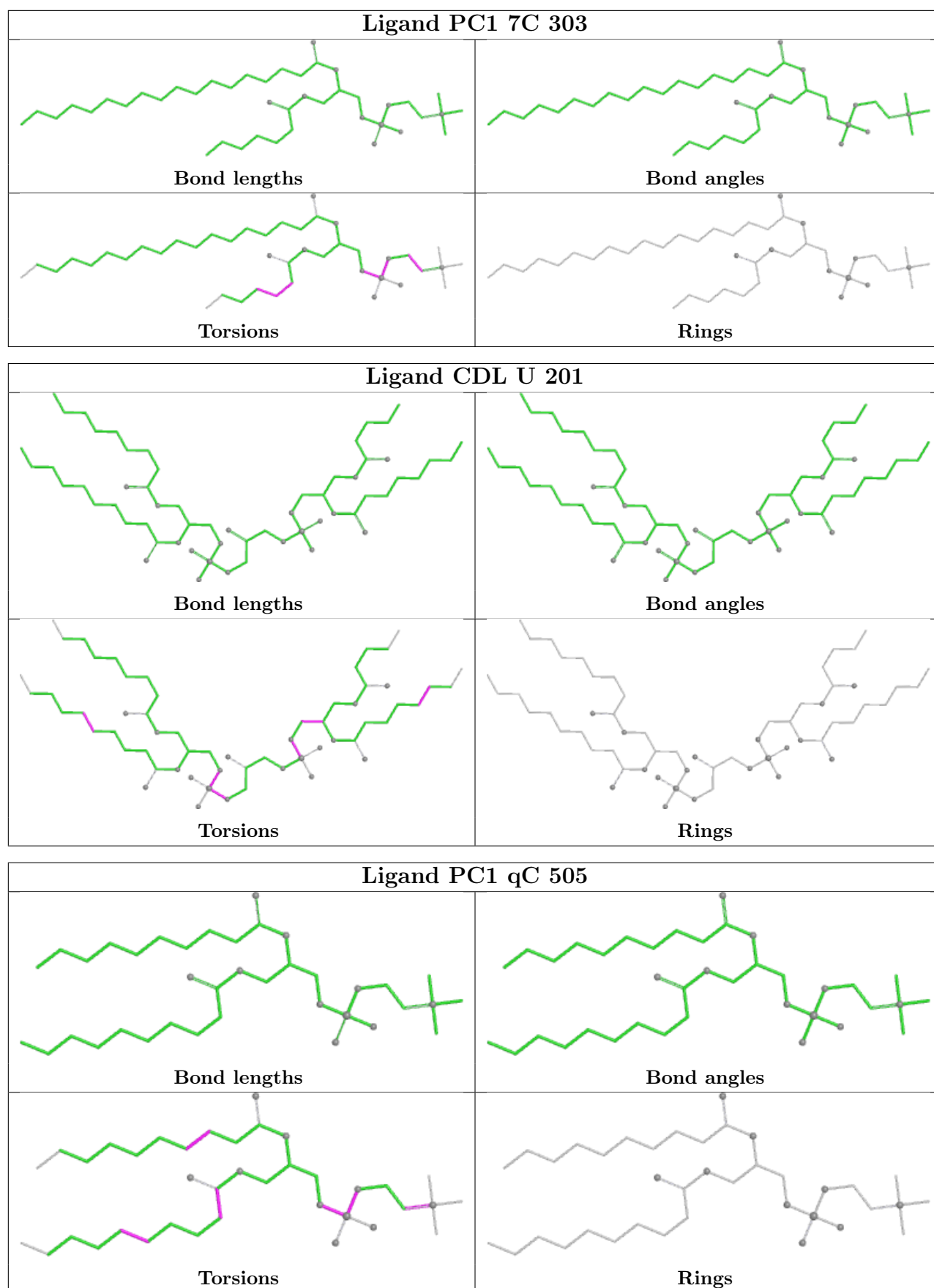


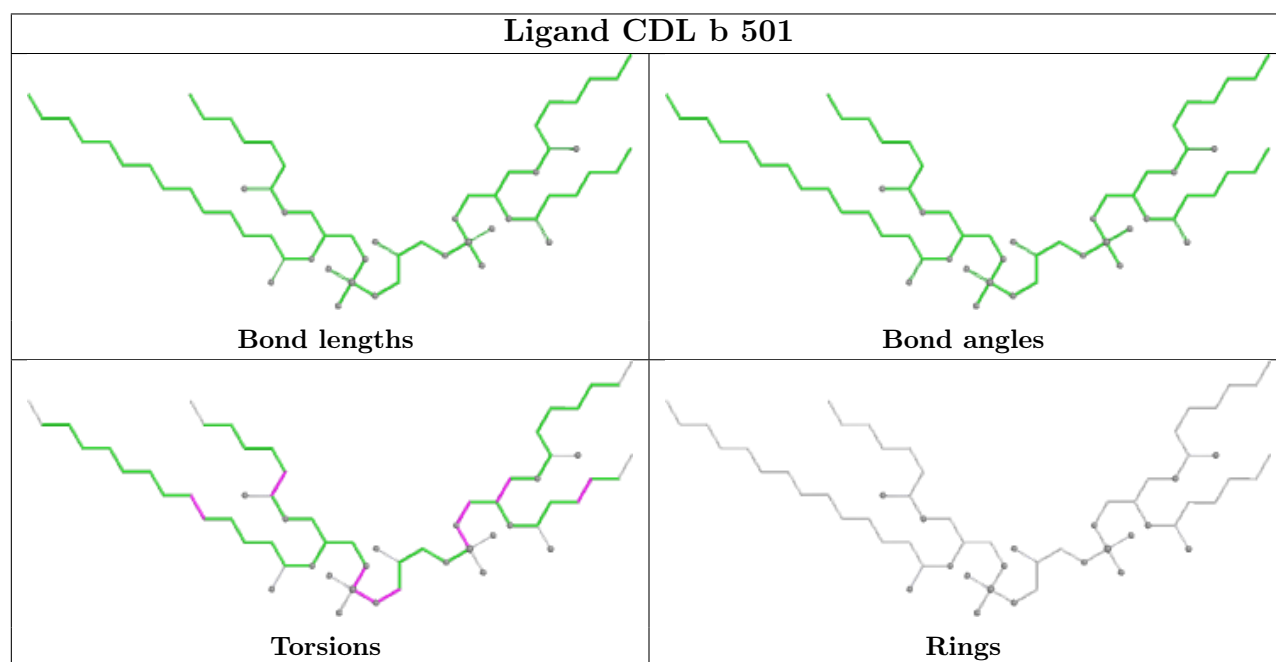
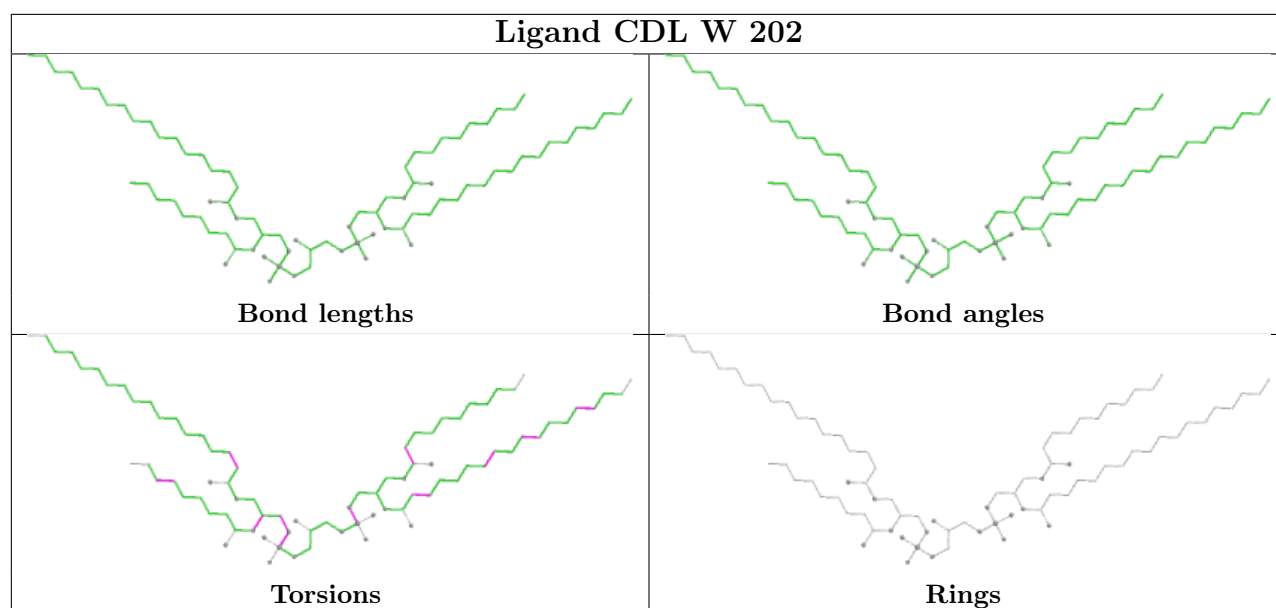


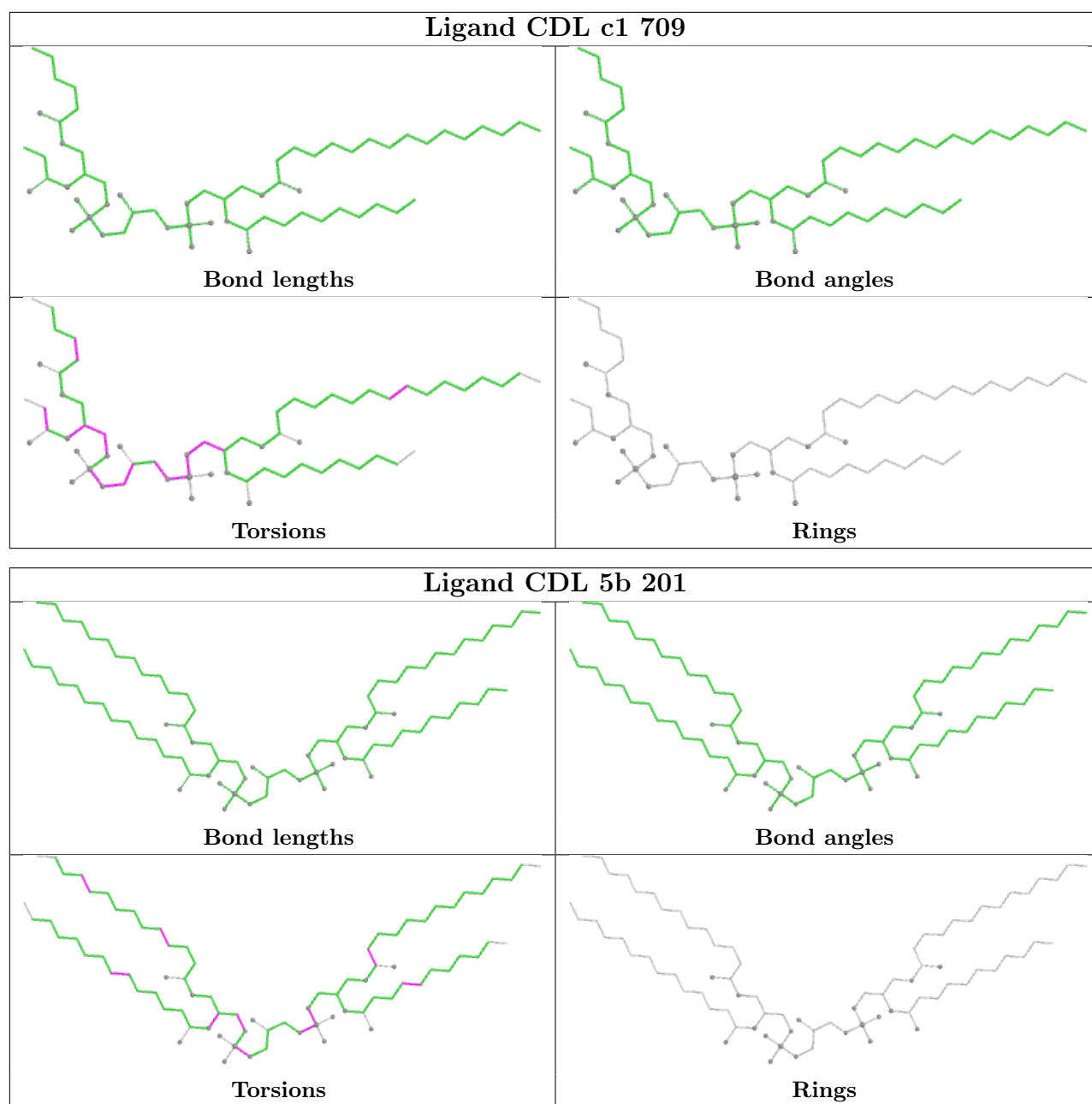


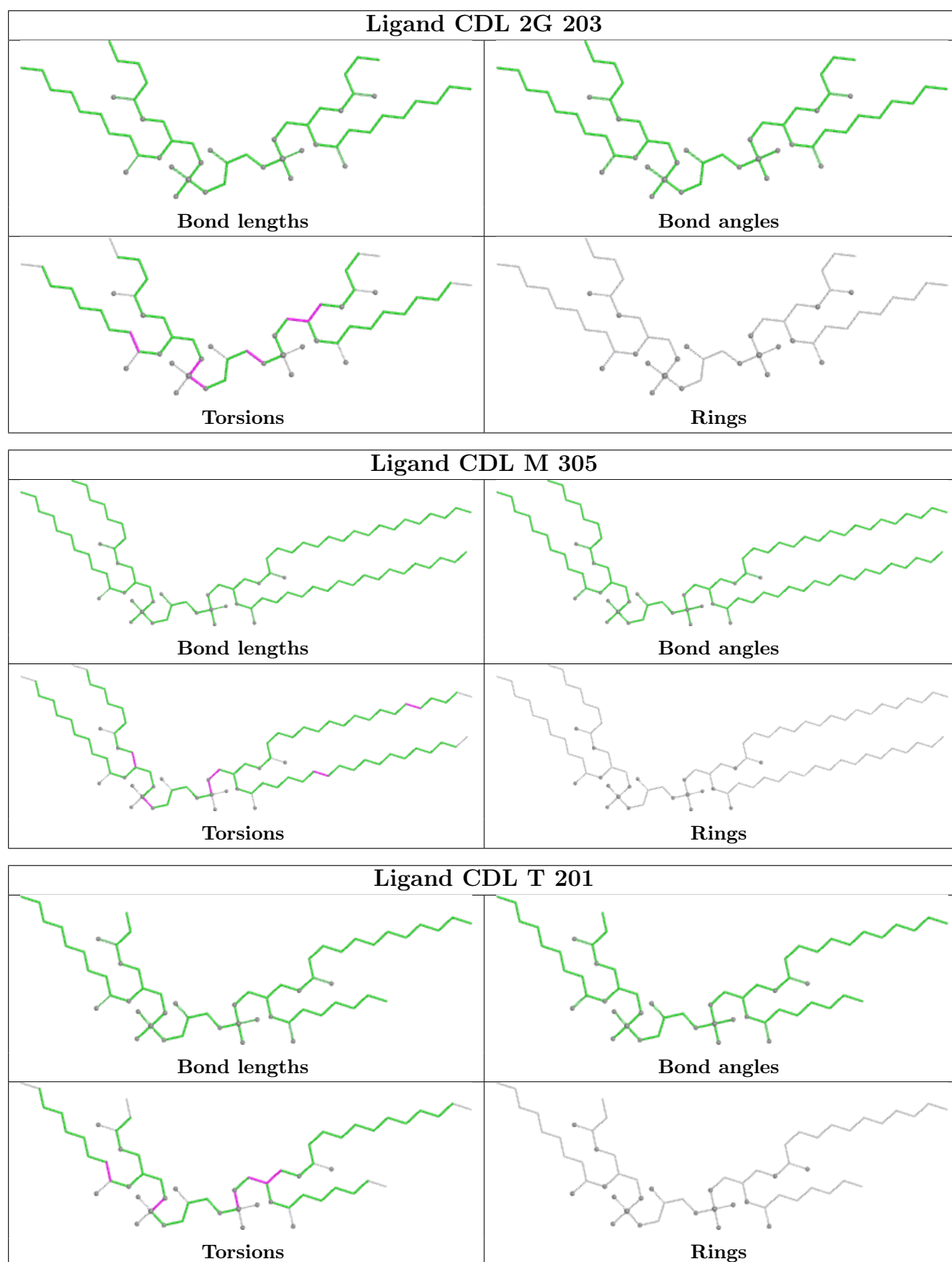


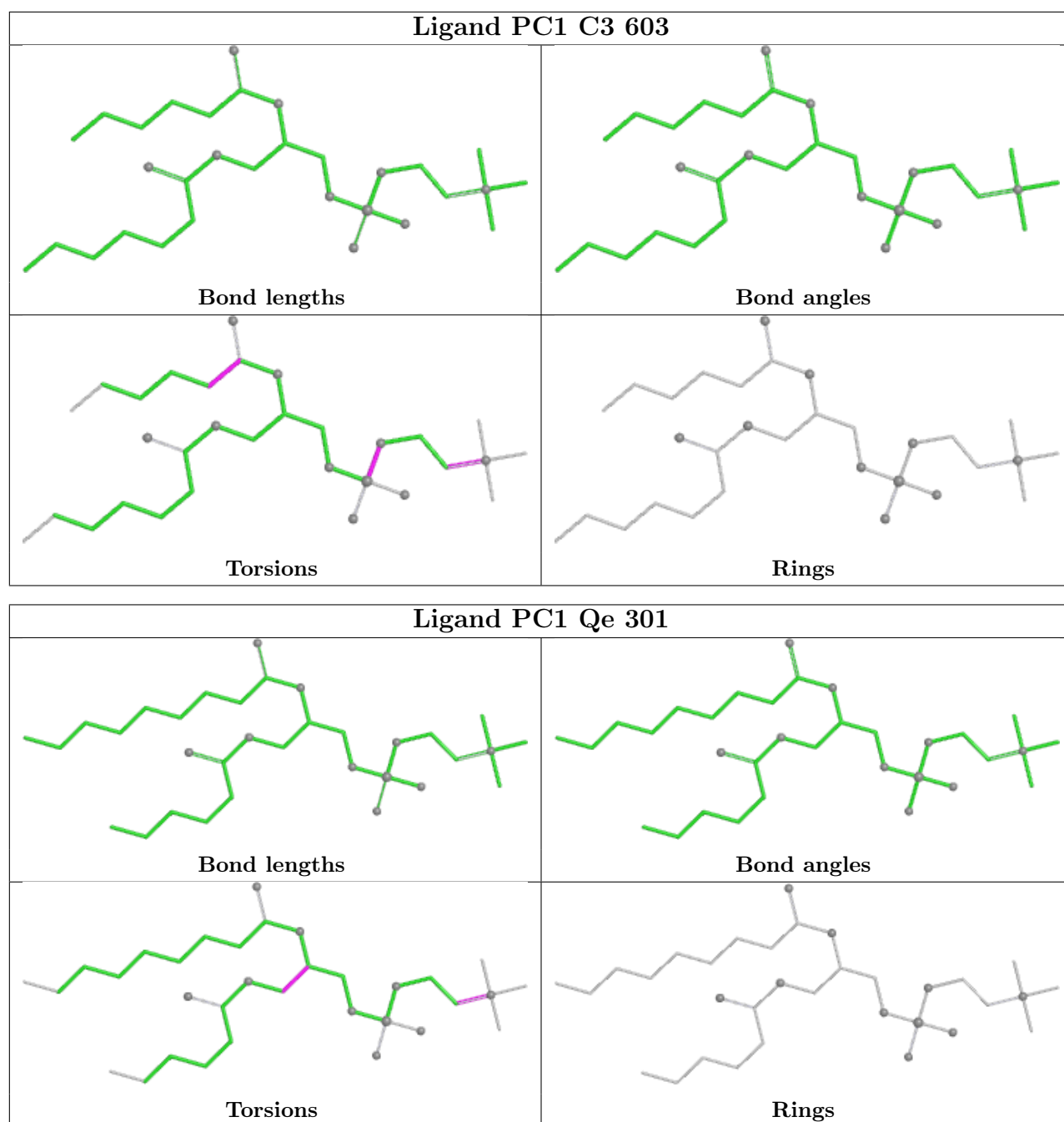


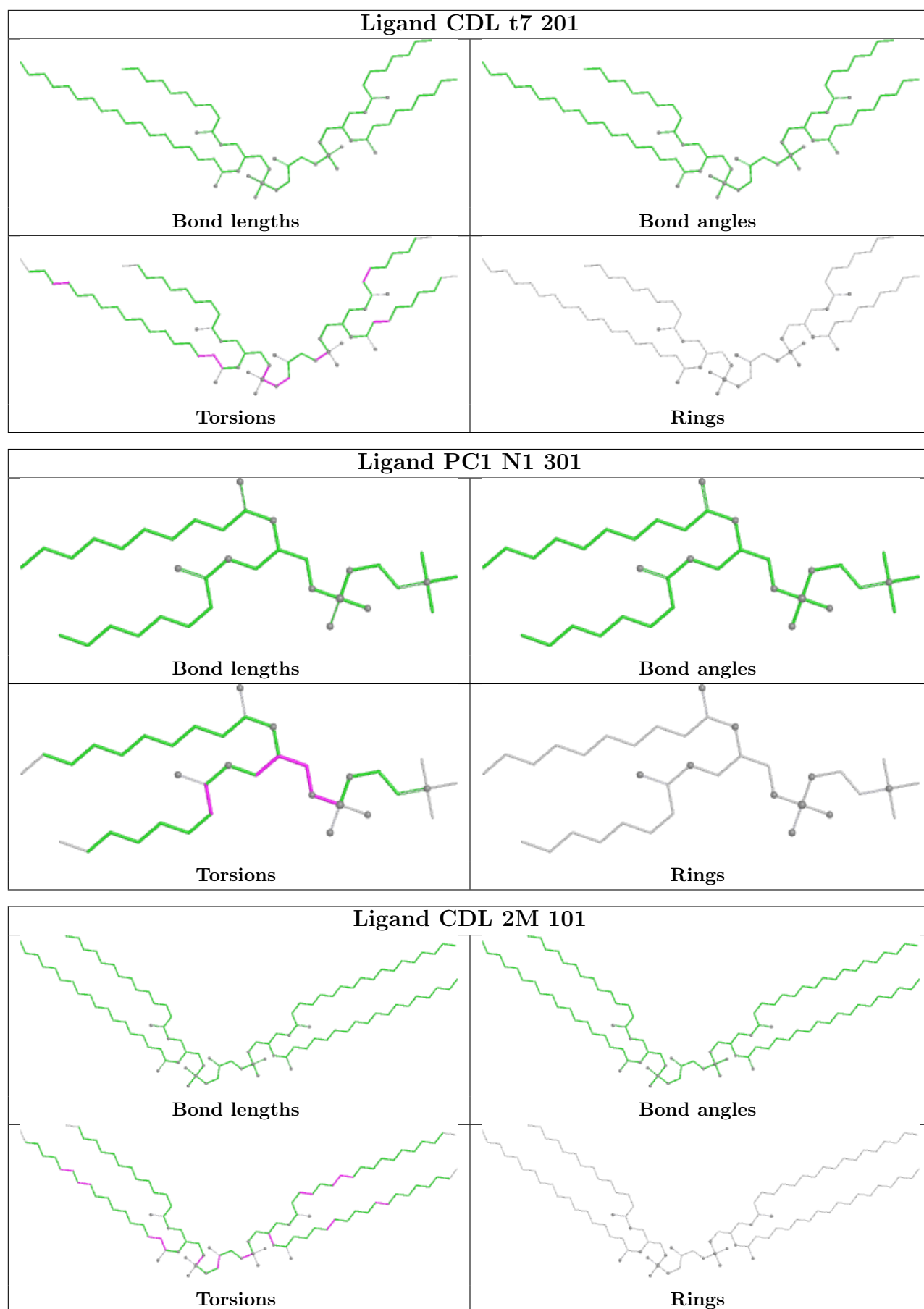


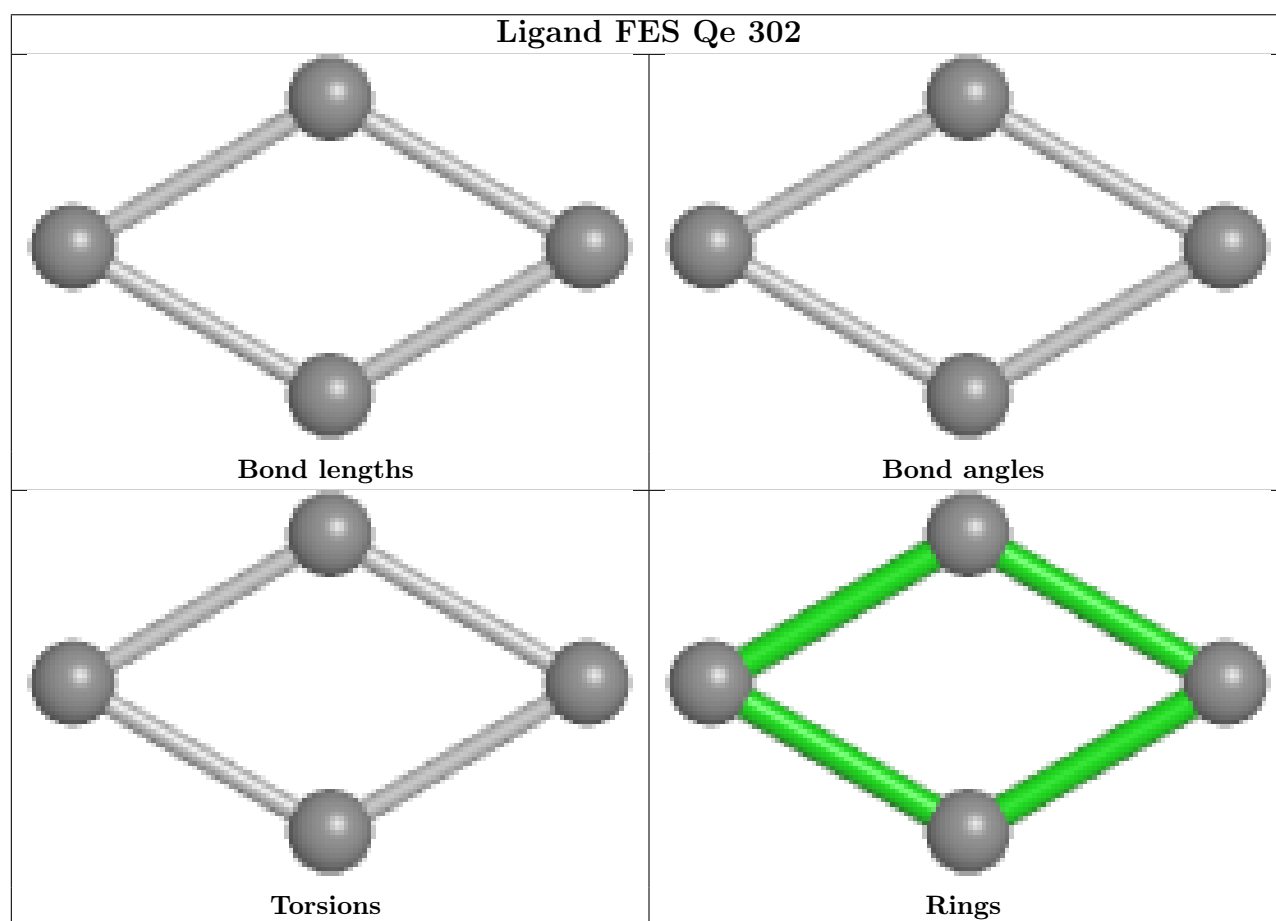
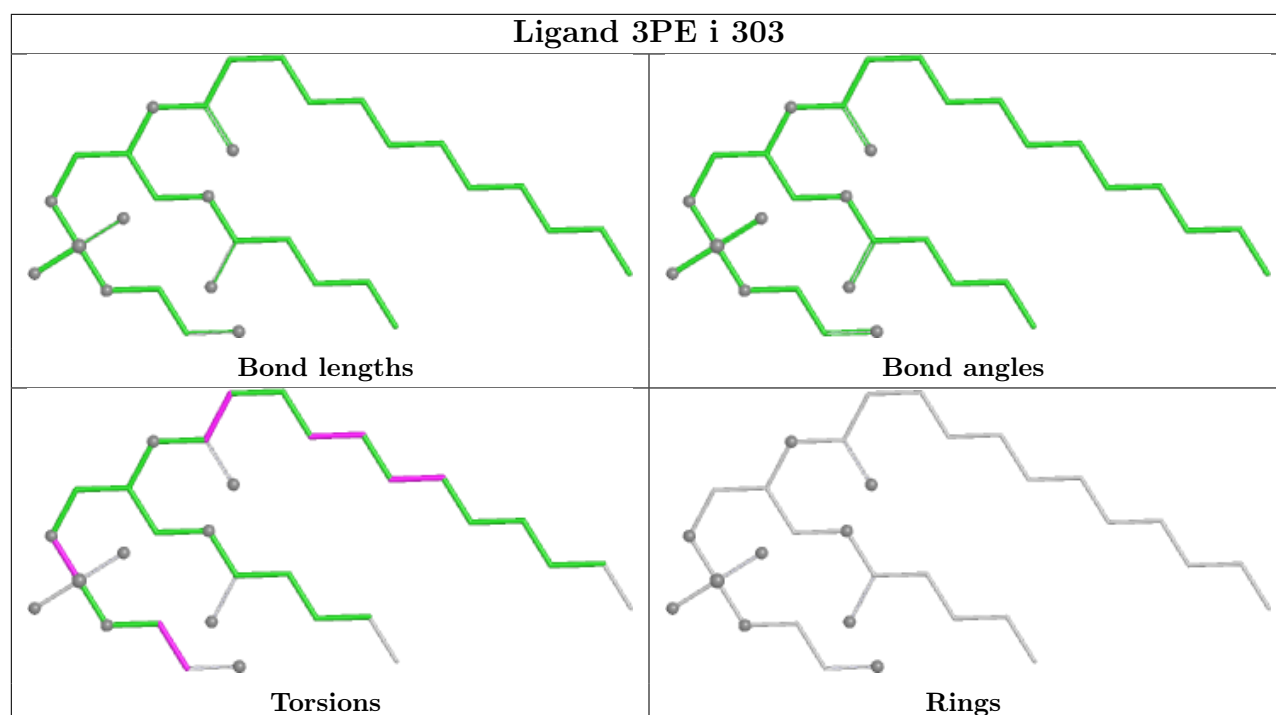


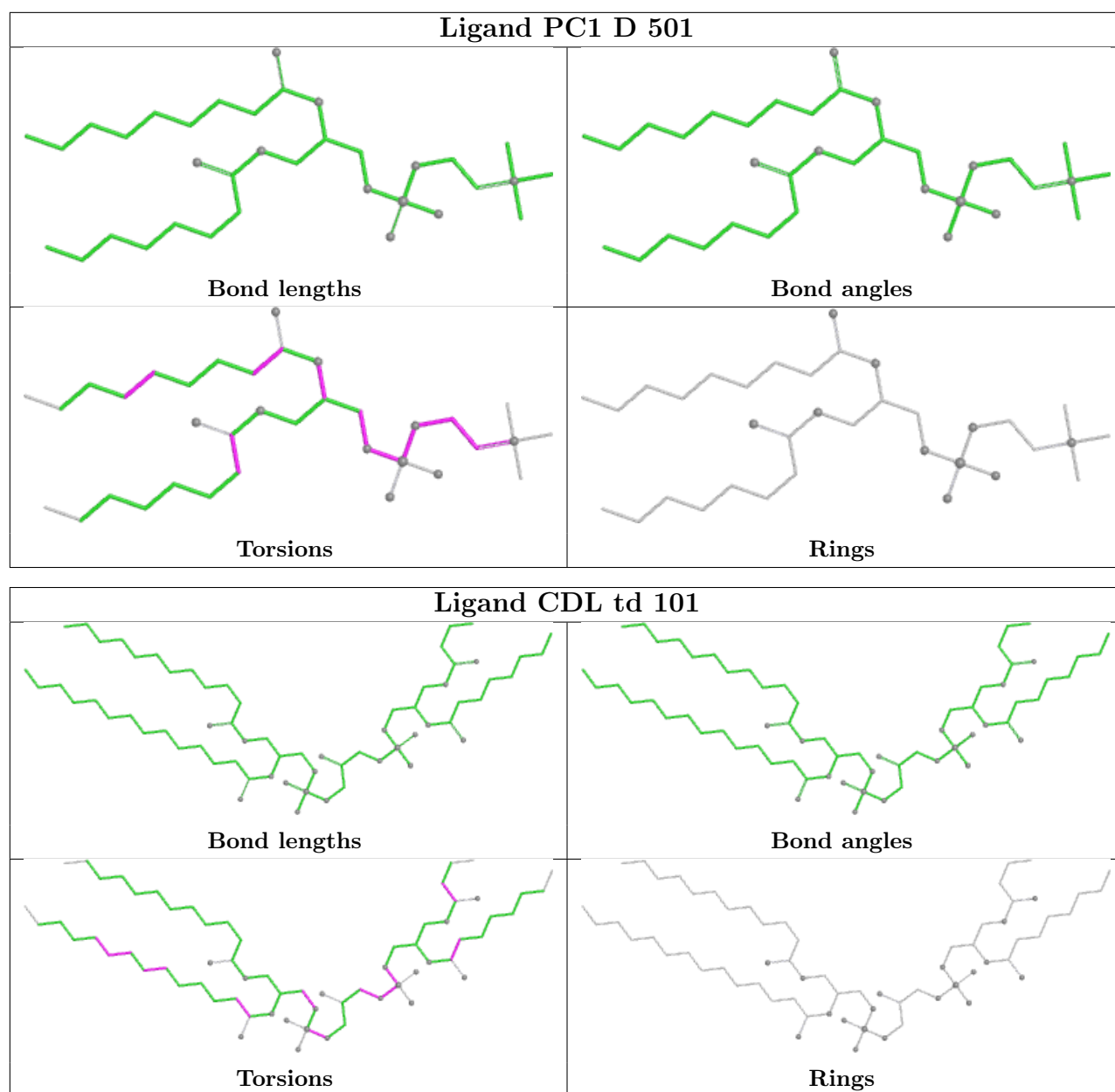


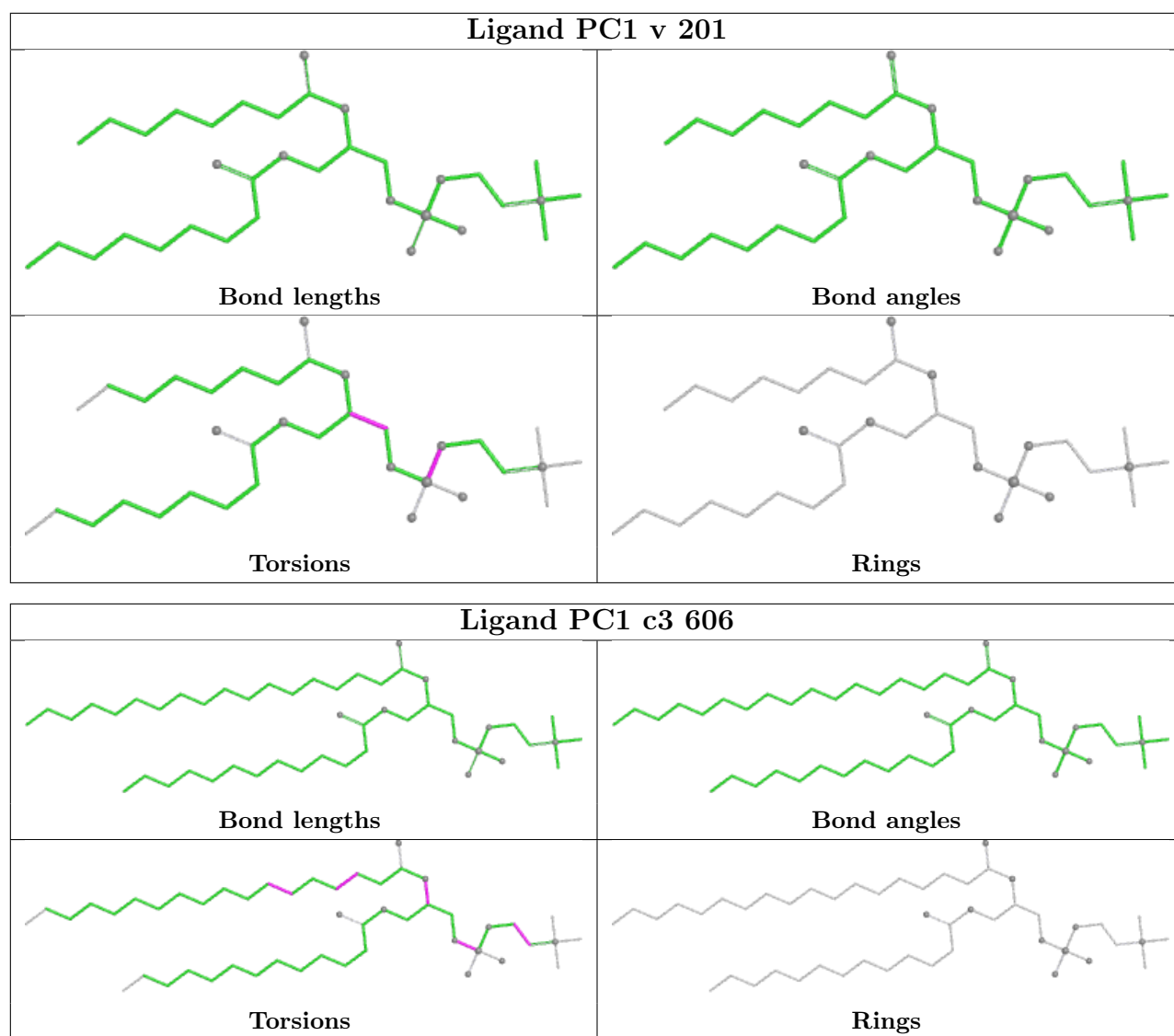




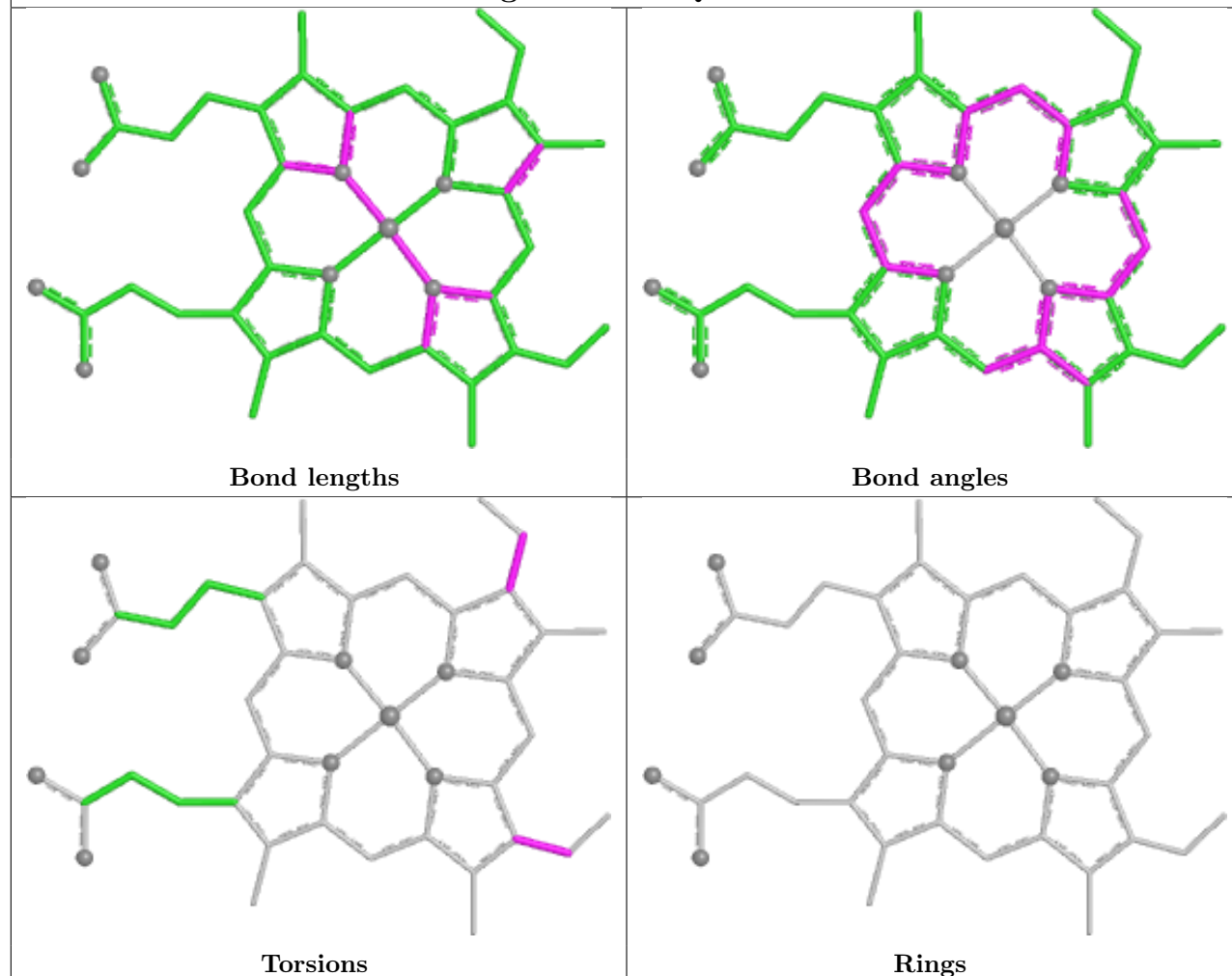




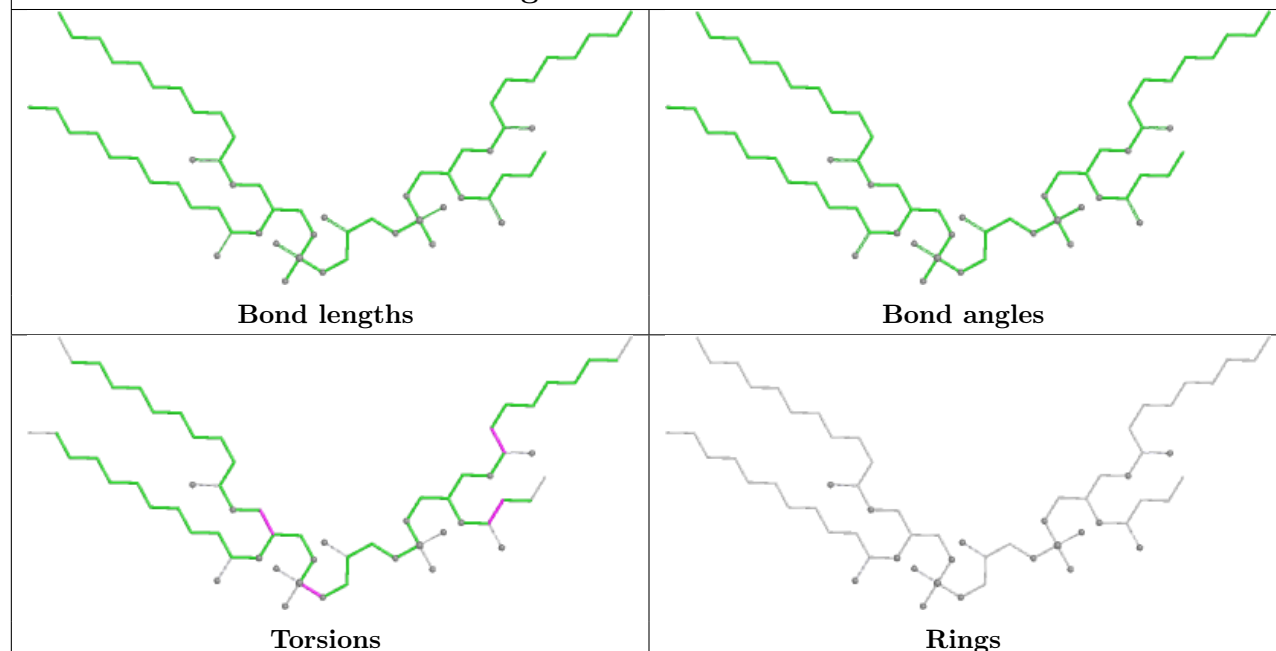


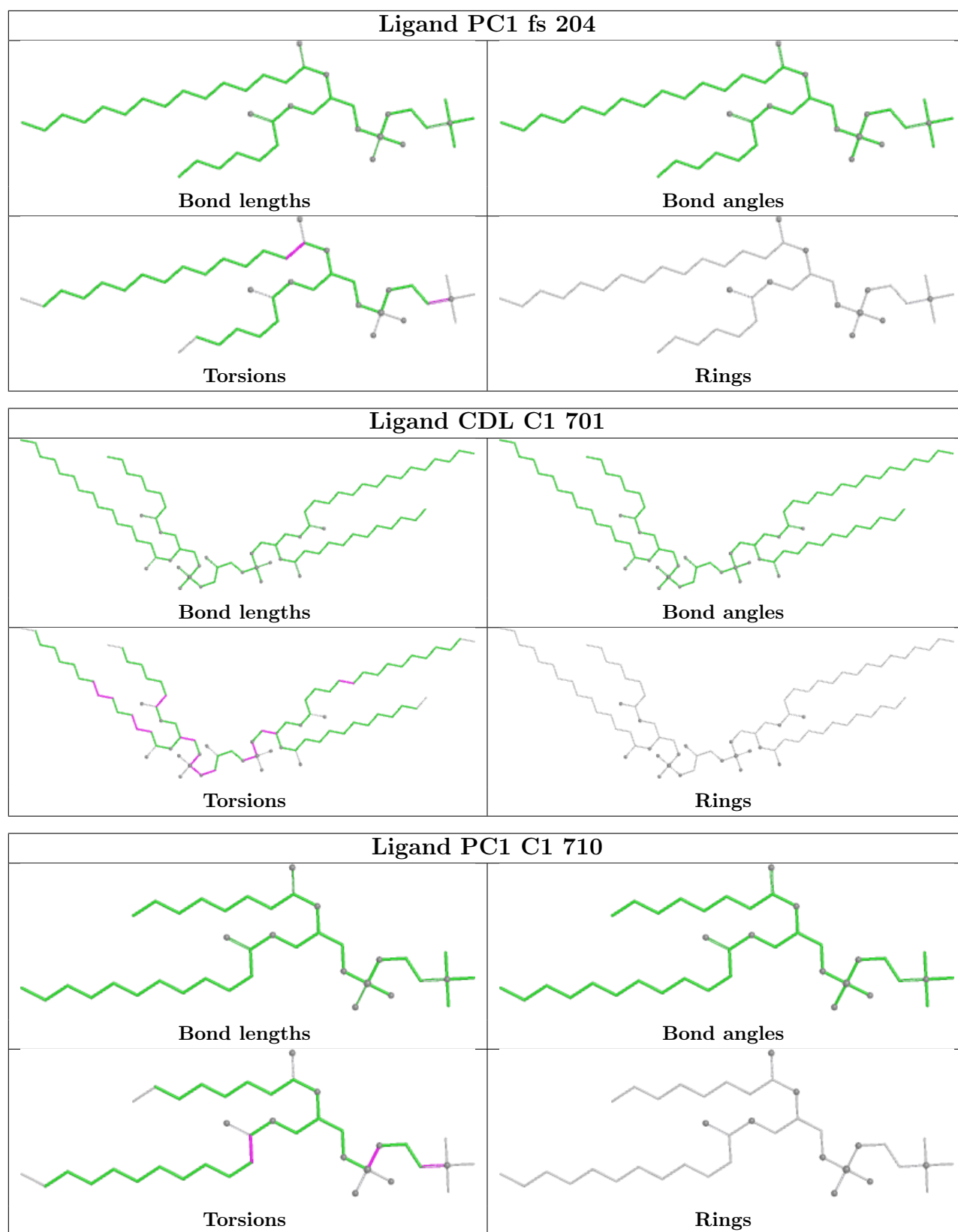


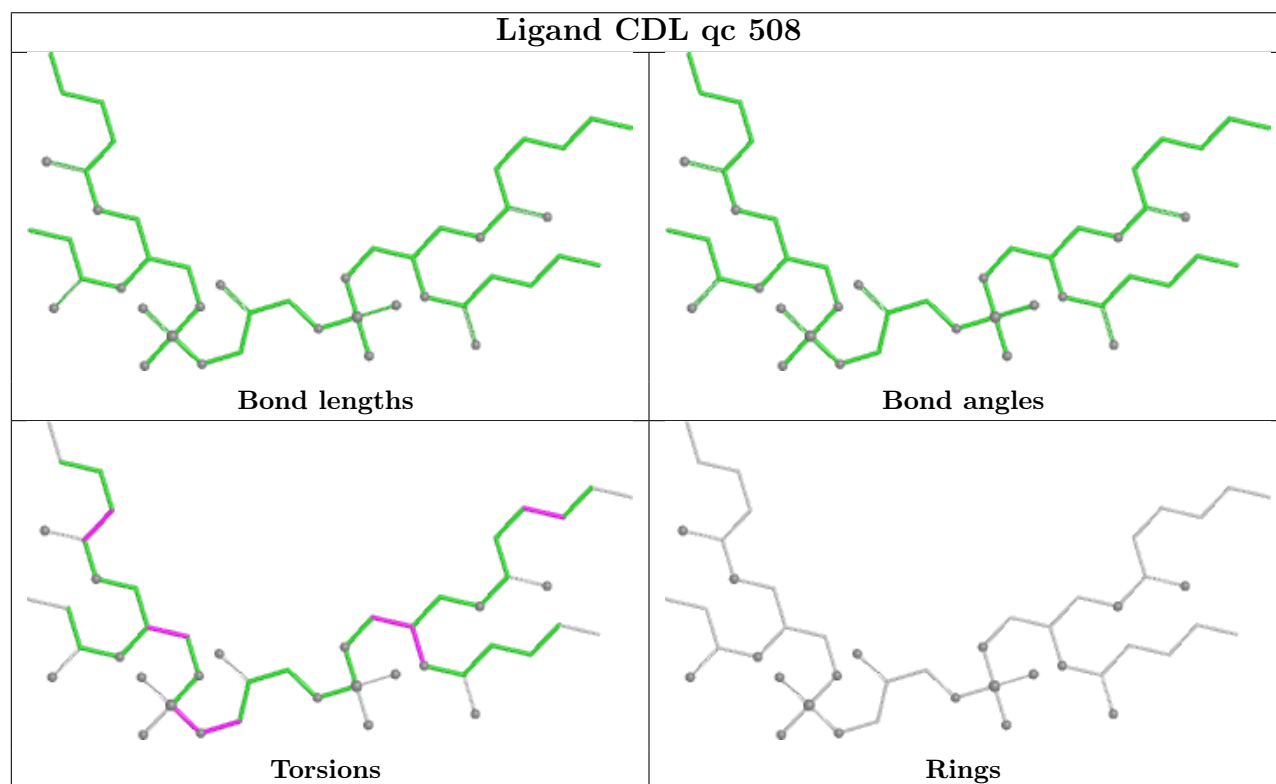
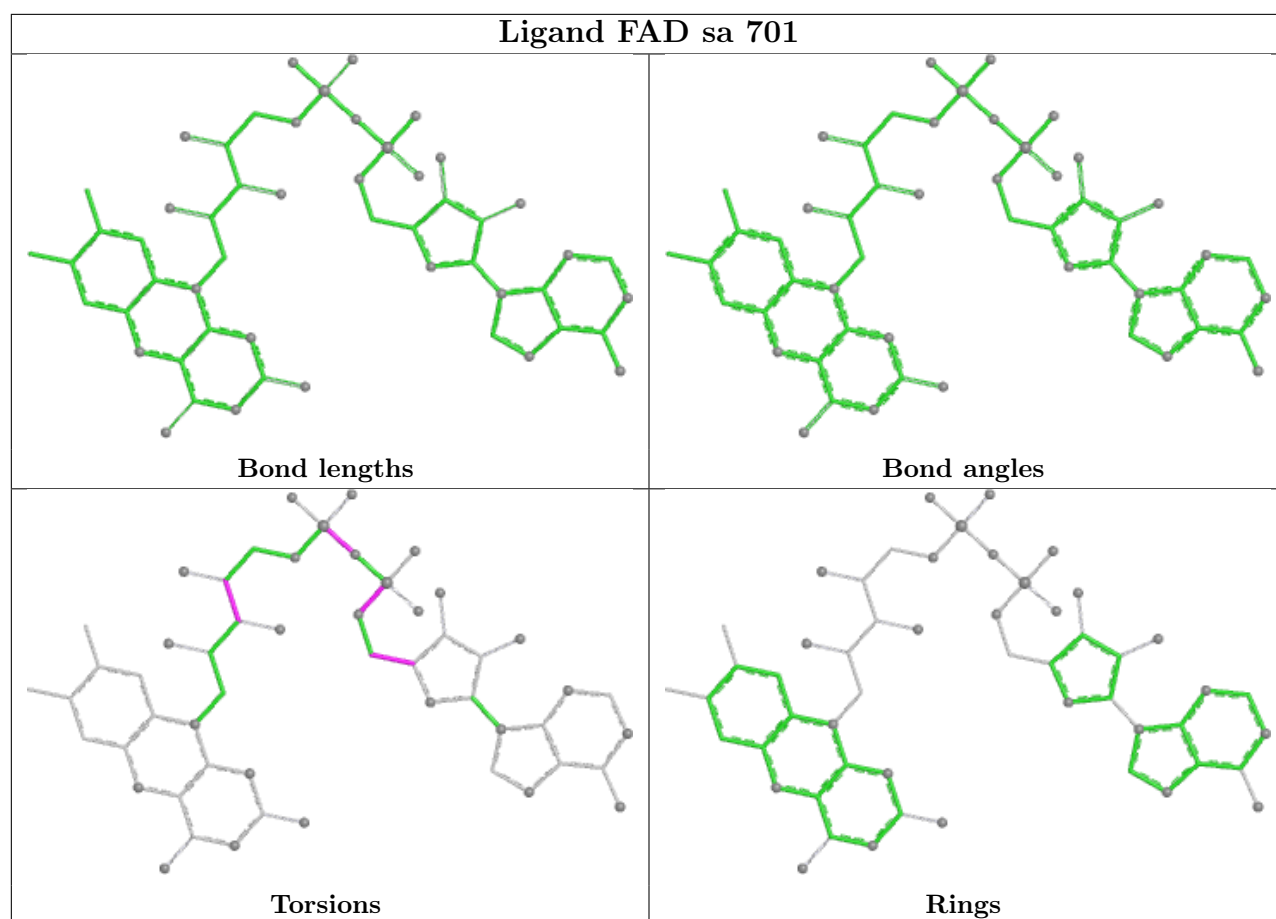
Ligand HEM Qc 502

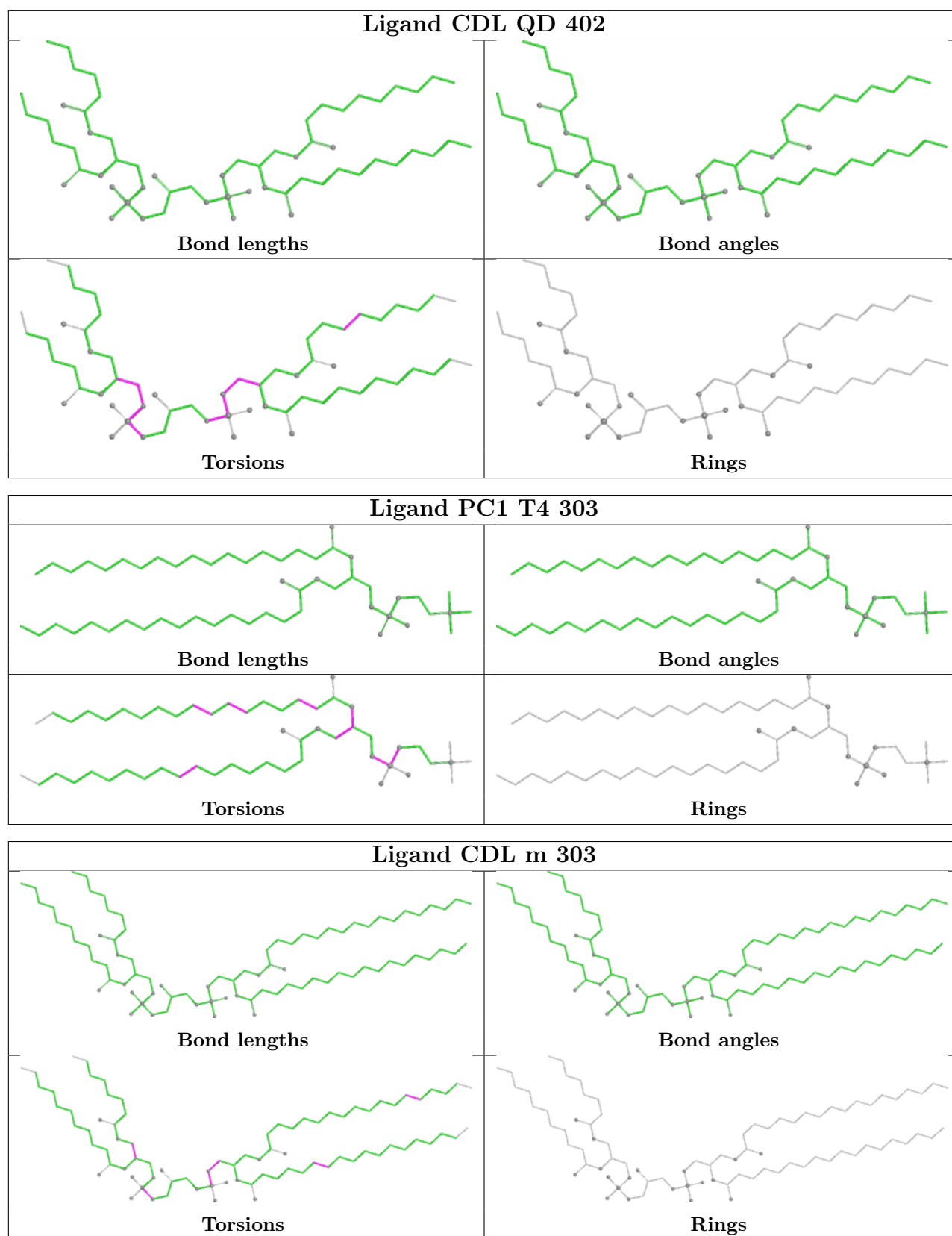


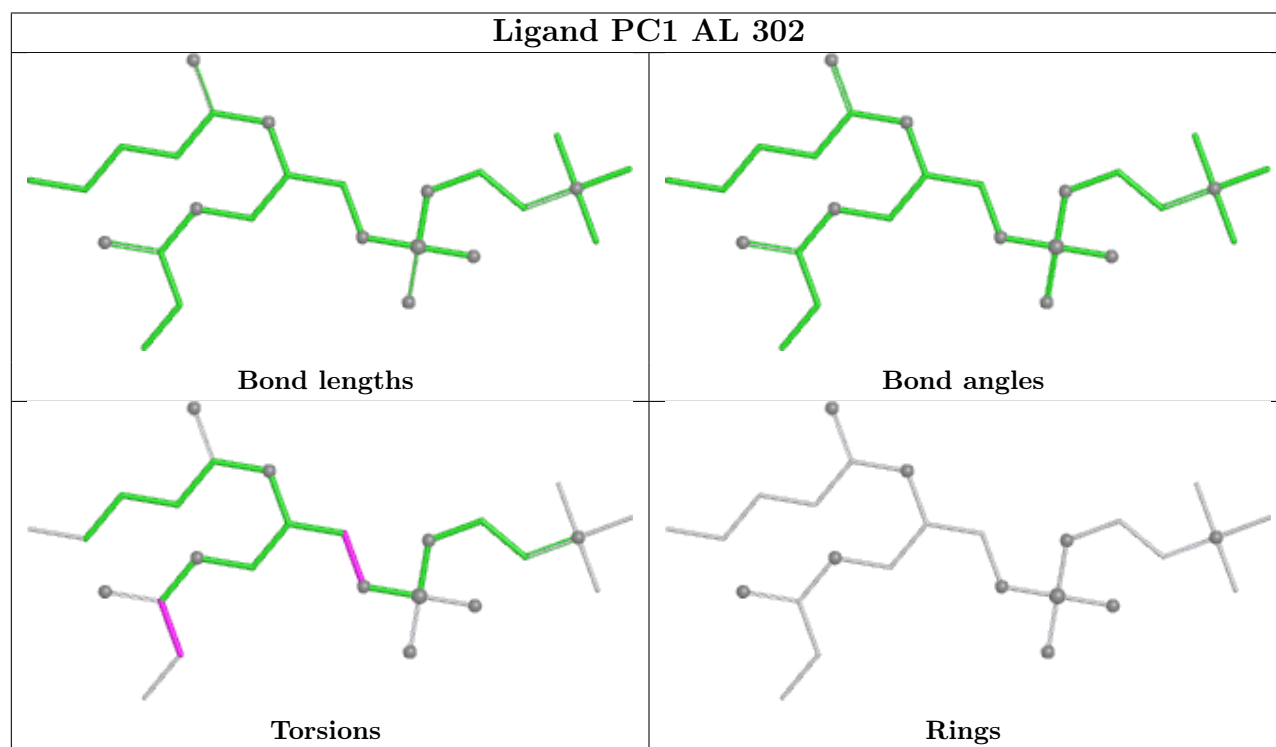
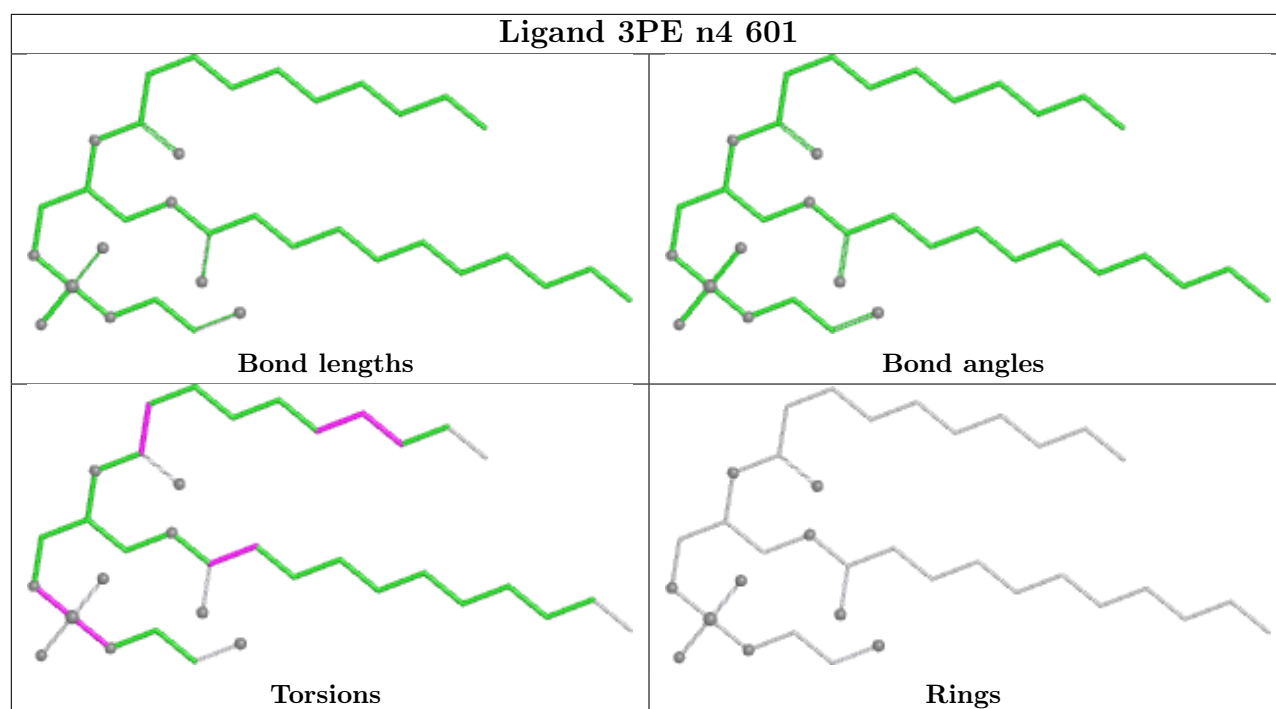
Ligand CDL m3 401

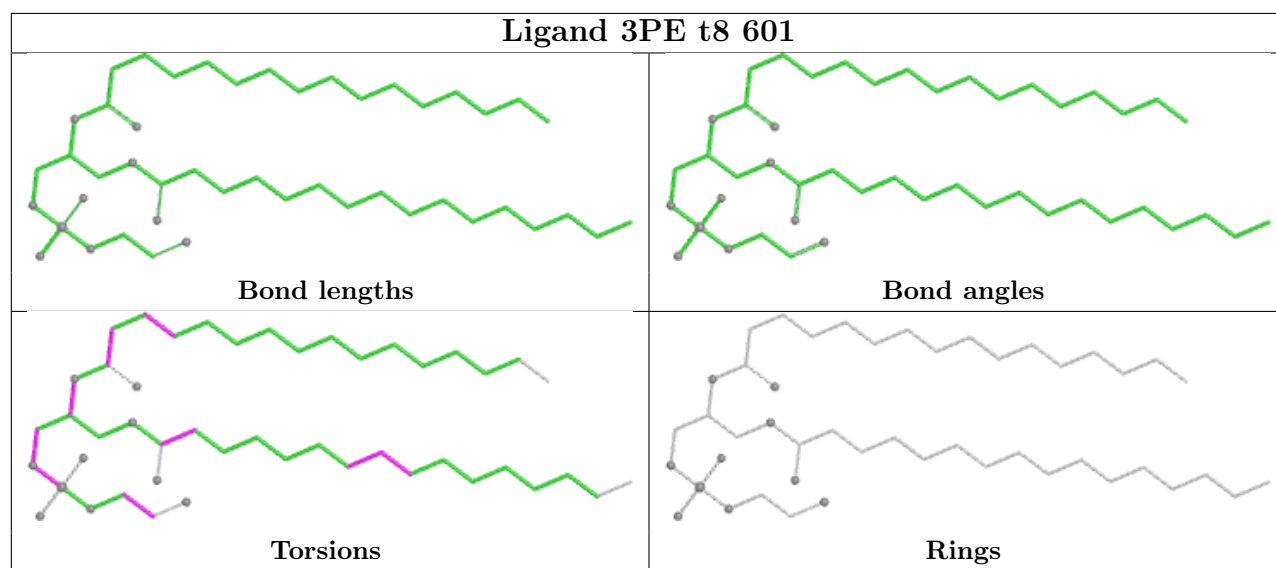
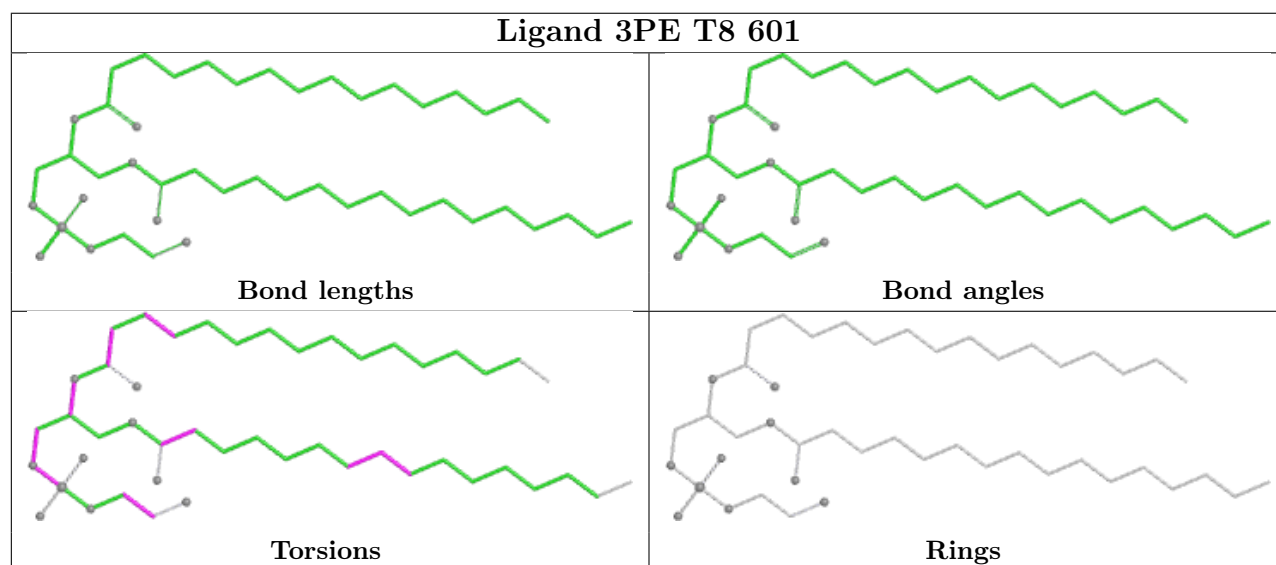
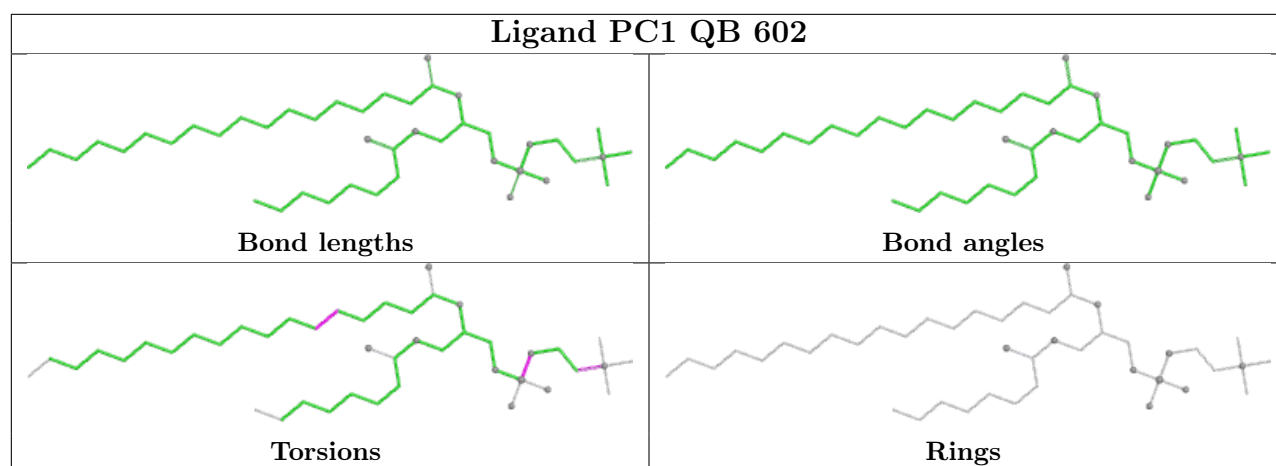


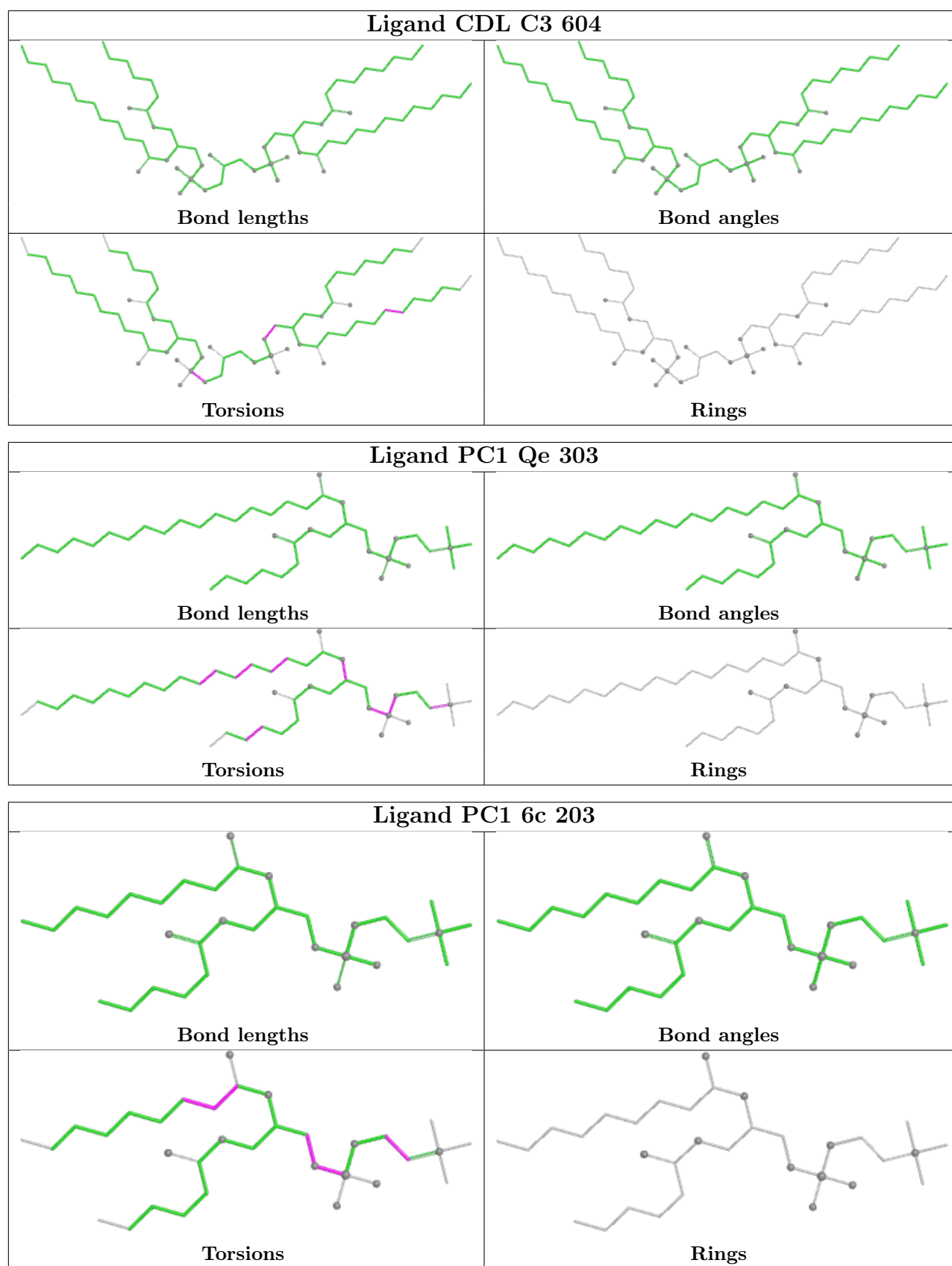


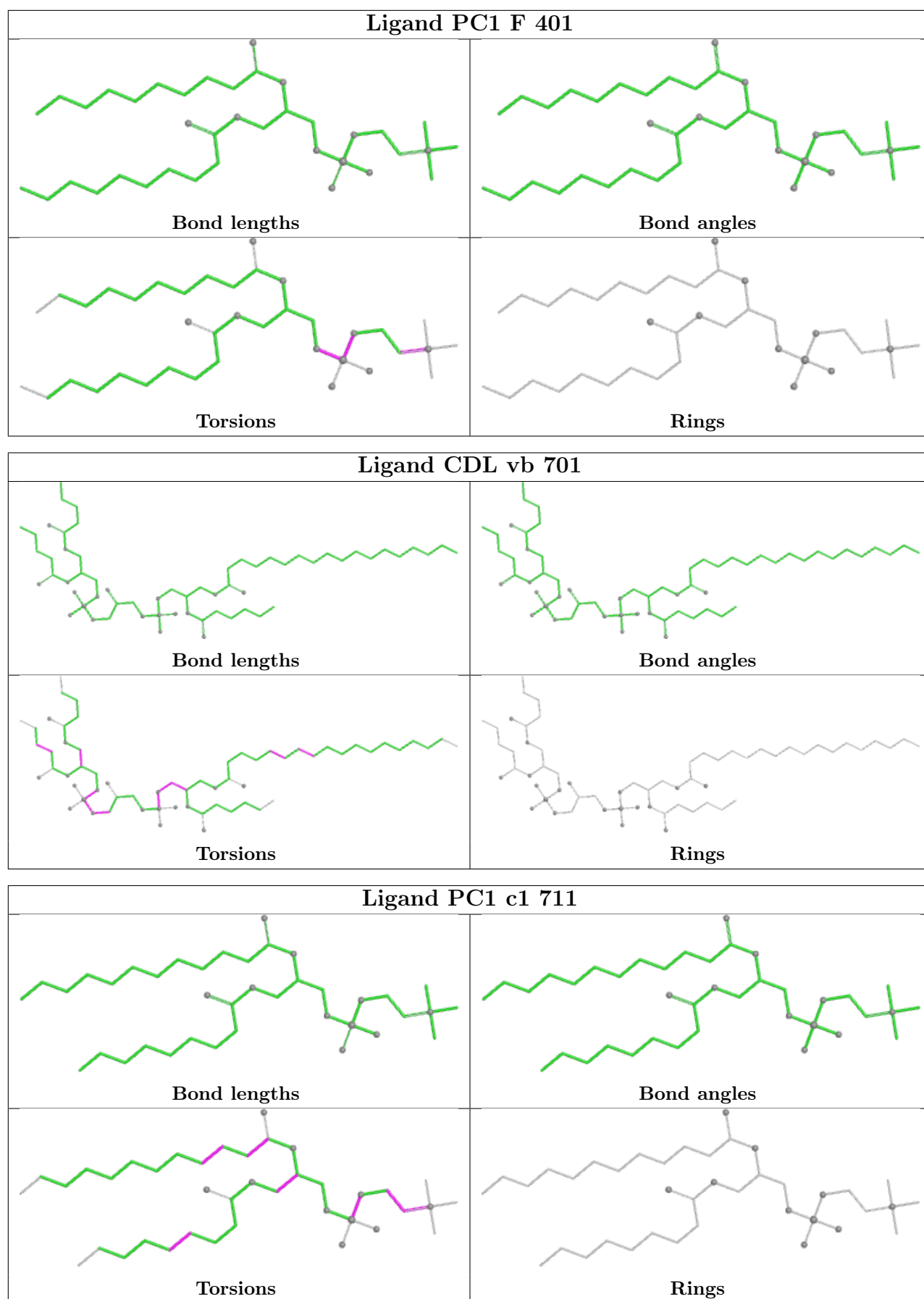


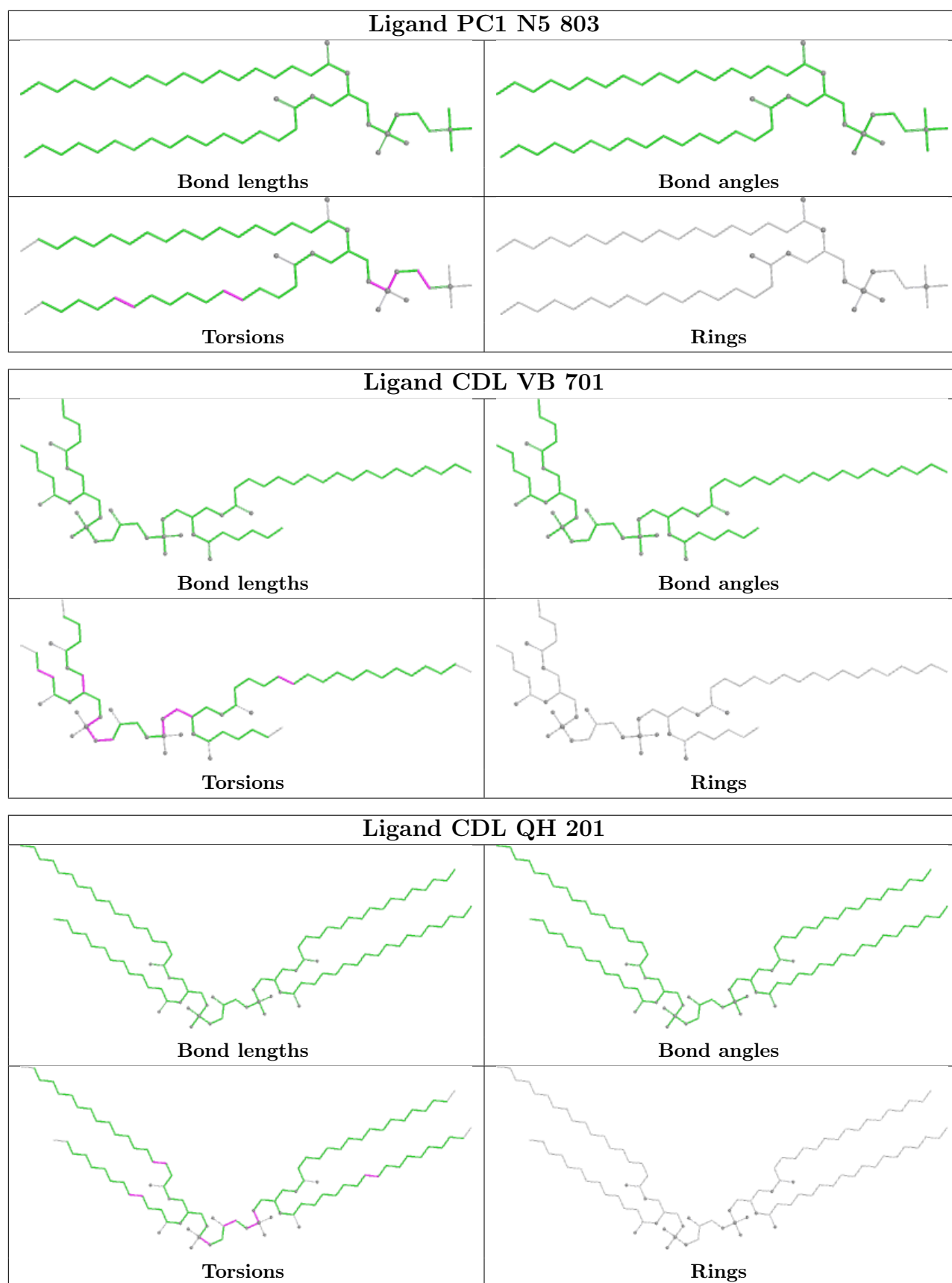


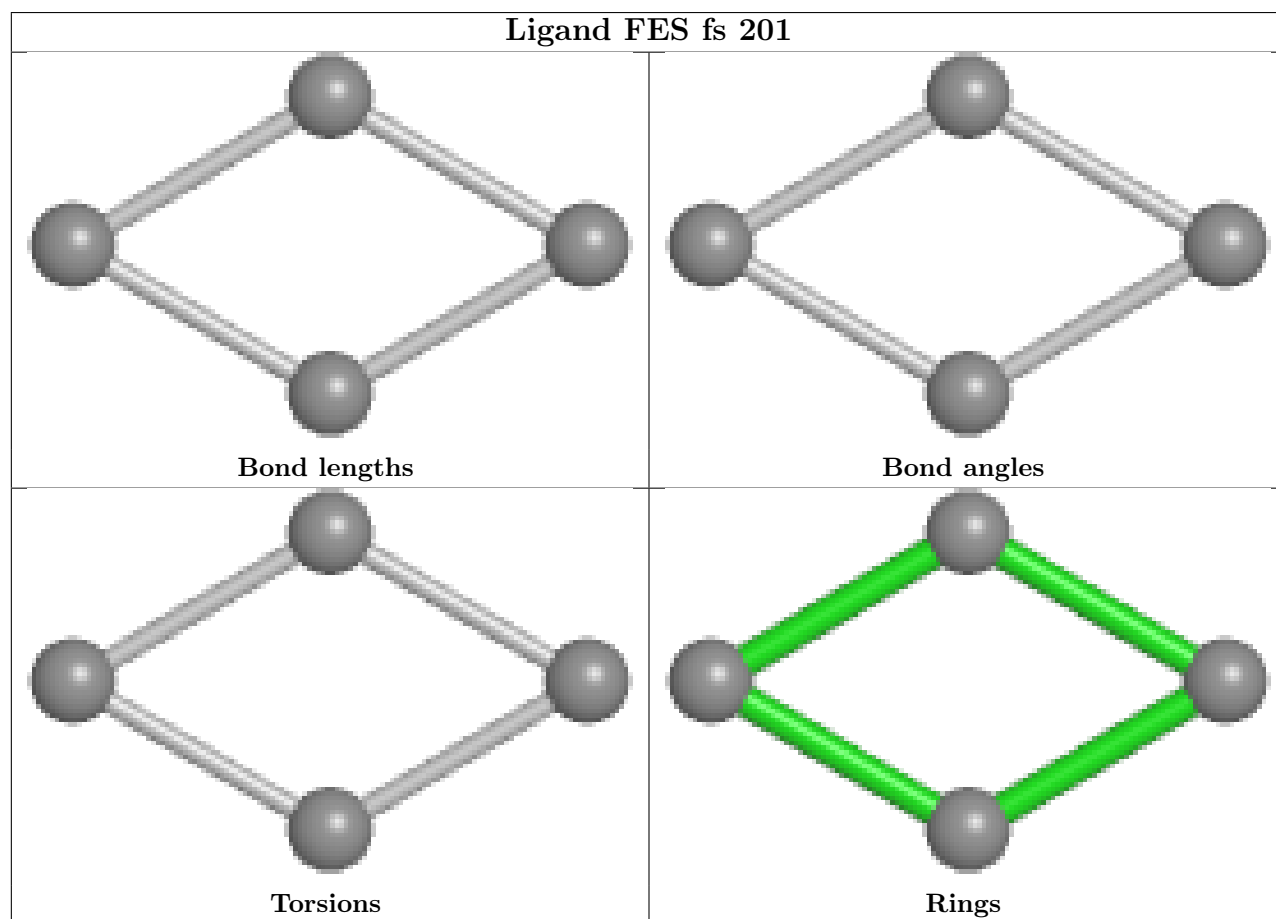
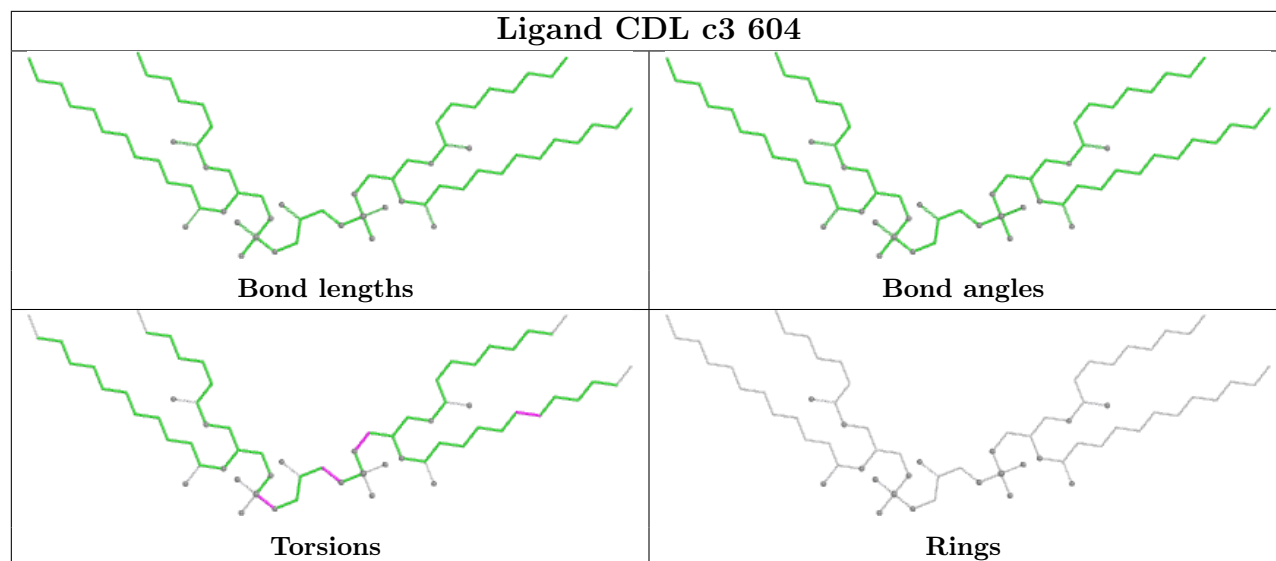




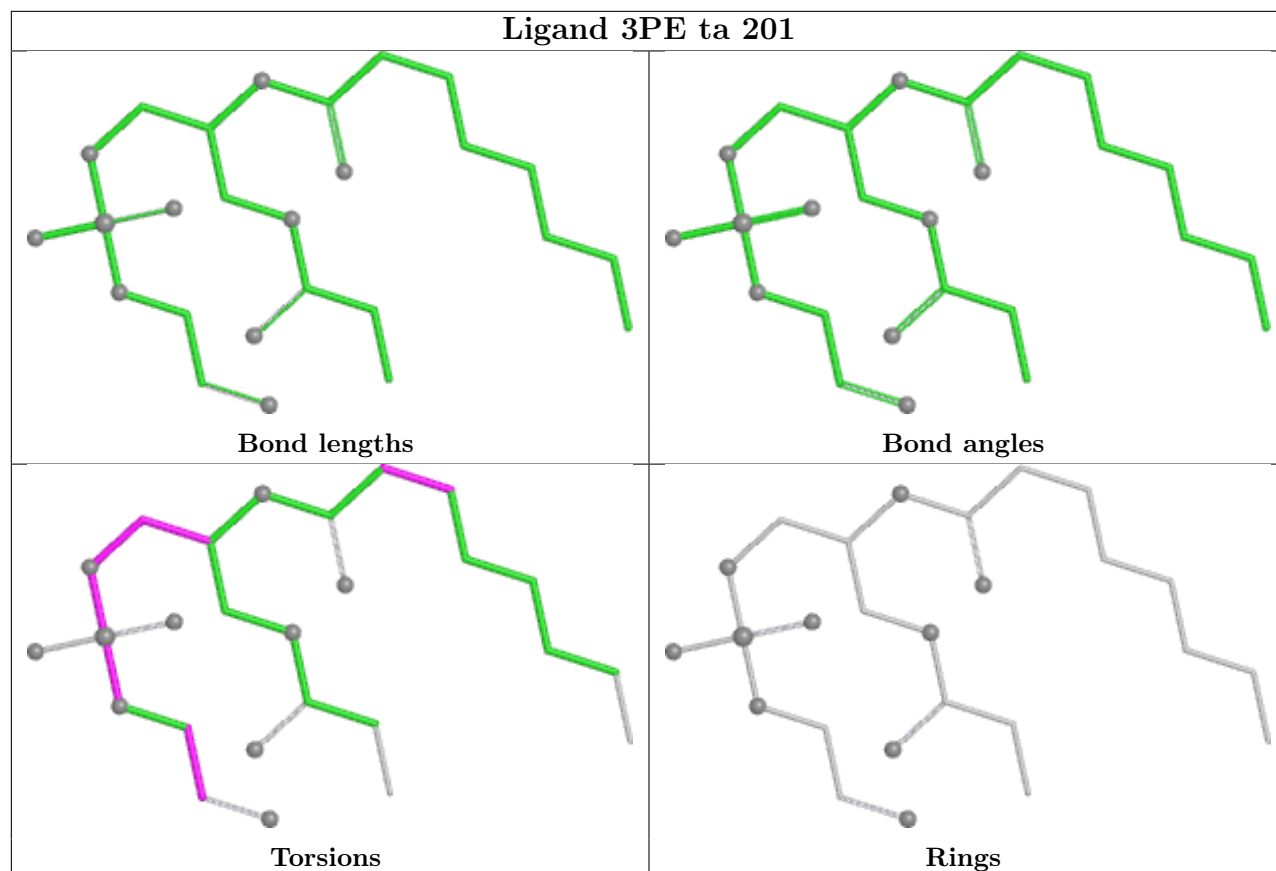




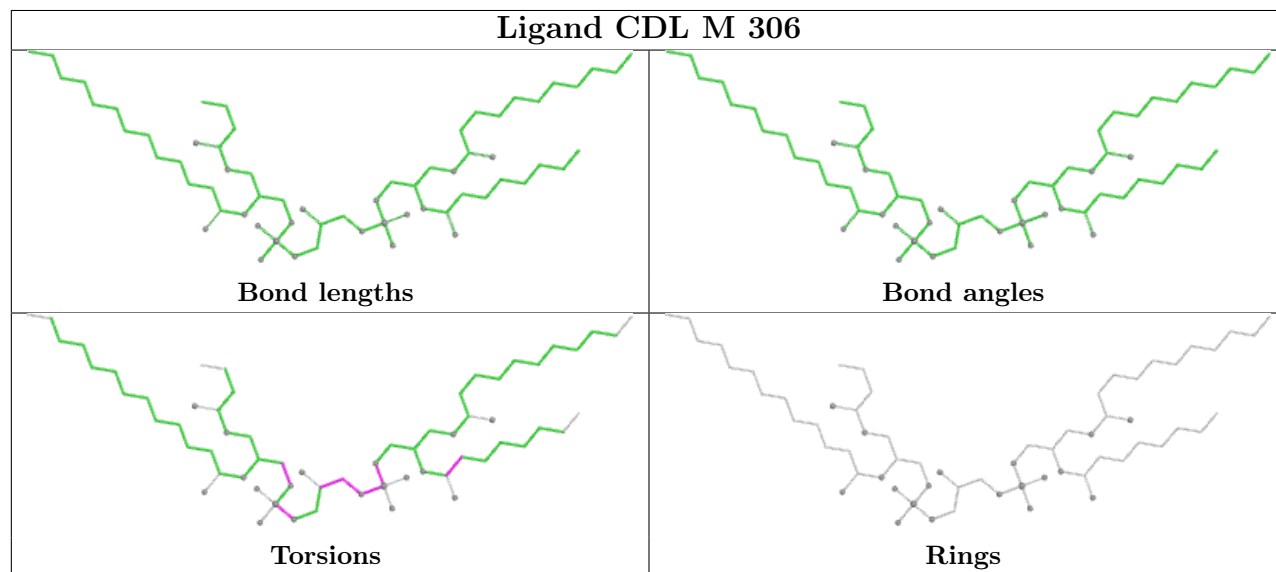


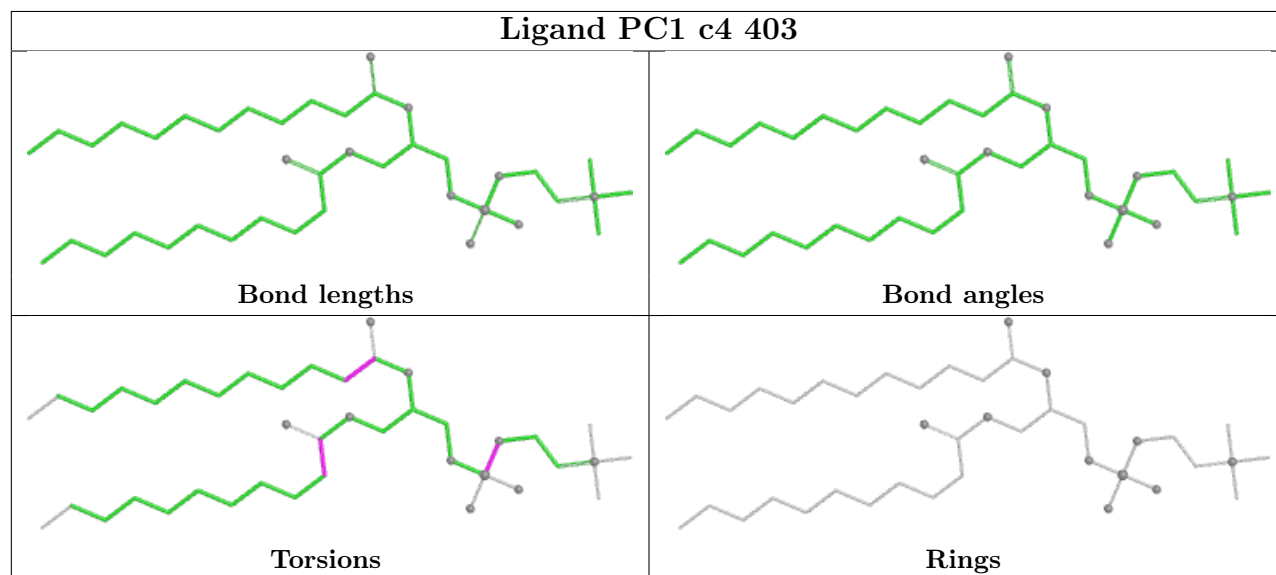
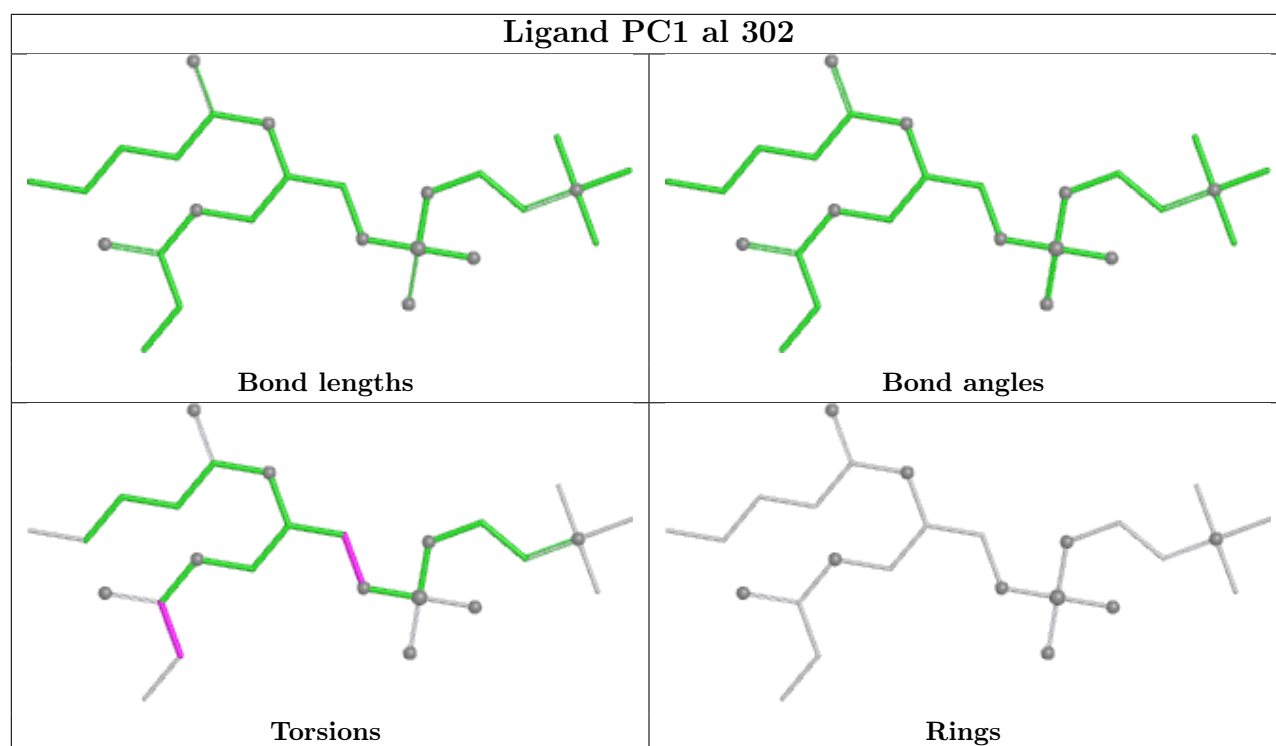


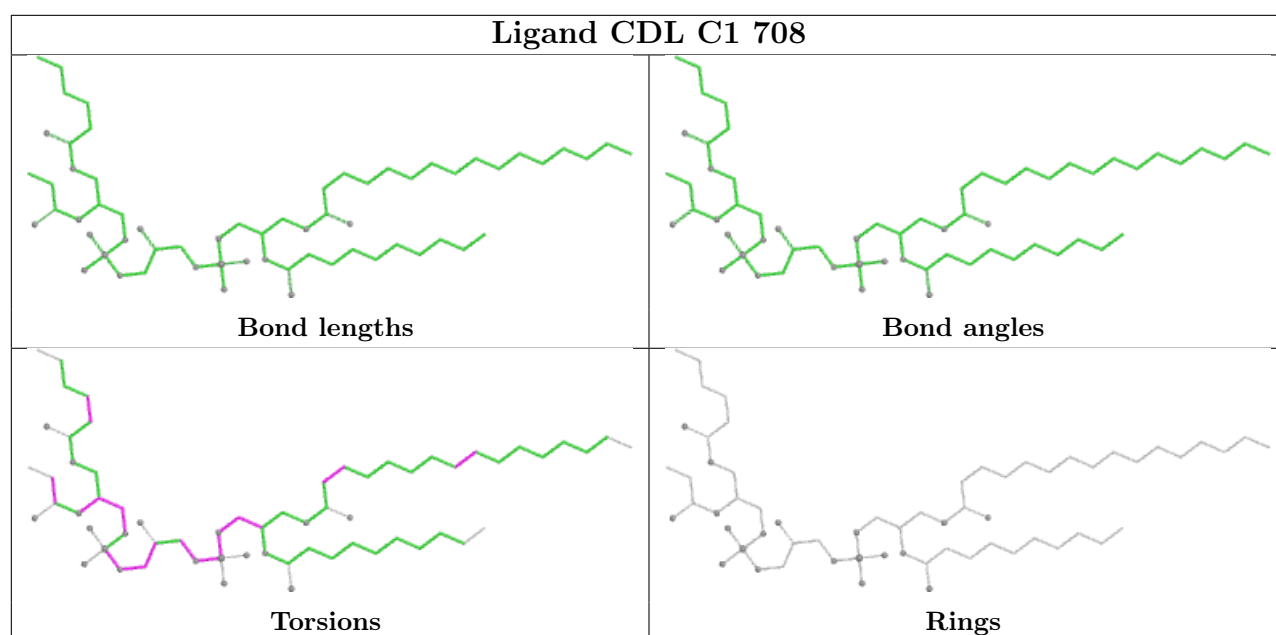
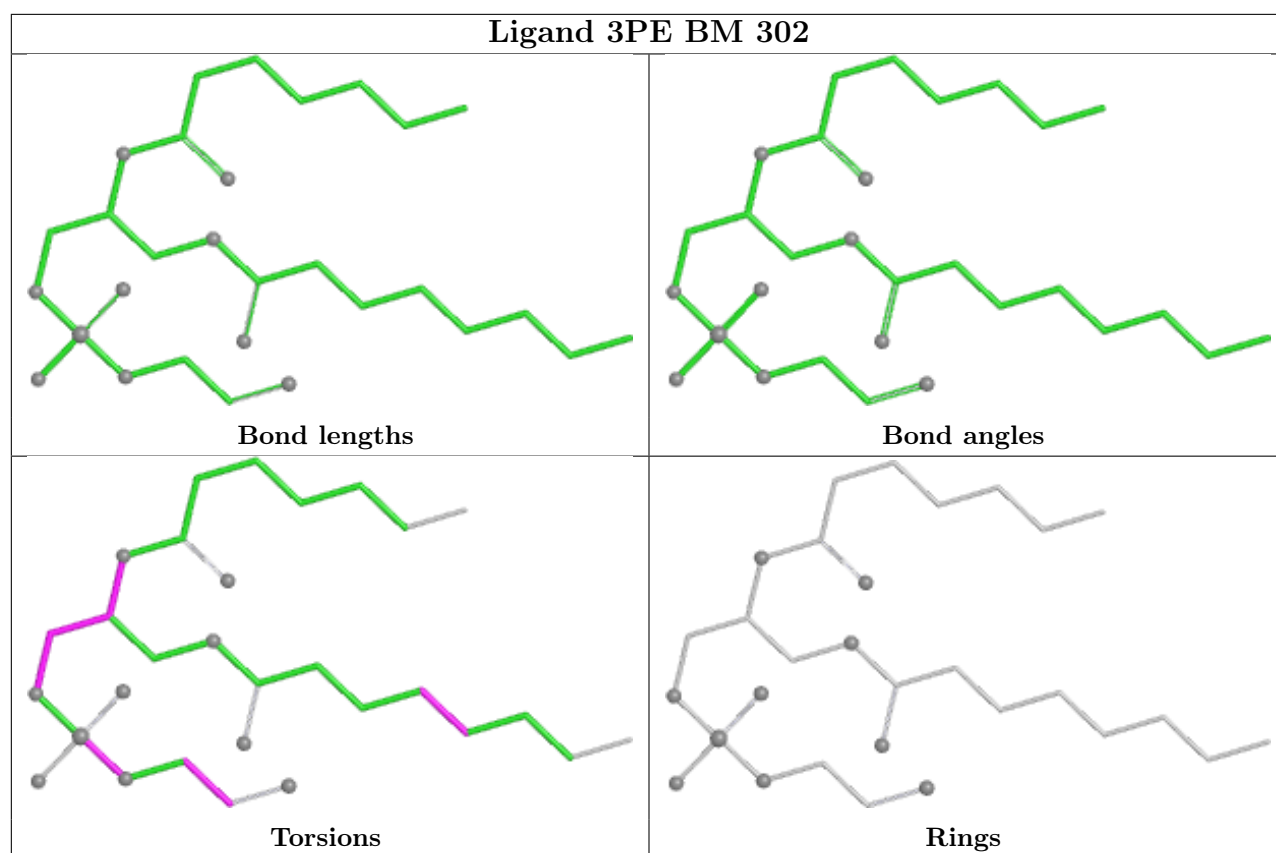
Ligand 3PE ta 201



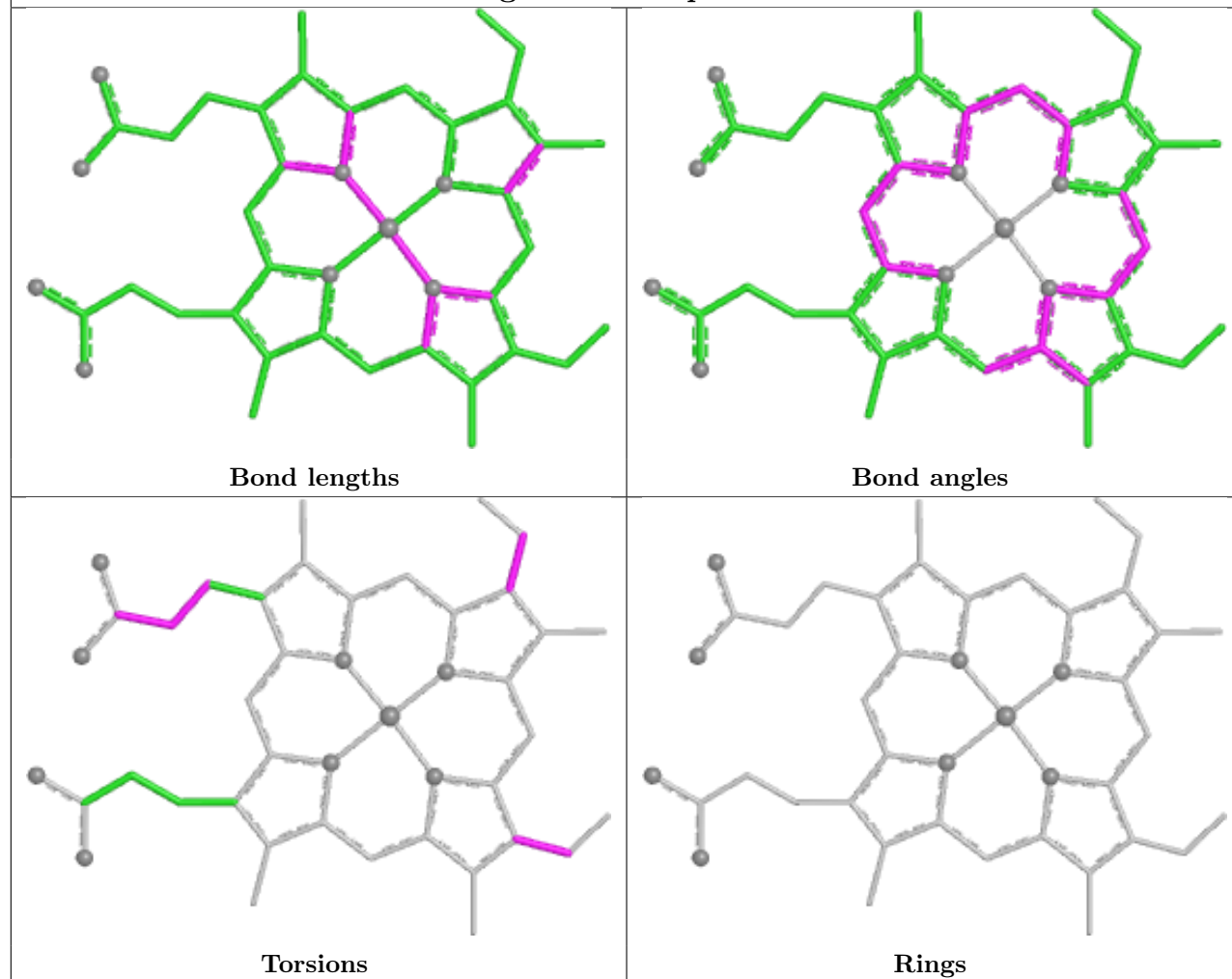
Ligand CDL M 306



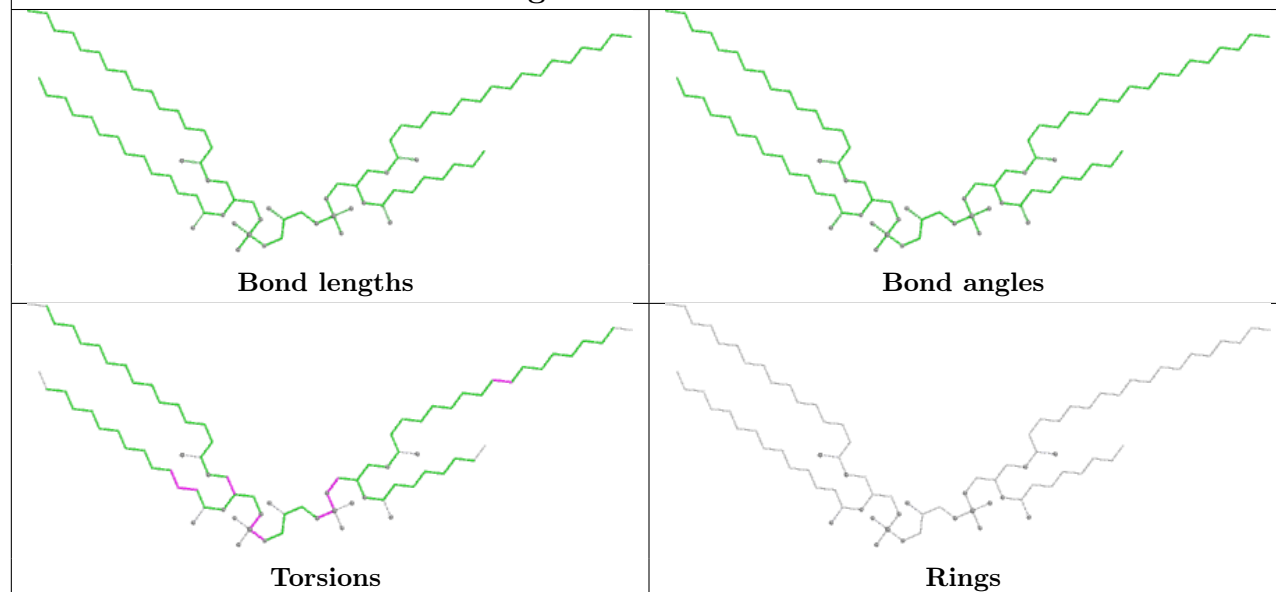


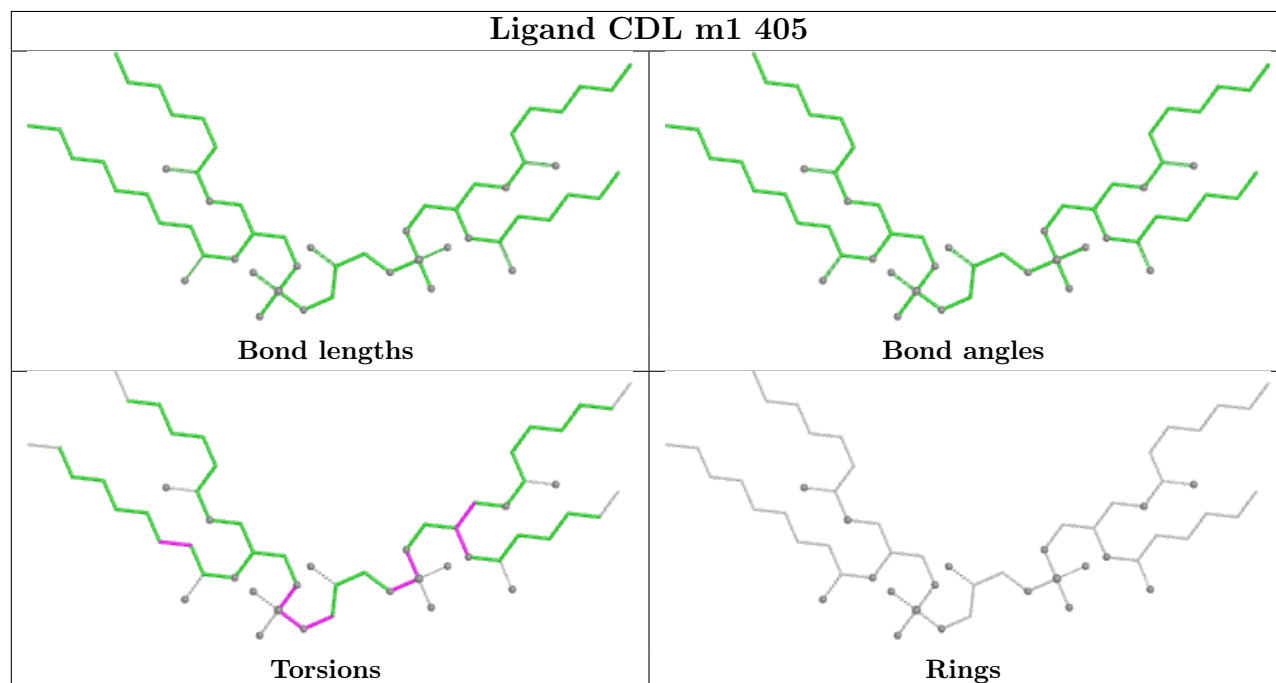
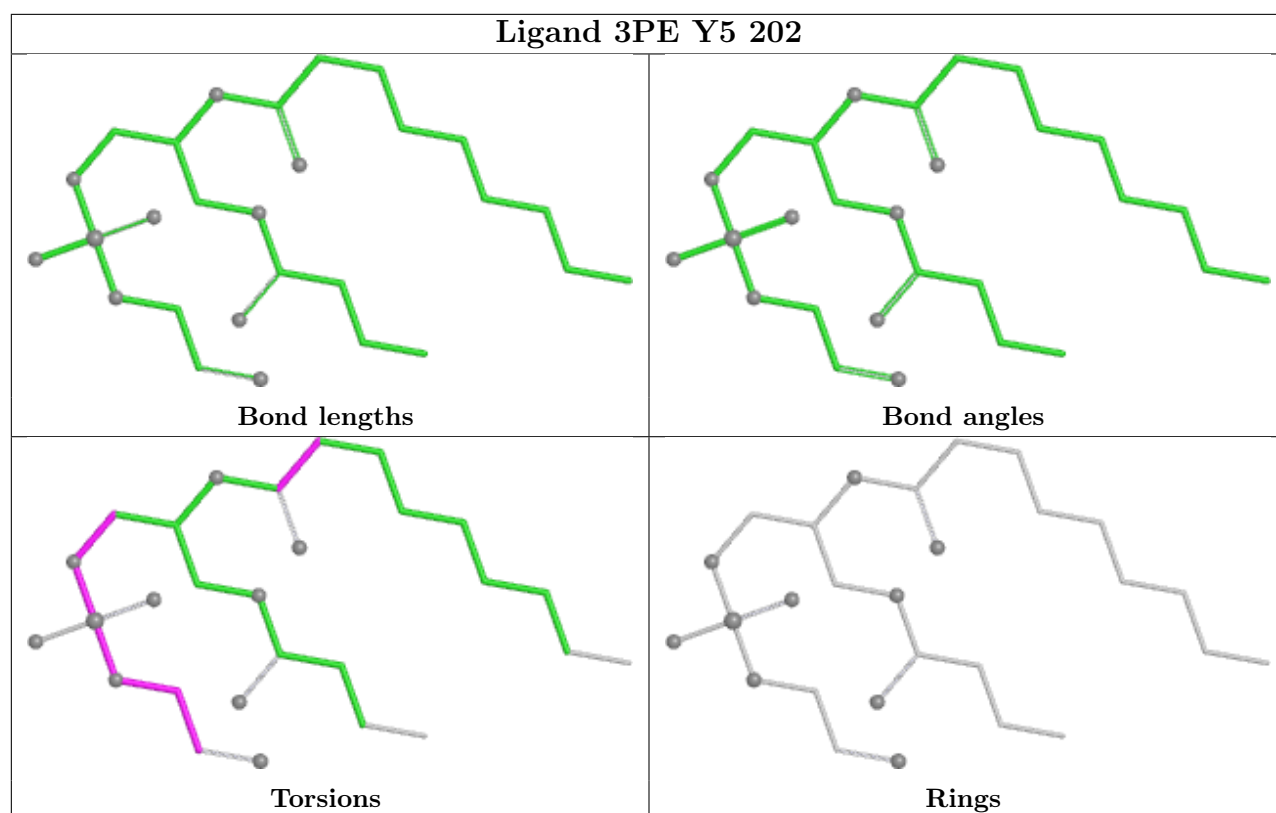


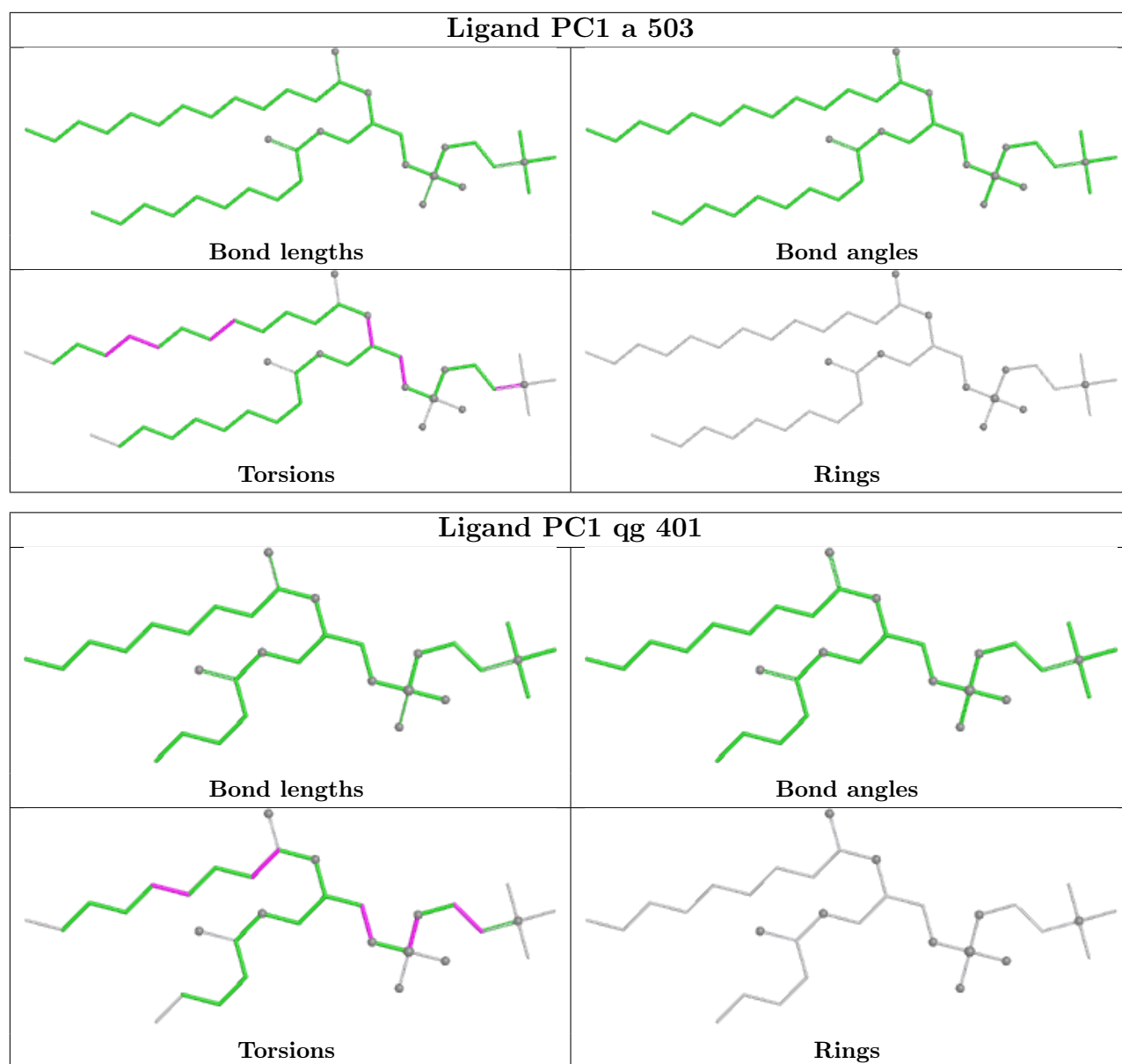
Ligand HEM qC 501

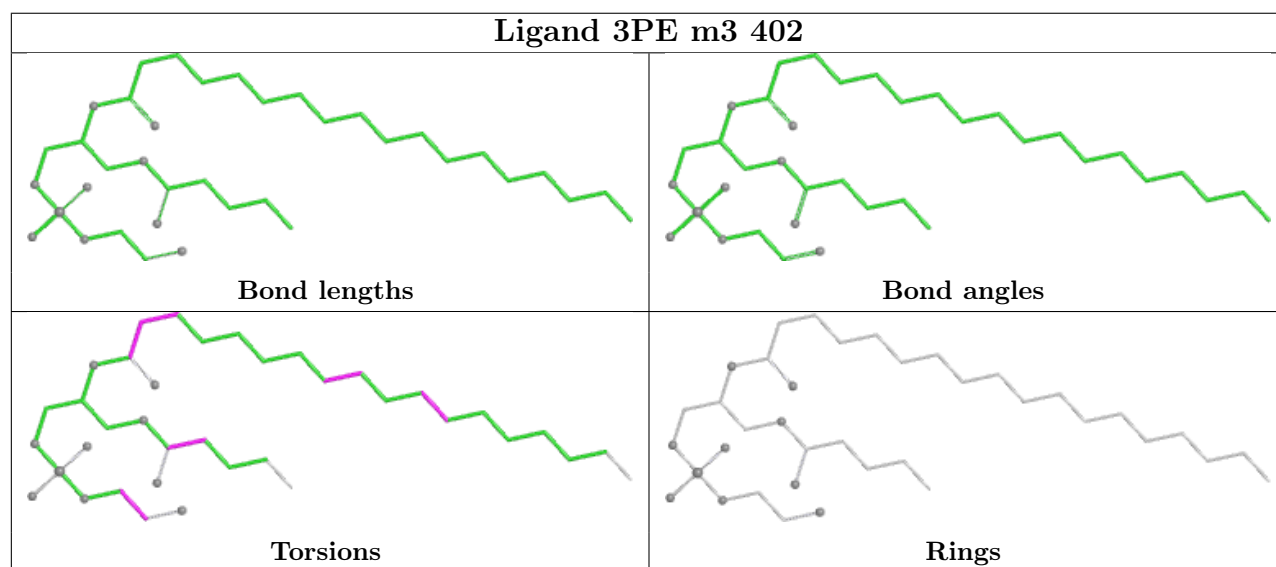
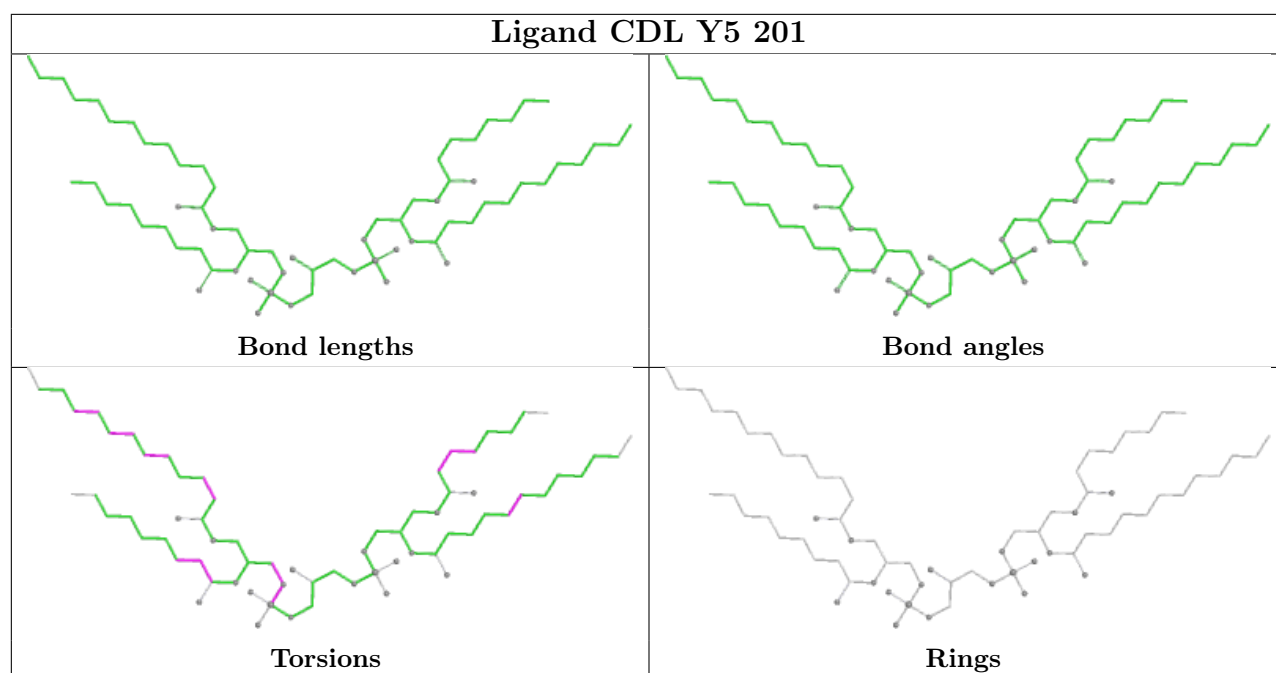


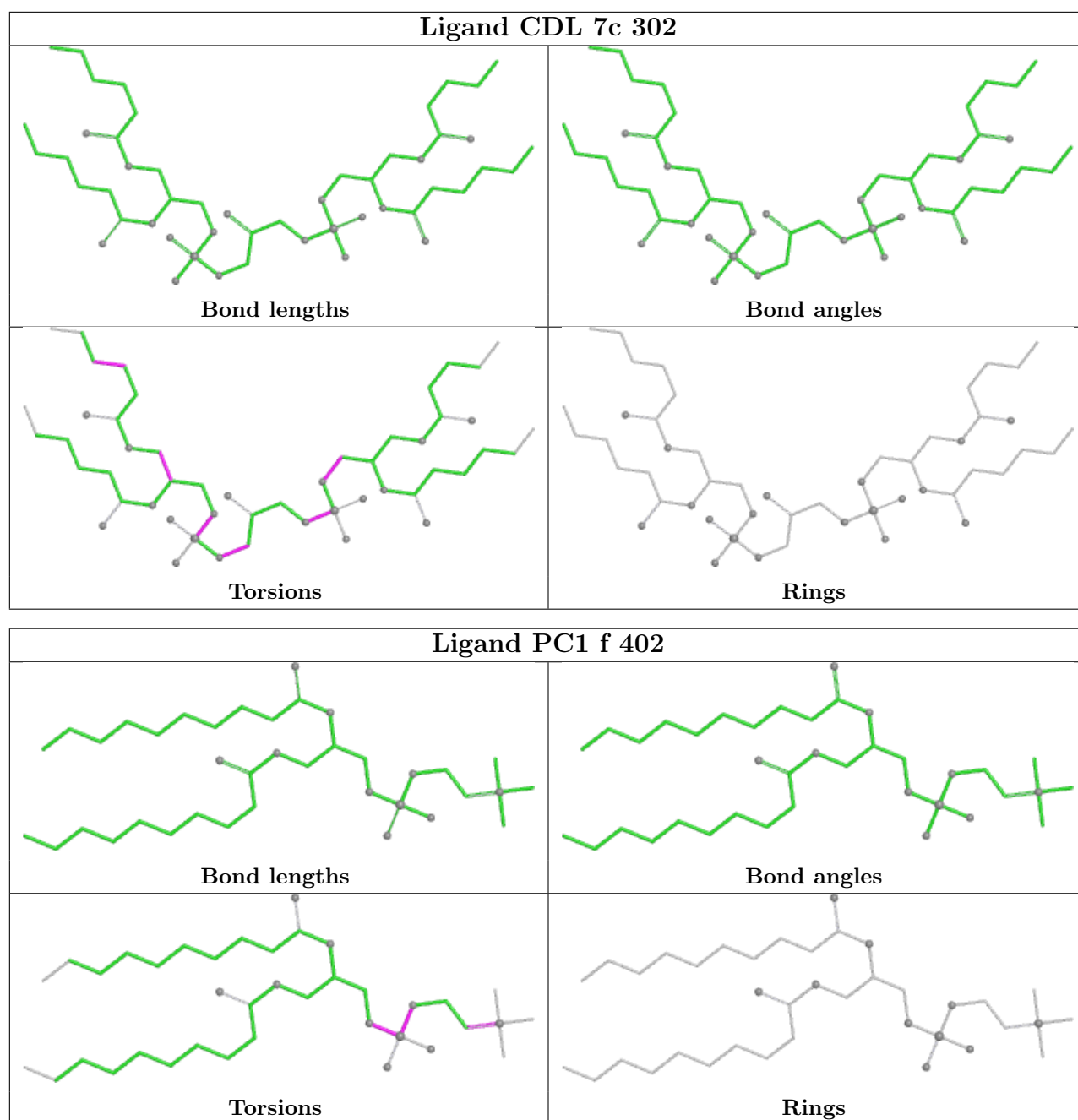
Ligand CDL th 200

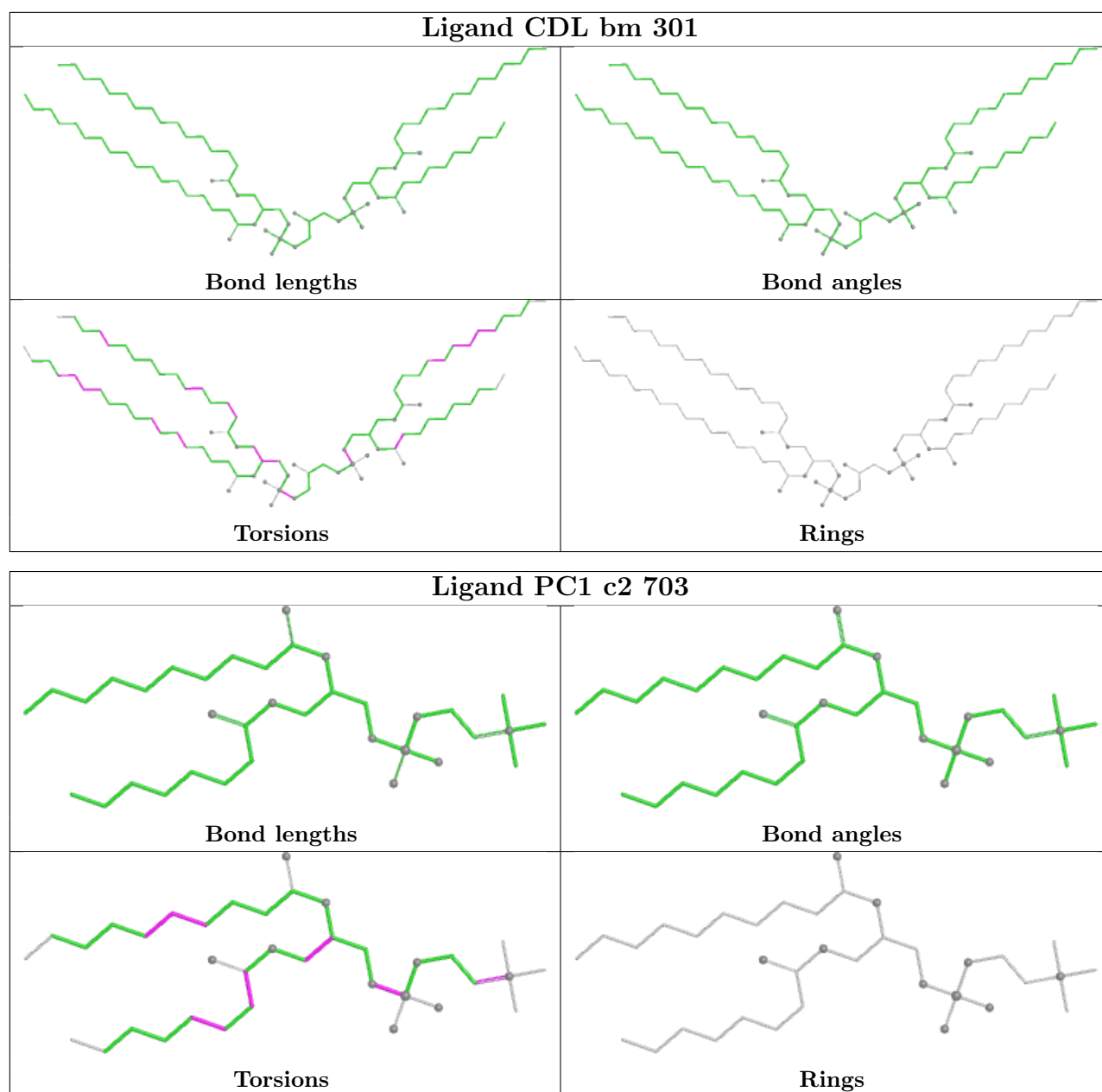


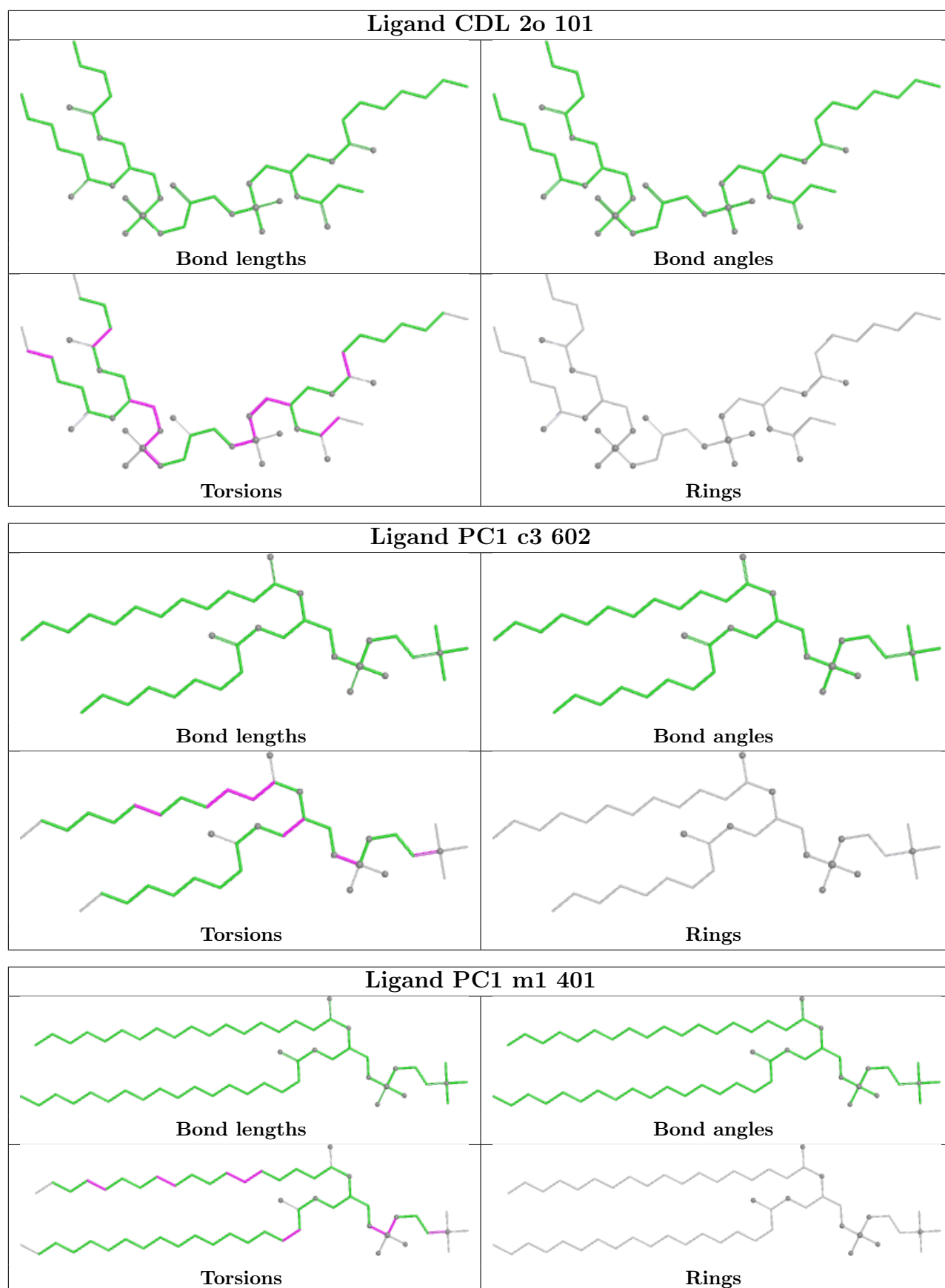


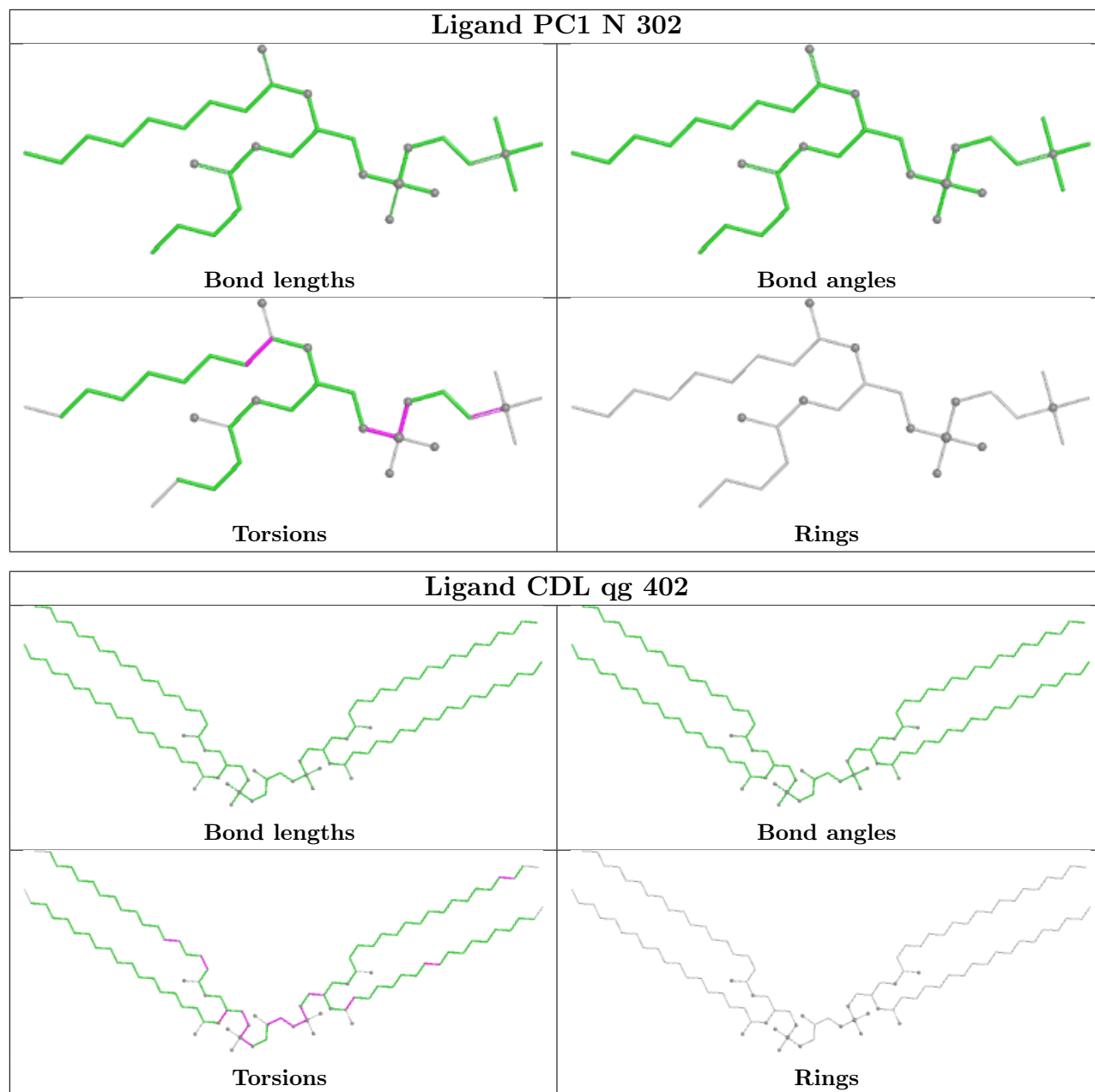


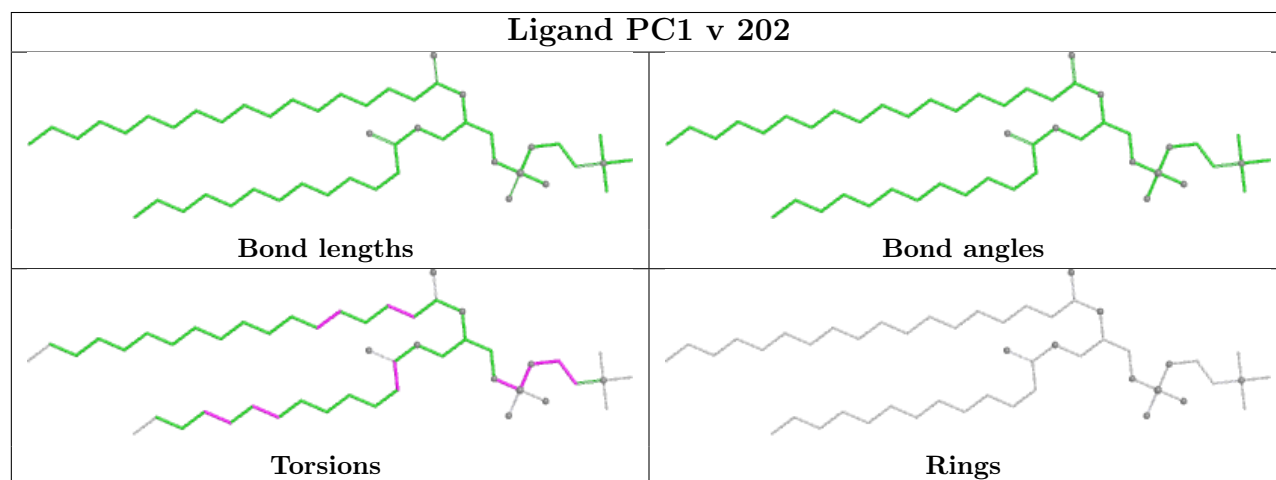
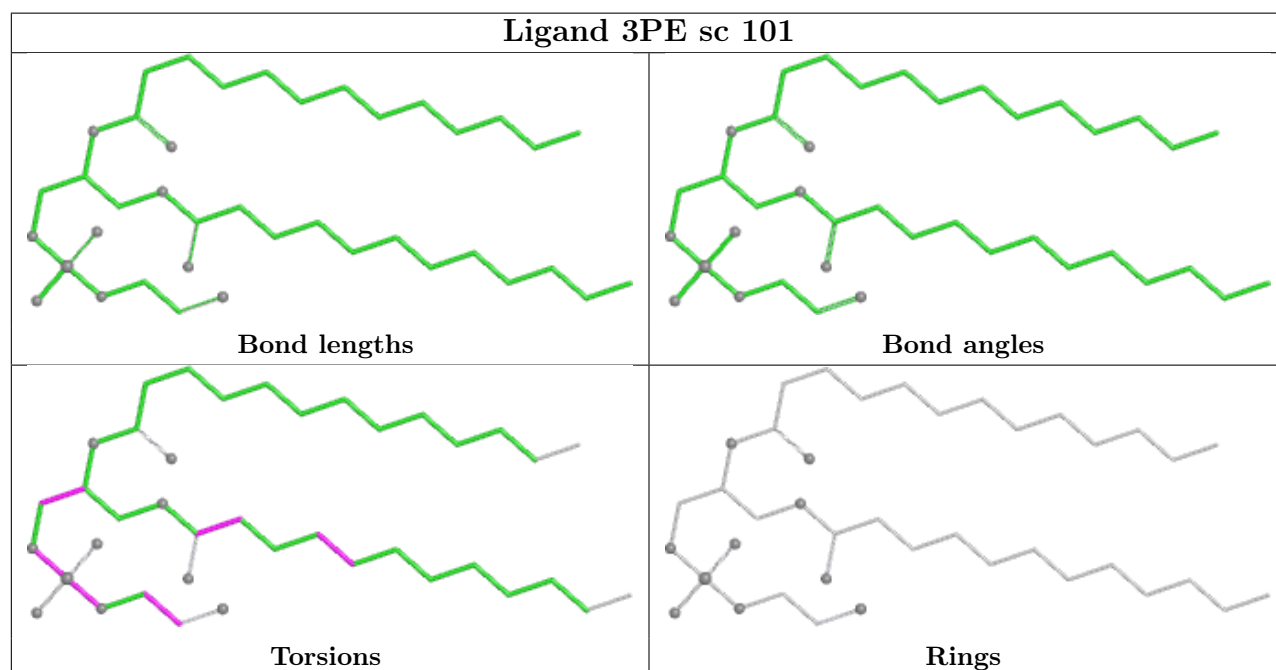
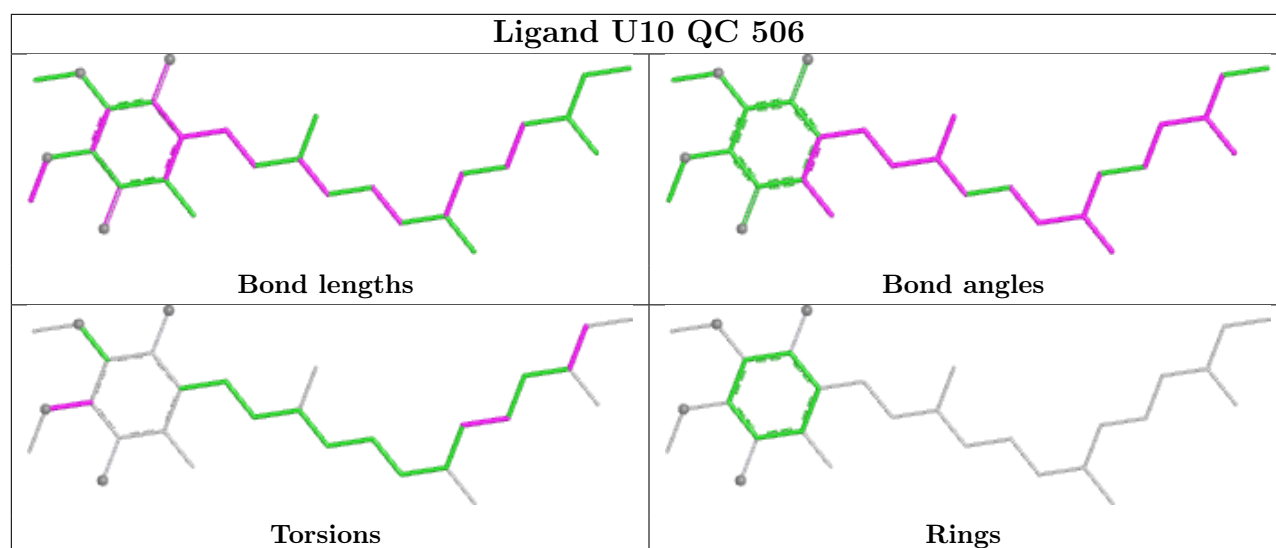


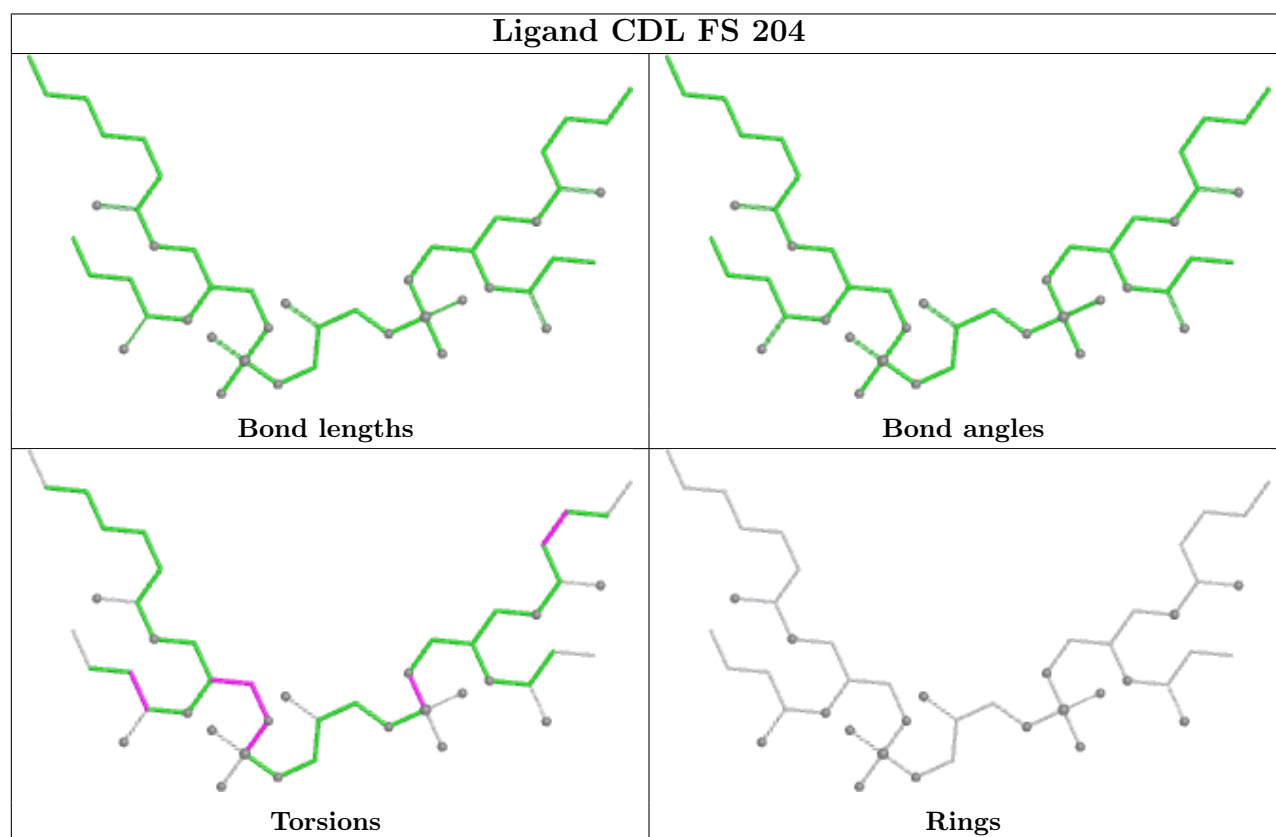
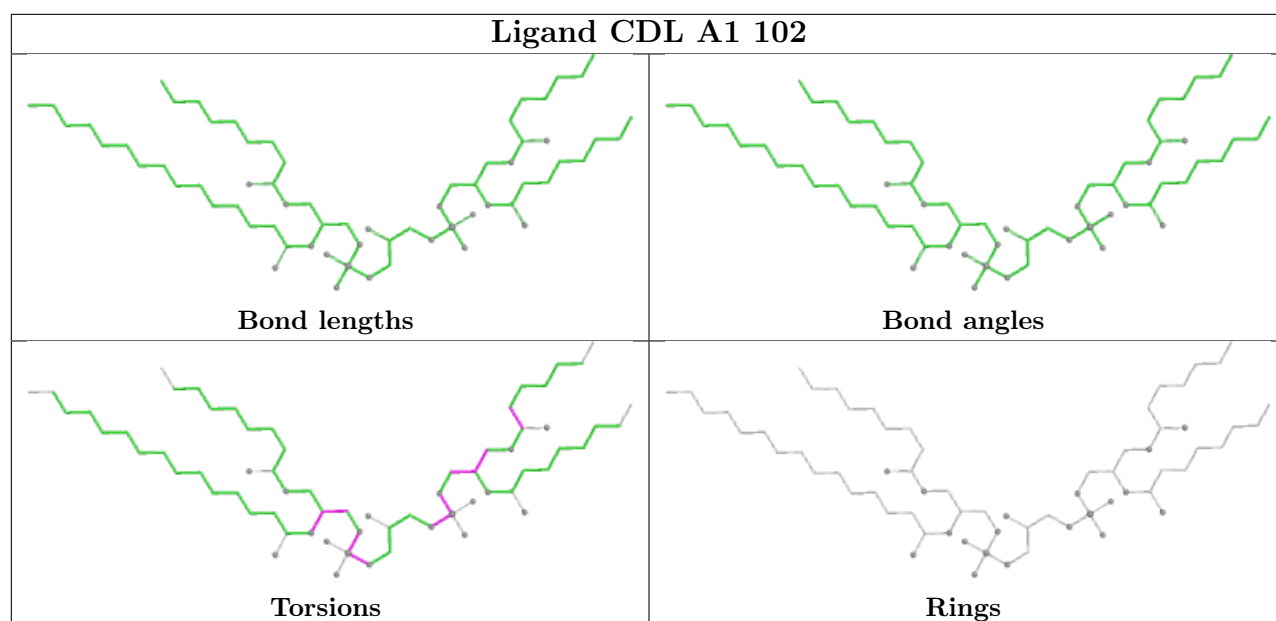


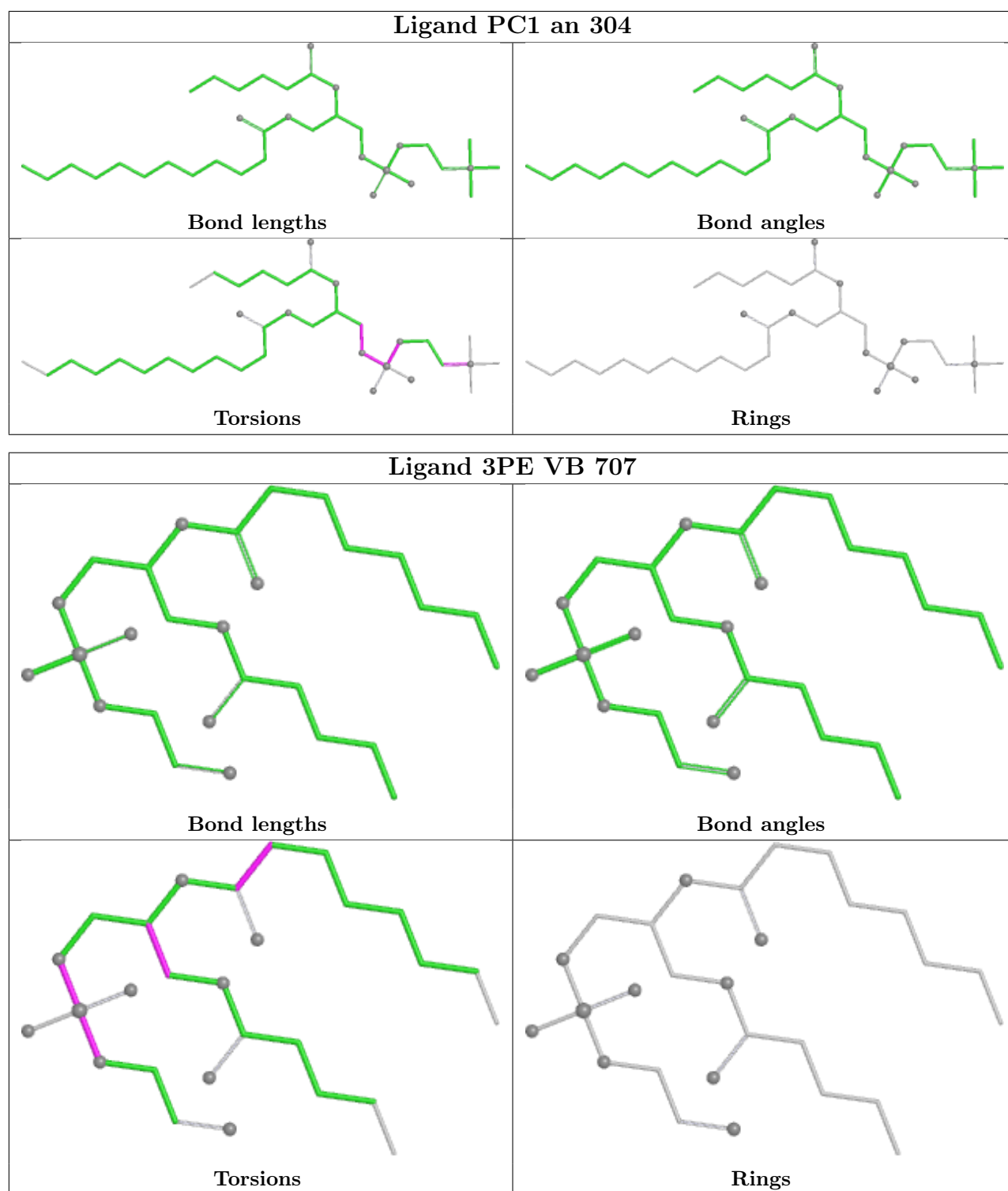


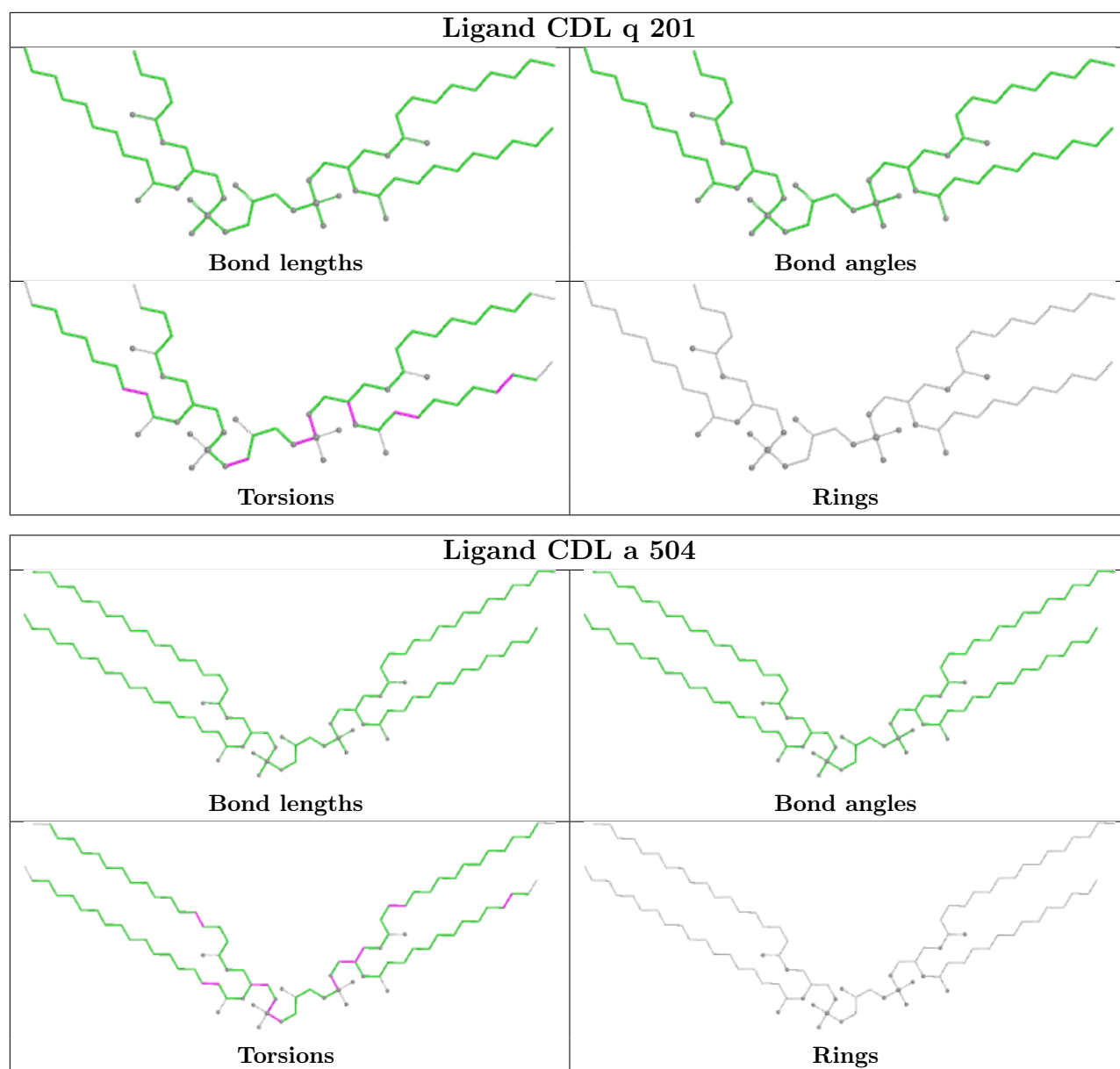


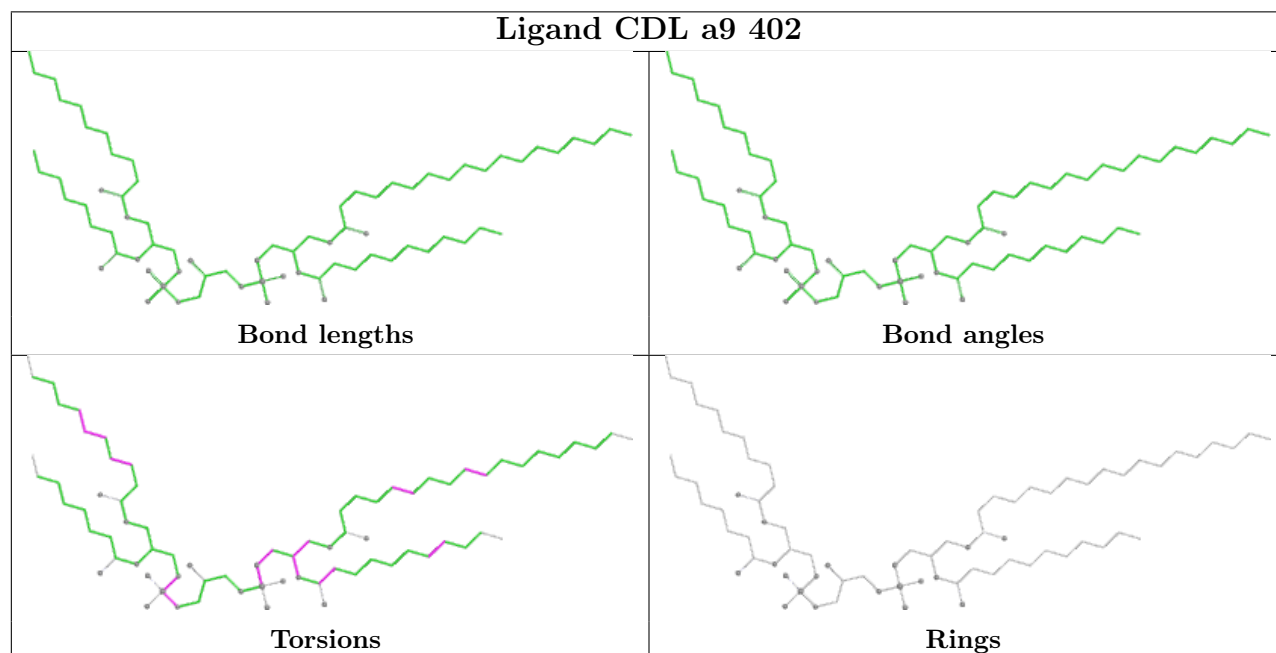
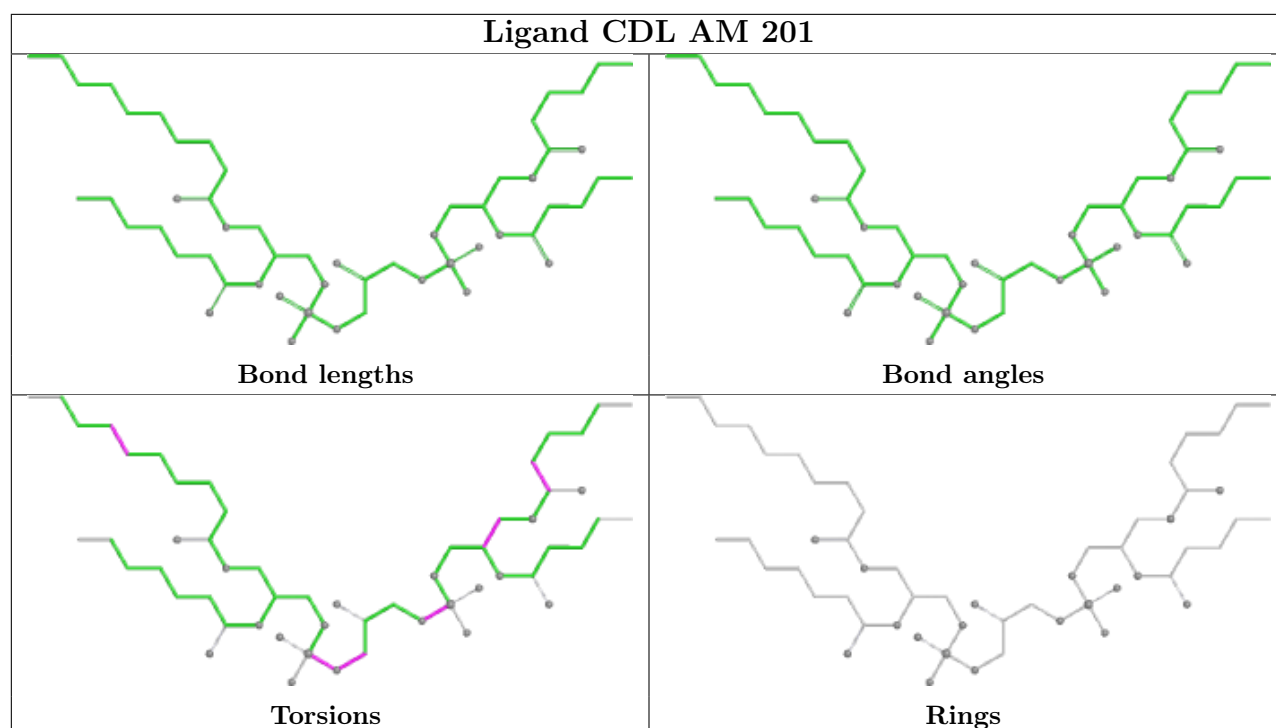


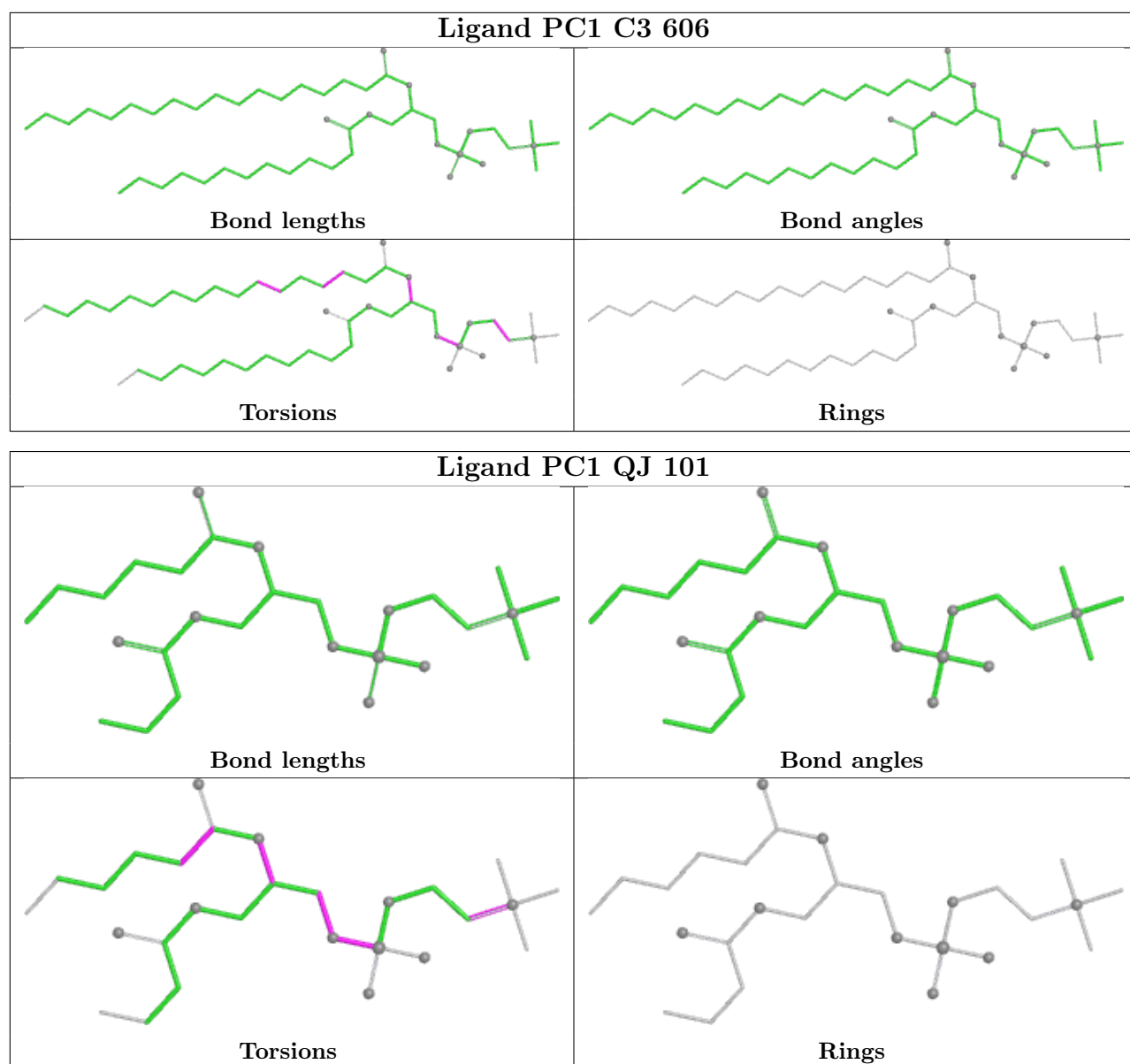


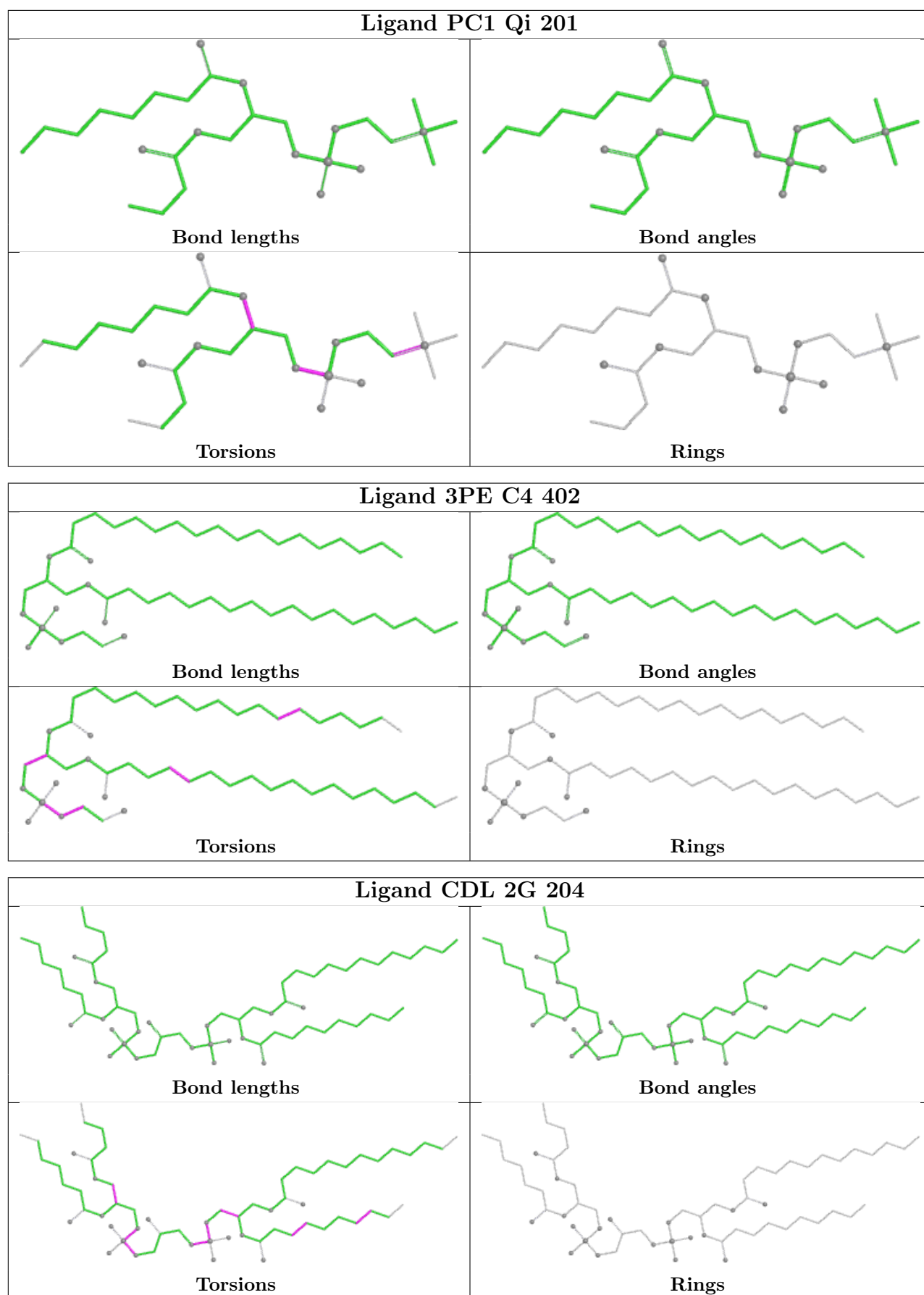


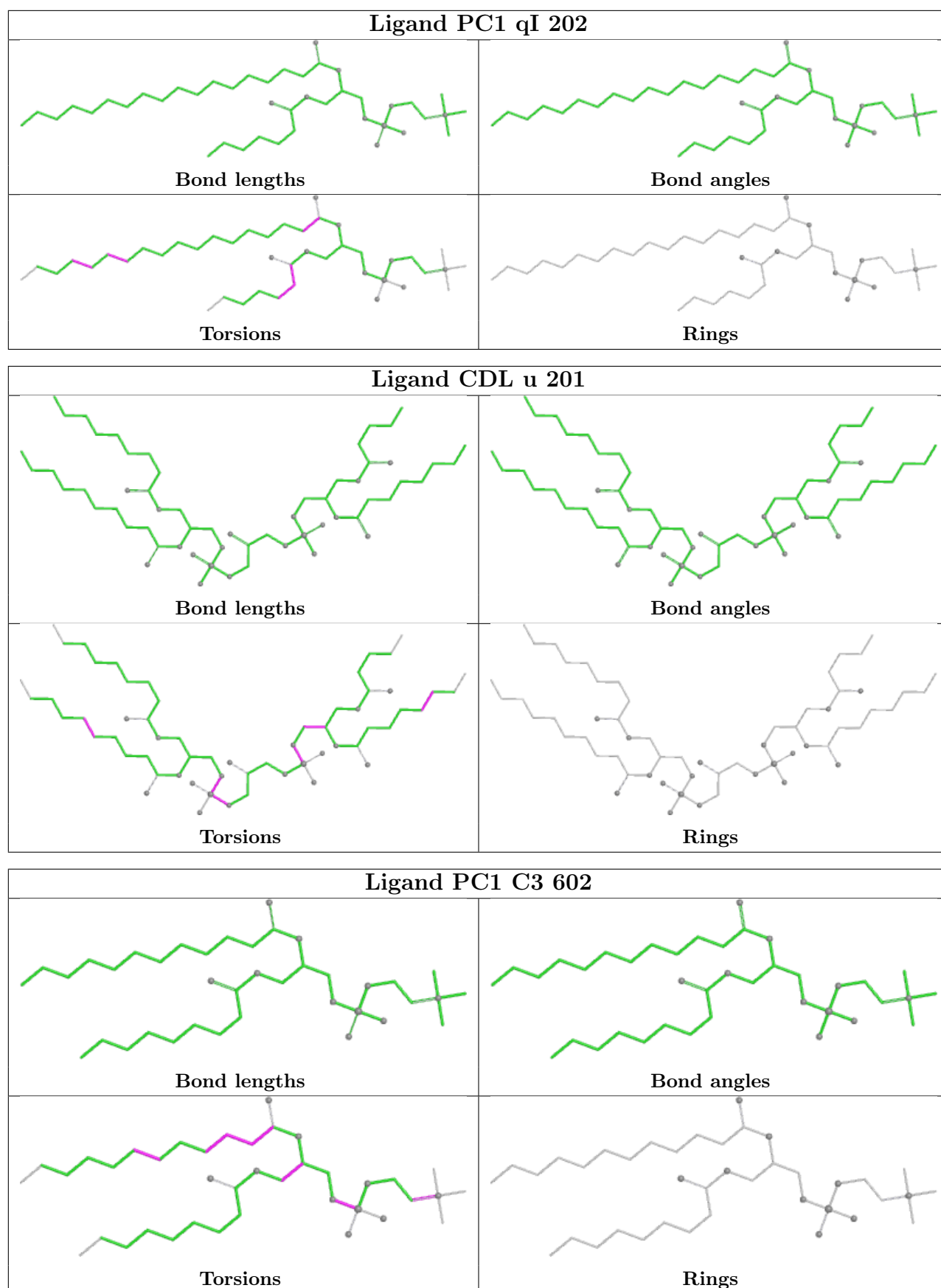


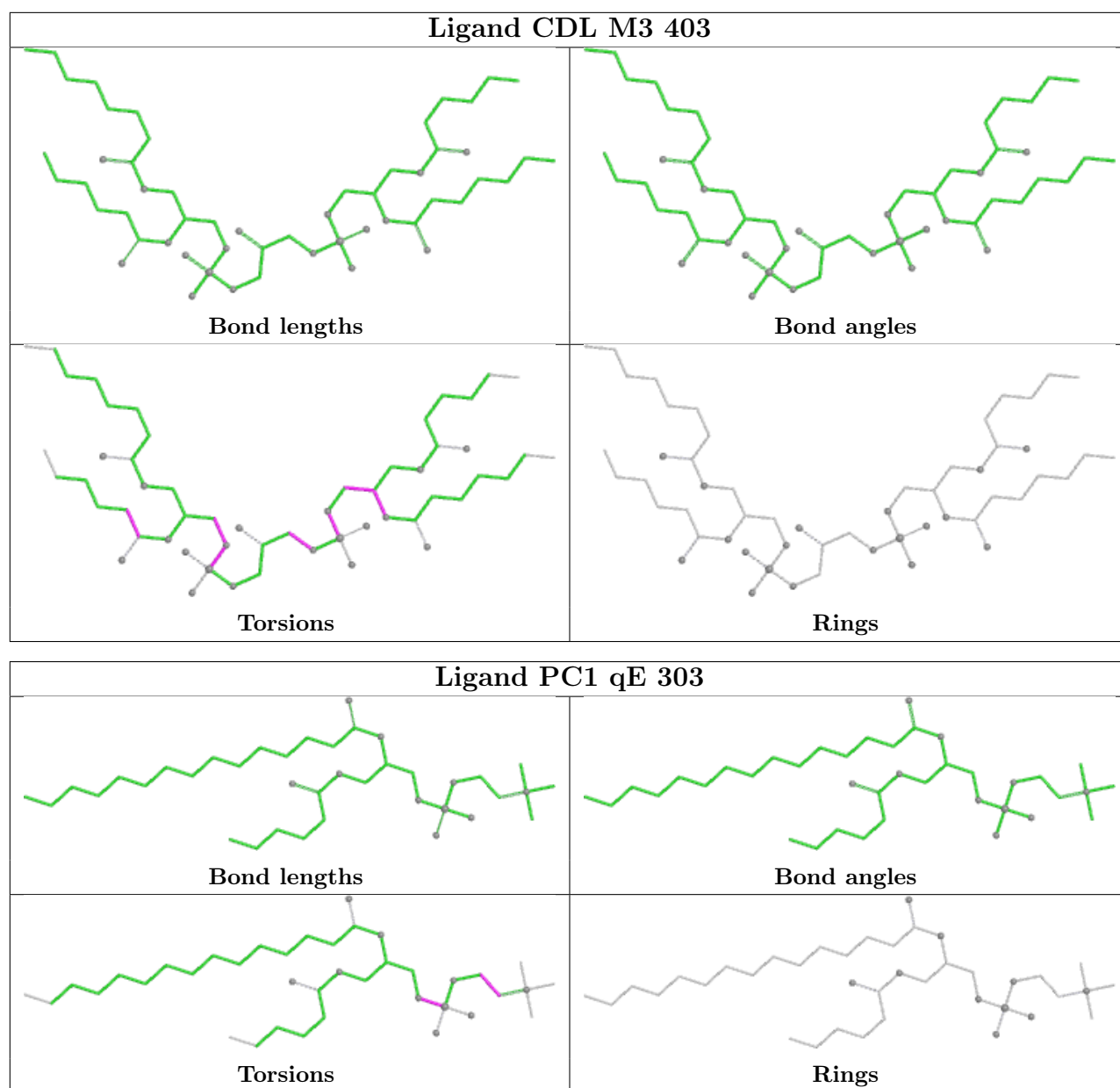


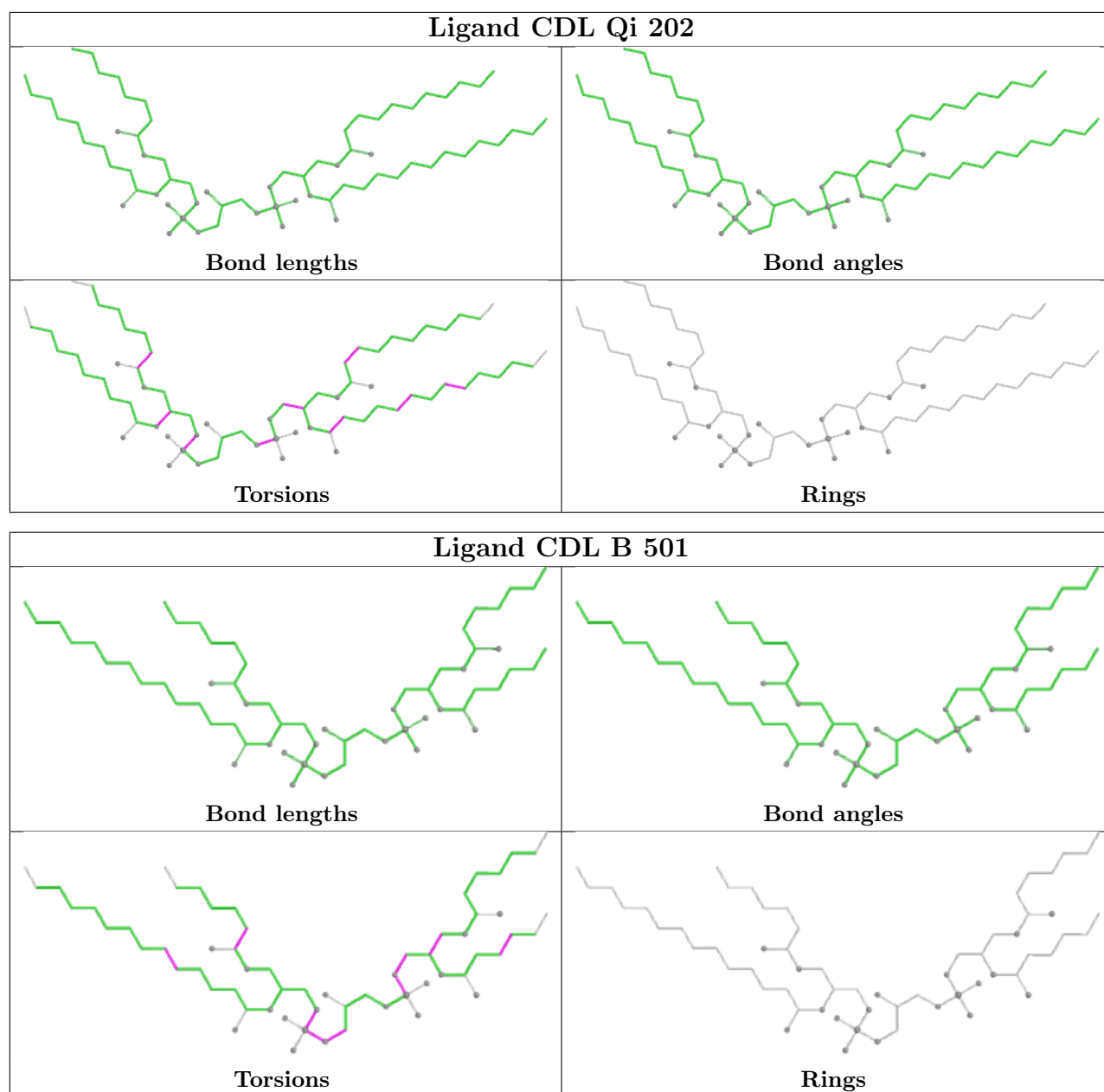


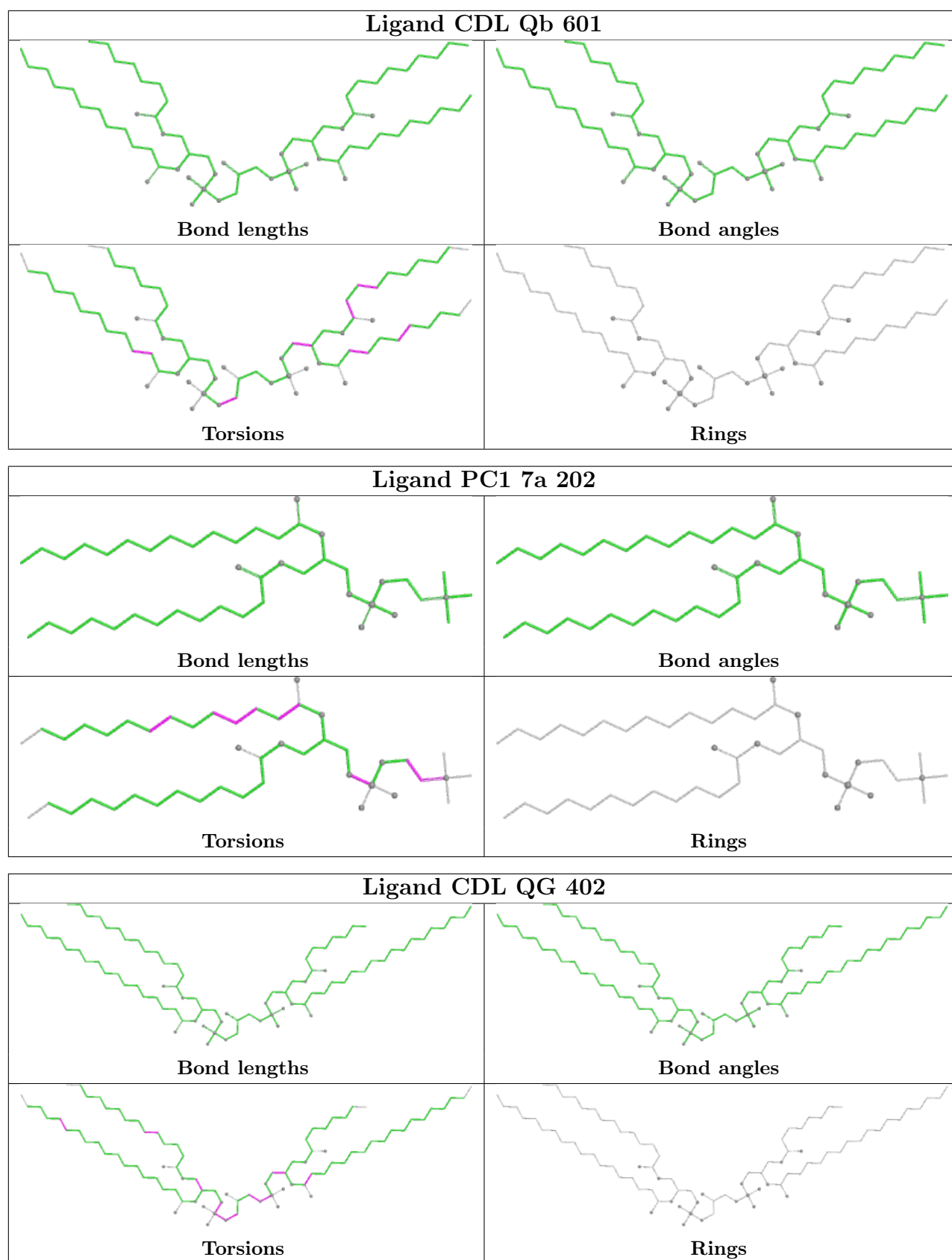


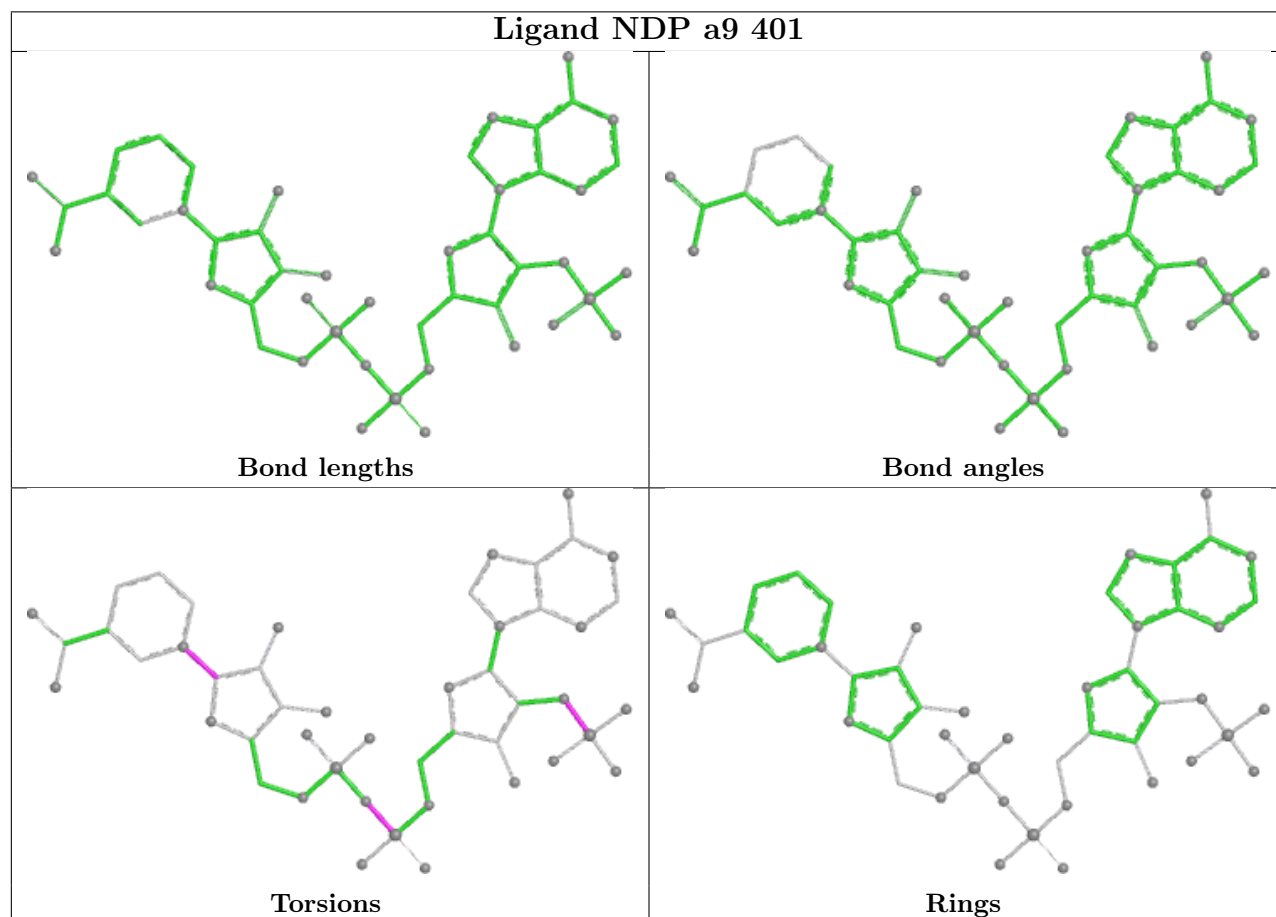
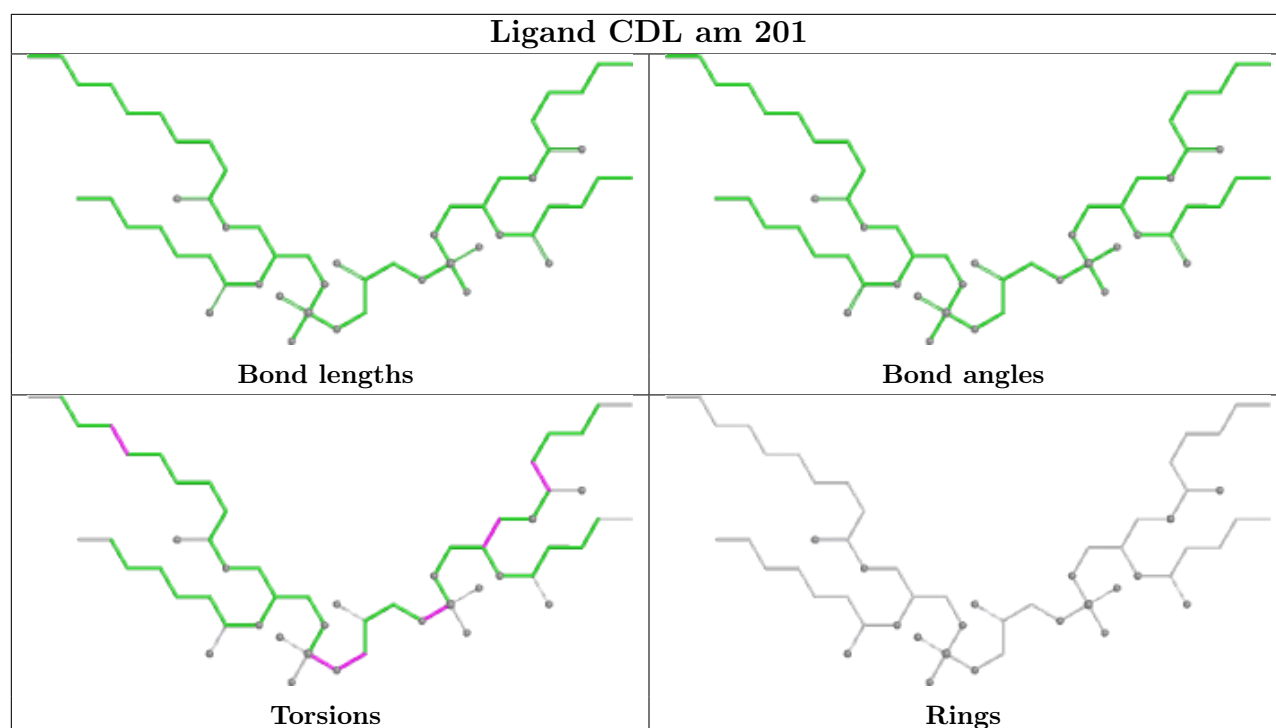




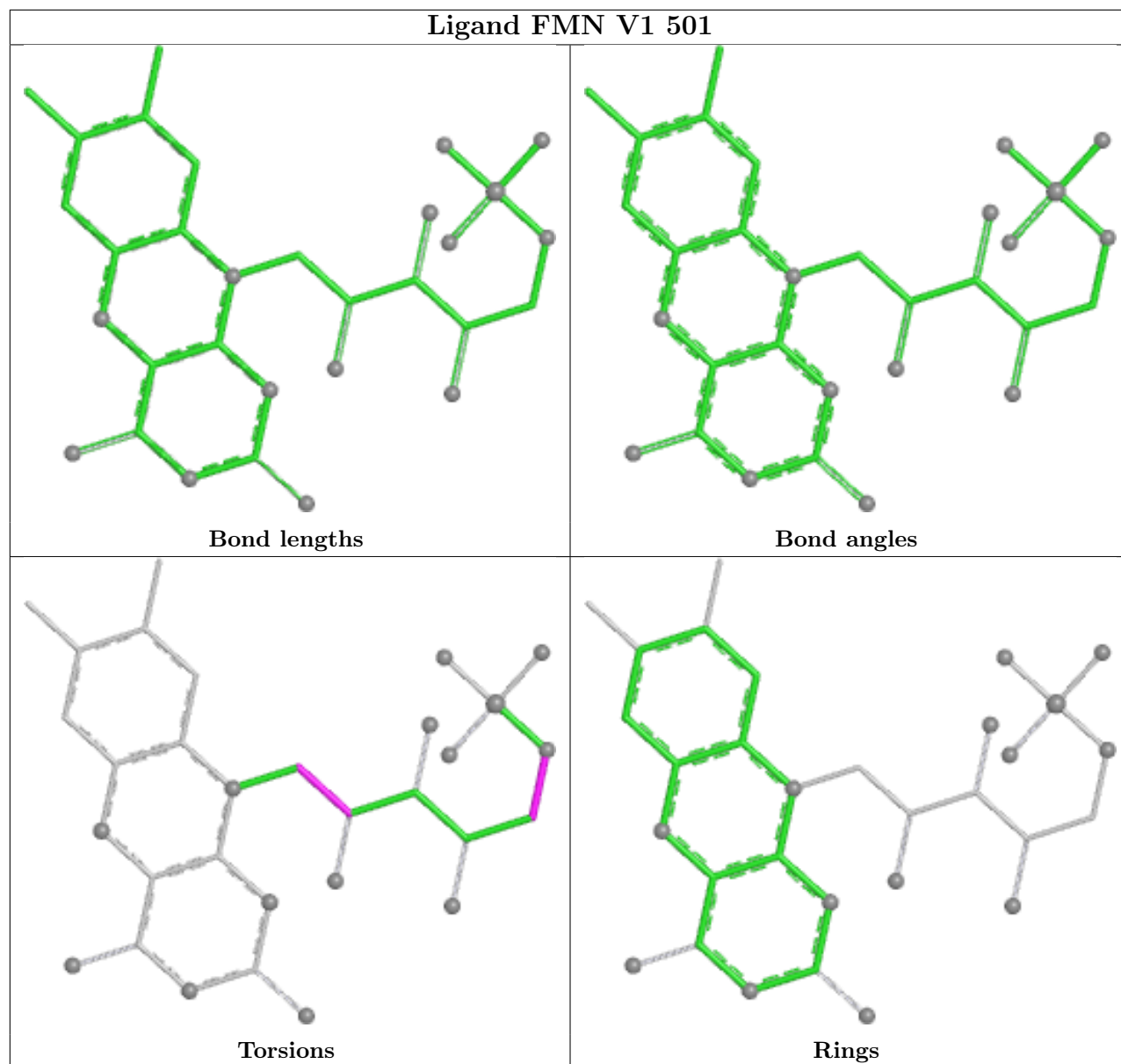


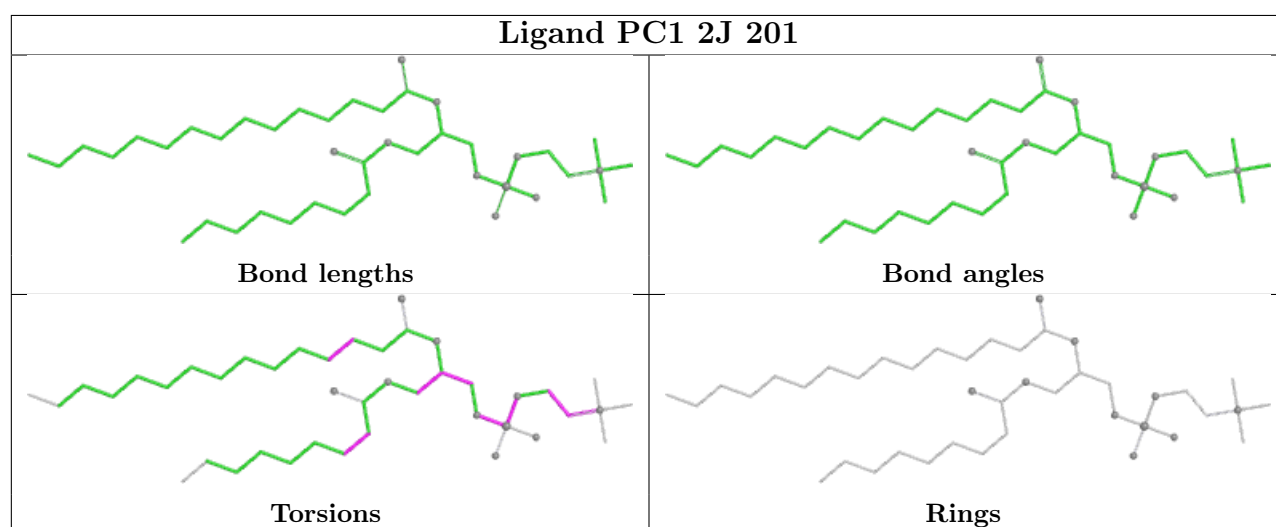
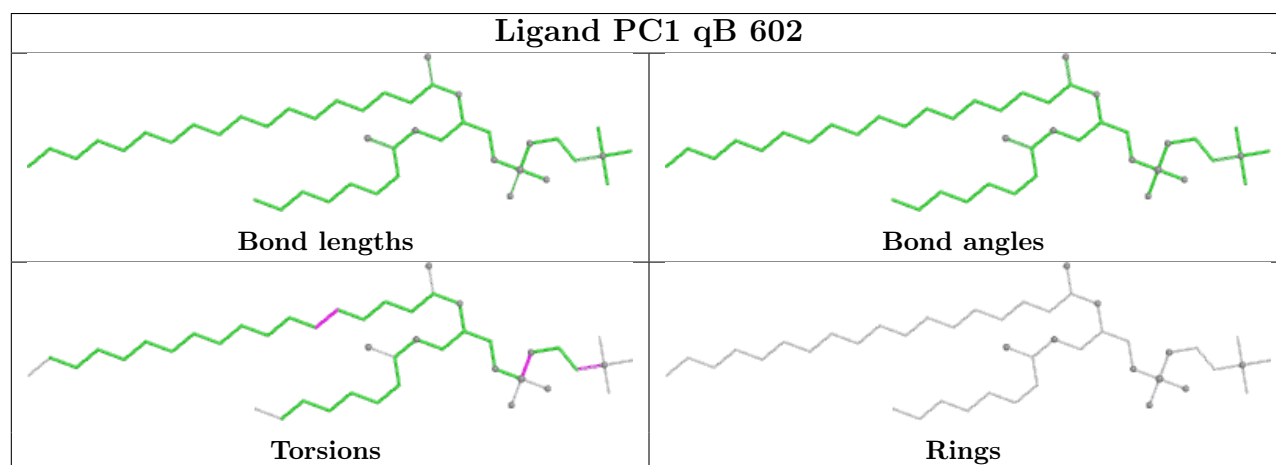
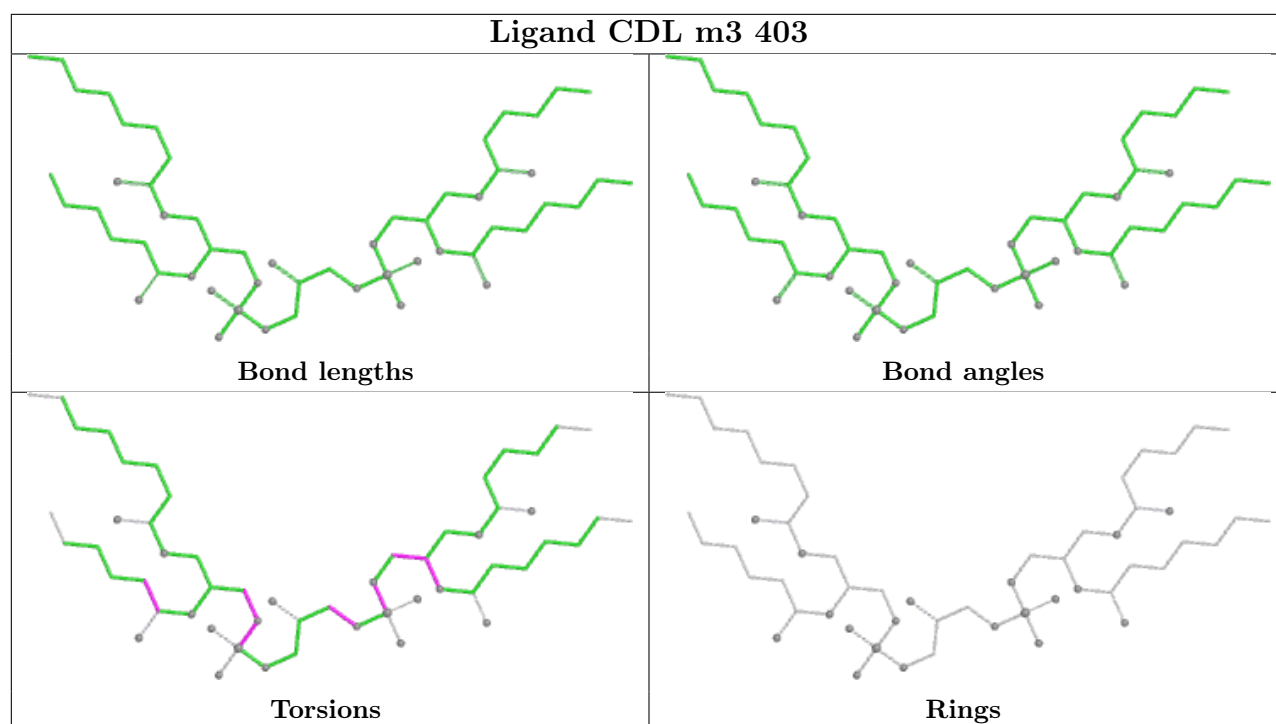




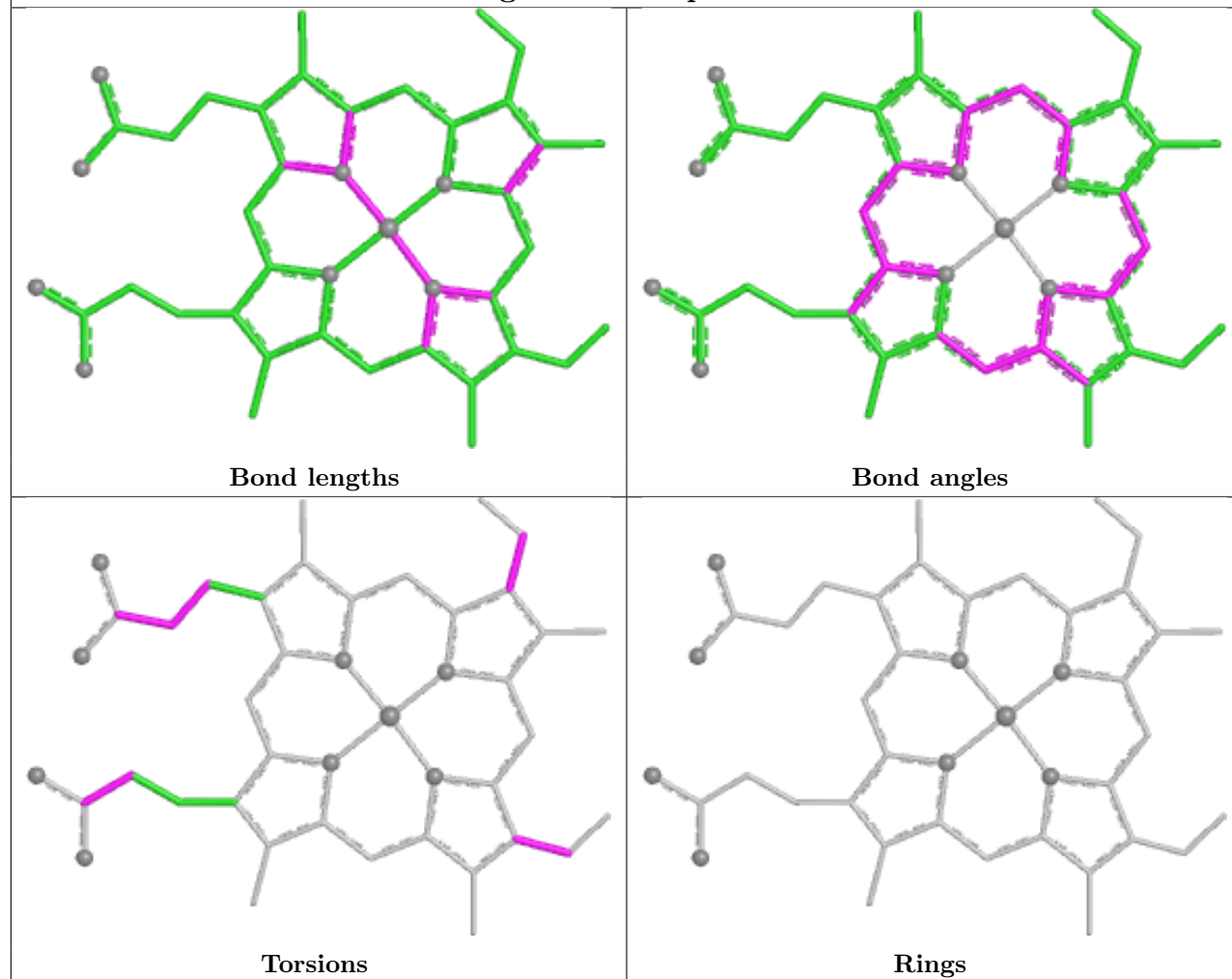


Ligand FMN V1 501

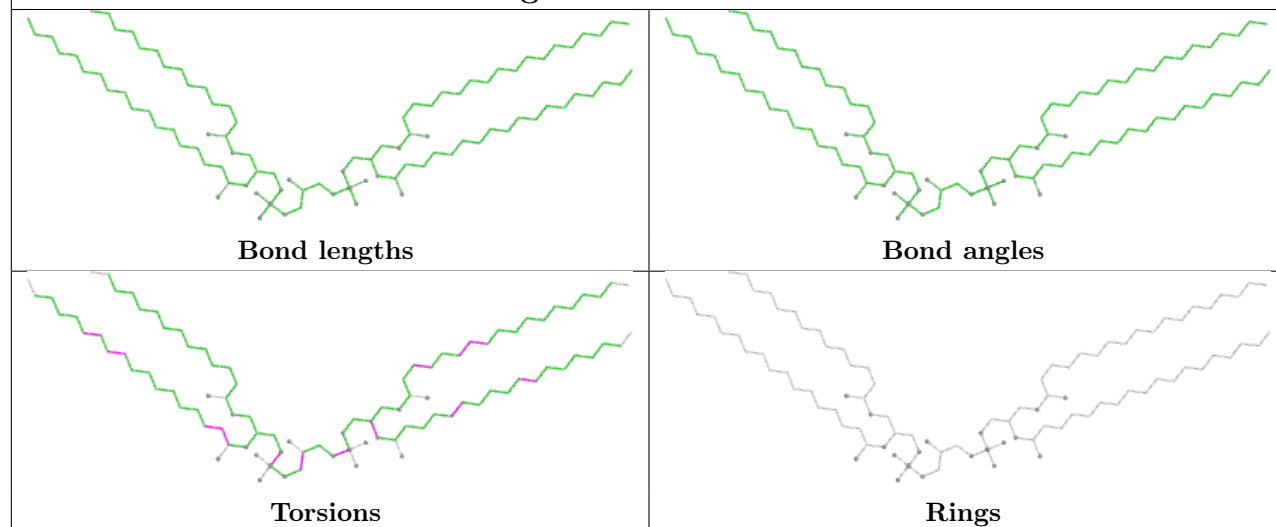


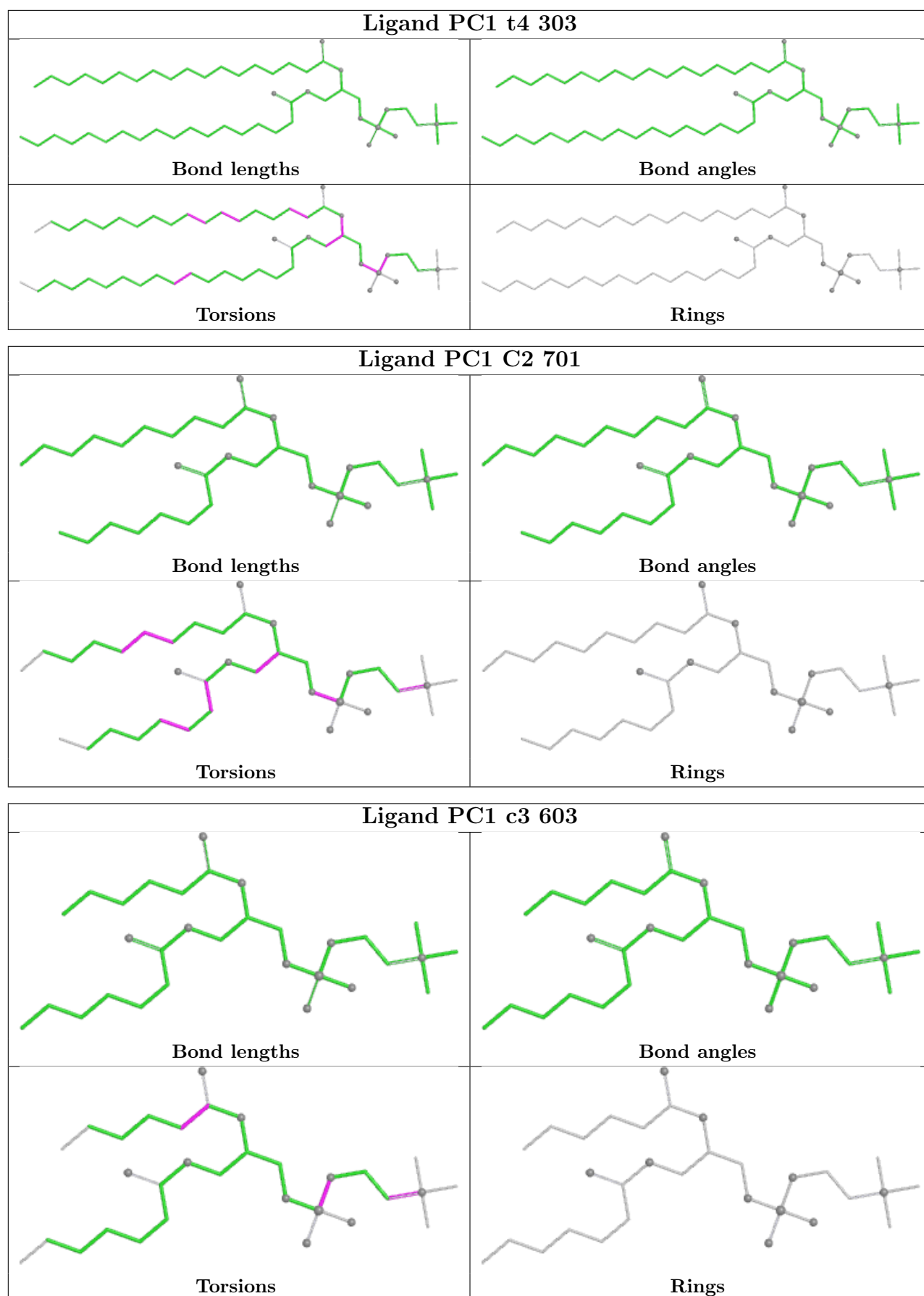


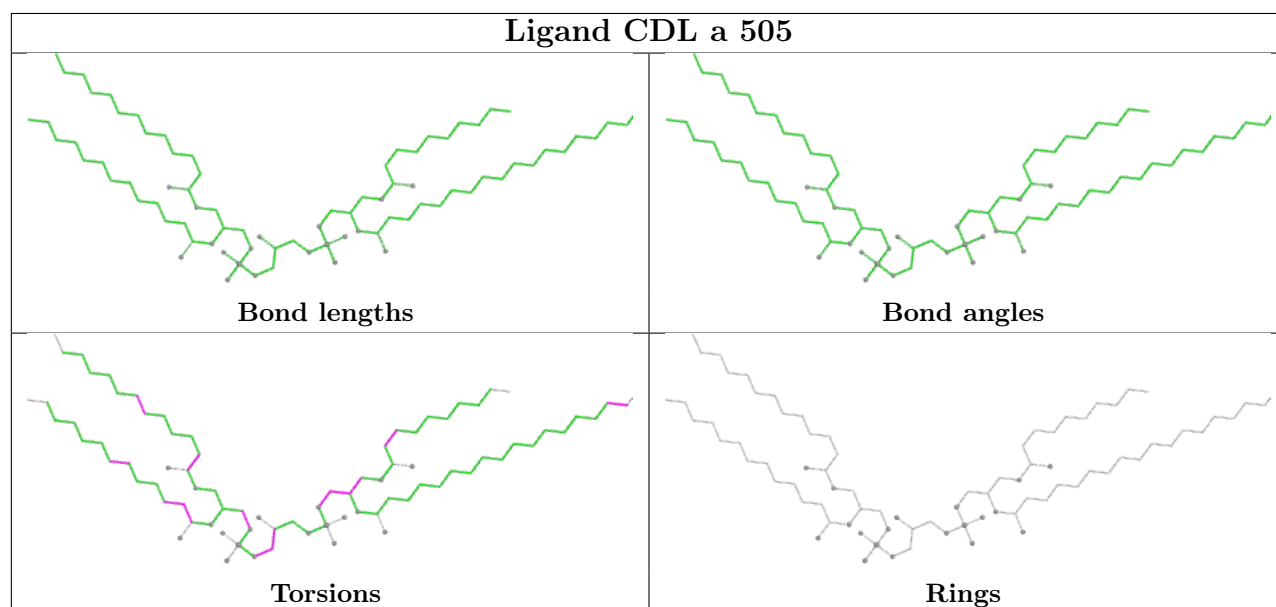
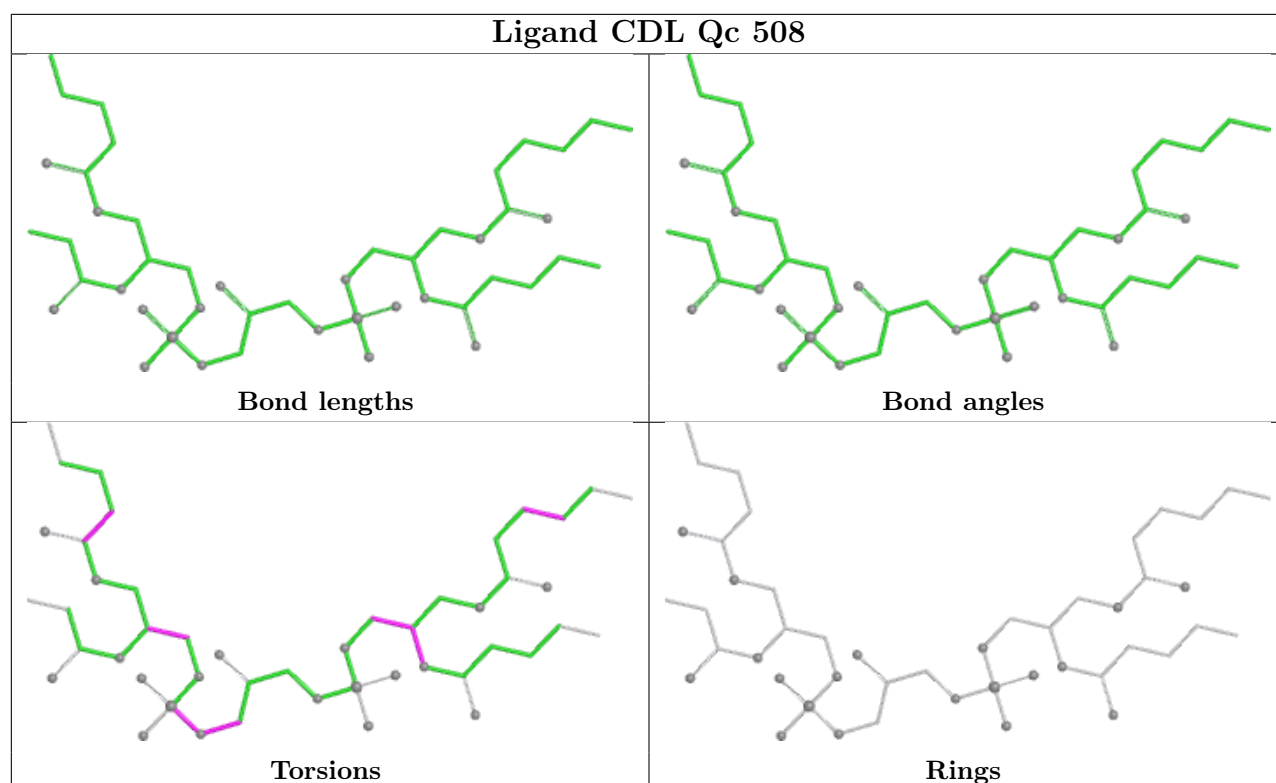
Ligand HEM qC 502

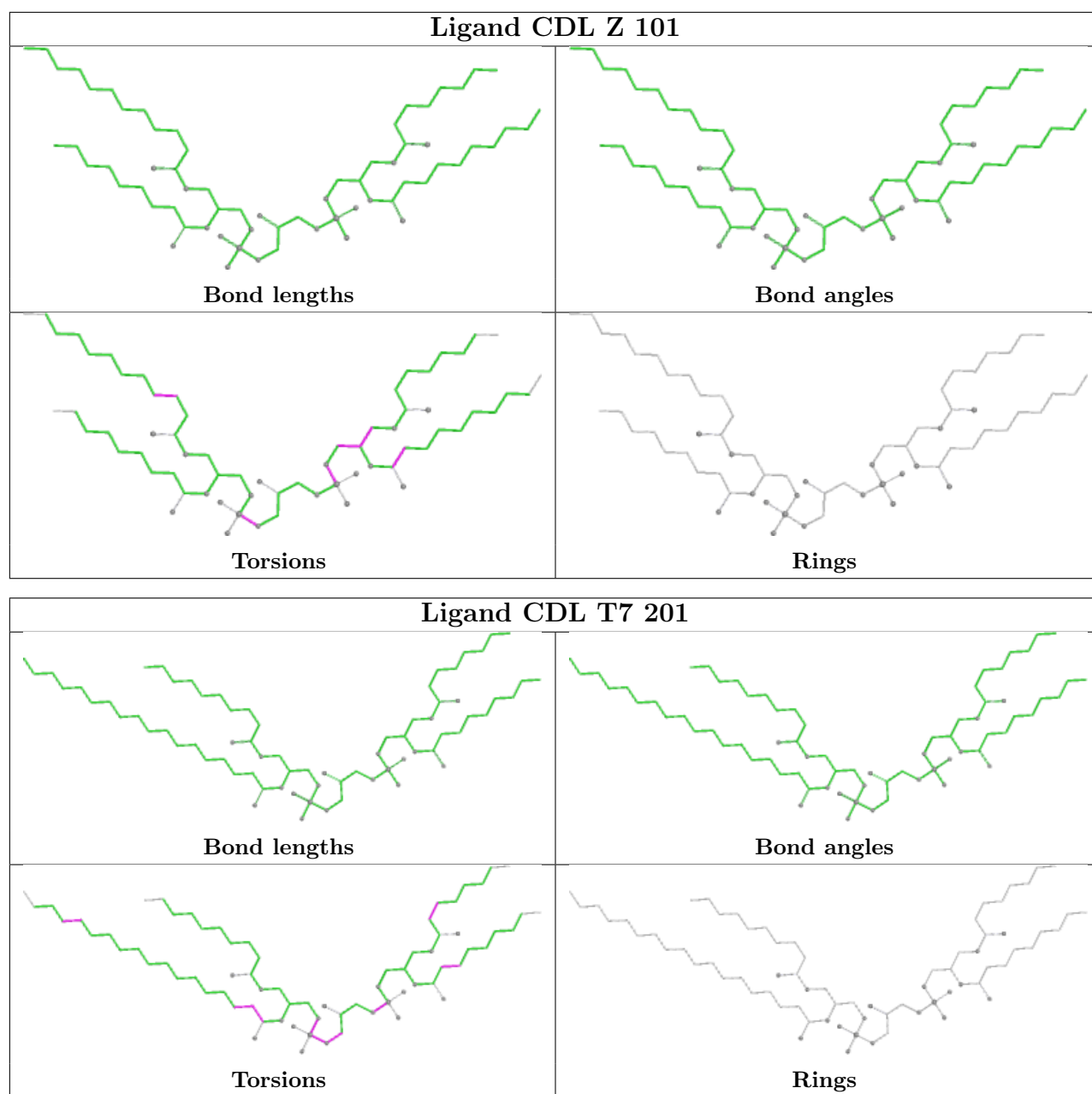


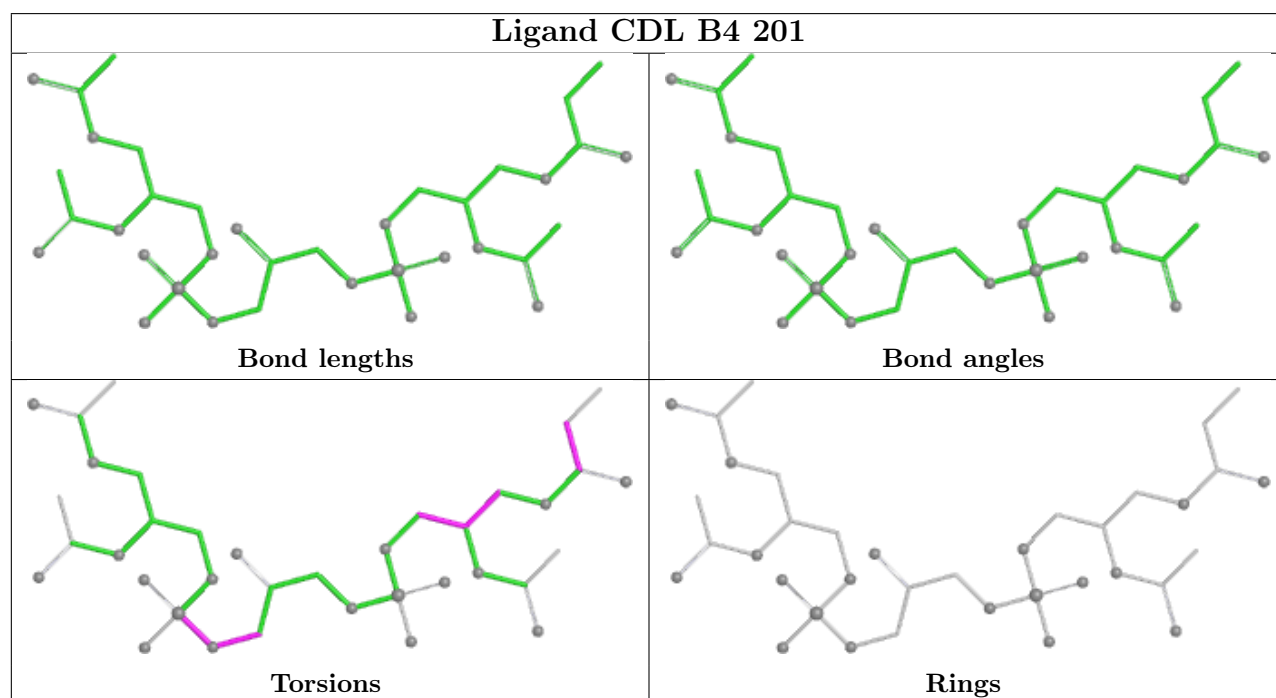
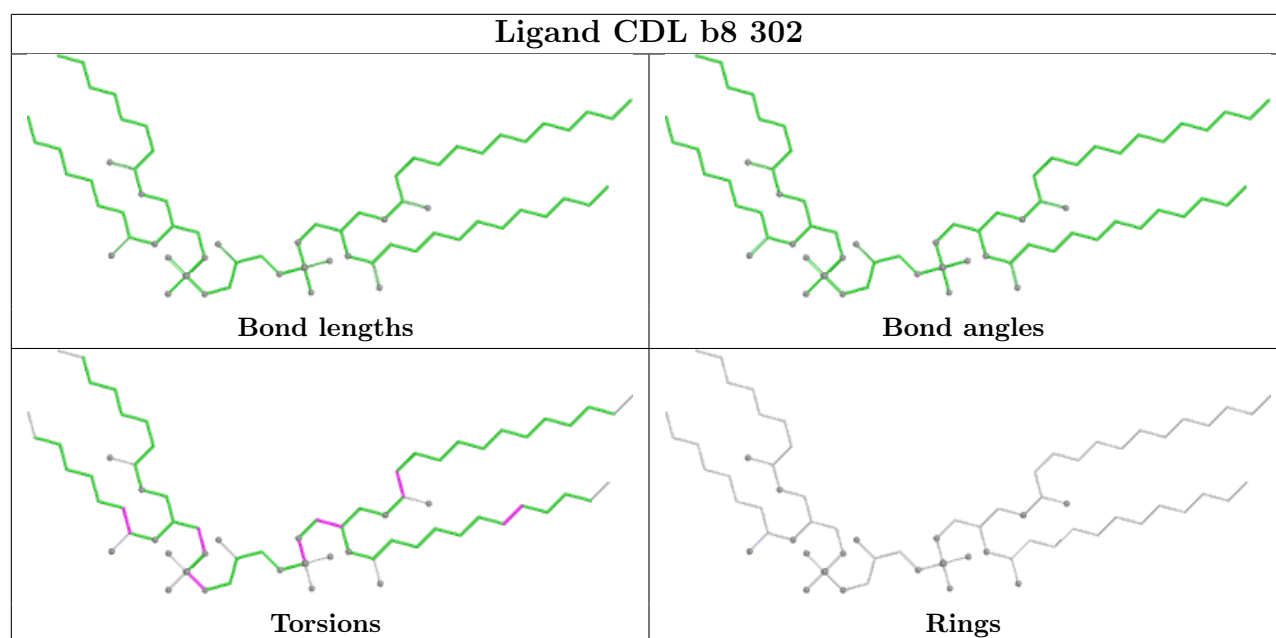
Ligand CDL 2m 101

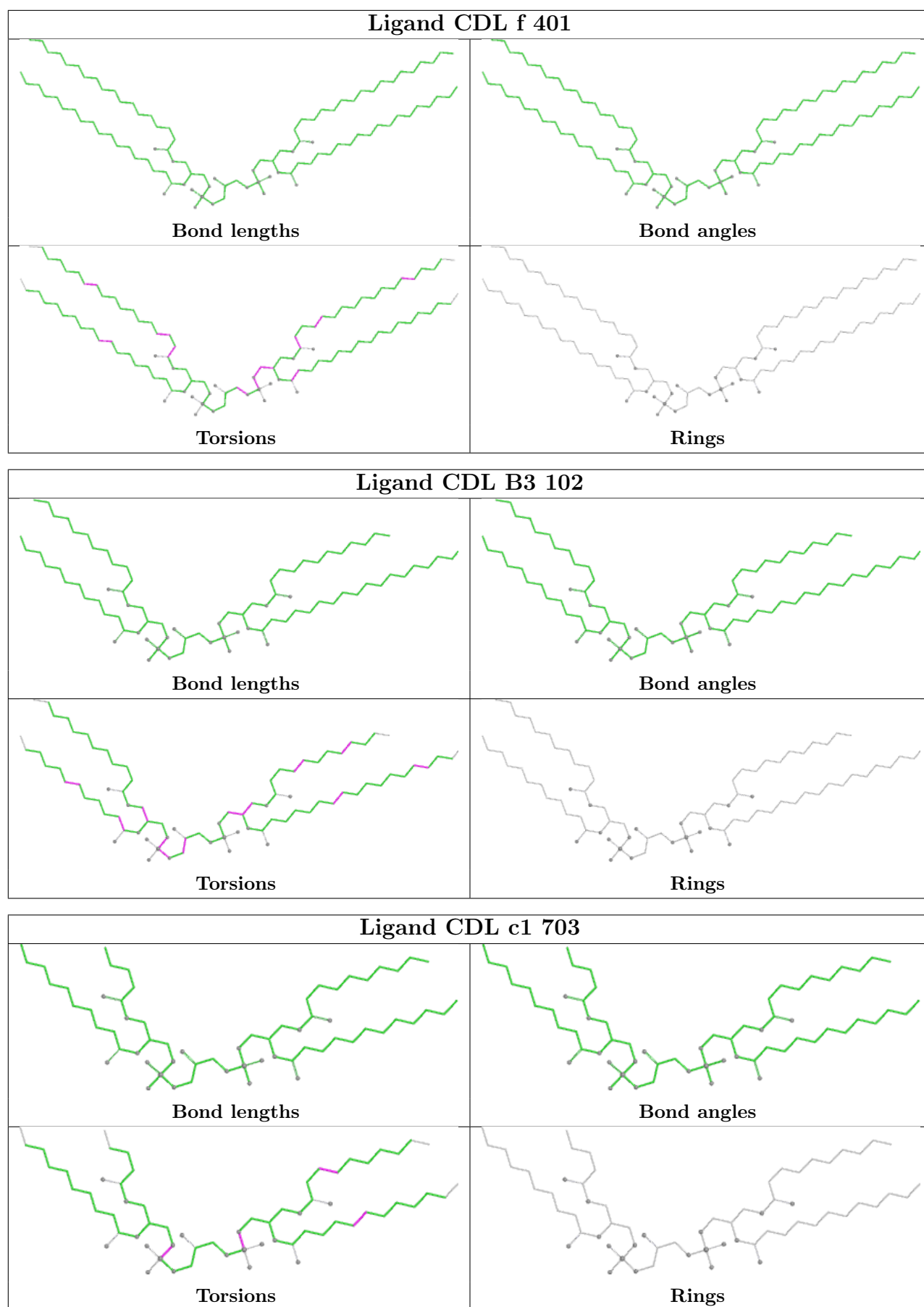


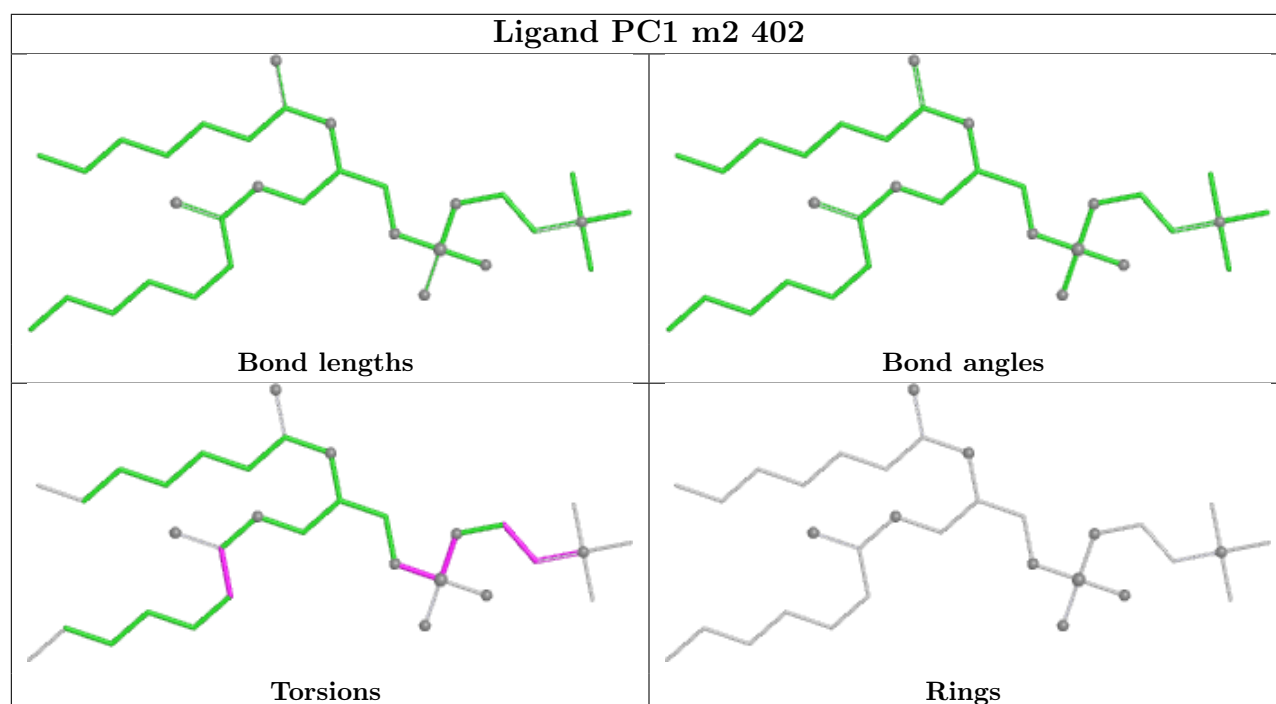
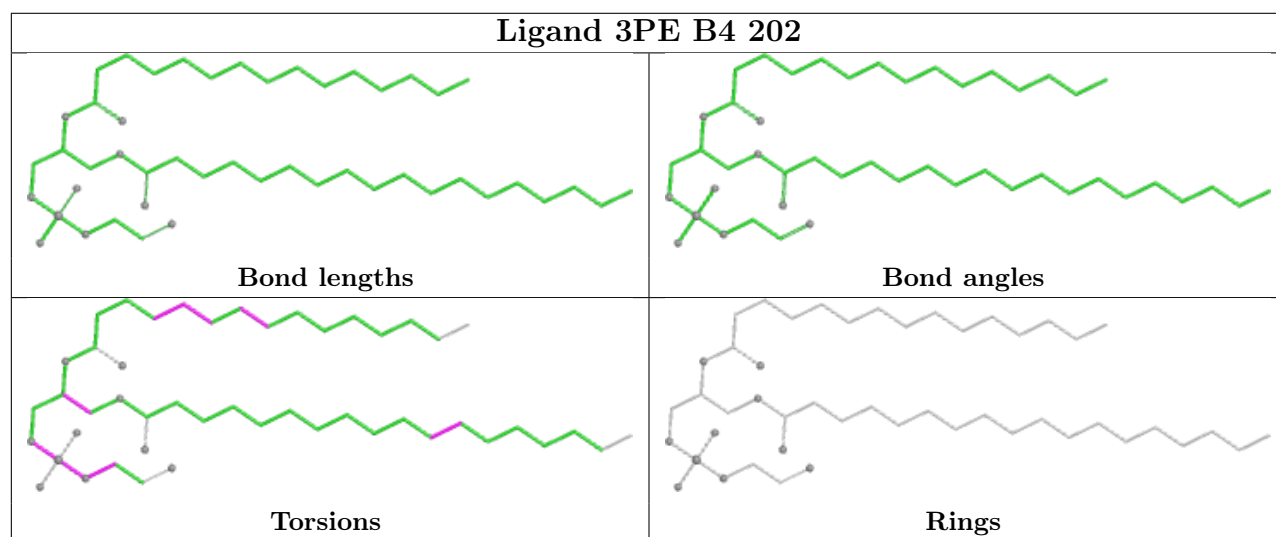
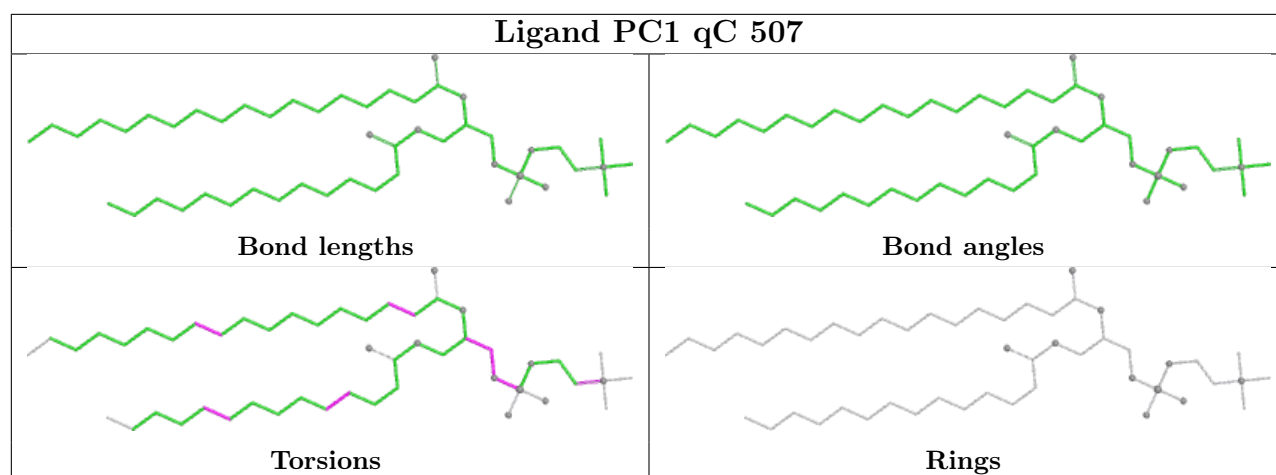




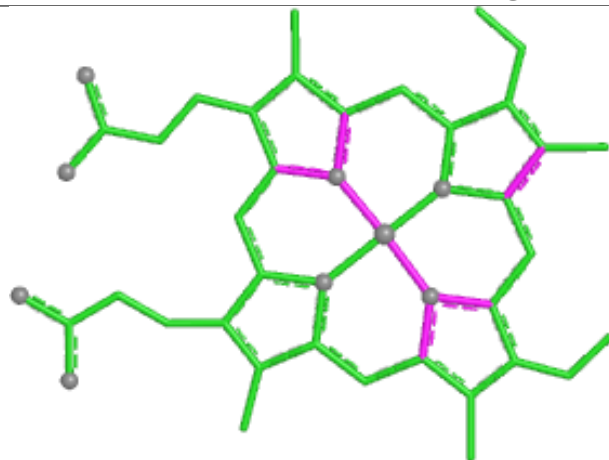




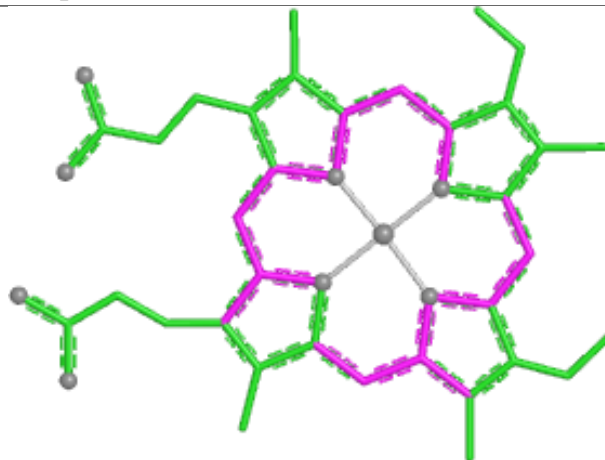




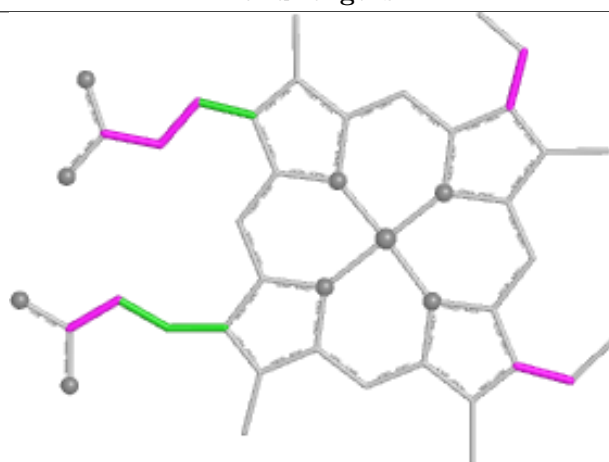
Ligand HEM qc 503



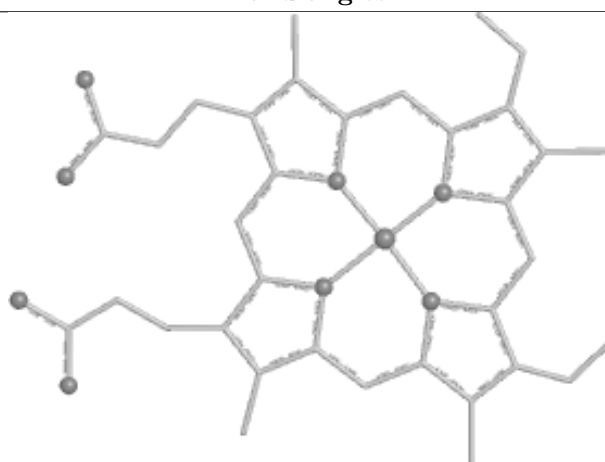
Bond lengths



Bond angles

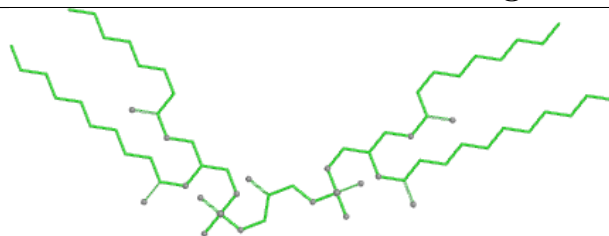


Torsions

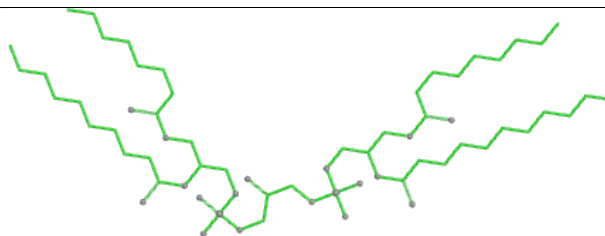


Rings

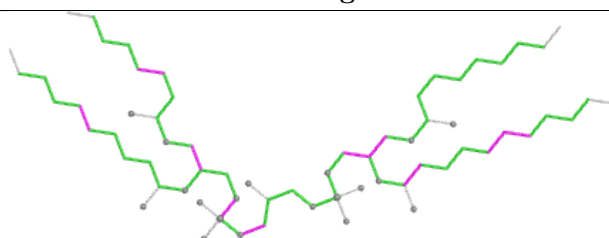
Ligand CDL m1 402



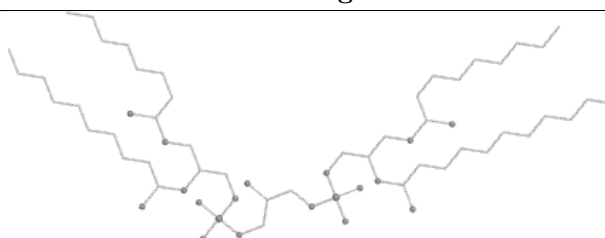
Bond lengths



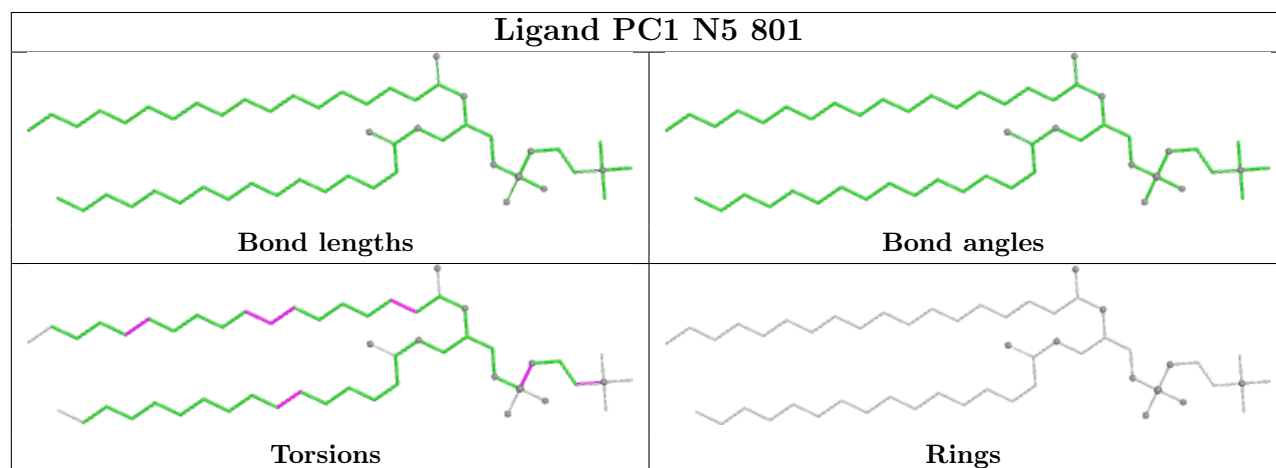
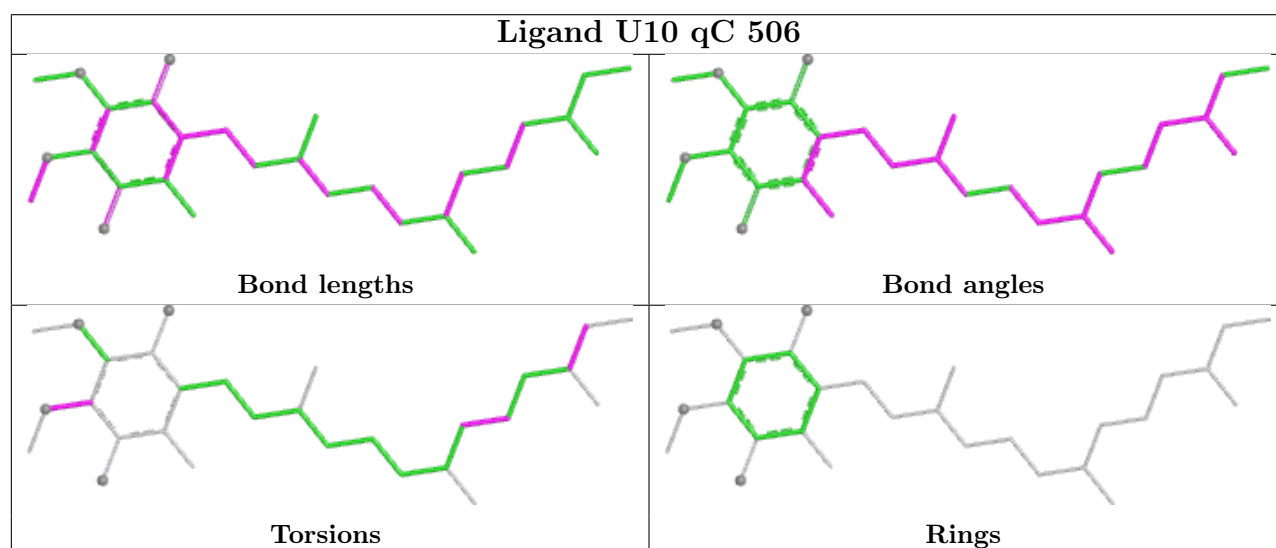
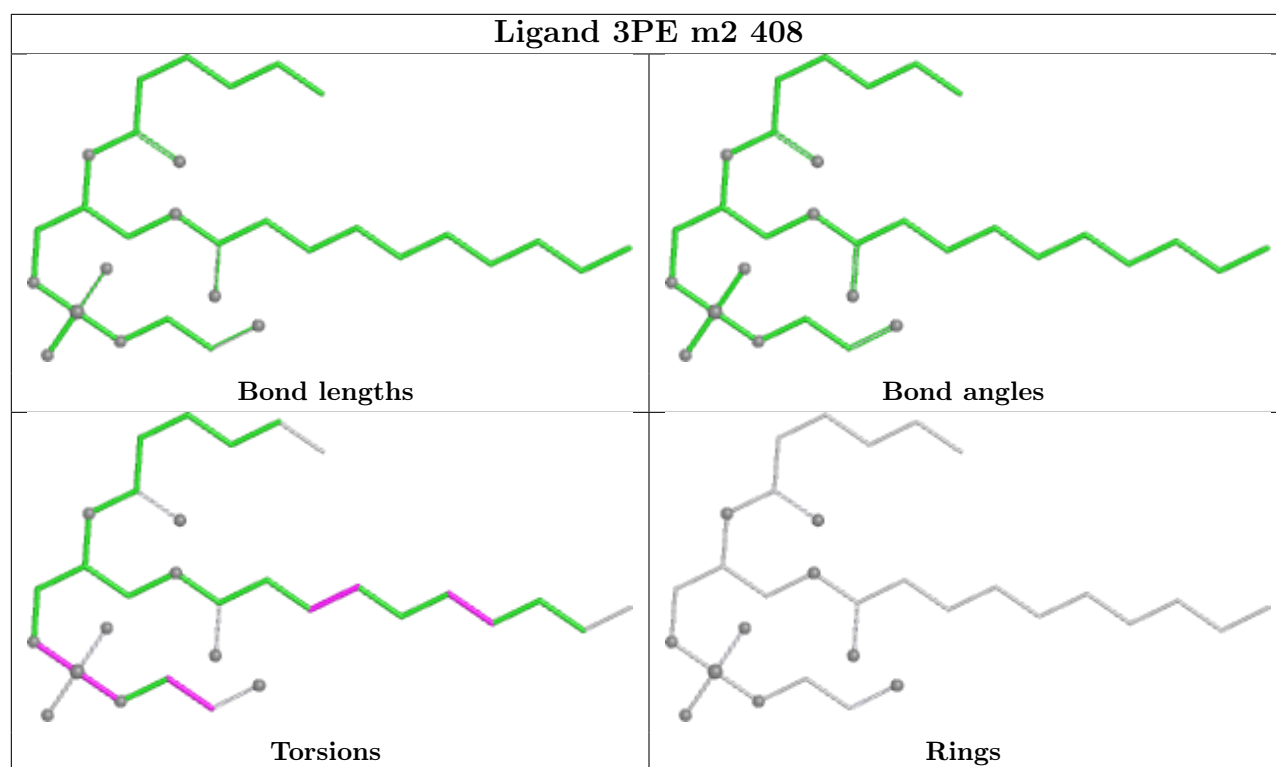
Bond angles

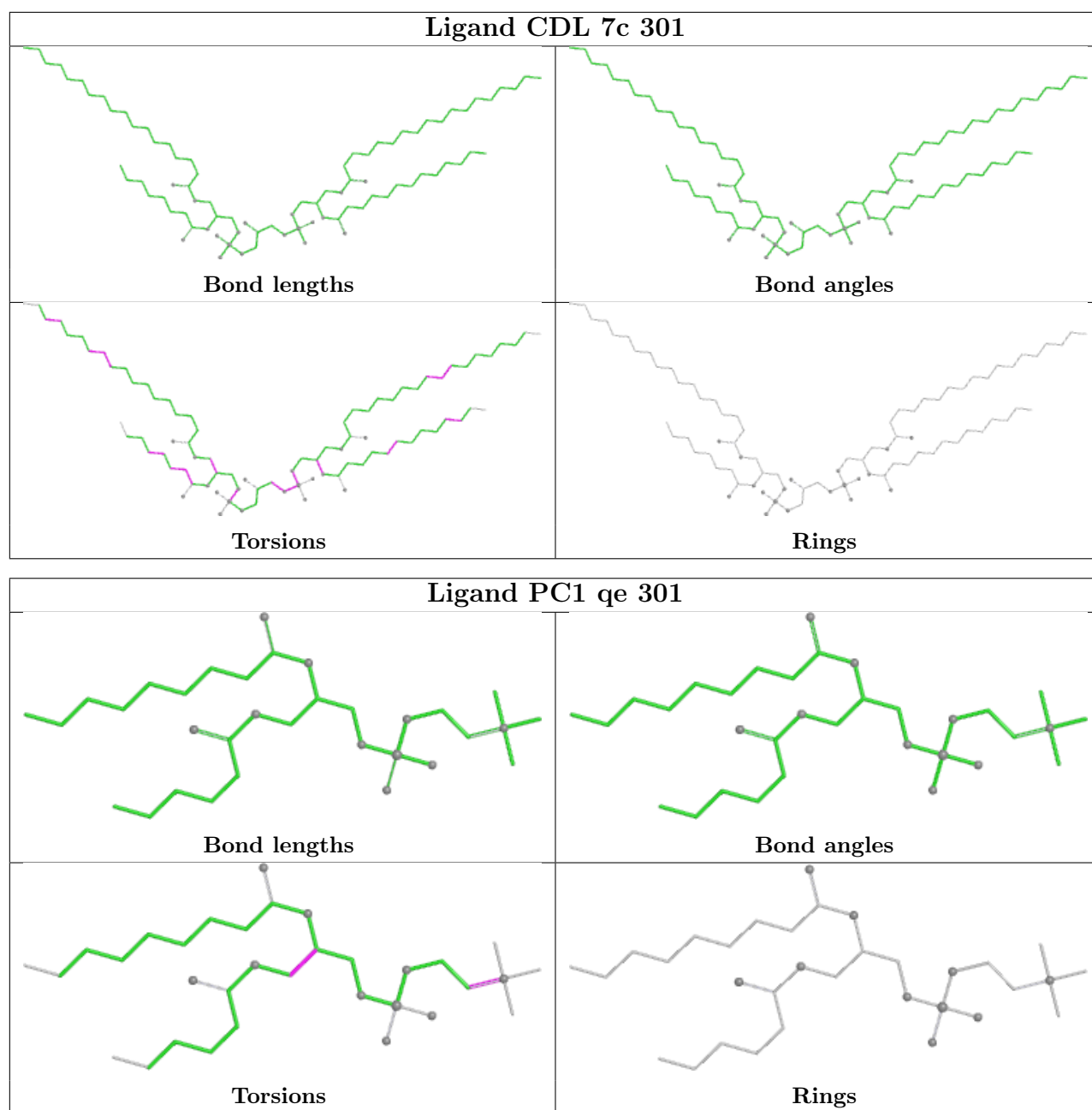


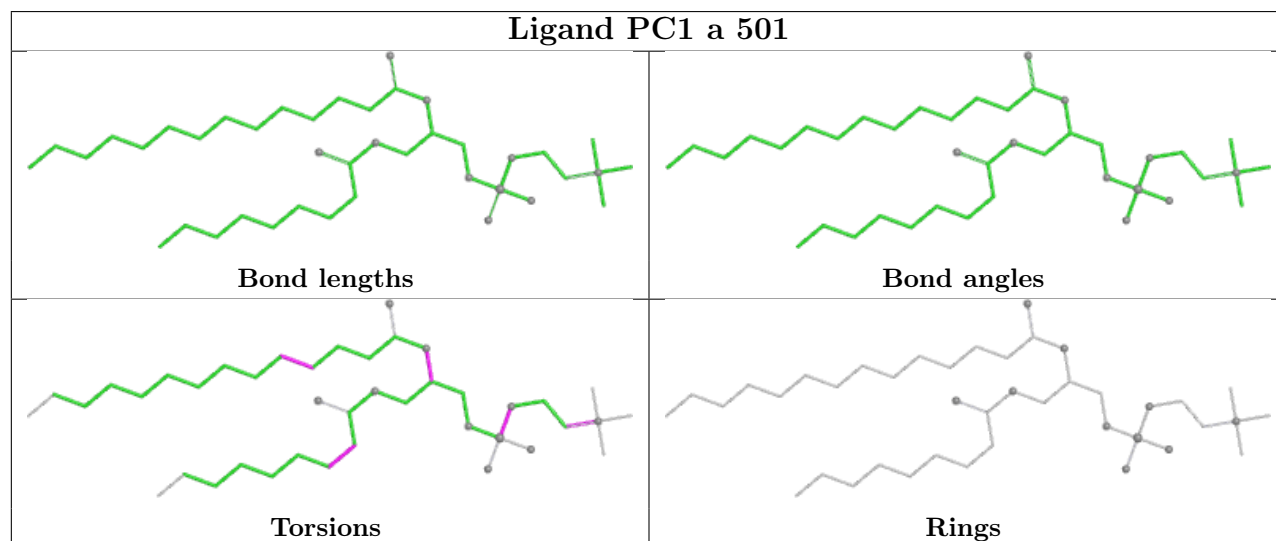
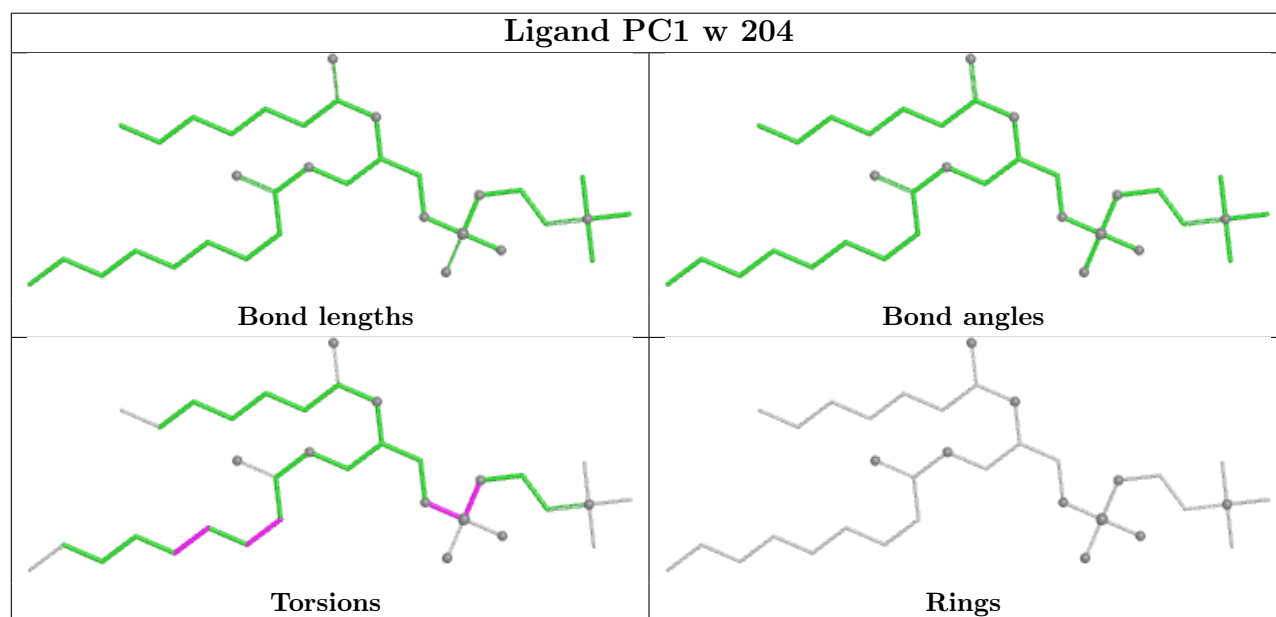
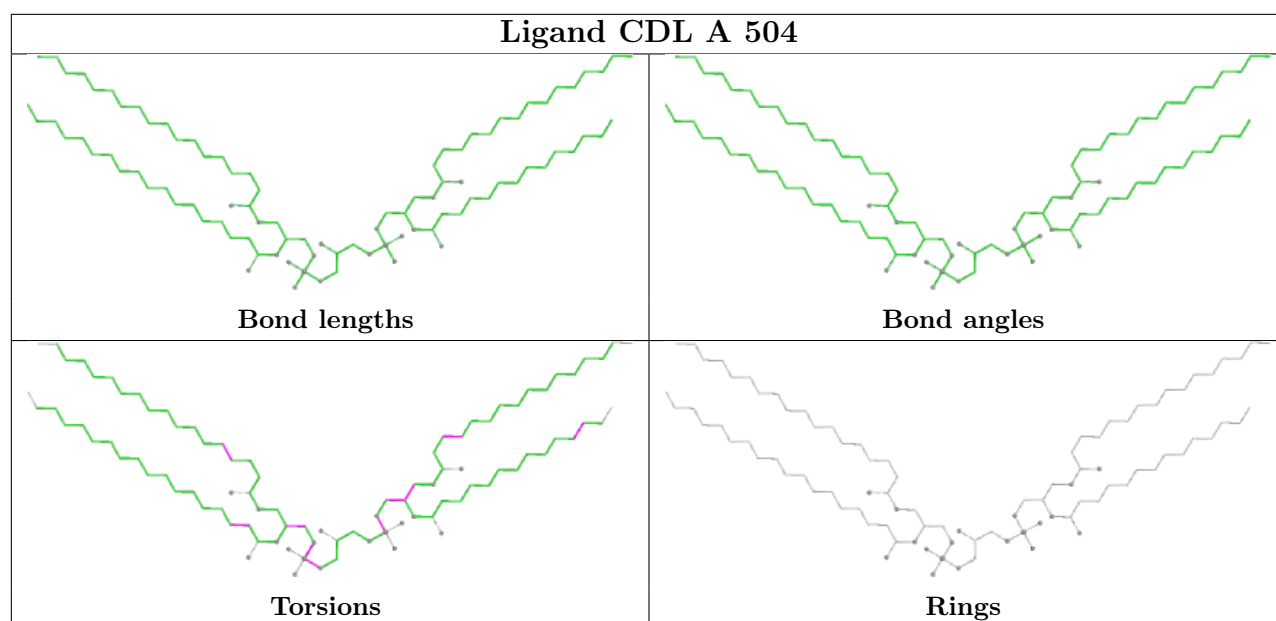
Torsions

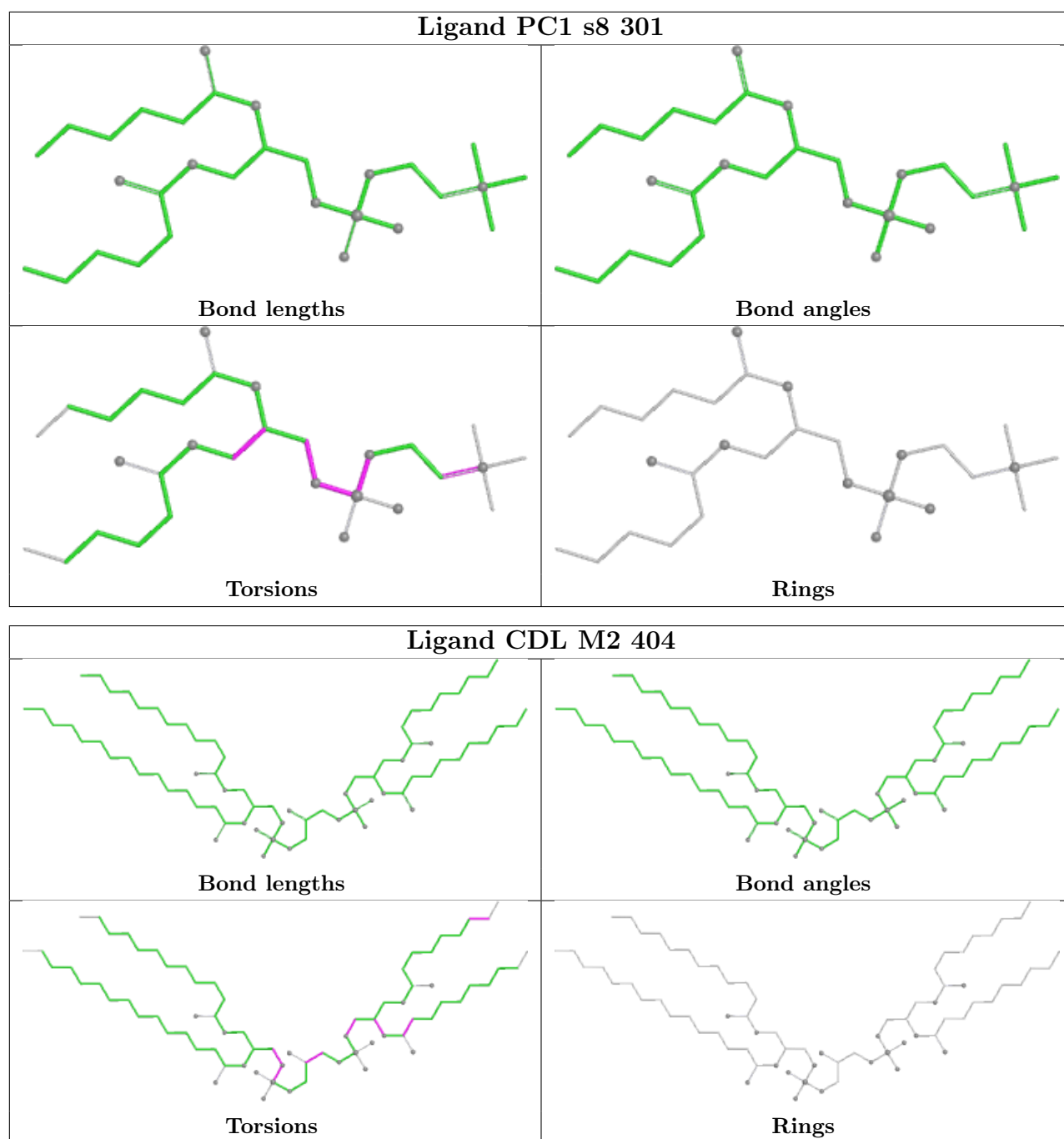


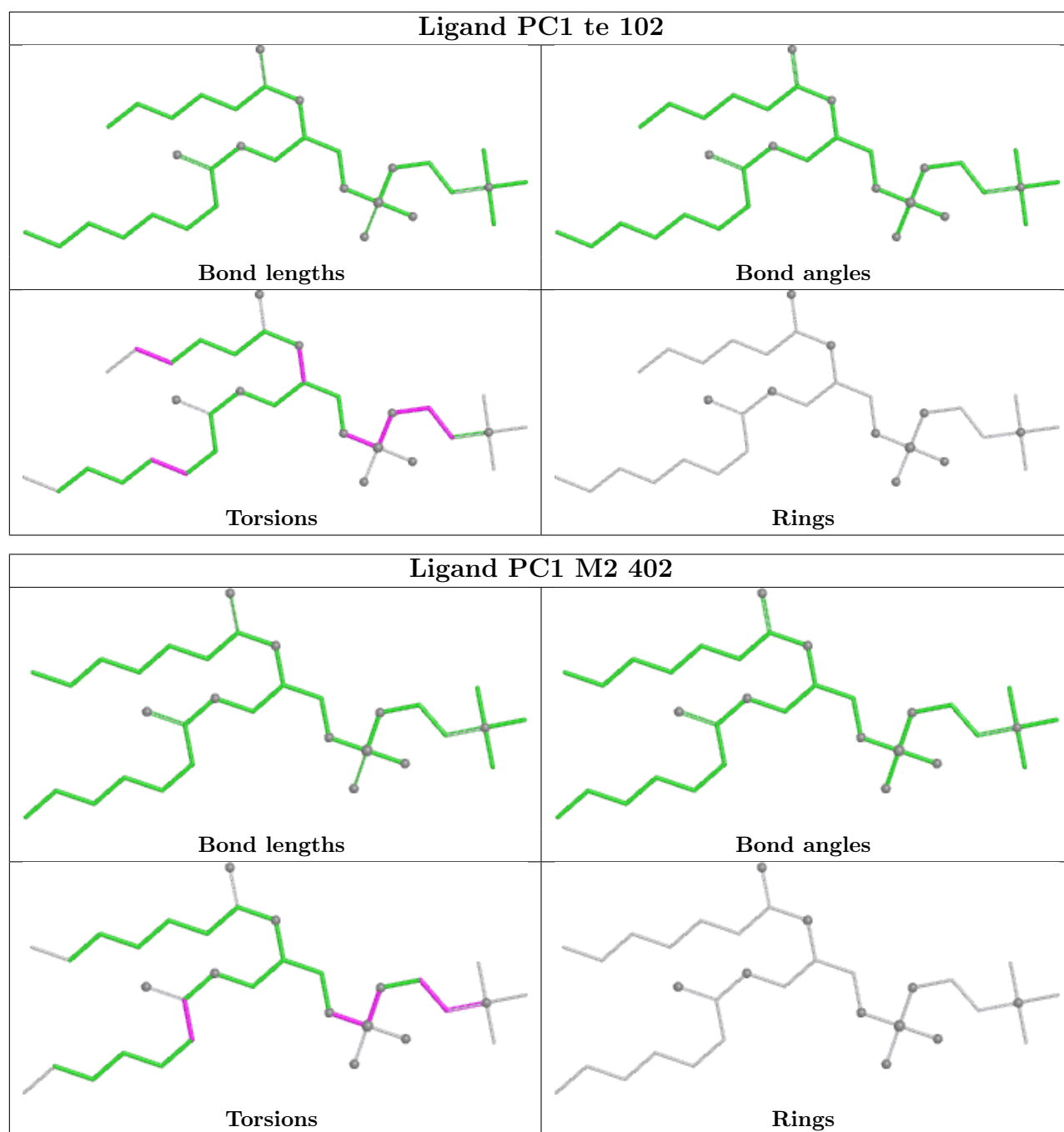
Rings

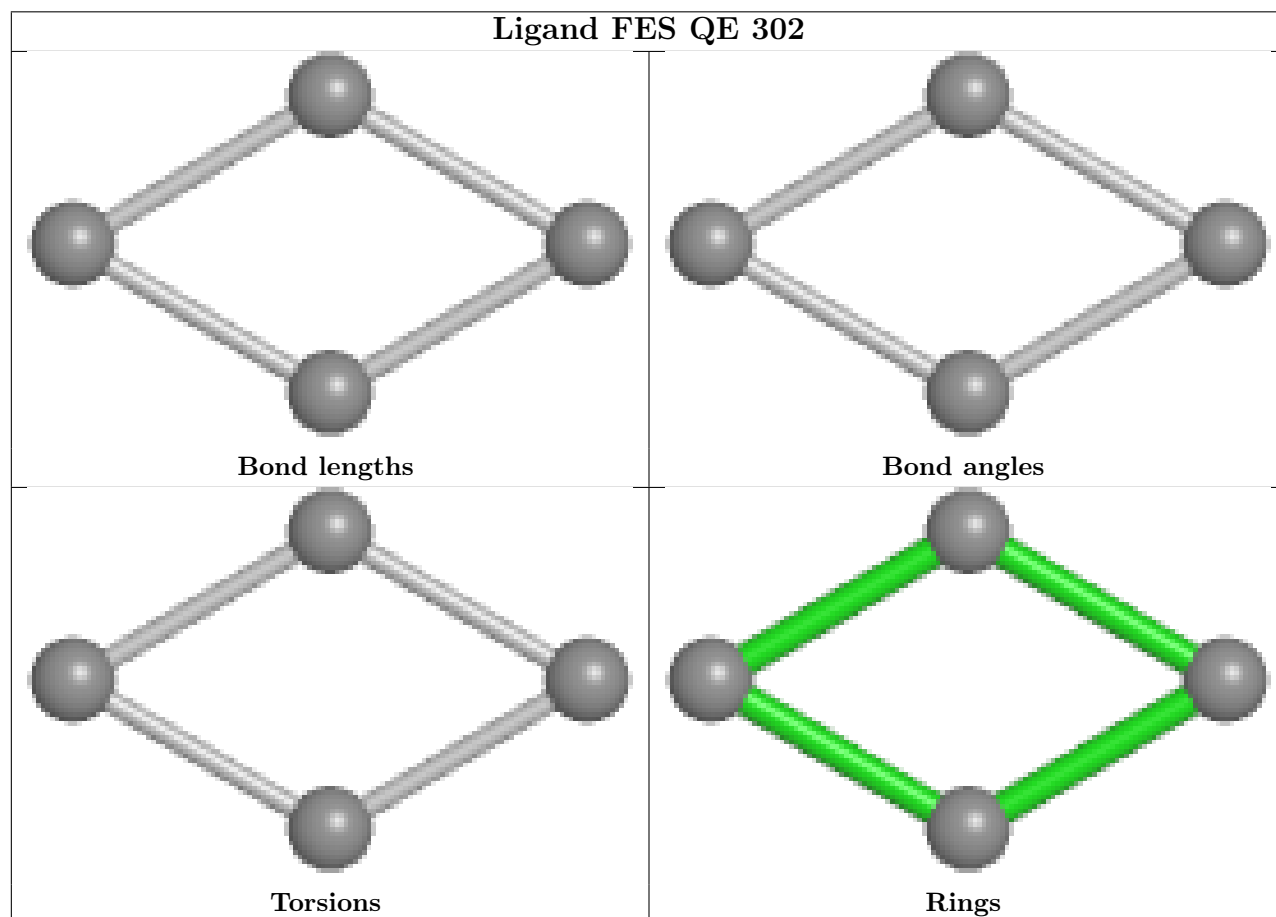
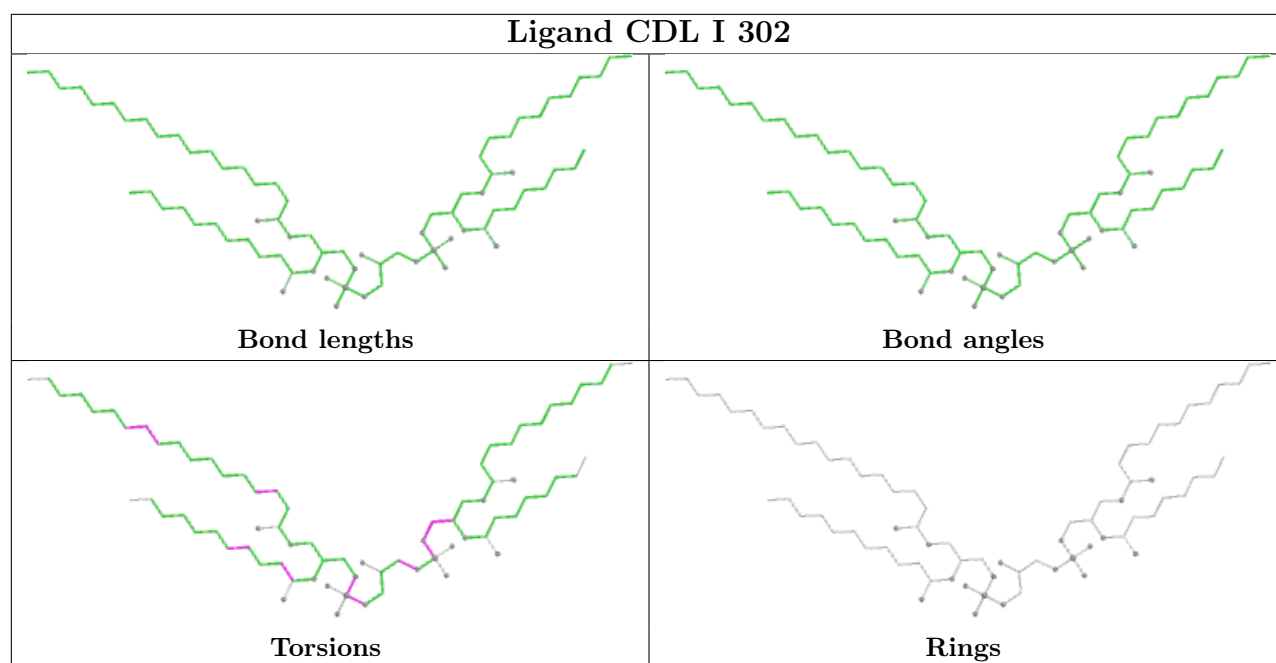


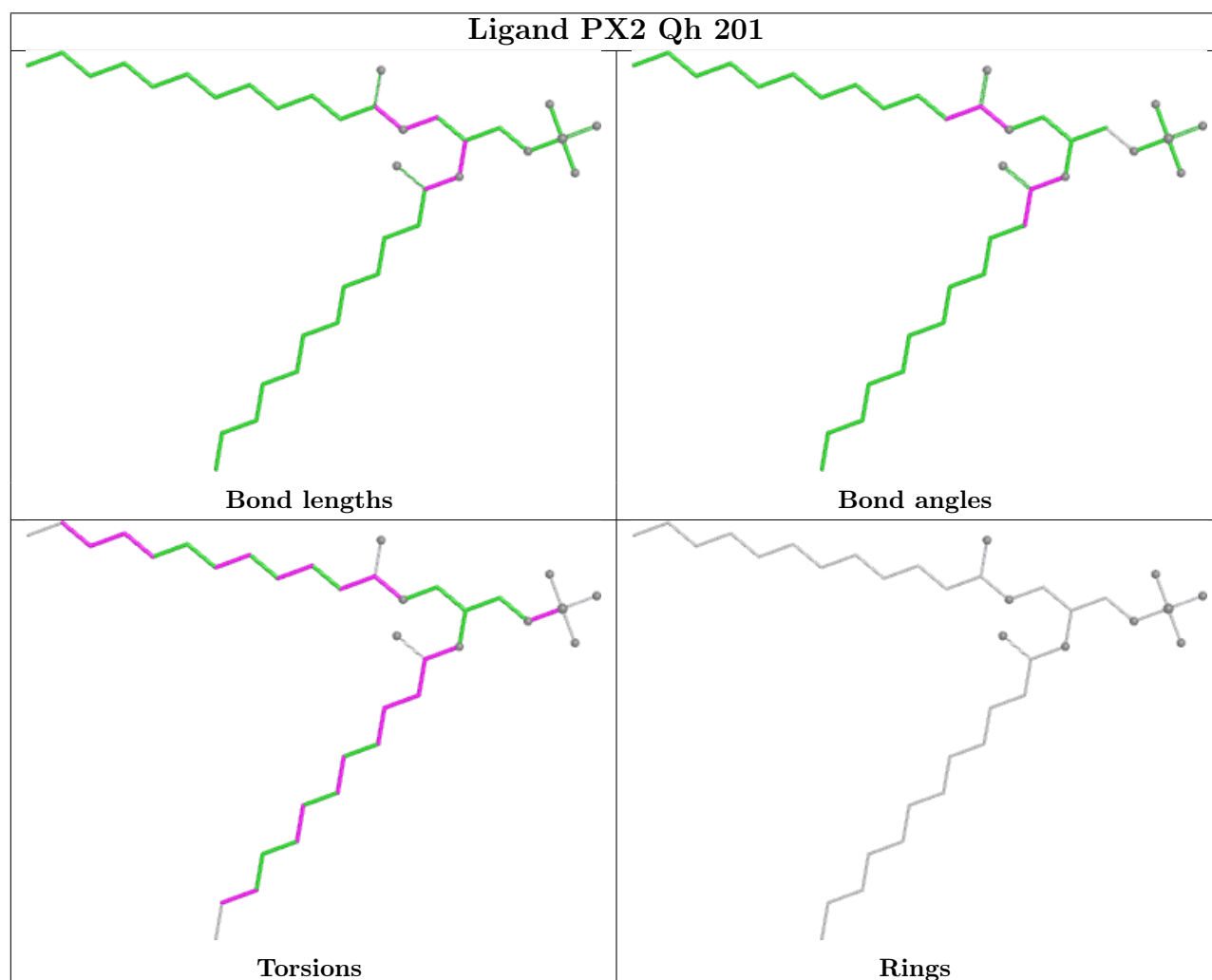
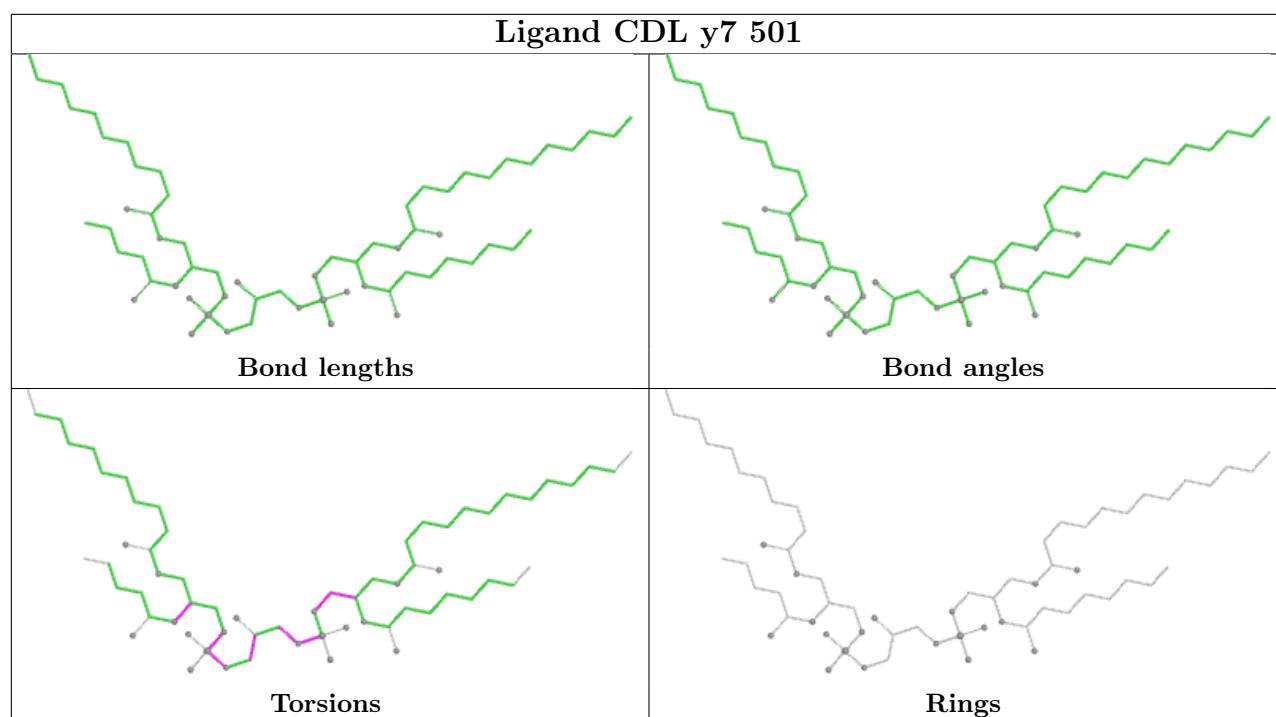


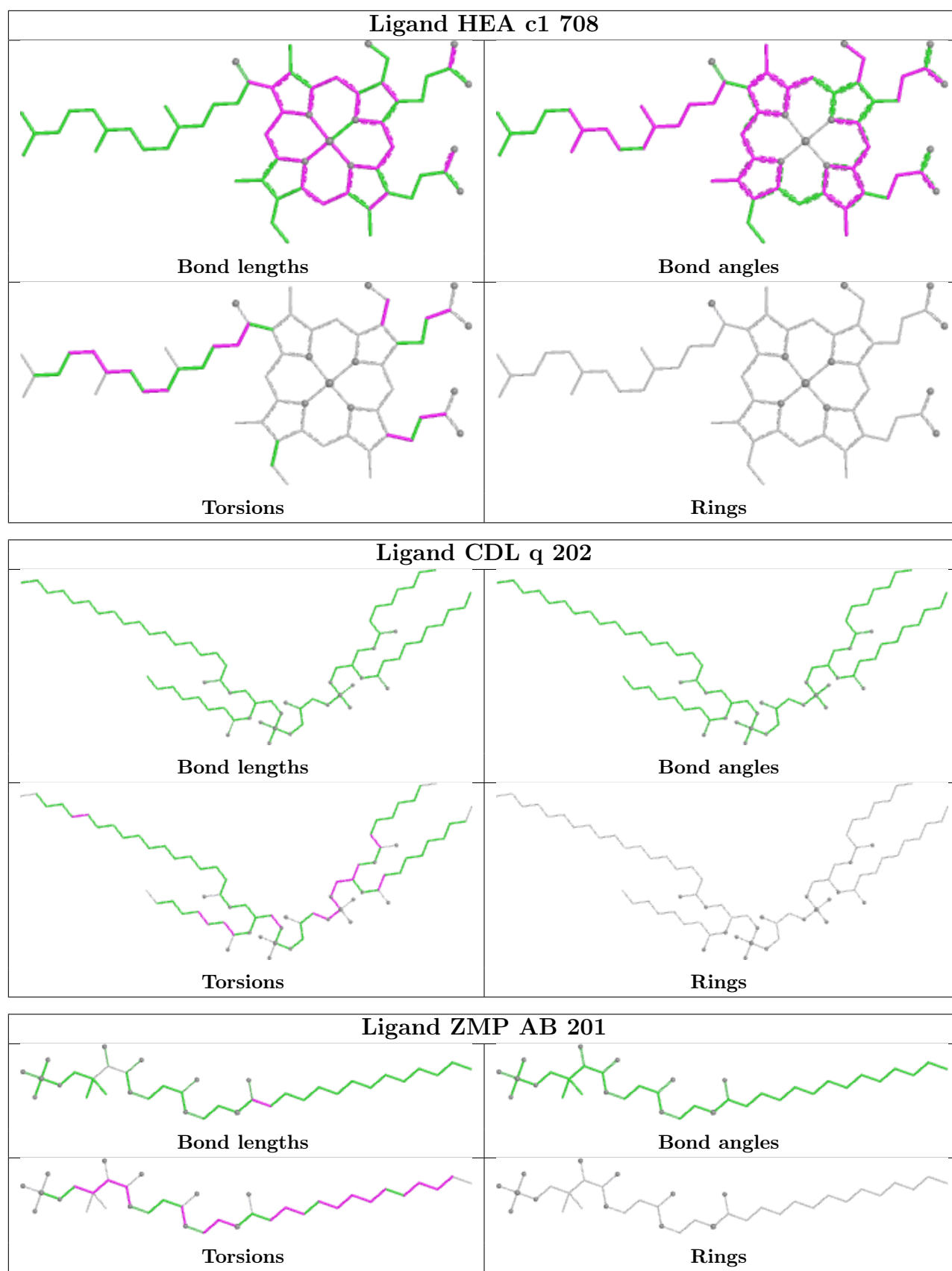


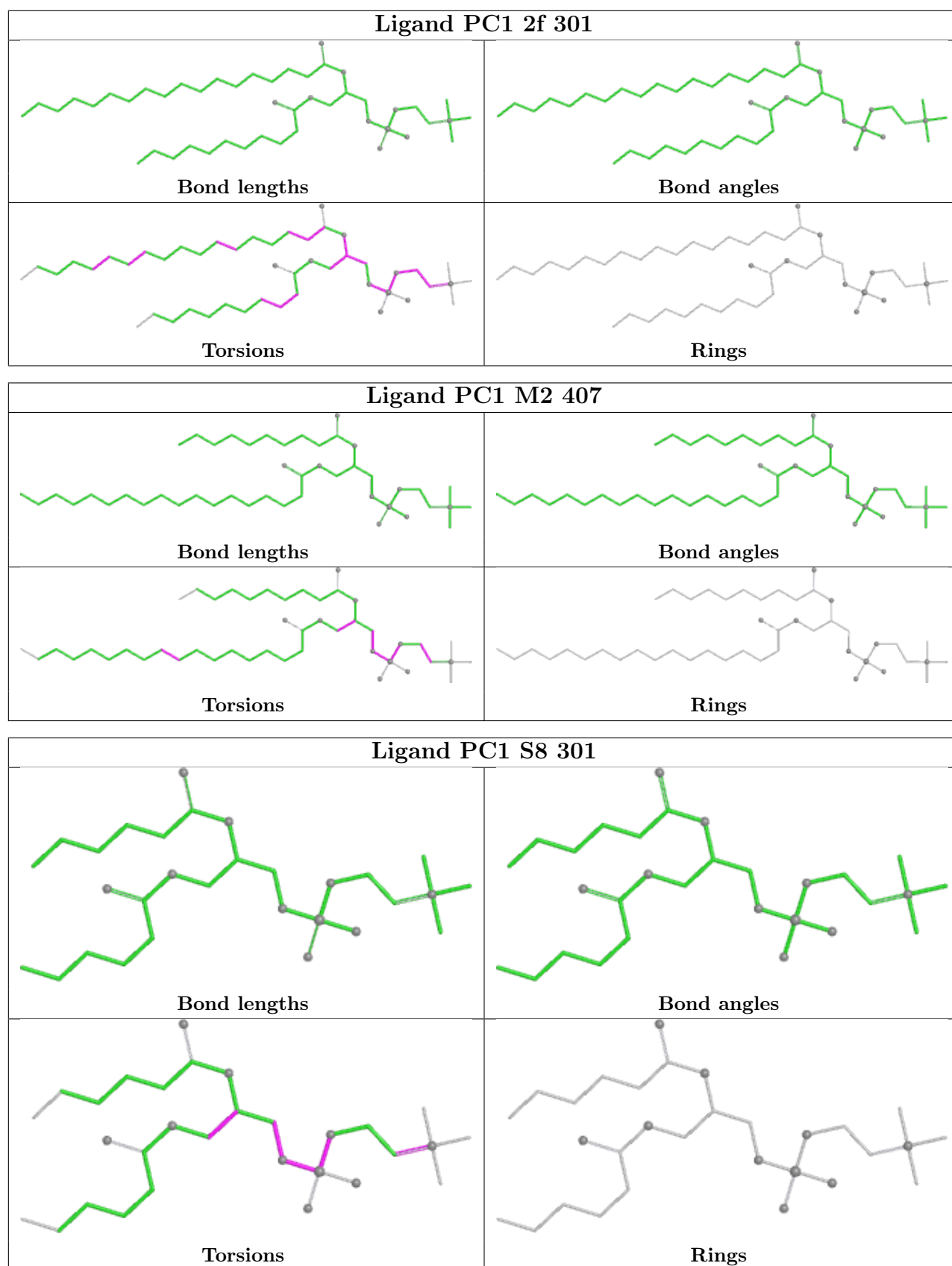


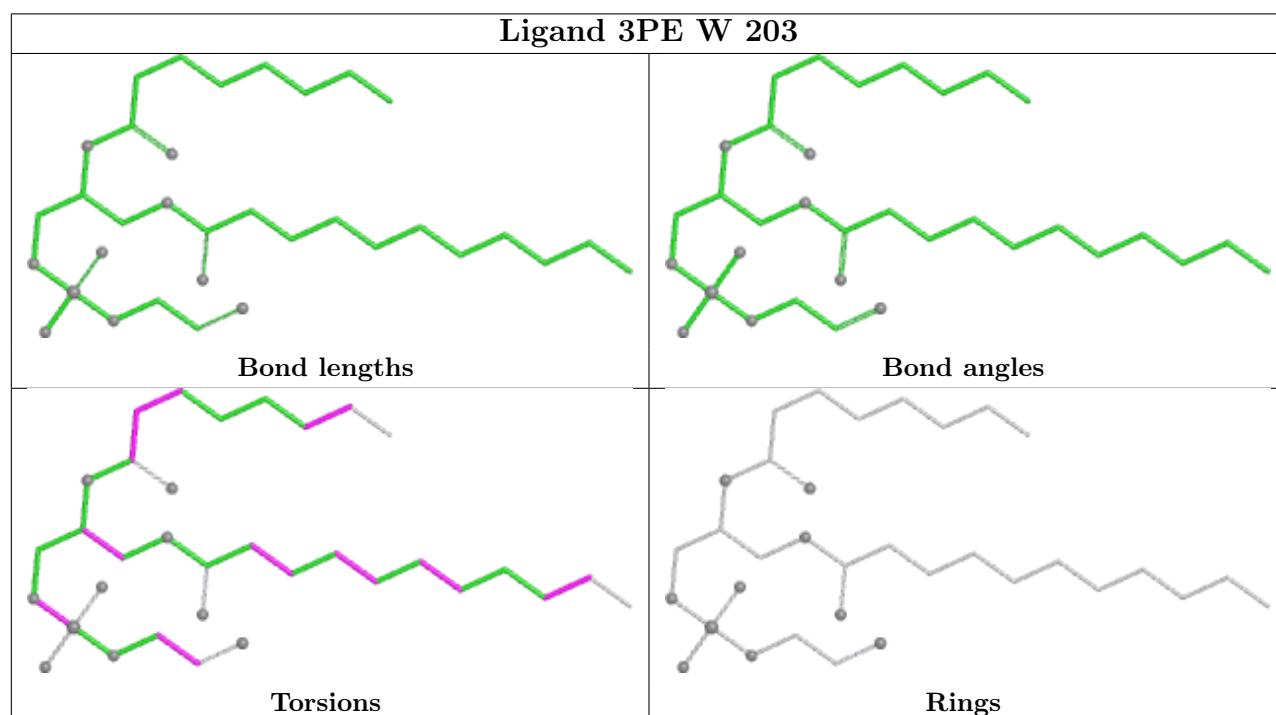
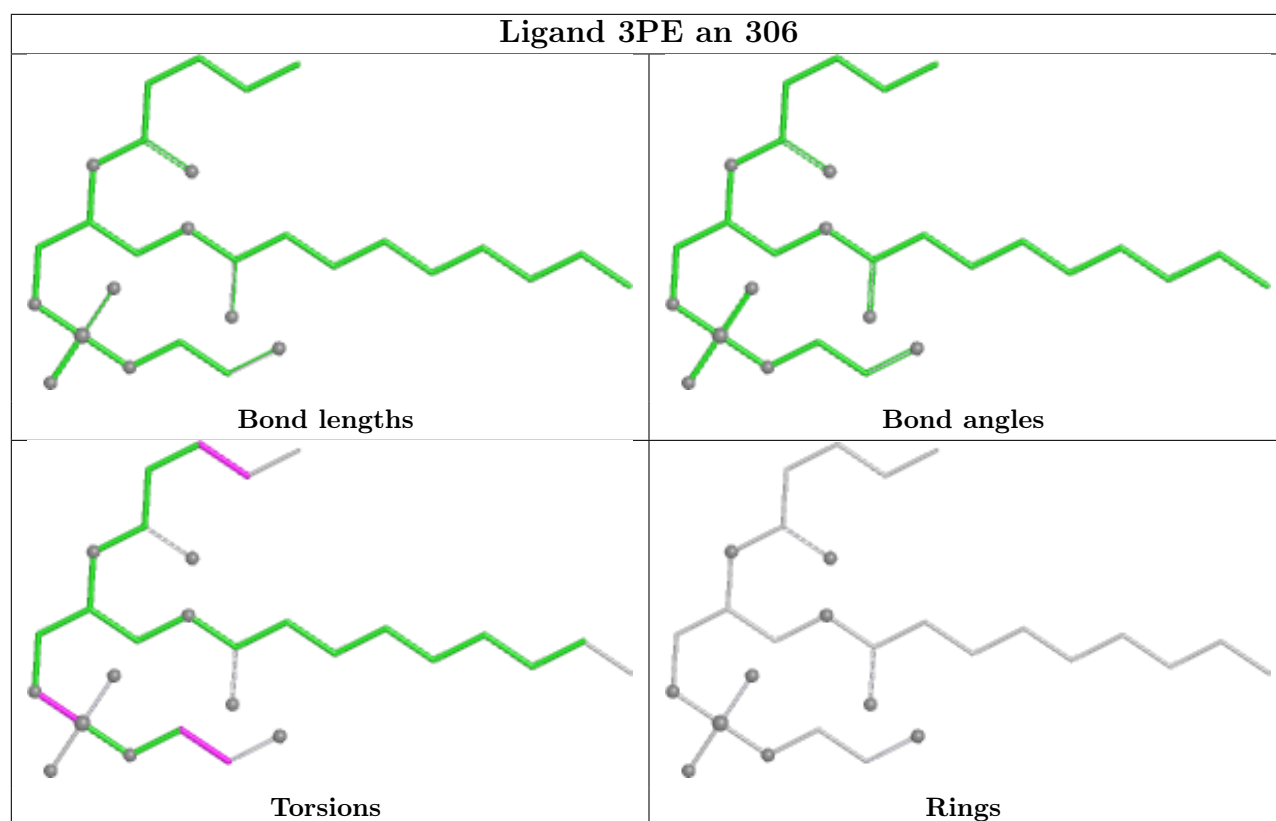


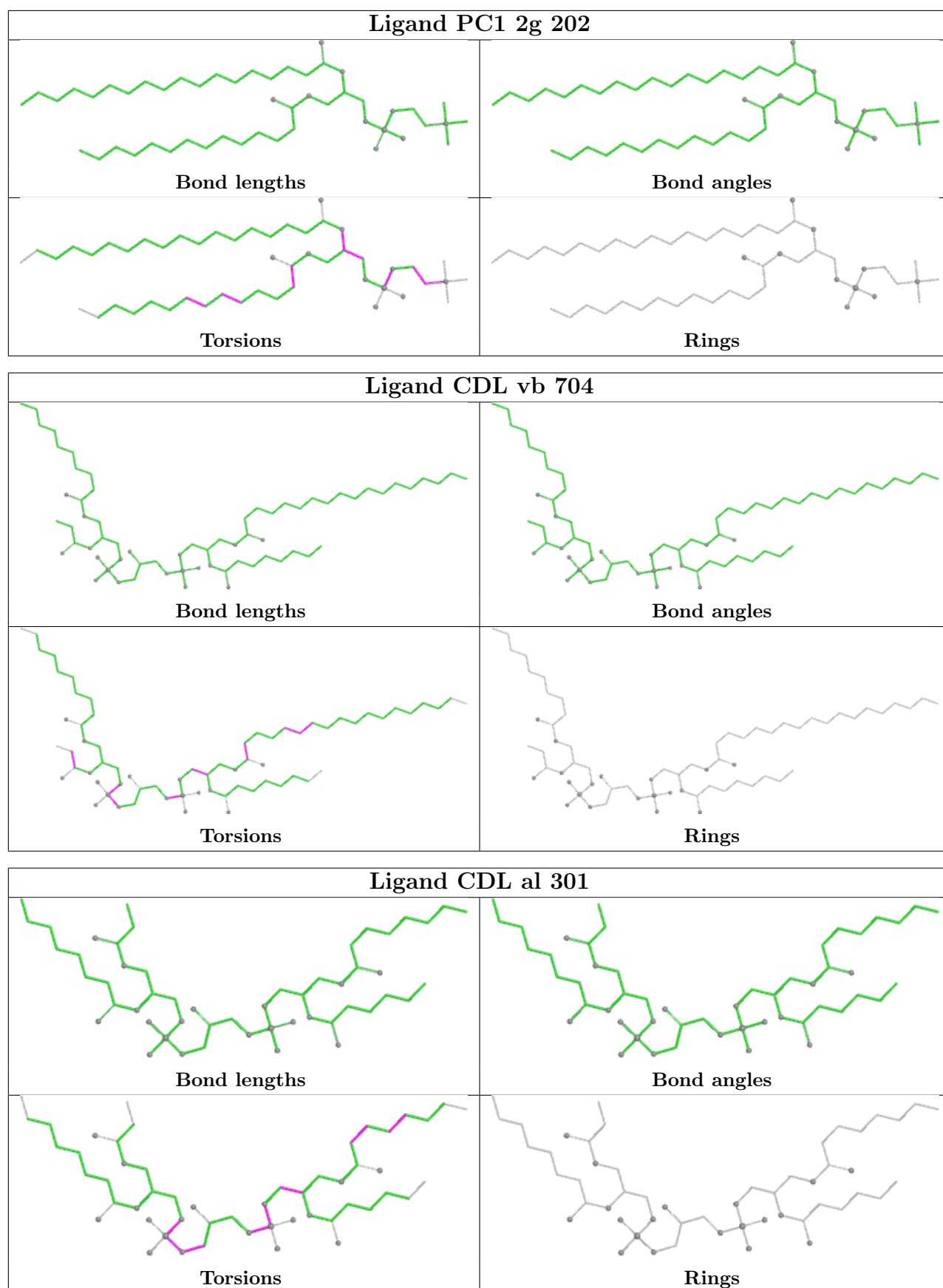


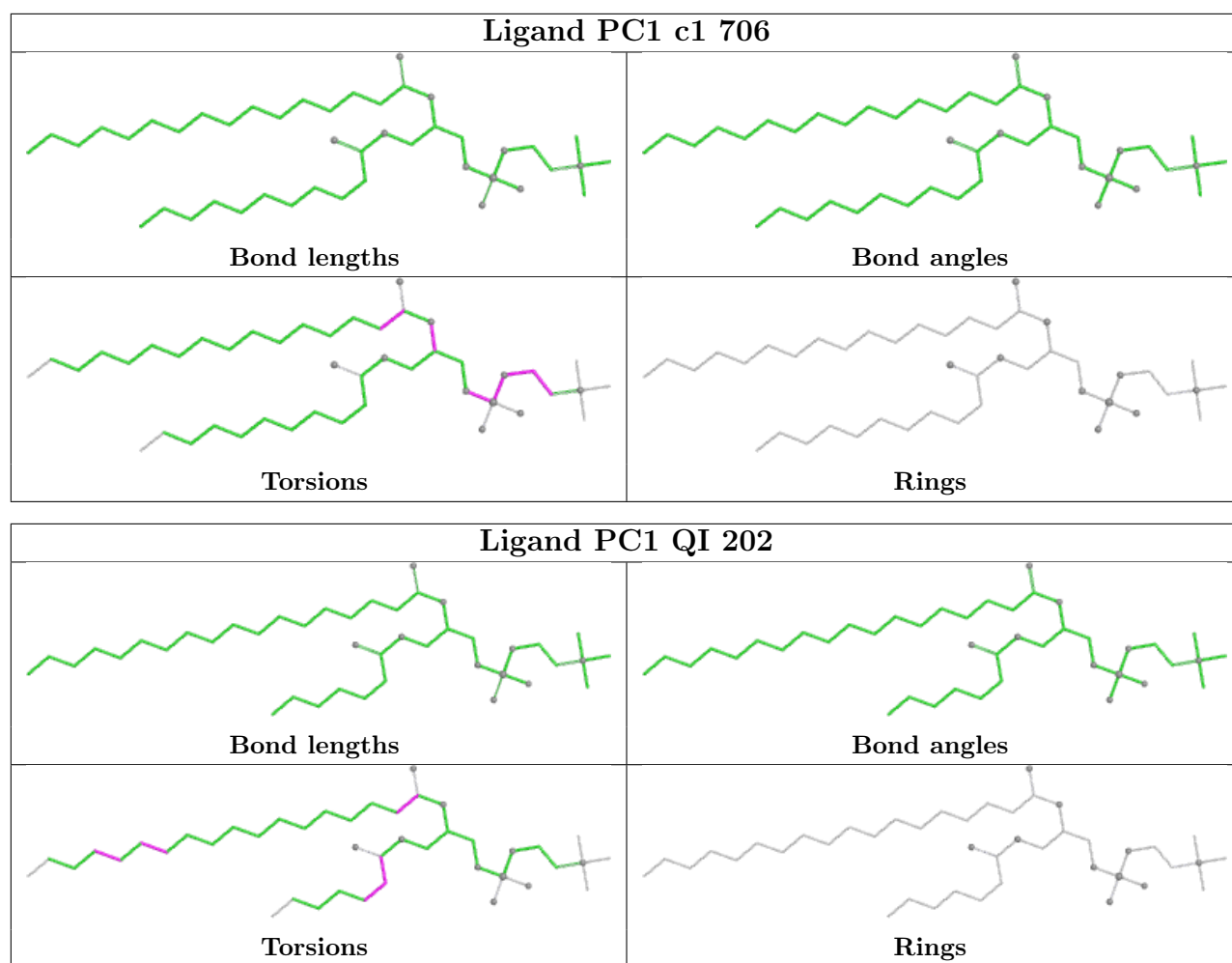


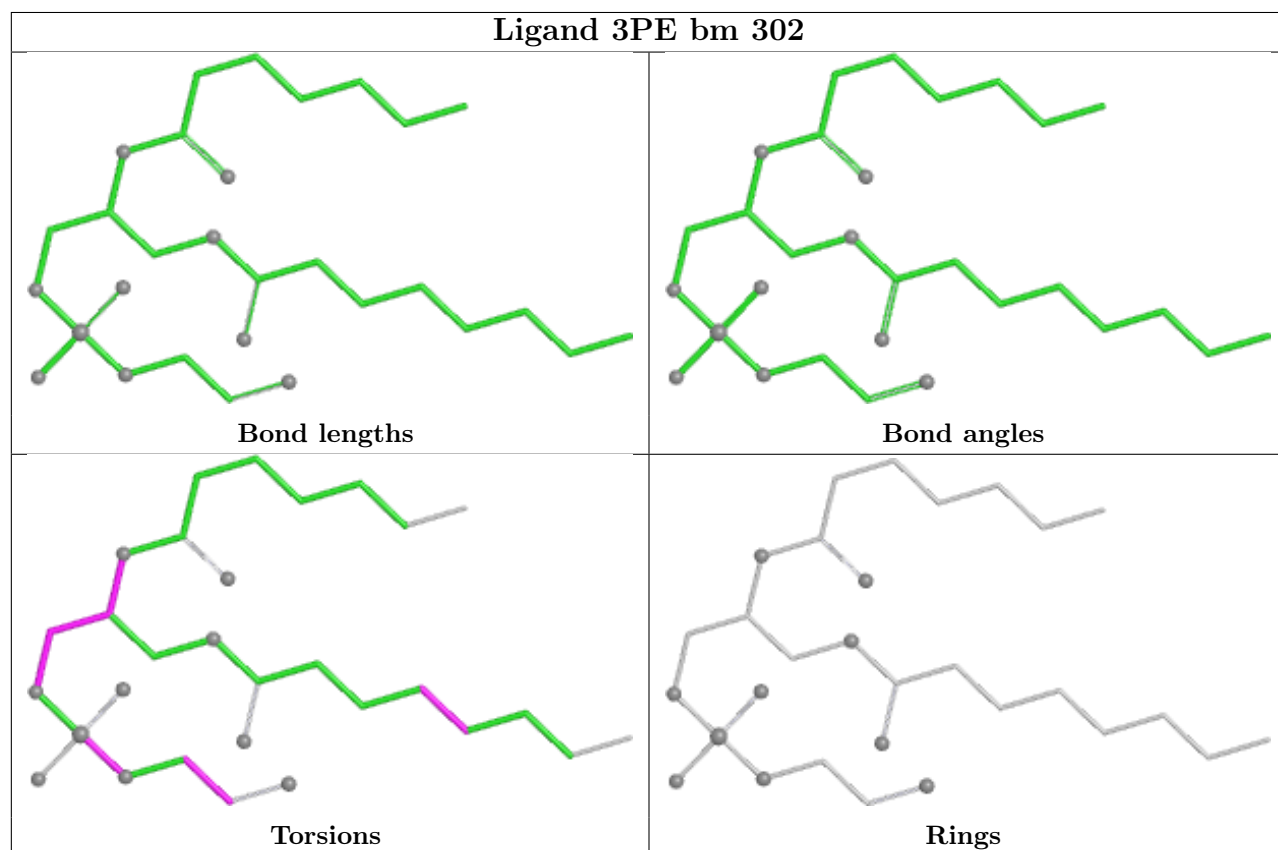
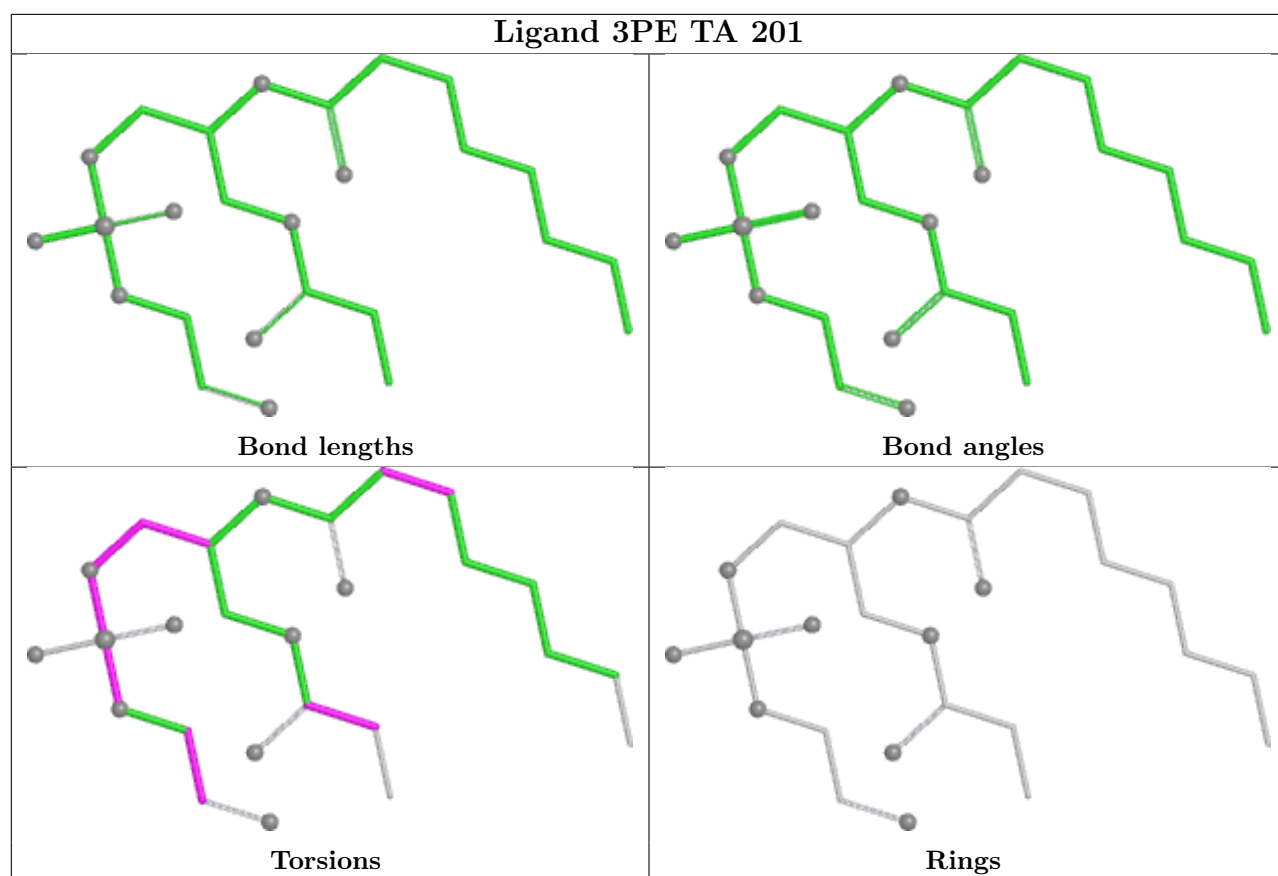


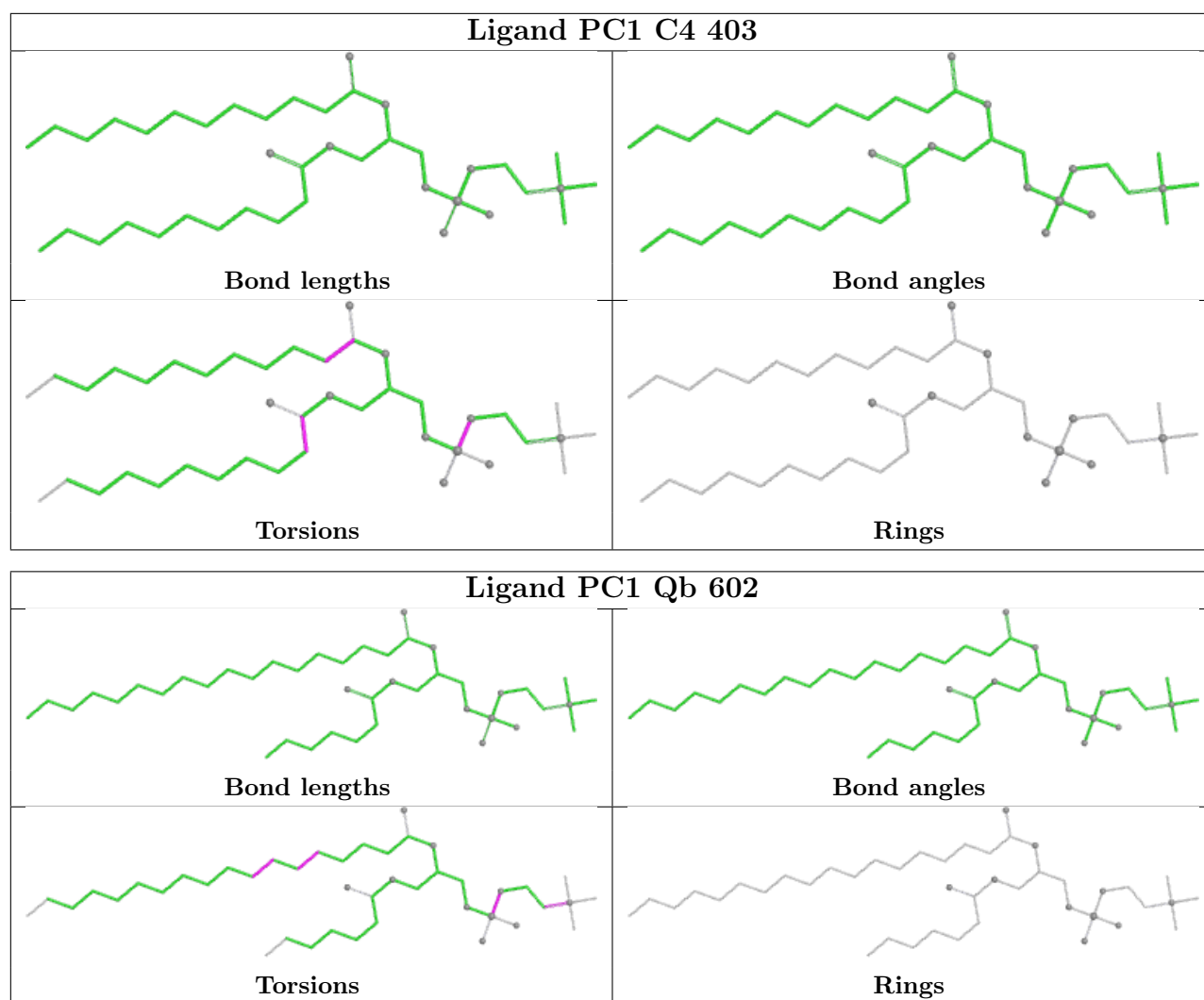


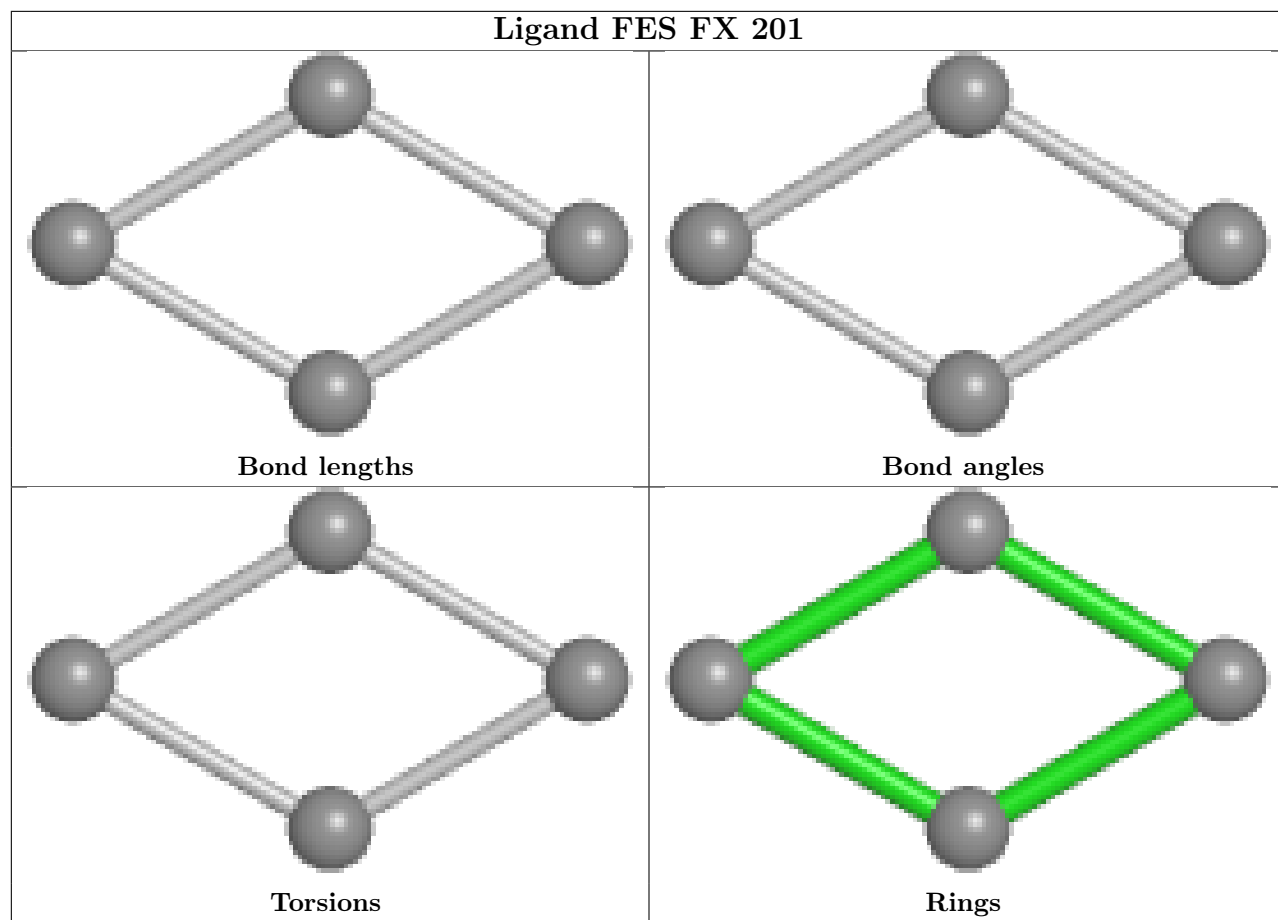




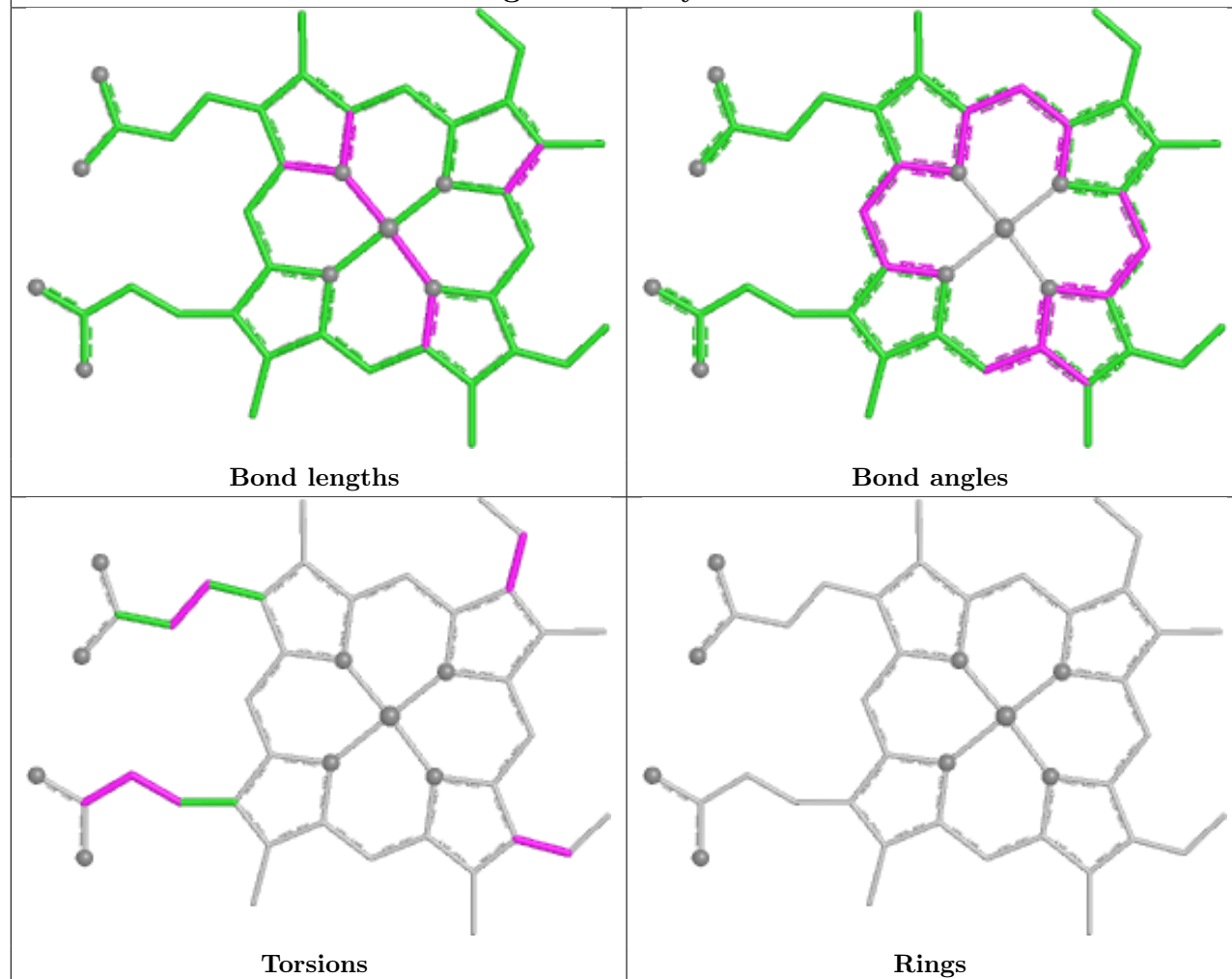




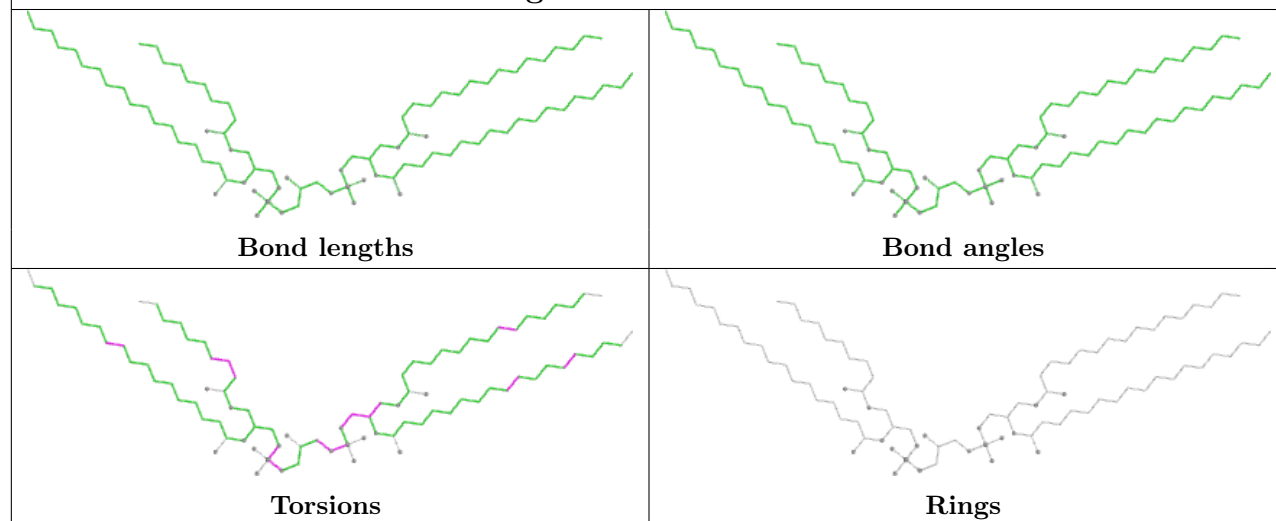




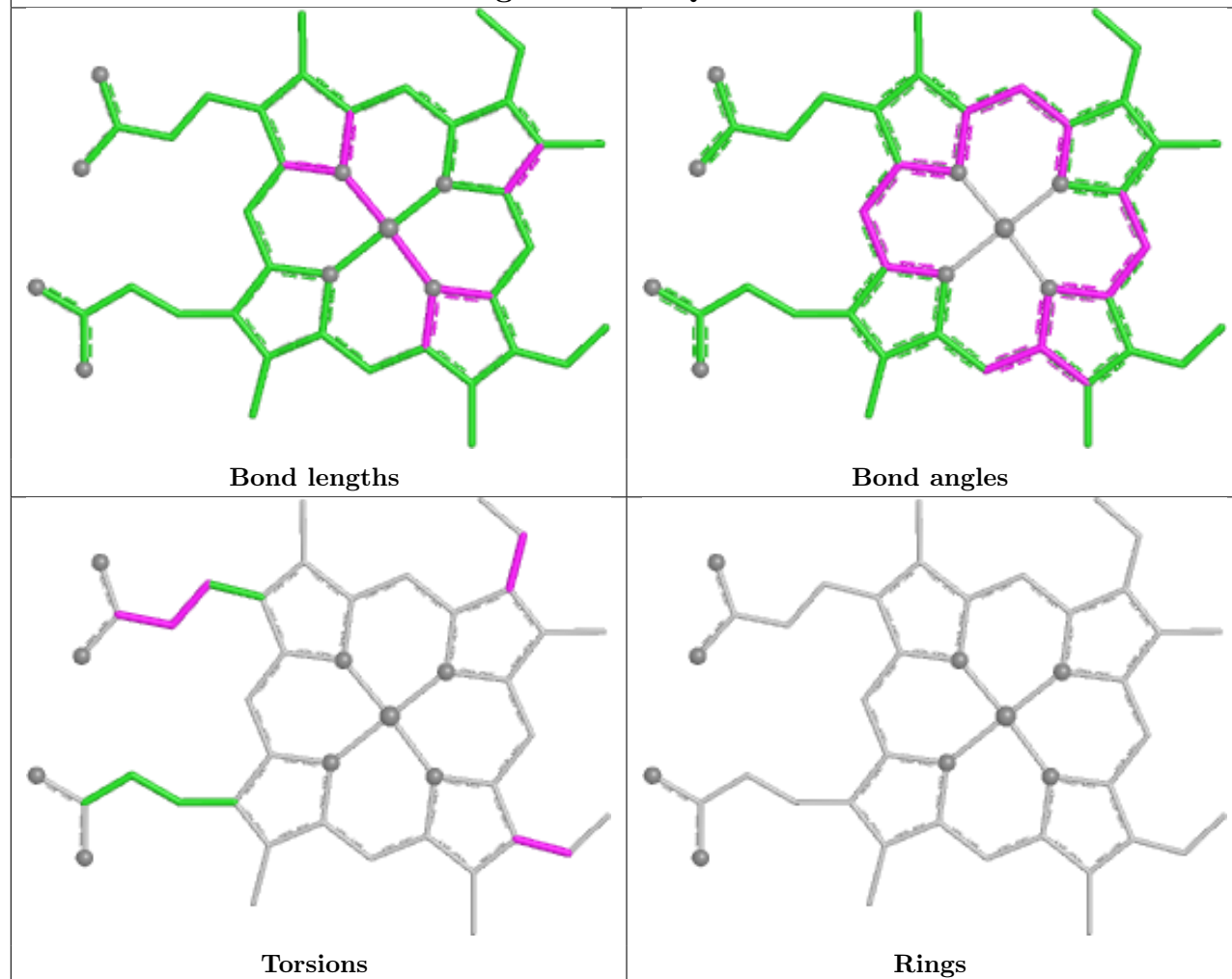
Ligand HEM y5 203



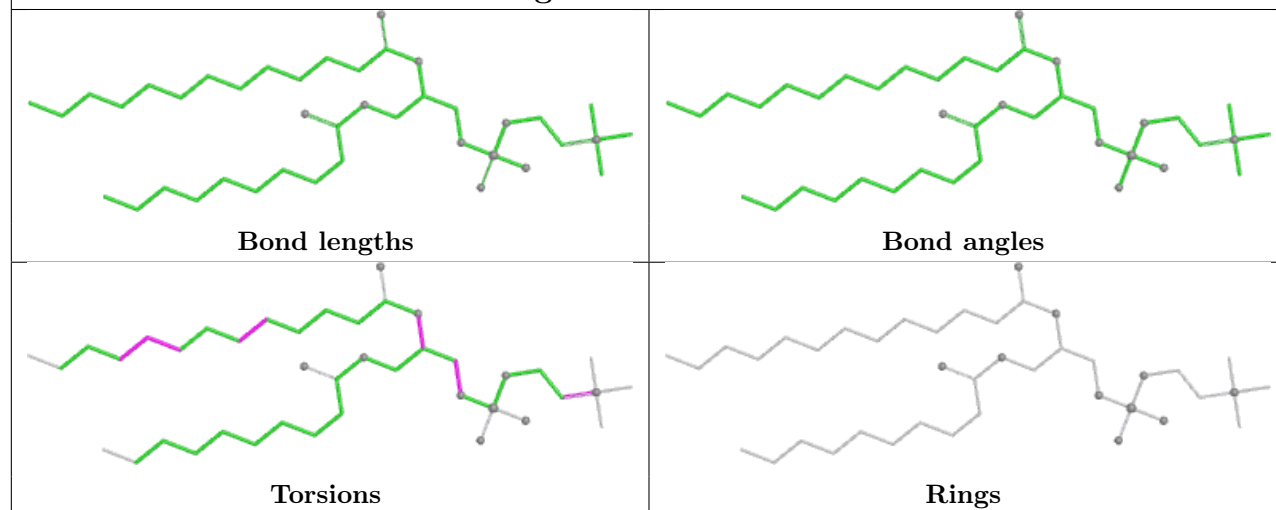
Ligand CDL n5 806

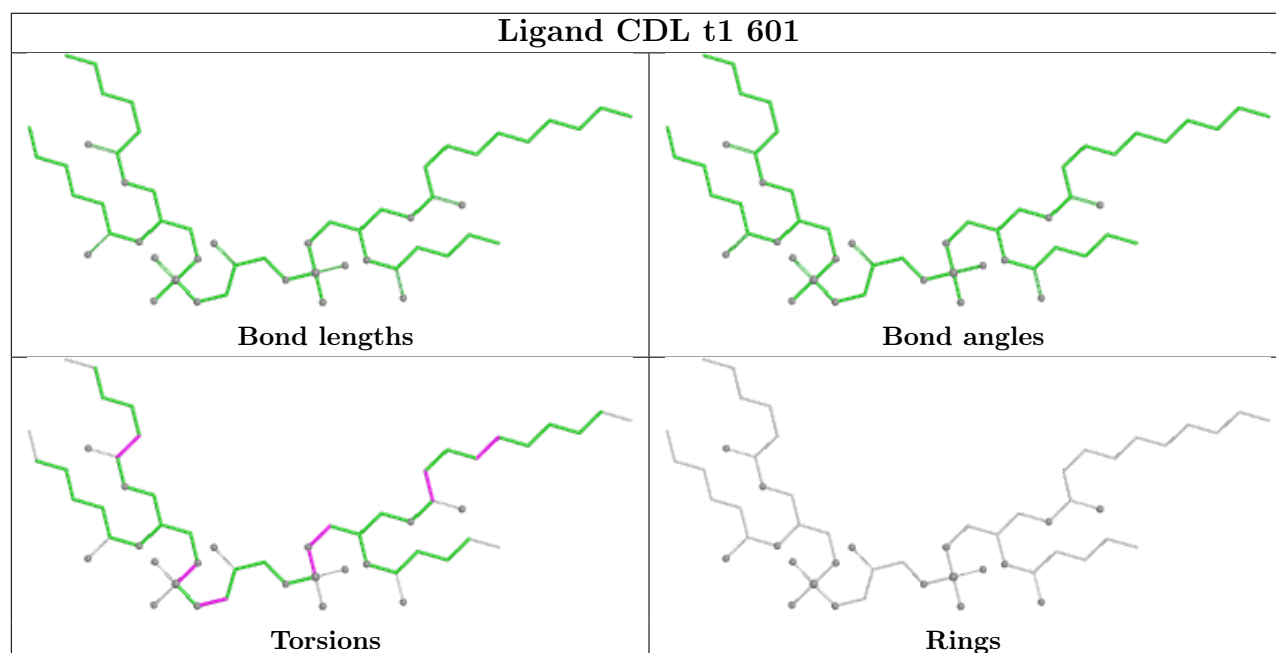
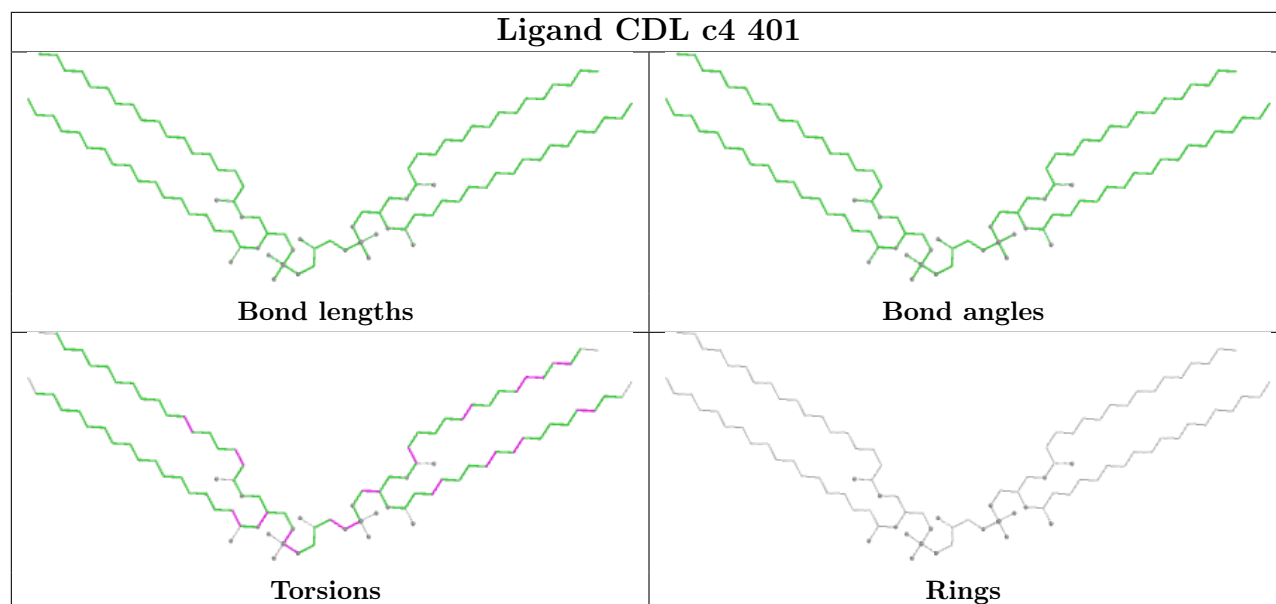
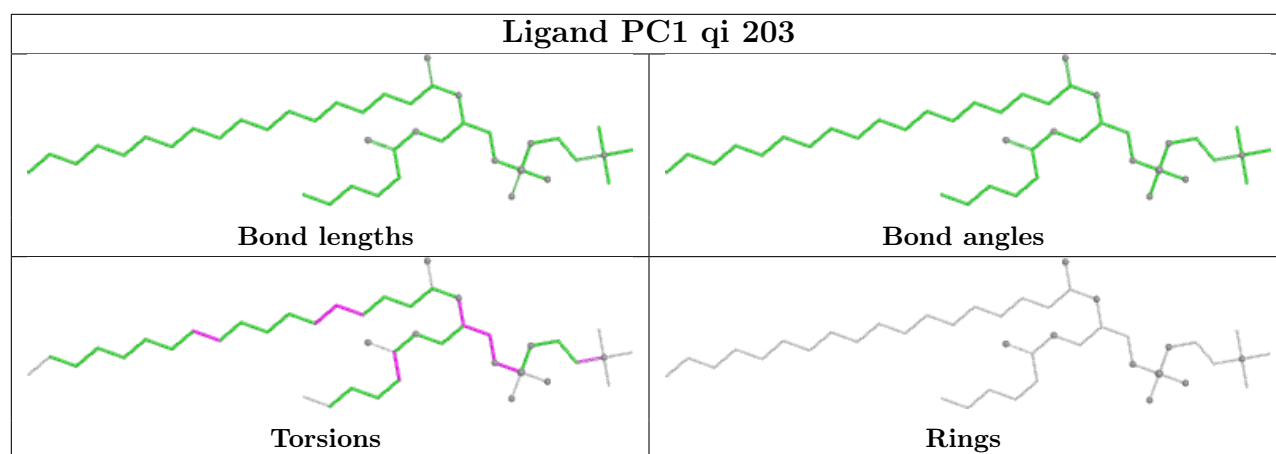


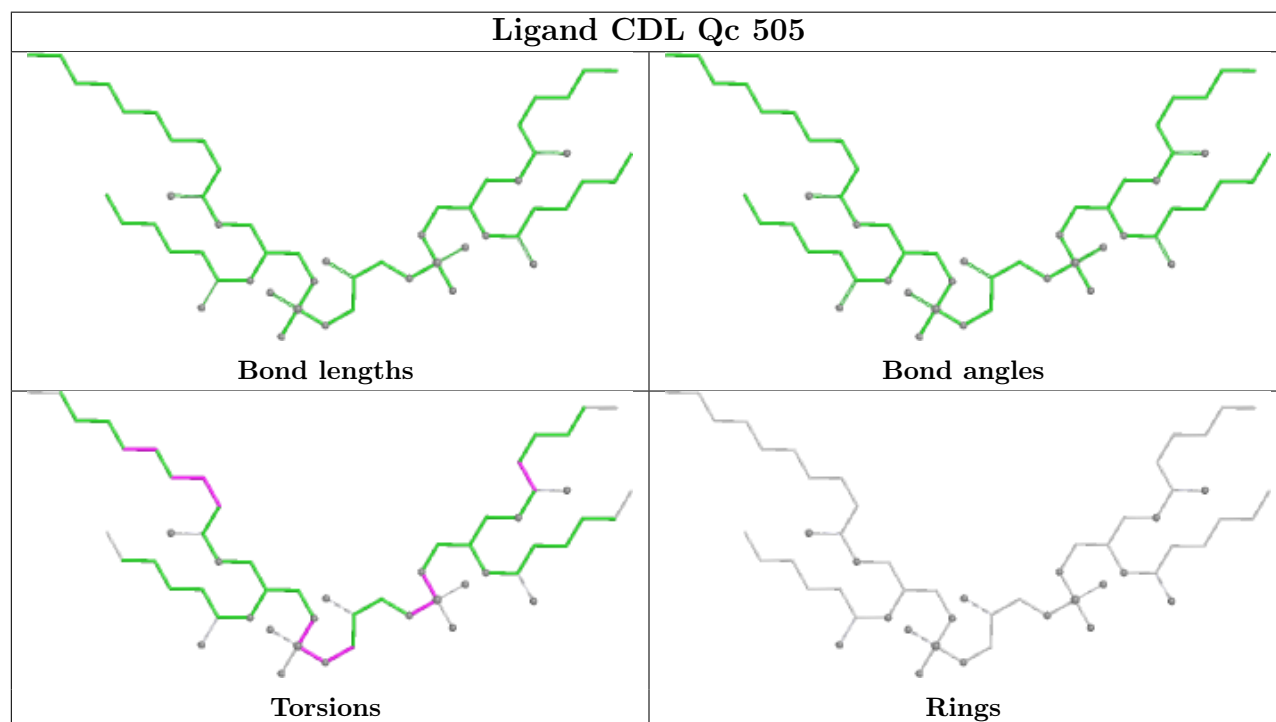
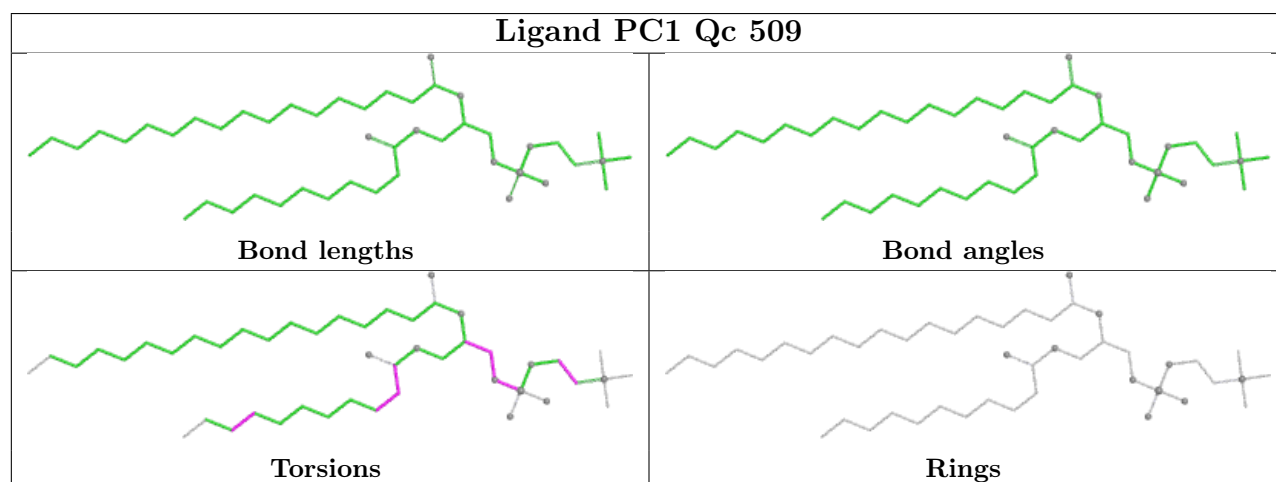
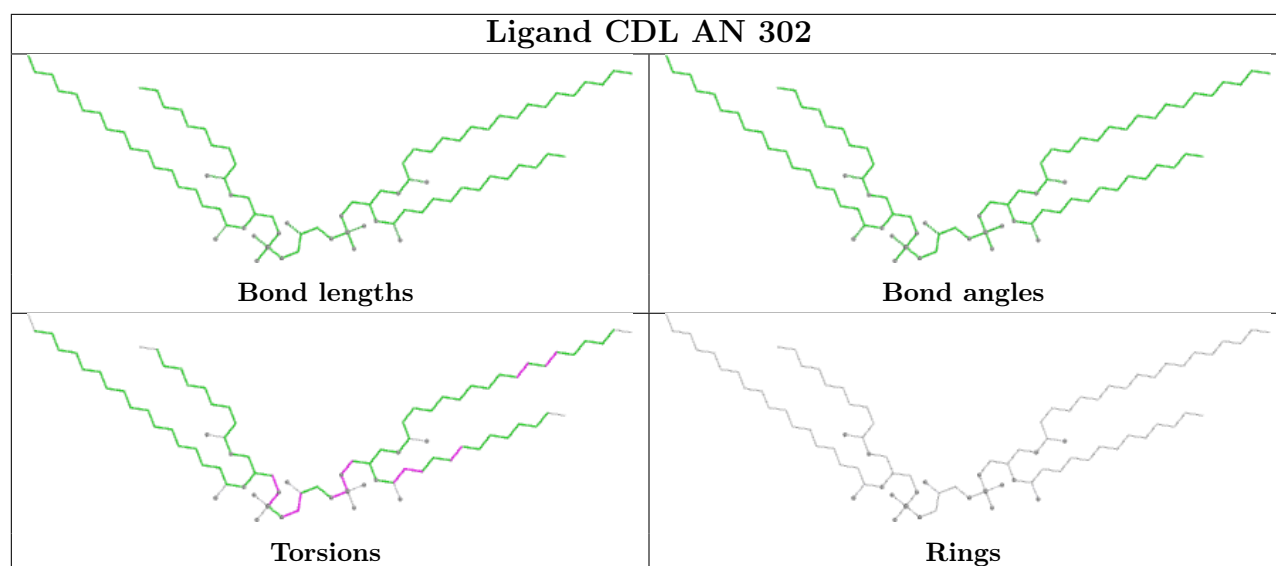
Ligand HEM QC 501

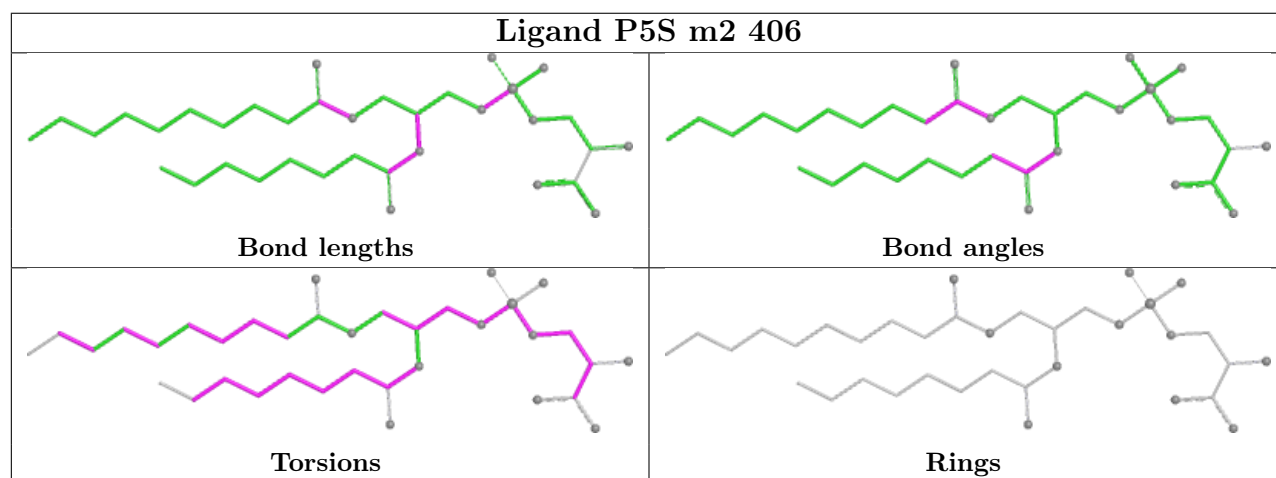
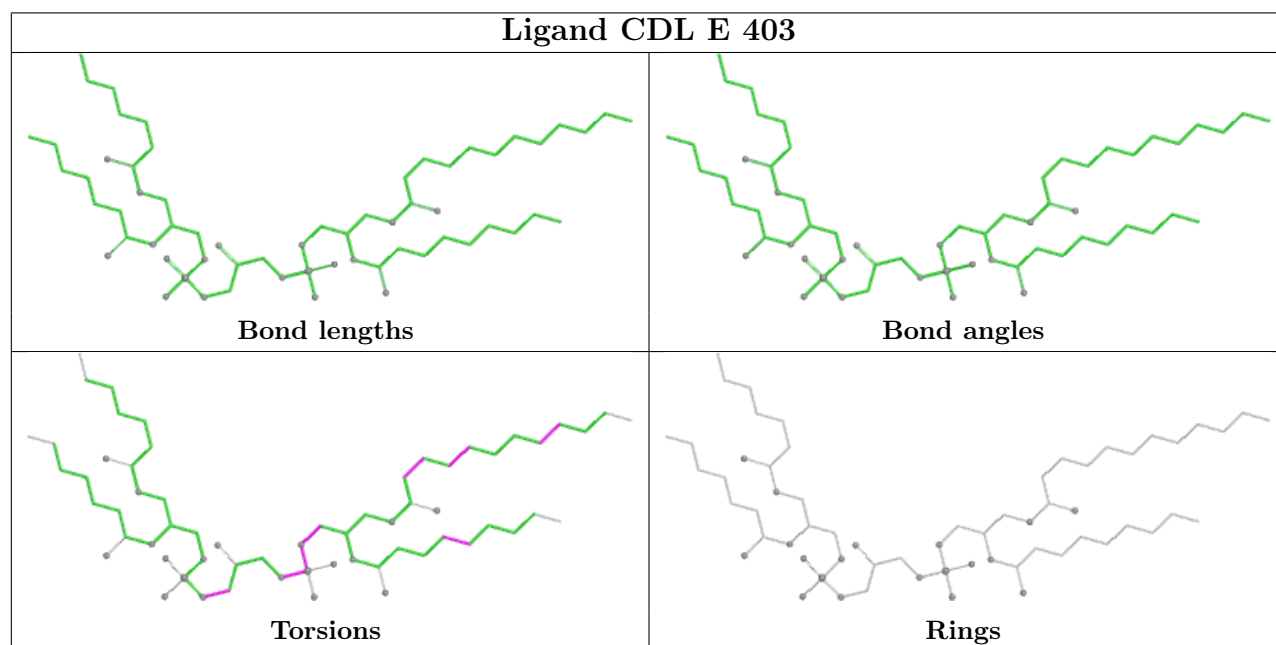
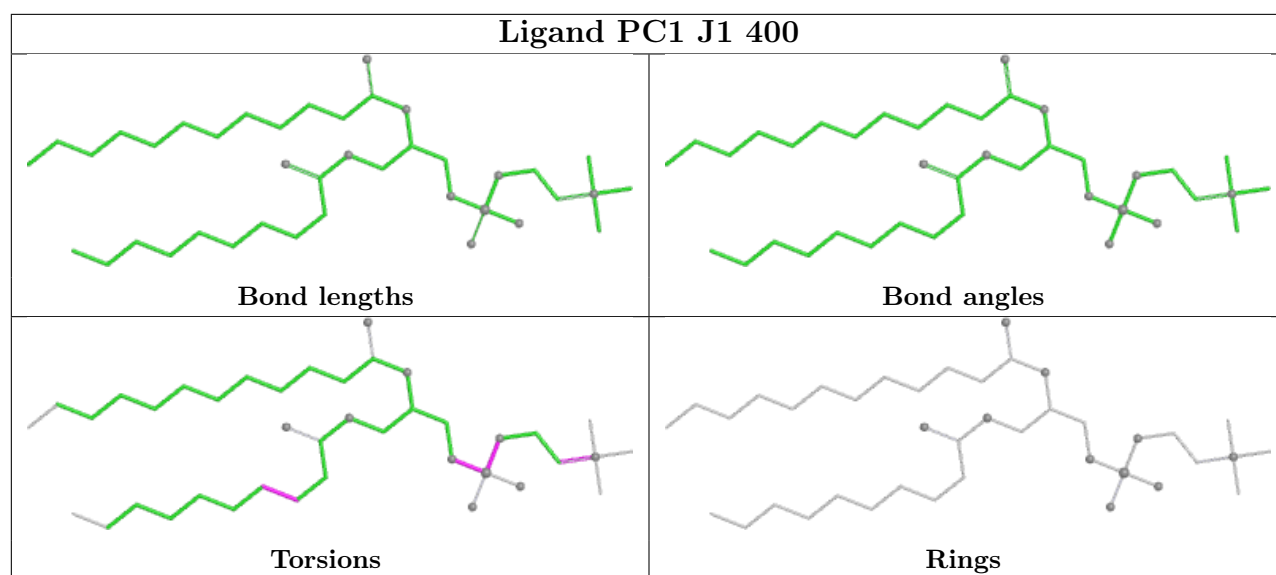


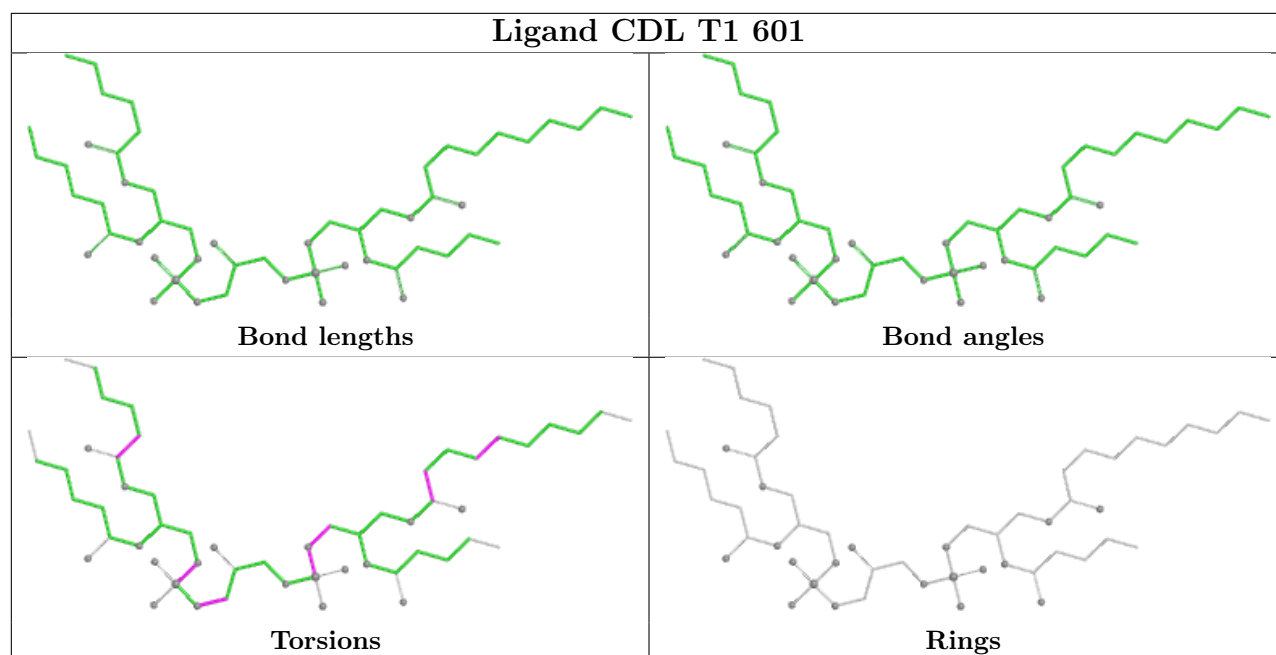
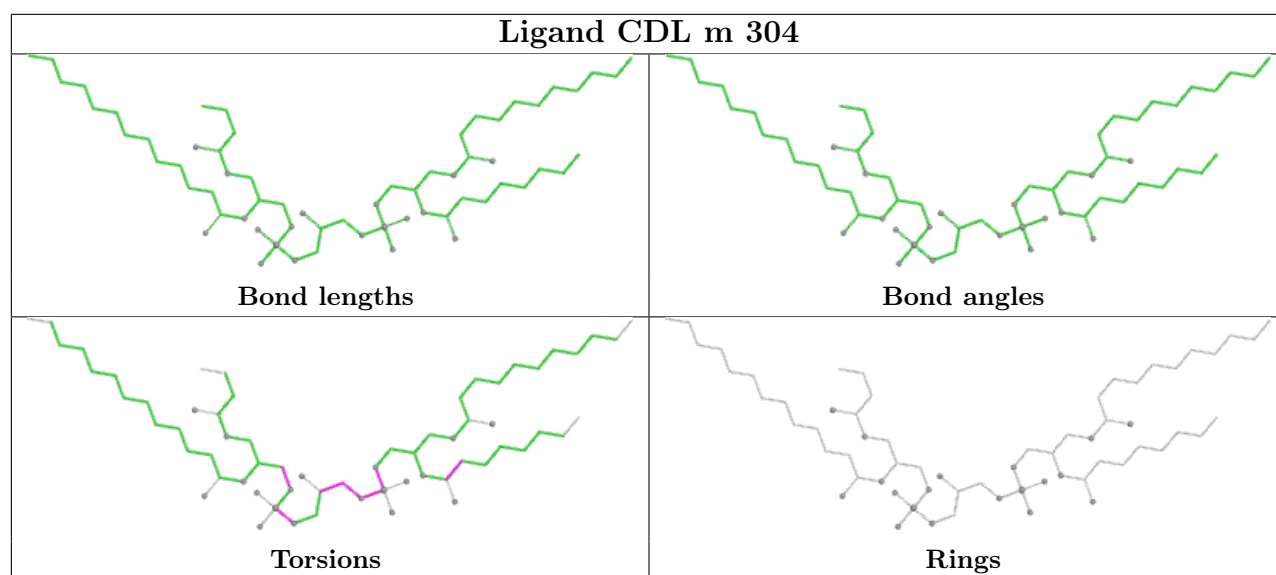
Ligand PC1 A 503

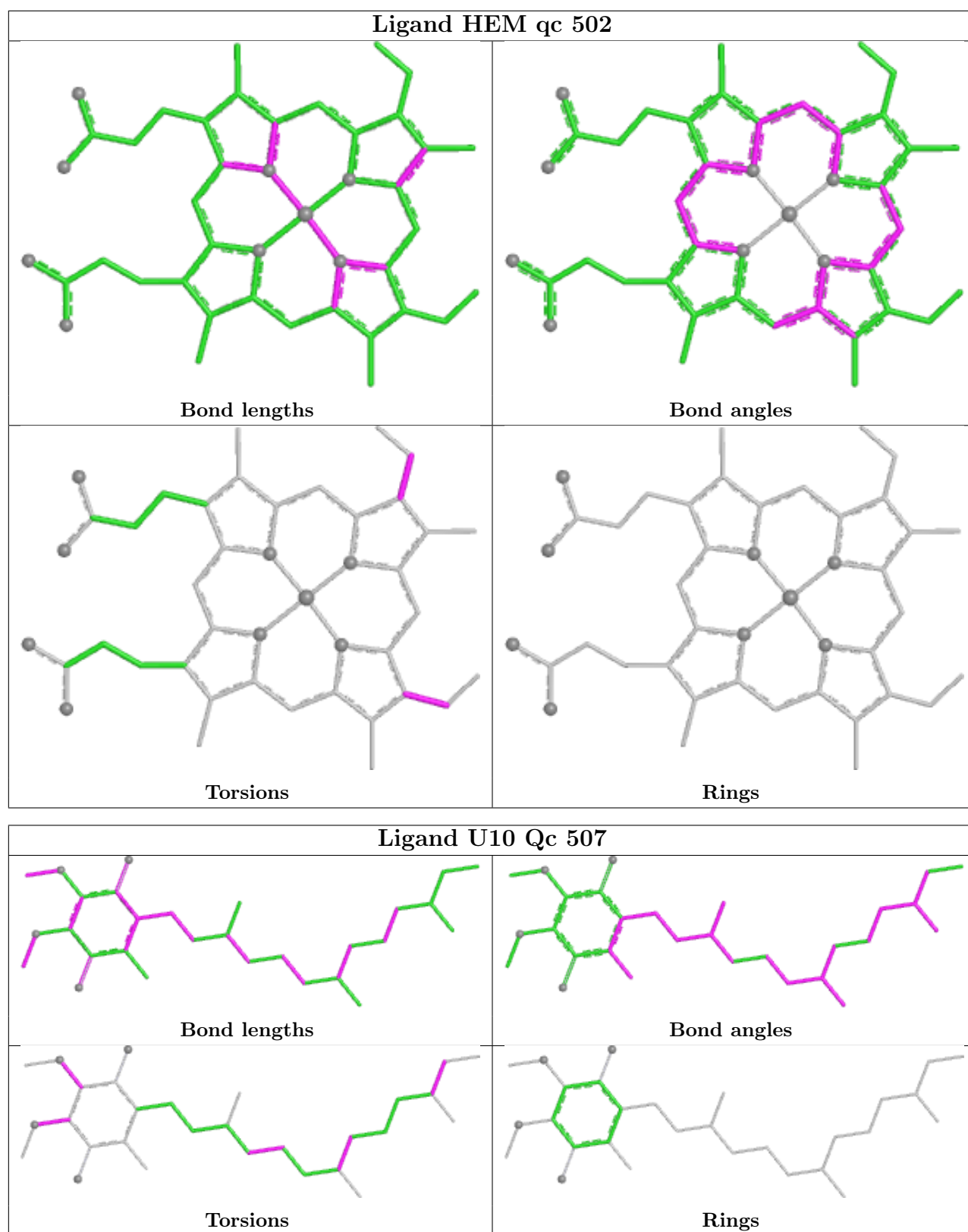


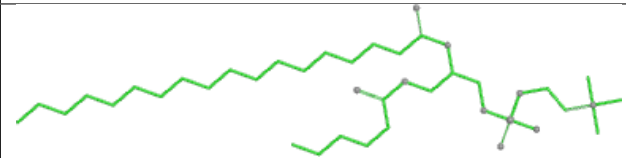
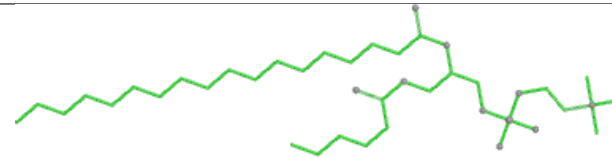
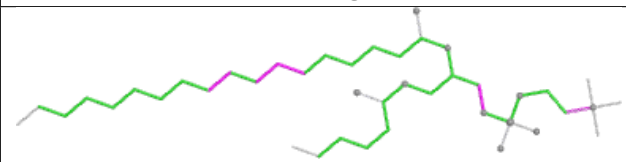
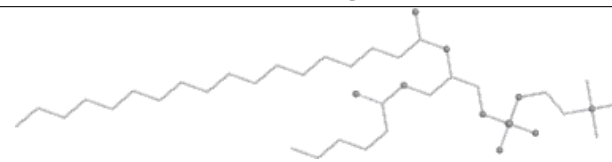
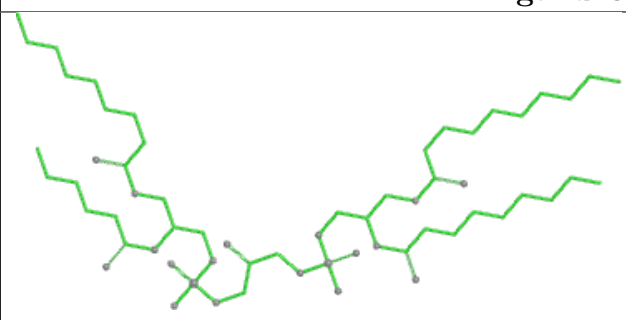
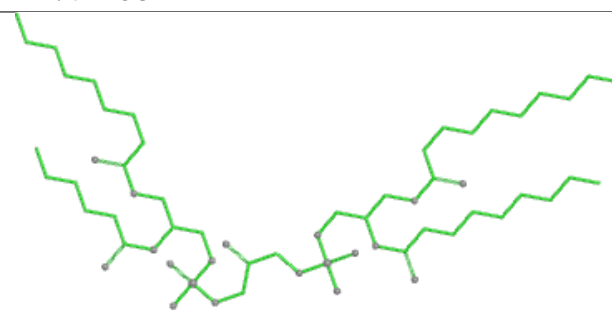
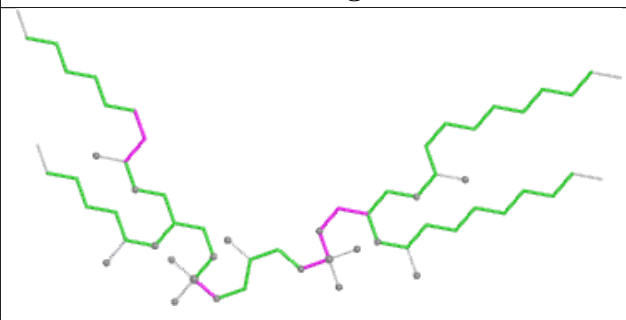
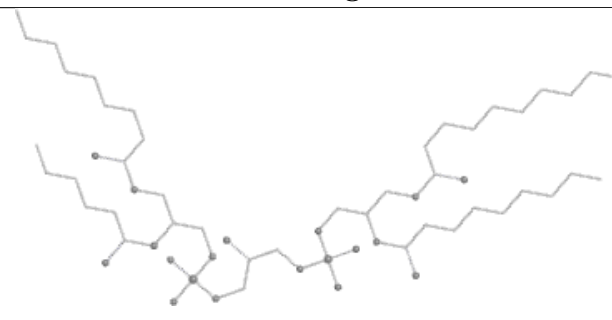
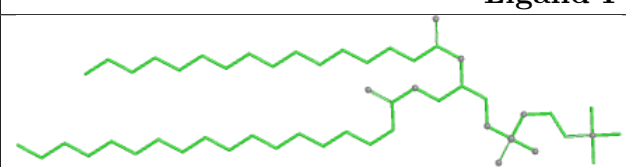
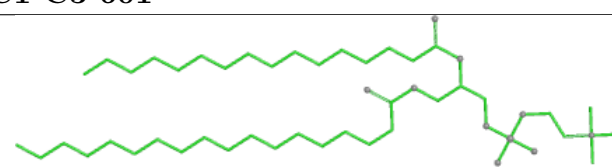
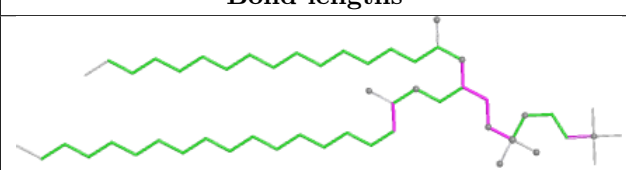
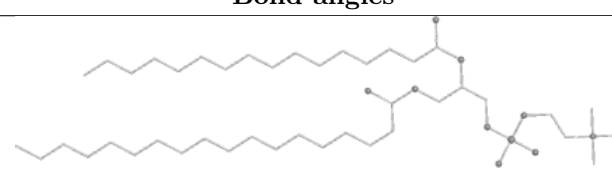


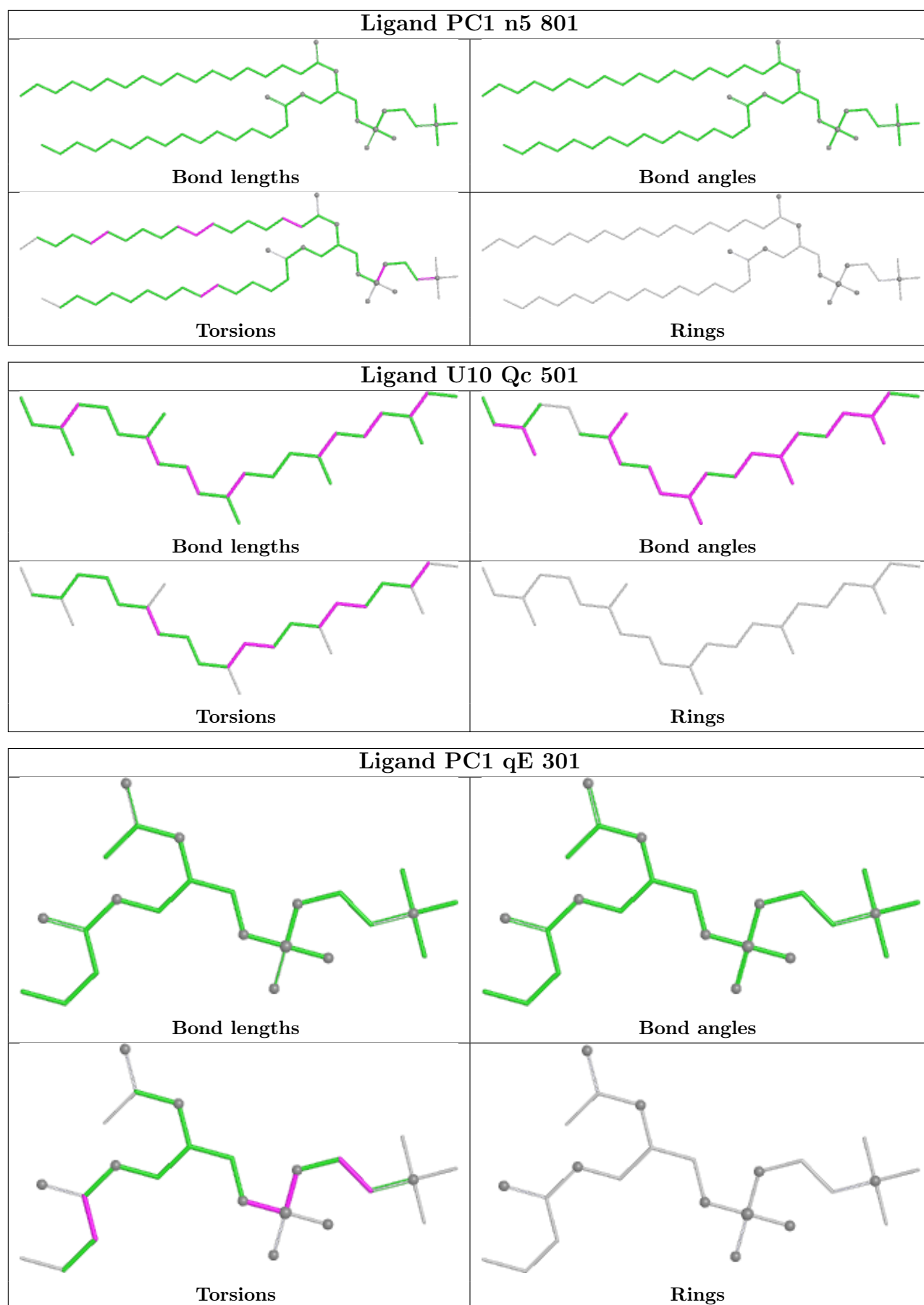


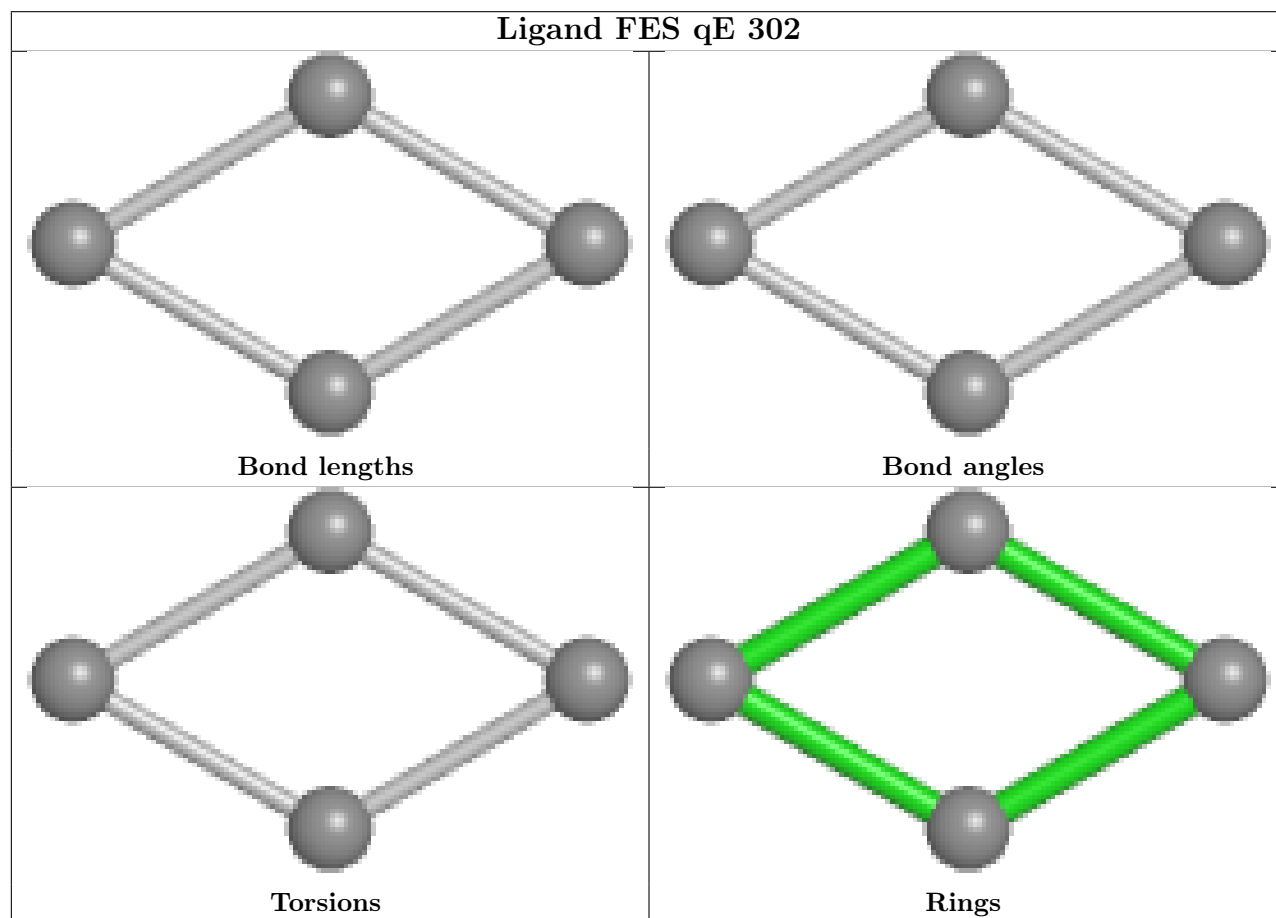
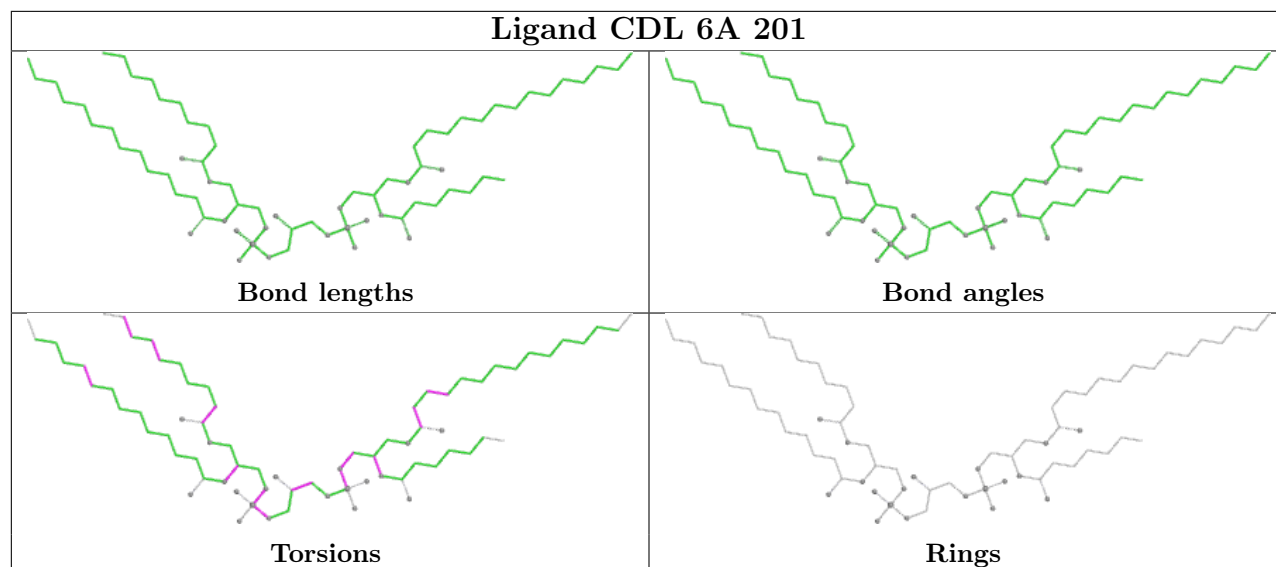


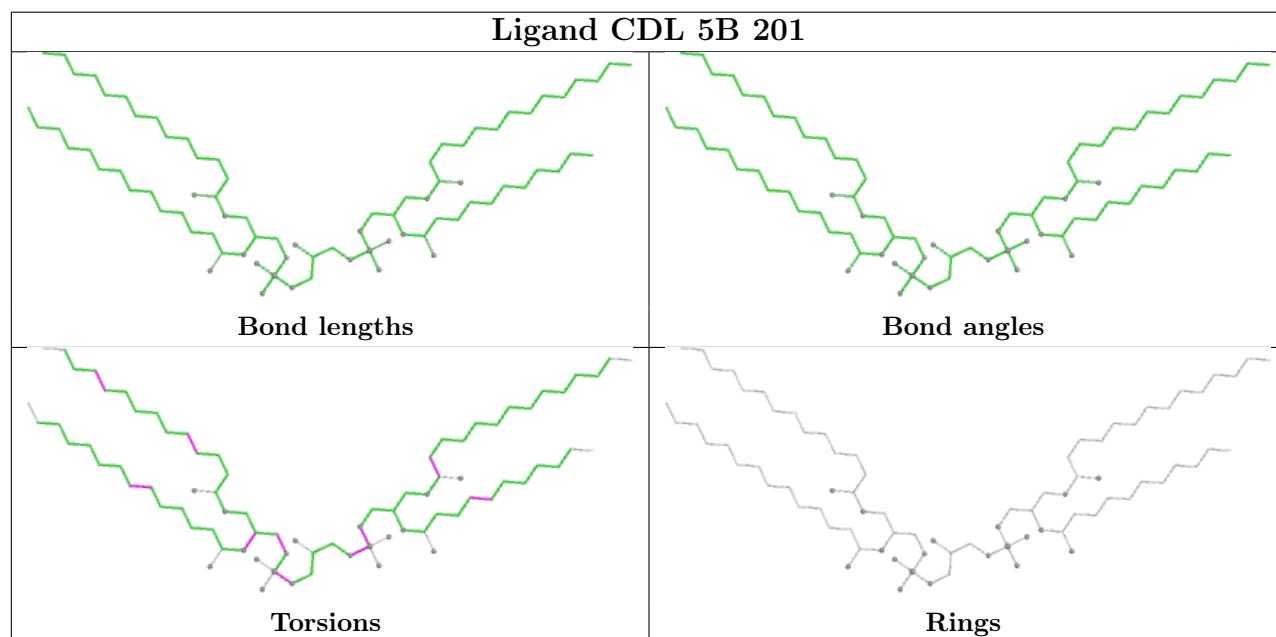
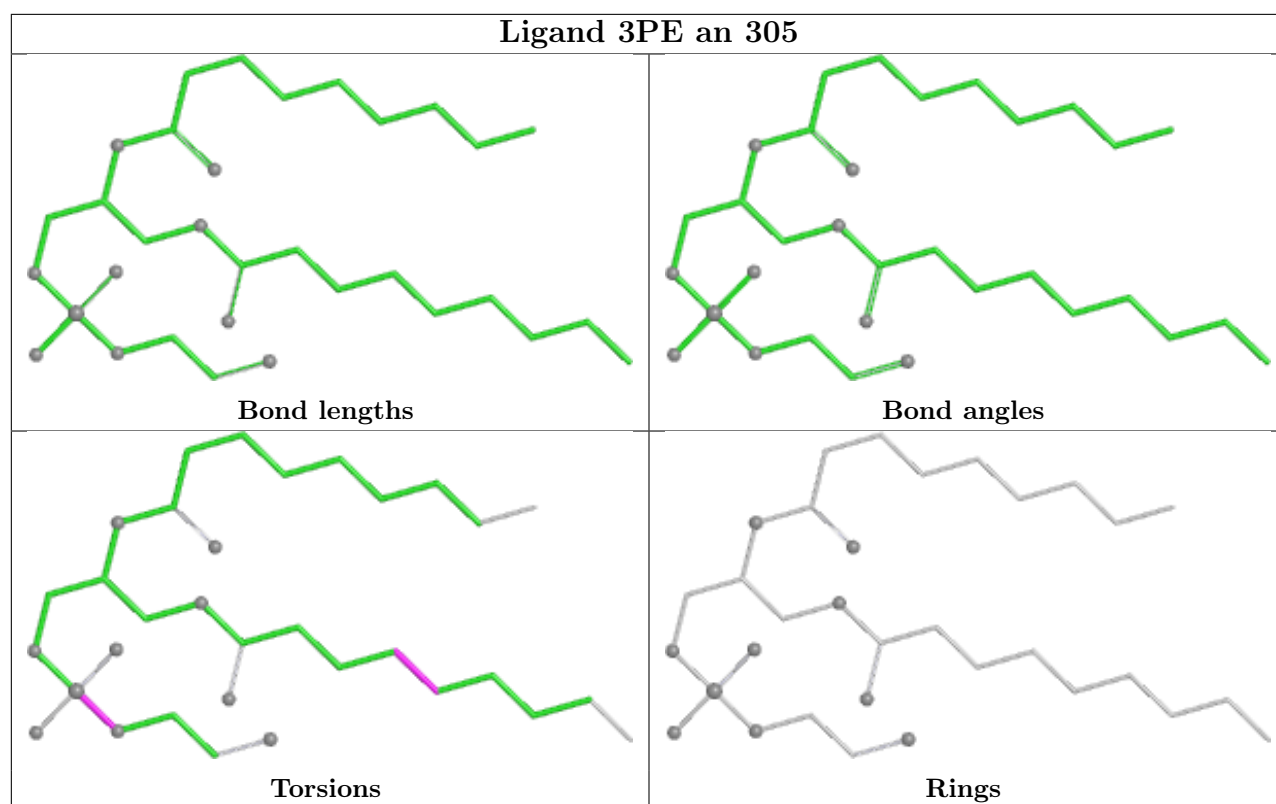


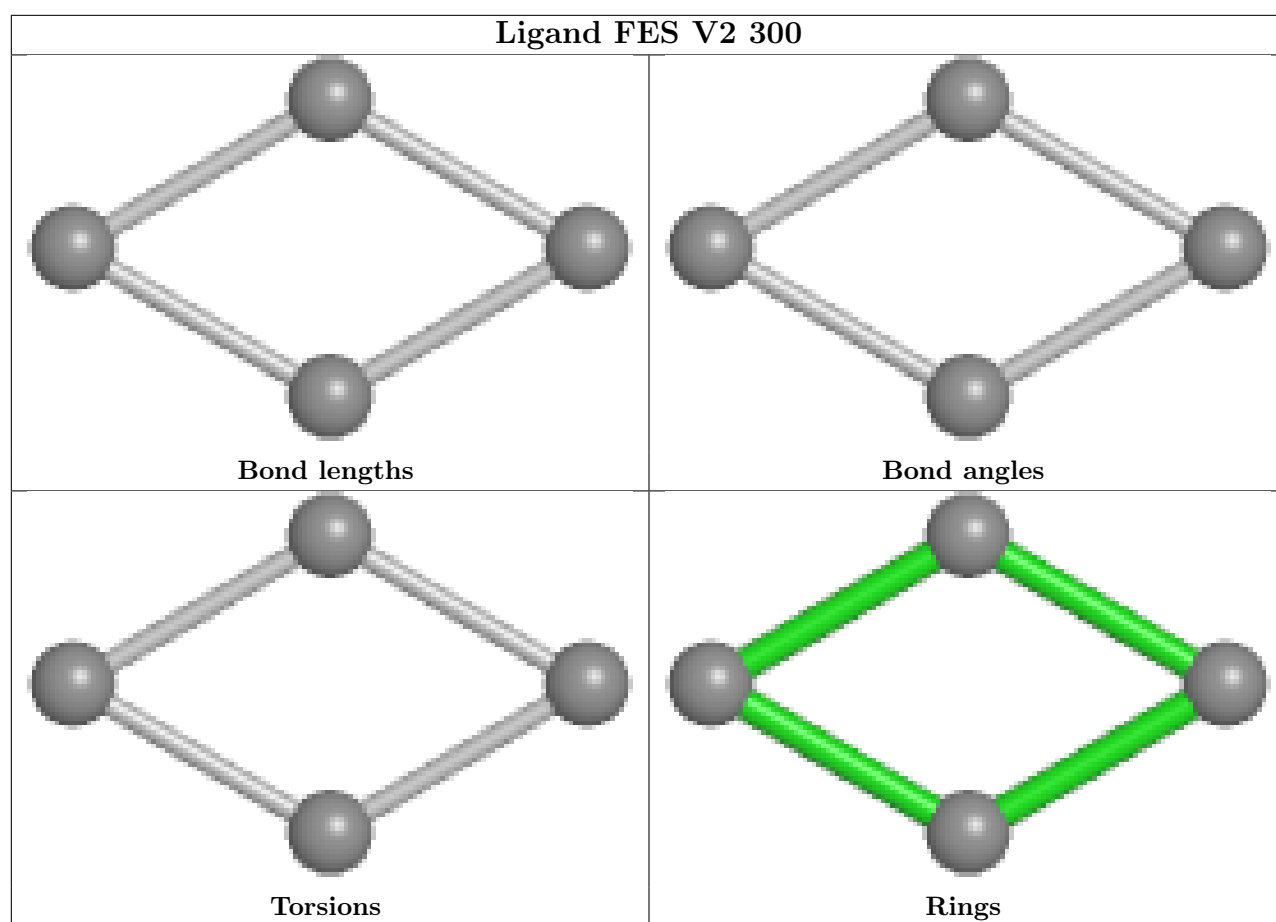
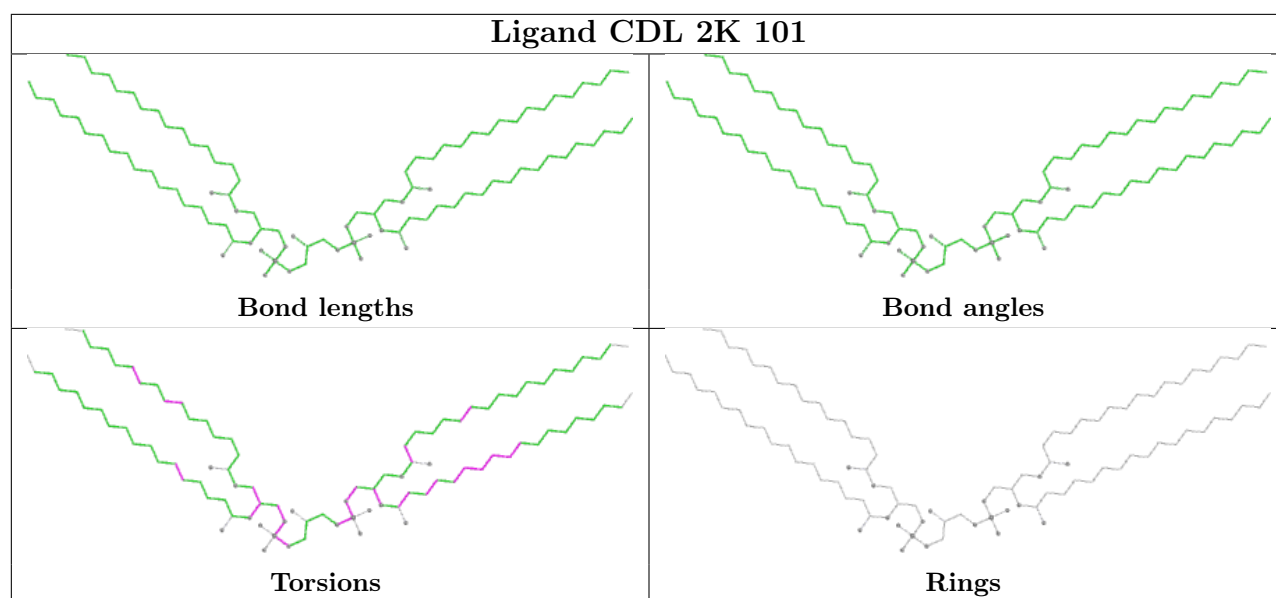


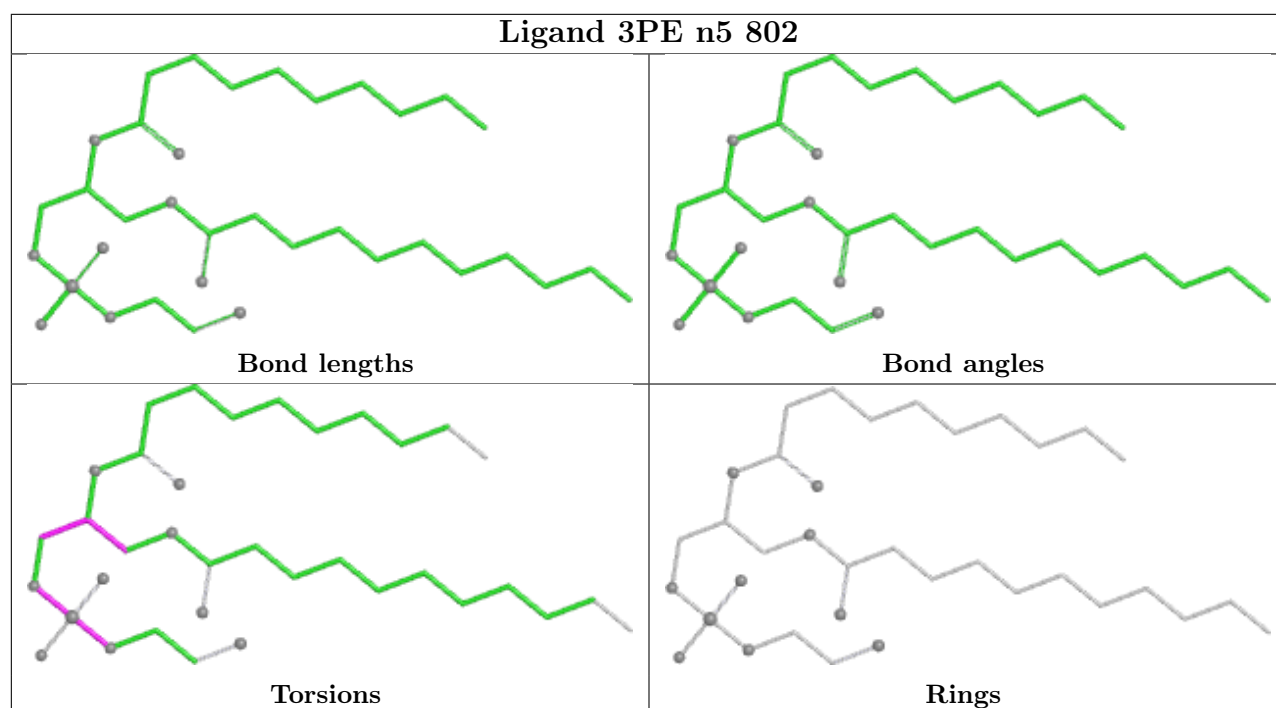
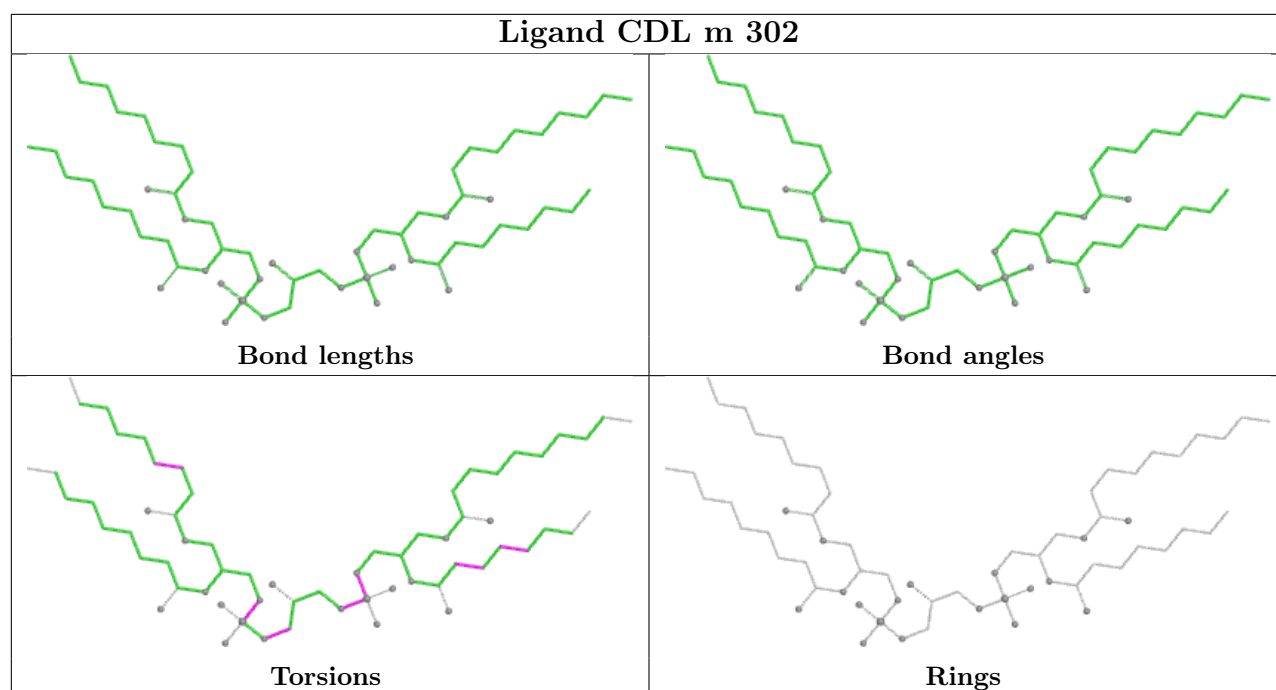
Ligand PC1 TC 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CDL 7a 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 C3 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

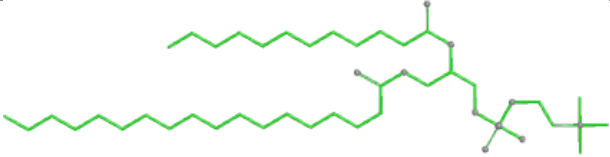
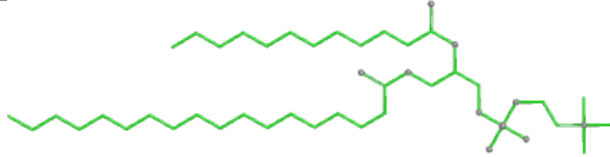
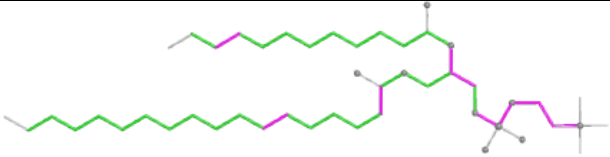
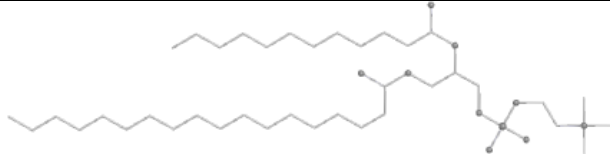
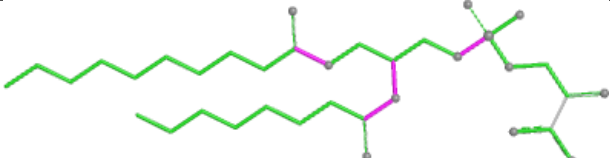
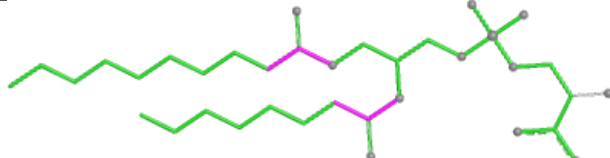
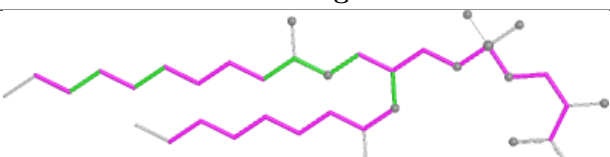
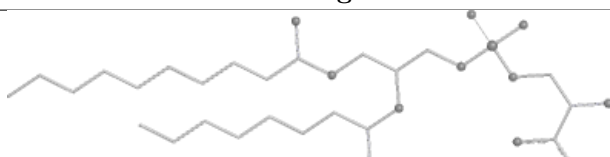
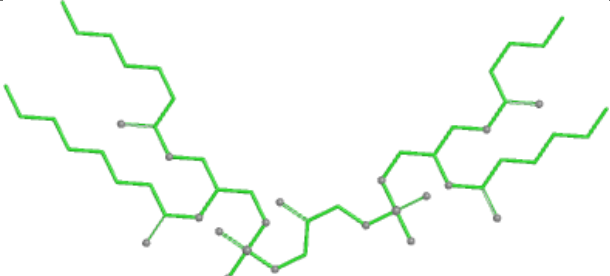
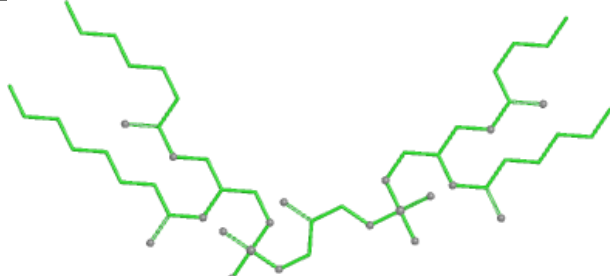
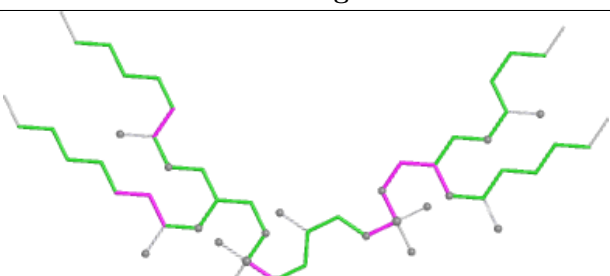
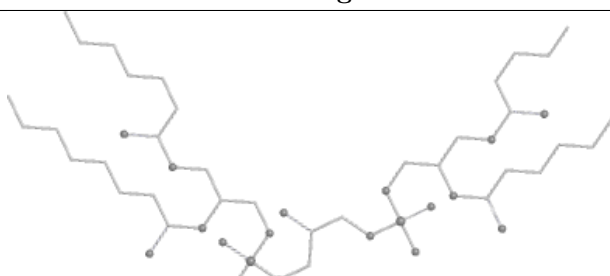


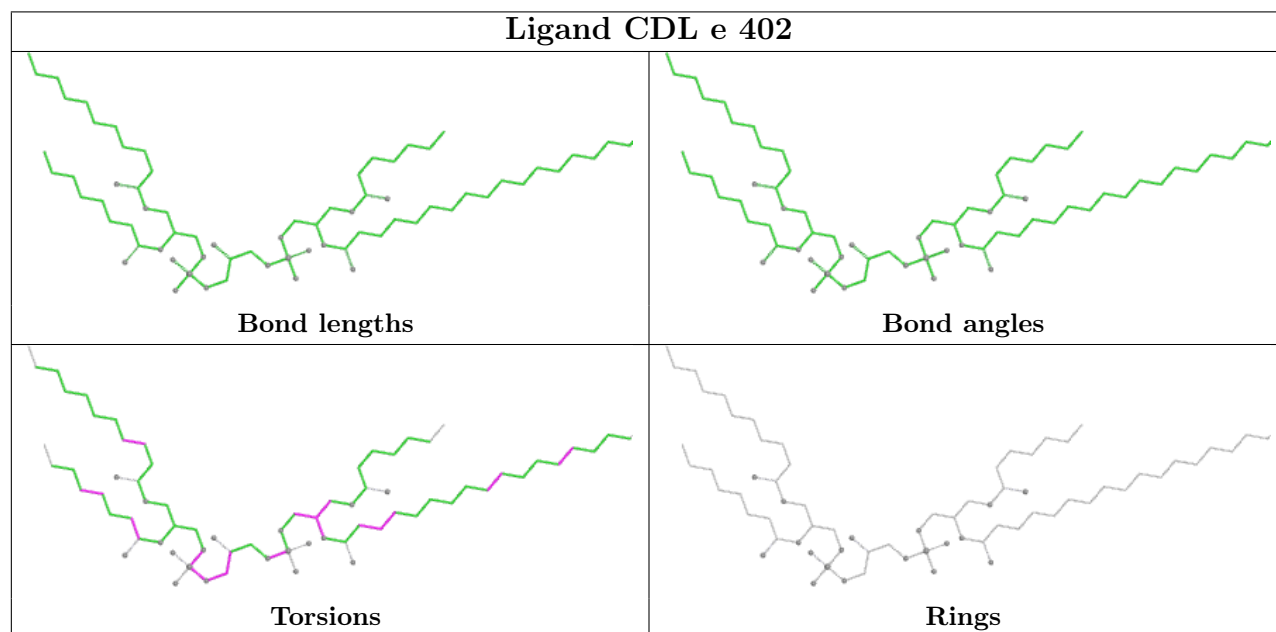
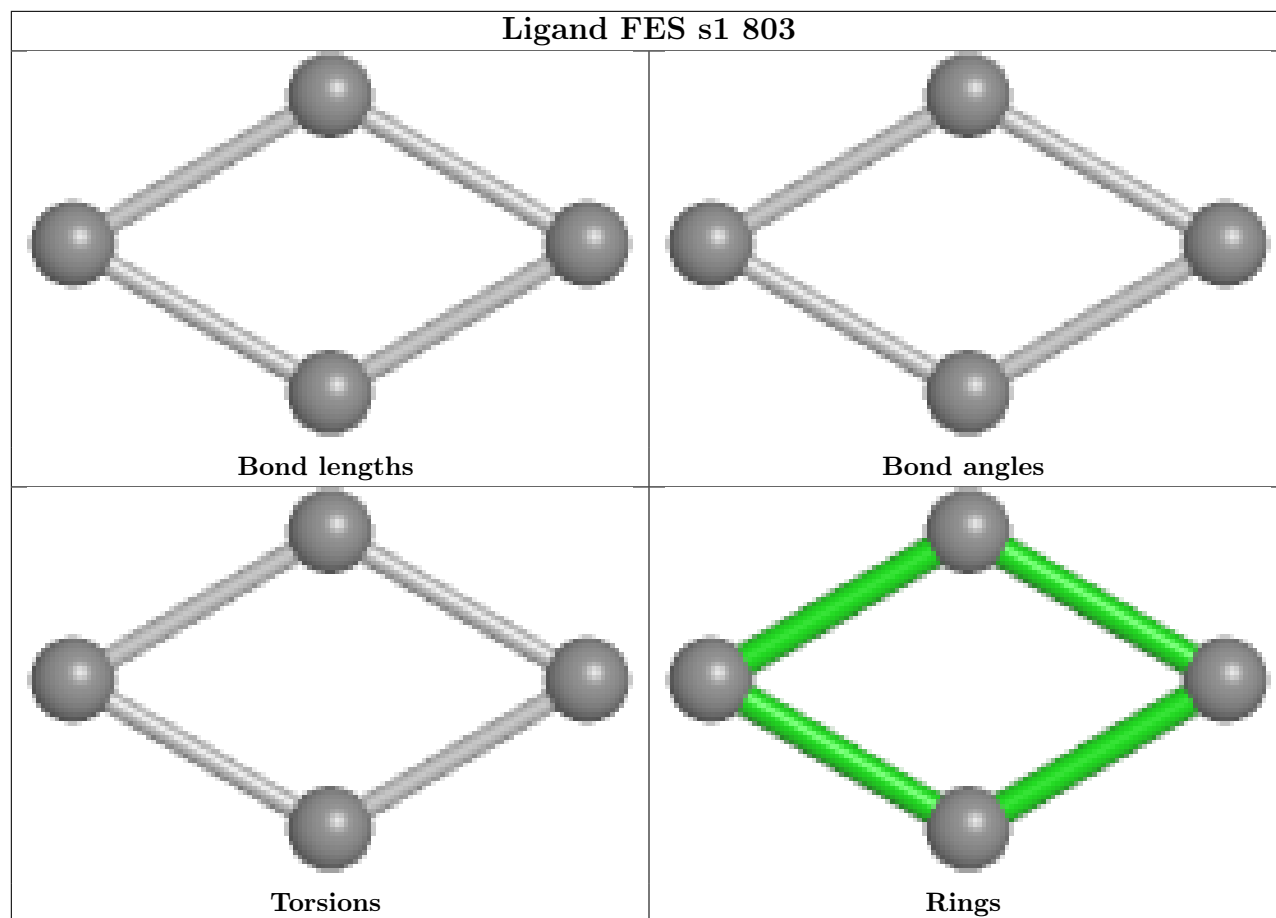


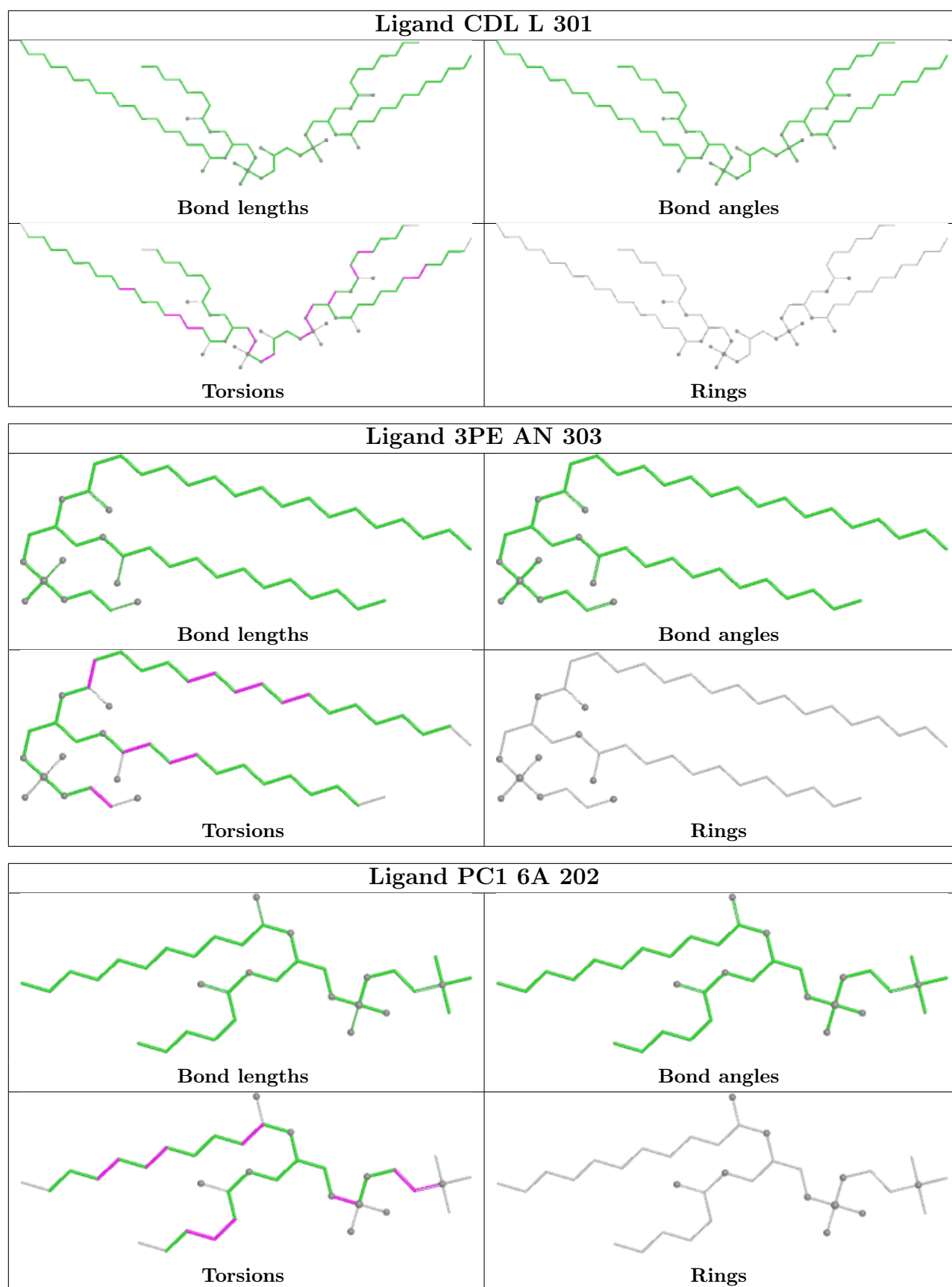


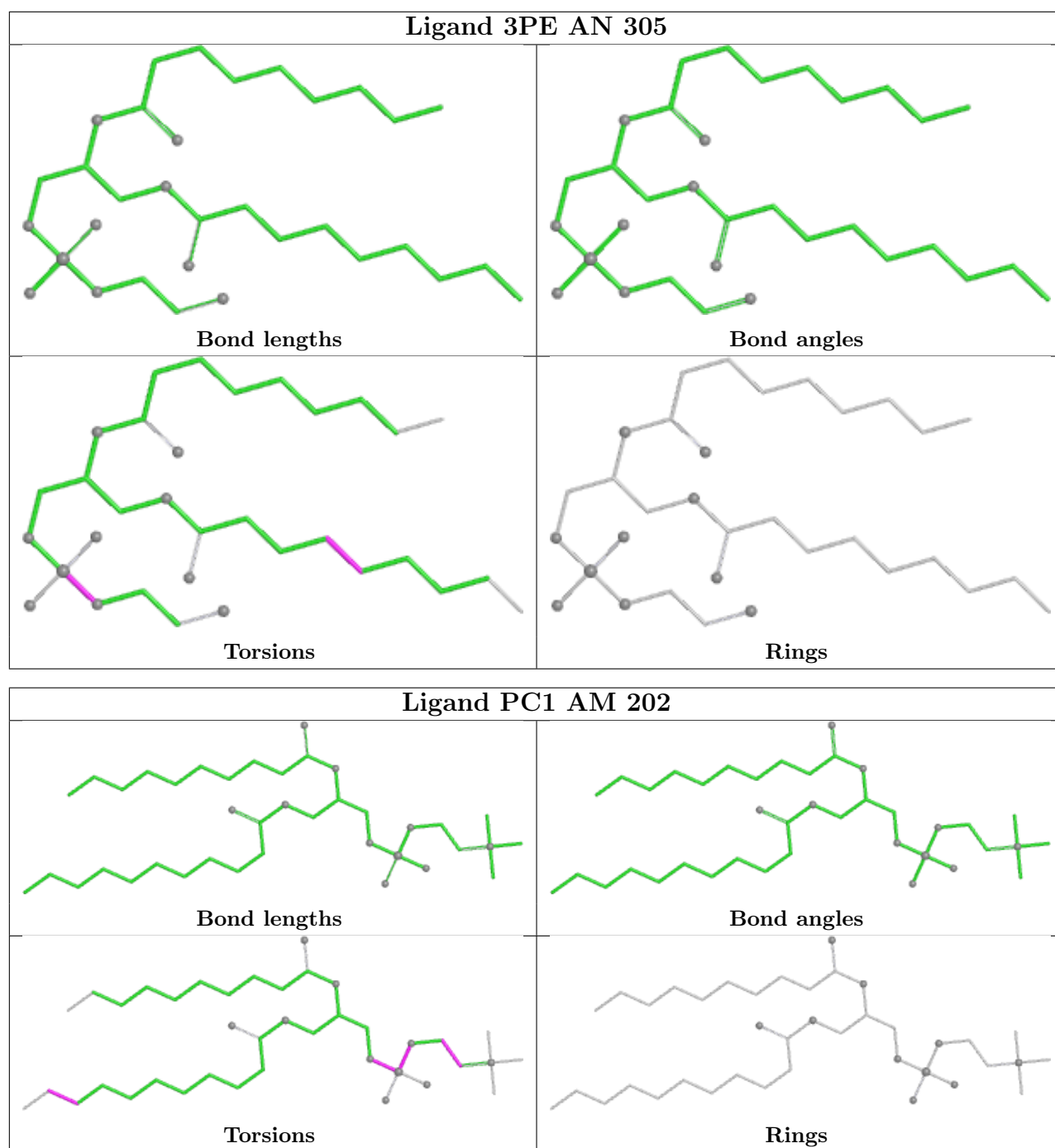


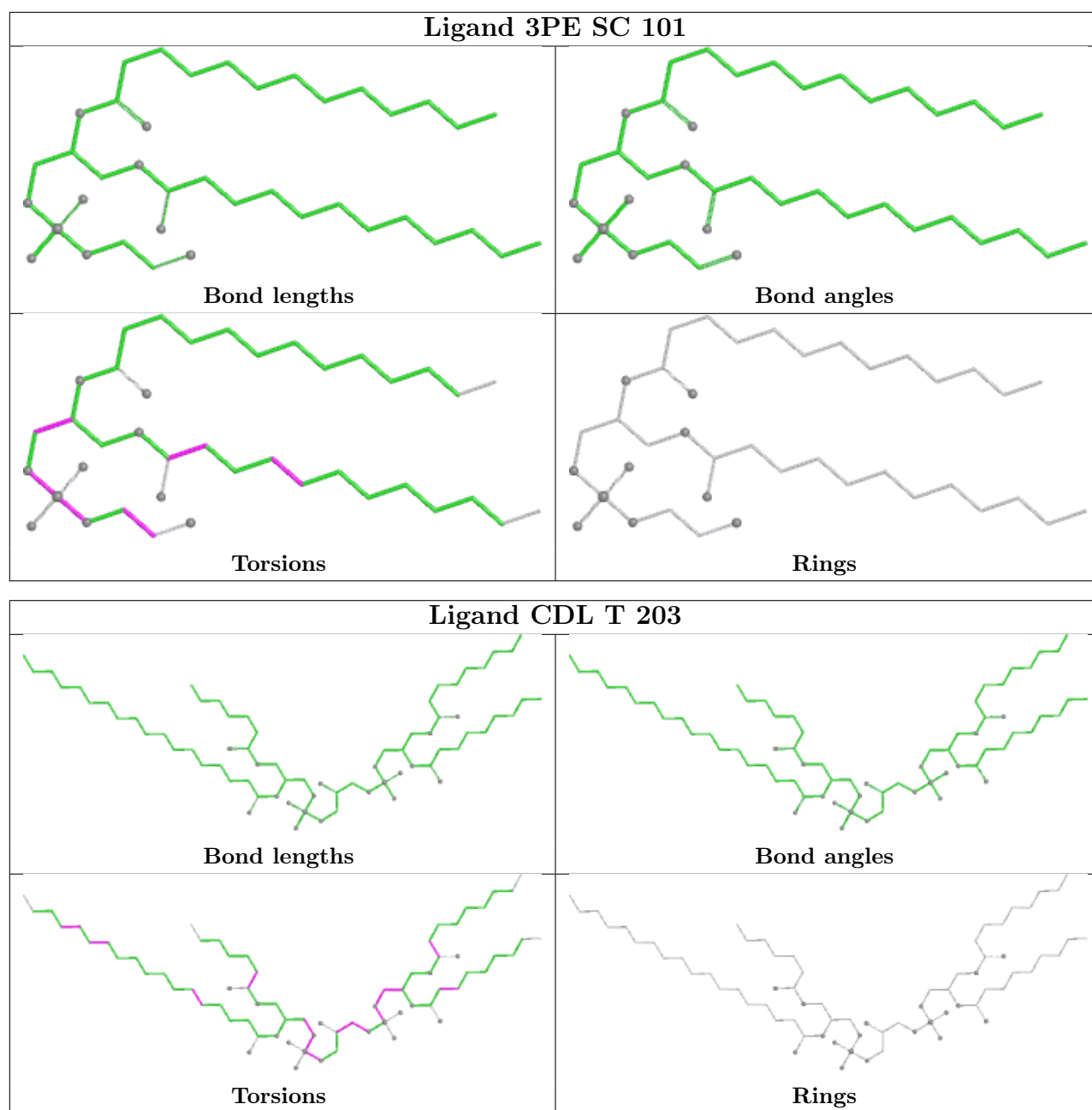


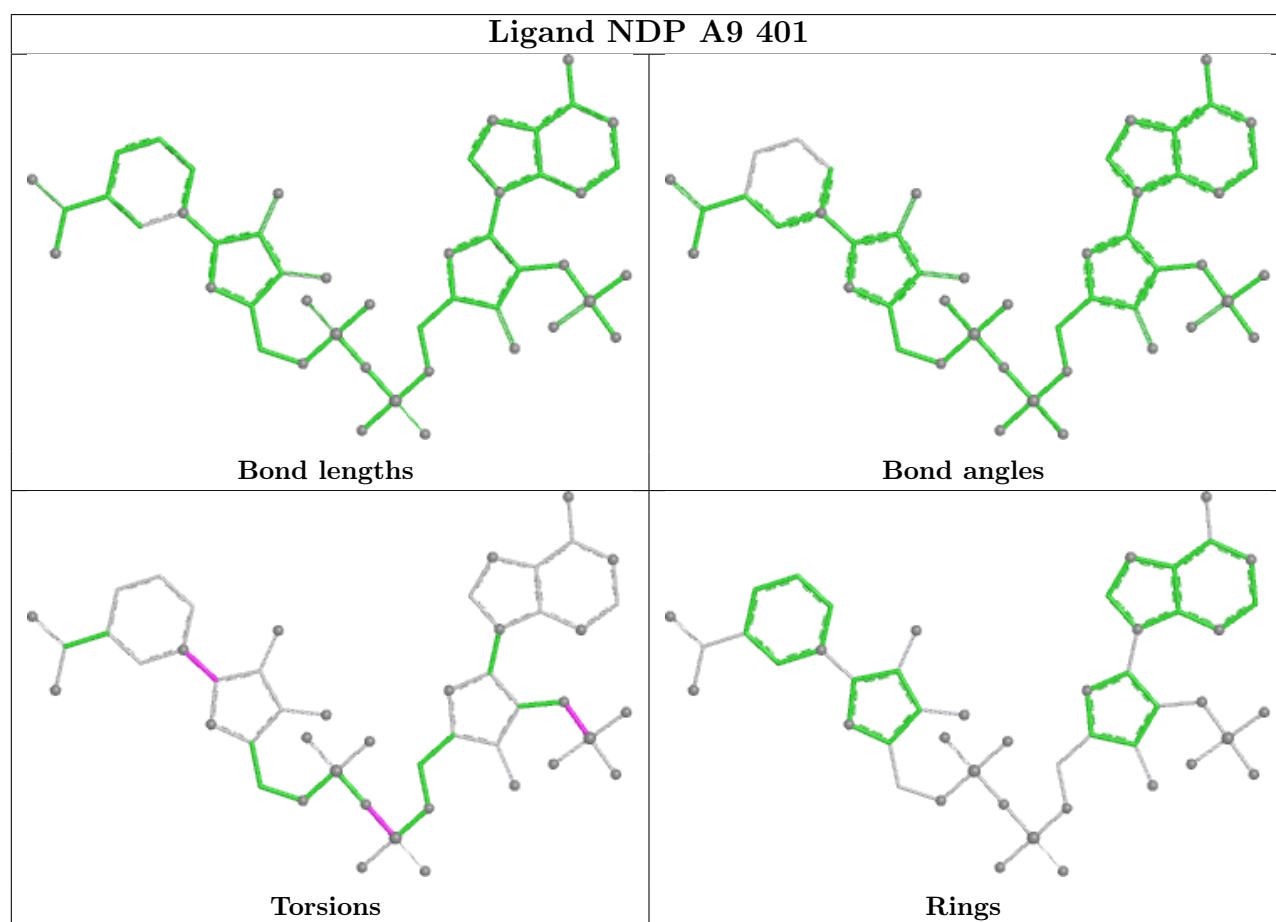
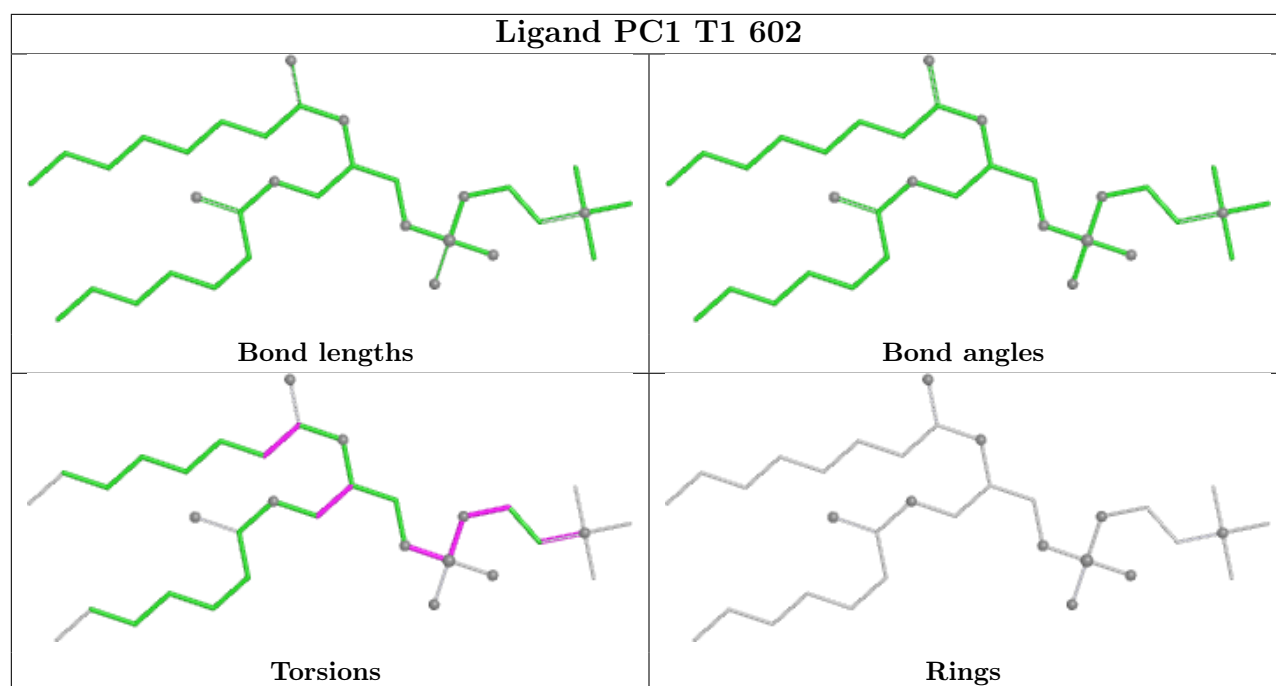
Ligand PC1 t4 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand P5S M2 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CDL m2 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

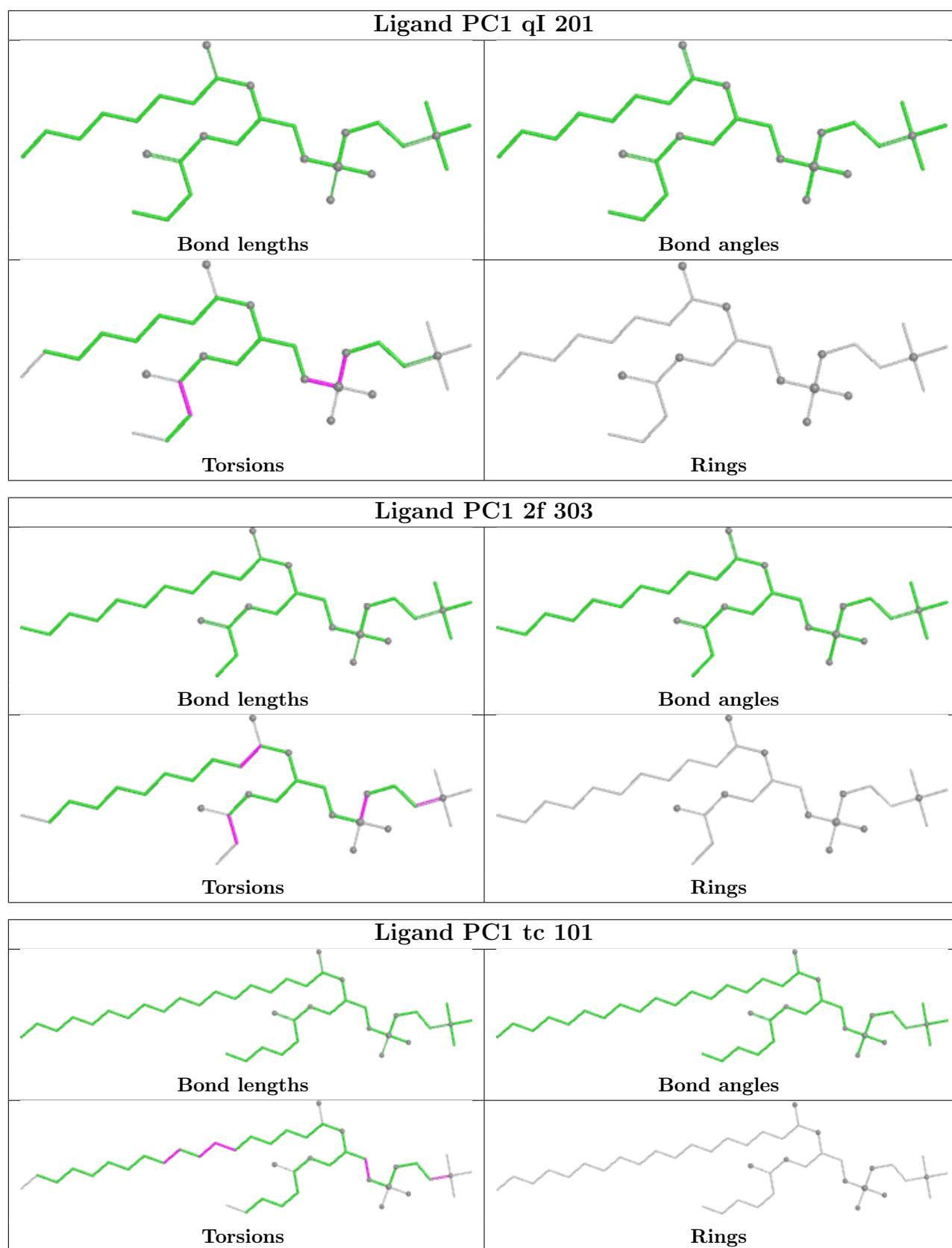


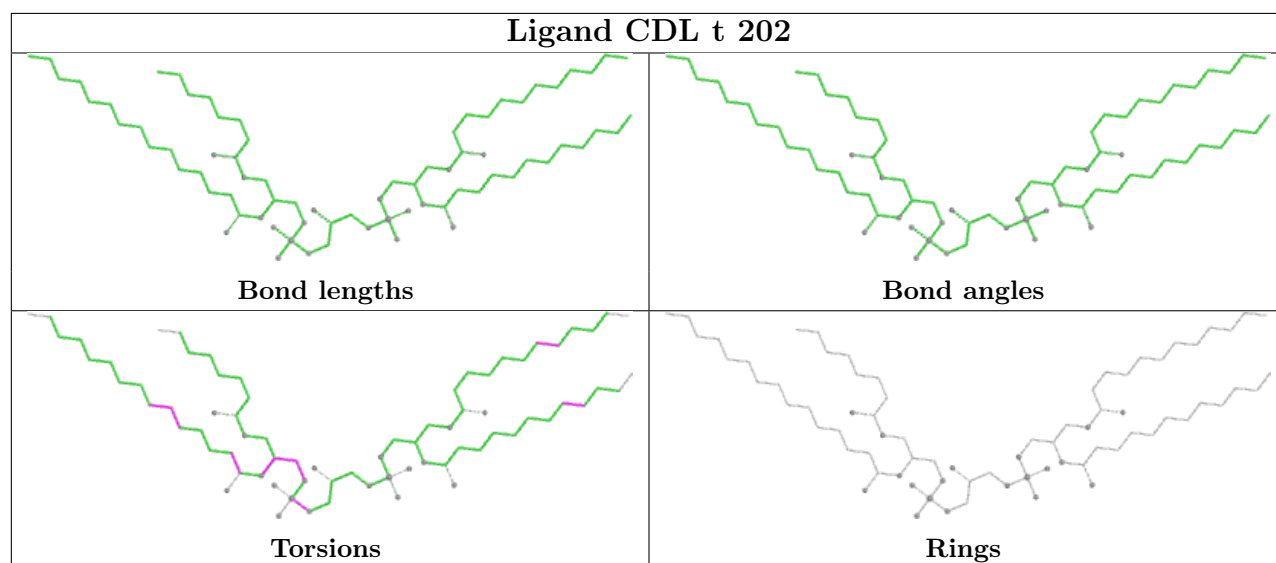
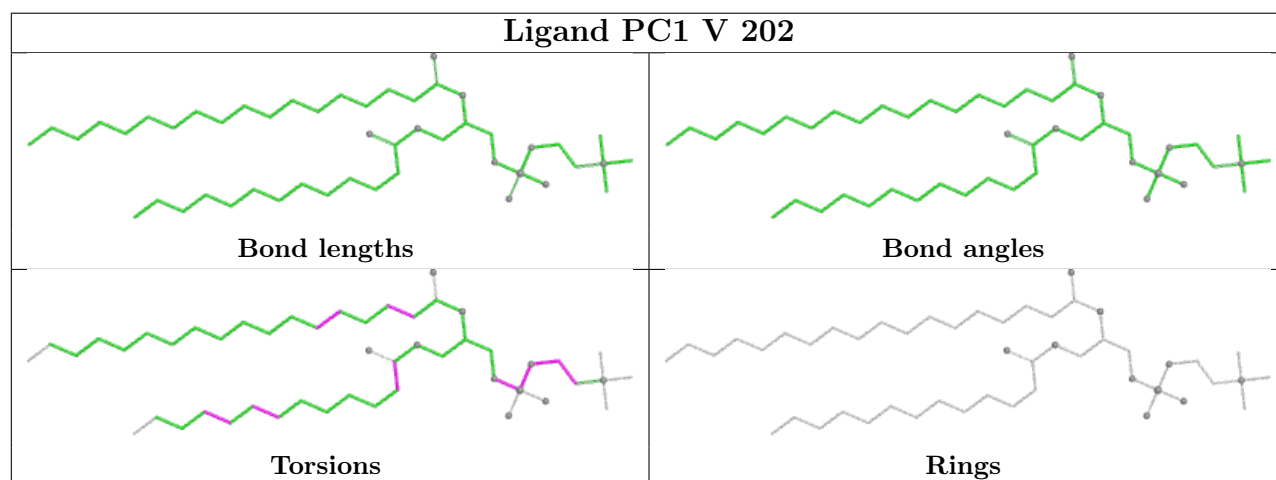
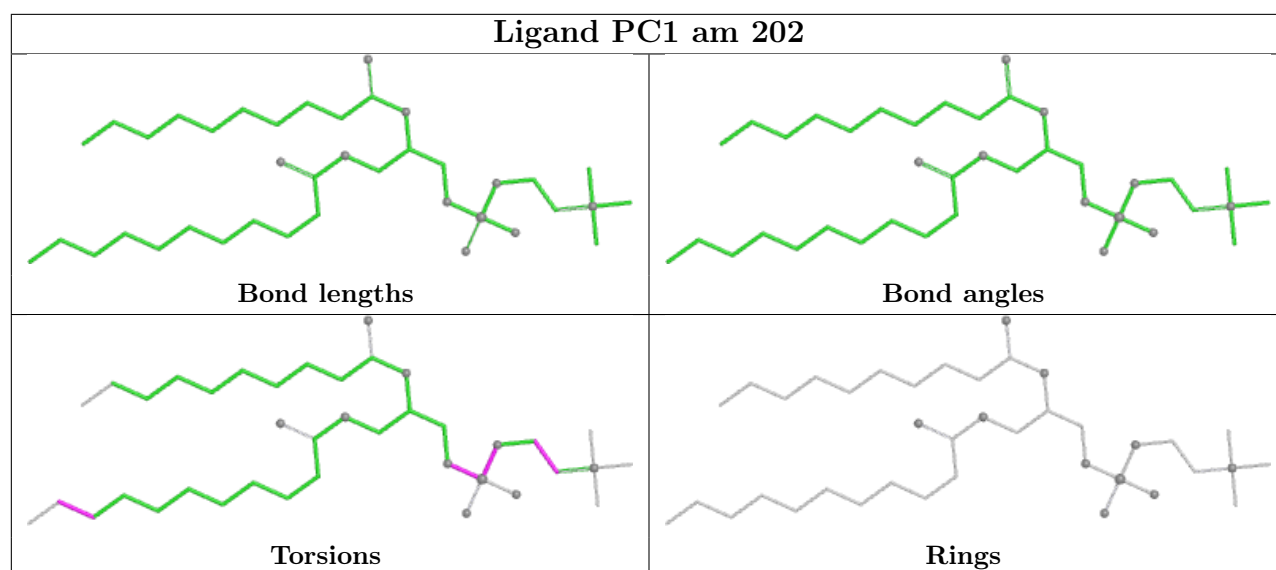


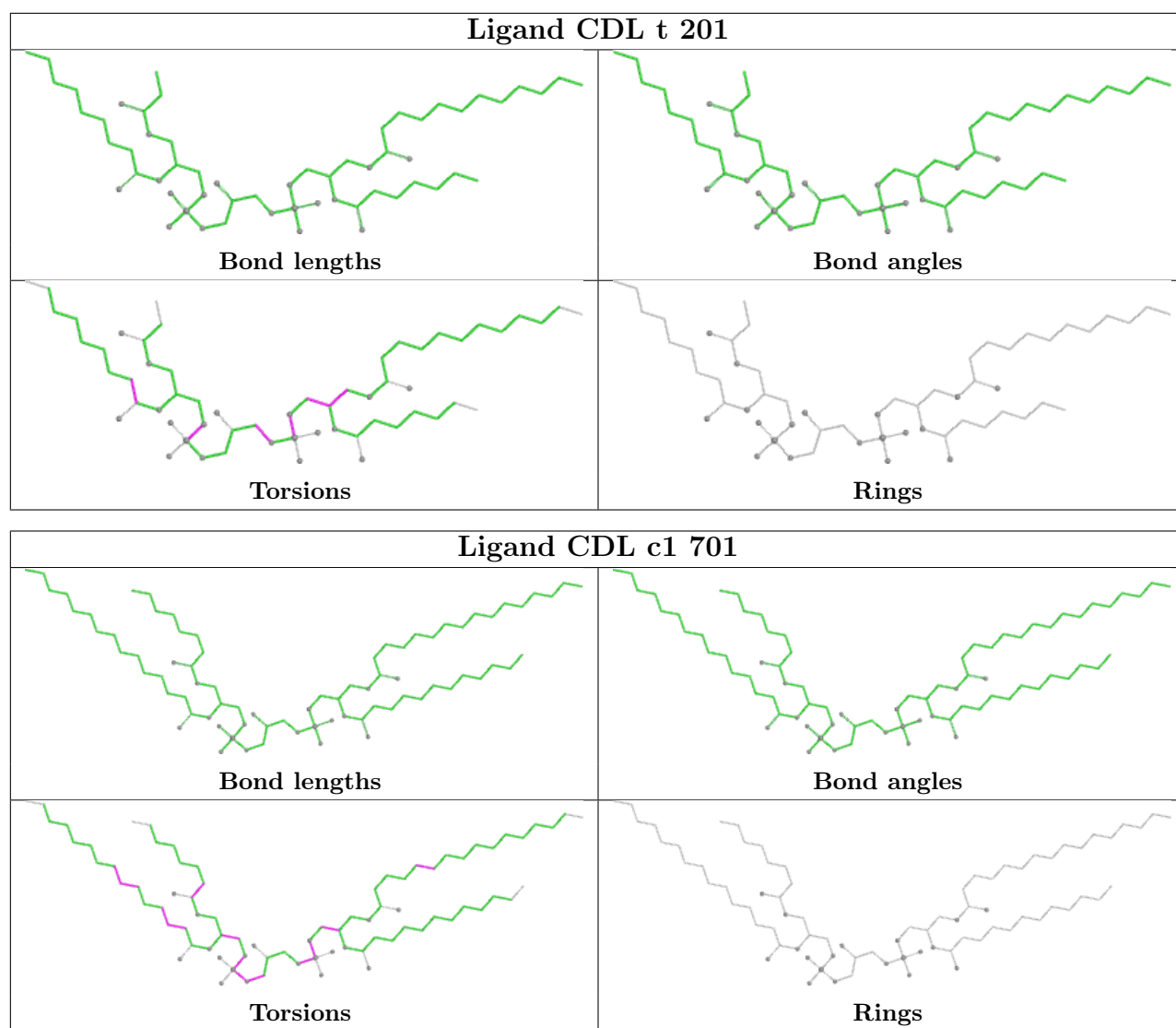




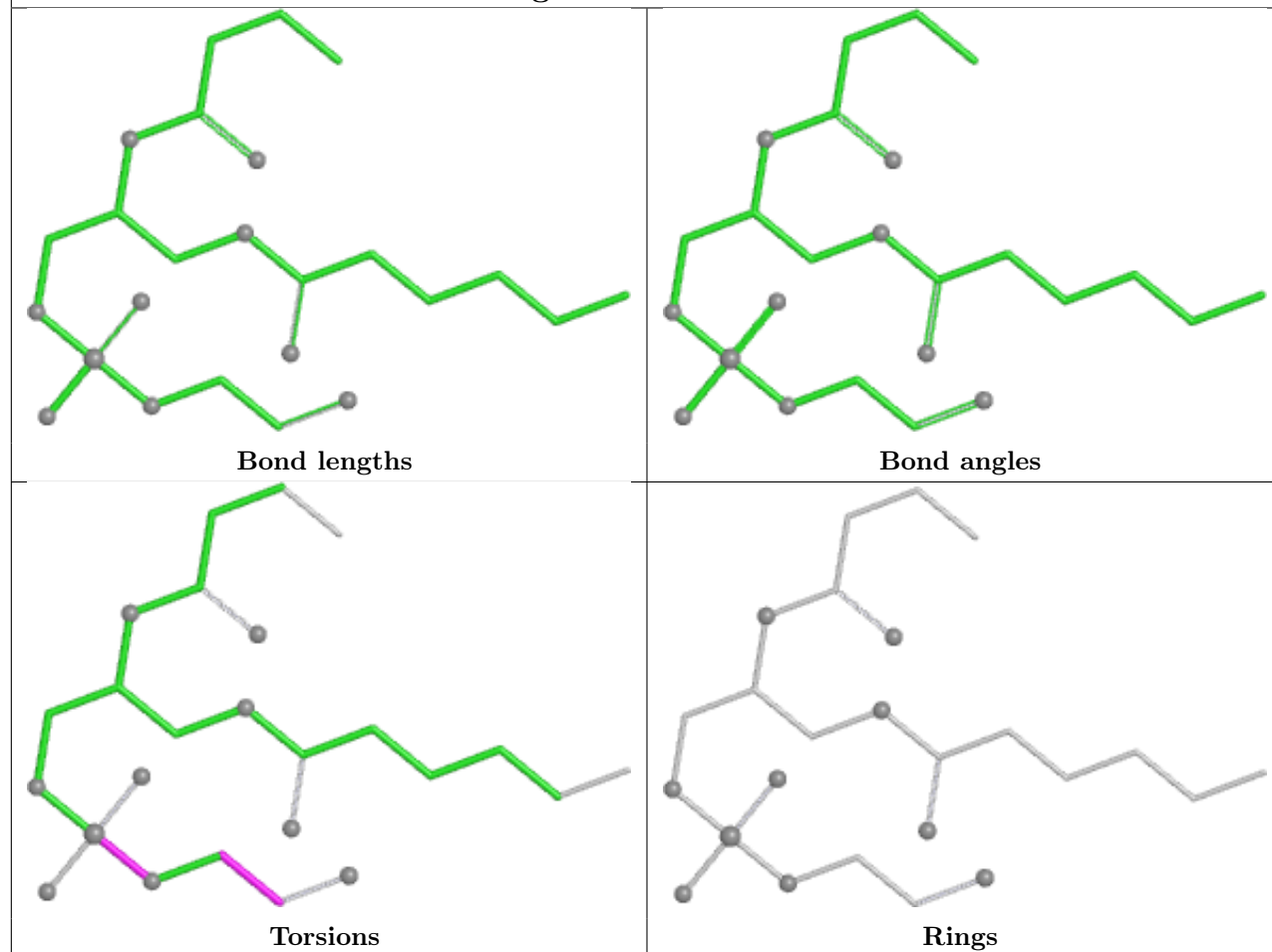




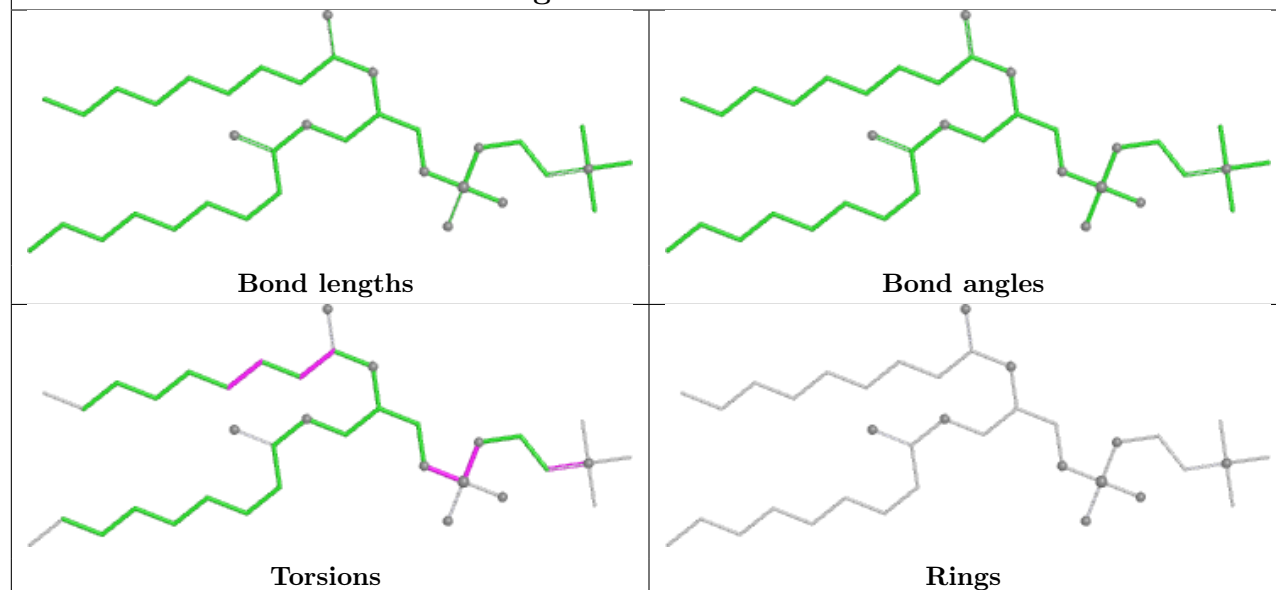


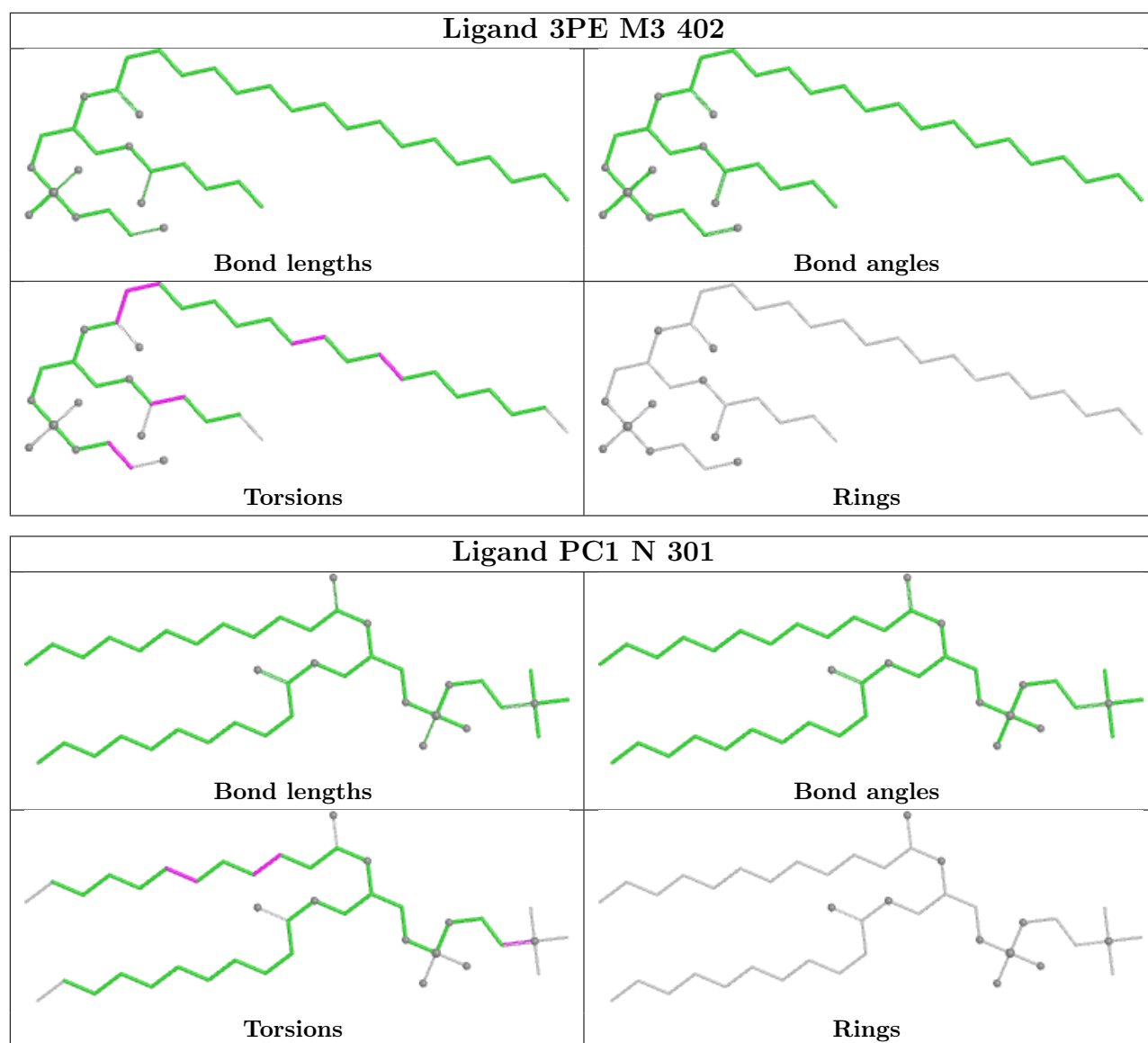


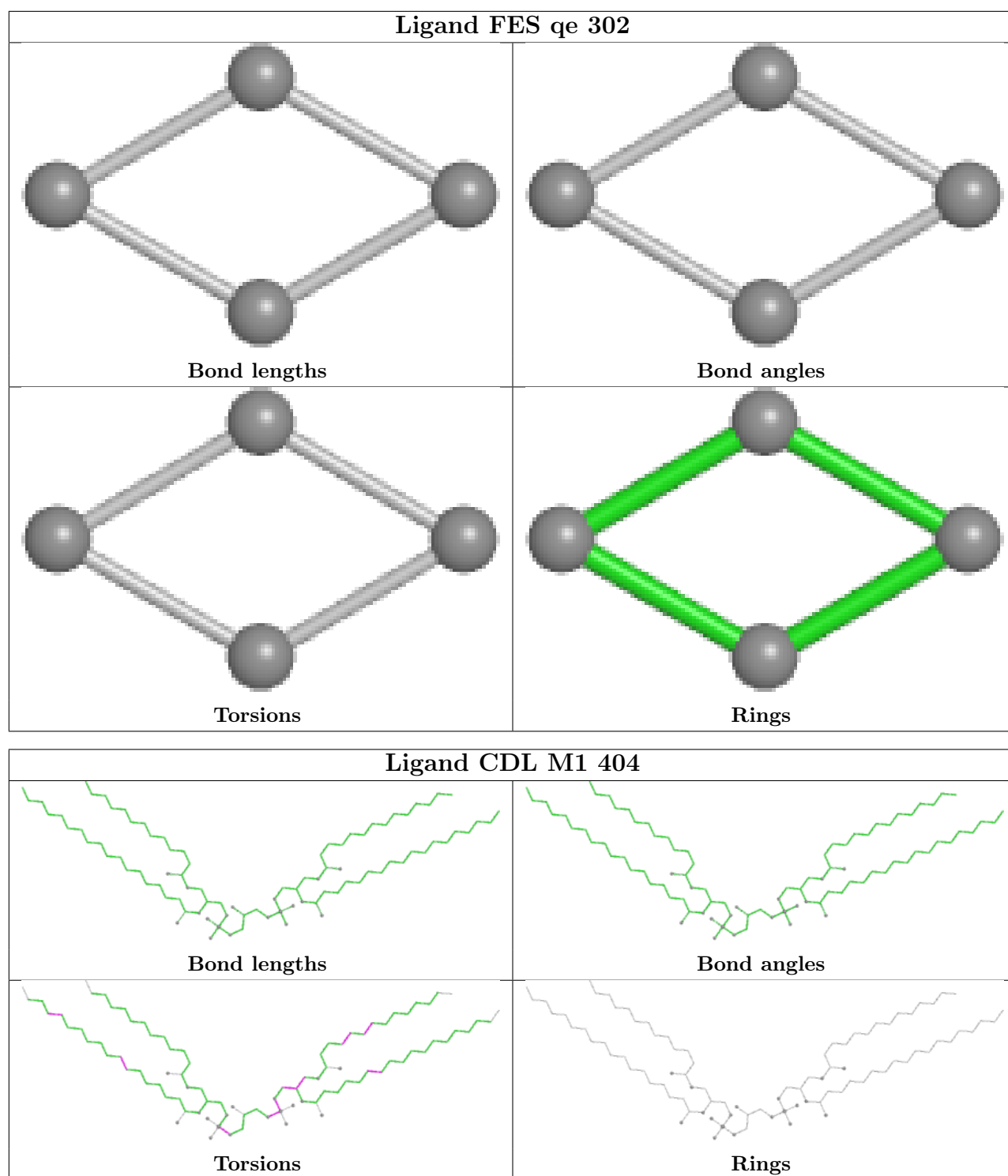
Ligand 3PE t4 302

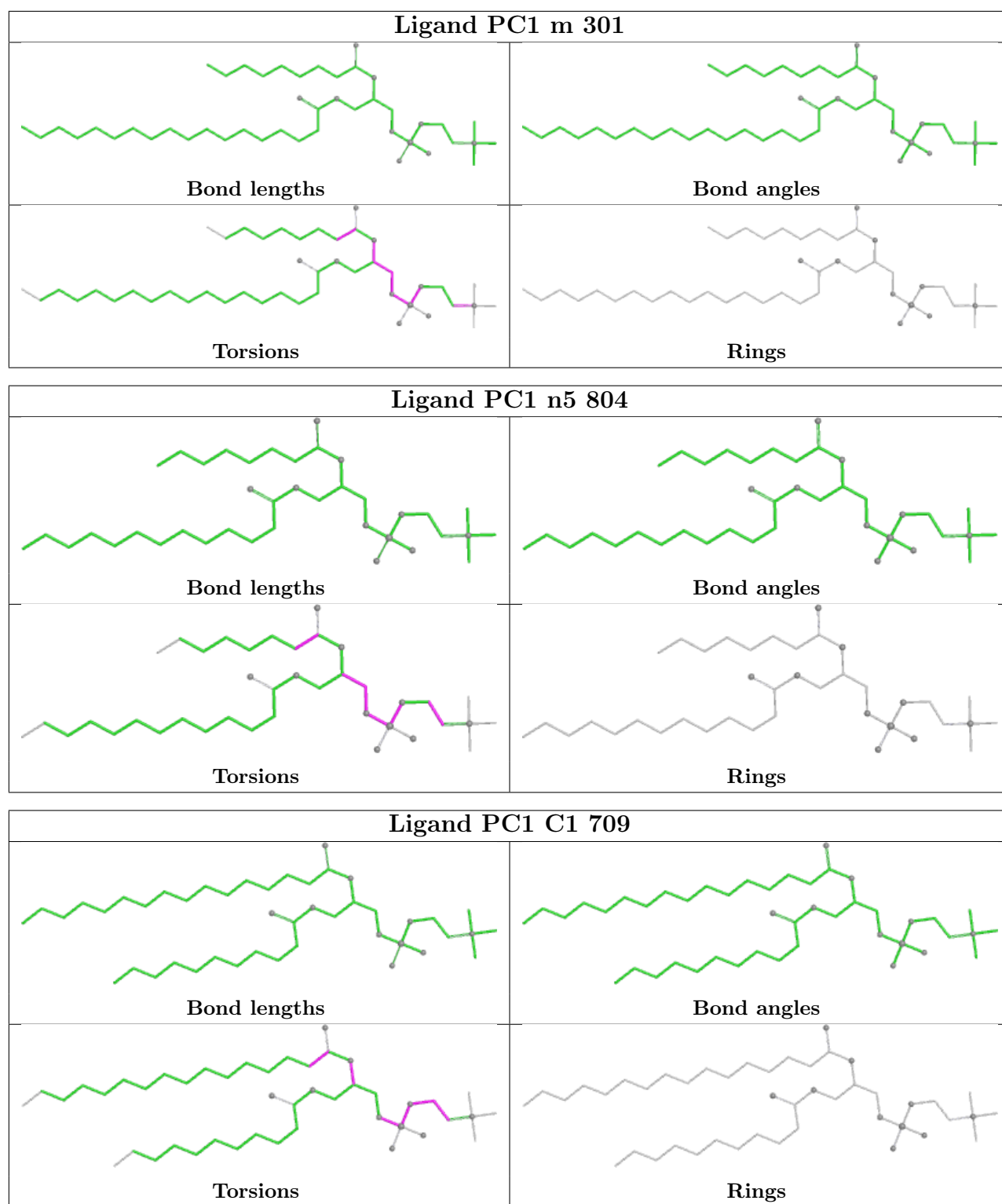


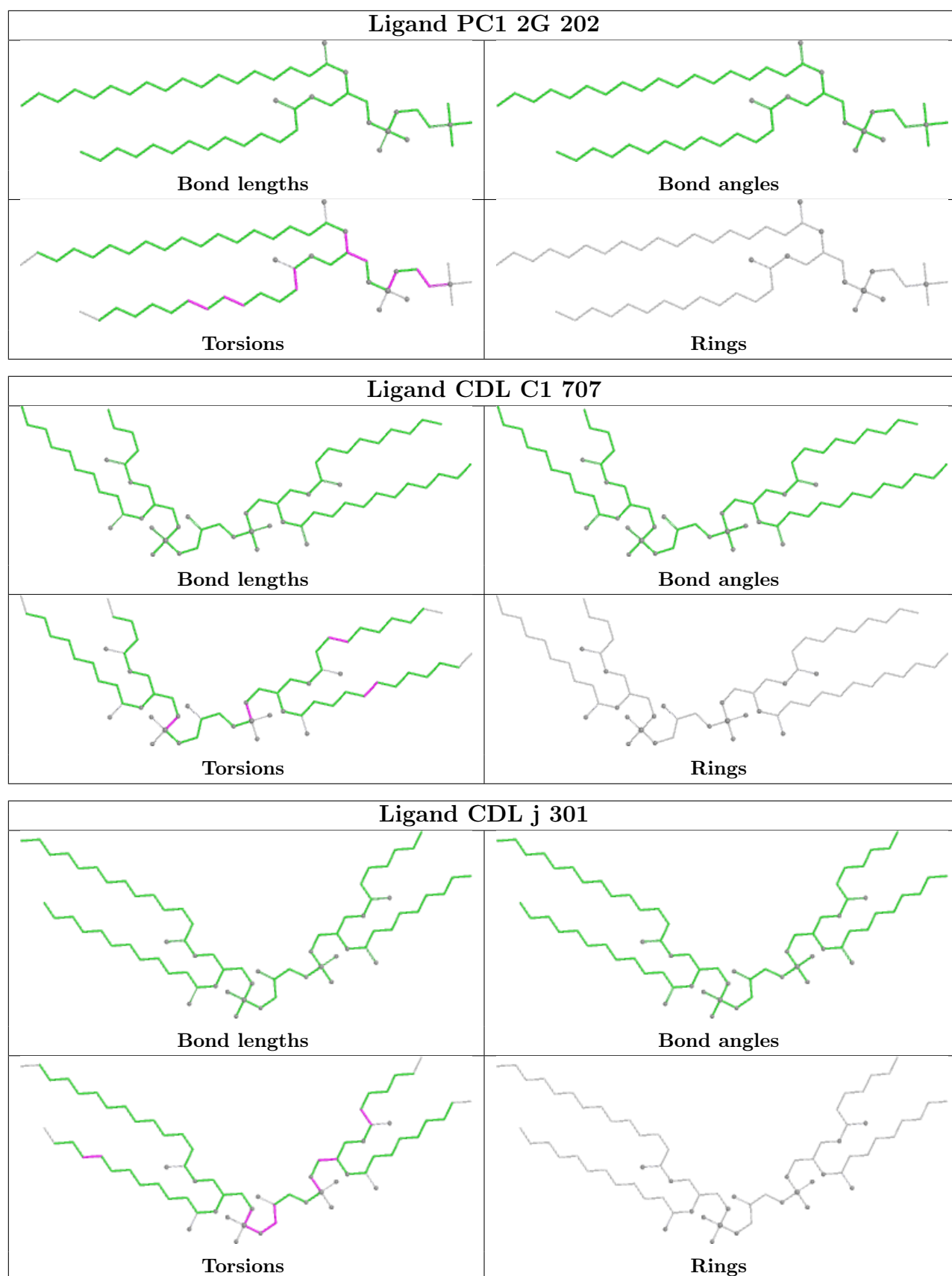
Ligand PC1 m 307

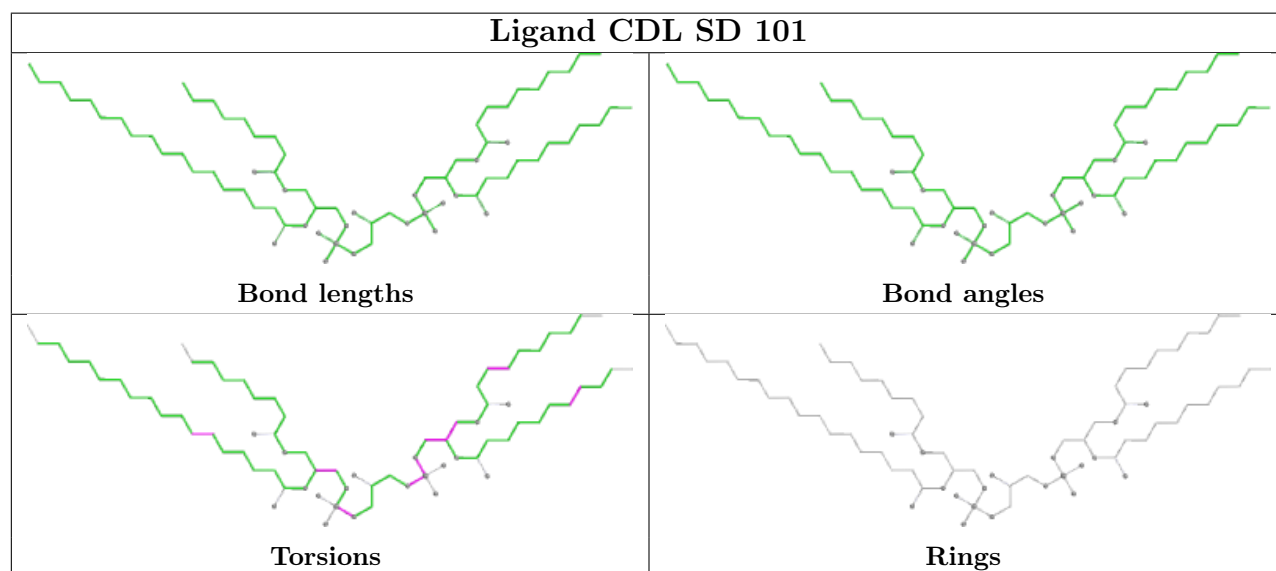
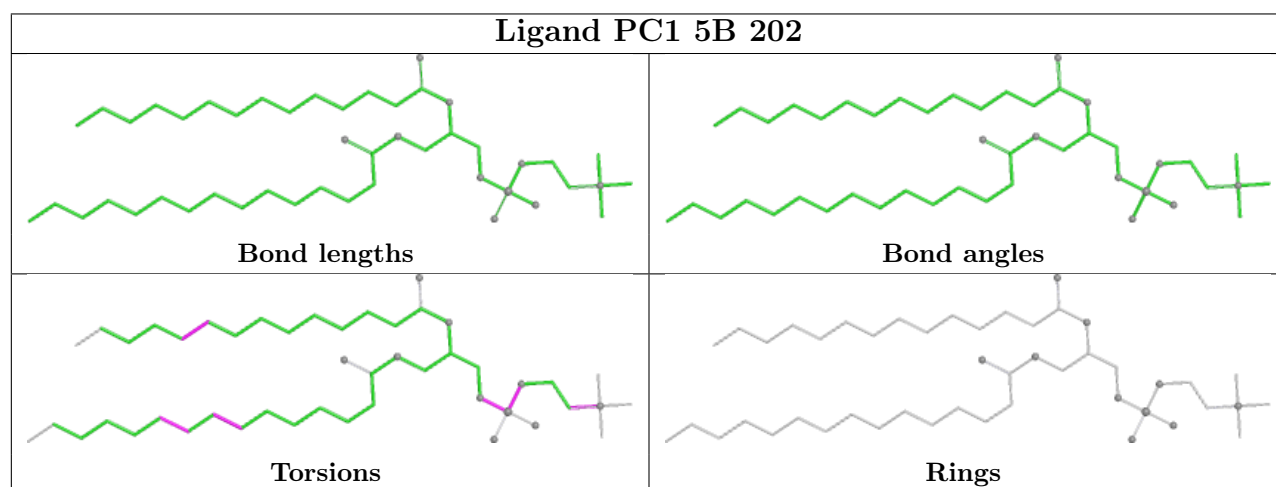
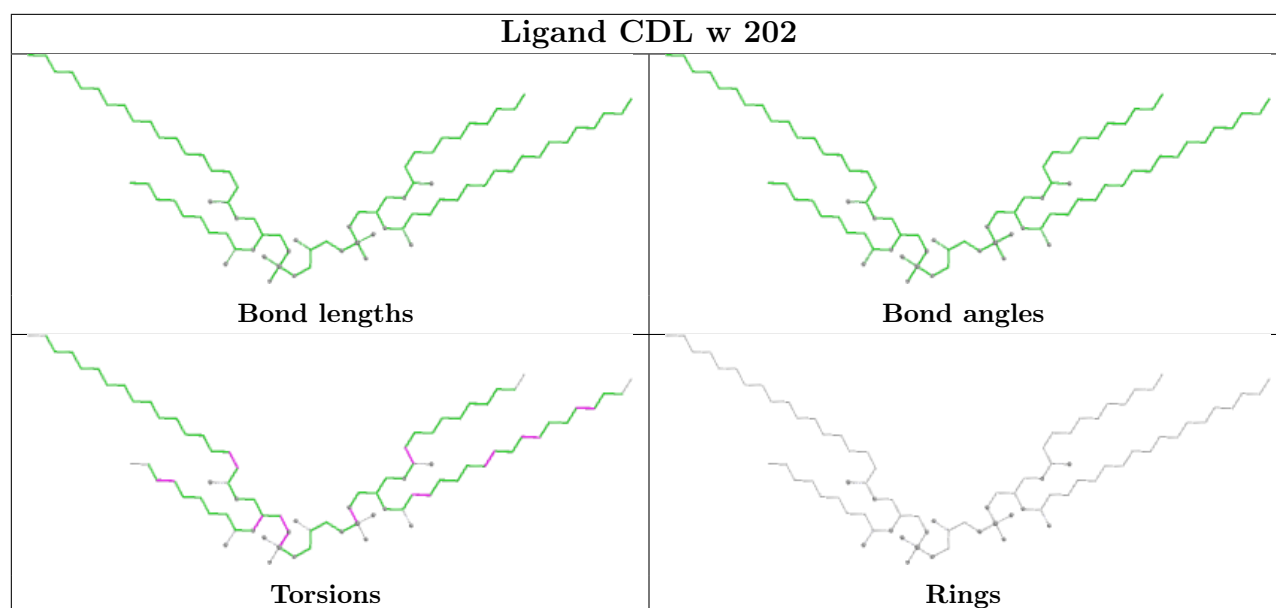


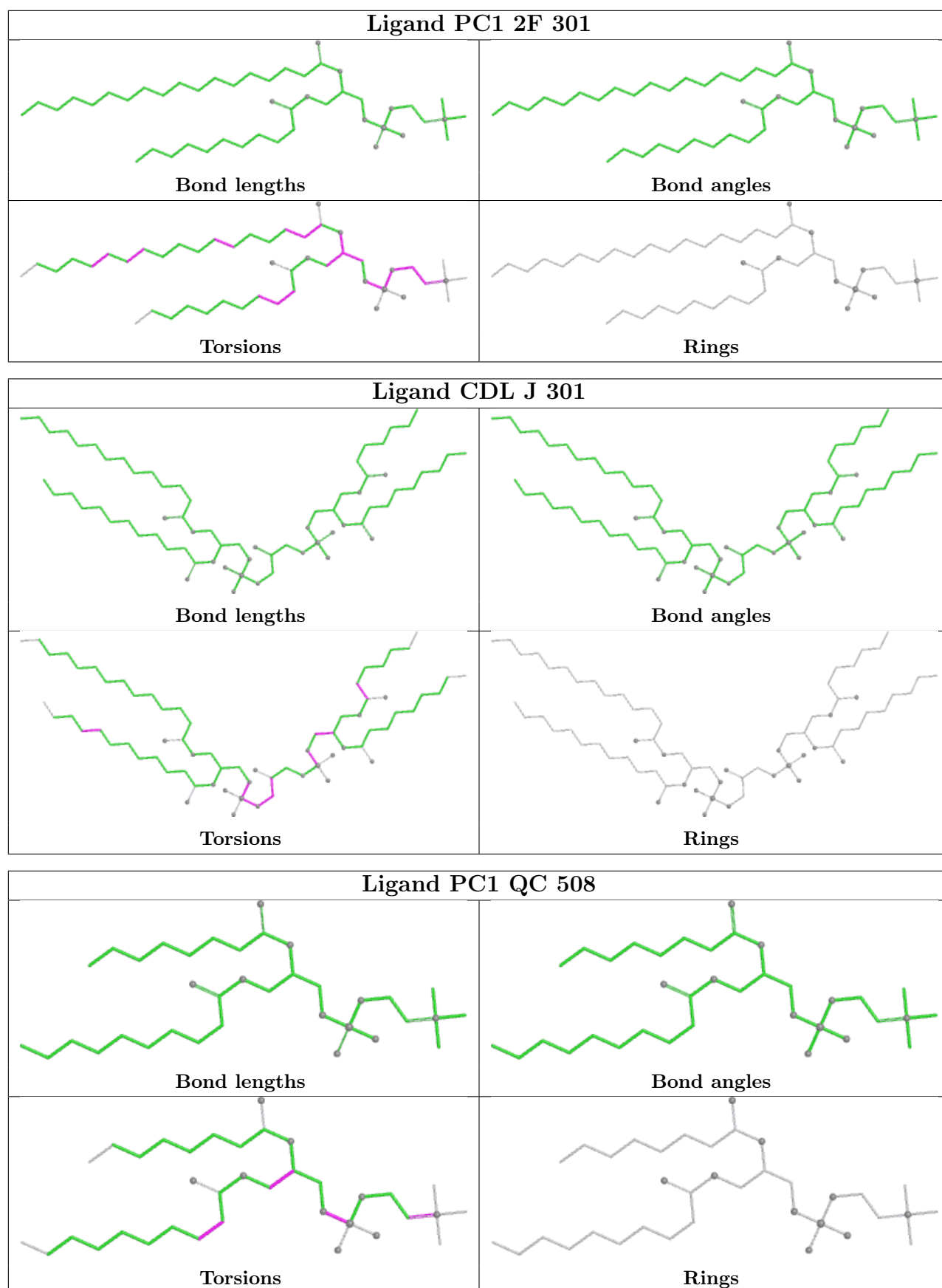


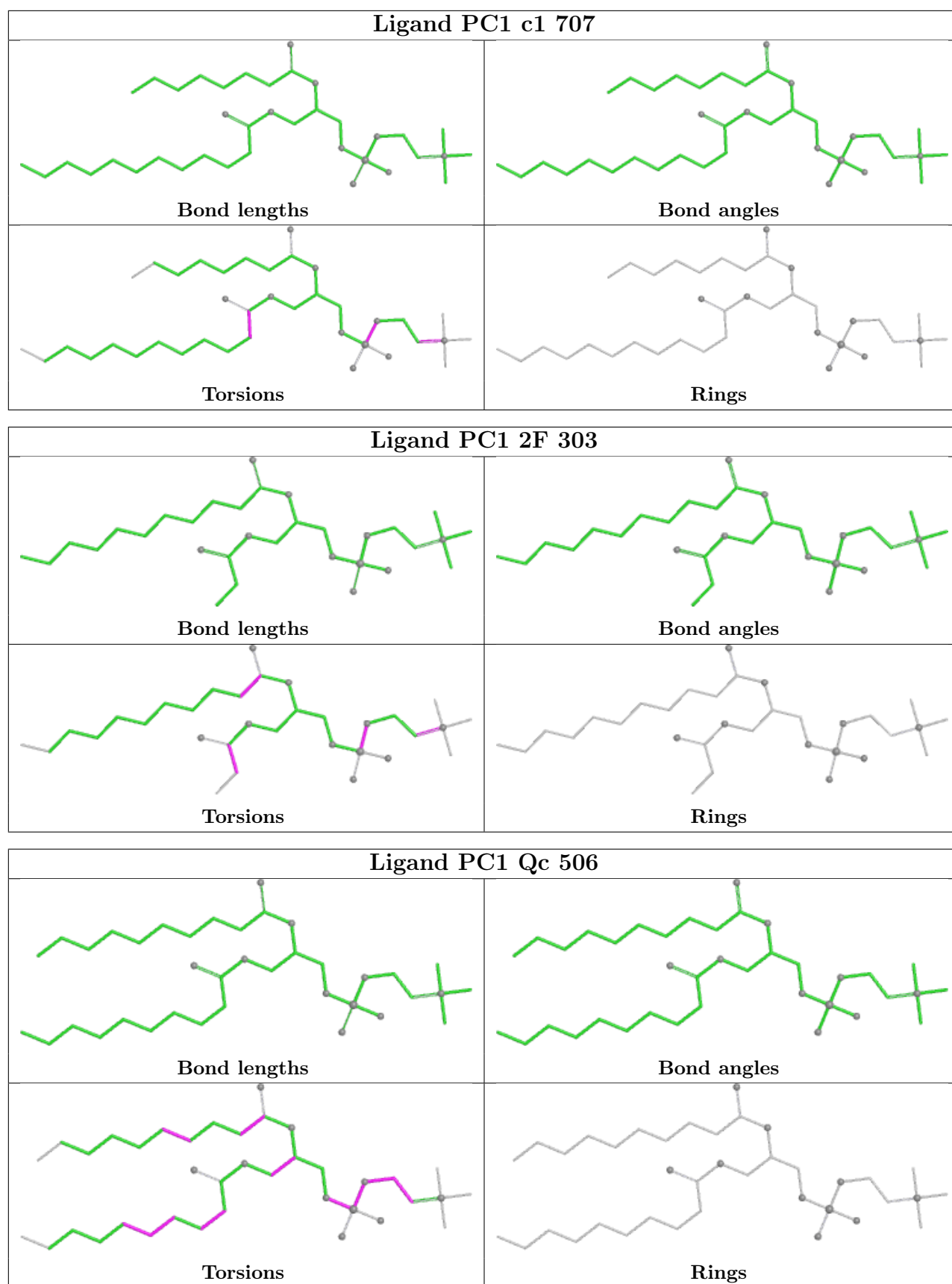


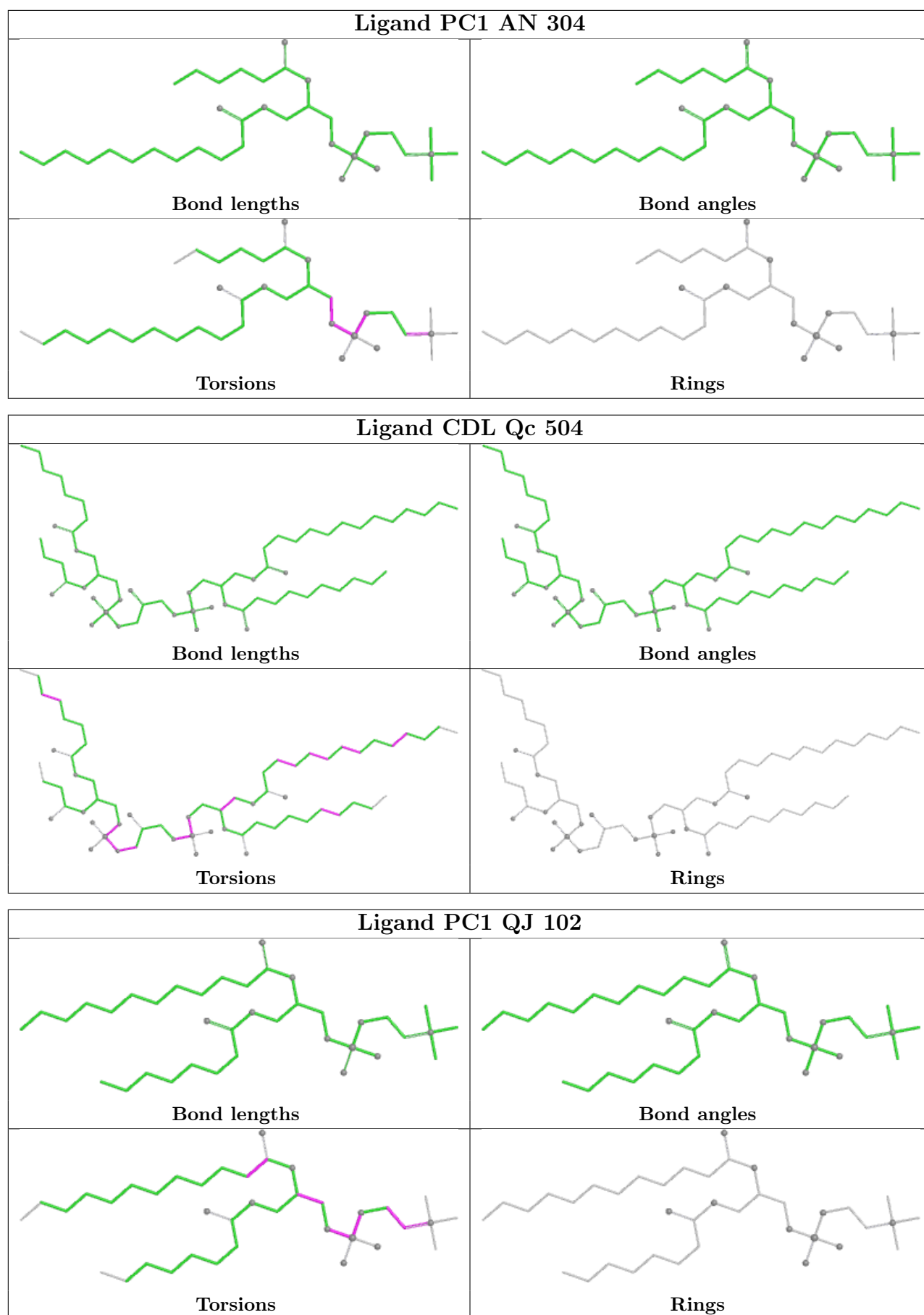


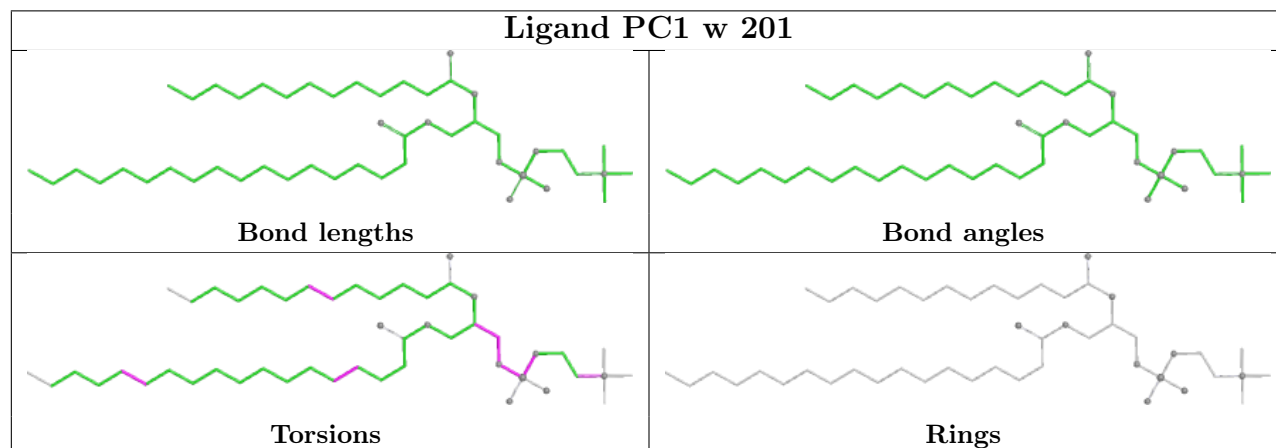
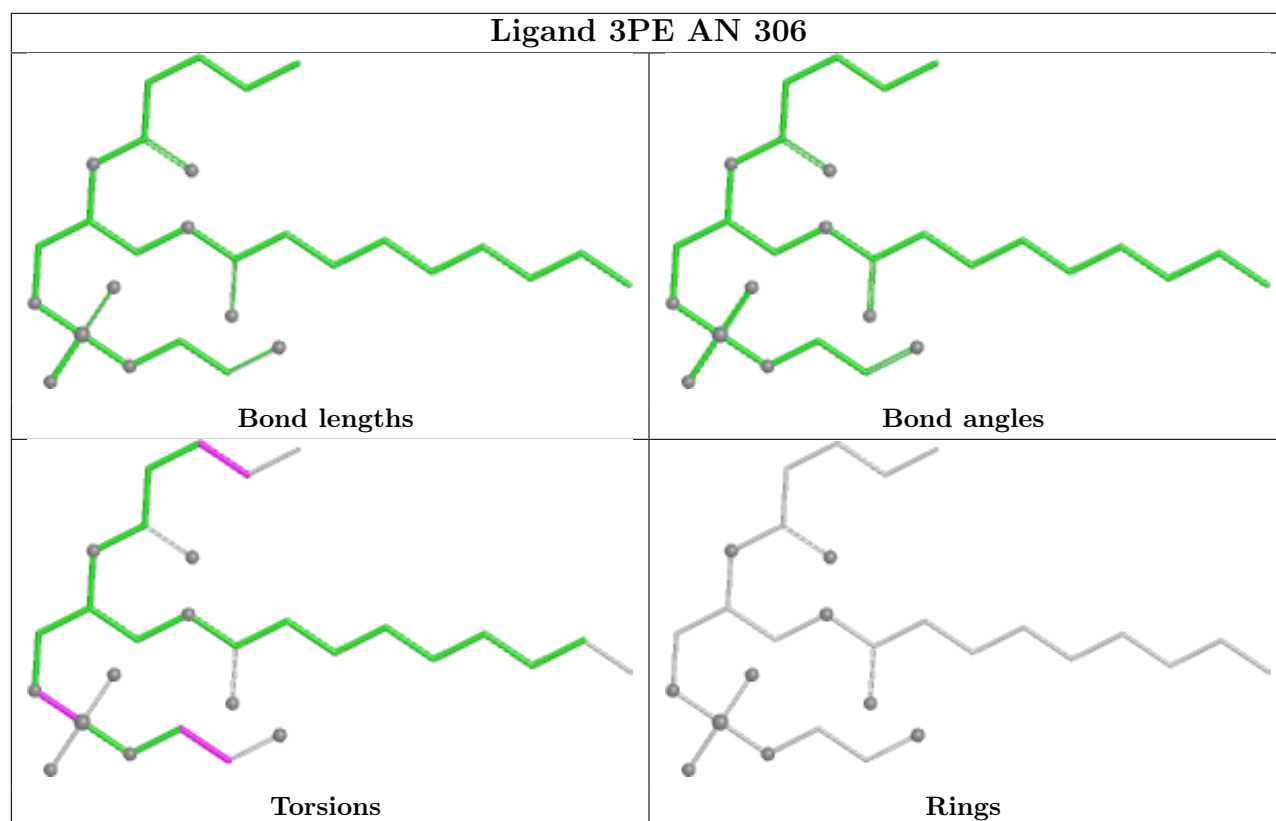
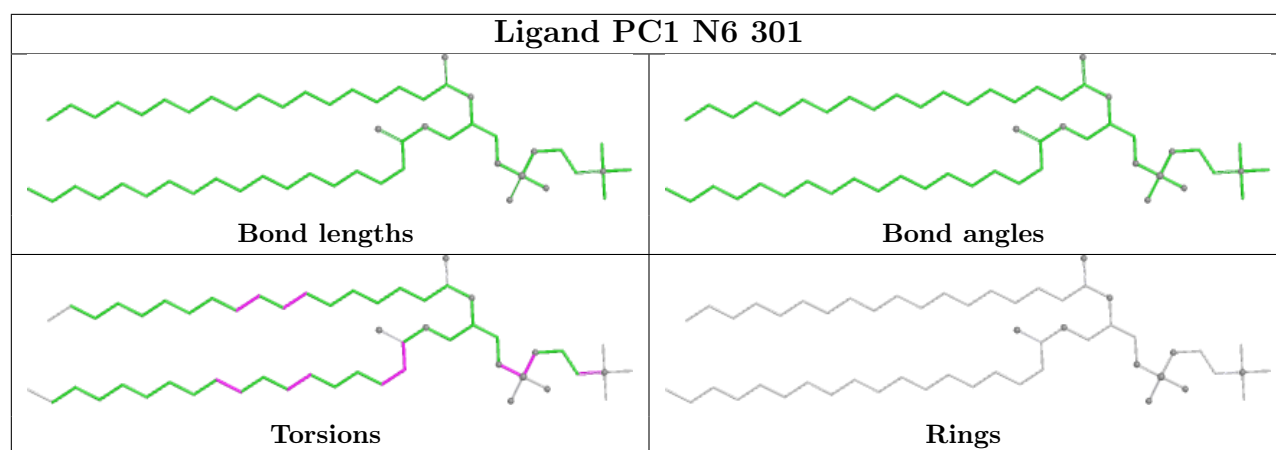


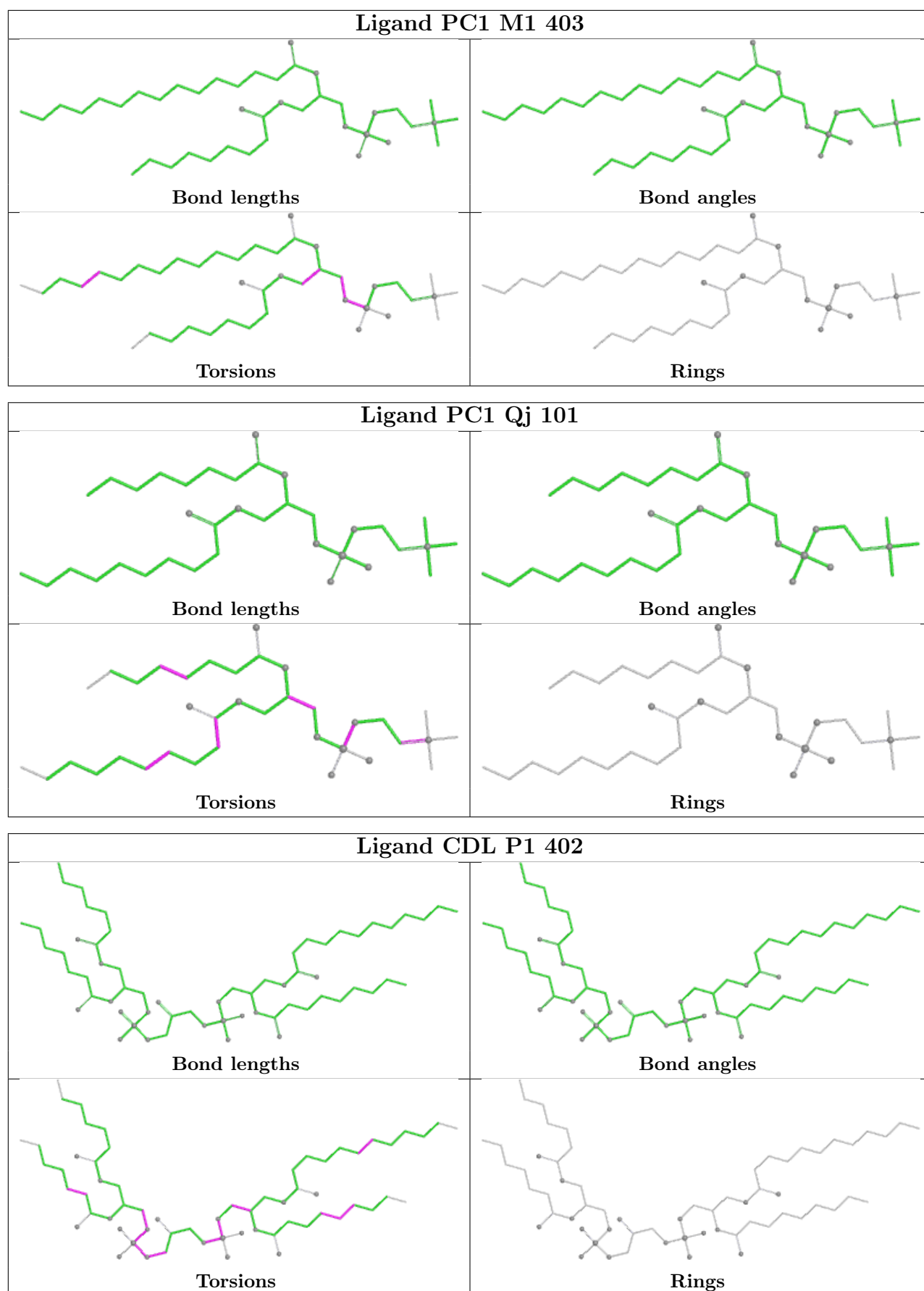


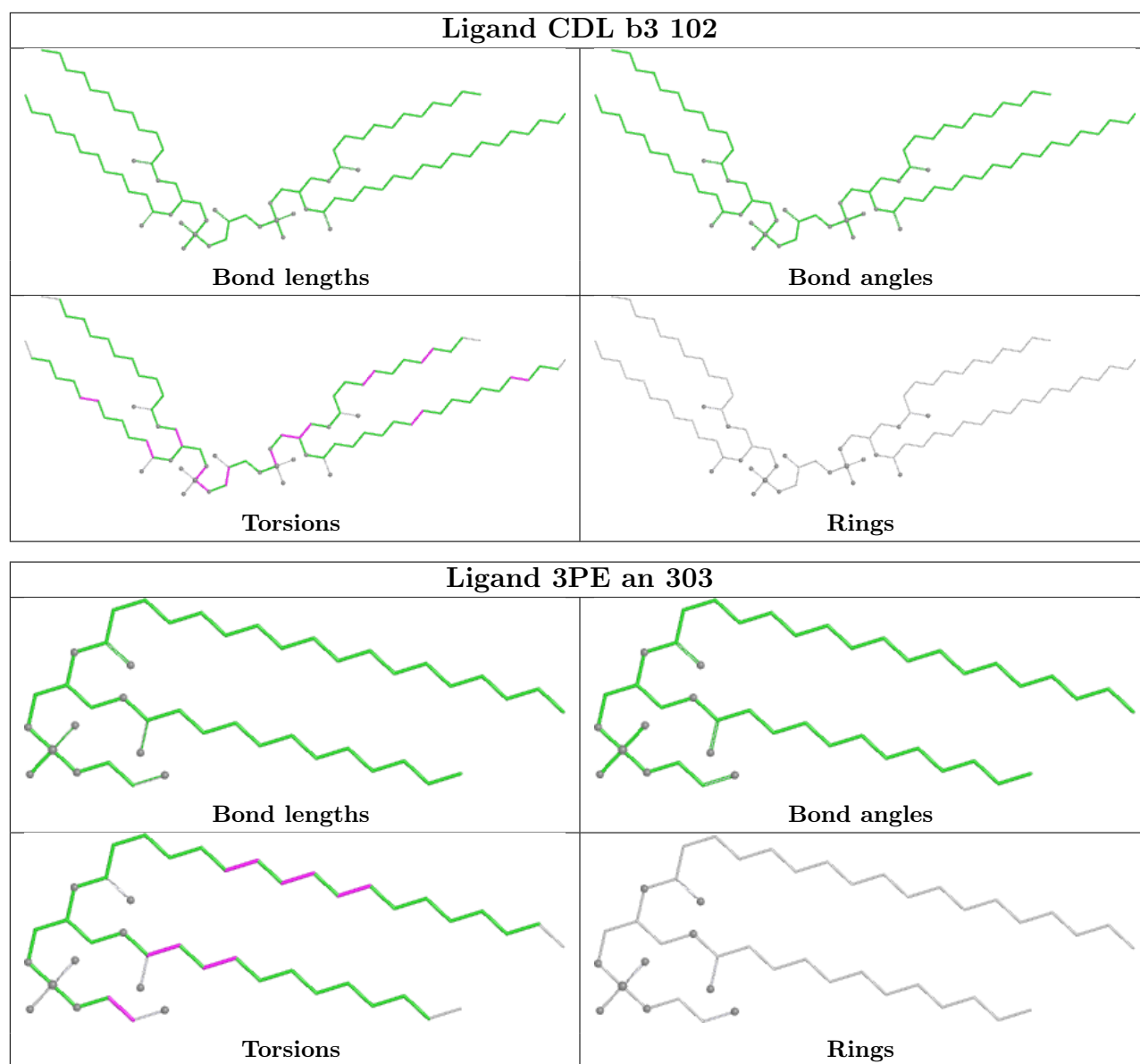


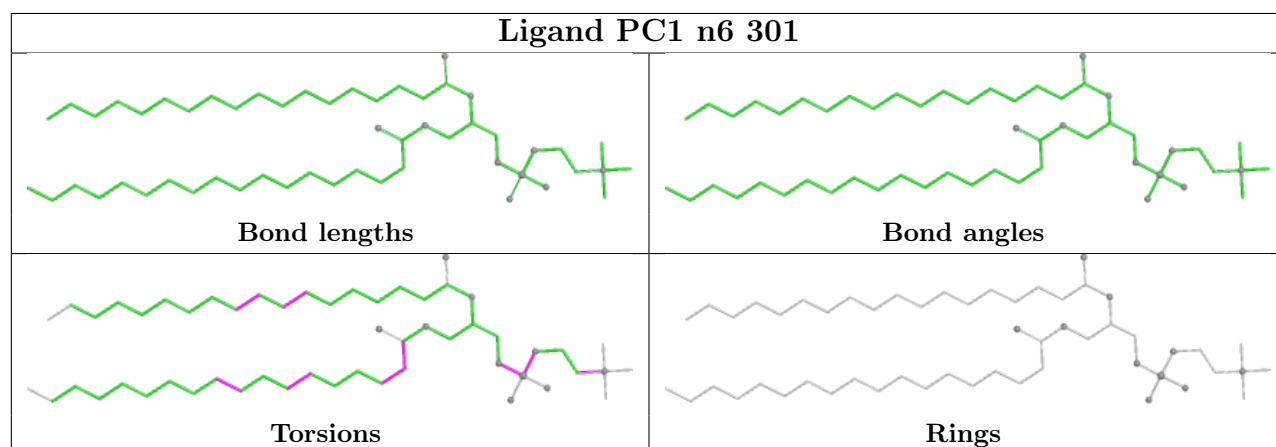
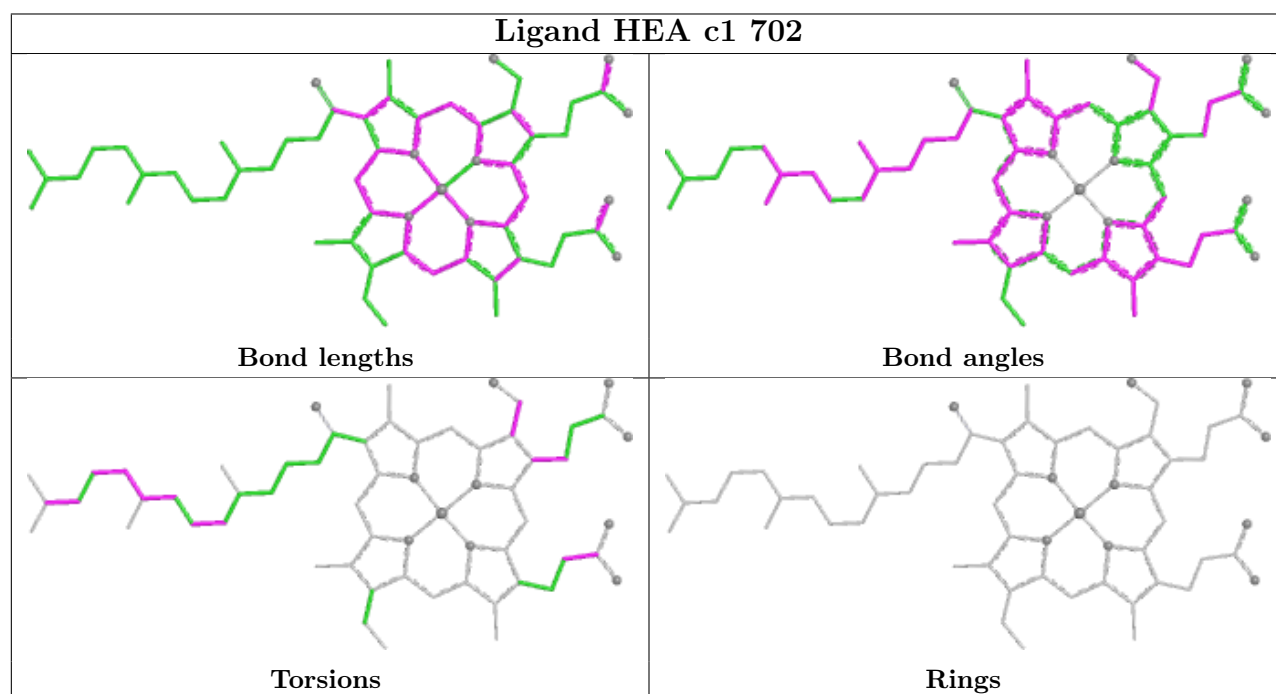
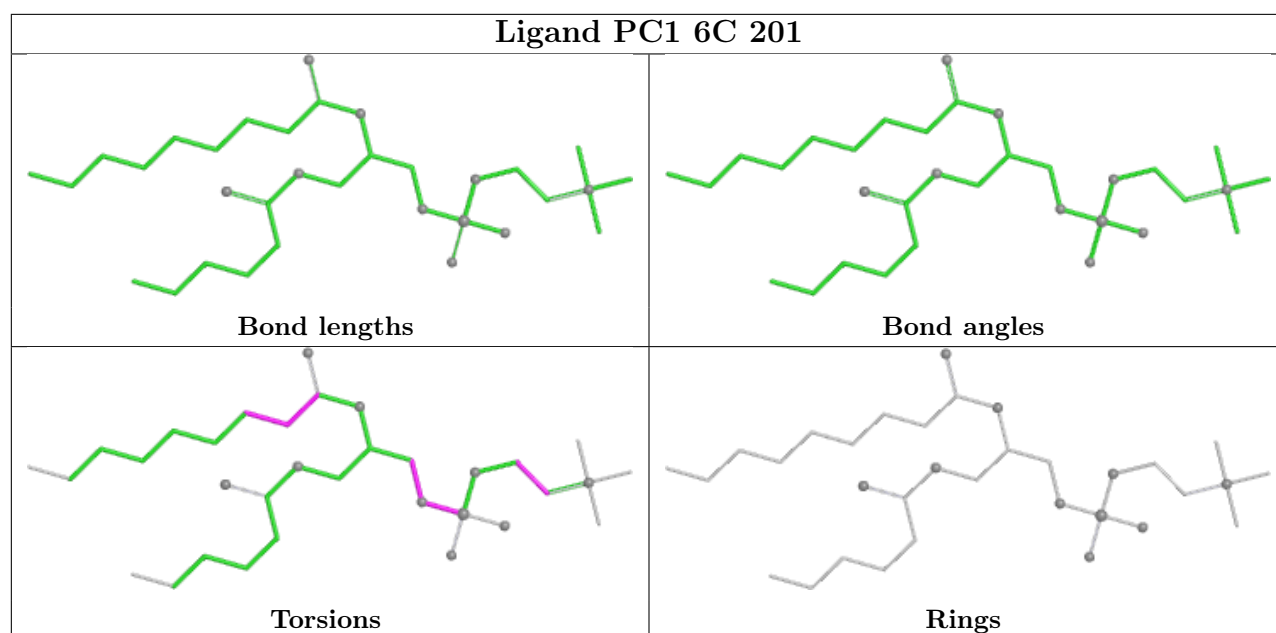


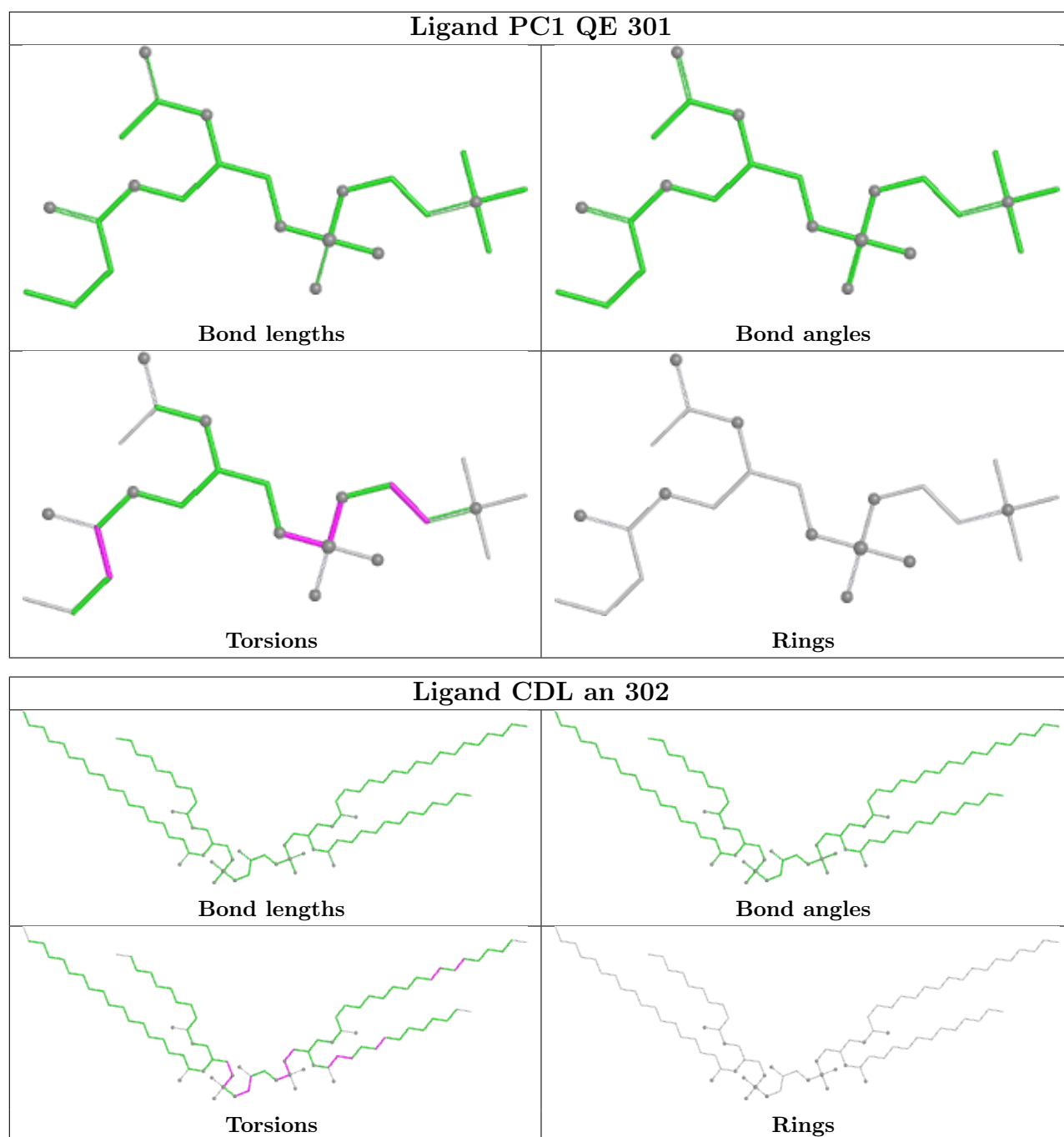


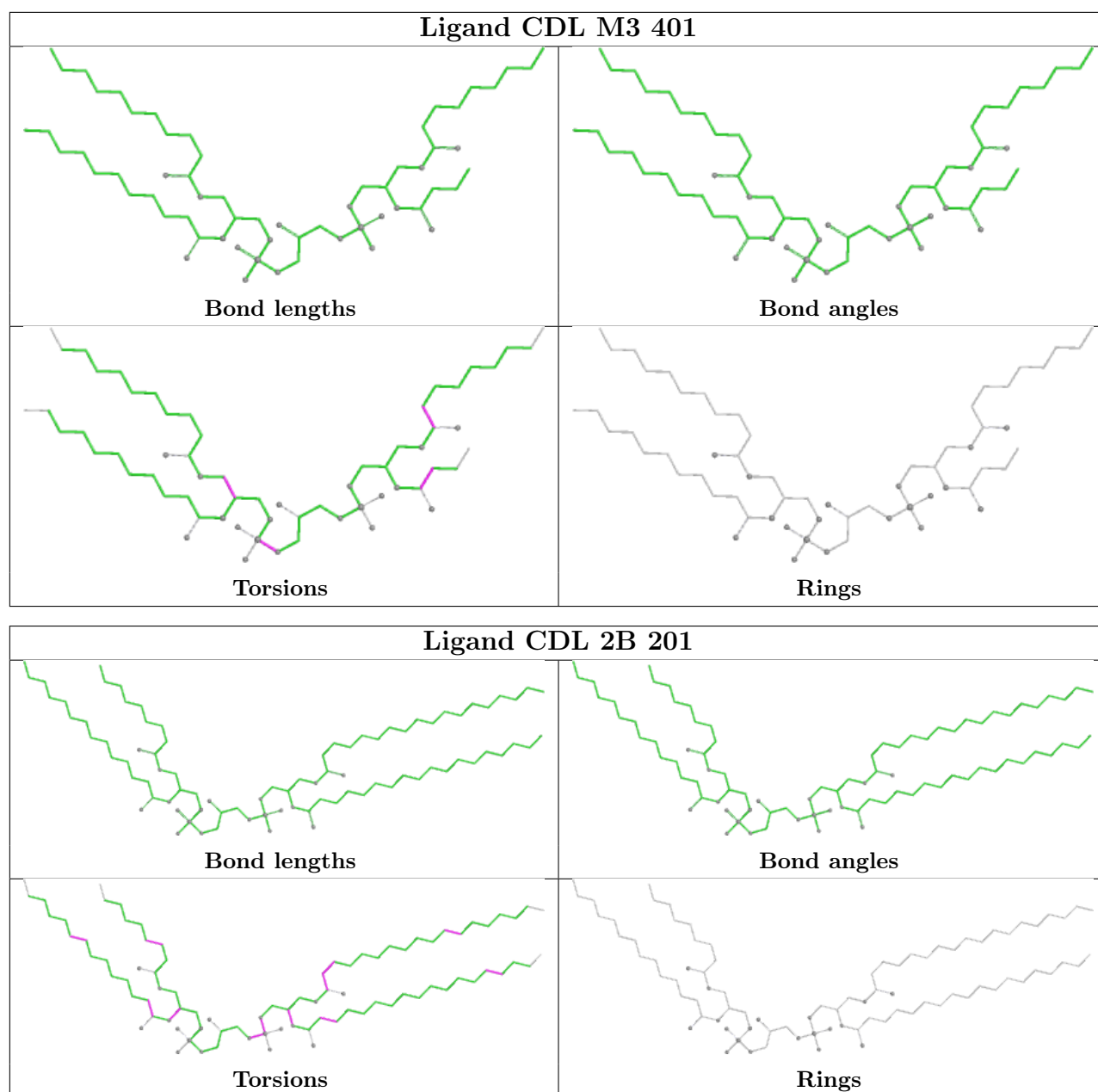




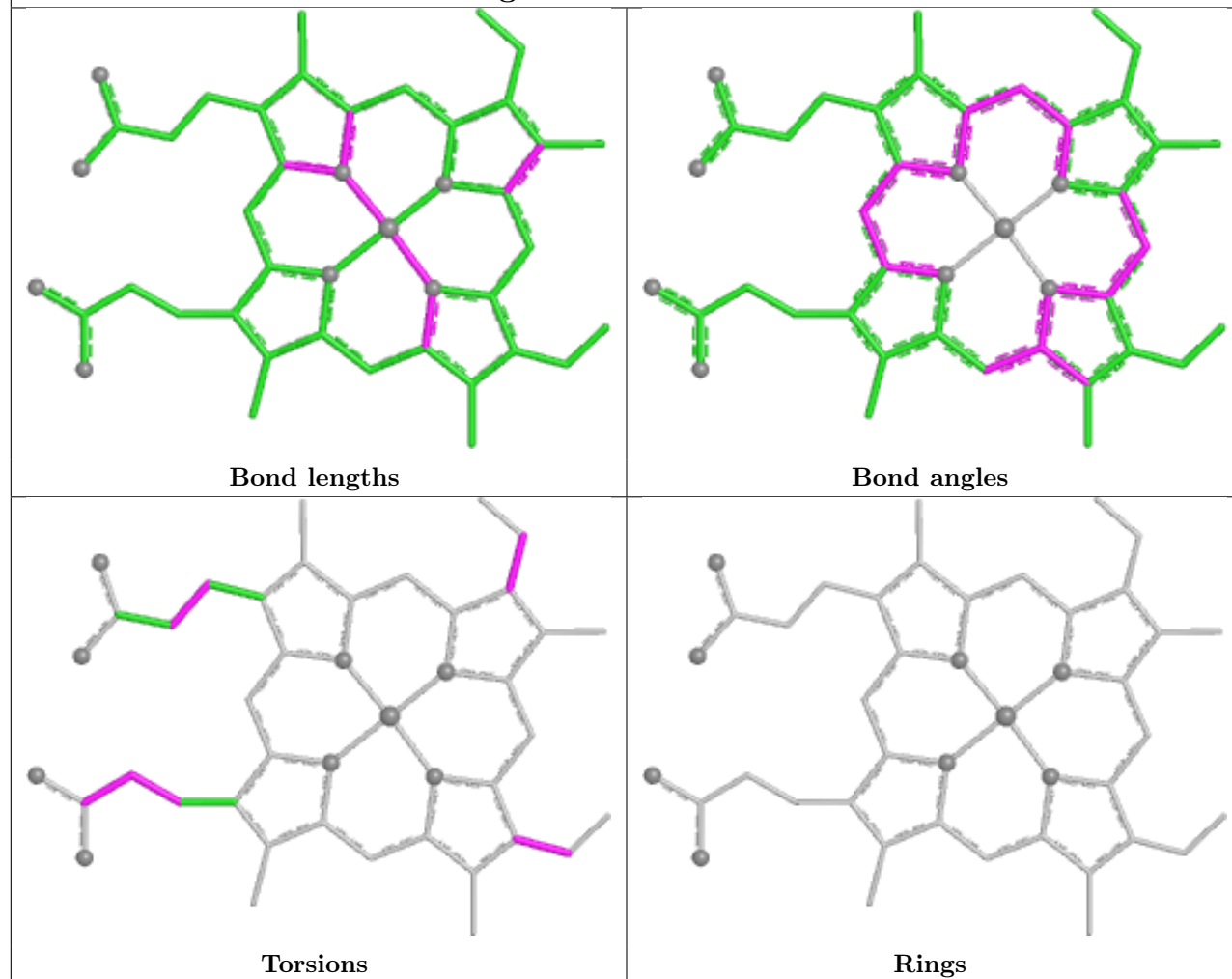




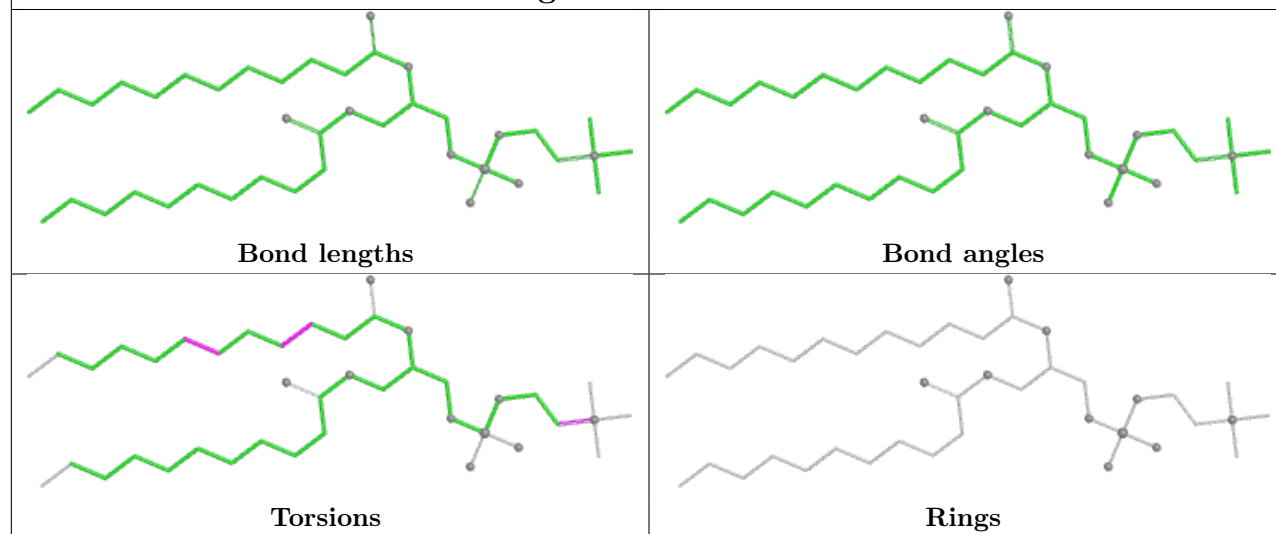


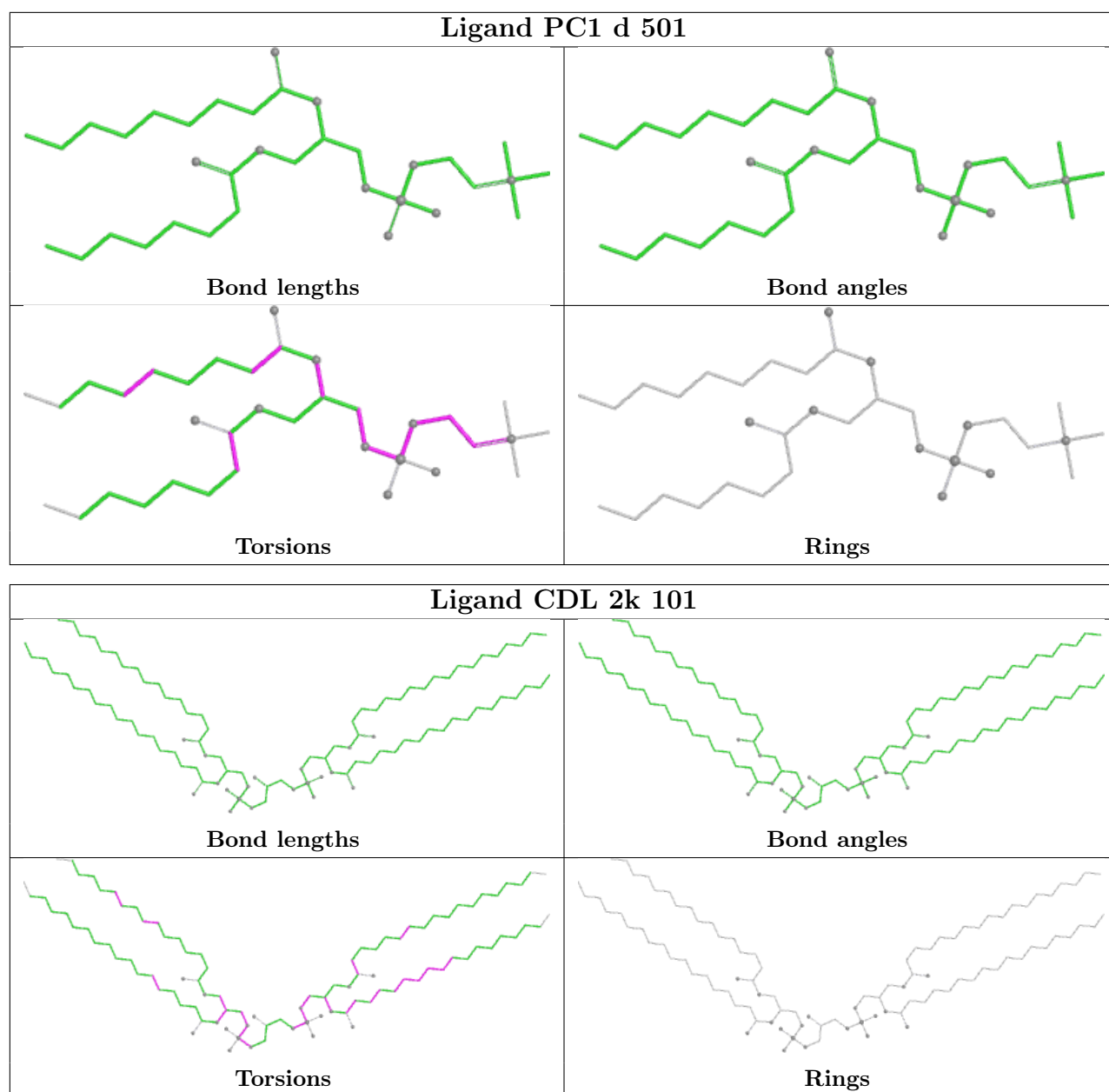


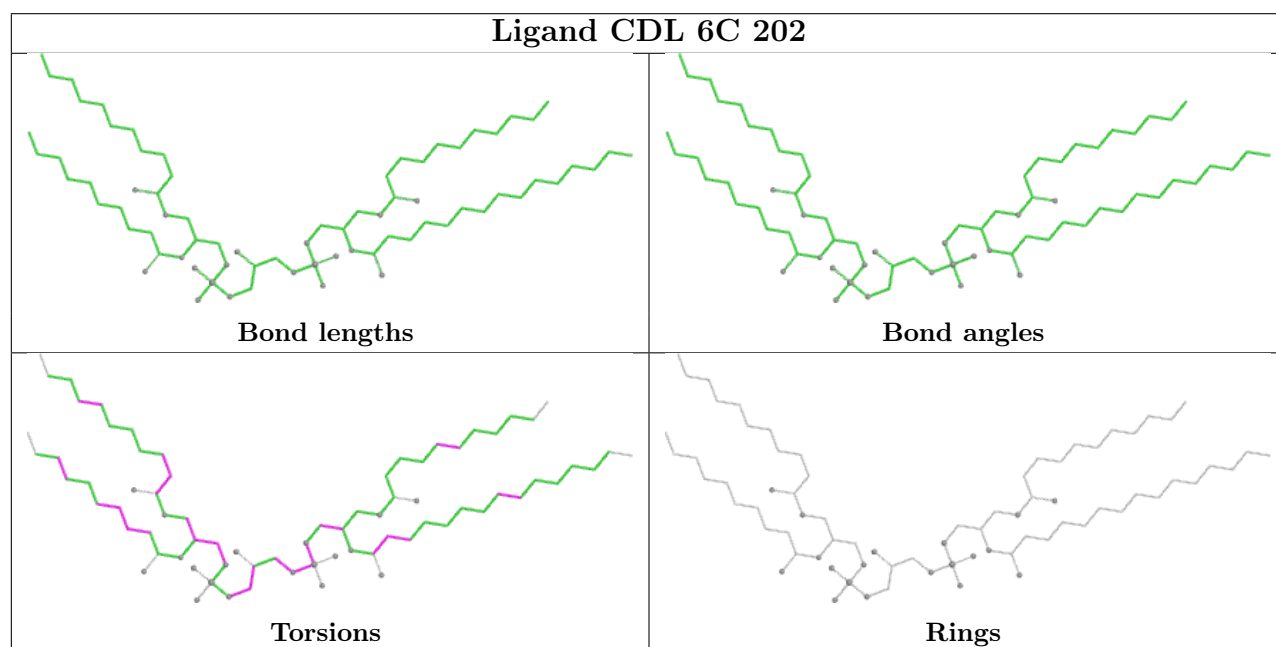
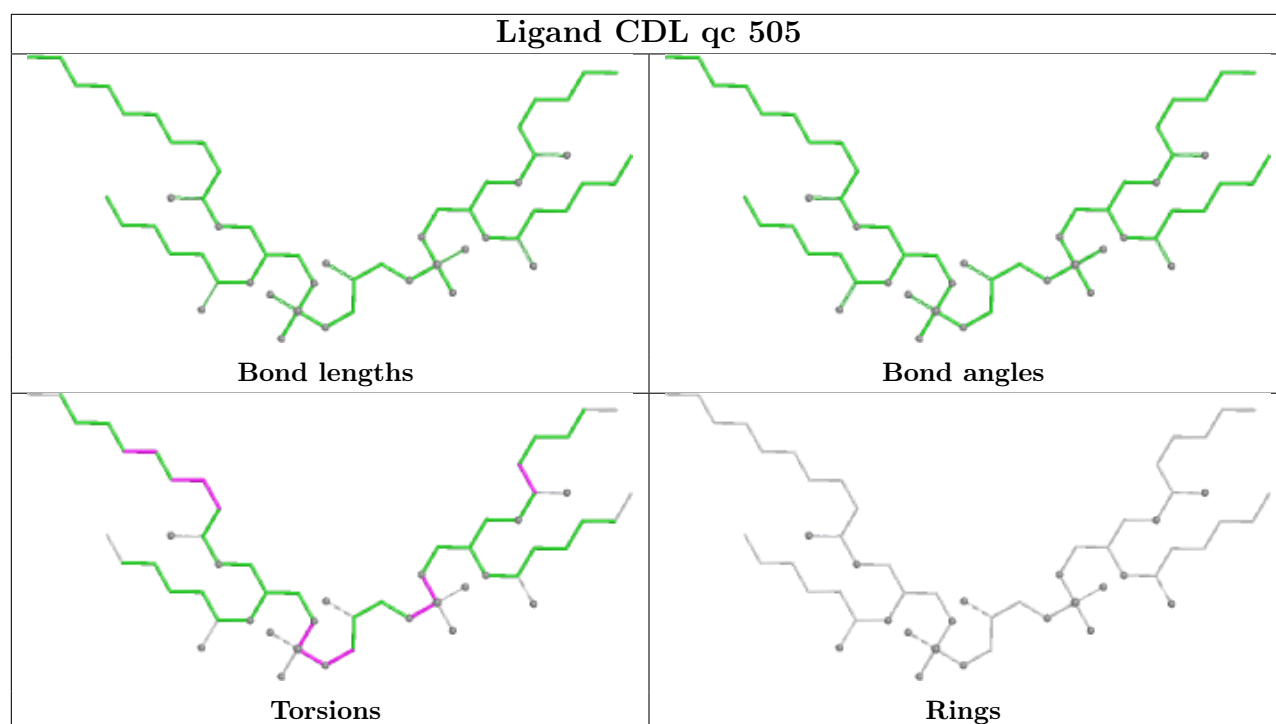
Ligand HEM Y5 203

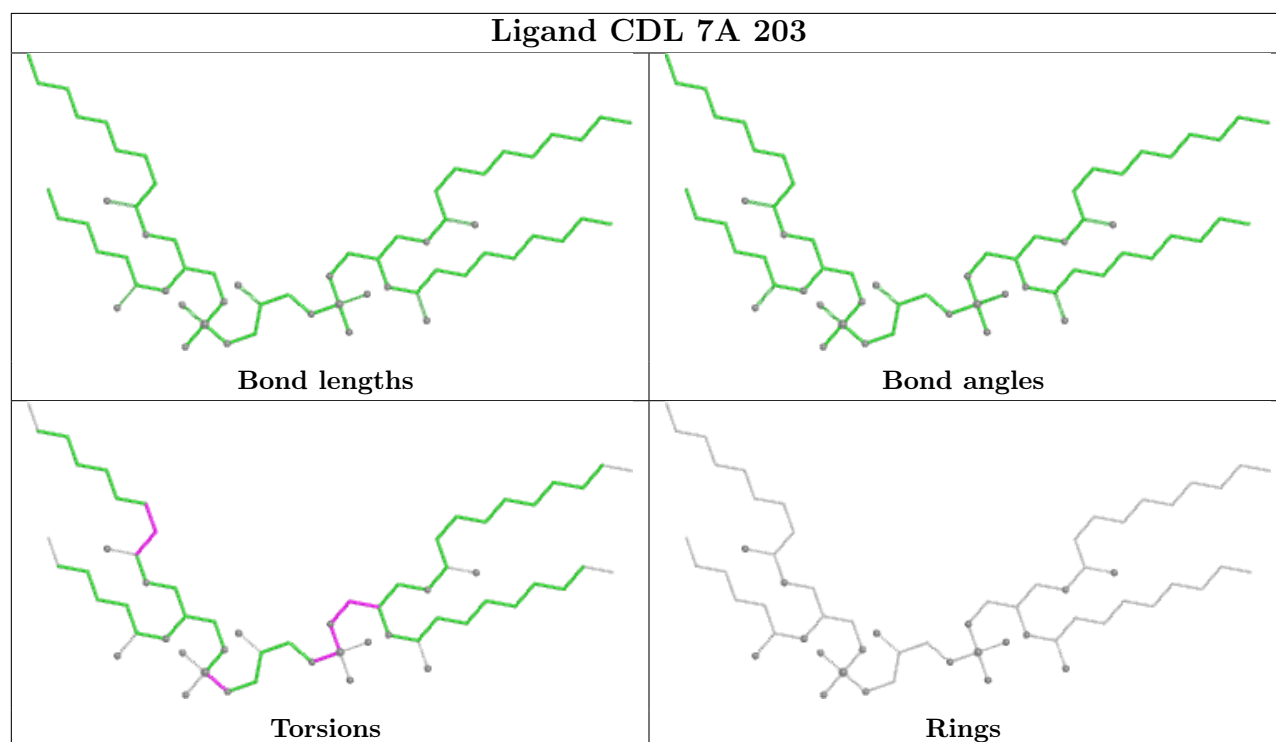
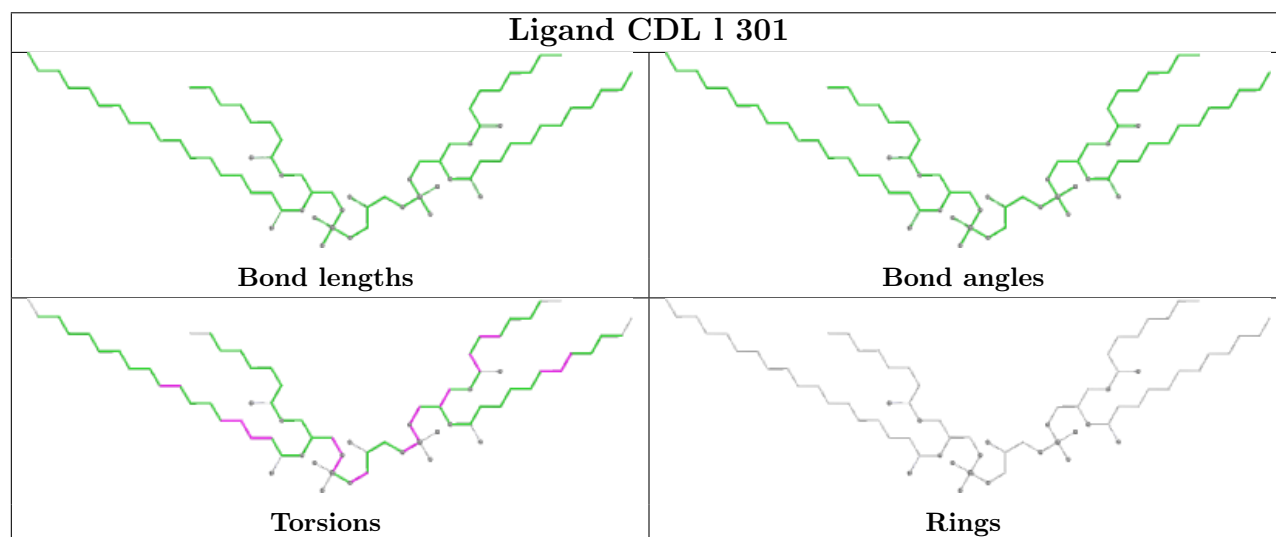
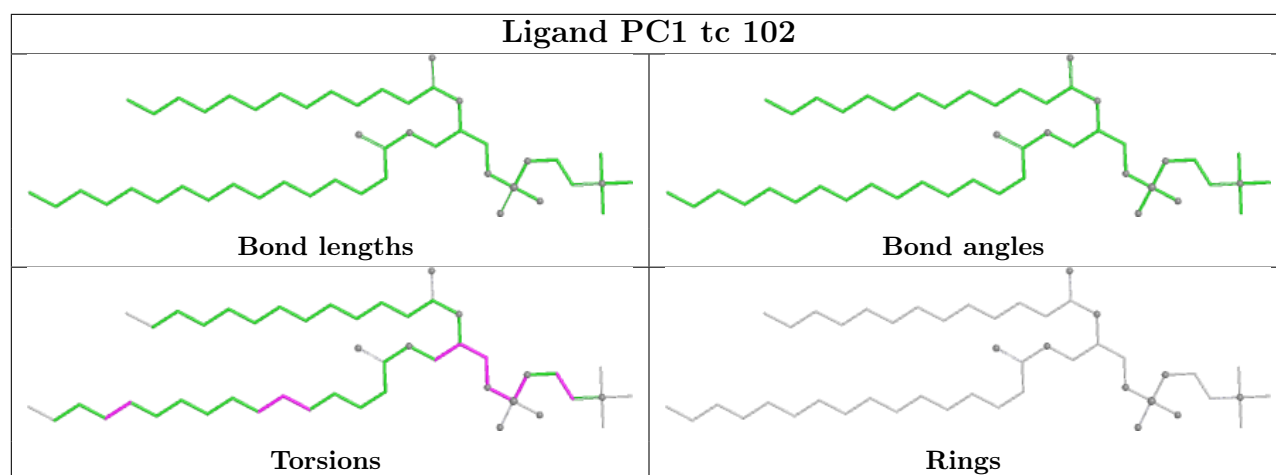


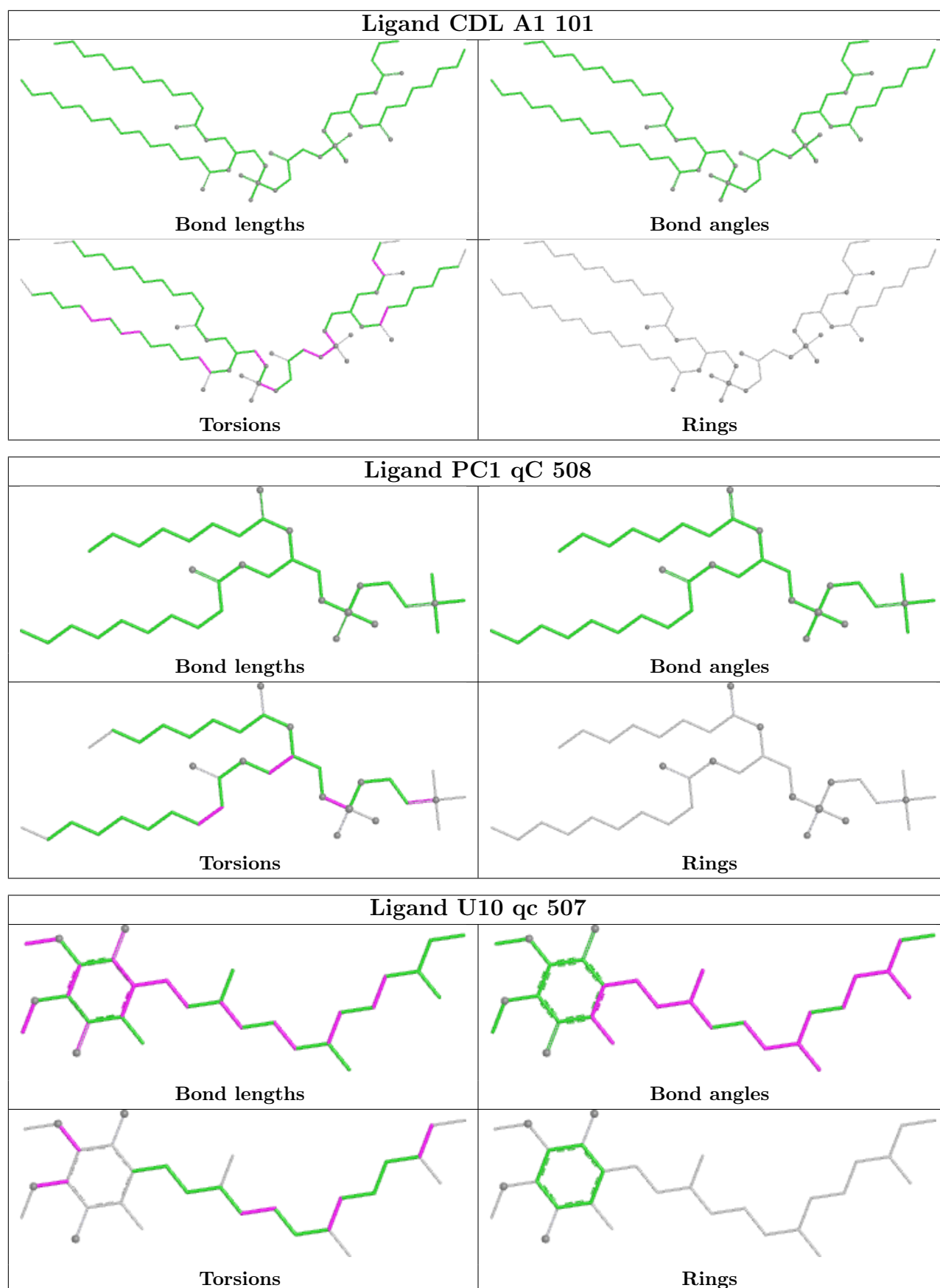
Ligand PC1 n 301

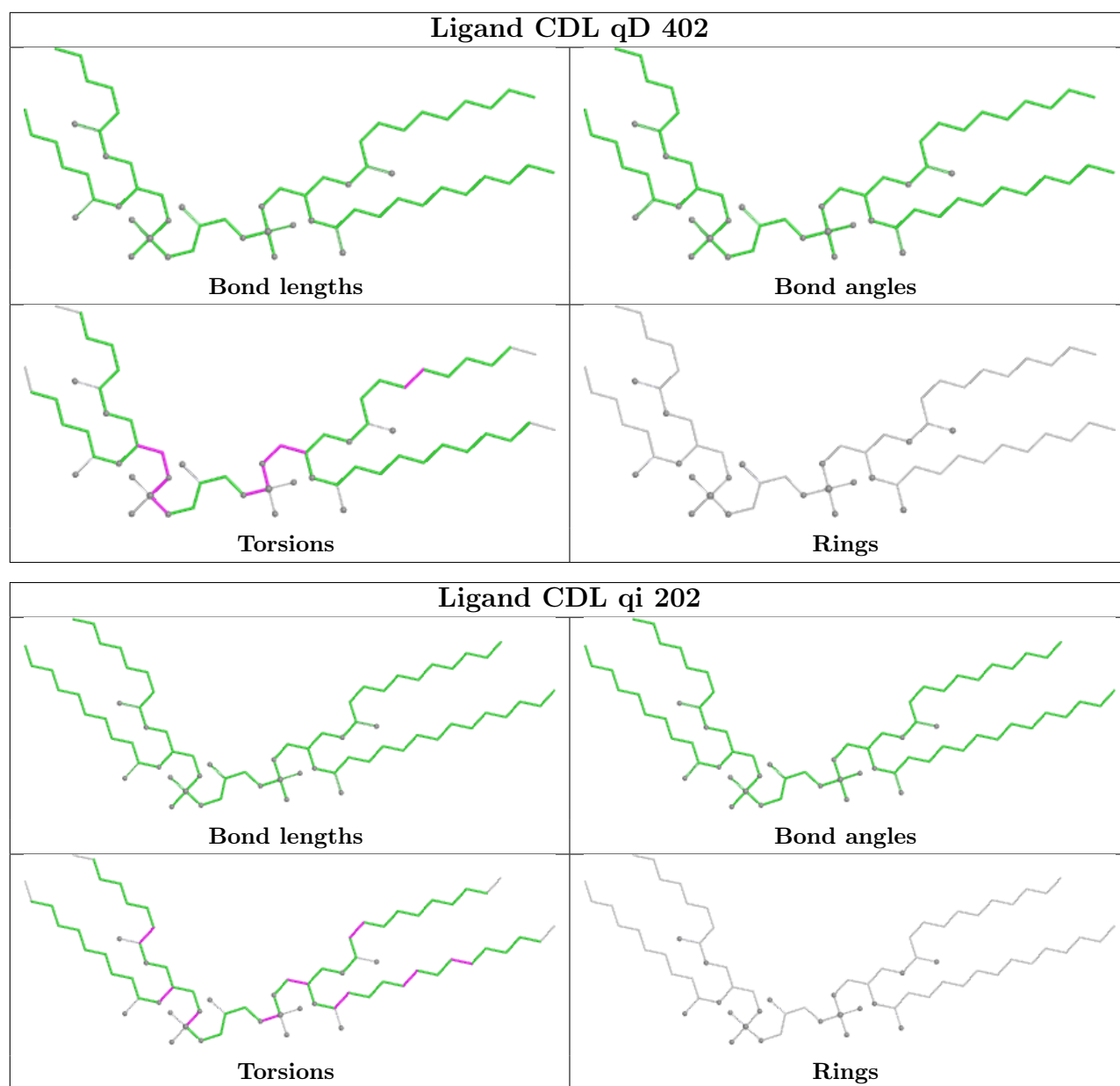


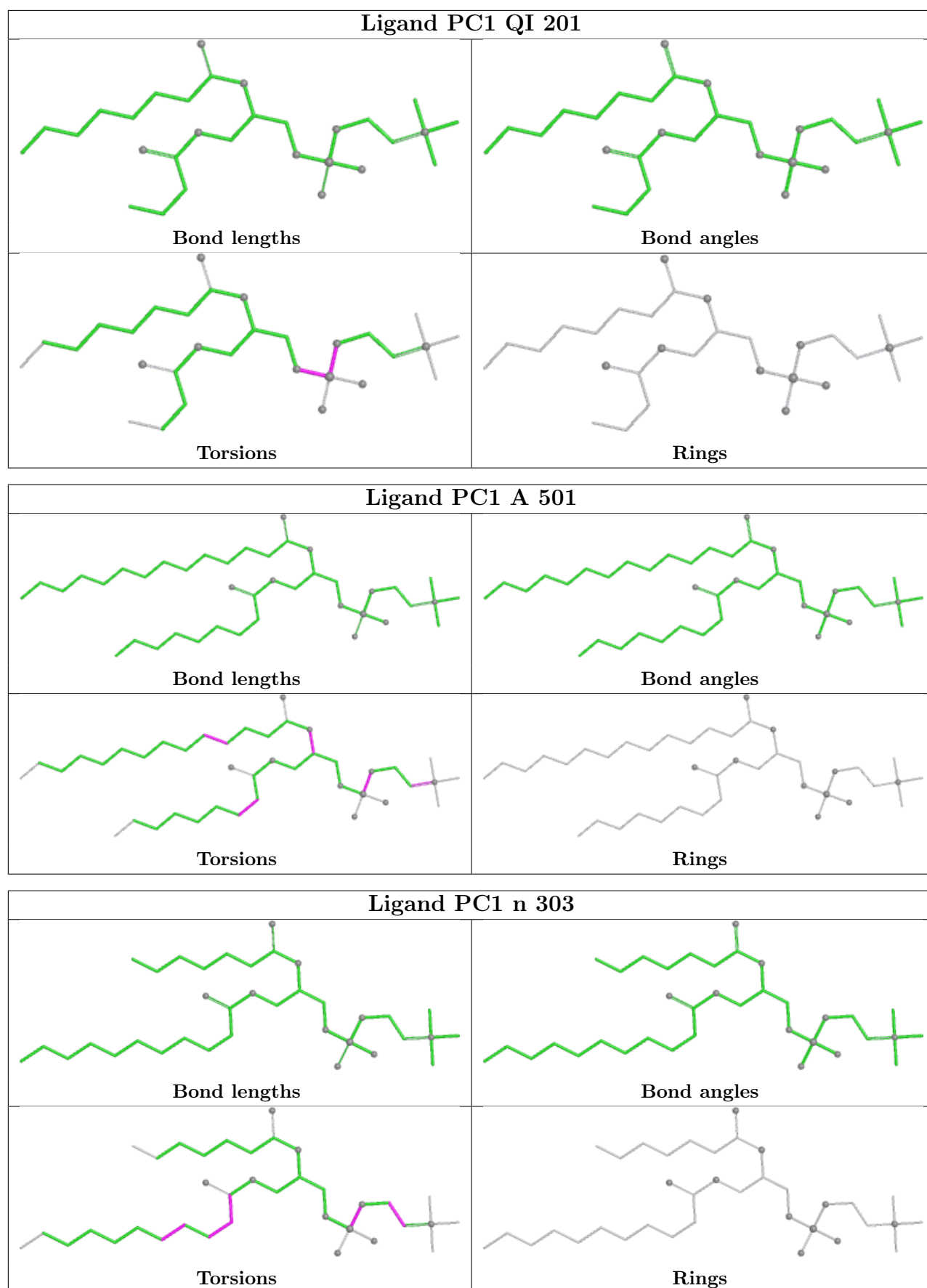


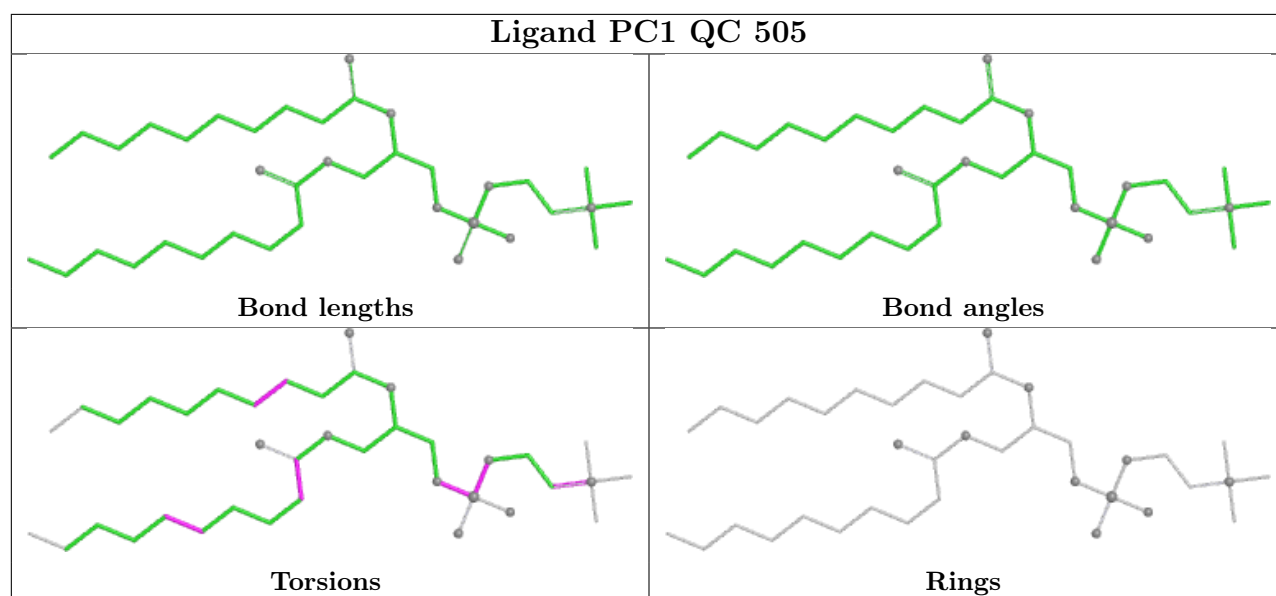
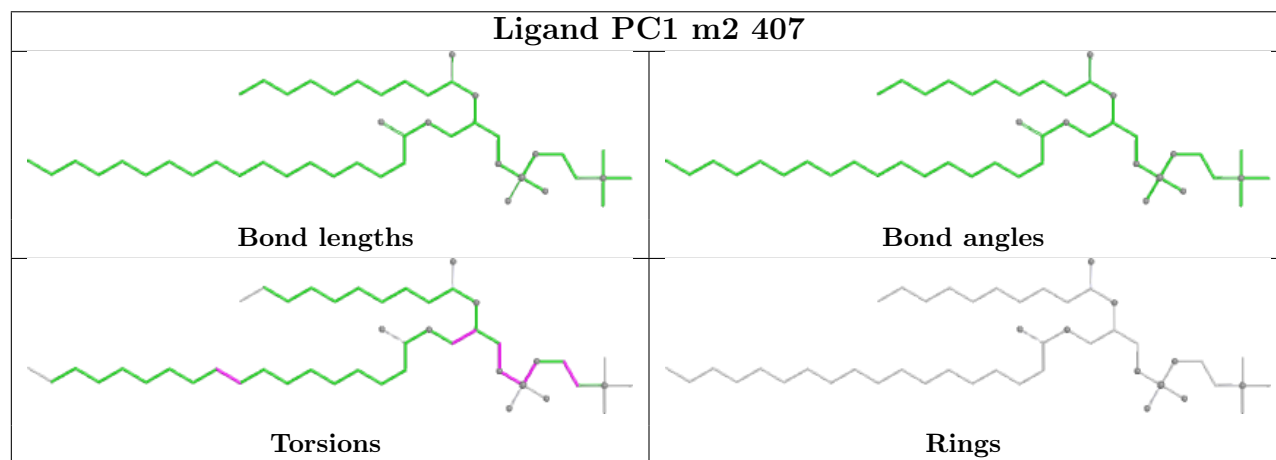
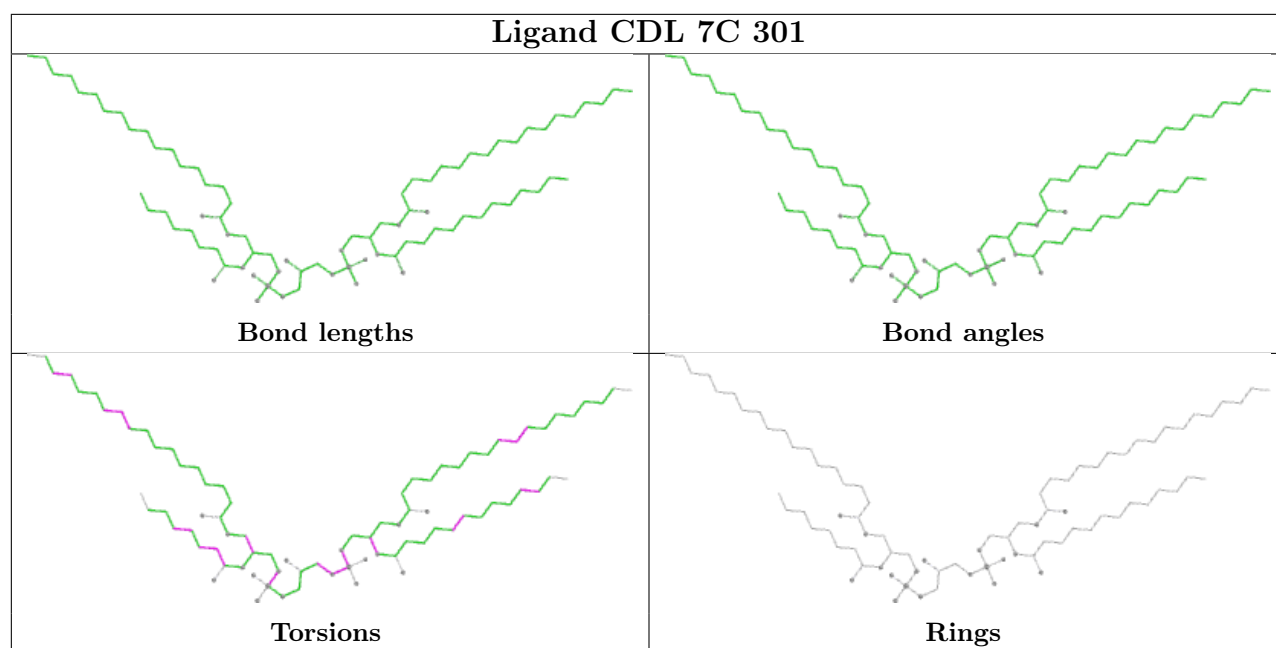


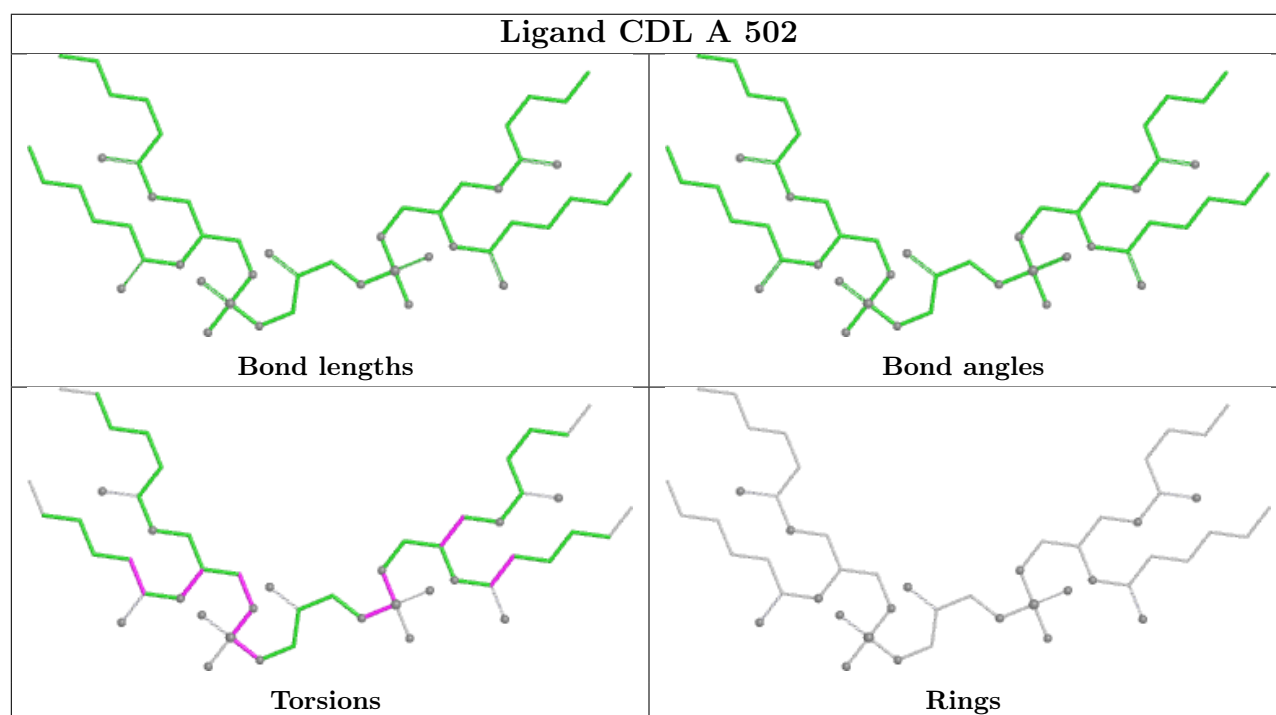
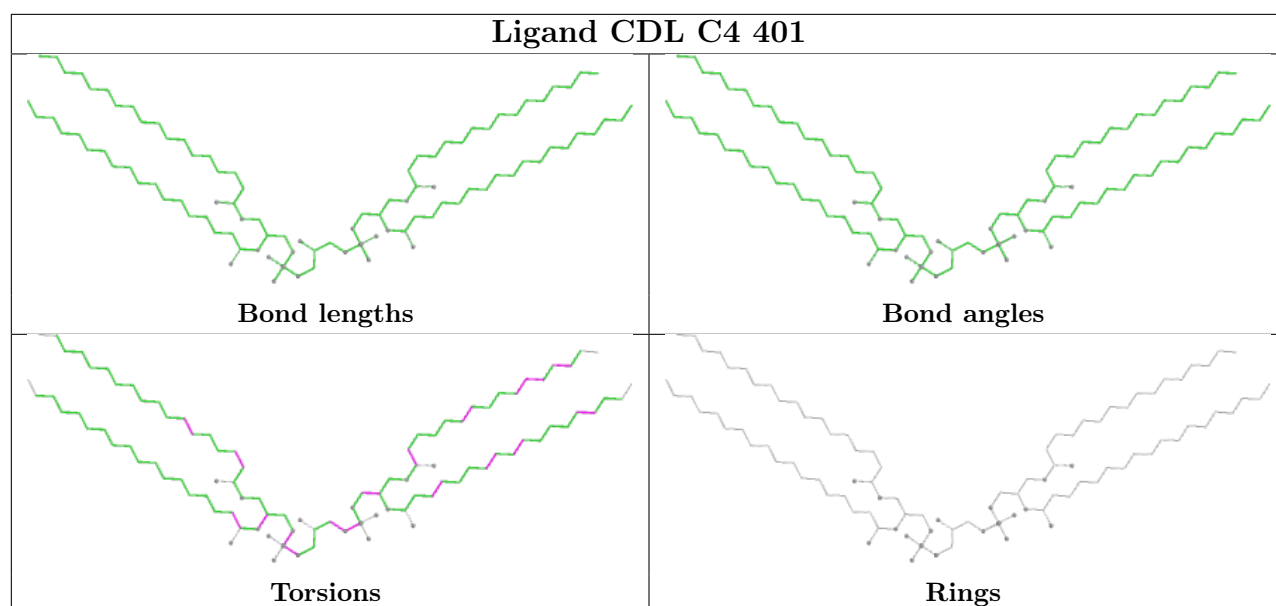


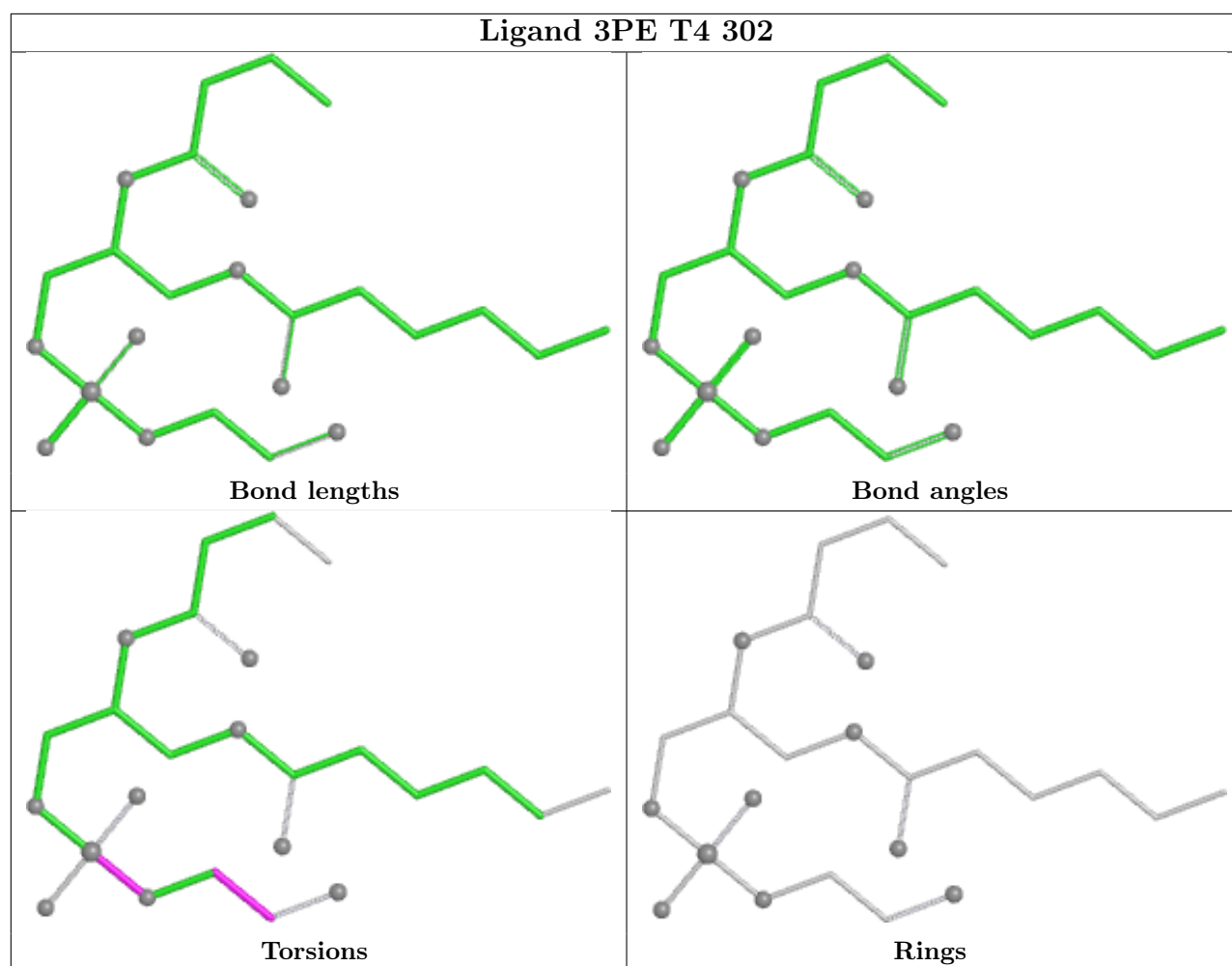


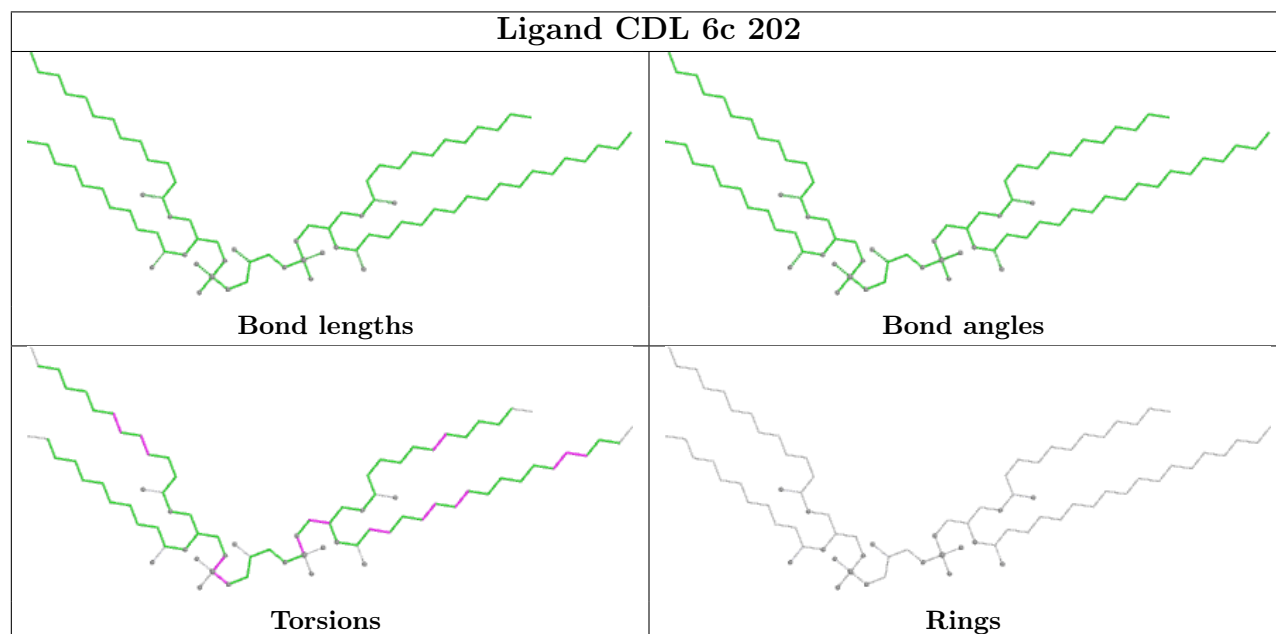
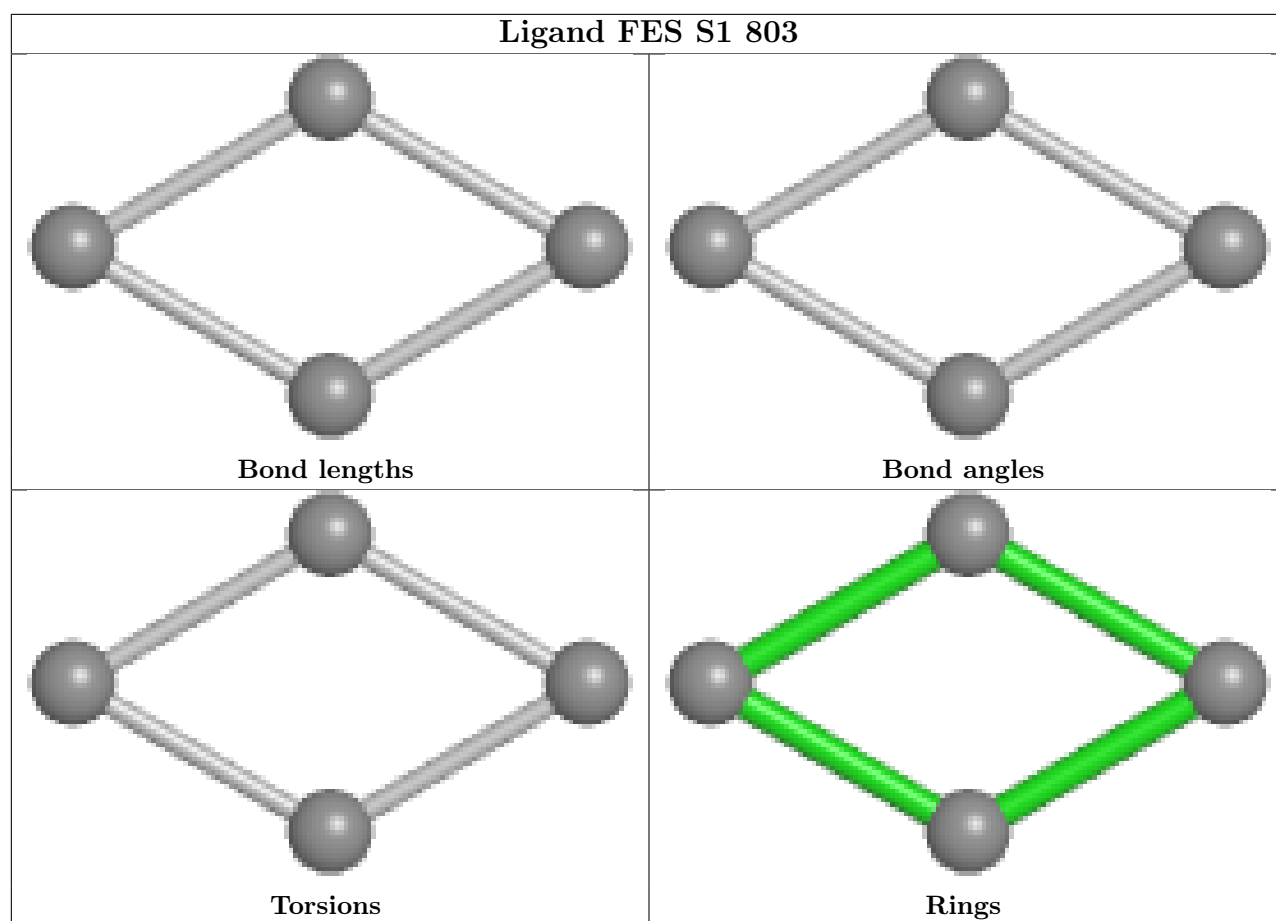


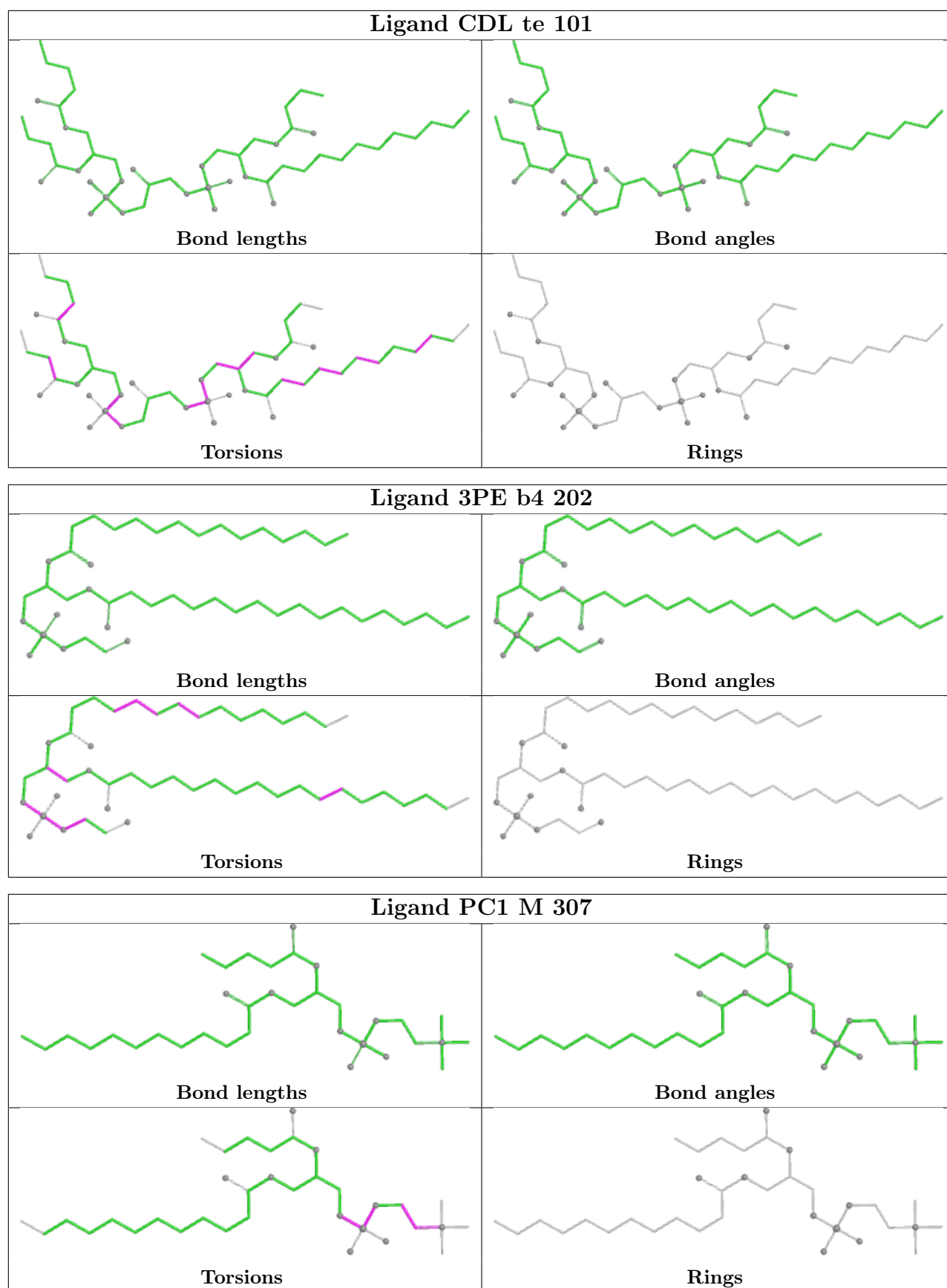


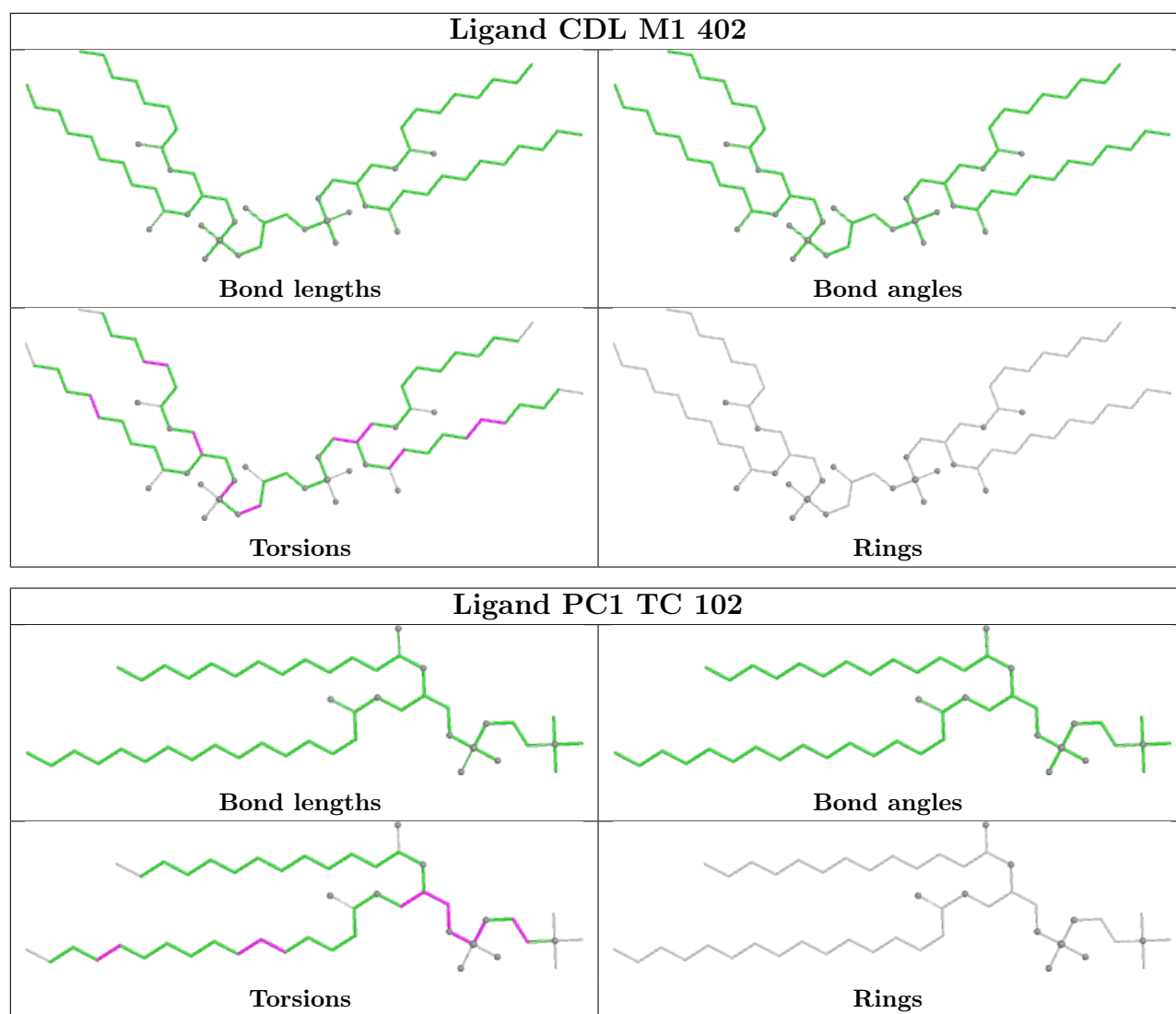




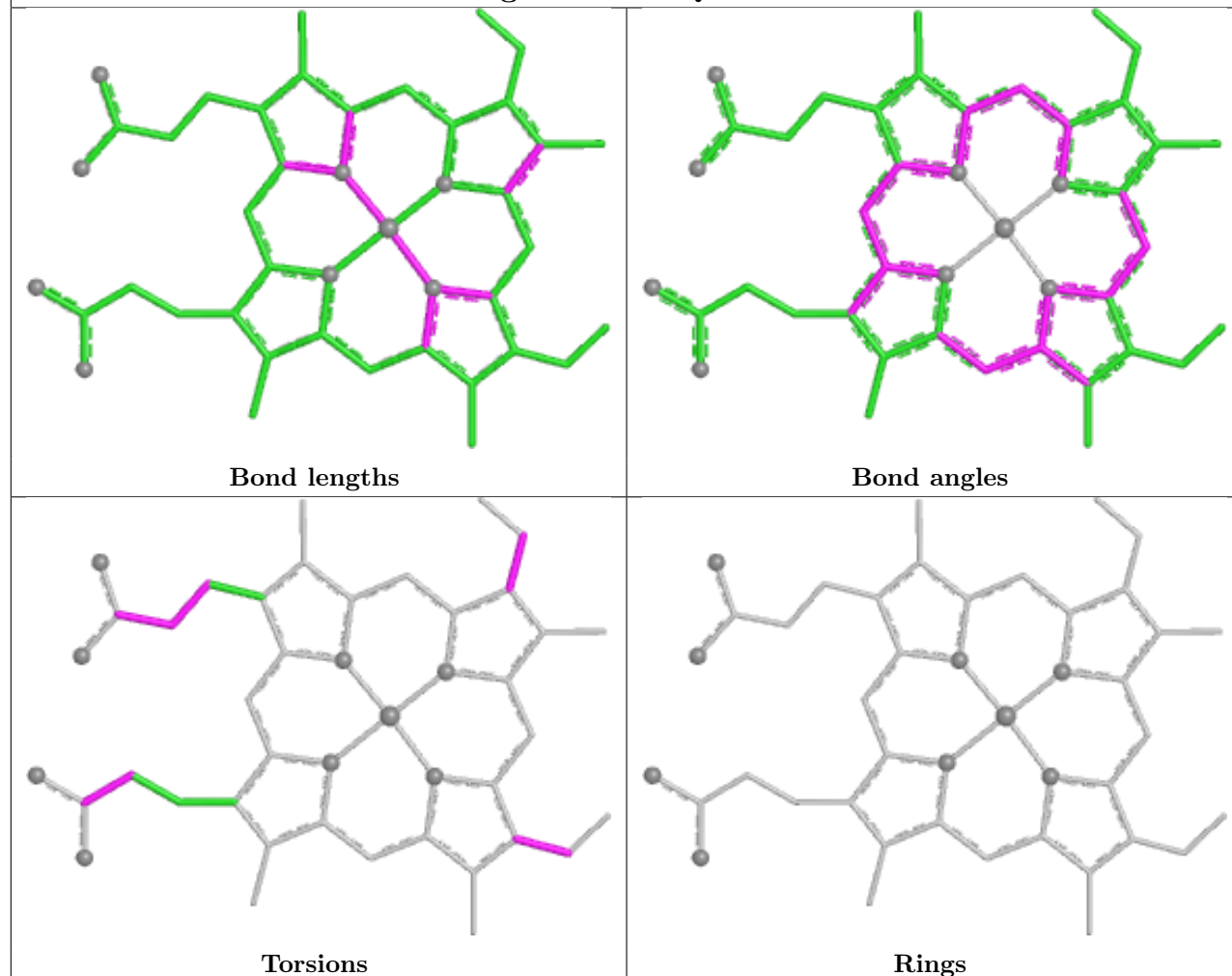




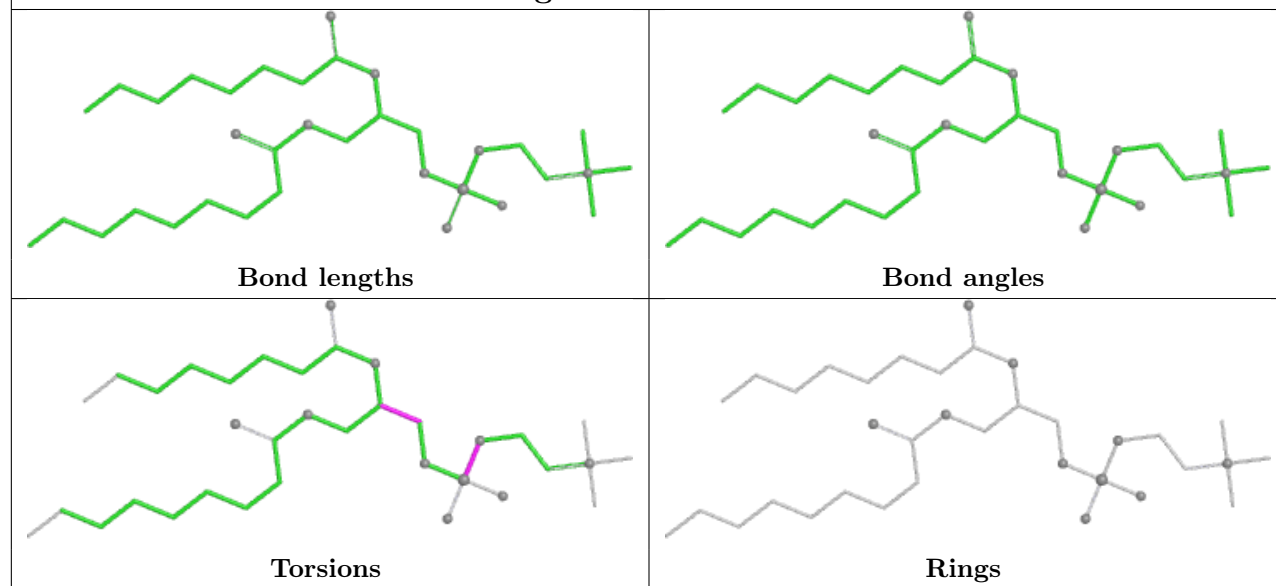


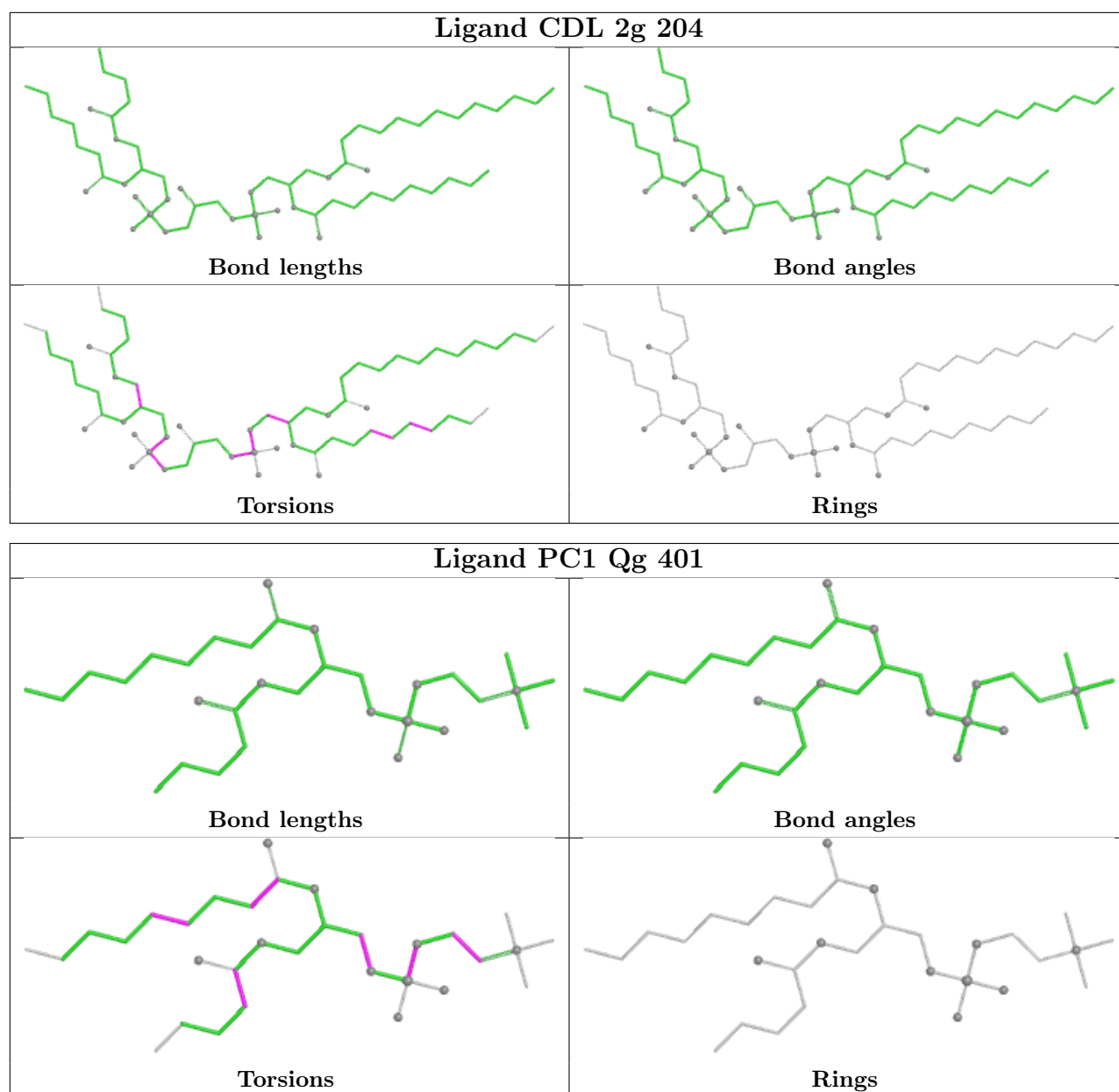


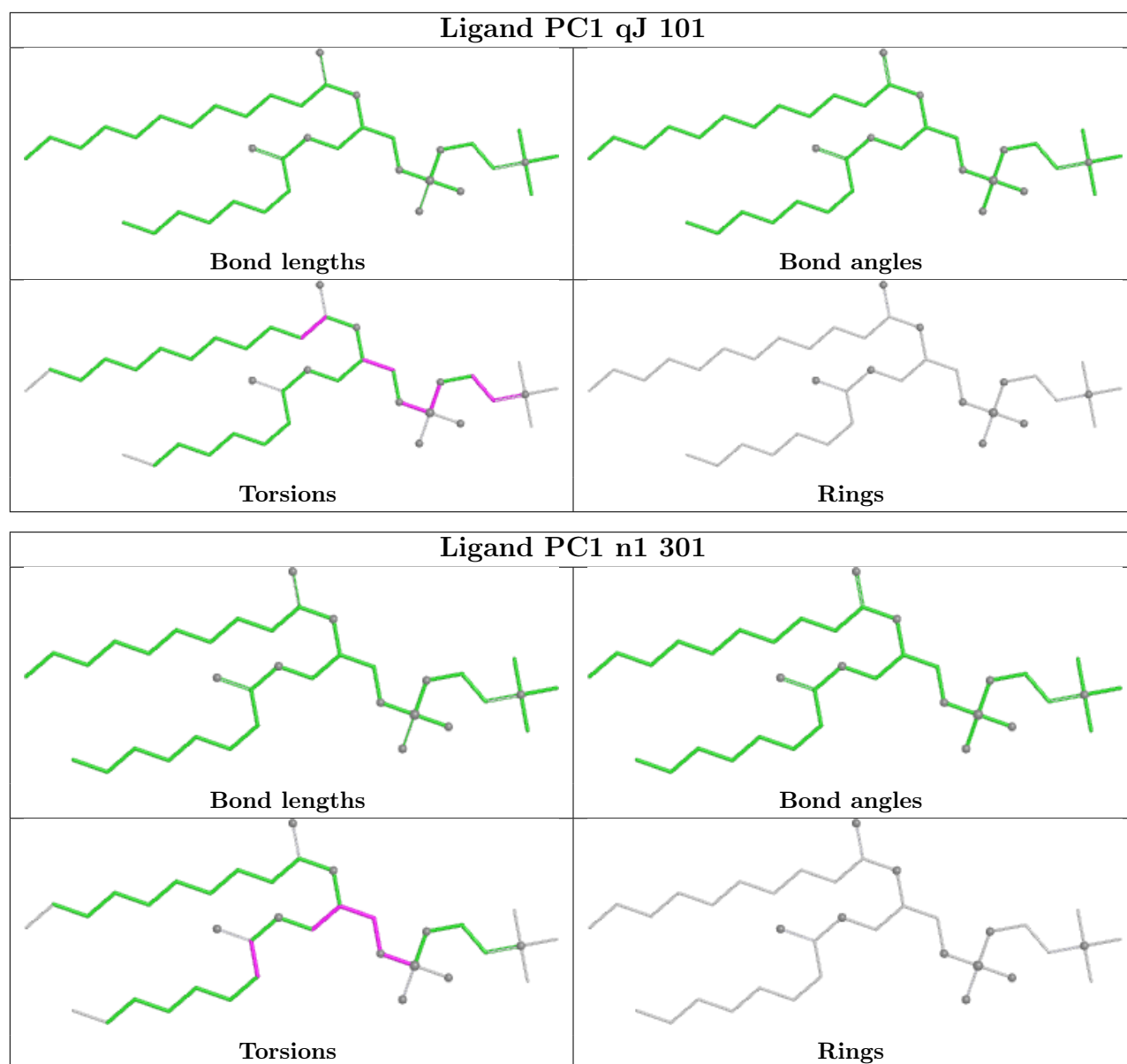
Ligand HEM Qc 503

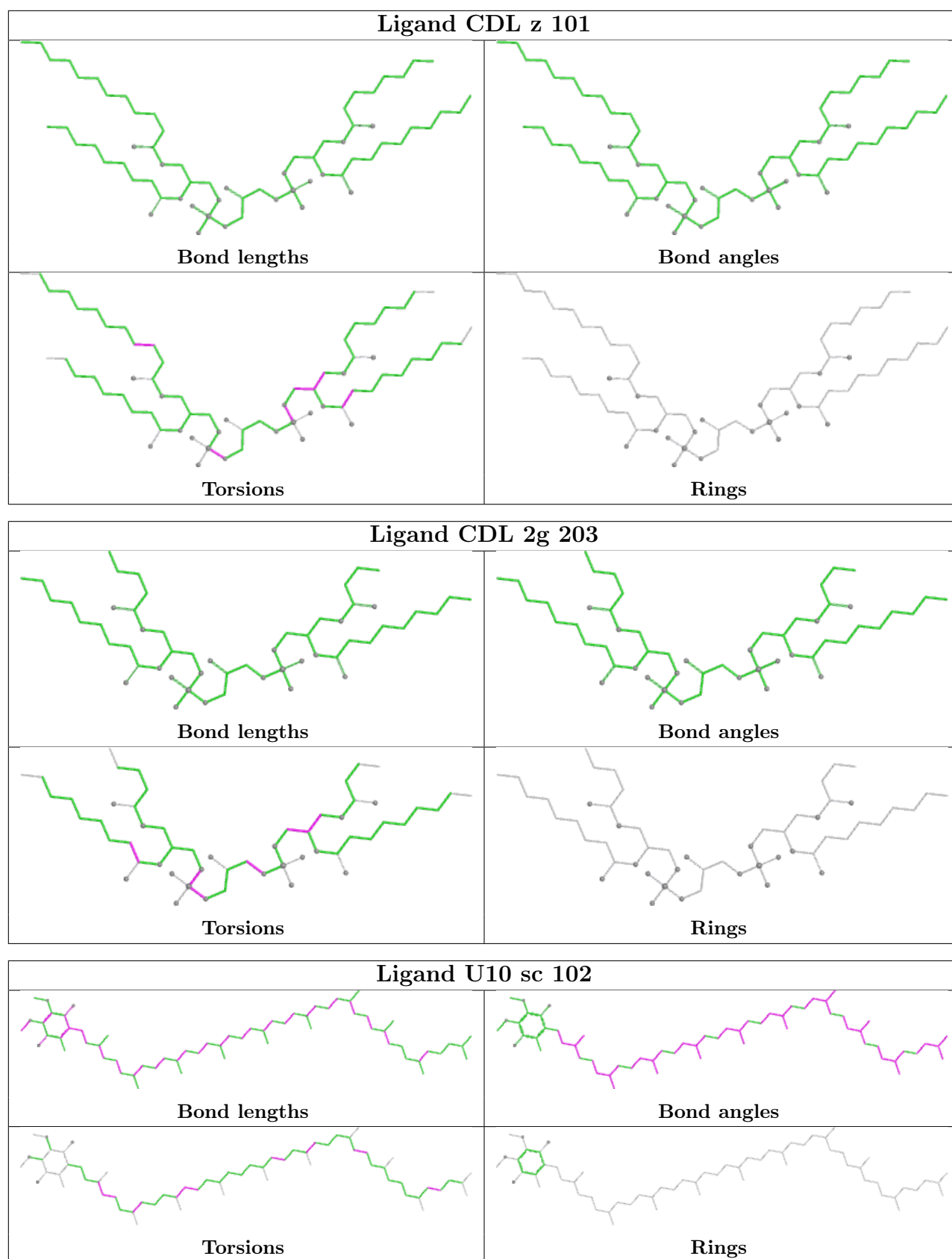


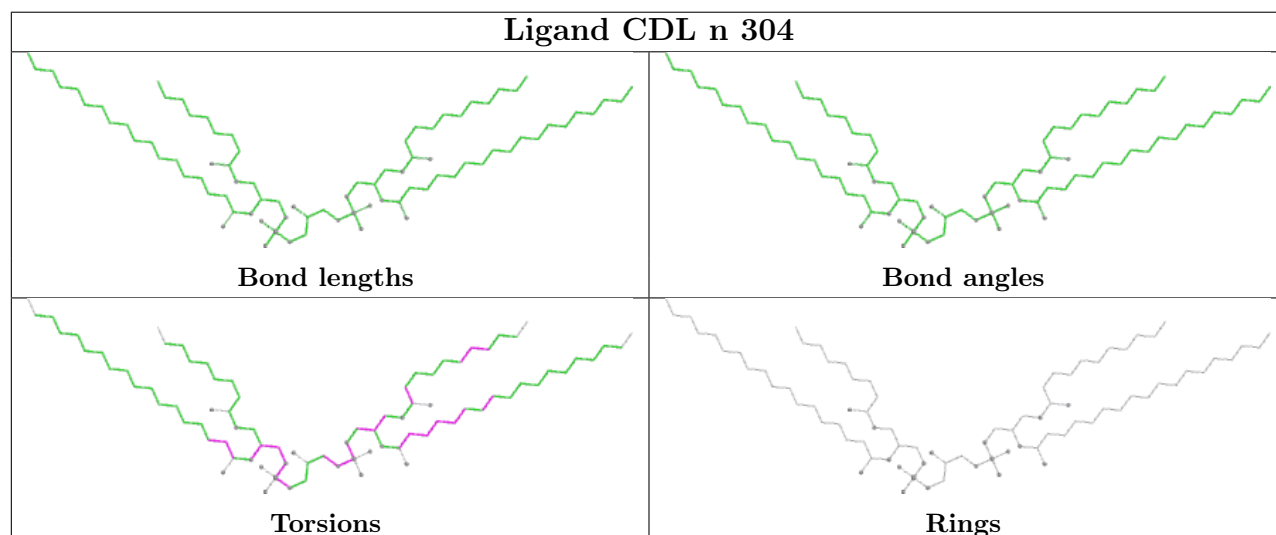
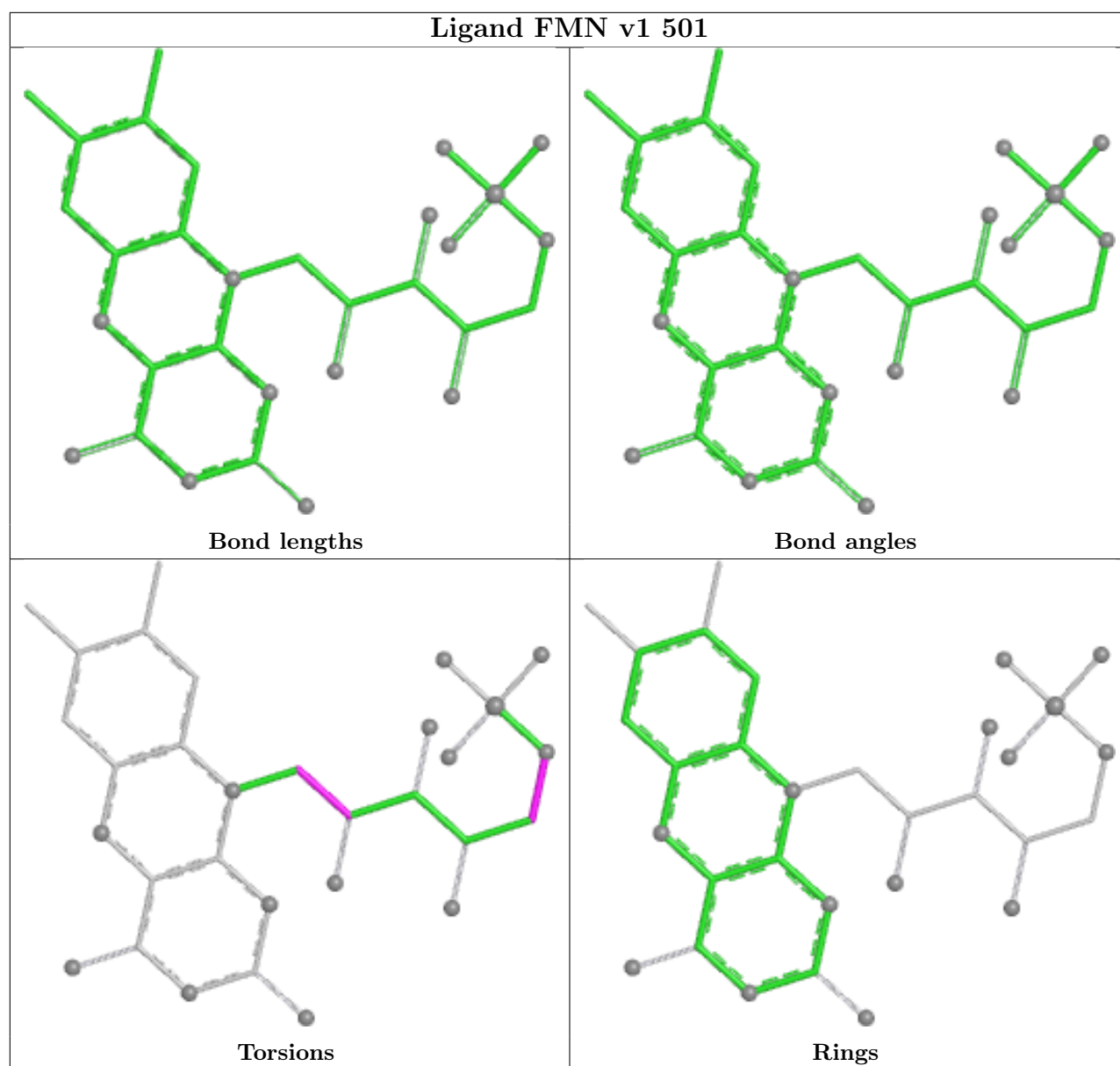
Ligand PC1 V 201

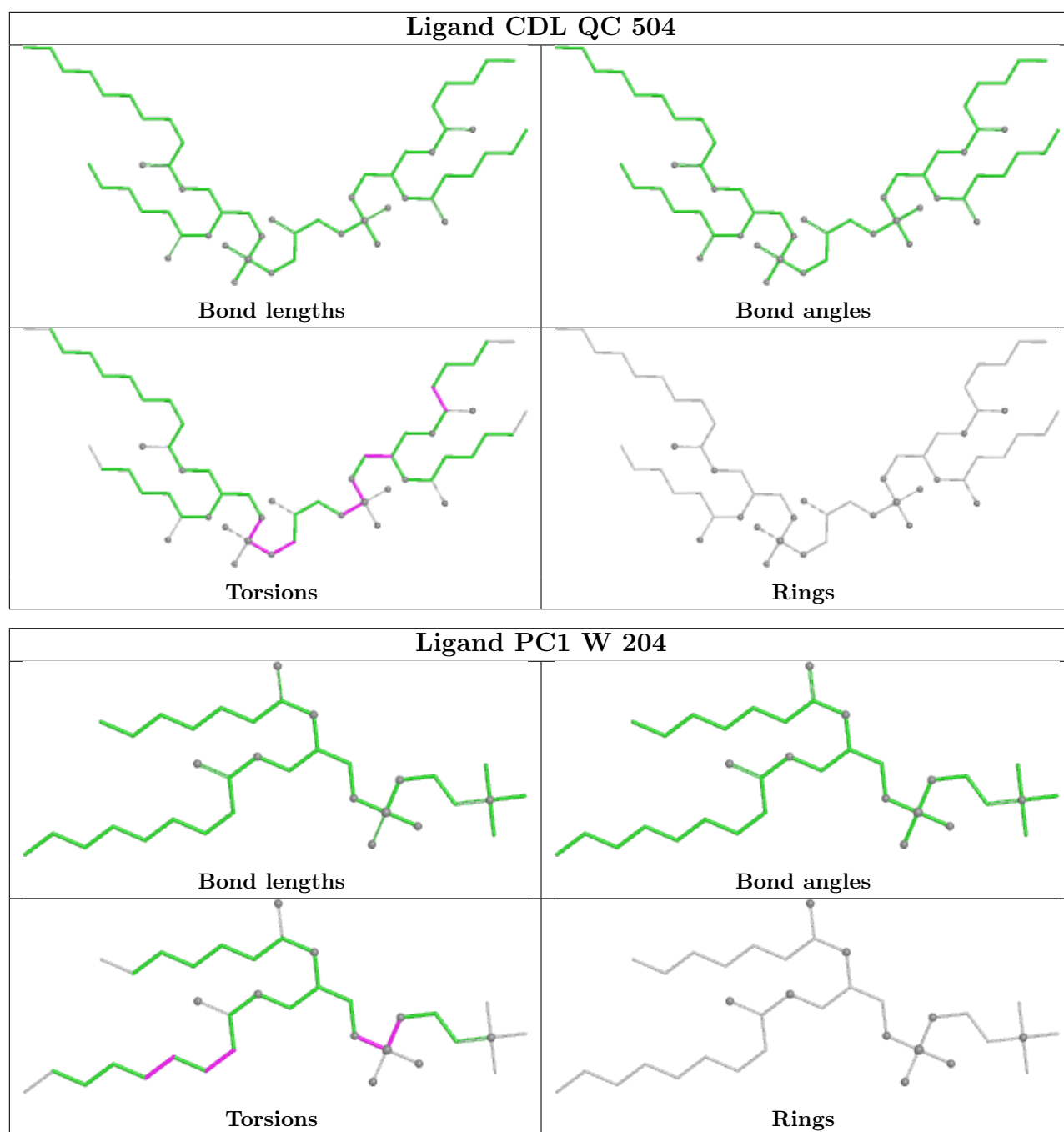


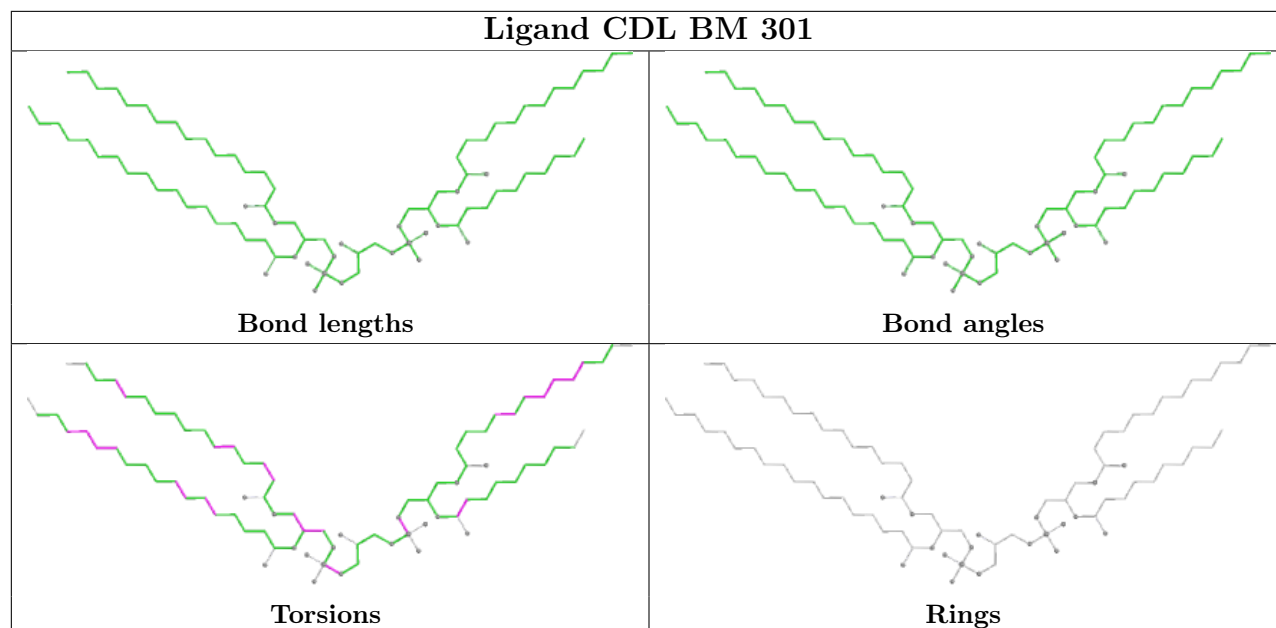
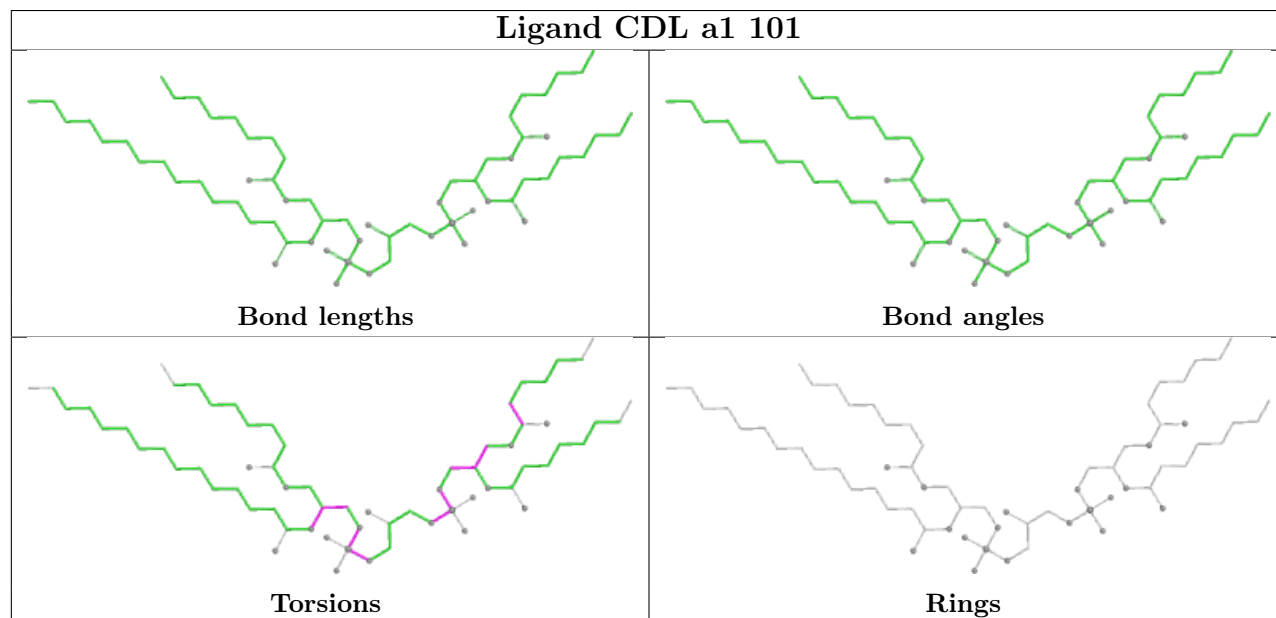


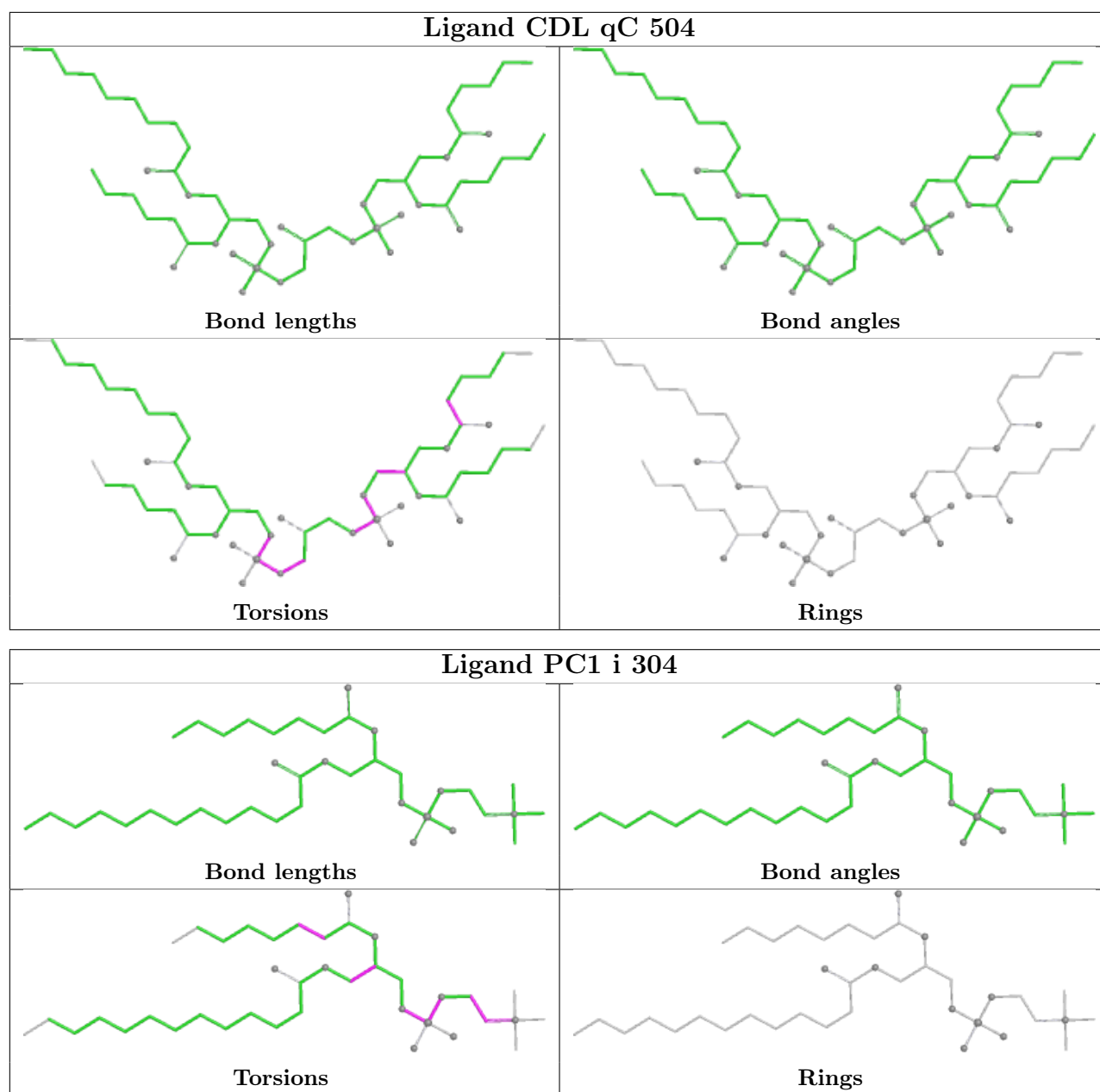


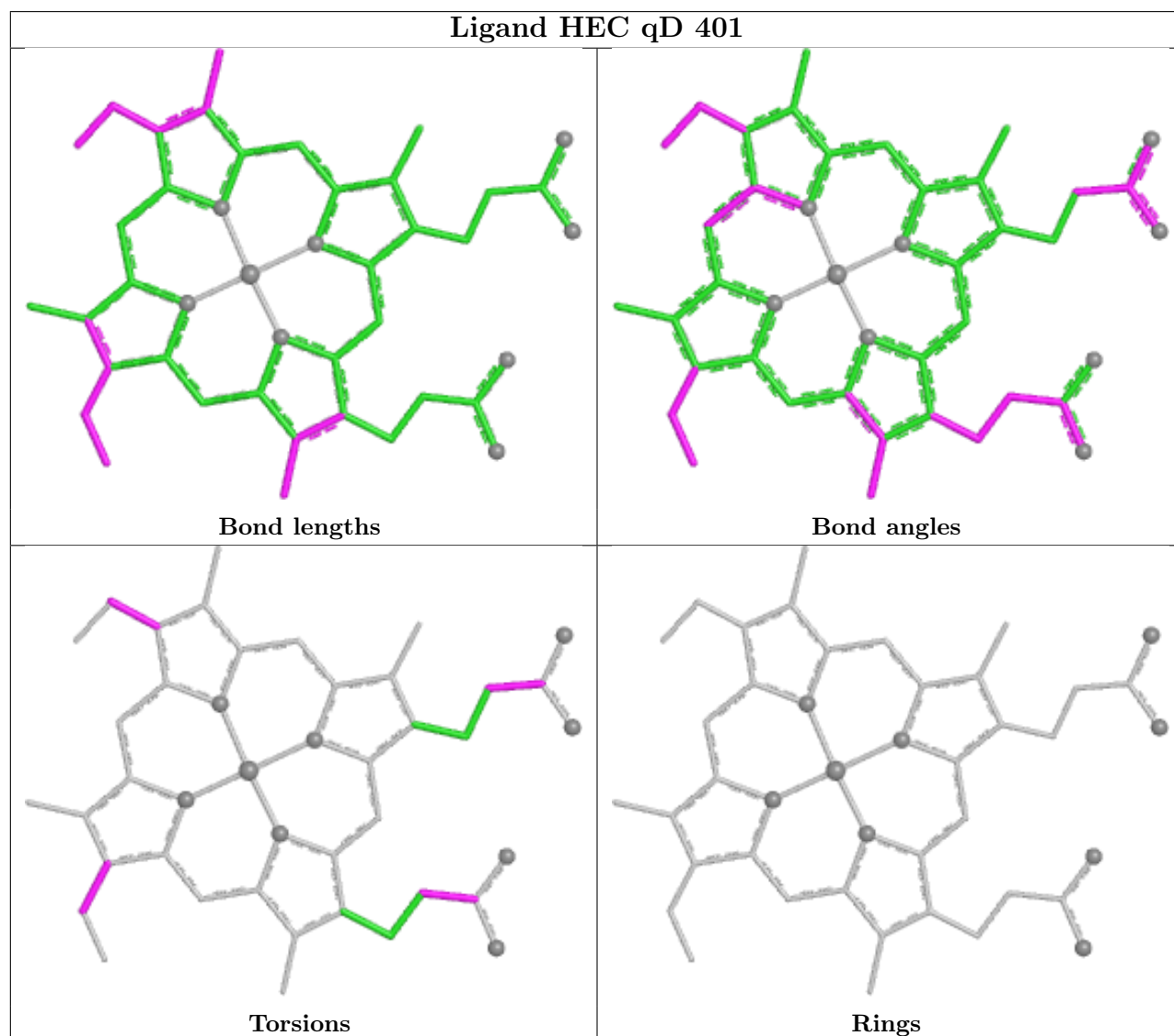
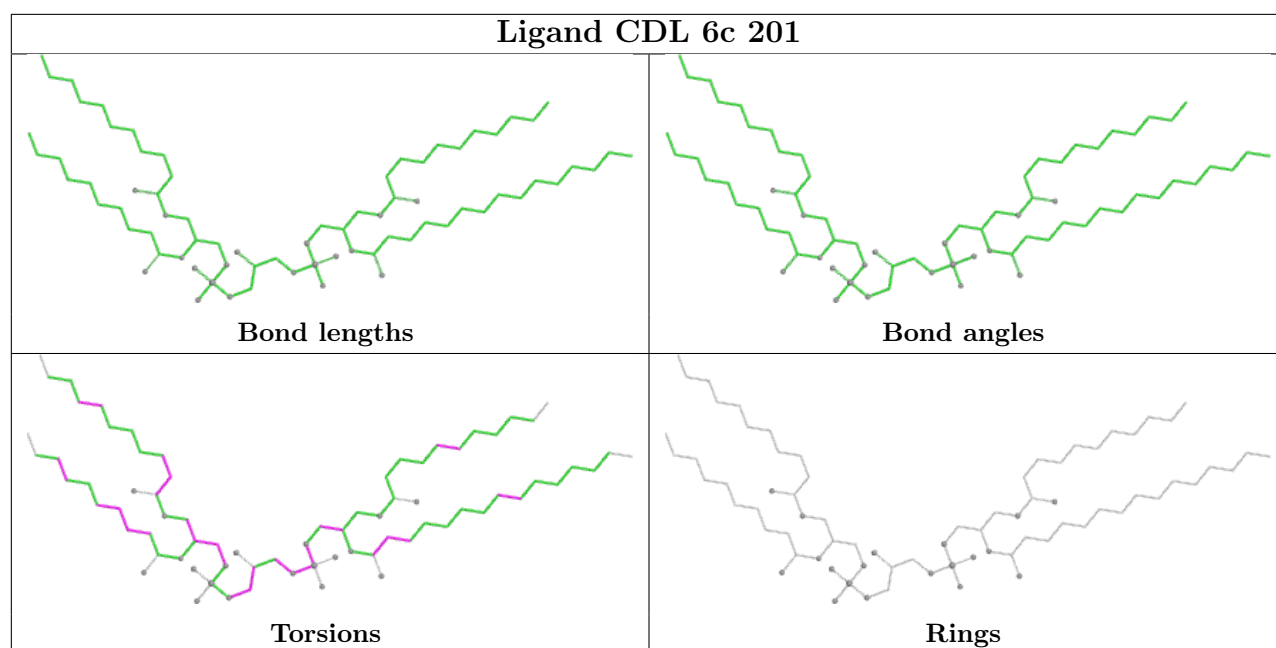


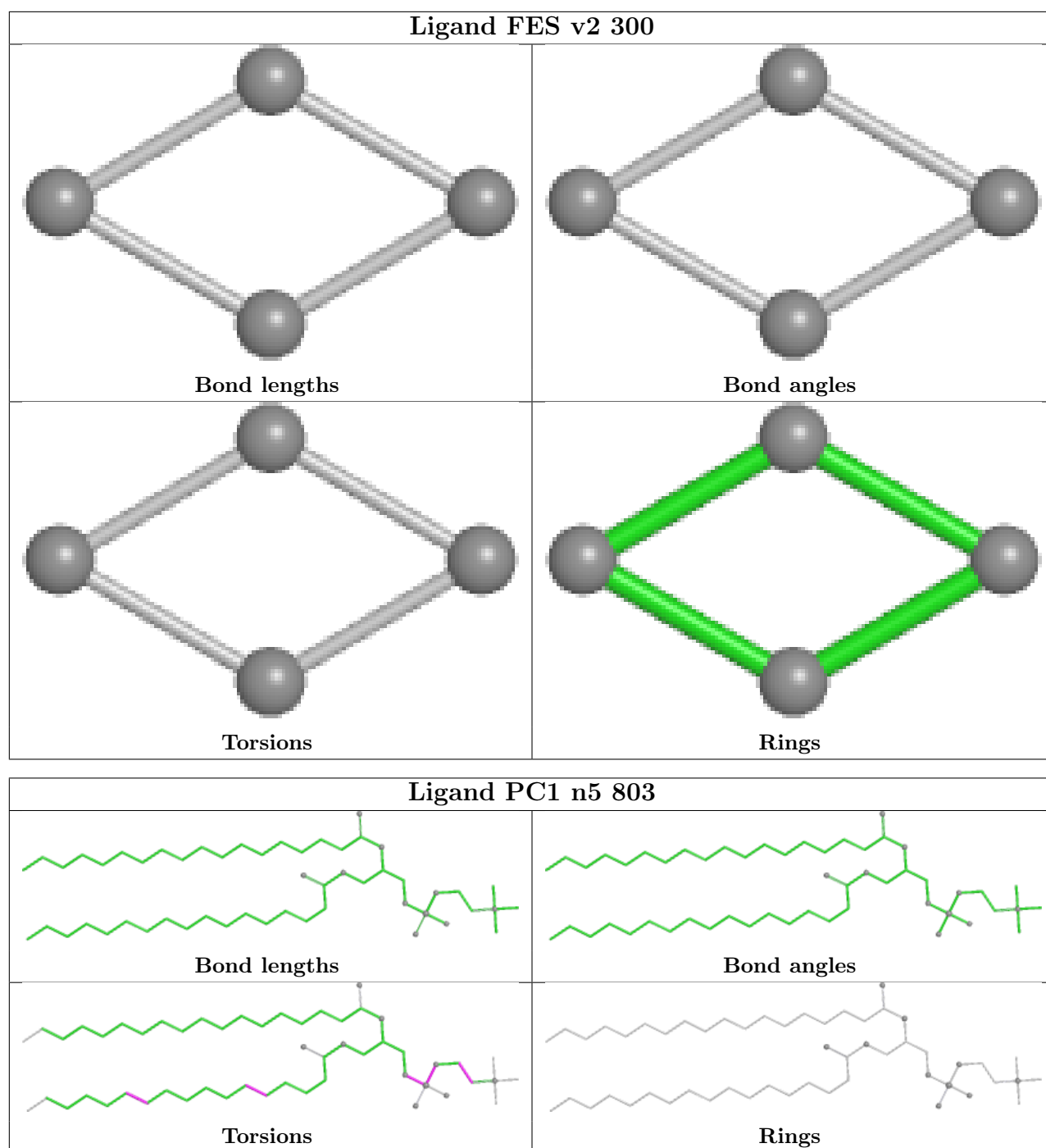


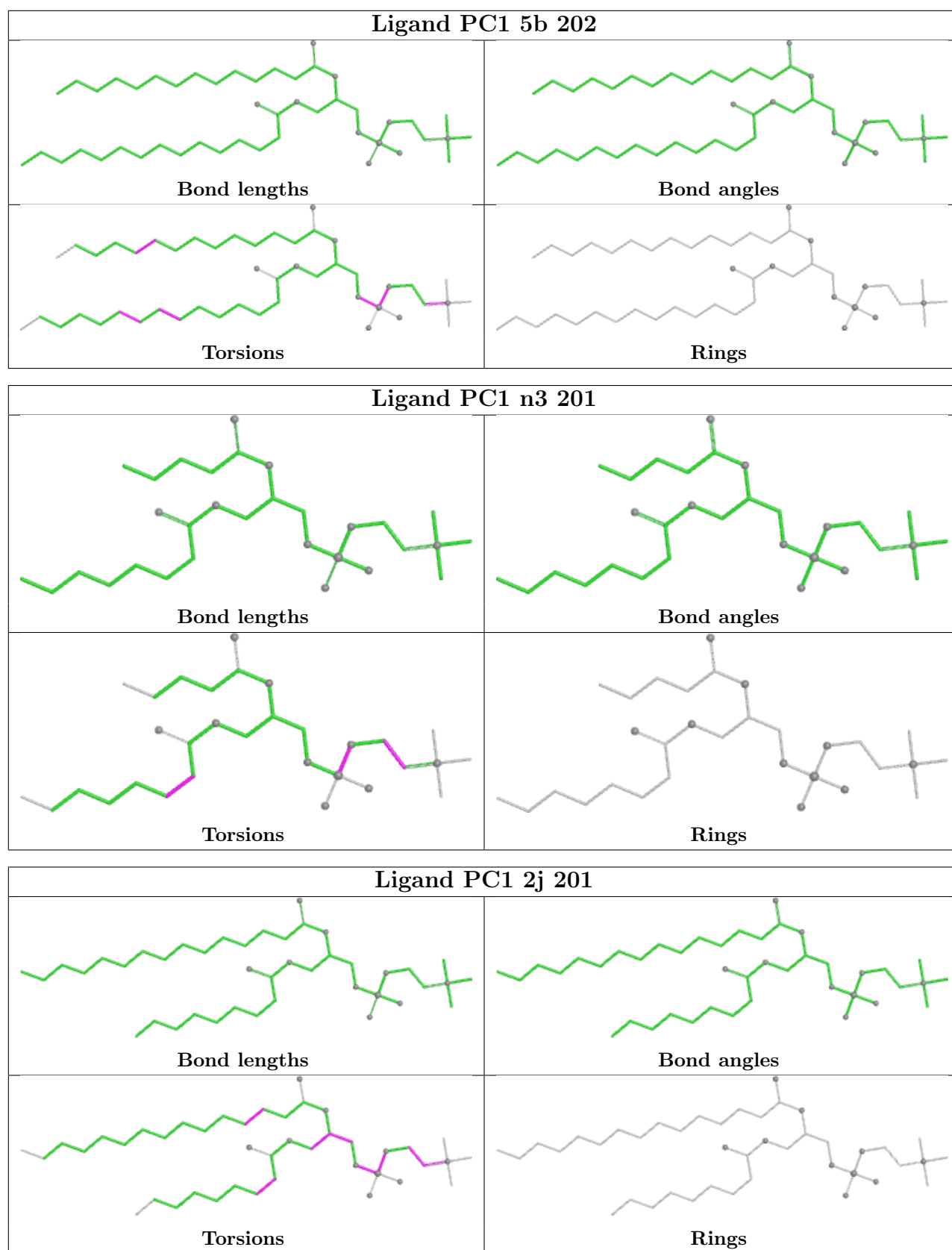


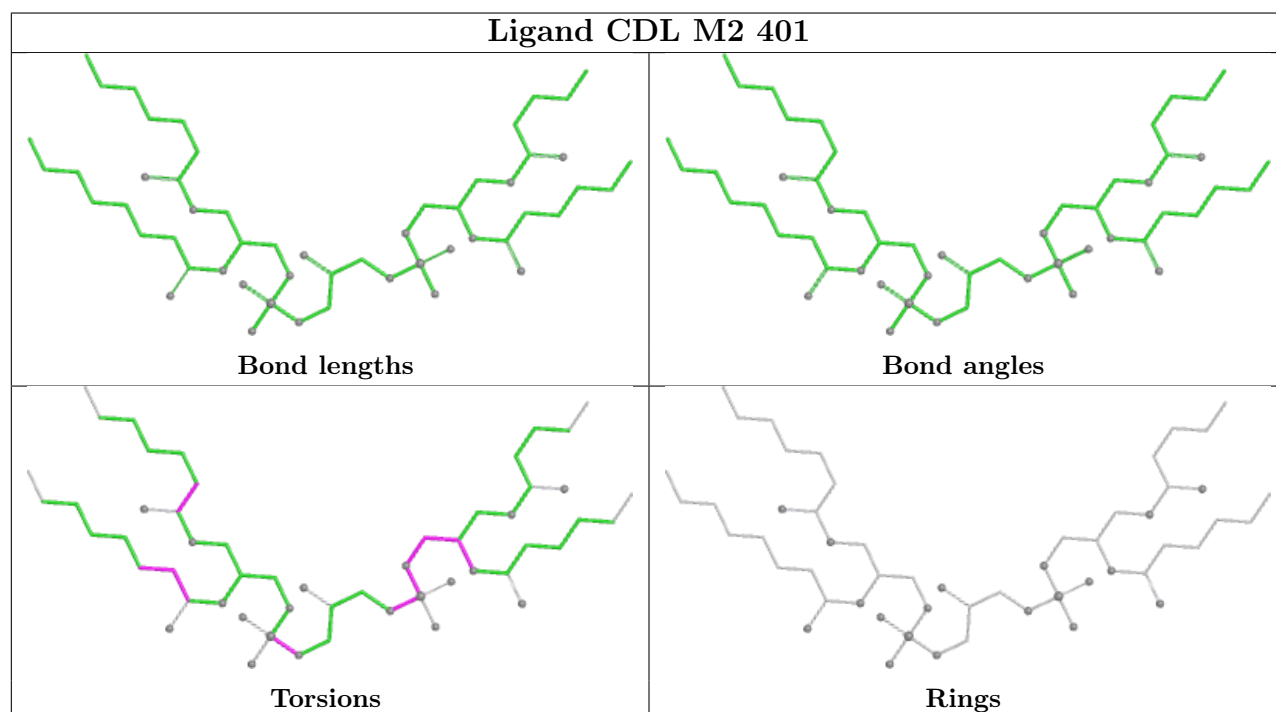
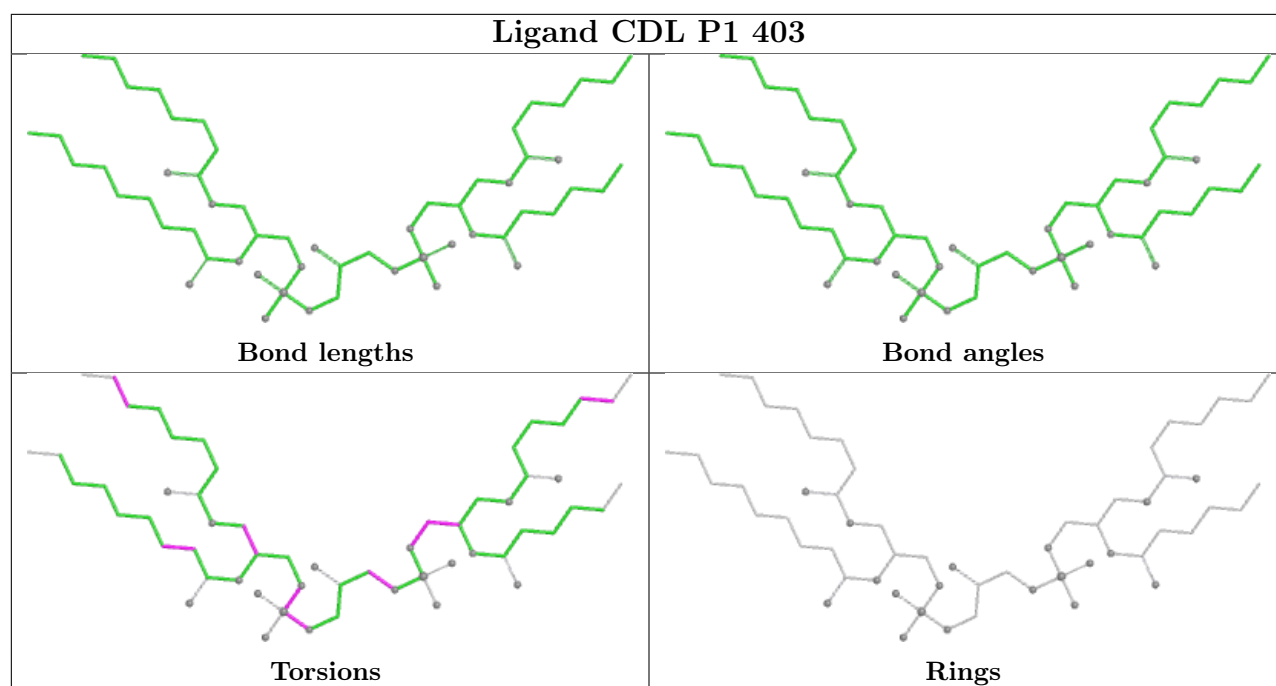
Ligand CDL BM 301**Ligand CDL a1 101**

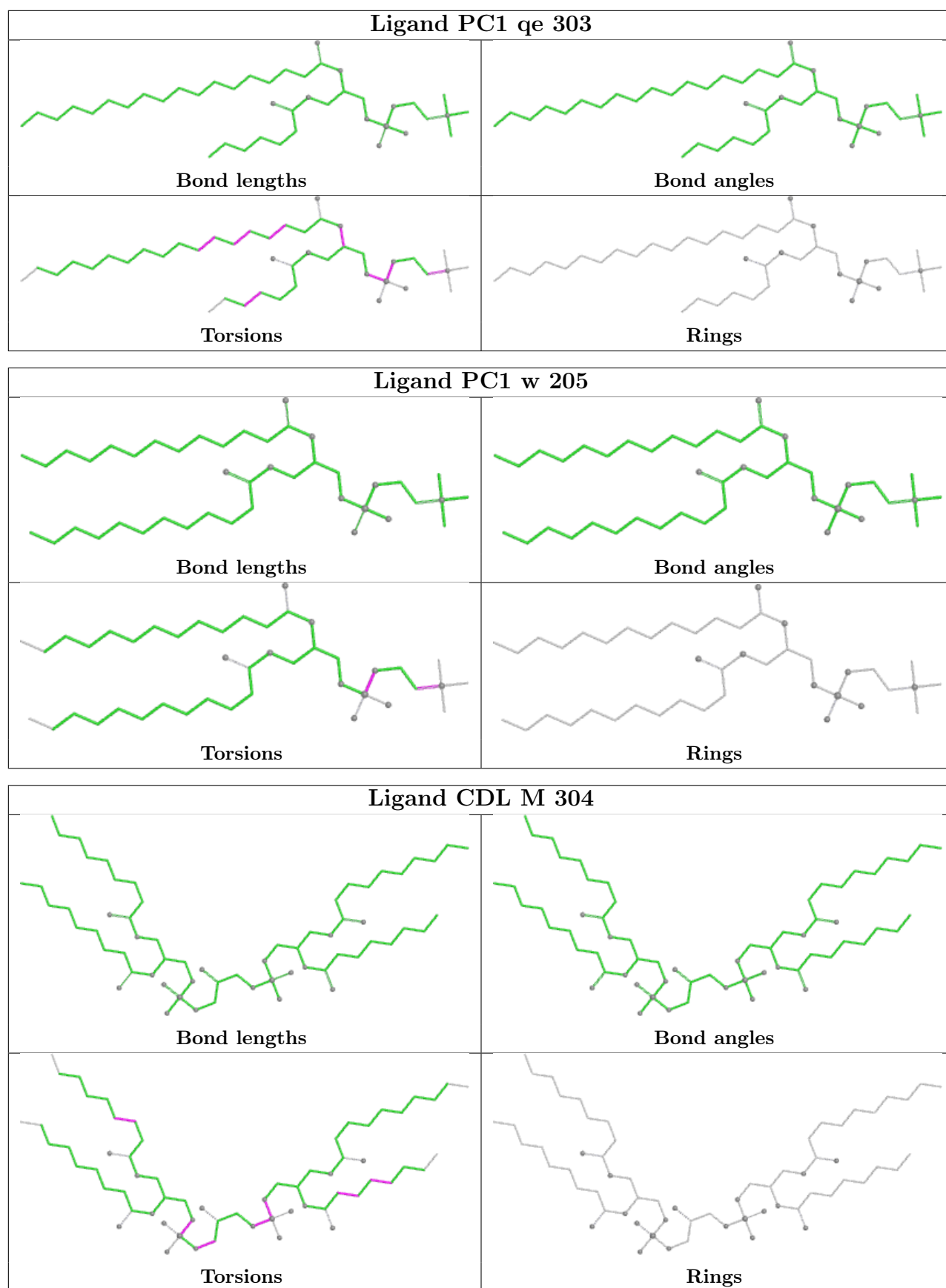


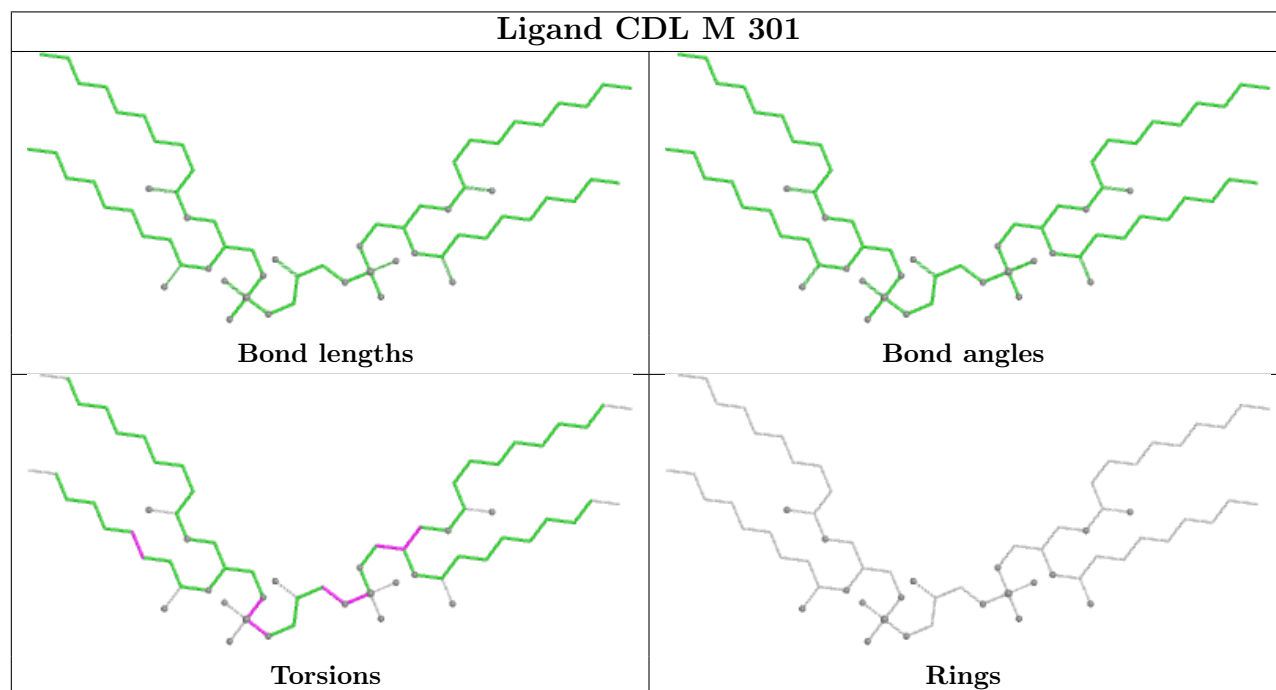
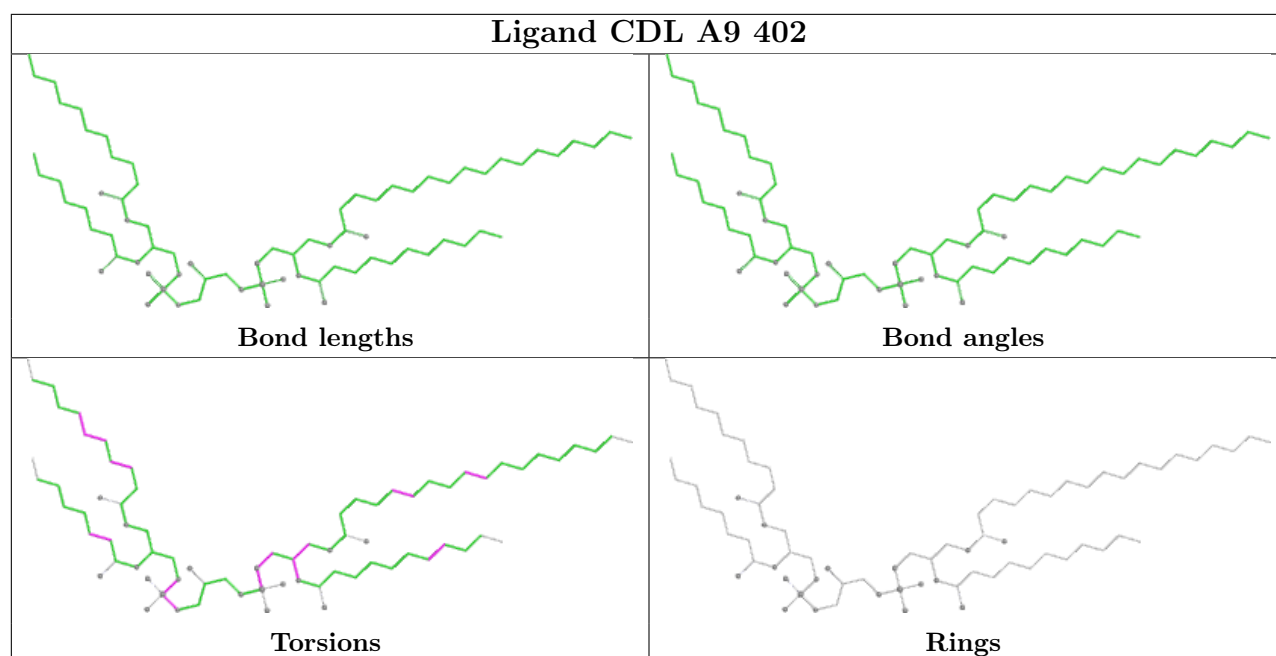


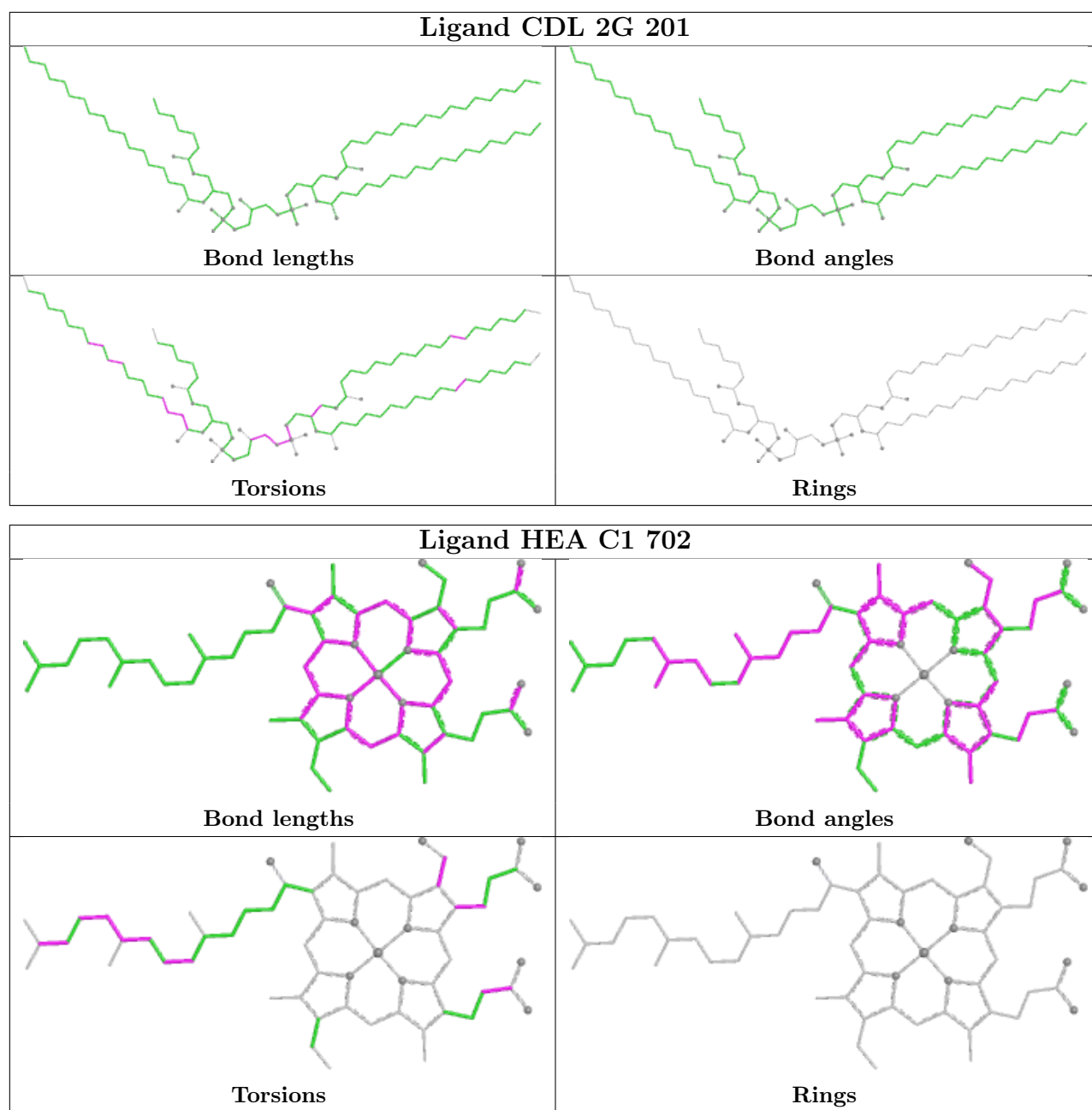


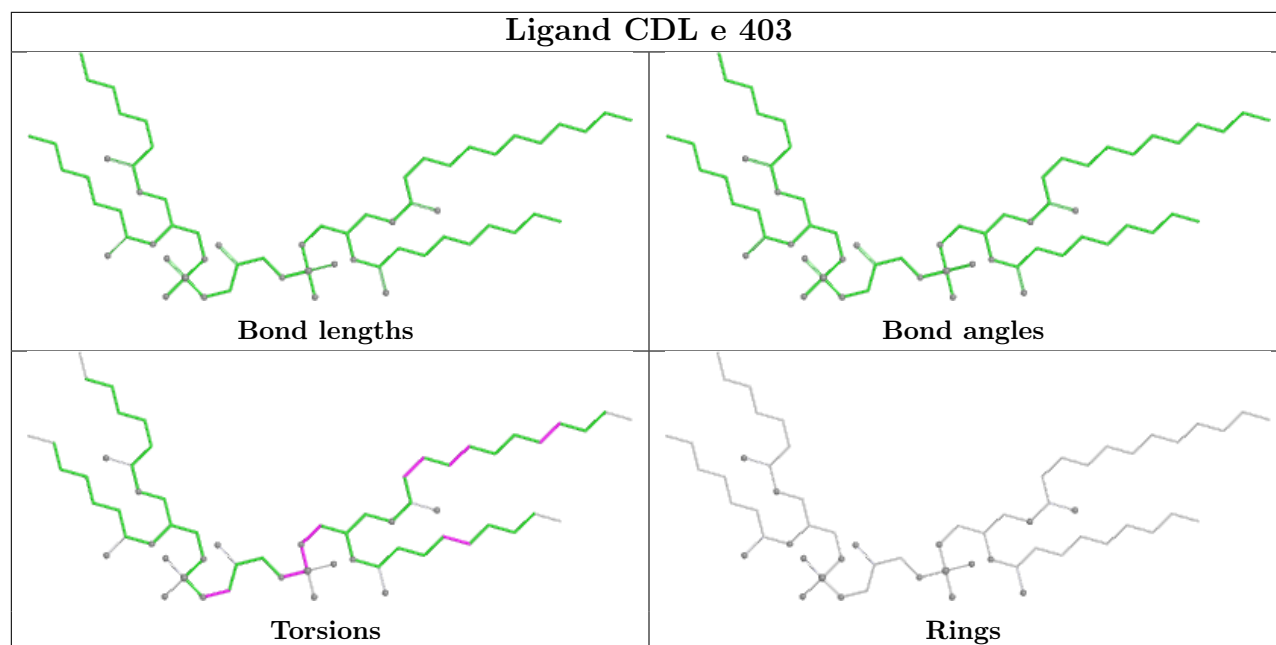
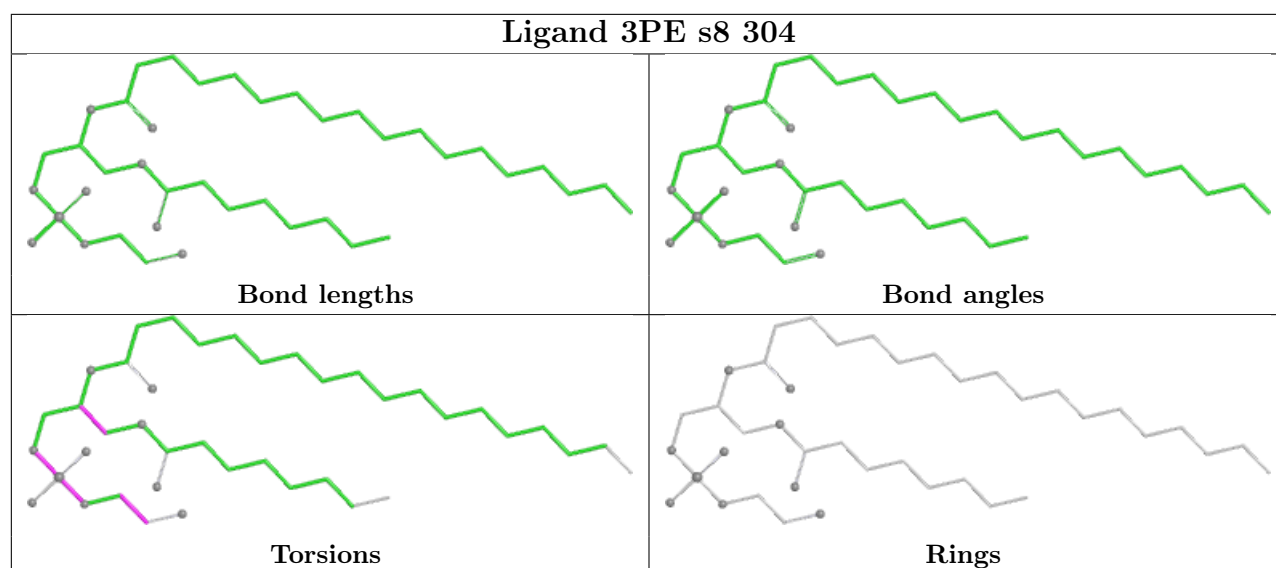


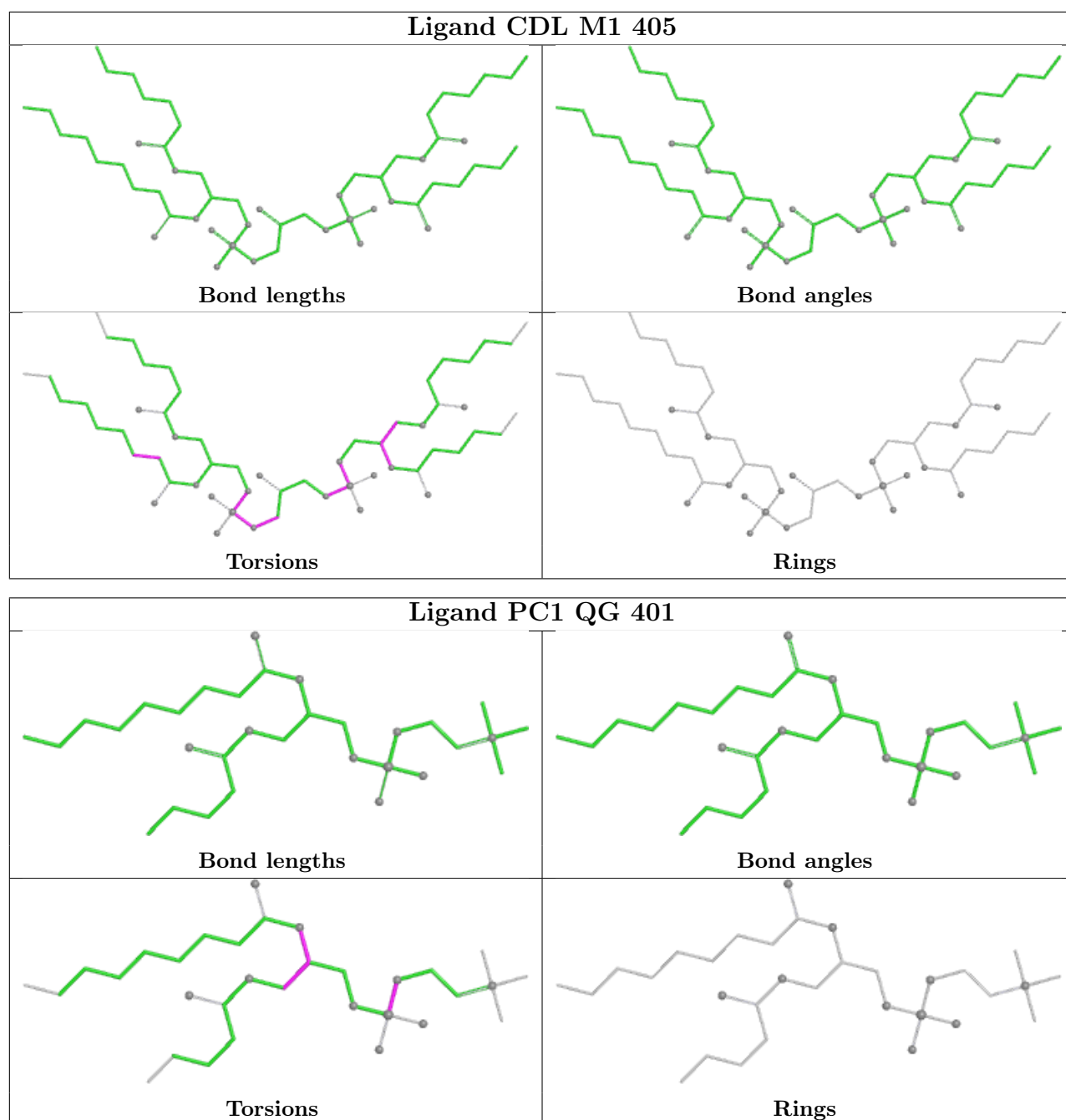


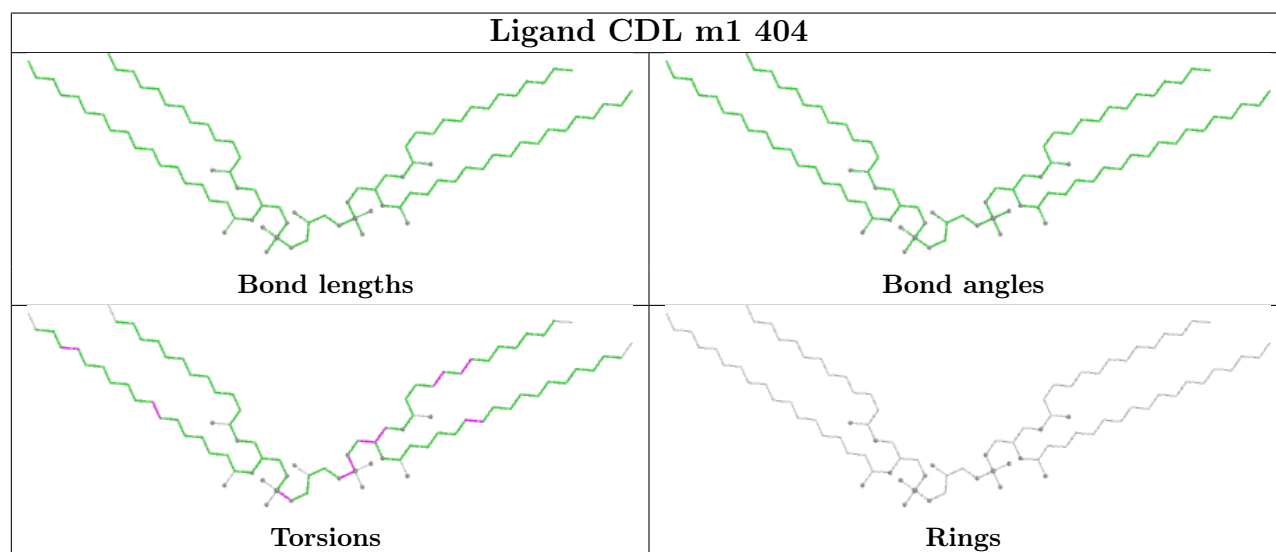
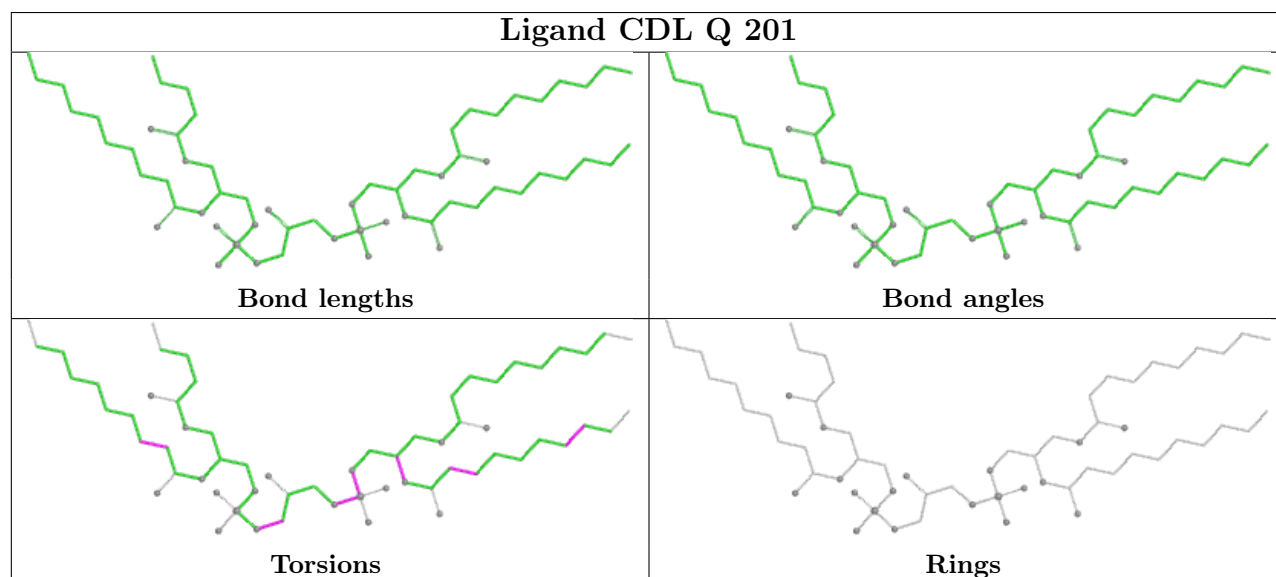
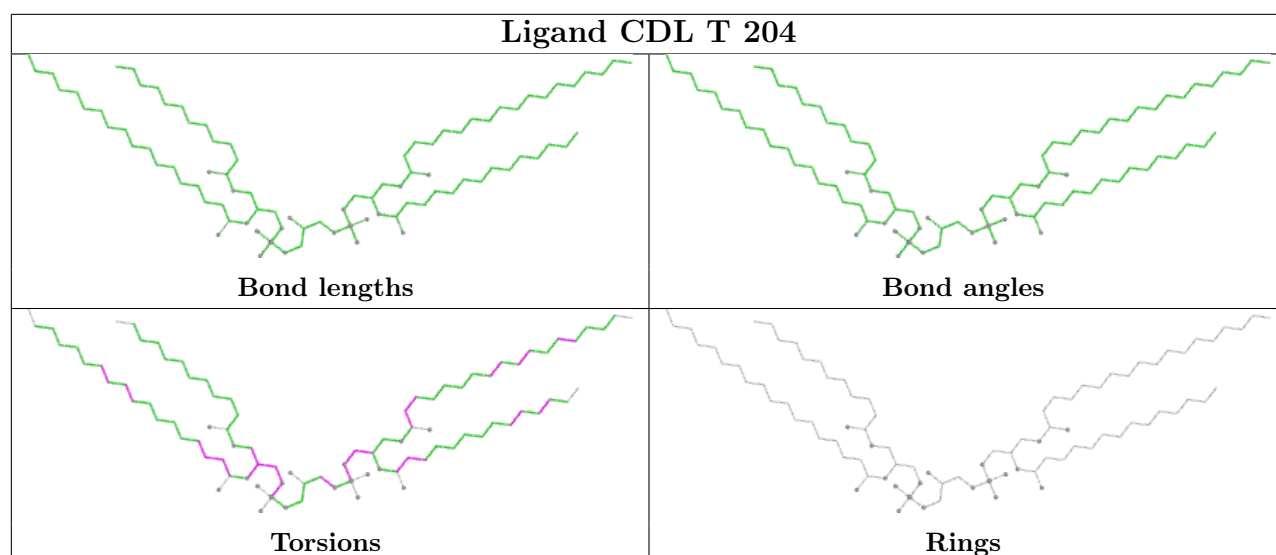


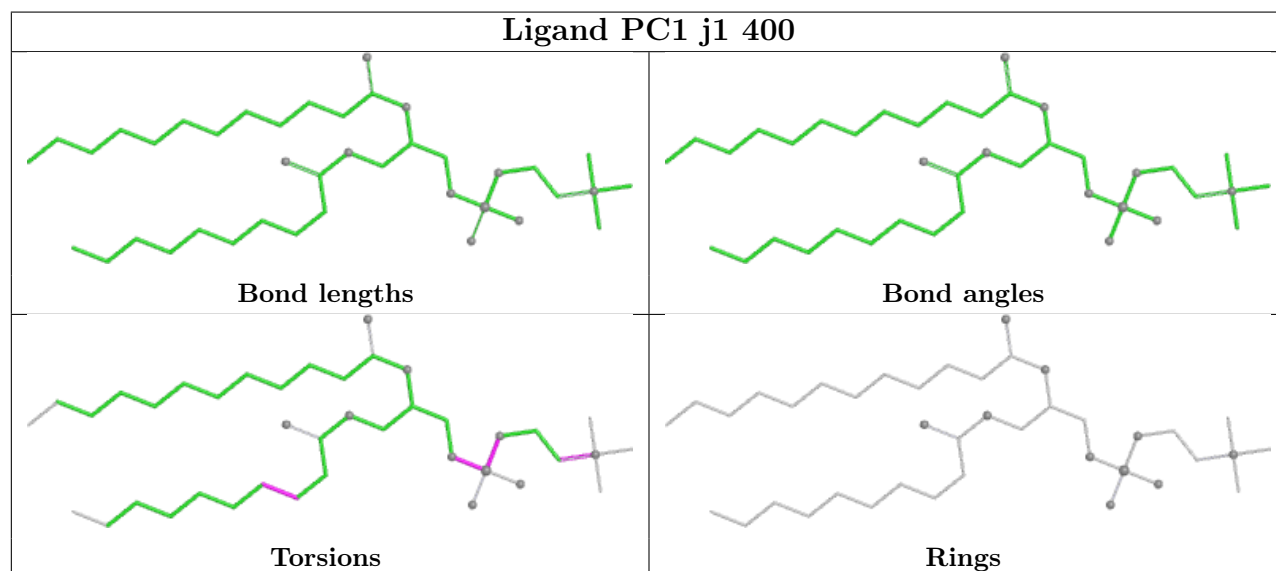
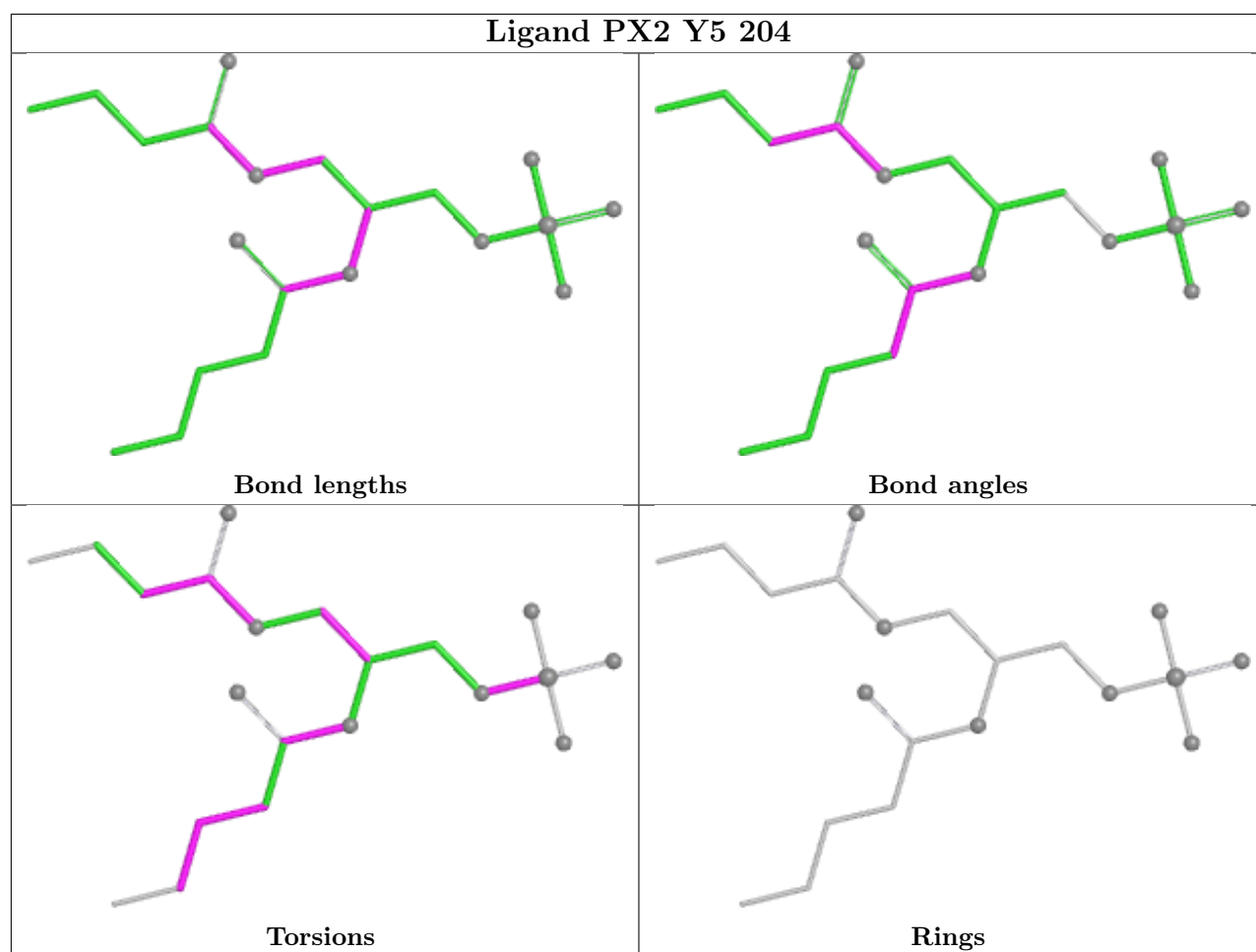


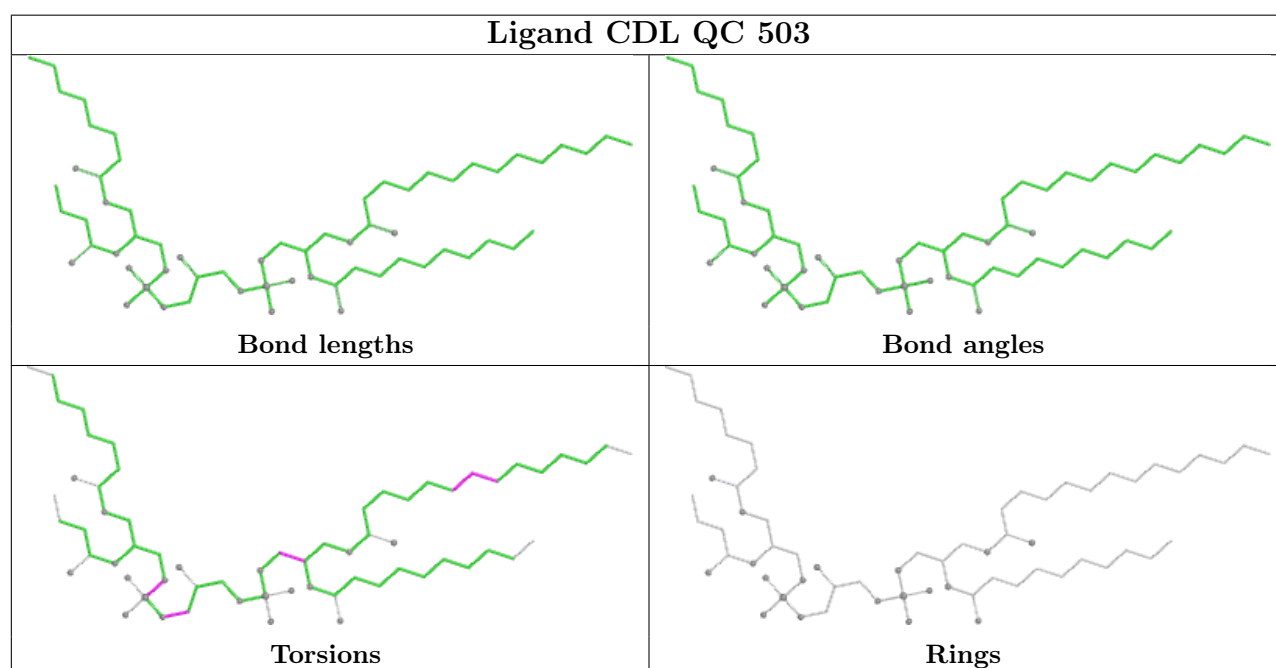
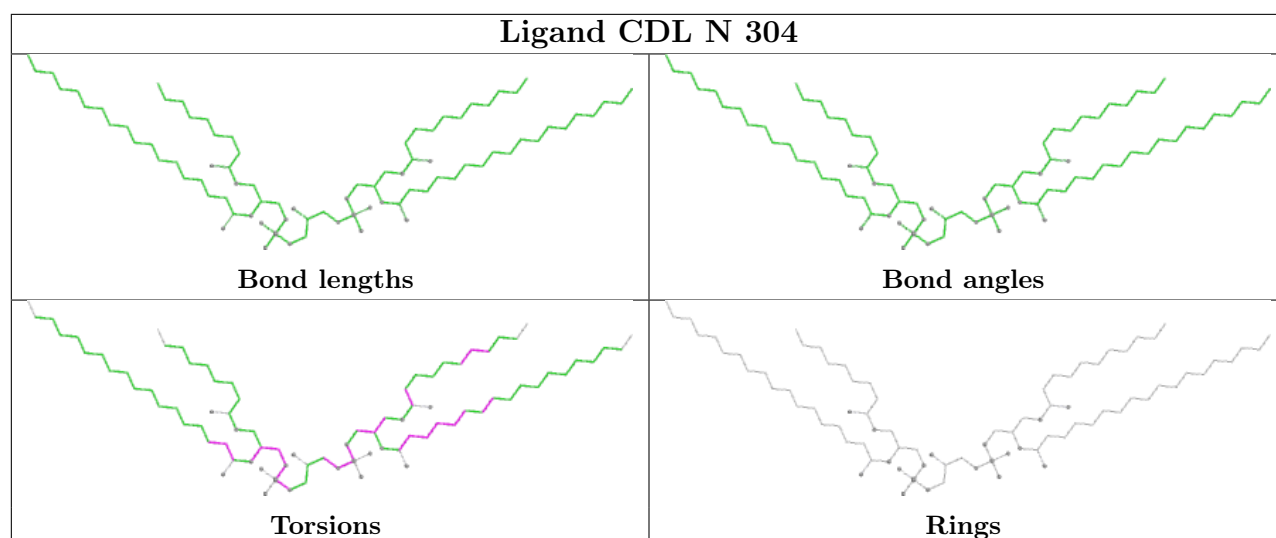




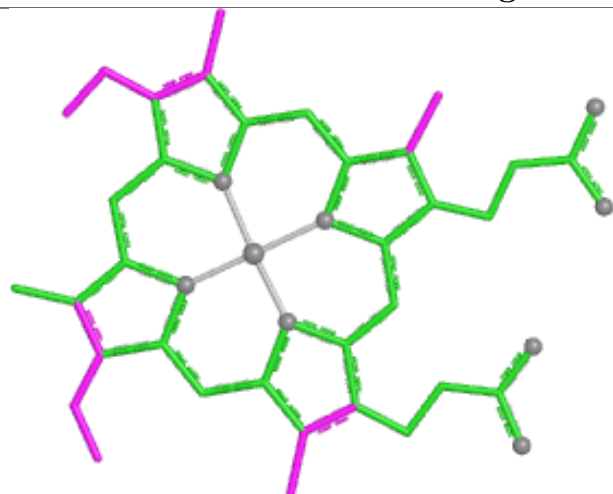




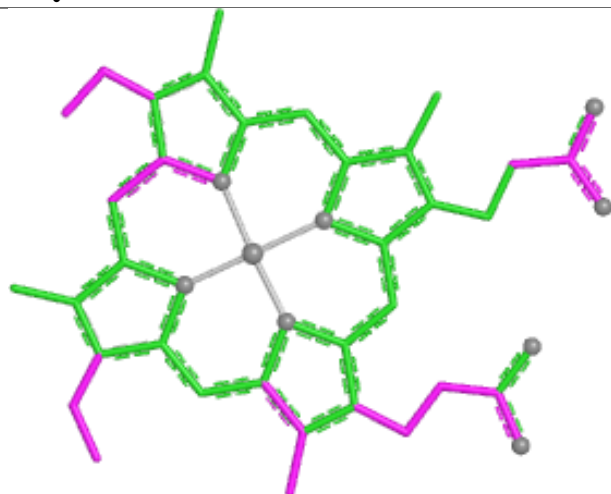




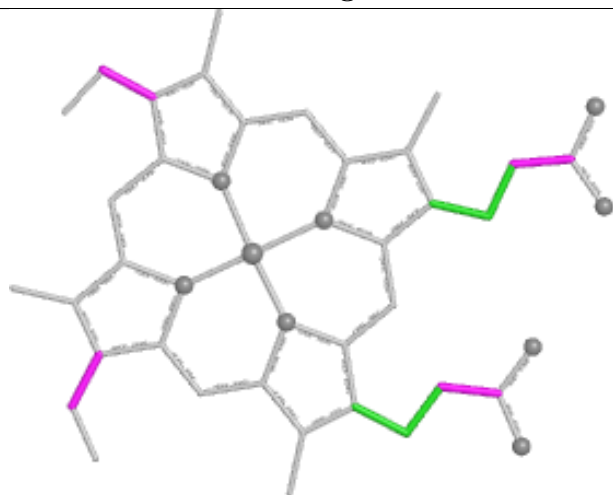
Ligand HEC QD 401



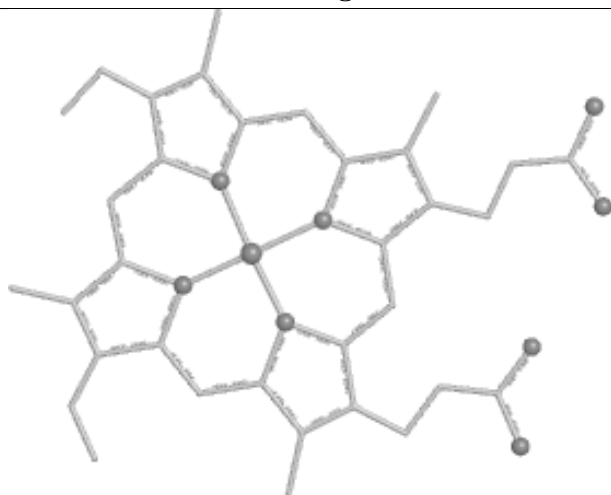
Bond lengths



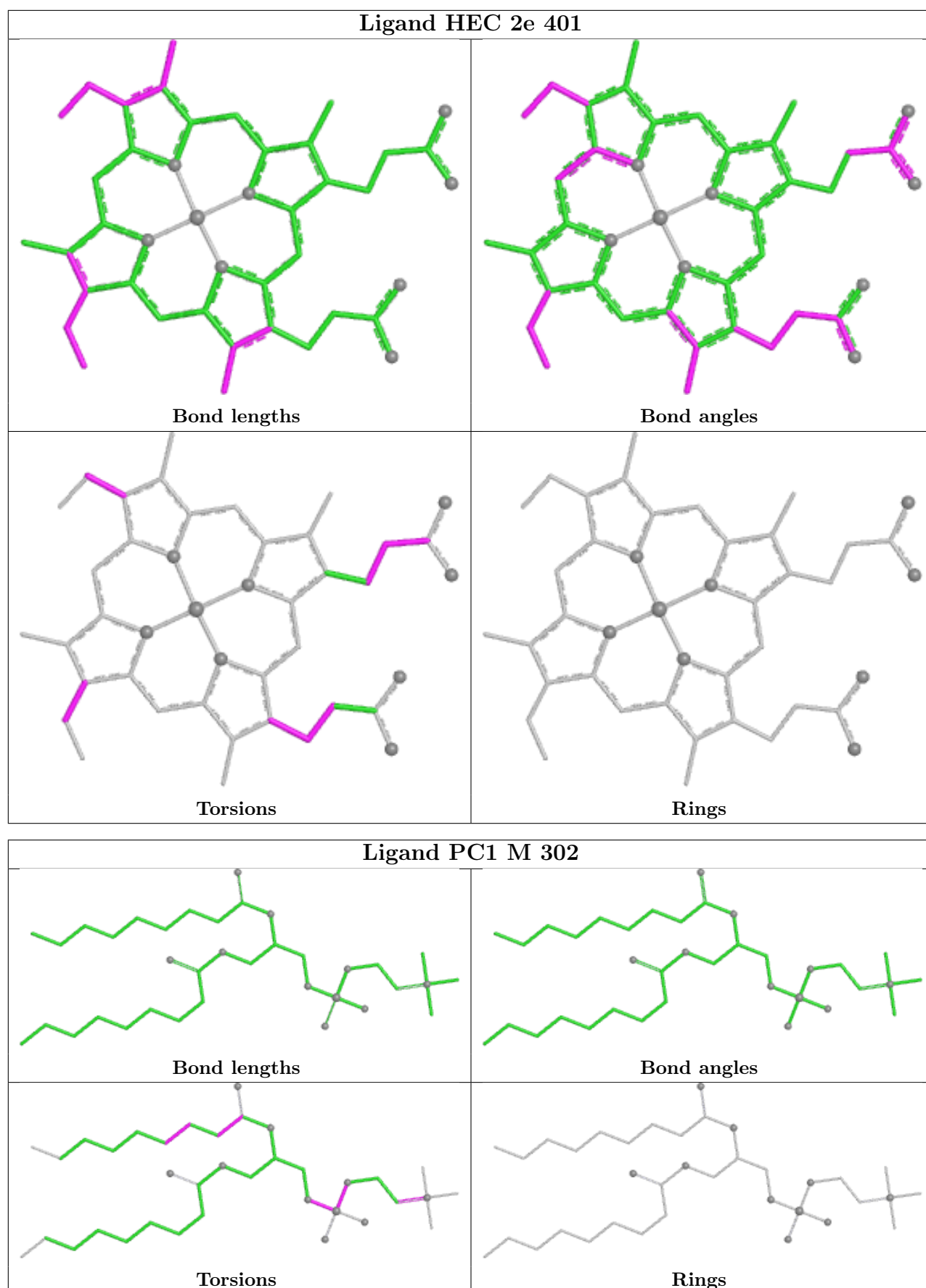
Bond angles

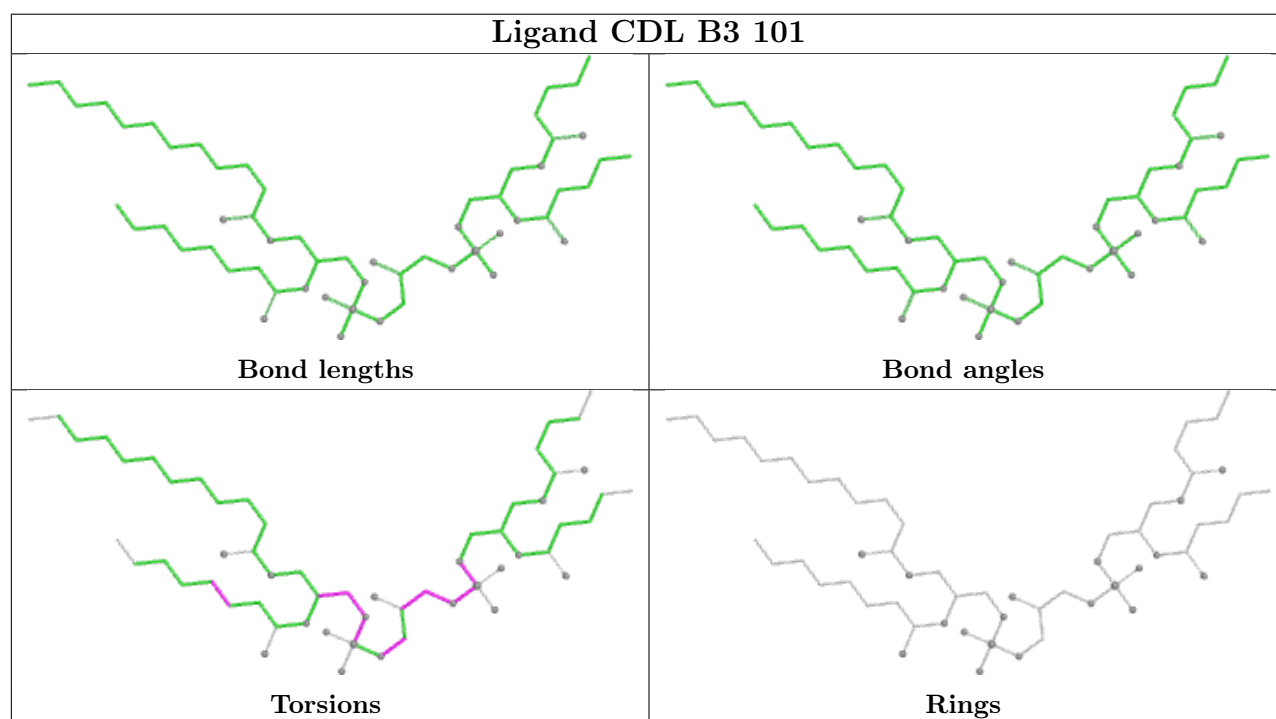
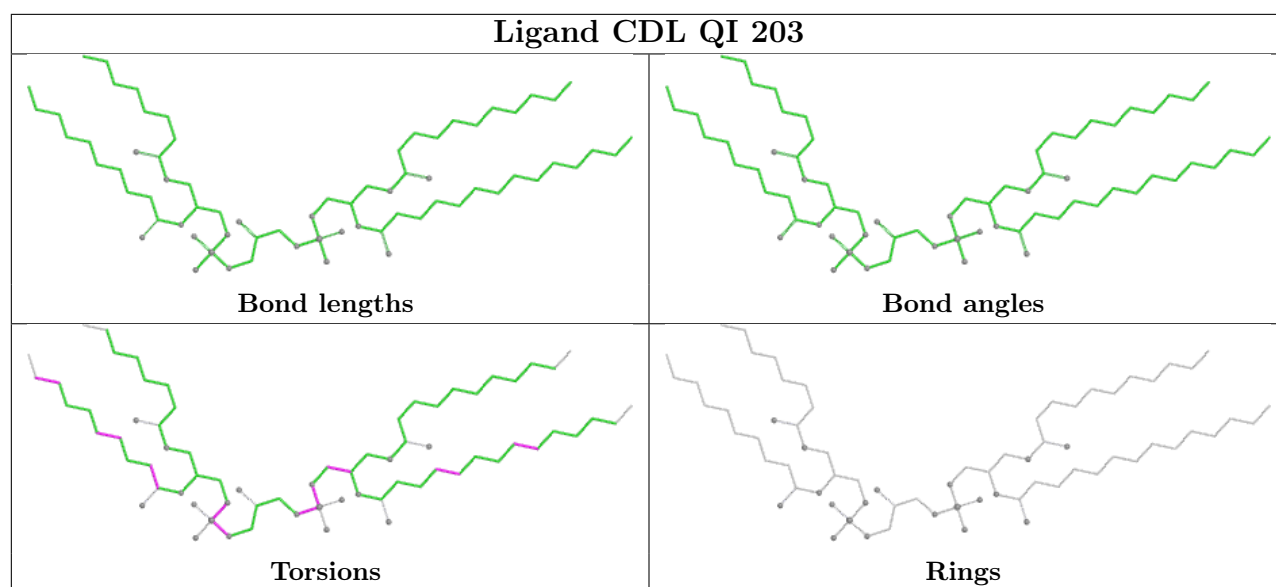


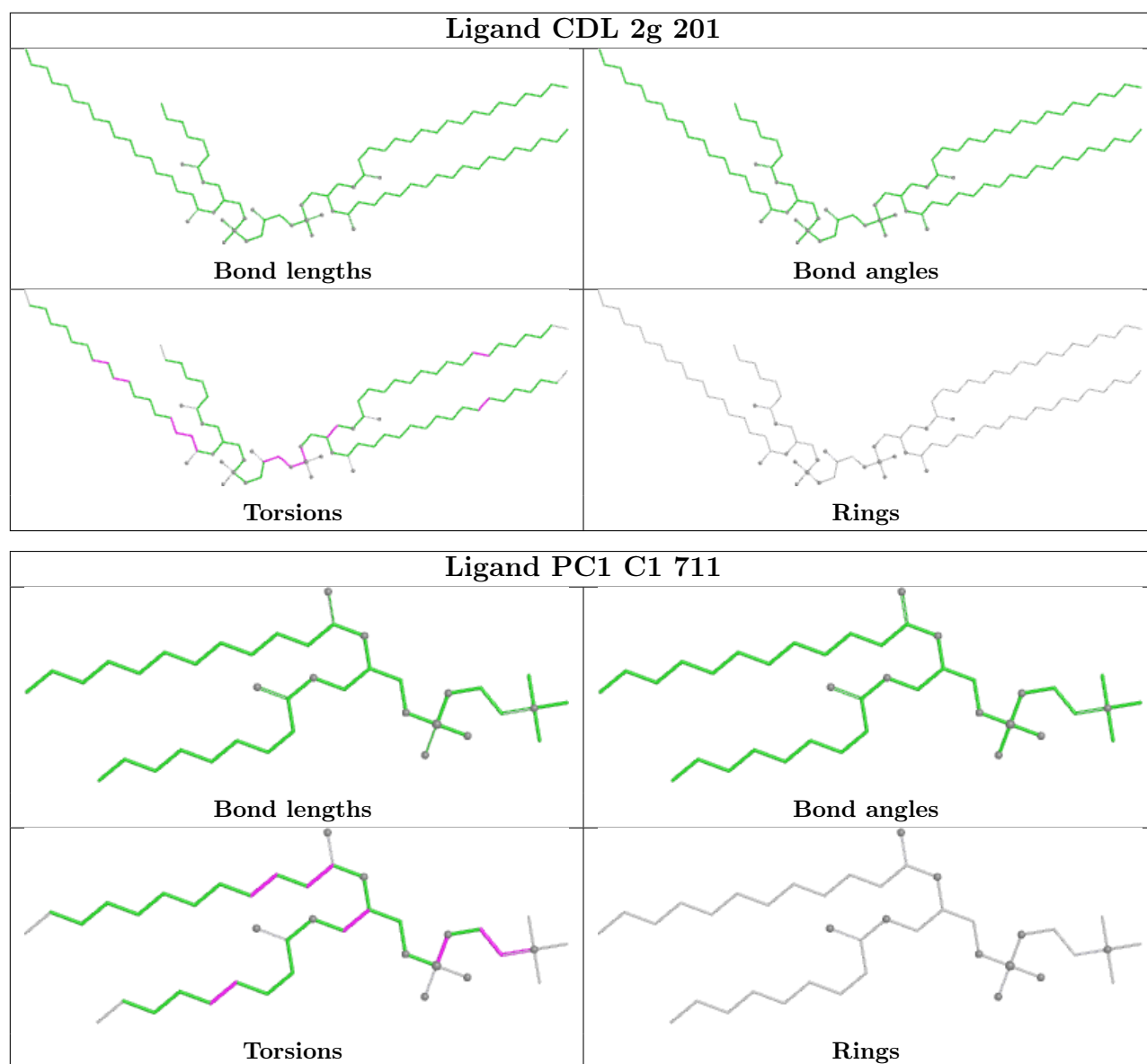
Torsions



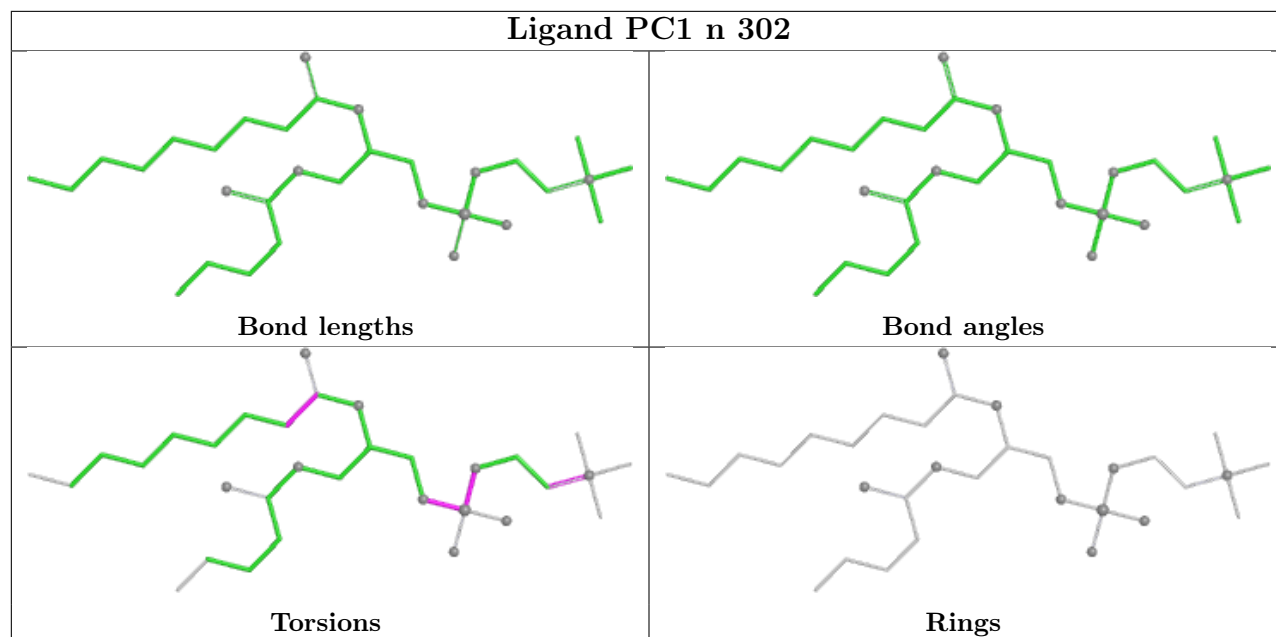
Rings



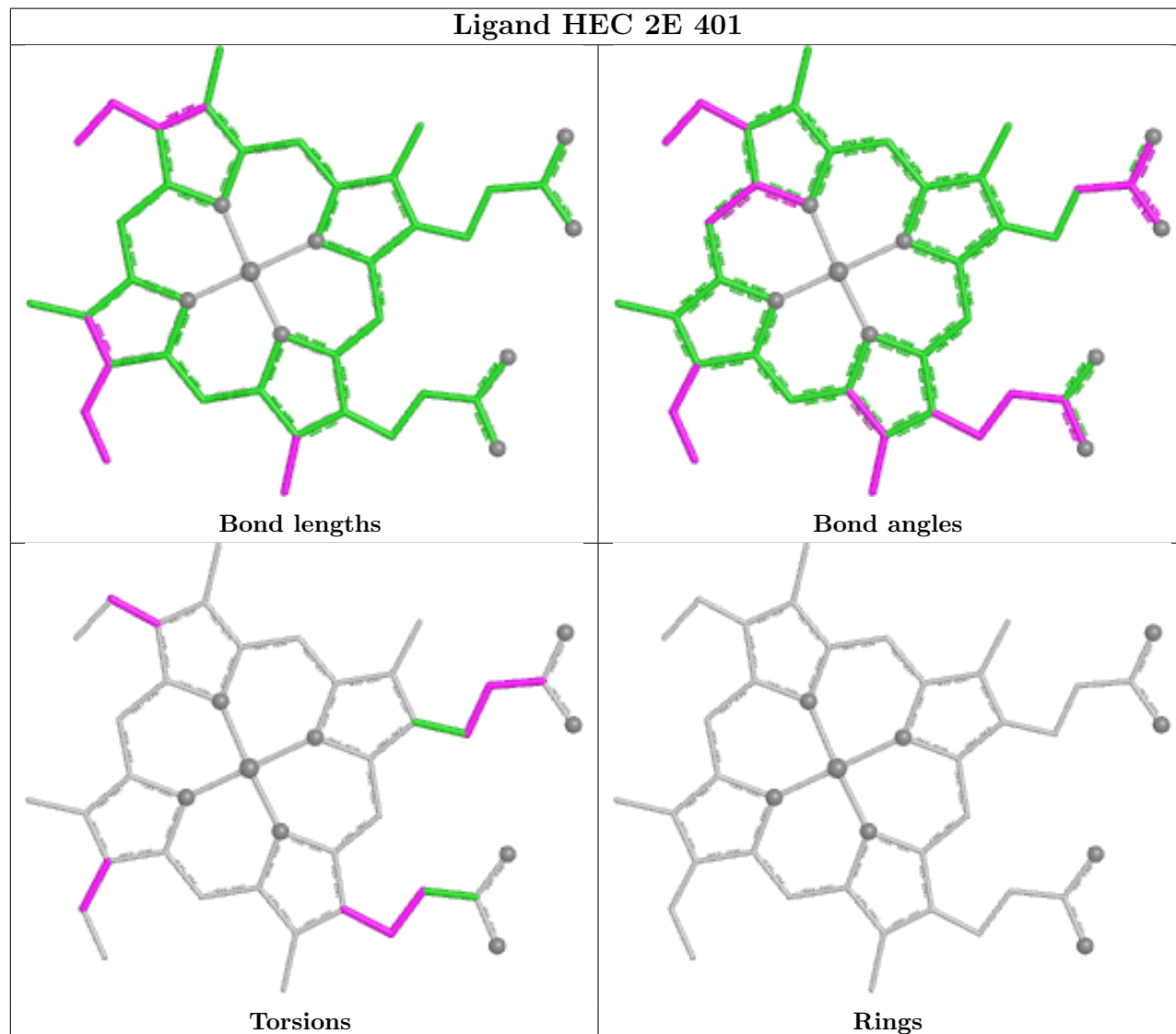


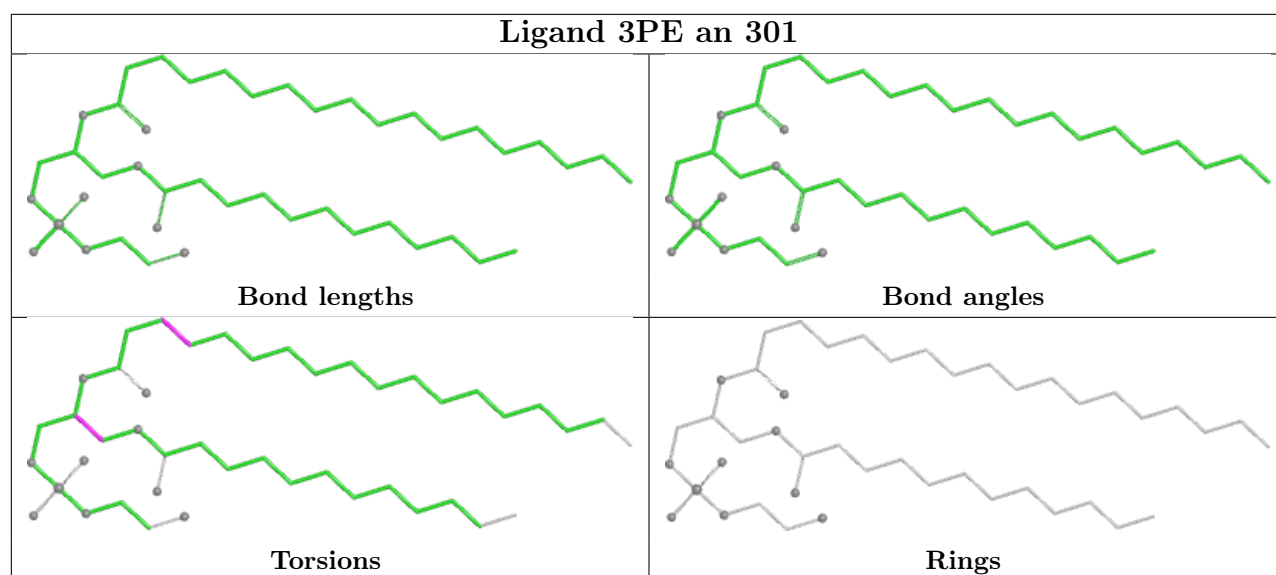


Ligand PC1 n 302



Ligand HEC 2E 401





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.

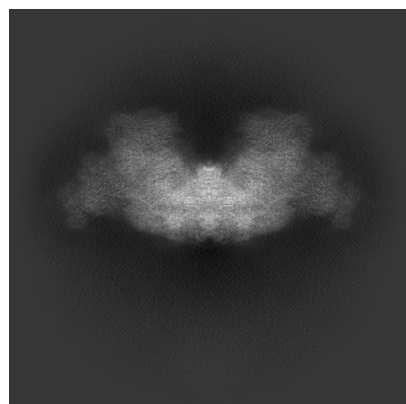
6 Map visualisation [i](#)

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.

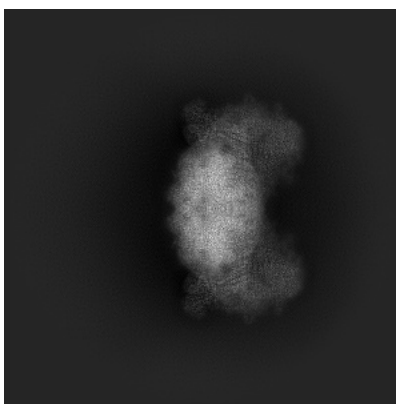
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

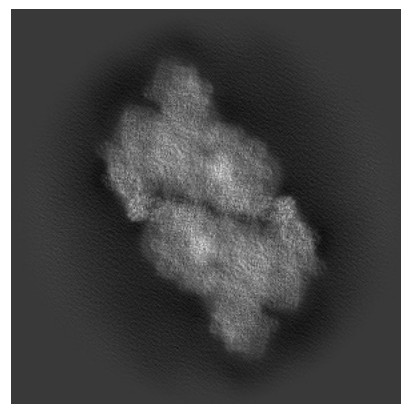
6.1.1 Primary map



X

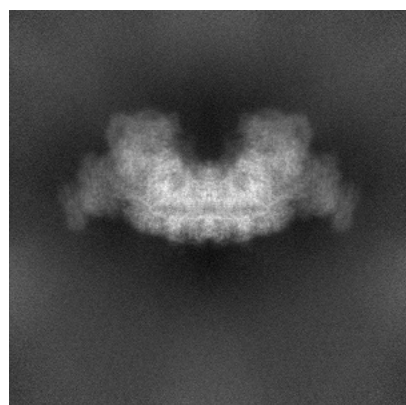


Y

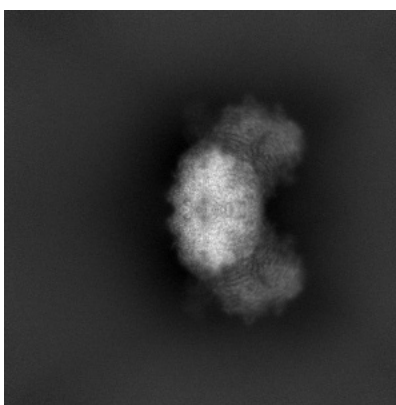


Z

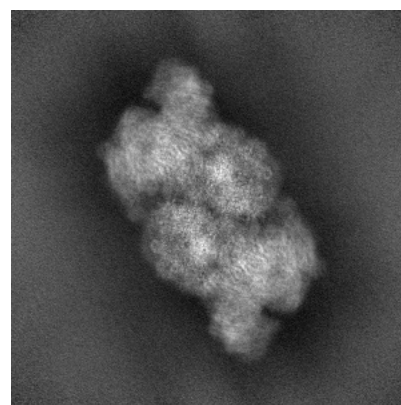
6.1.2 Raw map



X



Y

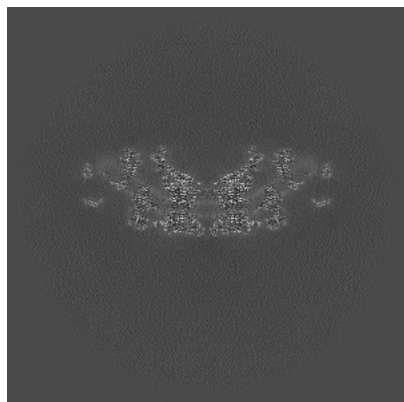


Z

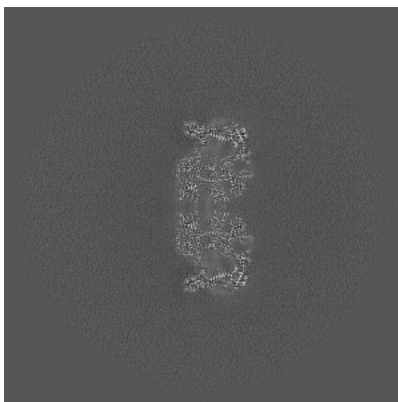
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

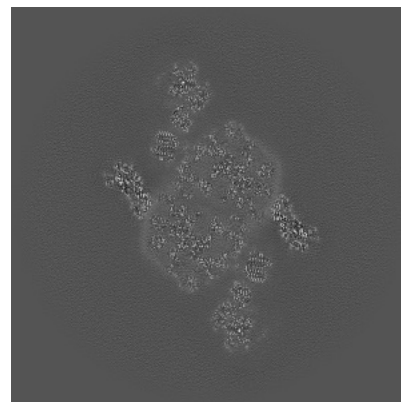
6.2.1 Primary map



X Index: 420

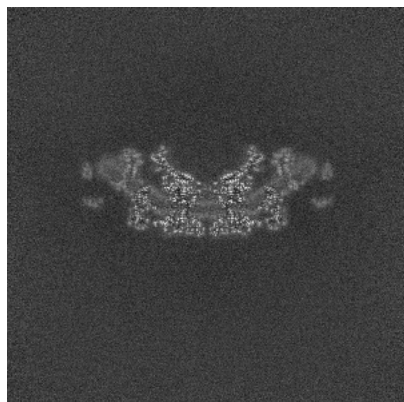


Y Index: 420

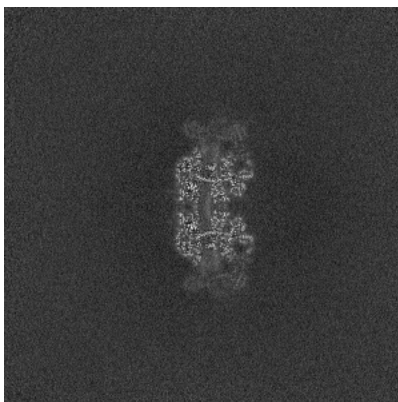


Z Index: 420

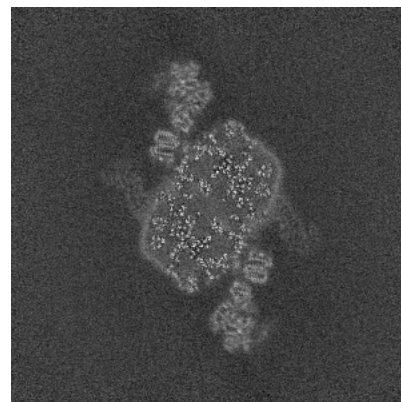
6.2.2 Raw map



X Index: 420



Y Index: 420

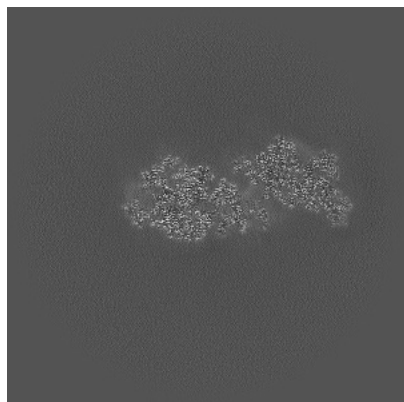


Z Index: 420

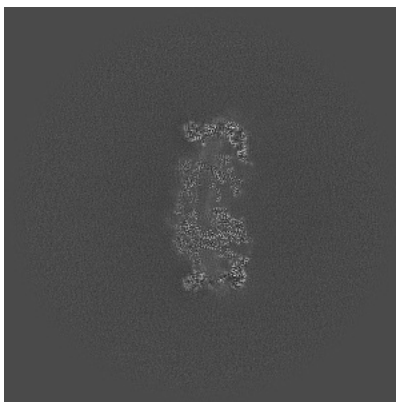
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

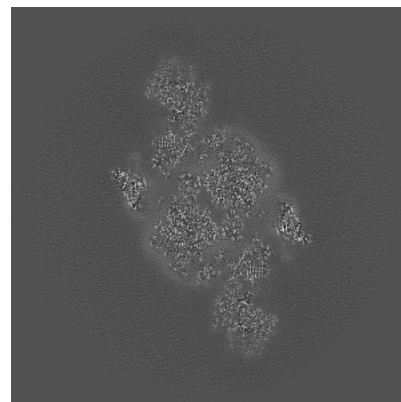
6.3.1 Primary map



X Index: 378

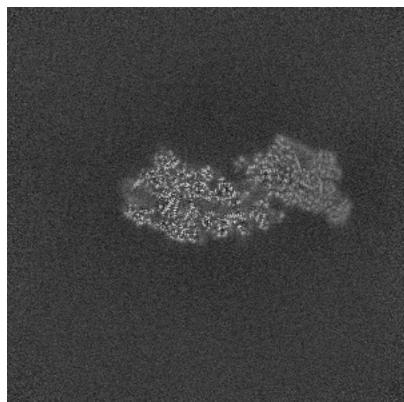


Y Index: 412

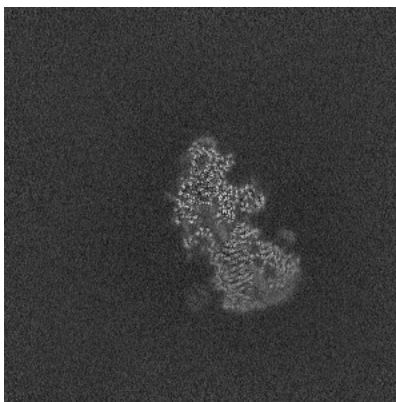


Z Index: 439

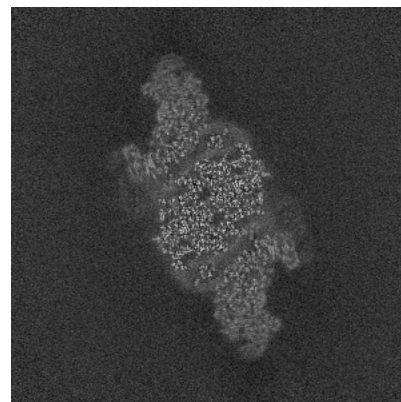
6.3.2 Raw map



X Index: 384



Y Index: 508

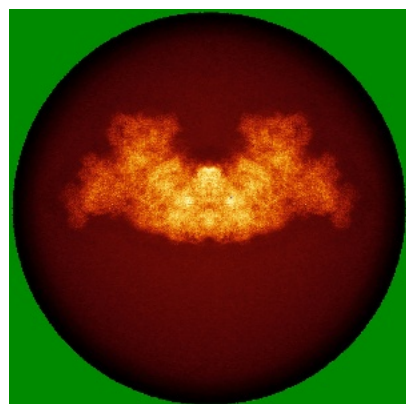


Z Index: 453

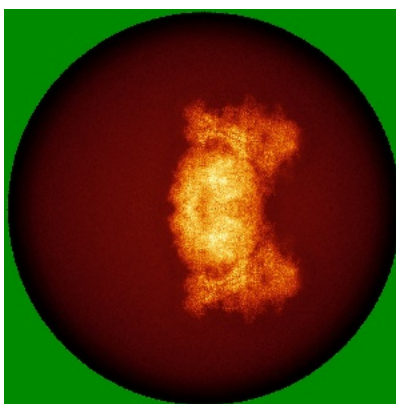
The images above show the largest variance slices of the map in three orthogonal directions.

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

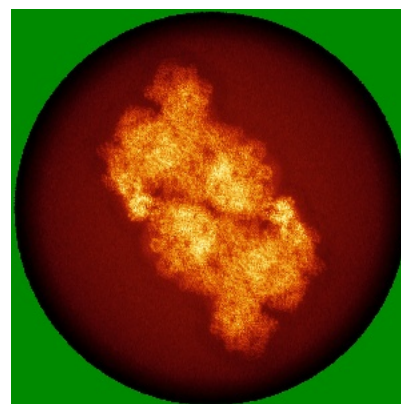
6.4.1 Primary map



X

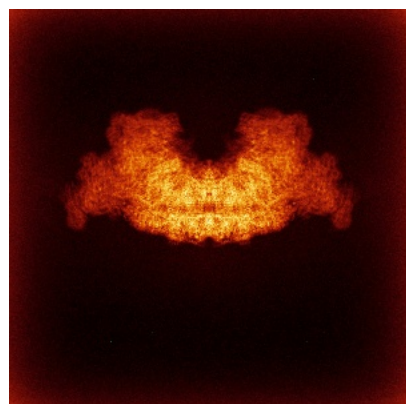


Y

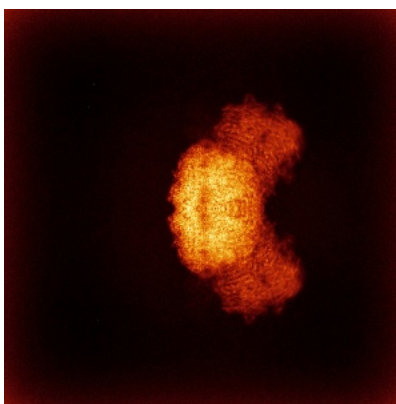


Z

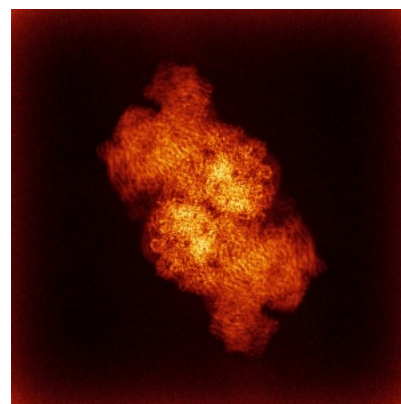
6.4.2 Raw map



X



Y

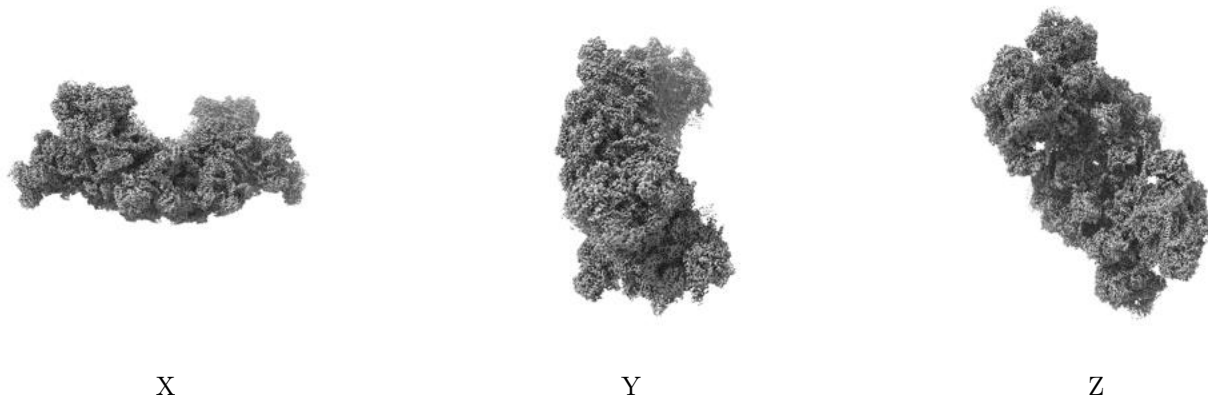


Z

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.

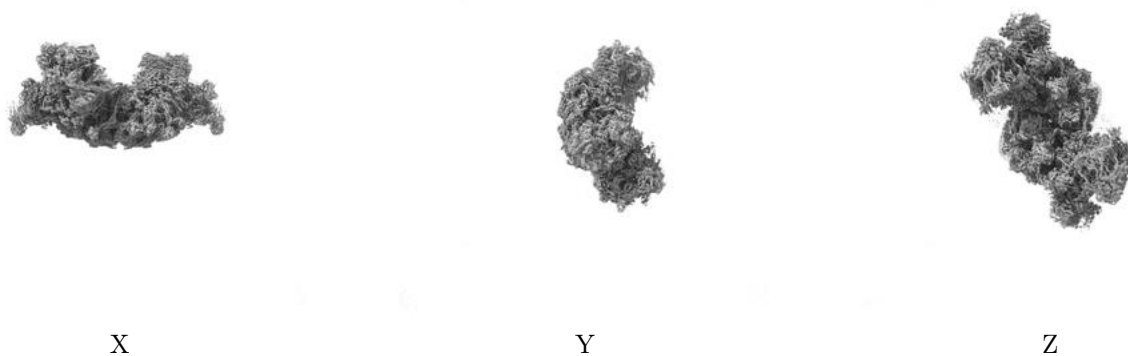
6.5 Orthogonal surface views [i](#)

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.

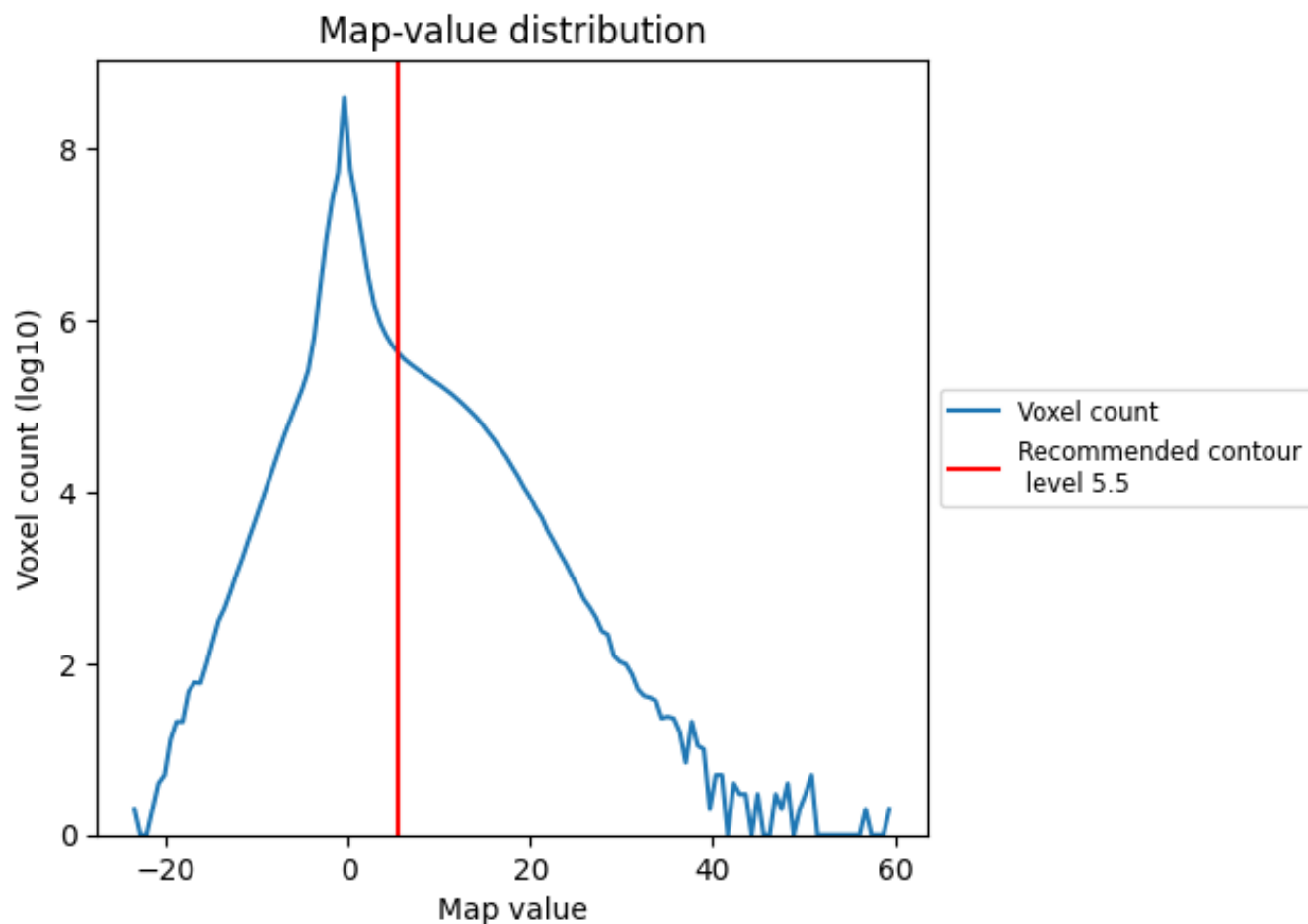
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

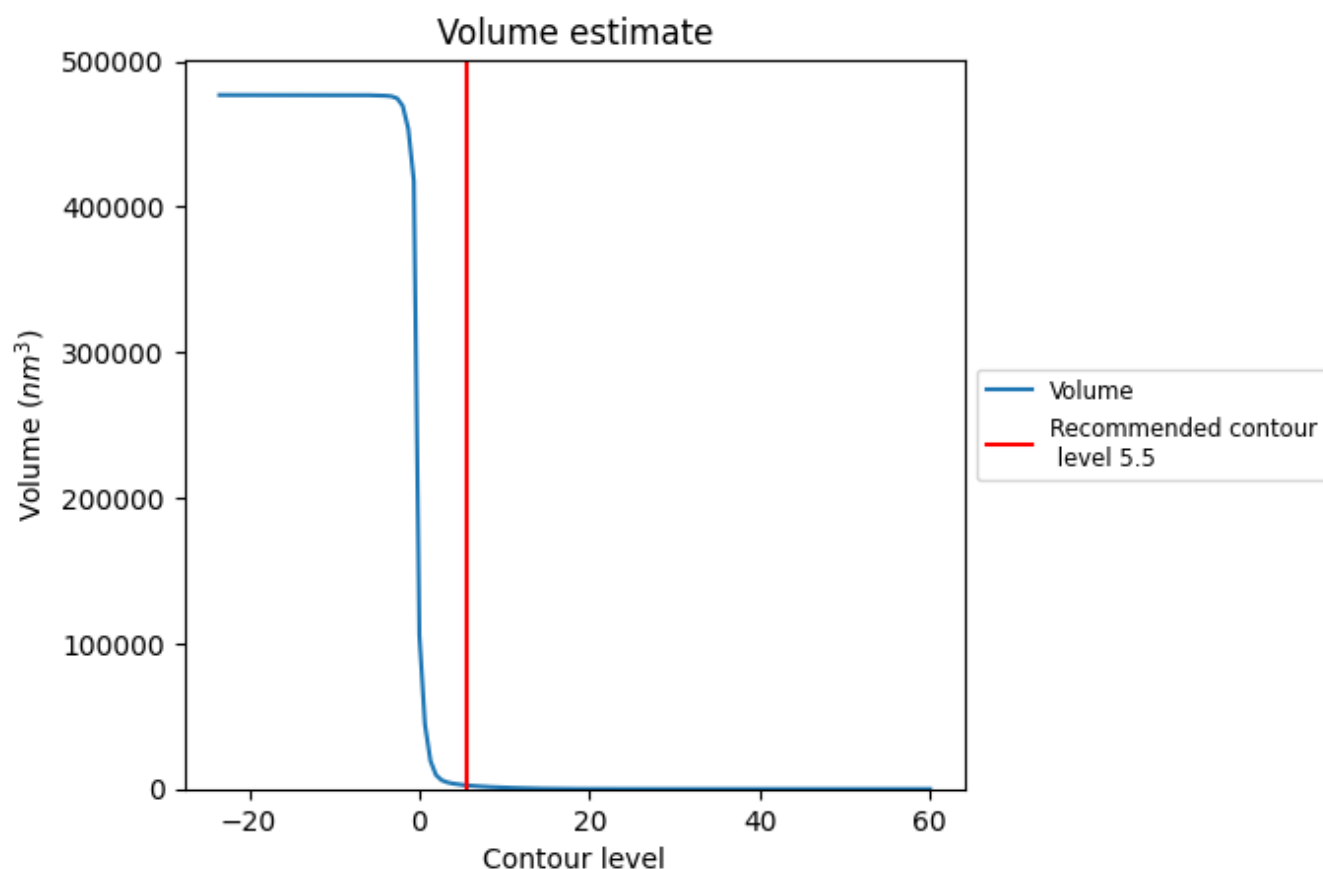
This section contains the results of statistical analysis of the map.

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.

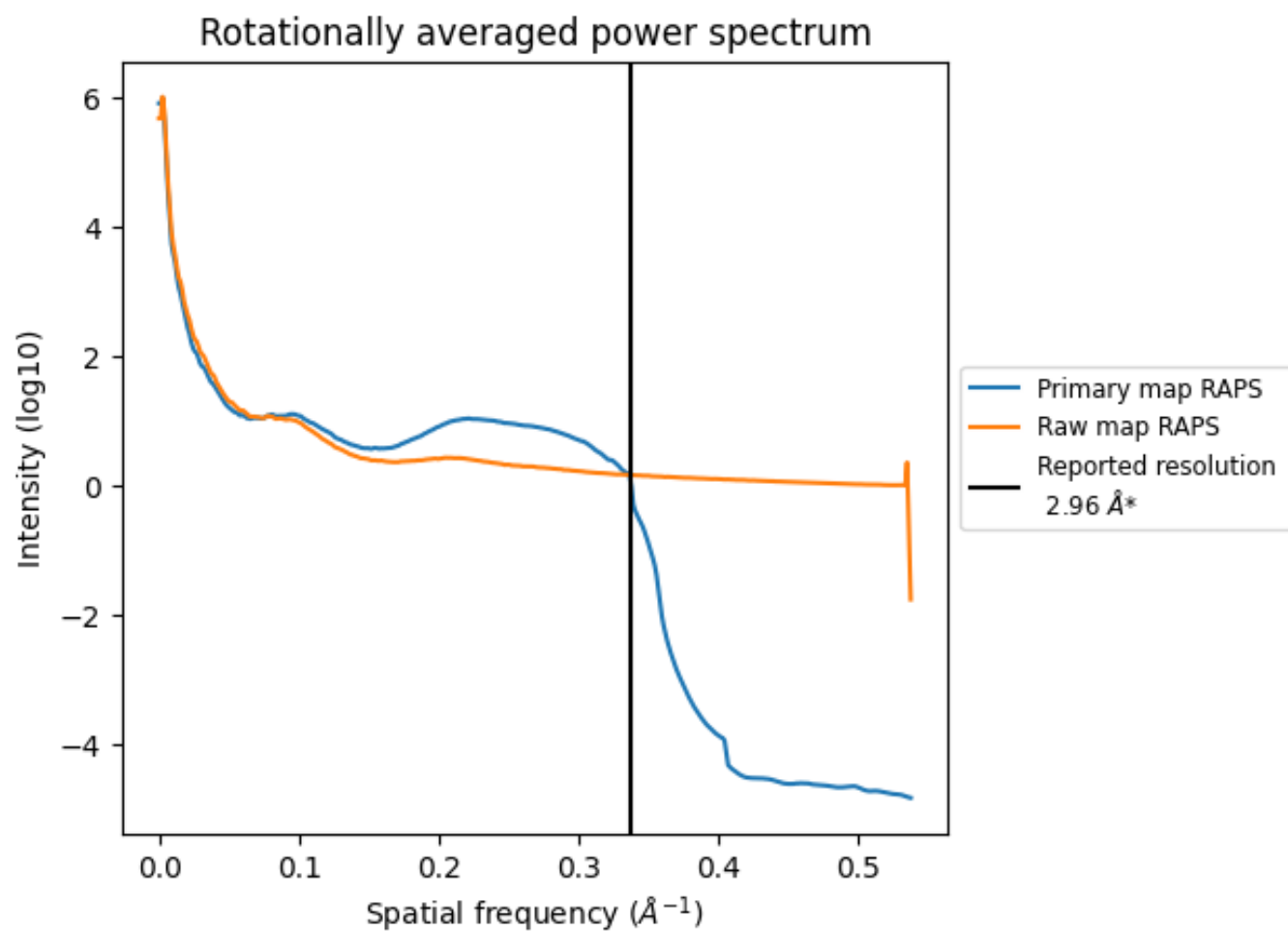
7.2 Volume estimate [i](#)



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 ⓘ

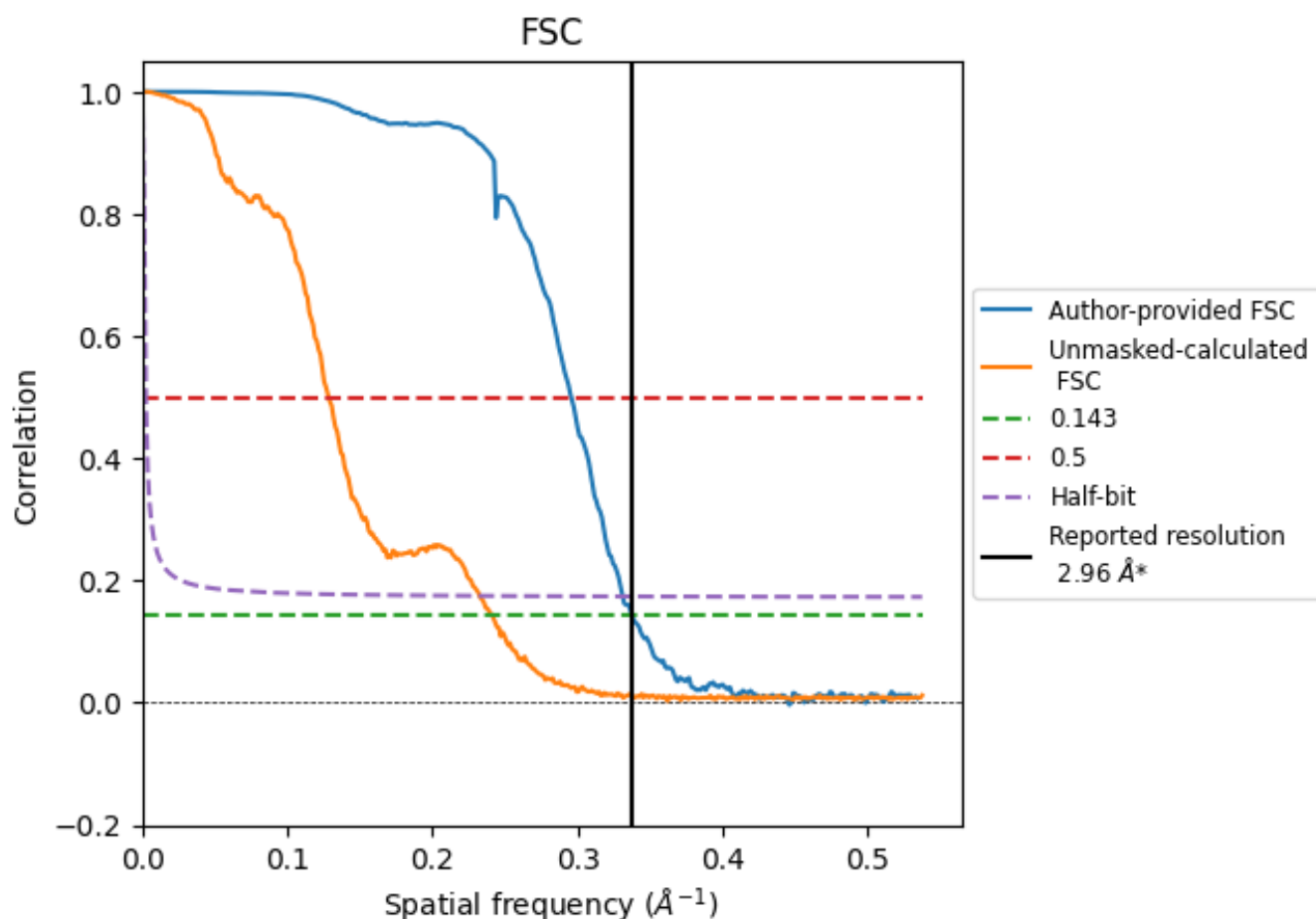


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

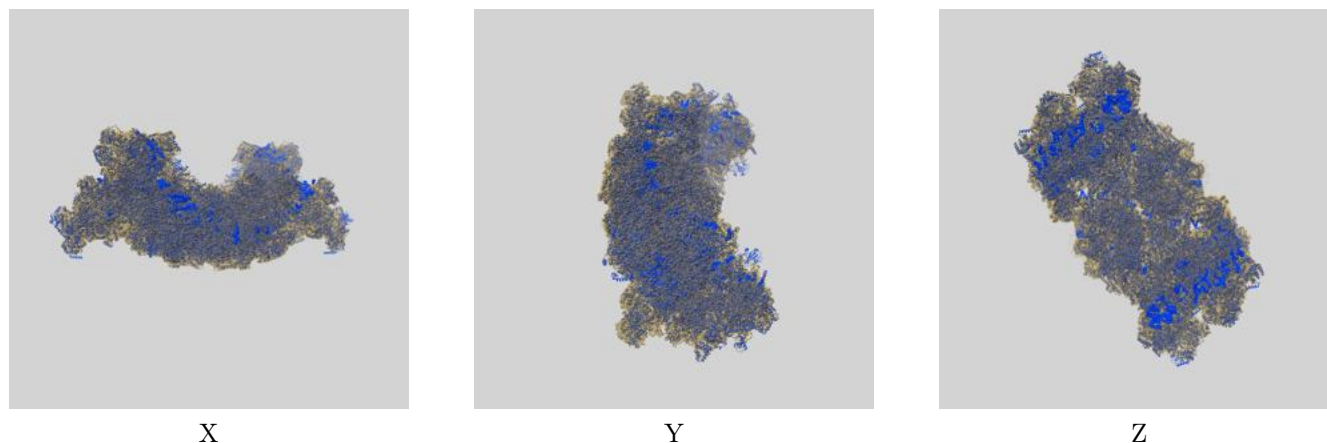
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.38	3.02
Unmasked-calculated*	4.15	7.78	4.30

*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](#)

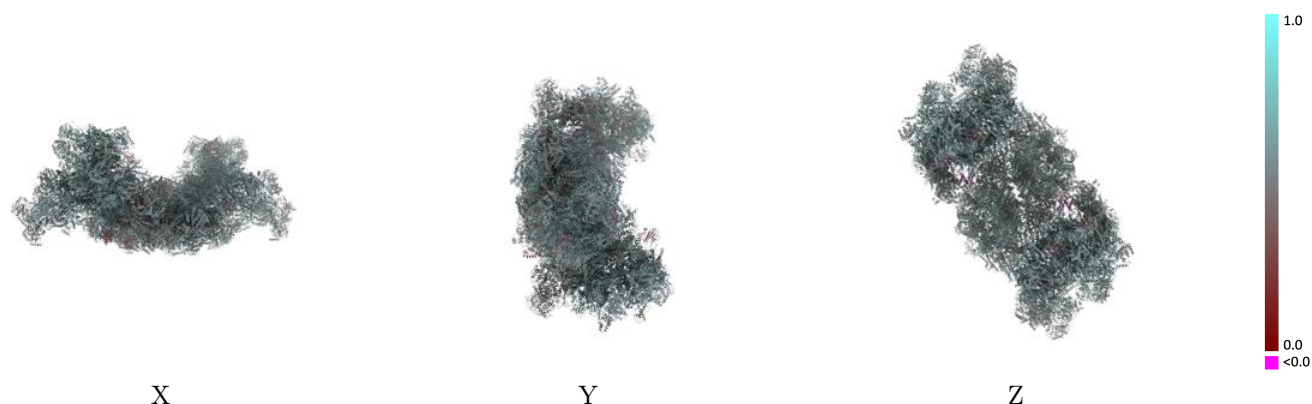
This section contains information regarding the fit between EMDB map EMD-34373 and PDB model 8GYM. Per-residue inclusion information can be found in [section 3](#) on [page 82](#).

9.1 Map-model overlay [i](#)



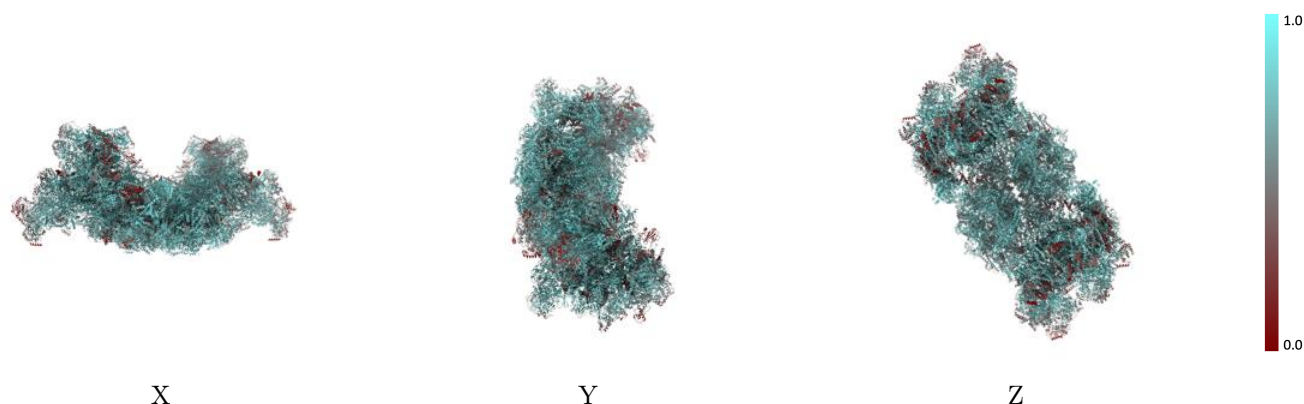
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



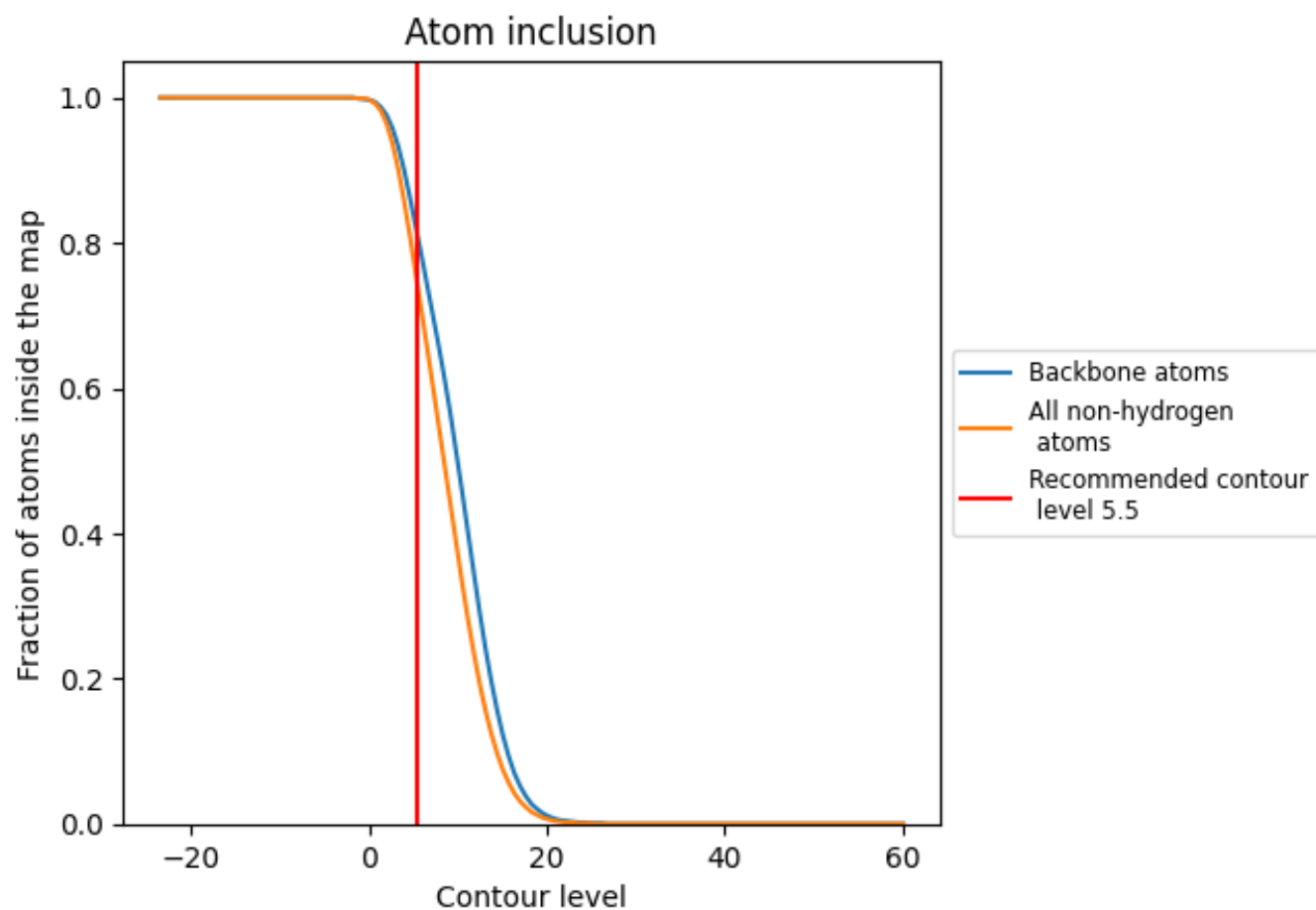
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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