



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 12:07 PM EST

PDB ID : 8B6H
EMDB ID : EMD-15867
Title : Cryo-EM structure of cytochrome c oxidase dimer (complex IV) from respiratory supercomplex of *Tetrahymena thermophila*
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2022-09-27
Resolution : 2.60 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:

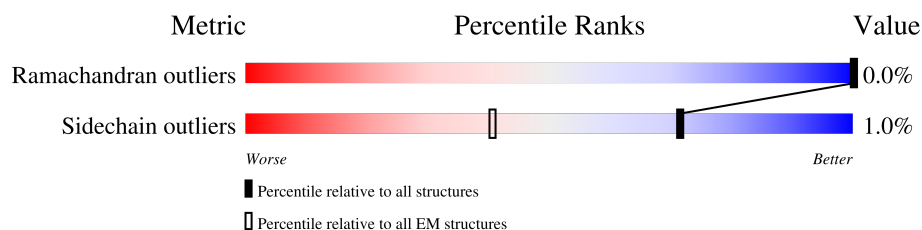
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



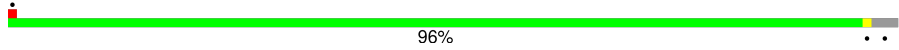
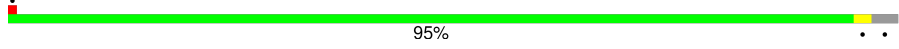
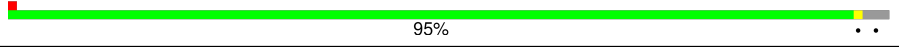
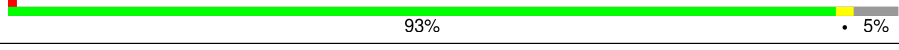
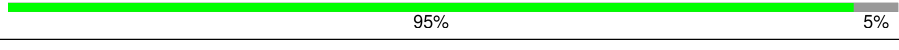
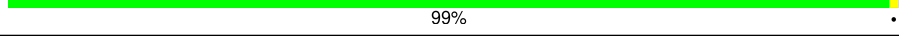
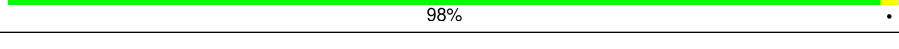
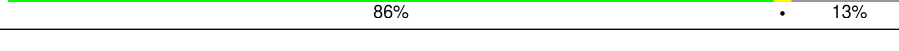
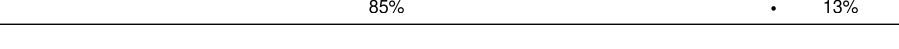
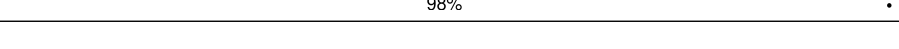
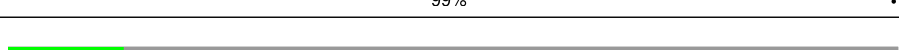

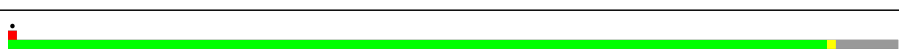
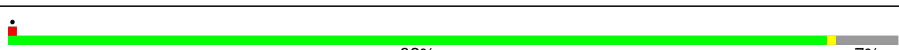
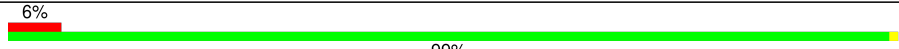
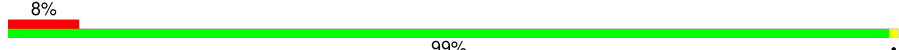

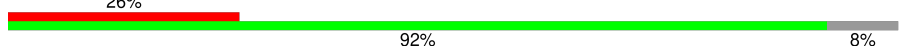


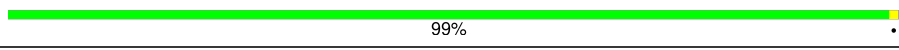
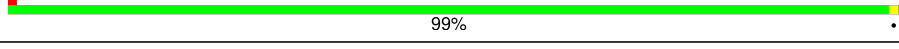



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	DA	688	96%
1	Da	688	96%
2	DB	604	98%
2	Db	604	98%
3	DC	594	6%
3	Dc	594	7%
4	DD	637	86%
4	Dd	637	86%
5	DE	130	97%











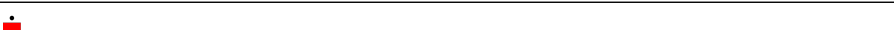

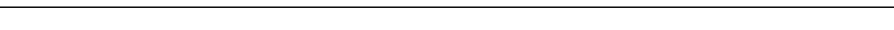
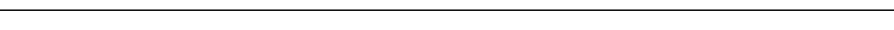





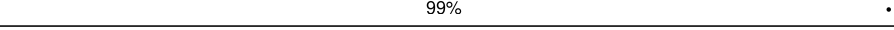
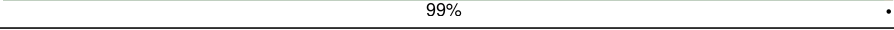
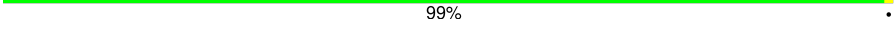
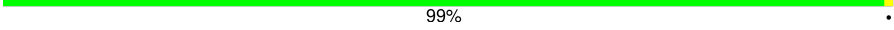
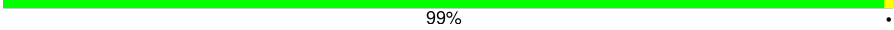
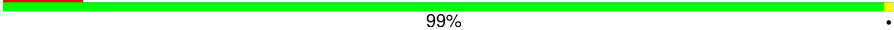
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Mol	Chain	Length	Quality of chain
5	De	130	
6	DF	230	
6	Df	230	
7	DG	103	
7	Dg	103	
8	DH	133	
8	Dh	133	
9	DI	236	
9	Di	236	
10	DJ	220	
10	Dj	220	
11	DK	990	
11	Dk	990	
12	DM	490	
12	Dm	490	
13	DN	453	
13	Dn	453	
14	DO	473	
14	Do	473	
15	DP	402	
15	Dp	402	
16	DQ	385	
16	Dq	385	
17	DR	348	
17	Dr	348	


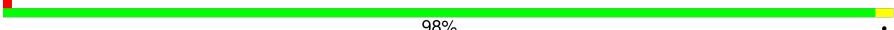
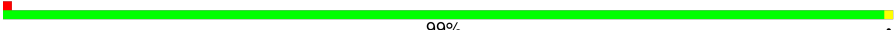
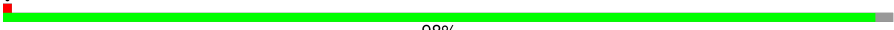






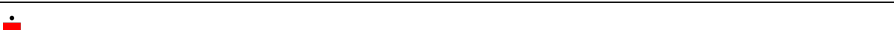

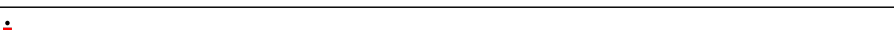
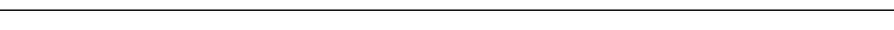
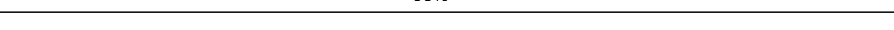
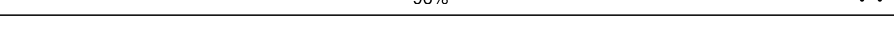
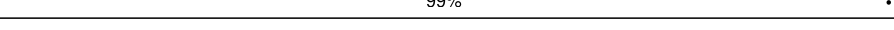
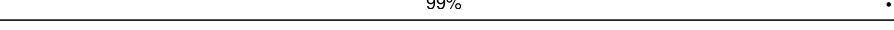
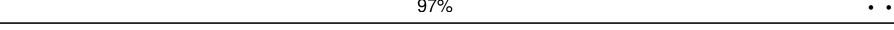
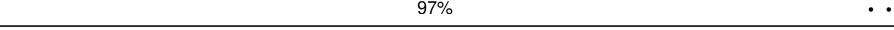
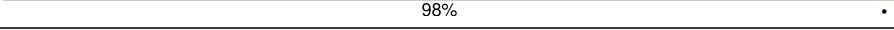
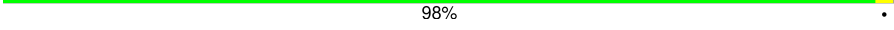


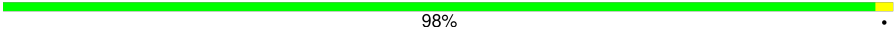
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Mol	Chain	Length	Quality of chain
18	DS	346	 99% .
18	Ds	346	 99% .
19	DT	318	 92% 8%
19	Dt	318	 92% 8%
20	DU	330	 99% .
20	Du	330	 99% .
21	DV	318	 99% .
21	Dv	318	 99% .
22	DW	318	 93% . 5%
22	Dw	318	 94% . 5%
23	DX	252	 99% .
23	Dx	252	 98% .
24	DY	234	 79% 20%
24	Dy	234	 79% 20%
25	DZ	231	 90% 10%
25	Dz	231	 90% 10%
26	EA	215	 89% 10%
26	Ea	215	 89% . 10%
27	EB	210	 99% .
27	Eb	210	 99% .
28	EC	212	 99% .
28	Ec	212	 99% .
29	ED	190	 99% .
29	Ed	190	 99% .
30	EE	193	 65% 35%

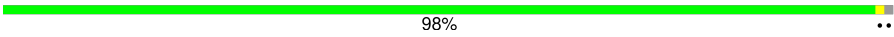
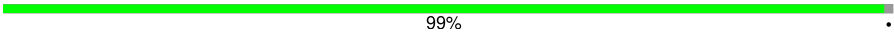
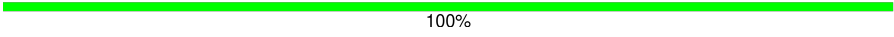
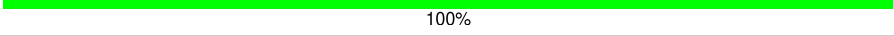


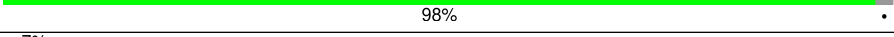
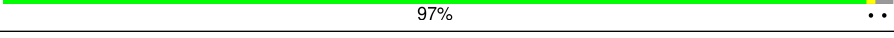
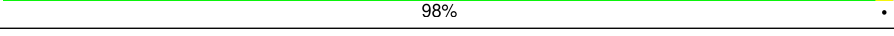
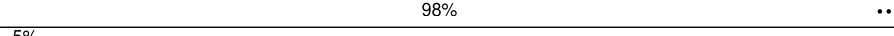

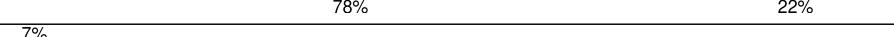
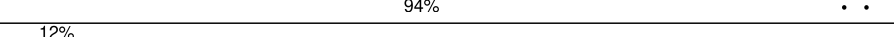
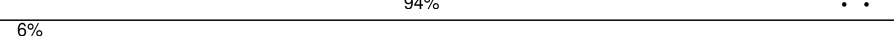
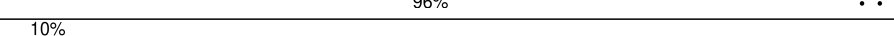
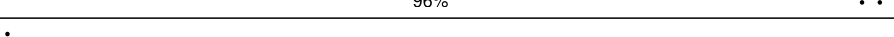
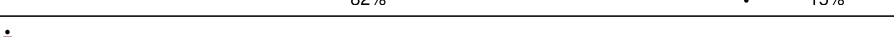

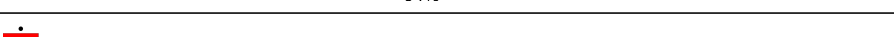



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Mol	Chain	Length	Quality of chain
30	Ee	193	 65% 35%
31	EF	188	 98% .
31	Ef	188	 99% .
32	EG	100	 98% .
32	Eg	100	 97% ..
33	EH	173	 99% .
33	Eh	173	 100%
34	EI	173	 97% ..
34	Ei	173	 97% ..
35	EV	88	 89% 11%
35	Ev	88	 89% 11%
36	EK	170	 98% ..
36	Ek	170	 98% ..
37	EL	158	 96% ..
37	El	158	 96% ..
38	EM	154	 99% ..
38	Em	154	 99% ..
39	EN	149	 97% ..
39	En	149	 97% ..
40	EO	124	 98% ..
40	Eo	124	 98% ..
41	EP	127	 77% . 21%
41	Ep	127	 77% . 21%
42	EQ	122	 98% .
42	Eq	122	 98% .

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Mol	Chain	Length	Quality of chain
43	ER	105	 98% ..
43	Er	105	 99% .
44	ES	89	 100%
44	Es	89	 100%
45	ET	93	 85% . 12%
45	Et	93	 85% . 12%
46	EU	90	 98% .
46	Eu	90	 97% ..
47	EJ	175	 98% .
47	Ej	175	 98% ..
48	EW	81	 78% 22%
48	Ew	81	 78% 22%
49	EX	72	 94% ..
49	Ex	72	 94% ..
50	EY	72	 96% ..
50	Ey	72	 96% ..
51	EZ	68	 82% . 15%
51	Ez	68	 84% . 15%
52	FA	72	 94% ..
52	Fa	72	 96% ..
53	DL	536	 71% 29%
53	Dl	536	 71% 29%

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 436035 atoms, of which 220788 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	DA	671	Total	C	H	N	O	S	0	0
			11168	3720	5609	907	896	36		
1	Da	671	Total	C	H	N	O	S	0	0
			11167	3720	5608	907	896	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	288	ALA	GLY	variant	UNP Q950Y4
Da	288	ALA	GLY	variant	UNP Q950Y4

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	DB	604	Total	C	H	N	O	S	0	0
			10232	3340	5101	888	892	11		
2	Db	604	Total	C	H	N	O	S	0	0
			10233	3340	5102	888	892	11		

- Molecule 3 is a protein called Ymf68.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	DC	582	Total	C	H	N	O	S	0	0
			10151	3451	5067	787	838	8		
3	Dc	582	Total	C	H	N	O	S	0	0
			10151	3451	5067	787	838	8		

- Molecule 4 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	DD	558	Total	C	H	N	O	P	S	0	0
			9076	2930	4424	782	921	2	17		

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Mol	Chain	Residues	Atoms							AltConf	Trace
4	Dd	558	Total	C	H	N	O	P	S	0	0
			9076	2930	4424	782	921	2	17		

- Molecule 5 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
5	DE	126	Total	C	H	N	O	S		0	0
			2104	698	1021	184	199	2			
5	De	126	Total	C	H	N	O	S		0	0
			2103	698	1020	184	199	2			

- Molecule 6 is a protein called Structural protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
6	DF	222	Total	C	H	N	O	S		0	0
			3681	1238	1768	312	350	13			
6	Df	222	Total	C	H	N	O	S		0	0
			3681	1238	1768	312	350	13			

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

Mol	Chain	Residues	Atoms							AltConf	Trace
7	DG	98	Total	C	H	N	O	S		0	0
			1659	567	788	155	147	2			
7	Dg	98	Total	C	H	N	O	S		0	0
			1659	567	788	155	147	2			

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

Mol	Chain	Residues	Atoms							AltConf	Trace
8	DH	133	Total	C	H	N	O	S		0	0
			2299	771	1129	197	201	1			
8	Dh	133	Total	C	H	N	O	S		0	0
			2299	771	1129	197	201	1			

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms							AltConf	Trace
9	DI	206	Total	C	H	N	O	P	S	0	0
			3381	1134	1604	286	348	1	8		

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Mol	Chain	Residues	Atoms							AltConf	Trace
9	Di	206	Total	C	H	N	O	P	S	0	0
			3381	1134	1604	286	348	1	8		

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

Mol	Chain	Residues	Atoms							AltConf	Trace
10	DJ	220	Total	C	H	N	O	S		0	0
			3653	1223	1772	316	330	12			
10	Dj	220	Total	C	H	N	O	S		0	0
			3653	1223	1772	316	330	12			

- Molecule 11 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
11	DK	130	Total	C	H	N	O	S		0	0
			2133	693	1062	174	196	8			
11	Dk	130	Total	C	H	N	O	S		0	0
			2133	693	1062	174	196	8			

- Molecule 12 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
12	DM	455	Total	C	H	N	O	S		0	0
			7385	2430	3592	645	709	9			
12	Dm	455	Total	C	H	N	O	S		0	0
			7385	2430	3592	645	709	9			

- Molecule 13 is a protein called Ymf67.

Mol	Chain	Residues	Atoms							AltConf	Trace
13	DN	453	Total	C	H	N	O	S		0	0
			7849	2578	3980	618	666	7			
13	Dn	453	Total	C	H	N	O	S		0	0
			7849	2578	3980	618	666	7			

- Molecule 14 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms							AltConf	Trace
14	DO	435	Total	C	H	N	O	S		0	0
			6956	2192	3508	603	650	3			
14	Do	435	Total	C	H	N	O	S		0	0
			6956	2192	3508	603	650	3			

- Molecule 15 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	DP	290	Total	C	H	N	O	S	0	0
			4660	1525	2291	400	439	5		
15	Dp	290	Total	C	H	N	O	S	0	0
			4660	1525	2291	400	439	5		

- Molecule 16 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	DQ	383	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		
16	Dq	383	Total	C	H	N	O	S	0	0
			6271	2041	3102	546	575	7		

- Molecule 17 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	DR	243	Total	C	H	N	O	S	0	0
			3982	1304	1958	335	380	5		
17	Dr	243	Total	C	H	N	O	S	0	0
			3982	1304	1958	335	380	5		

- Molecule 18 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	DS	346	Total	C	H	N	O	S	0	0
			5636	1892	2770	469	492	13		
18	Ds	346	Total	C	H	N	O	S	0	0
			5636	1892	2770	469	492	13		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	DT	293	Total	C	H	N	O	S	0	0
			4733	1555	2290	410	466	12		
19	Dt	293	Total	C	H	N	O	S	0	0
			4733	1555	2290	410	466	12		

- Molecule 20 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	DU	329	Total	C	H	N	O	S	0	0
			5204	1700	2584	446	470	4		
20	Du	329	Total	C	H	N	O	S	0	0
			5204	1700	2584	446	470	4		

- Molecule 21 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	DV	318	Total	C	H	N	O	S	0	0
			5114	1667	2552	440	451	4		
21	Dv	318	Total	C	H	N	O	S	0	0
			5114	1667	2552	440	451	4		

- Molecule 22 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	DW	301	Total	C	H	N	O	S	0	0
			4738	1515	2344	415	454	10		
22	Dw	301	Total	C	H	N	O	S	0	0
			4738	1515	2344	415	454	10		

- Molecule 23 is a protein called COXTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	DX	251	Total	C	H	N	O	S	0	0
			4126	1358	2018	368	377	5		
23	Dx	251	Total	C	H	N	O	S	0	0
			4126	1358	2018	368	377	5		

- Molecule 24 is a protein called COXTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	DY	187	Total	C	H	N	O	S	0	0
			3135	1023	1562	276	273	1		
24	Dy	187	Total	C	H	N	O	S	0	0
			3135	1023	1562	276	273	1		

- Molecule 25 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	DZ	208	Total	C	H	N	O	S	0	0
			3382	1089	1671	302	317	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
25	Dz	208	Total	C	H	N	O	S	0	0
			3383	1089	1672	302	317	3		

- Molecule 26 is a protein called COXTT12,Transmembrane protein,Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	EA	193	Total 3296	C 1084	H 1637	N 283	O 290	S 2	0	0
26	Ea	193	Total 3296	C 1084	H 1637	N 283	O 290	S 2	0	0

- Molecule 27 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	EB	209	Total	C	H	N	O	S	0	0
			3417	1131	1678	291	310	7		
27	Eb	209	Total	C	H	N	O	S	0	0
			3417	1131	1678	291	310	7		

- Molecule 28 is a protein called COXTT27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	EC	212	Total	C	H	N	O	S	0	0
			3307	1045	1660	276	324	2		
28	Ec	212	Total	C	H	N	O	S	0	0
			3307	1045	1660	276	324	2		

- Molecule 29 is a protein called Ymf75.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	ED	190	Total 3384	C 1141	H 1725	N 249	O 265	S 4	0	0
29	Ed	190	Total 3384	C 1141	H 1725	N 249	O 265	S 4	0	0

- Molecule 30 is a protein called Mobilization protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	EE	125	Total	C	H	N	O	S	0	0
			2073	656	1024	186	201	6		
30	Ee	125	Total	C	H	N	O	S	0	0
			2073	656	1024	186	201	6		

- Molecule 31 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	EF	188	Total	C	H	N	O	S	0	0
			2986	978	1477	260	257	14		
31	Ef	188	Total	C	H	N	O	S	0	0
			2986	978	1477	260	257	14		

- Molecule 32 is a protein called COXTT28.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	EG	98	Total	C	H	N	O	S	0	0
			1523	492	752	136	141	2		
32	Eg	98	Total	C	H	N	O	S	0	0
			1523	492	752	136	141	2		

- Molecule 33 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	EH	173	Total	C	H	N	O	S	0	0
			2820	929	1382	243	257	9		
33	Eh	173	Total	C	H	N	O	S	0	0
			2820	929	1382	243	257	9		

- Molecule 34 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	EI	172	Total	C	H	N	O	S	0	0
			2827	921	1419	231	253	3		
34	Ei	172	Total	C	H	N	O	S	0	0
			2827	921	1419	231	253	3		

- Molecule 35 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	EV	78	Total	C	H	N	O	S	0	0
			1276	411	633	109	117	6		
35	Ev	78	Total	C	H	N	O	S	0	0
			1276	411	633	109	117	6		

- Molecule 36 is a protein called Complex III subunit VII.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	EK	169	Total	C	H	N	O	S	0	0
			2796	878	1407	243	264	4		
36	Ek	169	Total	C	H	N	O	S	0	0
			2796	878	1407	243	264	4		

- Molecule 37 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	EL	153	Total	C	H	N	O	S	0	0
			2544	841	1253	226	220	4		
37	El	153	Total	C	H	N	O	S	0	0
			2544	841	1253	226	220	4		

- Molecule 38 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	EM	153	Total	C	H	N	O	S	0	0
			2603	848	1299	221	230	5		
38	Em	153	Total	C	H	N	O	S	0	0
			2603	848	1299	221	230	5		

- Molecule 39 is a protein called COXTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	EN	145	Total	C	H	N	O	S	0	0
			2417	798	1190	216	211	2		
39	En	145	Total	C	H	N	O	S	0	0
			2417	798	1190	216	211	2		

- Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	EO	123	Total	C	H	N	O	S	0	0
			2128	716	1031	183	194	4		
40	Eo	123	Total	C	H	N	O	S	0	0
			2128	716	1031	183	194	4		

- Molecule 41 is a protein called Phage protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	EP	100	Total	C	H	N	O	S	0	0
			1612	519	795	144	152	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
41	Ep	100	Total	C	H	N	O	S	0	0
			1612	519	795	144	152	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
42	EQ	122	Total	C	H	N	O	S	0	0
			2004	667	989	171	173	4		
42	Eq	122	Total	C	H	N	O	S	0	0
			2004	667	989	171	173	4		

- Molecule 43 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	ER	104	Total	C	H	N	O	S	0	0
			1651	535	800	156	152	8		
43	Er	104	Total	C	H	N	O	S	0	0
			1651	535	800	156	152	8		

- Molecule 44 is a protein called Ymf70.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	ES	89	Total	C	H	N	O	S	0	0
			1574	535	798	115	124	2		
44	Es	89	Total	C	H	N	O	S	0	0
			1574	535	798	115	124	2		

- Molecule 45 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	ET	82	Total	C	H	N	O	S	0	0
			1302	407	655	108	127	5		
45	Et	82	Total	C	H	N	O	S	0	0
			1302	407	655	108	127	5		

- Molecule 46 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	EU	88	Total	C	H	N	O	0	0
			1423	462	699	131	131		
46	Eu	88	Total	C	H	N	O	0	0
			1423	462	699	131	131		

- Molecule 47 is a protein called YftT domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	EJ	175	Total	C	H	N	O	S	0	0
			2802	889	1391	247	274	1		
47	Ej	175	Total	C	H	N	O	S	0	0
			2802	889	1391	247	274	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
48	EW	63	Total	C	H	N	O	S	0	0
			1025	327	510	90	96	2		
48	Ew	63	Total	C	H	N	O	S	0	0
			1025	327	510	90	96	2		

- Molecule 49 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	EX	69	Total	C	H	N	O	S	0	0
			1117	347	559	98	109	4		
49	Ex	69	Total	C	H	N	O	S	0	0
			1117	347	559	98	109	4		

- Molecule 50 is a protein called Annexin.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	EY	70	Total	C	H	N	O	S	0	0
			1123	362	562	90	105	4		
50	Ey	70	Total	C	H	N	O	S	0	0
			1123	362	562	90	105	4		

- Molecule 51 is a protein called Transposase.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	EZ	58	Total	C	H	N	O	S	0	0
			966	314	474	84	91	3		
51	Ez	58	Total	C	H	N	O	S	0	0
			966	314	474	84	91	3		

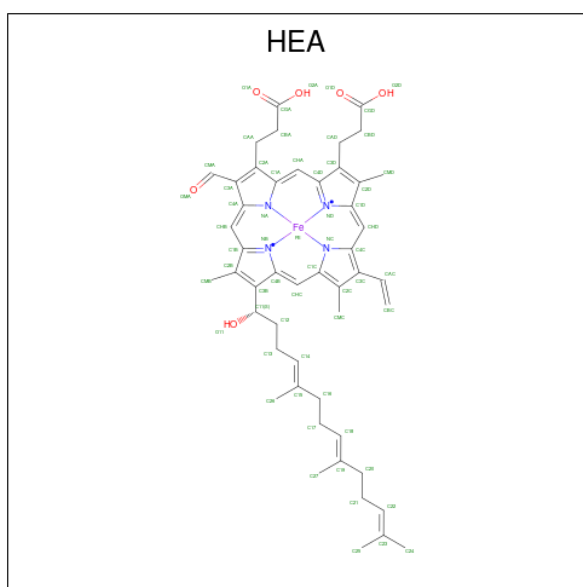
- Molecule 52 is a protein called Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	FA	71	Total	C	H	N	O	S	0	0
			1084	333	536	99	112	4		
52	Fa	71	Total	C	H	N	O	S	0	0
			1084	333	536	99	112	4		

- Molecule 53 is a protein called COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Dl	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		
53	DL	380	Total	C	H	N	O	S	0	0
			5730	1856	2814	492	566	2		

- Molecule 54 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
54	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
54	DA	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
54	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
54	Da	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 55 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand

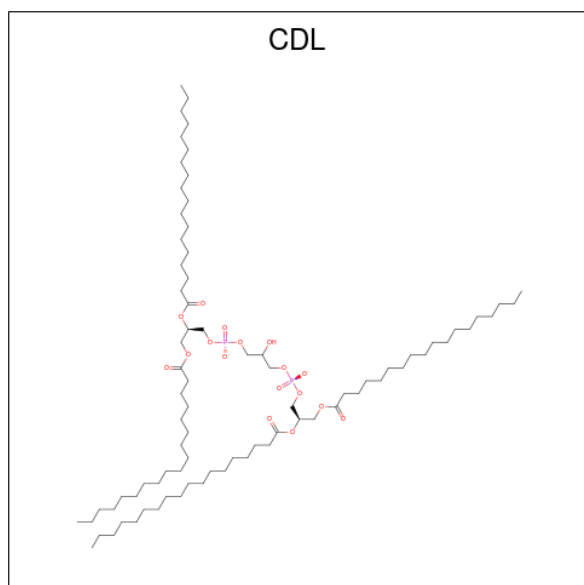
of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
55	DA	1	Total	Cu	0
			1	1	
55	Da	1	Total	Cu	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
56	DA	1	Total	Mg	0
			1	1	
56	Da	1	Total	Mg	0
			1	1	

- Molecule 57 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DA	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	DC	1	Total	C	H	O	P	0
			256	81	156	17	2	

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Mol	Chain	Residues	Atoms					AltConf
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DD	1	Total 256	C 81	H 156	O 17	P 2	0
57	DG	1	Total 256	C 81	H 156	O 17	P 2	0
57	DG	1	Total 256	C 81	H 156	O 17	P 2	0
57	DH	1	Total 256	C 81	H 156	O 17	P 2	0
57	DI	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DJ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DM	1	Total 256	C 81	H 156	O 17	P 2	0
57	DM	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DN	1	Total 256	C 81	H 156	O 17	P 2	0
57	DO	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0
57	DQ	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	DR	1	Total 256	C 81	H 156	O 17	P 2	0
57	DR	1	Total 256	C 81	H 156	O 17	P 2	0
57	DS	1	Total 256	C 81	H 156	O 17	P 2	0
57	DS	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DU	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DV	1	Total 256	C 81	H 156	O 17	P 2	0
57	DX	1	Total 256	C 81	H 156	O 17	P 2	0
57	DX	1	Total 256	C 81	H 156	O 17	P 2	0
57	DY	1	Total 256	C 81	H 156	O 17	P 2	0
57	DZ	1	Total 256	C 81	H 156	O 17	P 2	0
57	EA	1	Total 256	C 81	H 156	O 17	P 2	0
57	EB	1	Total 256	C 81	H 156	O 17	P 2	0
57	EB	1	Total 256	C 81	H 156	O 17	P 2	0
57	ED	1	Total 256	C 81	H 156	O 17	P 2	0
57	ED	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	EH	1	Total 256	C 81	H 156	O 17	P 2	0
57	EH	1	Total 255	C 81	H 155	O 17	P 2	0
57	EI	1	Total 256	C 81	H 156	O 17	P 2	0
57	EK	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EL	1	Total 256	C 81	H 156	O 17	P 2	0
57	EN	1	Total 256	C 81	H 156	O 17	P 2	0
57	EN	1	Total 256	C 81	H 156	O 17	P 2	0
57	EO	1	Total 256	C 81	H 156	O 17	P 2	0
57	EU	1	Total 256	C 81	H 156	O 17	P 2	0
57	Da	1	Total 256	C 81	H 156	O 17	P 2	0
57	Da	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dc	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dd	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dg	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dg	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	Dh	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dh	1	Total 256	C 81	H 156	O 17	P 2	0
57	Di	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dj	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dm	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dm	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dn	1	Total 256	C 81	H 156	O 17	P 2	0
57	Do	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dq	1	Total 256	C 81	H 156	O 17	P 2	0

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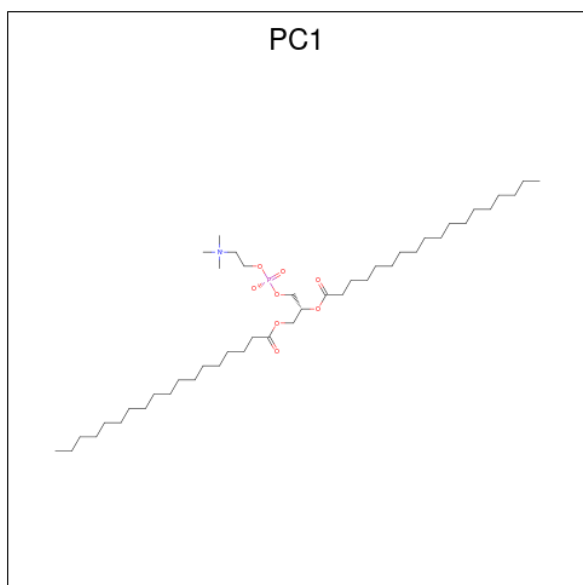
Mol	Chain	Residues	Atoms					AltConf
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57	Dr	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dv	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dx	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dx	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dy	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dz	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ea	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ed	1	Total 255	C 81	H 155	O 17	P 2	0
57	Ed	1	Total 256	C 81	H 156	O 17	P 2	0
57	Eg	1	Total 256	C 81	H 156	O 17	P 2	0
57	Eh	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
57	Ei	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Ek	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	El	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	En	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	En	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Ep	1	Total	C	H	O	P	0
			256	81	156	17	2	
57	Eu	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	DA	1	Total	C	H	N	O	P
			141	44	87	1	8	1
58	DA	1	Total	C	H	N	O	P
			142	44	88	1	8	1

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Mol	Chain	Residues	Atoms						AltConf
58	DB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DC	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	DG	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DI	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DJ	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DQ	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DS	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DS	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DV	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DX	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	DY	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EB	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

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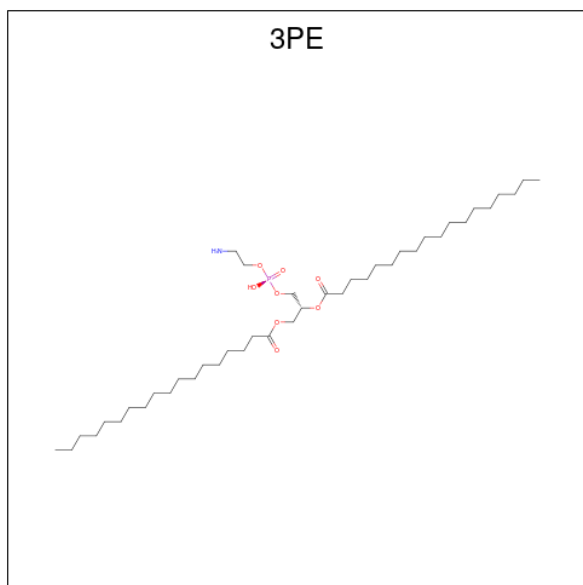
Mol	Chain	Residues	Atoms						AltConf
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Da	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	Da	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Db	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	Dg	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Di	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dq	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Ds	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dv	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dx	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dy	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eb	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eb	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Ef	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	El	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Eo	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 59 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
59	DA	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

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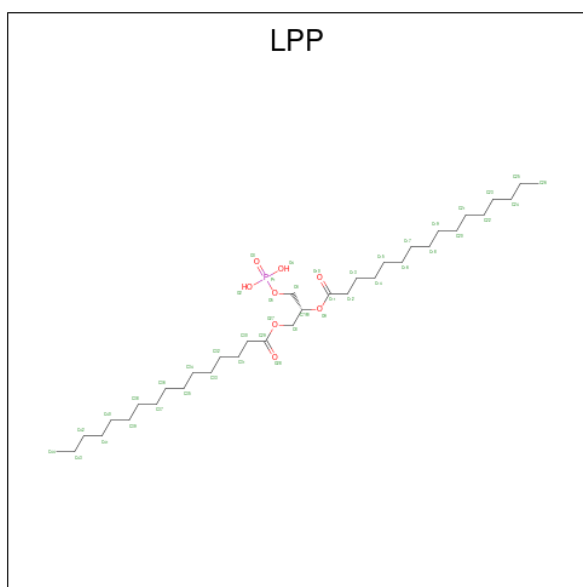
Mol	Chain	Residues	Atoms						AltConf
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DJ	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DR	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DS	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DS	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DX	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EL	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EM	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EN	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EO	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	EO	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Da	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dc	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dd	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dg	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dj	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
59	Dr	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dr	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Ds	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Dx	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	El	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Em	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Eo	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	Eo	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

- Molecule 60 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).

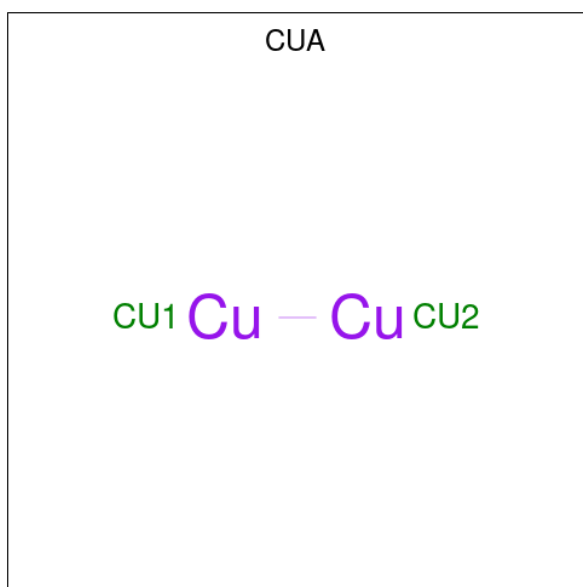


Mol	Chain	Residues	Atoms					AltConf
60	DA	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	EI	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Ed	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dl	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 61 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
61	DA	1	Total	Ca	0
			1	1	
61	Da	1	Total	Ca	0
			1	1	

- Molecule 62 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
62	DB	1	Total	Cu	0
			2	2	
62	Db	1	Total	Cu	0
			2	2	

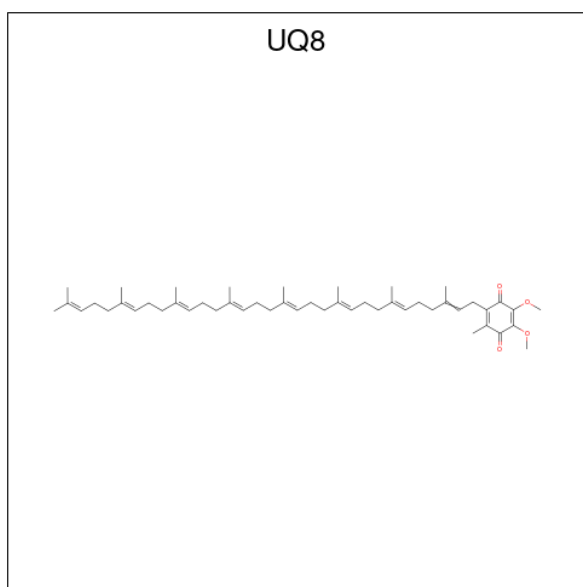
- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
63	DD	1	Total	Zn	0
			1	1	
63	Dd	1	Total	Zn	0
			1	1	

- Molecule 64 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

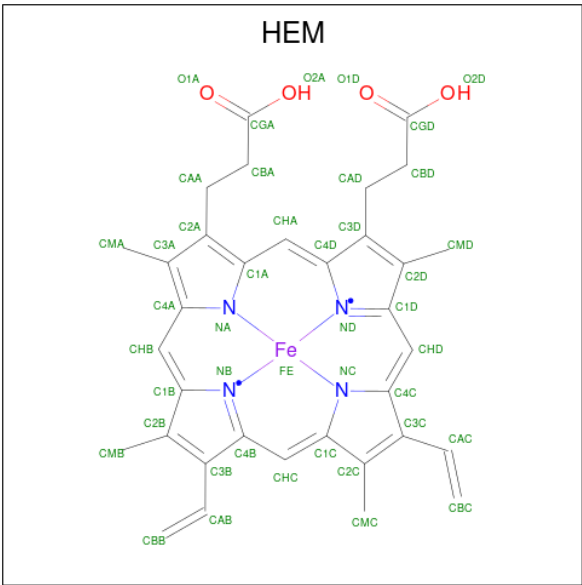
Mol	Chain	Residues	Atoms		AltConf
64	DD	1	Total	K	0
			1	1	

- Molecule 65 is Ubiquinone-8 (three-letter code: UQ8) (formula: C₄₉H₇₄O₄) (labeled as "Ligand of Interest" by depositor).



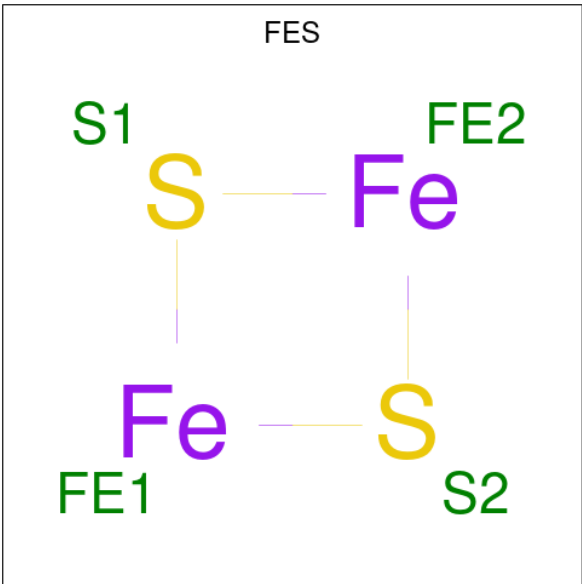
Mol	Chain	Residues	Atoms				AltConf
65	DS	1	Total	C	H	O	0
			127	49	74	4	
65	ED	1	Total	C	H	O	0
			127	49	74	4	
65	EL	1	Total	C	H	O	0
			127	49	74	4	
65	EN	1	Total	C	H	O	0
			127	49	74	4	
65	Ds	1	Total	C	H	O	0
			127	49	74	4	
65	Ed	1	Total	C	H	O	0
			127	49	74	4	
65	El	1	Total	C	H	O	0
			127	49	74	4	
65	En	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 66 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
66	ED	1	Total	C	Fe	H	N	O	0
			65	34	1	22	4	4	
66	Ed	1	Total	C	Fe	H	N	O	0
			67	34	1	24	4	4	

- Molecule 67 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



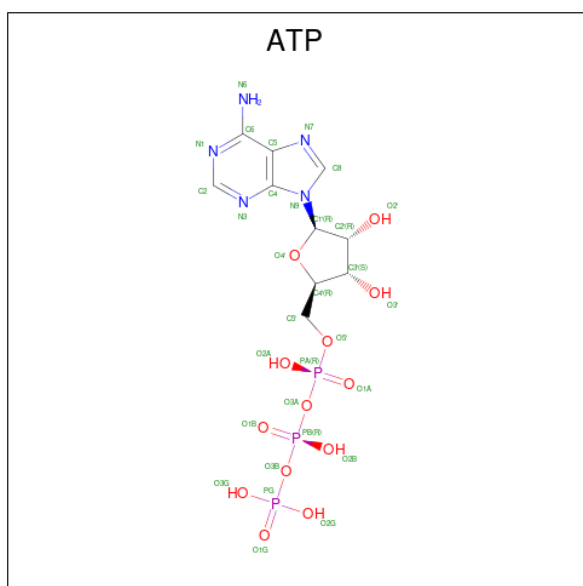
Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	Fe	S	0
			4	2	2	
67	Ef	1	Total	Fe	S	0
			4	2	2	
67	Ef	1	Total	Fe	S	0
			4	2	2	

- Molecule 68 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



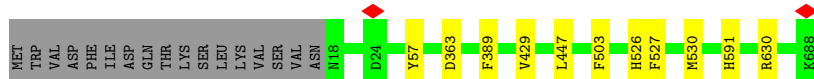
Mol	Chain	Residues	Atoms						AltConf
68	ER	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
68	Er	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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: Cytochrome c oxidase subunit 1

Chain DA:  96%



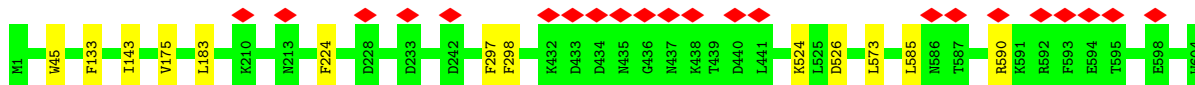
• Molecule 1: Cytochrome c oxidase subunit 1

Chain Da:  96%



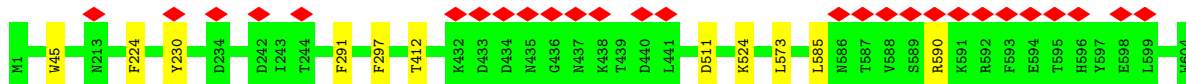
• Molecule 2: Cytochrome c oxidase subunit 2

Chain DB:  98%



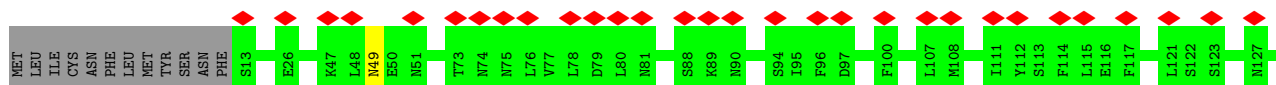
• Molecule 2: Cytochrome c oxidase subunit 2

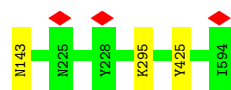
Chain Db:  98%



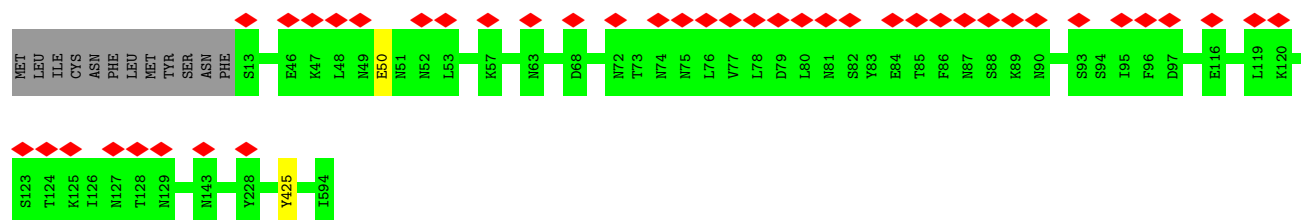
• Molecule 3: Ymf68

Chain DC:  97%

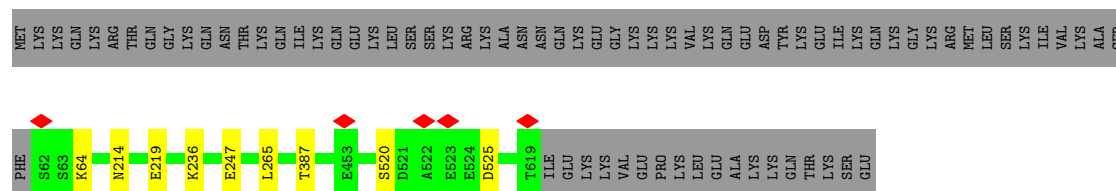




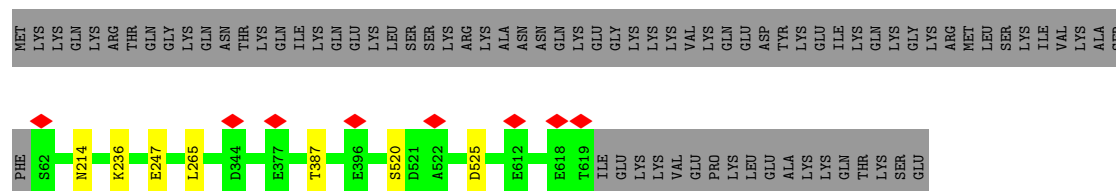
- Molecule 3: Ymf68



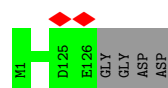
- Molecule 4: Cytochrome C oxidase subunit Vb protein



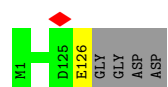
- Molecule 4: Cytochrome C oxidase subunit Vb protein



- Molecule 5: Transmembrane protein, putative

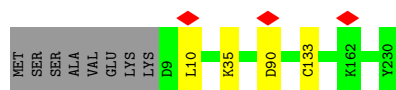


- Molecule 5: Transmembrane protein, putative



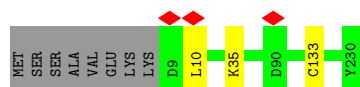
- Molecule 6: Structural protein

Chain DF:  95%



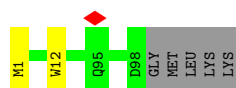
- Molecule 6: Structural protein

Chain Df:  95%



- Molecule 7: Transmembrane protein, putative

Chain DG:  93% 5%



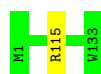
- Molecule 7: Transmembrane protein, putative

Chain Dg:  95% 5%



- Molecule 8: Transmembrane protein, putative

Chain DH:  99%




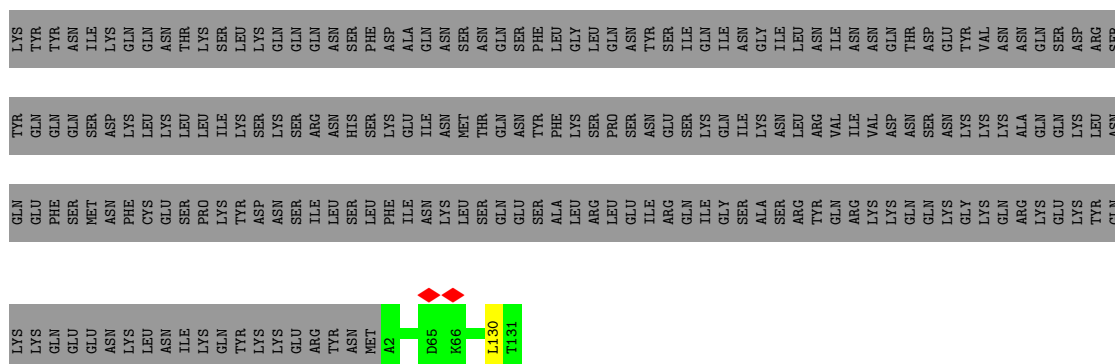
- Molecule 8: Transmembrane protein, putative

Chain Dh:  98%

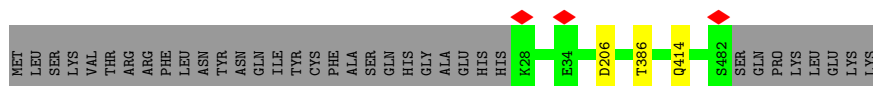


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

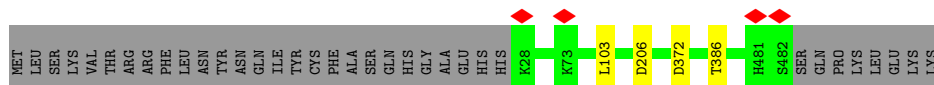
Chain DI:  86% 13%



- Molecule 12: Transmembrane protein, putative



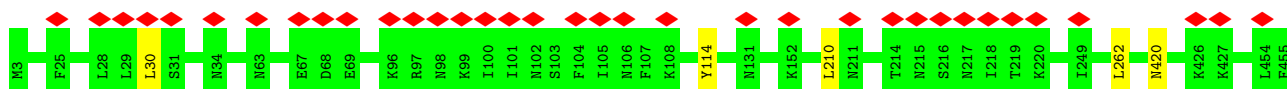
- Molecule 12: Transmembrane protein, putative



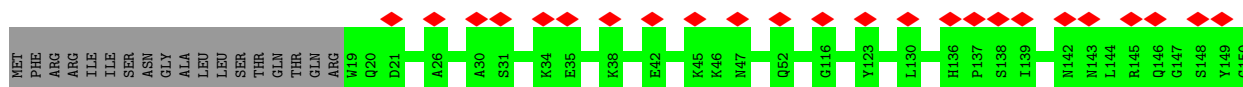
- Molecule 13: Ymf67

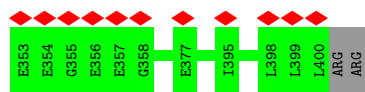


- Molecule 13: Ymf67

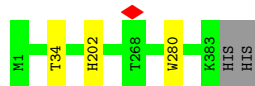


- Molecule 14: Protein phosphatase 2C, putative





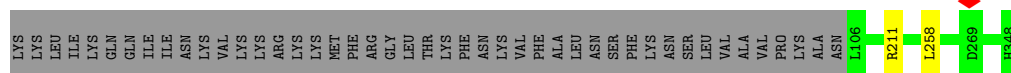
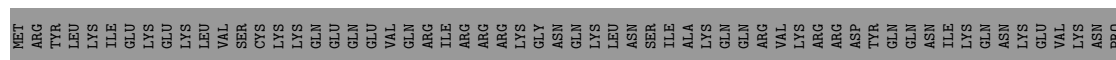
- Molecule 16: TraB family protein



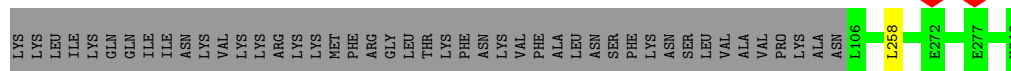
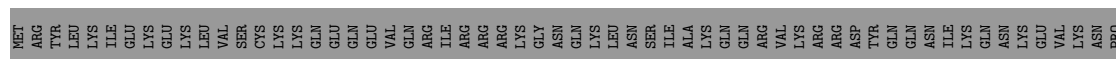
- Molecule 16: TraB family protein



- Molecule 17: Transmembrane protein, putative



- Molecule 17: Transmembrane protein, putative



- Molecule 18: Oxoglutarate/malate translocator protein, putative



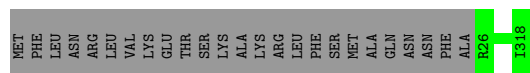
- Molecule 18: Oxoglutarate/malate translocator protein, putative





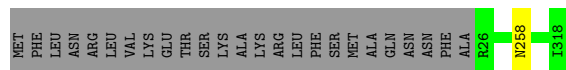
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain DT: 92% 8%



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt: 92% 8%



- Molecule 20: Carrier protein

Chain DU: 99% .



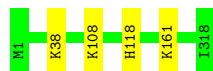
- Molecule 20: Carrier protein

Chain Du: 99% .



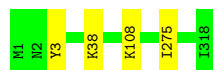
- Molecule 21: 2-oxoglutarate/malate carrier protein

Chain DV: 99% .



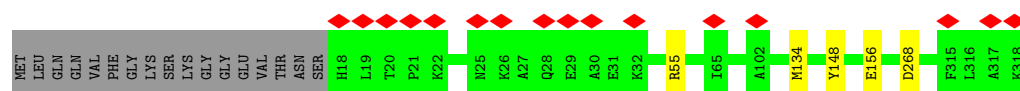
- Molecule 21: 2-oxoglutarate/malate carrier protein

Chain Dv: 99% .



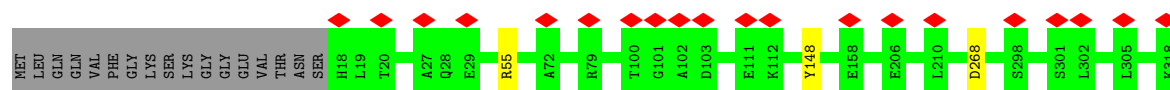
- Molecule 22: SURF1-like protein

Chain DW:  93% 5%



- Molecule 22: SURF1-like protein

Chain Dw:  94% 6% 5%



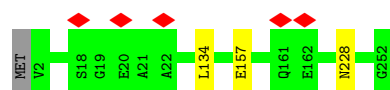
- Molecule 23: COXTT9

Chain DX:  99%




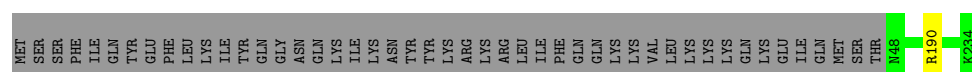
- Molecule 23: COXTT9

Chain Dx:  98%




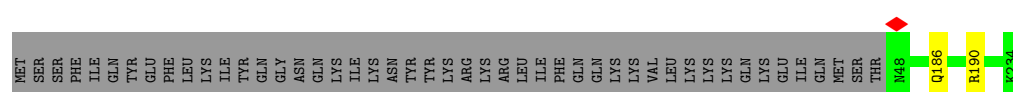
- Molecule 24: COXTT10

Chain DY:  79% 20%



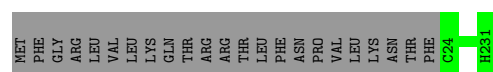
- Molecule 24: COXTT10

Chain Dy:  79% 20%



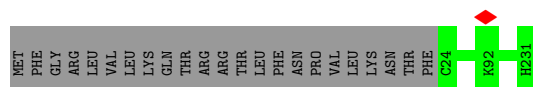
- Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain DZ:  90% 10%



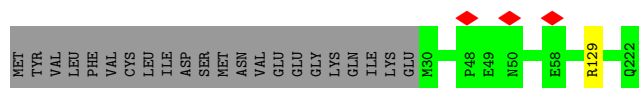
- Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain Dz:  90% 10%




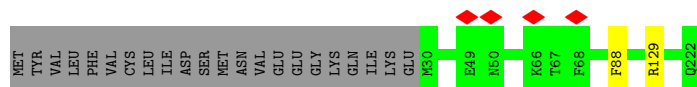
- Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain EA:  89% 10%



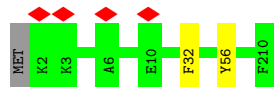
- Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain Ea:  89% 10%



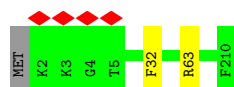
- Molecule 27: Transmembrane protein, putative

Chain EB:  99%



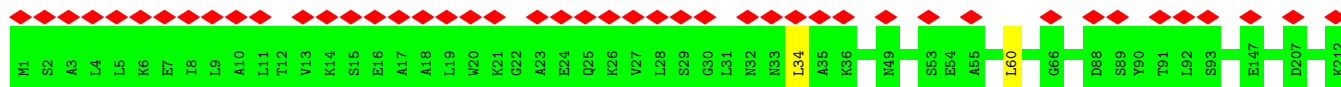
- Molecule 27: Transmembrane protein, putative

Chain Eb:  99%



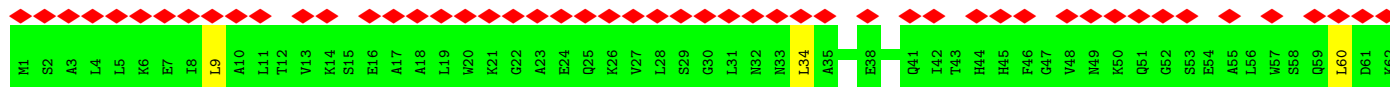
- Molecule 28: COXTT27

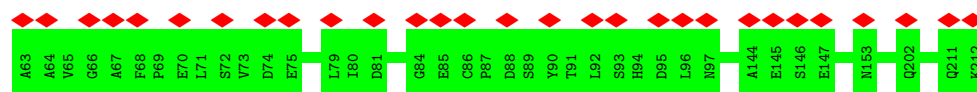
Chain EC:  21% 99%



- Molecule 28: COXTT27

Chain Ec:  38% 99%





- Molecule 29: Ymf75



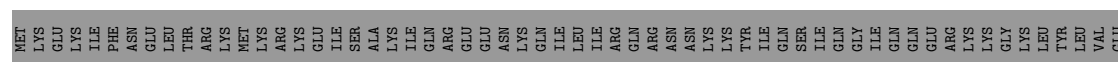
- Molecule 29: Ymf75



- Molecule 30: Mobilization protein



- Molecule 30: Mobilization protein

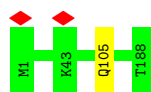


- Molecule 31: Iron-binding zinc finger CDGSH type protein

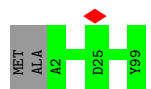


- Molecule 31: Iron-binding zinc finger CDGSH type protein

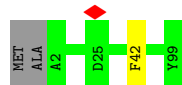




- Molecule 32: COXTT28



- Molecule 32: COXTT28



- Molecule 33: Transmembrane protein, putative



- Molecule 33: Transmembrane protein, putative

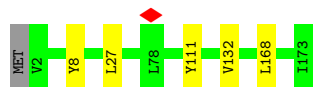


There are no outlier residues recorded for this chain.

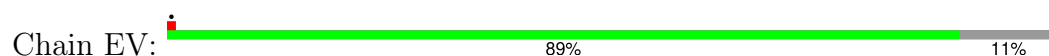
- Molecule 34: Transmembrane protein

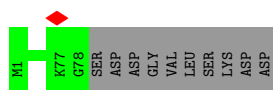


- Molecule 34: Transmembrane protein

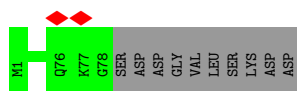
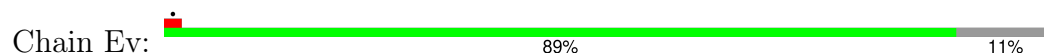


- Molecule 35: Decapping nuclease

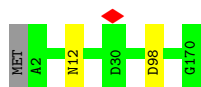




- Molecule 35: Decapping nuclease



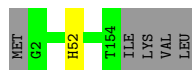
- Molecule 36: Complex III subunit VII



- Molecule 36: Complex III subunit VII



- Molecule 37: Transmembrane protein, putative



- Molecule 37: Transmembrane protein, putative



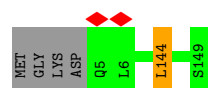
- Molecule 38: Transmembrane protein, putative



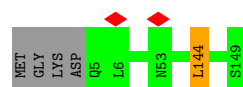
- Molecule 38: Transmembrane protein, putative

Diagram illustrating the interaction between MET, S2, F115, and F154. MET is a grey box, S2 is a green box, F115 is a yellow box, and F154 is a green box. S2 and F115 are connected by a green line, and F115 and F154 are connected by a green line.

- Chain EN: 



- Chain En:  97% ..



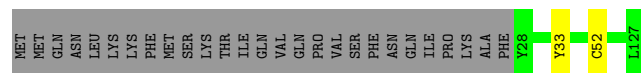
- Chain EO:  98% ...

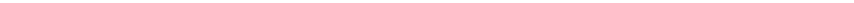


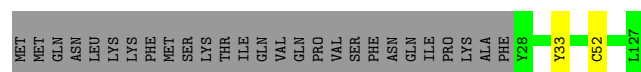
- Chain Eo:  98% ..



- Chain EP: 77% 21%



- Chain Ep:  77% • 21%



- 

Chain EQ:  98%



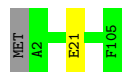
- Molecule 42: Transmembrane protein, putative

Chain Eq:  98%



- Molecule 43: Lysozyme

Chain ER:  98%



- Molecule 43: Lysozyme

Chain Er:  99%



- Molecule 44: Ymf70

Chain ES:  100%


There are no outlier residues recorded for this chain.

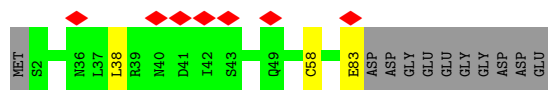
- Molecule 44: Ymf70

Chain Es:  100%




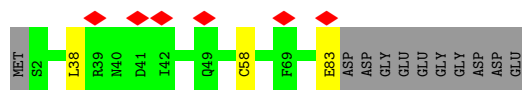
- Molecule 45: Zf-Tim10_DDP domain-containing protein

Chain ET:  8% 85% 12%

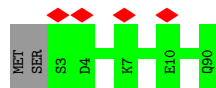


- Molecule 45: Zf-Tim10_DDP domain-containing protein

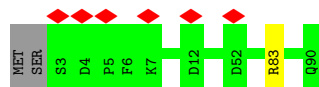
Chain Et:  6% 85% 12%



- Molecule 46: ABC transporter



- Molecule 46: ABC transporter



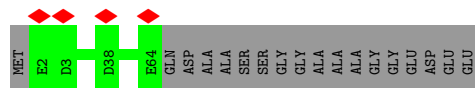
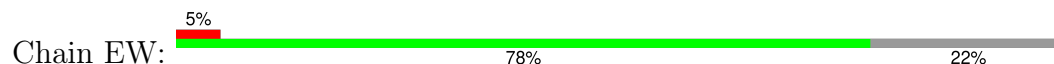
- Molecule 47: YfiT domain-containing protein



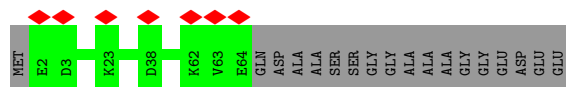
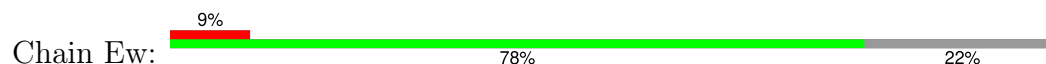
- Molecule 47: YfiT domain-containing protein



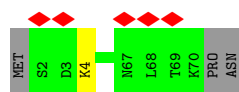
- Molecule 48: Cullin domain-containing protein



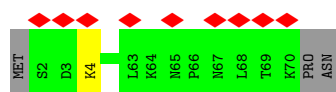
- Molecule 48: Cullin domain-containing protein



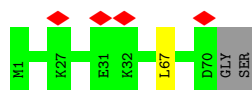
- Molecule 49: Zf-Tim10_DDP domain-containing protein



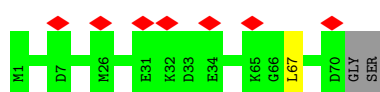
- Molecule 49: Zf-Tim10_DDP domain-containing protein



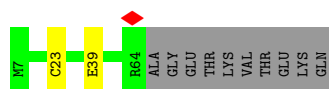
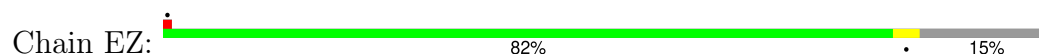
- Molecule 50: Annexin



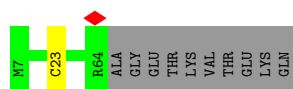
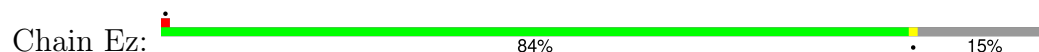
- Molecule 50: Annexin



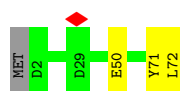
- Molecule 51: Transposase



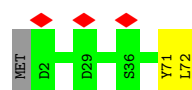
- Molecule 51: Transposase



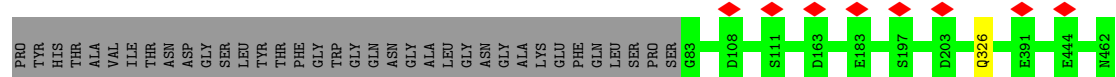
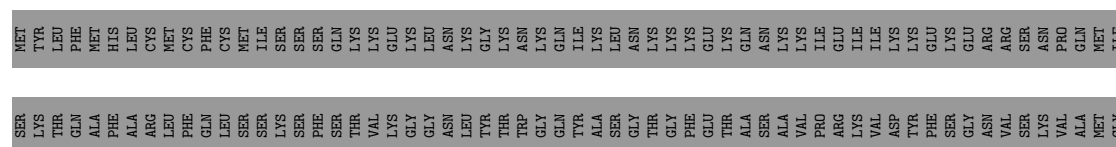
- Molecule 52: Tim10/DDP family zinc finger protein



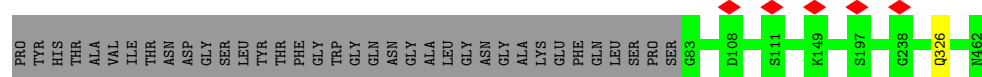
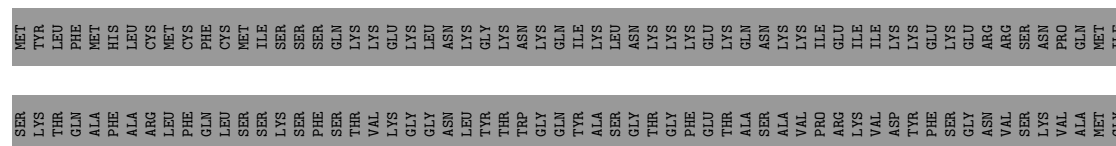
- Chain Fa:  96%



- Chain DL:  71% 29%



- Chain DL:  71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138746	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 ($e^-/\text{\AA}^2$)	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	7.005	Depositor
Minimum map value	-3.774	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.539	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	600.912, 600.912, 600.912	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2519, 1.2519, 1.2519	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CDL, UQ8, CU, PC1, FES, SEP, HEA, ATP, CUA, CA, HEM, 3PE, K, TPO, ZN, LPP, AME

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	DA	0.25	0/5748	0.44	0/7793
1	Da	0.25	0/5748	0.44	0/7793
2	DB	0.24	0/5282	0.46	2/7159 (0.0%)
2	Db	0.24	0/5282	0.46	2/7159 (0.0%)
3	DC	0.25	0/5256	0.42	0/7142
3	Dc	0.25	0/5256	0.41	0/7142
4	DD	0.24	0/4734	0.46	2/6387 (0.0%)
4	Dd	0.24	0/4734	0.46	2/6387 (0.0%)
5	DE	0.24	0/1116	0.41	0/1512
5	De	0.24	0/1116	0.41	0/1512
6	DF	0.25	0/1977	0.49	2/2673 (0.1%)
6	Df	0.25	0/1977	0.49	2/2673 (0.1%)
7	DG	0.24	0/906	0.46	0/1230
7	Dg	0.25	0/906	0.46	0/1230
8	DH	0.24	0/1199	0.46	0/1621
8	Dh	0.24	0/1199	0.46	0/1621
9	DI	0.24	0/1829	0.42	0/2486
9	Di	0.24	0/1829	0.42	0/2486
10	DJ	0.24	0/1950	0.43	0/2647
10	Dj	0.24	0/1950	0.43	0/2647
11	DK	0.24	0/1100	0.47	2/1495 (0.1%)
11	Dk	0.24	0/1100	0.47	2/1495 (0.1%)
12	DM	0.24	0/3910	0.44	0/5320
12	Dm	0.24	0/3910	0.44	0/5320
13	DN	0.24	0/3963	0.39	0/5359
13	Dn	0.24	0/3963	0.39	0/5359
14	DO	0.24	0/3505	0.42	0/4745
14	Do	0.24	0/3505	0.42	0/4745
15	DP	0.24	0/2433	0.46	0/3307
15	Dp	0.24	0/2433	0.46	0/3307
16	DQ	0.23	0/3247	0.44	0/4410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	Dq	0.24	0/3247	0.44	0/4410
17	DR	0.24	0/2077	0.46	2/2824 (0.1%)
17	Dr	0.24	0/2077	0.46	2/2824 (0.1%)
18	DS	0.25	0/2950	0.44	0/4003
18	Ds	0.25	0/2950	0.44	0/4003
19	DT	0.24	0/2518	0.45	0/3433
19	Dt	0.24	0/2518	0.45	0/3433
20	DU	0.24	0/2689	0.42	0/3657
20	Du	0.24	0/2689	0.42	0/3657
21	DV	0.24	0/2622	0.45	0/3554
21	Dv	0.24	0/2622	0.45	0/3554
22	DW	0.24	0/2449	0.45	0/3312
22	Dw	0.24	0/2449	0.45	0/3312
23	DX	0.24	0/2171	0.44	0/2930
23	Dx	0.24	0/2171	0.44	0/2930
24	DY	0.23	0/1619	0.45	0/2198
24	Dy	0.23	0/1619	0.44	0/2198
25	DZ	0.23	0/1752	0.41	0/2372
25	Dz	0.23	0/1752	0.41	0/2372
26	EA	0.24	0/1709	0.43	0/2321
26	Ea	0.24	0/1709	0.43	0/2321
27	EB	0.24	0/1793	0.42	0/2418
27	Eb	0.24	0/1793	0.42	0/2418
28	EC	0.25	0/1673	0.45	4/2258 (0.2%)
28	Ec	0.24	0/1673	0.46	4/2258 (0.2%)
29	ED	0.26	0/1708	0.38	0/2306
29	Ed	0.26	0/1708	0.38	0/2306
30	EE	0.24	0/1066	0.45	0/1432
30	Ee	0.24	0/1066	0.45	0/1432
31	EF	0.26	0/1562	0.45	0/2123
31	Ef	0.25	0/1562	0.45	0/2123
32	EG	0.25	0/786	0.44	0/1060
32	Eg	0.25	0/786	0.44	0/1060
33	EH	0.24	0/1471	0.44	0/1995
33	Uh	0.24	0/1471	0.44	0/1995
34	EI	0.25	0/1442	0.49	4/1952 (0.2%)
34	Ei	0.25	0/1442	0.49	4/1952 (0.2%)
35	EV	0.23	0/645	0.41	0/866
35	Ev	0.23	0/645	0.42	0/866
36	EK	0.23	0/1410	0.43	0/1900
36	Ek	0.24	0/1410	0.43	0/1900
37	EL	0.24	0/1335	0.44	0/1810
37	El	0.24	0/1335	0.44	0/1810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
38	EM	0.24	0/1335	0.46	0/1794
38	Em	0.24	0/1335	0.46	0/1794
39	EN	0.24	0/1270	0.50	2/1724 (0.1%)
39	En	0.24	0/1270	0.51	2/1724 (0.1%)
40	EO	0.23	0/1137	0.44	0/1545
40	Eo	0.23	0/1137	0.45	0/1545
41	EP	0.23	0/837	0.49	0/1133
41	Ep	0.23	0/837	0.48	0/1133
42	EQ	0.24	0/1035	0.42	0/1403
42	Eq	0.24	0/1035	0.43	0/1403
43	ER	0.24	0/874	0.46	0/1182
43	Er	0.24	0/874	0.46	0/1182
44	ES	0.25	0/802	0.41	0/1087
44	Es	0.25	0/802	0.41	0/1087
45	ET	0.24	0/654	0.43	0/878
45	Et	0.24	0/654	0.43	0/878
46	EU	0.23	0/744	0.44	0/1003
46	Eu	0.23	0/744	0.44	0/1003
47	EJ	0.24	0/1437	0.42	0/1941
47	Ej	0.24	0/1437	0.43	0/1941
48	EW	0.24	0/523	0.41	0/705
48	Ew	0.24	0/523	0.42	0/705
49	EX	0.23	0/564	0.41	0/757
49	Ex	0.24	0/564	0.42	0/757
50	EY	0.25	0/573	0.49	2/770 (0.3%)
50	Ey	0.25	0/573	0.49	2/770 (0.3%)
51	EZ	0.25	0/502	0.43	0/676
51	Ez	0.25	0/502	0.43	0/676
52	FA	0.23	0/554	0.40	0/746
52	Fa	0.23	0/554	0.40	0/746
53	DL	0.25	0/2984	0.45	0/4047
53	Dl	0.25	0/2984	0.45	0/4047
All	All	0.24	0/202854	0.44	44/274802 (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
47	Ej	0	1

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Ey	67	LEU	CB-CG-CD2	6.23	121.59	111.00
50	EY	67	LEU	CB-CG-CD2	6.17	121.50	111.00
4	DD	265	LEU	CB-CG-CD2	6.13	121.42	111.00
34	EI	168	LEU	CB-CG-CD2	6.03	121.26	111.00
2	Db	573	LEU	CB-CG-CD2	5.99	121.19	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Ej	99	PHE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	669/688 (97%)	654 (98%)	15 (2%)	0	100	100
1	Da	669/688 (97%)	657 (98%)	12 (2%)	0	100	100
2	DB	602/604 (100%)	586 (97%)	16 (3%)	0	100	100
2	Db	602/604 (100%)	592 (98%)	10 (2%)	0	100	100
3	DC	580/594 (98%)	569 (98%)	9 (2%)	2 (0%)	37	59
3	Dc	580/594 (98%)	569 (98%)	11 (2%)	0	100	100
4	DD	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
4	Dd	554/637 (87%)	551 (100%)	3 (0%)	0	100	100
5	DE	124/130 (95%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	De	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
6	DF	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
6	Df	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
7	DG	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
7	Dg	96/103 (93%)	95 (99%)	1 (1%)	0	100	100
8	DH	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
8	Dh	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
9	DI	203/236 (86%)	198 (98%)	4 (2%)	1 (0%)	25	47
9	Di	203/236 (86%)	196 (97%)	6 (3%)	1 (0%)	25	47
10	DJ	218/220 (99%)	218 (100%)	0	0	100	100
10	Dj	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
11	DK	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
11	Dk	128/990 (13%)	121 (94%)	7 (6%)	0	100	100
12	DM	453/490 (92%)	446 (98%)	7 (2%)	0	100	100
12	Dm	453/490 (92%)	446 (98%)	7 (2%)	0	100	100
13	DN	451/453 (100%)	444 (98%)	7 (2%)	0	100	100
13	Dn	451/453 (100%)	444 (98%)	7 (2%)	0	100	100
14	DO	431/473 (91%)	429 (100%)	2 (0%)	0	100	100
14	Do	431/473 (91%)	427 (99%)	4 (1%)	0	100	100
15	DP	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
15	Dp	288/402 (72%)	283 (98%)	5 (2%)	0	100	100
16	DQ	381/385 (99%)	368 (97%)	13 (3%)	0	100	100
16	Dq	381/385 (99%)	370 (97%)	11 (3%)	0	100	100
17	DR	241/348 (69%)	237 (98%)	4 (2%)	0	100	100
17	Dr	241/348 (69%)	238 (99%)	3 (1%)	0	100	100
18	DS	344/346 (99%)	343 (100%)	1 (0%)	0	100	100
18	Ds	344/346 (99%)	343 (100%)	1 (0%)	0	100	100
19	DT	291/318 (92%)	290 (100%)	1 (0%)	0	100	100
19	Dt	291/318 (92%)	290 (100%)	1 (0%)	0	100	100
20	DU	327/330 (99%)	321 (98%)	6 (2%)	0	100	100
20	Du	327/330 (99%)	321 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	DV	316/318 (99%)	312 (99%)	4 (1%)	0	100	100
21	Dv	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
22	DW	299/318 (94%)	298 (100%)	1 (0%)	0	100	100
22	Dw	299/318 (94%)	297 (99%)	2 (1%)	0	100	100
23	DX	249/252 (99%)	246 (99%)	3 (1%)	0	100	100
23	Dx	249/252 (99%)	248 (100%)	1 (0%)	0	100	100
24	DY	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
24	Dy	185/234 (79%)	184 (100%)	1 (0%)	0	100	100
25	DZ	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
25	Dz	206/231 (89%)	205 (100%)	1 (0%)	0	100	100
26	EA	191/215 (89%)	187 (98%)	4 (2%)	0	100	100
26	Ea	191/215 (89%)	189 (99%)	2 (1%)	0	100	100
27	EB	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
27	Eb	207/210 (99%)	207 (100%)	0	0	100	100
28	EC	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
28	Ec	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
29	ED	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
29	Ed	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
30	EE	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
30	Ee	123/193 (64%)	121 (98%)	2 (2%)	0	100	100
31	EF	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
31	Ef	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
32	EG	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
32	Eg	96/100 (96%)	96 (100%)	0	0	100	100
33	EH	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
33	Eh	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
34	EI	170/173 (98%)	166 (98%)	4 (2%)	0	100	100
34	Ei	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
35	EV	76/88 (86%)	75 (99%)	1 (1%)	0	100	100
35	Ev	76/88 (86%)	75 (99%)	1 (1%)	0	100	100
36	EK	167/170 (98%)	166 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Ek	167/170 (98%)	166 (99%)	1 (1%)	0	100	100
37	EL	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
37	El	151/158 (96%)	150 (99%)	1 (1%)	0	100	100
38	EM	151/154 (98%)	150 (99%)	1 (1%)	0	100	100
38	Em	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
39	EN	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
39	En	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
40	EO	121/124 (98%)	118 (98%)	3 (2%)	0	100	100
40	Eo	121/124 (98%)	119 (98%)	2 (2%)	0	100	100
41	EP	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
41	Ep	98/127 (77%)	98 (100%)	0	0	100	100
42	EQ	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
42	Eq	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
43	ER	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
43	Er	102/105 (97%)	101 (99%)	1 (1%)	0	100	100
44	ES	87/89 (98%)	87 (100%)	0	0	100	100
44	Es	87/89 (98%)	87 (100%)	0	0	100	100
45	ET	80/93 (86%)	80 (100%)	0	0	100	100
45	Et	80/93 (86%)	80 (100%)	0	0	100	100
46	EU	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
46	Eu	86/90 (96%)	85 (99%)	1 (1%)	0	100	100
47	EJ	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
47	Ej	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
48	EW	61/81 (75%)	61 (100%)	0	0	100	100
48	Ew	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
49	EX	67/72 (93%)	67 (100%)	0	0	100	100
49	Ex	67/72 (93%)	67 (100%)	0	0	100	100
50	EY	68/72 (94%)	68 (100%)	0	0	100	100
50	Ey	68/72 (94%)	68 (100%)	0	0	100	100
51	EZ	56/68 (82%)	55 (98%)	1 (2%)	0	100	100
51	Ez	56/68 (82%)	56 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	FA	69/72 (96%)	69 (100%)	0	0	100	100
52	Fa	69/72 (96%)	69 (100%)	0	0	100	100
53	DL	378/536 (70%)	364 (96%)	14 (4%)	0	100	100
53	Dl	378/536 (70%)	364 (96%)	14 (4%)	0	100	100
All	All	23566/27324 (86%)	23198 (98%)	364 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	DC	143	ASN
9	Di	119	GLU
9	DI	119	GLU
3	DC	49	ASN

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	DA	596/613 (97%)	585 (98%)	11 (2%)	54	77
1	Da	596/613 (97%)	586 (98%)	10 (2%)	56	78
2	DB	569/569 (100%)	557 (98%)	12 (2%)	48	73
2	Db	569/569 (100%)	559 (98%)	10 (2%)	54	77
3	DC	553/565 (98%)	551 (100%)	2 (0%)	89	96
3	Dc	553/565 (98%)	551 (100%)	2 (0%)	89	96
4	DD	506/579 (87%)	500 (99%)	6 (1%)	67	85
4	Dd	506/579 (87%)	502 (99%)	4 (1%)	79	91
5	DE	114/116 (98%)	114 (100%)	0	100	100
5	De	114/116 (98%)	113 (99%)	1 (1%)	75	90
6	DF	200/207 (97%)	197 (98%)	3 (2%)	60	81
6	Df	200/207 (97%)	198 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	DG	84/88 (96%)	82 (98%)	2 (2%)	44	70
7	Dg	84/88 (96%)	84 (100%)	0	100	100
8	DH	119/119 (100%)	118 (99%)	1 (1%)	79	91
8	Dh	119/119 (100%)	117 (98%)	2 (2%)	56	78
9	DI	193/218 (88%)	191 (99%)	2 (1%)	73	88
9	Di	193/218 (88%)	190 (98%)	3 (2%)	58	79
10	DJ	199/199 (100%)	195 (98%)	4 (2%)	50	74
10	Dj	199/199 (100%)	197 (99%)	2 (1%)	73	88
11	DK	121/943 (13%)	121 (100%)	0	100	100
11	Dk	121/943 (13%)	121 (100%)	0	100	100
12	DM	413/447 (92%)	410 (99%)	3 (1%)	81	93
12	Dm	413/447 (92%)	409 (99%)	4 (1%)	73	88
13	DN	442/442 (100%)	437 (99%)	5 (1%)	70	86
13	Dn	442/442 (100%)	437 (99%)	5 (1%)	70	86
14	DO	380/413 (92%)	380 (100%)	0	100	100
14	Do	380/413 (92%)	380 (100%)	0	100	100
15	DP	253/358 (71%)	251 (99%)	2 (1%)	79	91
15	Dp	253/358 (71%)	251 (99%)	2 (1%)	79	91
16	DQ	340/342 (99%)	337 (99%)	3 (1%)	75	90
16	Dq	340/342 (99%)	338 (99%)	2 (1%)	84	94
17	DR	219/318 (69%)	218 (100%)	1 (0%)	86	95
17	Dr	219/318 (69%)	219 (100%)	0	100	100
18	DS	293/293 (100%)	288 (98%)	5 (2%)	56	78
18	Ds	293/293 (100%)	288 (98%)	5 (2%)	56	78
19	DT	267/289 (92%)	267 (100%)	0	100	100
19	Dt	267/289 (92%)	266 (100%)	1 (0%)	89	96
20	DU	275/276 (100%)	273 (99%)	2 (1%)	81	93
20	Du	275/276 (100%)	272 (99%)	3 (1%)	70	86
21	DV	259/259 (100%)	255 (98%)	4 (2%)	60	81
21	Dv	259/259 (100%)	255 (98%)	4 (2%)	60	81
22	DW	258/272 (95%)	253 (98%)	5 (2%)	52	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Dw	258/272 (95%)	255 (99%)	3 (1%)	67	85
23	DX	218/219 (100%)	216 (99%)	2 (1%)	75	90
23	Dx	218/219 (100%)	215 (99%)	3 (1%)	62	82
24	DY	169/216 (78%)	168 (99%)	1 (1%)	84	94
24	Dy	169/216 (78%)	167 (99%)	2 (1%)	67	85
25	DZ	189/213 (89%)	189 (100%)	0	100	100
25	Dz	189/213 (89%)	189 (100%)	0	100	100
26	EA	180/201 (90%)	179 (99%)	1 (1%)	84	94
26	Ea	180/201 (90%)	178 (99%)	2 (1%)	70	86
27	EB	180/181 (99%)	178 (99%)	2 (1%)	70	86
27	Eb	180/181 (99%)	178 (99%)	2 (1%)	70	86
28	EC	178/178 (100%)	178 (100%)	0	100	100
28	Ec	178/178 (100%)	177 (99%)	1 (1%)	84	94
29	ED	185/185 (100%)	183 (99%)	2 (1%)	70	86
29	Ed	185/185 (100%)	183 (99%)	2 (1%)	70	86
30	EE	116/180 (64%)	116 (100%)	0	100	100
30	Ee	116/180 (64%)	116 (100%)	0	100	100
31	EF	164/164 (100%)	161 (98%)	3 (2%)	54	77
31	Ef	164/164 (100%)	163 (99%)	1 (1%)	84	94
32	EG	77/78 (99%)	77 (100%)	0	100	100
32	Eg	77/78 (99%)	76 (99%)	1 (1%)	65	84
33	EH	156/156 (100%)	155 (99%)	1 (1%)	84	94
33	Eh	156/156 (100%)	156 (100%)	0	100	100
34	EI	156/157 (99%)	153 (98%)	3 (2%)	52	75
34	Ei	156/157 (99%)	153 (98%)	3 (2%)	52	75
35	EV	71/80 (89%)	71 (100%)	0	100	100
35	Ev	71/80 (89%)	71 (100%)	0	100	100
36	EK	153/154 (99%)	151 (99%)	2 (1%)	65	84
36	Ek	153/154 (99%)	150 (98%)	3 (2%)	50	74
37	EL	134/139 (96%)	133 (99%)	1 (1%)	81	93
37	El	134/139 (96%)	133 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	EM	137/138 (99%)	136 (99%)	1 (1%)	81	93
38	Em	137/138 (99%)	136 (99%)	1 (1%)	81	93
39	EN	132/135 (98%)	131 (99%)	1 (1%)	79	91
39	En	132/135 (98%)	131 (99%)	1 (1%)	79	91
40	EO	112/113 (99%)	110 (98%)	2 (2%)	54	77
40	Eo	112/113 (99%)	110 (98%)	2 (2%)	54	77
41	EP	87/113 (77%)	85 (98%)	2 (2%)	45	71
41	Ep	87/113 (77%)	85 (98%)	2 (2%)	45	71
42	EQ	104/104 (100%)	101 (97%)	3 (3%)	37	64
42	Eq	104/104 (100%)	101 (97%)	3 (3%)	37	64
43	ER	87/88 (99%)	86 (99%)	1 (1%)	70	86
43	Er	87/88 (99%)	87 (100%)	0	100	100
44	ES	84/84 (100%)	84 (100%)	0	100	100
44	Es	84/84 (100%)	84 (100%)	0	100	100
45	ET	75/83 (90%)	72 (96%)	3 (4%)	27	52
45	Et	75/83 (90%)	72 (96%)	3 (4%)	27	52
46	EU	78/80 (98%)	78 (100%)	0	100	100
46	Eu	78/80 (98%)	77 (99%)	1 (1%)	65	84
47	EJ	157/157 (100%)	154 (98%)	3 (2%)	52	75
47	Ej	157/157 (100%)	154 (98%)	3 (2%)	52	75
48	EW	57/66 (86%)	57 (100%)	0	100	100
48	Ew	57/66 (86%)	57 (100%)	0	100	100
49	EX	64/67 (96%)	63 (98%)	1 (2%)	58	79
49	Ex	64/67 (96%)	63 (98%)	1 (2%)	58	79
50	EY	62/63 (98%)	62 (100%)	0	100	100
50	Ey	62/63 (98%)	62 (100%)	0	100	100
51	EZ	55/63 (87%)	53 (96%)	2 (4%)	30	56
51	Ez	55/63 (87%)	54 (98%)	1 (2%)	54	77
52	FA	62/63 (98%)	59 (95%)	3 (5%)	21	44
52	Fa	62/63 (98%)	60 (97%)	2 (3%)	34	60
53	DL	308/441 (70%)	307 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Dl	308/441 (70%)	307 (100%)	1 (0%)	91	97
All	All	21280/24568 (87%)	21059 (99%)	221 (1%)	71	88

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Da	429	VAL
8	Dh	122	GLU
53	Dl	326	GLN
38	Em	115	PHE
1	Da	521	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
13	Dn	298	ASN
53	DL	260	ASN
17	Dr	262	GLN
28	Ec	194	GLN
24	DY	226	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 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	$\# Z > 2$
16	AME	Dq	1	16	9,10,11	0.27	0	9,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	AME	DV	1	21	9,10,11	0.26	0	9,11,13	0.54	0
33	AME	EH	1	33	9,10,11	0.25	0	9,11,13	0.41	0
21	AME	Dv	1	21	9,10,11	0.26	0	9,11,13	0.55	0
4	SEP	Dd	520	4	8,9,10	1.61	1 (12%)	7,12,14	1.44	1 (14%)
33	AME	Eh	1	33	9,10,11	0.26	0	9,11,13	0.41	0
9	SEP	Di	120	9	8,9,10	1.60	1 (12%)	7,12,14	1.27	1 (14%)
4	SEP	DD	520	4	8,9,10	1.60	1 (12%)	7,12,14	1.41	1 (14%)
35	AME	EV	1	35	9,10,11	0.27	0	9,11,13	0.43	0
4	TPO	Dd	387	4	8,10,11	1.63	1 (12%)	10,14,16	2.08	1 (10%)
18	AME	Ds	1	18	9,10,11	0.27	0	9,11,13	0.47	0
35	AME	Ev	1	35	9,10,11	0.26	0	9,11,13	0.43	0
16	AME	DQ	1	16	9,10,11	0.26	0	9,11,13	0.43	0
8	AME	DH	1	8	9,10,11	0.28	0	9,11,13	0.44	0
42	AME	Eq	1	42	9,10,11	0.28	0	9,11,13	0.43	0
4	TPO	DD	387	4	8,10,11	1.63	1 (12%)	10,14,16	2.09	1 (10%)
8	AME	Dh	1	8	9,10,11	0.27	0	9,11,13	0.45	0
18	AME	DS	1	18	9,10,11	0.27	0	9,11,13	0.47	0
42	AME	EQ	1	42	9,10,11	0.26	0	9,11,13	0.45	0
9	SEP	DI	120	9	8,9,10	1.60	1 (12%)	7,12,14	1.29	1 (14%)

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
16	AME	Dq	1	16	-	2/9/10/12	-
21	AME	DV	1	21	-	0/9/10/12	-
33	AME	EH	1	33	-	0/9/10/12	-
21	AME	Dv	1	21	-	0/9/10/12	-
4	SEP	Dd	520	4	-	0/6/8/10	-
33	AME	Eh	1	33	-	2/9/10/12	-
9	SEP	Di	120	9	-	0/6/8/10	-
4	SEP	DD	520	4	-	0/6/8/10	-
35	AME	EV	1	35	-	1/9/10/12	-
4	TPO	Dd	387	4	-	2/9/11/13	-
18	AME	Ds	1	18	-	1/9/10/12	-
35	AME	Ev	1	35	-	1/9/10/12	-
16	AME	DQ	1	16	-	2/9/10/12	-
8	AME	DH	1	8	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	Eq	1	42	-	2/9/10/12	-
4	TPO	DD	387	4	-	2/9/11/13	-
8	AME	Dh	1	8	-	0/9/10/12	-
18	AME	DS	1	18	-	0/9/10/12	-
42	AME	EQ	1	42	-	2/9/10/12	-
9	SEP	DI	120	9	-	1/6/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Dd	520	SEP	P-O1P	3.53	1.61	1.50
9	Di	120	SEP	P-O1P	3.52	1.61	1.50
4	Dd	387	TPO	P-O1P	3.51	1.61	1.50
4	DD	520	SEP	P-O1P	3.50	1.61	1.50
9	DI	120	SEP	P-O1P	3.49	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Dd	387	TPO	P-OG1-CB	-6.03	106.95	123.33
4	DD	387	TPO	P-OG1-CB	-6.00	107.02	123.33
4	Dd	520	SEP	OG-CB-CA	3.22	111.28	108.14
4	DD	520	SEP	OG-CB-CA	3.15	111.21	108.14
9	DI	120	SEP	OG-CB-CA	2.76	110.83	108.14

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	EQ	1	AME	O-C-CA-CB
33	EH	1	AME	O-C-CA-CB
42	Eq	1	AME	O-C-CA-CB
42	Eq	1	AME	CB-CG-SD-CE
42	EQ	1	AME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 245 ligands modelled in this entry, 9 are monoatomic - leaving 236 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	$\# Z > 2$
57	CDL	DV	401	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dl	1101	-	43,43,43	0.22	0	46,48,48	0.26	0
58	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.28	0
59	3PE	Dj	407	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Dv	405	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	Dj	402	-	99,99,99	0.29	0	105,111,111	0.25	0
68	ATP	Er	201	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
57	CDL	Dn	503	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dx	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DV	406	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dj	406	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	205	-	53,53,53	0.28	0	59,61,61	0.28	0
59	3PE	Dd	703	-	50,50,50	0.26	0	53,55,55	0.20	0
57	CDL	DC	601	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dn	506	-	43,43,43	0.21	0	46,48,48	0.28	0
57	CDL	El	903	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ds	405	-	99,99,99	0.30	0	105,111,111	0.24	0
65	UQ8	Ds	404	-	53,53,53	0.51	0	66,67,67	0.68	2 (3%)
57	CDL	DD	703	-	99,99,99	0.29	0	105,111,111	0.25	0
60	LPP	Ed	203	-	43,43,43	0.21	0	46,48,48	0.26	0
58	PC1	El	904	-	53,53,53	0.27	0	59,61,61	0.29	0
62	CUA	DB	701	2	0,1,1	-	-	-	-	-
57	CDL	En	1202	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DR	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dy	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	EH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dr	403	-	99,99,99	0.29	0	105,111,111	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	DH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DS	407	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	EH	202	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ed	204	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EL	903	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dd	706	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DV	405	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	DS	401	-	50,50,50	0.26	0	53,55,55	0.23	0
60	LPP	EI	402	-	43,43,43	0.21	0	46,48,48	0.26	0
67	FES	EF	201	31	0,4,4	-	-	-	-	-
57	CDL	Dj	408	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ed	205	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	El	902	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DC	608	-	53,53,53	0.27	0	59,61,61	0.27	0
57	CDL	DN	501	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EA	301	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DS	406	-	53,53,53	0.28	0	59,61,61	0.26	0
59	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.23	0
57	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DZ	501	-	99,99,99	0.29	0	105,111,111	0.24	0
59	3PE	Dc	606	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Dq	402	-	99,99,99	0.29	0	105,111,111	0.25	0
65	UQ8	En	1203	-	53,53,53	0.52	0	66,67,67	0.64	3 (4%)
57	CDL	Dm	502	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DG	204	-	50,50,50	0.26	0	53,55,55	0.20	0
57	CDL	DJ	303	-	99,99,99	0.29	0	105,111,111	0.26	0
57	CDL	DQ	1504	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	501	-	99,99,99	0.29	0	105,111,111	0.26	0
57	CDL	Eu	101	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DR	401	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DJ	307	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	El	905	-	50,50,50	0.28	0	53,55,55	0.21	0
58	PC1	Dq	405	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Dr	401	-	50,50,50	0.26	0	53,55,55	0.22	0
66	HEM	ED	602	-	42,50,50	1.29	5 (11%)	46,82,82	1.74	8 (17%)
57	CDL	Dq	403	-	99,99,99	0.29	0	105,111,111	0.26	0
59	3PE	Ds	401	-	50,50,50	0.26	0	53,55,55	0.23	0
58	PC1	DA	706	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DA	705	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	Em	901	-	50,50,50	0.27	0	53,55,55	0.19	0
58	PC1	Ds	406	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	Dh	202	-	99,99,99	0.29	0	105,111,111	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Da	709	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dx	1202	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Dx	1205	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DX	307	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dj	403	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EB	302	-	99,99,99	0.29	0	105,111,111	0.27	0
60	LPP	DN	503	-	43,43,43	0.21	0	46,48,48	0.28	0
57	CDL	El	901	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DI	702	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	EU	101	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DD	702	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DA	710	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dx	1204	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DJ	305	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Ep	701	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	507	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DC	606	-	50,50,50	0.26	0	53,55,55	0.22	0
57	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EB	304	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dm	501	-	99,99,99	0.29	0	105,111,111	0.25	0
65	UQ8	El	906	-	53,53,53	0.54	0	66,67,67	0.84	4 (6%)
58	PC1	DY	302	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	DN	505	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dr	402	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	EO	206	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dv	406	-	53,53,53	0.28	0	59,61,61	0.27	0
54	HEA	DA	701	1	58,67,67	2.31	21 (36%)	63,103,103	2.26	26 (41%)
62	CUA	Db	701	2	0,1,1	-	-	-	-	-
57	CDL	DV	404	-	99,99,99	0.29	0	105,111,111	0.26	0
58	PC1	Dc	605	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Ds	407	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Ek	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DA	709	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DY	301	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dc	602	-	53,53,53	0.27	0	59,61,61	0.28	0
57	CDL	Dd	705	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	505	-	99,99,99	0.29	0	105,111,111	0.27	0
57	CDL	DG	202	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DC	603	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	207	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	DM	502	-	99,99,99	0.29	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	3PE	DA	708	-	50,50,50	0.26	0	53,55,55	0.19	0
57	CDL	Ea	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DJ	304	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DX	305	-	50,50,50	0.27	0	53,55,55	0.20	0
59	3PE	Dx	1206	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	EN	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dz	501	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	Dn	504	-	43,43,43	0.21	0	46,48,48	0.29	0
57	CDL	En	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Eb	302	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dx	1208	-	53,53,53	0.28	0	59,61,61	0.28	0
54	HEA	DA	702	-	58,67,67	2.30	20 (34%)	63,103,103	2.30	24 (38%)
57	CDL	EL	904	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.26	0
60	LPP	DA	711	-	43,43,43	0.21	0	46,48,48	0.26	0
57	CDL	Dh	201	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dd	704	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.27	0
60	LPP	DN	502	-	43,43,43	0.22	0	46,48,48	0.30	0
57	CDL	Dq	401	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dg	202	-	99,99,99	0.29	0	105,111,111	0.24	0
65	UQ8	EL	906	-	53,53,53	0.53	0	66,67,67	0.80	3 (4%)
57	CDL	Dq	404	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DC	605	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	DA	707	-	53,53,53	0.29	0	59,61,61	0.28	0
57	CDL	ED	604	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DQ	1502	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dj	401	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	DJ	301	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	Du	402	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DR	402	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EN	1202	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dv	408	-	53,53,53	0.28	0	59,61,61	0.27	0
58	PC1	EO	205	-	53,53,53	0.27	0	59,61,61	0.29	0
57	CDL	DQ	1501	-	99,99,99	0.29	0	105,111,111	0.26	0
59	3PE	EL	905	-	50,50,50	0.27	0	53,55,55	0.22	0
59	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
65	UQ8	Ed	202	-	53,53,53	0.53	0	66,67,67	0.72	2 (3%)
58	PC1	DX	302	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	DX	306	-	53,53,53	0.28	0	59,61,61	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Dg	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ds	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	EI	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dc	601	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Da	705	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dv	404	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Du	404	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DQ	1503	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	EL	901	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DU	403	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Do	501	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dv	407	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DS	405	-	99,99,99	0.29	0	105,111,111	0.24	0
59	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	DO	501	-	99,99,99	0.29	0	105,111,111	0.24	0
66	HEM	Ed	201	-	42,50,50	1.29	6 (14%)	46,82,82	1.74	8 (17%)
59	3PE	Eo	203	-	50,50,50	0.26	0	53,55,55	0.21	0
59	3PE	Ds	403	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	DN	504	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DV	407	-	53,53,53	0.28	0	59,61,61	0.27	0
54	HEA	Da	701	1	58,67,67	2.31	21 (36%)	63,103,103	2.26	27 (42%)
57	CDL	Dj	405	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Di	701	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Eh	1601	-	99,99,99	0.30	0	105,111,111	0.23	0
58	PC1	DG	203	-	53,53,53	0.28	0	59,61,61	0.28	0
59	3PE	DC	607	-	50,50,50	0.26	0	53,55,55	0.20	0
59	3PE	EO	204	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	DS	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	EO	202	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	EM	901	-	50,50,50	0.26	0	53,55,55	0.20	0
59	3PE	EN	1203	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	Dd	702	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DU	404	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	EO	203	-	50,50,50	0.26	0	53,55,55	0.20	0
67	FES	Ef	1002	31	0,4,4	-	-	-	-	-
58	PC1	Dc	607	-	53,53,53	0.27	0	59,61,61	0.28	0
57	CDL	DD	704	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	Db	702	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	Dx	1203	-	99,99,99	0.30	0	105,111,111	0.24	0
67	FES	Ef	1003	31	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	DG	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DX	301	-	99,99,99	0.30	0	105,111,111	0.25	0
67	FES	EF	202	31	0,4,4	-	-	-		
58	PC1	DC	602	-	53,53,53	0.27	0	59,61,61	0.28	0
58	PC1	EB	301	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	DI	701	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dv	401	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	DJ	306	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Da	708	-	50,50,50	0.25	0	53,55,55	0.21	0
59	3PE	Dx	1207	-	50,50,50	0.27	0	53,55,55	0.19	0
65	UQ8	DS	404	-	53,53,53	0.51	0	66,67,67	0.68	2 (3%)
57	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.28	0
65	UQ8	ED	603	-	53,53,53	0.52	0	66,67,67	0.71	2 (3%)
54	HEA	Da	702	-	58,67,67	2.31	21 (36%)	63,103,103	2.29	23 (36%)
57	CDL	DU	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DJ	302	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	EK	201	-	99,99,99	0.29	0	105,111,111	0.25	0
68	ATP	ER	201	-	28,33,33	0.66	0	34,52,52	0.92	1 (2%)
58	PC1	Eo	201	-	53,53,53	0.29	0	59,61,61	0.28	0
57	CDL	Dj	404	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Du	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DV	403	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	ED	601	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DM	501	-	99,99,99	0.29	0	105,111,111	0.24	0
58	PC1	Ef	1001	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	DX	304	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	EL	902	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Eg	101	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.18	0
59	3PE	Eo	202	-	50,50,50	0.26	0	53,55,55	0.19	0
58	PC1	Dg	203	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Di	702	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	DS	403	-	50,50,50	0.27	0	53,55,55	0.20	0
65	UQ8	EN	1204	-	53,53,53	0.52	0	66,67,67	0.68	2 (3%)
57	CDL	DU	402	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	EO	201	-	53,53,53	0.29	0	59,61,61	0.28	0
58	PC1	Da	706	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dc	604	-	53,53,53	0.27	0	59,61,61	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
57	CDL	DV	401	-	-	28/110/110/110	-
60	LPP	Dl	1101	-	-	8/45/45/45	-
58	PC1	Da	707	-	-	12/57/57/57	-
59	3PE	Dj	407	-	-	5/54/54/54	-
58	PC1	Dv	405	-	-	10/57/57/57	-
57	CDL	Dj	402	-	-	29/110/110/110	-
68	ATP	Er	201	-	-	2/18/38/38	0/3/3/3
57	CDL	Dn	503	-	-	22/110/110/110	-
57	CDL	Dx	1201	-	-	28/110/110/110	-
58	PC1	DV	406	-	-	11/57/57/57	-
58	PC1	Dj	406	-	-	10/57/57/57	-
58	PC1	Eo	205	-	-	14/57/57/57	-
59	3PE	Dd	703	-	-	17/54/54/54	-
57	CDL	DC	601	-	-	26/110/110/110	-
60	LPP	Dn	506	-	-	7/45/45/45	-
57	CDL	El	903	-	-	31/110/110/110	-
57	CDL	Ds	405	-	-	28/110/110/110	-
65	UQ8	Ds	404	-	-	11/51/75/75	0/1/1/1
57	CDL	DD	703	-	-	25/110/110/110	-
60	LPP	Ed	203	-	-	2/45/45/45	-
58	PC1	El	904	-	-	10/57/57/57	-
57	CDL	En	1202	-	-	23/110/110/110	-
57	CDL	DR	403	-	-	27/110/110/110	-
57	CDL	Dy	301	-	-	25/110/110/110	-
57	CDL	EH	201	-	-	22/110/110/110	-
57	CDL	Dr	403	-	-	23/110/110/110	-
57	CDL	DH	201	-	-	22/110/110/110	-
58	PC1	DS	407	-	-	16/57/57/57	-
57	CDL	EH	202	-	-	24/110/110/110	-
57	CDL	Ed	204	-	-	24/110/110/110	-
57	CDL	EL	903	-	-	37/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	Dd	706	-	-	24/110/110/110	-
58	PC1	DV	405	-	-	13/57/57/57	-
59	3PE	DS	401	-	-	16/54/54/54	-
60	LPP	EI	402	-	-	8/45/45/45	-
67	FES	EF	201	31	-	-	0/1/1/1
57	CDL	Dj	408	-	-	33/110/110/110	-
57	CDL	Ed	205	-	-	25/110/110/110	-
57	CDL	El	902	-	-	38/110/110/110	-
58	PC1	DC	608	-	-	18/57/57/57	-
57	CDL	DN	501	-	-	16/110/110/110	-
57	CDL	EA	301	-	-	27/110/110/110	-
58	PC1	DS	406	-	-	19/57/57/57	-
59	3PE	Dg	204	-	-	11/54/54/54	-
57	CDL	Dn	502	-	-	27/110/110/110	-
57	CDL	DZ	501	-	-	28/110/110/110	-
59	3PE	Dc	606	-	-	18/54/54/54	-
57	CDL	Dq	402	-	-	27/110/110/110	-
65	UQ8	En	1203	-	-	10/51/75/75	0/1/1/1
57	CDL	Dm	502	-	-	18/110/110/110	-
59	3PE	DG	204	-	-	16/54/54/54	-
57	CDL	DJ	303	-	-	33/110/110/110	-
57	CDL	DQ	1504	-	-	33/110/110/110	-
57	CDL	Dn	501	-	-	35/110/110/110	-
57	CDL	Eu	101	-	-	27/110/110/110	-
59	3PE	DR	401	-	-	8/54/54/54	-
57	CDL	DJ	307	-	-	29/110/110/110	-
59	3PE	El	905	-	-	16/54/54/54	-
58	PC1	Dq	405	-	-	10/57/57/57	-
59	3PE	Dr	401	-	-	15/54/54/54	-
66	HEM	ED	602	-	-	2/12/54/54	-
57	CDL	Dq	403	-	-	23/110/110/110	-
59	3PE	Ds	401	-	-	16/54/54/54	-
58	PC1	DA	706	-	-	14/57/57/57	-
57	CDL	DA	705	-	-	26/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Em	901	-	-	13/54/54/54	-
58	PC1	Ds	406	-	-	7/57/57/57	-
57	CDL	Dh	202	-	-	33/110/110/110	-
57	CDL	Da	709	-	-	33/110/110/110	-
58	PC1	Dx	1202	-	-	13/57/57/57	-
59	3PE	Dx	1205	-	-	17/54/54/54	-
57	CDL	DX	307	-	-	26/110/110/110	-
57	CDL	Dj	403	-	-	32/110/110/110	-
57	CDL	EB	302	-	-	24/110/110/110	-
60	LPP	DN	503	-	-	1/45/45/45	-
57	CDL	El	901	-	-	39/110/110/110	-
58	PC1	DI	702	-	-	18/57/57/57	-
57	CDL	EU	101	-	-	30/110/110/110	-
57	CDL	DD	702	-	-	25/110/110/110	-
57	CDL	DA	710	-	-	22/110/110/110	-
58	PC1	Dx	1204	-	-	14/57/57/57	-
57	CDL	DJ	305	-	-	23/110/110/110	-
57	CDL	Ep	701	-	-	28/110/110/110	-
57	CDL	Dn	507	-	-	20/110/110/110	-
59	3PE	DC	606	-	-	9/54/54/54	-
57	CDL	Dv	403	-	-	24/110/110/110	-
57	CDL	EB	304	-	-	34/110/110/110	-
57	CDL	Dm	501	-	-	38/110/110/110	-
65	UQ8	El	906	-	-	12/51/75/75	0/1/1/1
58	PC1	DY	302	-	-	10/57/57/57	-
57	CDL	DN	505	-	-	29/110/110/110	-
57	CDL	Dr	402	-	-	33/110/110/110	-
58	PC1	EO	206	-	-	26/57/57/57	-
57	CDL	Du	403	-	-	29/110/110/110	-
58	PC1	Dv	406	-	-	19/57/57/57	-
54	HEA	DA	701	1	-	3/32/76/76	-
57	CDL	DV	404	-	-	36/110/110/110	-
58	PC1	Dc	605	-	-	16/57/57/57	-
59	3PE	Ds	407	-	-	11/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	Ek	201	-	-	26/110/110/110	-
57	CDL	DA	709	-	-	35/110/110/110	-
57	CDL	DY	301	-	-	27/110/110/110	-
58	PC1	Dc	602	-	-	17/57/57/57	-
57	CDL	Dd	705	-	-	30/110/110/110	-
57	CDL	Dn	505	-	-	25/110/110/110	-
57	CDL	DG	202	-	-	18/110/110/110	-
58	PC1	DC	603	-	-	14/57/57/57	-
58	PC1	EO	207	-	-	17/57/57/57	-
57	CDL	DM	502	-	-	15/110/110/110	-
59	3PE	DA	708	-	-	12/54/54/54	-
57	CDL	Ea	301	-	-	24/110/110/110	-
57	CDL	DJ	304	-	-	33/110/110/110	-
59	3PE	DX	305	-	-	13/54/54/54	-
59	3PE	Dx	1206	-	-	20/54/54/54	-
57	CDL	EN	1201	-	-	28/110/110/110	-
57	CDL	Dz	501	-	-	27/110/110/110	-
60	LPP	Dn	504	-	-	9/45/45/45	-
57	CDL	En	1201	-	-	23/110/110/110	-
58	PC1	Eb	302	-	-	4/57/57/57	-
58	PC1	Dx	1208	-	-	5/57/57/57	-
54	HEA	DA	702	-	-	9/32/76/76	-
57	CDL	EL	904	-	-	29/110/110/110	-
58	PC1	Eb	301	-	-	9/57/57/57	-
60	LPP	DA	711	-	-	7/45/45/45	-
57	CDL	Dh	201	-	-	22/110/110/110	-
57	CDL	Dd	704	-	-	34/110/110/110	-
58	PC1	Dy	302	-	-	10/57/57/57	-
60	LPP	DN	502	-	-	8/45/45/45	-
57	CDL	Dq	401	-	-	23/110/110/110	-
57	CDL	Dg	202	-	-	23/110/110/110	-
65	UQ8	EL	906	-	-	10/51/75/75	0/1/1/1
57	CDL	Dq	404	-	-	20/110/110/110	-
58	PC1	DC	605	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	DC	604	-	-	16/57/57/57	-
58	PC1	DA	707	-	-	11/57/57/57	-
57	CDL	ED	604	-	-	25/110/110/110	-
57	CDL	DQ	1502	-	-	22/110/110/110	-
57	CDL	Dj	401	-	-	31/110/110/110	-
58	PC1	DB	702	-	-	23/57/57/57	-
59	3PE	DJ	301	-	-	15/54/54/54	-
57	CDL	Du	402	-	-	18/110/110/110	-
57	CDL	DR	402	-	-	35/110/110/110	-
57	CDL	EN	1202	-	-	29/110/110/110	-
58	PC1	Dv	408	-	-	9/57/57/57	-
58	PC1	EO	205	-	-	10/57/57/57	-
57	CDL	DQ	1501	-	-	30/110/110/110	-
59	3PE	EL	905	-	-	16/54/54/54	-
59	3PE	Dr	404	-	-	10/54/54/54	-
65	UQ8	Ed	202	-	-	9/51/75/75	0/1/1/1
58	PC1	DX	302	-	-	13/57/57/57	-
58	PC1	DX	306	-	-	9/57/57/57	-
57	CDL	Dg	201	-	-	38/110/110/110	-
57	CDL	Ds	402	-	-	30/110/110/110	-
57	CDL	EI	401	-	-	22/110/110/110	-
57	CDL	Dc	601	-	-	28/110/110/110	-
57	CDL	Da	705	-	-	32/110/110/110	-
57	CDL	Dv	404	-	-	40/110/110/110	-
57	CDL	Du	404	-	-	27/110/110/110	-
58	PC1	DQ	1503	-	-	11/57/57/57	-
57	CDL	EL	901	-	-	33/110/110/110	-
57	CDL	DU	403	-	-	20/110/110/110	-
57	CDL	Do	501	-	-	29/110/110/110	-
58	PC1	Dv	407	-	-	12/57/57/57	-
57	CDL	DS	405	-	-	31/110/110/110	-
59	3PE	DG	205	-	-	14/54/54/54	-
57	CDL	DO	501	-	-	26/110/110/110	-
66	HEM	Ed	201	-	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Eo	203	-	-	6/54/54/54	-
59	3PE	Ds	403	-	-	19/54/54/54	-
57	CDL	DN	504	-	-	27/110/110/110	-
58	PC1	DV	407	-	-	10/57/57/57	-
54	HEA	Da	701	1	-	4/32/76/76	-
57	CDL	Dj	405	-	-	22/110/110/110	-
57	CDL	Di	701	-	-	30/110/110/110	-
57	CDL	Eh	1601	-	-	32/110/110/110	-
58	PC1	DG	203	-	-	8/57/57/57	-
59	3PE	DC	607	-	-	15/54/54/54	-
59	3PE	EO	204	-	-	8/54/54/54	-
57	CDL	DS	402	-	-	30/110/110/110	-
57	CDL	EO	202	-	-	30/110/110/110	-
59	3PE	EM	901	-	-	13/54/54/54	-
59	3PE	EN	1203	-	-	14/54/54/54	-
58	PC1	Eo	204	-	-	19/57/57/57	-
57	CDL	Dd	702	-	-	27/110/110/110	-
57	CDL	DU	404	-	-	22/110/110/110	-
58	PC1	Dc	603	-	-	14/57/57/57	-
59	3PE	EO	203	-	-	17/54/54/54	-
67	FES	Ef	1002	31	-	-	0/1/1/1
58	PC1	Dc	607	-	-	16/57/57/57	-
57	CDL	DD	704	-	-	32/110/110/110	-
58	PC1	Db	702	-	-	21/57/57/57	-
57	CDL	Dx	1203	-	-	31/110/110/110	-
67	FES	Ef	1003	31	-	-	0/1/1/1
57	CDL	DG	201	-	-	36/110/110/110	-
57	CDL	DX	301	-	-	30/110/110/110	-
67	FES	EF	202	31	-	-	0/1/1/1
58	PC1	DC	602	-	-	16/57/57/57	-
58	PC1	EB	301	-	-	11/57/57/57	-
57	CDL	DI	701	-	-	25/110/110/110	-
57	CDL	Dv	401	-	-	26/110/110/110	-
58	PC1	DJ	306	-	-	12/57/57/57	-
59	3PE	Da	708	-	-	16/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Dx	1207	-	-	14/54/54/54	-
65	UQ8	DS	404	-	-	8/51/75/75	0/1/1/1
57	CDL	DV	402	-	-	40/110/110/110	-
57	CDL	Ei	401	-	-	21/110/110/110	-
58	PC1	EB	303	-	-	3/57/57/57	-
65	UQ8	ED	603	-	-	8/51/75/75	0/1/1/1
54	HEA	Da	702	-	-	9/32/76/76	-
57	CDL	DU	401	-	-	32/110/110/110	-
57	CDL	DJ	302	-	-	17/110/110/110	-
57	CDL	EK	201	-	-	26/110/110/110	-
68	ATP	ER	201	-	-	7/18/38/38	0/3/3/3
58	PC1	Eo	201	-	-	15/57/57/57	-
57	CDL	Dj	404	-	-	33/110/110/110	-
57	CDL	Du	401	-	-	28/110/110/110	-
57	CDL	DV	403	-	-	25/110/110/110	-
57	CDL	ED	601	-	-	24/110/110/110	-
57	CDL	DM	501	-	-	31/110/110/110	-
58	PC1	Ef	1001	-	-	15/57/57/57	-
59	3PE	DX	304	-	-	18/54/54/54	-
57	CDL	EL	902	-	-	25/110/110/110	-
57	CDL	Dv	402	-	-	37/110/110/110	-
57	CDL	Eg	101	-	-	32/110/110/110	-
59	3PE	DX	303	-	-	13/54/54/54	-
59	3PE	Eo	202	-	-	15/54/54/54	-
58	PC1	Dg	203	-	-	12/57/57/57	-
58	PC1	Di	702	-	-	19/57/57/57	-
59	3PE	DS	403	-	-	19/54/54/54	-
65	UQ8	EN	1204	-	-	15/51/75/75	0/1/1/1
57	CDL	DU	402	-	-	18/110/110/110	-
58	PC1	EO	201	-	-	12/57/57/57	-
58	PC1	Da	706	-	-	17/57/57/57	-
58	PC1	Dc	604	-	-	12/57/57/57	-

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Da	701	HEA	C3A-C2A	6.62	1.49	1.40
54	DA	701	HEA	C3A-C2A	6.53	1.49	1.40
54	Da	702	HEA	C3A-C2A	6.51	1.49	1.40
54	DA	702	HEA	C3A-C2A	6.49	1.49	1.40
54	Da	701	HEA	C3B-C2B	5.46	1.47	1.34

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	701	HEA	C3D-C4D-ND	6.01	116.16	110.35
54	DA	702	HEA	C3D-C4D-ND	5.95	116.10	110.35
54	Da	702	HEA	C3D-C4D-ND	5.93	116.09	110.35
54	Da	701	HEA	C3D-C4D-ND	5.90	116.06	110.35
54	DA	702	HEA	C2D-C1D-ND	5.52	116.19	109.84

There are no chirality outliers.

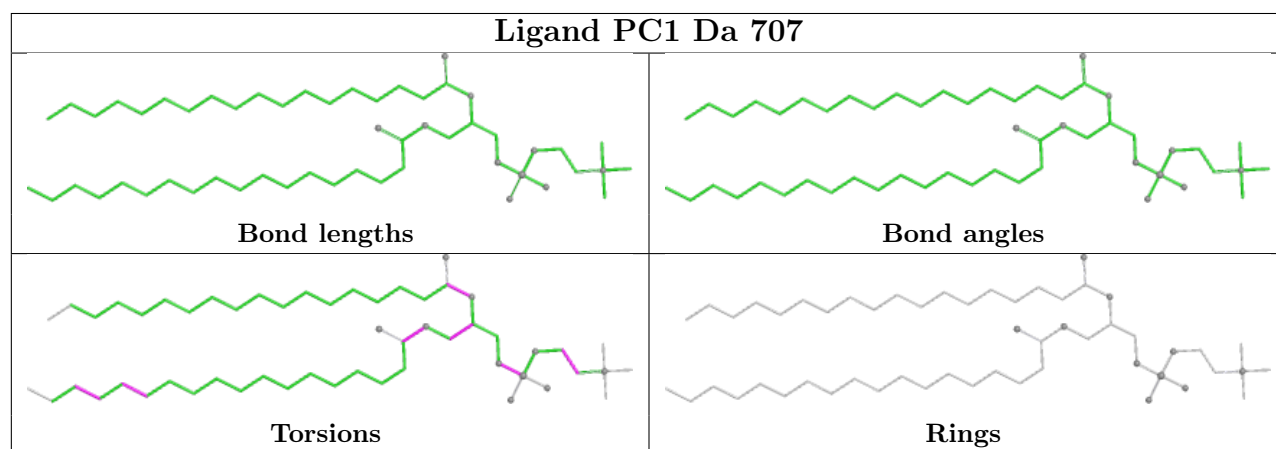
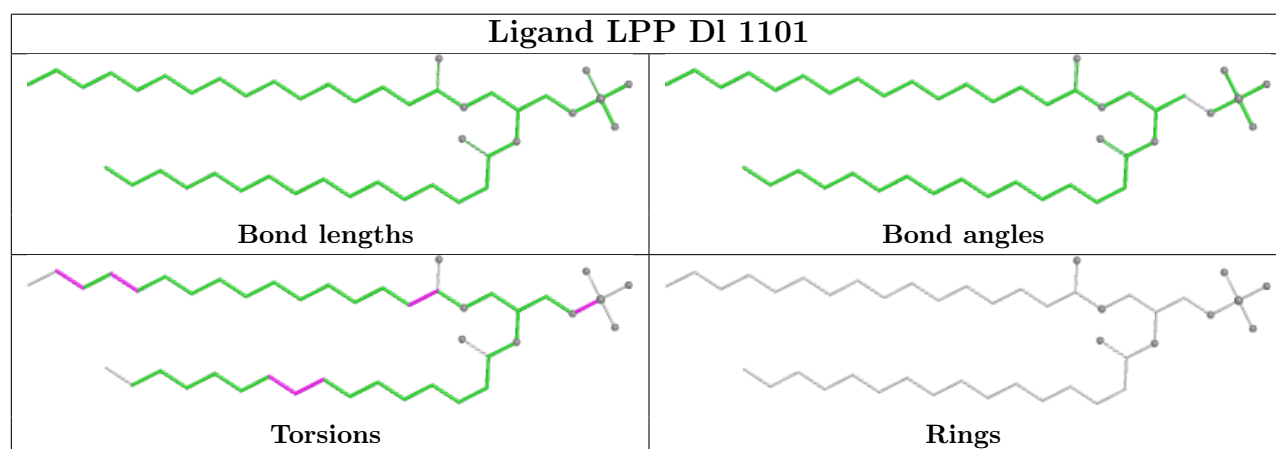
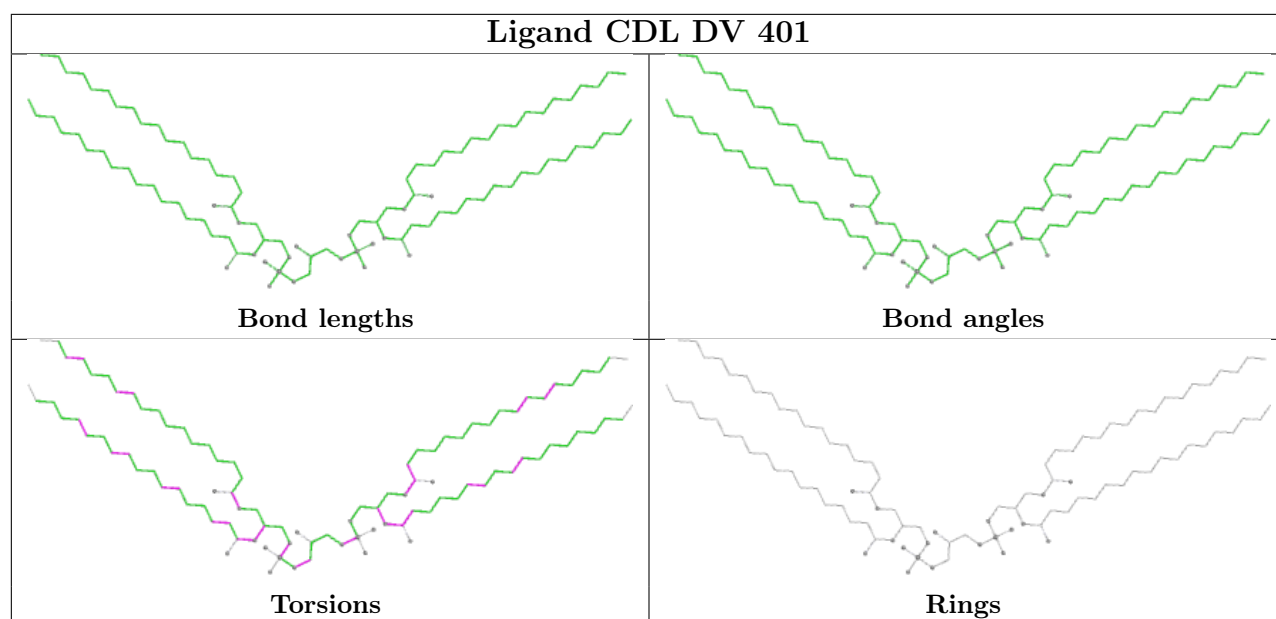
5 of 4627 torsion outliers are listed below:

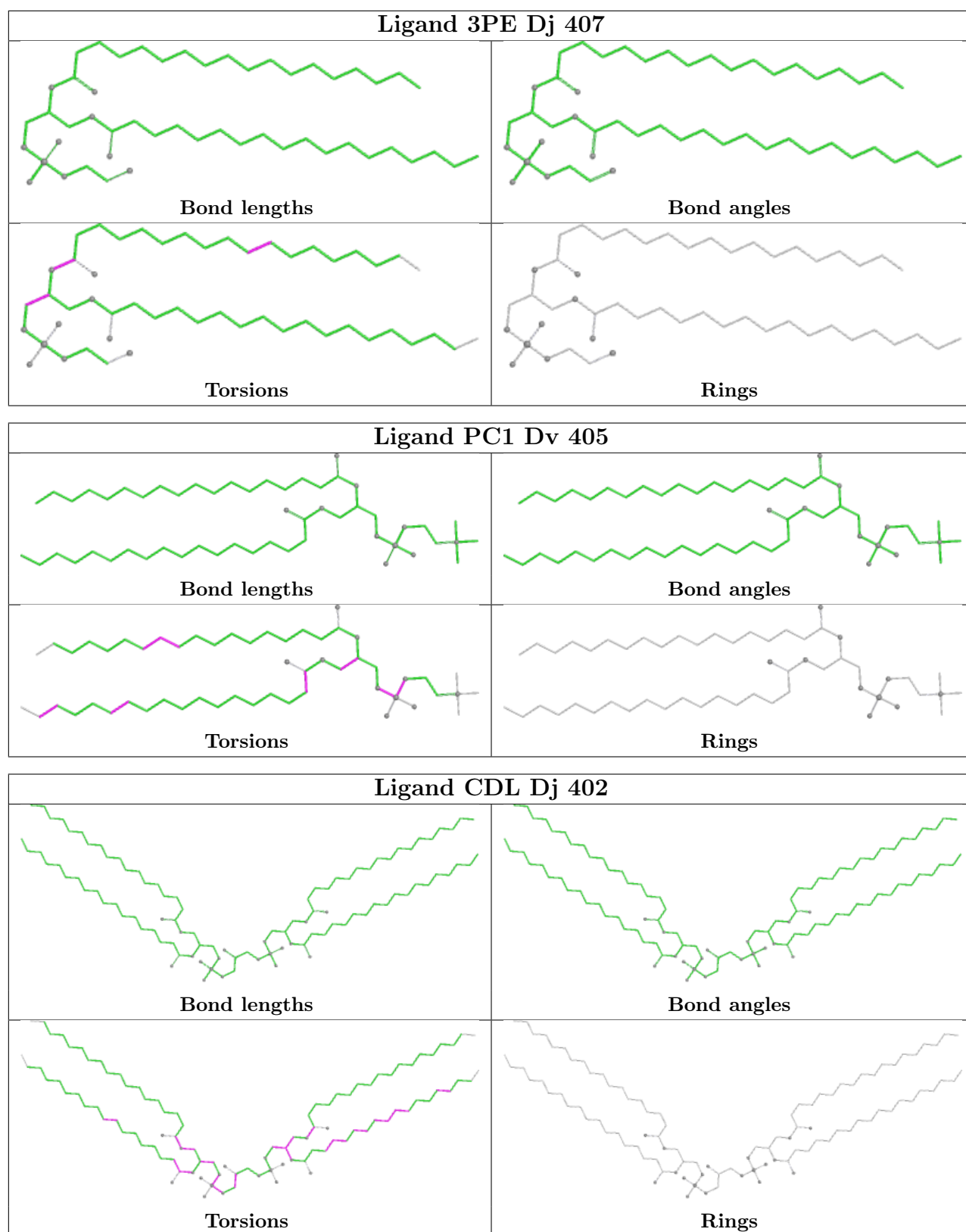
Mol	Chain	Res	Type	Atoms
57	DA	709	CDL	CA2-OA2-PA1-OA3
57	DA	709	CDL	CA2-OA2-PA1-OA4
57	DA	709	CDL	CA2-OA2-PA1-OA5
57	DA	709	CDL	CA3-OA5-PA1-OA4
57	DA	709	CDL	CB2-OB2-PB2-OB3

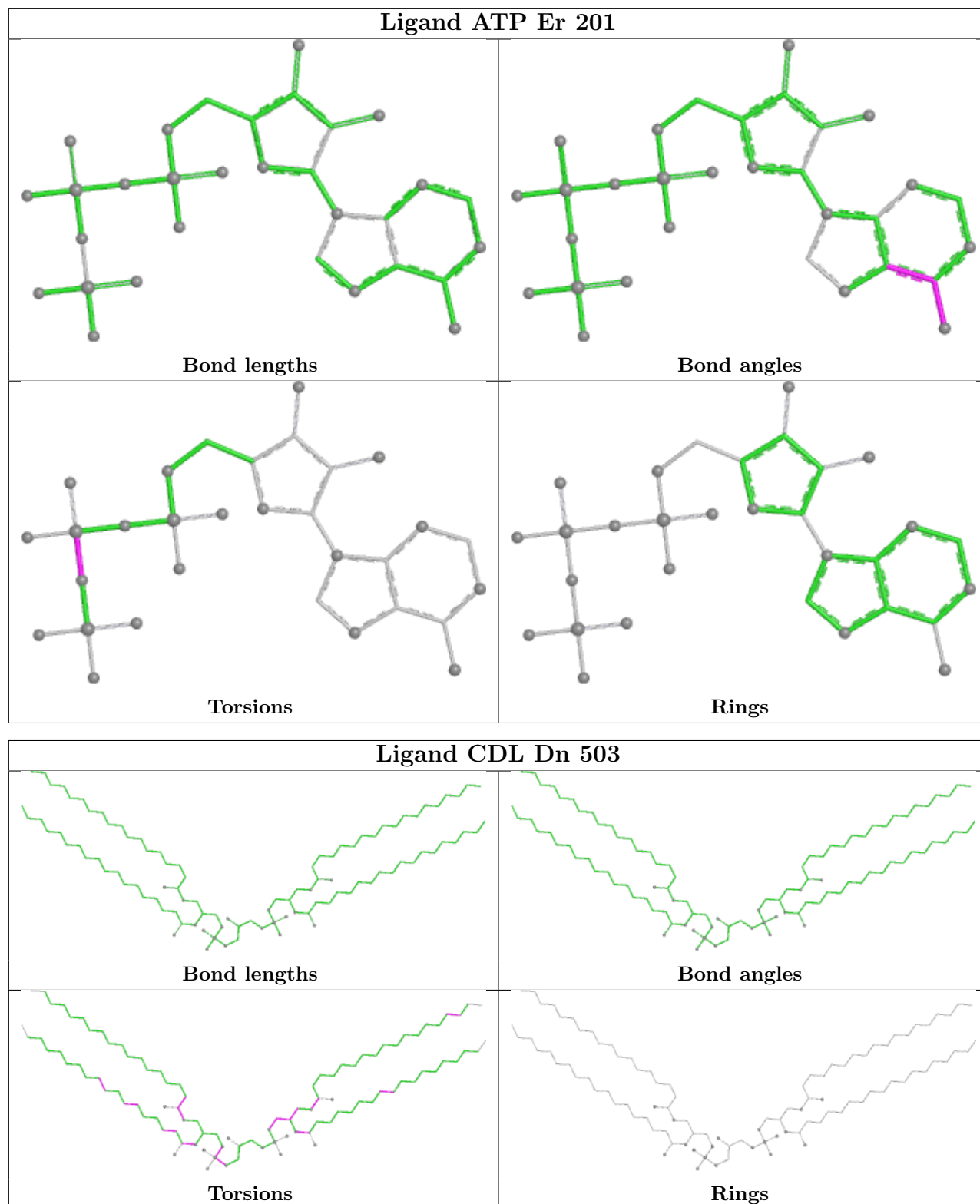
There are no ring outliers.

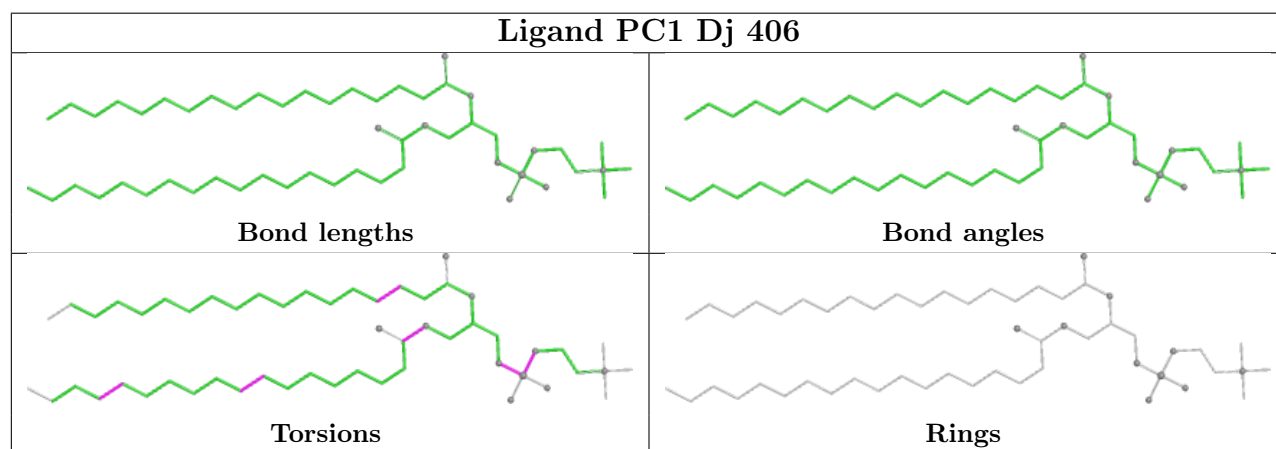
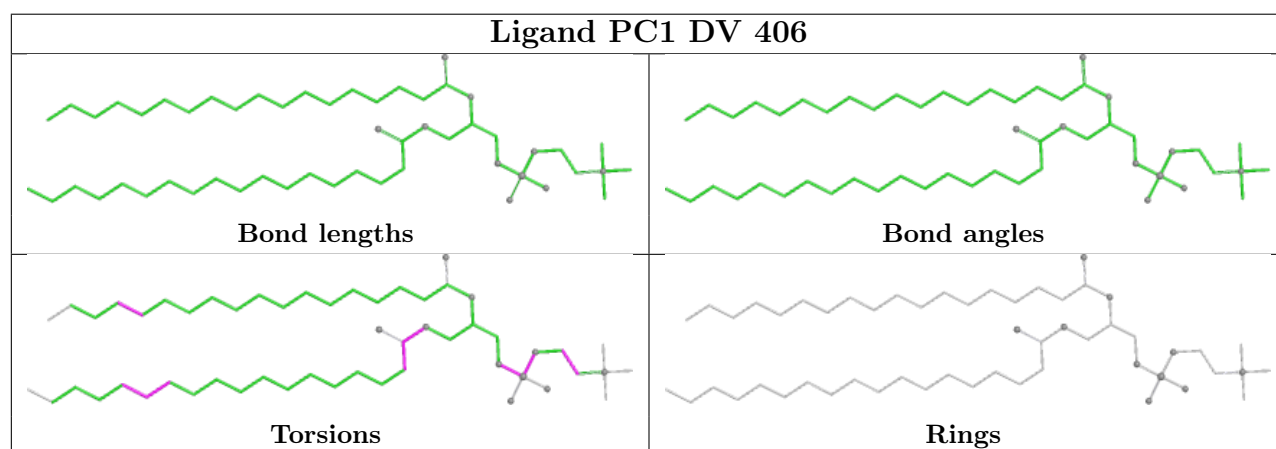
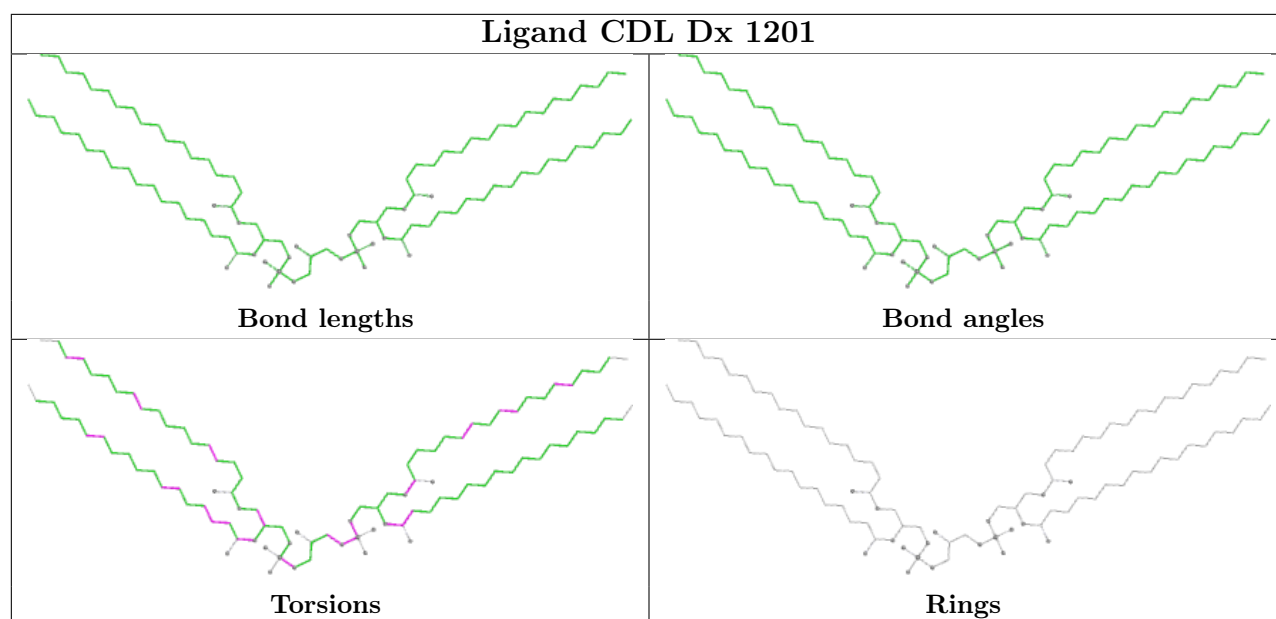
No monomer is involved in short contacts.

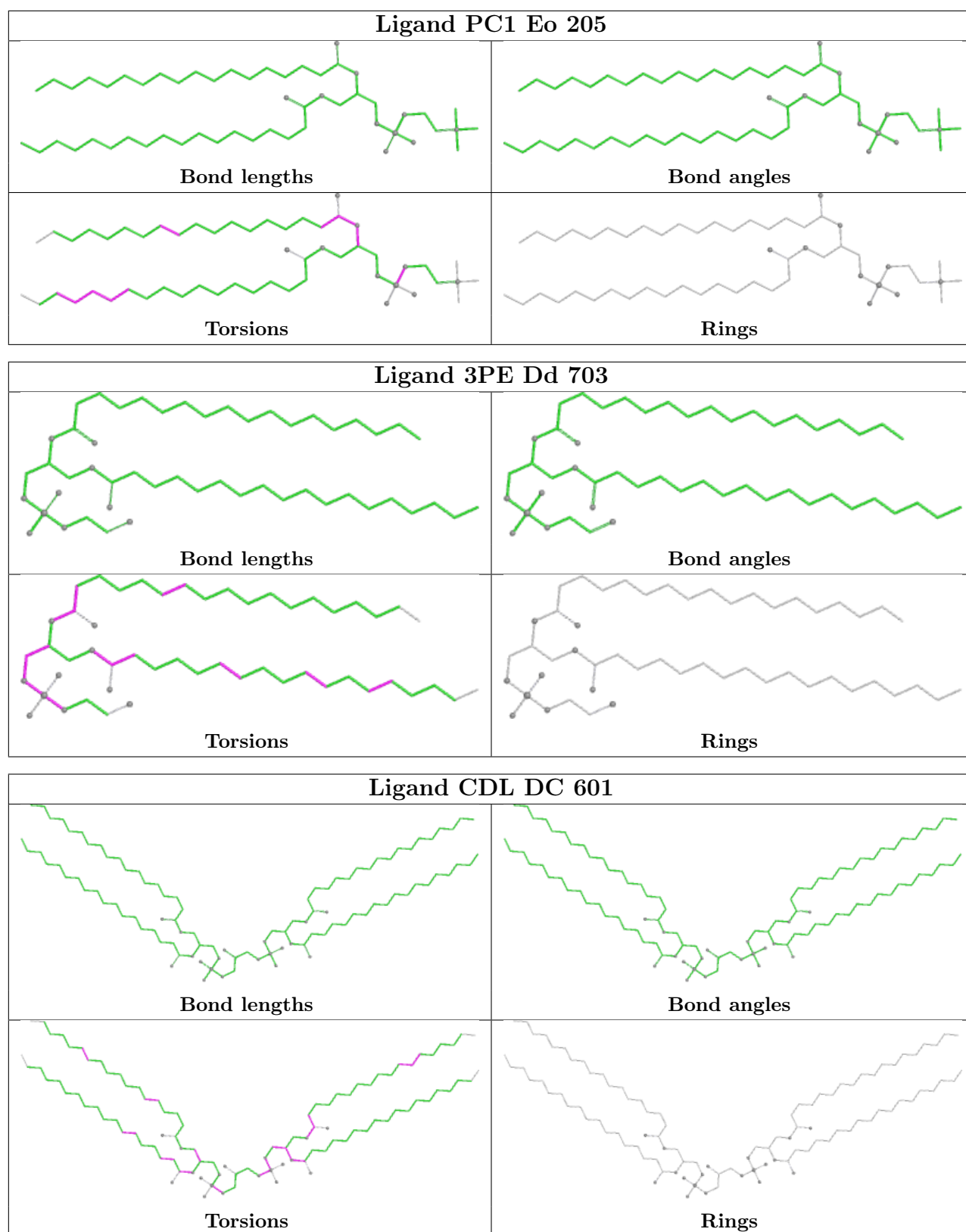
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

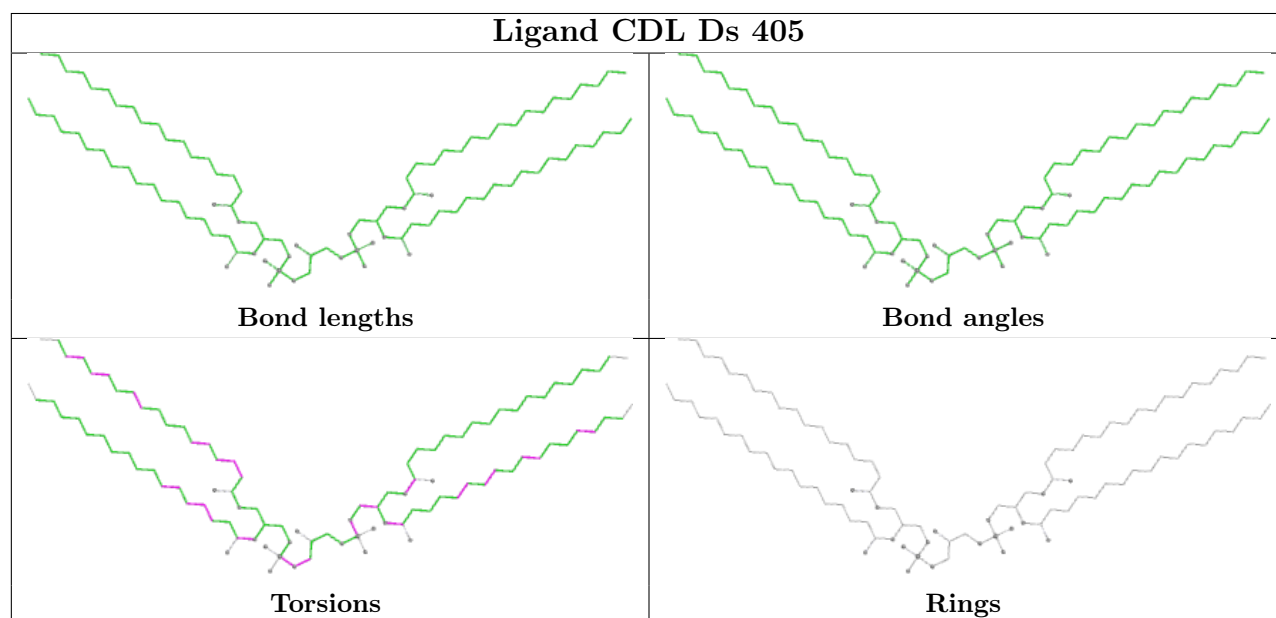
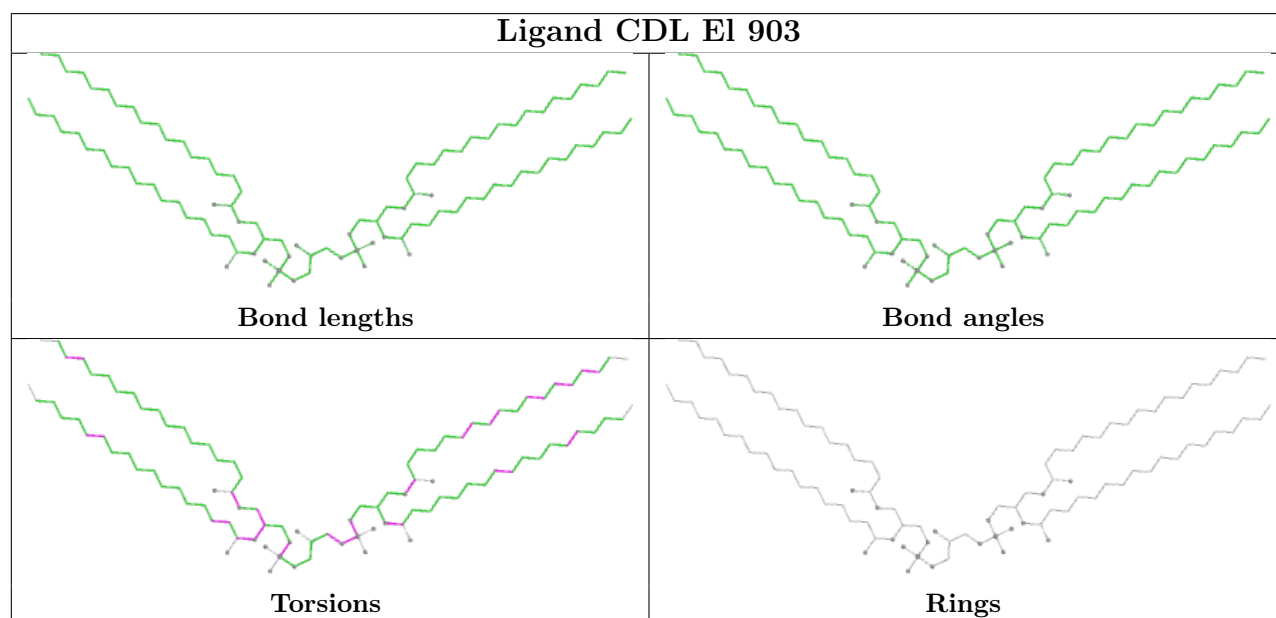
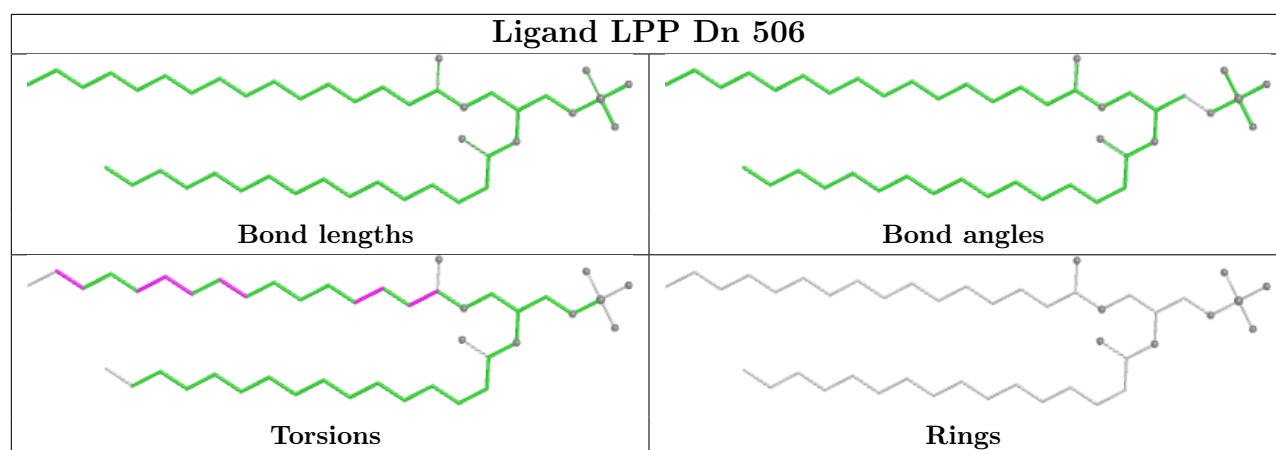


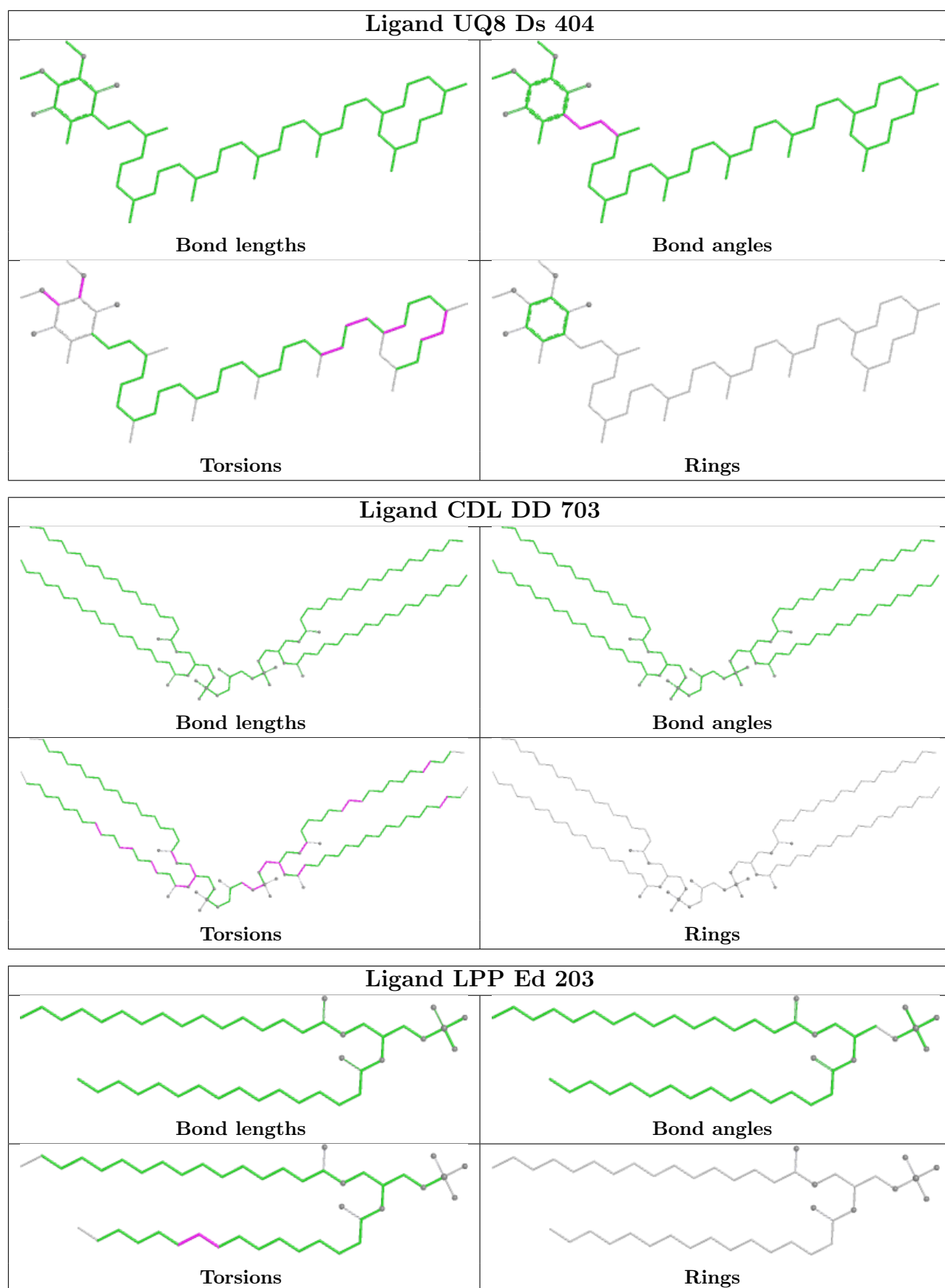


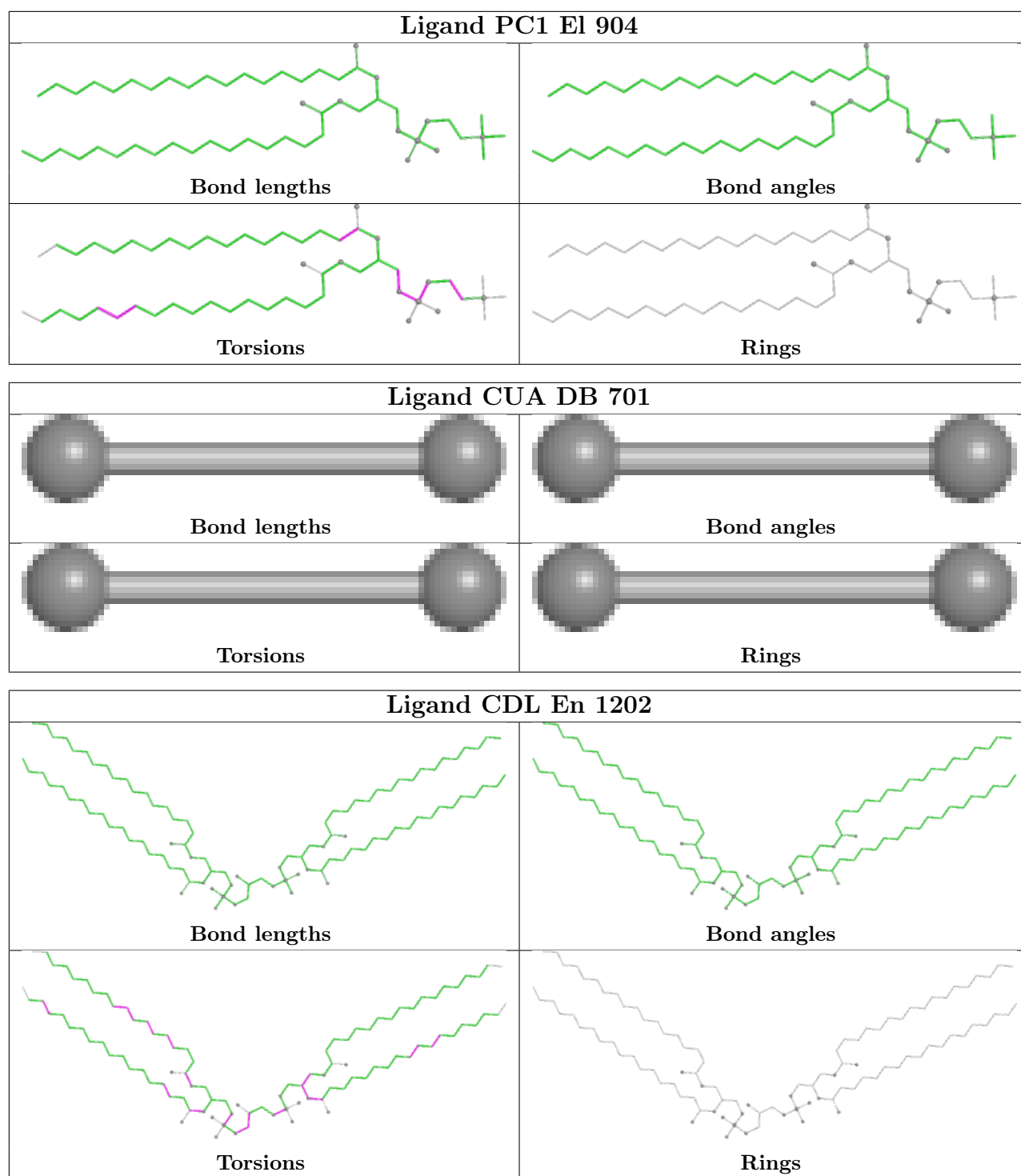


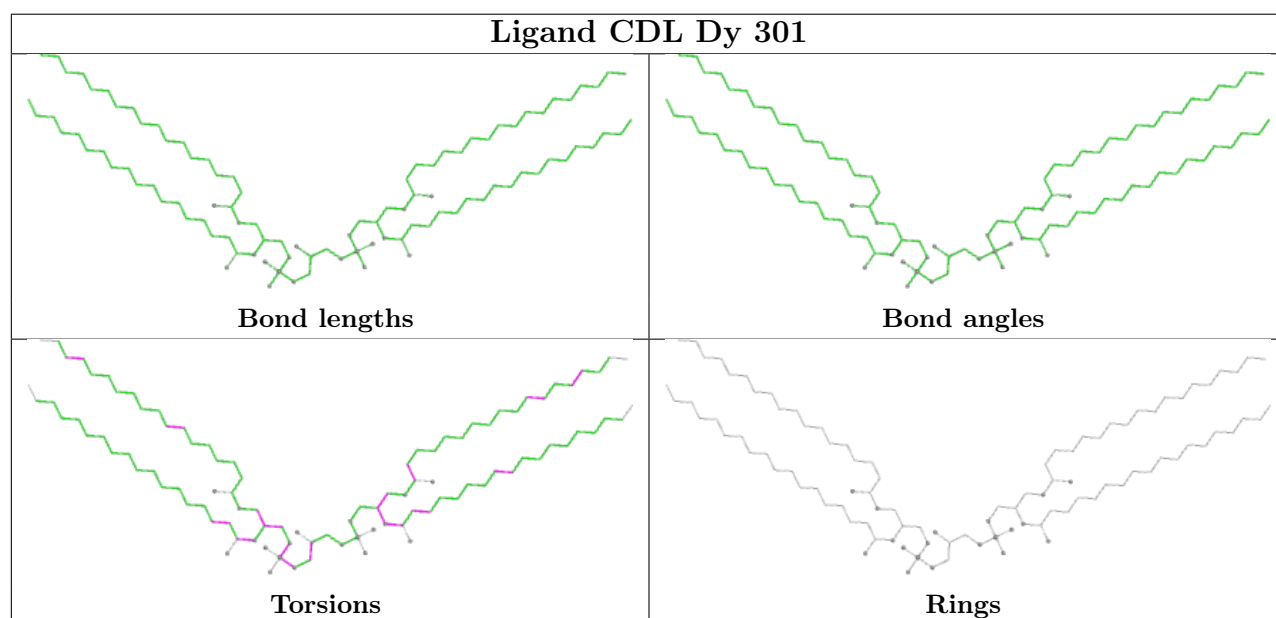
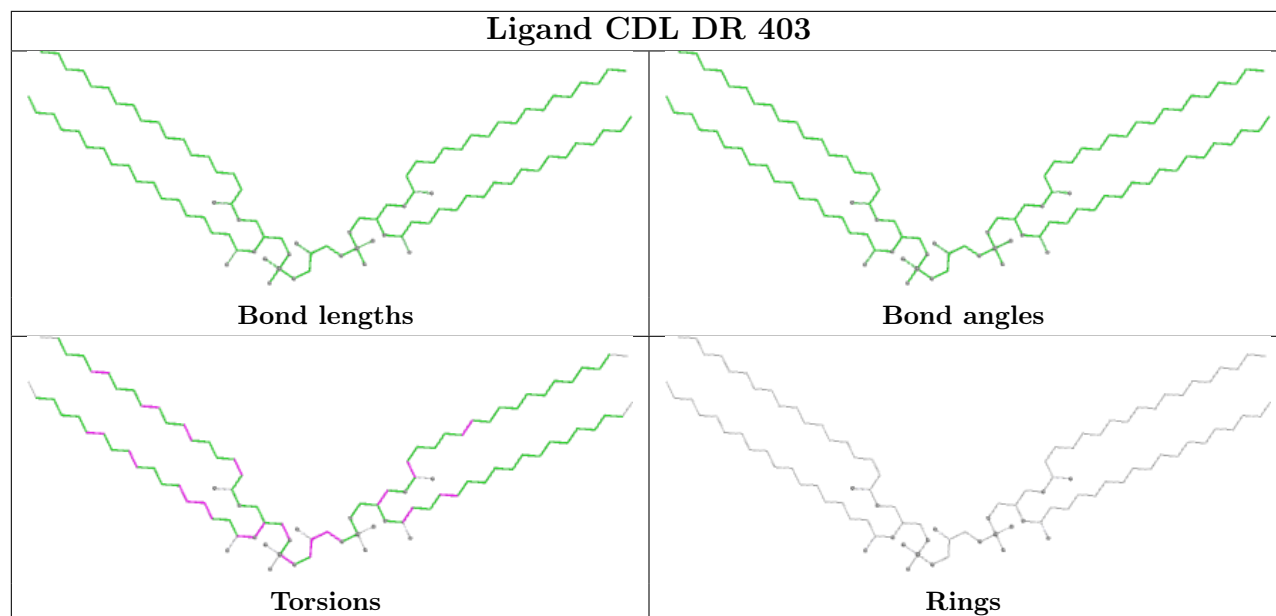


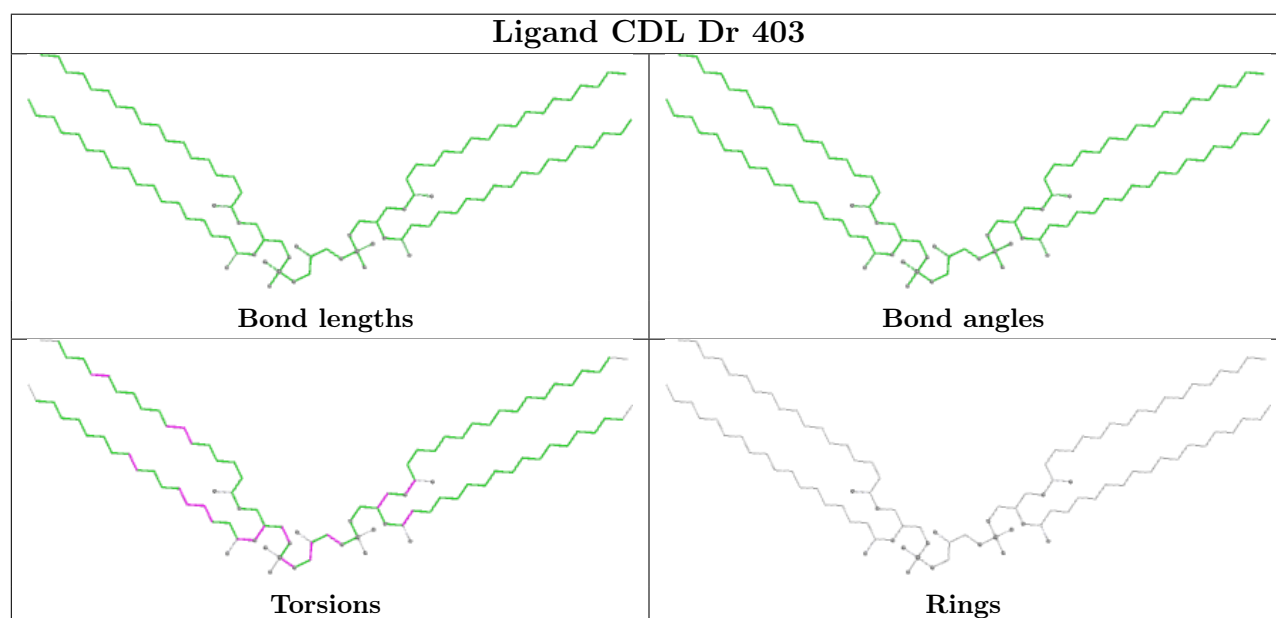
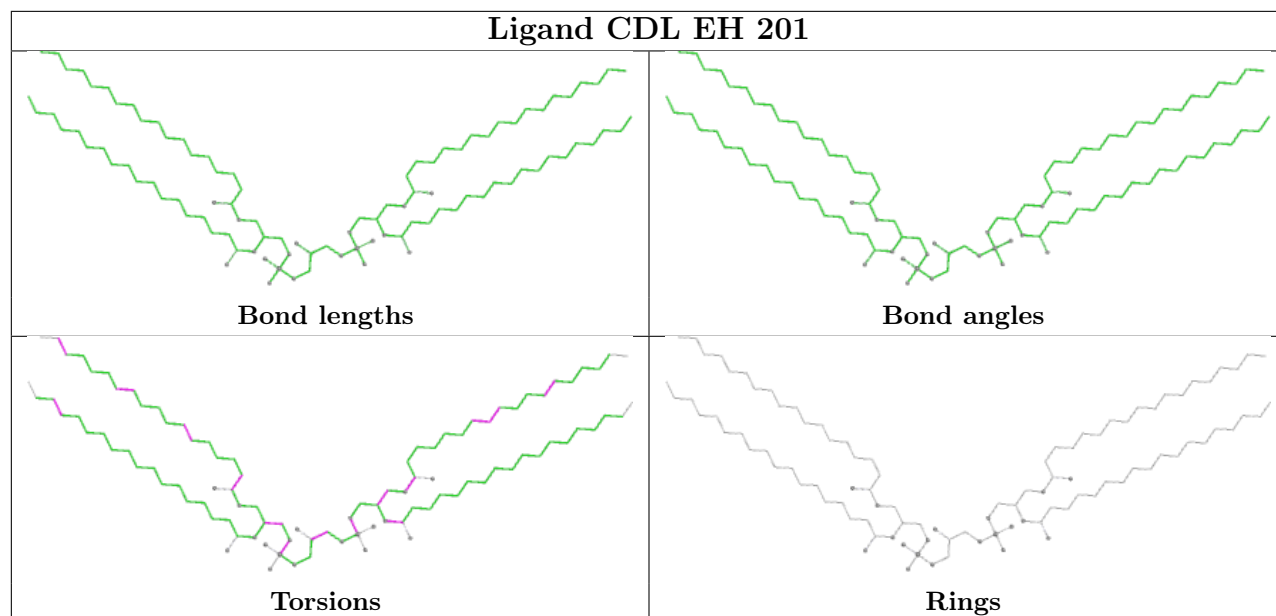


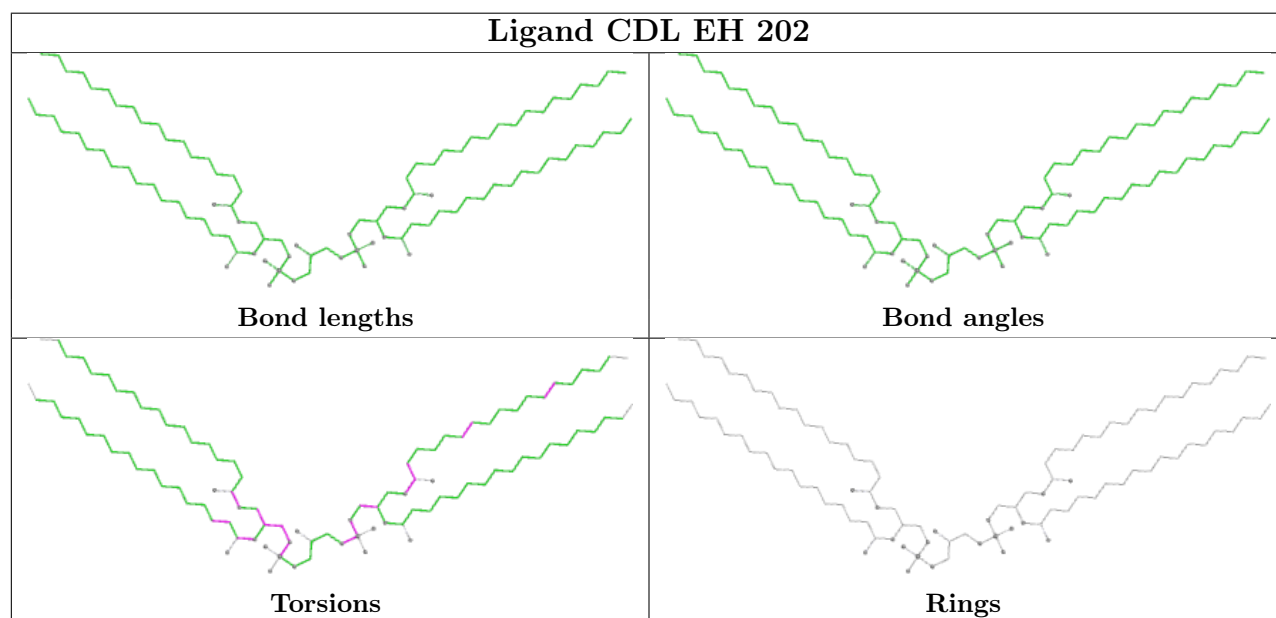
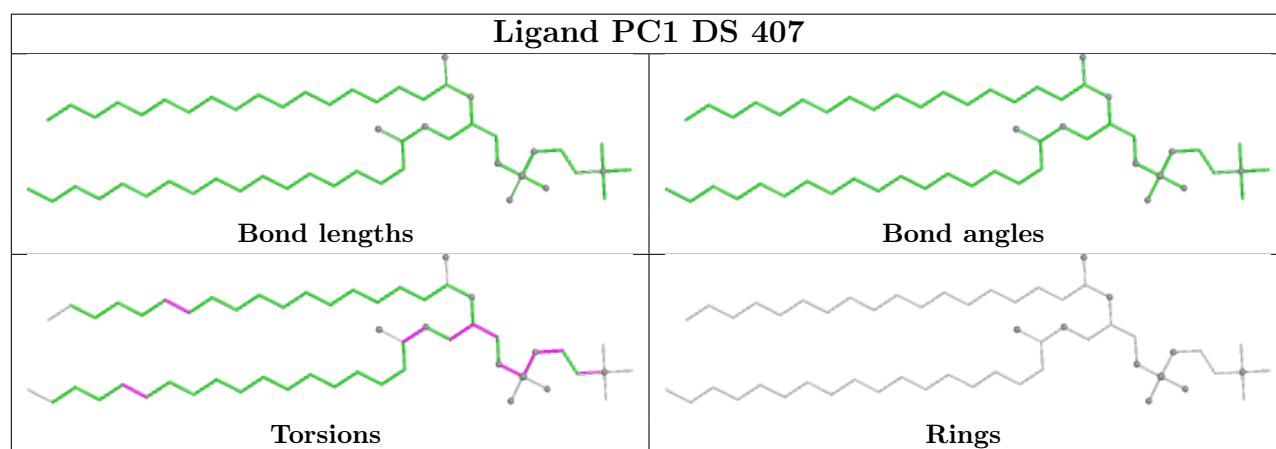
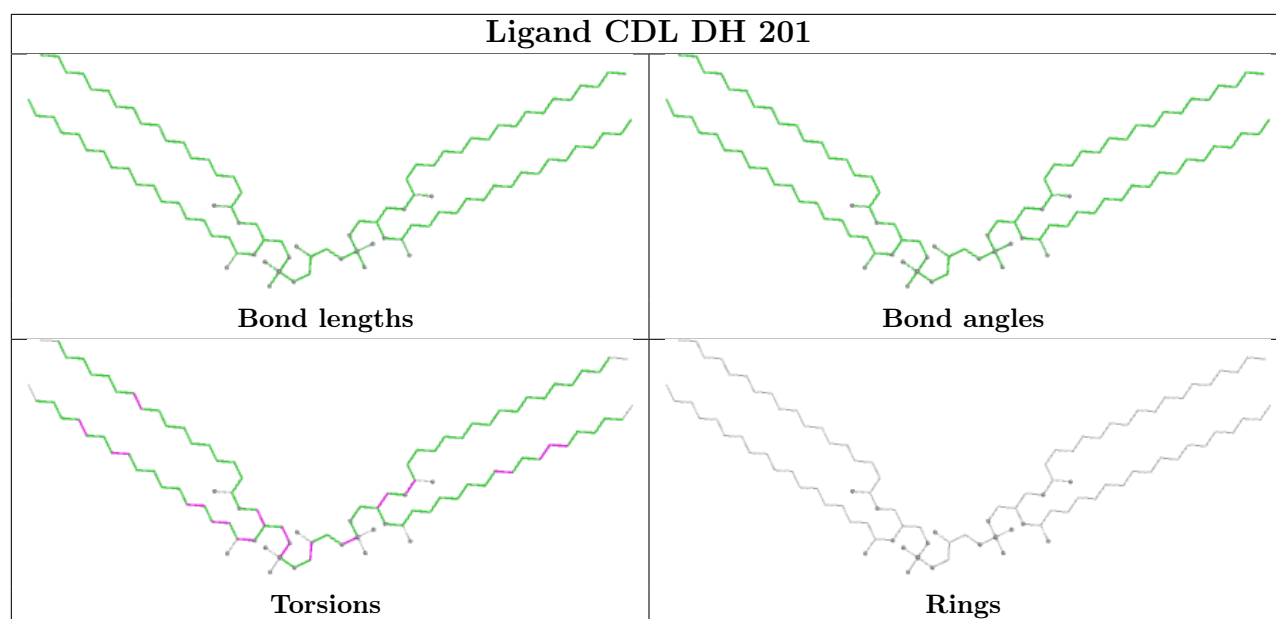


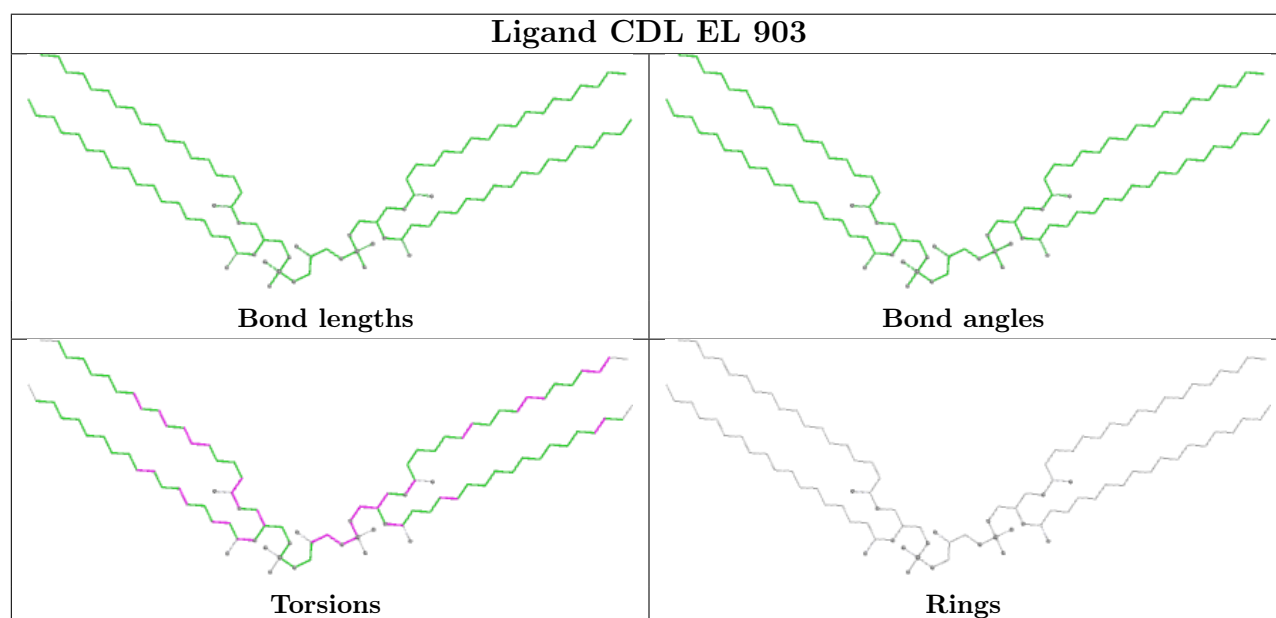
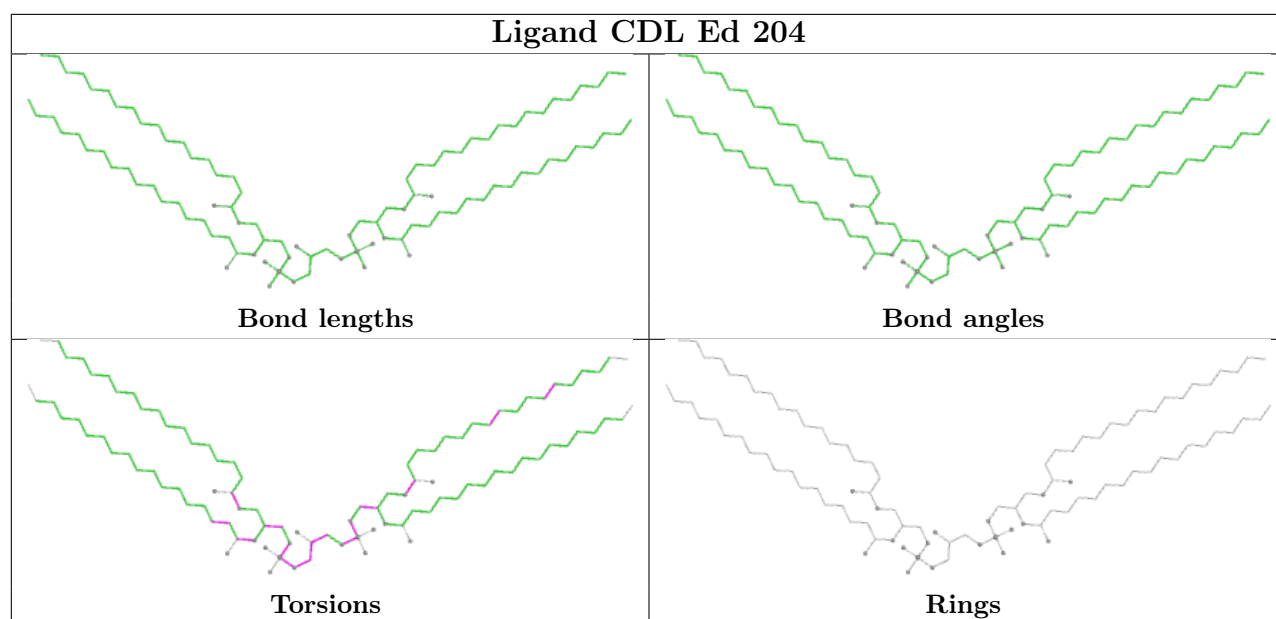


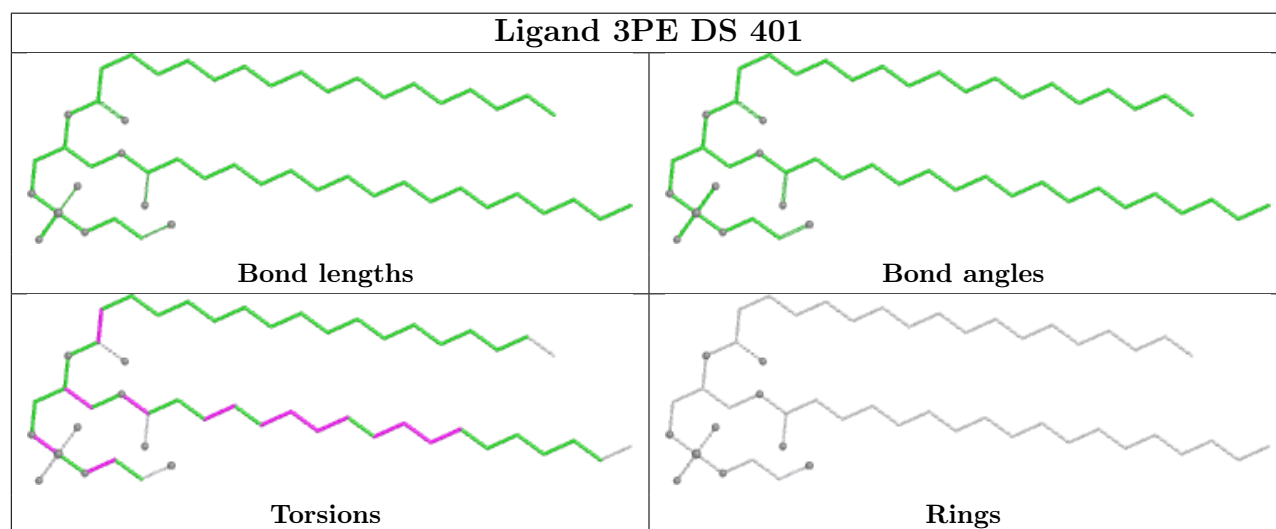
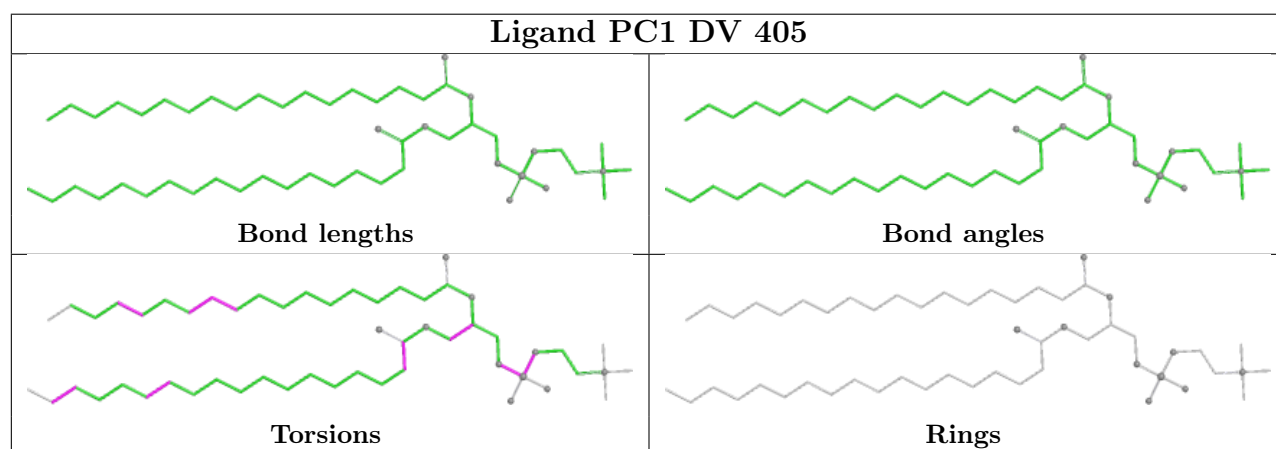
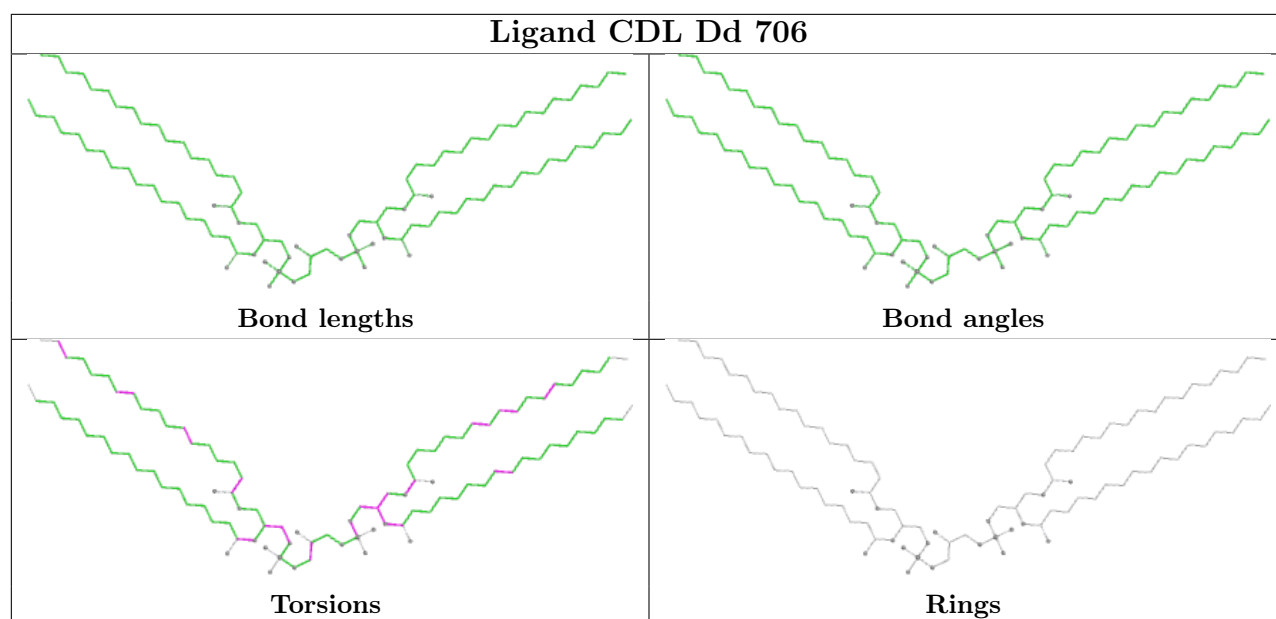


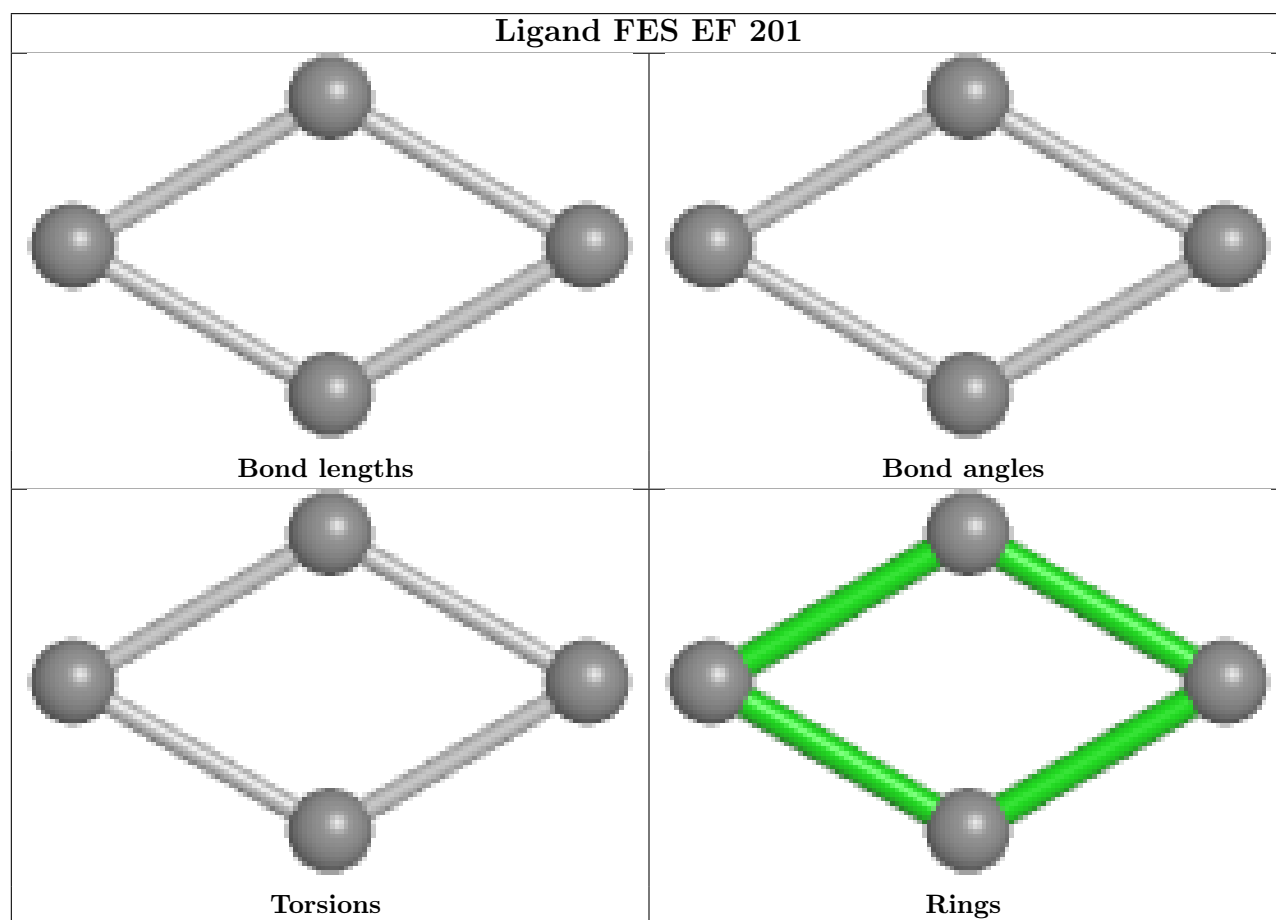
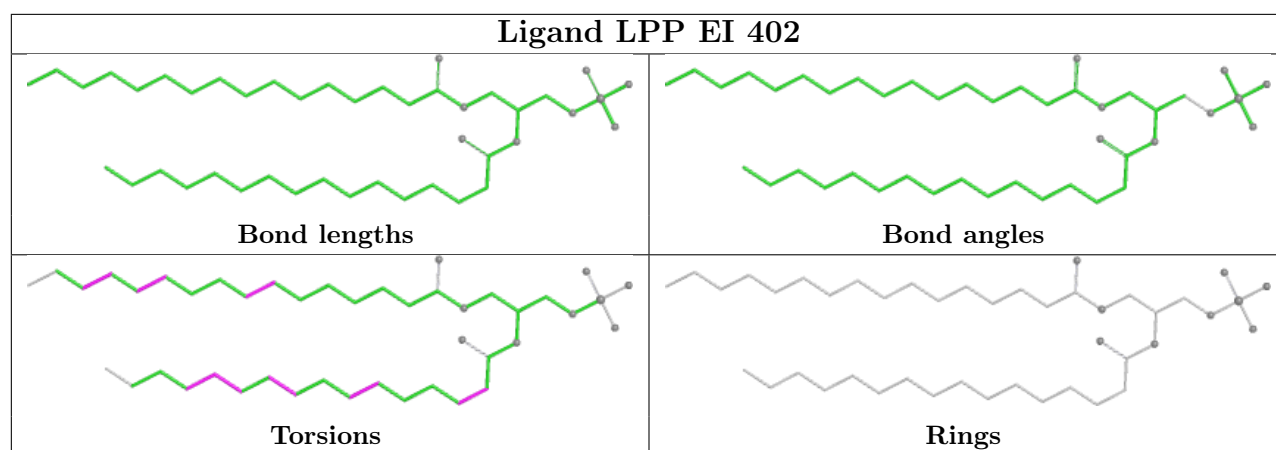


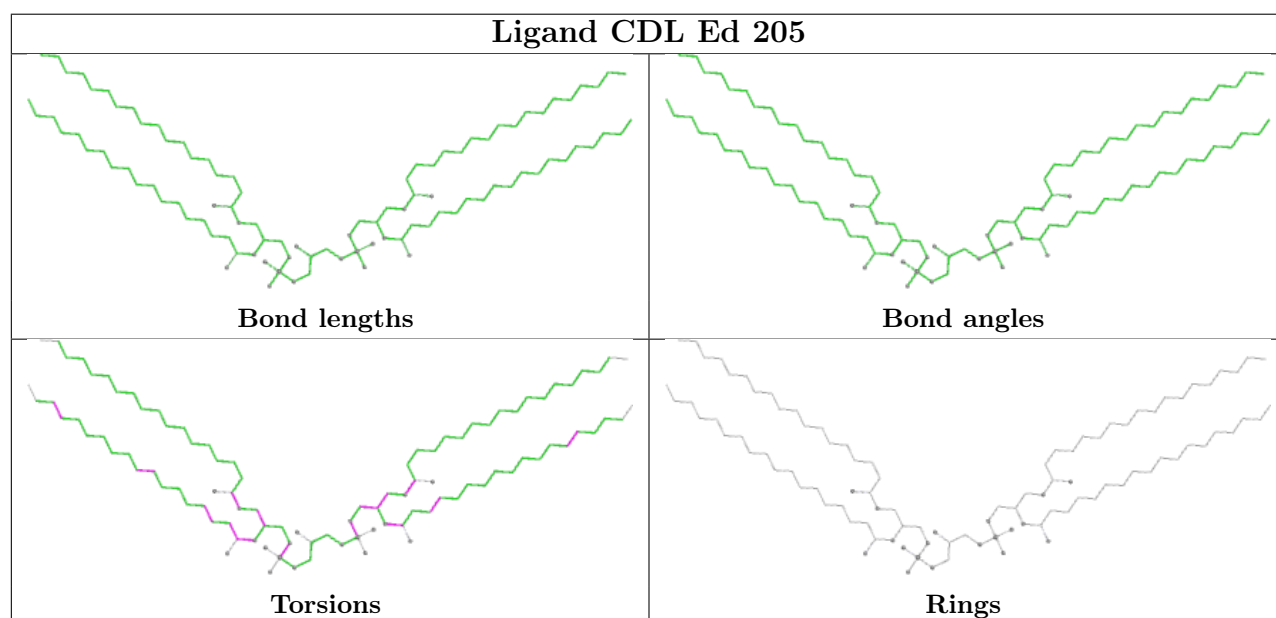
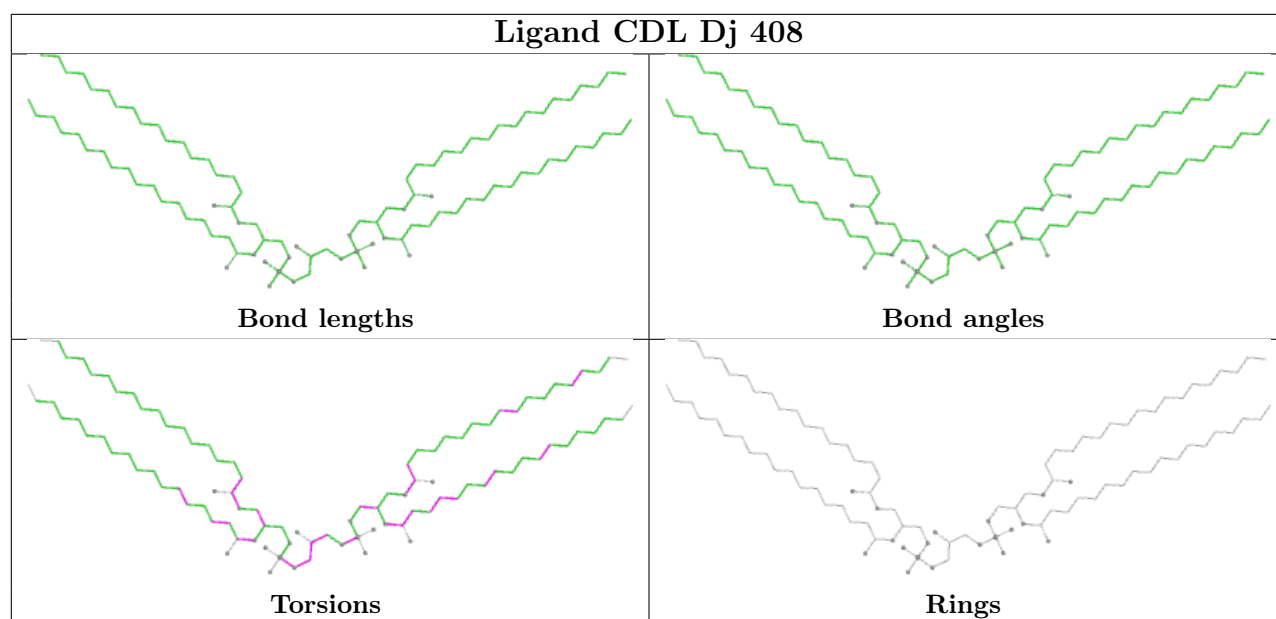


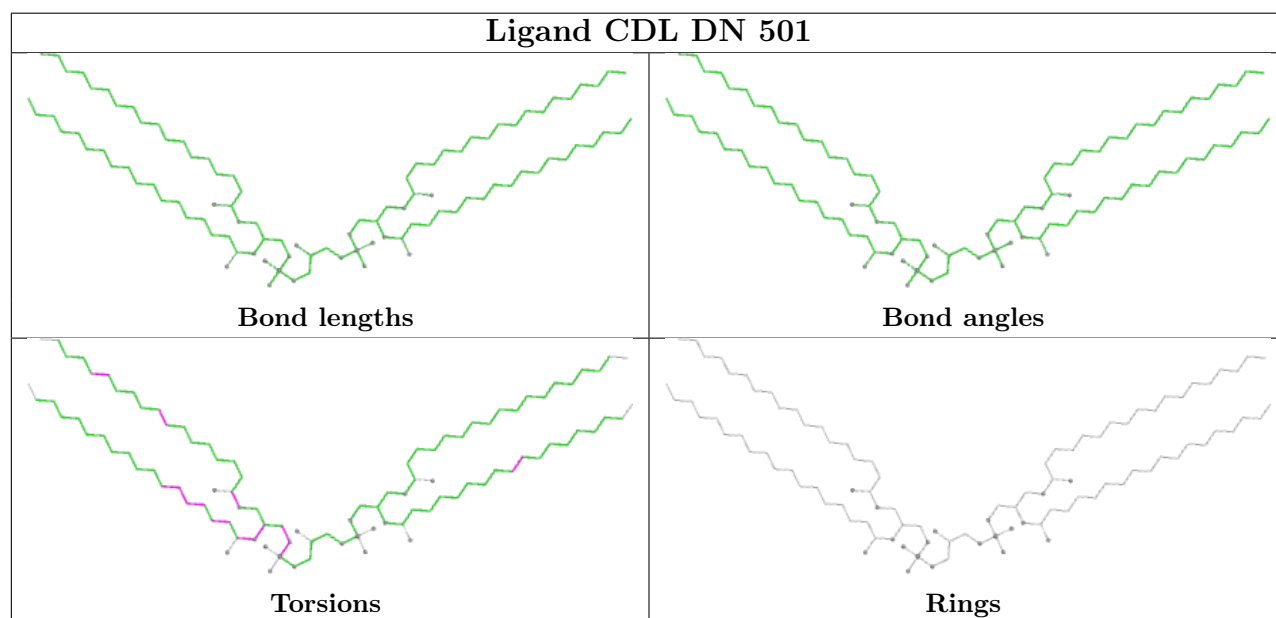
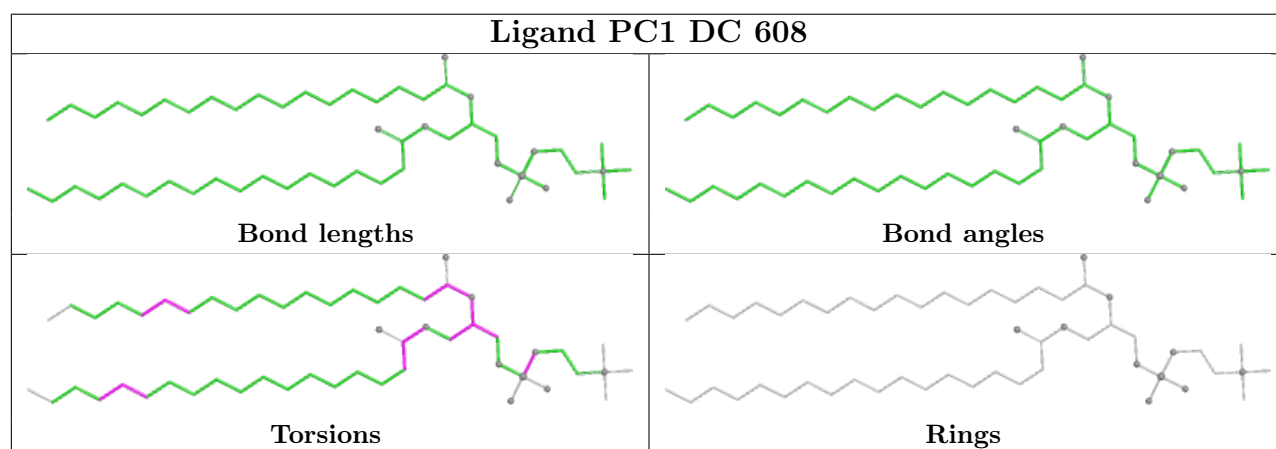
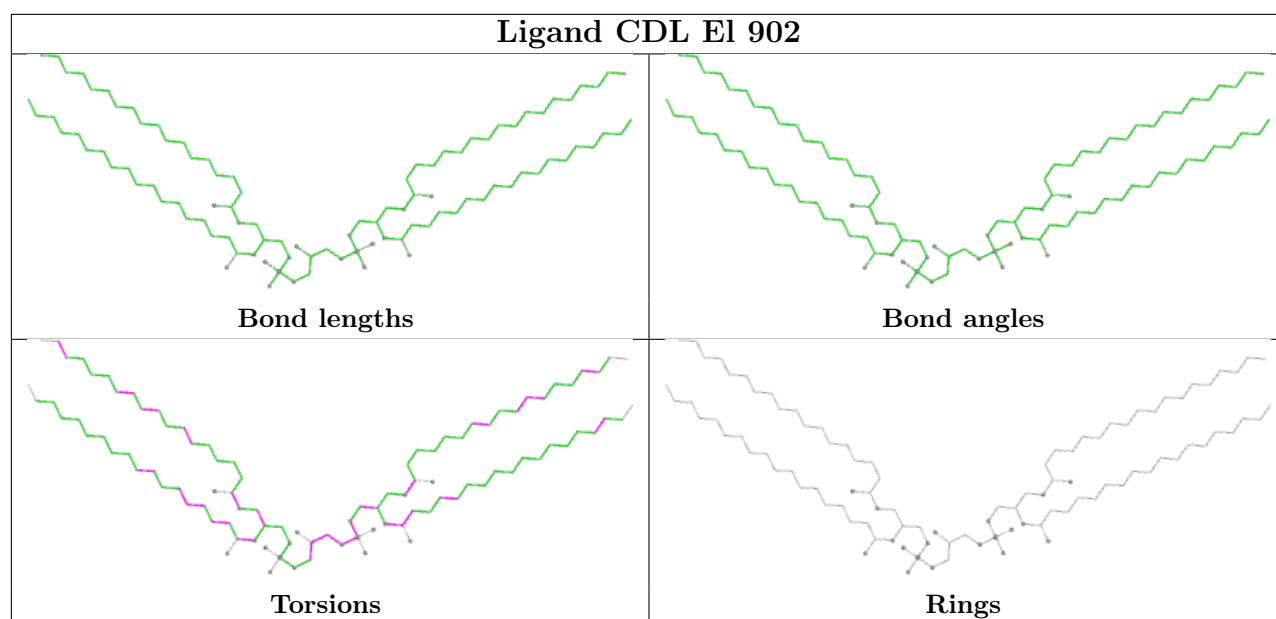


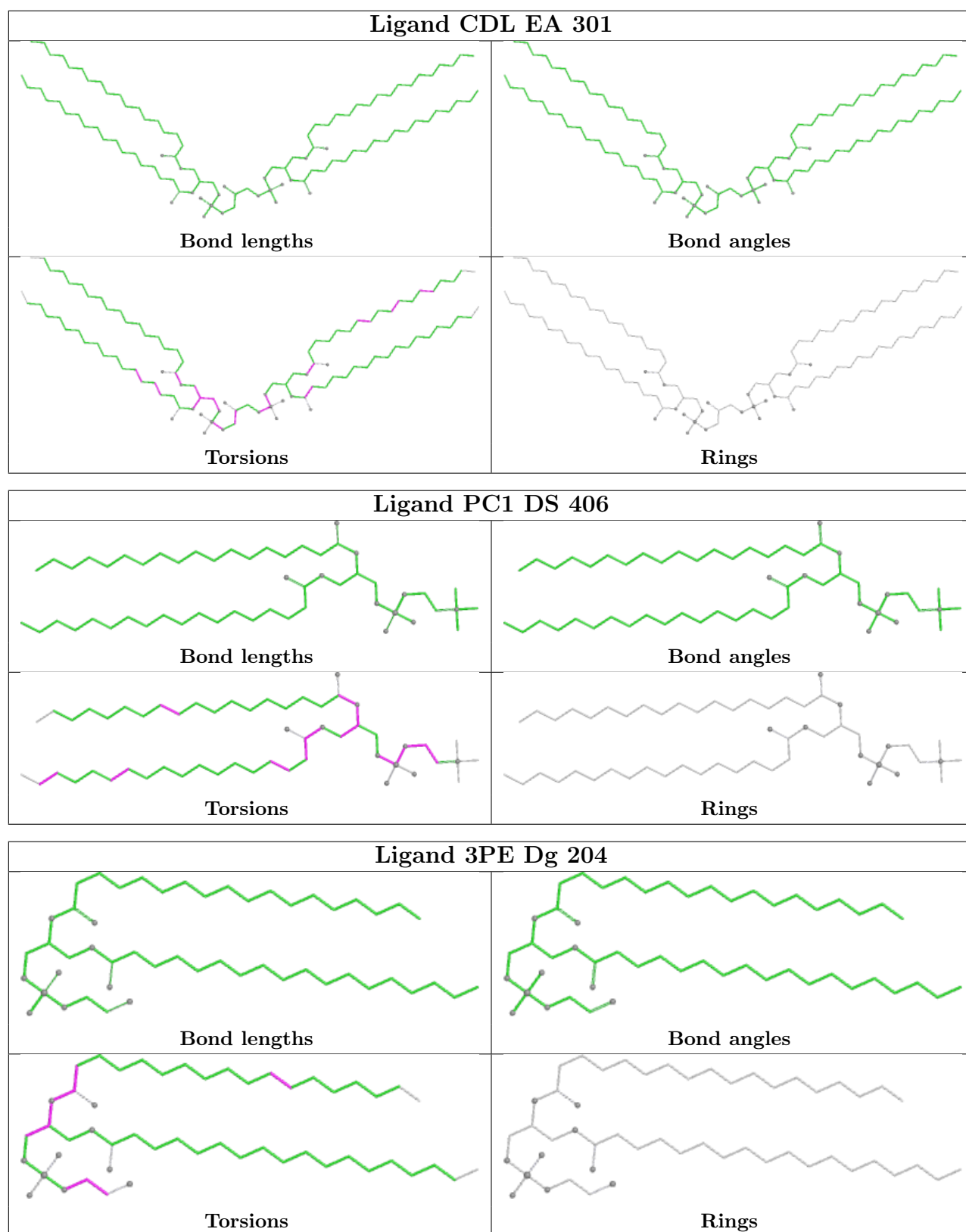


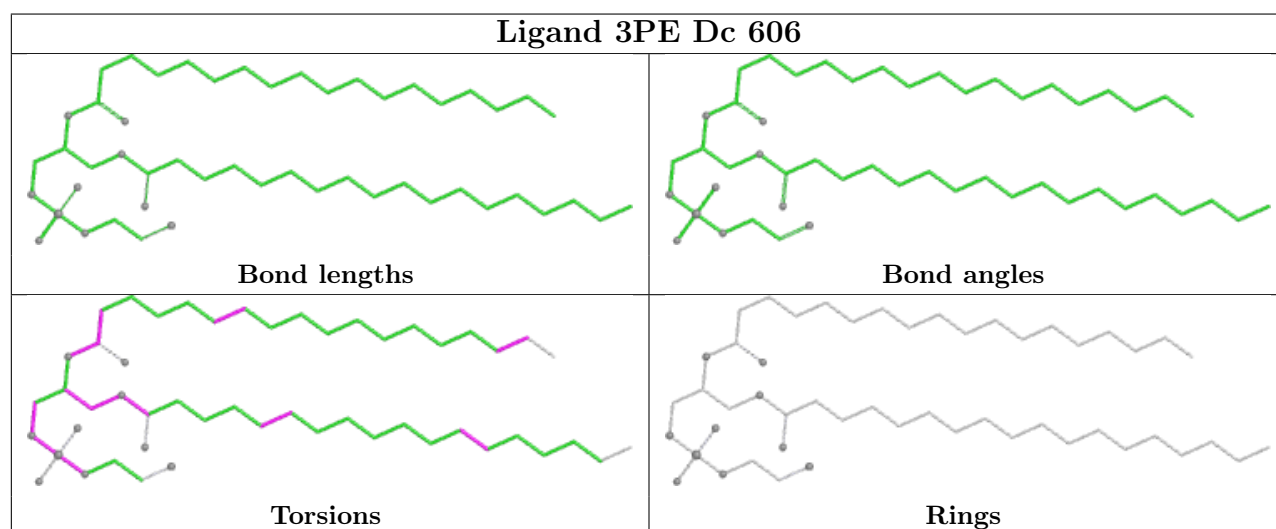
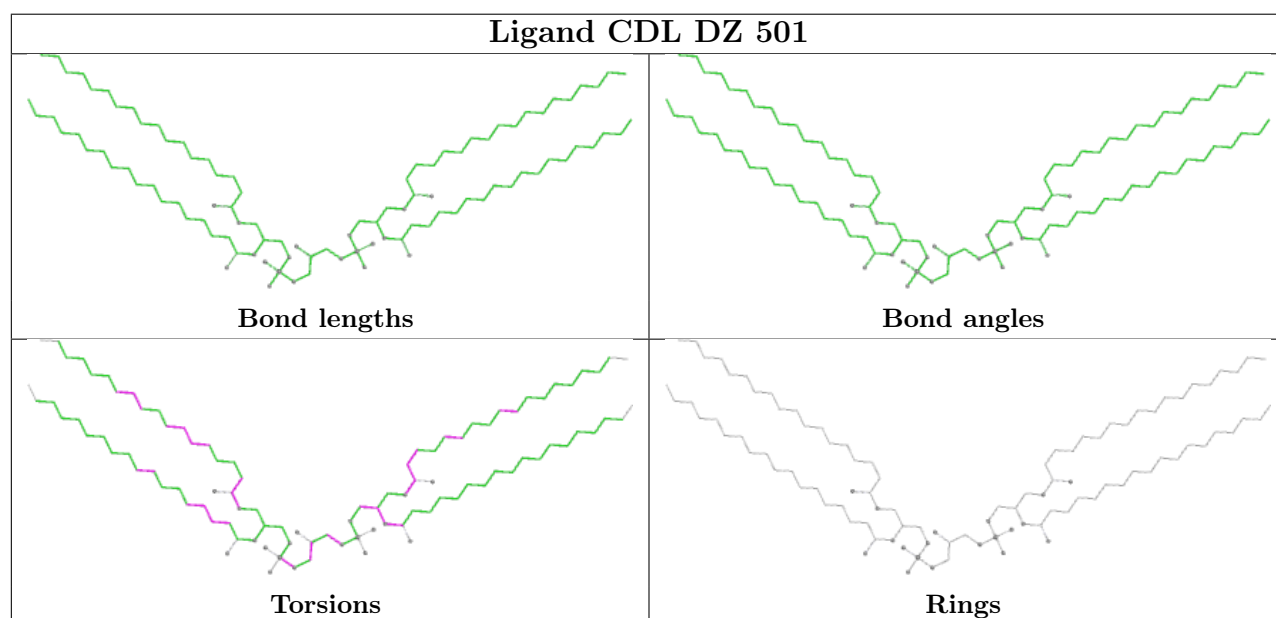
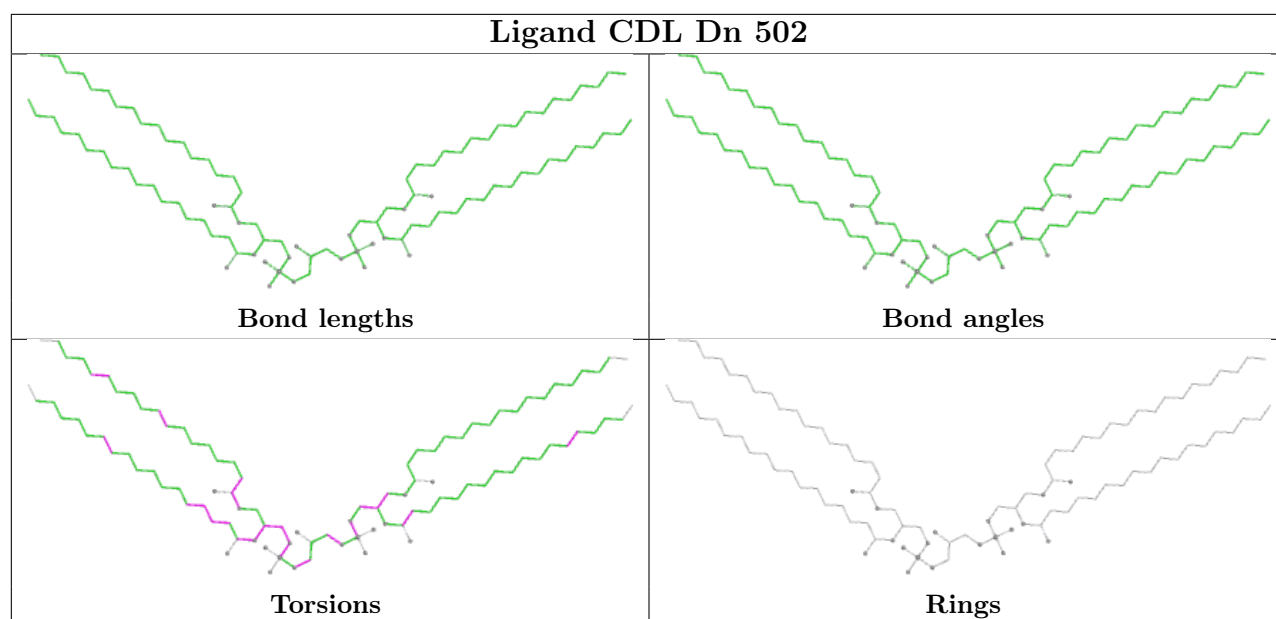


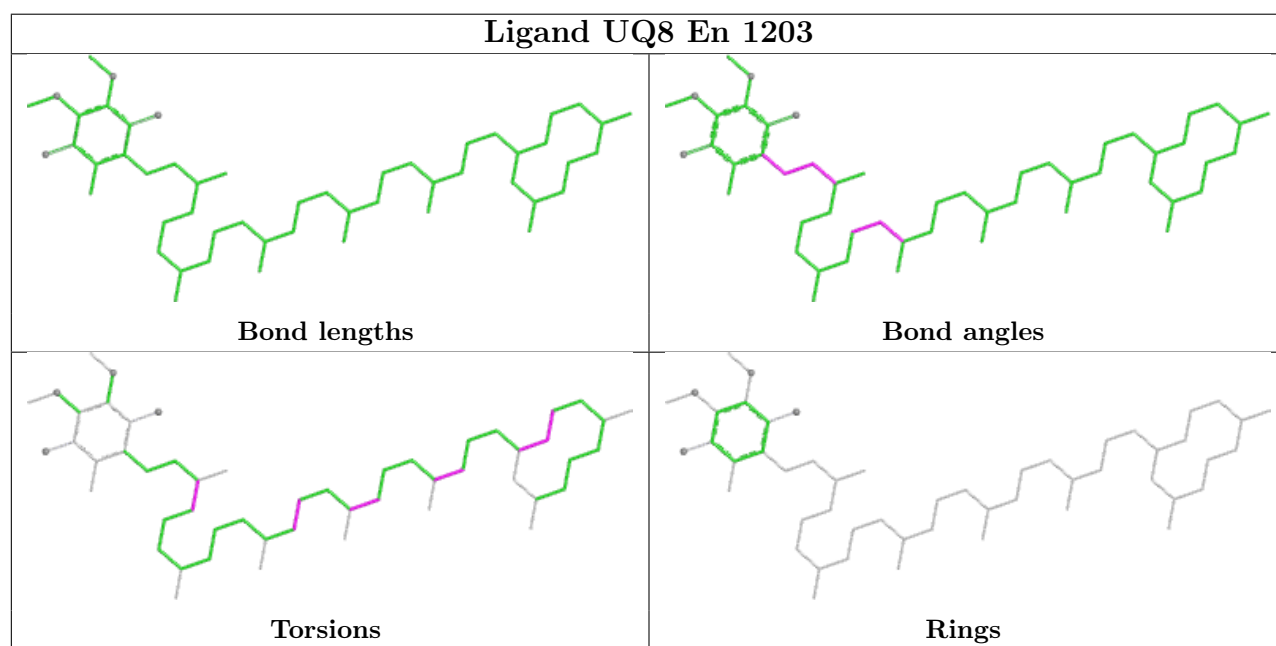
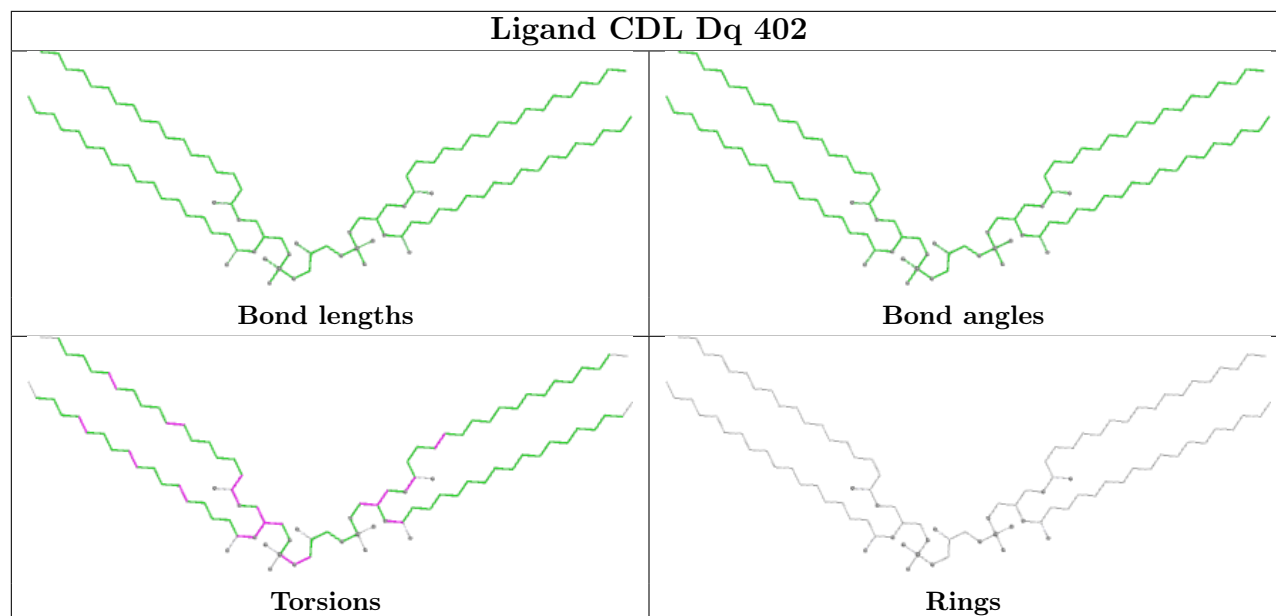


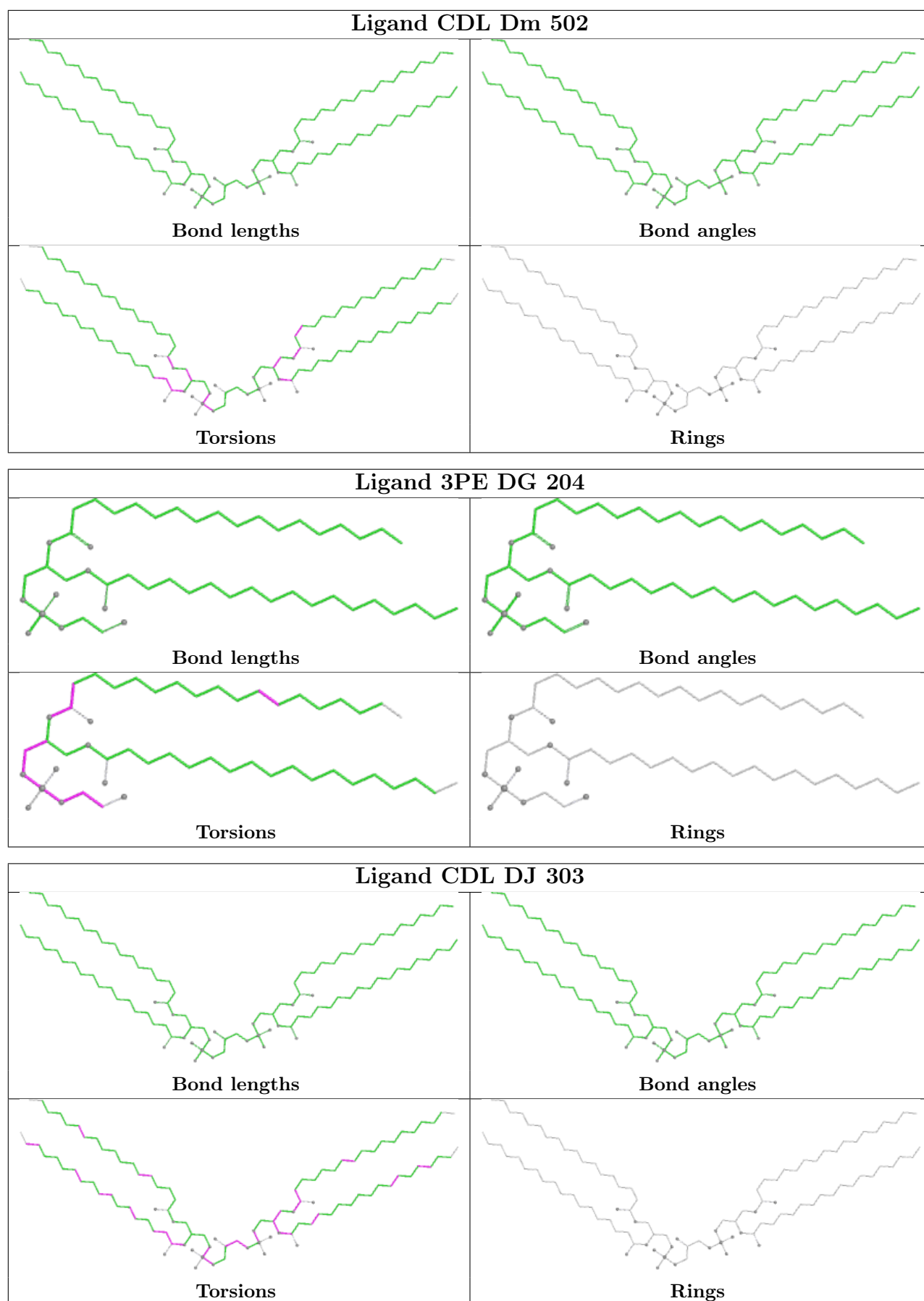


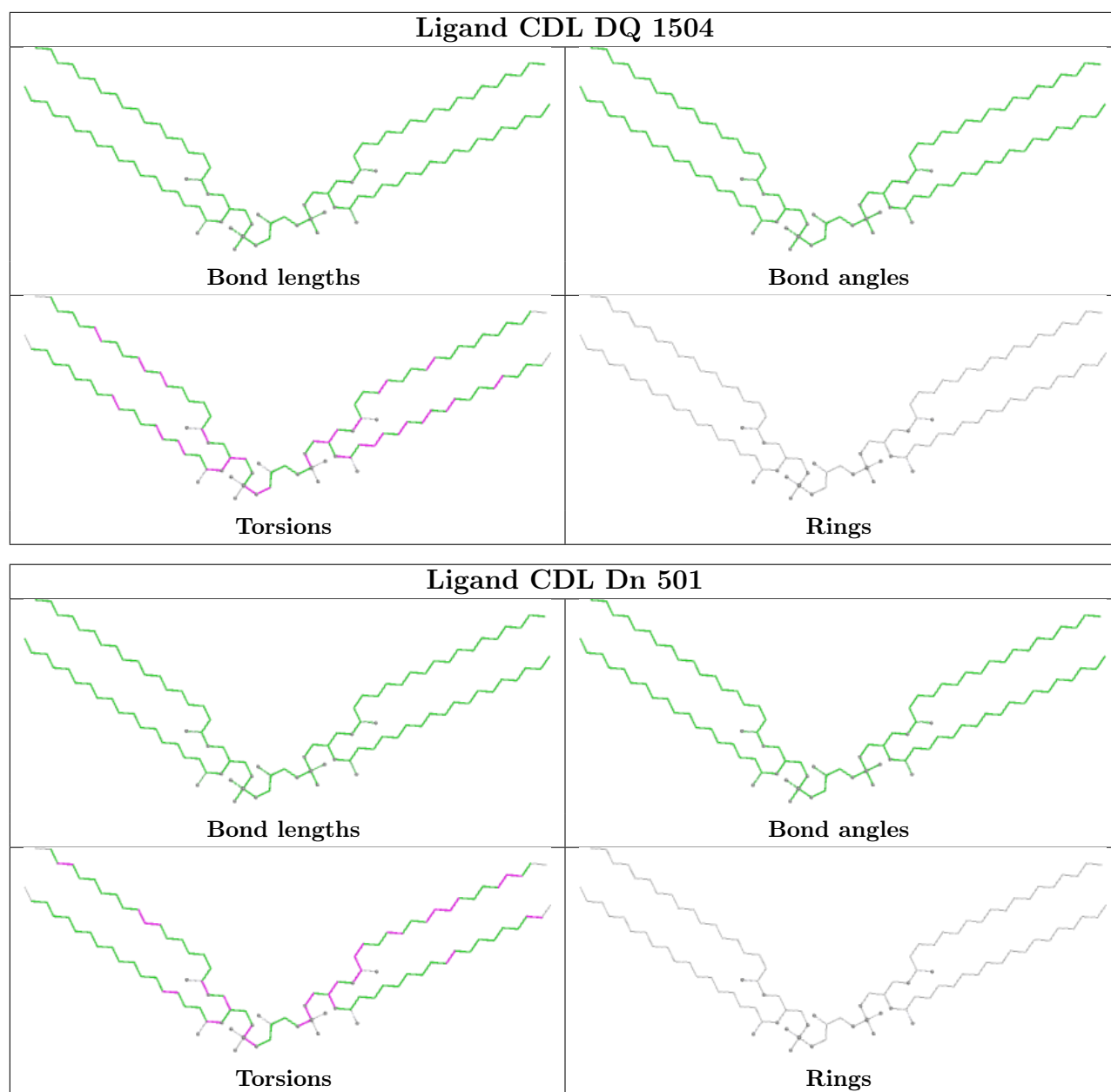


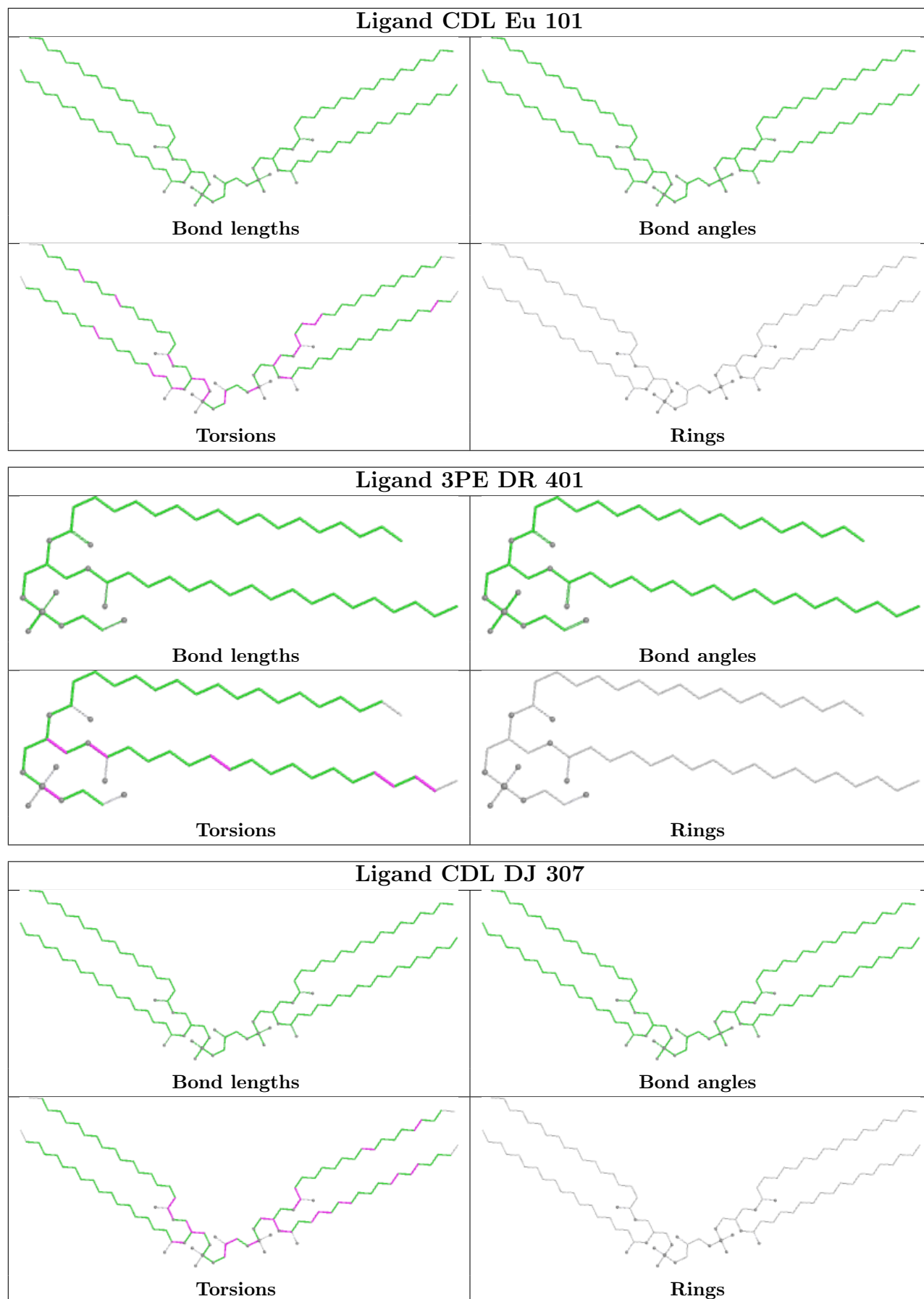


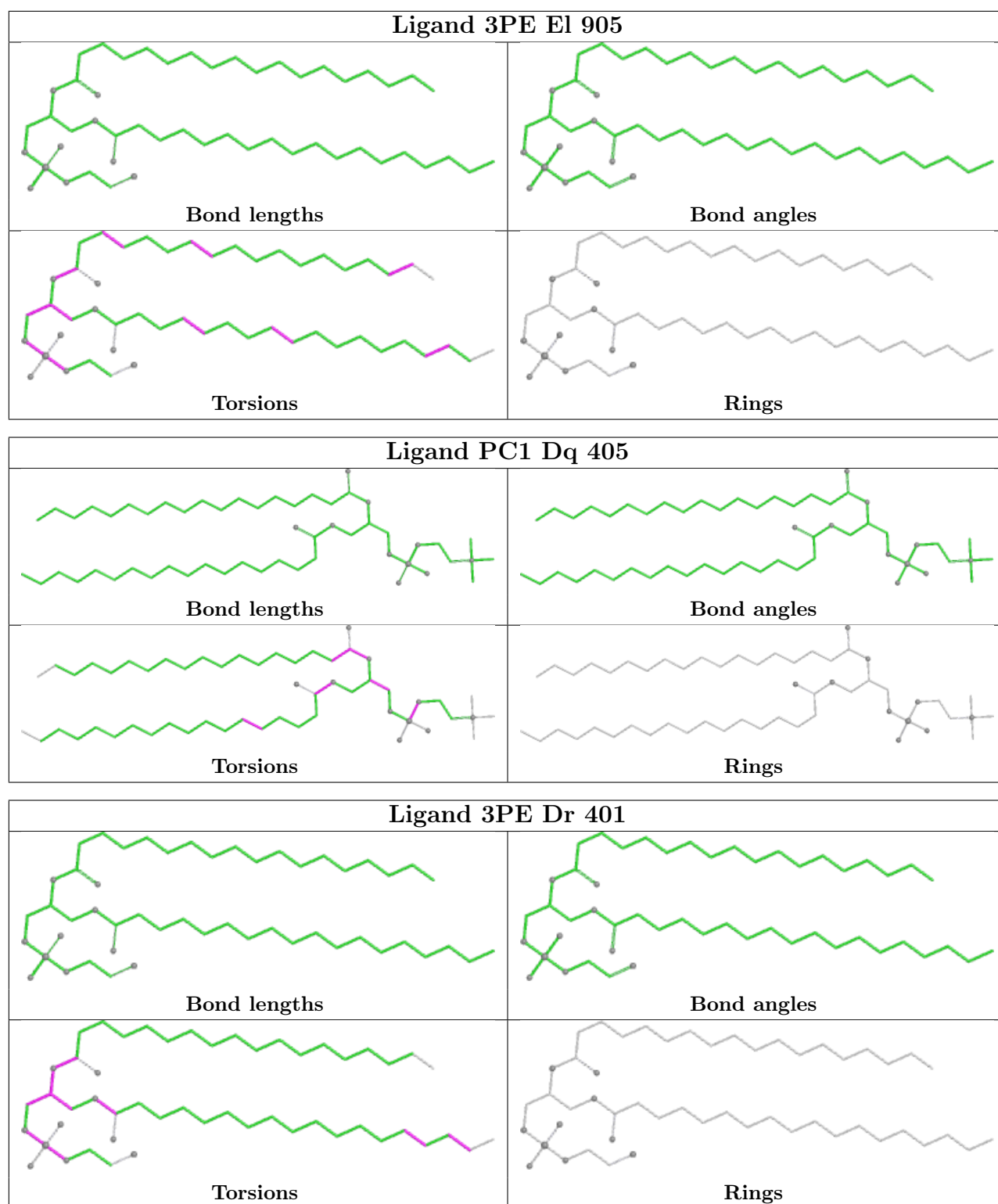




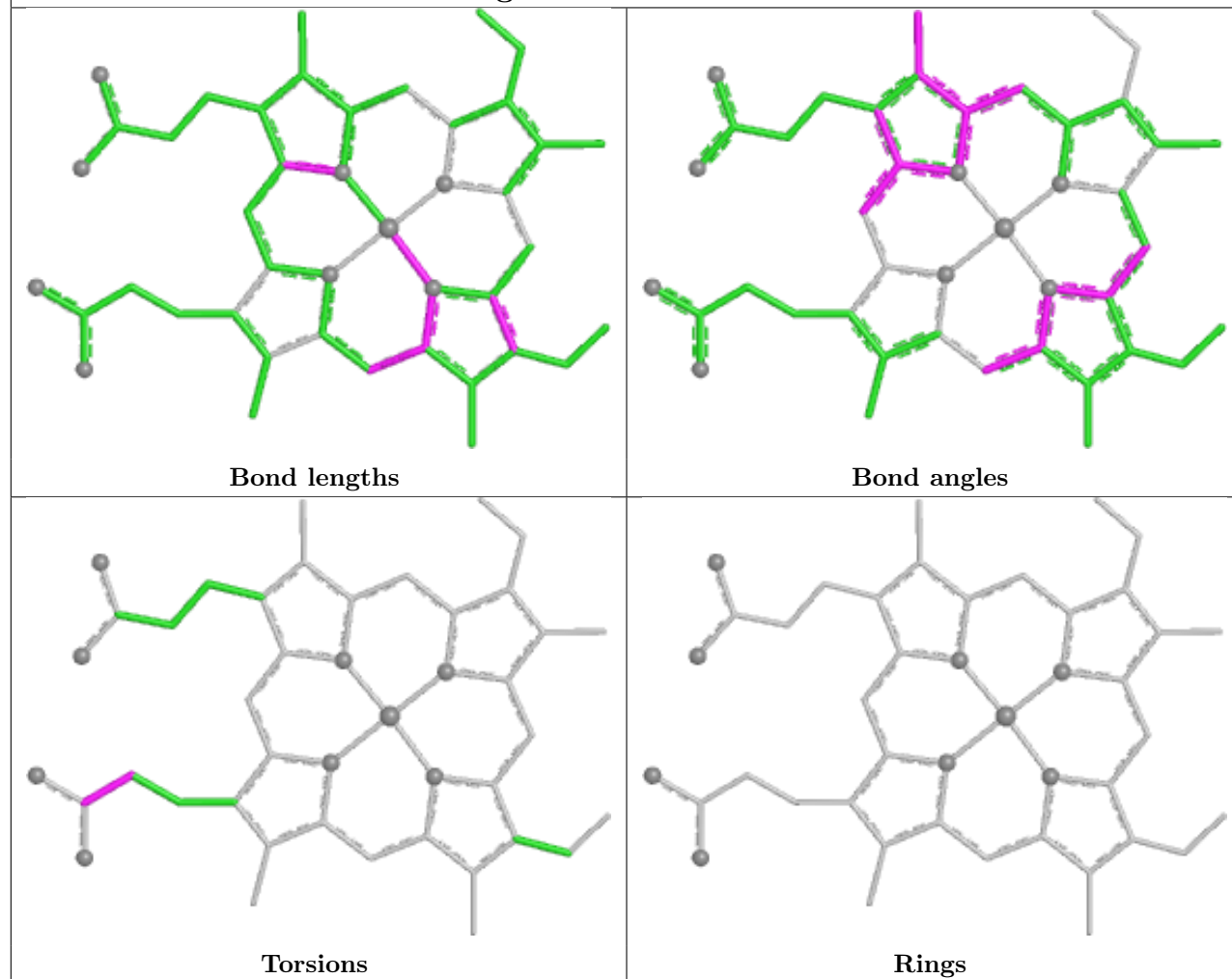




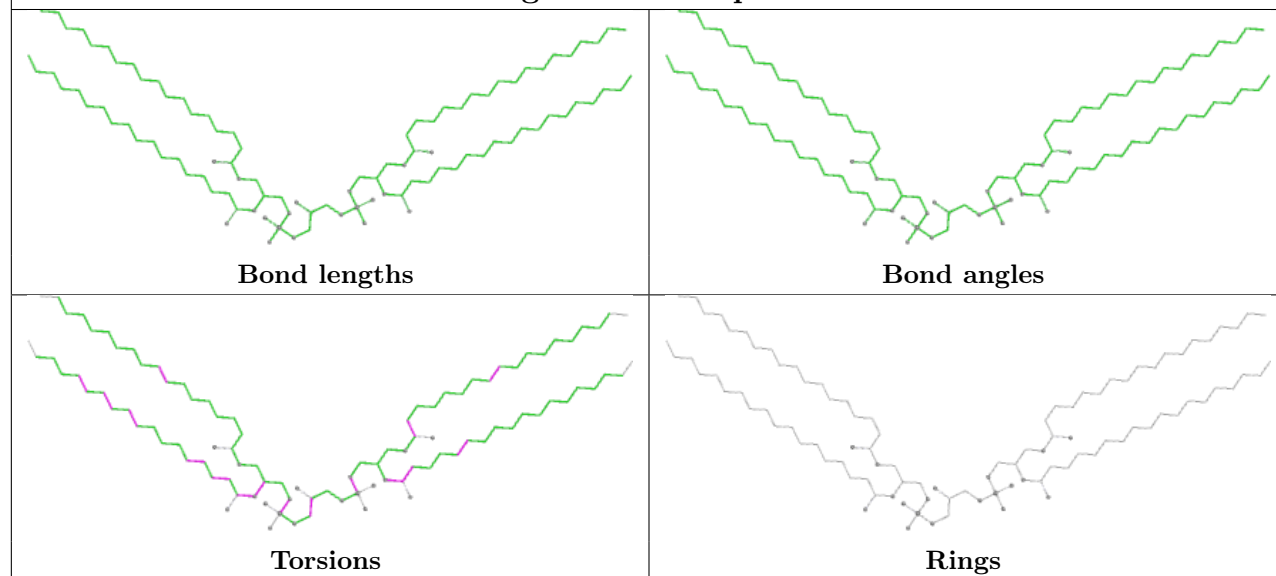


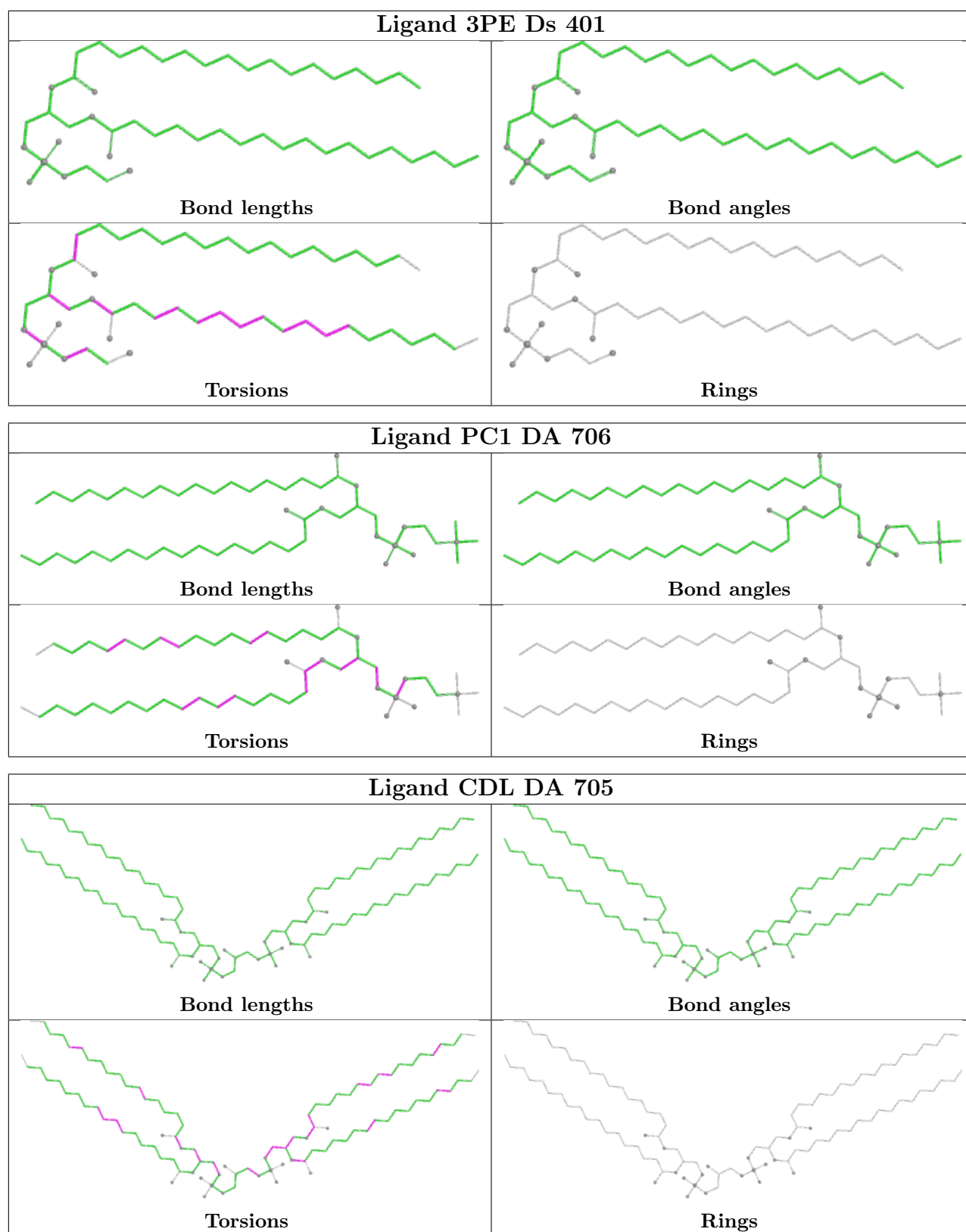


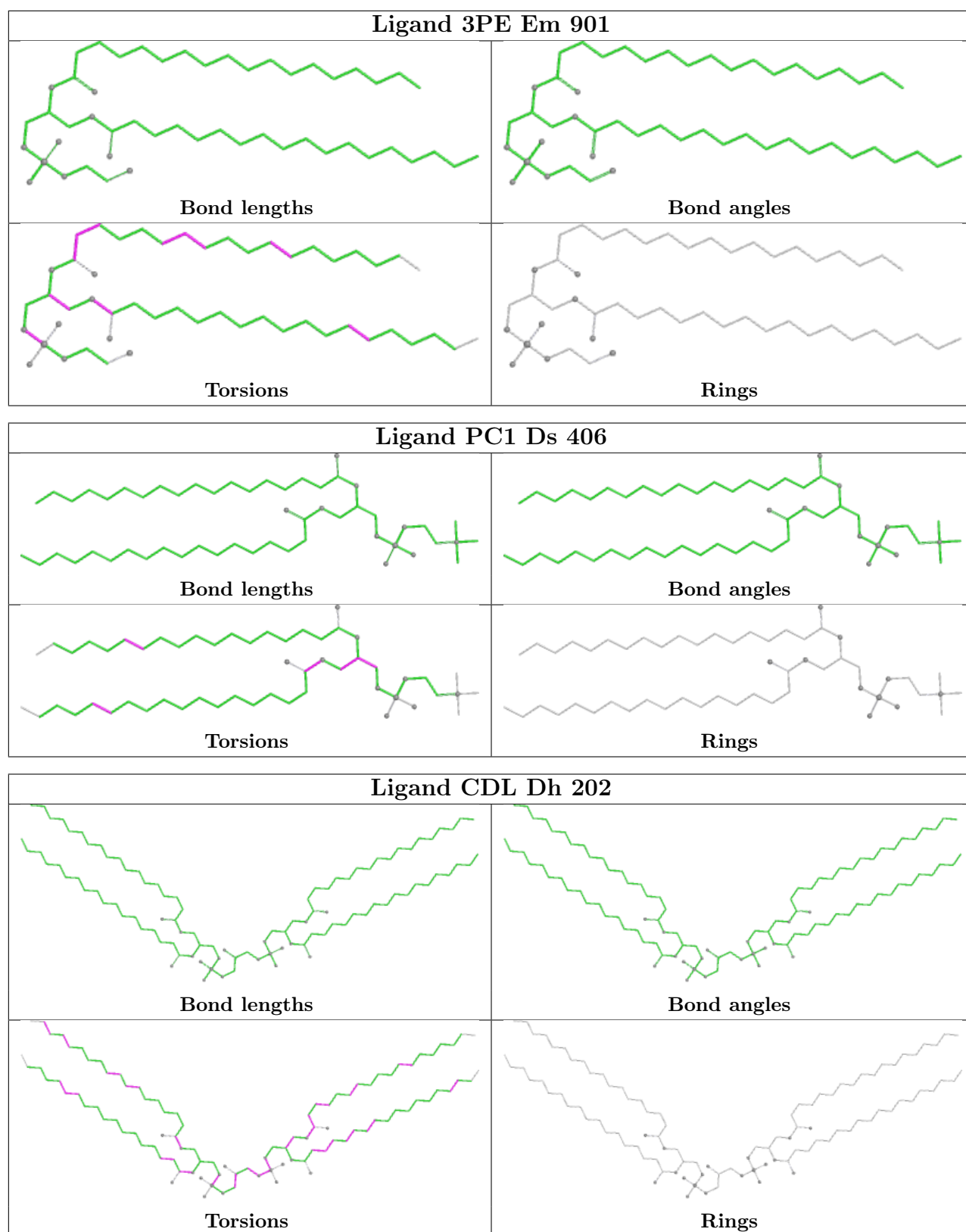
Ligand HEM ED 602

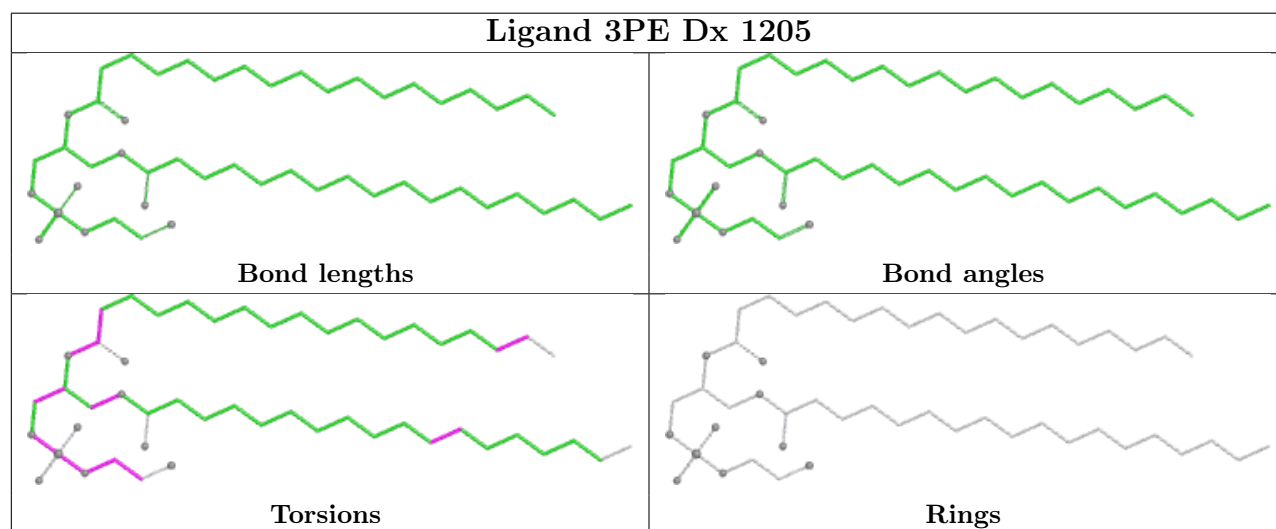
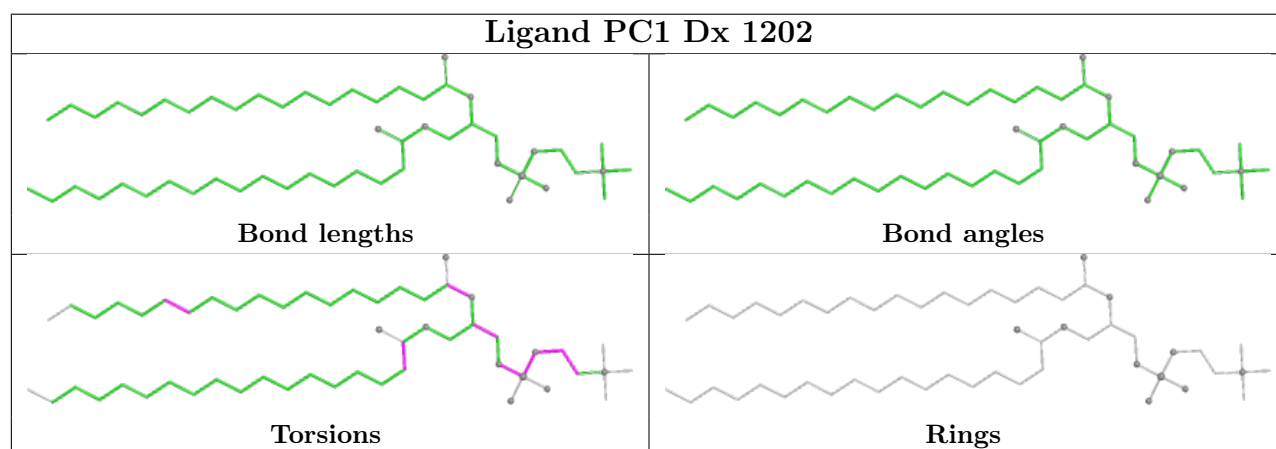
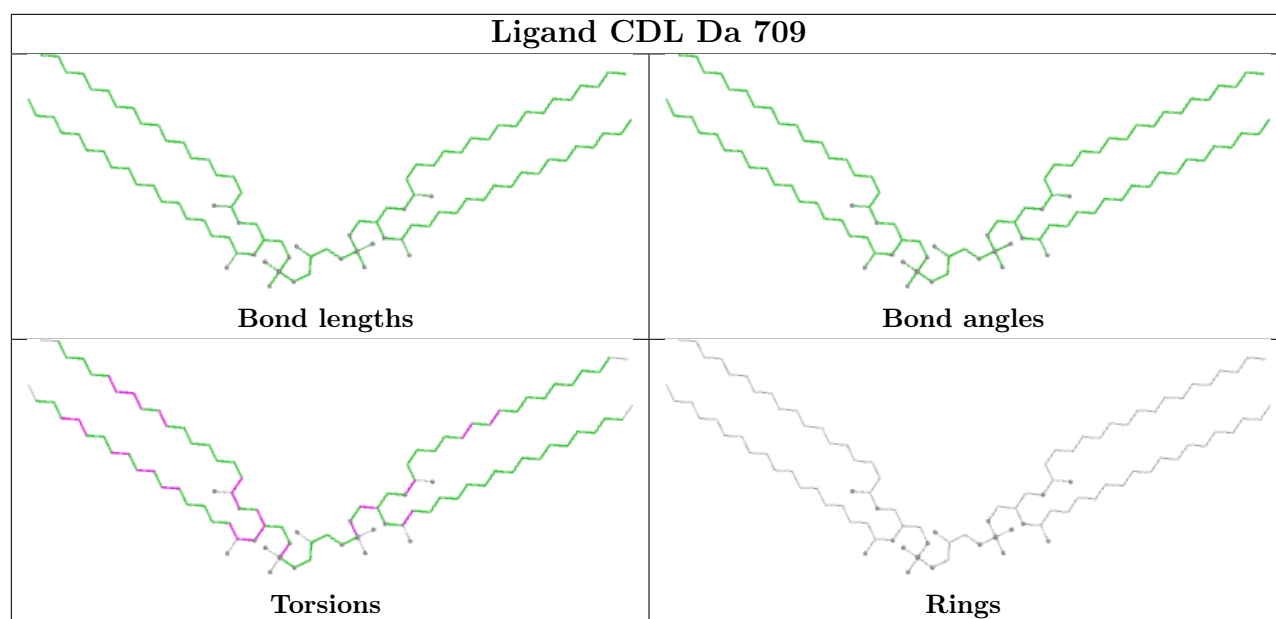


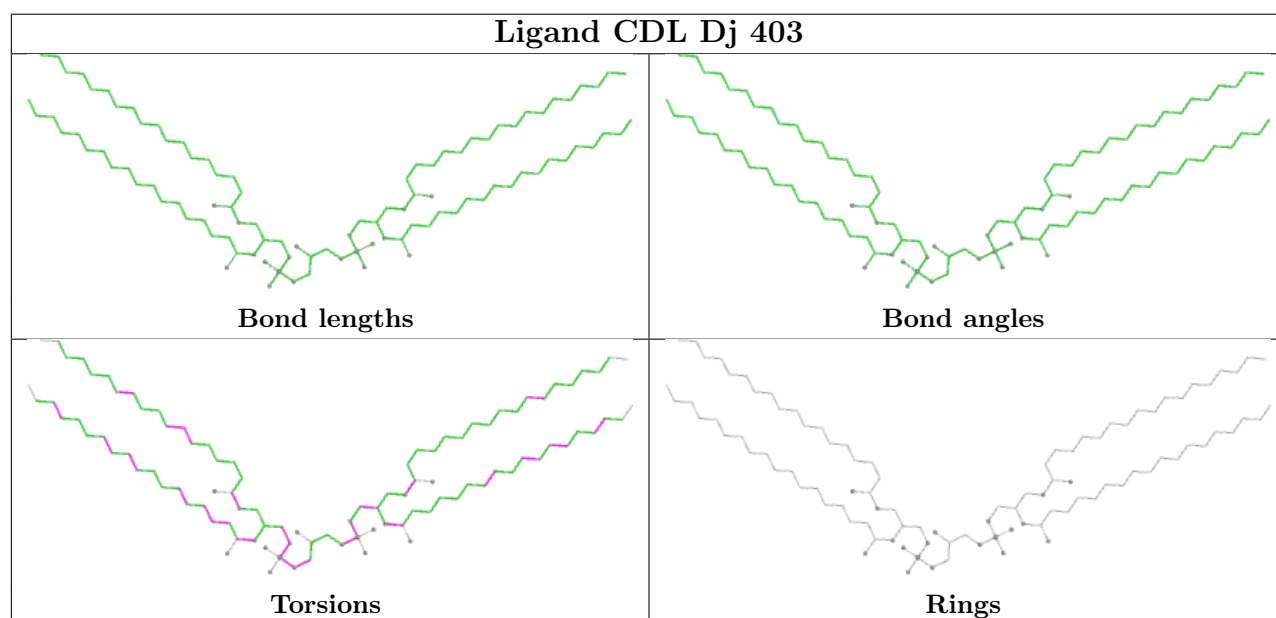
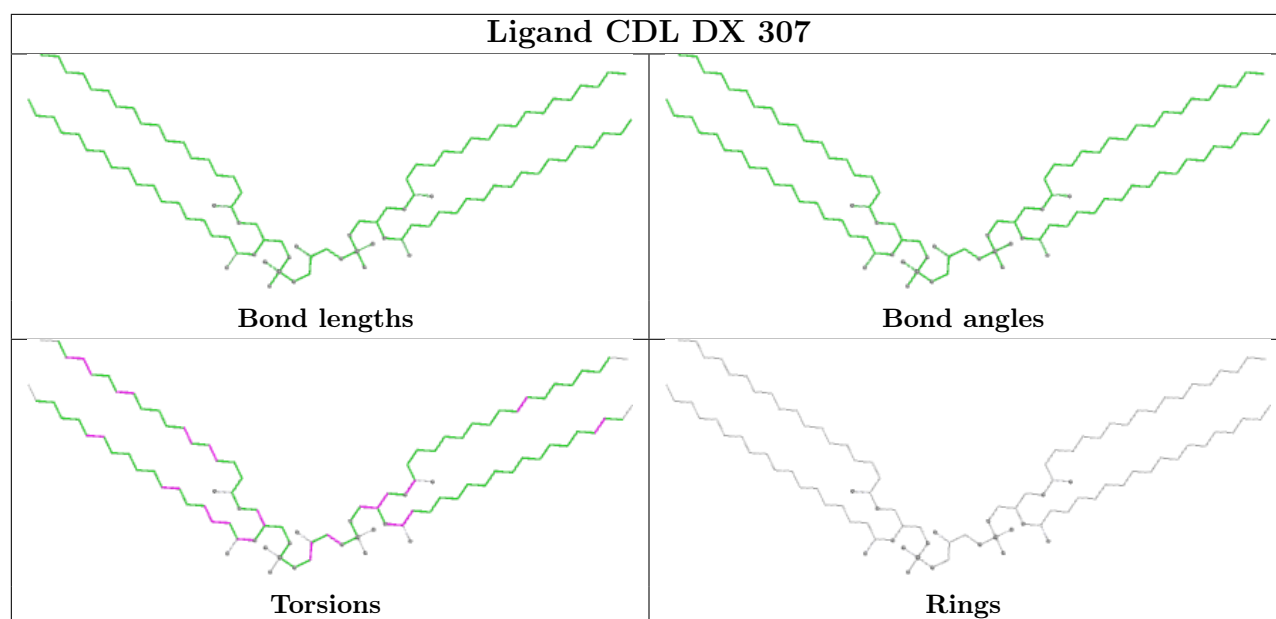
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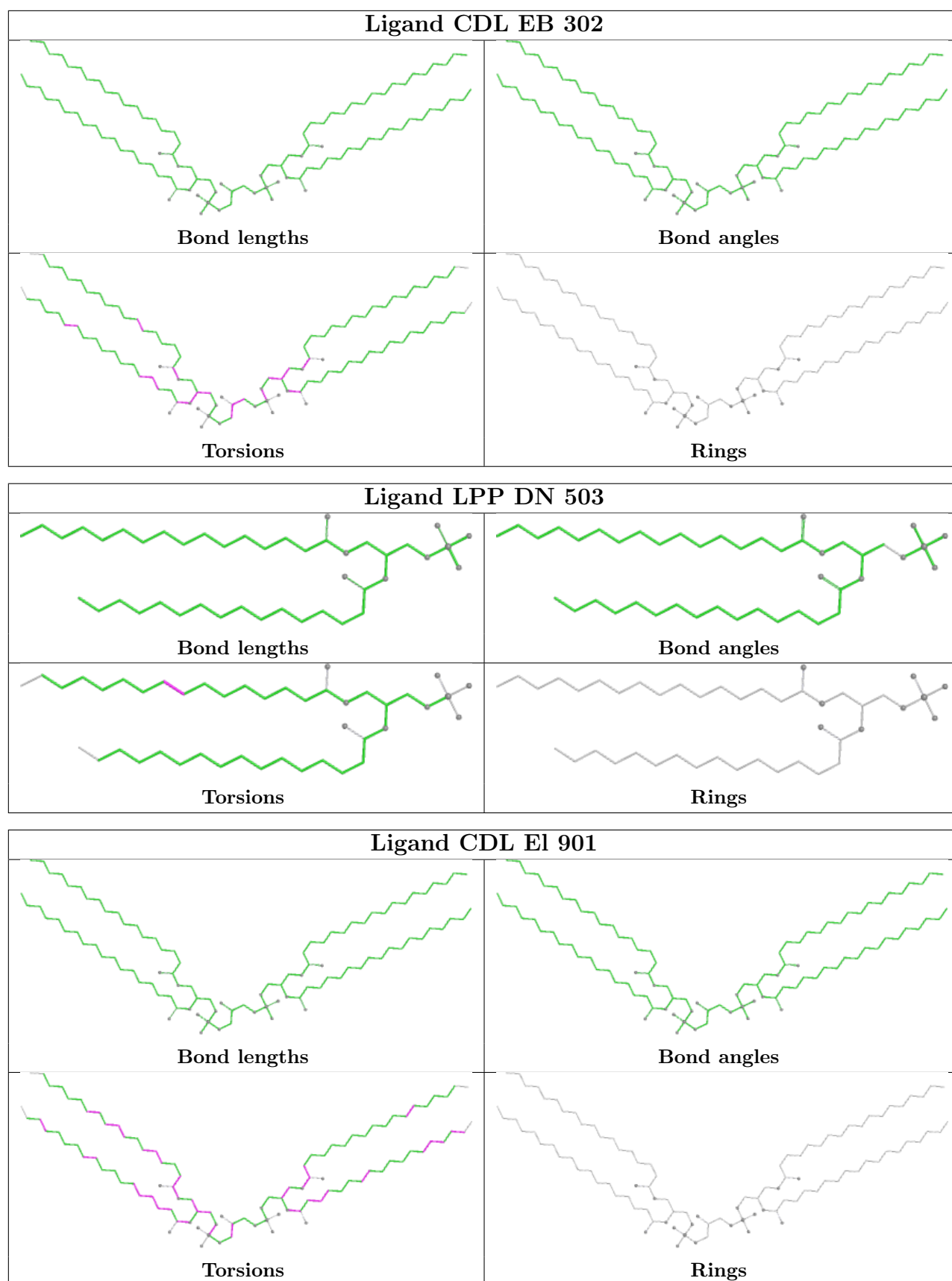


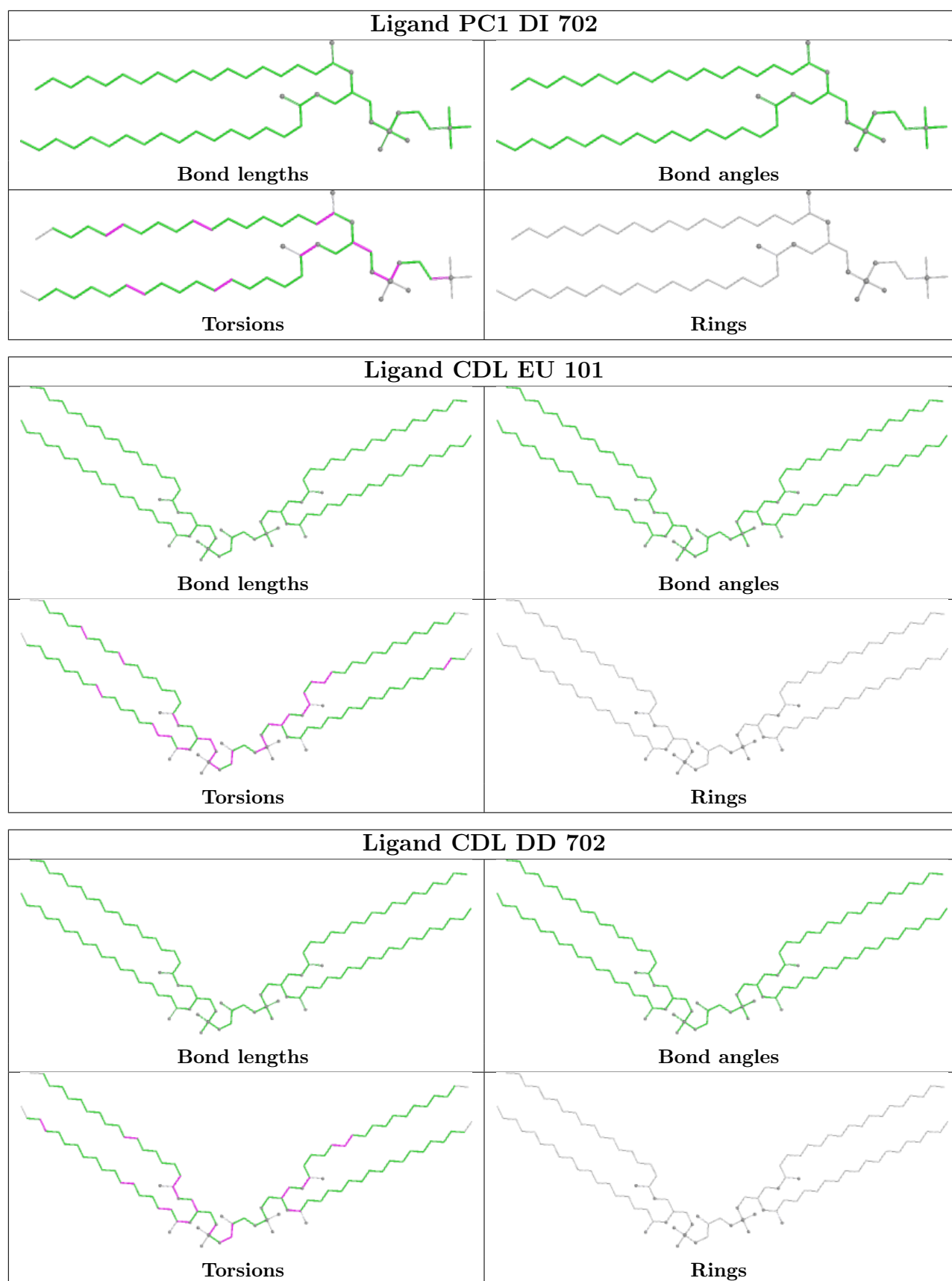


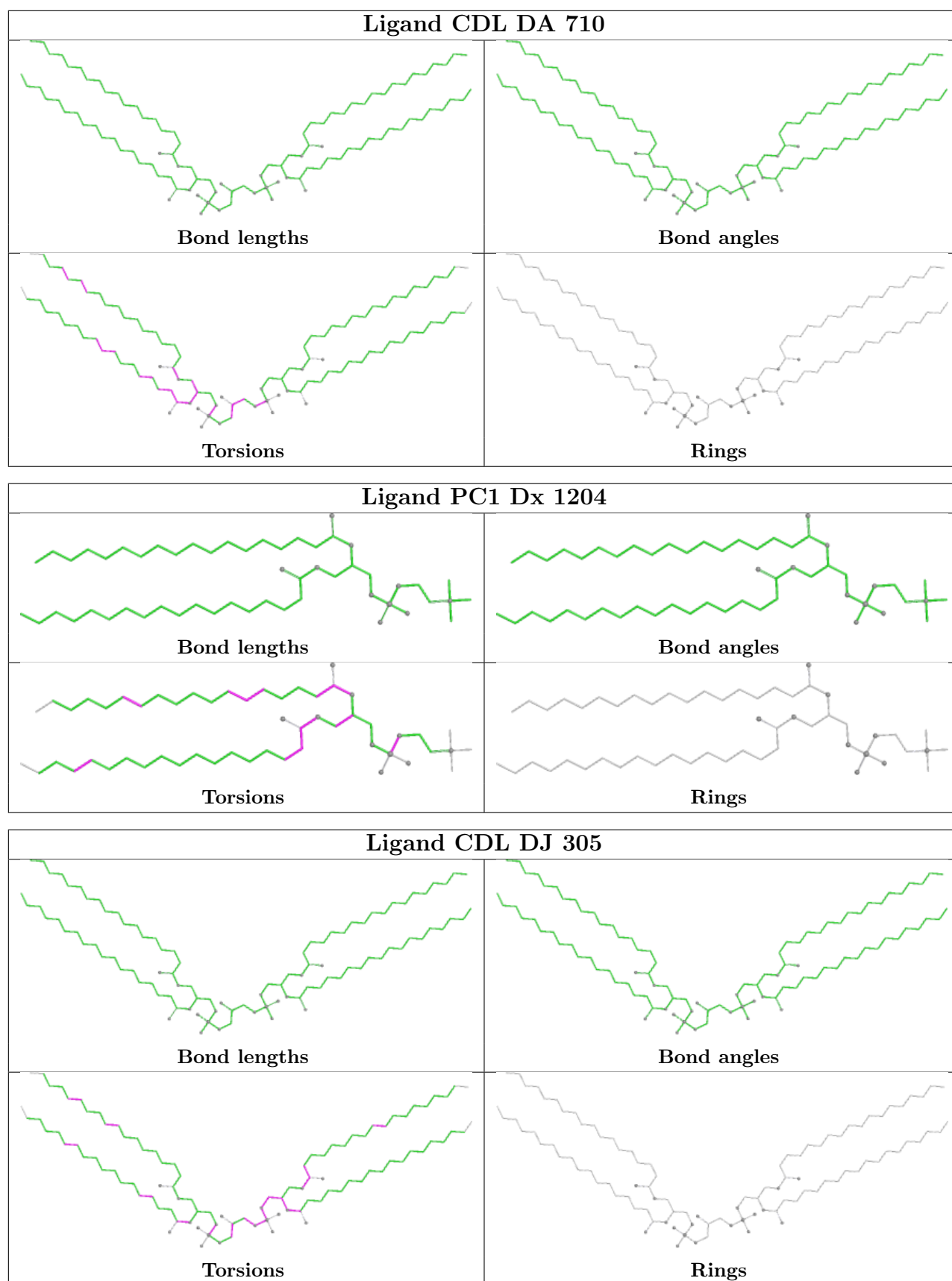


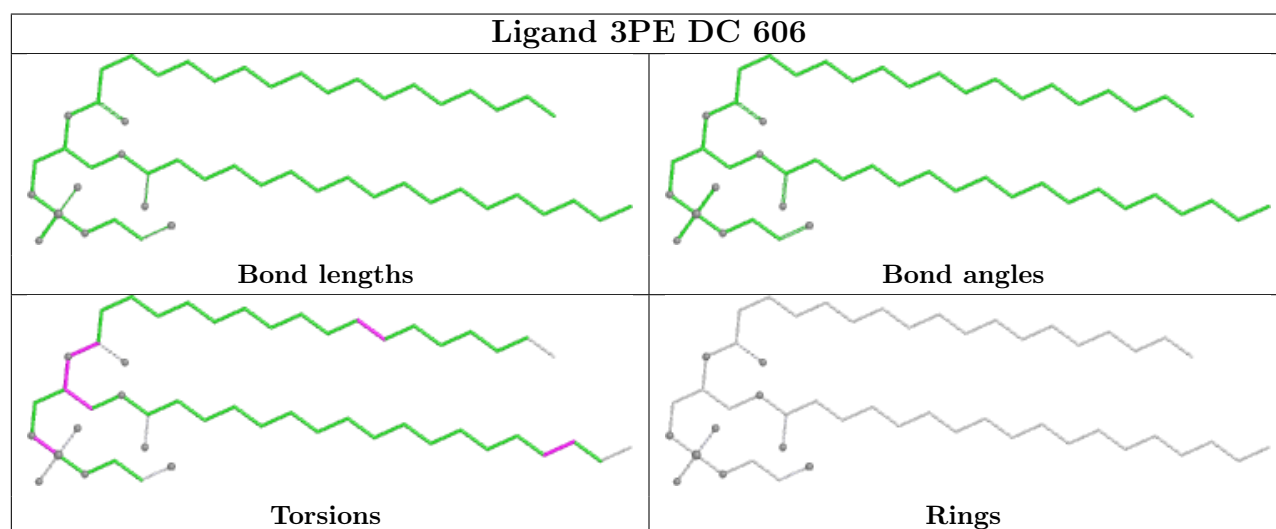
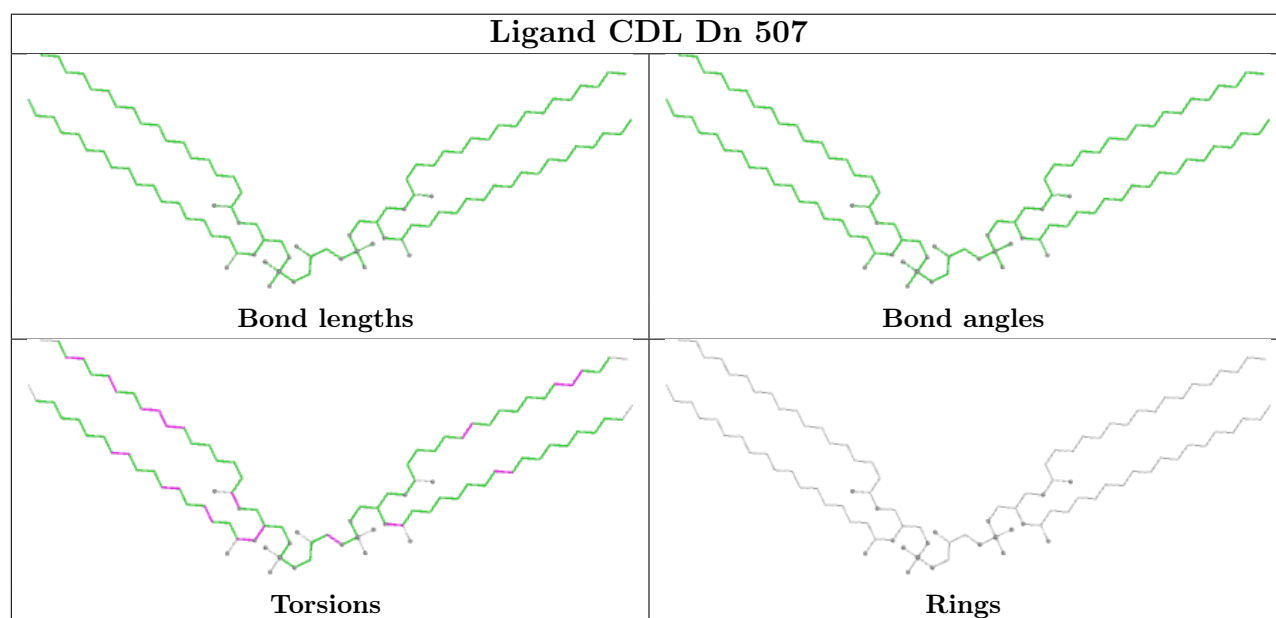
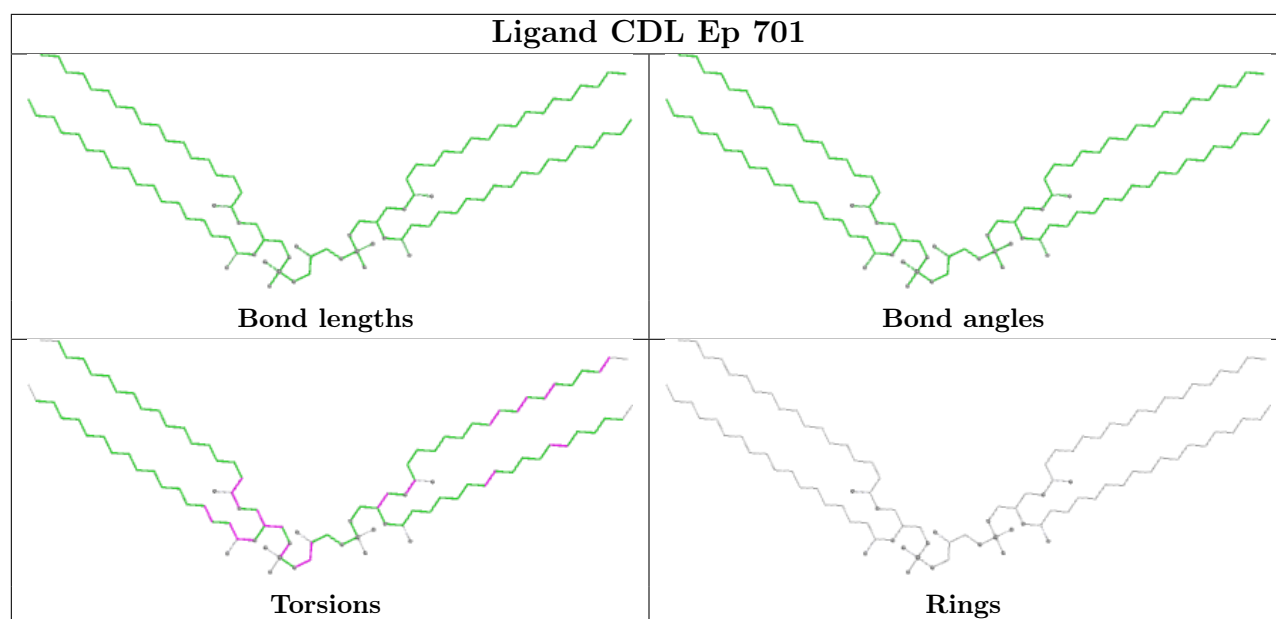


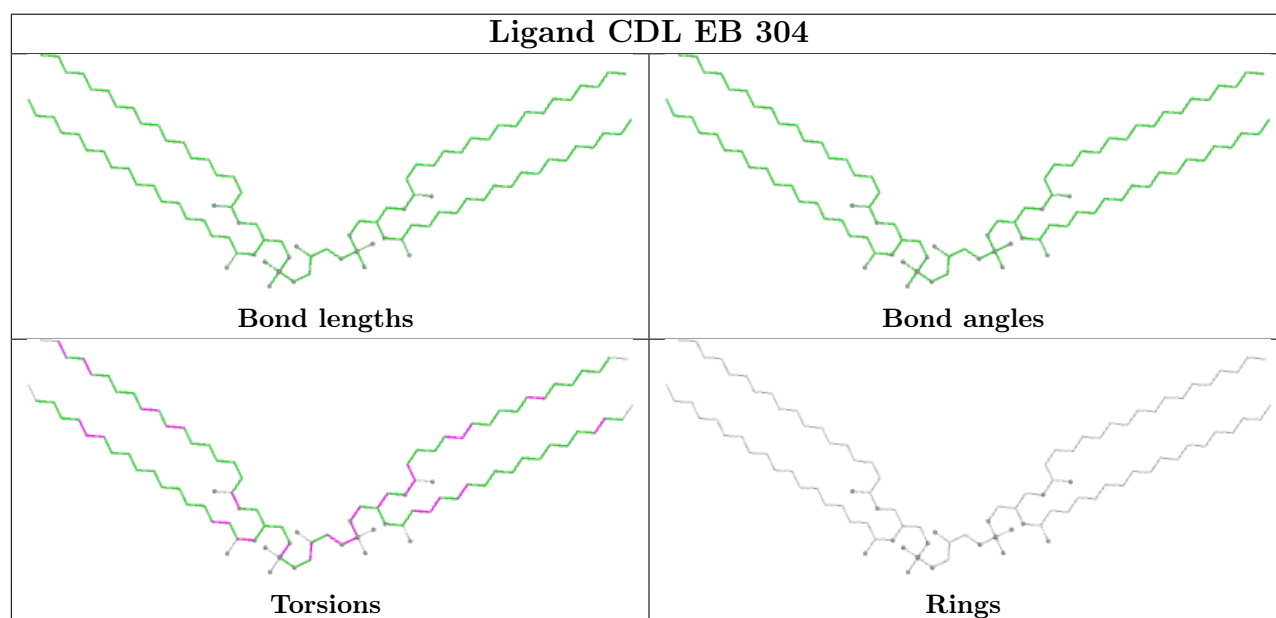
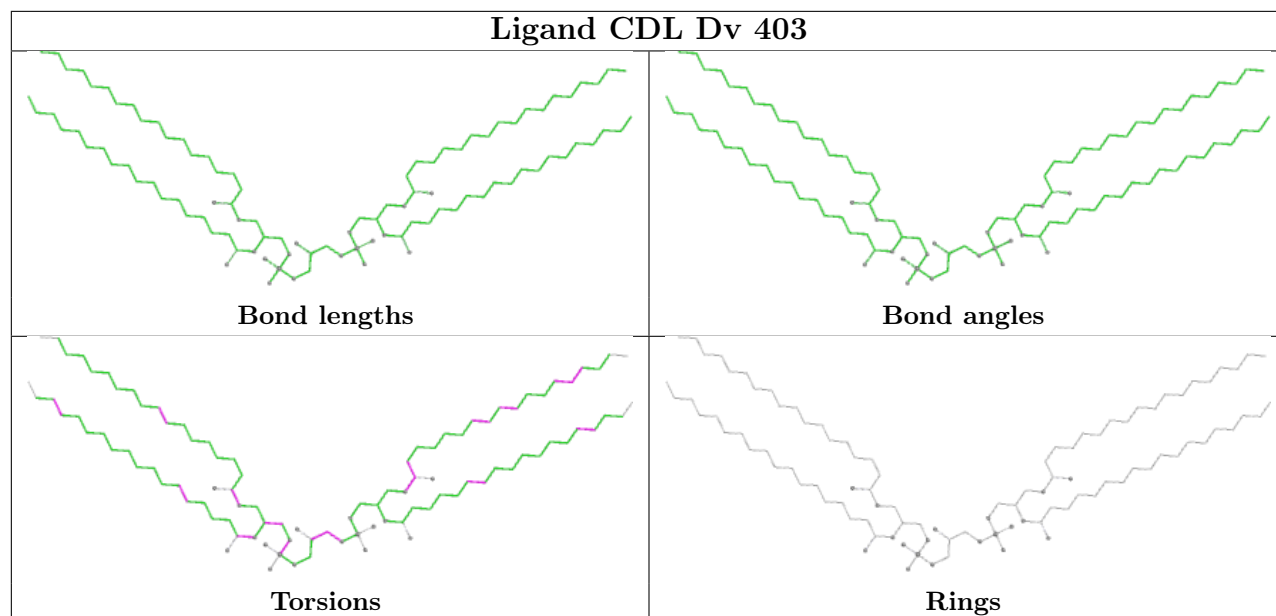


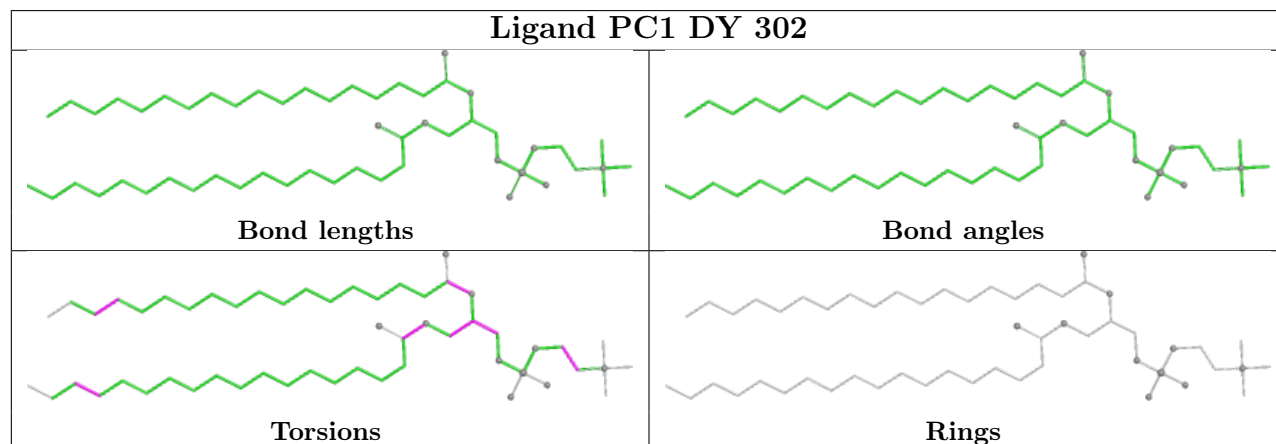
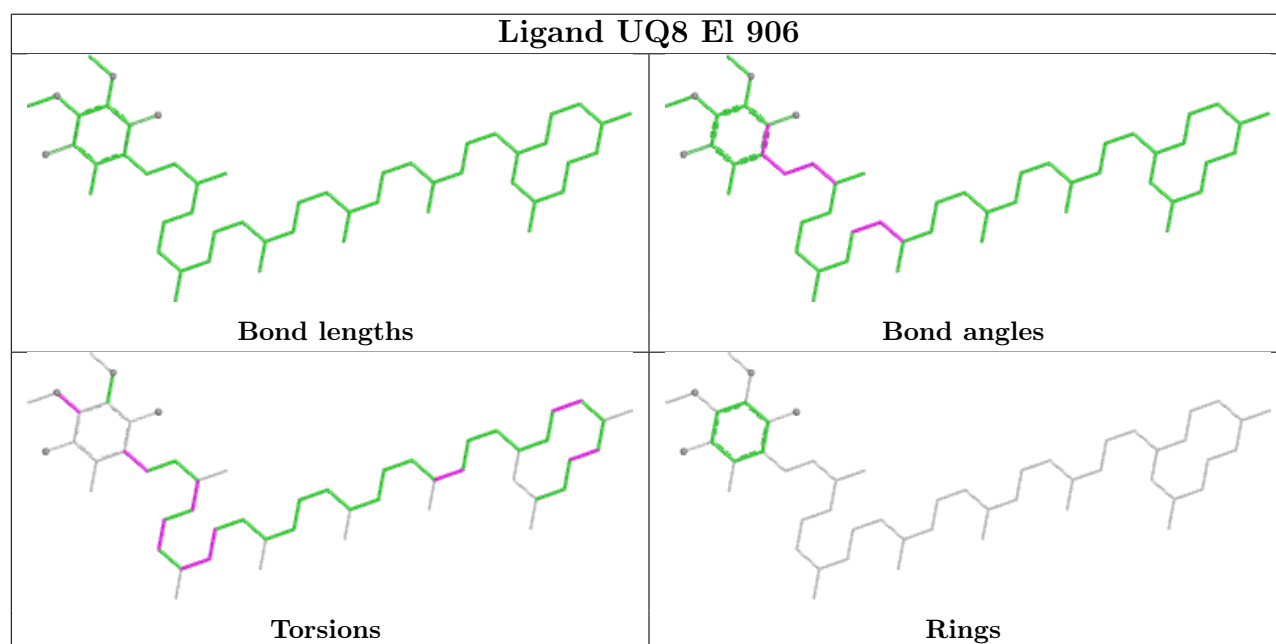
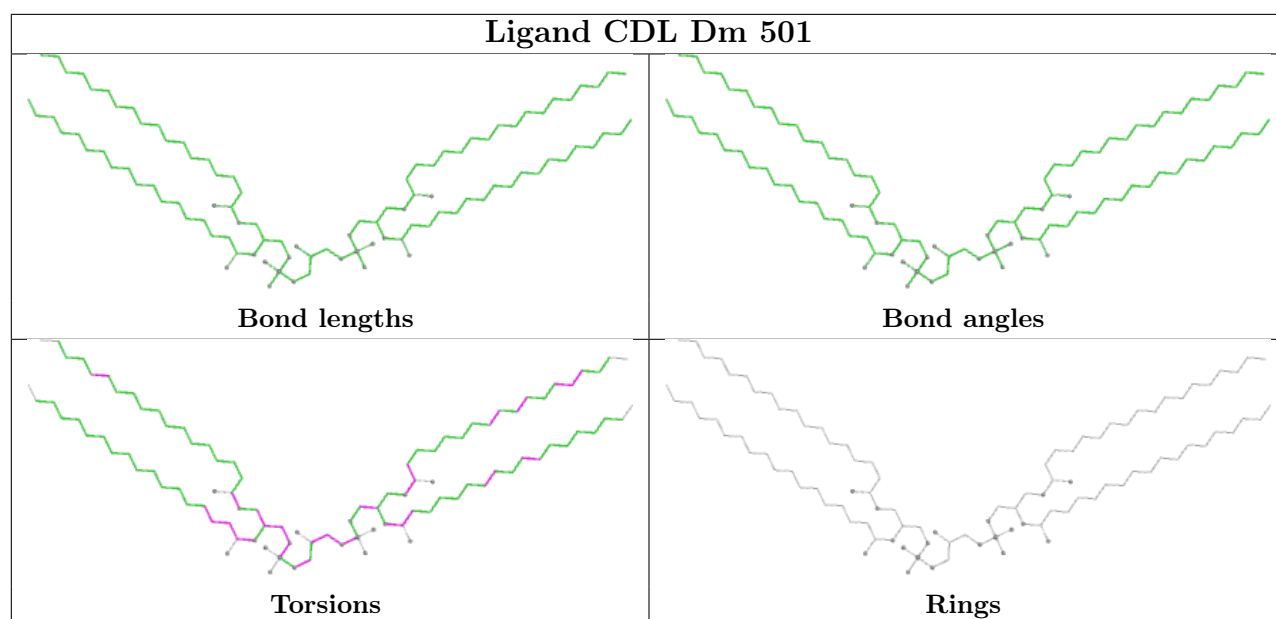


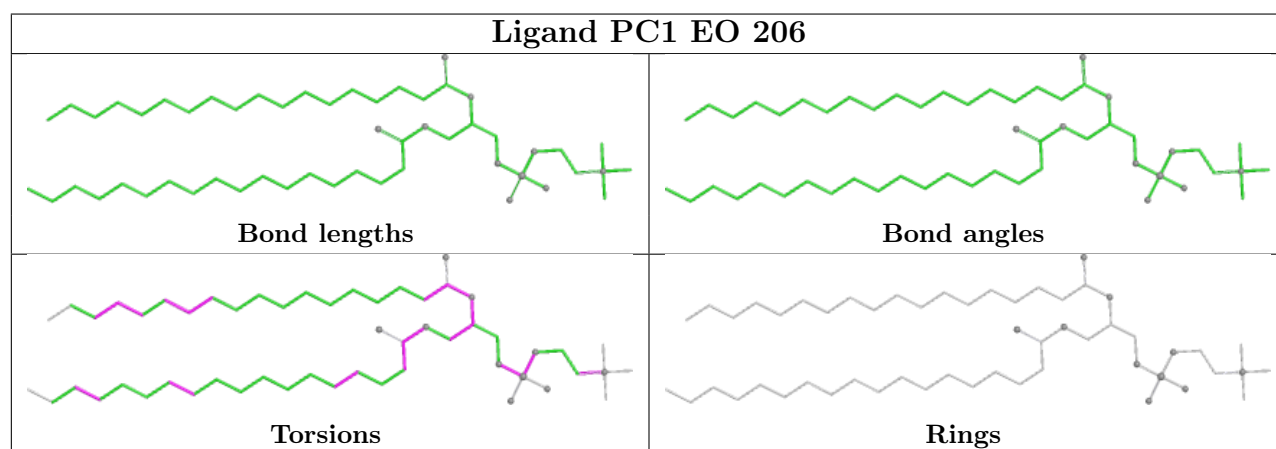
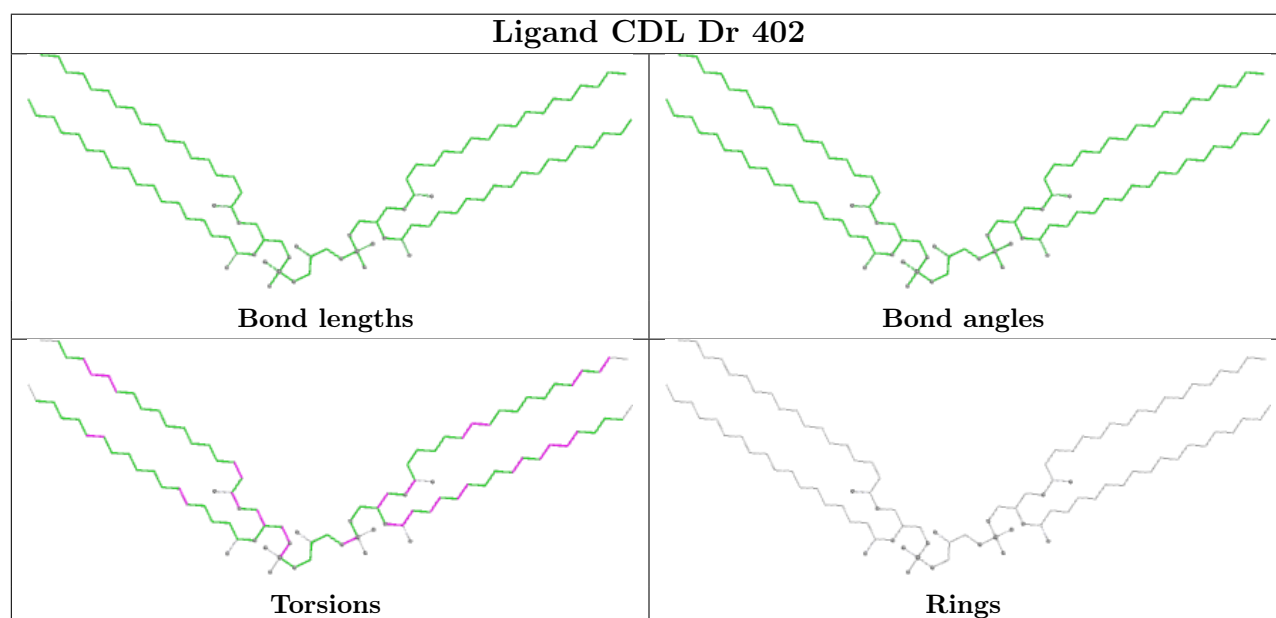
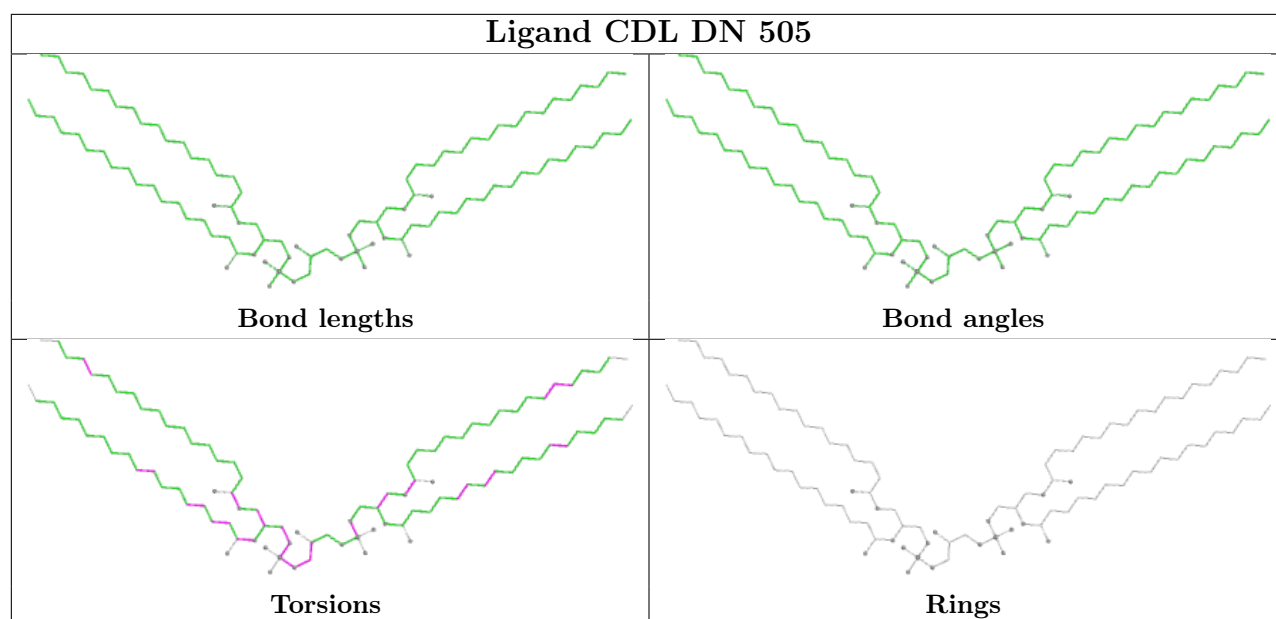


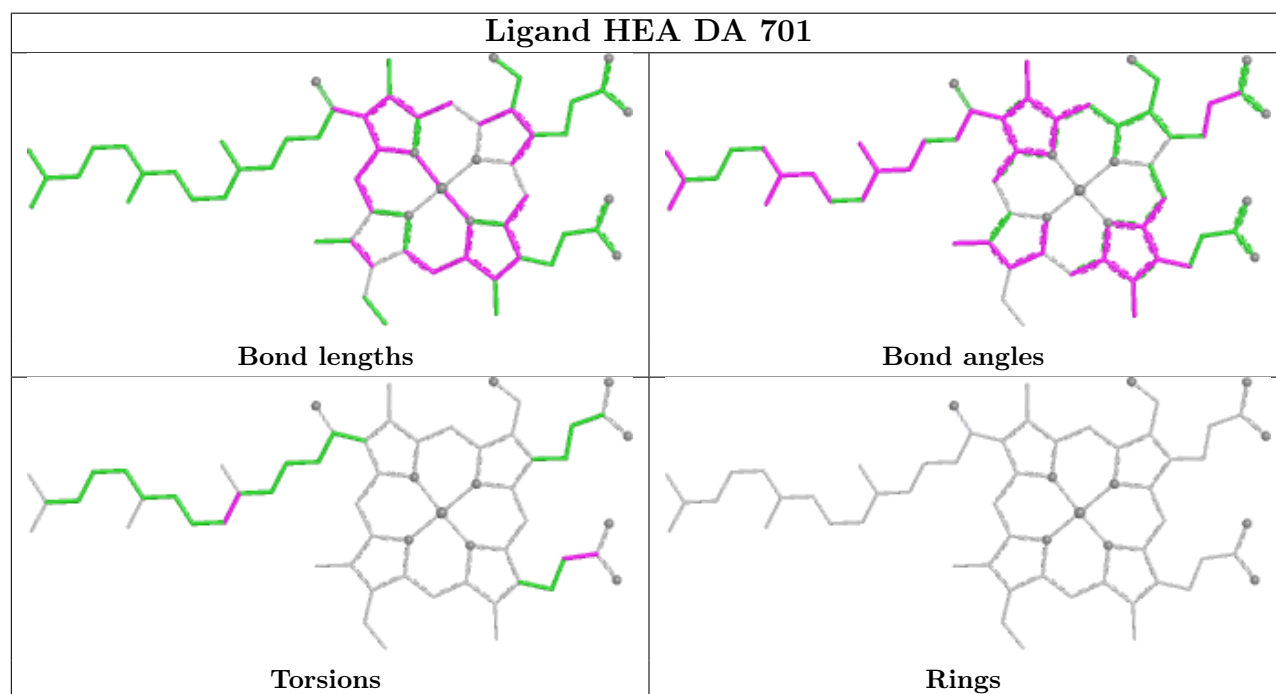
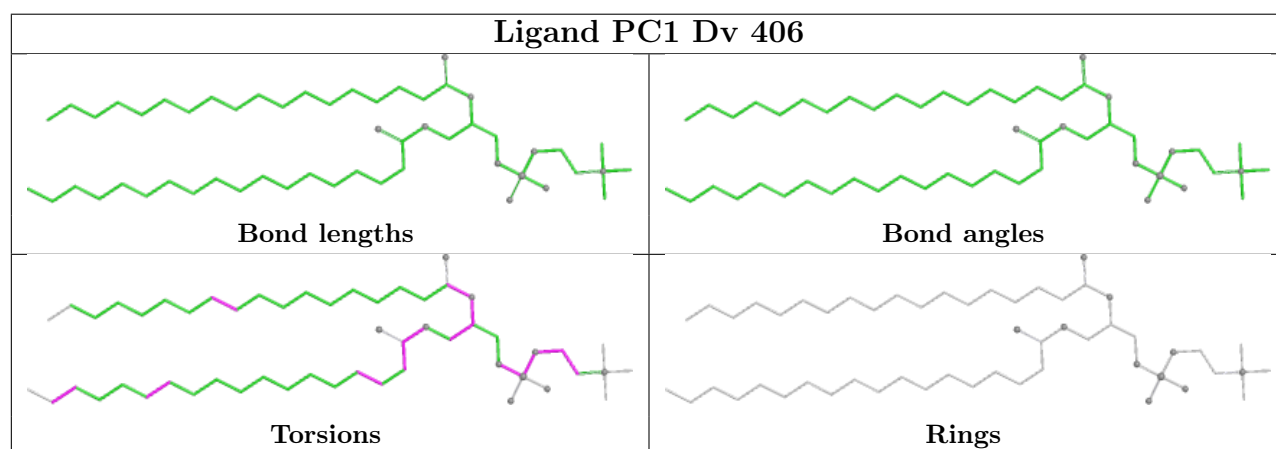
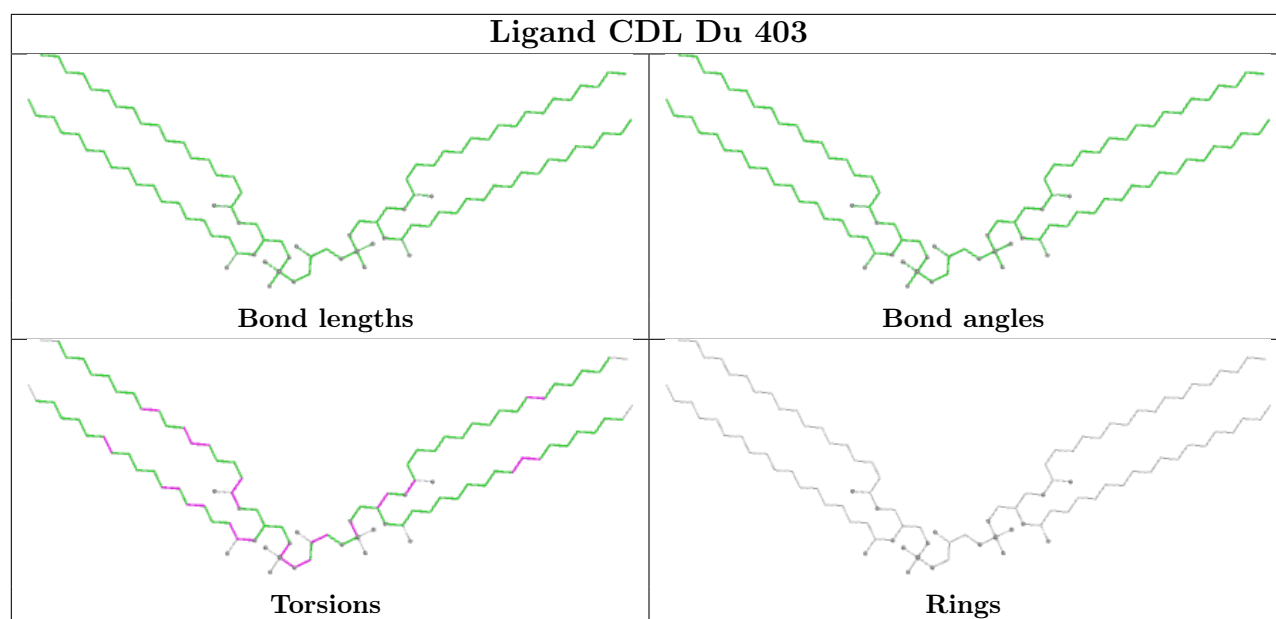


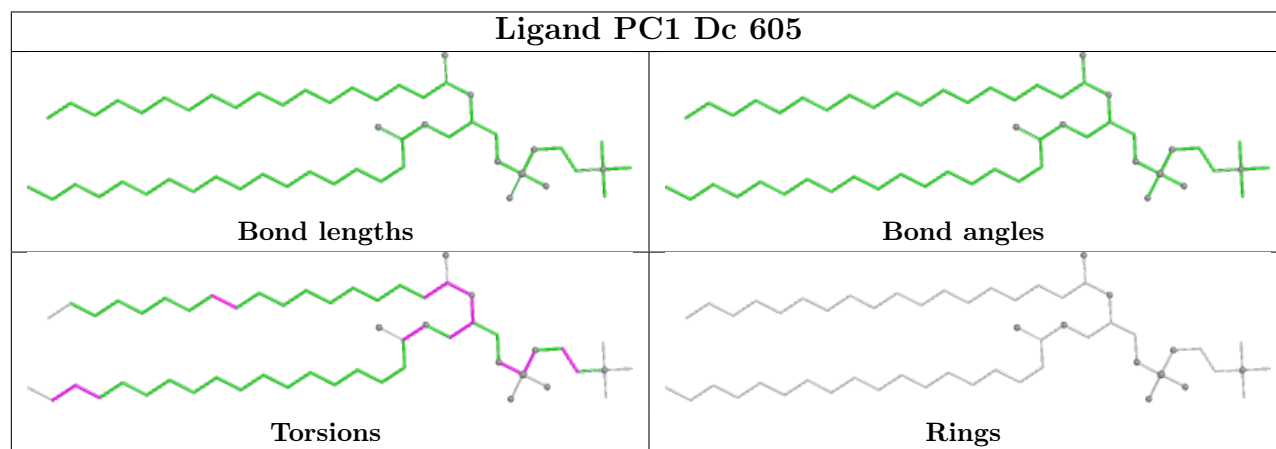
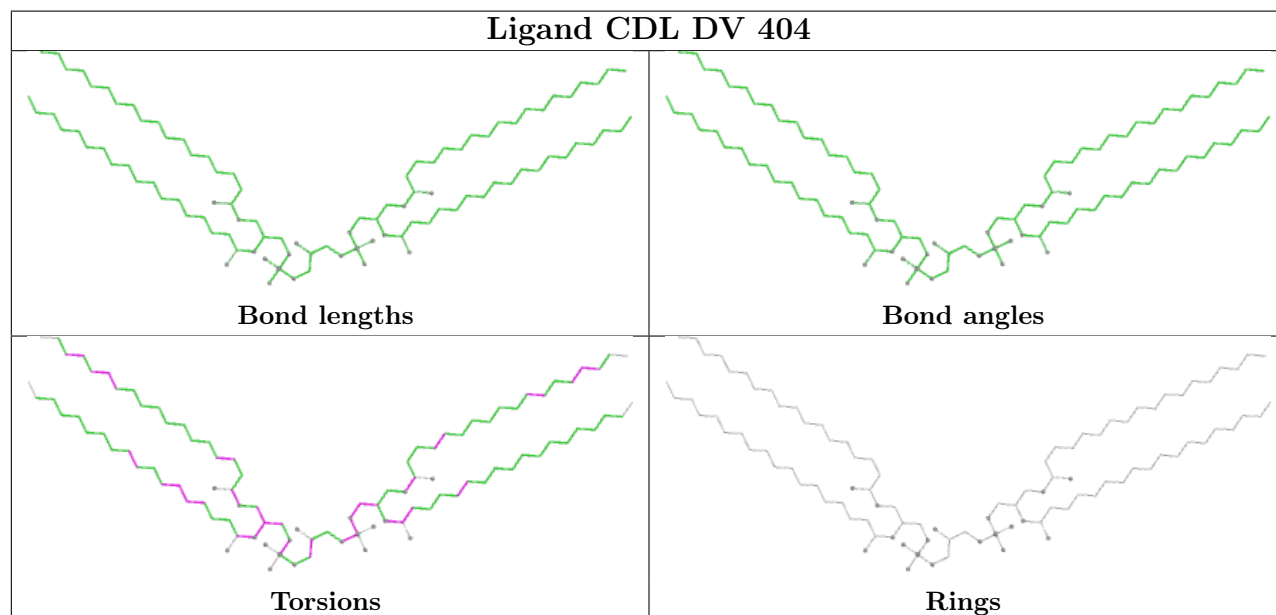
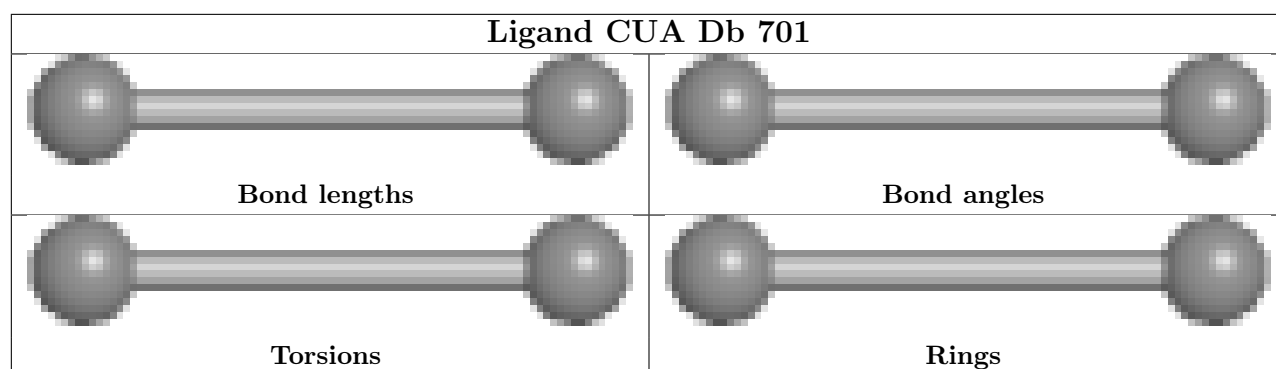


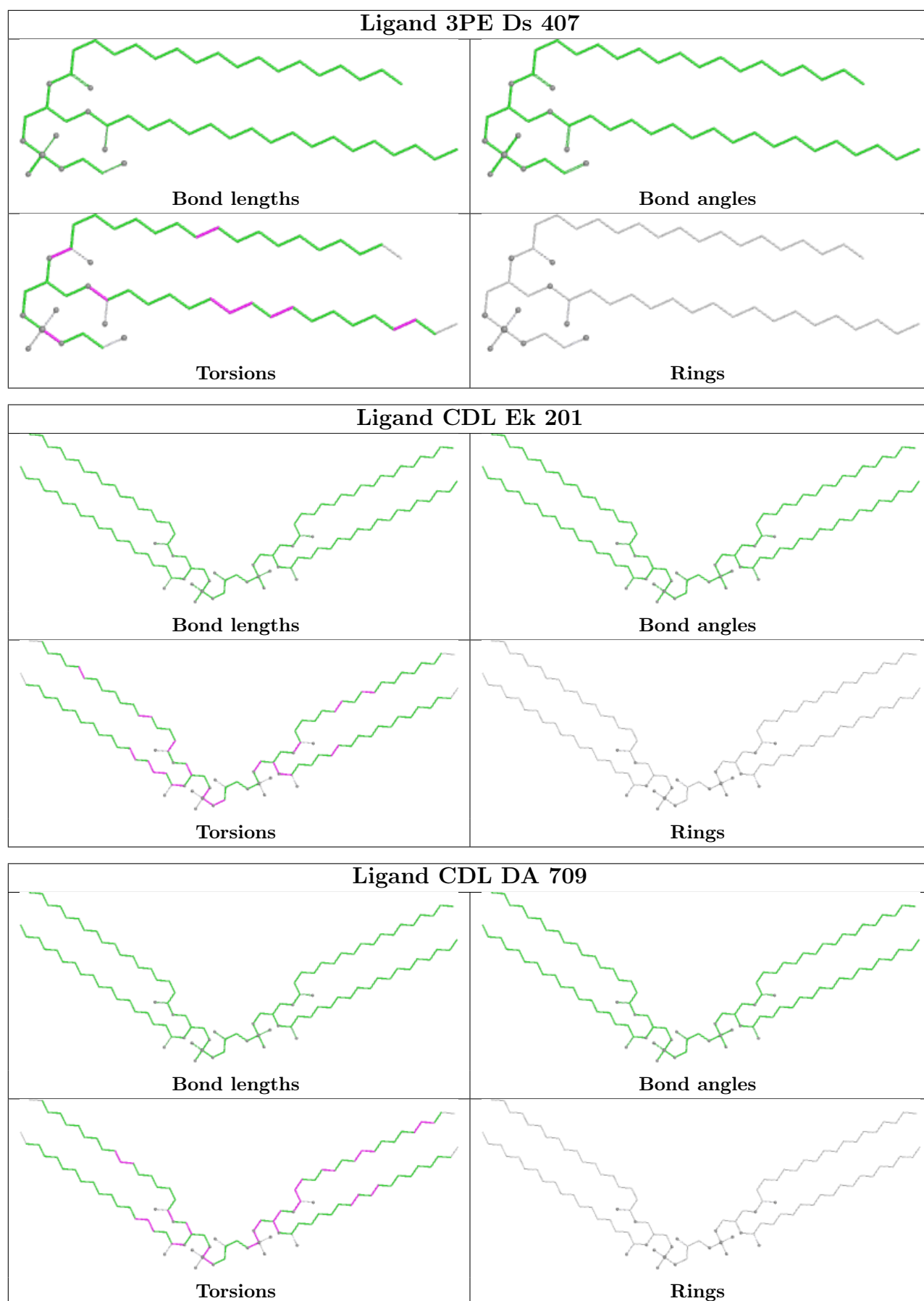


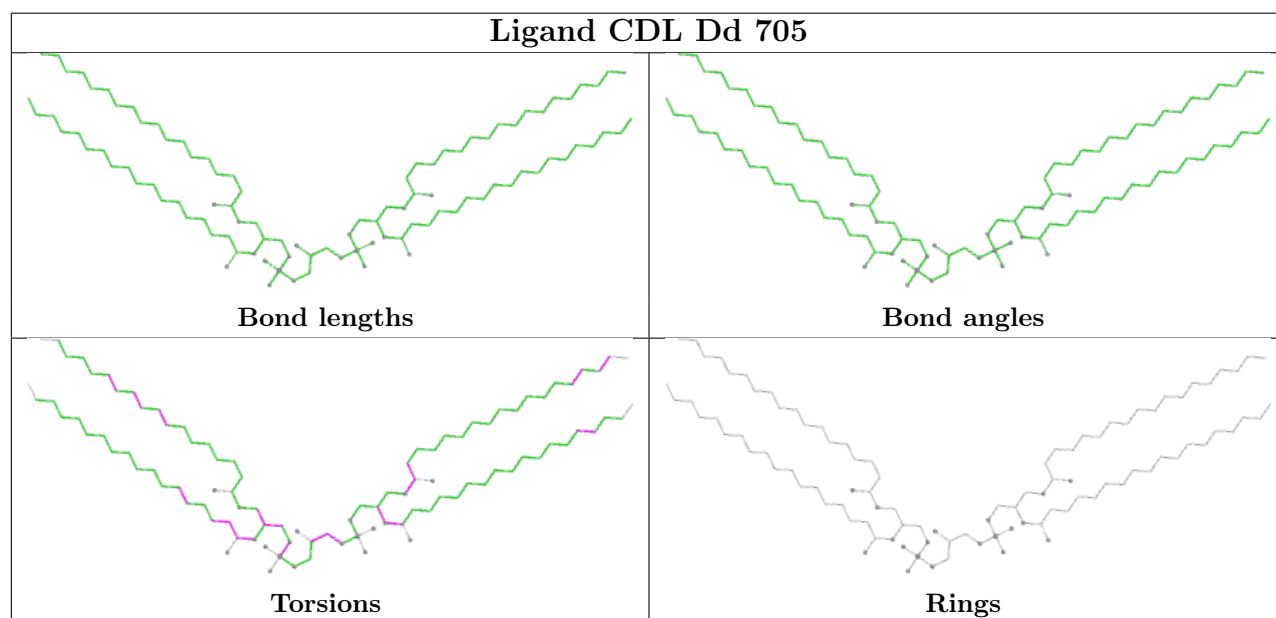
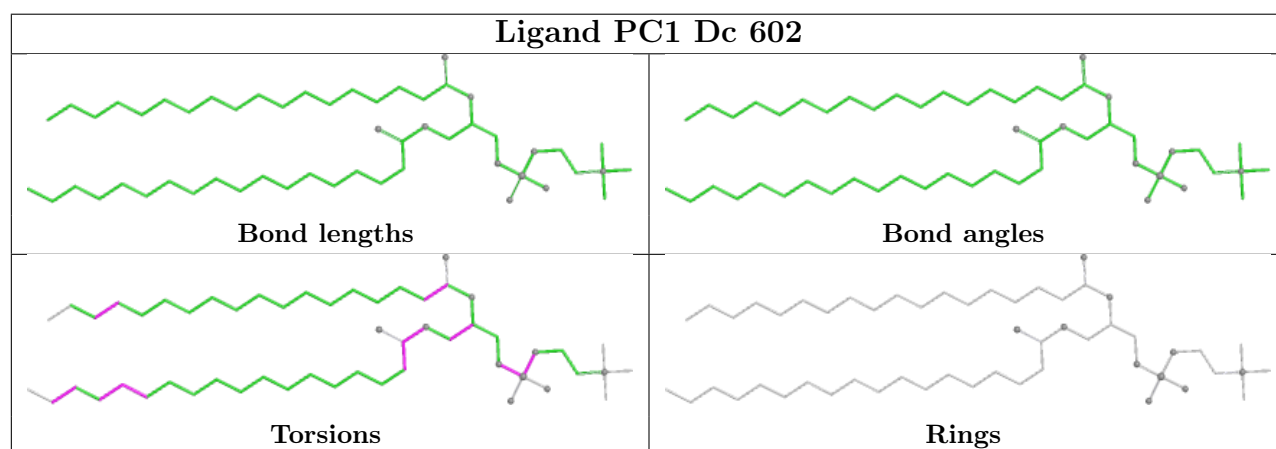
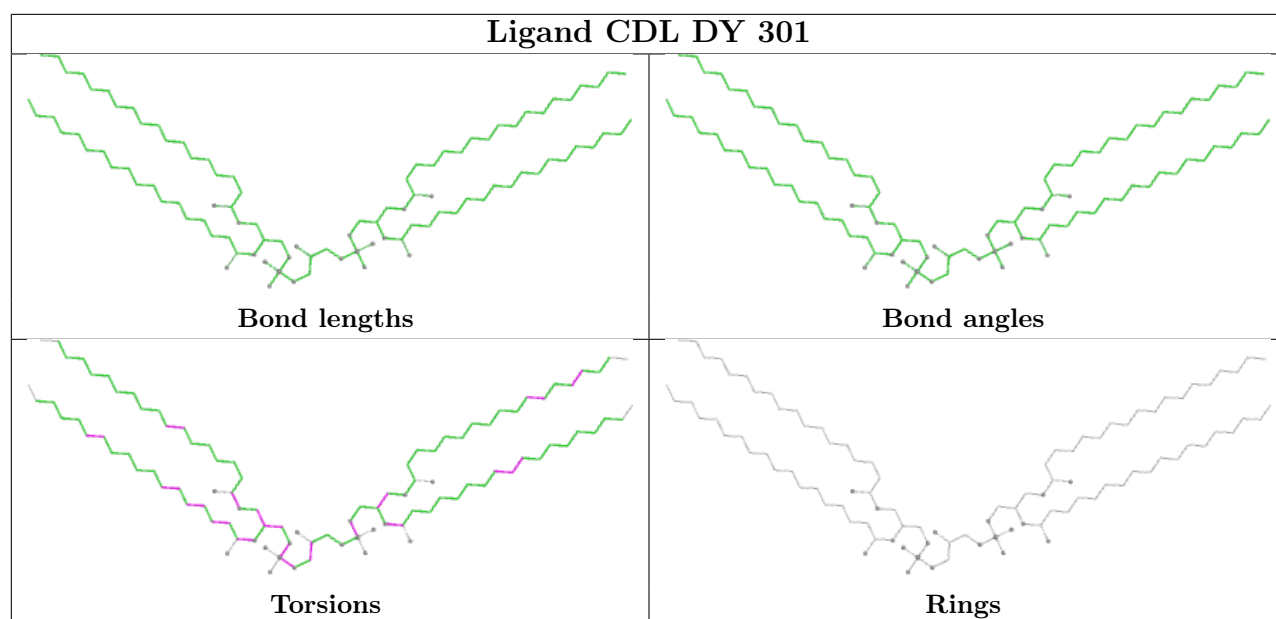


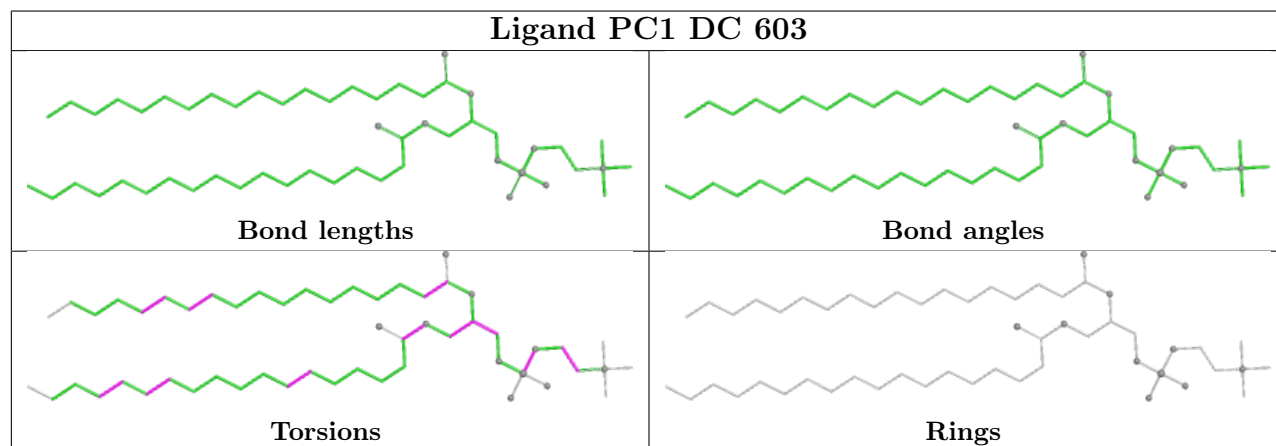
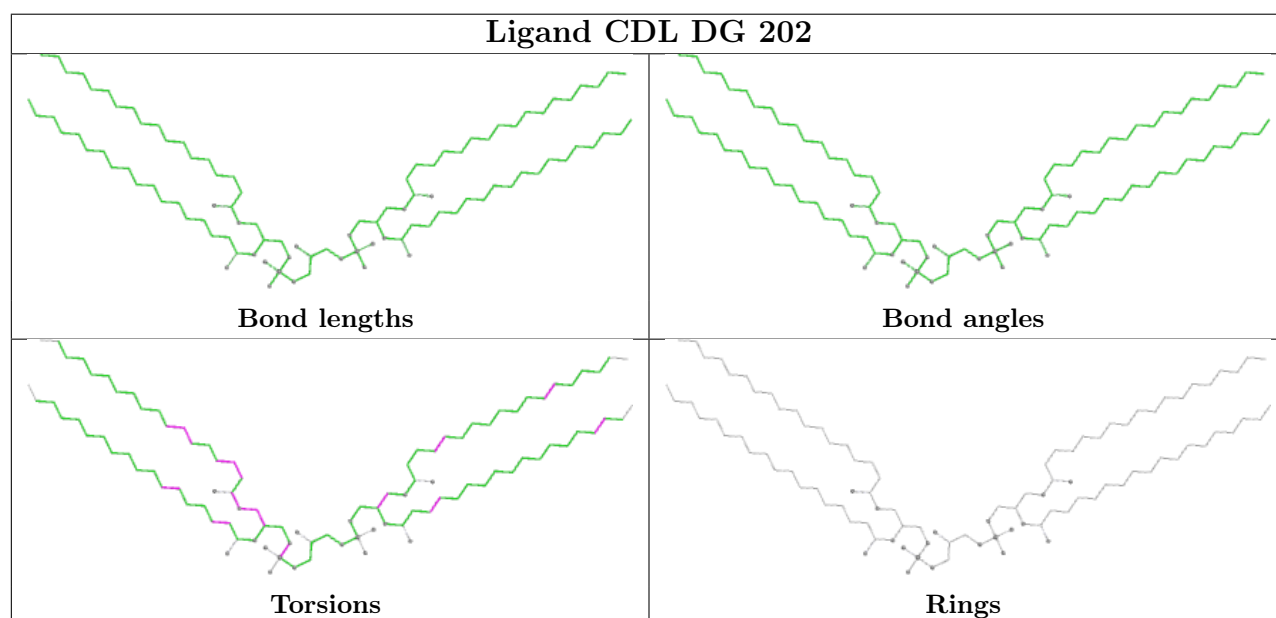
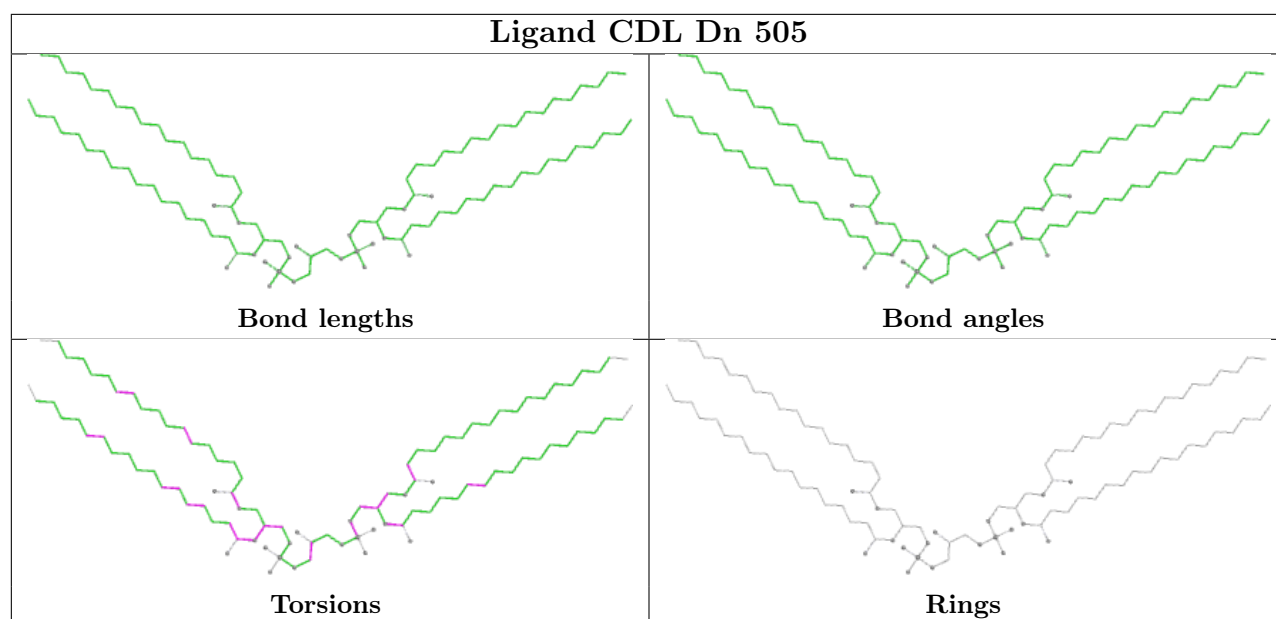


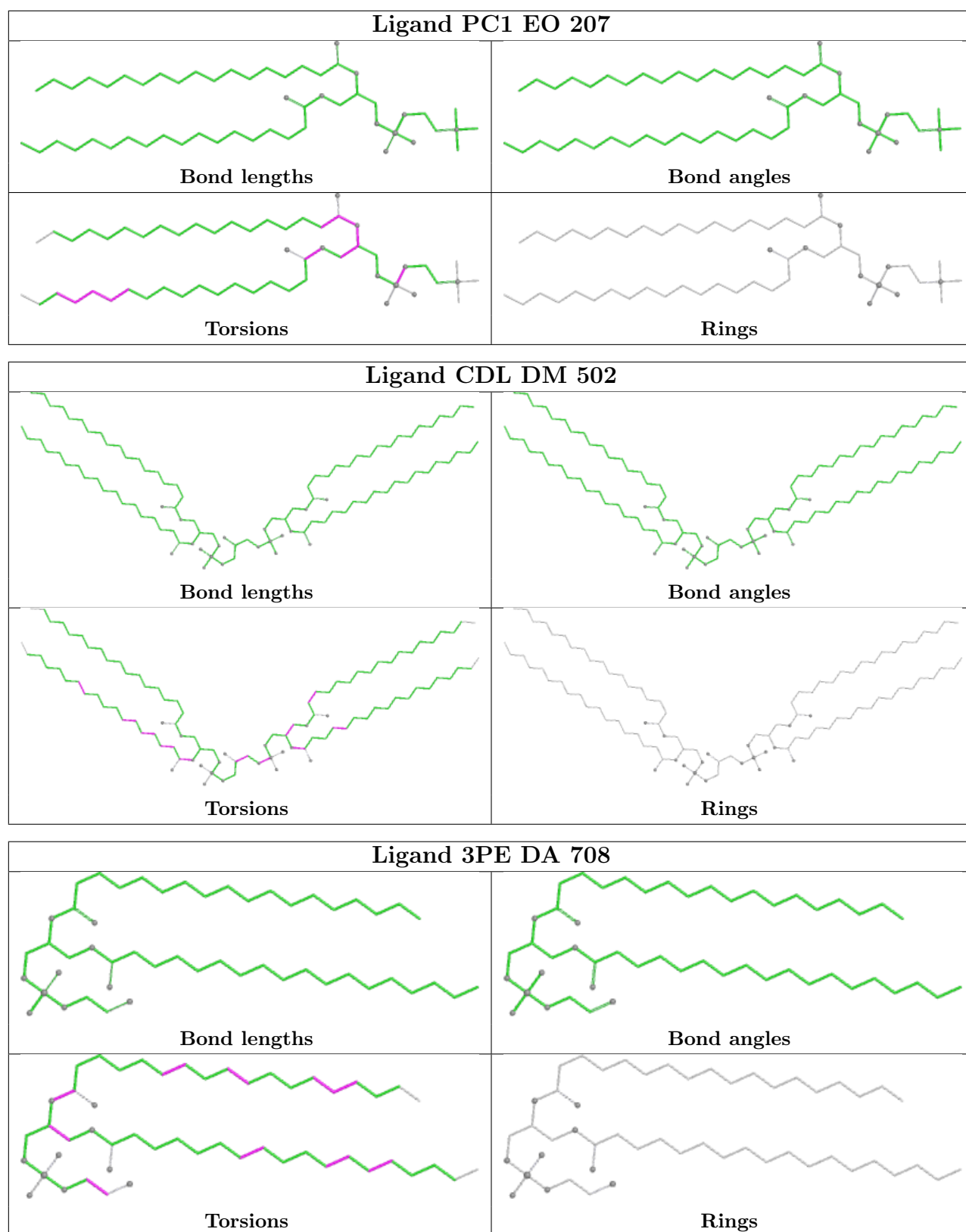


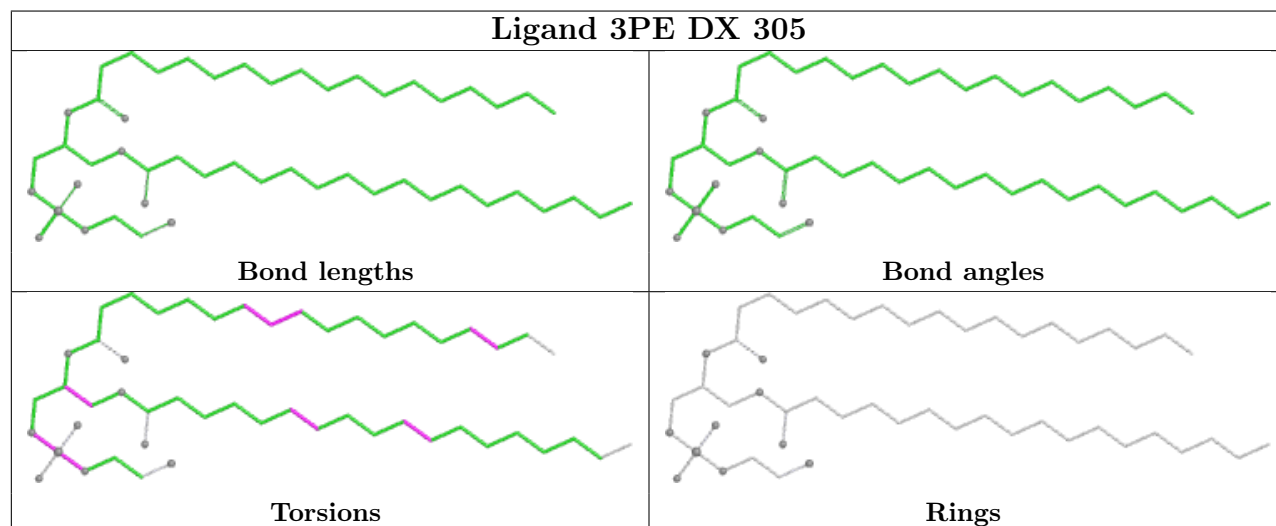
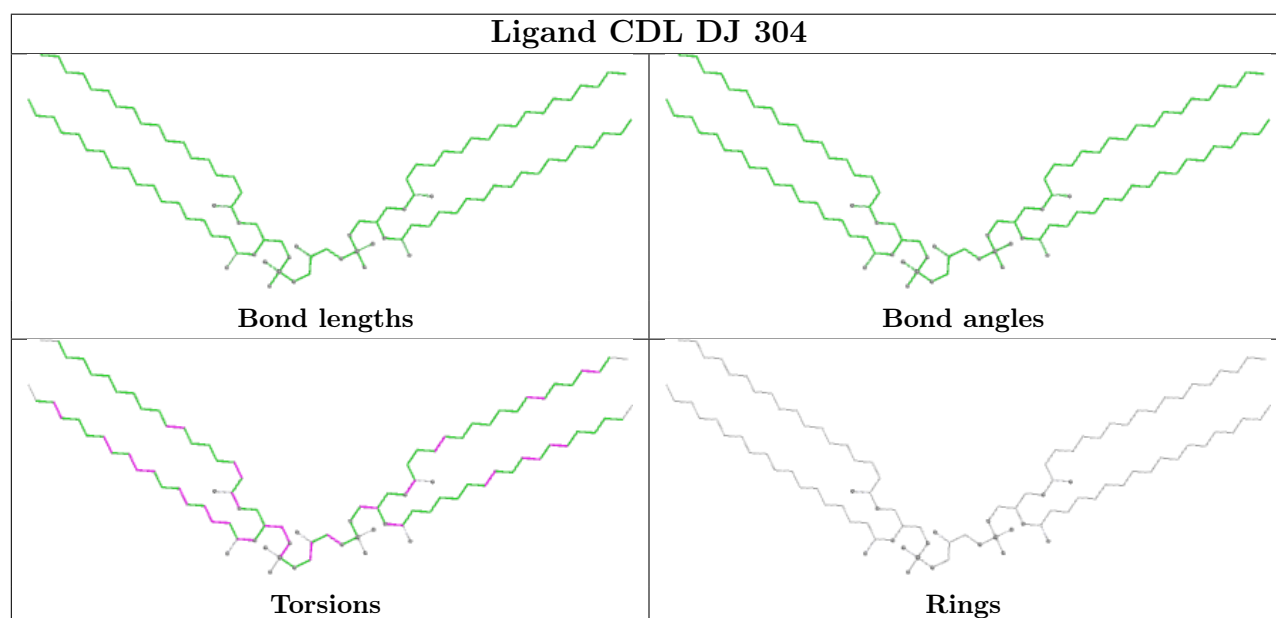
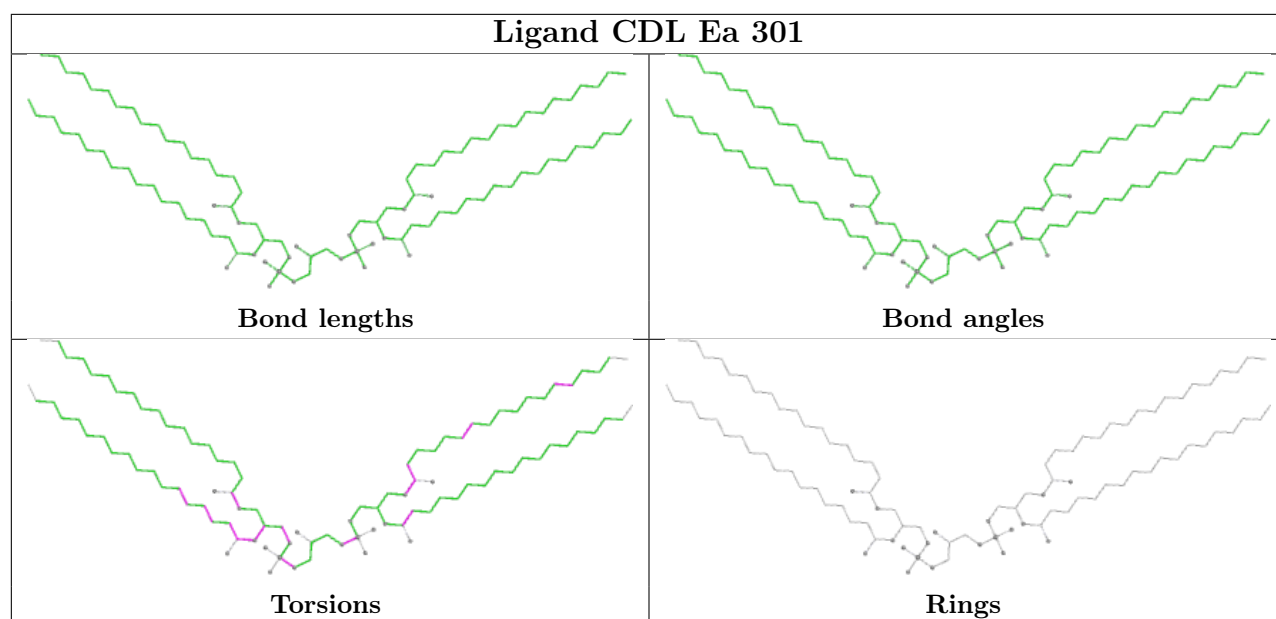


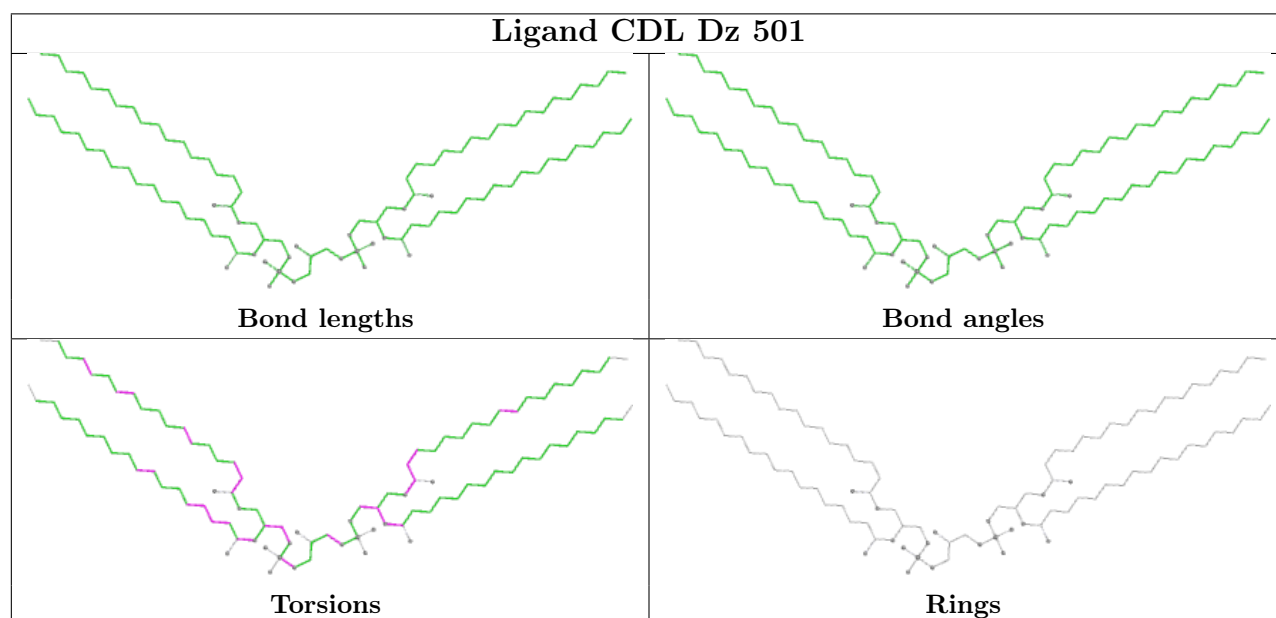
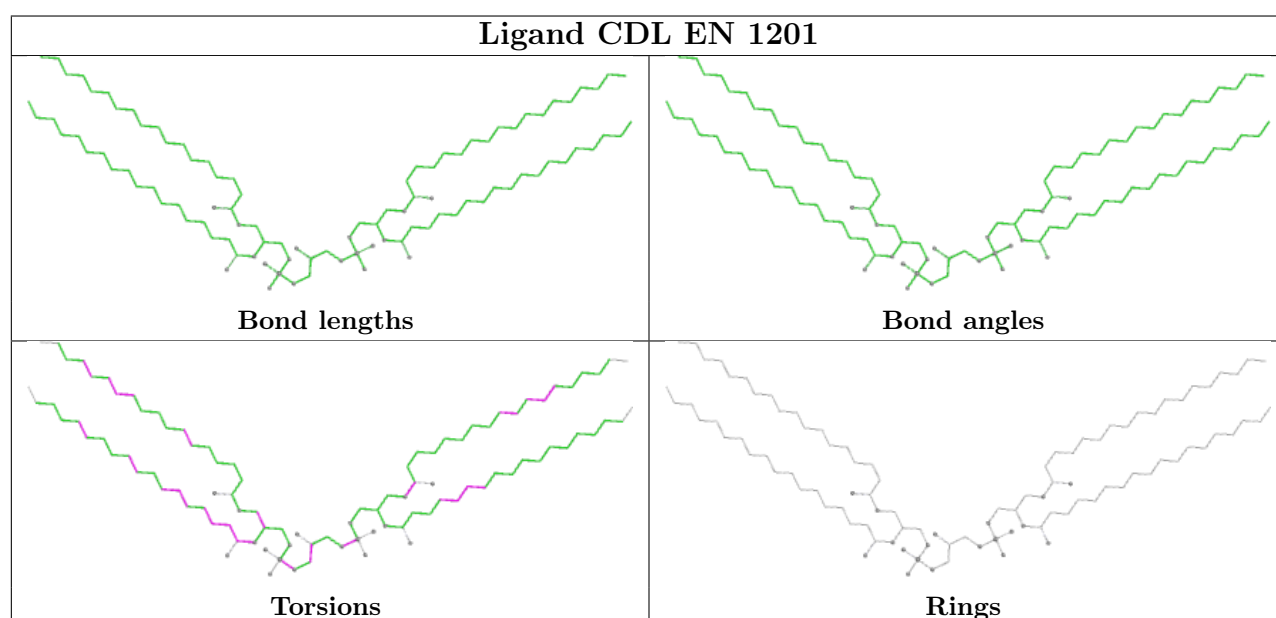
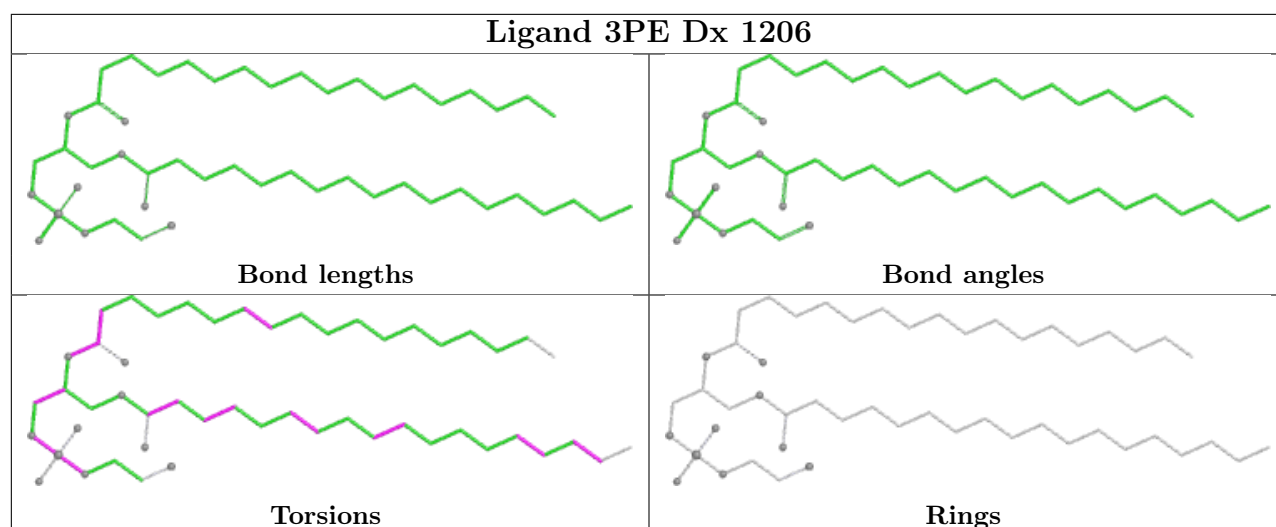


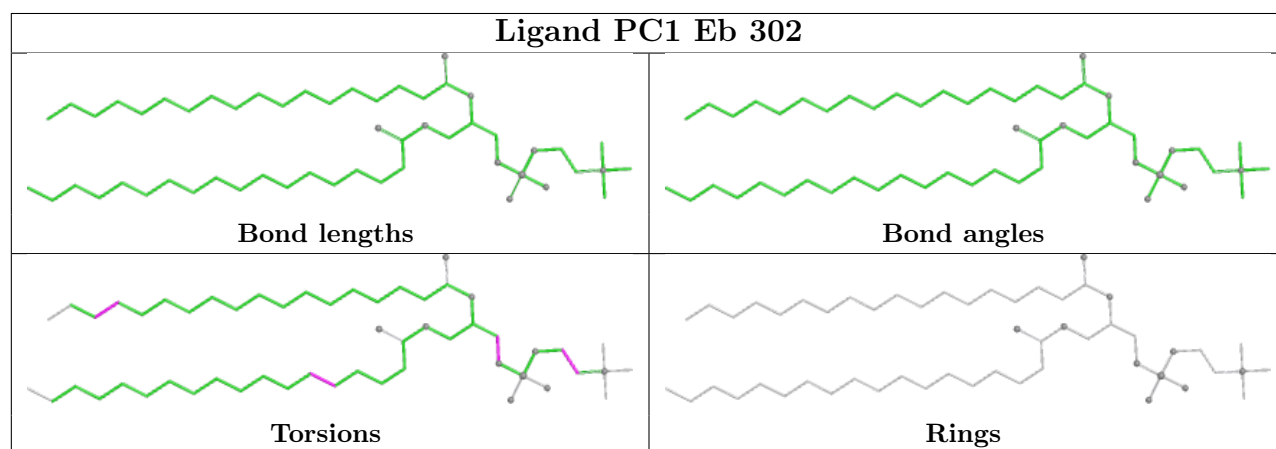
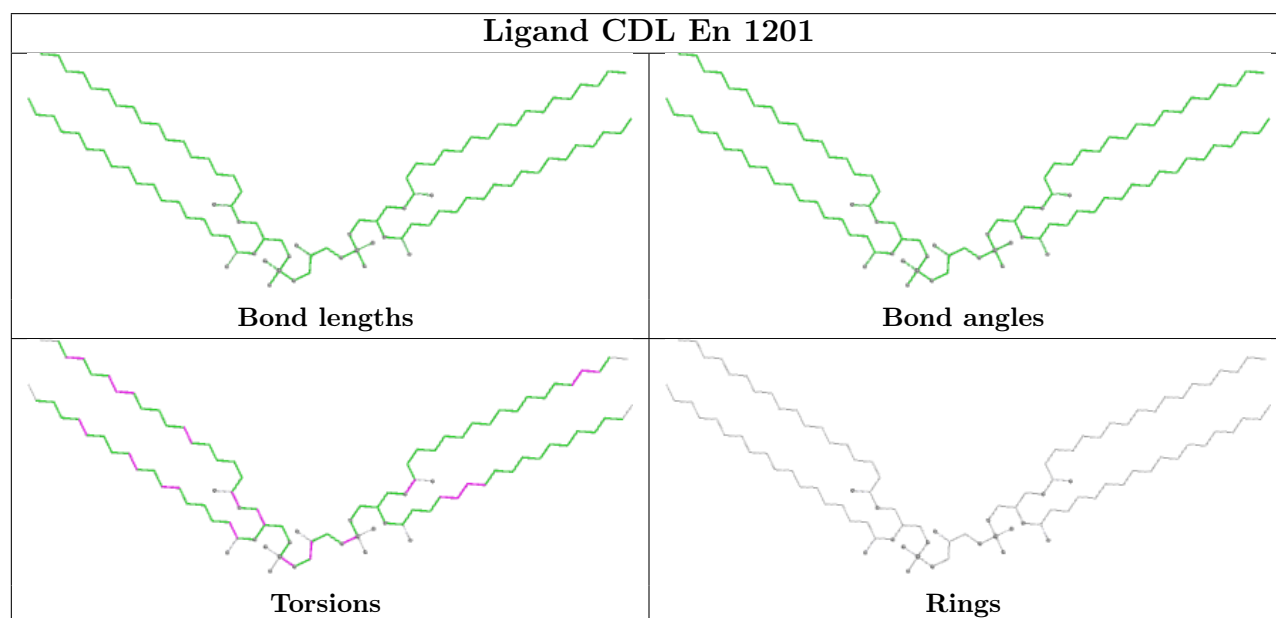
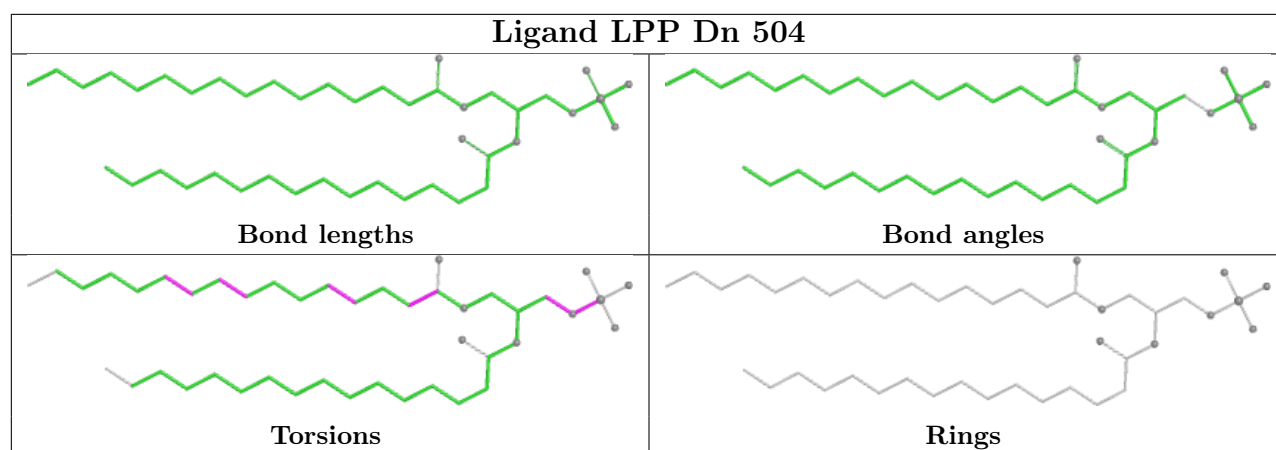


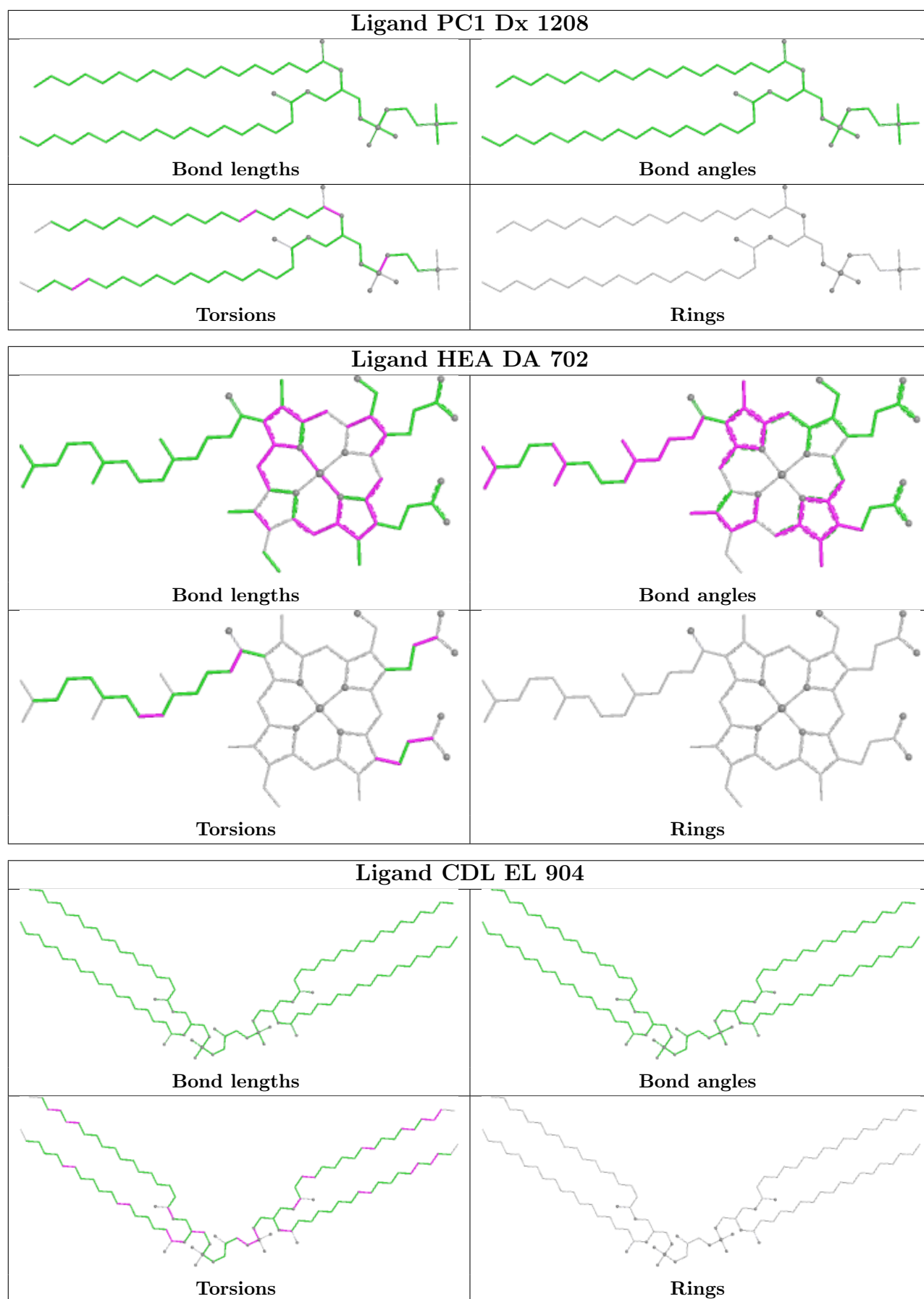


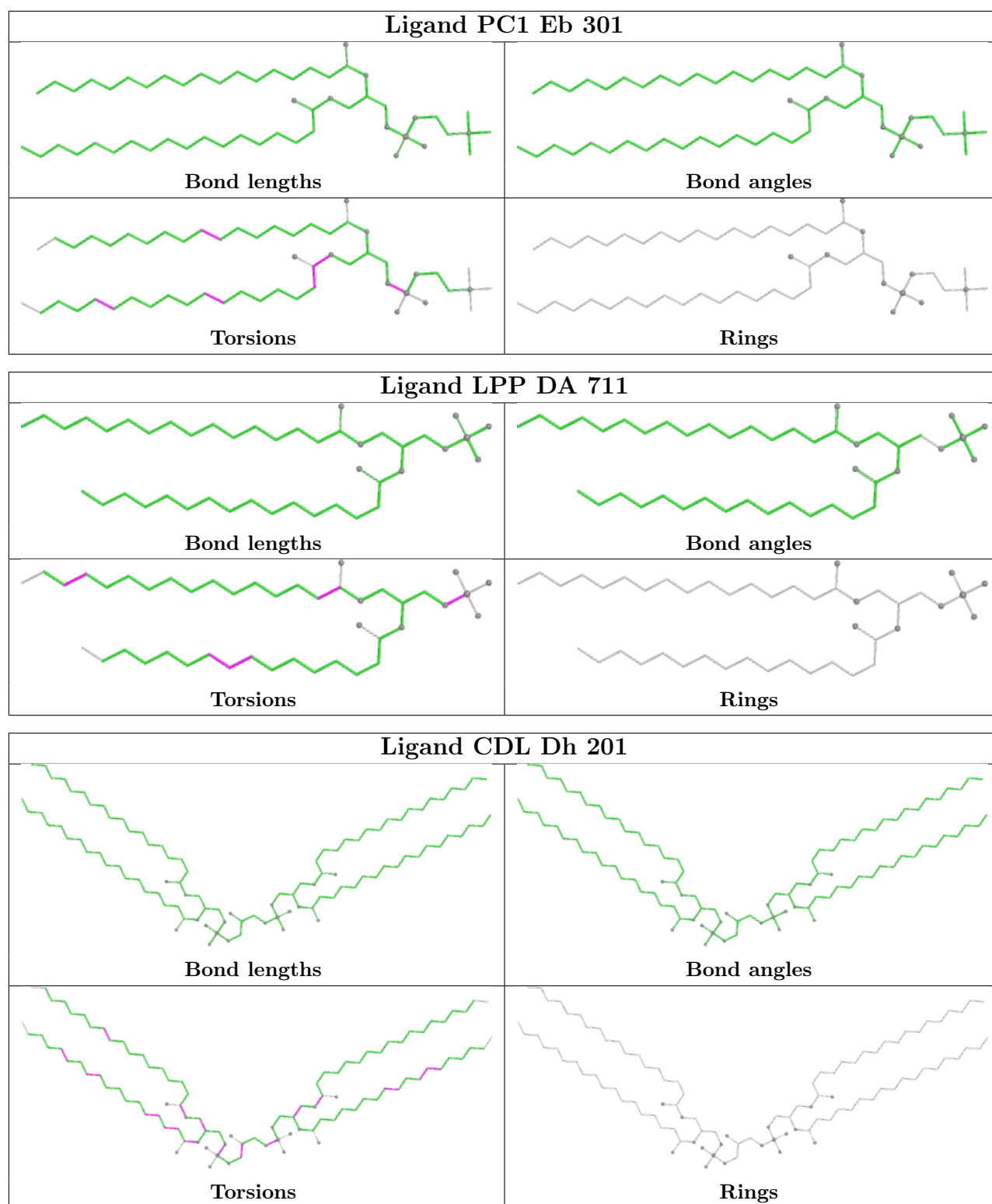


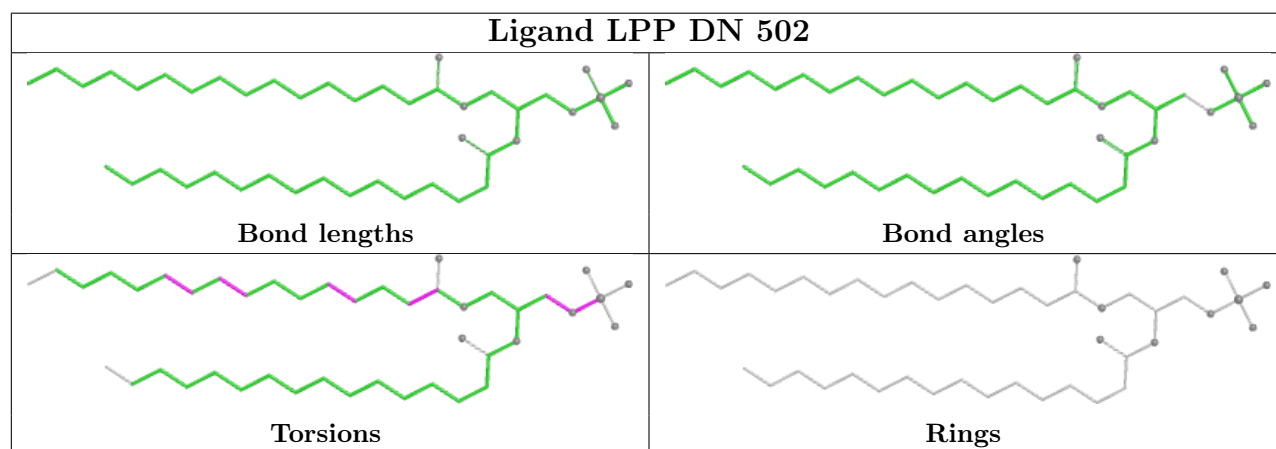
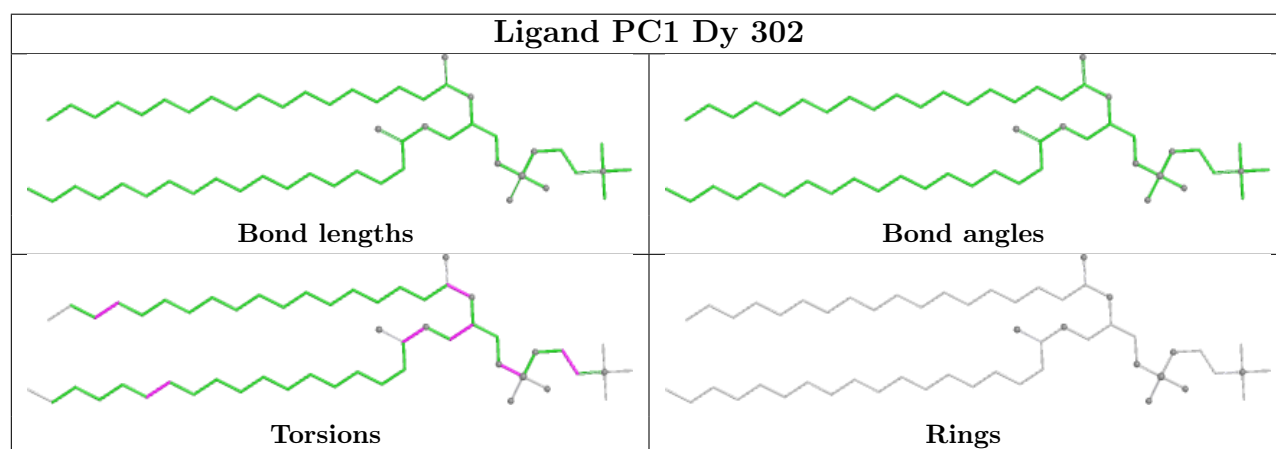
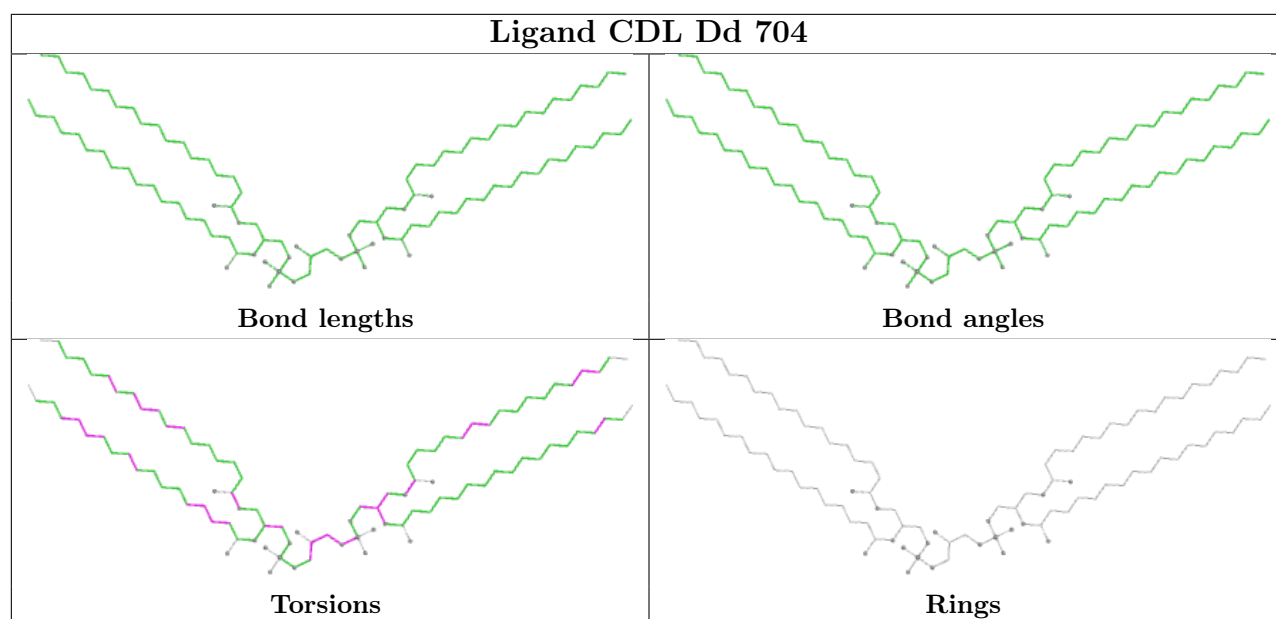


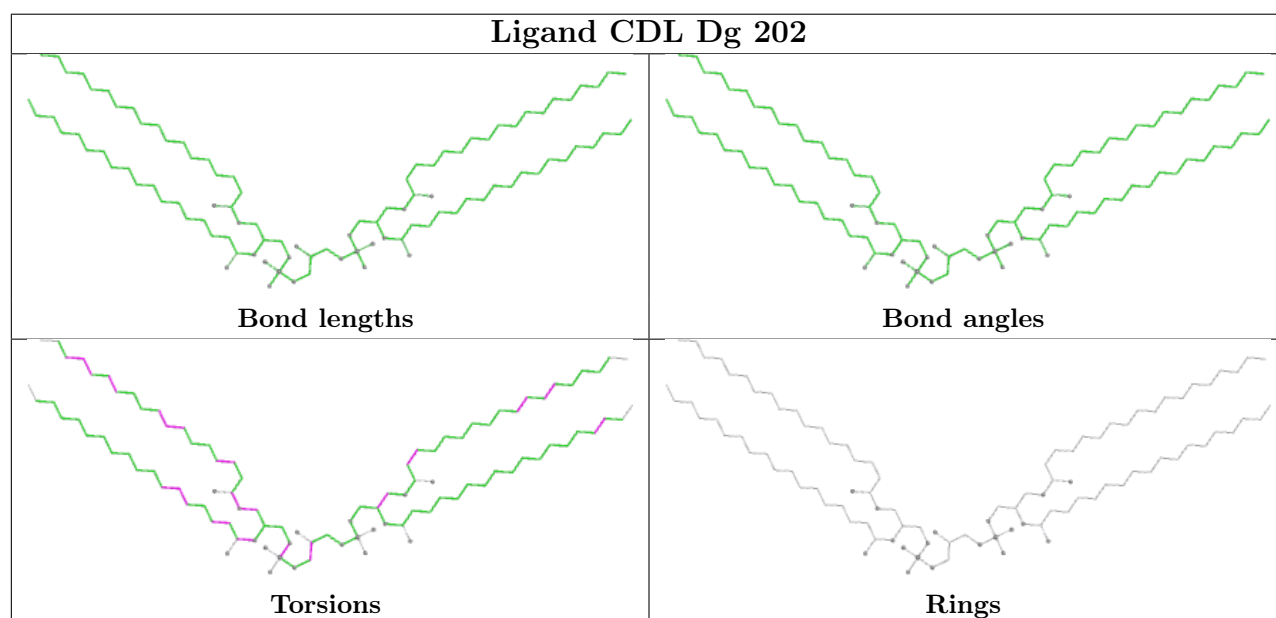
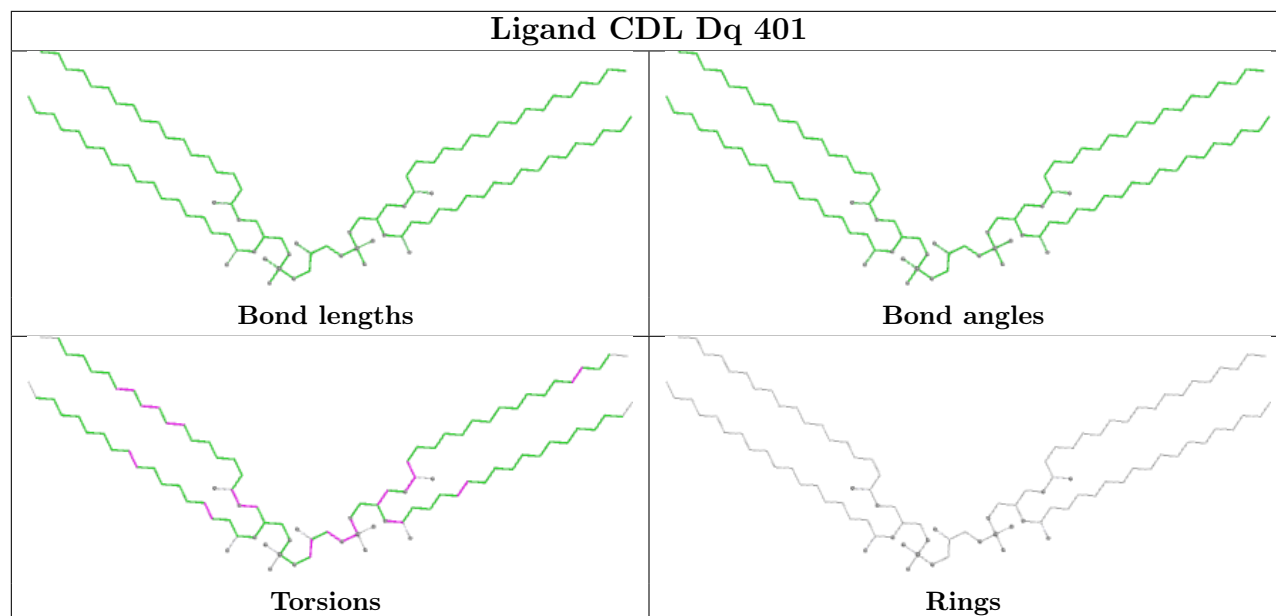


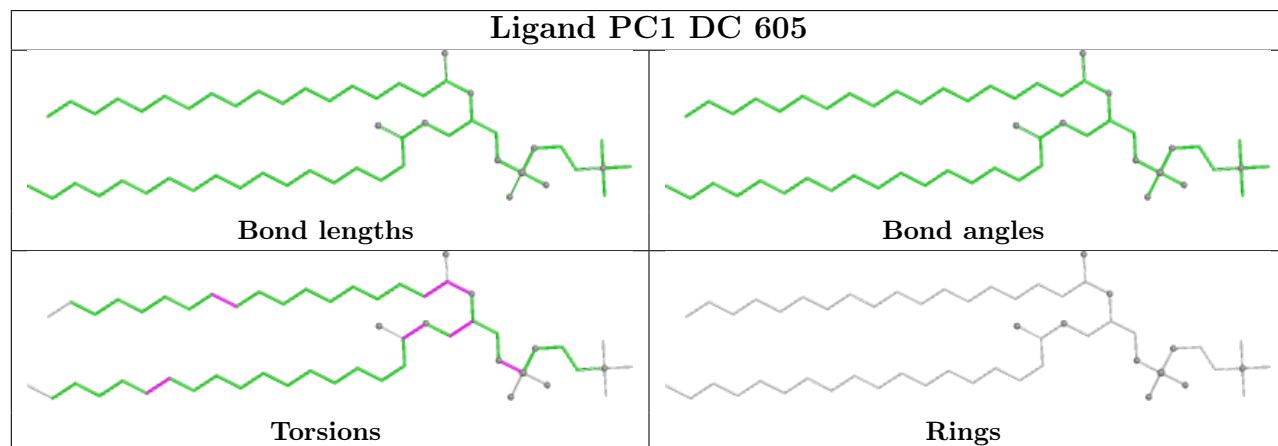
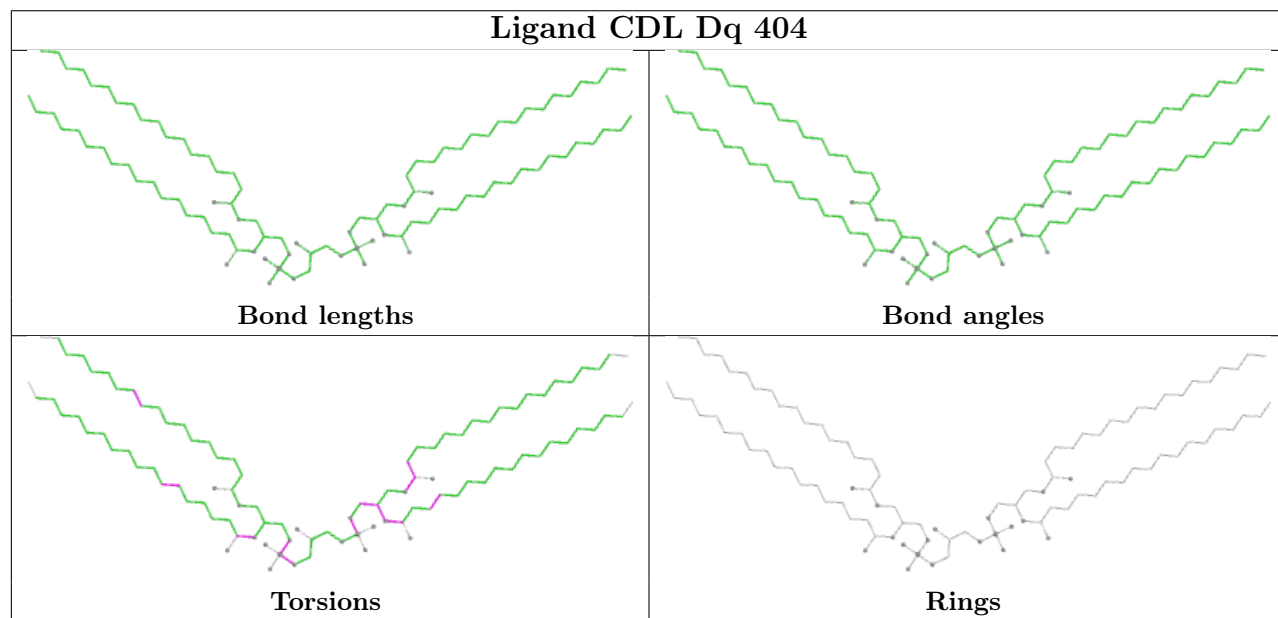
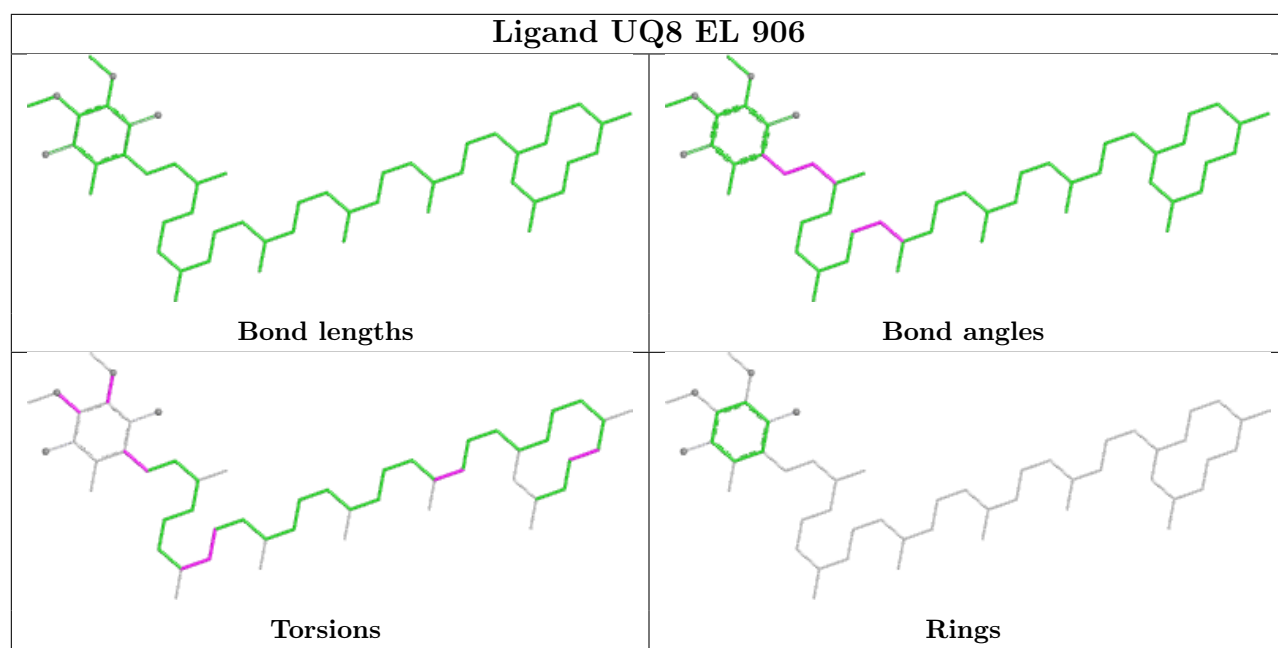


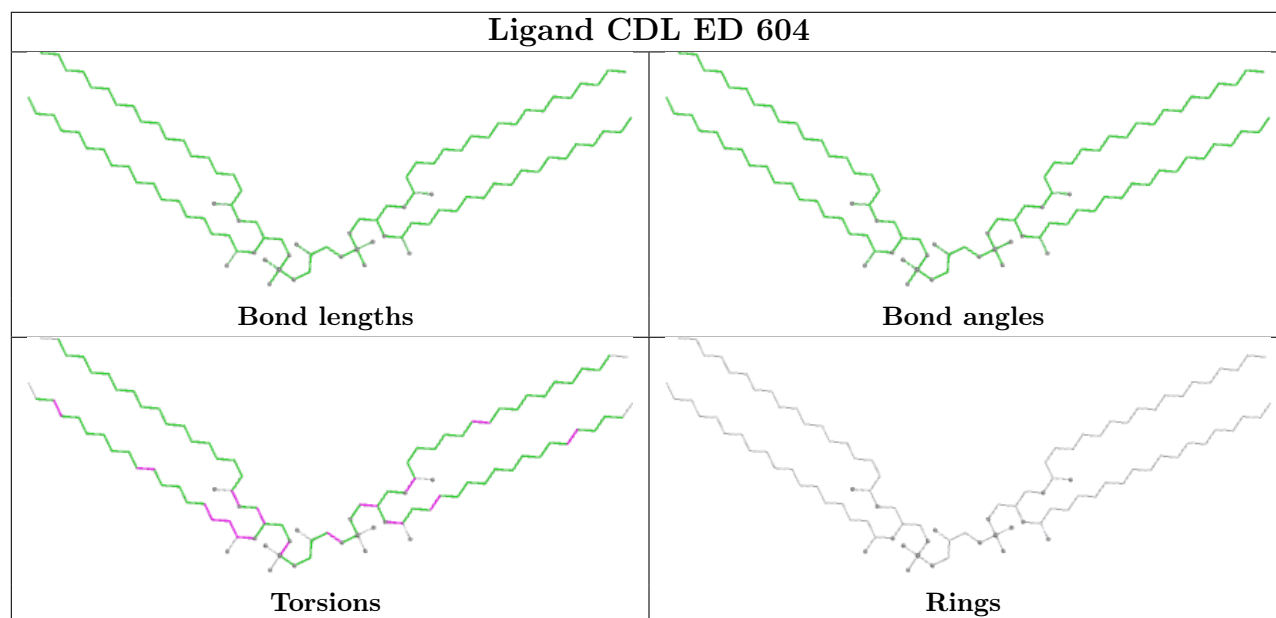
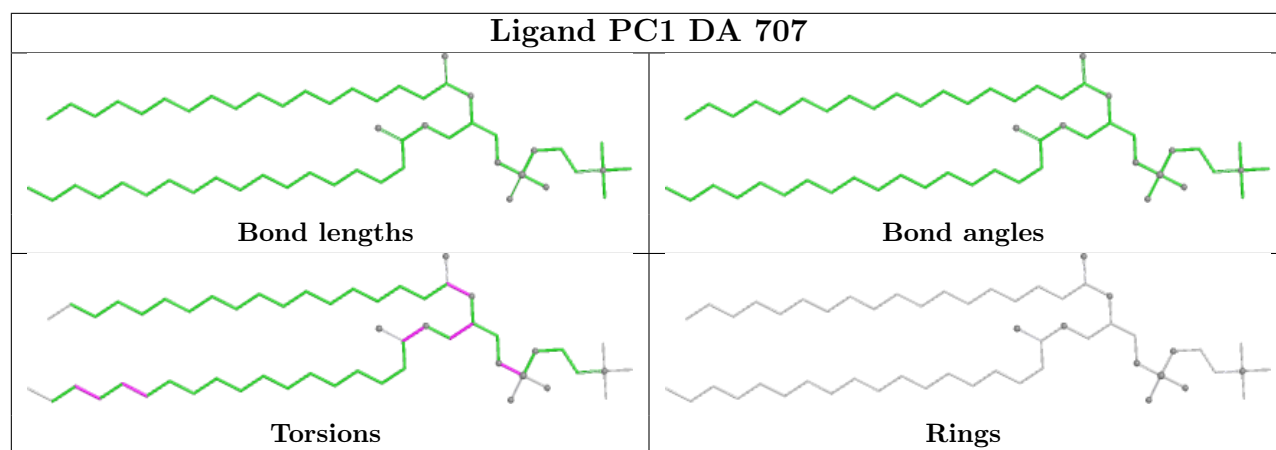
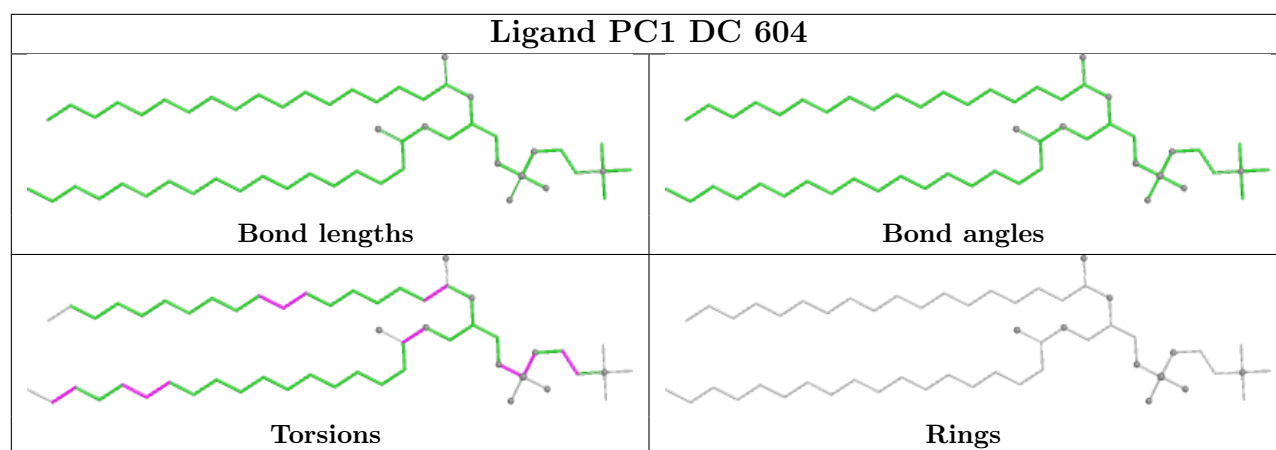


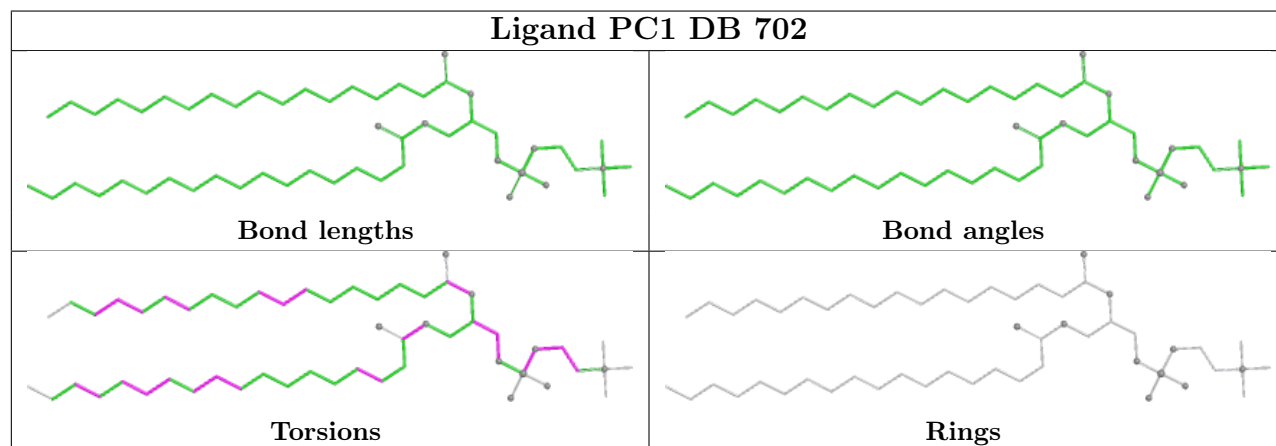
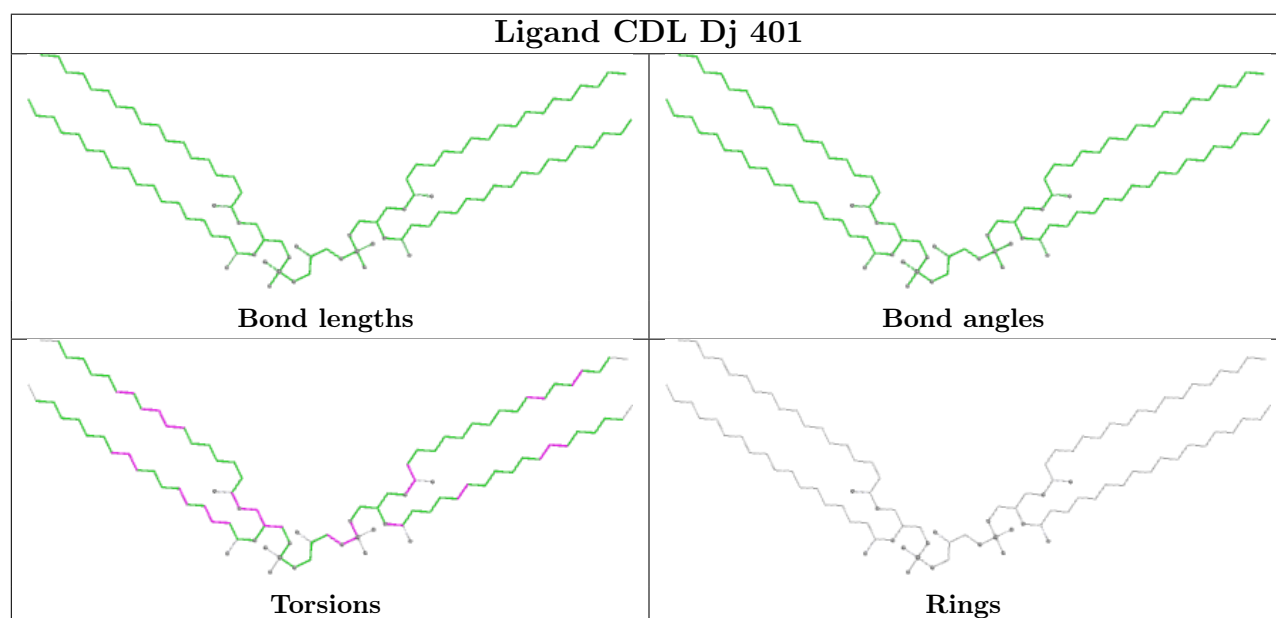
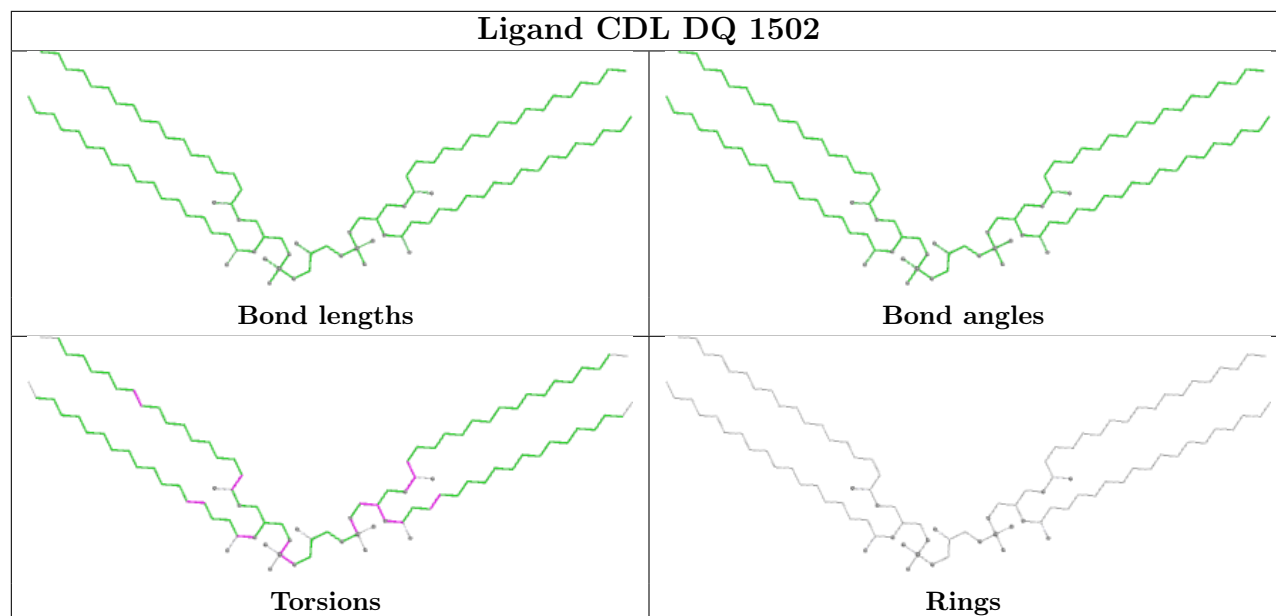


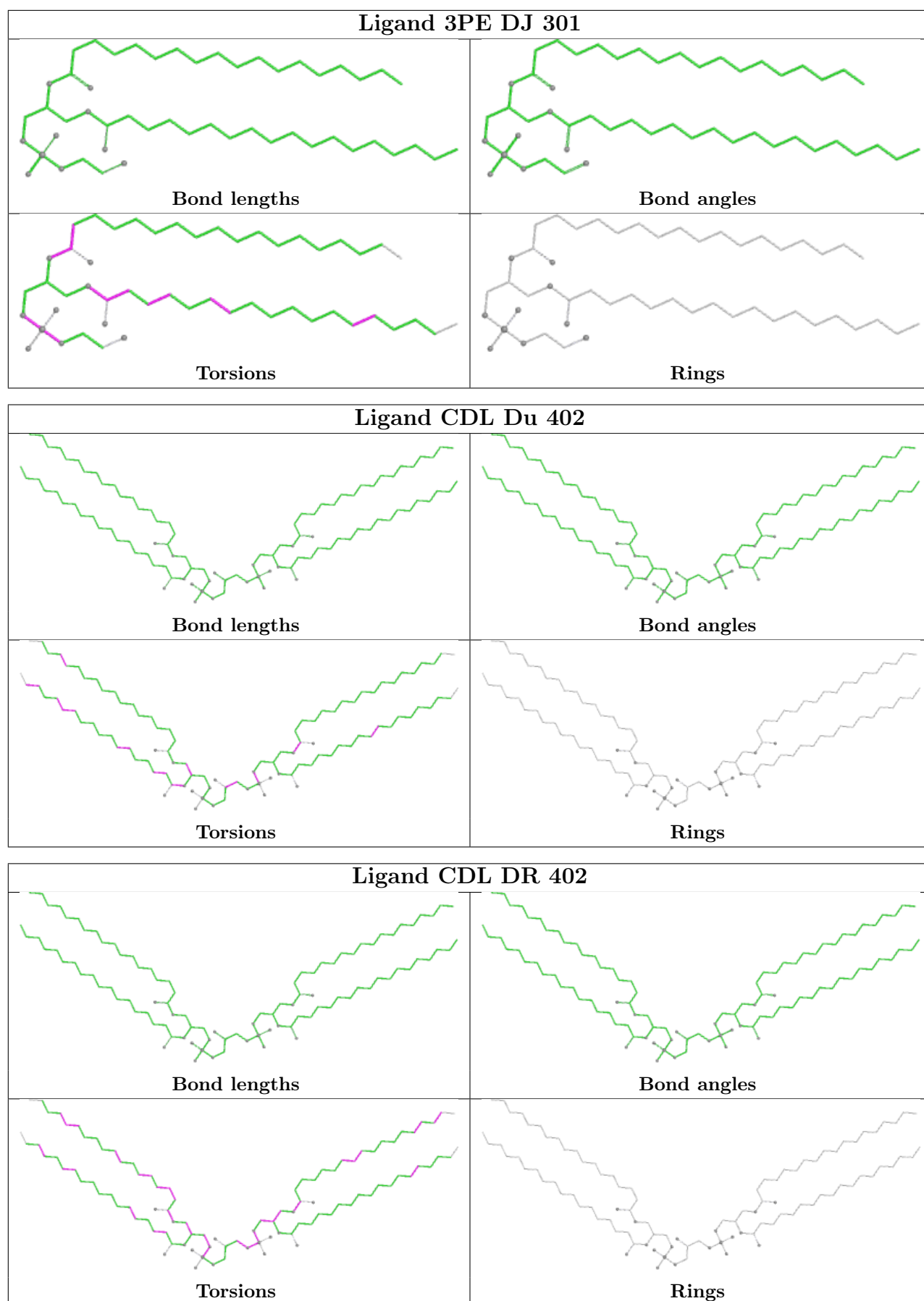


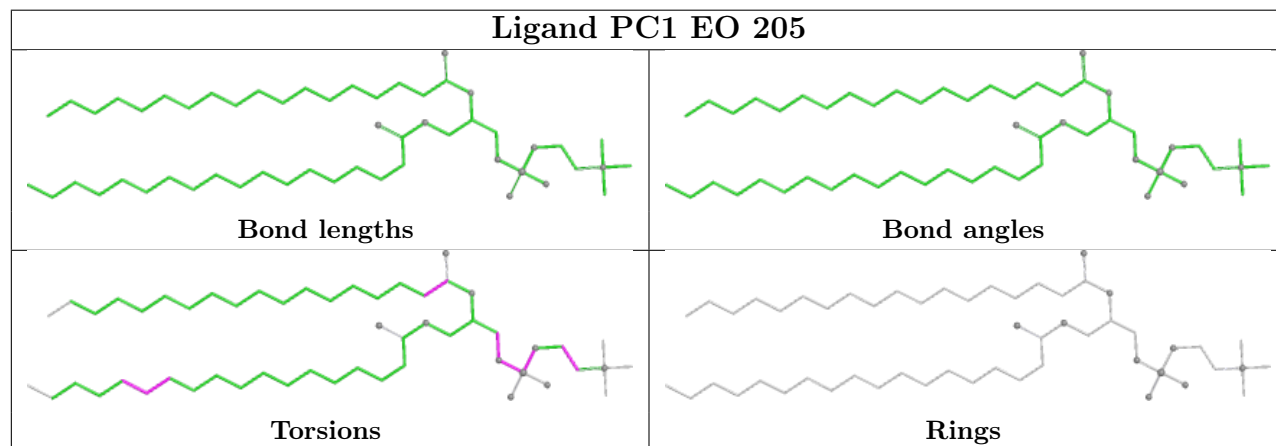
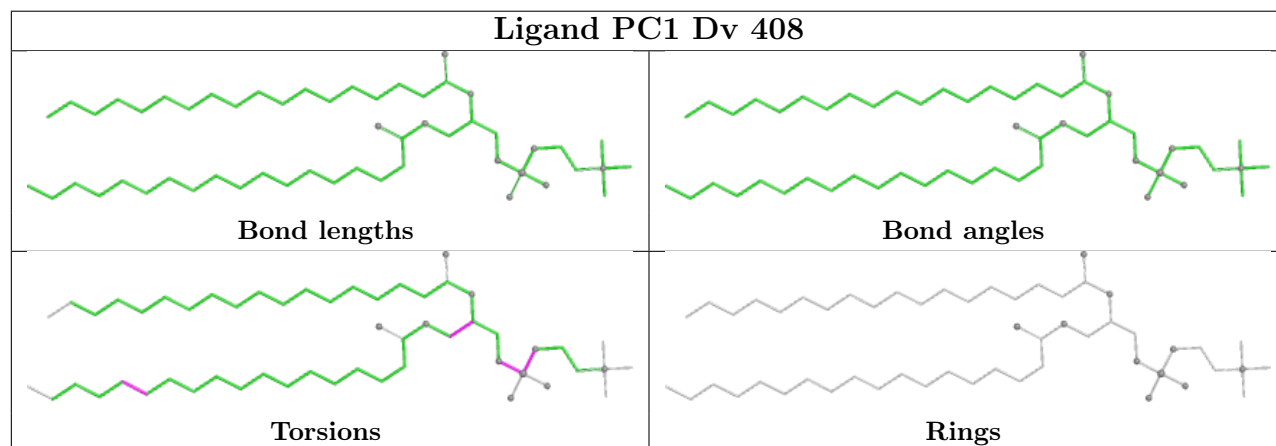
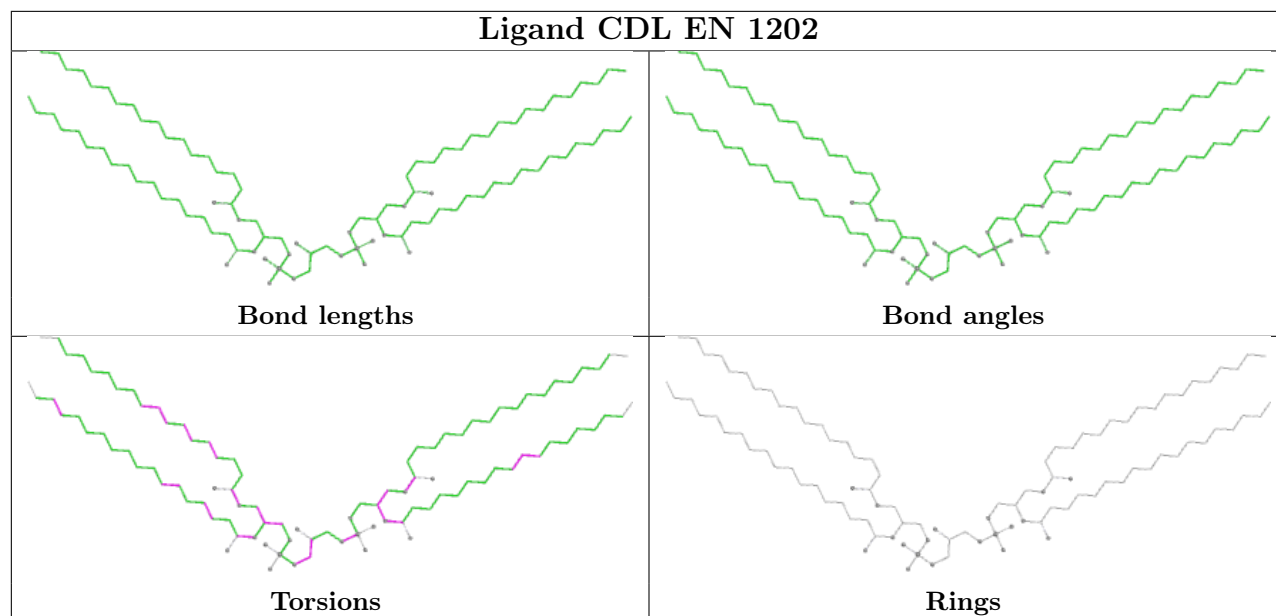


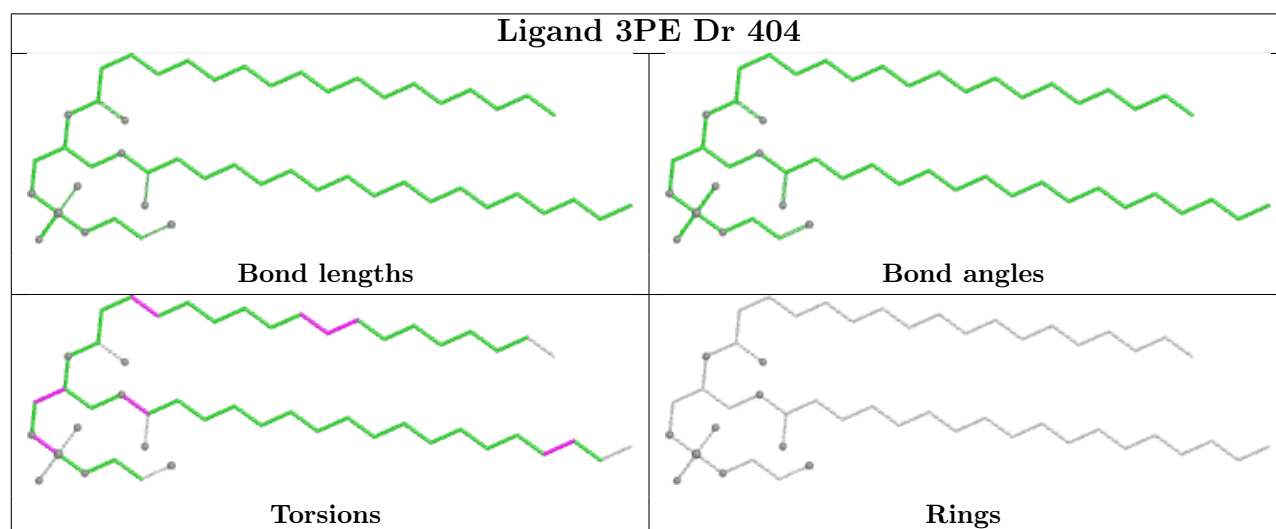
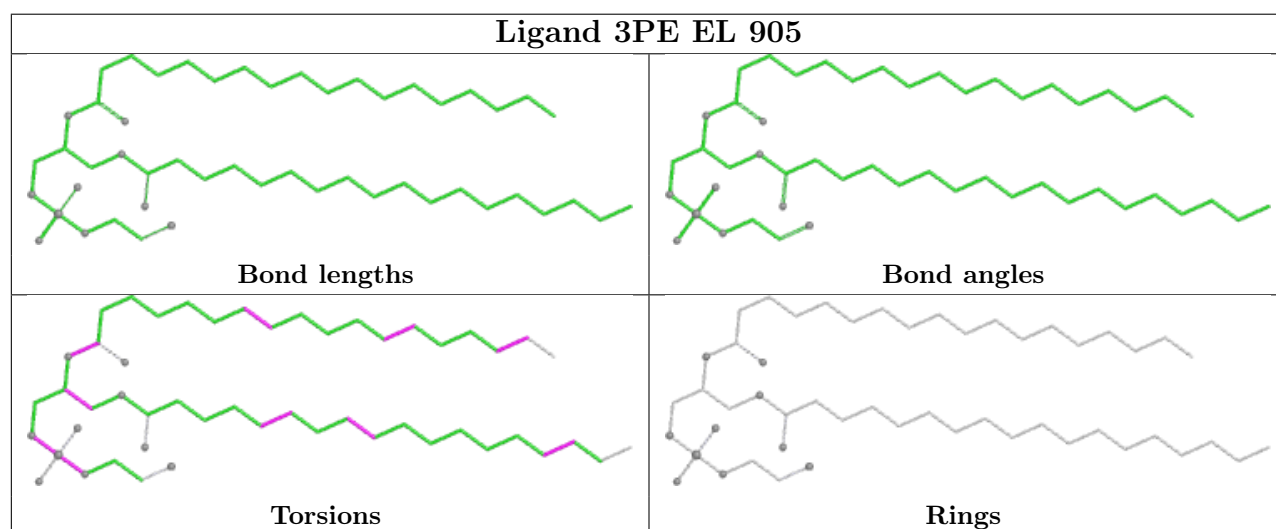
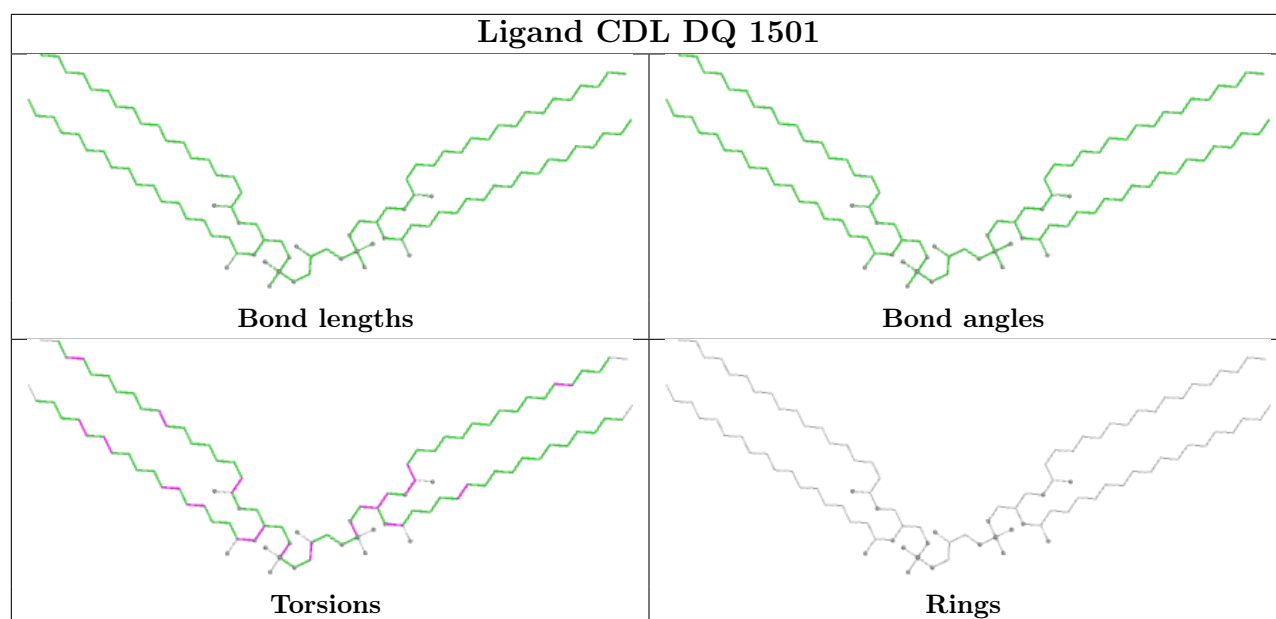


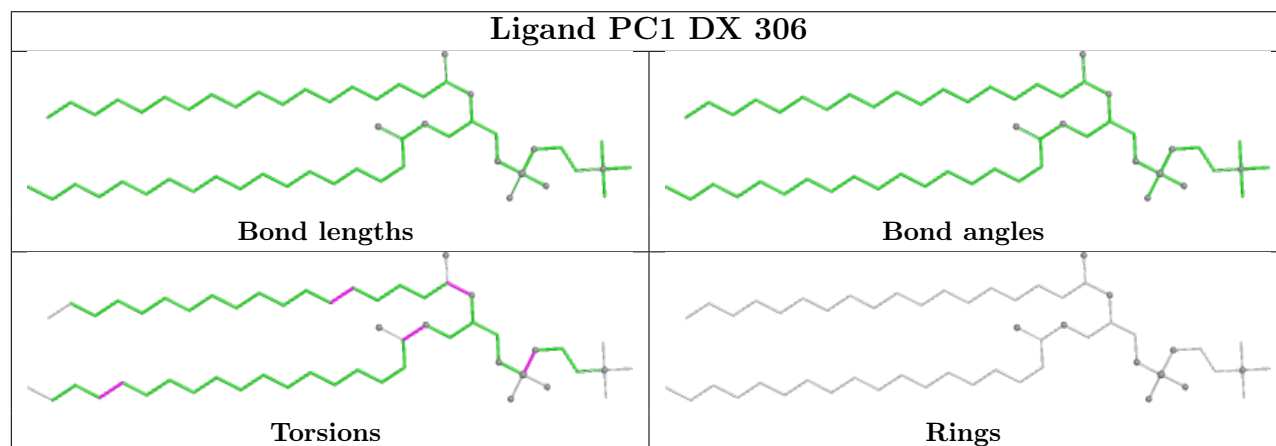
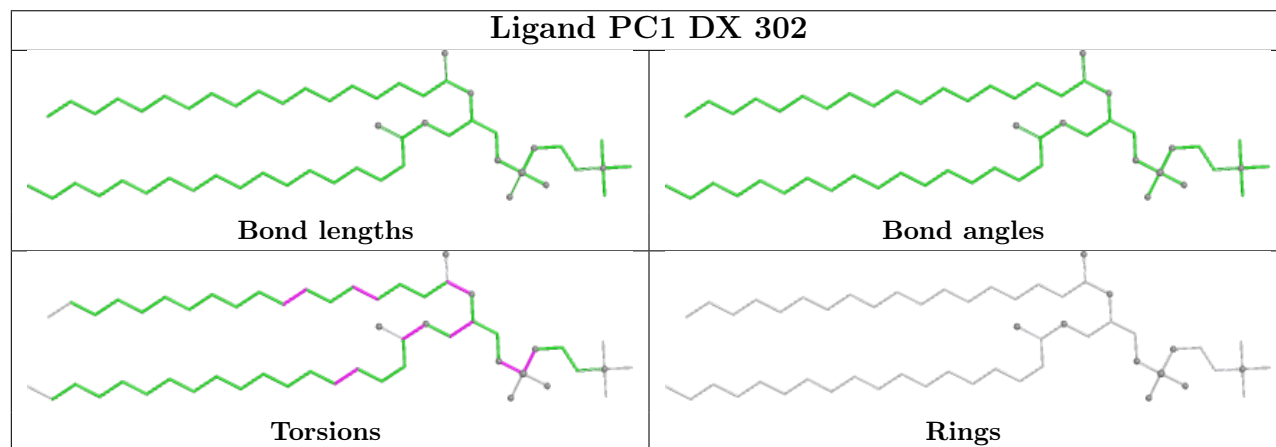
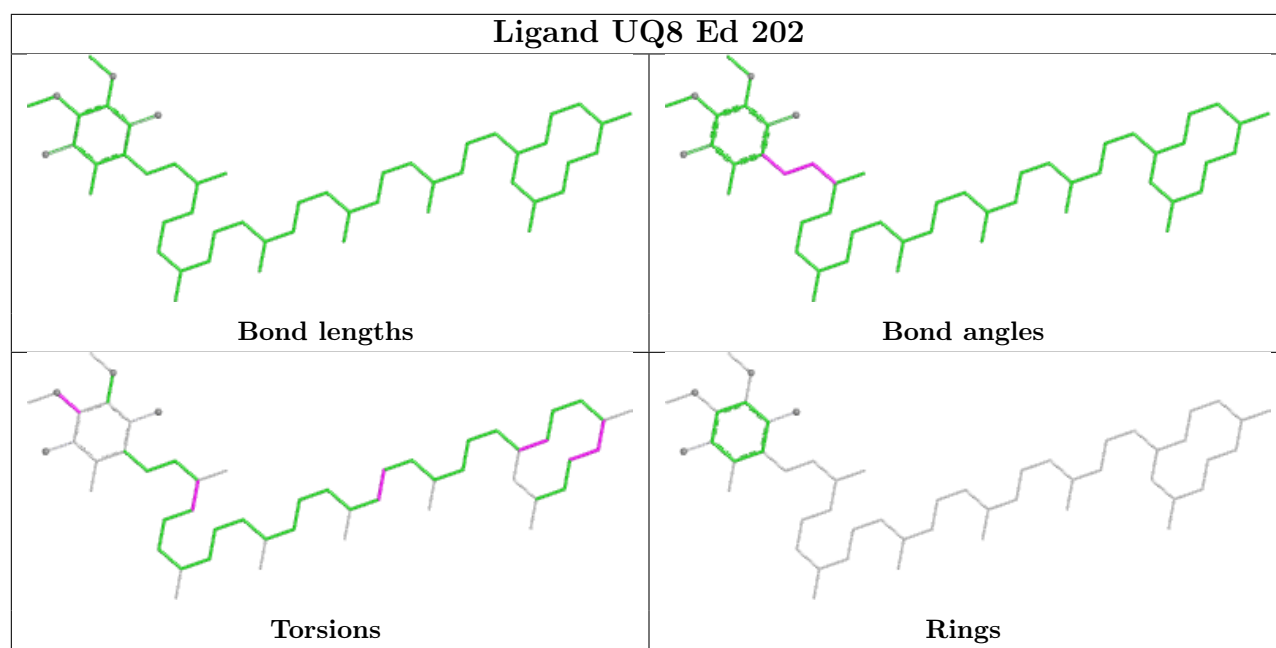


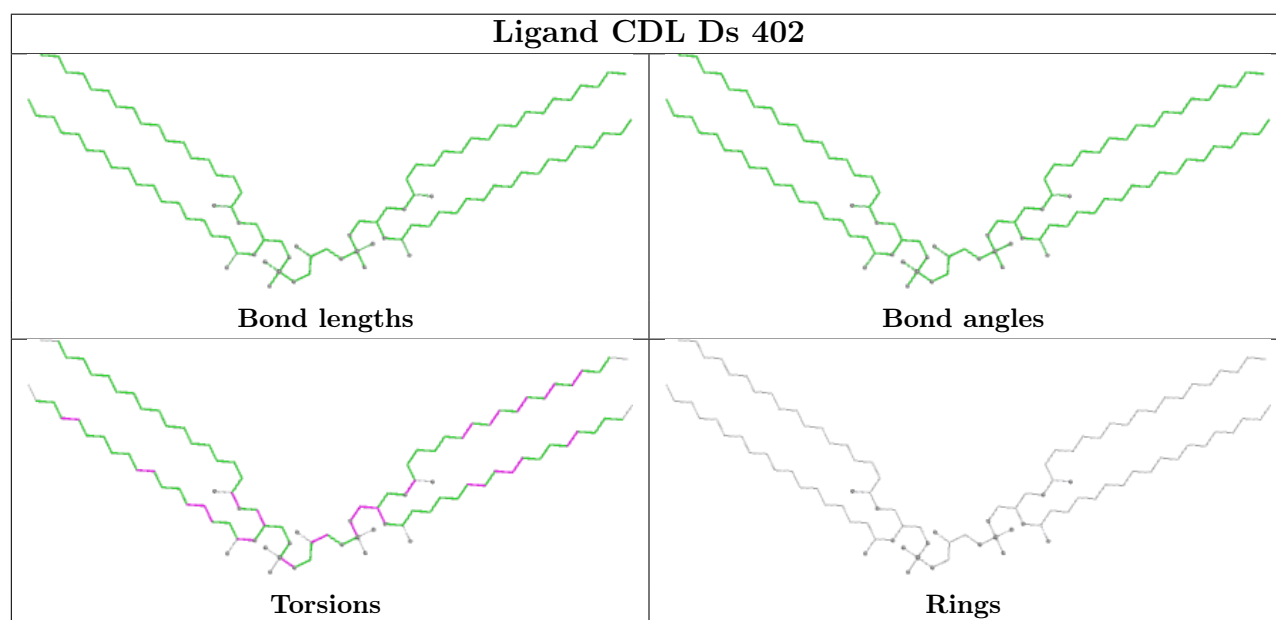
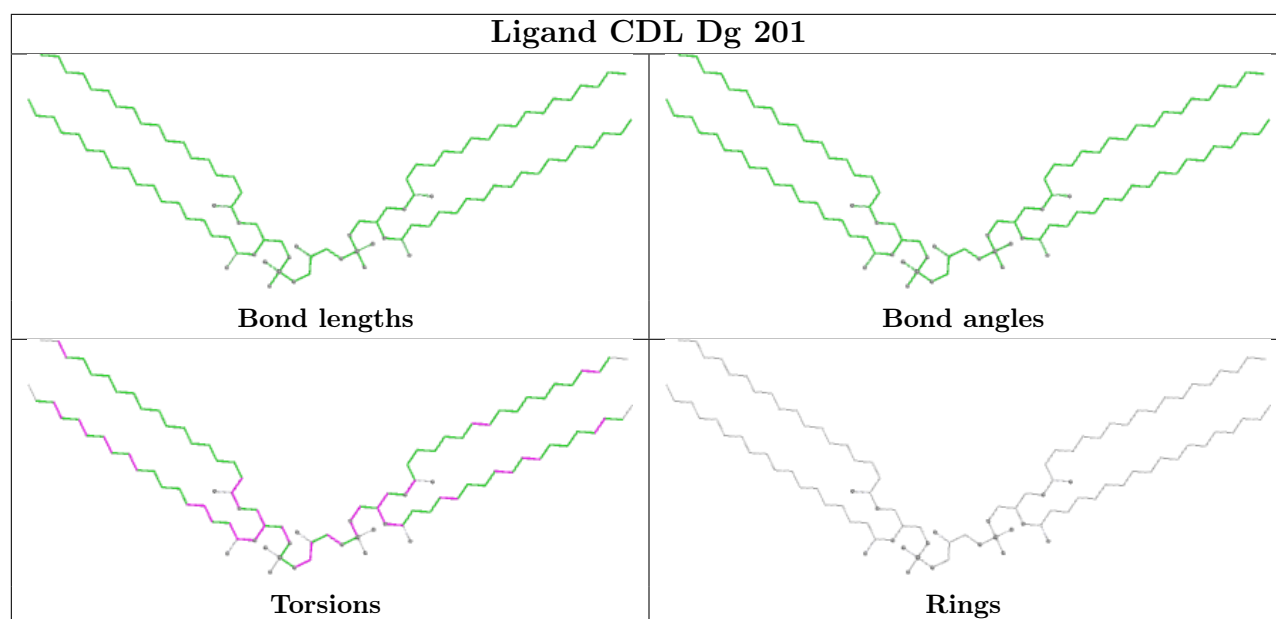


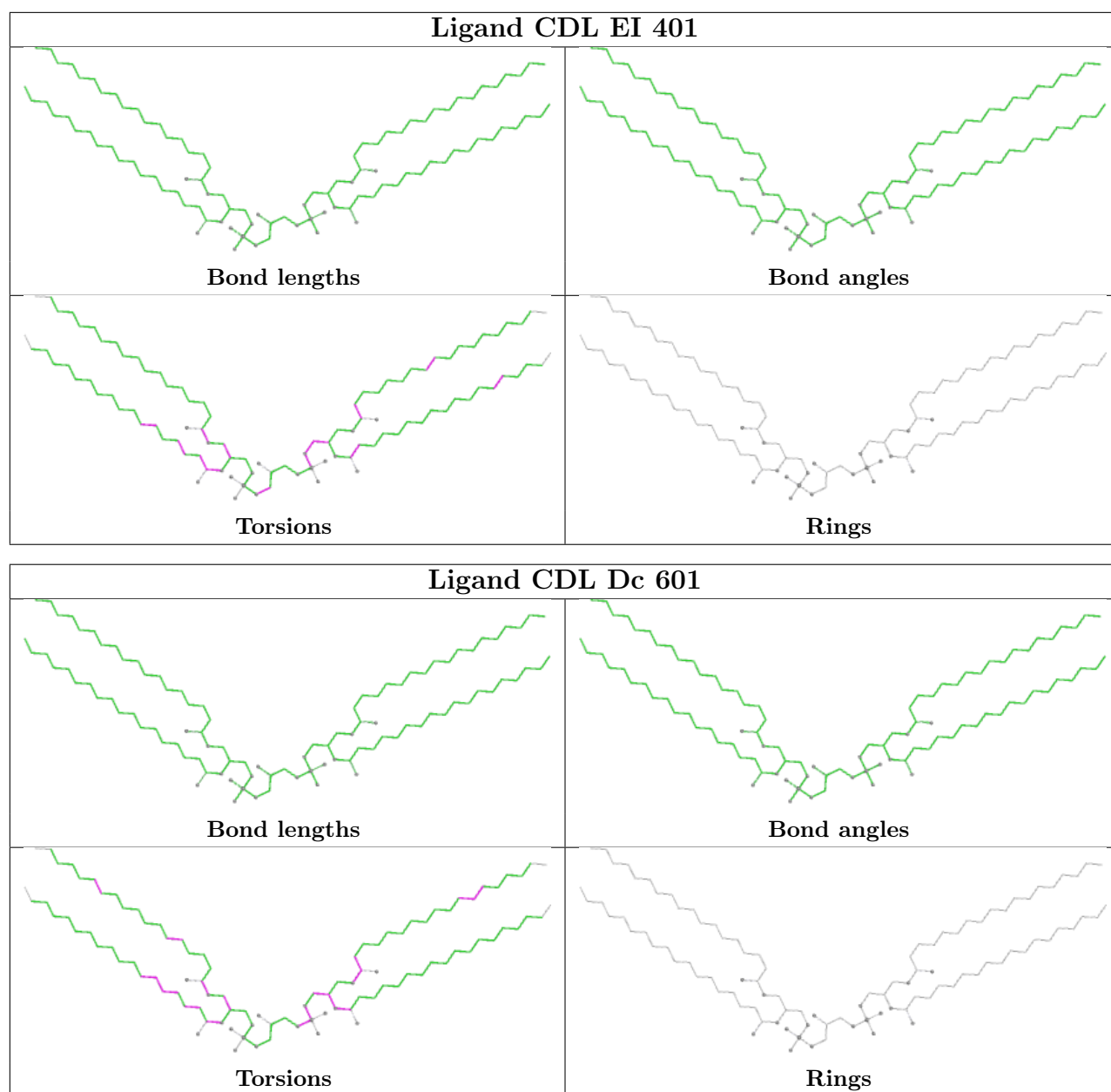


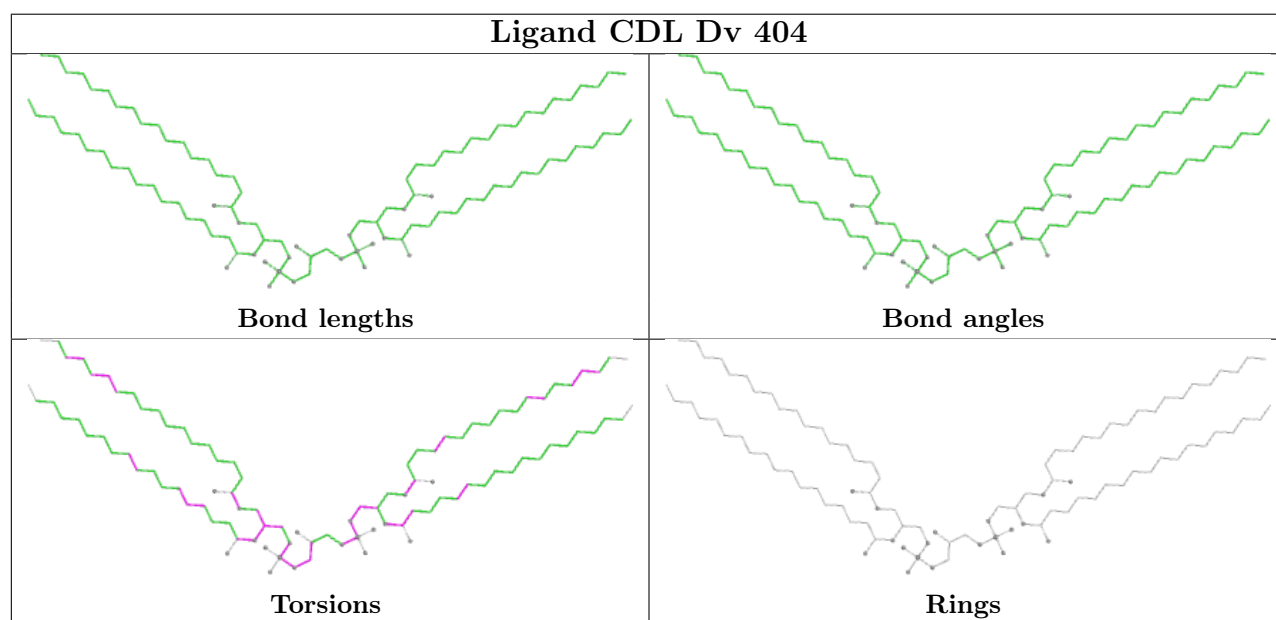
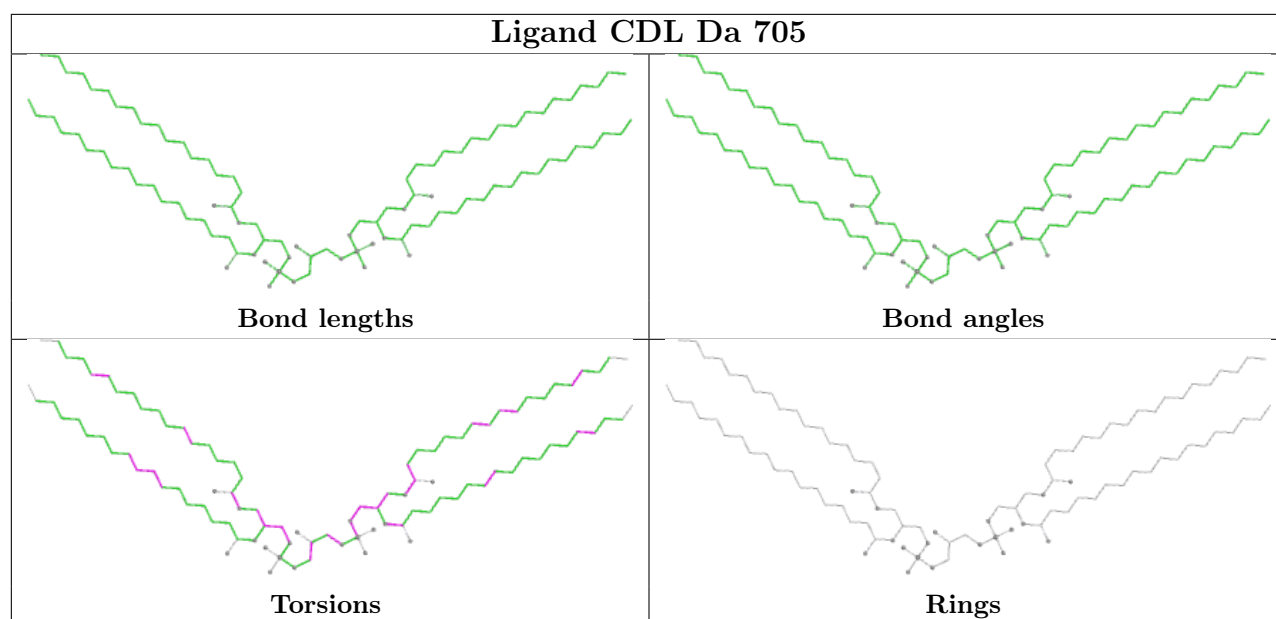


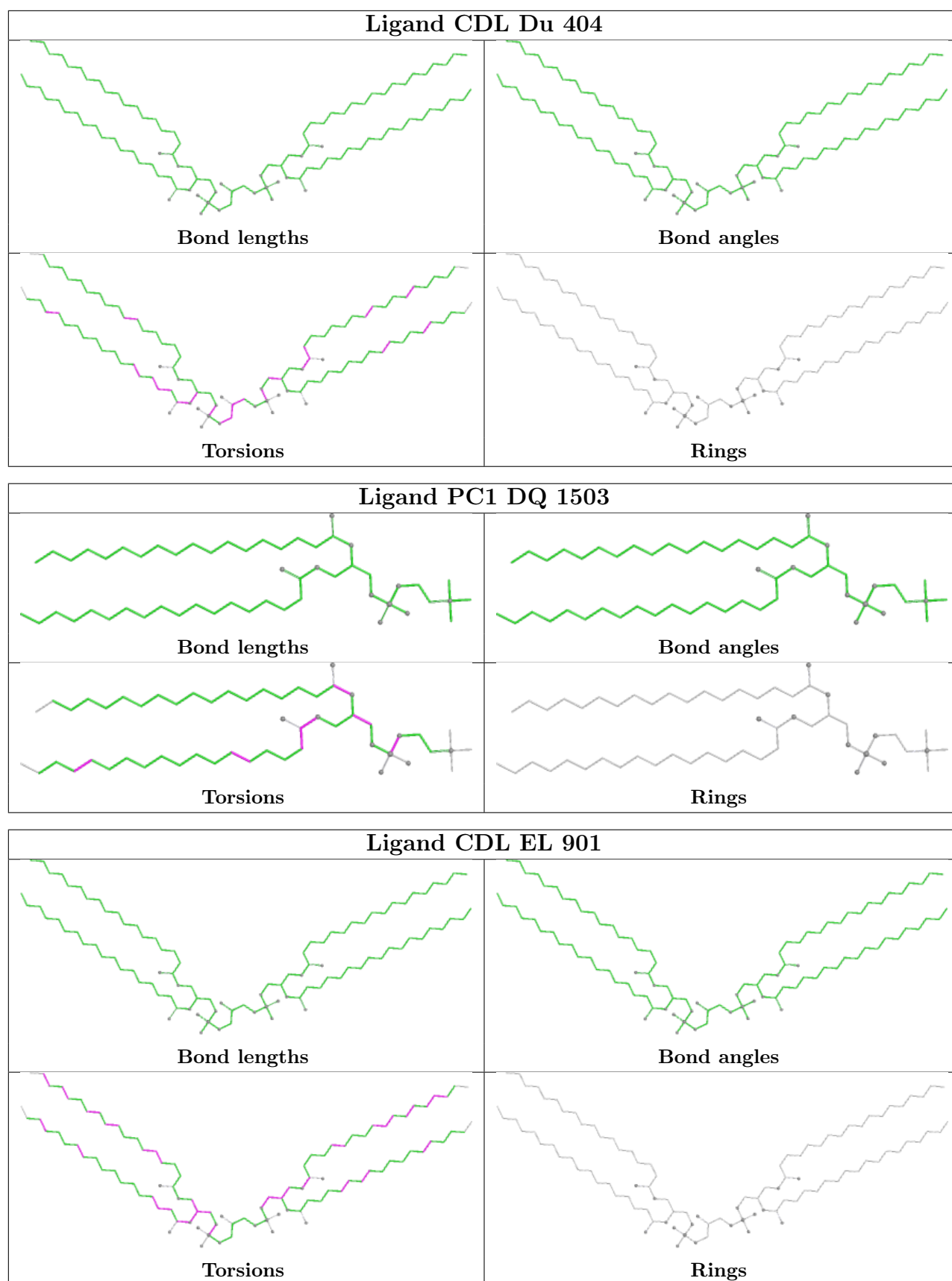


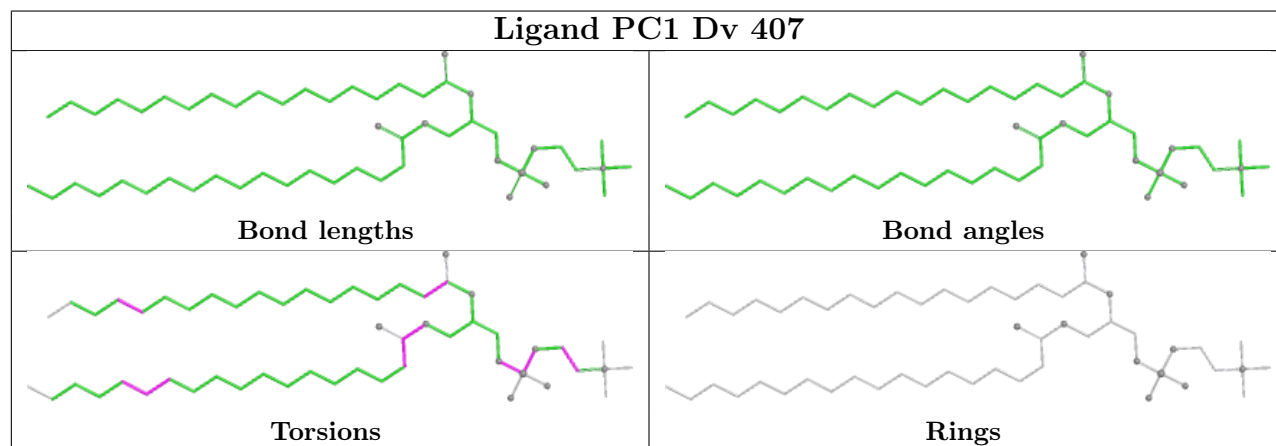
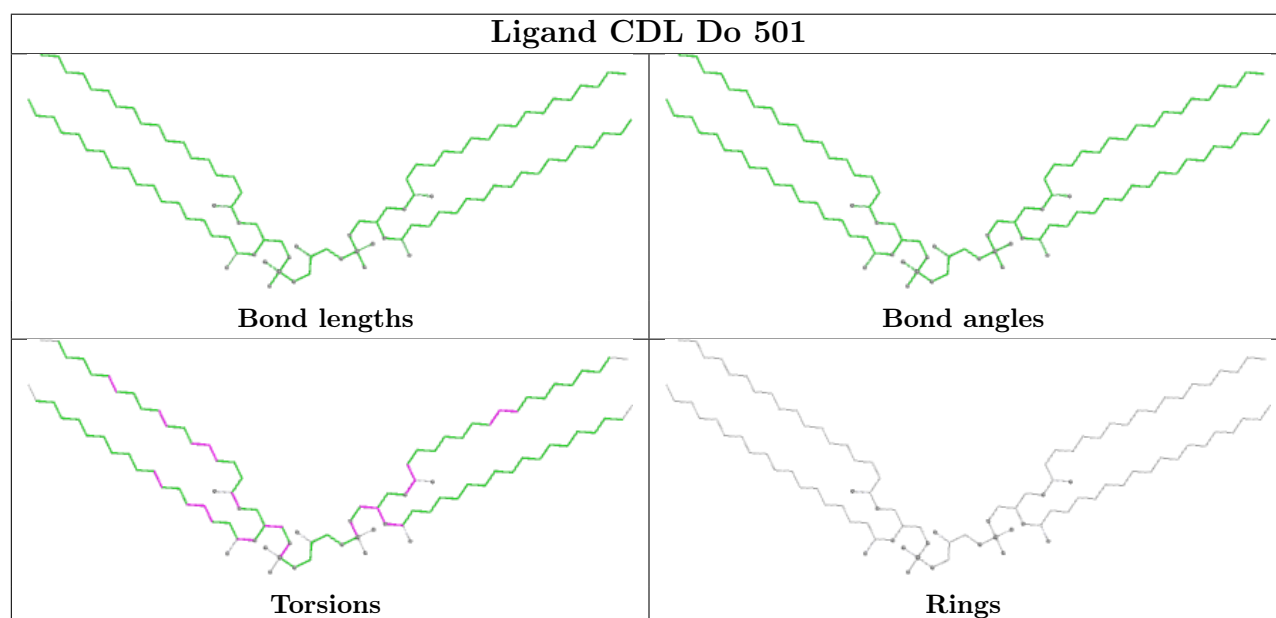
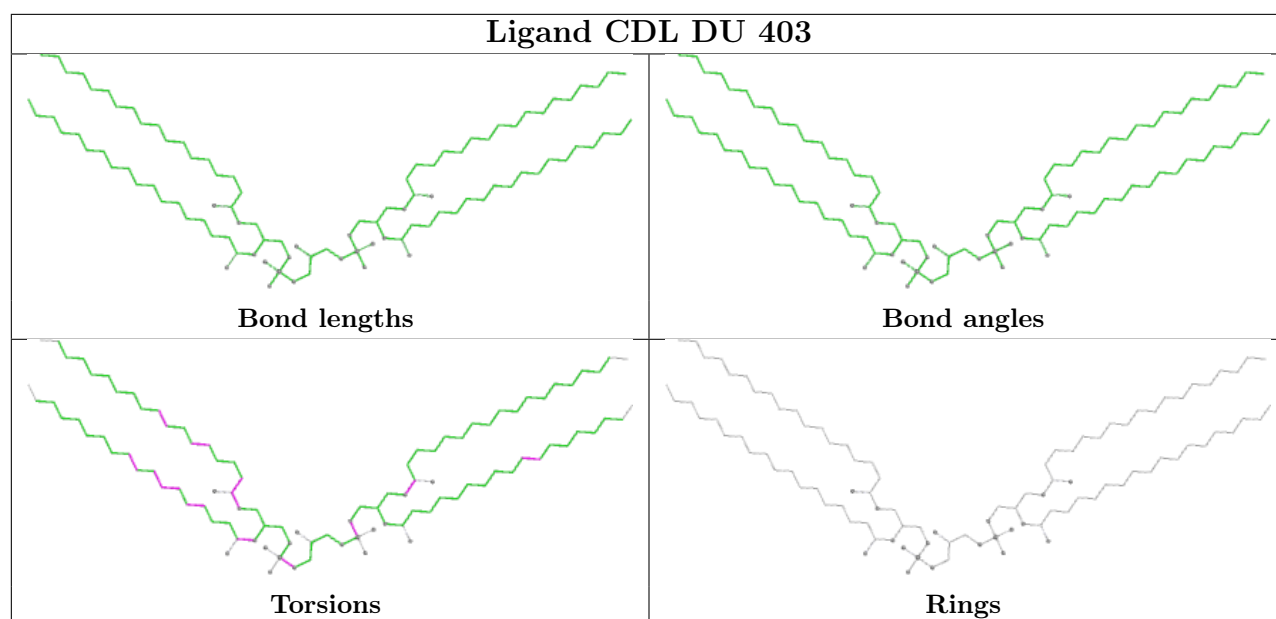


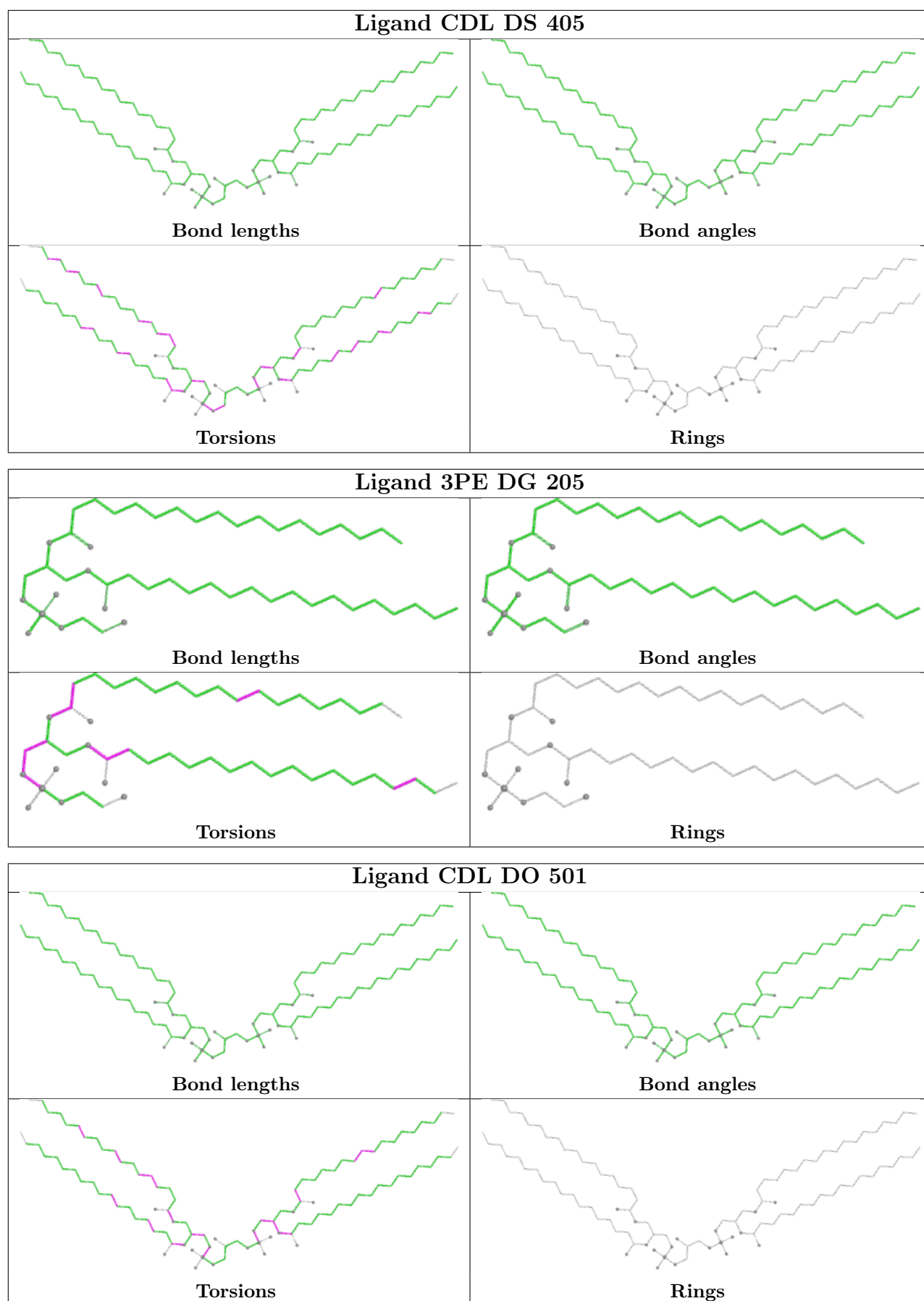




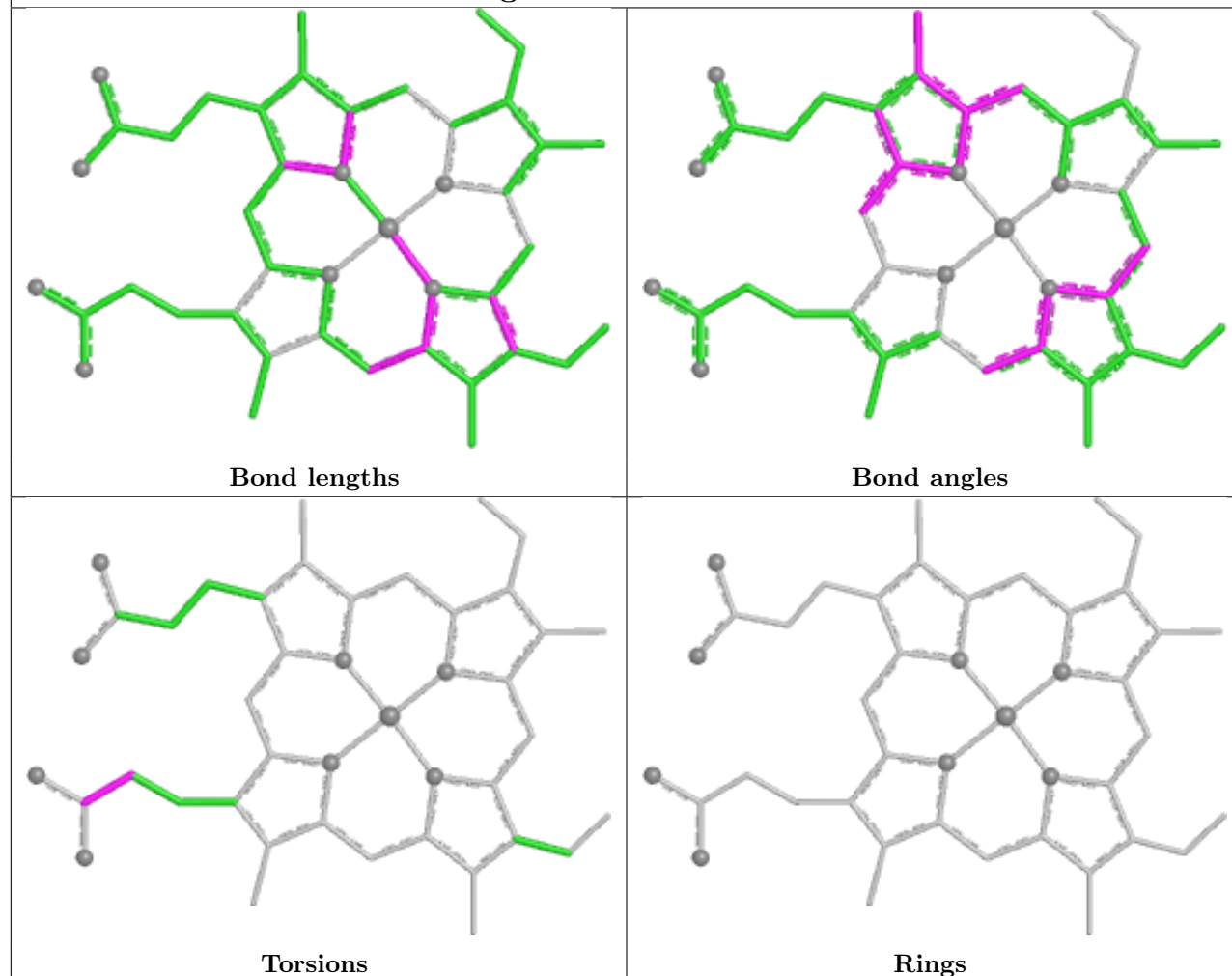




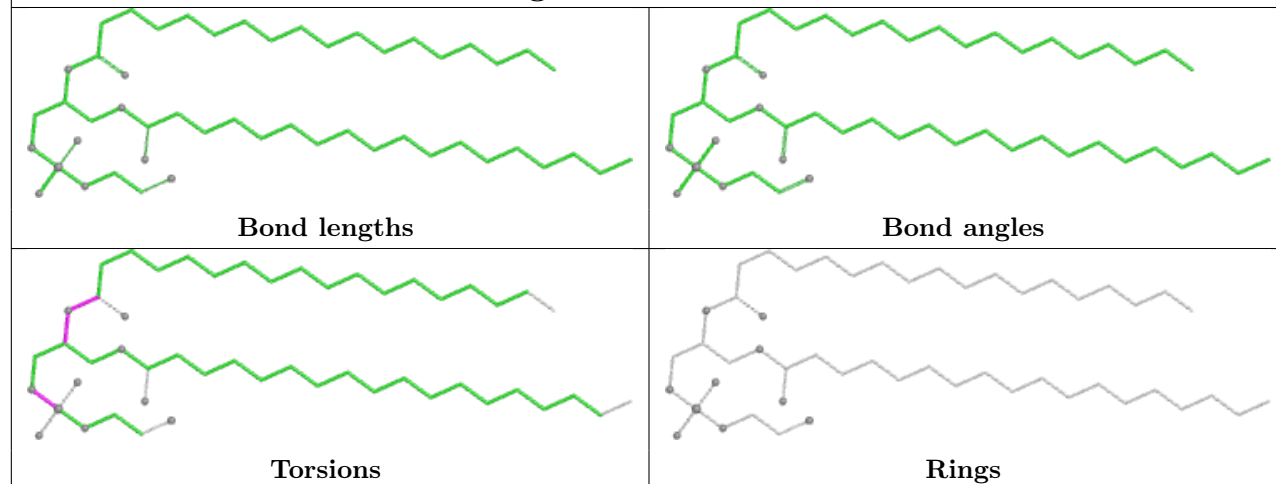


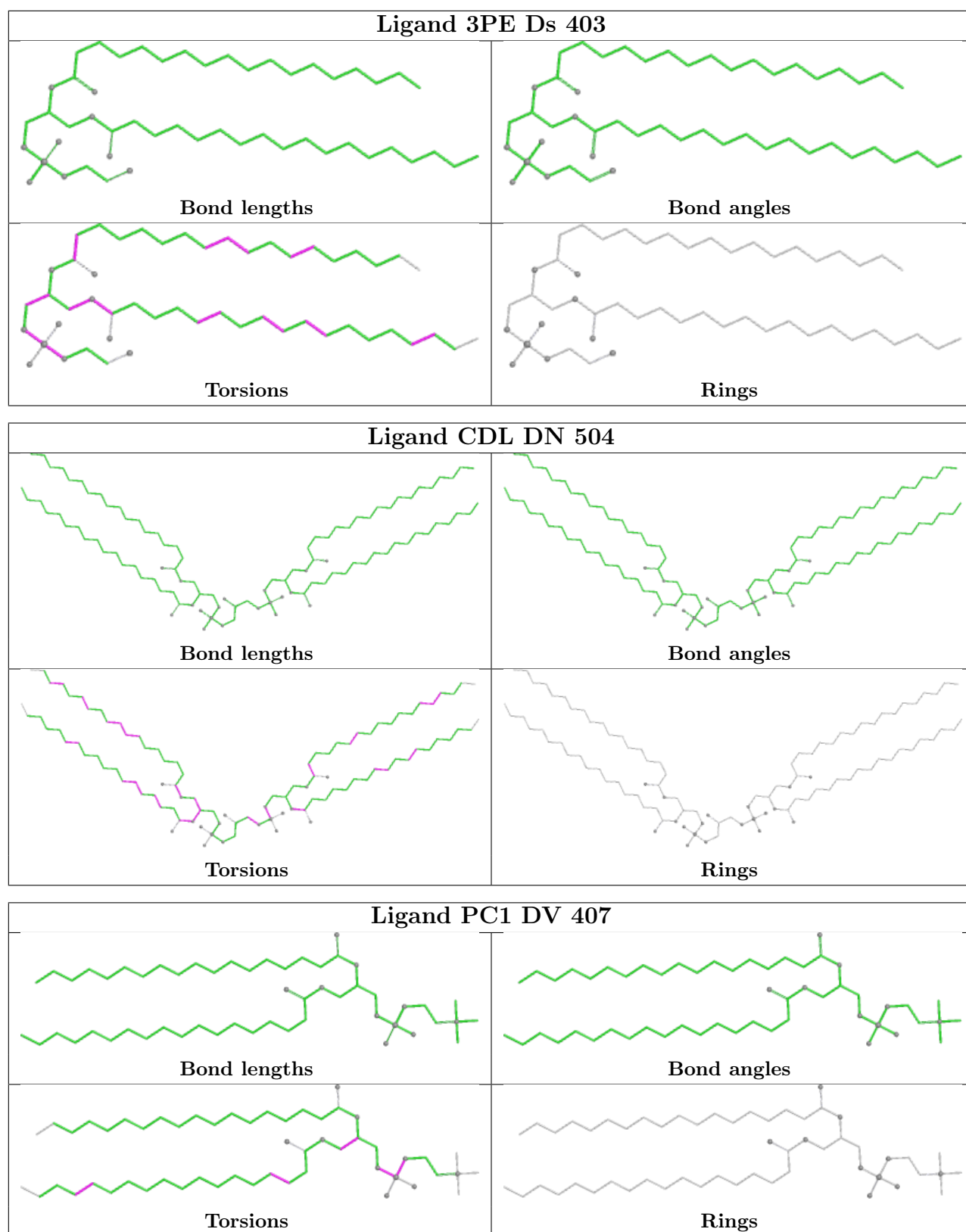


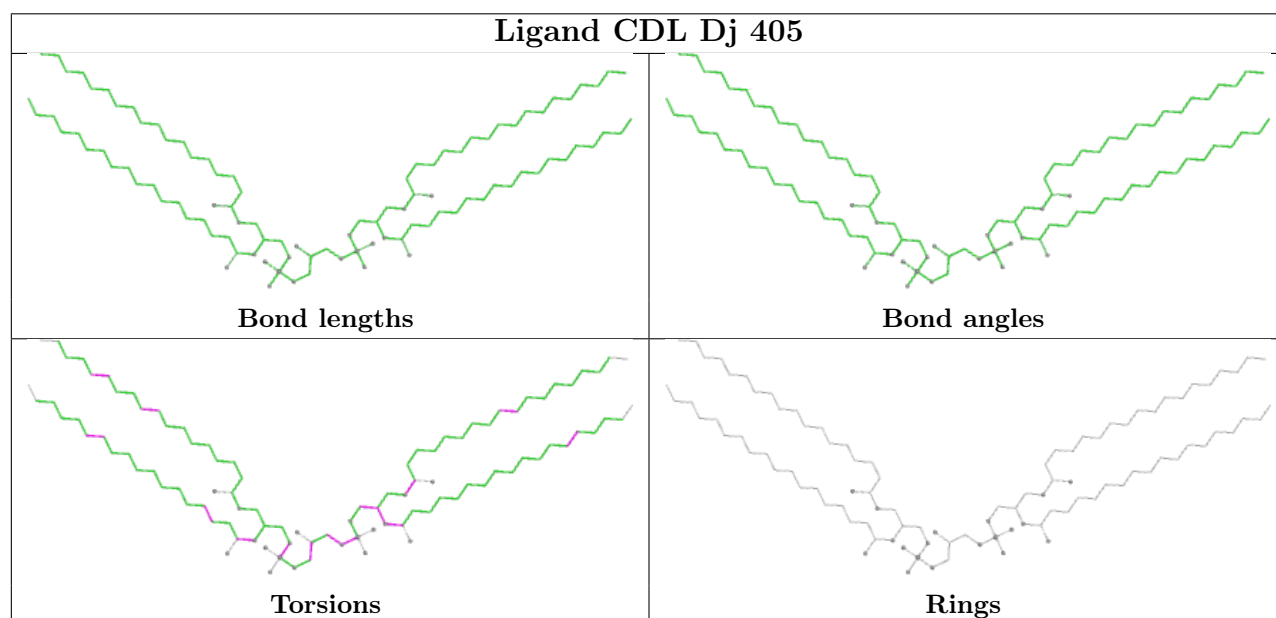
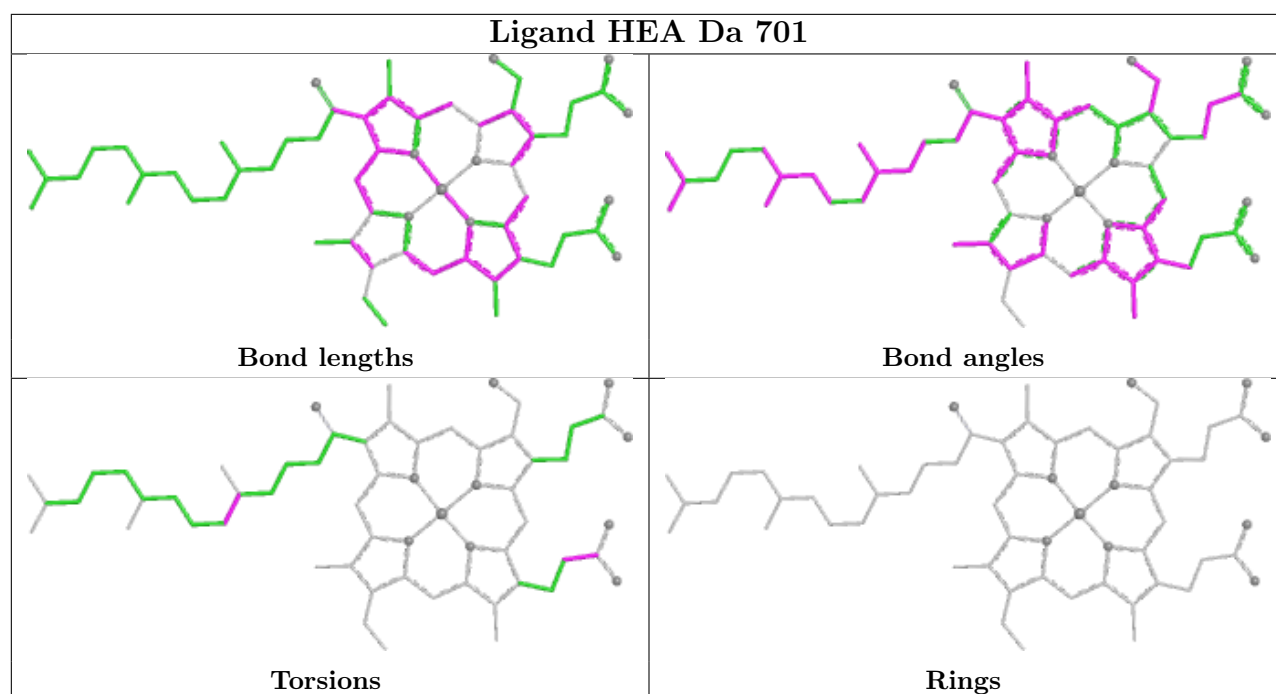
Ligand HEM Ed 201

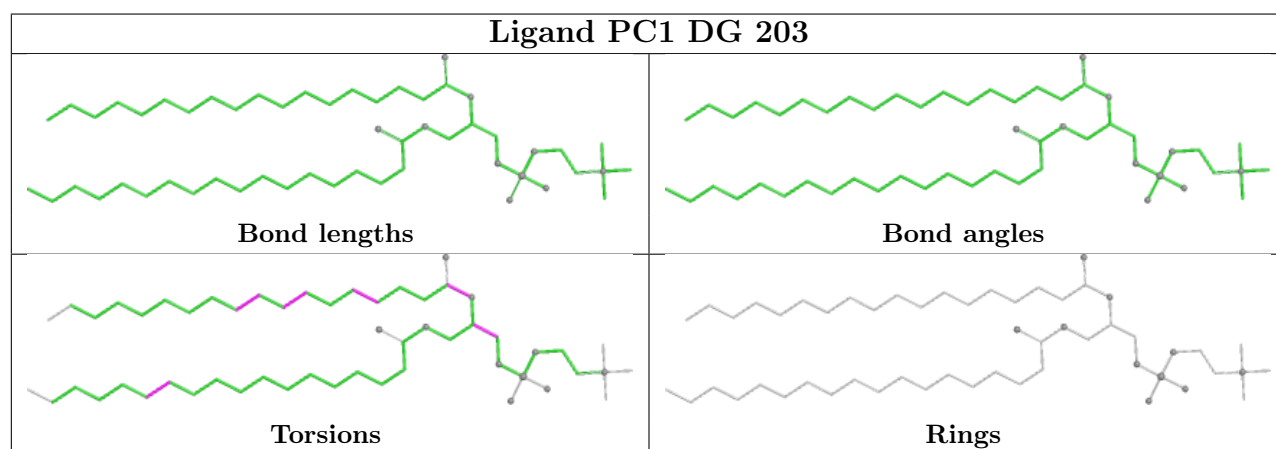
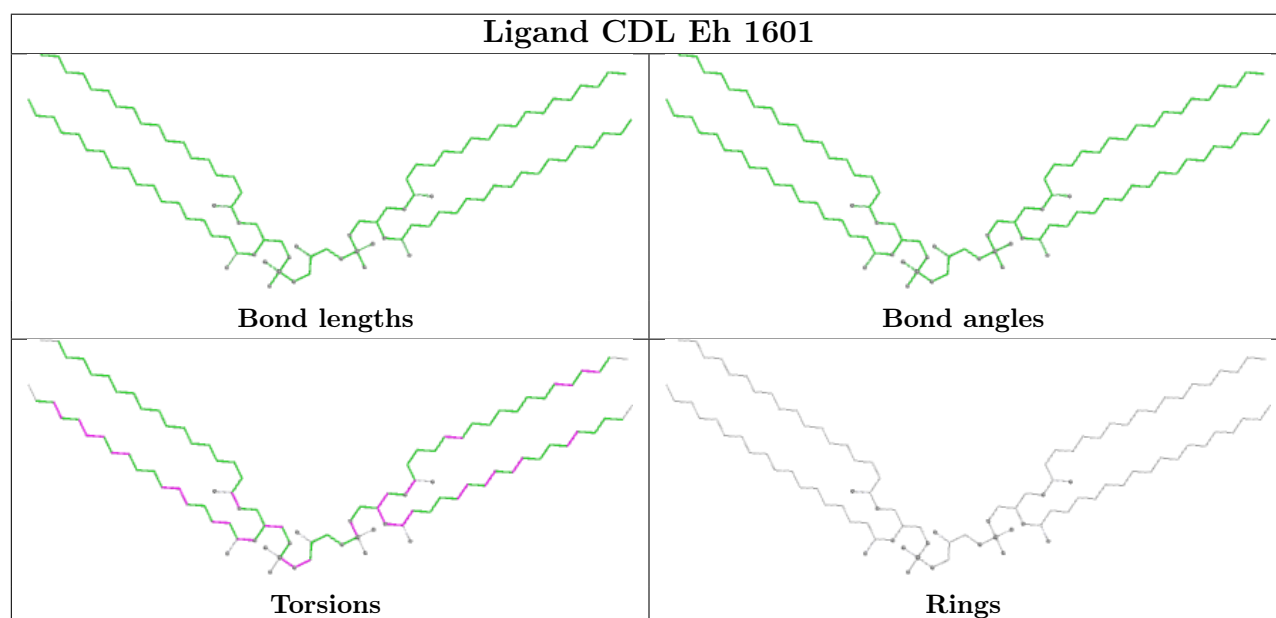
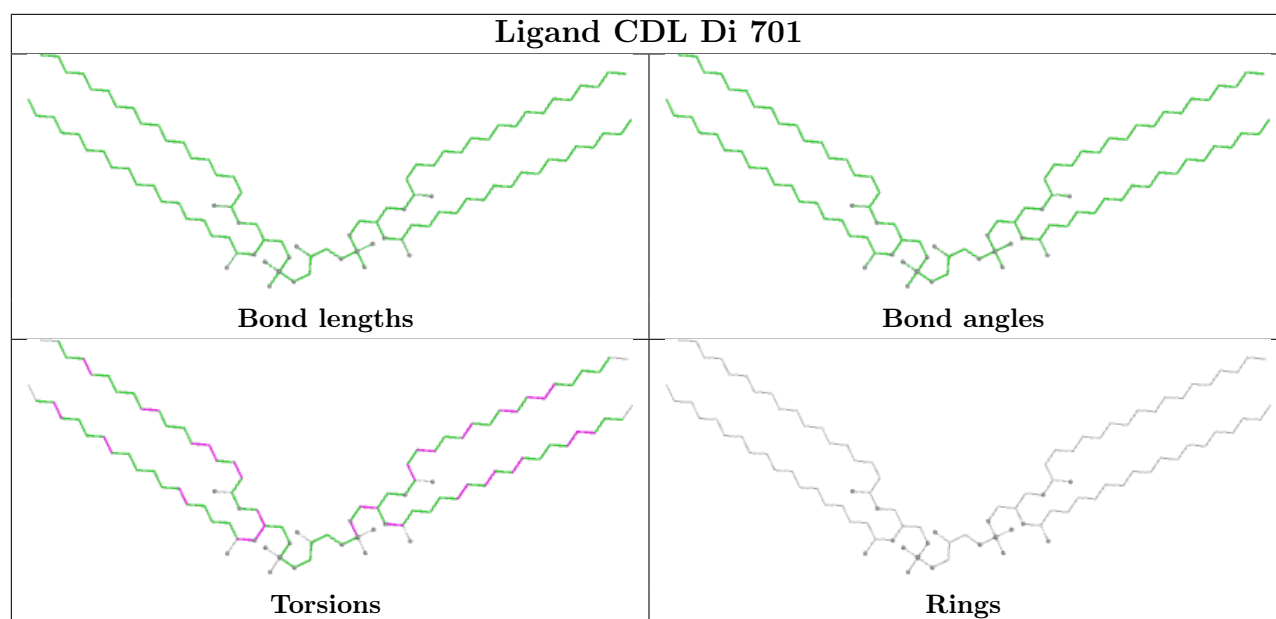


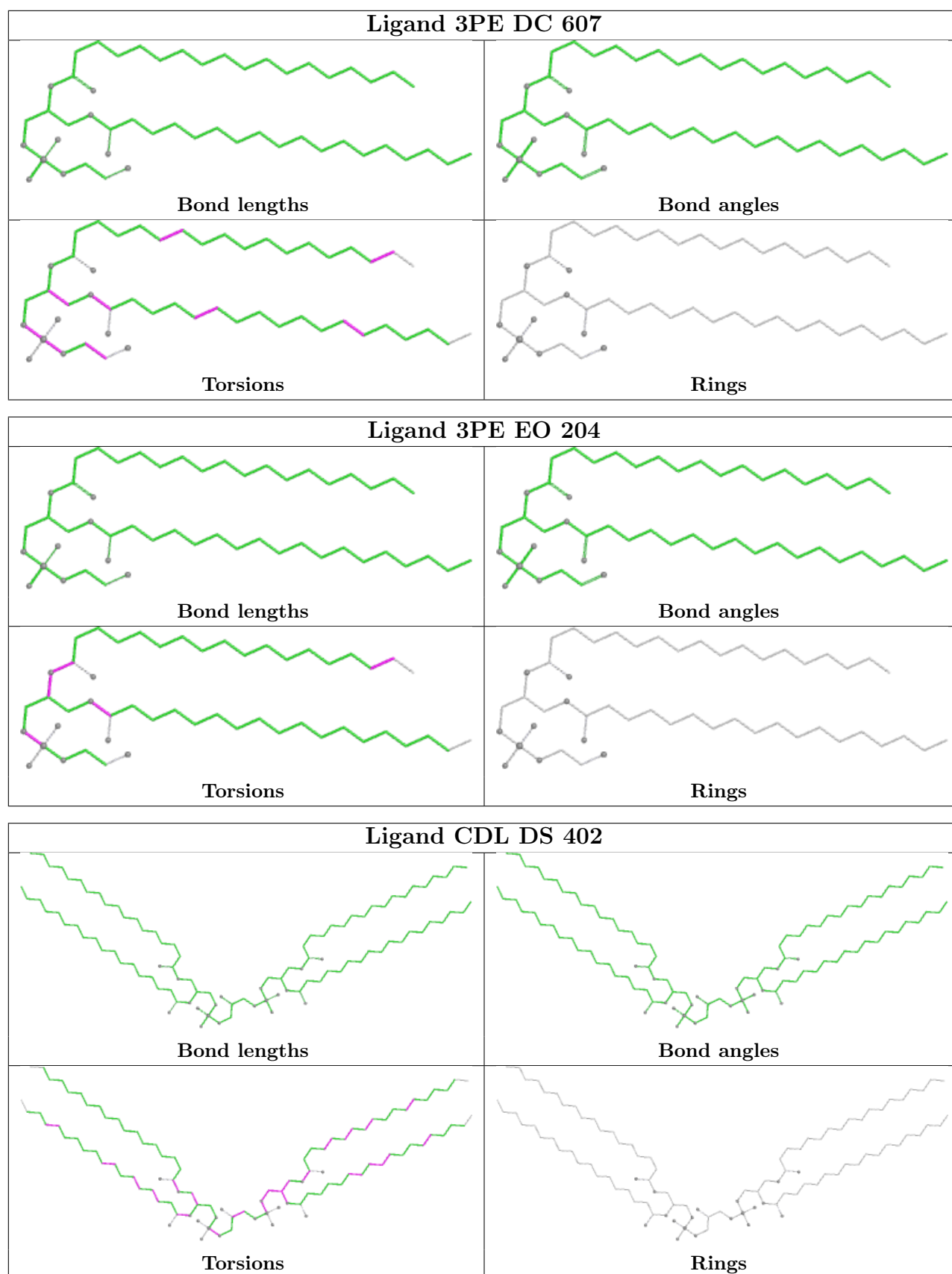
Ligand 3PE Eo 203

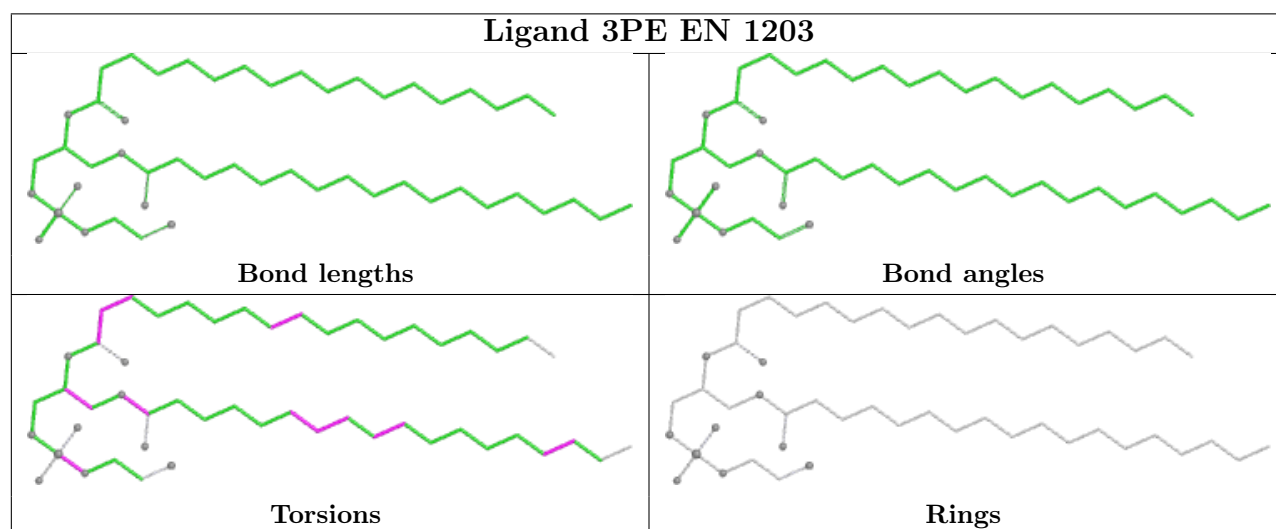
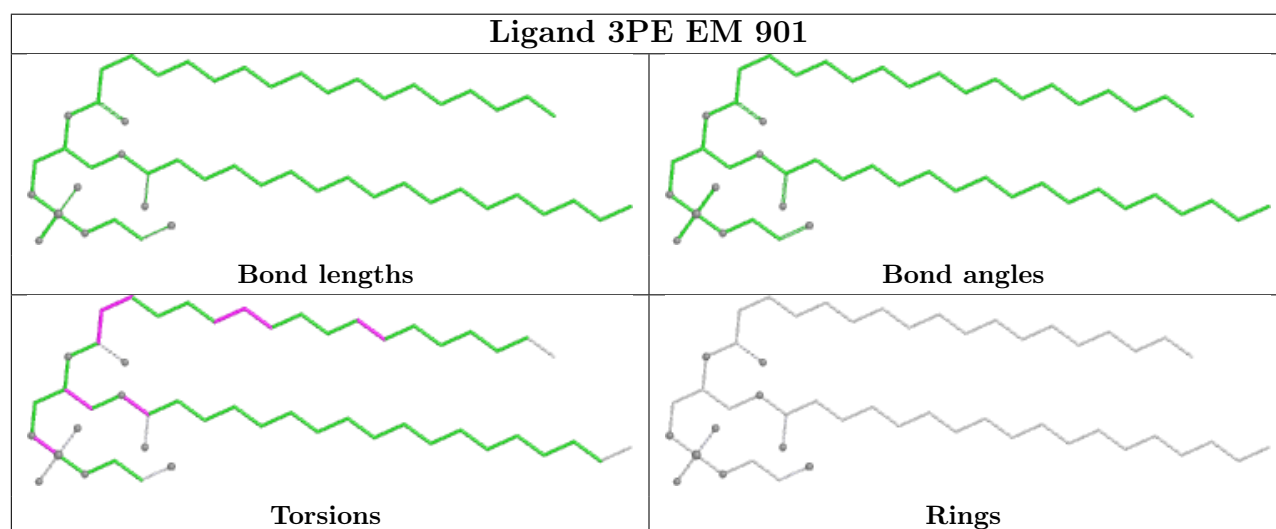
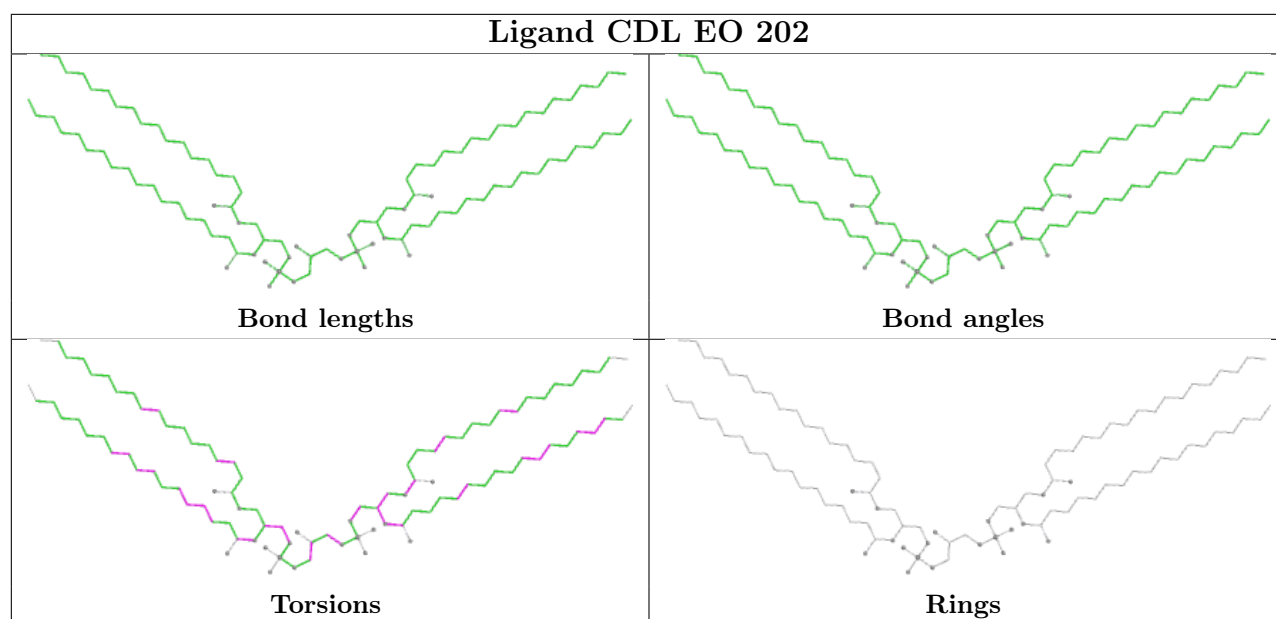


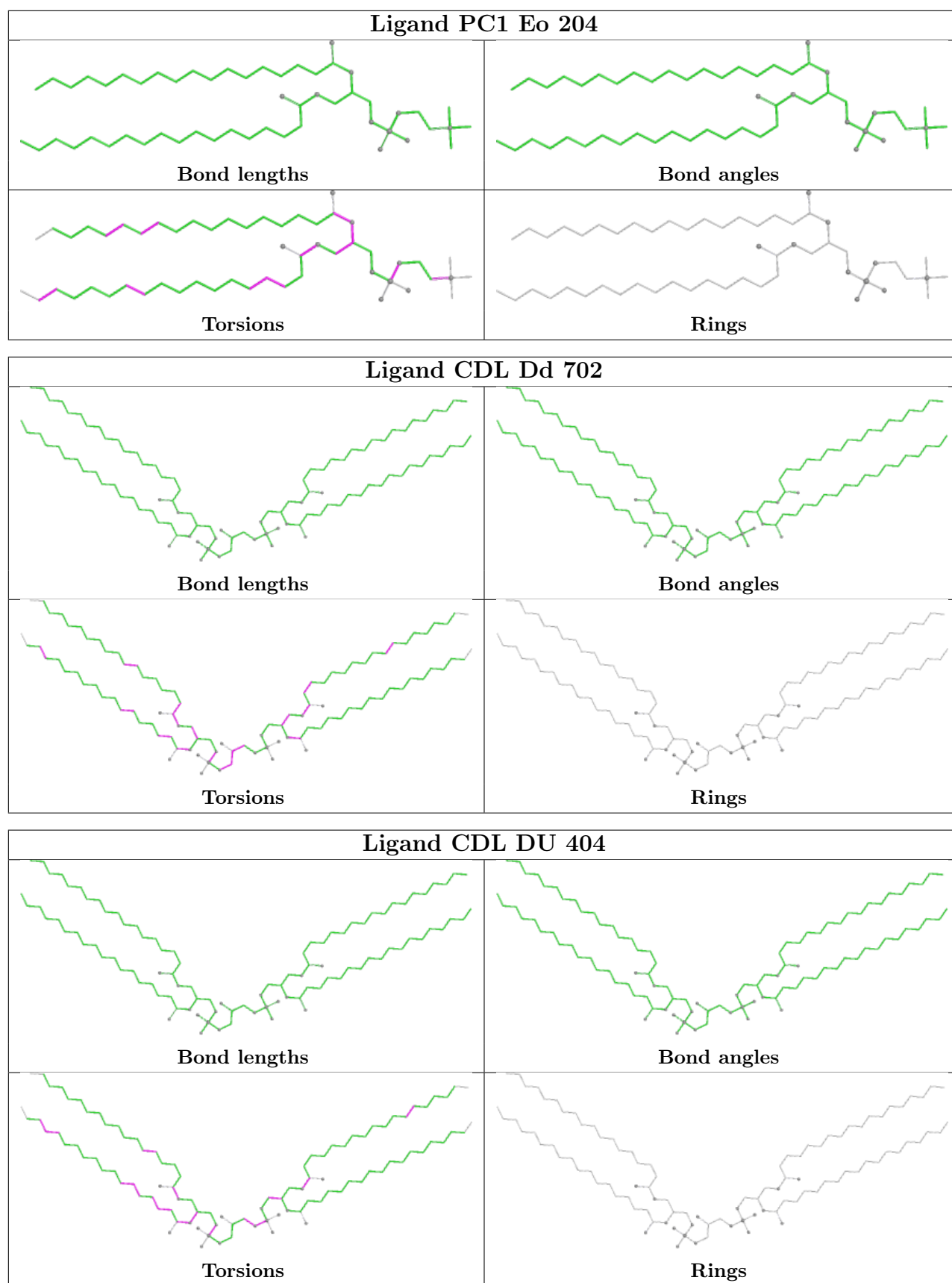


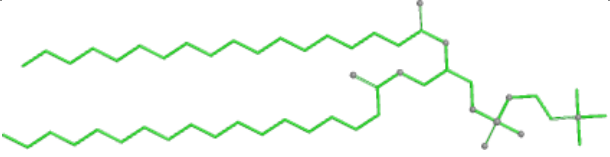
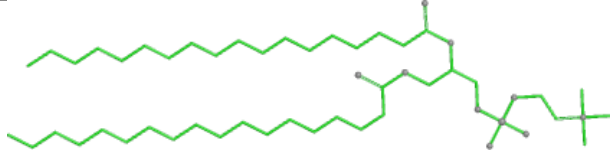
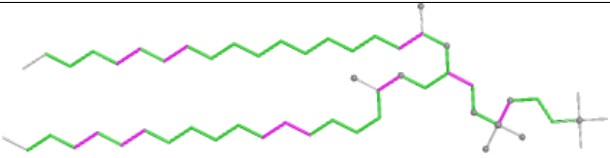
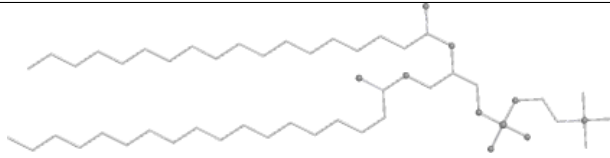



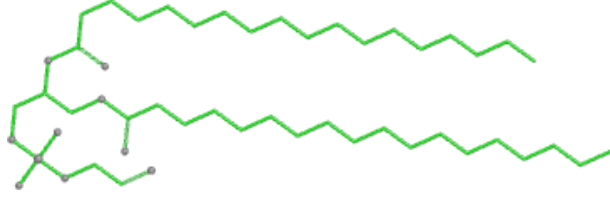

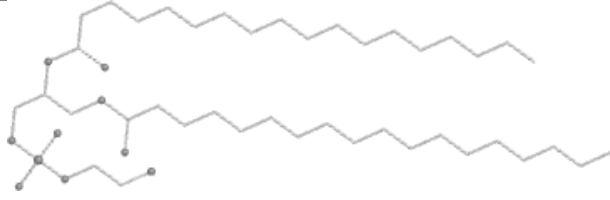


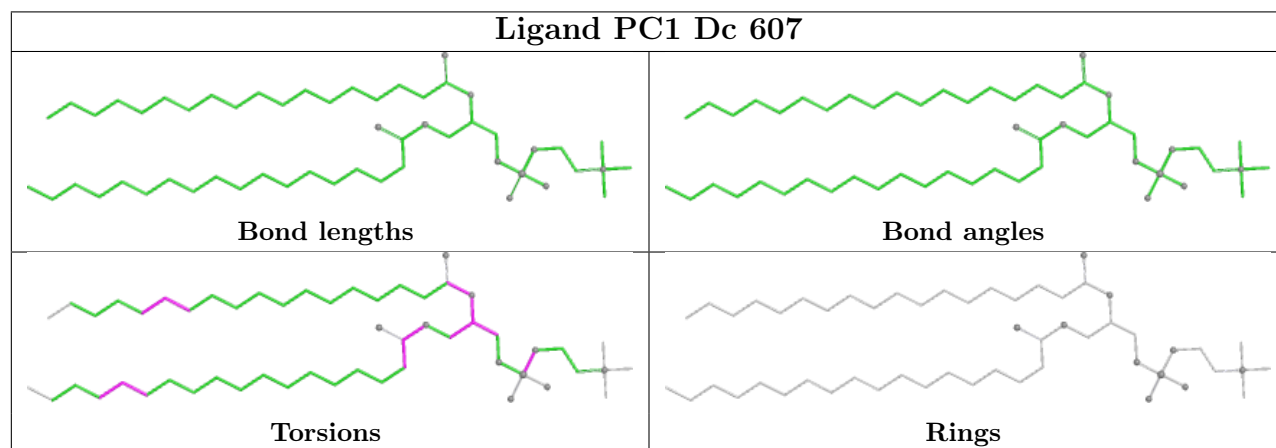
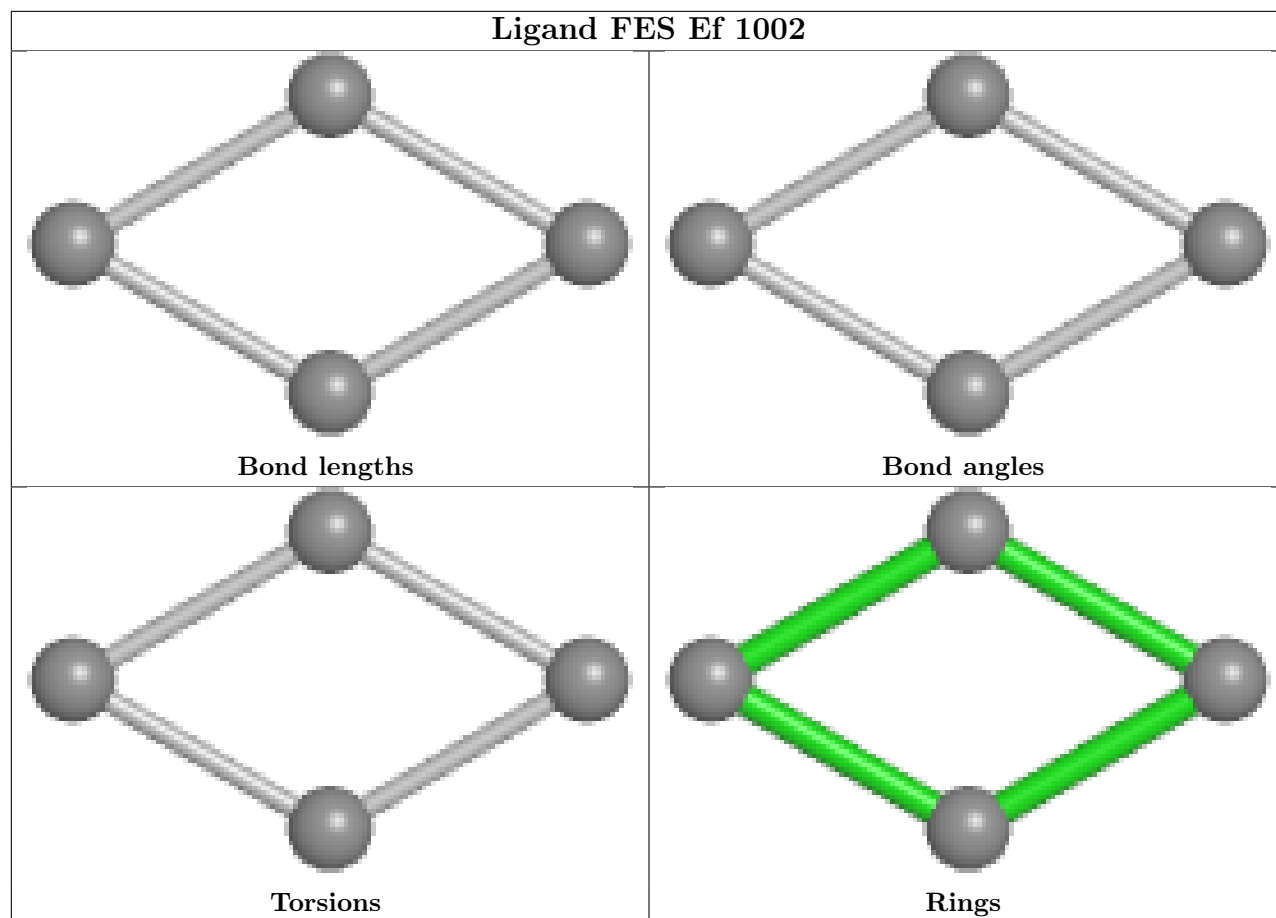


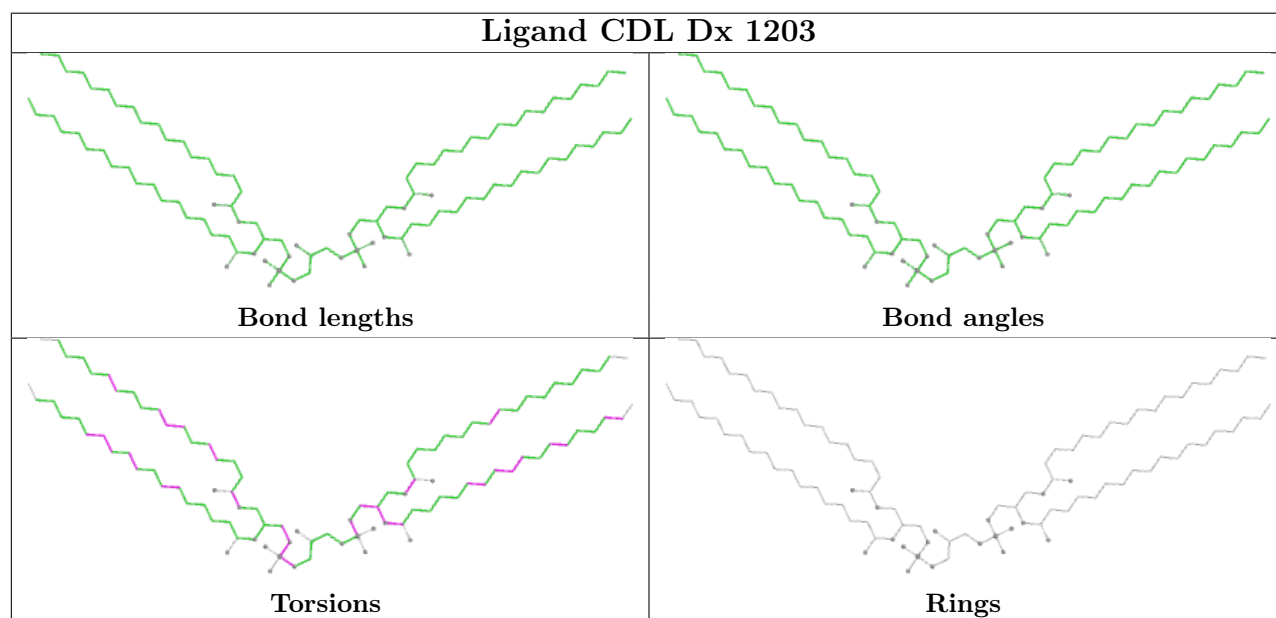
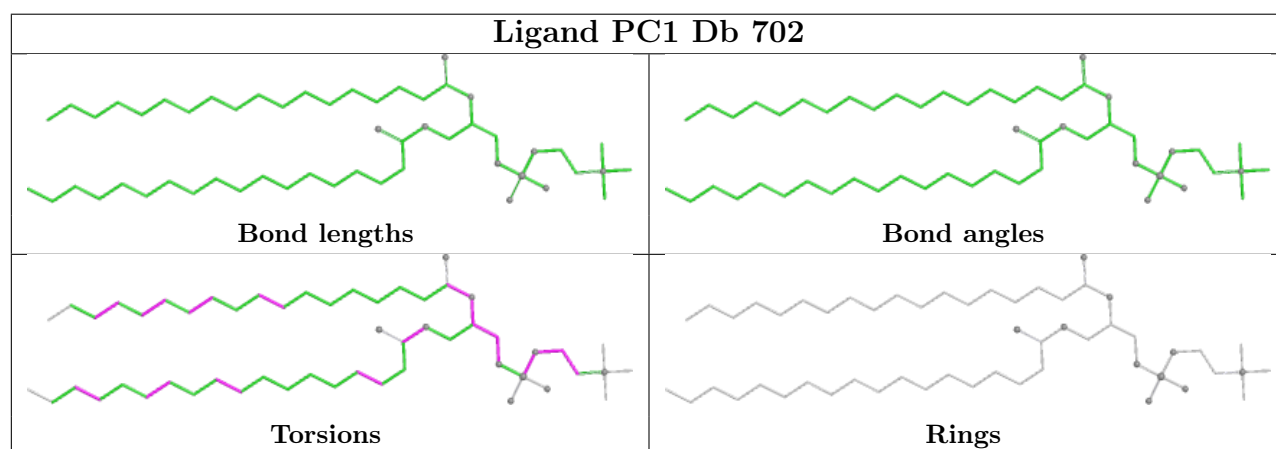
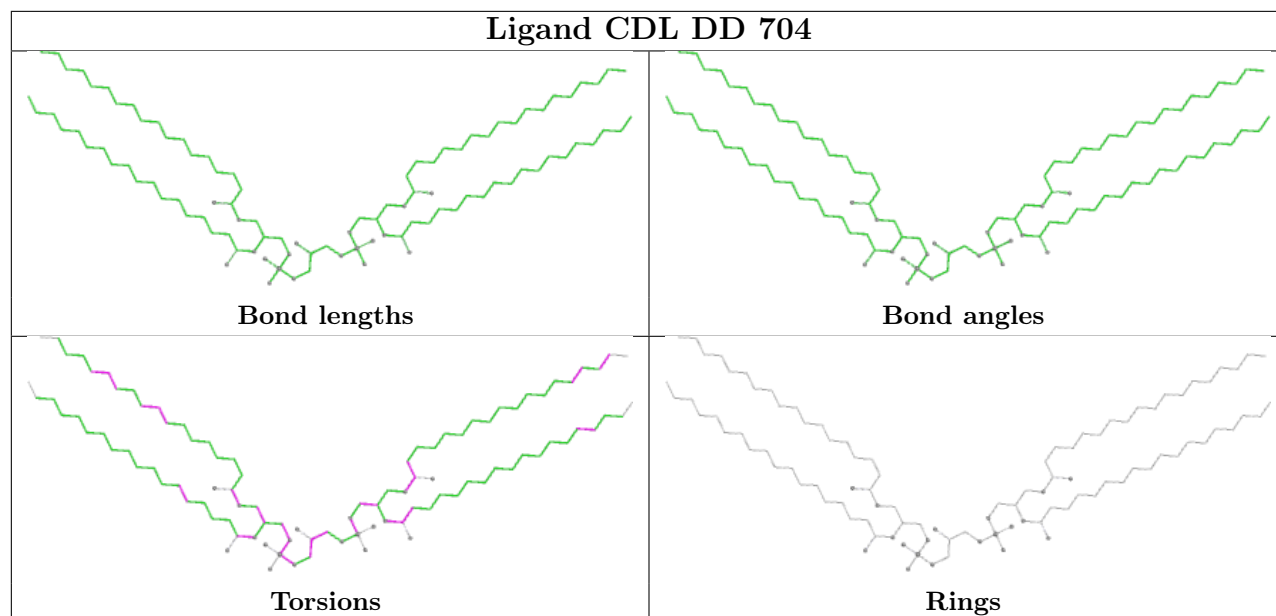


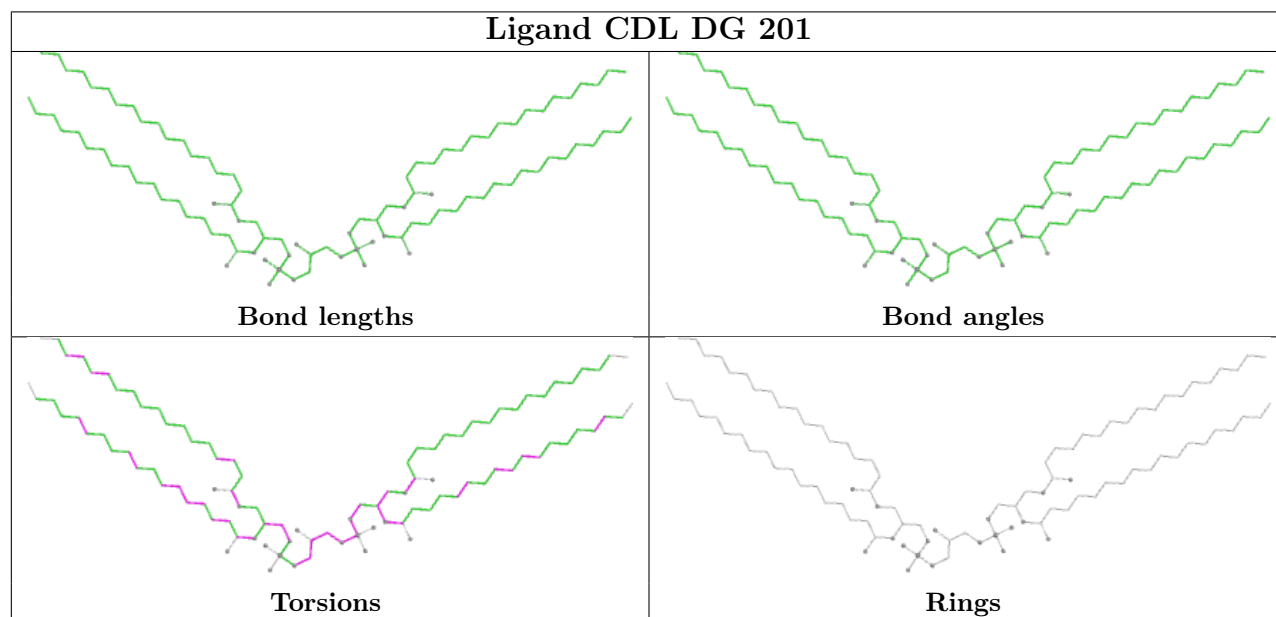
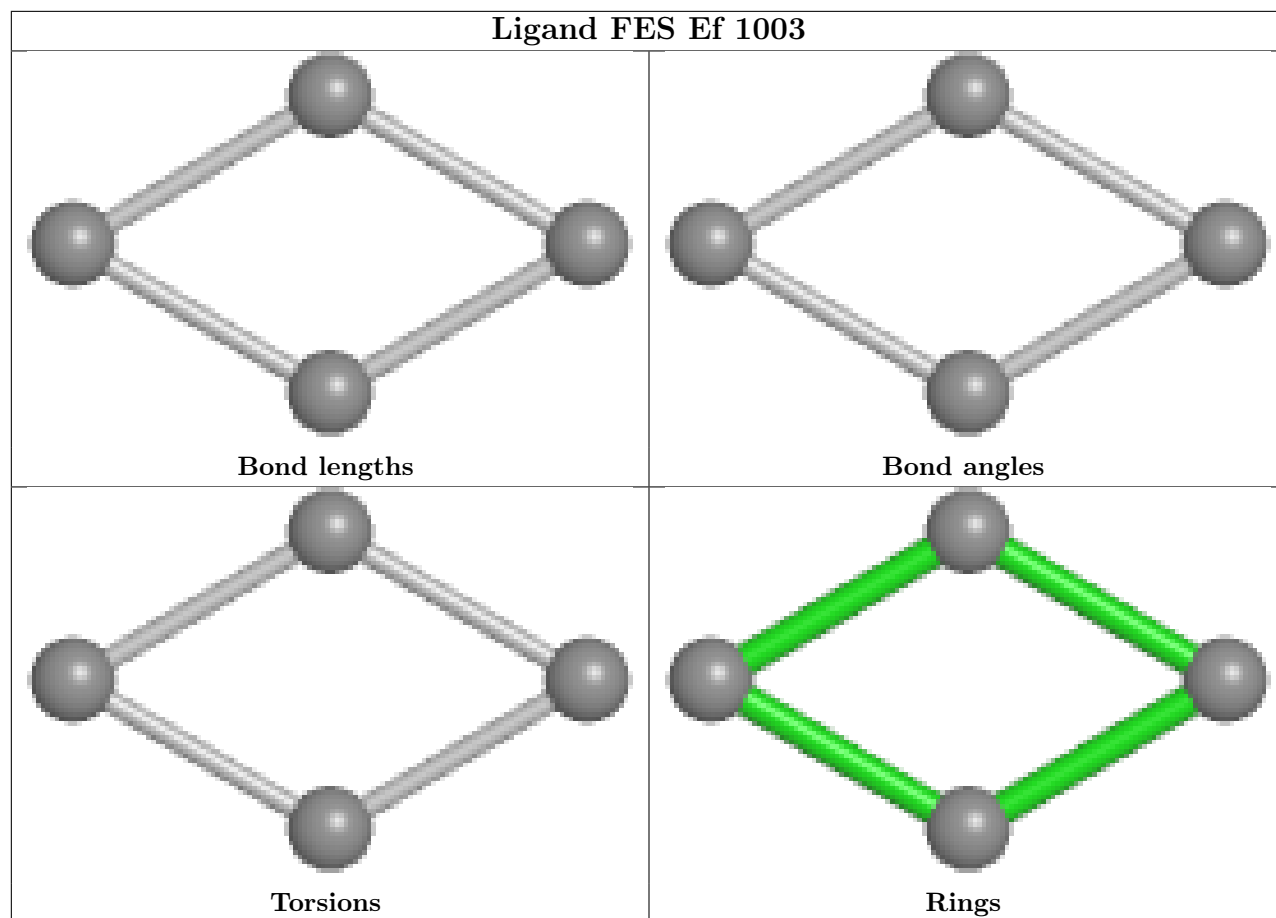


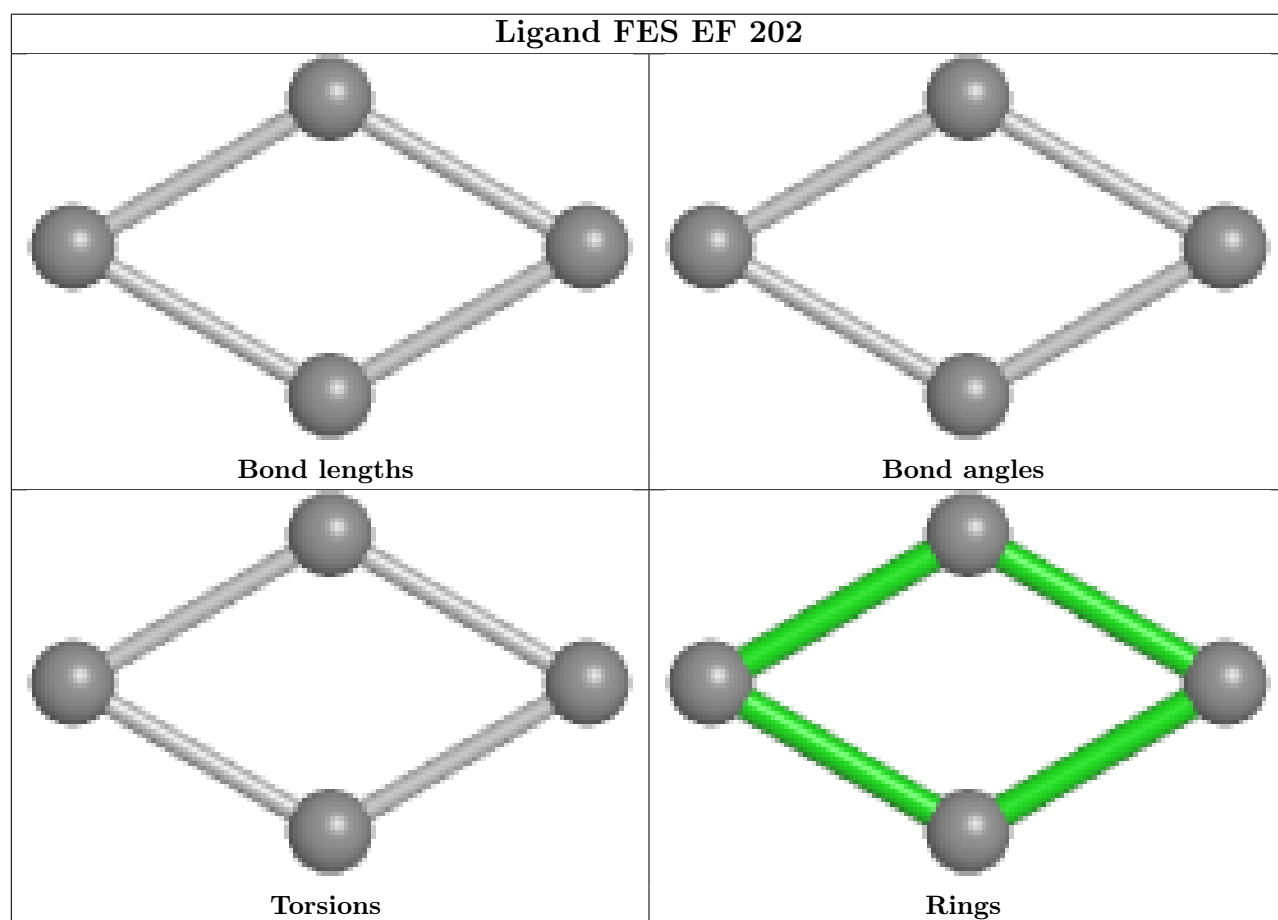
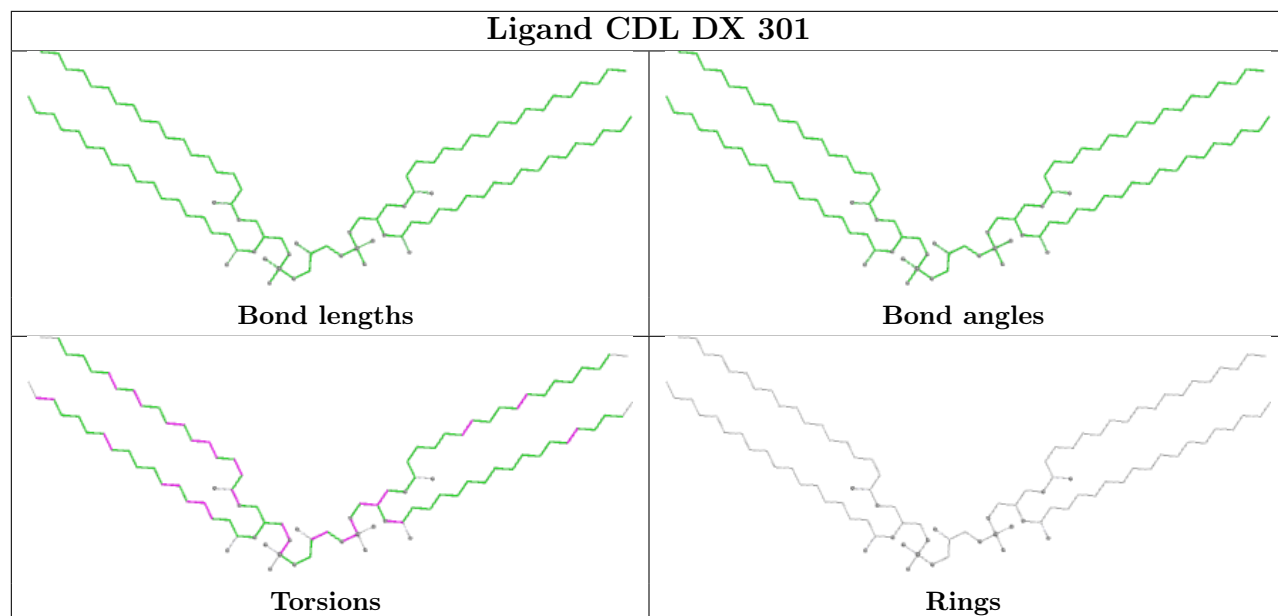
Ligand PC1 Dc 603			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

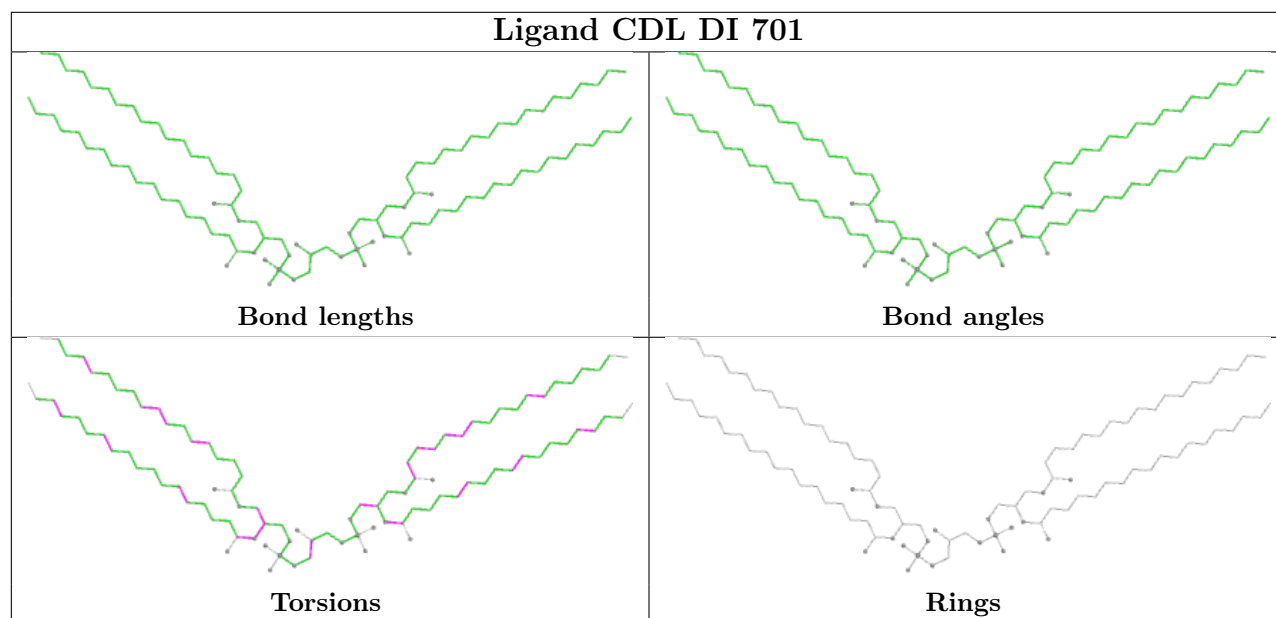
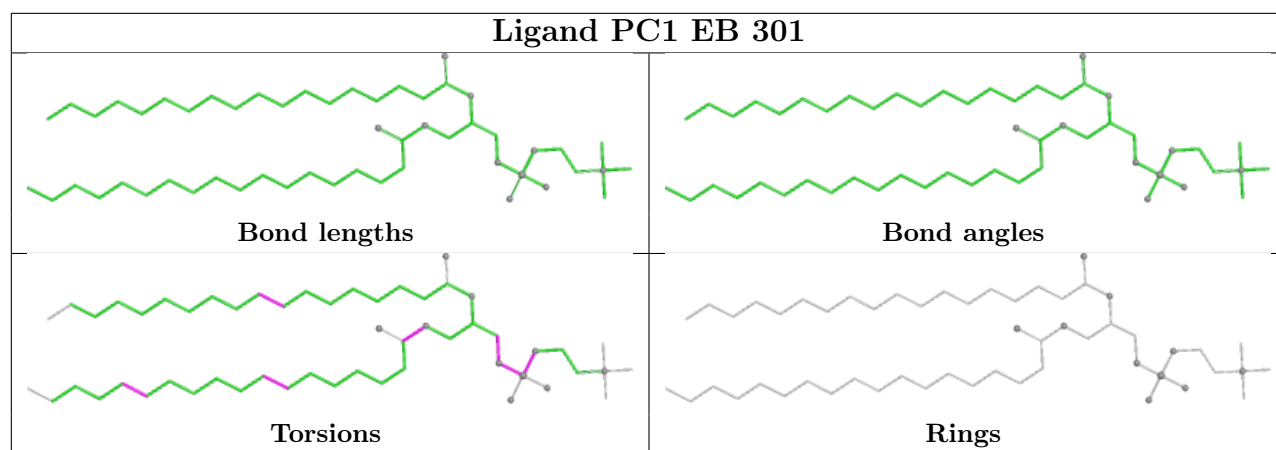
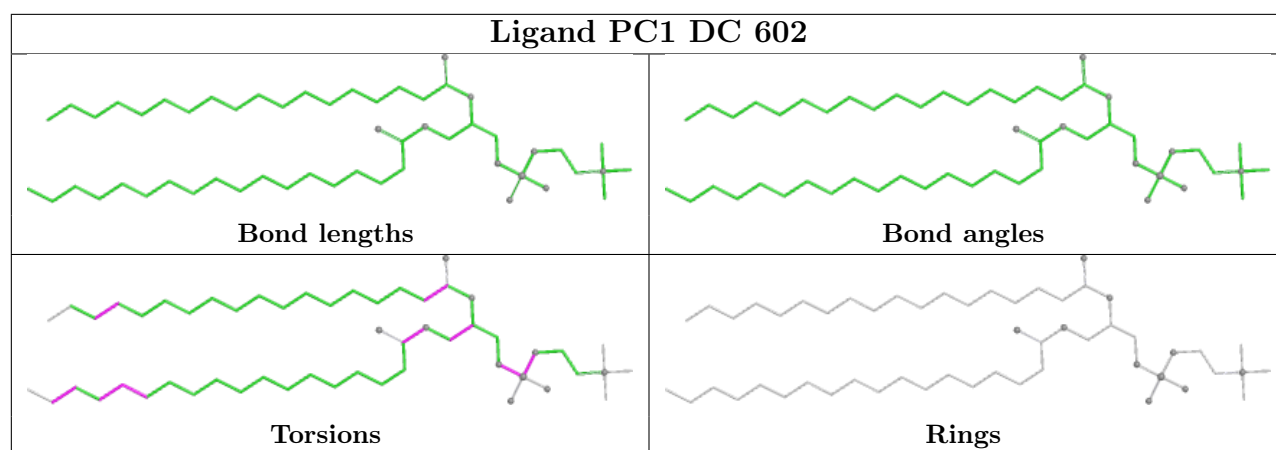
Ligand 3PE EO 203			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

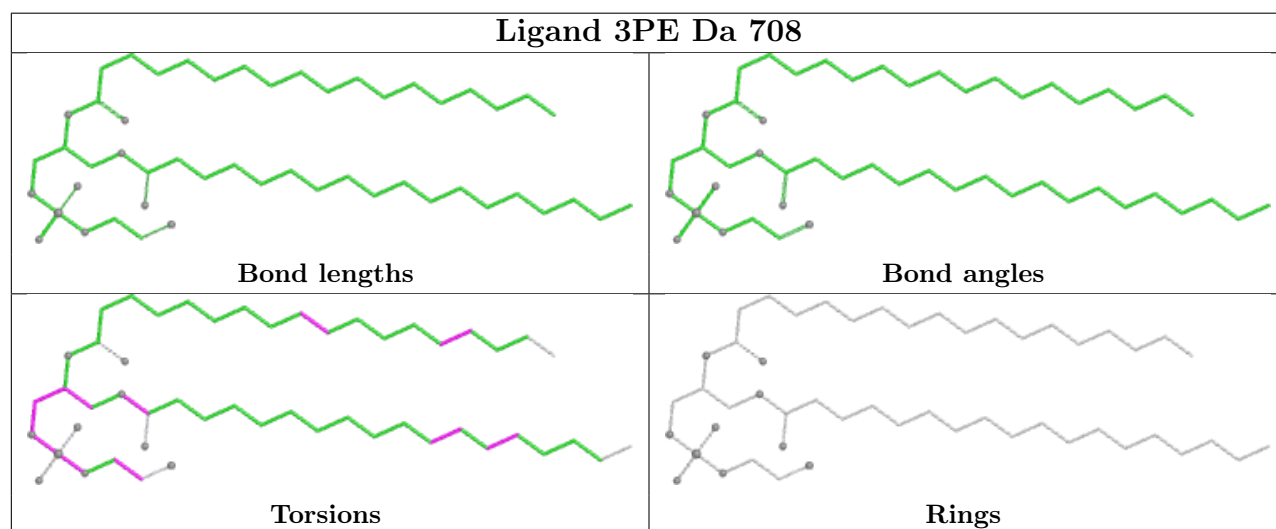
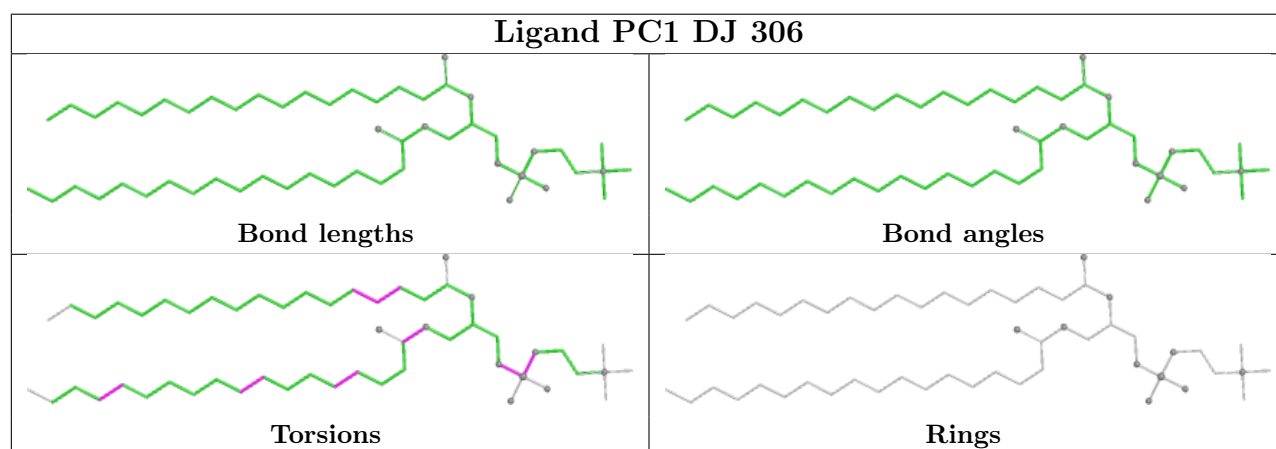
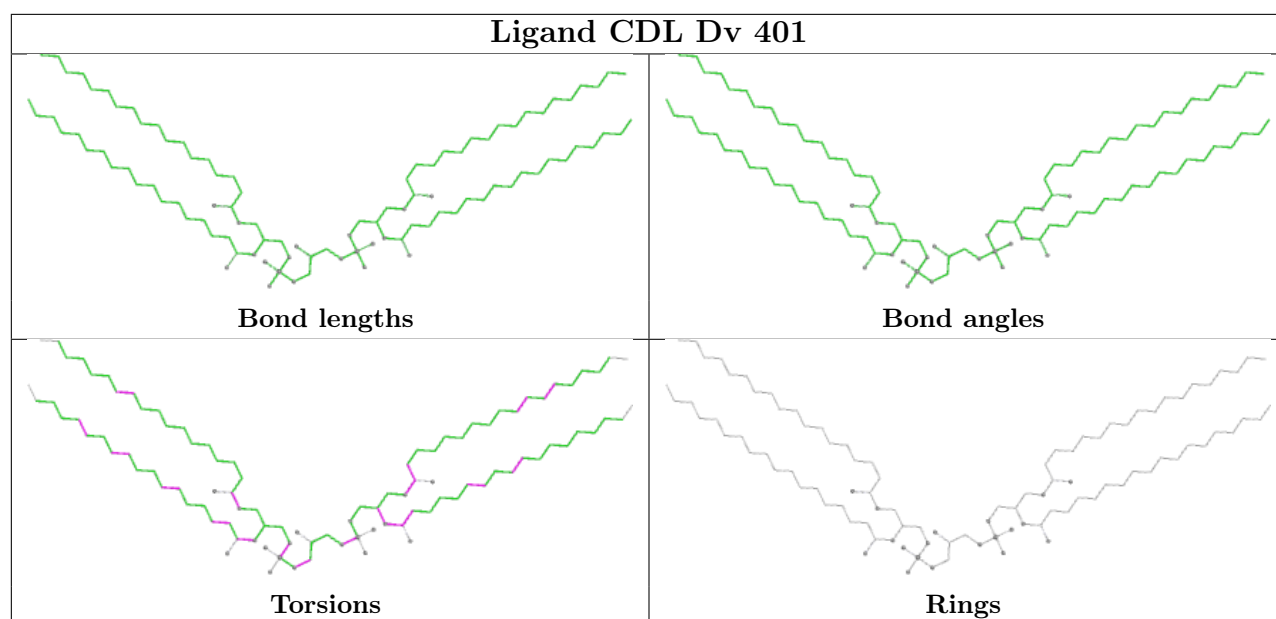


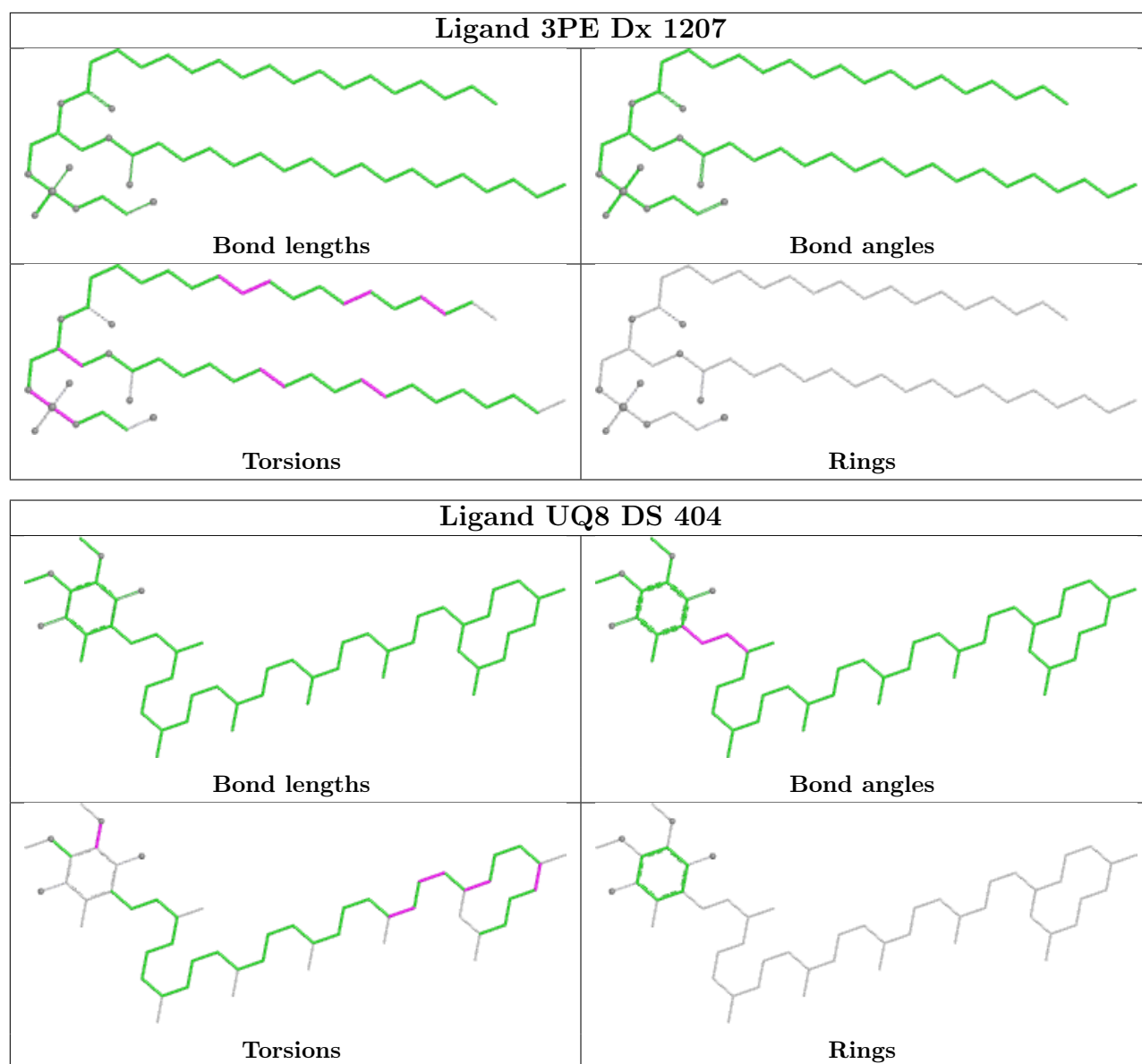


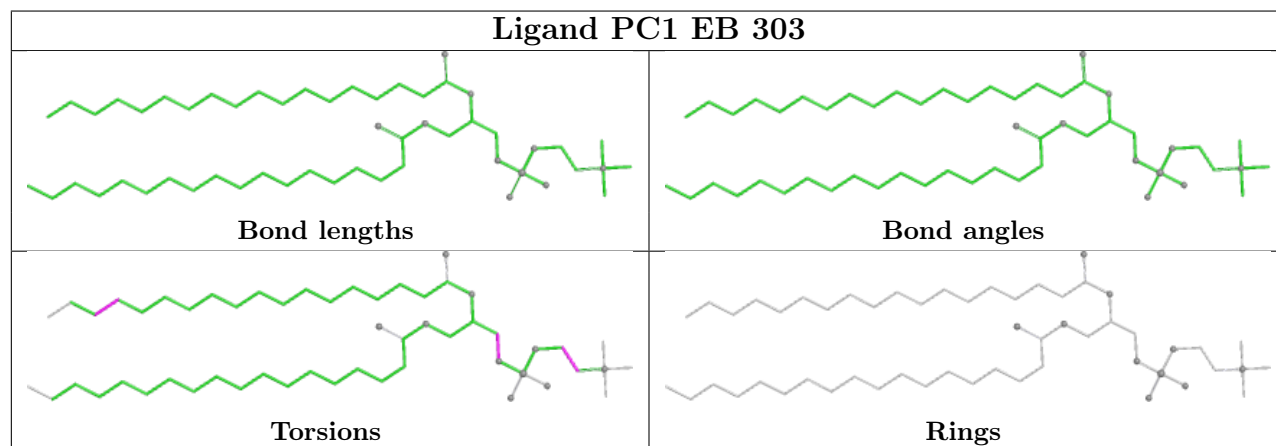
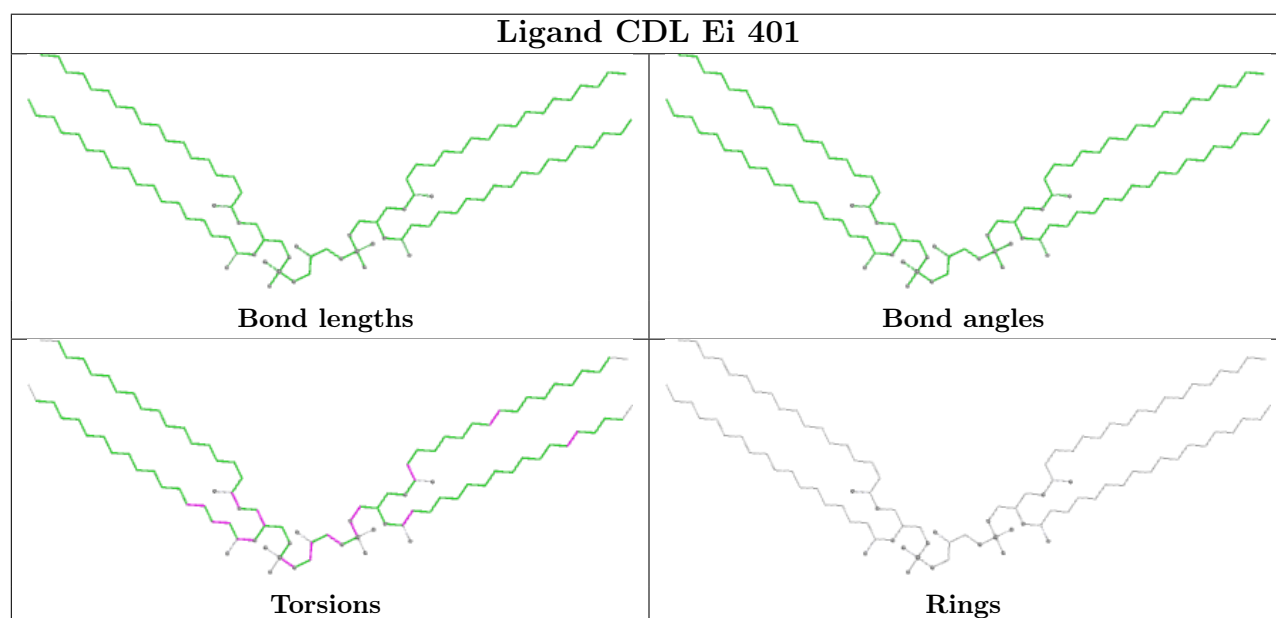
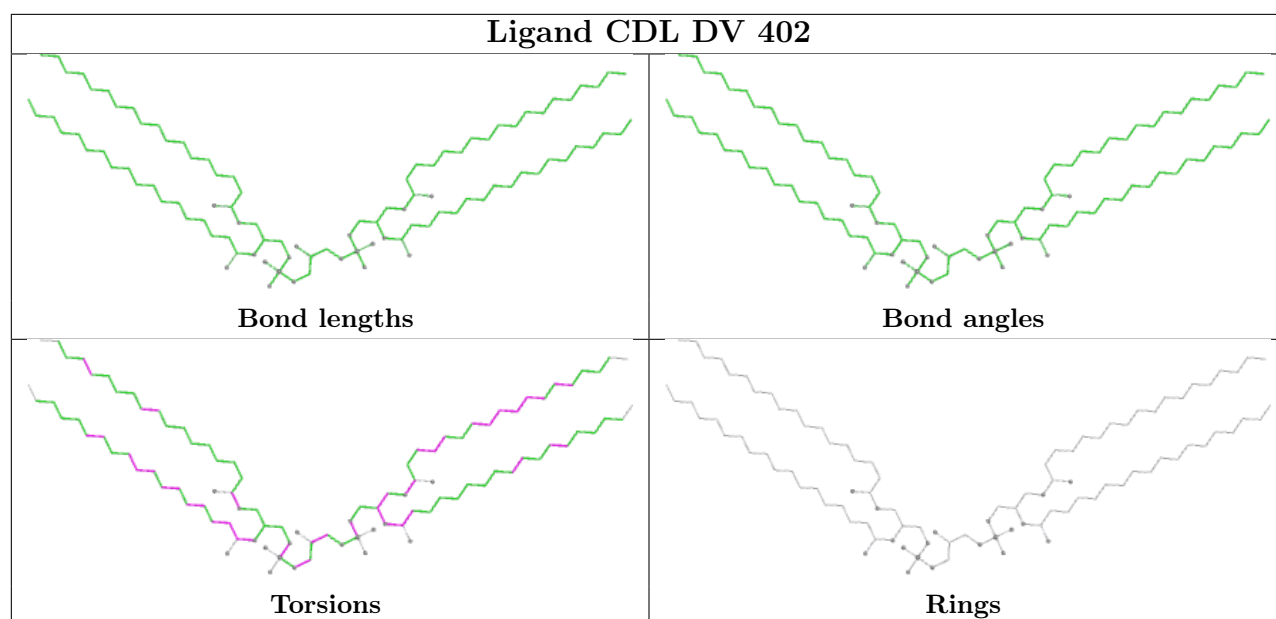


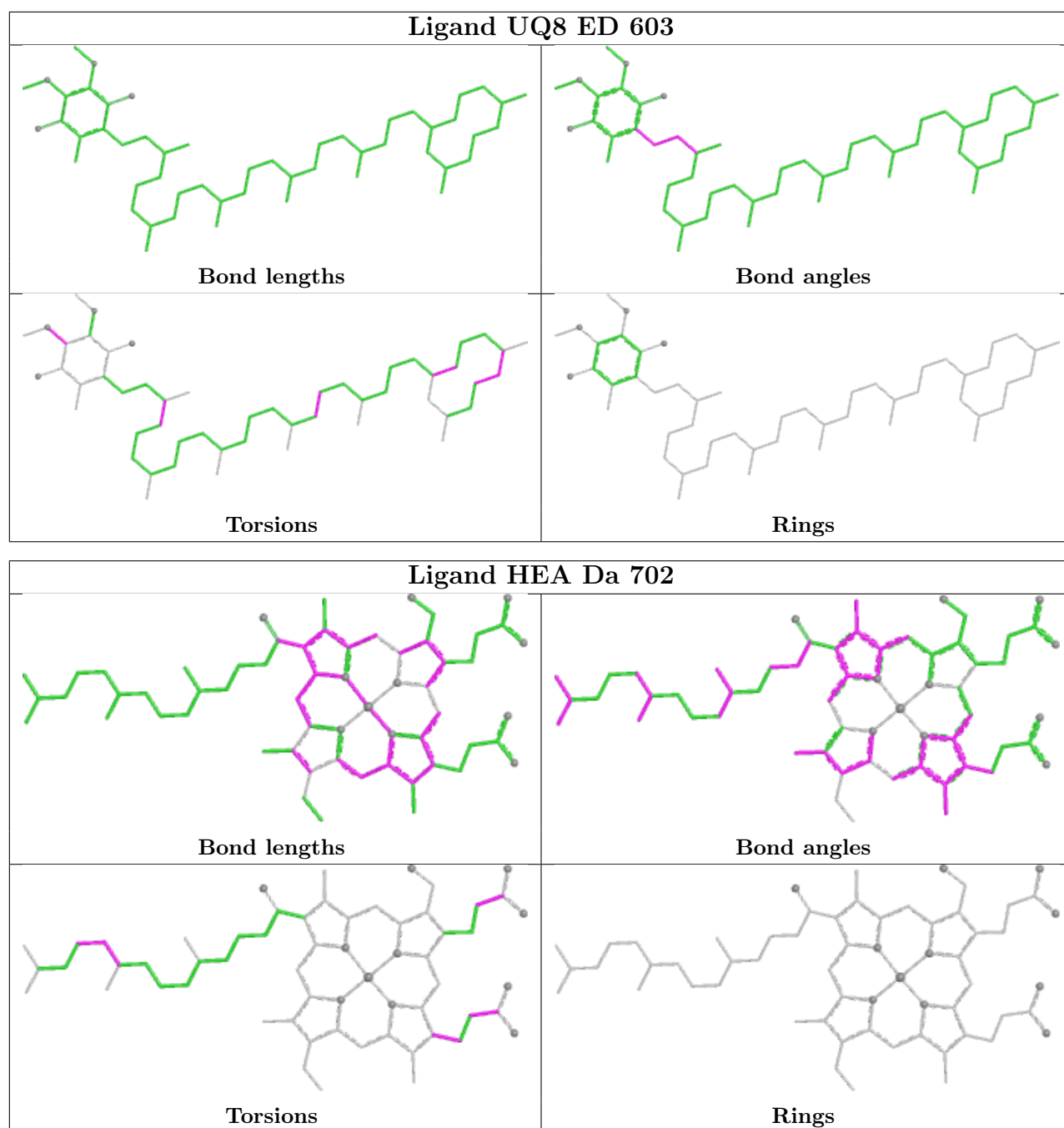


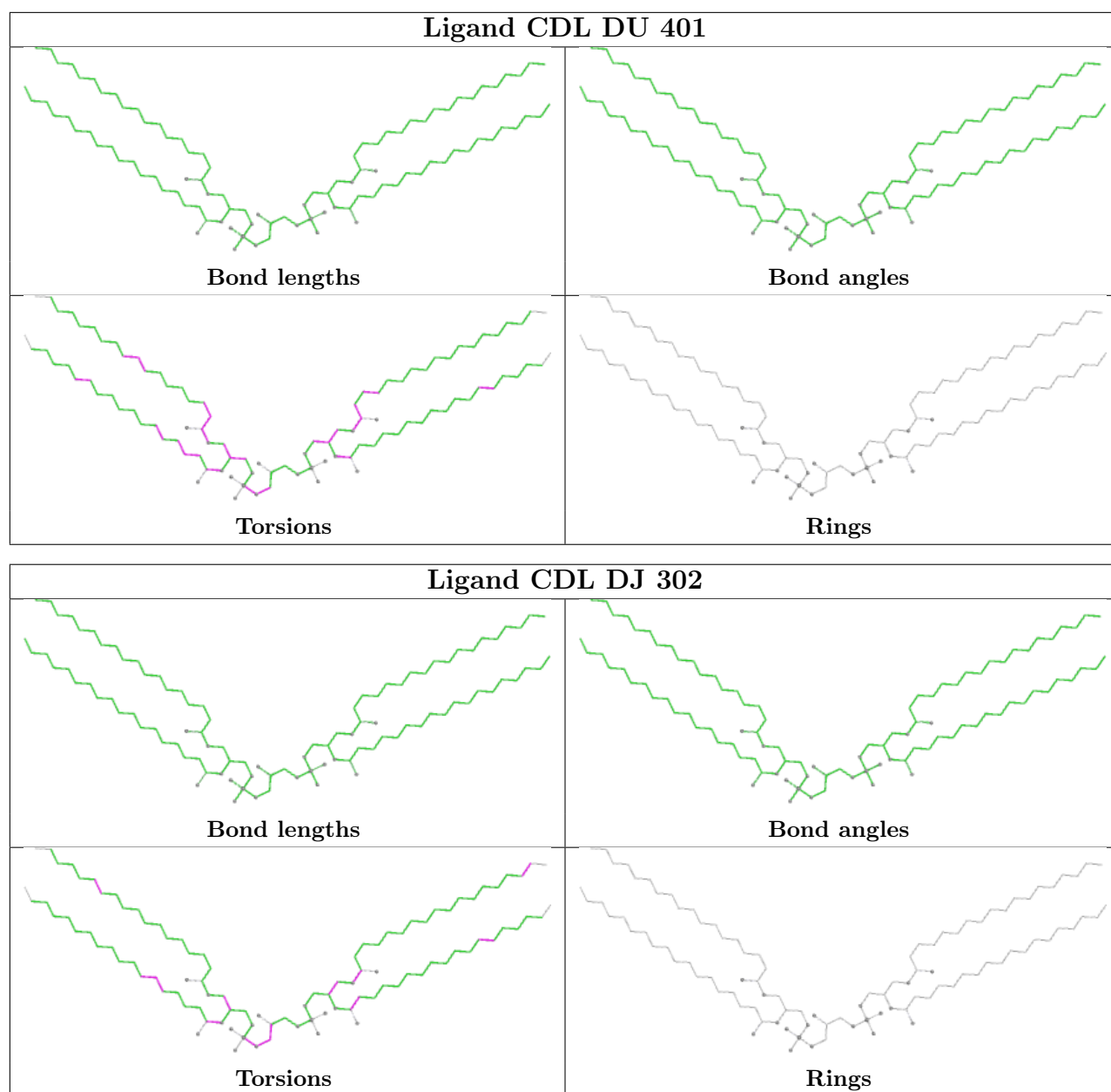


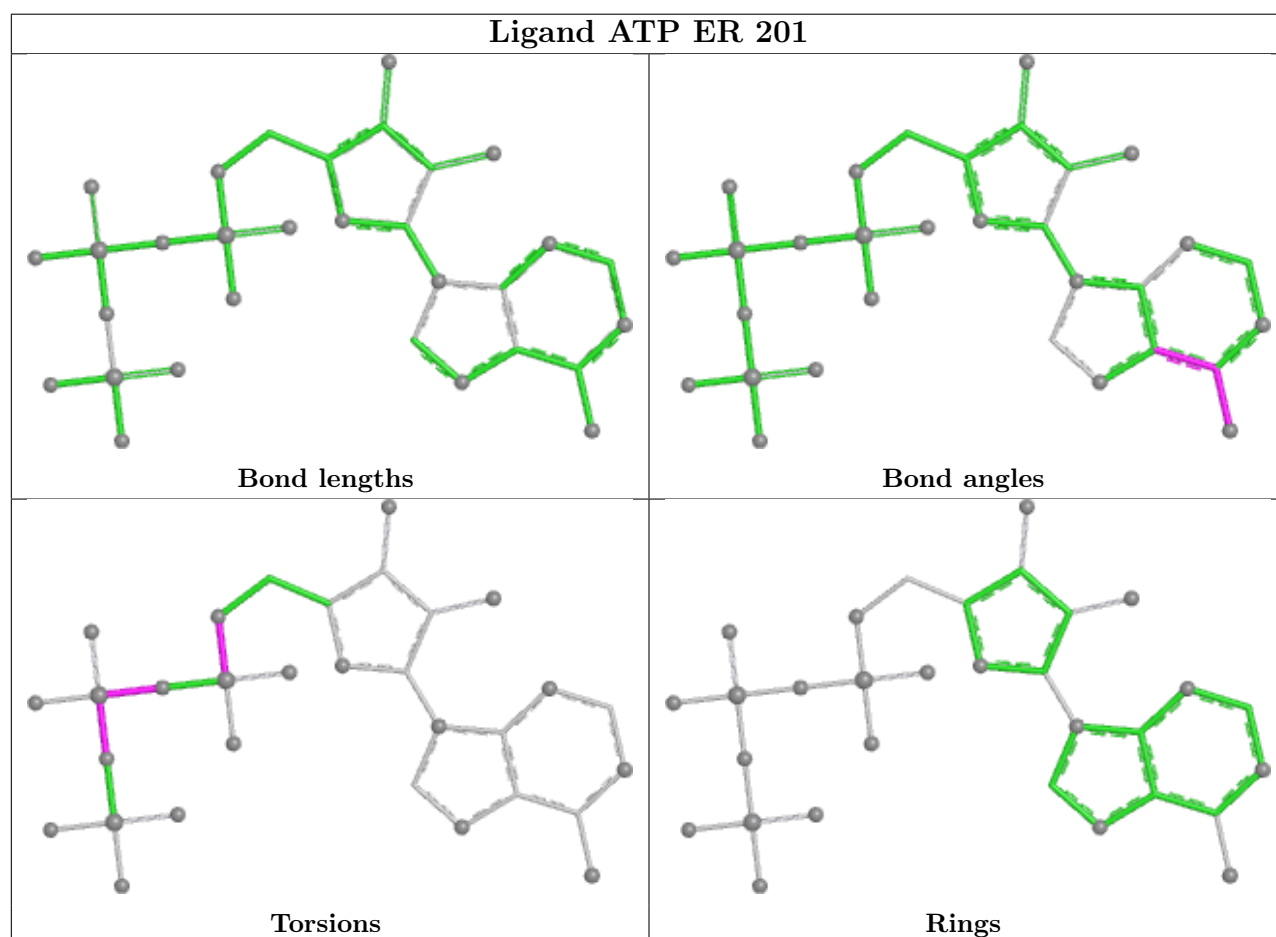
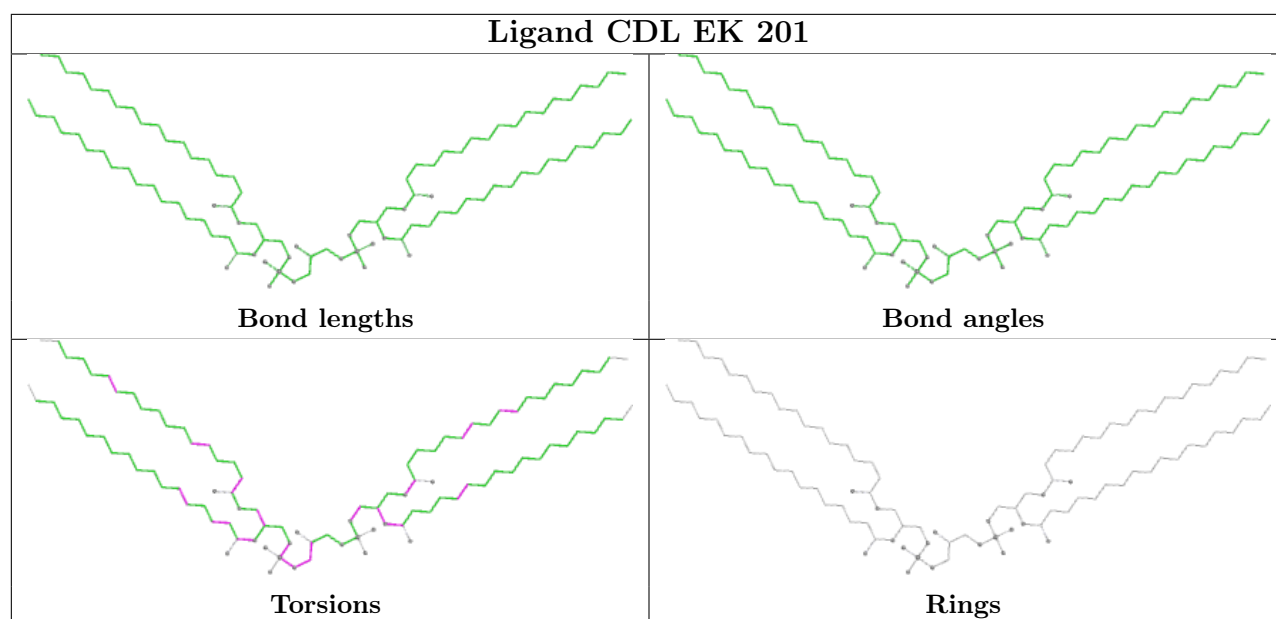


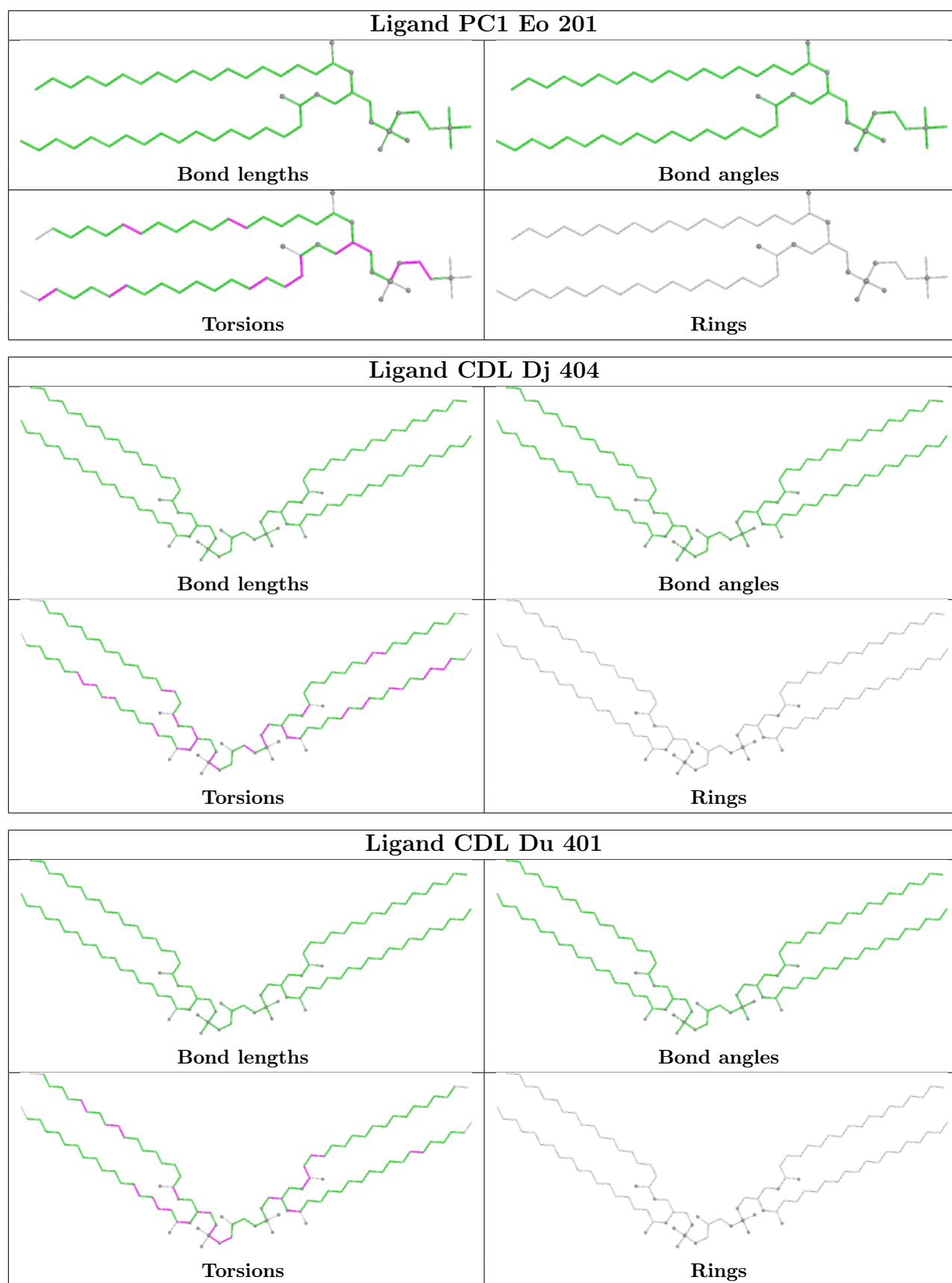


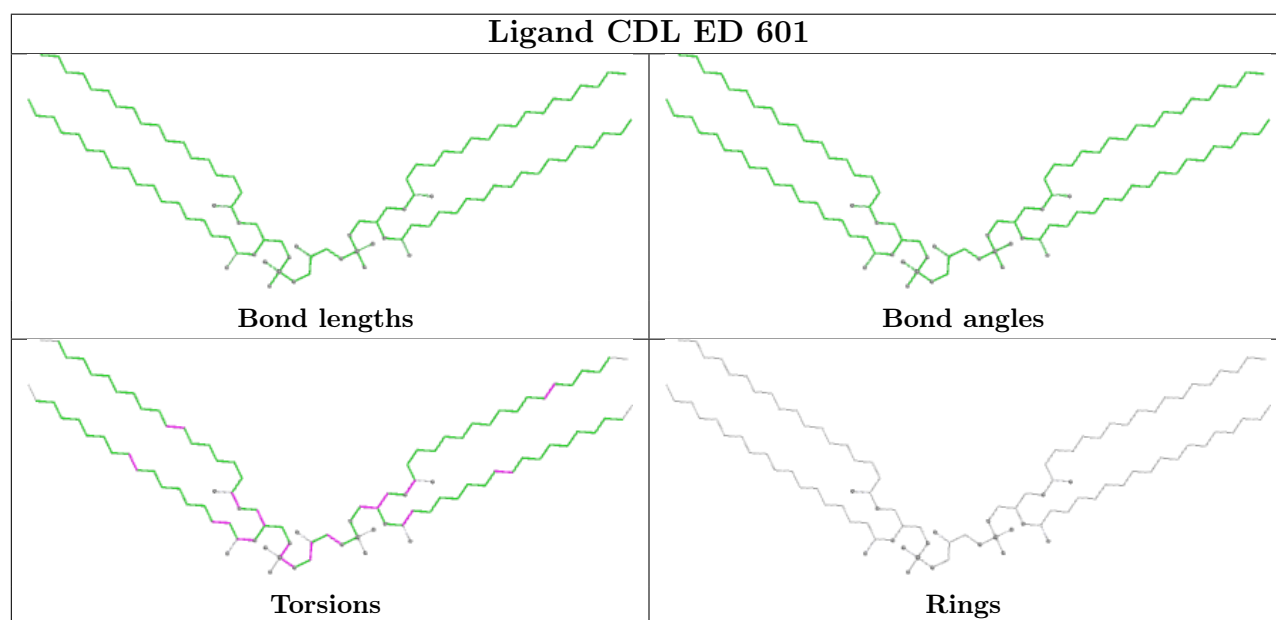
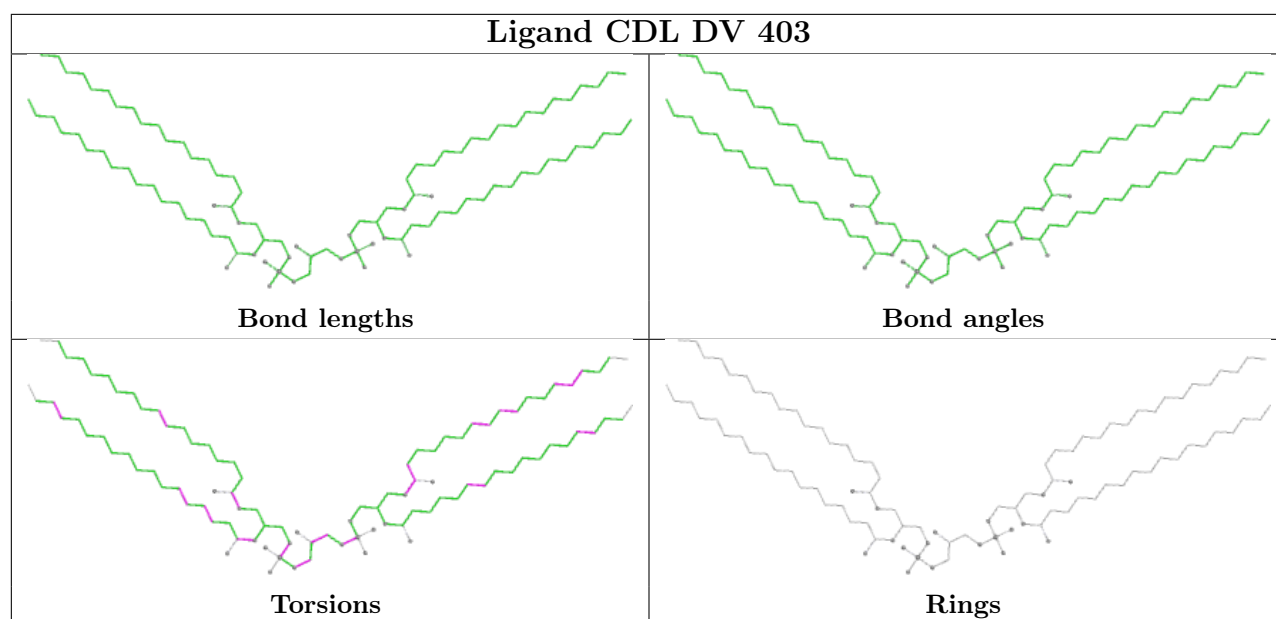


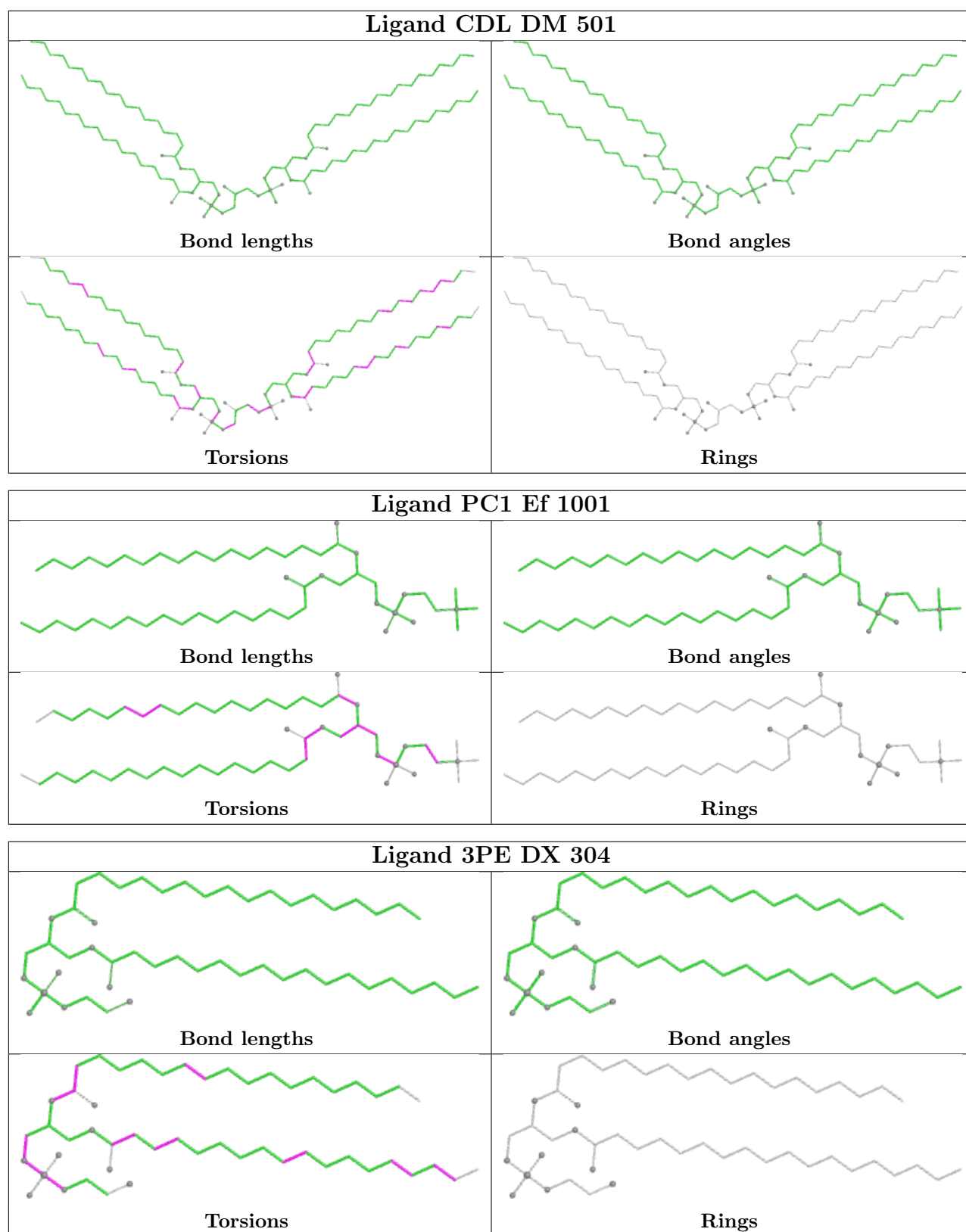


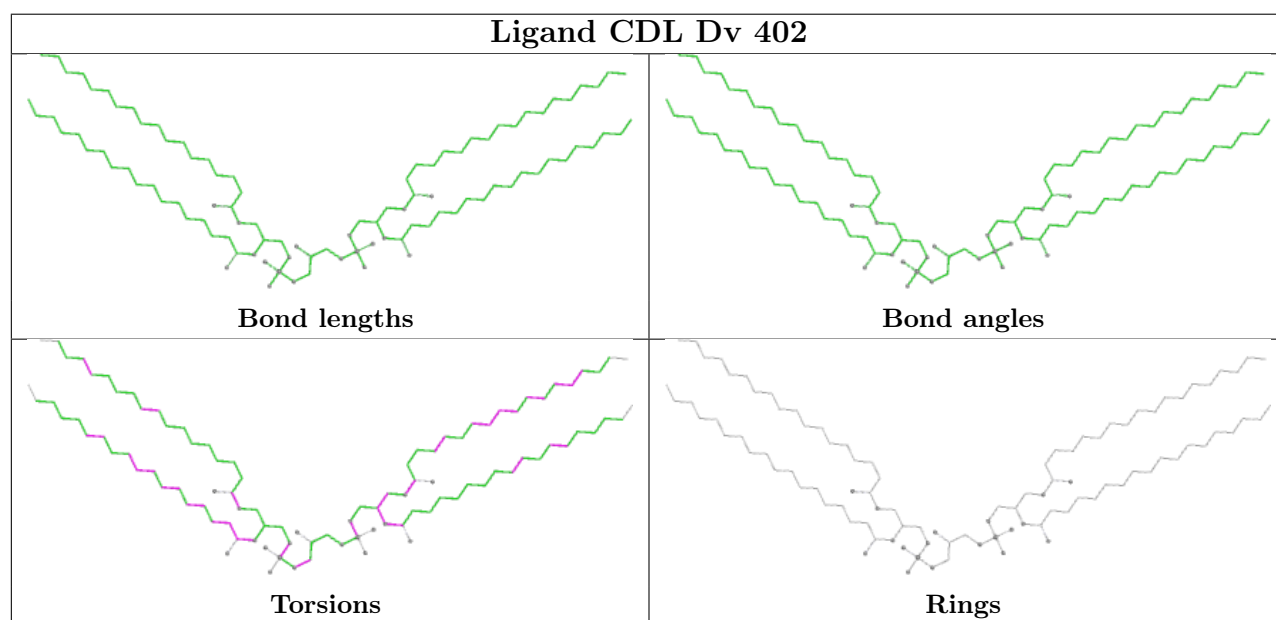
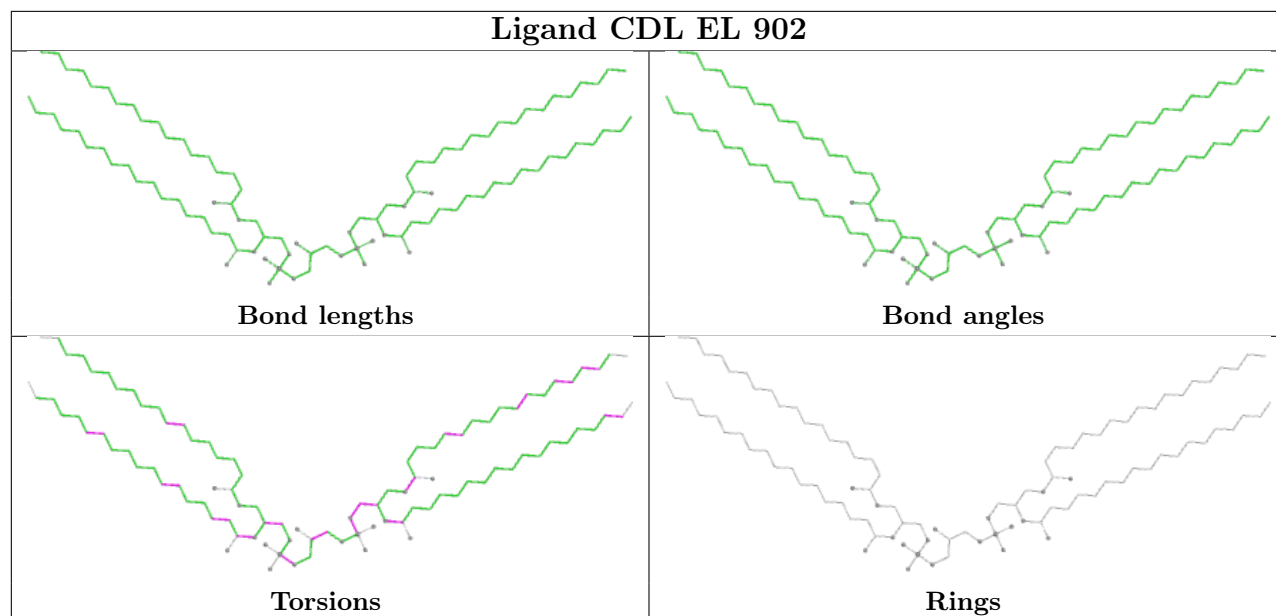


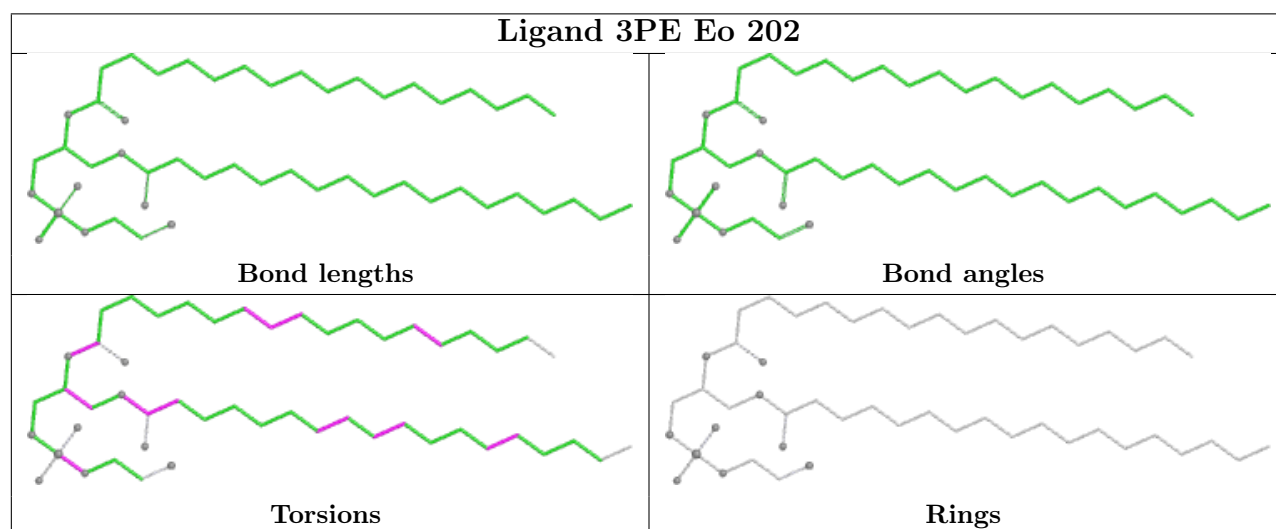
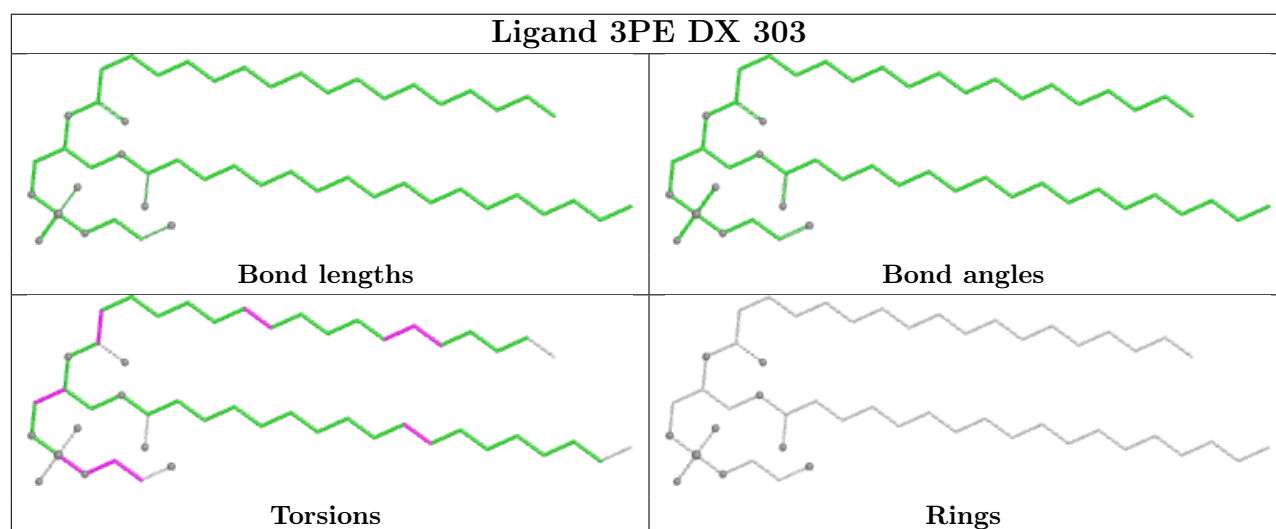
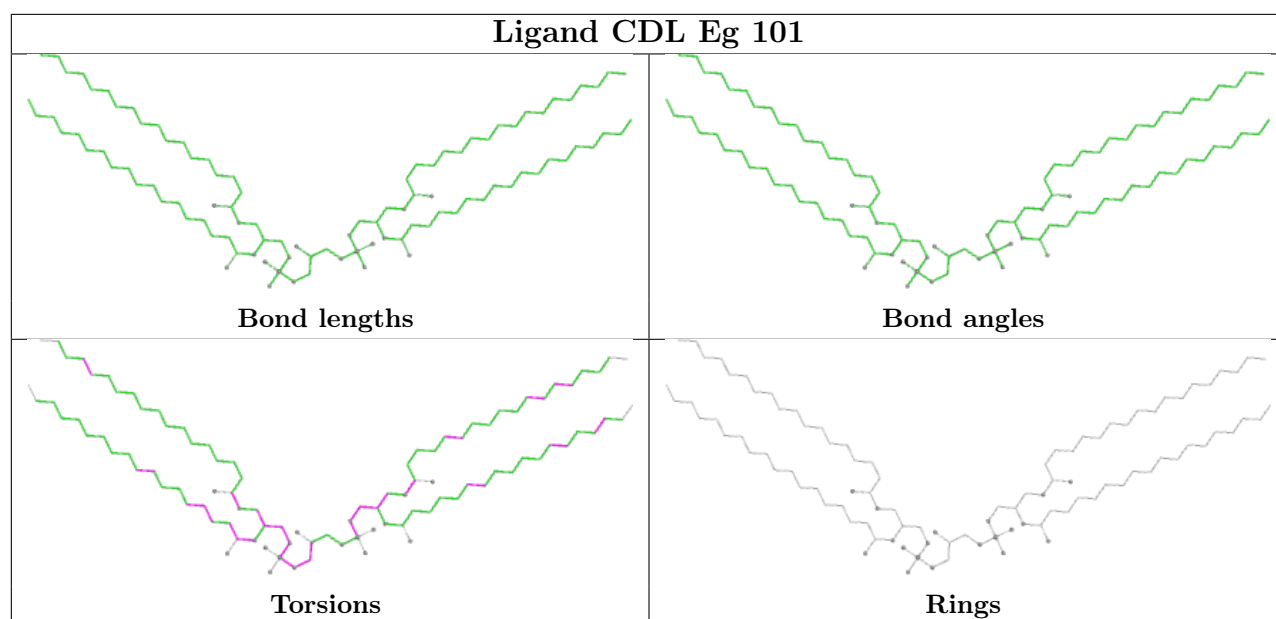


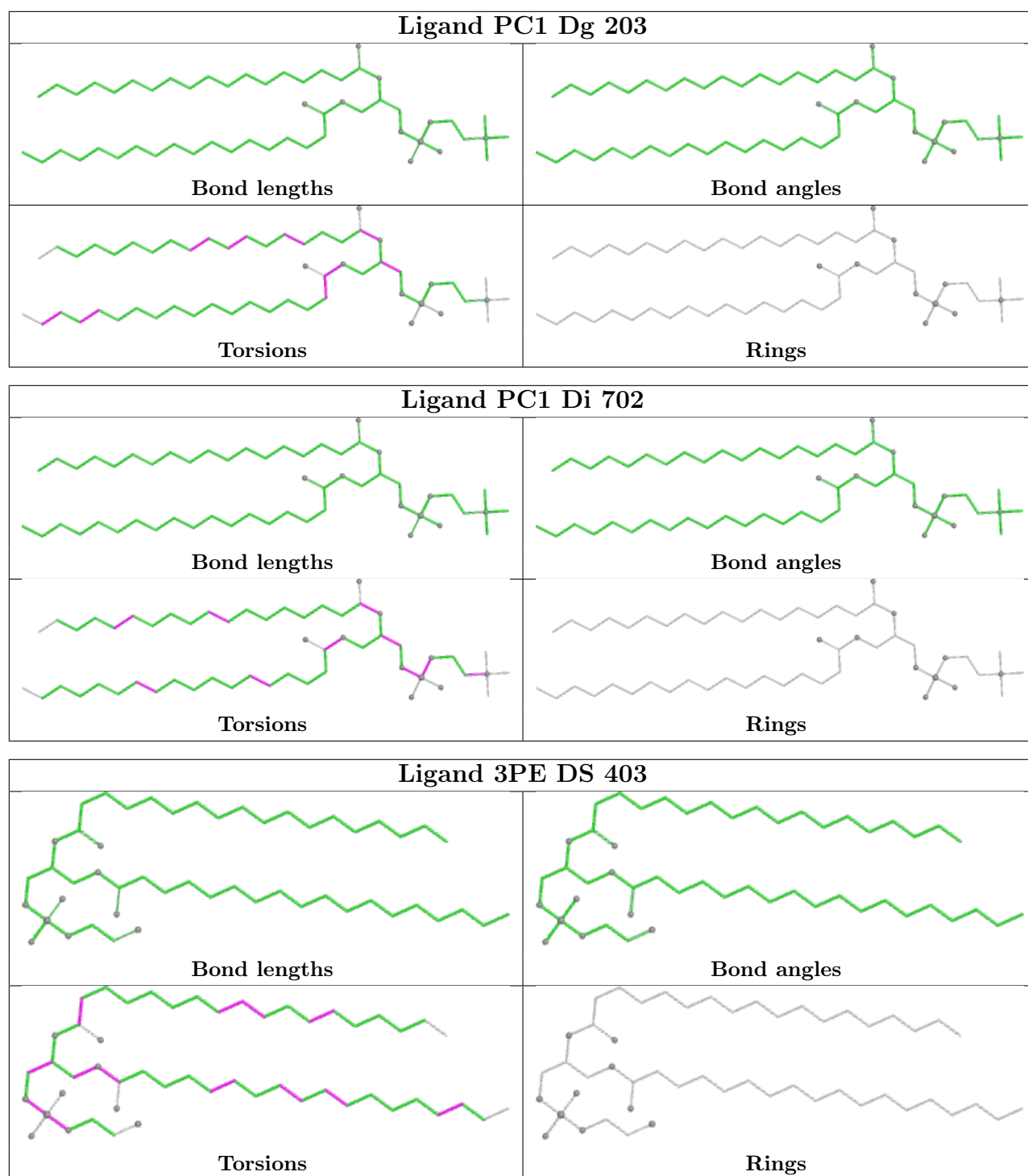


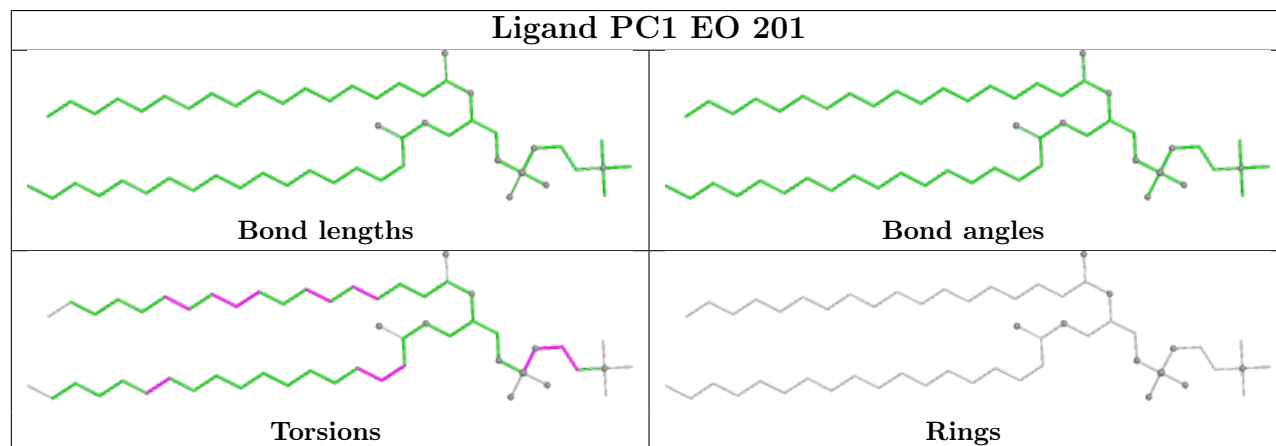
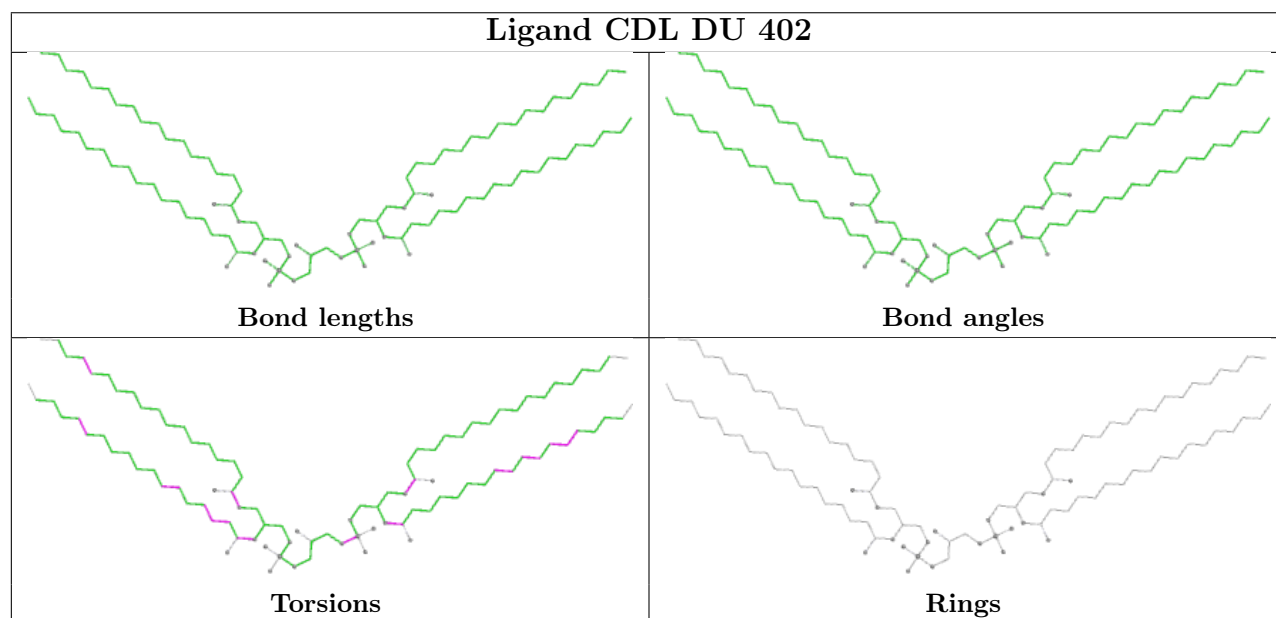
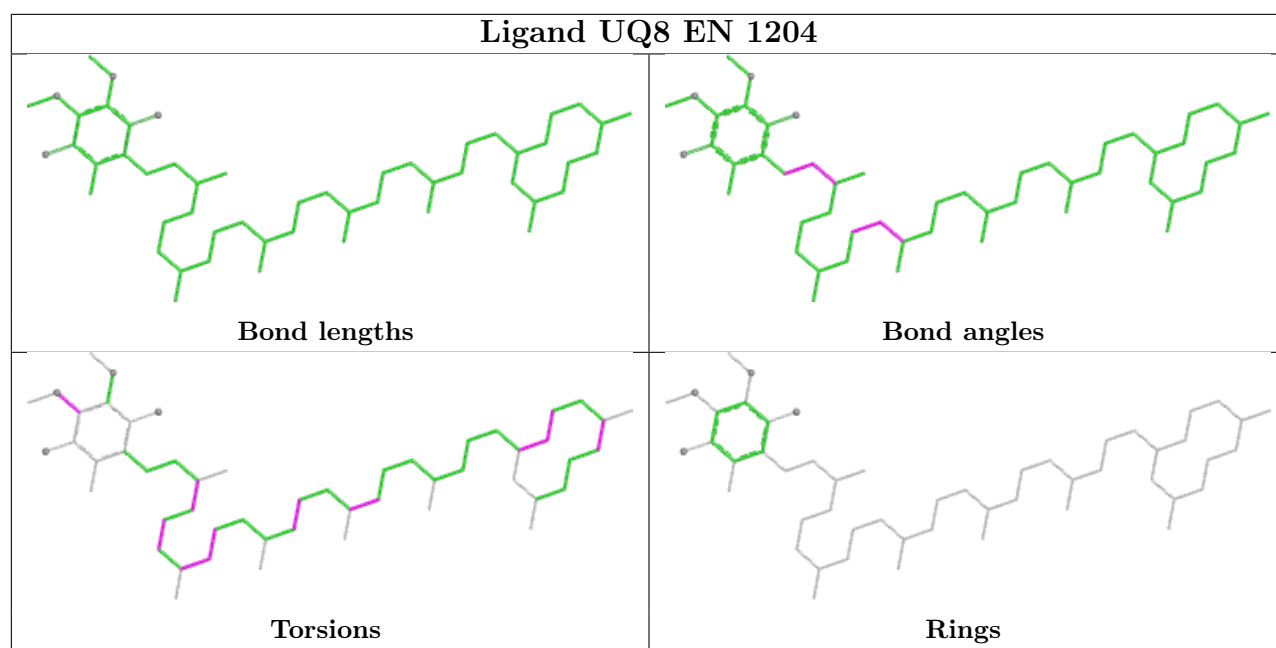


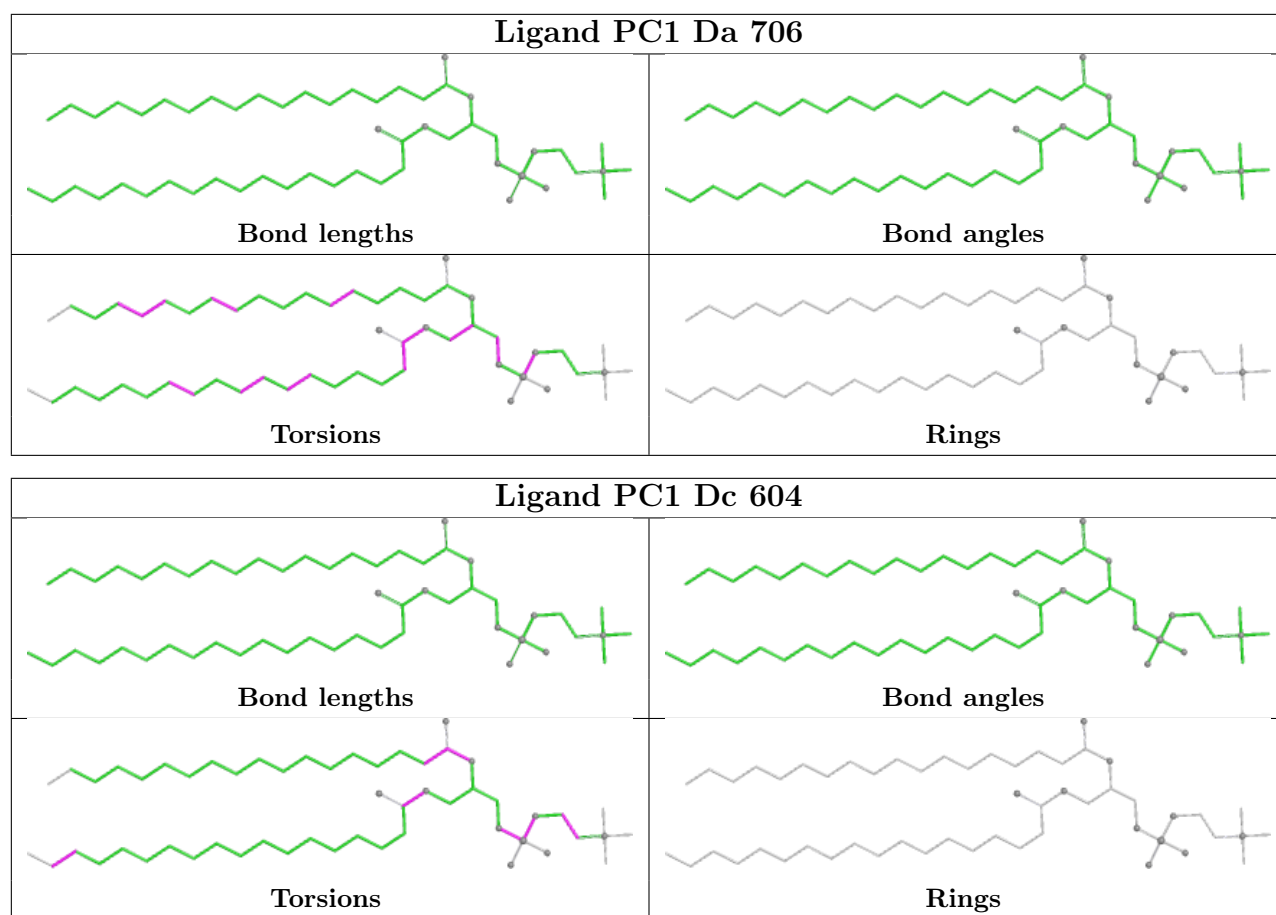












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

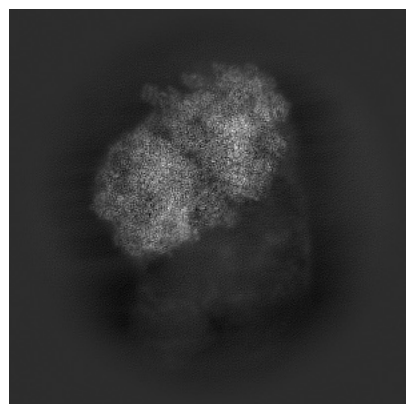
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15867. These allow visual inspection of the internal detail of the map and identification of artifacts.

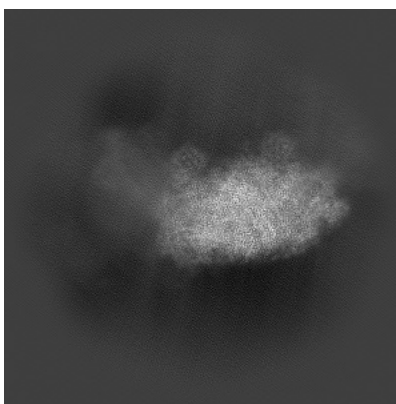
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

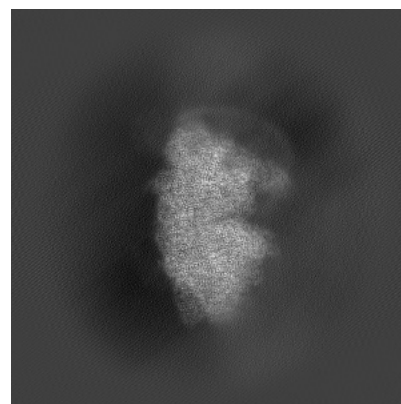
6.1.1 Primary map



X

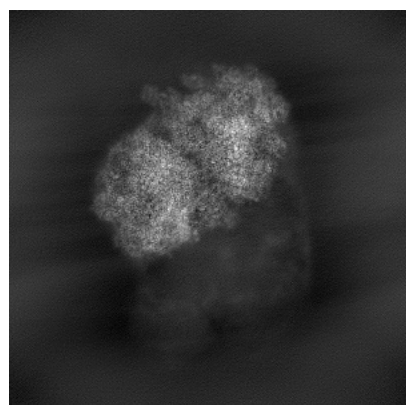


Y

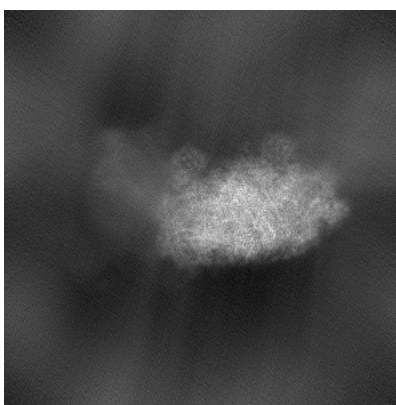


Z

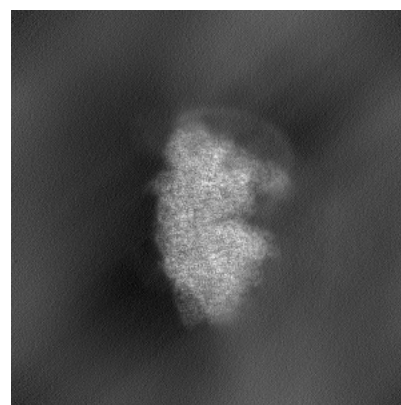
6.1.2 Raw map



X



Y

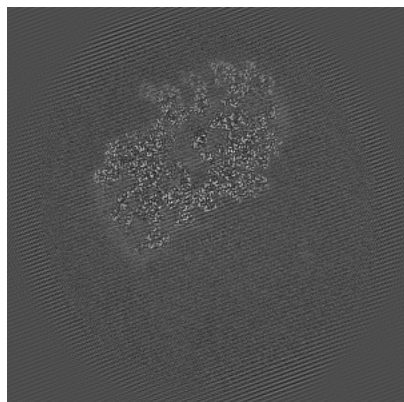


Z

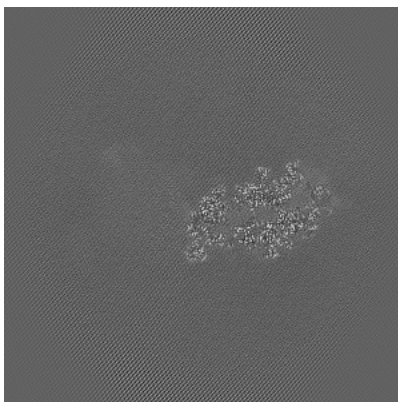
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

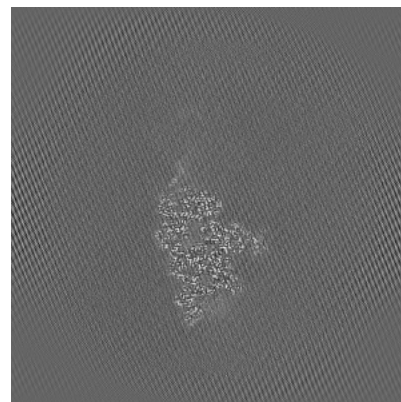
6.2.1 Primary map



X Index: 240

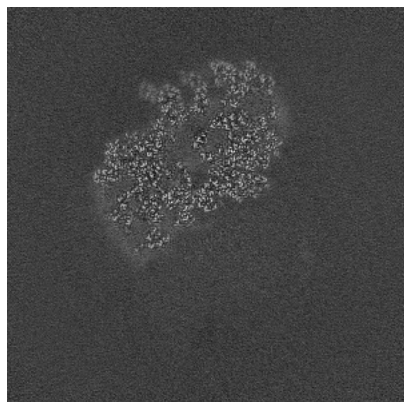


Y Index: 240

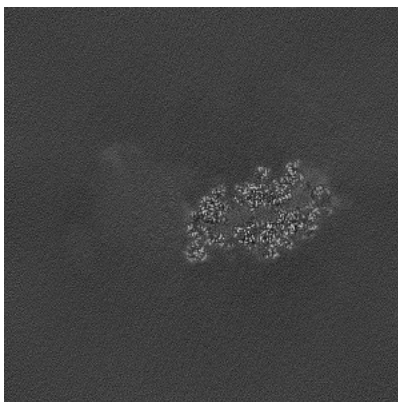


Z Index: 240

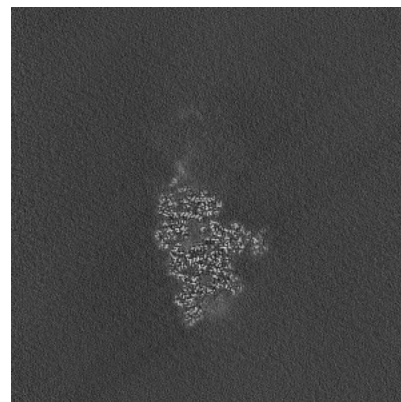
6.2.2 Raw map



X Index: 240



Y Index: 240

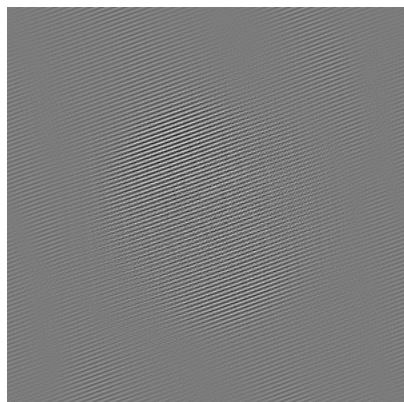


Z Index: 240

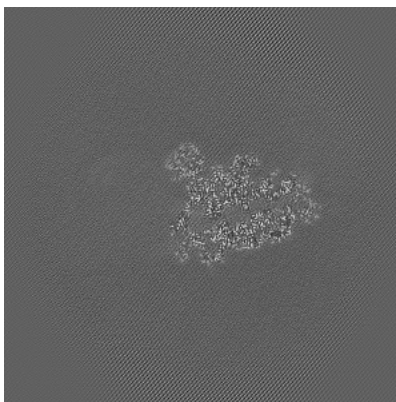
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

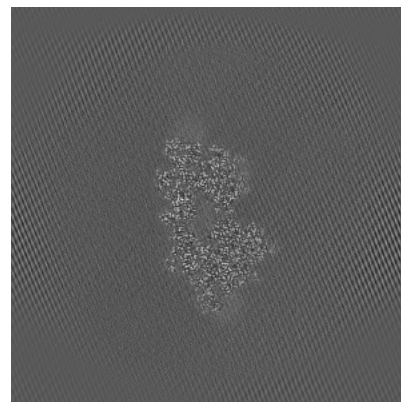
6.3.1 Primary map



X Index: 444

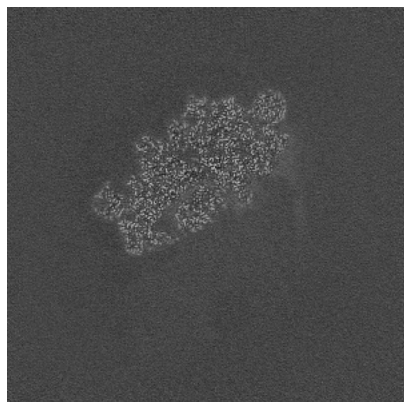


Y Index: 204

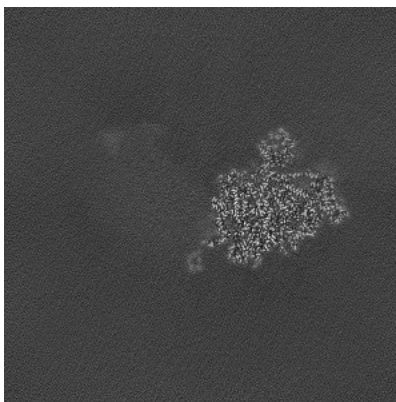


Z Index: 287

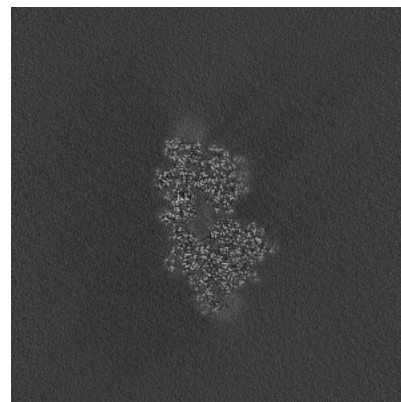
6.3.2 Raw map



X Index: 206



Y Index: 271

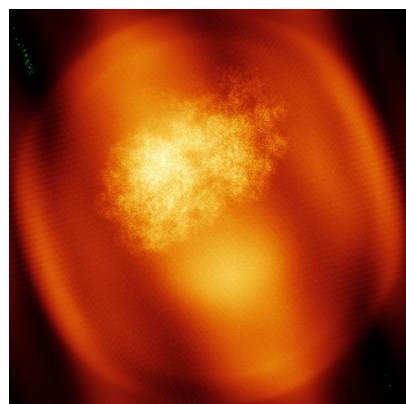


Z Index: 287

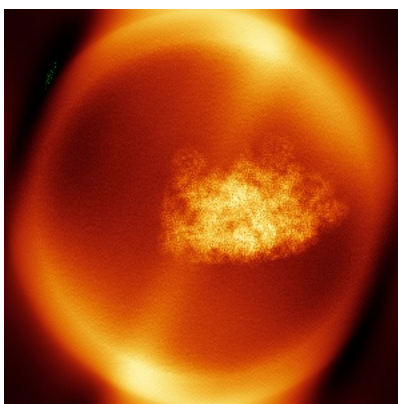
The images above show the largest variance slices of the map in three orthogonal directions.

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

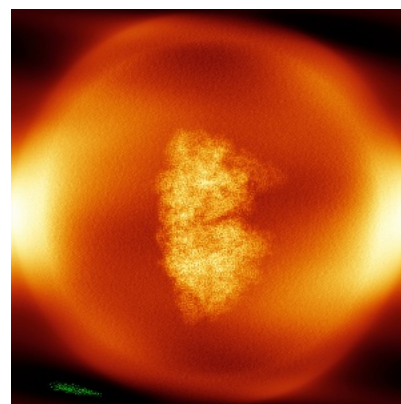
6.4.1 Primary map



X

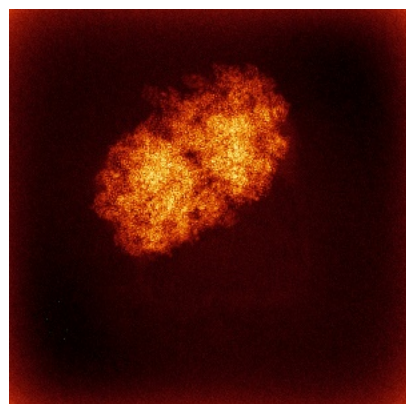


Y

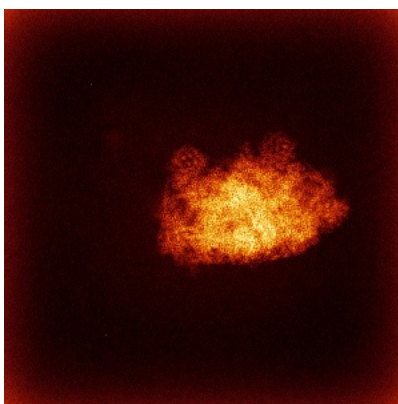


Z

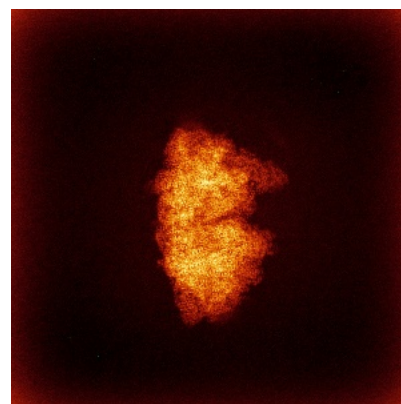
6.4.2 Raw map



X



Y

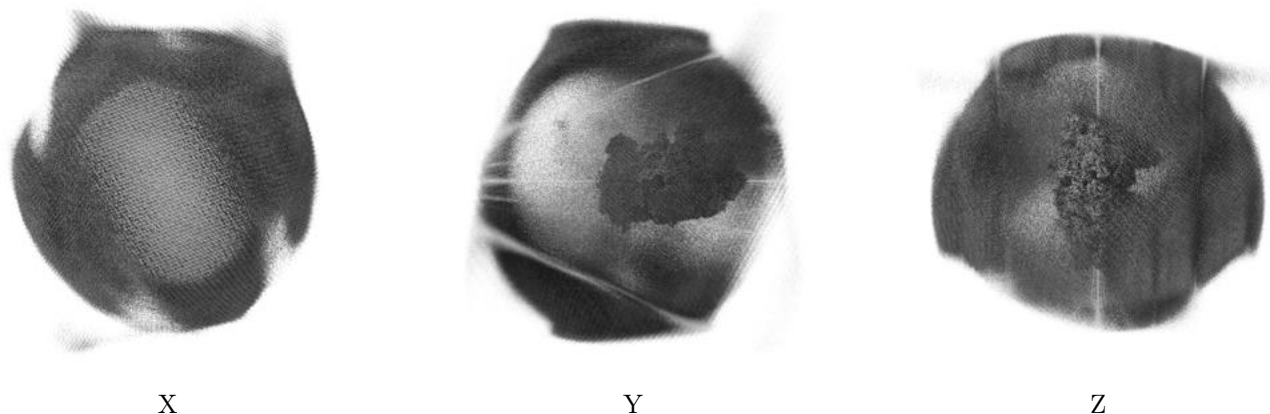


Z

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.

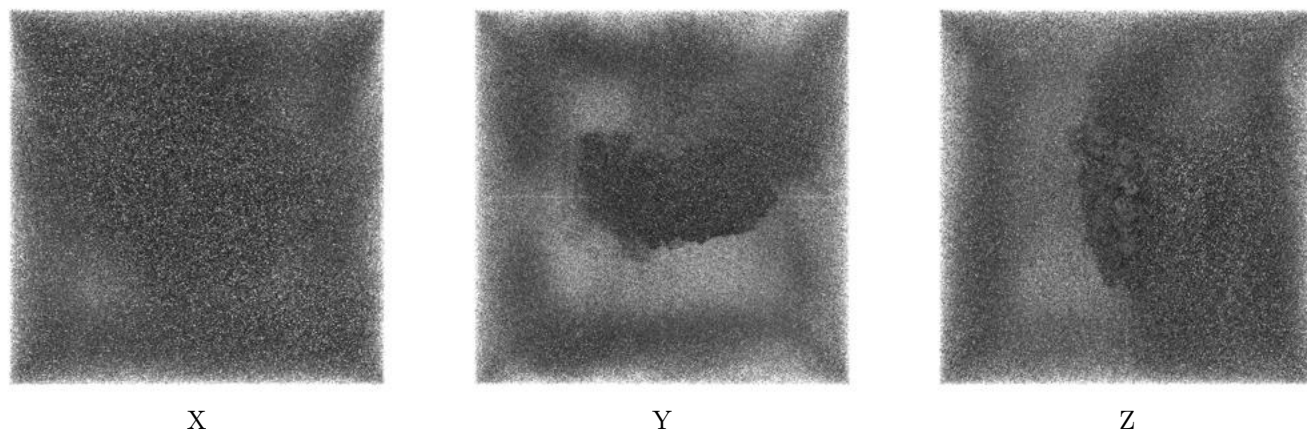
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. 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.

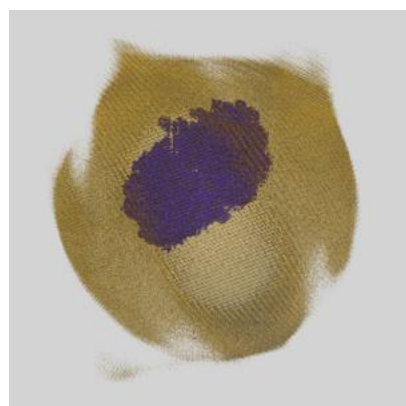
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

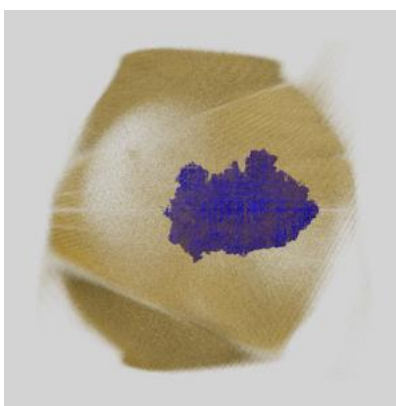
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

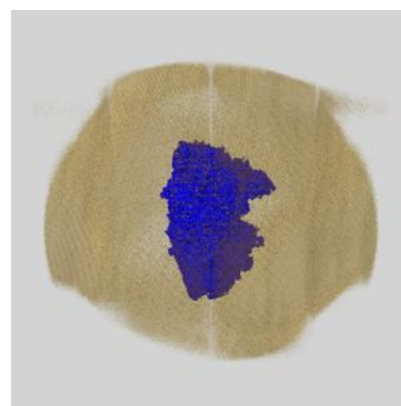
6.6.1 emd_15867_msk_1.map [i](#)



X



Y

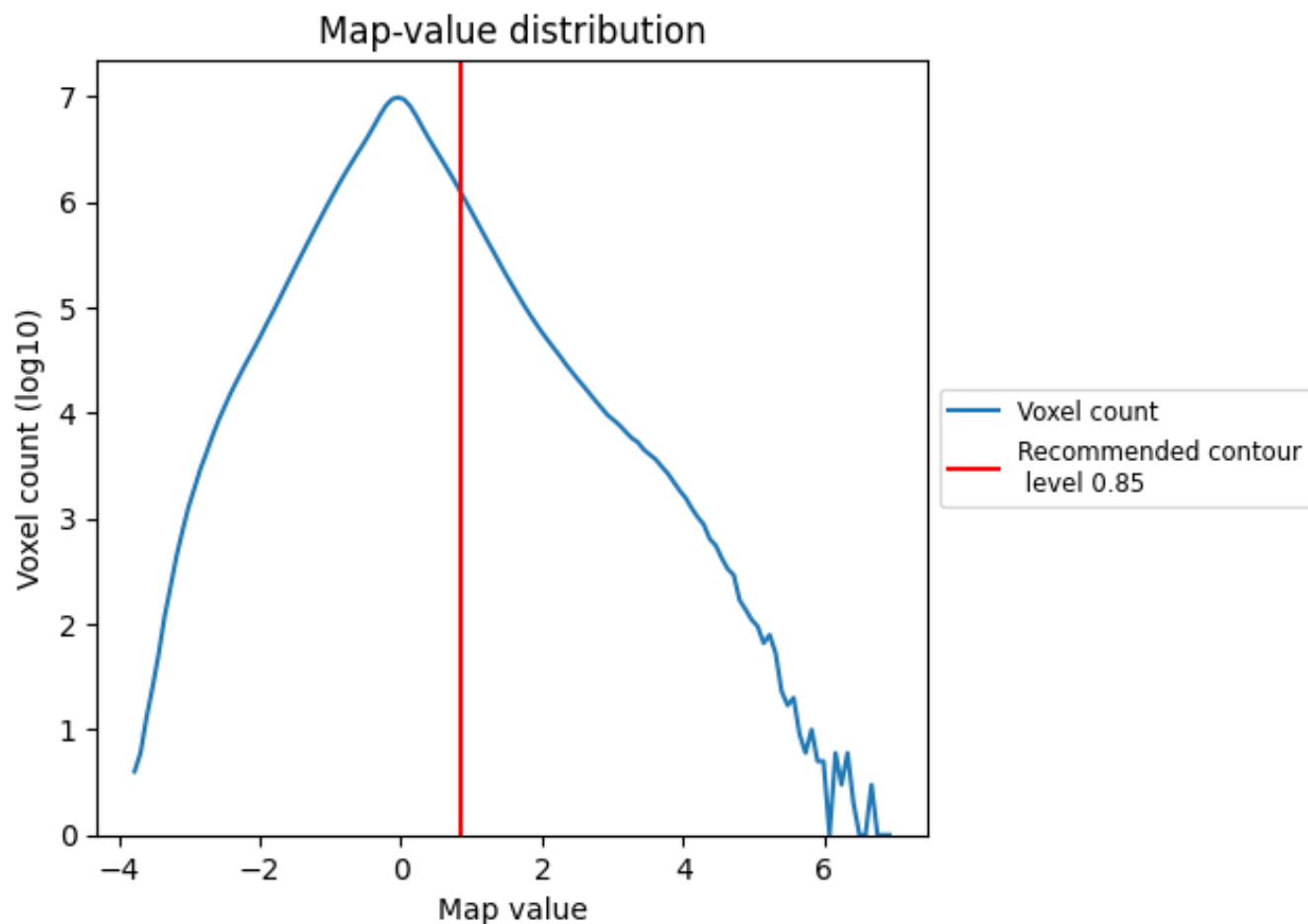


Z

7 Map analysis [i](#)

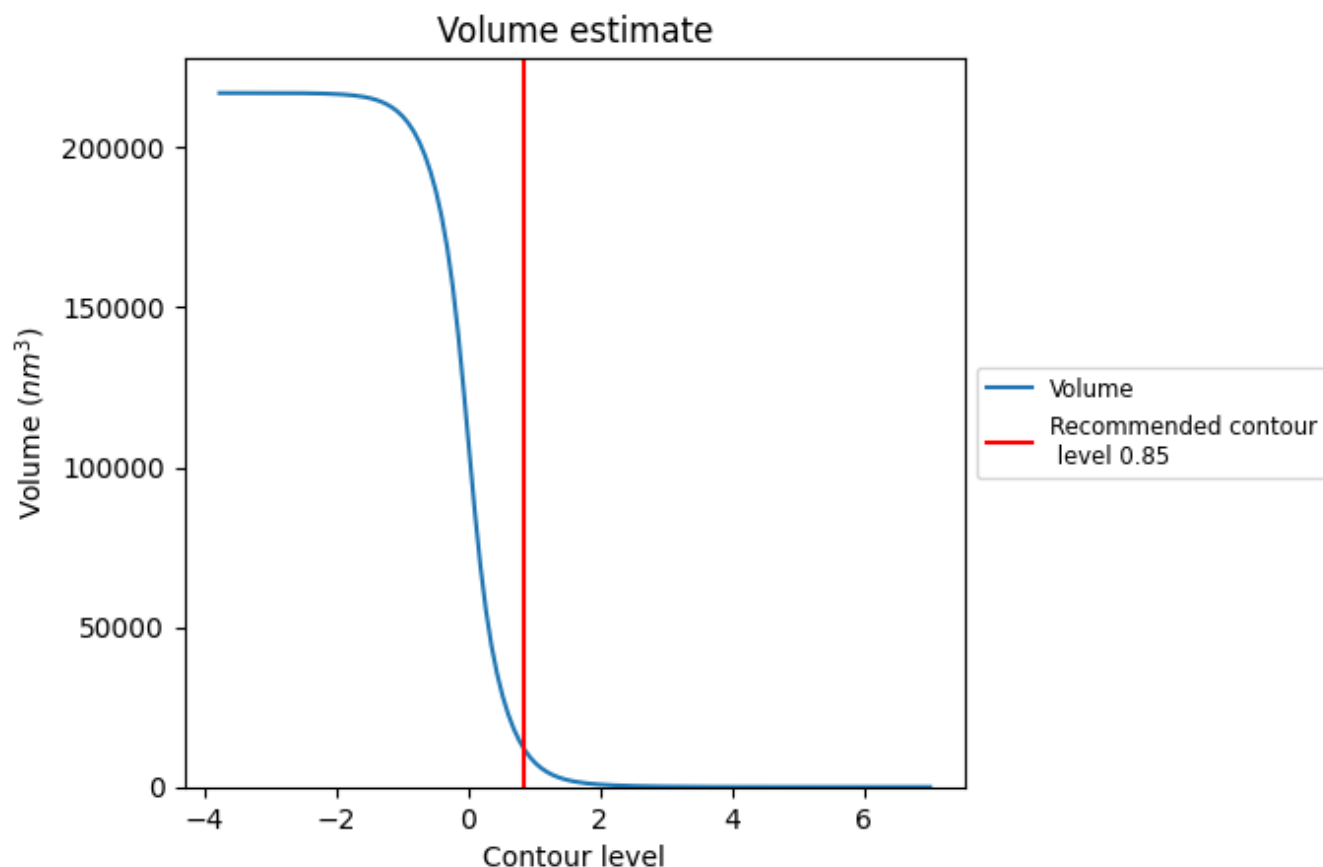
This section contains the results of statistical analysis of the map.

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.

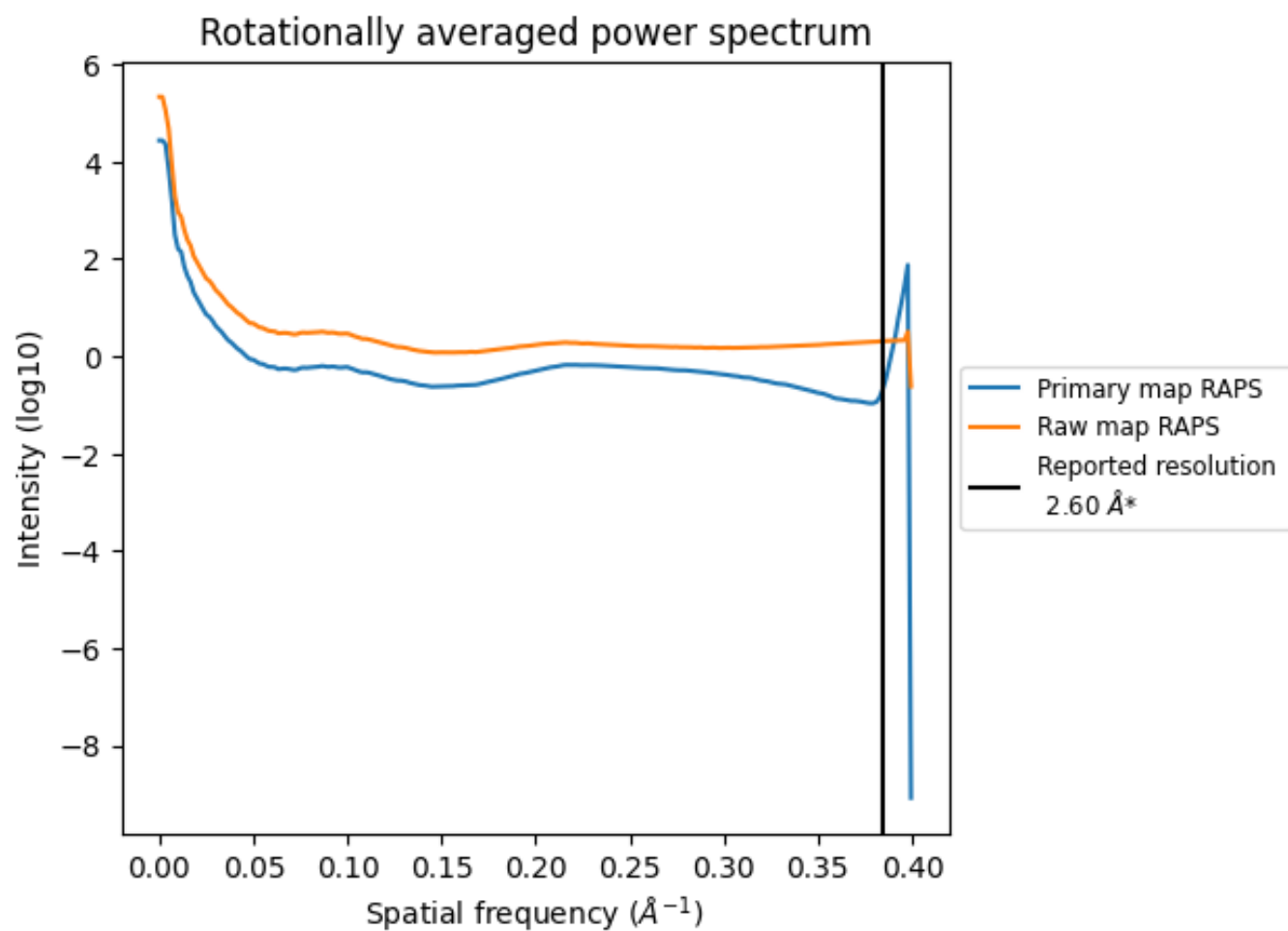
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11769 nm³; this corresponds to an approximate mass of 10631 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 ⓘ

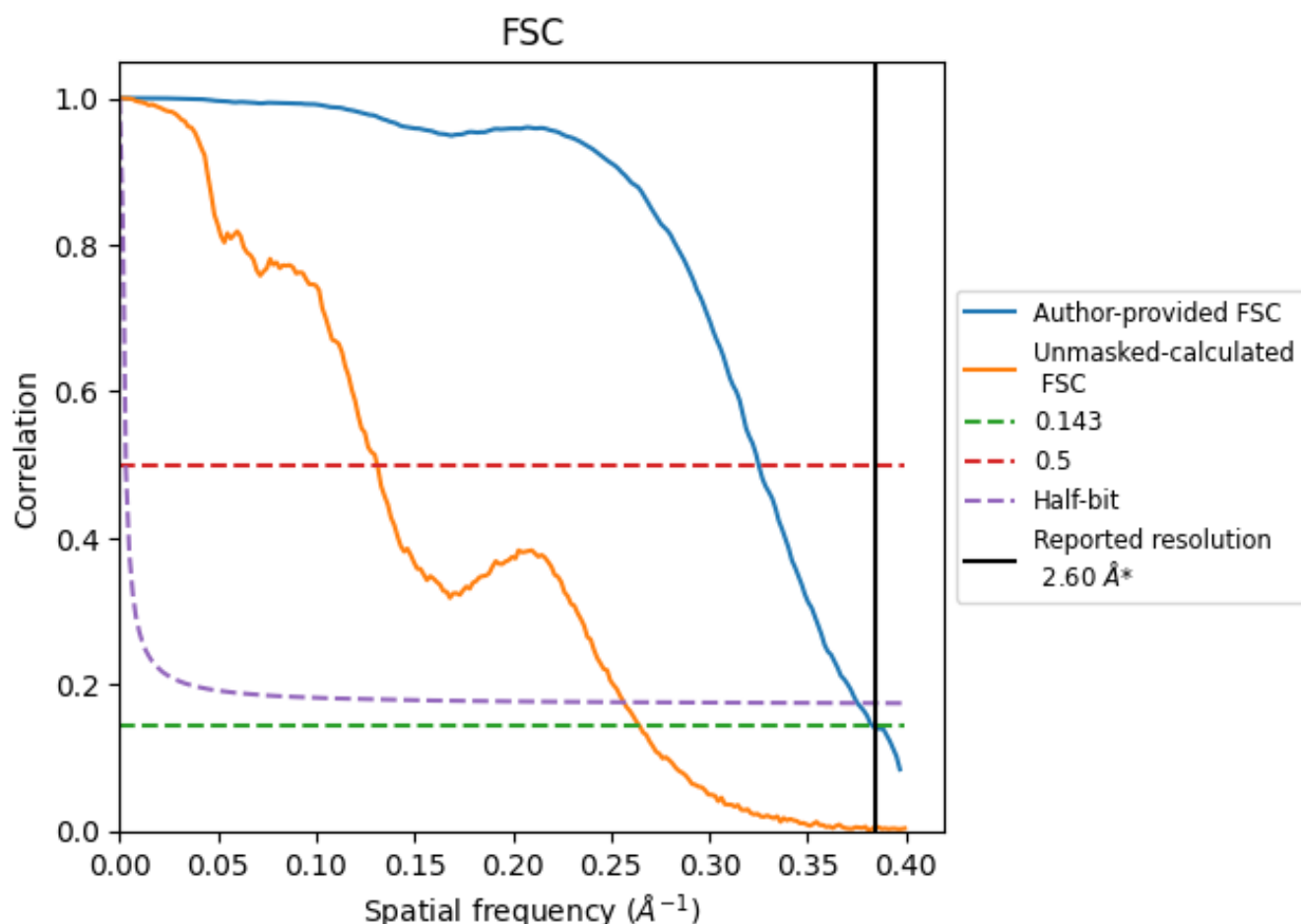


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

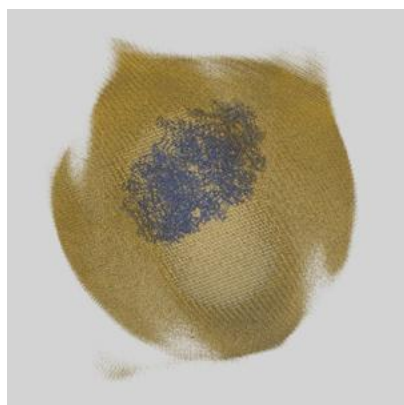
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	3.08	2.66
Unmasked-calculated*	3.78	7.63	3.90

*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 3.78 differs from the reported value 2.6 by more than 10 %

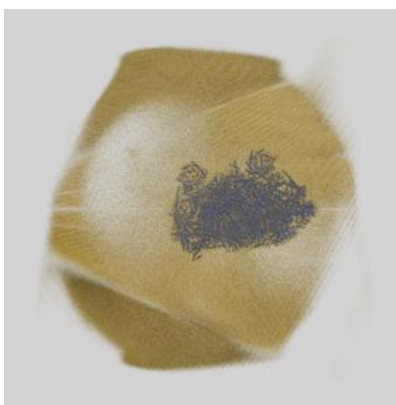
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15867 and PDB model 8B6H. Per-residue inclusion information can be found in section [3](#) on page [35](#).

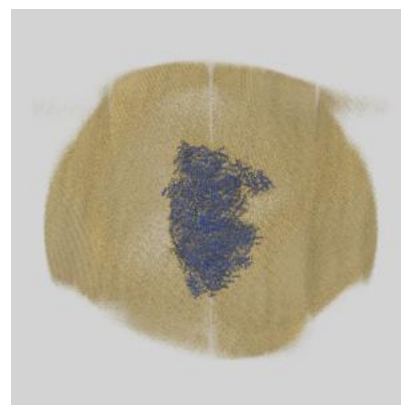
9.1 Map-model overlay [i](#)



X



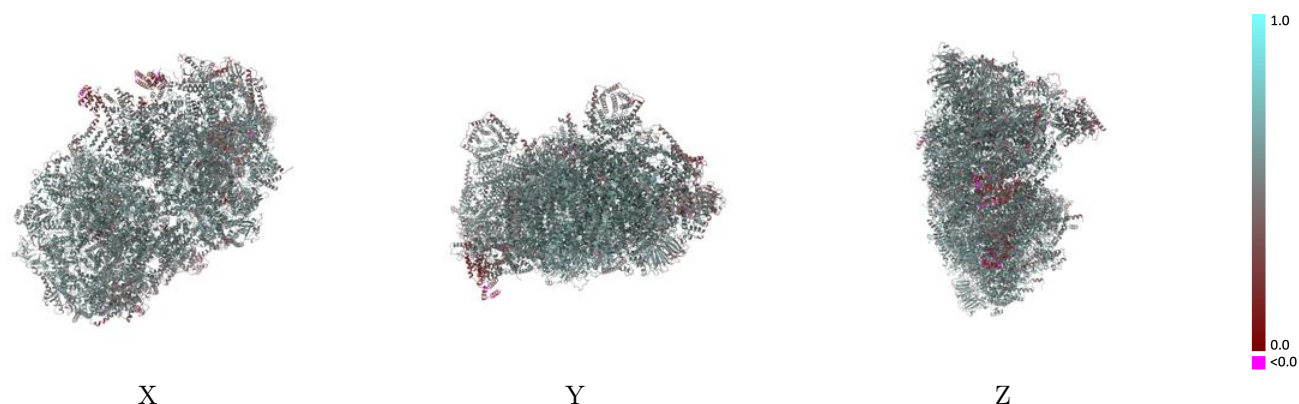
Y



Z

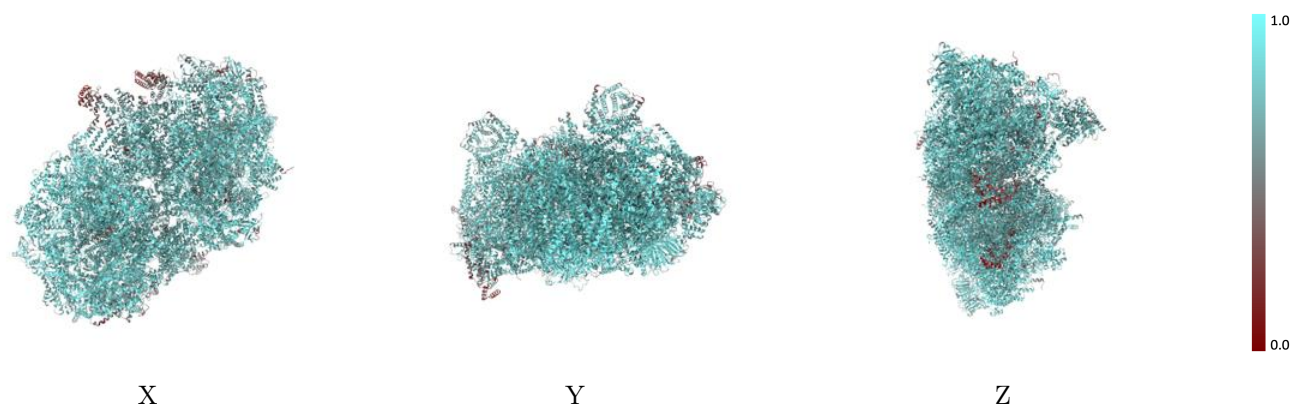
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



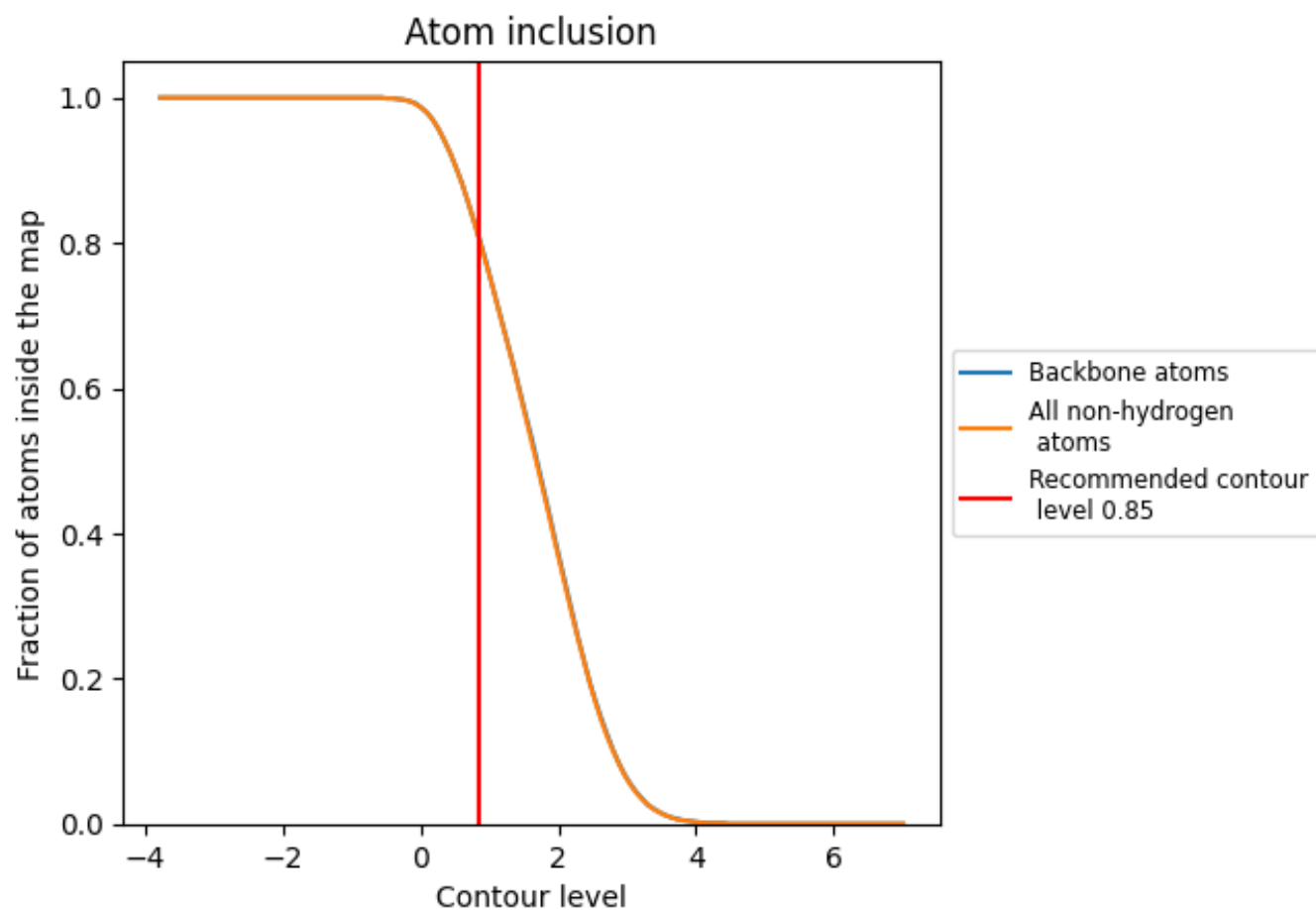
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.5310
DA	 0.8810	 0.5710
DB	 0.8500	 0.5430
DC	 0.8300	 0.5390
DD	 0.8510	 0.5550
DE	 0.8880	 0.5740
DF	 0.8890	 0.5670
DG	 0.7980	 0.5330
DH	 0.8850	 0.5740
DI	 0.8520	 0.5570
DJ	 0.7770	 0.5310
DK	 0.8630	 0.5500
DL	 0.8360	 0.5440
DM	 0.8640	 0.5680
DN	 0.7760	 0.5020
DO	 0.6980	 0.4450
DP	 0.8050	 0.5130
DQ	 0.8430	 0.5560
DR	 0.8460	 0.5530
DS	 0.8390	 0.5470
DT	 0.9000	 0.5850
DU	 0.8200	 0.5360
DV	 0.8040	 0.5240
DW	 0.7730	 0.4920
DX	 0.7740	 0.5200
DY	 0.8330	 0.5420
DZ	 0.8440	 0.5570
Da	 0.8890	 0.5800
Db	 0.8280	 0.5440
Dc	 0.8030	 0.5240
Dd	 0.8080	 0.5320
De	 0.8870	 0.5650
Df	 0.8780	 0.5640
Dg	 0.8040	 0.5350
Dh	 0.8330	 0.5540































































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Chain	Atom inclusion	Q-score
Di	 0.8280	 0.5500
Dj	 0.7660	 0.5300
Dk	 0.8440	 0.5420
Dl	 0.8090	 0.5110
Dm	 0.8380	 0.5440
Dn	 0.7040	 0.4610
Do	 0.5570	 0.3840
Dp	 0.7700	 0.4890
Dq	 0.8230	 0.5440
Dr	 0.8630	 0.5640
Ds	 0.8650	 0.5640
Dt	 0.8970	 0.5890
Du	 0.7640	 0.5150
Dv	 0.7940	 0.5110
Dw	 0.7680	 0.5000
Dx	 0.7520	 0.5130
Dy	 0.8110	 0.5200
Dz	 0.8030	 0.5230
EA	 0.8070	 0.5260
EB	 0.8090	 0.5290
EC	 0.6260	 0.3840
ED	 0.7530	 0.5100
EE	 0.8440	 0.5340
EF	 0.9090	 0.5870
EG	 0.8710	 0.5720
EH	 0.8430	 0.5530
EI	 0.8310	 0.5470
EJ	 0.8560	 0.5500
EK	 0.8080	 0.5280
EL	 0.7890	 0.5330
EM	 0.8530	 0.5510
EN	 0.8270	 0.5410
EO	 0.7610	 0.5170
EP	 0.8910	 0.5920
EQ	 0.9210	 0.5850
ER	 0.9190	 0.5840
ES	 0.9060	 0.5920
ET	 0.6820	 0.4310
EU	 0.7770	 0.5170
EV	 0.8080	 0.5100
EW	 0.7410	 0.4740
EX	 0.7180	 0.4750

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Continued from previous page...

Chain	Atom inclusion	Q-score
EY	 0.7590	 0.4680
EZ	 0.8090	 0.5170
Ea	 0.7830	 0.5220
Eb	 0.8310	 0.5440
Ec	 0.4840	 0.3370
Ed	 0.6940	 0.4880
Ee	 0.8170	 0.5240
Ef	 0.8900	 0.5800
Eg	 0.7810	 0.5430
Eh	 0.8540	 0.5680
Ei	 0.7960	 0.5310
Ej	 0.7740	 0.4980
Ek	 0.7820	 0.5210
El	 0.7810	 0.5470
Em	 0.8570	 0.5550
En	 0.8240	 0.5480
Eo	 0.7860	 0.5290
Ep	 0.8270	 0.5520
Eq	 0.8960	 0.5810
Er	 0.9110	 0.6000
Es	 0.8860	 0.5860
Et	 0.6830	 0.4060
Eu	 0.7390	 0.5030
Ev	 0.8100	 0.5100
Ew	 0.7000	 0.4350
Ex	 0.6710	 0.4530
Ey	 0.7090	 0.4490
Ez	 0.7880	 0.5110
FA	 0.8150	 0.5050
Fa	 0.7740	 0.4920