



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 02:02 pm BST

PDB ID : 8B6H / pdb_00008b6h
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:

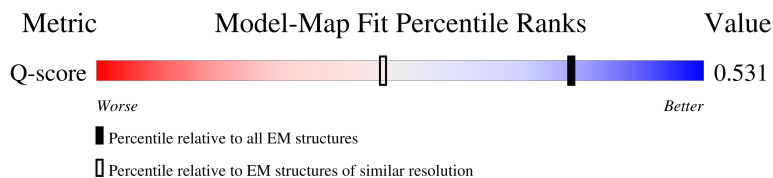
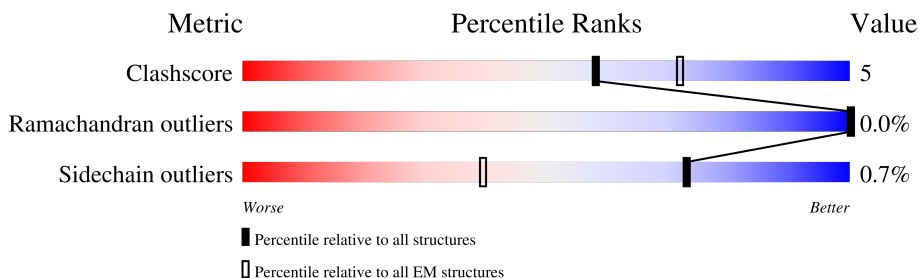
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	
1	Da	688	
2	DB	604	
2	Db	604	

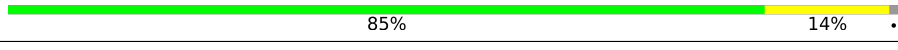
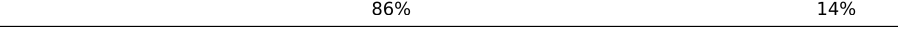
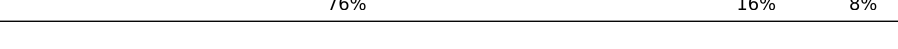
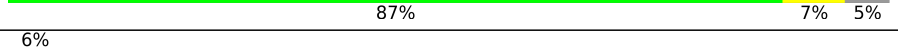
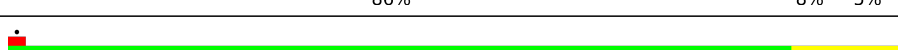
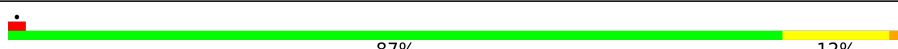
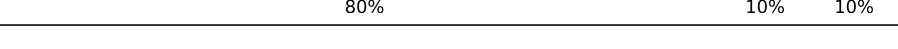
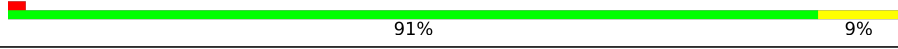
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Mol	Chain	Length	Quality of chain
3	DC	594	
3	Dc	594	
4	DD	637	
4	Dd	637	
5	DE	130	
5	De	130	
6	DF	230	
6	Df	230	
7	DG	103	
7	Dg	103	
8	DH	133	
8	Dh	133	
9	DI	236	
9	Di	236	
10	DJ	220	
10	Dj	220	
11	DK	990	
11	Dk	990	
12	DM	490	
12	Dm	490	
13	DN	453	
13	Dn	453	
14	DO	473	
14	Do	473	
15	DP	402	

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Mol	Chain	Length	Quality of chain
15	Dp	402	
16	DQ	385	
16	Dq	385	
17	DR	348	
17	Dr	348	
18	DS	346	
18	Ds	346	
19	DT	318	
19	Dt	318	
20	DU	330	
20	Du	330	
21	DV	318	
21	Dv	318	
22	DW	318	
22	Dw	318	
23	DX	252	
23	Dx	252	
24	DY	234	
24	Dy	234	
25	DZ	231	
25	Dz	231	
26	EA	215	
26	Ea	215	
27	EB	210	
27	Eb	210	

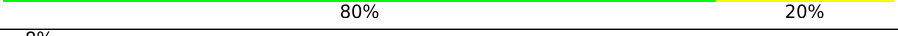
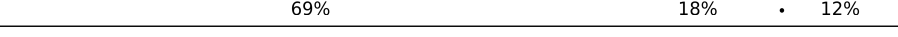
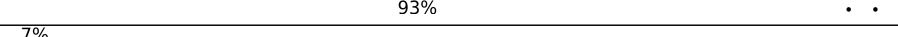
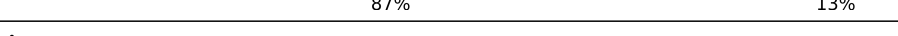
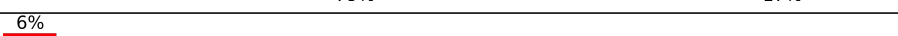
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Mol	Chain	Length	Quality of chain
28	EC	212	
28	Ec	212	
29	ED	190	
29	Ed	190	
30	EE	193	
30	Ee	193	
31	EF	188	
31	Ef	188	
32	EG	100	
32	Eg	100	
33	EH	173	
33	Eh	173	
34	EI	173	
34	Ei	173	
35	EV	88	
35	Ev	88	
36	EK	170	
36	Ek	170	
37	EL	158	
37	El	158	
38	EM	154	
38	Em	154	
39	EN	149	
39	En	149	
40	EO	124	

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Mol	Chain	Length	Quality of chain
40	Eo	124	
41	EP	127	
41	Ep	127	
42	EQ	122	
42	Eq	122	
43	ER	105	
43	Er	105	
44	ES	89	
44	Es	89	
45	ET	93	
45	Et	93	
46	EU	90	
46	Eu	90	
47	EJ	175	
47	Ej	175	
48	EW	81	
48	Ew	81	
49	EX	72	
49	Ex	72	
50	EY	72	
50	Ey	72	
51	EZ	68	
51	Ez	68	
52	FA	72	
52	Fa	72	

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Mol	Chain	Length	Quality of chain
53	DL	536	 63% 8% 29%
53	Dl	536	 62% 9% 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	C	H	N	O	S	0	0
			3296	1084	1637	283	290	2		
26	Ea	193	Total	C	H	N	O	S	0	0
			3296	1084	1637	283	290	2		

- 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 Yft 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		

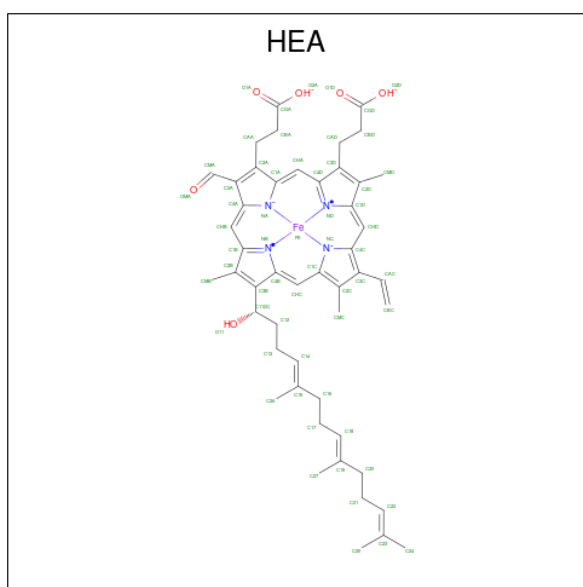
- Molecule 52 is a protein called Tim10/DDP family zinc finger protein.

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 (CCD ID: 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 (CCD ID: CU) (formula: Cu) (labeled as "Ligand of

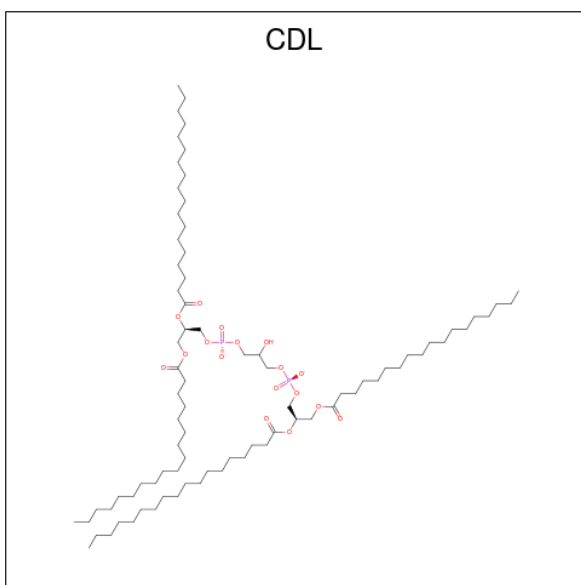
Interest" by depositor).

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 (CCD ID: 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 (CCD ID: 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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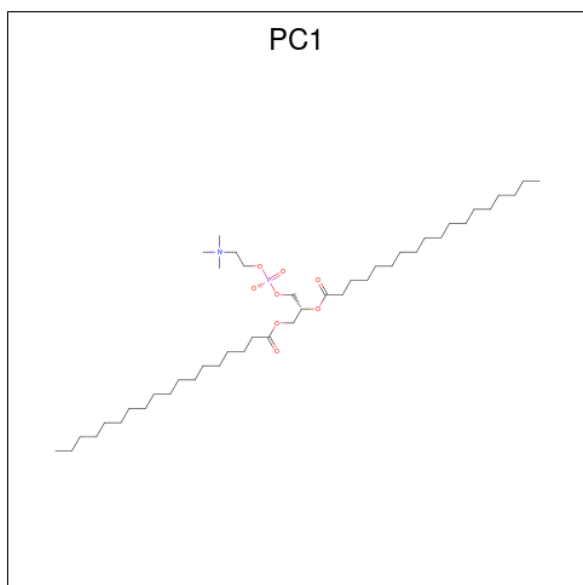
Mol	Chain	Residues	Atoms					AltConf
57	Dr	1	Total 256	C 81	H 156	O 17	P 2	0
57	Dr	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17	P 2	0
57	Ds	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 156	O 17	P 2	0
57	Du	1	Total 256	C 81	H 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	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 (CCD ID: 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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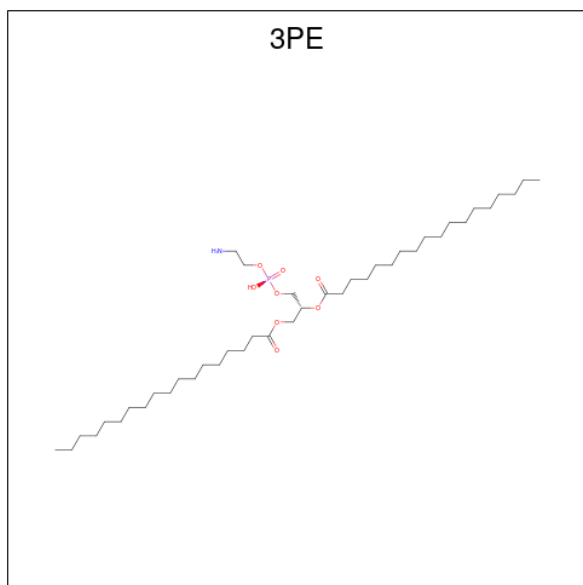
Mol	Chain	Residues	Atoms						AltConf
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	EO	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Da	1	Total 141	C 44	H 87	N 1	O 8	P 1	0
58	Da	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Db	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
58	Dc	1	Total 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 (CCD ID: 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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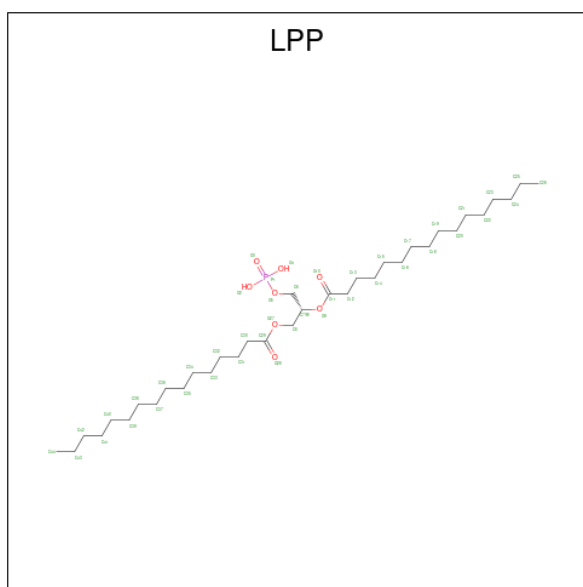
Mol	Chain	Residues	Atoms						AltConf
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DC	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DG	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DJ	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DR	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
59	DS	1	Total 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 (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).

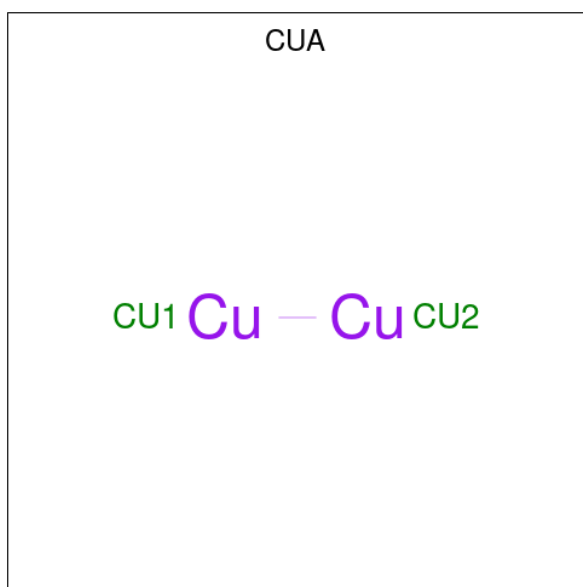


Mol	Chain	Residues	Atoms					AltConf
60	DA	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	DN	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	EI	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Dn	1	Total	C	H	O	P	0
			111	35	67	8	1	
60	Ed	1	Total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

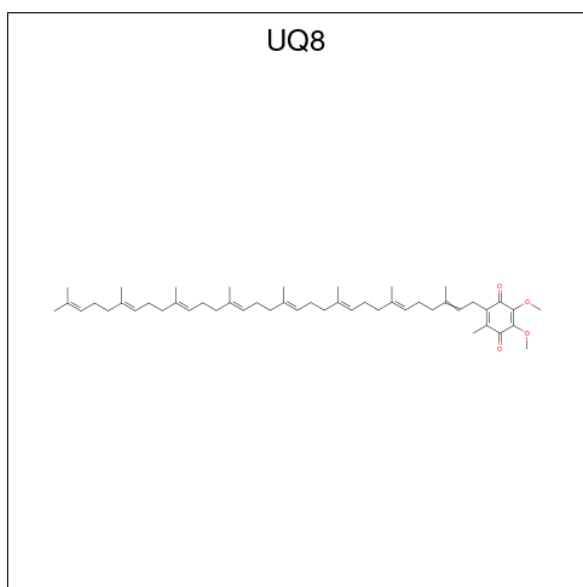
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

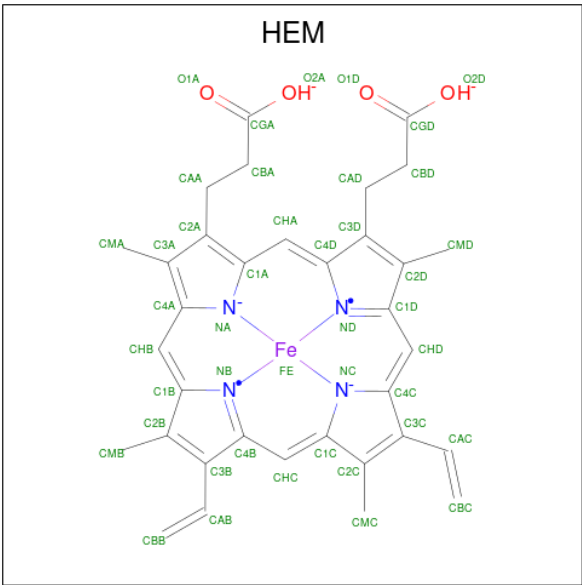
Mol	Chain	Residues	Atoms		AltConf
64	DD	1	Total	K	0
			1	1	

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



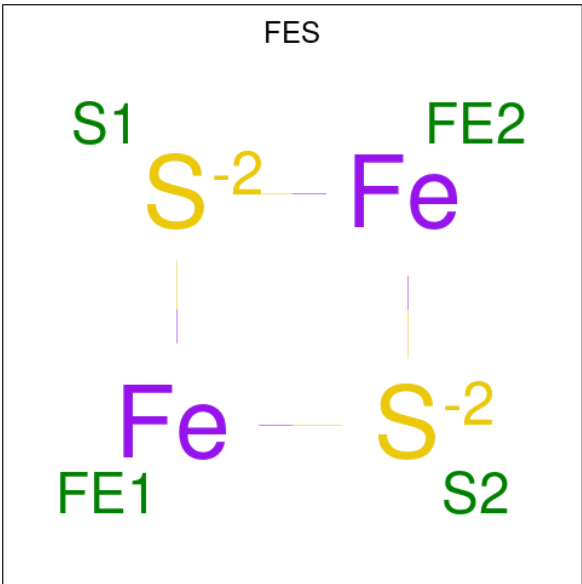
Mol	Chain	Residues	Atoms				AltConf
65	DS	1	Total	C	H	O	0
			127	49	74	4	
65	ED	1	Total	C	H	O	0
			127	49	74	4	
65	EL	1	Total	C	H	O	0
			127	49	74	4	
65	EN	1	Total	C	H	O	0
			127	49	74	4	
65	Ds	1	Total	C	H	O	0
			127	49	74	4	
65	Ed	1	Total	C	H	O	0
			127	49	74	4	
65	El	1	Total	C	H	O	0
			127	49	74	4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

- Molecule 66 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



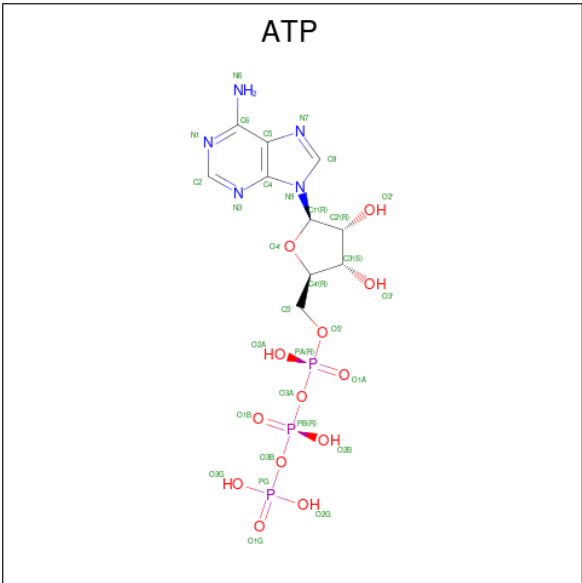
Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

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	

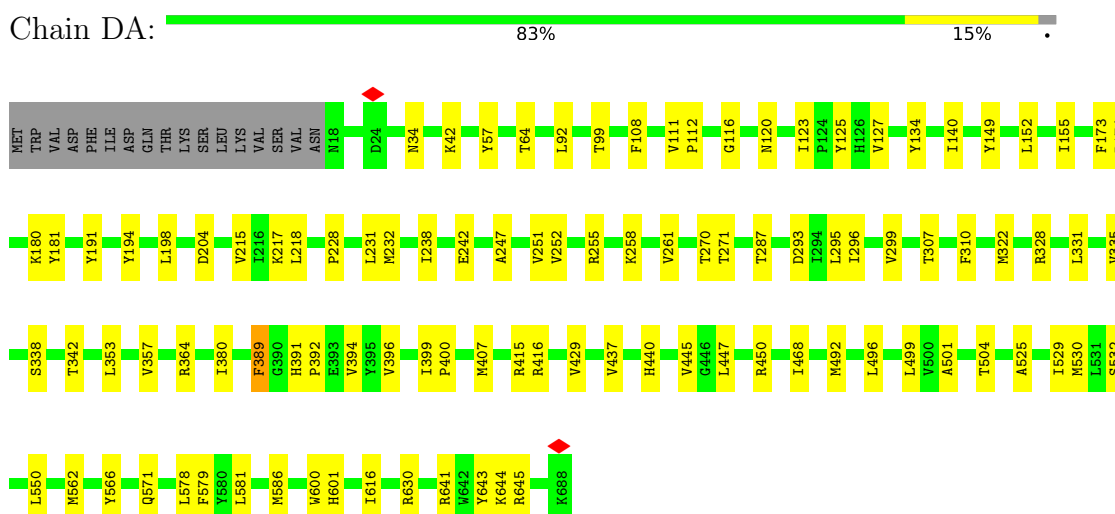
- Molecule 68 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



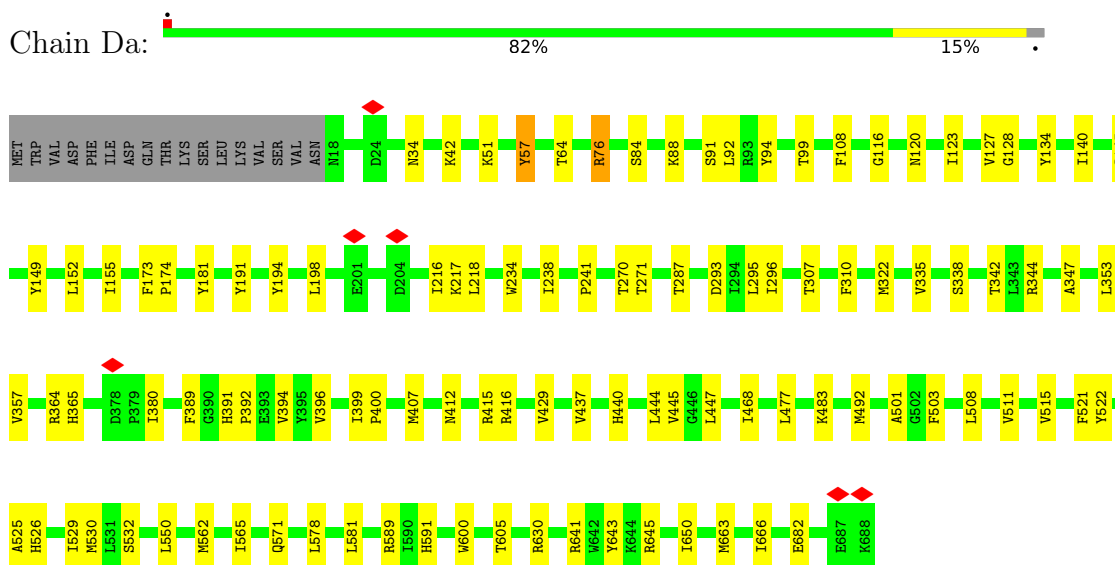
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

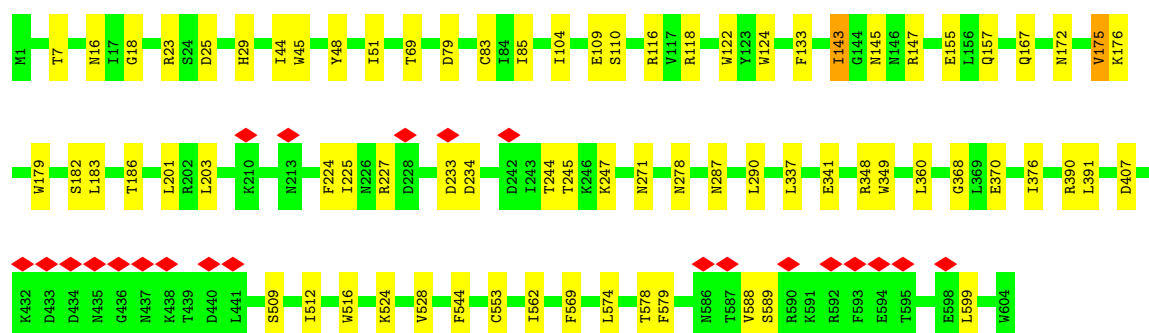


• Molecule 1: Cytochrome c oxidase subunit 1



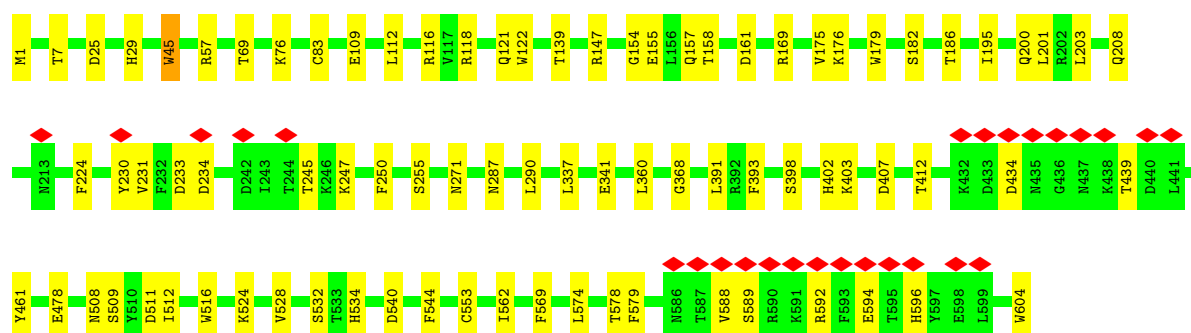
• Molecule 2: Cytochrome c oxidase subunit 2

Chain DB:  88% 12%



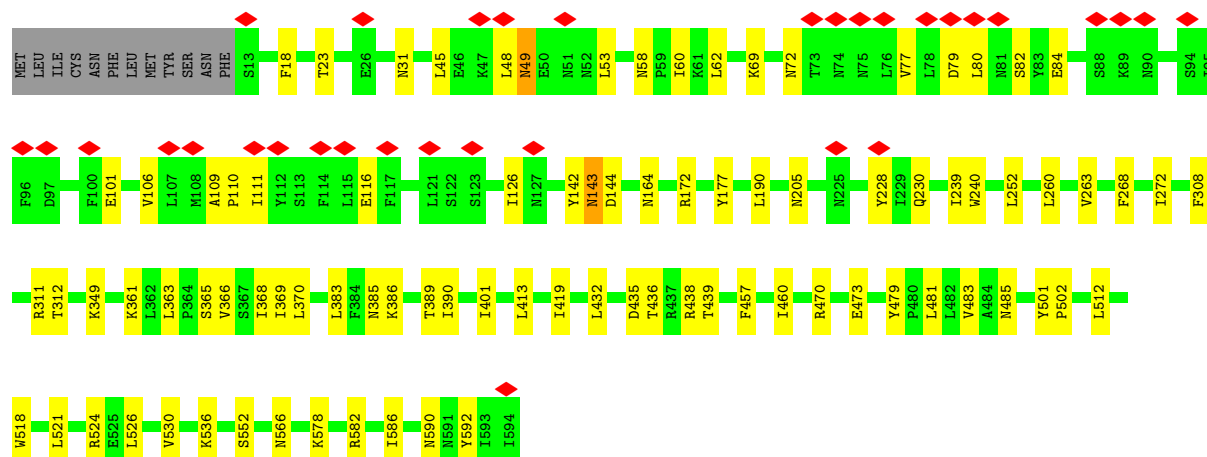
• Molecule 2: Cytochrome c oxidase subunit 2

Chain Db:  86% 14%



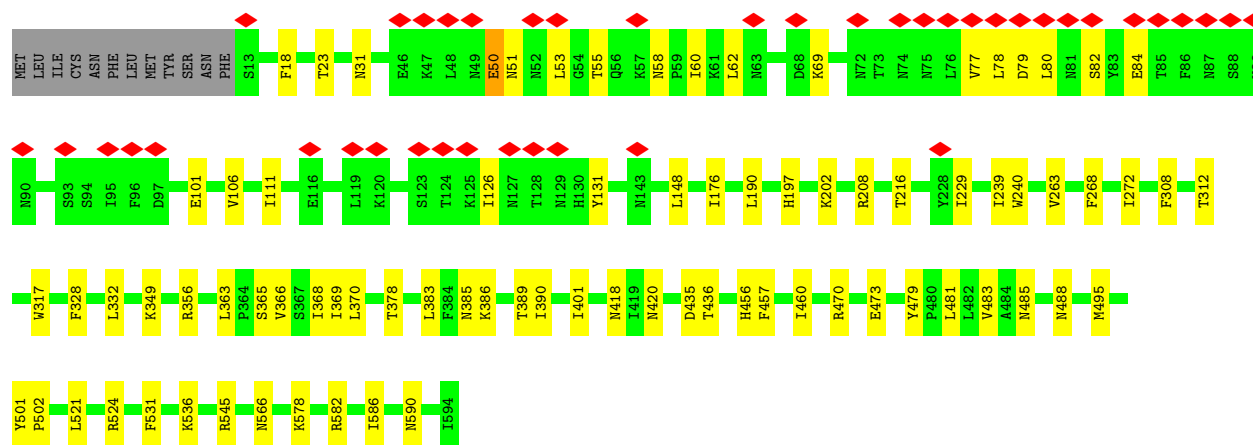
• Molecule 3: Ymf68

Chain DC:  6% 83% 15%



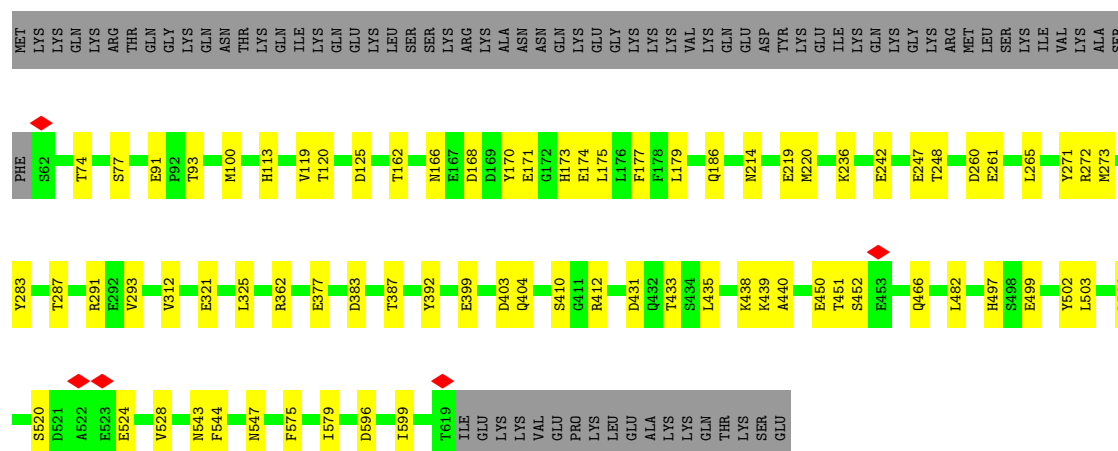
• Molecule 3: Ymf68

Chain Dc:  7% 84% 14%



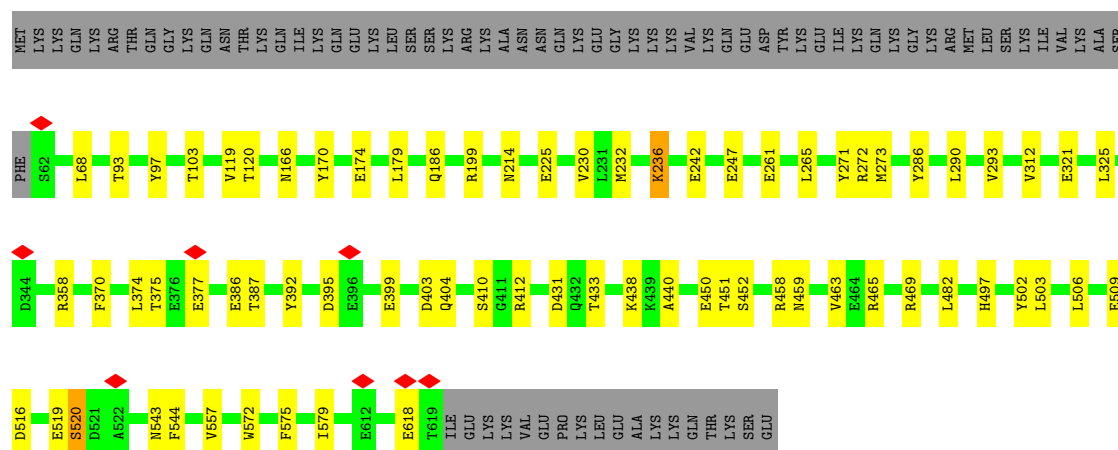
• Molecule 4: Cytochrome C oxidase subunit Vb protein

Chain DD: 76% 12% 12%

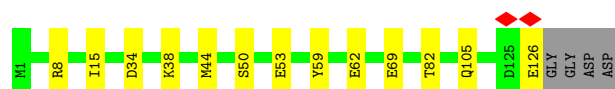


• Molecule 4: Cytochrome C oxidase subunit Vb protein

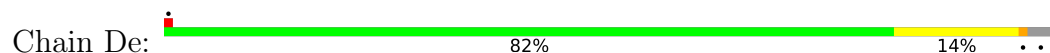
Chain Dd: 76% 11% 12%



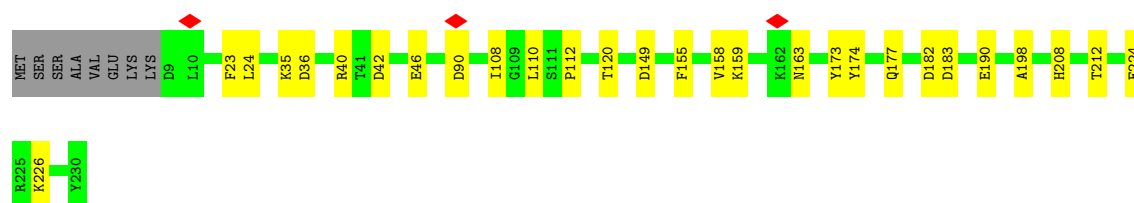
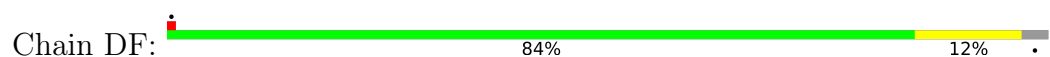
• Molecule 5: Transmembrane protein, putative



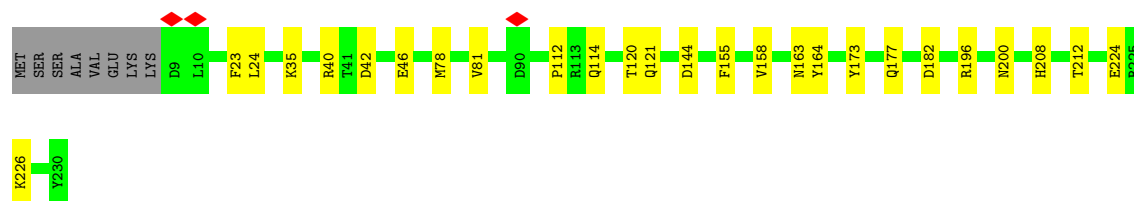
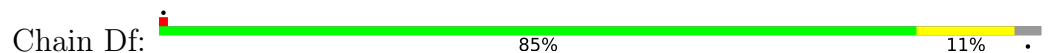
- Molecule 5: Transmembrane protein, putative



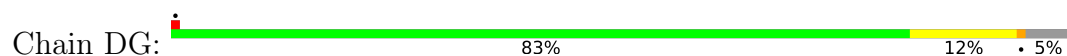
- Molecule 6: Structural protein



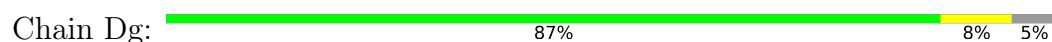
- Molecule 6: Structural protein



- Molecule 7: Transmembrane protein, putative

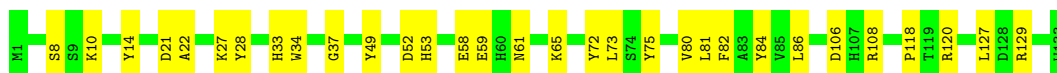


- Molecule 7: Transmembrane protein, putative



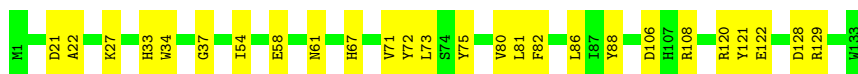
- Molecule 8: Transmembrane protein, putative

Chain DH:  77% 23%



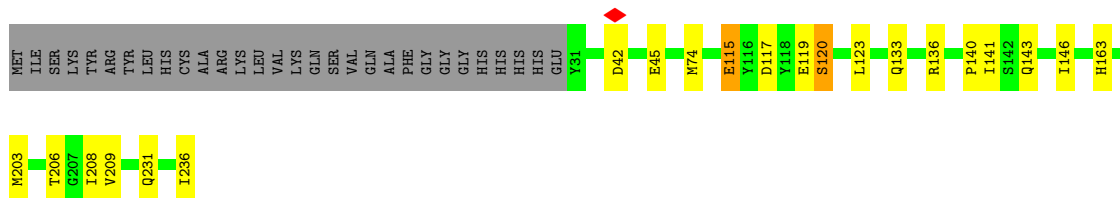
- Molecule 8: Transmembrane protein, putative

Chain Dh:  80% 20%



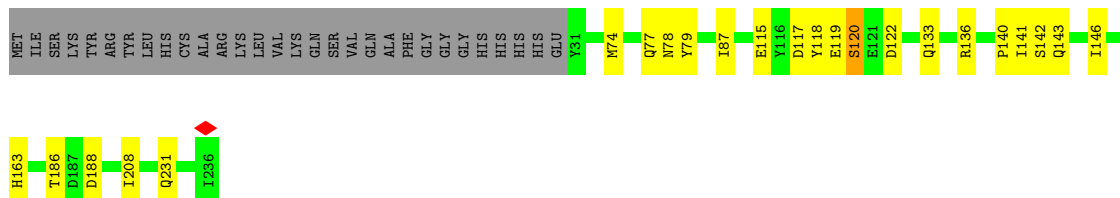
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:  78% 8% 13%



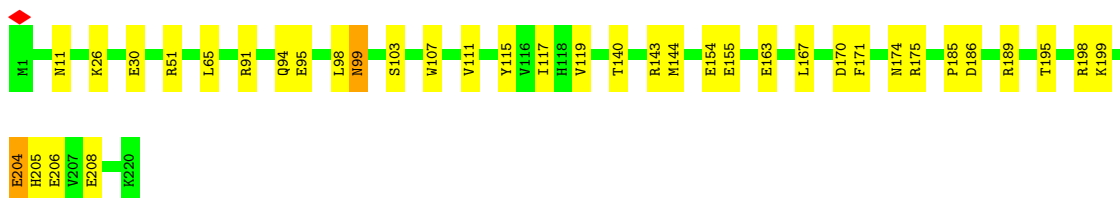
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Di:  78% 9% 13%



- Molecule 10: Transmembrane protein, putative

Chain DJ:  83% 16% 1%



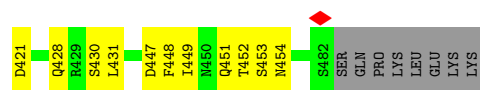
- Molecule 10: Transmembrane protein, putative

Chain Dj:  87% 13%

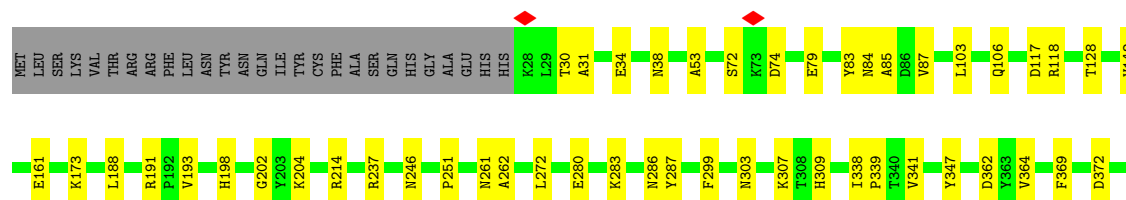
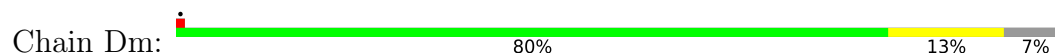
[illegible]

Chain DM: 81% 12% 7%

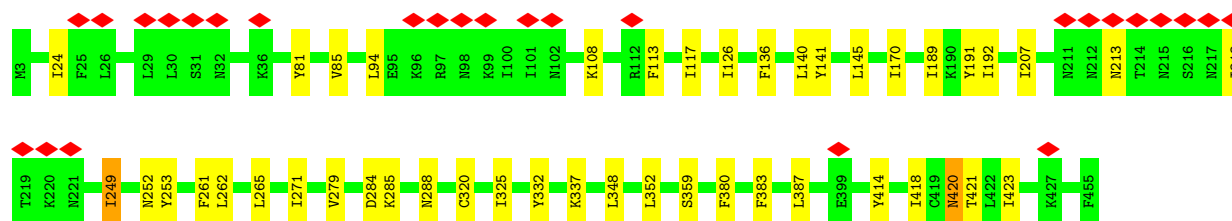
MET	LEU	SER	VAL	THR	ARG	ARG	PHE	LEU	ASN	TTR	ASN	ASN	GLN	TTR	CYS	PHE	ALA	SER	GLN	HIS	GLY	ALA	GLU	HIS	HIS									
Y158	R163	D166	K173	L188	R191	H198	G202	R237	N246	D249	S263	E274	E280	Y298	F299	N303	D317	I338	P339	D362	Y363	V364	V365	R366	V378	T379	R380	T386	E390	V391	Y392	E393	R405	Q414



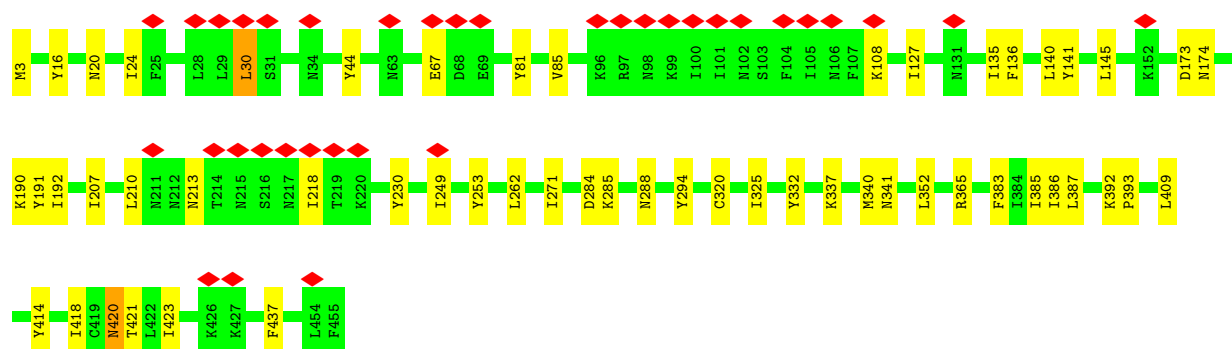
- Molecule 12: Transmembrane protein, putative



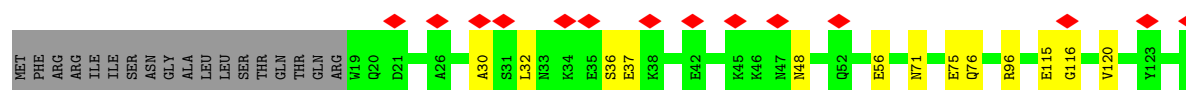
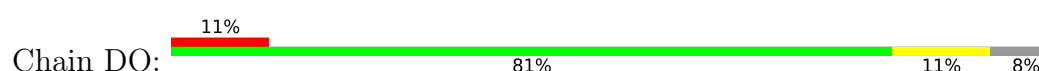
- Molecule 13: Ymf67



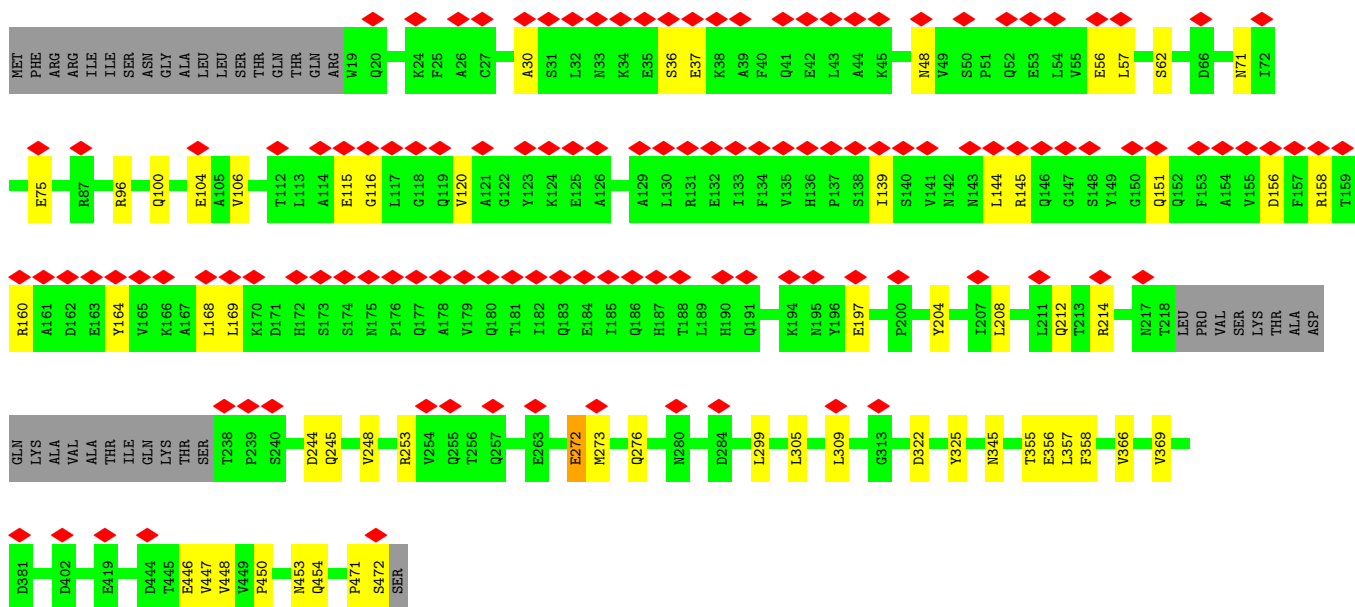
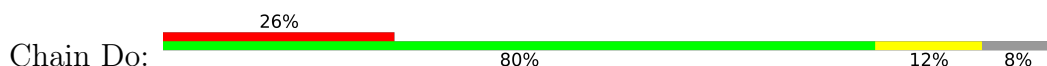
- Molecule 13: Ymf67



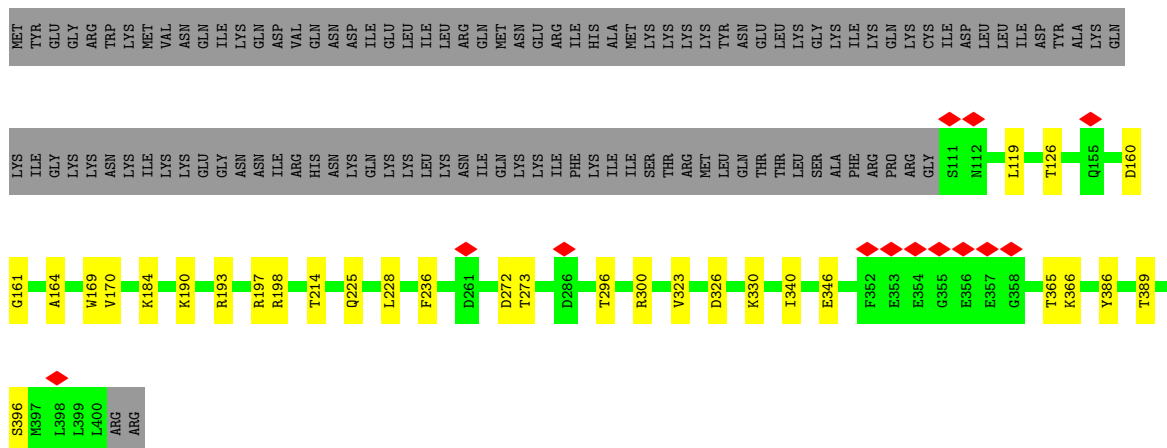
- Molecule 14: Protein phosphatase 2C, putative

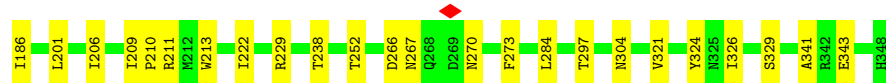


- Molecule 14: Protein phosphatase 2C, putative

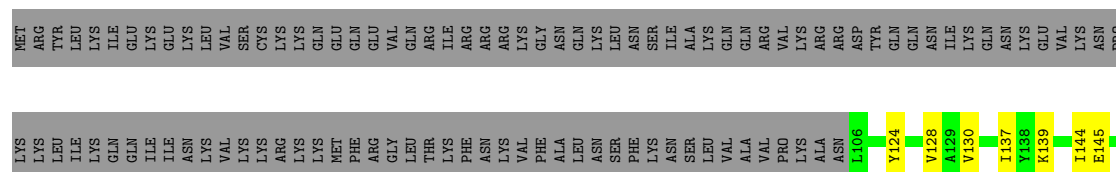


- Molecule 15: SURF1-like protein

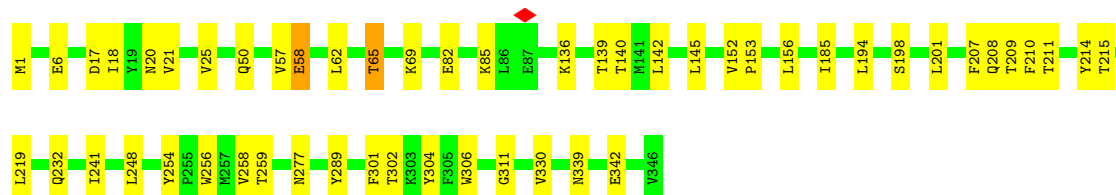
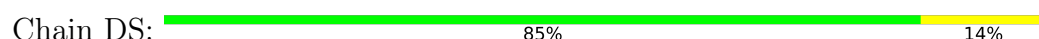




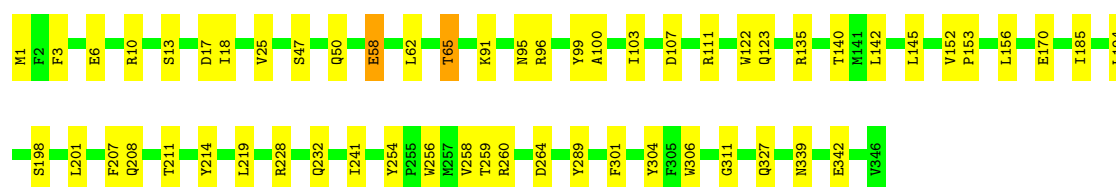
- Molecule 17: Transmembrane protein, putative



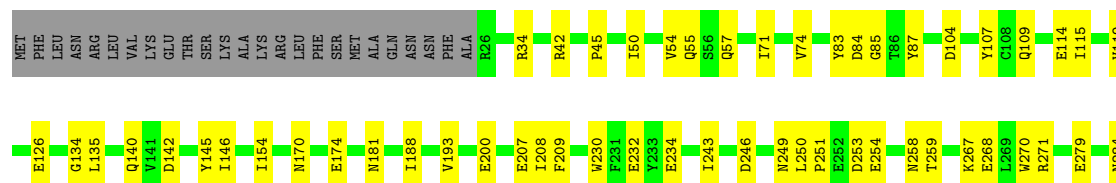
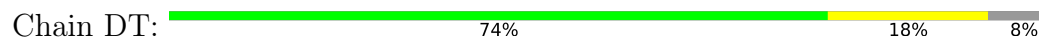
- Molecule 18: Oxoglutarate/malate translocator protein, putative



- Molecule 18: Oxoglutarate/malate translocator protein, putative



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





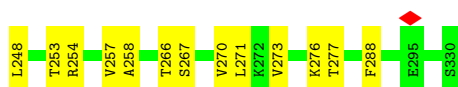
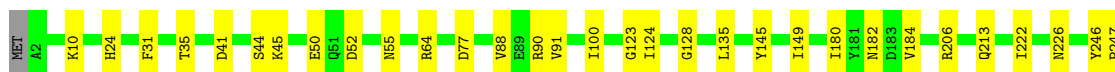
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt: 76% 16% 8%



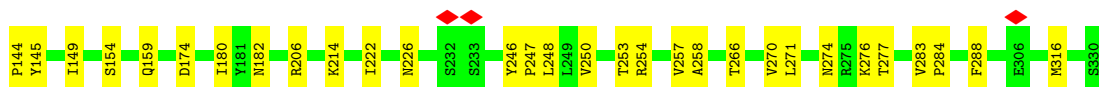
- Molecule 20: Carrier protein

Chain DU: 86% 13%



- Molecule 20: Carrier protein

Chain Du: 81% 18%



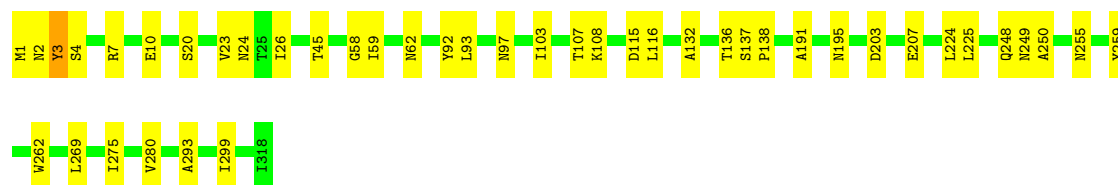
- Molecule 21: 2-oxoglutarate/malate carrier protein

Chain DV: 87% 13%

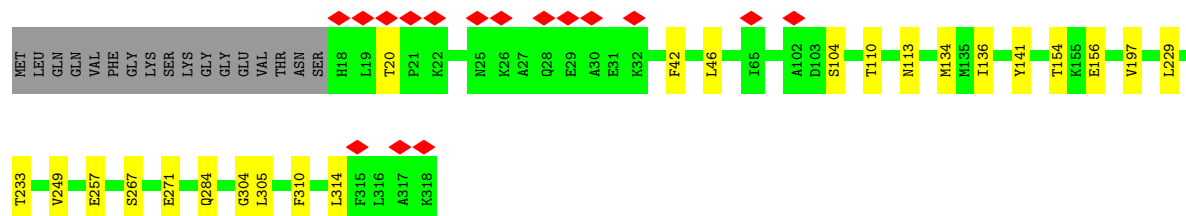
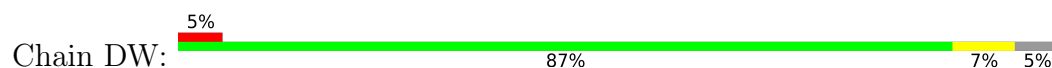


- Molecule 21: 2-oxoglutarate/malate carrier protein

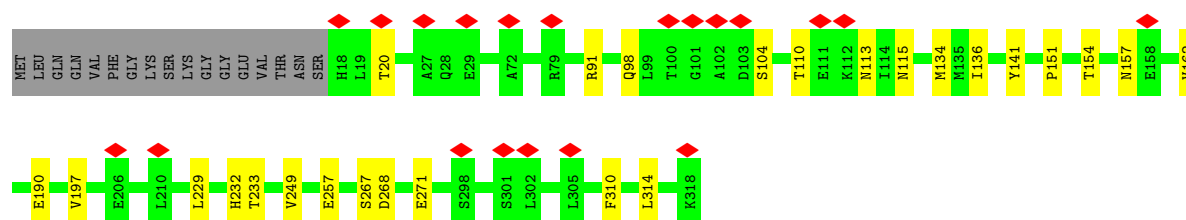
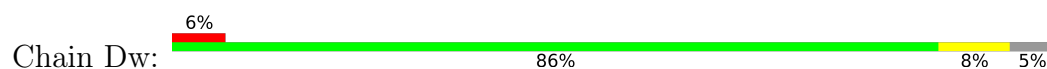
Chain Dv: 86% 13%



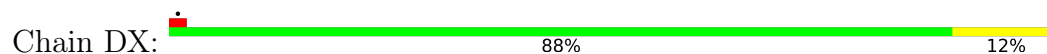
• Molecule 22: SURF1-like protein



• Molecule 22: SURF1-like protein



• Molecule 23: COXTT9

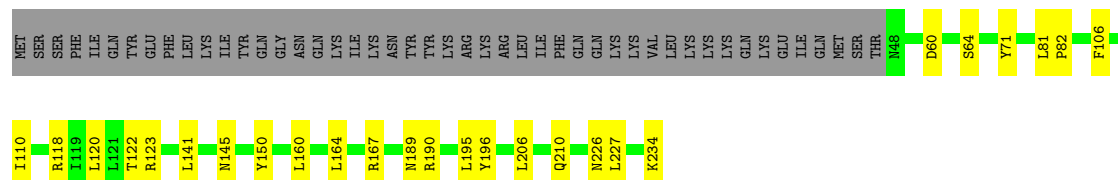


• Molecule 23: COXTT9



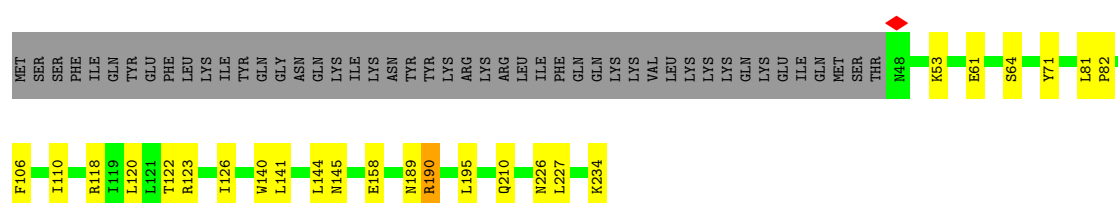
- Molecule 24: COXTT10

Chain DY:  69% 11% 20%



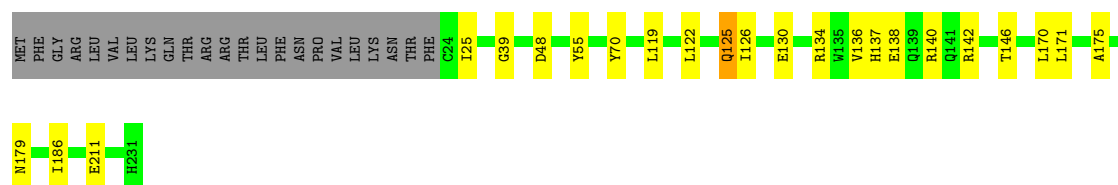
- Molecule 24: COXTT10

Chain Dy:  69% 10% 20%



- Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain DZ:  80% 10% 10%



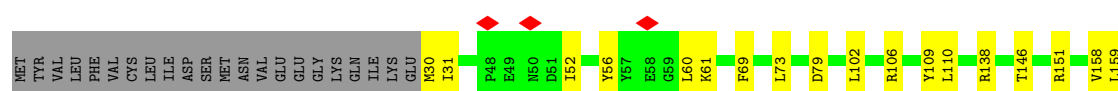
- Molecule 25: 39S ribosomal protein L9, mitochondrial

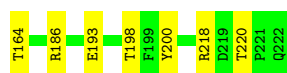
Chain Dz:  75% 15% 10%



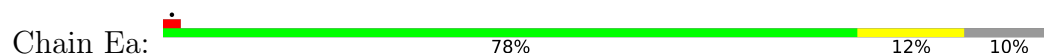
- Molecule 26: COXTT12, Transmembrane protein, Transmembrane protein

Chain EA:  78% 12% 10%





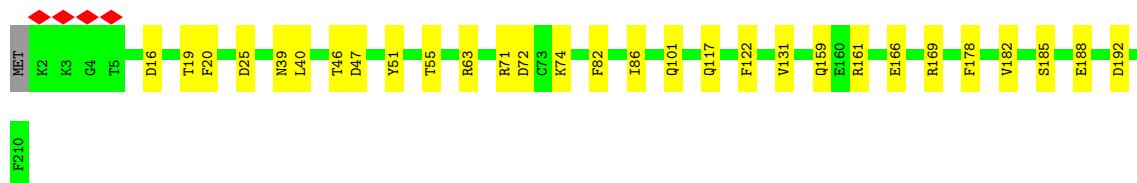
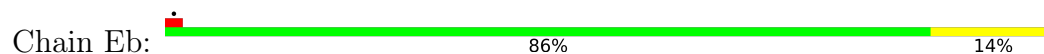
- Molecule 26: COXTT12, Transmembrane protein, Transmembrane protein



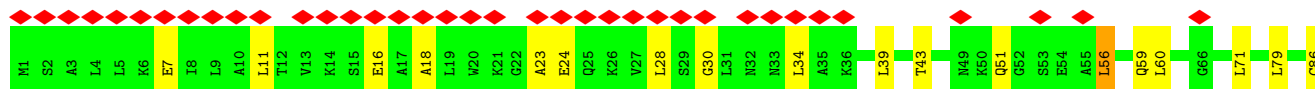
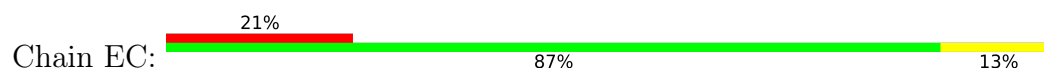
- Molecule 27: Transmembrane protein, putative



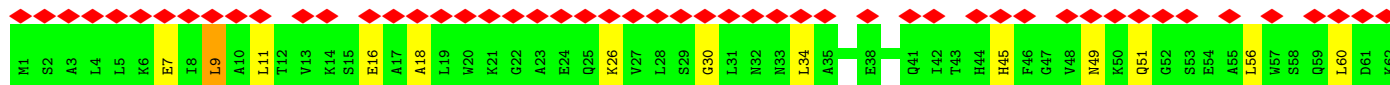
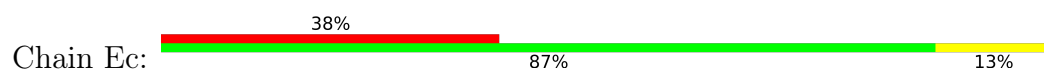
- Molecule 27: Transmembrane protein, putative

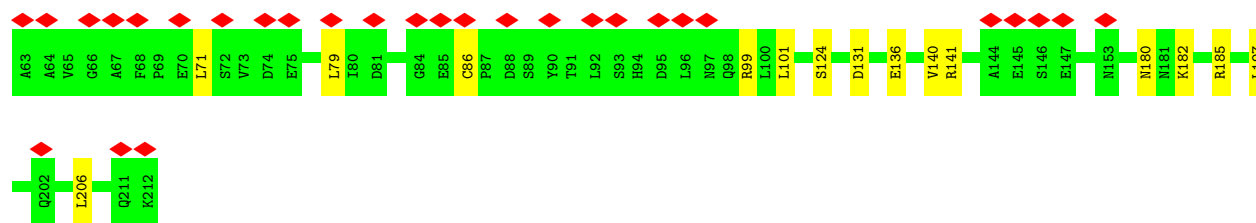


- Molecule 28: COXTT27

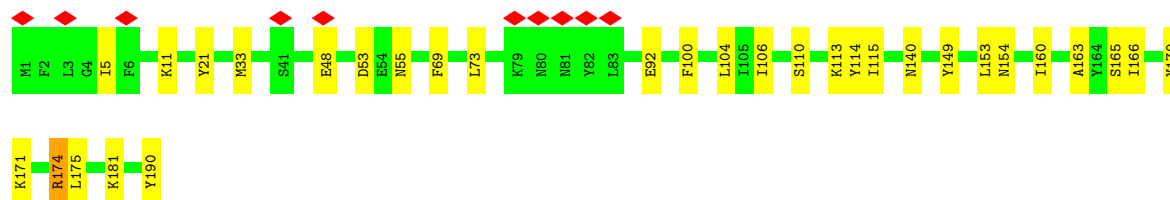
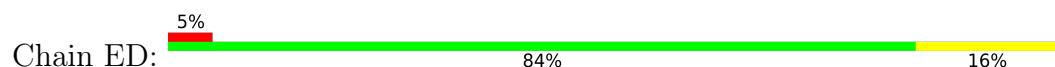


- Molecule 28: COXTT27

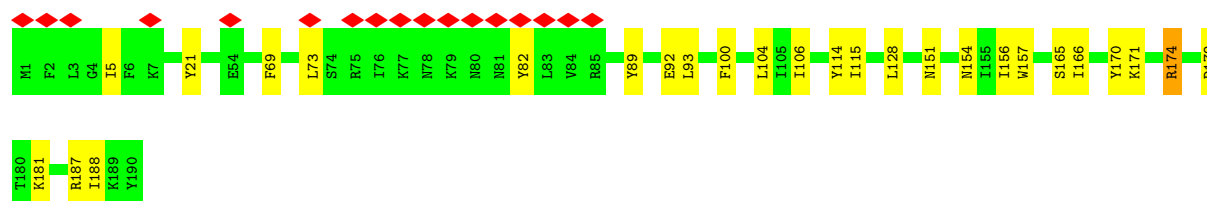
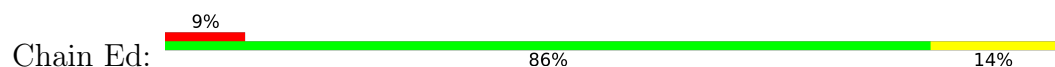




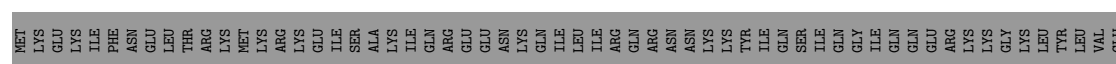
• Molecule 29: Ymf75



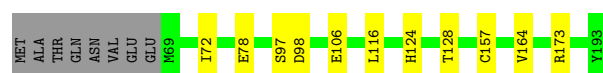
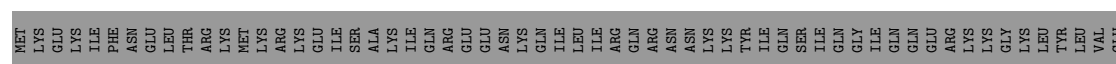
• Molecule 29: Ymf75



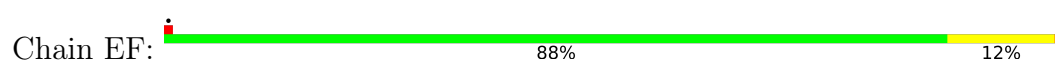
• Molecule 30: Mobilization protein



• Molecule 30: Mobilization protein

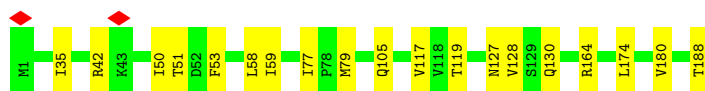


• Molecule 31: Iron-binding zinc finger CDGSH type protein





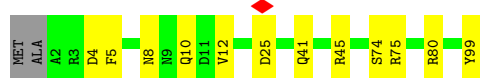
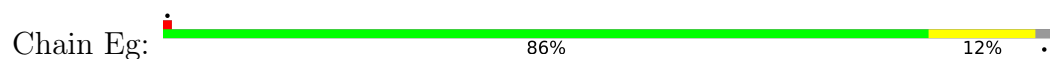
- Molecule 31: Iron-binding zinc finger CDGSH type protein



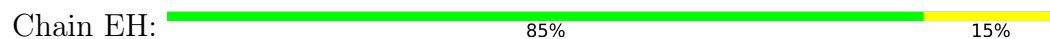
- Molecule 32: COXTT28



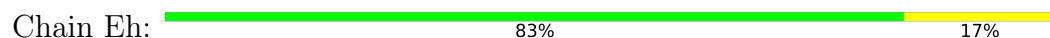
- Molecule 32: COXTT28



- Molecule 33: Transmembrane protein, putative



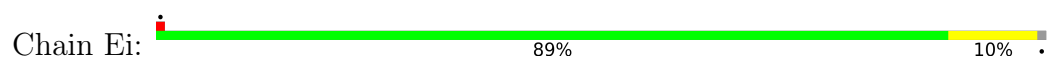
- Molecule 33: Transmembrane protein, putative

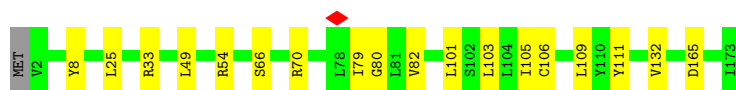


- Molecule 34: Transmembrane protein

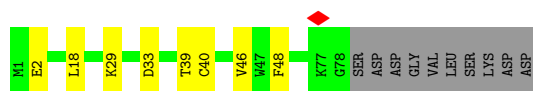
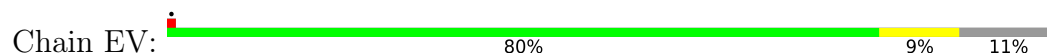


- Molecule 34: Transmembrane protein

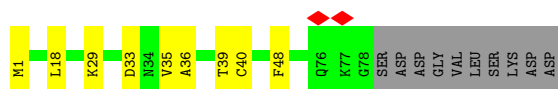
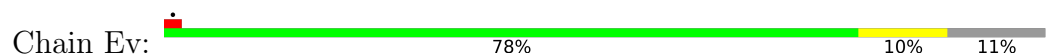




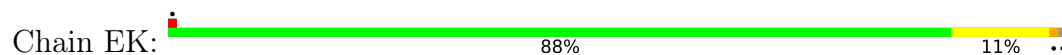
- Molecule 35: Decapping nuclease



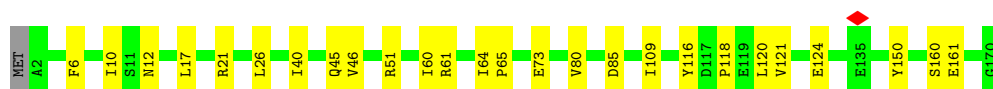
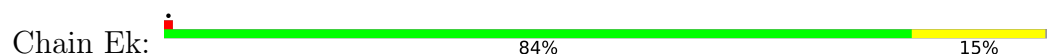
- Molecule 35: Decapping nuclease



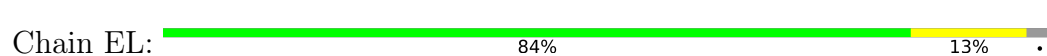
- Molecule 36: Complex III subunit VII



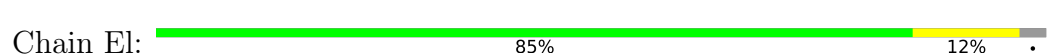
- Molecule 36: Complex III subunit VII



- Molecule 37: Transmembrane protein, putative



- Molecule 37: Transmembrane protein, putative



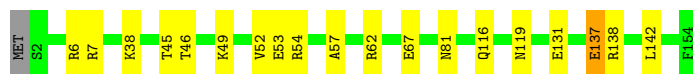
- Molecule 38: Transmembrane protein, putative

Chain EM:  87% 12% ..



- Molecule 38: Transmembrane protein, putative

Chain Em:  87% 12% ..



- Molecule 39: COXTT22

Chain EN:  89% 8% ..



- Molecule 39: COXTT22

Chain En:  91% 6% .



- Molecule 40: Transmembrane protein, putative

Chain EO:  87% 12% .



- Molecule 40: Transmembrane protein, putative

Chain Eo:  85% 14% .



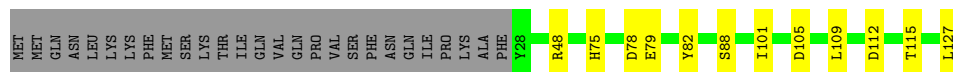
- Molecule 41: Phage protein

Chain EP:  68% 11% 21%



- Molecule 41: Phage protein

Chain Ep:  69% 9% 21%



- Molecule 42: Transmembrane protein, putative

Chain EQ:  81% 19%



- Molecule 42: Transmembrane protein, putative

Chain Eq:  84% 16%



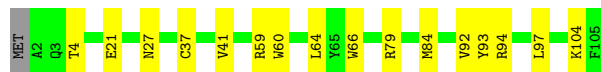
- Molecule 43: Lysozyme

Chain ER:  85% 14%



- Molecule 43: Lysozyme

Chain Er:  84% 15%



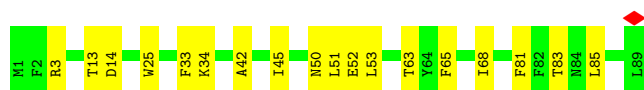
- Molecule 44: Ymf70

Chain ES:  81% 19%

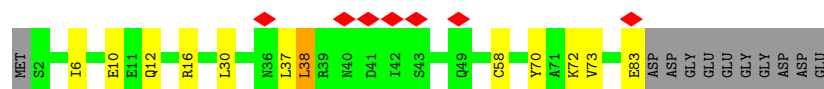
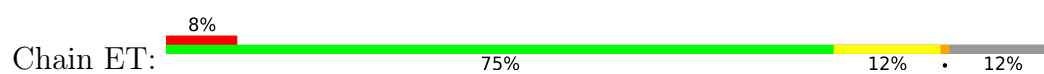


- Molecule 44: Ymf70

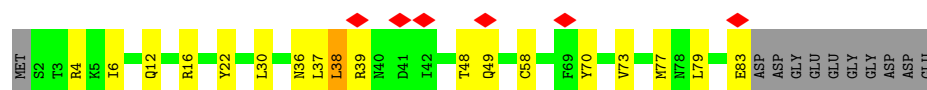
Chain Es:  80% 20%



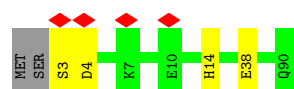
- Molecule 45: Zf-Tim10_DDP domain-containing protein



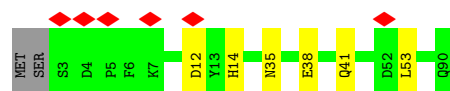
- Molecule 45: Zf-Tim10_DDP domain-containing protein



- Molecule 46: ABC transporter



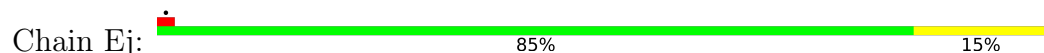
- Molecule 46: ABC transporter



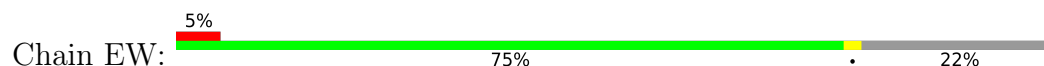
- Molecule 47: YfIT domain-containing protein

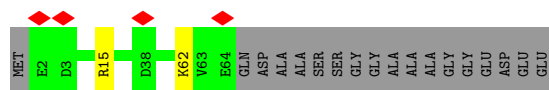


- Molecule 47: YfIT domain-containing protein

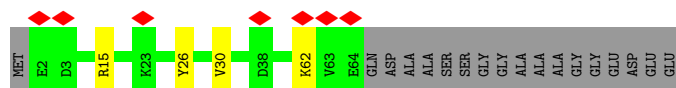
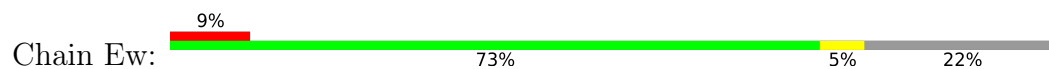


- Molecule 48: Cullin domain-containing protein

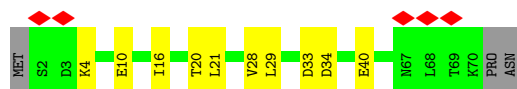
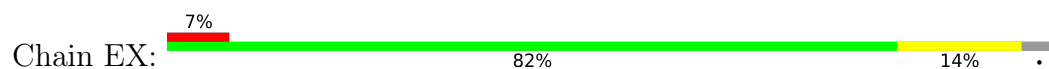




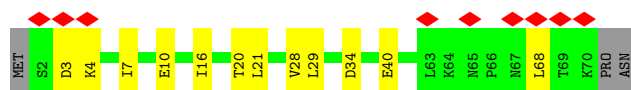
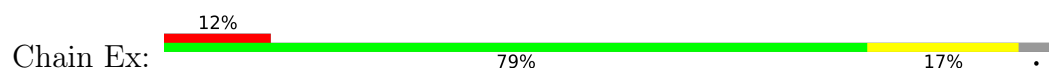
- Molecule 48: Cullin domain-containing protein



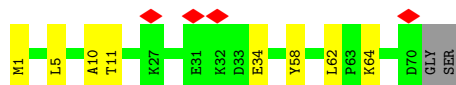
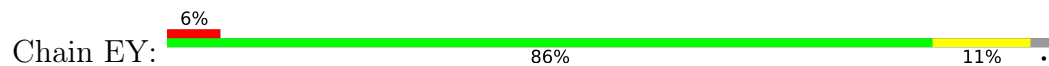
- Molecule 49: Zf-Tim10_DDP domain-containing protein



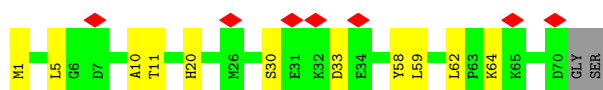
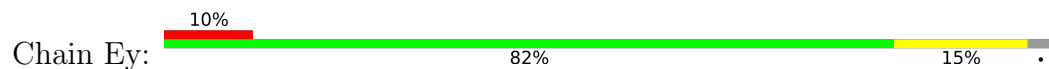
- Molecule 49: Zf-Tim10_DDP domain-containing protein



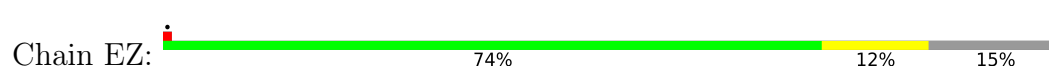
- Molecule 50: Annexin



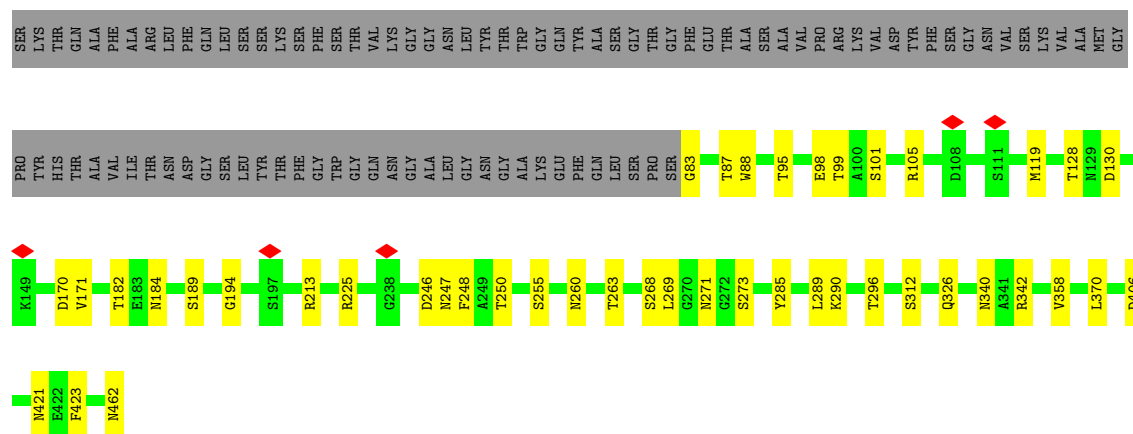
- Molecule 50: Annexin



- Molecule 51: Transposase



- Molecule 51: Transposase



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: AME, ATP, CDL, SEP, HEA, MG, LPP, CUA, PC1, K, TPO, HEM, ZN, CU, 3PE, FES, CA, UQ8

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	0.09	0/5748	0.23	0/7793
1	Da	0.09	0/5748	0.23	0/7793
2	DB	0.08	0/5282	0.22	0/7159
2	Db	0.07	0/5282	0.22	0/7159
3	DC	0.08	0/5256	0.22	0/7142
3	Dc	0.08	0/5256	0.22	0/7142
4	DD	0.08	0/4734	0.21	0/6387
4	Dd	0.08	0/4734	0.20	0/6387
5	DE	0.08	0/1116	0.19	0/1512
5	De	0.09	0/1116	0.20	0/1512
6	DF	0.08	0/1977	0.22	0/2673
6	Df	0.08	0/1977	0.22	0/2673
7	DG	0.09	0/906	0.23	0/1230
7	Dg	0.09	0/906	0.20	0/1230
8	DH	0.07	0/1199	0.20	0/1621
8	Dh	0.06	0/1199	0.20	0/1621
9	DI	0.07	0/1829	0.19	0/2486
9	Di	0.07	0/1829	0.19	0/2486
10	DJ	0.07	0/1950	0.20	0/2647
10	Dj	0.07	0/1950	0.19	0/2647
11	DK	0.08	0/1100	0.26	0/1495
11	Dk	0.08	0/1100	0.24	0/1495
12	DM	0.07	0/3910	0.20	0/5320
12	Dm	0.07	0/3910	0.20	0/5320
13	DN	0.08	0/3963	0.20	0/5359
13	Dn	0.08	0/3963	0.21	0/5359
14	DO	0.06	0/3505	0.17	0/4745
14	Do	0.06	0/3505	0.17	0/4745
15	DP	0.07	0/2433	0.19	0/3307
15	Dp	0.07	0/2433	0.18	0/3307
16	DQ	0.08	0/3247	0.21	0/4410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	Dq	0.07	0/3247	0.21	0/4410
17	DR	0.07	0/2077	0.23	0/2824
17	Dr	0.08	0/2077	0.23	0/2824
18	DS	0.08	0/2950	0.21	0/4003
18	Ds	0.08	0/2950	0.21	0/4003
19	DT	0.07	0/2518	0.20	0/3433
19	Dt	0.07	0/2518	0.20	0/3433
20	DU	0.08	0/2689	0.21	0/3657
20	Du	0.08	0/2689	0.20	0/3657
21	DV	0.09	0/2622	0.20	0/3554
21	Dv	0.09	0/2622	0.20	0/3554
22	DW	0.07	0/2449	0.19	0/3312
22	Dw	0.07	0/2449	0.19	0/3312
23	DX	0.07	0/2171	0.19	0/2930
23	Dx	0.07	0/2171	0.19	0/2930
24	DY	0.07	0/1619	0.21	0/2198
24	Dy	0.07	0/1619	0.20	0/2198
25	DZ	0.07	0/1752	0.18	0/2372
25	Dz	0.07	0/1752	0.18	0/2372
26	EA	0.07	0/1709	0.18	0/2321
26	Ea	0.07	0/1709	0.18	0/2321
27	EB	0.07	0/1793	0.19	0/2418
27	Eb	0.07	0/1793	0.19	0/2418
28	EC	0.08	0/1673	0.24	0/2258
28	Ec	0.08	0/1673	0.23	0/2258
29	ED	0.08	0/1708	0.18	0/2306
29	Ed	0.08	0/1708	0.18	0/2306
30	EE	0.08	0/1066	0.20	0/1432
30	Ee	0.10	0/1066	0.21	0/1432
31	EF	0.09	0/1562	0.23	0/2123
31	Ef	0.08	0/1562	0.22	0/2123
32	EG	0.11	0/786	0.20	0/1060
32	Eg	0.09	0/786	0.18	0/1060
33	EH	0.08	0/1471	0.21	0/1995
33	Eh	0.08	0/1471	0.21	0/1995
34	EI	0.10	0/1442	0.27	0/1952
34	Ei	0.10	0/1442	0.26	0/1952
35	EV	0.07	0/645	0.20	0/866
35	Ev	0.07	0/645	0.20	0/866
36	EK	0.09	0/1410	0.22	0/1900
36	Ek	0.09	0/1410	0.21	0/1900
37	EL	0.08	0/1335	0.20	0/1810
37	El	0.08	0/1335	0.21	0/1810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	EM	0.09	0/1335	0.22	0/1794
38	Em	0.09	0/1335	0.22	0/1794
39	EN	0.08	0/1270	0.25	0/1724
39	En	0.08	0/1270	0.25	0/1724
40	EO	0.07	0/1137	0.20	0/1545
40	Eo	0.07	0/1137	0.21	0/1545
41	EP	0.07	0/837	0.20	0/1133
41	Ep	0.07	0/837	0.19	0/1133
42	EQ	0.09	0/1035	0.20	0/1403
42	Eq	0.09	0/1035	0.20	0/1403
43	ER	0.07	0/874	0.18	0/1182
43	Er	0.07	0/874	0.18	0/1182
44	ES	0.07	0/802	0.20	0/1087
44	Es	0.07	0/802	0.20	0/1087
45	ET	0.07	0/654	0.18	0/878
45	Et	0.07	0/654	0.17	0/878
46	EU	0.06	0/744	0.18	0/1003
46	Eu	0.06	0/744	0.17	0/1003
47	EJ	0.07	0/1437	0.20	0/1941
47	Ej	0.08	0/1437	0.20	0/1941
48	EW	0.07	0/523	0.19	0/705
48	Ew	0.09	0/523	0.21	0/705
49	EX	0.07	0/564	0.18	0/757
49	Ex	0.06	0/564	0.17	0/757
50	EY	0.10	0/573	0.28	0/770
50	Ey	0.09	0/573	0.28	0/770
51	EZ	0.08	0/502	0.20	0/676
51	Ez	0.08	0/502	0.20	0/676
52	FA	0.08	0/554	0.18	0/746
52	Fa	0.08	0/554	0.19	0/746
53	DL	0.07	0/2984	0.22	0/4047
53	Dl	0.07	0/2984	0.22	0/4047
All	All	0.08	0/202854	0.21	0/274802

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.

There are no bond angle outliers.

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DA	5559	5609	5607	78	0
1	Da	5559	5608	5606	82	0
2	DB	5131	5101	5104	57	0
2	Db	5131	5102	5104	63	0
3	DC	5084	5067	5067	78	0
3	Dc	5084	5067	5067	74	0
4	DD	4652	4424	4424	64	0
4	Dd	4652	4424	4424	59	0
5	DE	1083	1021	1020	14	0
5	De	1083	1020	1020	17	0
6	DF	1913	1768	1768	24	0
6	Df	1913	1768	1768	20	0
7	DG	871	788	788	12	0
7	Dg	871	788	788	7	0
8	DH	1170	1129	1130	23	0
8	Dh	1170	1129	1130	19	0
9	DI	1777	1604	1603	16	0
9	Di	1777	1604	1603	17	0
10	DJ	1881	1772	1772	29	0
10	Dj	1881	1772	1772	24	0
11	DK	1071	1062	1062	15	0
11	Dk	1071	1062	1062	10	0
12	DM	3793	3592	3592	42	0
12	Dm	3793	3592	3592	41	0
13	DN	3869	3980	3980	40	0
13	Dn	3869	3980	3980	46	0
14	DO	3448	3508	3508	37	0
14	Do	3448	3508	3508	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	DP	2369	2291	2291	18	0
15	Dp	2369	2291	2291	19	0
16	DQ	3169	3102	3102	41	0
16	Dq	3169	3102	3102	43	0
17	DR	2024	1958	1958	25	0
17	Dr	2024	1958	1958	29	0
18	DS	2866	2770	2782	37	0
18	Ds	2866	2770	2782	38	0
19	DT	2443	2290	2290	46	0
19	Dt	2443	2290	2290	42	0
20	DU	2620	2584	2584	33	0
20	Du	2620	2584	2584	39	0
21	DV	2562	2552	2553	28	0
21	Dv	2562	2552	2553	28	0
22	DW	2394	2344	2344	16	0
22	Dw	2394	2344	2344	19	0
23	DX	2108	2018	2018	21	0
23	Dx	2108	2018	2018	21	0
24	DY	1573	1562	1562	19	0
24	Dy	1573	1562	1562	18	0
25	DZ	1711	1671	1670	19	0
25	Dz	1711	1672	1670	29	0
26	EA	1659	1637	1637	17	0
26	Ea	1659	1637	1637	17	0
27	EB	1739	1678	1677	13	0
27	Eb	1739	1678	1677	24	0
28	EC	1647	1660	1660	18	0
28	Ec	1647	1660	1660	18	0
29	ED	1659	1725	1726	28	0
29	Ed	1659	1725	1726	21	0
30	EE	1049	1024	1026	13	0
30	Ee	1049	1024	1026	13	0
31	EF	1509	1477	1477	22	0
31	Ef	1509	1477	1477	18	0
32	EG	771	752	752	7	0
32	Eg	771	752	752	9	0
33	EH	1438	1382	1394	16	0
33	EH	1438	1382	1394	22	0
34	EI	1408	1419	1419	11	0
34	Ei	1408	1419	1419	10	0
35	EV	643	633	645	6	0
35	Ev	643	633	645	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	EK	1389	1407	1406	17	0
36	Ek	1389	1407	1407	24	0
37	EL	1291	1253	1253	17	0
37	El	1291	1253	1253	16	0
38	EM	1304	1299	1299	14	0
38	Em	1304	1299	1299	14	0
39	EN	1227	1190	1190	9	0
39	En	1227	1190	1190	8	0
40	EO	1097	1031	1031	12	0
40	Eo	1097	1031	1031	17	0
41	EP	817	795	795	10	0
41	Ep	817	795	795	9	0
42	EQ	1015	989	1001	15	0
42	Eq	1015	989	1001	14	0
43	ER	851	800	800	13	0
43	Er	851	800	800	13	0
44	ES	776	798	798	14	0
44	Es	776	798	798	15	0
45	ET	647	655	655	10	0
45	Et	647	655	655	13	0
46	EU	724	699	699	3	0
46	Eu	724	699	699	5	0
47	EJ	1411	1391	1391	15	0
47	Ej	1411	1391	1391	21	0
48	EW	515	510	510	1	0
48	Ew	515	510	510	2	0
49	EX	558	559	559	9	0
49	Ex	558	559	559	11	0
50	EY	561	562	562	8	0
50	Ey	561	562	562	10	0
51	EZ	492	474	473	9	0
51	Ez	492	474	473	9	0
52	FA	548	536	536	8	0
52	Fa	548	536	536	6	0
53	DL	2916	2814	2814	24	0
53	Dl	2916	2814	2814	27	0
54	DA	120	108	108	2	0
54	Da	120	108	108	3	0
55	DA	1	0	0	0	0
55	Da	1	0	0	0	0
56	DA	1	0	0	0	0
56	Da	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DA	300	468	468	1	0
57	DC	100	156	156	1	0
57	DD	300	468	468	3	0
57	DG	200	312	312	1	0
57	DH	100	156	156	4	0
57	DI	100	156	156	1	0
57	DJ	500	780	780	5	0
57	DM	200	312	312	2	0
57	DN	300	468	468	3	0
57	DO	100	156	156	1	0
57	DQ	300	468	468	6	0
57	DR	200	312	312	0	0
57	DS	200	312	312	3	0
57	DU	400	624	624	0	0
57	DV	400	624	624	5	0
57	DX	200	312	312	3	0
57	DY	100	156	156	1	0
57	DZ	100	156	156	1	0
57	Da	200	312	312	3	0
57	Dc	100	156	156	1	0
57	Dd	400	624	624	7	0
57	Dg	200	312	312	7	0
57	Dh	200	312	312	4	0
57	Di	100	156	156	1	0
57	Dj	600	936	936	4	0
57	Dm	200	312	312	1	0
57	Dn	500	780	780	8	0
57	Do	100	156	156	1	0
57	Dq	400	624	624	1	0
57	Dr	200	312	312	3	0
57	Ds	200	312	312	2	0
57	Du	400	624	624	3	0
57	Dv	400	624	624	8	0
57	Dx	200	312	312	5	0
57	Dy	100	156	156	0	0
57	Dz	100	156	156	0	0
57	EA	100	156	156	1	0
57	EB	200	312	312	4	0
57	ED	200	312	312	1	0
57	EH	200	311	312	0	0
57	EI	100	156	156	0	0
57	EK	100	156	156	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	EL	400	624	624	9	0
57	EN	200	312	312	3	0
57	EO	100	156	156	0	0
57	EU	100	156	156	0	0
57	Ea	100	156	156	0	0
57	Ed	200	311	312	0	0
57	Eg	100	156	156	2	0
57	Eh	100	156	156	2	0
57	Ei	100	156	156	0	0
57	Ek	100	156	156	1	0
57	El	300	468	468	4	0
57	En	200	312	312	4	0
57	Ep	100	156	156	1	0
57	Eu	100	156	156	0	0
58	DA	108	175	176	1	0
58	DB	54	88	88	0	0
58	DC	270	439	440	3	0
58	DG	54	88	88	2	0
58	DI	54	88	88	1	0
58	DJ	54	88	88	0	0
58	DQ	54	88	88	1	0
58	DS	108	176	176	0	0
58	DV	162	264	264	0	0
58	DX	108	176	176	2	0
58	DY	54	88	88	0	0
58	Da	108	175	176	1	0
58	Db	54	88	88	0	0
58	Dc	270	439	440	2	0
58	Dg	54	88	88	0	0
58	Di	54	88	88	1	0
58	Dj	54	88	88	0	0
58	Dq	54	88	88	0	0
58	Ds	54	88	88	0	0
58	Dv	216	352	352	2	0
58	Dx	162	264	264	3	0
58	Dy	54	88	88	0	0
58	EB	108	176	176	1	0
58	EO	216	352	352	5	0
58	Eb	108	176	176	1	0
58	Ef	54	88	88	1	0
58	El	54	88	88	0	0
58	Eo	162	264	264	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DA	51	82	82	0	0
59	DC	102	164	164	3	0
59	DG	102	164	164	1	0
59	DJ	51	82	82	0	0
59	DR	51	82	82	2	0
59	DS	102	164	164	3	0
59	DX	153	246	246	1	0
59	Da	51	82	82	0	0
59	Dc	51	82	82	0	0
59	Dd	51	82	82	0	0
59	Dg	51	82	82	1	0
59	Dj	51	82	82	2	0
59	Dr	102	164	164	1	0
59	Ds	153	246	246	1	0
59	Dx	153	246	246	3	0
59	EL	51	82	82	2	0
59	EM	51	82	82	2	0
59	EN	51	82	82	0	0
59	EO	102	164	164	1	0
59	El	51	82	82	1	0
59	Em	51	82	82	0	0
59	Eo	102	164	164	0	0
60	DA	44	67	67	0	0
60	DN	88	134	134	0	0
60	DI	44	67	67	0	0
60	Dn	88	134	134	0	0
60	EI	44	67	67	1	0
60	Ed	44	67	67	1	0
61	DA	1	0	0	0	0
61	Da	1	0	0	0	0
62	DB	2	0	0	0	0
62	Db	2	0	0	0	0
63	DD	1	0	0	0	0
63	Dd	1	0	0	0	0
64	DD	1	0	0	0	0
65	DS	53	74	74	2	0
65	Ds	53	74	74	3	0
65	ED	53	74	74	5	0
65	EL	53	74	74	2	0
65	EN	53	74	74	2	0
65	Ed	53	74	74	5	0
65	El	53	74	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	En	53	74	74	4	0
66	ED	43	22	30	5	0
66	Ed	43	24	30	4	0
67	EF	8	0	0	0	0
67	Ef	8	0	0	0	0
68	ER	31	12	12	2	0
68	Er	31	12	12	2	0
All	All	215247	220788	220904	2060	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2060 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ed:201:HEM:HBB2	66:Ed:201:HEM:HMB1	1.53	0.91
4:DD:497:HIS:HD1	13:DN:191:TYR:HH	1.19	0.89
66:ED:602:HEM:HMB2	66:ED:602:HEM:HBB2	1.54	0.89
26:EA:138:ARG:O	26:EA:151:ARG:NH2	2.09	0.86
20:Du:48:ARG:NH1	20:Du:52:ASP:OD2	2.11	0.84

There are no symmetry-related clashes.

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DC	580/594 (98%)	569 (98%)	9 (2%)	2 (0%)	36	58
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
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%)	24	46
9	Di	203/236 (86%)	196 (97%)	6 (3%)	1 (0%)	24	46
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	590 (99%)	6 (1%)	68	86
1	Da	596/613 (97%)	588 (99%)	8 (1%)	61	82
2	DB	569/569 (100%)	561 (99%)	8 (1%)	59	81
2	Db	569/569 (100%)	563 (99%)	6 (1%)	65	84
3	DC	553/565 (98%)	553 (100%)	0	100	100
3	Dc	553/565 (98%)	552 (100%)	1 (0%)	87	95
4	DD	506/579 (87%)	503 (99%)	3 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Dd	506/579 (87%)	503 (99%)	3 (1%)	78	91
5	DE	114/116 (98%)	114 (100%)	0	100	100
5	De	114/116 (98%)	113 (99%)	1 (1%)	70	87
6	DF	200/207 (97%)	198 (99%)	2 (1%)	68	86
6	Df	200/207 (97%)	199 (100%)	1 (0%)	81	92
7	DG	84/88 (96%)	83 (99%)	1 (1%)	63	83
7	Dg	84/88 (96%)	84 (100%)	0	100	100
8	DH	119/119 (100%)	118 (99%)	1 (1%)	73	88
8	Dh	119/119 (100%)	117 (98%)	2 (2%)	53	78
9	DI	193/218 (88%)	191 (99%)	2 (1%)	68	86
9	Di	193/218 (88%)	191 (99%)	2 (1%)	68	86
10	DJ	199/199 (100%)	195 (98%)	4 (2%)	48	74
10	Dj	199/199 (100%)	196 (98%)	3 (2%)	57	80
11	DK	121/943 (13%)	120 (99%)	1 (1%)	73	88
11	Dk	121/943 (13%)	121 (100%)	0	100	100
12	DM	413/447 (92%)	411 (100%)	2 (0%)	81	92
12	Dm	413/447 (92%)	410 (99%)	3 (1%)	76	89
13	DN	442/442 (100%)	439 (99%)	3 (1%)	76	89
13	Dn	442/442 (100%)	438 (99%)	4 (1%)	70	87
14	DO	380/413 (92%)	379 (100%)	1 (0%)	86	94
14	Do	380/413 (92%)	379 (100%)	1 (0%)	86	94
15	DP	253/358 (71%)	252 (100%)	1 (0%)	84	93
15	Dp	253/358 (71%)	252 (100%)	1 (0%)	84	93
16	DQ	340/342 (99%)	339 (100%)	1 (0%)	86	94
16	Dq	340/342 (99%)	340 (100%)	0	100	100
17	DR	219/318 (69%)	218 (100%)	1 (0%)	81	92
17	Dr	219/318 (69%)	219 (100%)	0	100	100
18	DS	293/293 (100%)	289 (99%)	4 (1%)	59	81
18	Ds	293/293 (100%)	288 (98%)	5 (2%)	53	78
19	DT	267/289 (92%)	267 (100%)	0	100	100
19	Dt	267/289 (92%)	267 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	DU	275/276 (100%)	273 (99%)	2 (1%)	76	89
20	Du	275/276 (100%)	271 (98%)	4 (2%)	57	80
21	DV	259/259 (100%)	258 (100%)	1 (0%)	84	93
21	Dv	259/259 (100%)	256 (99%)	3 (1%)	63	83
22	DW	258/272 (95%)	257 (100%)	1 (0%)	84	93
22	Dw	258/272 (95%)	257 (100%)	1 (0%)	84	93
23	DX	218/219 (100%)	217 (100%)	1 (0%)	81	92
23	Dx	218/219 (100%)	215 (99%)	3 (1%)	59	81
24	DY	169/216 (78%)	169 (100%)	0	100	100
24	Dy	169/216 (78%)	168 (99%)	1 (1%)	78	91
25	DZ	189/213 (89%)	188 (100%)	1 (0%)	81	92
25	Dz	189/213 (89%)	188 (100%)	1 (0%)	81	92
26	EA	180/201 (90%)	179 (99%)	1 (1%)	78	91
26	Ea	180/201 (90%)	180 (100%)	0	100	100
27	EB	180/181 (99%)	180 (100%)	0	100	100
27	Eb	180/181 (99%)	179 (99%)	1 (1%)	78	91
28	EC	178/178 (100%)	177 (99%)	1 (1%)	78	91
28	Ec	178/178 (100%)	177 (99%)	1 (1%)	78	91
29	ED	185/185 (100%)	183 (99%)	2 (1%)	65	84
29	Ed	185/185 (100%)	183 (99%)	2 (1%)	65	84
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%)	51	76
31	Ef	164/164 (100%)	163 (99%)	1 (1%)	78	91
32	EG	77/78 (99%)	77 (100%)	0	100	100
32	Eg	77/78 (99%)	77 (100%)	0	100	100
33	EH	156/156 (100%)	155 (99%)	1 (1%)	78	91
33	Uh	156/156 (100%)	156 (100%)	0	100	100
34	EI	156/157 (99%)	154 (99%)	2 (1%)	61	82
34	Ei	156/157 (99%)	153 (98%)	3 (2%)	50	75
35	EV	71/80 (89%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Ev	71/80 (89%)	71 (100%)	0	100	100
36	EK	153/154 (99%)	151 (99%)	2 (1%)	61	82
36	Ek	153/154 (99%)	150 (98%)	3 (2%)	48	74
37	EL	134/139 (96%)	134 (100%)	0	100	100
37	El	134/139 (96%)	134 (100%)	0	100	100
38	EM	137/138 (99%)	136 (99%)	1 (1%)	76	89
38	Em	137/138 (99%)	136 (99%)	1 (1%)	76	89
39	EN	132/135 (98%)	131 (99%)	1 (1%)	73	88
39	En	132/135 (98%)	131 (99%)	1 (1%)	73	88
40	EO	112/113 (99%)	111 (99%)	1 (1%)	70	87
40	Eo	112/113 (99%)	111 (99%)	1 (1%)	70	87
41	EP	87/113 (77%)	87 (100%)	0	100	100
41	Ep	87/113 (77%)	87 (100%)	0	100	100
42	EQ	104/104 (100%)	101 (97%)	3 (3%)	37	65
42	Eq	104/104 (100%)	101 (97%)	3 (3%)	37	65
43	ER	87/88 (99%)	87 (100%)	0	100	100
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%)	28	55
45	Et	75/83 (90%)	72 (96%)	3 (4%)	28	55
46	EU	78/80 (98%)	78 (100%)	0	100	100
46	Eu	78/80 (98%)	78 (100%)	0	100	100
47	EJ	157/157 (100%)	156 (99%)	1 (1%)	78	91
47	Ej	157/157 (100%)	155 (99%)	2 (1%)	61	82
48	EW	57/66 (86%)	56 (98%)	1 (2%)	51	76
48	Ew	57/66 (86%)	56 (98%)	1 (2%)	51	76
49	EX	64/67 (96%)	63 (98%)	1 (2%)	55	79
49	Ex	64/67 (96%)	63 (98%)	1 (2%)	55	79
50	EY	62/63 (98%)	62 (100%)	0	100	100
50	Ey	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	EZ	55/63 (87%)	54 (98%)	1 (2%)	51	76
51	Ez	55/63 (87%)	54 (98%)	1 (2%)	51	76
52	FA	62/63 (98%)	60 (97%)	2 (3%)	34	62
52	Fa	62/63 (98%)	60 (97%)	2 (3%)	34	62
53	DL	308/441 (70%)	307 (100%)	1 (0%)	86	94
53	Dl	308/441 (70%)	307 (100%)	1 (0%)	86	94
All	All	21280/24568 (87%)	21123 (99%)	157 (1%)	73	89

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	Du	10	LYS
42	Eq	65	PHE
21	Dv	3	TYR
29	Ed	82	TYR
48	Ew	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
21	Dv	24	ASN
47	Ej	105	GLN
22	Dw	203	HIS
34	Ei	166	ASN
53	Dl	271	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	$\# Z > 2$
4	TPO	Dd	387	4	8,10,11	1.58	1 (12%)	10,14,16	1.87	1 (10%)
33	AME	EH	1	33	9,10,11	0.21	0	9,11,13	0.47	0
9	SEP	DI	120	9	8,9,10	1.54	1 (12%)	8,12,14	1.55	2 (25%)
4	SEP	Dd	520	4	8,9,10	1.55	1 (12%)	8,12,14	1.73	2 (25%)
33	AME	Eh	1	33	9,10,11	0.23	0	9,11,13	0.46	0
42	AME	Eq	1	42	9,10,11	0.24	0	9,11,13	0.50	0
4	TPO	DD	387	4	8,10,11	1.57	1 (12%)	10,14,16	1.88	1 (10%)
9	SEP	Di	120	9	8,9,10	1.54	1 (12%)	8,12,14	1.56	2 (25%)
4	SEP	DD	520	4	8,9,10	1.54	1 (12%)	8,12,14	1.70	2 (25%)
35	AME	Ev	1	35	9,10,11	0.23	0	9,11,13	0.49	0
16	AME	DQ	1	16	9,10,11	0.23	0	9,11,13	0.47	0
8	AME	Dh	1	8	9,10,11	0.23	0	9,11,13	0.50	0
21	AME	DV	1	21	9,10,11	0.23	0	9,11,13	0.57	0
21	AME	Dv	1	21	9,10,11	0.22	0	9,11,13	0.58	0
18	AME	Ds	1	18	9,10,11	0.23	0	9,11,13	0.52	0
8	AME	DH	1	8	9,10,11	0.24	0	9,11,13	0.49	0
18	AME	DS	1	18	9,10,11	0.24	0	9,11,13	0.52	0
35	AME	EV	1	35	9,10,11	0.23	0	9,11,13	0.47	0
42	AME	EQ	1	42	9,10,11	0.22	0	9,11,13	0.51	0
16	AME	Dq	1	16	9,10,11	0.24	0	9,11,13	0.47	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
4	TPO	Dd	387	4	-	2/9/11/13	-
33	AME	EH	1	33	-	0/9/10/12	-
9	SEP	DI	120	9	-	1/5/8/10	-
4	SEP	Dd	520	4	-	0/5/8/10	-
33	AME	Eh	1	33	-	2/9/10/12	-
42	AME	Eq	1	42	-	2/9/10/12	-
4	TPO	DD	387	4	-	2/9/11/13	-
9	SEP	Di	120	9	-	0/5/8/10	-
4	SEP	DD	520	4	-	0/5/8/10	-
35	AME	Ev	1	35	-	1/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	AME	DQ	1	16	-	1/9/10/12	-
8	AME	Dh	1	8	-	0/9/10/12	-
21	AME	DV	1	21	-	0/9/10/12	-
21	AME	Dv	1	21	-	0/9/10/12	-
18	AME	Ds	1	18	-	1/9/10/12	-
8	AME	DH	1	8	-	0/9/10/12	-
18	AME	DS	1	18	-	1/9/10/12	-
35	AME	EV	1	35	-	1/9/10/12	-
42	AME	EQ	1	42	-	2/9/10/12	-
16	AME	Dq	1	16	-	2/9/10/12	-

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	3.38	1.61	1.50
9	Di	120	SEP	P-O1P	3.37	1.61	1.50
4	Dd	387	TPO	P-O1P	3.37	1.61	1.50
4	DD	520	SEP	P-O1P	3.35	1.61	1.50
9	DI	120	SEP	P-O1P	3.35	1.61	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Dd	387	TPO	P-OG1-CB	-5.38	106.95	123.21
4	DD	387	TPO	P-OG1-CB	-5.36	107.02	123.21
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
4	Dd	520	SEP	P-OG-CB	-3.14	109.66	118.30

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.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	EH	1	AME	2	0
9	DI	120	SEP	1	0
4	Dd	520	SEP	1	0
33	Eh	1	AME	3	0
42	Eq	1	AME	4	0
9	Di	120	SEP	1	0
35	Ev	1	AME	1	0
16	DQ	1	AME	2	0
21	DV	1	AME	2	0
21	Dv	1	AME	2	0
18	Ds	1	AME	2	0
18	DS	1	AME	1	0
42	EQ	1	AME	4	0
16	Dq	1	AME	1	0

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	DC	601	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DA	710	-	99,99,99	0.29	0	105,111,111	0.25	0
68	ATP	ER	201	-	29,33,33	0.28	0	44,52,52	0.78	1 (2%)
57	CDL	En	1202	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	El	901	-	99,99,99	0.30	0	105,111,111	0.25	0
54	HEA	DA	701	1	66,67,67	2.50	26 (39%)	78,103,103	2.34	31 (39%)
58	PC1	Dv	408	-	53,53,53	0.29	0	59,61,61	0.26	0
66	HEM	Ed	201	-	50,50,50	1.54	5 (10%)	66,82,82	1.61	11 (16%)
57	CDL	Dm	502	-	99,99,99	0.30	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Du	403	-	99,99,99	0.30	0	105,111,111	0.24	0
59	3PE	DA	708	-	50,50,50	0.26	0	53,55,55	0.20	0
57	CDL	DZ	501	-	99,99,99	0.30	0	105,111,111	0.24	0
59	3PE	Dr	404	-	50,50,50	0.26	0	53,55,55	0.20	0
58	PC1	DC	608	-	53,53,53	0.28	0	59,61,61	0.26	0
58	PC1	Dj	406	-	53,53,53	0.29	0	59,61,61	0.26	0
58	PC1	DC	604	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	Dd	704	-	99,99,99	0.30	0	105,111,111	0.25	0
54	HEA	Da	702	-	66,67,67	2.49	26 (39%)	78,103,103	2.37	32 (41%)
60	LPP	DN	503	-	43,43,43	0.22	0	47,48,48	0.28	0
62	CUA	DB	701	2	0,1,1	-	-	-	-	-
57	CDL	Dn	505	-	99,99,99	0.30	0	105,111,111	0.27	0
58	PC1	DA	706	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	Ds	405	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dm	501	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DN	504	-	99,99,99	0.29	0	105,111,111	0.25	0
59	3PE	Dx	1206	-	50,50,50	0.27	0	53,55,55	0.21	0
58	PC1	Eo	204	-	53,53,53	0.29	0	59,61,61	0.26	0
58	PC1	DV	406	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	DV	404	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DA	705	-	99,99,99	0.30	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	EU	101	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dg	202	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dx	1208	-	53,53,53	0.29	0	59,61,61	0.27	0
60	LPP	DI	1101	-	43,43,43	0.23	0	47,48,48	0.27	0
57	CDL	Dj	403	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Eh	1601	-	99,99,99	0.31	0	105,111,111	0.23	0
57	CDL	ED	604	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	DX	306	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	El	902	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dd	702	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Do	501	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dj	401	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DD	704	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dy	302	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	DI	701	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	DG	203	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	EA	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dq	402	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DS	406	-	53,53,53	0.29	0	59,61,61	0.25	0
57	CDL	EL	901	-	99,99,99	0.30	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Eu	101	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	Ds	401	-	50,50,50	0.26	0	53,55,55	0.23	0
59	3PE	Da	708	-	50,50,50	0.26	0	53,55,55	0.21	0
65	UQ8	ED	603	-	53,53,53	0.51	0	64,67,67	0.72	3 (4%)
58	PC1	DC	602	-	53,53,53	0.28	0	59,61,61	0.27	0
57	CDL	DR	403	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dg	203	-	53,53,53	0.29	0	59,61,61	0.27	0
58	PC1	EB	301	-	53,53,53	0.28	0	59,61,61	0.25	0
59	3PE	DR	401	-	50,50,50	0.27	0	53,55,55	0.21	0
60	LPP	DA	711	-	43,43,43	0.22	0	47,48,48	0.28	0
58	PC1	Eb	301	-	53,53,53	0.28	0	59,61,61	0.25	0
57	CDL	DS	402	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	DC	607	-	50,50,50	0.27	0	53,55,55	0.21	0
58	PC1	DV	405	-	53,53,53	0.29	0	59,61,61	0.26	0
68	ATP	Er	201	-	29,33,33	0.28	0	44,52,52	0.78	1 (2%)
57	CDL	EL	902	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dn	501	-	99,99,99	0.30	0	105,111,111	0.26	0
59	3PE	Ds	407	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Di	702	-	53,53,53	0.29	0	59,61,61	0.26	0
60	LPP	Dn	504	-	43,43,43	0.22	0	47,48,48	0.33	0
58	PC1	Eo	205	-	53,53,53	0.29	0	59,61,61	0.27	0
57	CDL	Dx	1203	-	99,99,99	0.31	0	105,111,111	0.24	0
57	CDL	DO	501	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dx	1204	-	53,53,53	0.29	0	59,61,61	0.27	0
65	UQ8	EN	1204	-	53,53,53	0.50	0	64,67,67	0.67	2 (3%)
57	CDL	DQ	1502	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	DX	302	-	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
57	CDL	DR	402	-	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	0.26	0
57	CDL	Dy	301	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dd	706	-	99,99,99	0.29	0	105,111,111	0.24	0
65	UQ8	El	906	-	53,53,53	0.52	0	64,67,67	0.83	3 (4%)
59	3PE	Ds	403	-	50,50,50	0.27	0	53,55,55	0.20	0
59	3PE	Eo	202	-	50,50,50	0.27	0	53,55,55	0.20	0
65	UQ8	Ed	202	-	53,53,53	0.52	0	64,67,67	0.72	3 (4%)
57	CDL	Du	401	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dv	405	-	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
58	PC1	Dc	604	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	EN	1203	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Dj	404	-	99,99,99	0.30	0	105,111,111	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PC1	EB	303	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	ED	601	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Dr	402	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	EO	207	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	DU	401	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dh	201	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DG	201	-	99,99,99	0.30	0	105,111,111	0.25	0
65	UQ8	EL	906	-	53,53,53	0.51	0	64,67,67	0.78	3 (4%)
57	CDL	Dn	507	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dj	405	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DS	407	-	53,53,53	0.29	0	59,61,61	0.25	0
57	CDL	DJ	305	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dc	603	-	53,53,53	0.28	0	59,61,61	0.26	0
58	PC1	Eo	201	-	53,53,53	0.29	0	59,61,61	0.27	0
58	PC1	DC	603	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	DX	307	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EL	903	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EN	1202	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	Dx	1207	-	50,50,50	0.27	0	53,55,55	0.20	0
59	3PE	EO	203	-	50,50,50	0.27	0	53,55,55	0.21	0
59	3PE	DX	305	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	DV	402	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Ek	201	-	99,99,99	0.30	0	105,111,111	0.25	0
67	FES	EF	202	31	0,4,4	-	-	-	-	-
59	3PE	DX	303	-	50,50,50	0.26	0	53,55,55	0.19	0
59	3PE	Dx	1205	-	50,50,50	0.27	0	53,55,55	0.21	0
60	LPP	DN	502	-	43,43,43	0.23	0	47,48,48	0.36	0
57	CDL	Du	402	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Dn	502	-	99,99,99	0.30	0	105,111,111	0.24	0
59	3PE	DC	606	-	50,50,50	0.27	0	53,55,55	0.22	0
59	3PE	EO	204	-	50,50,50	0.27	0	53,55,55	0.22	0
58	PC1	Dq	405	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	Da	705	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DI	702	-	53,53,53	0.29	0	59,61,61	0.26	0
58	PC1	Dc	607	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	Eo	203	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	Dr	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EB	304	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	El	903	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	Dr	401	-	50,50,50	0.27	0	53,55,55	0.22	0
57	CDL	Dj	408	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	Dg	204	-	50,50,50	0.26	0	53,55,55	0.23	0
58	PC1	Da	706	-	53,53,53	0.29	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	Dj	402	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Db	702	-	53,53,53	0.29	0	59,61,61	0.25	0
58	PC1	El	904	-	53,53,53	0.28	0	59,61,61	0.28	0
57	CDL	DG	202	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Ea	301	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	En	1201	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	DJ	306	-	53,53,53	0.29	0	59,61,61	0.26	0
62	CUA	Db	701	2	0,1,1	-	-	-		
65	UQ8	DS	404	-	53,53,53	0.50	0	64,67,67	0.66	2 (3%)
60	LPP	Ed	203	-	43,43,43	0.22	0	47,48,48	0.27	0
58	PC1	Ds	406	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	Dd	705	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dv	401	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DQ	1501	-	99,99,99	0.29	0	105,111,111	0.26	0
57	CDL	Dq	401	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DJ	302	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	Dv	406	-	53,53,53	0.29	0	59,61,61	0.25	0
59	3PE	DG	204	-	50,50,50	0.27	0	53,55,55	0.20	0
67	FES	Ef	1002	31	0,4,4	-	-	-		
58	PC1	DA	707	-	53,53,53	0.29	0	59,61,61	0.27	0
67	FES	Ef	1003	31	0,4,4	-	-	-		
57	CDL	Dc	601	-	99,99,99	0.30	0	105,111,111	0.24	0
65	UQ8	En	1203	-	53,53,53	0.51	0	64,67,67	0.62	2 (3%)
57	CDL	Dx	1201	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Du	404	-	99,99,99	0.30	0	105,111,111	0.24	0
67	FES	EF	201	31	0,4,4	-	-	-		
57	CDL	DU	402	-	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
58	PC1	EO	206	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	DU	404	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	EO	205	-	53,53,53	0.28	0	59,61,61	0.28	0
58	PC1	Dv	407	-	53,53,53	0.29	0	59,61,61	0.26	0
59	3PE	DJ	301	-	50,50,50	0.27	0	53,55,55	0.21	0
60	LPP	Dn	506	-	43,43,43	0.22	0	47,48,48	0.28	0
58	PC1	EO	201	-	53,53,53	0.30	0	59,61,61	0.27	0
59	3PE	Em	901	-	50,50,50	0.27	0	53,55,55	0.19	0
57	CDL	Di	701	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	DY	302	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	EI	401	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DU	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DN	505	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	EK	201	-	99,99,99	0.30	0	105,111,111	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	Eg	101	-	99,99,99	0.29	0	105,111,111	0.25	0
66	HEM	ED	602	-	50,50,50	1.55	6 (12%)	66,82,82	1.60	10 (15%)
54	HEA	Da	701	1	66,67,67	2.50	26 (39%)	78,103,103	2.36	31 (39%)
57	CDL	Ds	402	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	Ed	205	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	Dq	404	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	EL	904	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Eb	302	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	DG	205	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	Dv	403	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Dx	1202	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	Dz	501	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DX	301	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	Dd	703	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Dh	202	-	99,99,99	0.30	0	105,111,111	0.24	0
59	3PE	EM	901	-	50,50,50	0.27	0	53,55,55	0.20	0
57	CDL	Da	709	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	EB	302	-	99,99,99	0.30	0	105,111,111	0.27	0
59	3PE	Dj	407	-	50,50,50	0.27	0	53,55,55	0.21	0
57	CDL	Ei	401	-	99,99,99	0.29	0	105,111,111	0.24	0
57	CDL	DA	709	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	Da	707	-	53,53,53	0.29	0	59,61,61	0.27	0
59	3PE	EL	905	-	50,50,50	0.27	0	53,55,55	0.22	0
57	CDL	DS	405	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DN	501	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	DX	304	-	50,50,50	0.26	0	53,55,55	0.21	0
57	CDL	EH	202	-	99,99,99	0.29	0	105,111,111	0.25	0
58	PC1	Dc	602	-	53,53,53	0.28	0	59,61,61	0.27	0
59	3PE	El	905	-	50,50,50	0.28	0	53,55,55	0.21	0
57	CDL	EH	201	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DD	703	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	Ep	701	-	99,99,99	0.29	0	105,111,111	0.25	0
57	CDL	DJ	307	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dq	403	-	99,99,99	0.29	0	105,111,111	0.26	0
59	3PE	Dc	606	-	50,50,50	0.27	0	53,55,55	0.20	0
58	PC1	Dc	605	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	DY	301	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DQ	1504	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DQ	1503	-	53,53,53	0.28	0	59,61,61	0.26	0
57	CDL	Dv	404	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	DV	403	-	99,99,99	0.30	0	105,111,111	0.24	0
57	CDL	DM	501	-	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	EO	202	-	99,99,99	0.30	0	105,111,111	0.25	0
57	CDL	Dg	201	-	99,99,99	0.30	0	105,111,111	0.25	0
58	PC1	DB	702	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	DV	401	-	99,99,99	0.30	0	105,111,111	0.24	0
58	PC1	Ef	1001	-	53,53,53	0.28	0	59,61,61	0.26	0
58	PC1	DC	605	-	53,53,53	0.29	0	59,61,61	0.26	0
57	CDL	Dv	402	-	99,99,99	0.30	0	105,111,111	0.25	0
59	3PE	DS	401	-	50,50,50	0.26	0	53,55,55	0.23	0
57	CDL	DJ	304	-	99,99,99	0.30	0	105,111,111	0.25	0
65	UQ8	Ds	404	-	53,53,53	0.50	0	64,67,67	0.66	1 (1%)
57	CDL	DJ	303	-	99,99,99	0.30	0	105,111,111	0.26	0
57	CDL	Dn	503	-	99,99,99	0.29	0	105,111,111	0.24	0
60	LPP	EI	402	-	43,43,43	0.22	0	47,48,48	0.27	0
57	CDL	EN	1201	-	99,99,99	0.30	0	105,111,111	0.25	0
54	HEA	DA	702	-	66,67,67	2.49	26 (39%)	78,103,103	2.38	31 (39%)

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	DC	601	-	-	27/110/110/110	-
57	CDL	DA	710	-	-	25/110/110/110	-
68	ATP	ER	201	-	-	6/22/38/38	0/3/3/3
57	CDL	En	1202	-	-	25/110/110/110	-
57	CDL	El	901	-	-	40/110/110/110	-
54	HEA	DA	701	1	-	3/36/76/76	-
58	PC1	Dv	408	-	-	9/57/57/57	-
66	HEM	Ed	201	-	-	2/14/54/54	-
57	CDL	Dm	502	-	-	20/110/110/110	-
57	CDL	Du	403	-	-	30/110/110/110	-
59	3PE	DA	708	-	-	13/54/54/54	-
57	CDL	DZ	501	-	-	28/110/110/110	-
59	3PE	Dr	404	-	-	10/54/54/54	-
58	PC1	DC	608	-	-	18/57/57/57	-
58	PC1	Dj	406	-	-	10/57/57/57	-
58	PC1	DC	604	-	-	16/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	Dd	704	-	-	34/110/110/110	-
54	HEA	Da	702	-	-	9/36/76/76	-
60	LPP	DN	503	-	-	1/45/45/45	-
57	CDL	Dn	505	-	-	27/110/110/110	-
58	PC1	DA	706	-	-	14/57/57/57	-
57	CDL	Ds	405	-	-	28/110/110/110	-
57	CDL	Dm	501	-	-	39/110/110/110	-
57	CDL	DN	504	-	-	28/110/110/110	-
59	3PE	Dx	1206	-	-	20/54/54/54	-
58	PC1	Eo	204	-	-	20/57/57/57	-
58	PC1	DV	406	-	-	11/57/57/57	-
57	CDL	DV	404	-	-	38/110/110/110	-
57	CDL	DA	705	-	-	28/110/110/110	-
57	CDL	DD	702	-	-	25/110/110/110	-
57	CDL	EU	101	-	-	33/110/110/110	-
57	CDL	Dg	202	-	-	22/110/110/110	-
58	PC1	Dx	1208	-	-	5/57/57/57	-
60	LPP	Dl	1101	-	-	8/45/45/45	-
57	CDL	Dj	403	-	-	36/110/110/110	-
57	CDL	Eh	1601	-	-	35/110/110/110	-
57	CDL	ED	604	-	-	27/110/110/110	-
58	PC1	DX	306	-	-	10/57/57/57	-
57	CDL	El	902	-	-	37/110/110/110	-
57	CDL	Dd	702	-	-	28/110/110/110	-
57	CDL	Do	501	-	-	29/110/110/110	-
57	CDL	Dj	401	-	-	32/110/110/110	-
57	CDL	DH	201	-	-	22/110/110/110	-
57	CDL	DD	704	-	-	34/110/110/110	-
58	PC1	Dy	302	-	-	11/57/57/57	-
57	CDL	DI	701	-	-	26/110/110/110	-
58	PC1	DG	203	-	-	8/57/57/57	-
57	CDL	EA	301	-	-	26/110/110/110	-
57	CDL	Dq	402	-	-	26/110/110/110	-
58	PC1	DS	406	-	-	19/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	EL	901	-	-	36/110/110/110	-
57	CDL	Eu	101	-	-	30/110/110/110	-
59	3PE	Ds	401	-	-	17/54/54/54	-
59	3PE	Da	708	-	-	17/54/54/54	-
65	UQ8	ED	603	-	-	8/51/75/75	0/1/1/1
58	PC1	DC	602	-	-	17/57/57/57	-
57	CDL	DR	403	-	-	27/110/110/110	-
58	PC1	Dg	203	-	-	12/57/57/57	-
58	PC1	EB	301	-	-	12/57/57/57	-
59	3PE	DR	401	-	-	9/54/54/54	-
60	LPP	DA	711	-	-	7/45/45/45	-
58	PC1	Eb	301	-	-	11/57/57/57	-
57	CDL	DS	402	-	-	30/110/110/110	-
59	3PE	DC	607	-	-	16/54/54/54	-
58	PC1	DV	405	-	-	14/57/57/57	-
68	ATP	Er	201	-	-	5/22/38/38	0/3/3/3
57	CDL	EL	902	-	-	26/110/110/110	-
57	CDL	Dn	501	-	-	35/110/110/110	-
59	3PE	Ds	407	-	-	12/54/54/54	-
58	PC1	Di	702	-	-	19/57/57/57	-
60	LPP	Dn	504	-	-	9/45/45/45	-
58	PC1	Eo	205	-	-	14/57/57/57	-
57	CDL	Dx	1203	-	-	31/110/110/110	-
57	CDL	DO	501	-	-	26/110/110/110	-
58	PC1	Dx	1204	-	-	14/57/57/57	-
65	UQ8	EN	1204	-	-	16/51/75/75	0/1/1/1
57	CDL	DQ	1502	-	-	23/110/110/110	-
58	PC1	DX	302	-	-	14/57/57/57	-
57	CDL	DM	502	-	-	17/110/110/110	-
57	CDL	DR	402	-	-	35/110/110/110	-
58	PC1	DV	407	-	-	10/57/57/57	-
57	CDL	Dy	301	-	-	29/110/110/110	-
57	CDL	Dd	706	-	-	26/110/110/110	-
65	UQ8	El	906	-	-	12/51/75/75	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Ds	403	-	-	19/54/54/54	-
59	3PE	Eo	202	-	-	16/54/54/54	-
65	UQ8	Ed	202	-	-	9/51/75/75	0/1/1/1
57	CDL	Du	401	-	-	30/110/110/110	-
58	PC1	Dv	405	-	-	12/57/57/57	-
59	3PE	DS	403	-	-	19/54/54/54	-
58	PC1	Dc	604	-	-	12/57/57/57	-
59	3PE	EN	1203	-	-	14/54/54/54	-
57	CDL	Dj	404	-	-	33/110/110/110	-
58	PC1	EB	303	-	-	4/57/57/57	-
57	CDL	ED	601	-	-	27/110/110/110	-
57	CDL	Dr	402	-	-	32/110/110/110	-
58	PC1	EO	207	-	-	17/57/57/57	-
57	CDL	DU	401	-	-	32/110/110/110	-
57	CDL	Dh	201	-	-	25/110/110/110	-
57	CDL	DG	201	-	-	38/110/110/110	-
65	UQ8	EL	906	-	-	10/51/75/75	0/1/1/1
57	CDL	Dn	507	-	-	22/110/110/110	-
57	CDL	Dj	405	-	-	23/110/110/110	-
58	PC1	DS	407	-	-	16/57/57/57	-
57	CDL	DJ	305	-	-	25/110/110/110	-
58	PC1	Dc	603	-	-	14/57/57/57	-
58	PC1	Eo	201	-	-	15/57/57/57	-
58	PC1	DC	603	-	-	13/57/57/57	-
57	CDL	DX	307	-	-	25/110/110/110	-
57	CDL	EL	903	-	-	37/110/110/110	-
57	CDL	EN	1202	-	-	31/110/110/110	-
59	3PE	Dx	1207	-	-	13/54/54/54	-
59	3PE	EO	203	-	-	18/54/54/54	-
59	3PE	DX	305	-	-	13/54/54/54	-
57	CDL	DV	402	-	-	42/110/110/110	-
57	CDL	Ek	201	-	-	26/110/110/110	-
67	FES	EF	202	31	-	-	0/1/1/1
59	3PE	DX	303	-	-	14/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	Dx	1205	-	-	16/54/54/54	-
60	LPP	DN	502	-	-	8/45/45/45	-
57	CDL	Du	402	-	-	19/110/110/110	-
57	CDL	Dn	502	-	-	27/110/110/110	-
59	3PE	DC	606	-	-	9/54/54/54	-
59	3PE	EO	204	-	-	8/54/54/54	-
58	PC1	Dq	405	-	-	9/57/57/57	-
57	CDL	Da	705	-	-	32/110/110/110	-
58	PC1	DI	702	-	-	19/57/57/57	-
58	PC1	Dc	607	-	-	17/57/57/57	-
59	3PE	Eo	203	-	-	7/54/54/54	-
57	CDL	Dr	403	-	-	23/110/110/110	-
57	CDL	EB	304	-	-	34/110/110/110	-
57	CDL	El	903	-	-	31/110/110/110	-
59	3PE	Dr	401	-	-	16/54/54/54	-
57	CDL	Dj	408	-	-	33/110/110/110	-
59	3PE	Dg	204	-	-	12/54/54/54	-
58	PC1	Da	706	-	-	16/57/57/57	-
57	CDL	Dj	402	-	-	29/110/110/110	-
58	PC1	Db	702	-	-	21/57/57/57	-
58	PC1	El	904	-	-	10/57/57/57	-
57	CDL	DG	202	-	-	19/110/110/110	-
57	CDL	Ea	301	-	-	24/110/110/110	-
57	CDL	En	1201	-	-	24/110/110/110	-
58	PC1	DJ	306	-	-	11/57/57/57	-
65	UQ8	DS	404	-	-	9/51/75/75	0/1/1/1
60	LPP	Ed	203	-	-	2/45/45/45	-
58	PC1	Ds	406	-	-	9/57/57/57	-
57	CDL	Dd	705	-	-	31/110/110/110	-
57	CDL	Dv	401	-	-	28/110/110/110	-
57	CDL	DQ	1501	-	-	31/110/110/110	-
57	CDL	Dq	401	-	-	25/110/110/110	-
57	CDL	DJ	302	-	-	19/110/110/110	-
58	PC1	Dv	406	-	-	19/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PE	DG	204	-	-	16/54/54/54	-
67	FES	Ef	1002	31	-	-	0/1/1/1
58	PC1	DA	707	-	-	11/57/57/57	-
67	FES	Ef	1003	31	-	-	0/1/1/1
57	CDL	Dc	601	-	-	31/110/110/110	-
65	UQ8	En	1203	-	-	9/51/75/75	0/1/1/1
57	CDL	Dx	1201	-	-	29/110/110/110	-
57	CDL	Du	404	-	-	26/110/110/110	-
67	FES	EF	201	31	-	-	0/1/1/1
57	CDL	DU	402	-	-	19/110/110/110	-
57	CDL	Ed	204	-	-	25/110/110/110	-
58	PC1	EO	206	-	-	26/57/57/57	-
57	CDL	DU	404	-	-	23/110/110/110	-
58	PC1	EO	205	-	-	10/57/57/57	-
58	PC1	Dv	407	-	-	13/57/57/57	-
59	3PE	DJ	301	-	-	15/54/54/54	-
60	LPP	Dn	506	-	-	7/45/45/45	-
58	PC1	EO	201	-	-	12/57/57/57	-
59	3PE	Em	901	-	-	14/54/54/54	-
57	CDL	Di	701	-	-	32/110/110/110	-
58	PC1	DY	302	-	-	10/57/57/57	-
57	CDL	EI	401	-	-	24/110/110/110	-
57	CDL	DU	403	-	-	19/110/110/110	-
57	CDL	DN	505	-	-	30/110/110/110	-
57	CDL	EK	201	-	-	26/110/110/110	-
57	CDL	Eg	101	-	-	34/110/110/110	-
66	HEM	ED	602	-	-	2/14/54/54	-
54	HEA	Da	701	1	-	5/36/76/76	-
57	CDL	Ds	402	-	-	32/110/110/110	-
57	CDL	Ed	205	-	-	25/110/110/110	-
57	CDL	Dq	404	-	-	21/110/110/110	-
57	CDL	EL	904	-	-	33/110/110/110	-
58	PC1	Eb	302	-	-	5/57/57/57	-
59	3PE	DG	205	-	-	14/54/54/54	-
57	CDL	Dv	403	-	-	24/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	Dx	1202	-	-	14/57/57/57	-
57	CDL	Dz	501	-	-	28/110/110/110	-
57	CDL	DX	301	-	-	33/110/110/110	-
59	3PE	Dd	703	-	-	17/54/54/54	-
57	CDL	Dh	202	-	-	32/110/110/110	-
59	3PE	EM	901	-	-	13/54/54/54	-
57	CDL	Da	709	-	-	33/110/110/110	-
57	CDL	EB	302	-	-	27/110/110/110	-
59	3PE	Dj	407	-	-	5/54/54/54	-
57	CDL	Ei	401	-	-	23/110/110/110	-
57	CDL	DA	709	-	-	35/110/110/110	-
58	PC1	Da	707	-	-	13/57/57/57	-
59	3PE	EL	905	-	-	16/54/54/54	-
57	CDL	DS	405	-	-	32/110/110/110	-
57	CDL	DN	501	-	-	20/110/110/110	-
59	3PE	DX	304	-	-	17/54/54/54	-
57	CDL	EH	202	-	-	24/110/110/110	-
58	PC1	Dc	602	-	-	18/57/57/57	-
59	3PE	El	905	-	-	17/54/54/54	-
57	CDL	EH	201	-	-	26/110/110/110	-
57	CDL	DD	703	-	-	25/110/110/110	-
57	CDL	Ep	701	-	-	30/110/110/110	-
57	CDL	DJ	307	-	-	32/110/110/110	-
57	CDL	Dq	403	-	-	24/110/110/110	-
59	3PE	Dc	606	-	-	18/54/54/54	-
58	PC1	Dc	605	-	-	16/57/57/57	-
57	CDL	DY	301	-	-	29/110/110/110	-
57	CDL	DQ	1504	-	-	33/110/110/110	-
58	PC1	DQ	1503	-	-	11/57/57/57	-
57	CDL	Dv	404	-	-	41/110/110/110	-
57	CDL	DV	403	-	-	24/110/110/110	-
57	CDL	DM	501	-	-	31/110/110/110	-
57	CDL	EO	202	-	-	31/110/110/110	-
57	CDL	Dg	201	-	-	40/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	DB	702	-	-	21/57/57/57	-
57	CDL	DV	401	-	-	28/110/110/110	-
58	PC1	Ef	1001	-	-	18/57/57/57	-
58	PC1	DC	605	-	-	11/57/57/57	-
57	CDL	Dv	402	-	-	40/110/110/110	-
59	3PE	DS	401	-	-	17/54/54/54	-
57	CDL	DJ	304	-	-	37/110/110/110	-
65	UQ8	Ds	404	-	-	12/51/75/75	0/1/1/1
57	CDL	DJ	303	-	-	36/110/110/110	-
57	CDL	Dn	503	-	-	24/110/110/110	-
60	LPP	EI	402	-	-	8/45/45/45	-
57	CDL	EN	1201	-	-	27/110/110/110	-
54	HEA	DA	702	-	-	8/36/76/76	-

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	Da	701	HEA	C3A-C2A	5.89	1.49	1.36
54	DA	701	HEA	C3A-C2A	5.83	1.49	1.36
54	Da	702	HEA	C3A-C2A	5.82	1.49	1.36
54	DA	702	HEA	C3A-C2A	5.80	1.49	1.36
54	DA	702	HEA	FE-NB	5.55	2.12	1.94

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	701	HEA	C3C-C4C-NC	6.87	114.47	110.25
54	Da	702	HEA	C3C-C4C-NC	6.84	114.46	110.25
54	Da	701	HEA	C3C-C4C-NC	6.79	114.43	110.25
54	DA	702	HEA	C3C-C4C-NC	6.71	114.37	110.25
54	DA	701	HEA	C3D-C4D-ND	5.99	116.16	110.36

There are no chirality outliers.

5 of 4794 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

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Mol	Chain	Res	Type	Atoms
57	DA	709	CDL	CB2-OB2-PB2-OB3
57	DA	710	CDL	CA3-OA5-PA1-OA2
57	DA	710	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

132 monomers are involved in 215 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DC	601	CDL	1	0
68	ER	201	ATP	2	0
57	En	1202	CDL	2	0
57	El	901	CDL	1	0
54	DA	701	HEA	1	0
58	Dv	408	PC1	1	0
66	Ed	201	HEM	4	0
57	Dm	502	CDL	1	0
57	DZ	501	CDL	1	0
58	DC	608	PC1	2	0
57	Dd	704	CDL	1	0
57	Ds	405	CDL	1	0
57	DN	504	CDL	2	0
59	Dx	1206	3PE	1	0
58	Eo	204	PC1	3	0
57	DD	702	CDL	2	0
57	Dg	202	CDL	2	0
57	Dj	403	CDL	2	0
57	Eh	1601	CDL	2	0
57	ED	604	CDL	1	0
58	DX	306	PC1	1	0
57	El	902	CDL	2	0
57	Dd	702	CDL	2	0
57	Do	501	CDL	1	0
57	Dj	401	CDL	1	0
57	DH	201	CDL	4	0
57	DI	701	CDL	1	0
58	DG	203	PC1	2	0
57	EA	301	CDL	1	0
57	EL	901	CDL	3	0
65	ED	603	UQ8	5	0
59	DR	401	3PE	2	0
57	DS	402	CDL	2	0
59	DC	607	3PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	Er	201	ATP	2	0
57	EL	902	CDL	5	0
57	Dn	501	CDL	1	0
58	Di	702	PC1	1	0
57	Dx	1203	CDL	2	0
57	DO	501	CDL	1	0
58	Dx	1204	PC1	1	0
65	EN	1204	UQ8	2	0
57	DQ	1502	CDL	2	0
58	DX	302	PC1	1	0
57	Dd	706	CDL	1	0
65	El	906	UQ8	2	0
59	Ds	403	3PE	1	0
65	Ed	202	UQ8	5	0
57	Du	401	CDL	1	0
58	Dv	405	PC1	1	0
59	DS	403	3PE	2	0
57	Dj	404	CDL	1	0
58	EB	303	PC1	1	0
57	Dr	402	CDL	3	0
57	Dh	201	CDL	3	0
57	DG	201	CDL	1	0
65	EL	906	UQ8	2	0
57	Dn	507	CDL	2	0
58	Eo	201	PC1	3	0
57	DX	307	CDL	2	0
57	EL	903	CDL	1	0
57	EN	1202	CDL	3	0
57	DV	402	CDL	2	0
57	Ek	201	CDL	1	0
59	Dx	1205	3PE	2	0
57	Du	402	CDL	2	0
57	Dn	502	CDL	3	0
59	DC	606	3PE	2	0
59	EO	204	3PE	1	0
58	DI	702	PC1	1	0
58	Dc	607	PC1	2	0
57	EB	304	CDL	3	0
57	El	903	CDL	1	0
59	Dr	401	3PE	1	0
59	Dg	204	3PE	1	0
57	En	1201	CDL	2	0

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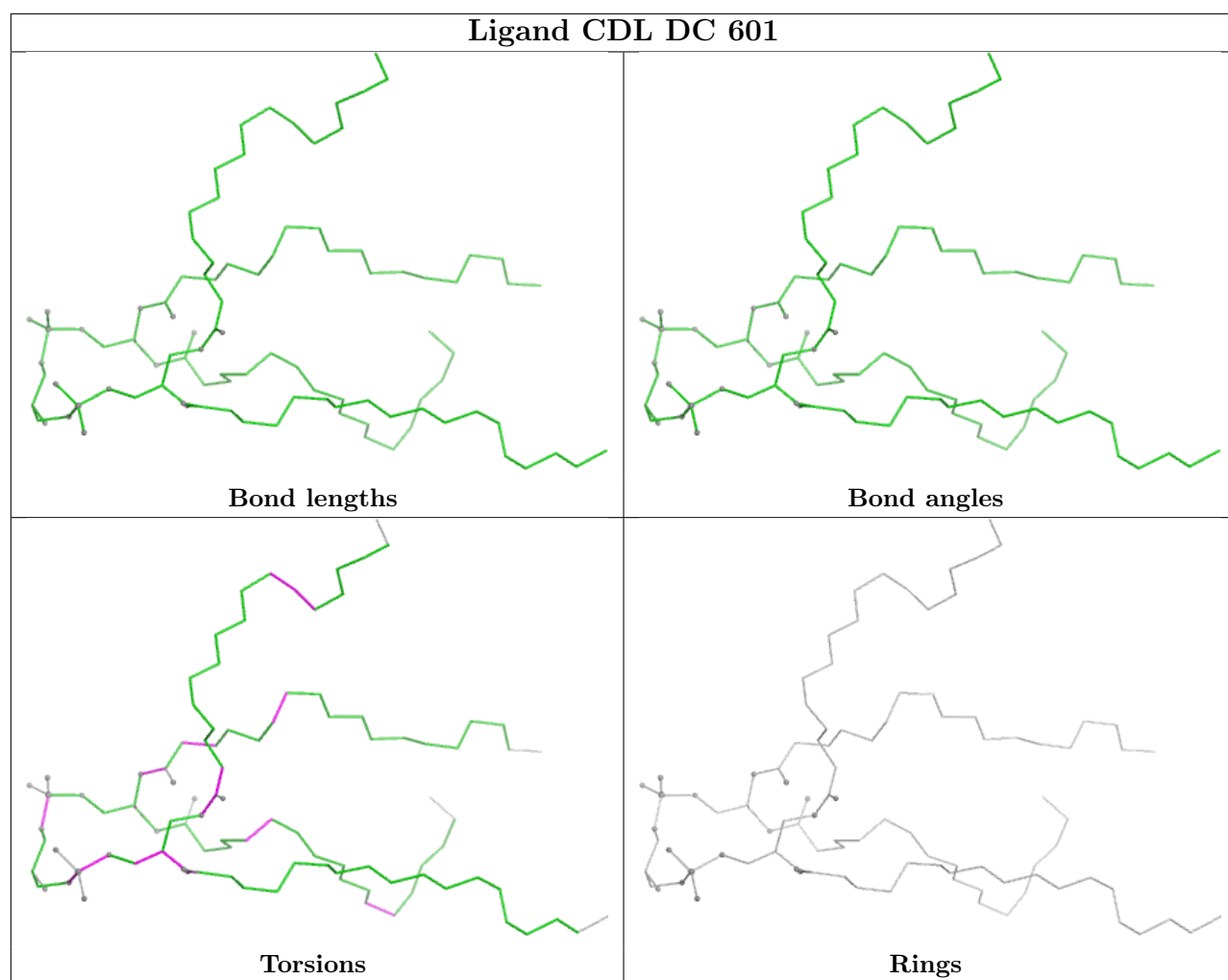
Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	DS	404	UQ8	2	0
60	Ed	203	LPP	1	0
57	Dd	705	CDL	3	0
57	Dv	401	CDL	2	0
57	DQ	1501	CDL	3	0
57	Dq	401	CDL	1	0
57	DJ	302	CDL	2	0
59	DG	204	3PE	1	0
58	DA	707	PC1	1	0
57	Dc	601	CDL	1	0
65	En	1203	UQ8	4	0
57	Dx	1201	CDL	3	0
58	EO	206	PC1	1	0
58	EO	205	PC1	2	0
58	EO	201	PC1	2	0
57	Di	701	CDL	1	0
57	DN	505	CDL	1	0
57	Eg	101	CDL	2	0
66	ED	602	HEM	5	0
54	Da	701	HEA	3	0
57	Ds	402	CDL	1	0
58	Eb	302	PC1	1	0
57	Dv	403	CDL	2	0
58	Dx	1202	PC1	2	0
57	DX	301	CDL	1	0
57	Dh	202	CDL	2	0
59	EM	901	3PE	2	0
57	Da	709	CDL	3	0
57	EB	302	CDL	1	0
59	Dj	407	3PE	2	0
57	DA	709	CDL	1	0
58	Da	707	PC1	1	0
59	EL	905	3PE	2	0
57	DS	405	CDL	1	0
59	DX	304	3PE	1	0
59	El	905	3PE	1	0
57	DD	703	CDL	1	0
57	Ep	701	CDL	1	0
57	DY	301	CDL	1	0
57	DQ	1504	CDL	1	0
58	DQ	1503	PC1	1	0
57	Dv	404	CDL	1	0

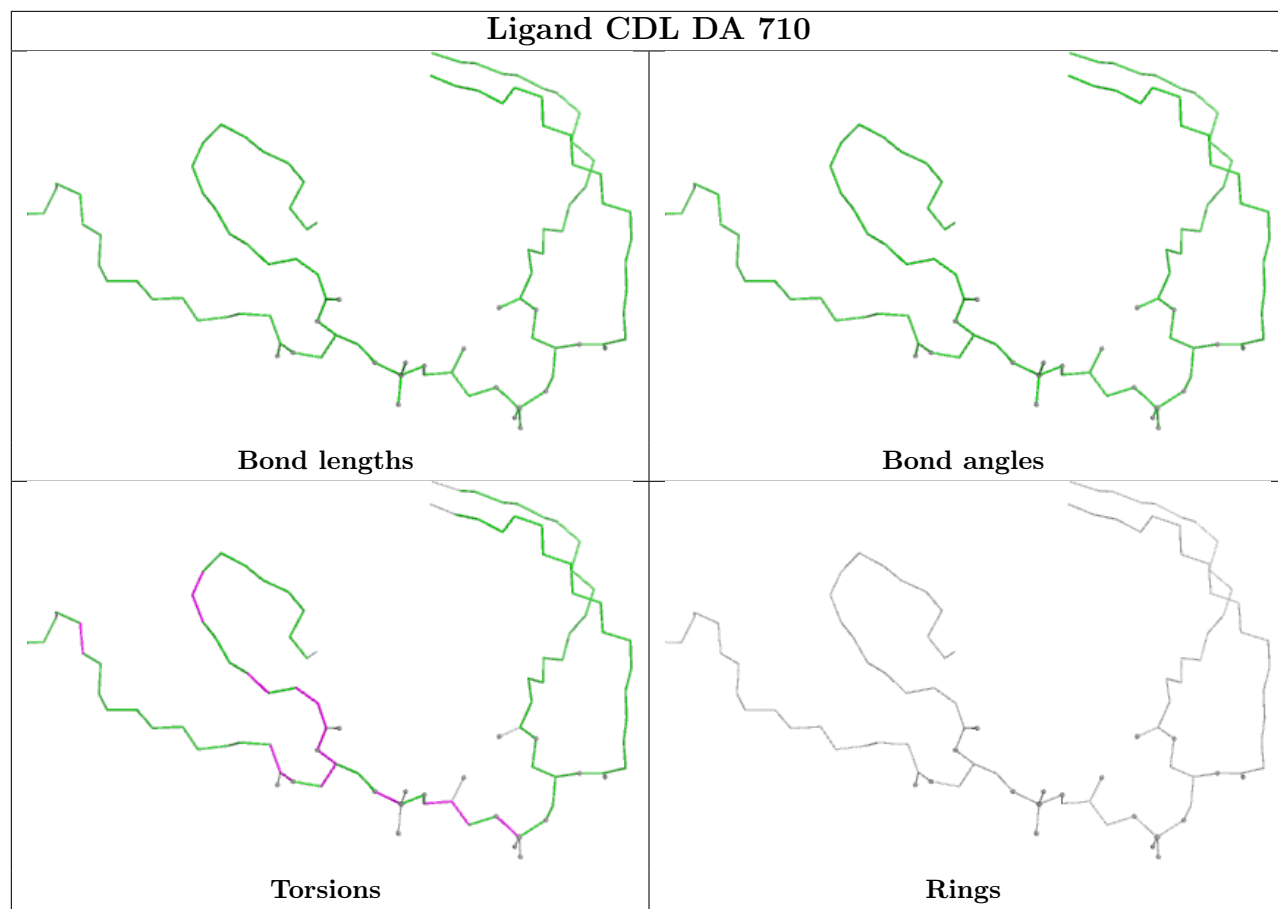
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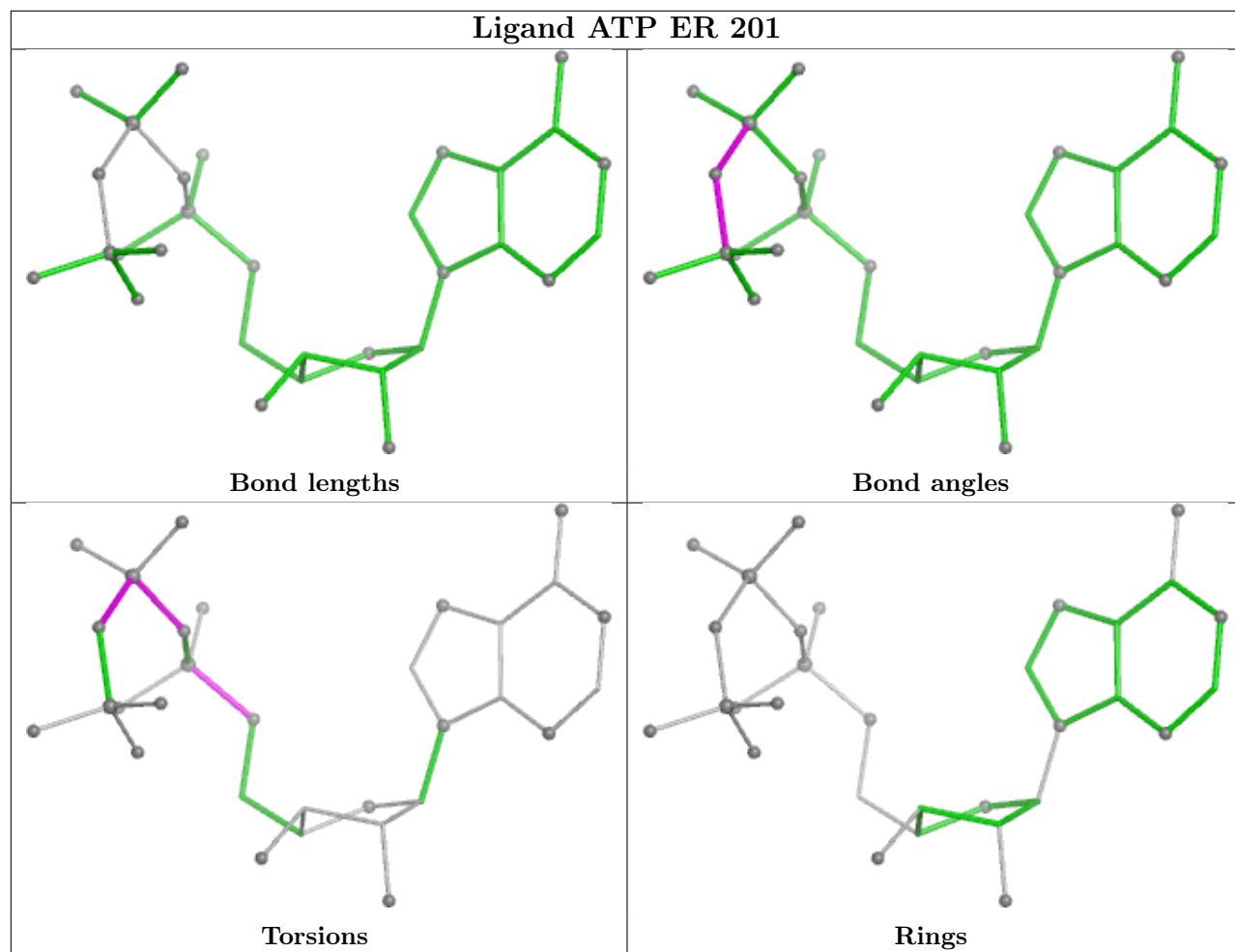
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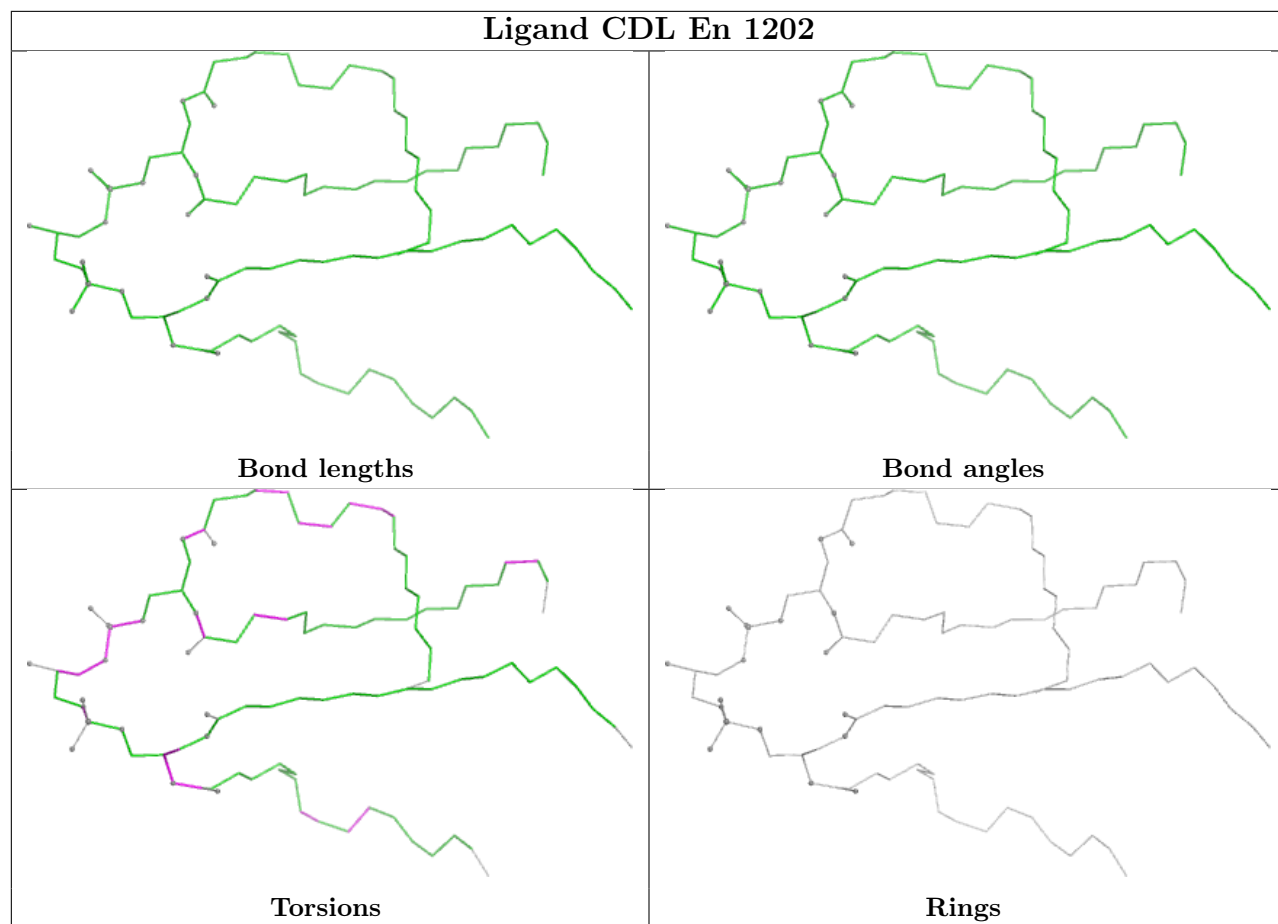
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DV	403	CDL	1	0
57	DM	501	CDL	2	0
57	Dg	201	CDL	5	0
57	DV	401	CDL	2	0
58	Ef	1001	PC1	1	0
58	DC	605	PC1	1	0
57	Dv	402	CDL	3	0
59	DS	401	3PE	1	0
57	DJ	304	CDL	1	0
65	Ds	404	UQ8	3	0
57	DJ	303	CDL	2	0
57	Dn	503	CDL	2	0
60	EI	402	LPP	1	0
54	DA	702	HEA	1	0

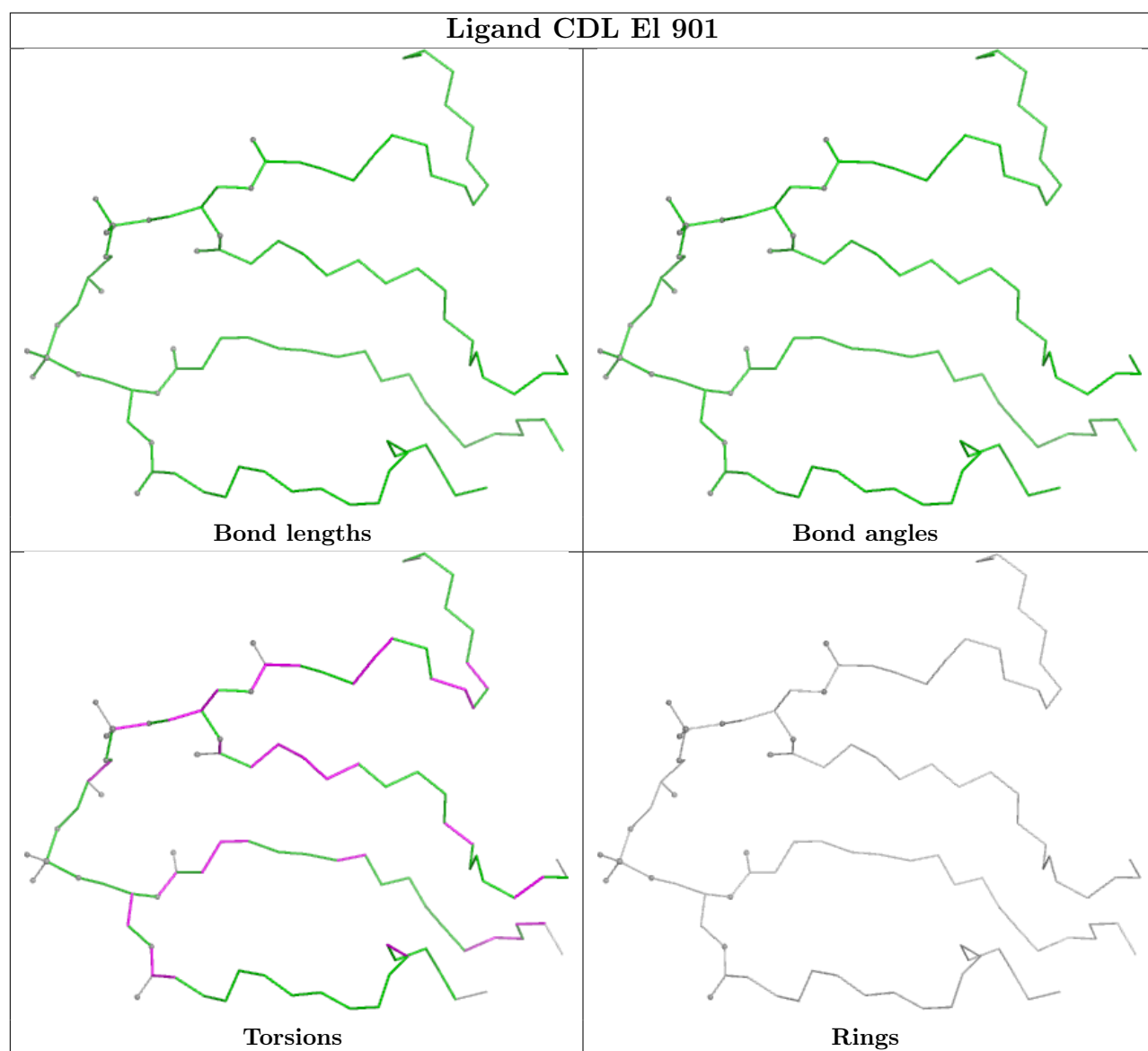
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

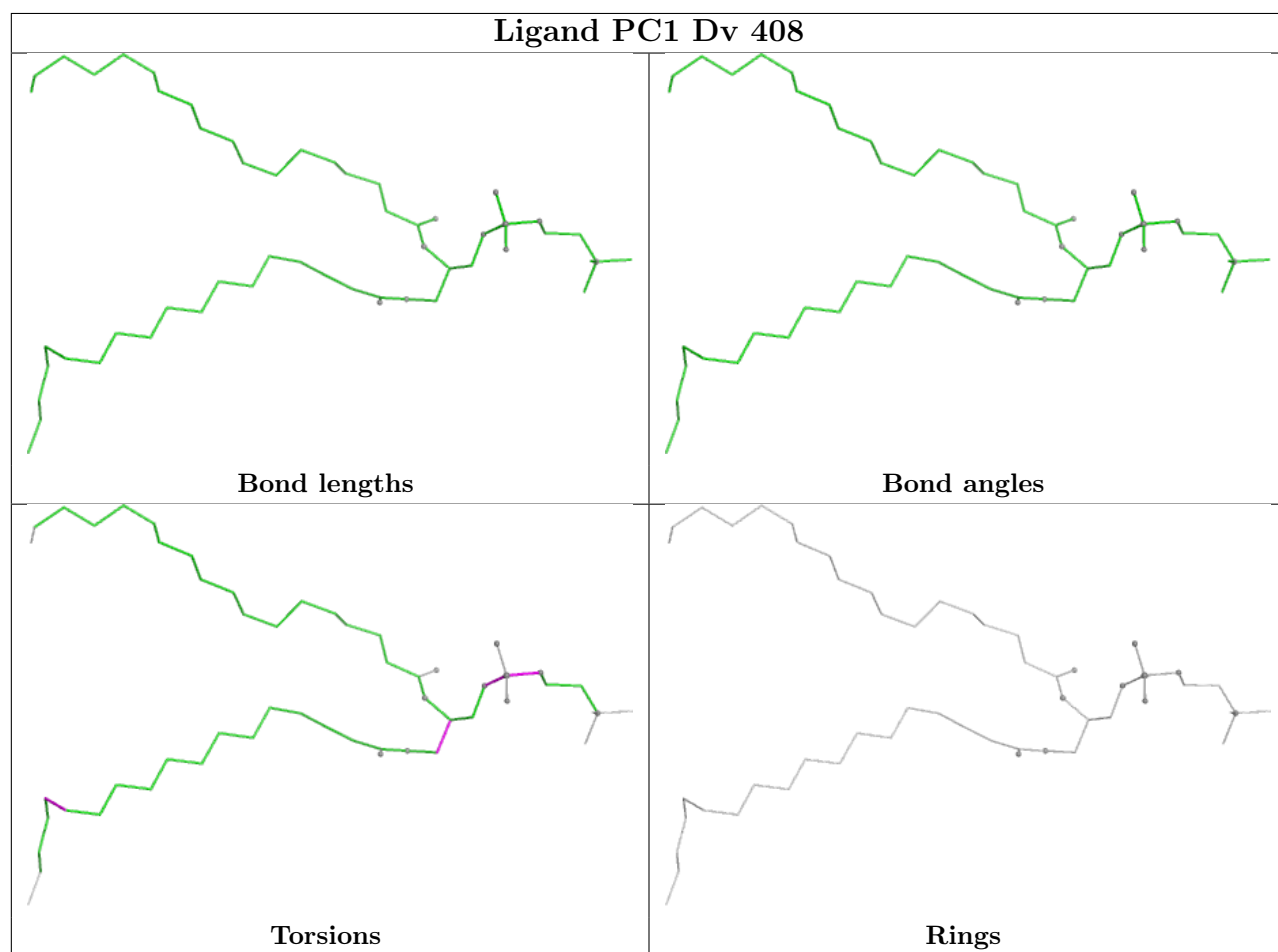
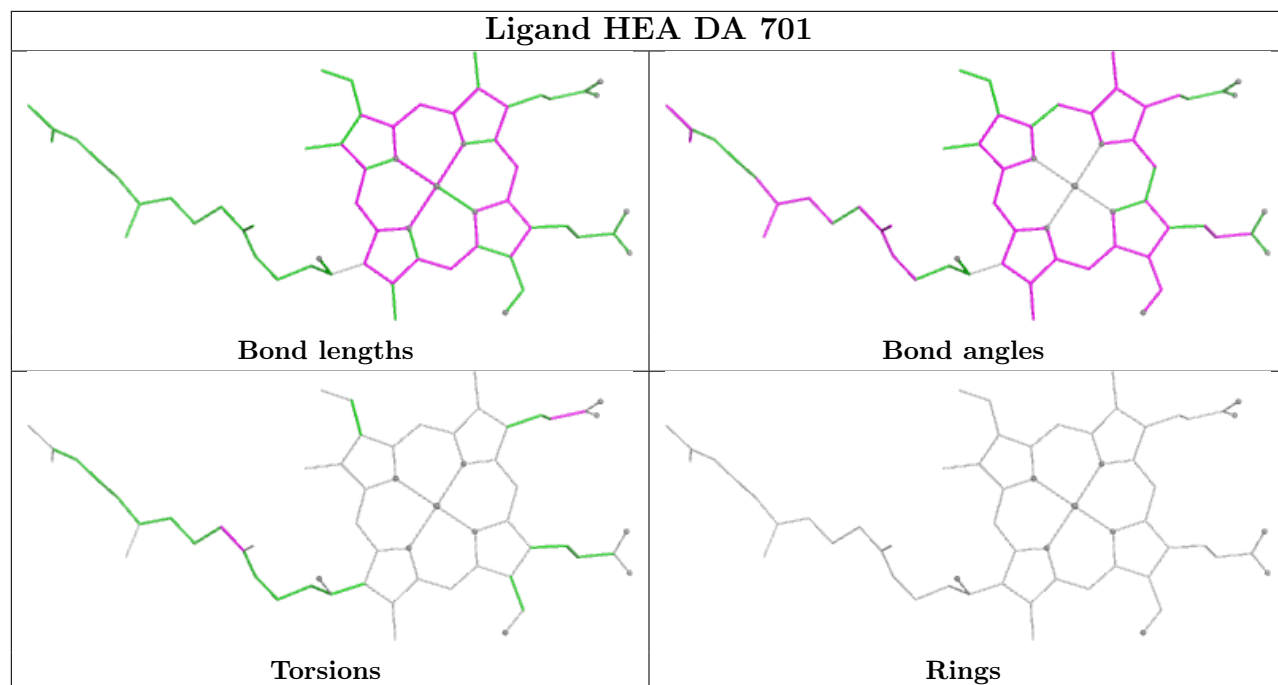




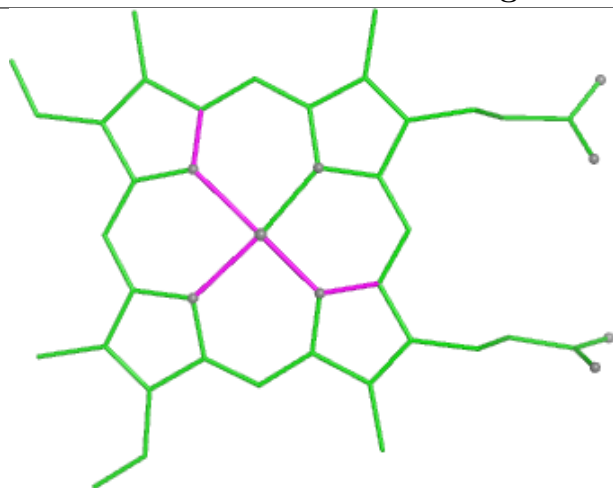




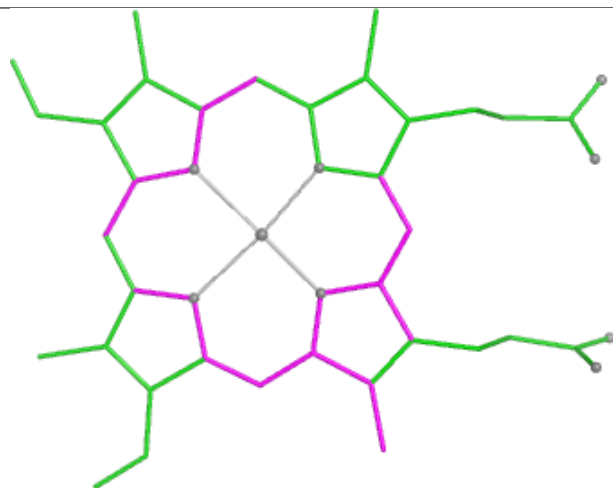




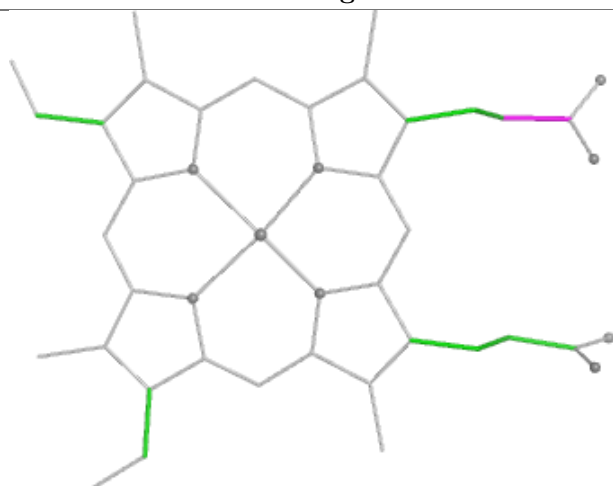
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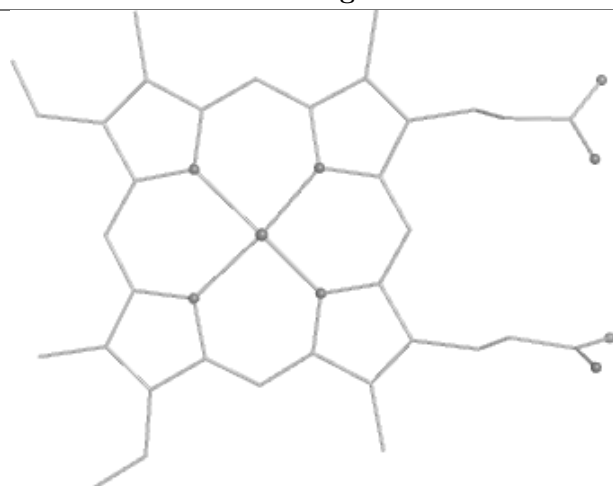
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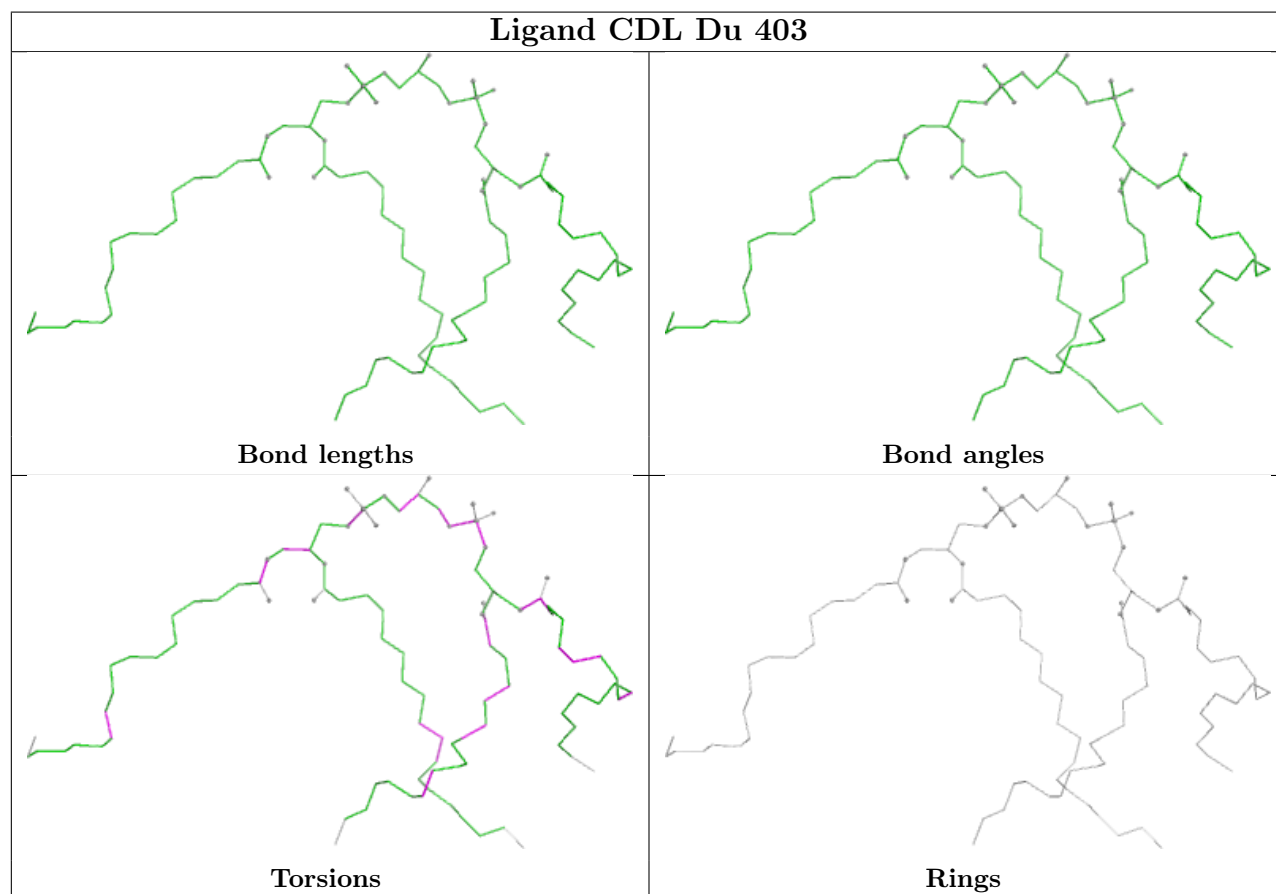
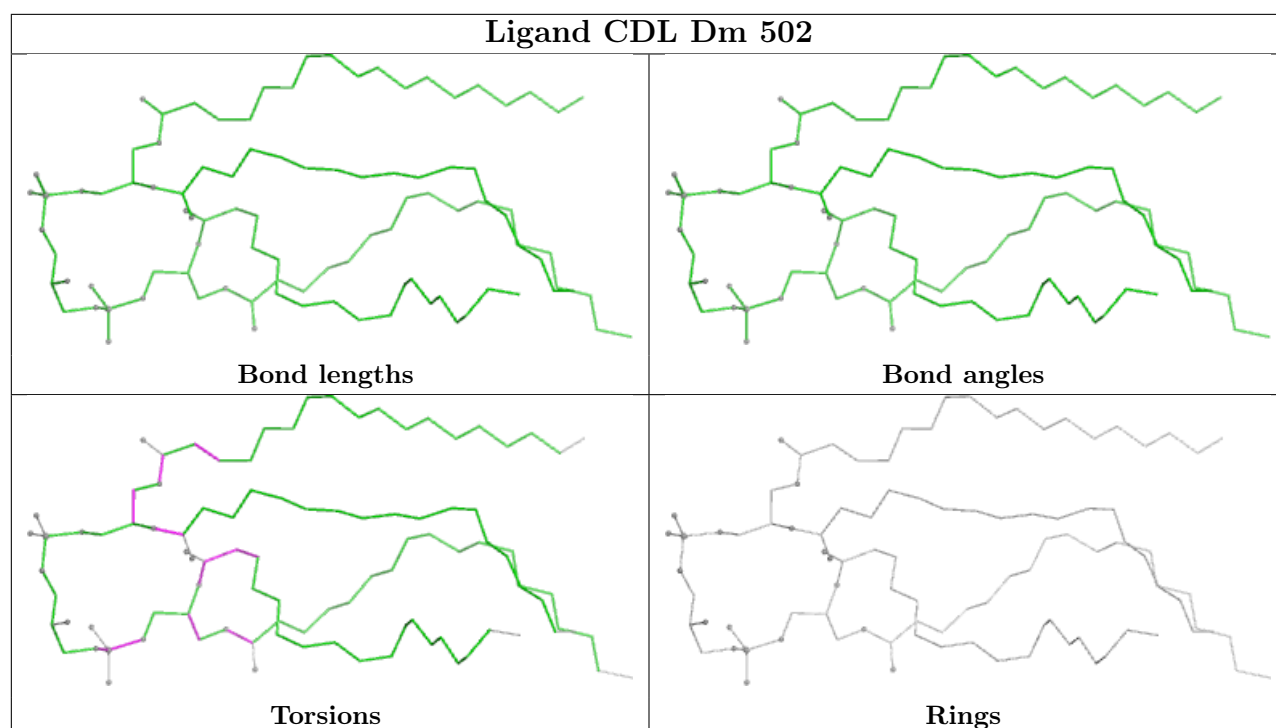
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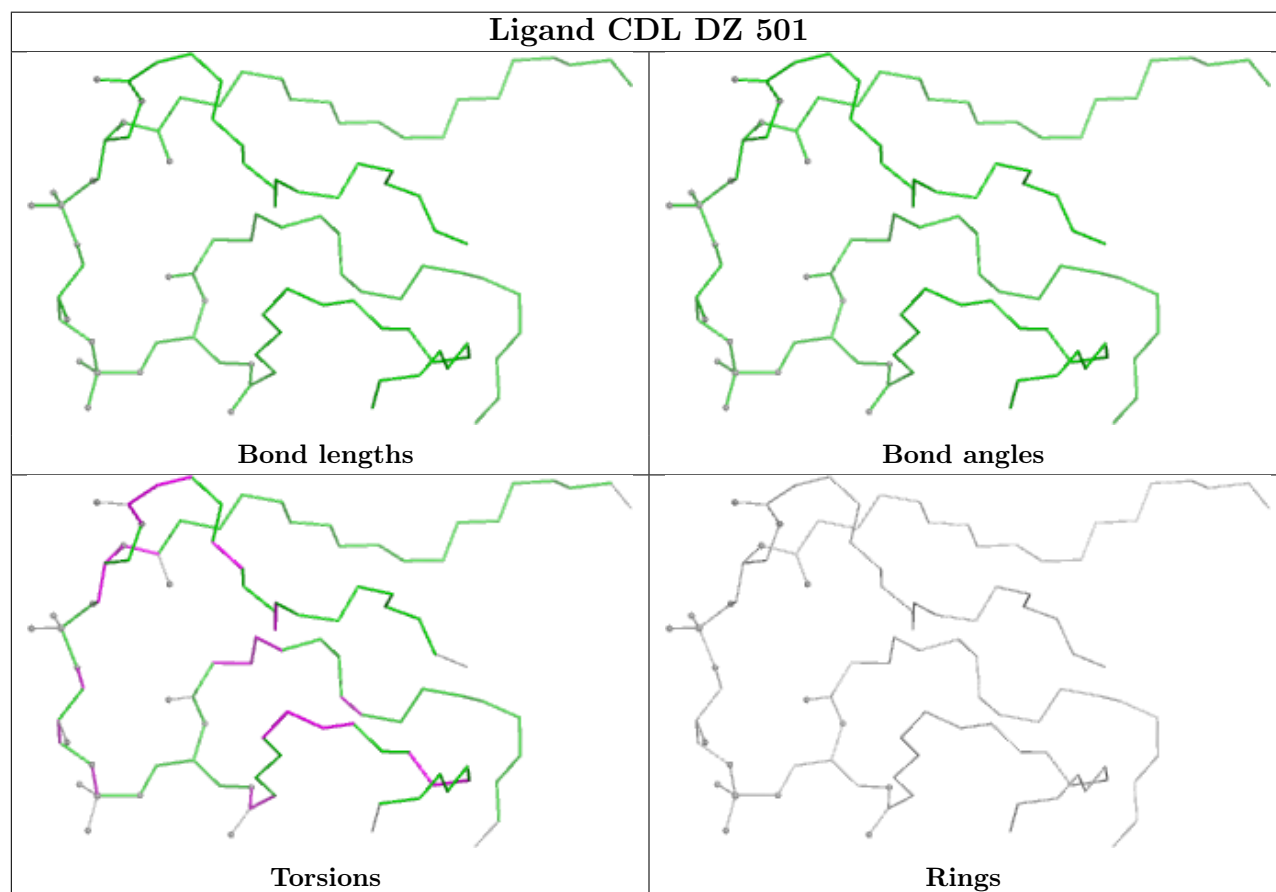
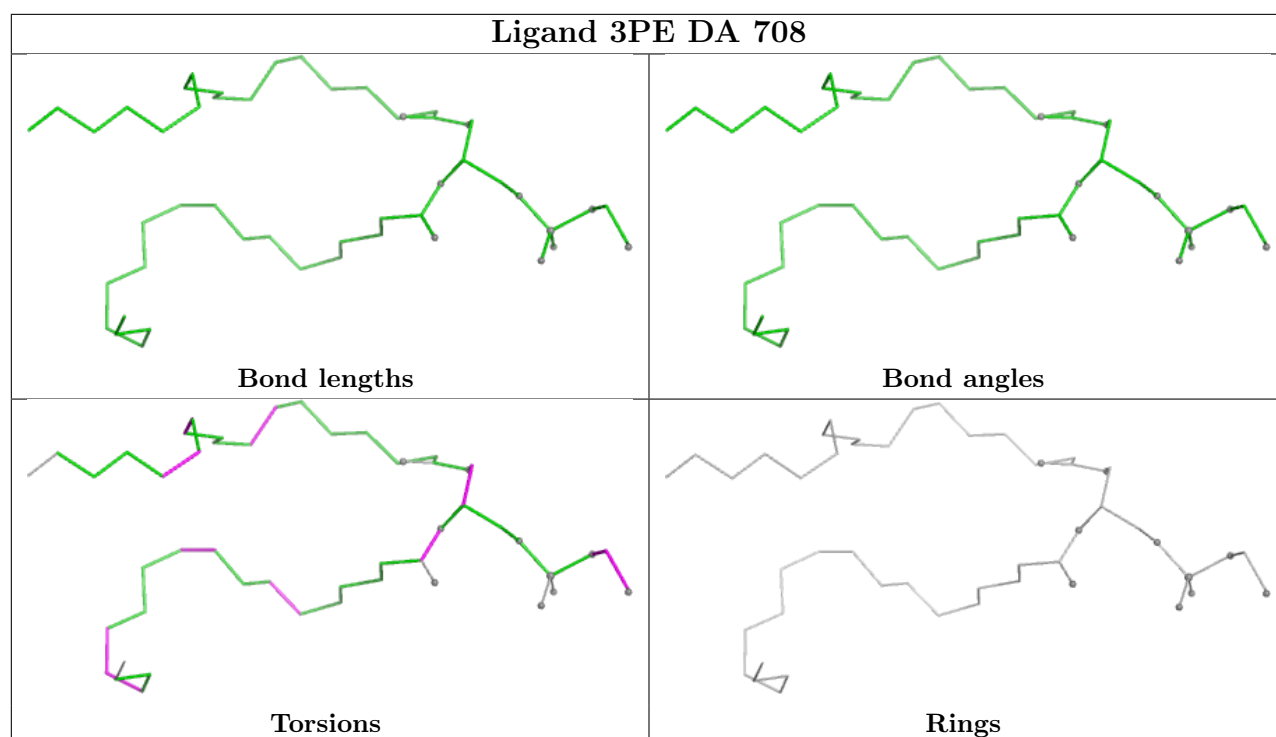


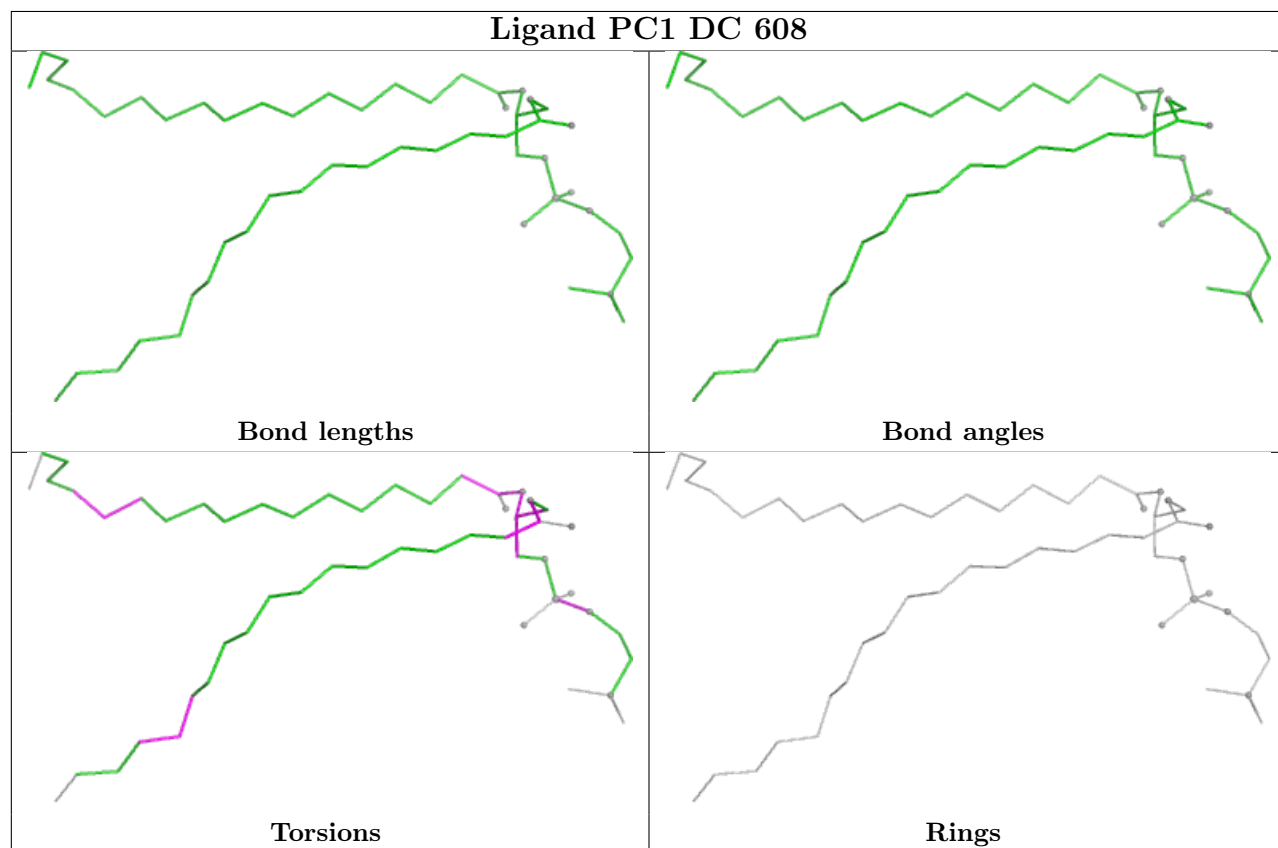
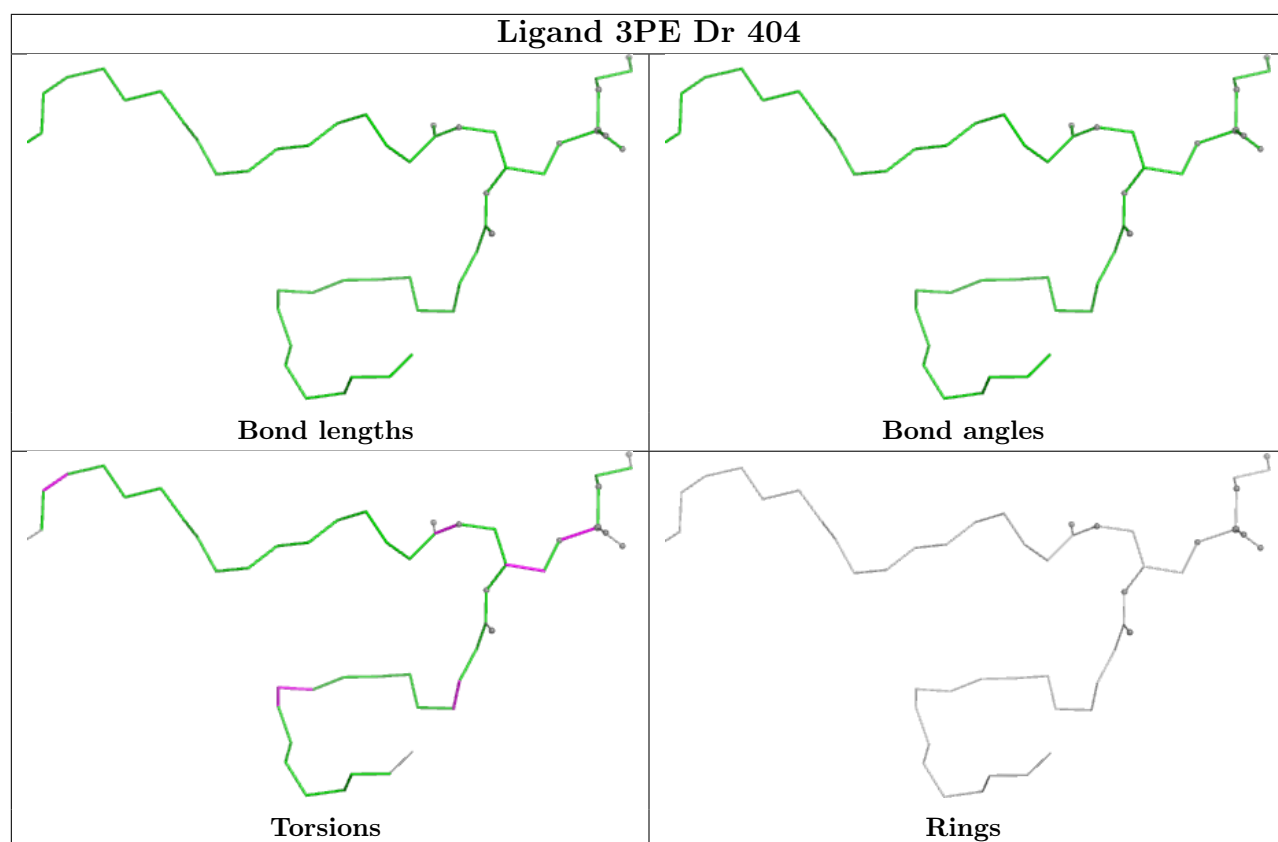
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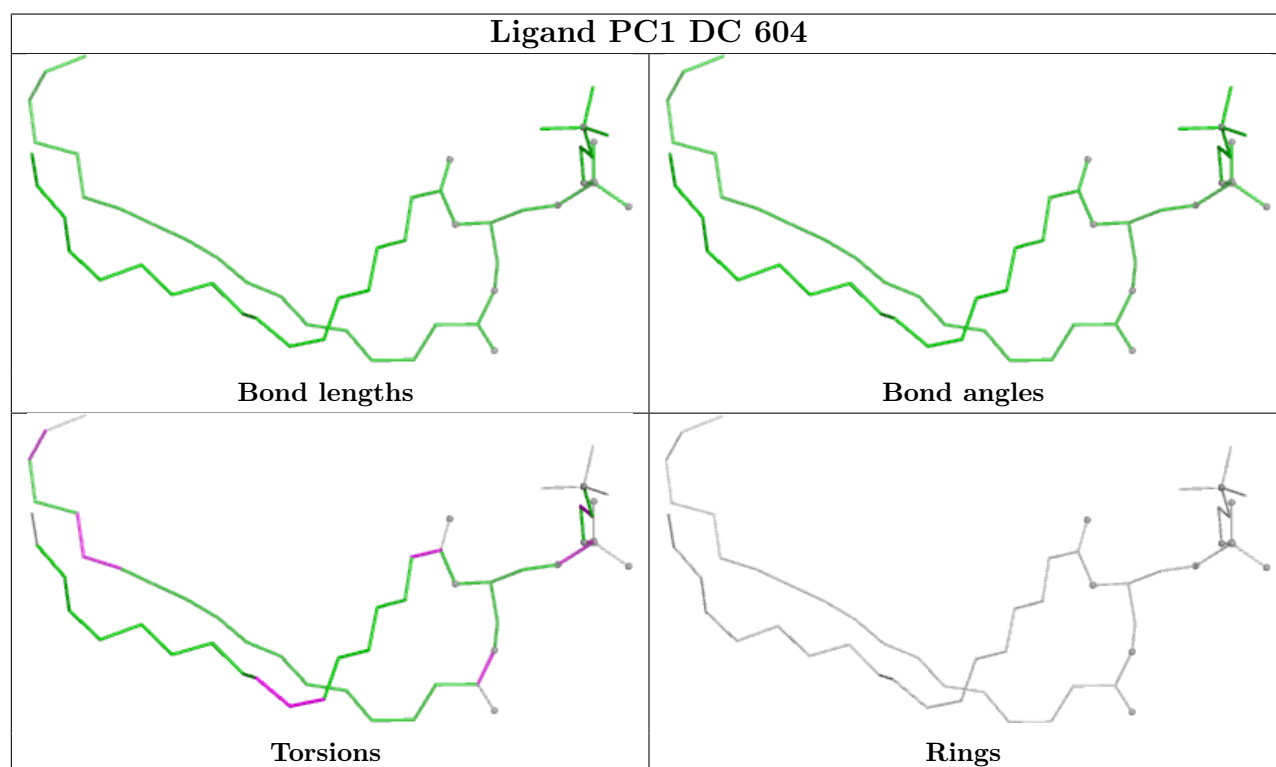
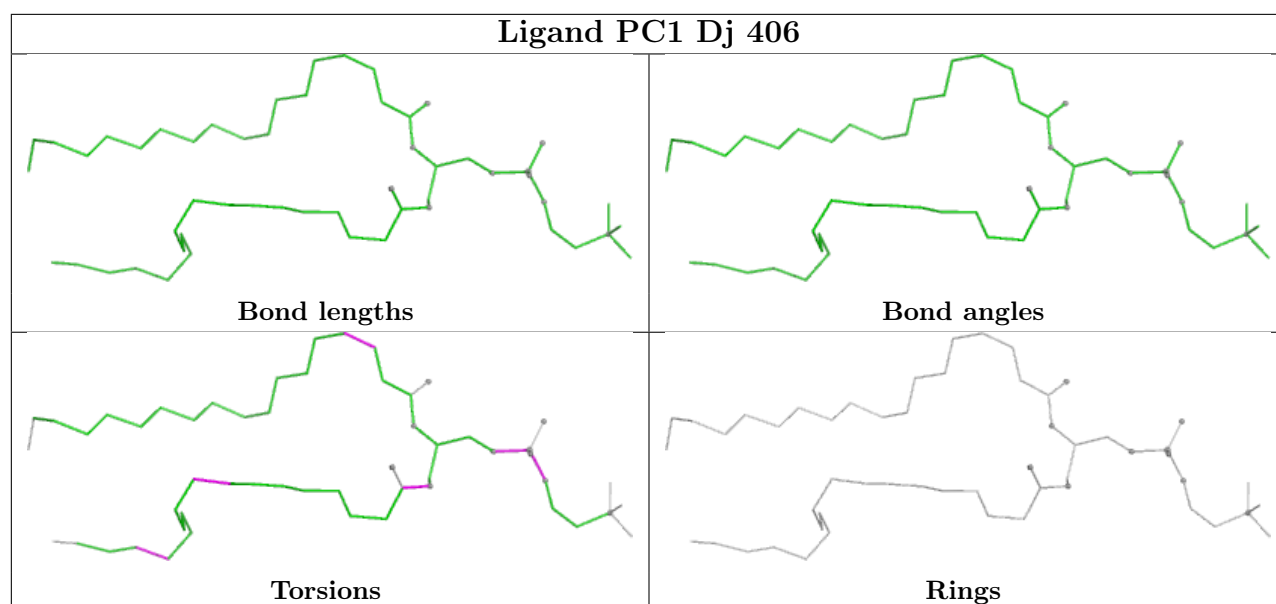


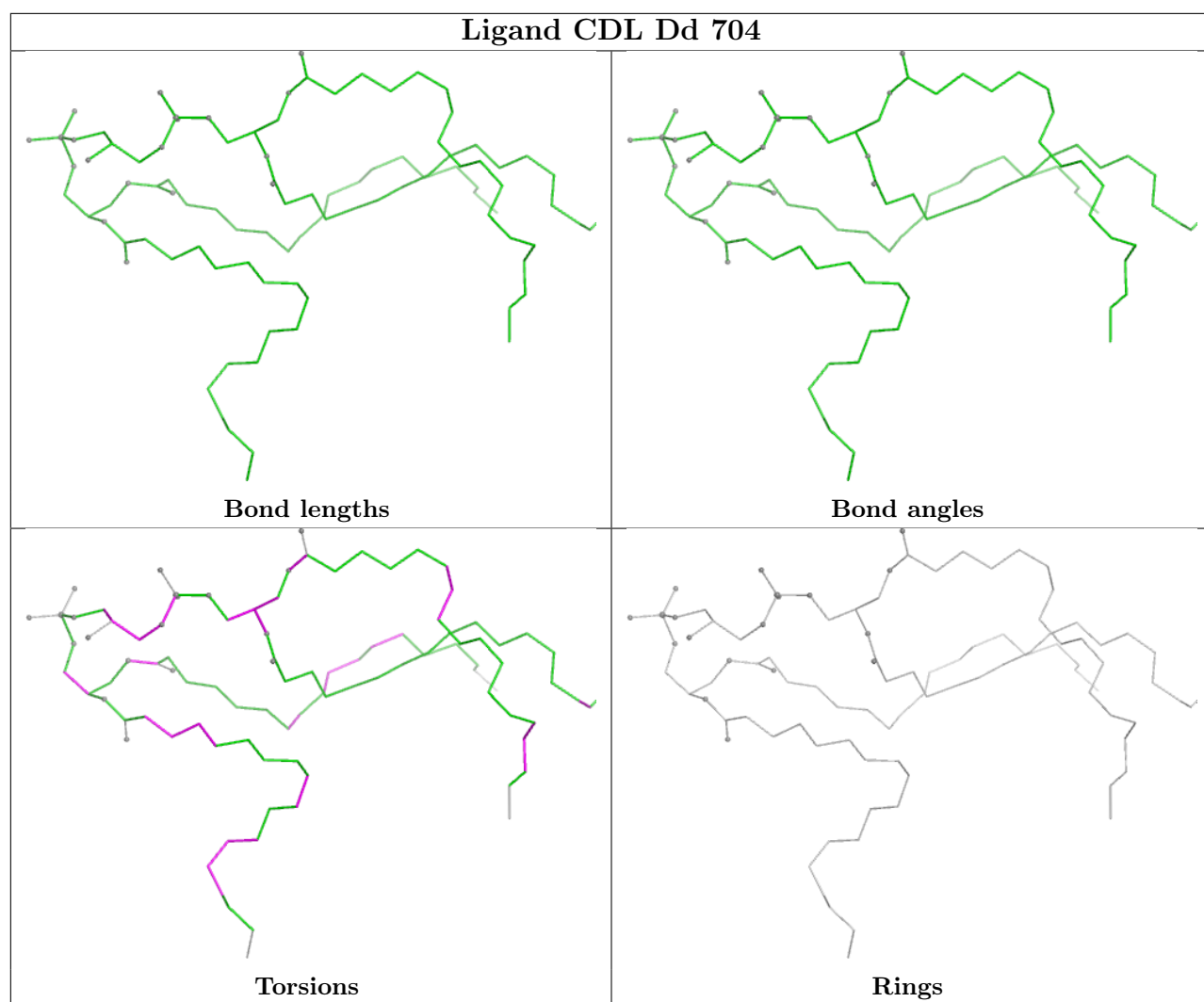
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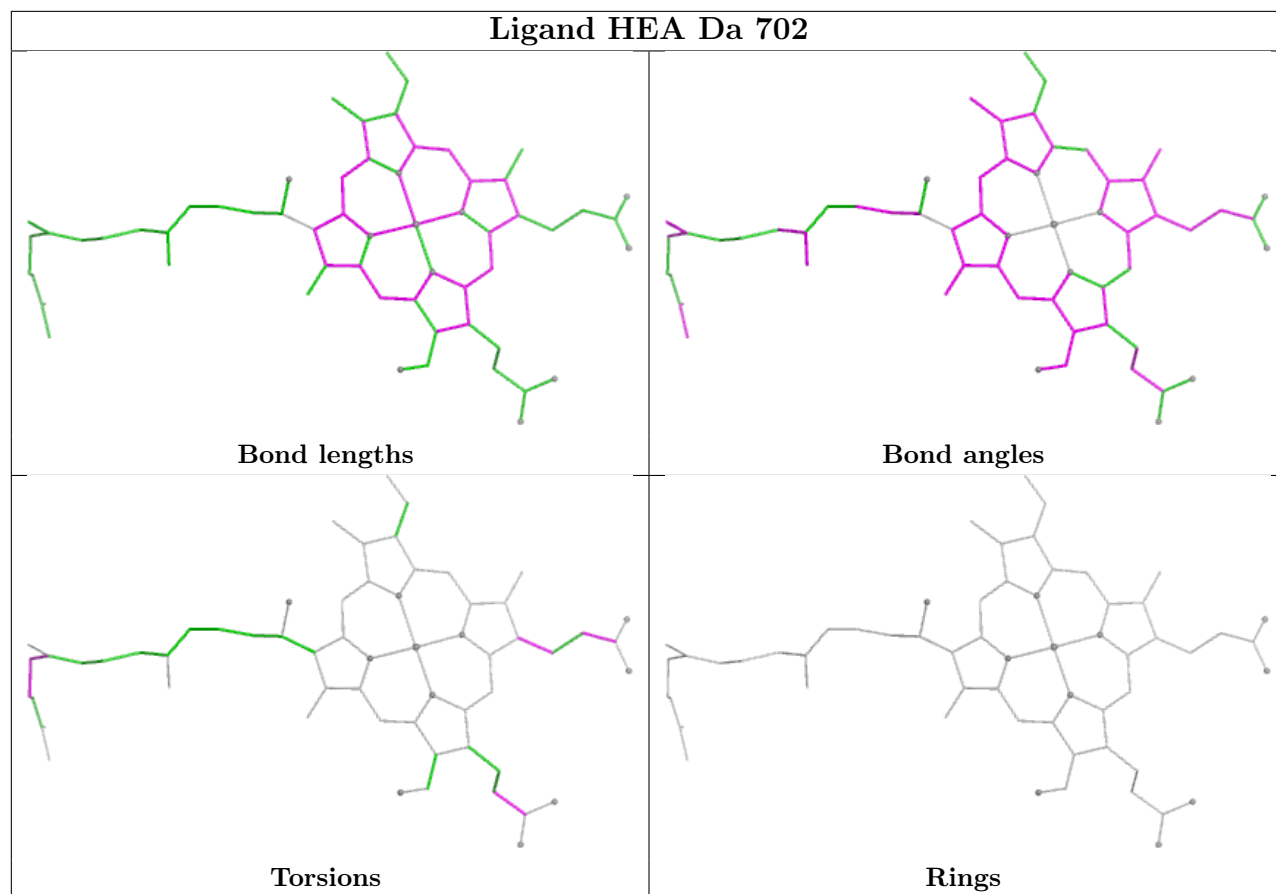


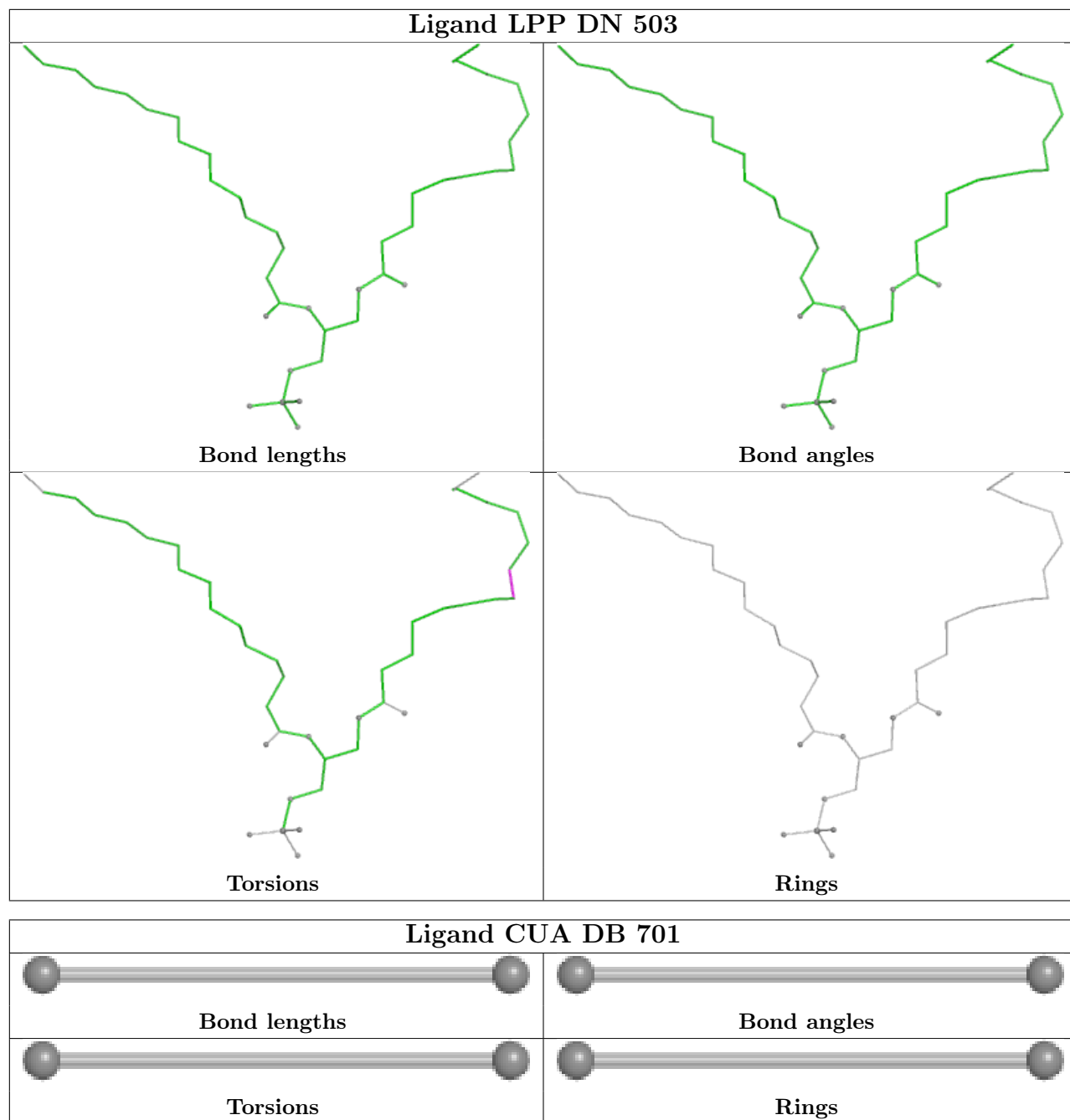


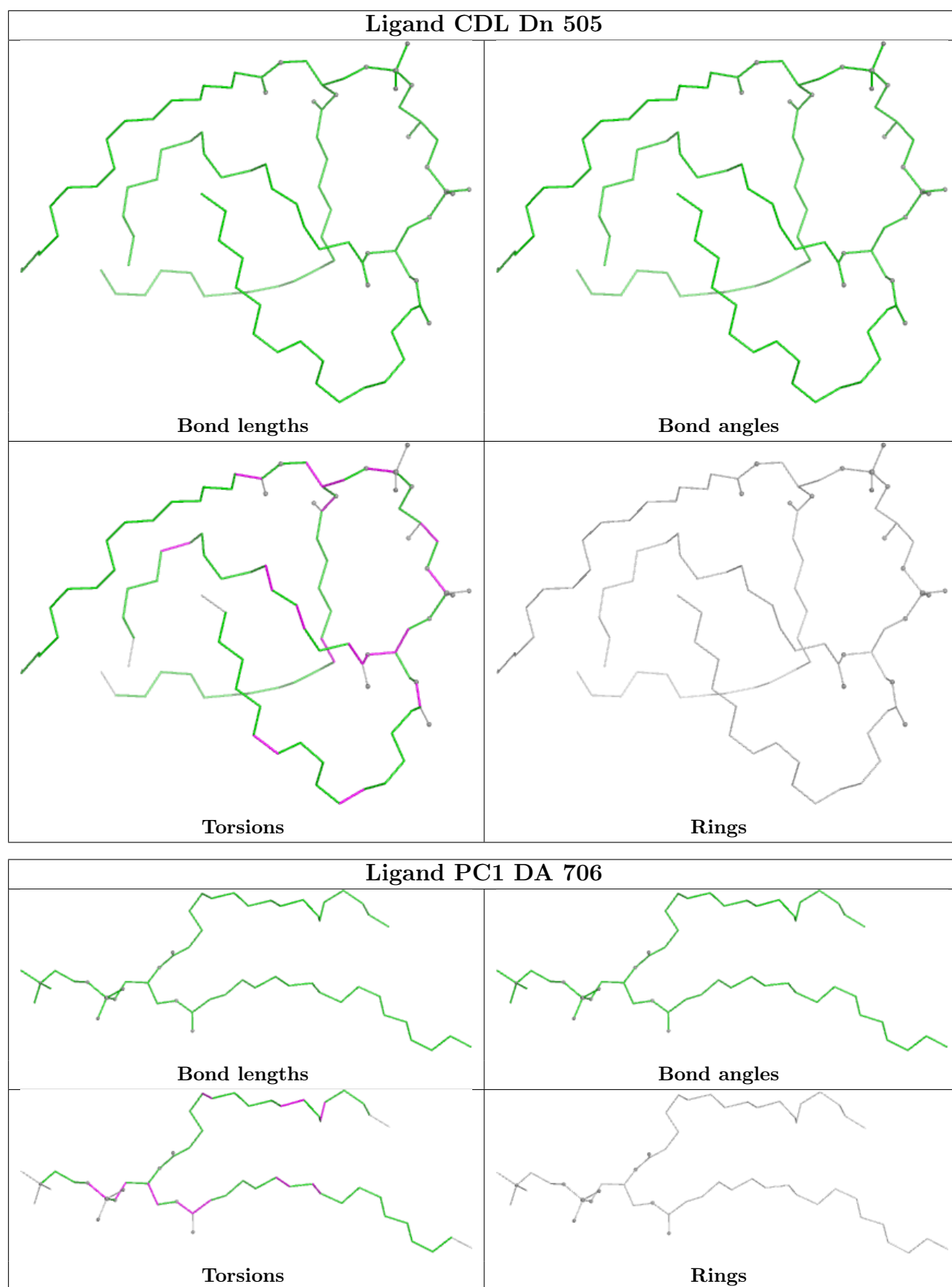


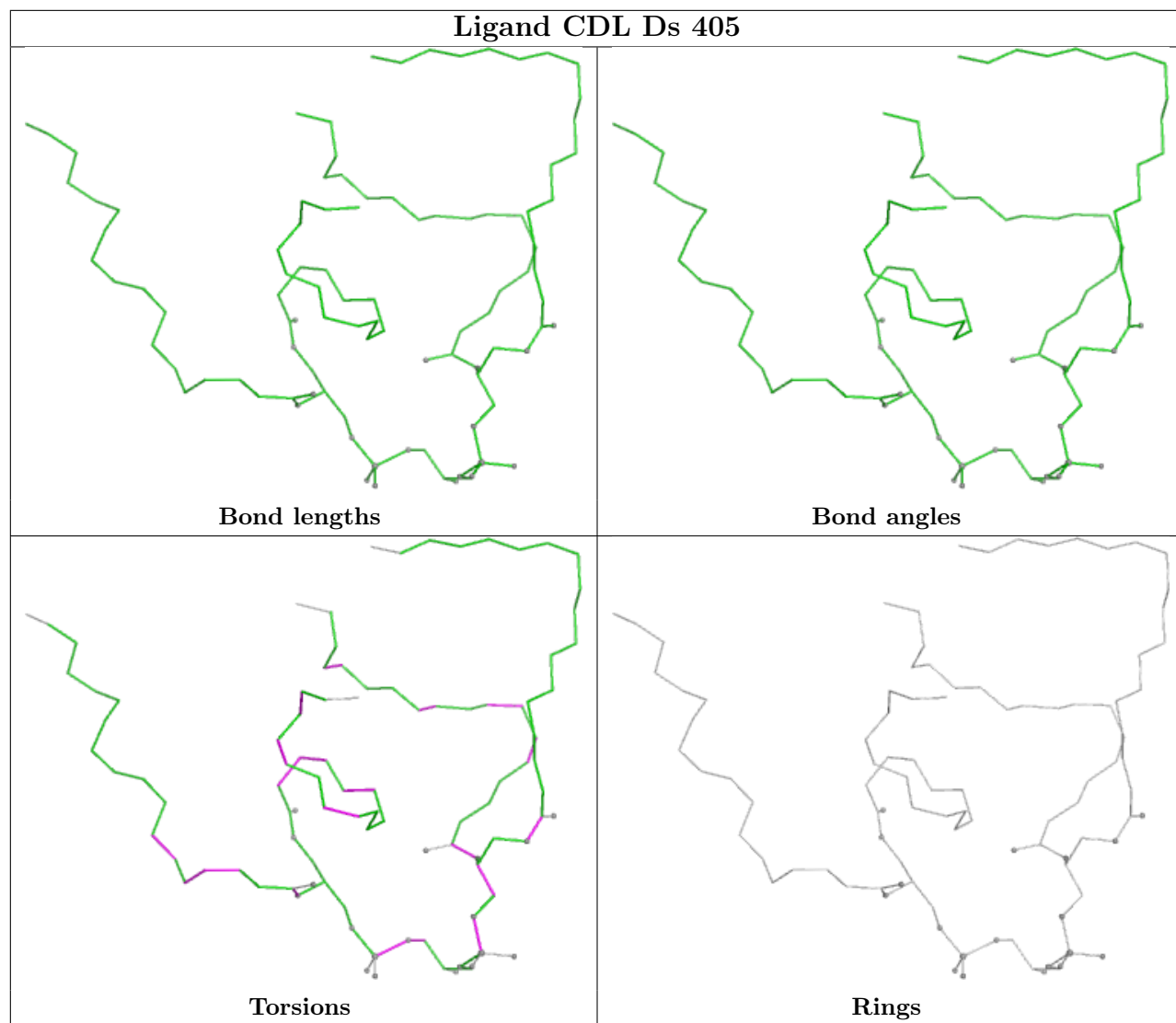


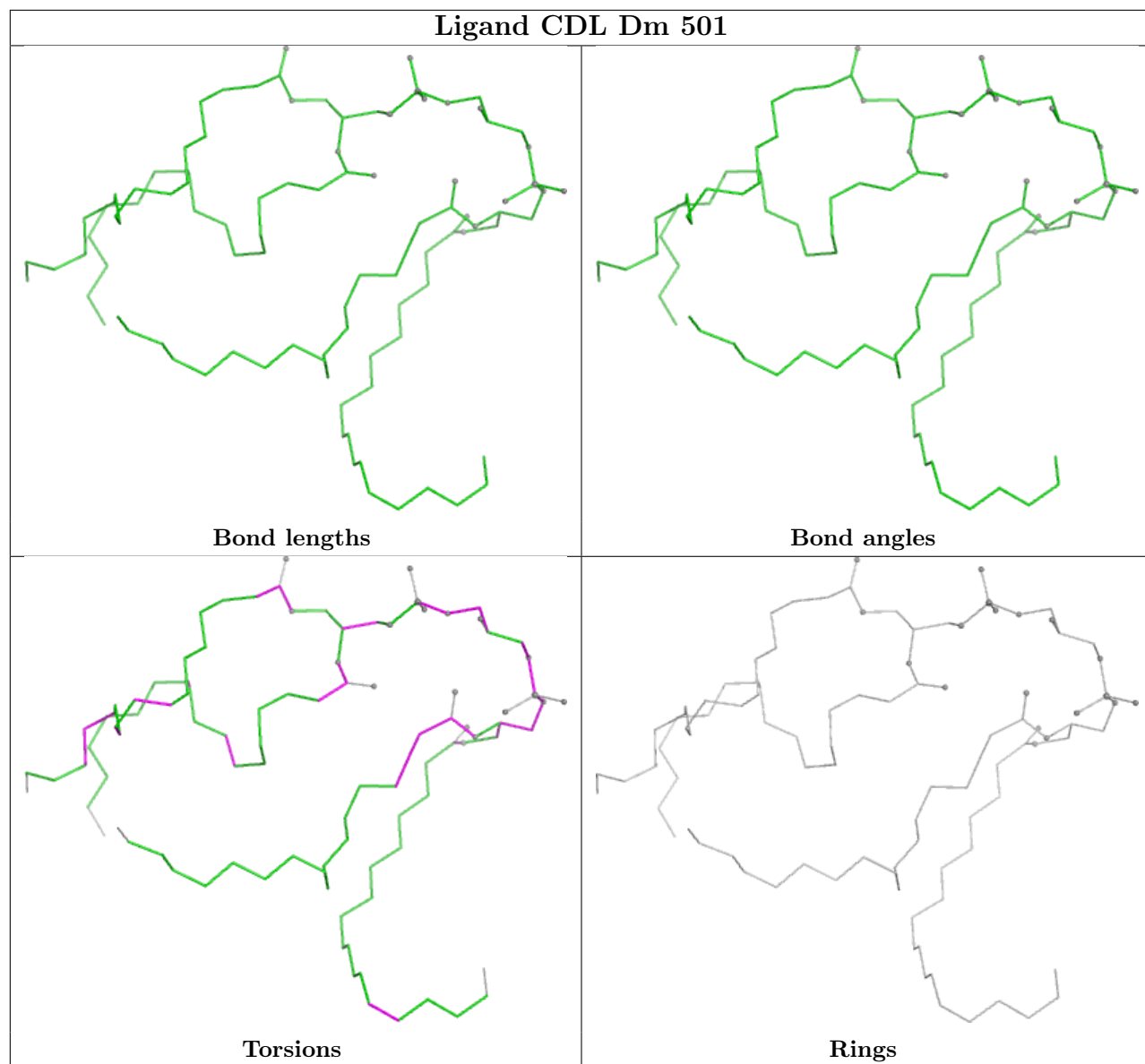


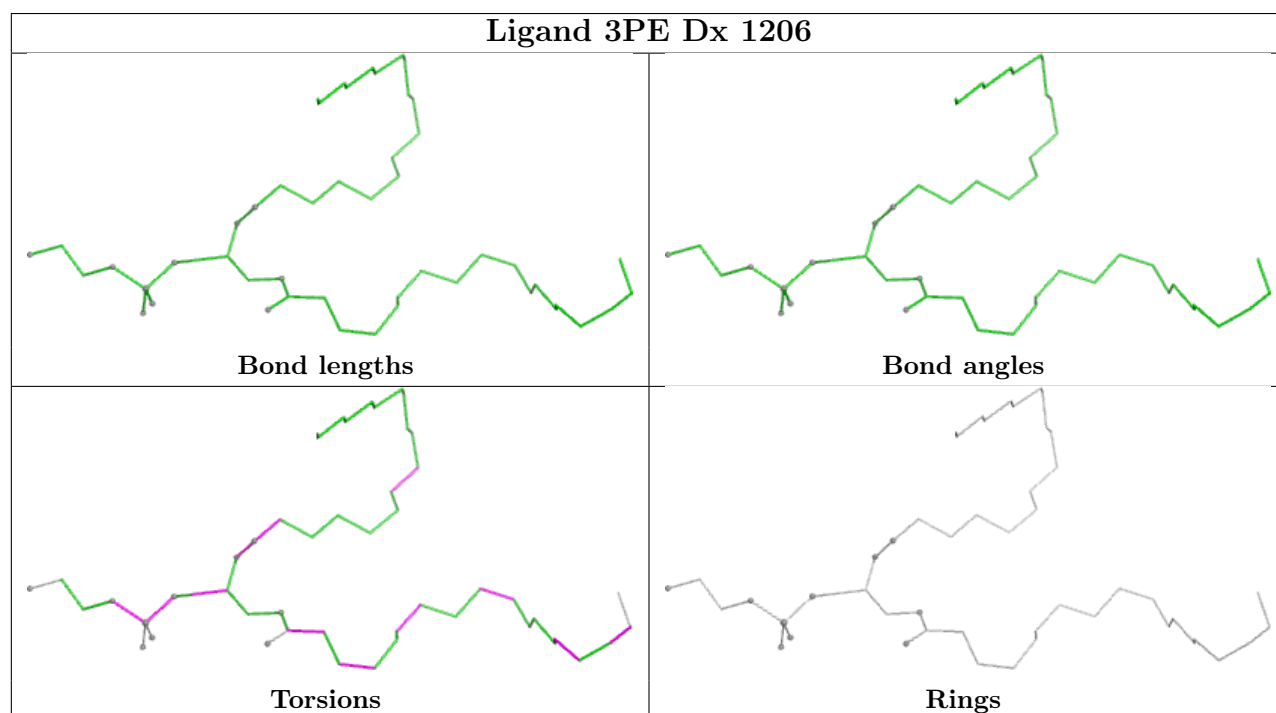
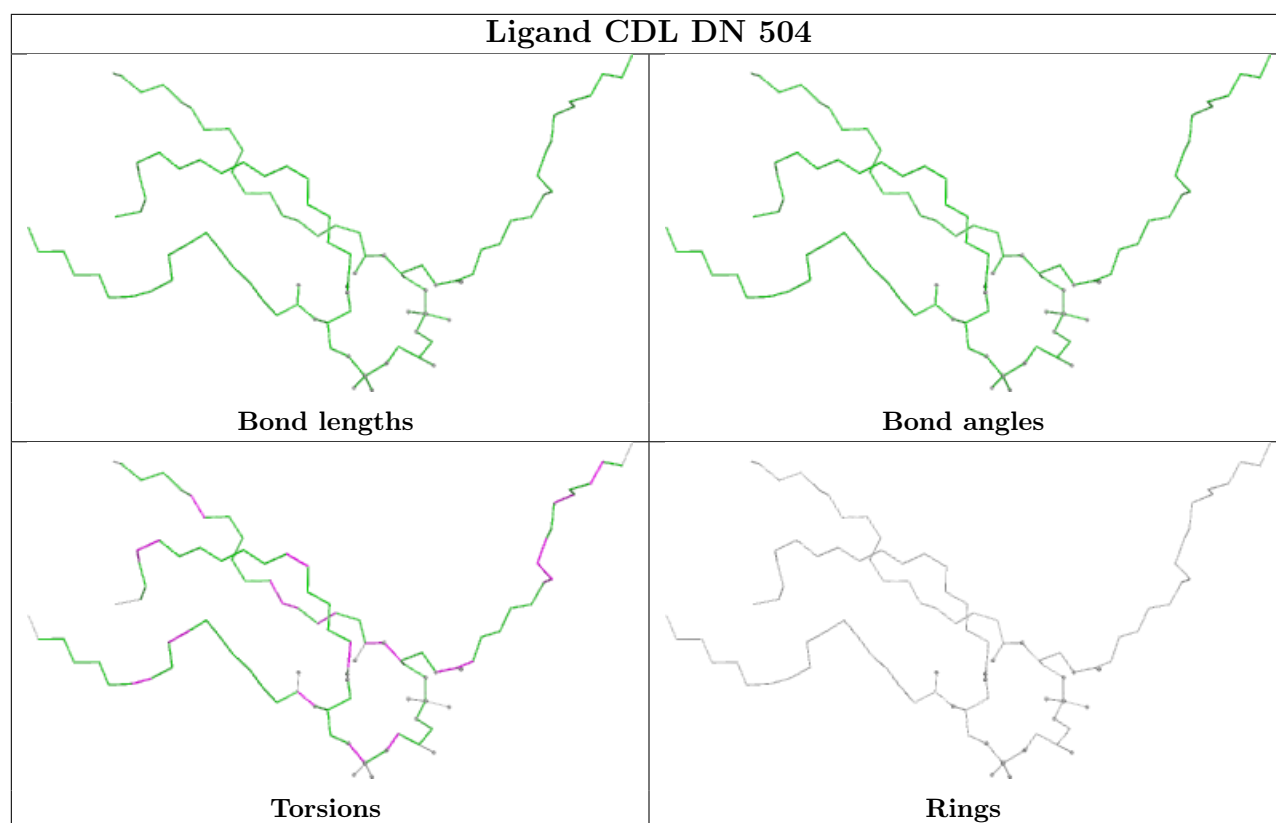


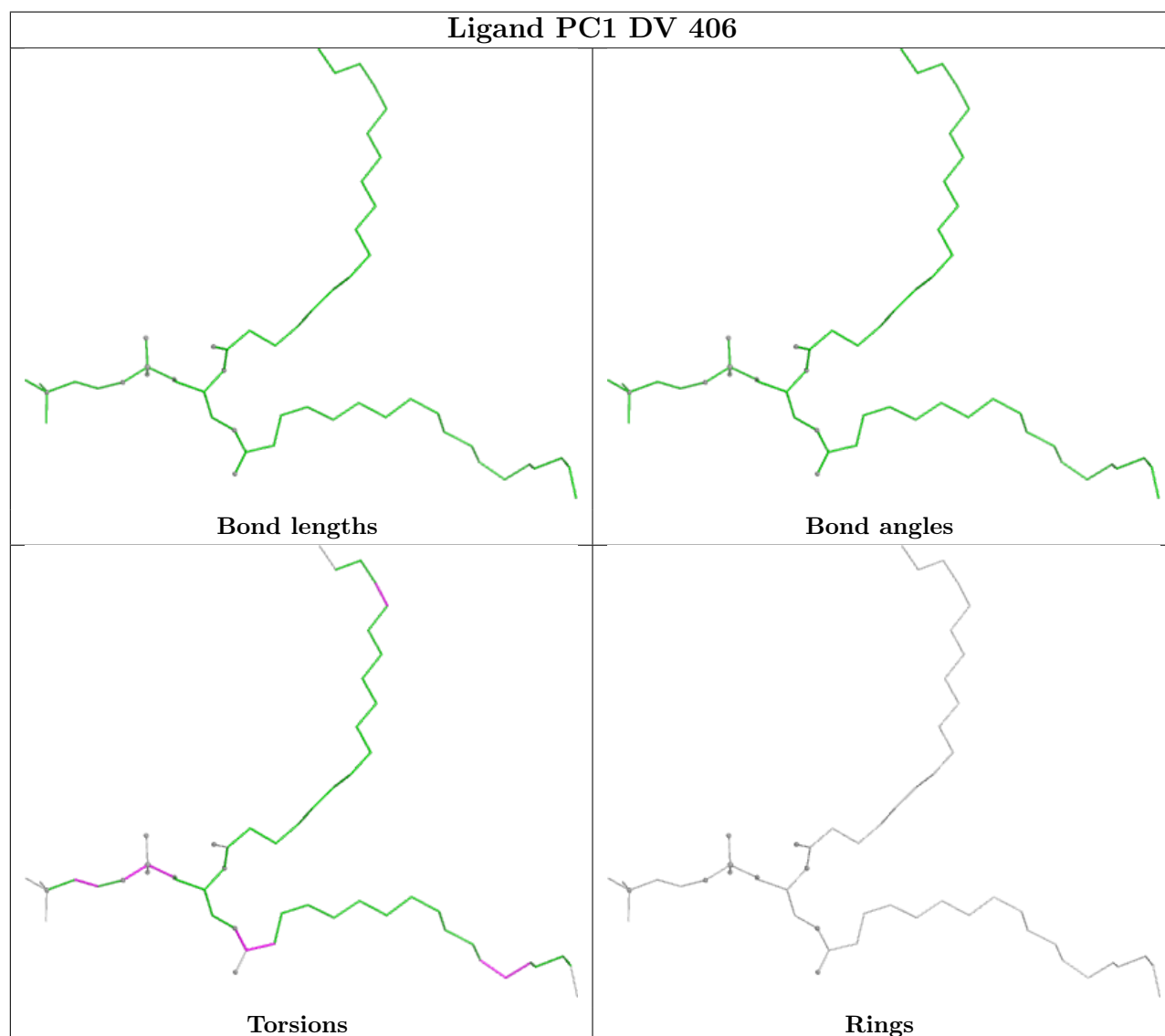
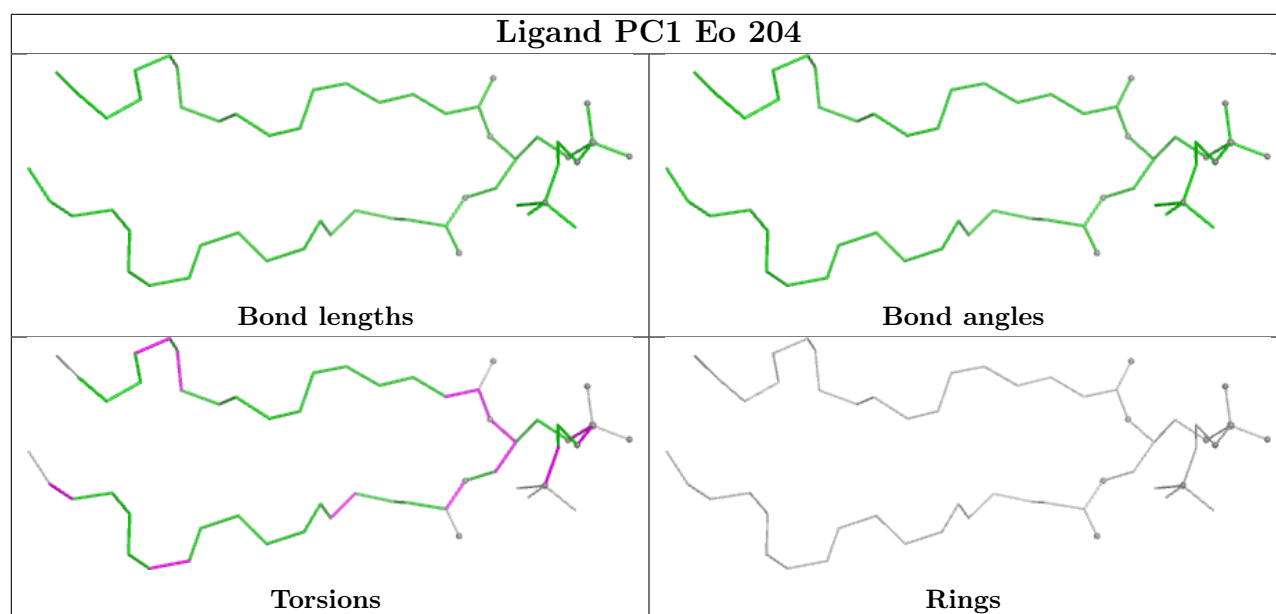


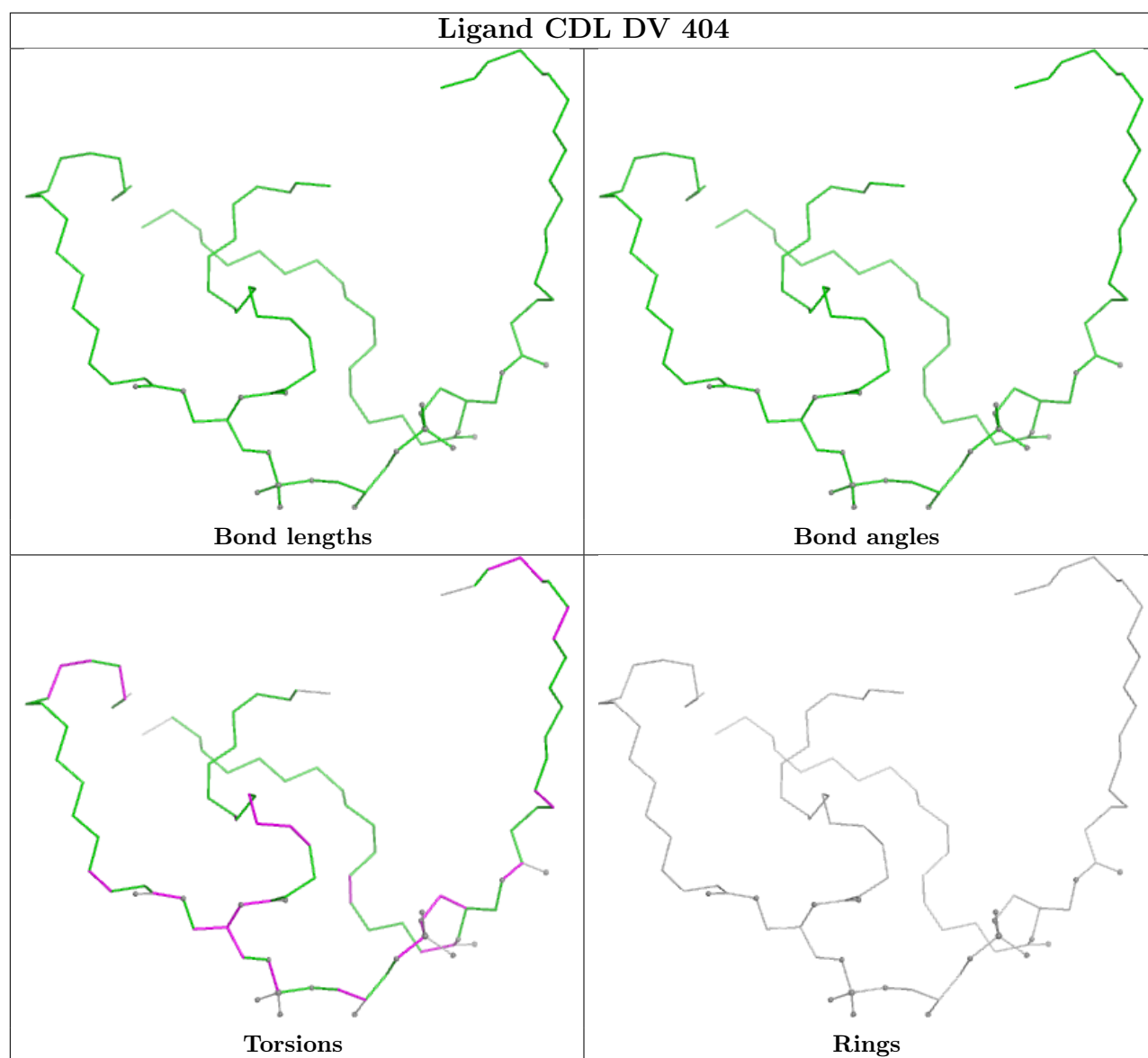


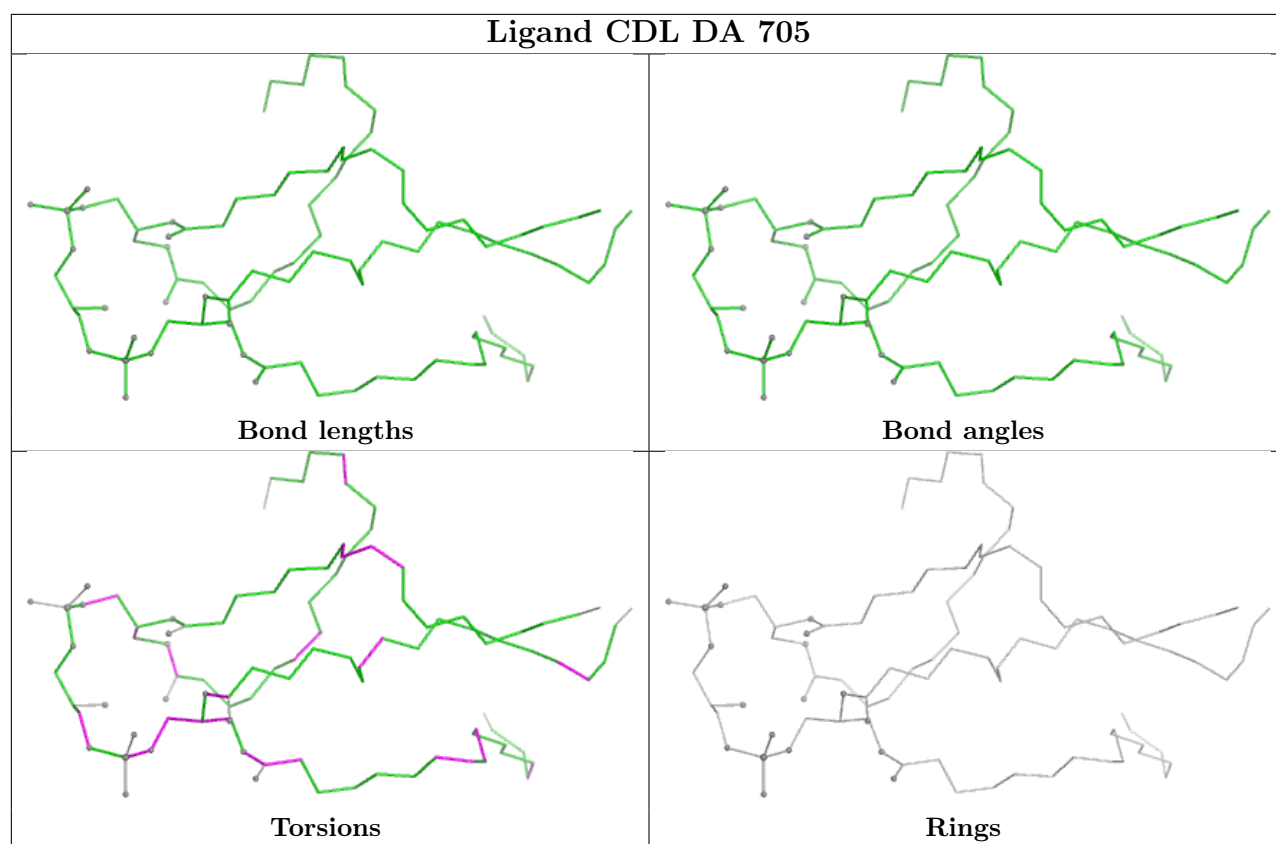


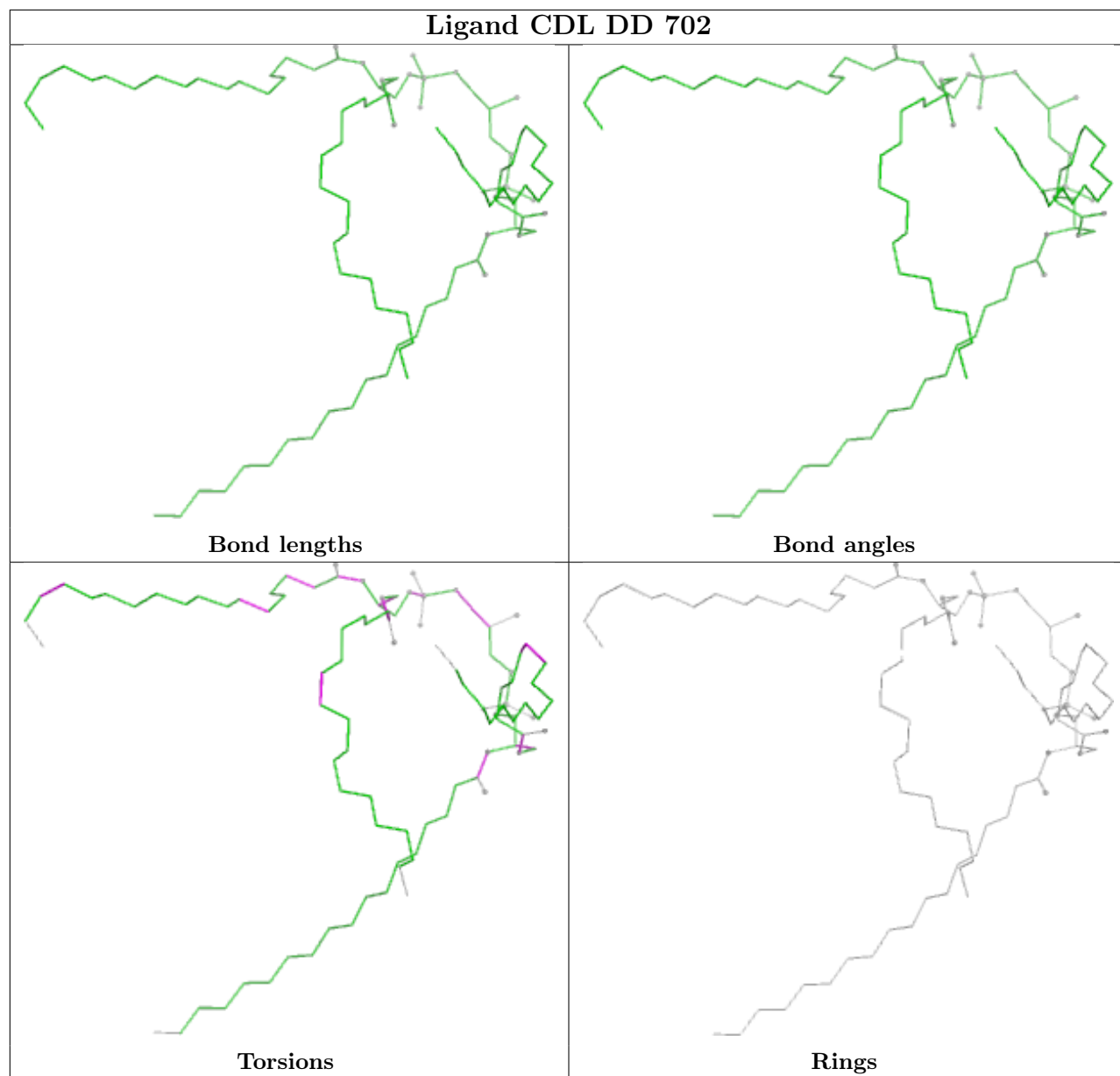


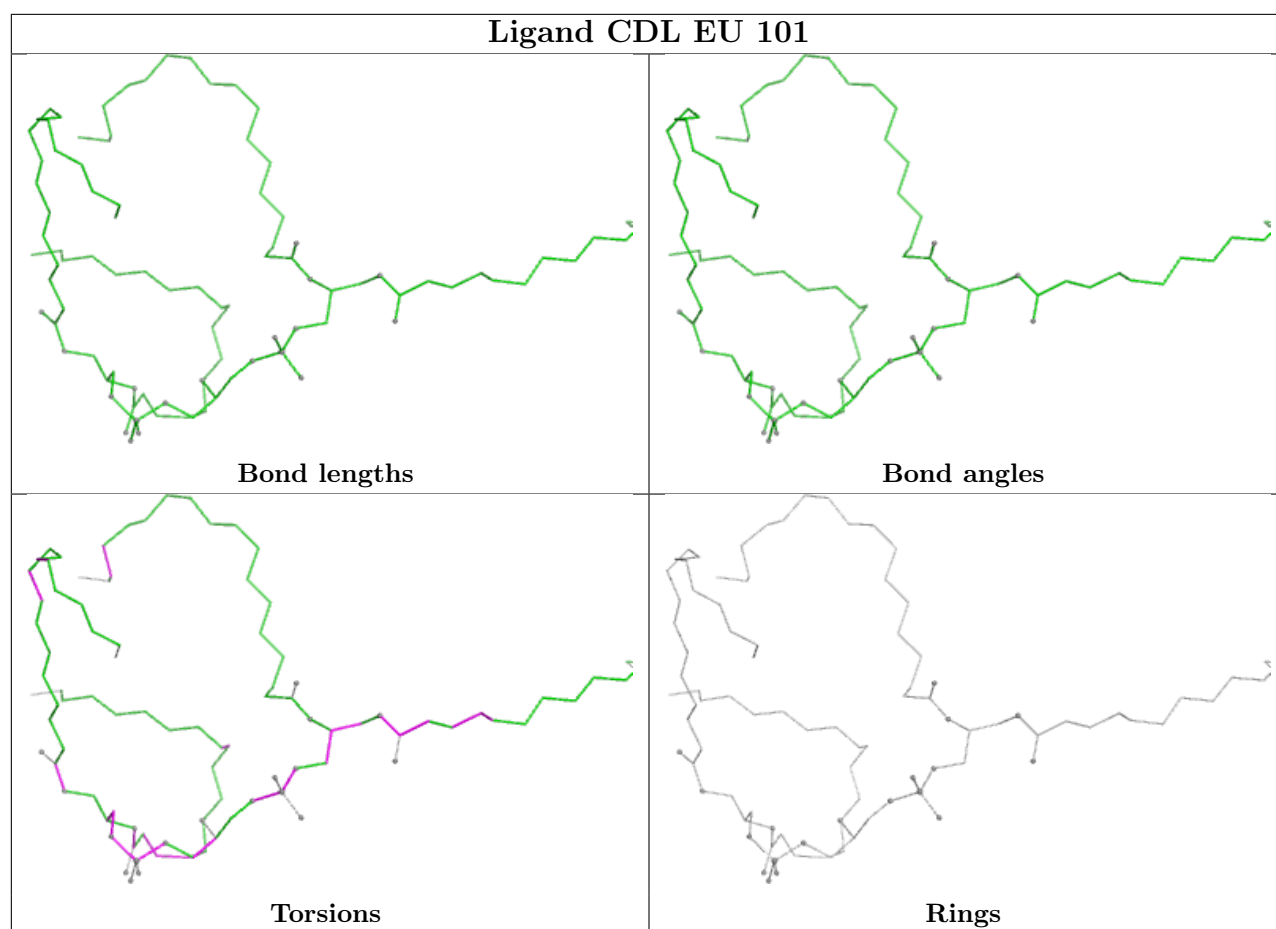


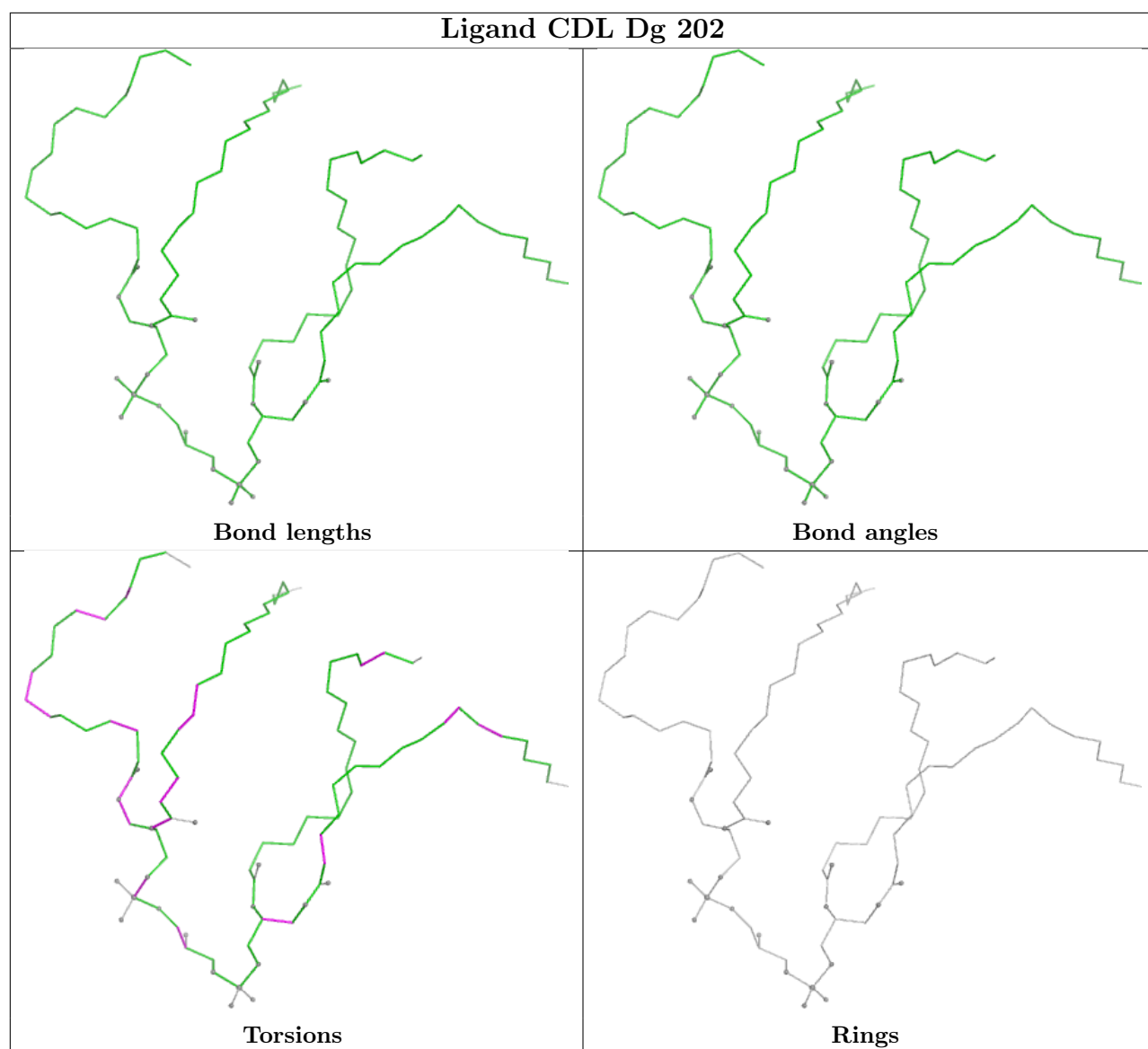


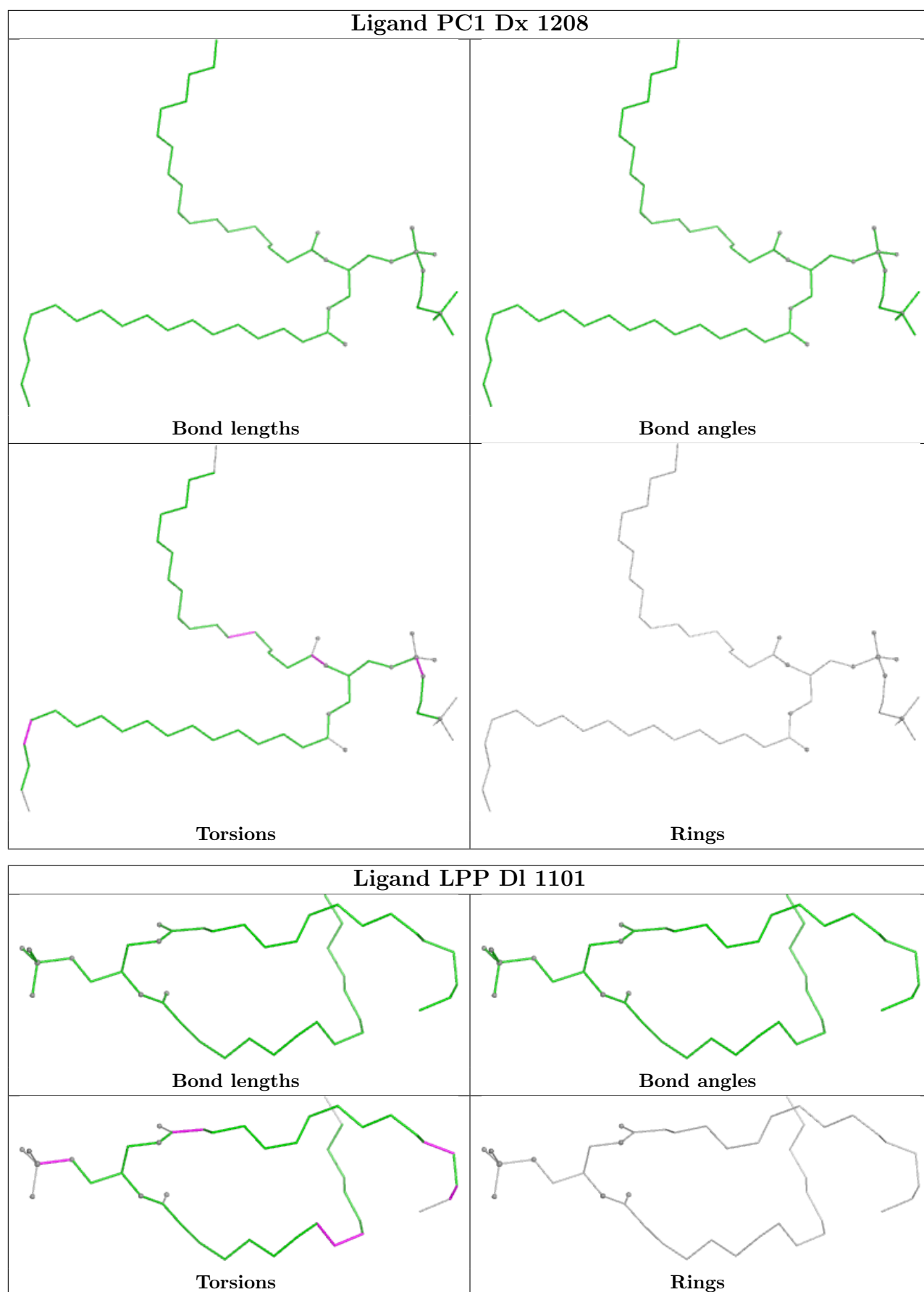


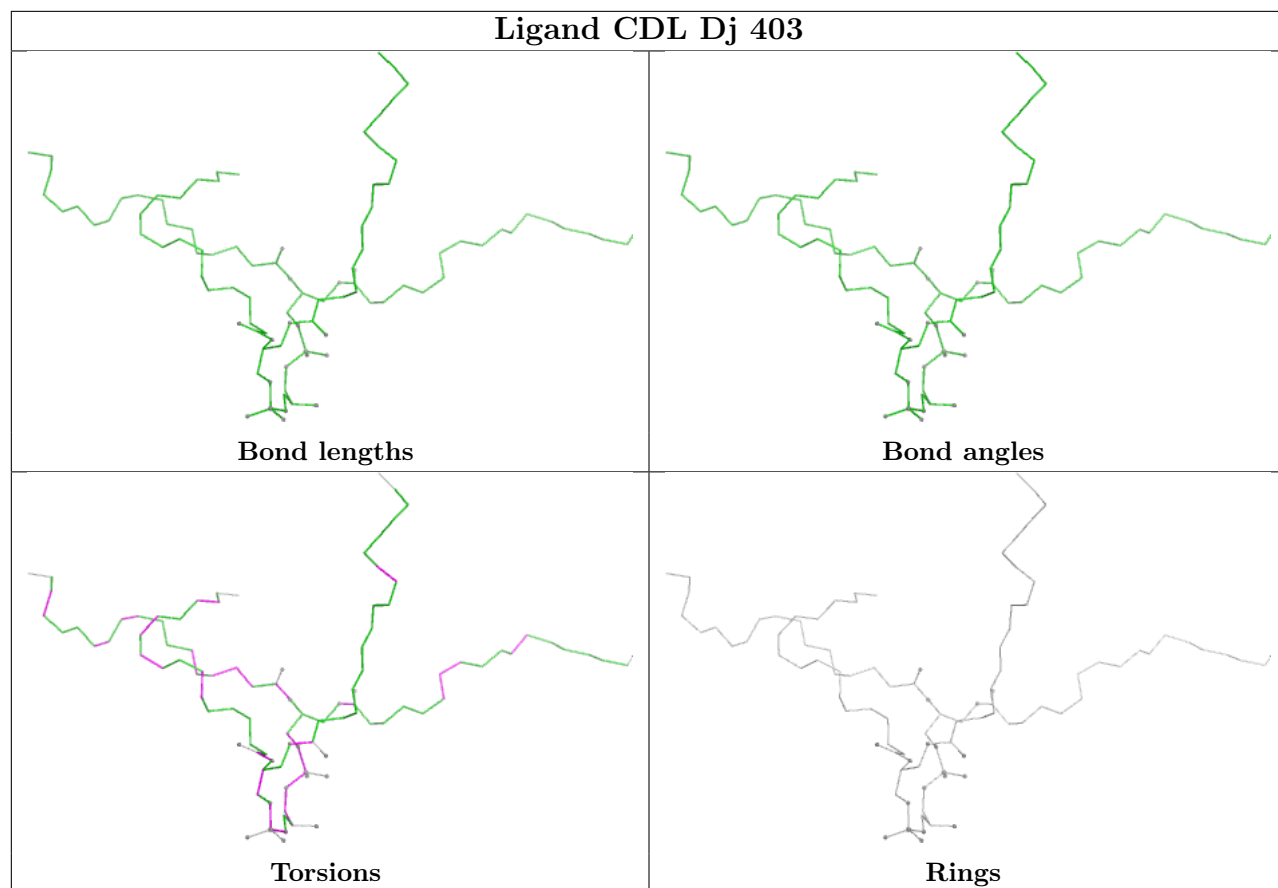


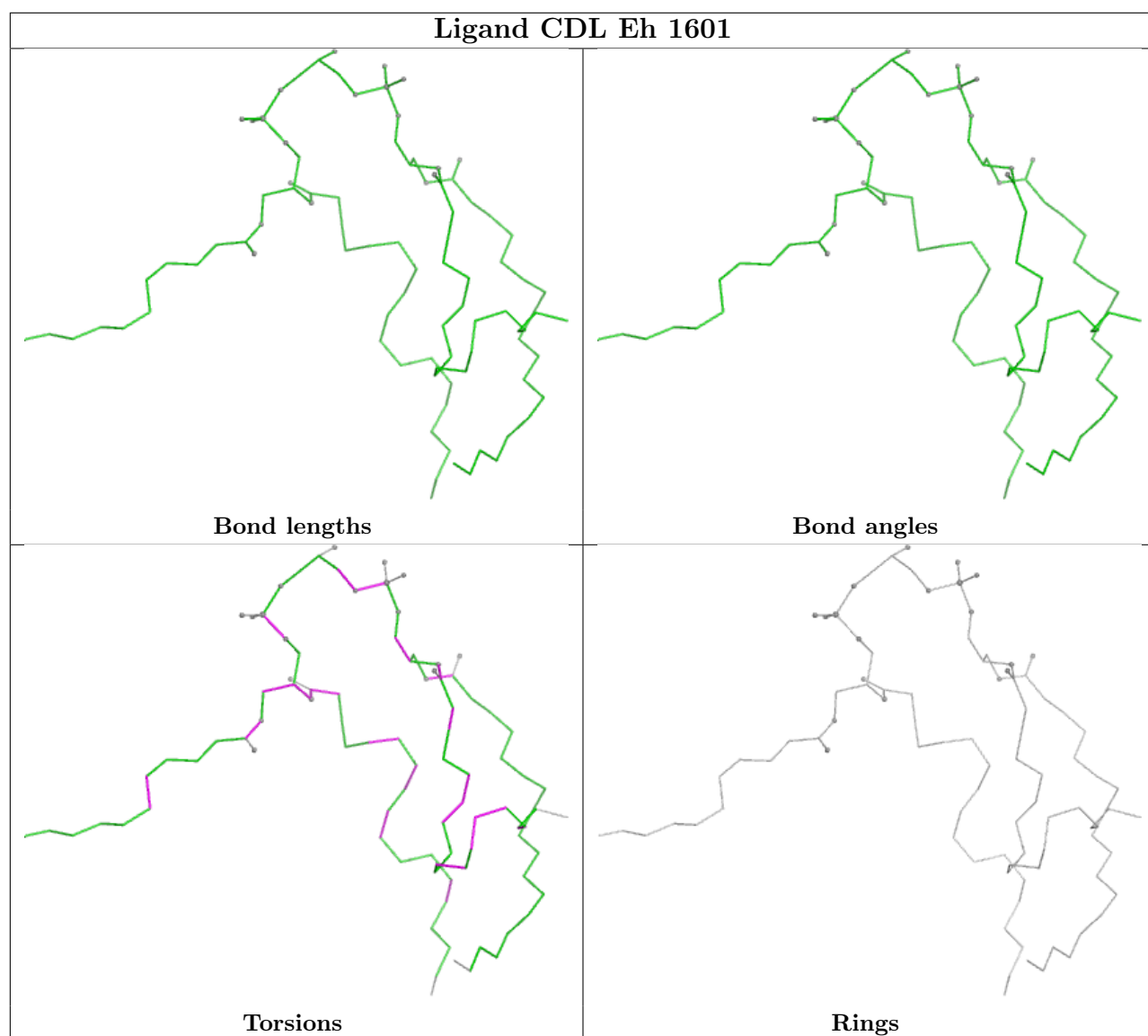


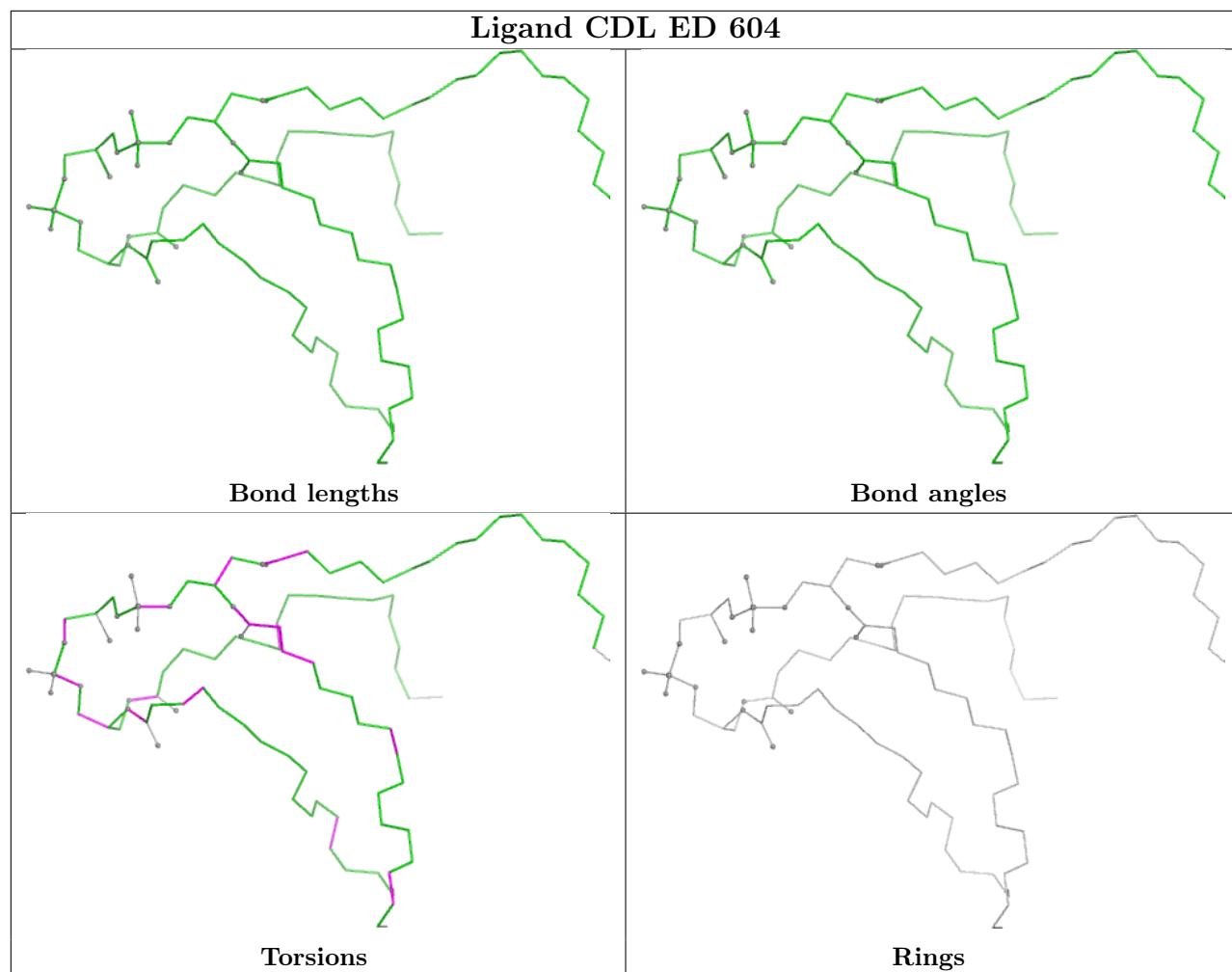


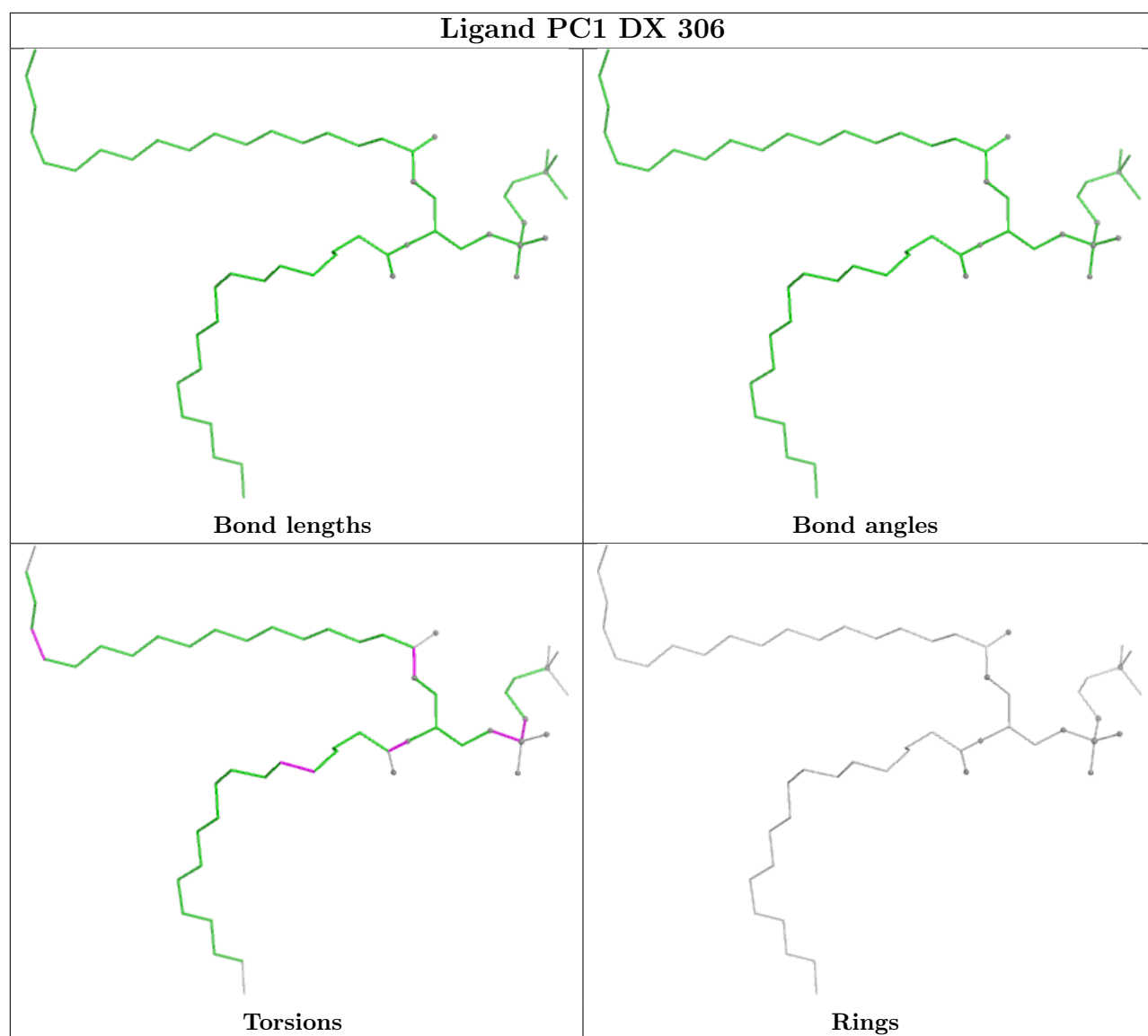


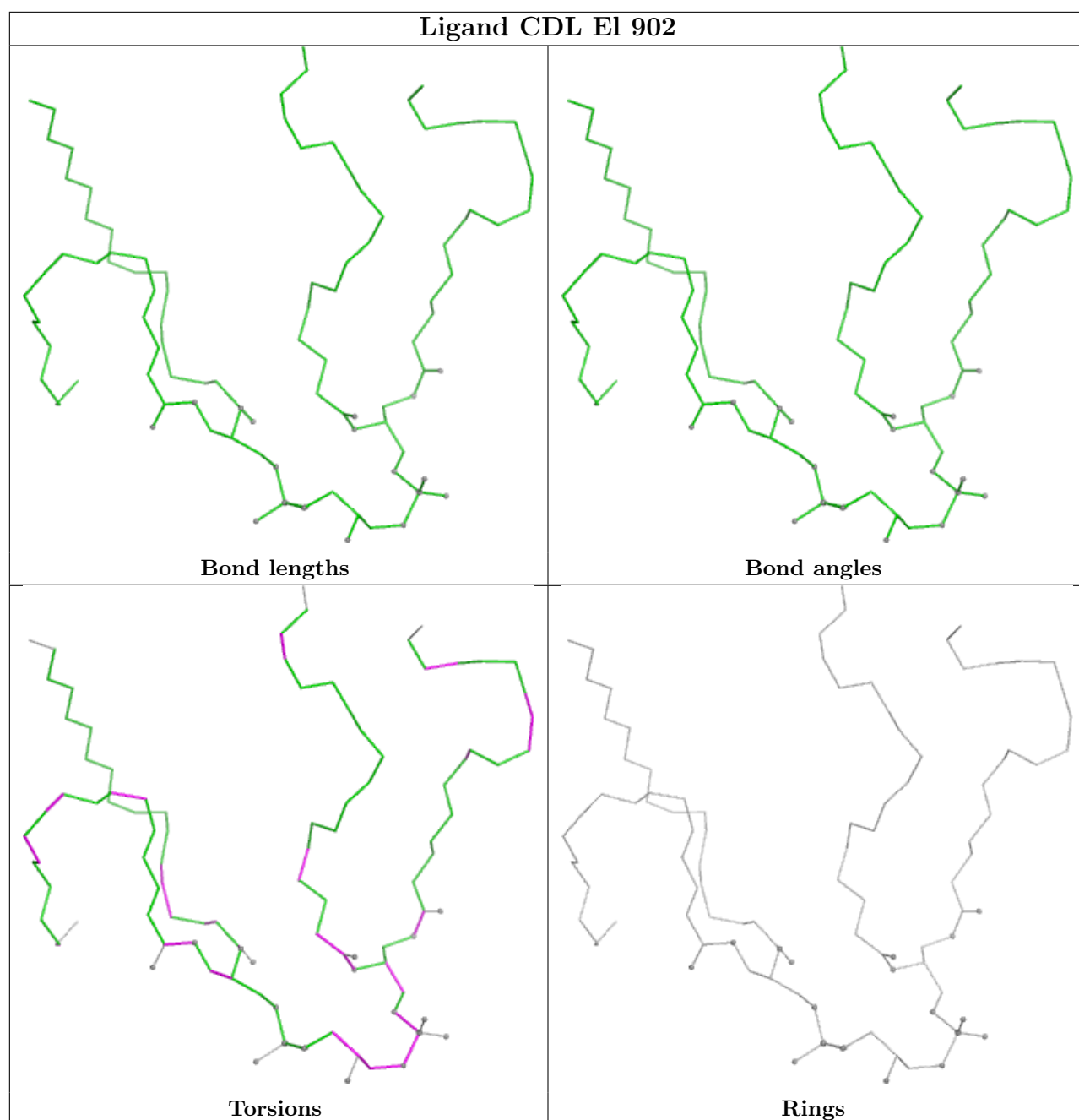


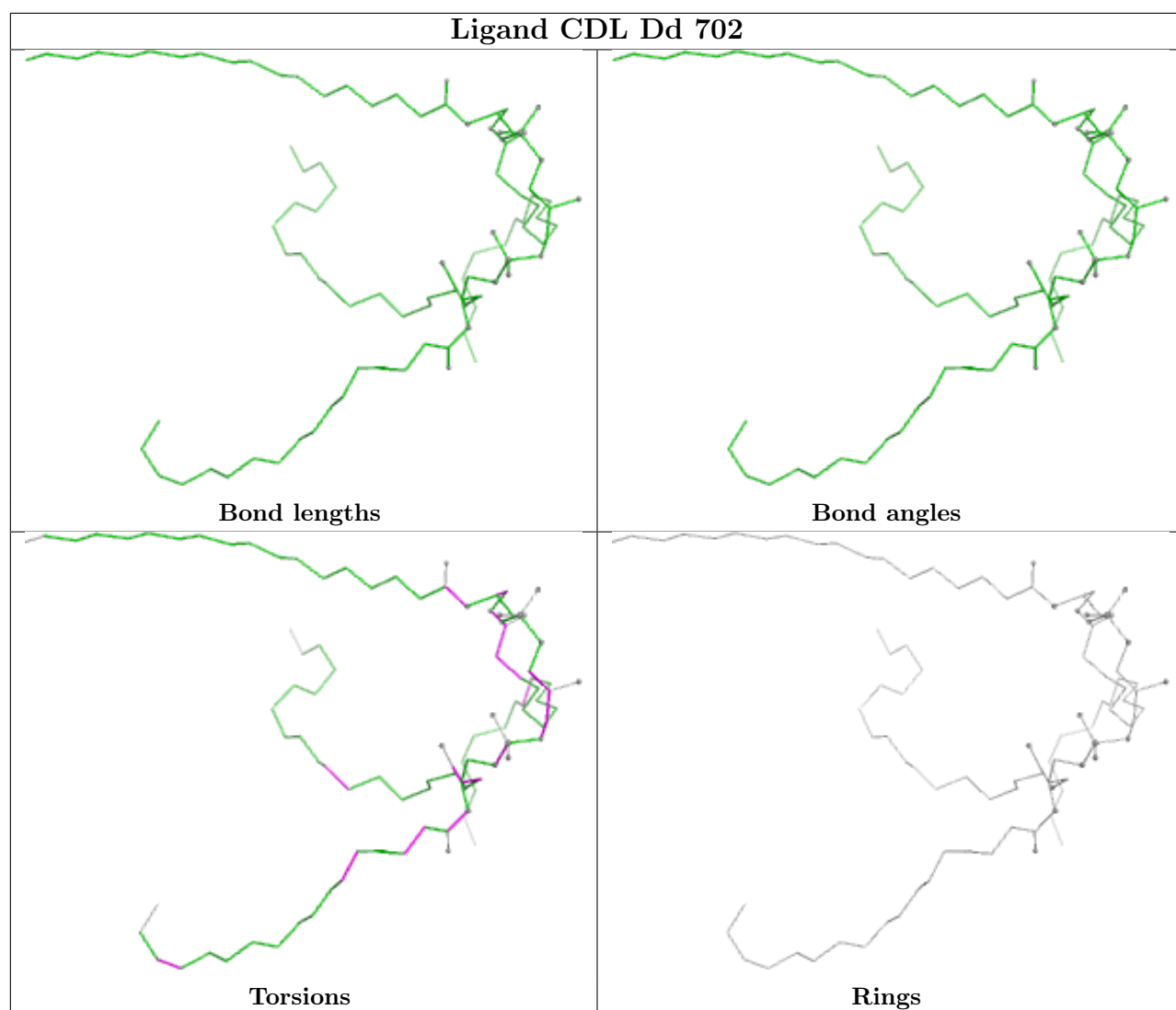


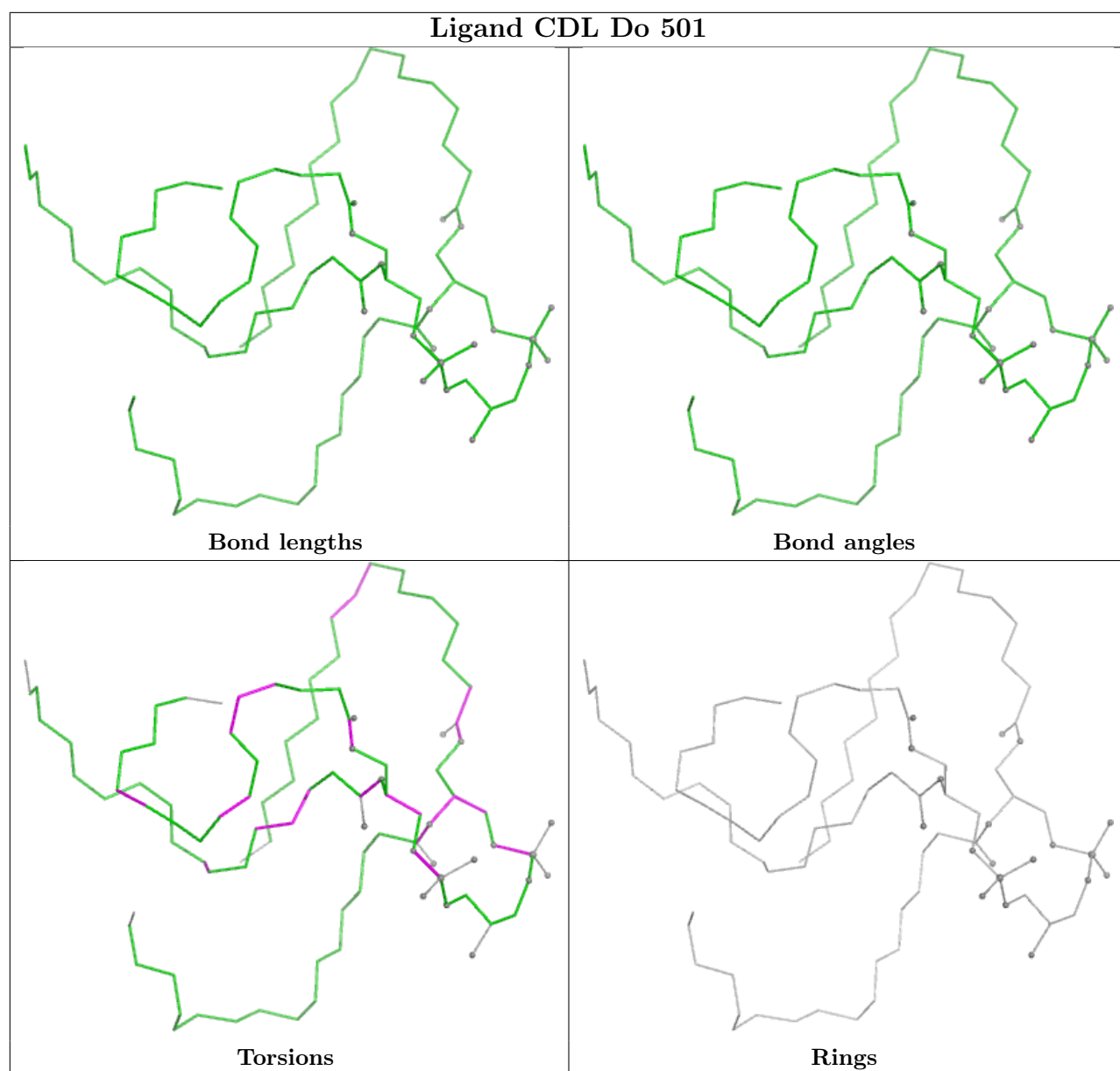


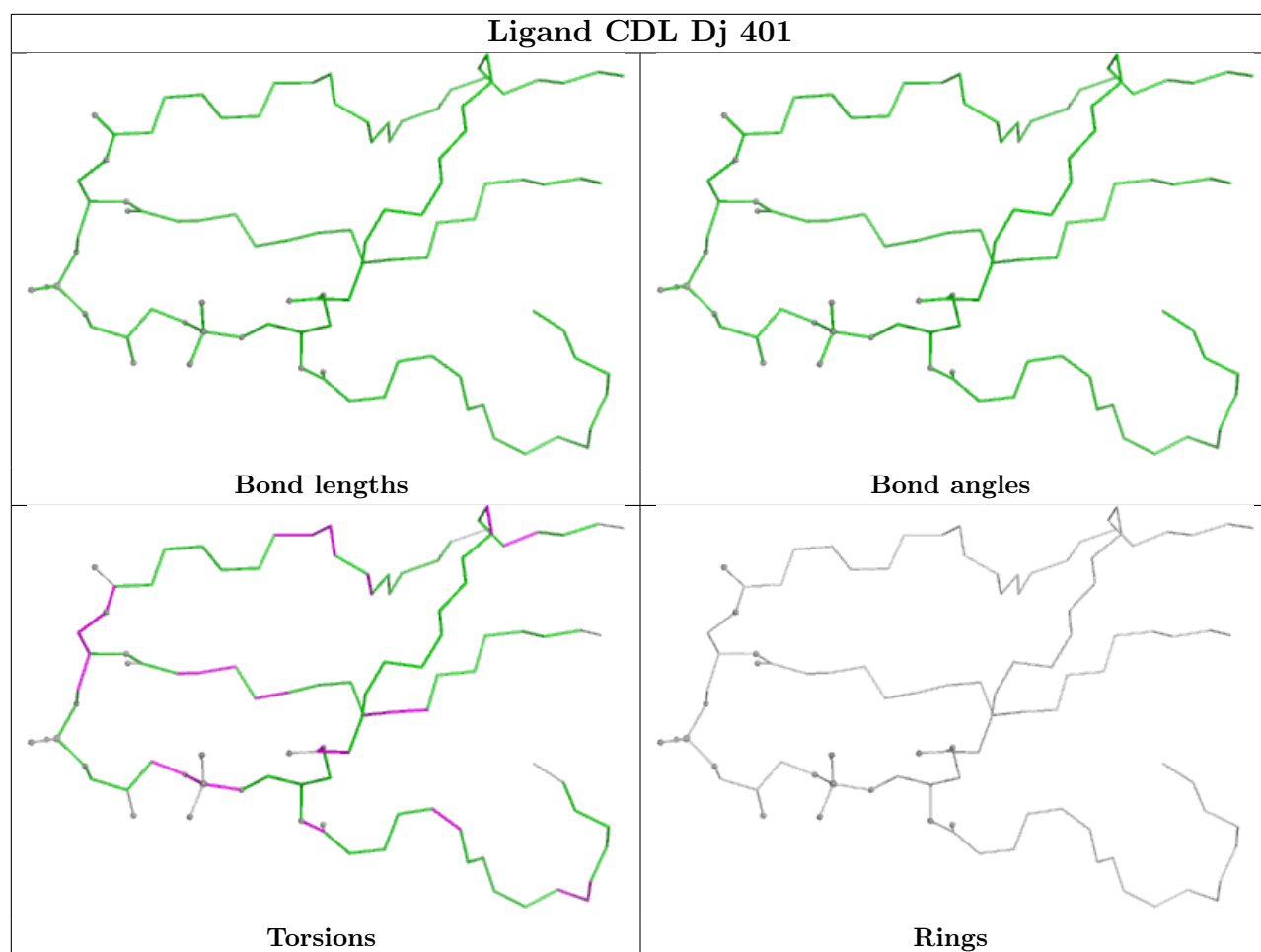


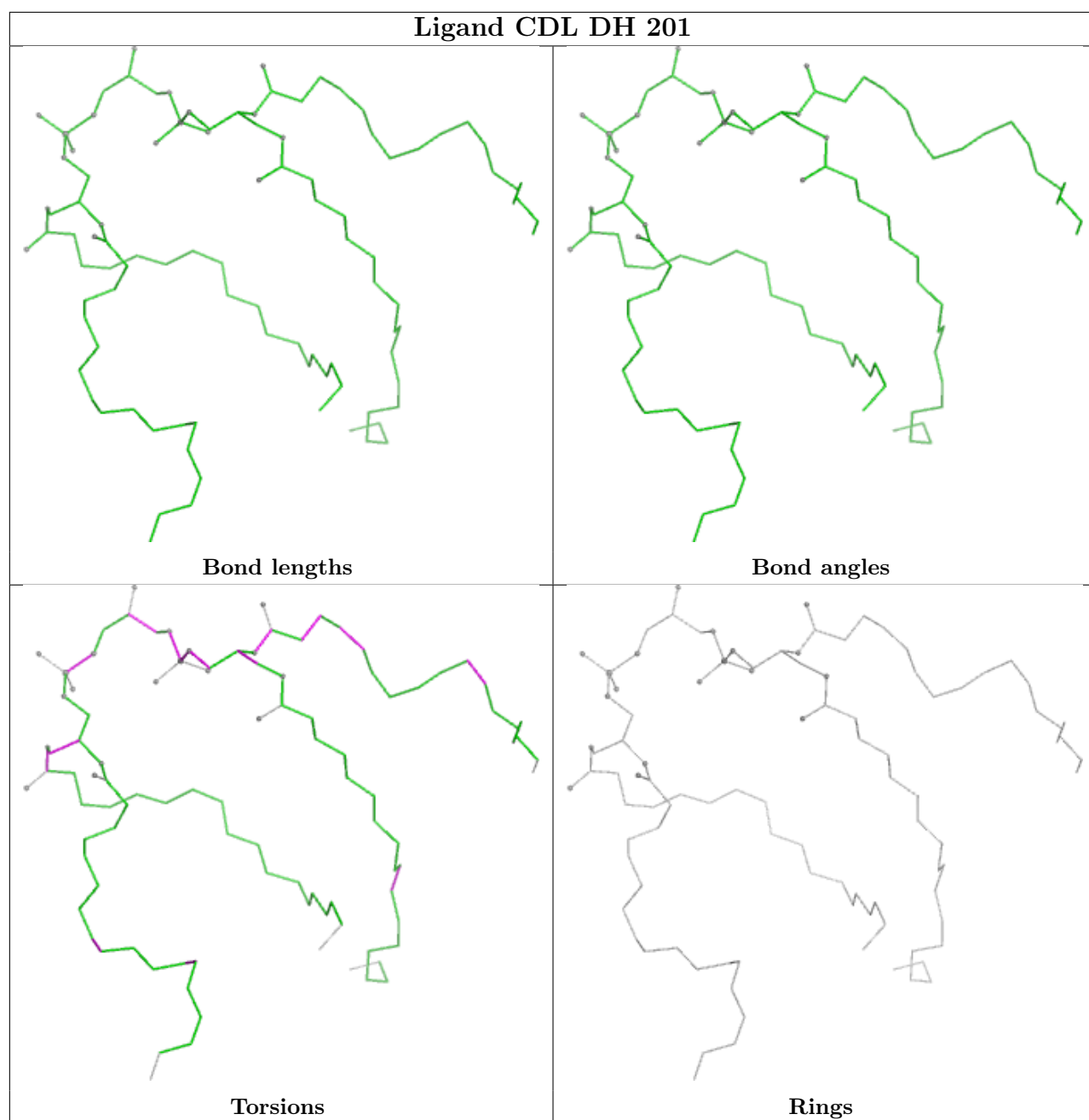


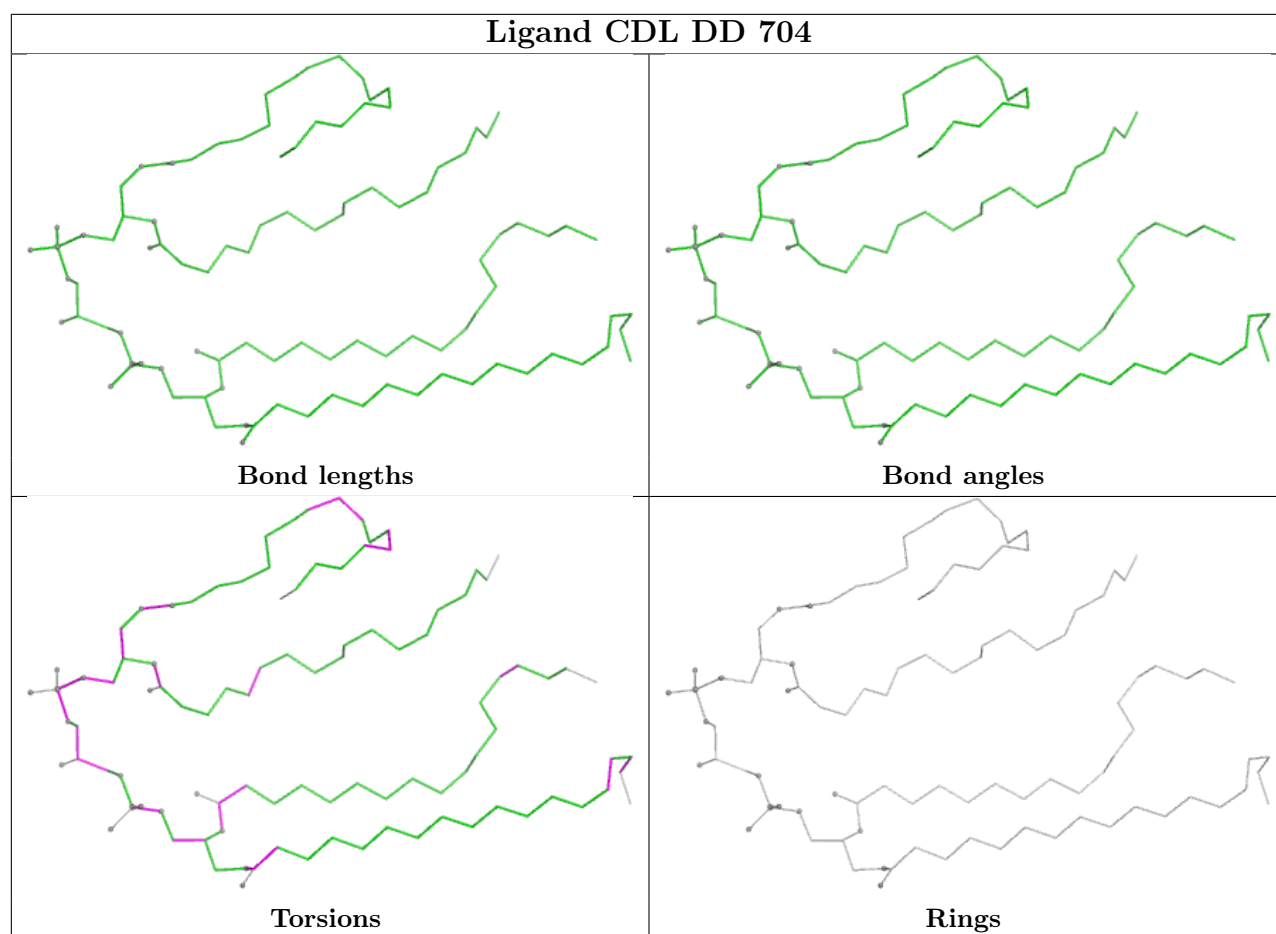


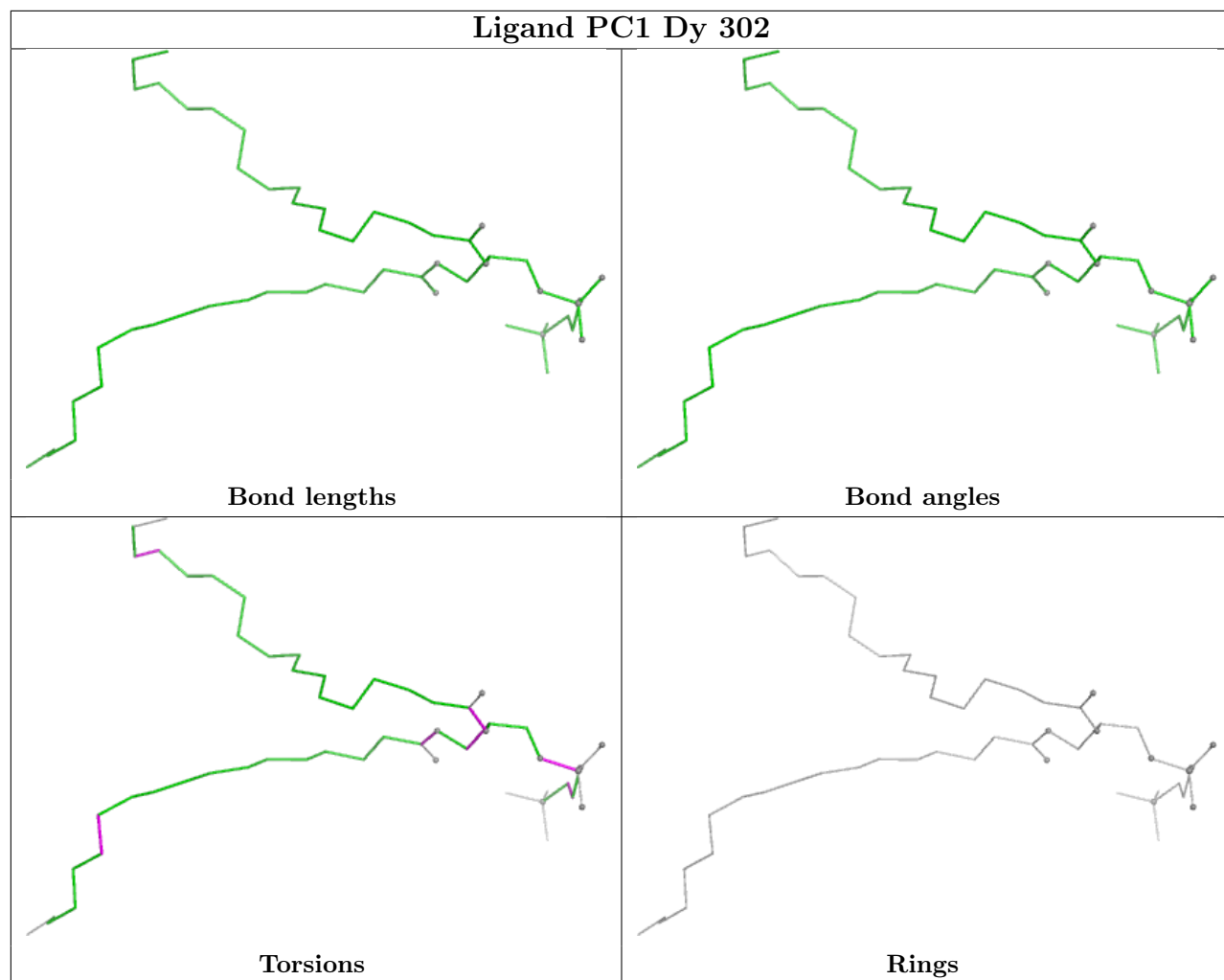


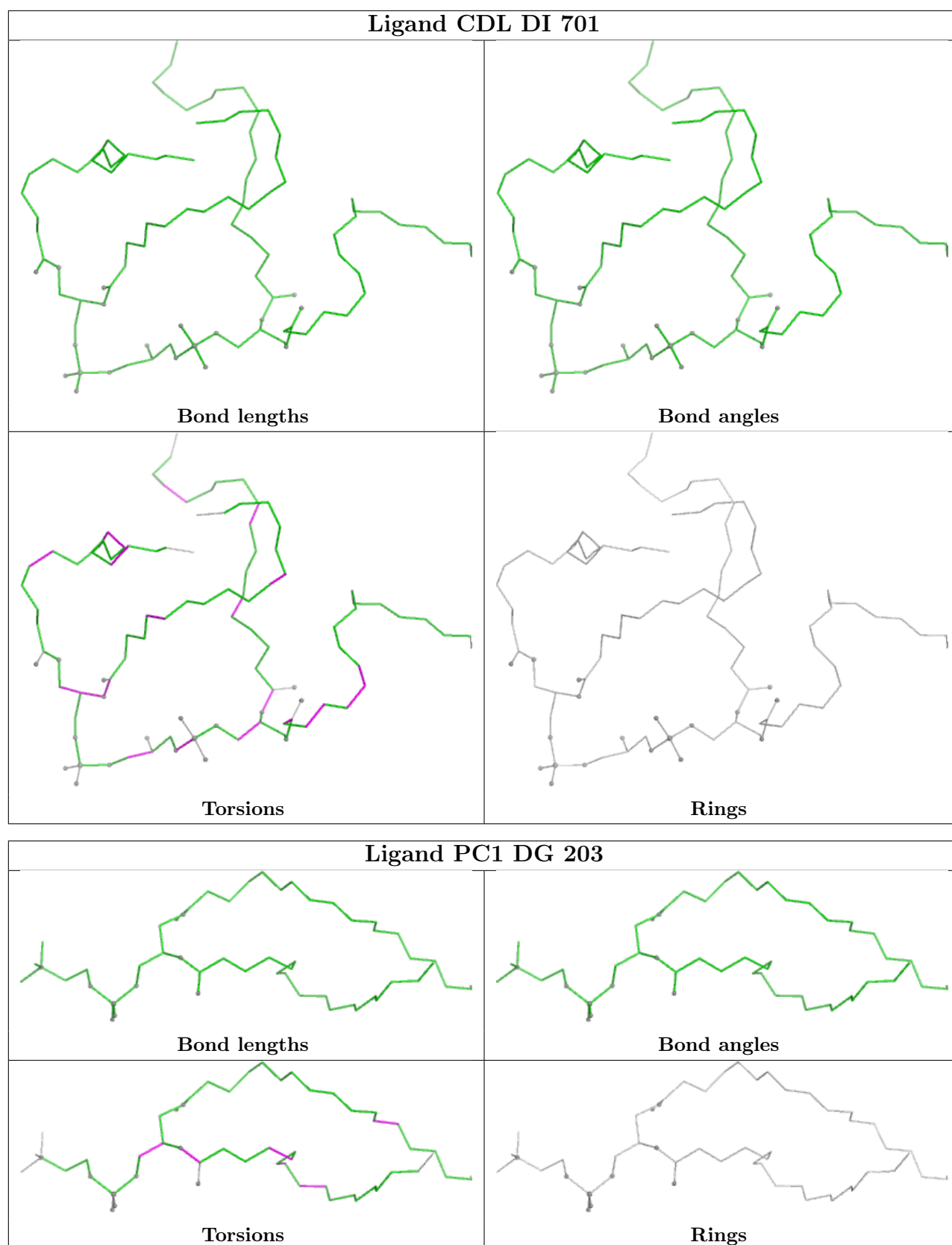


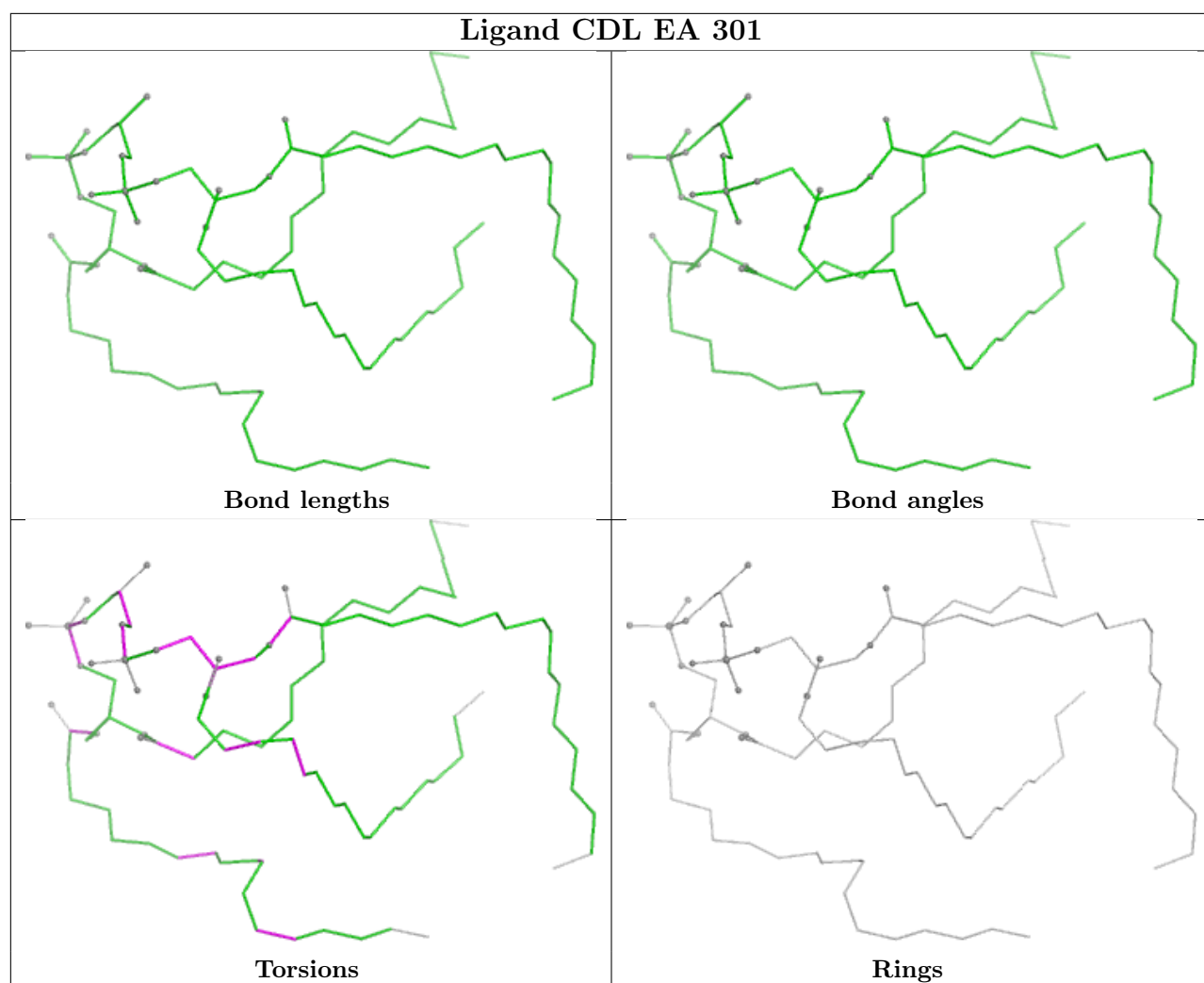


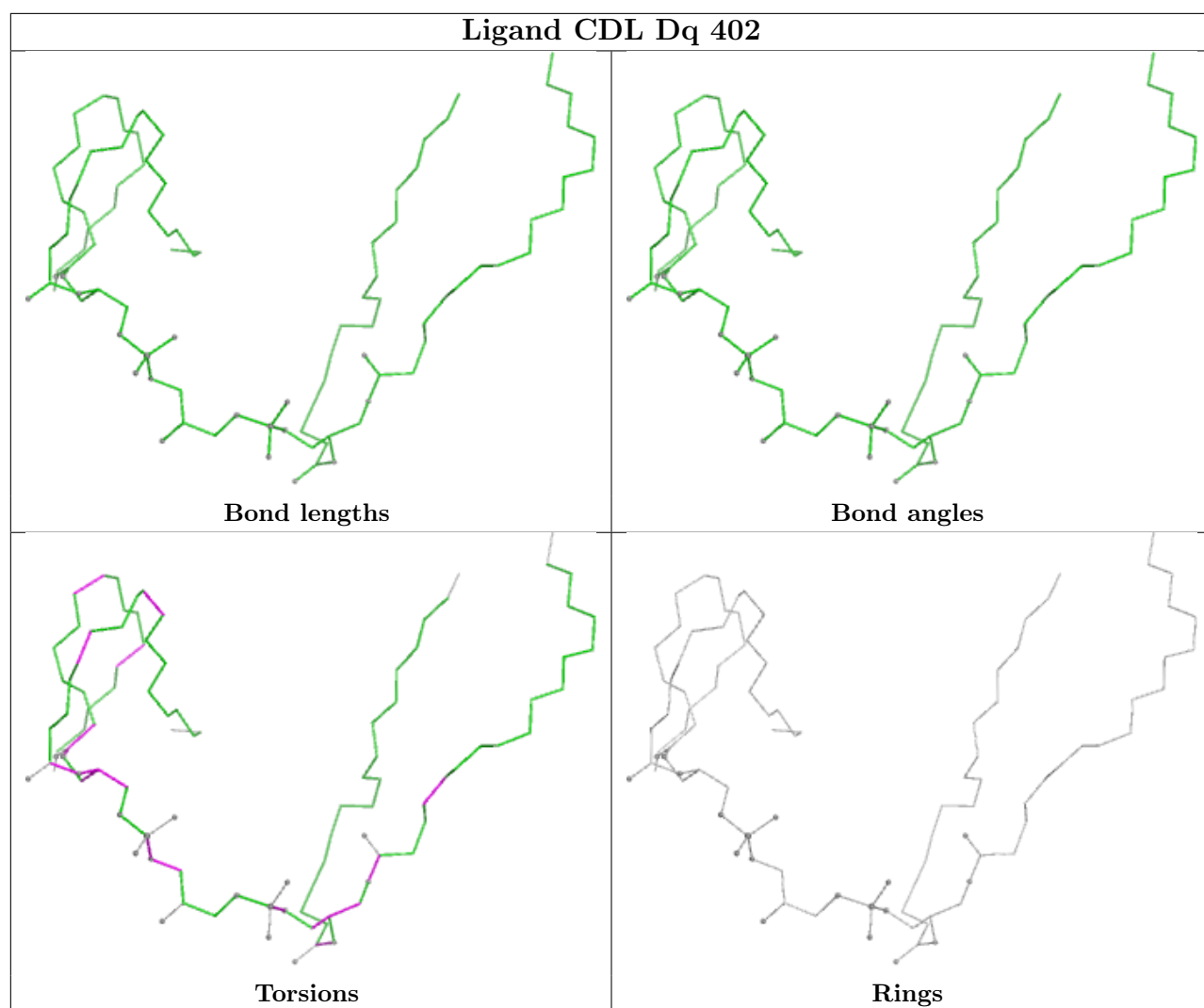


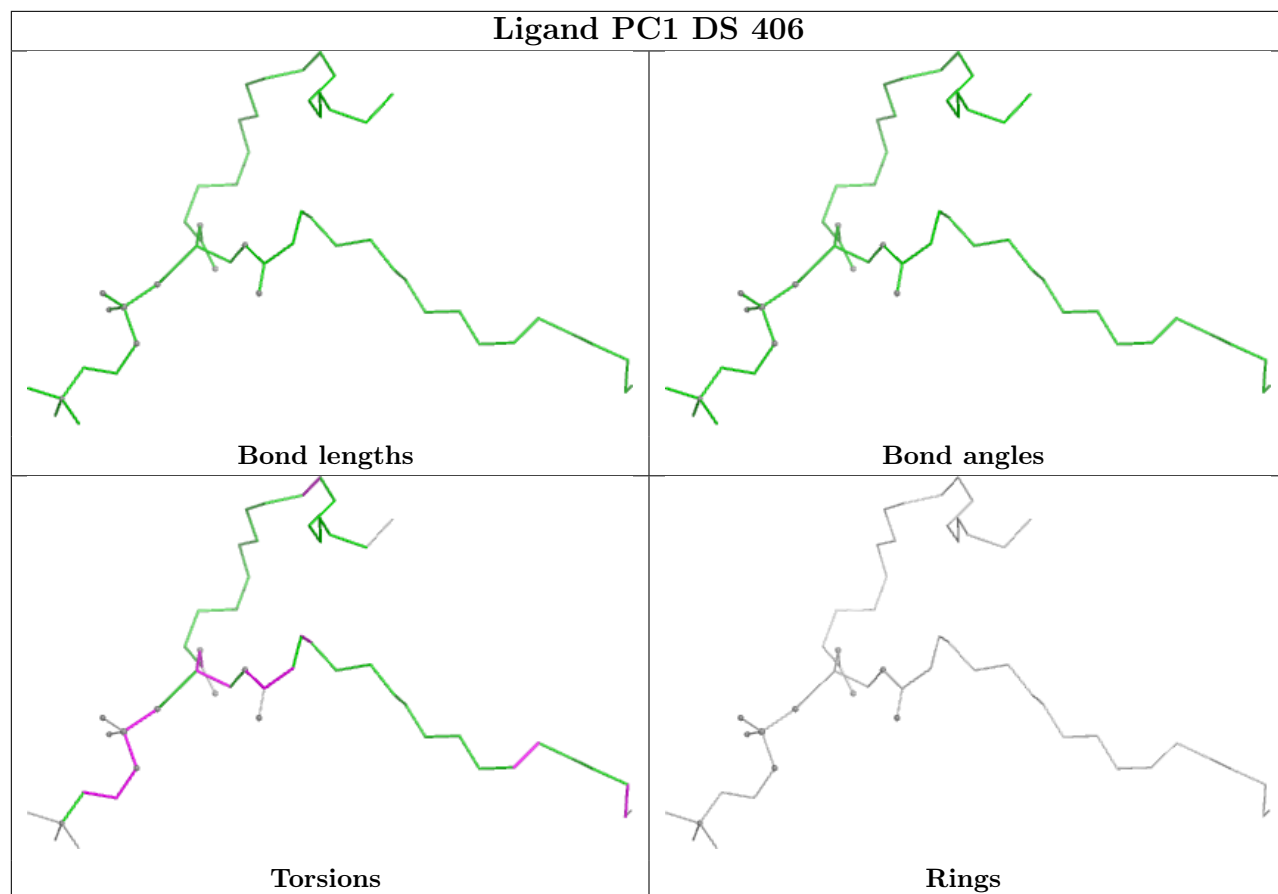


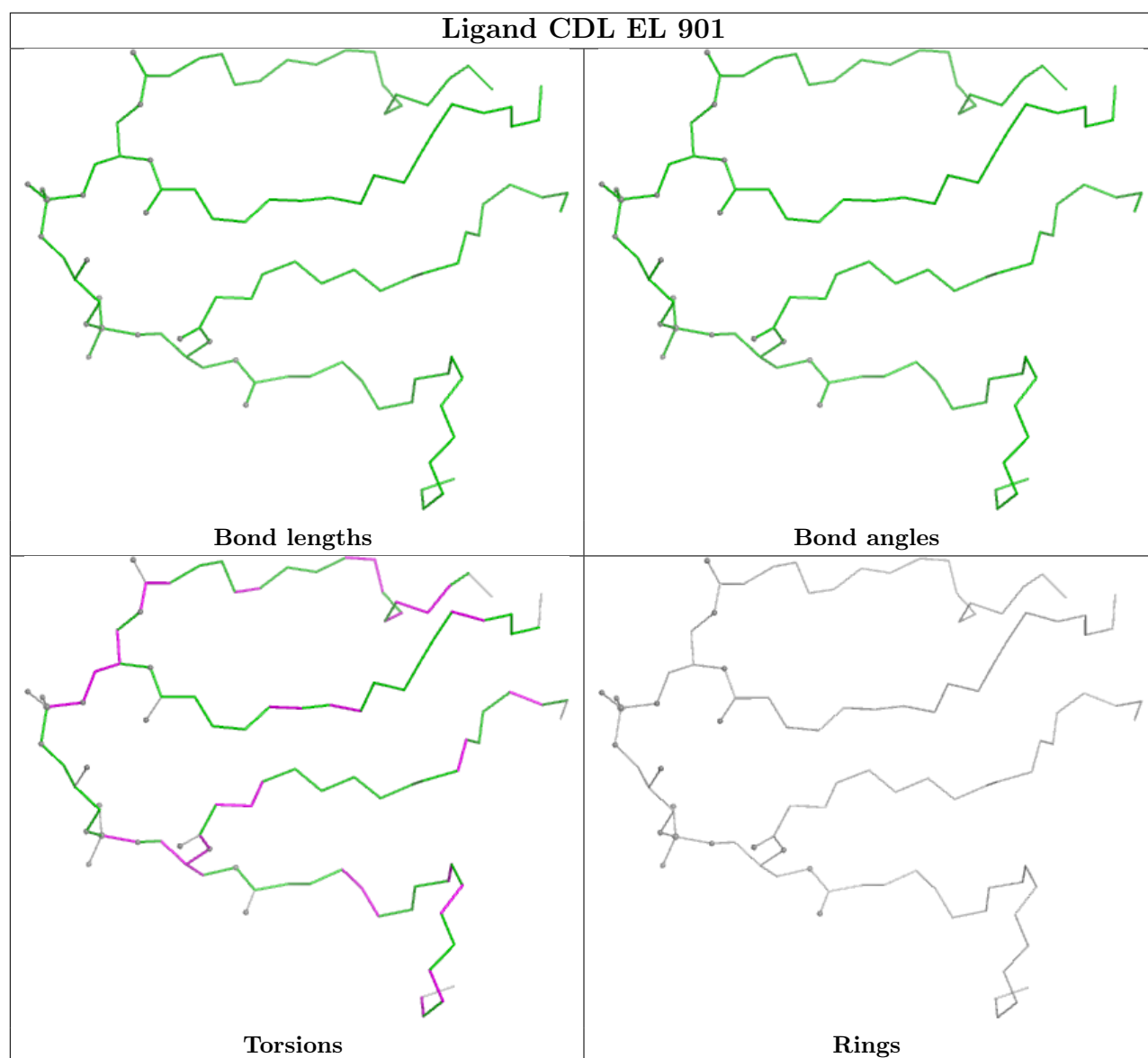


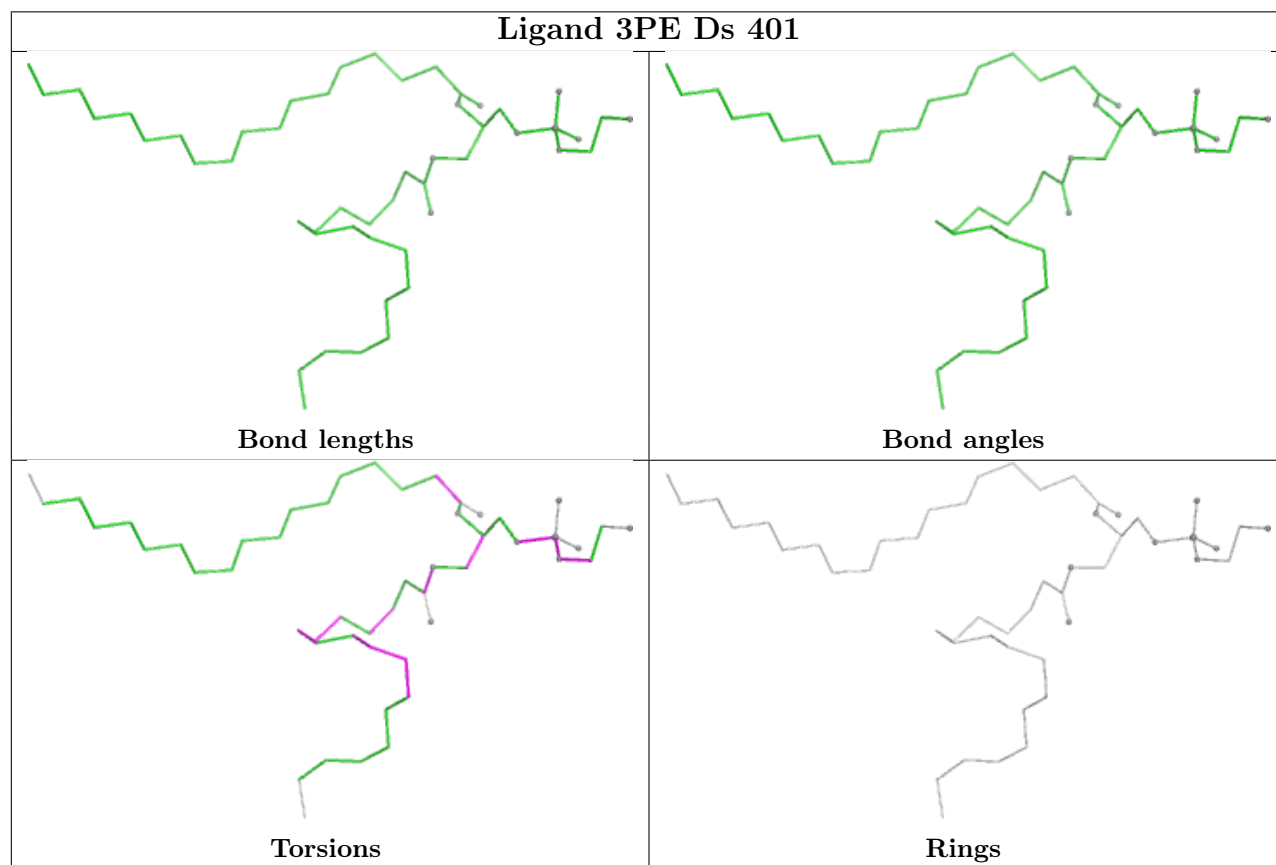
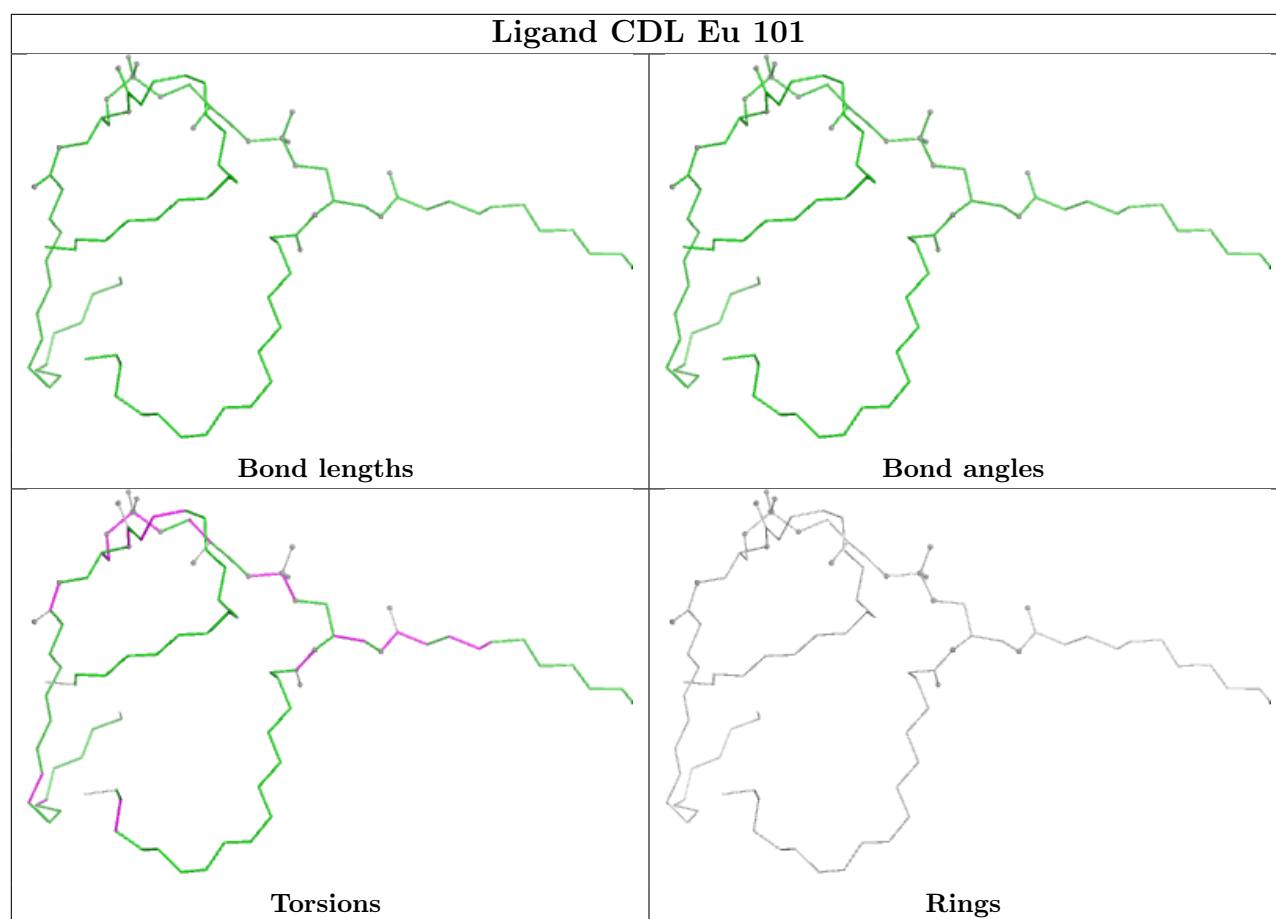


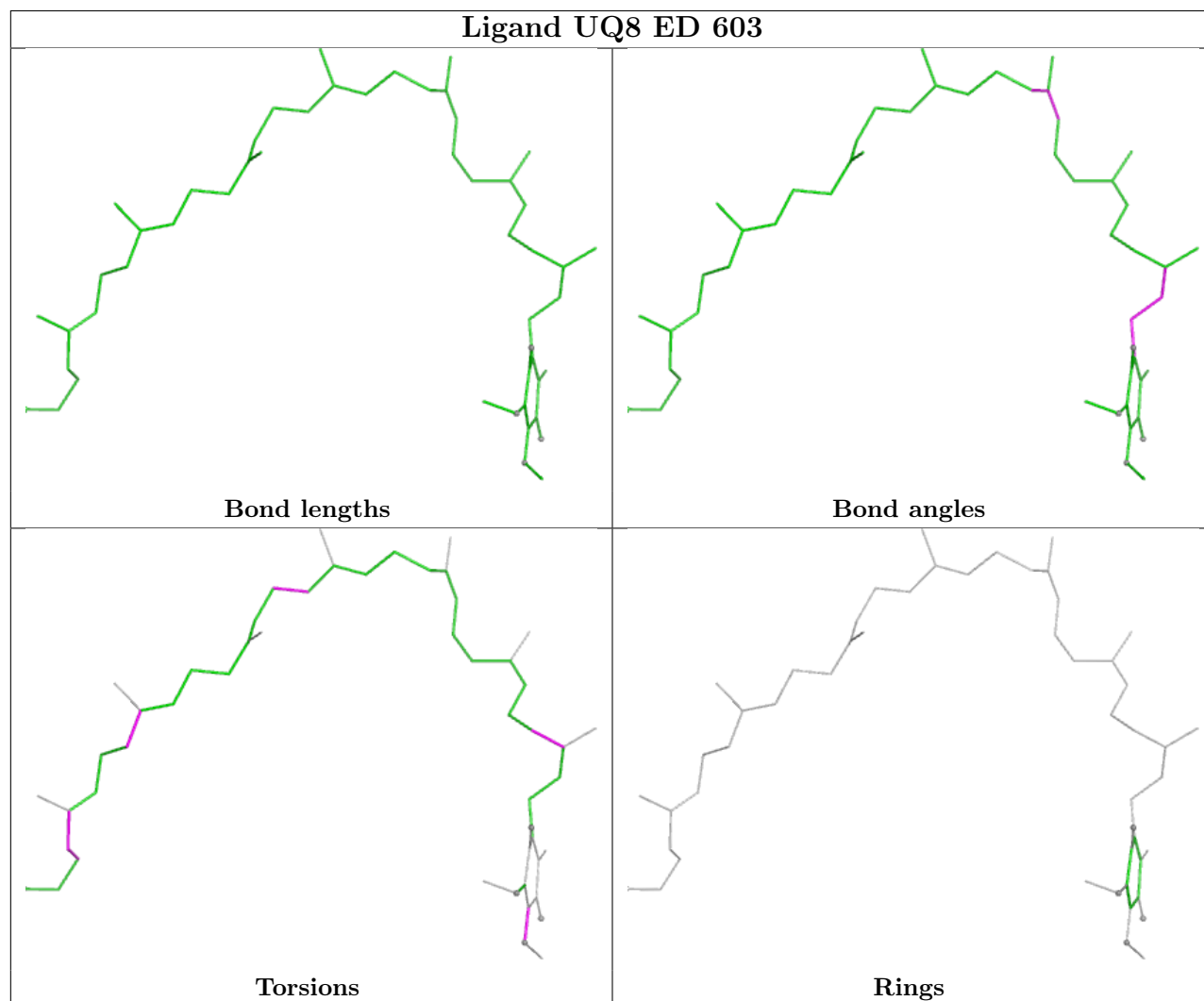
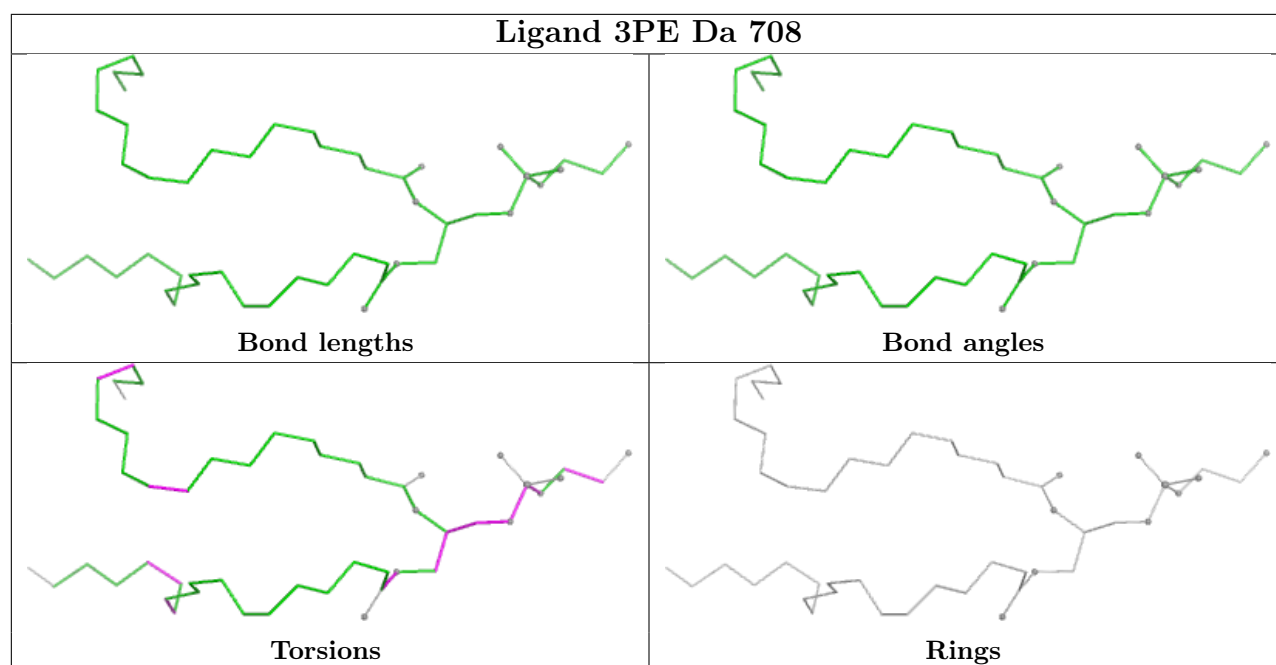


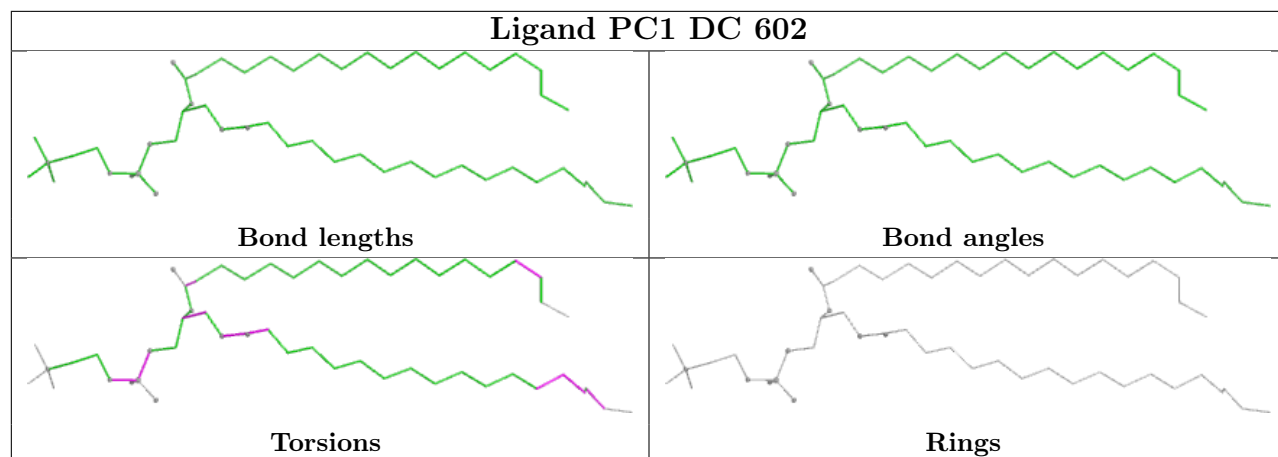


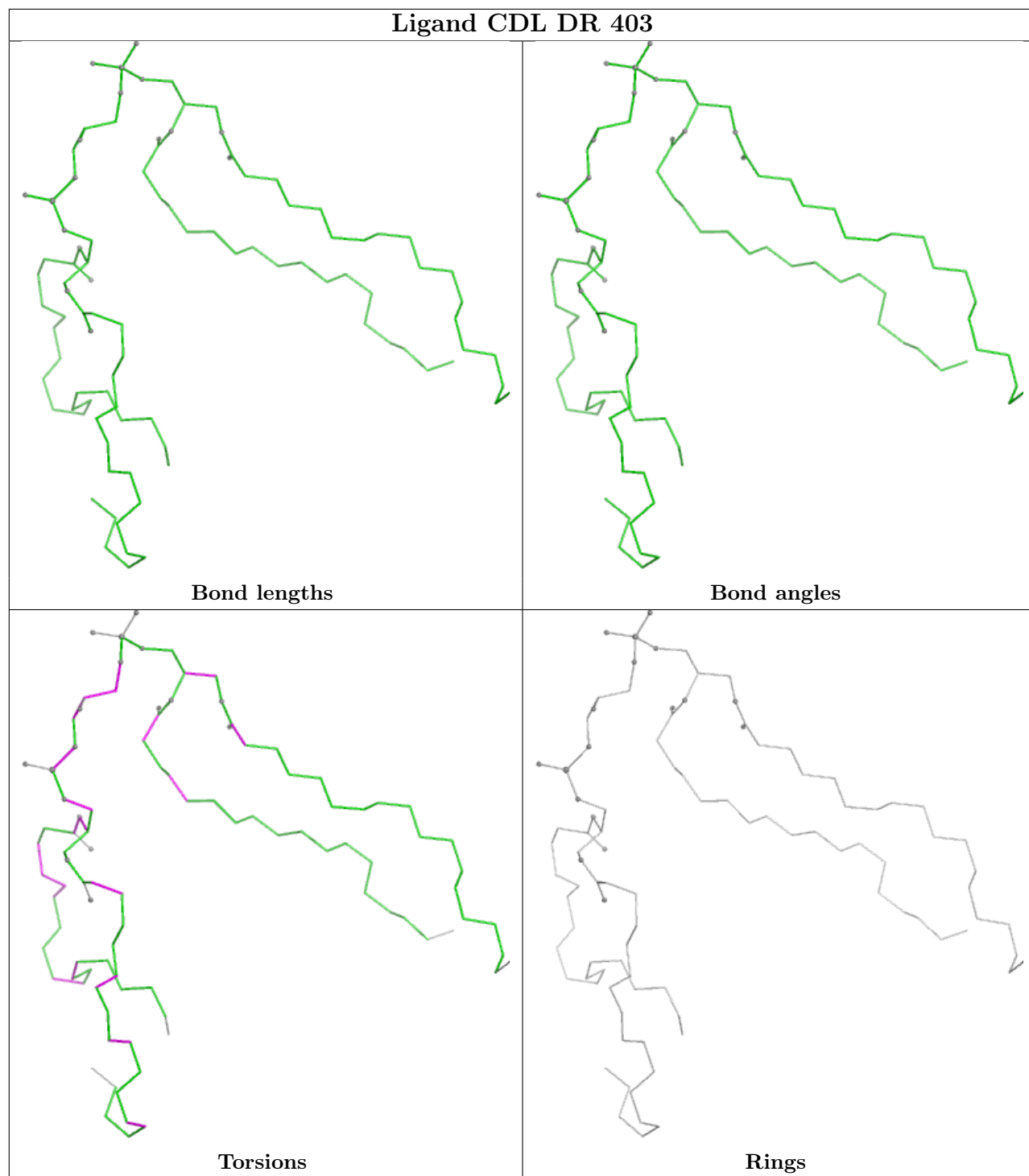


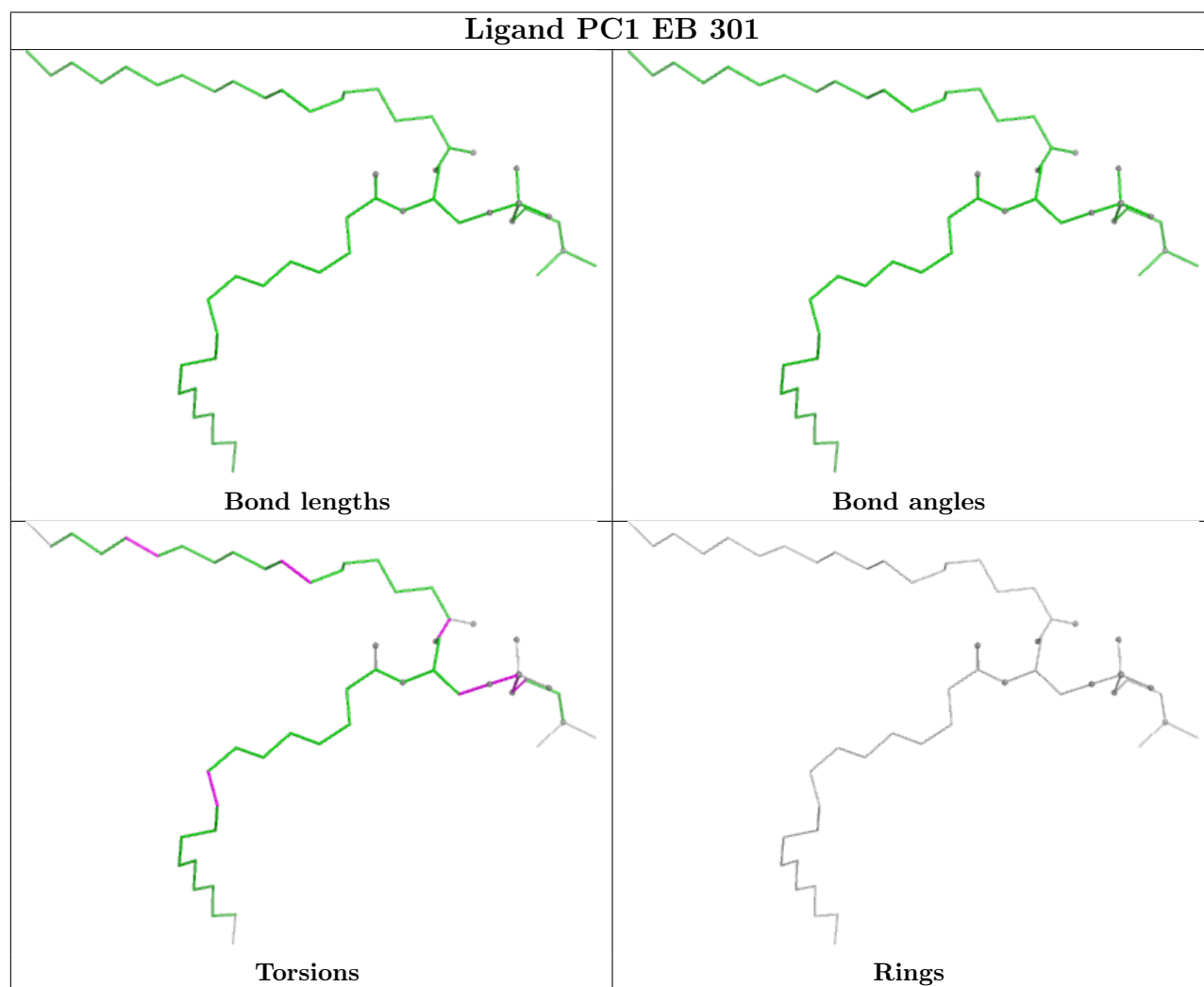
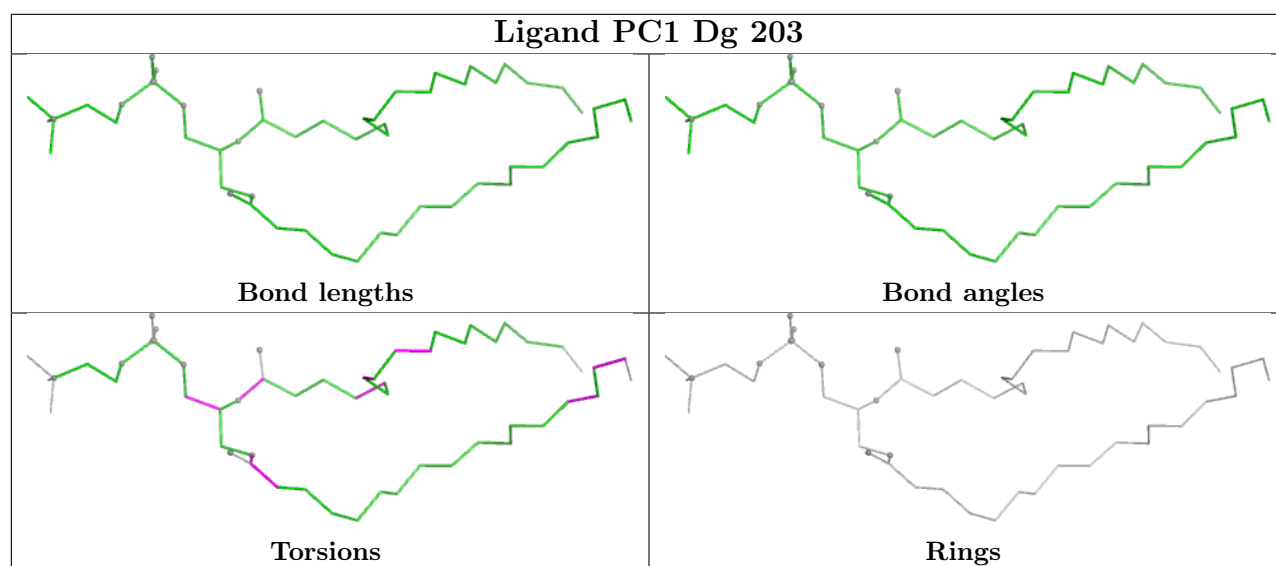


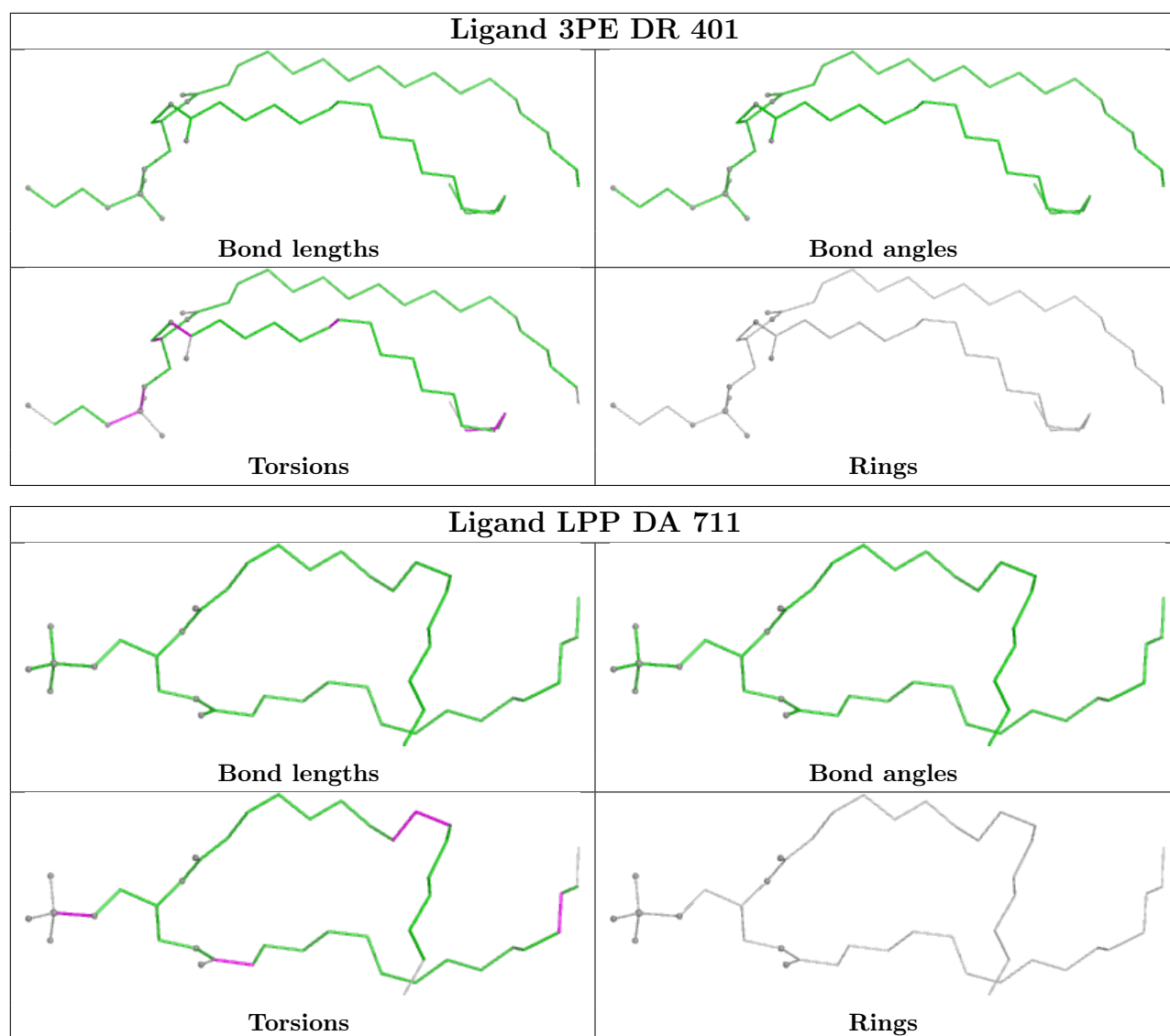


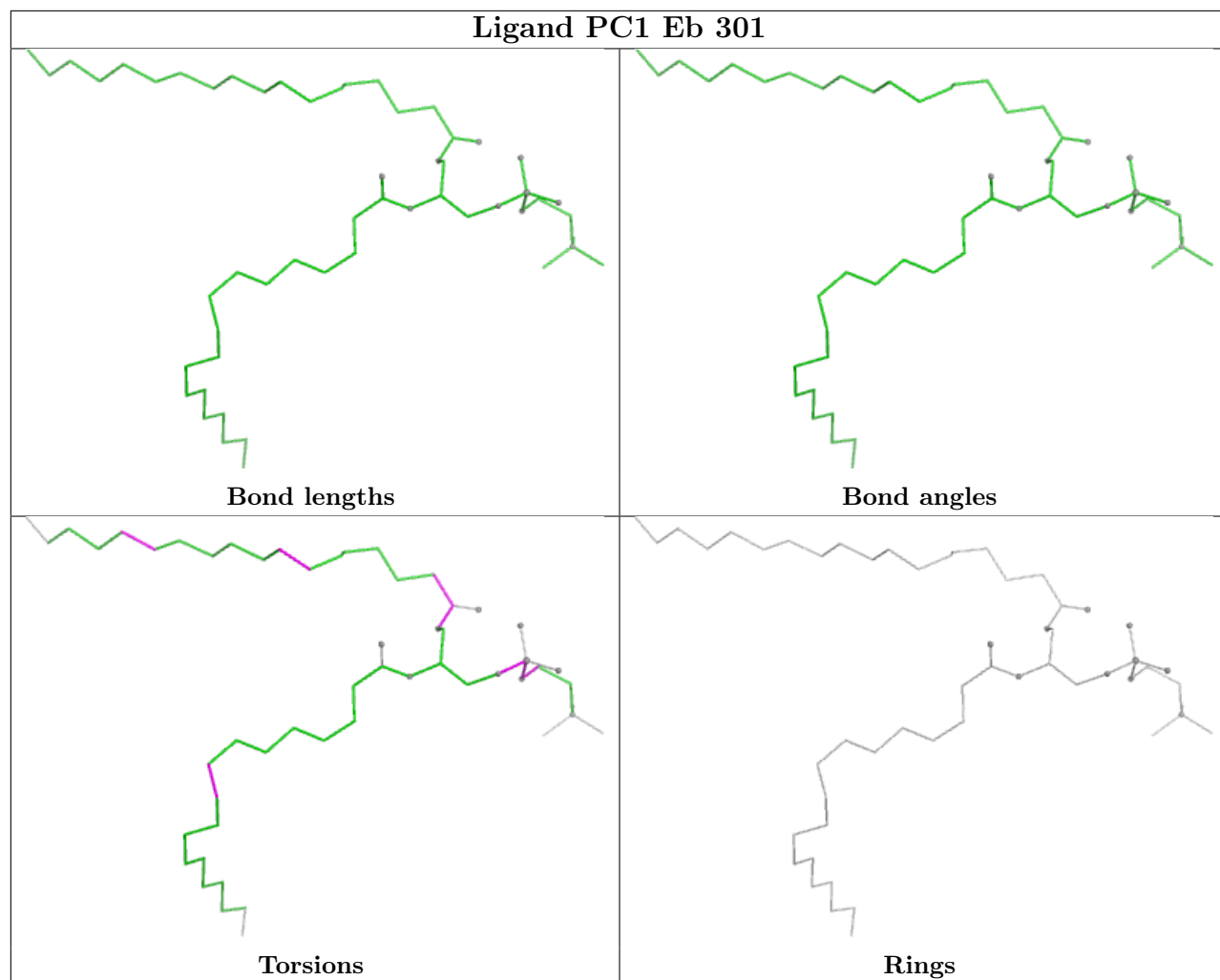


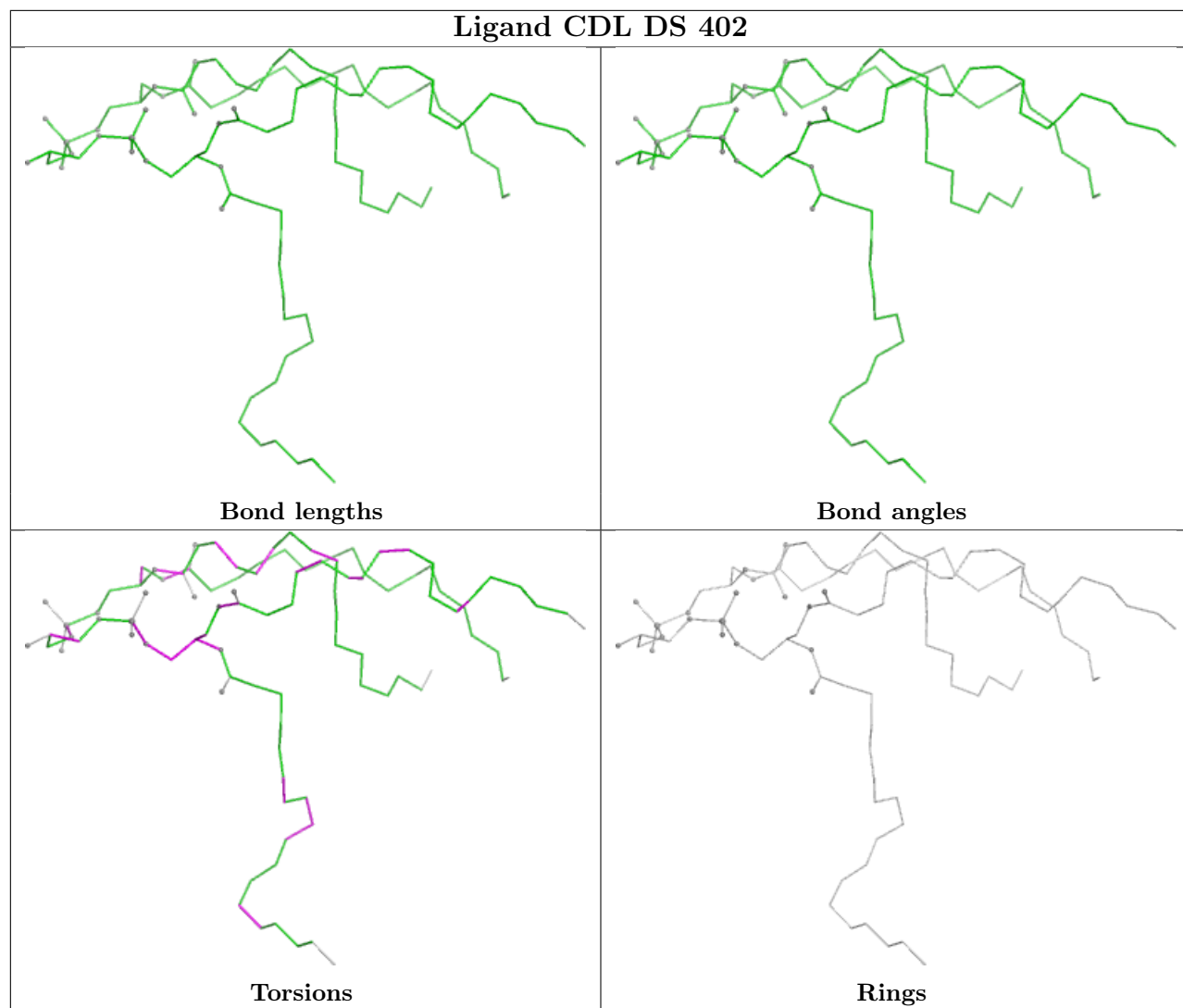


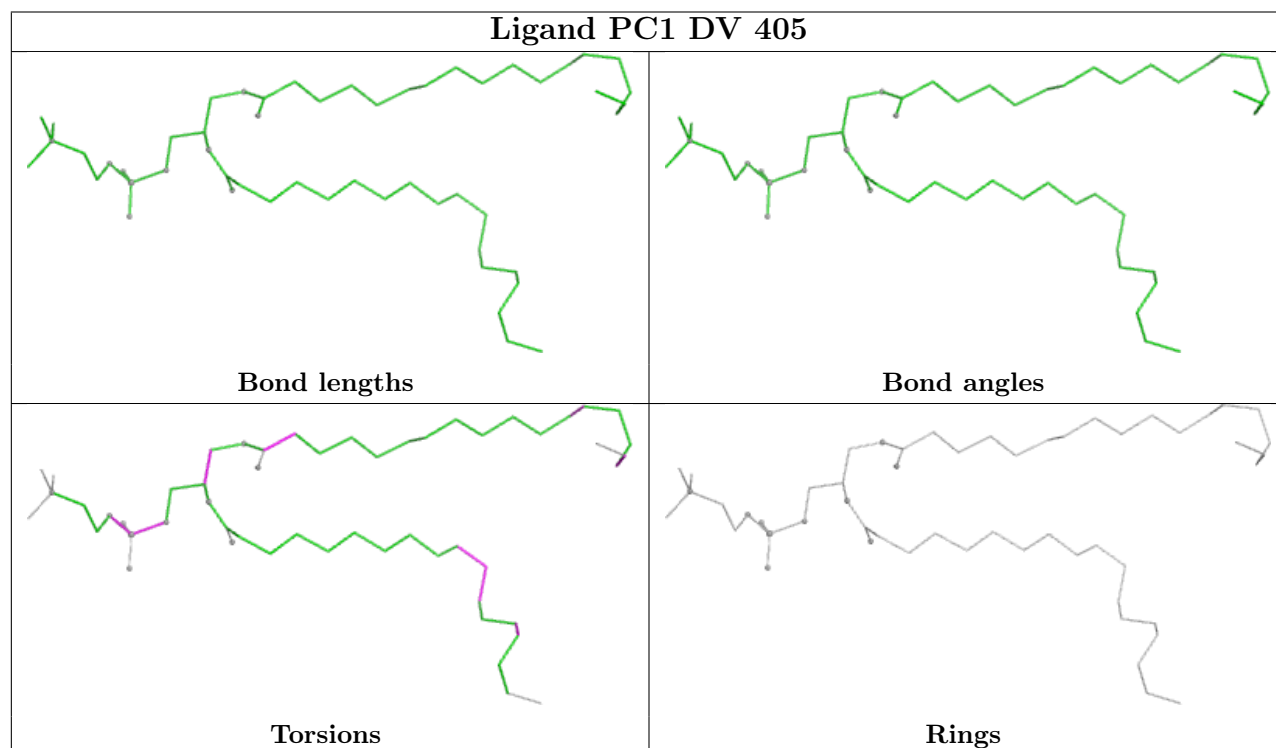
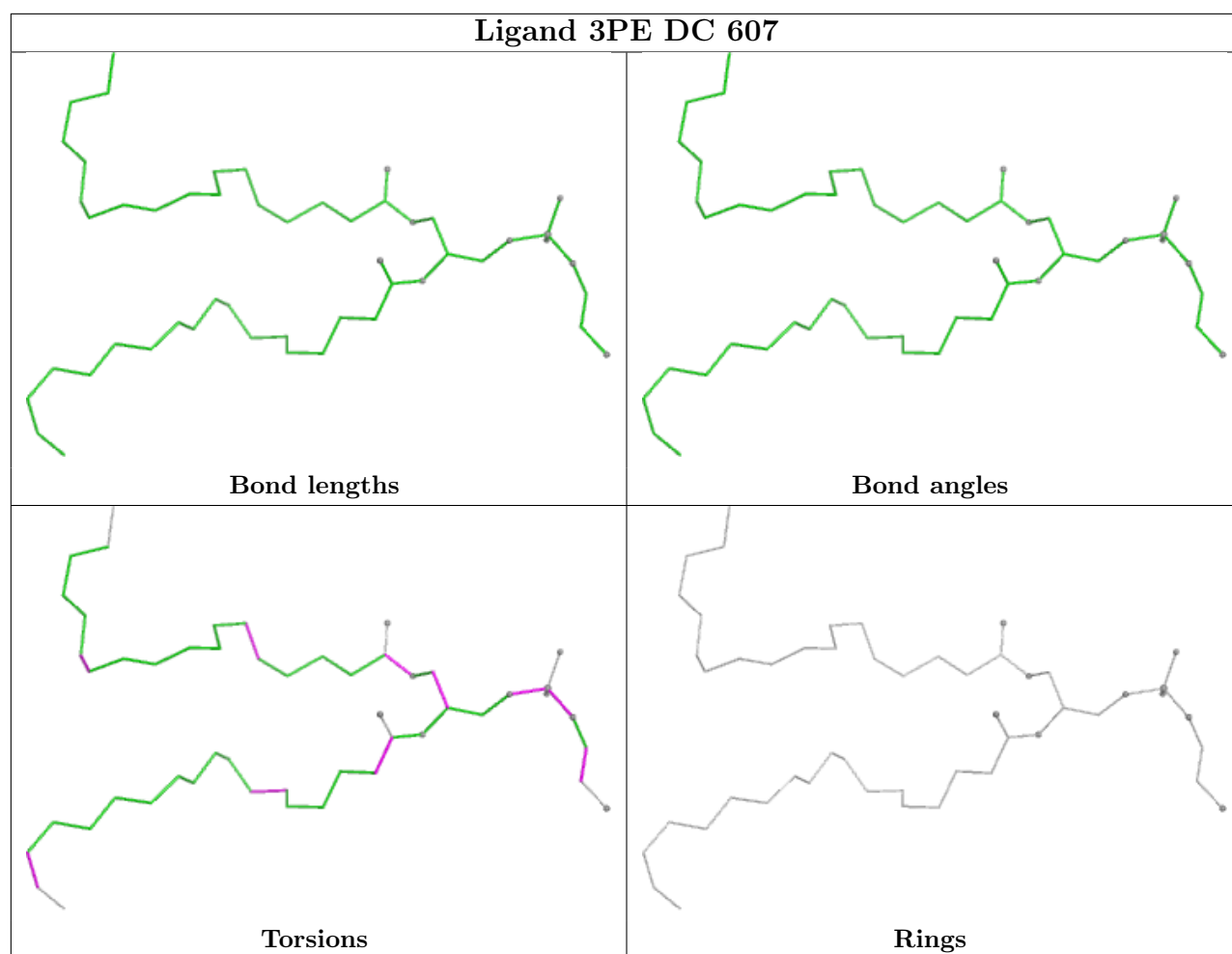


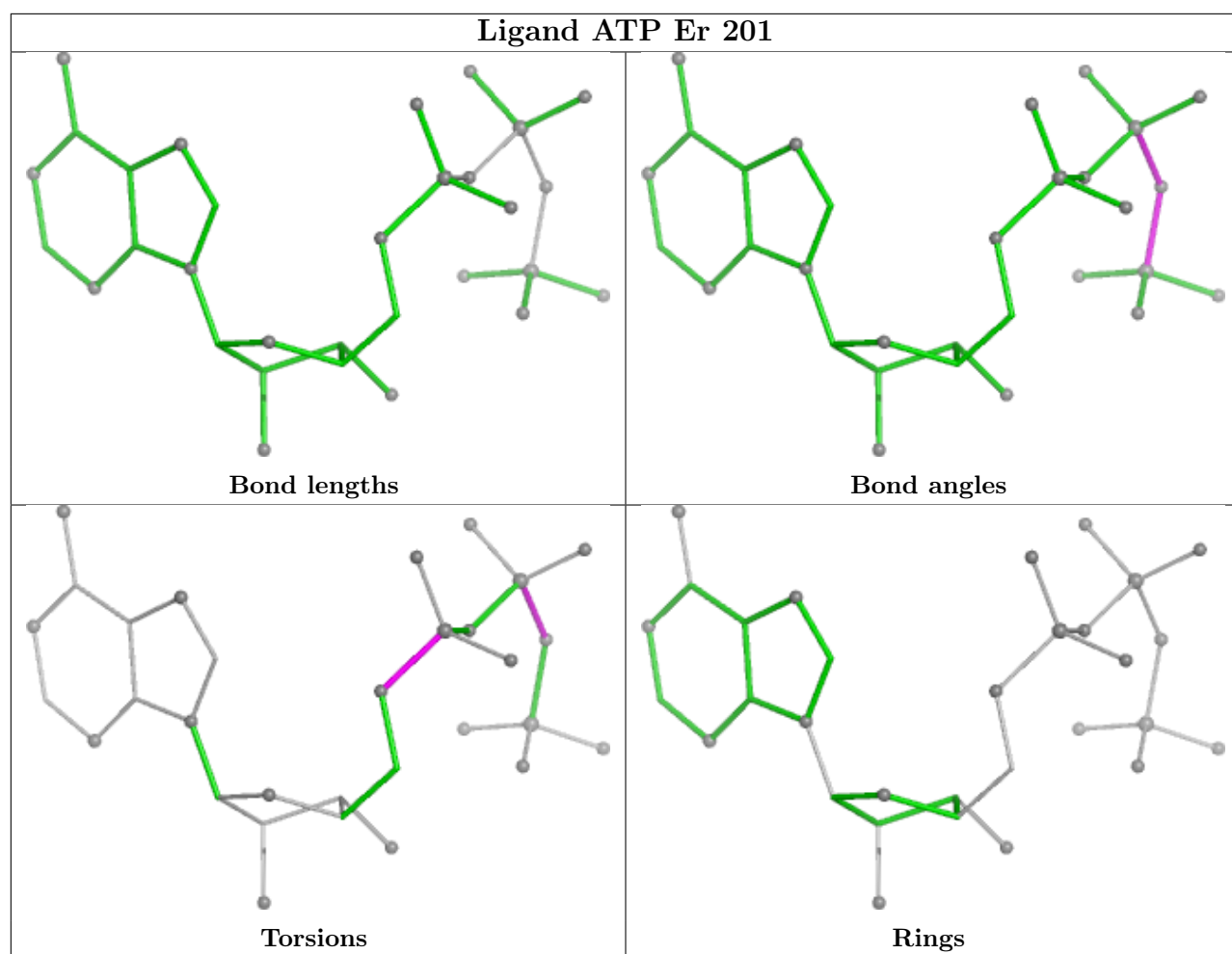


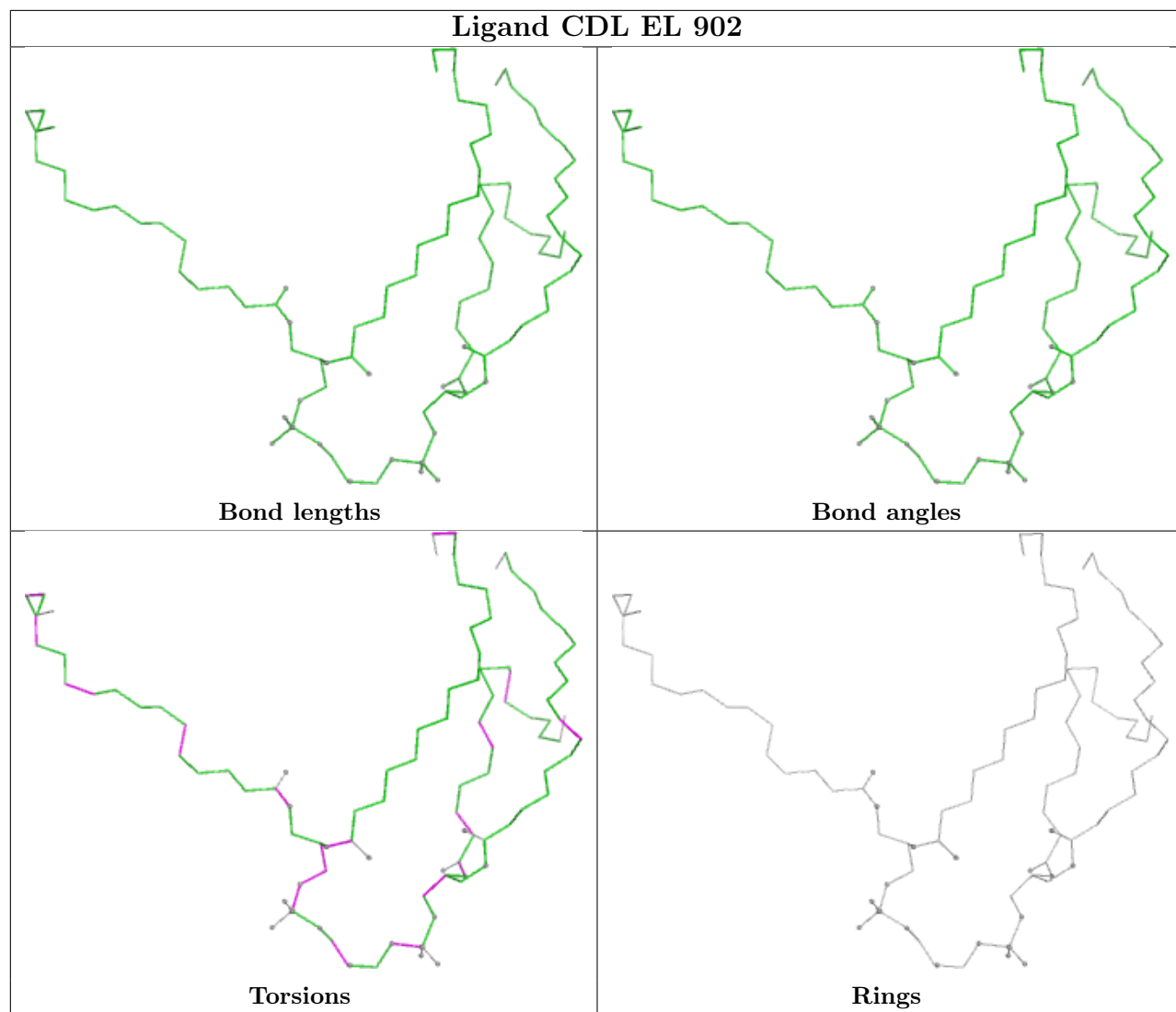


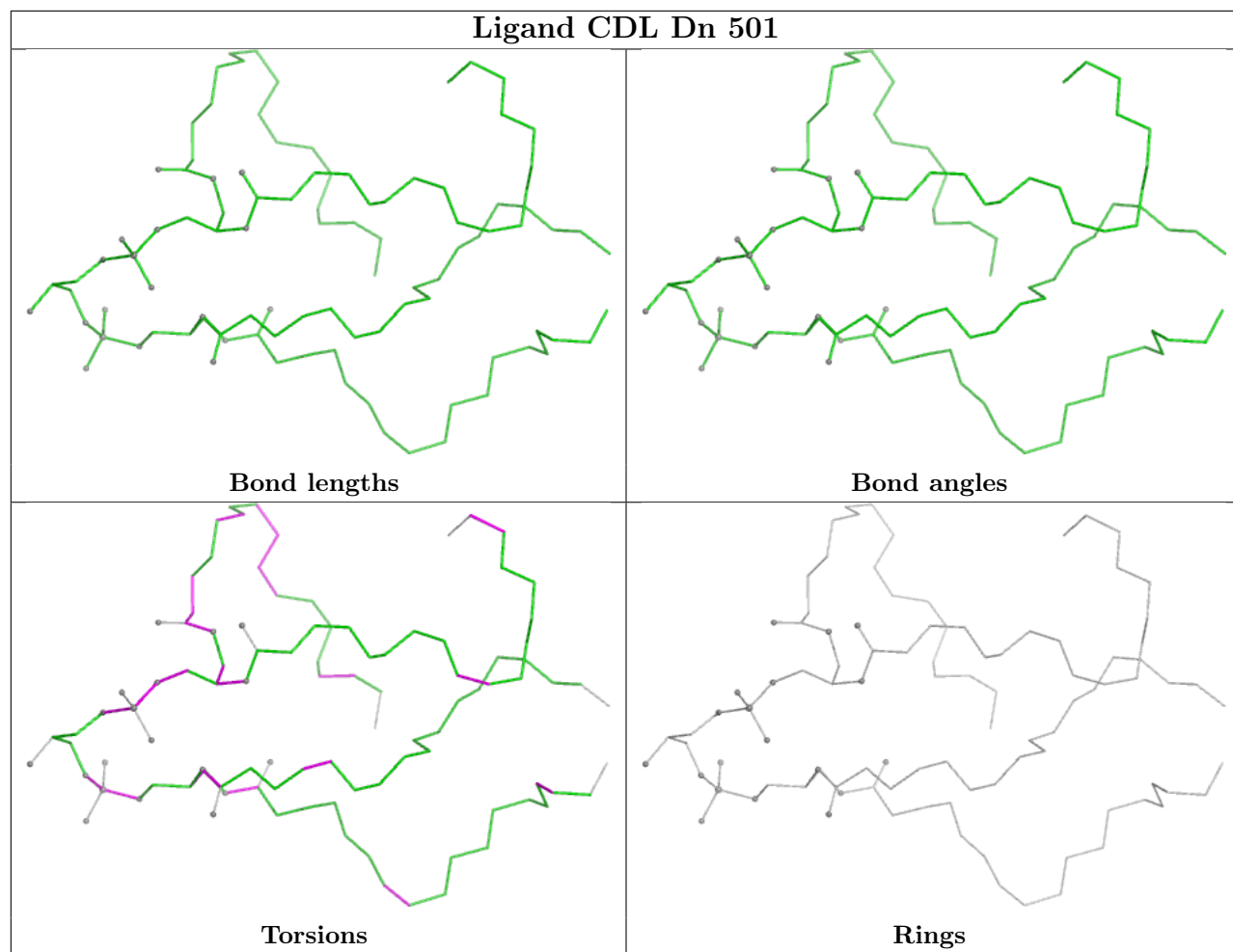


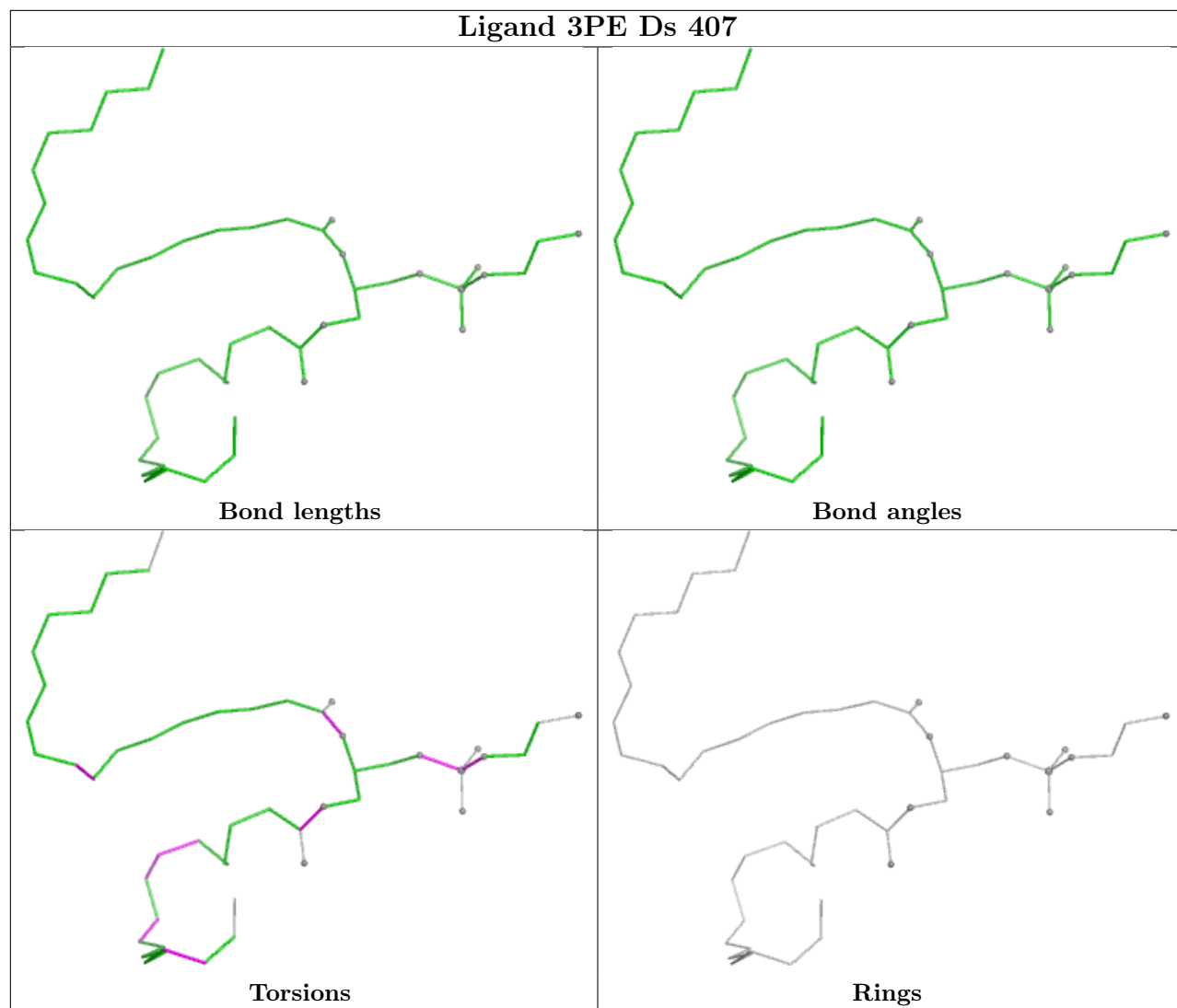


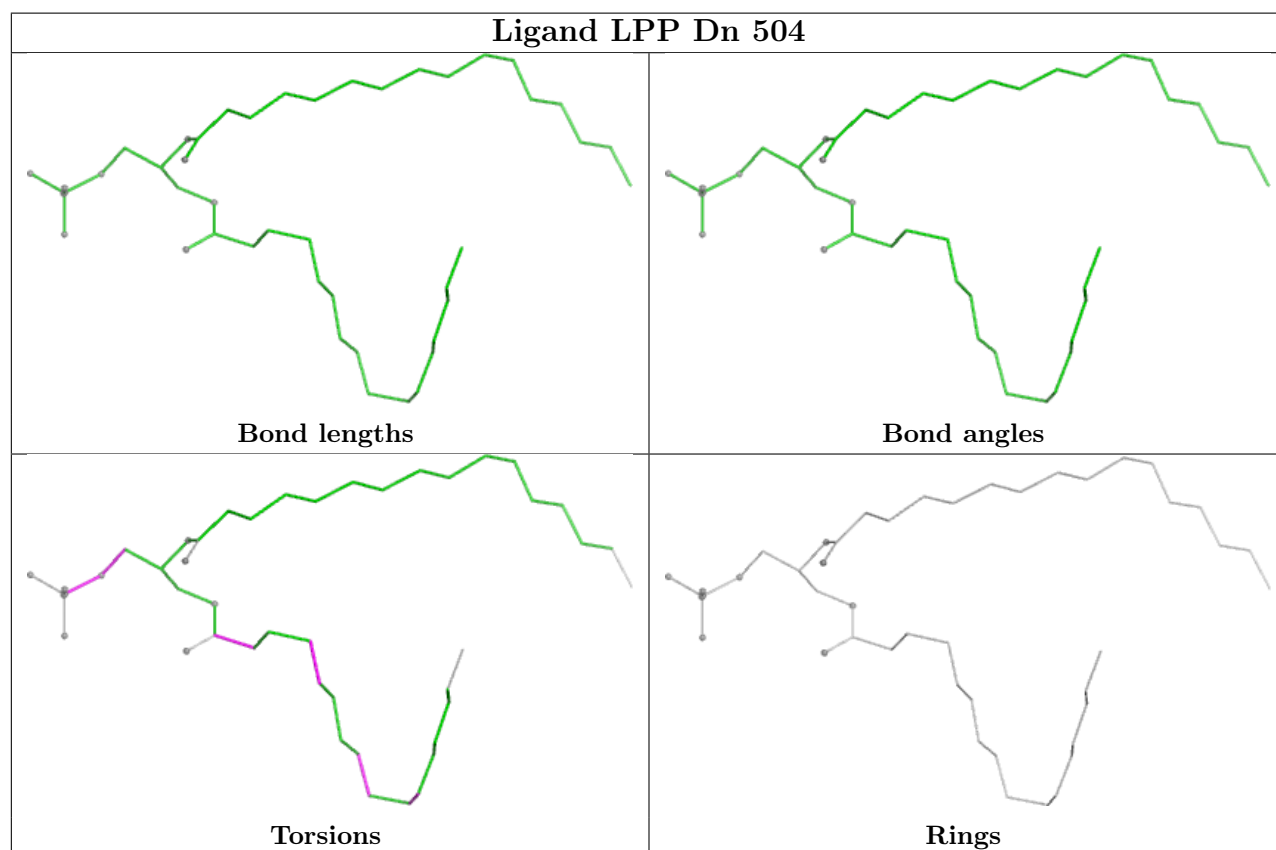
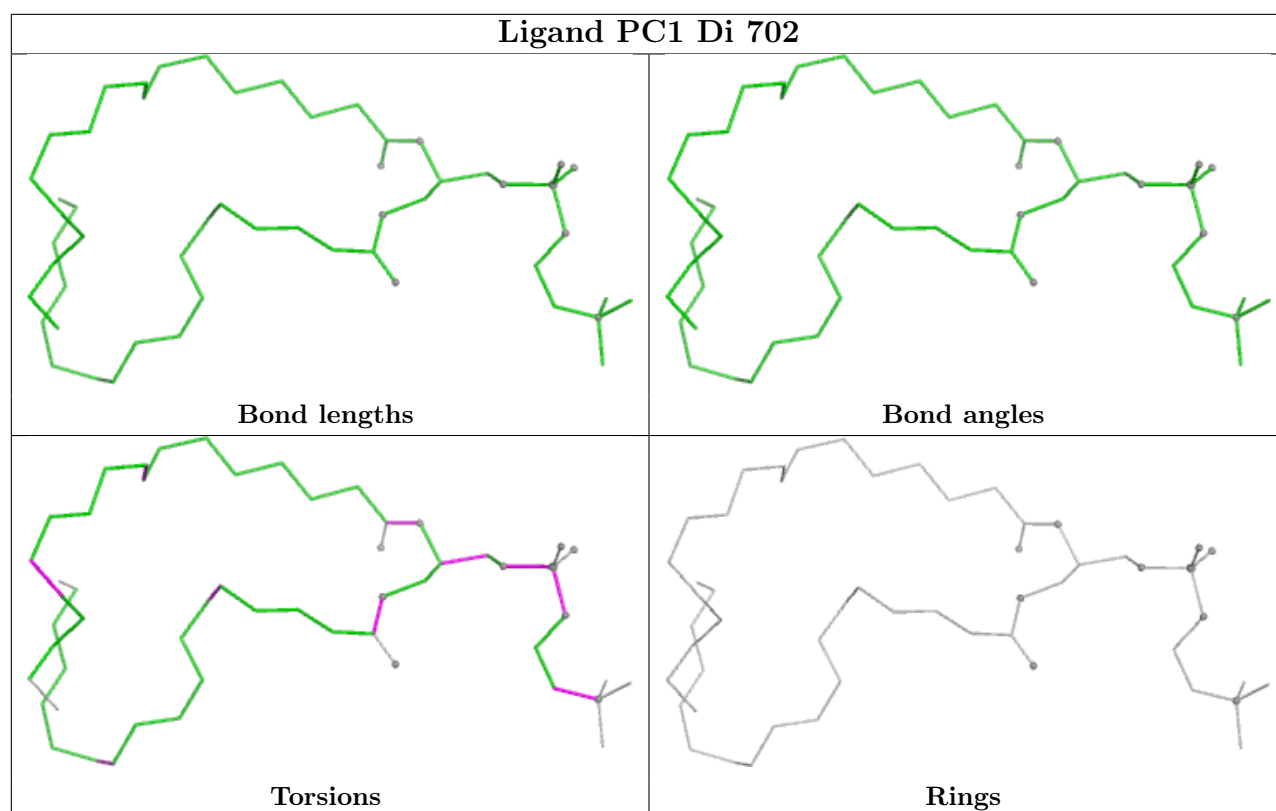


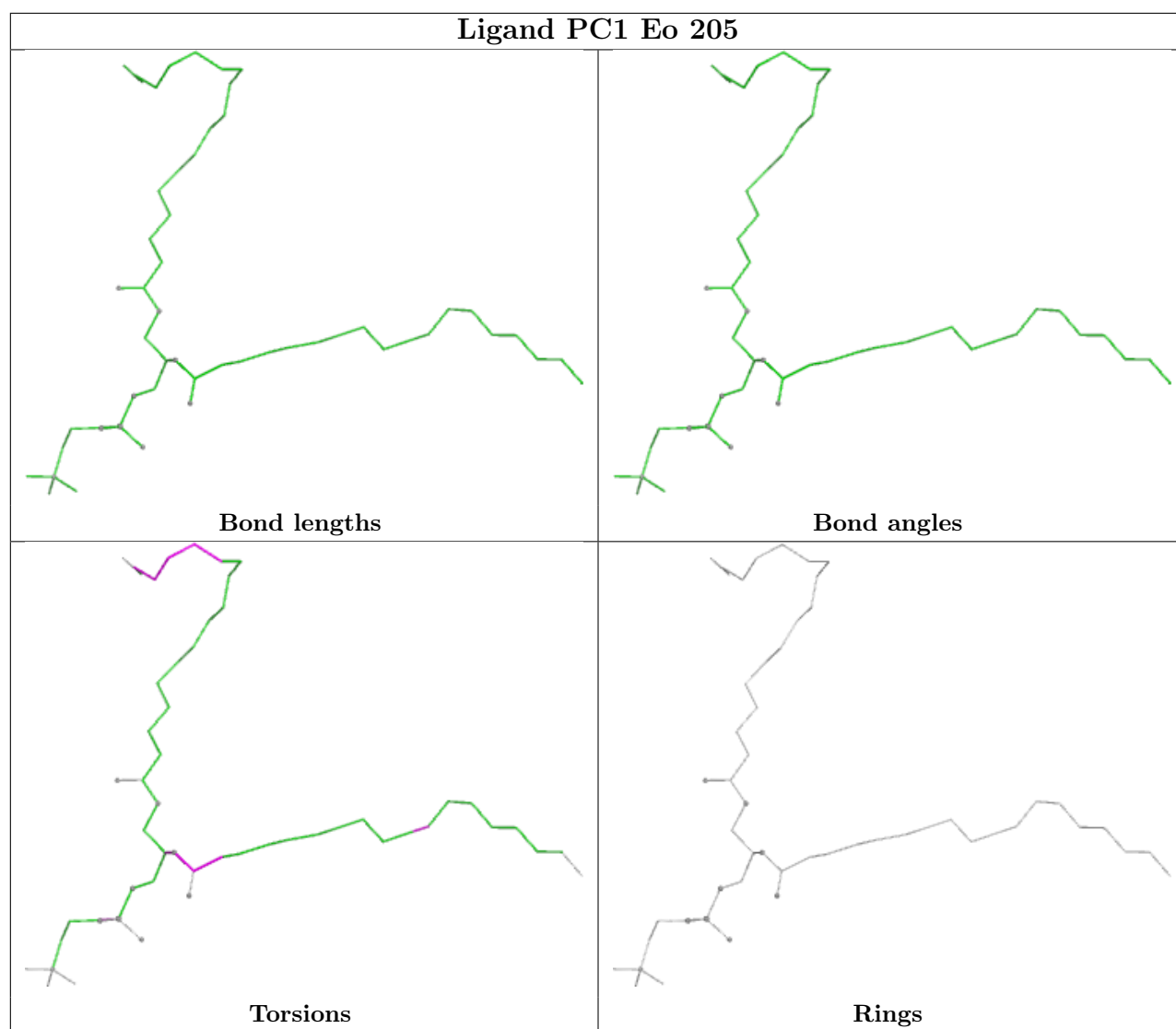


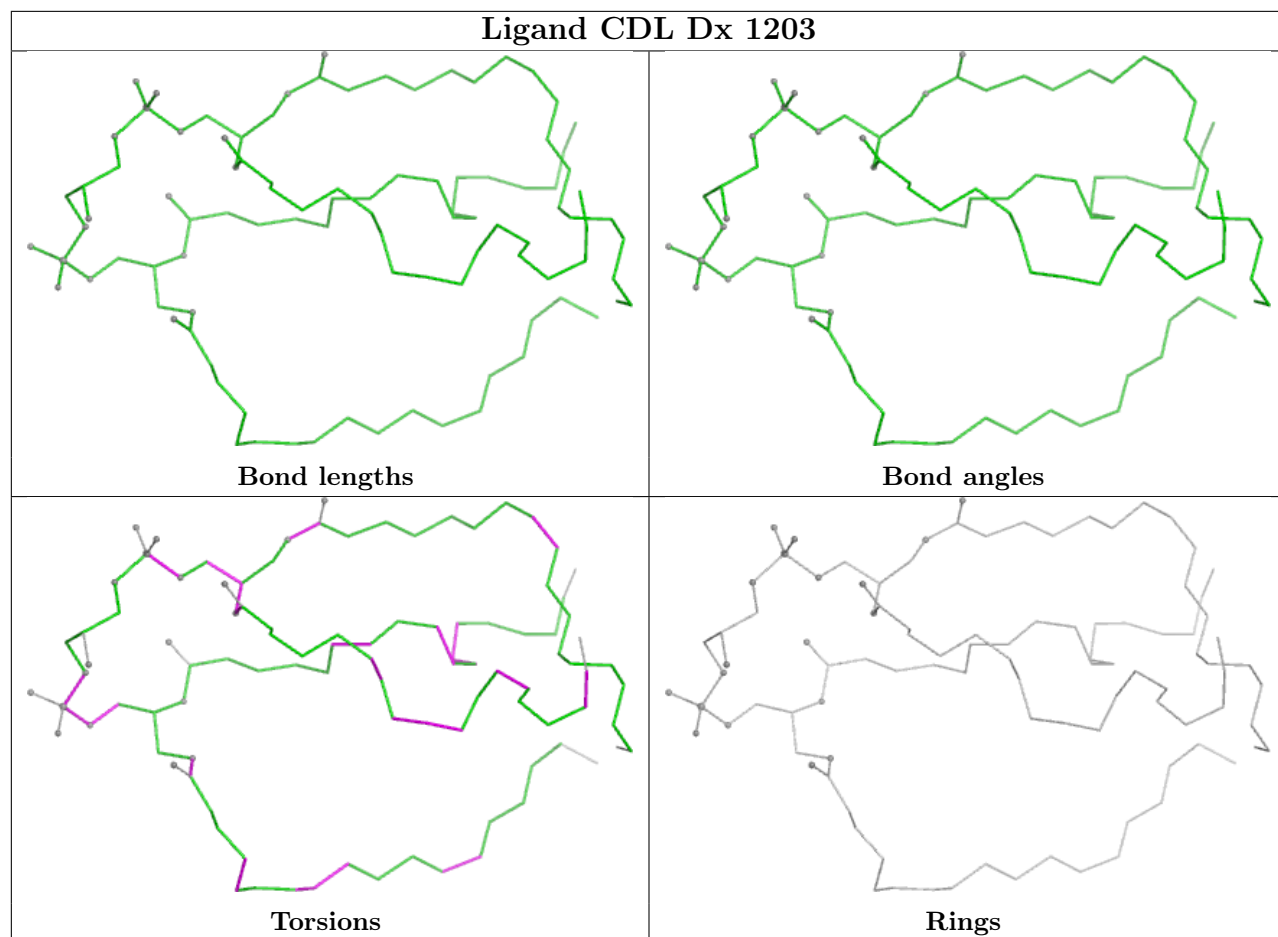


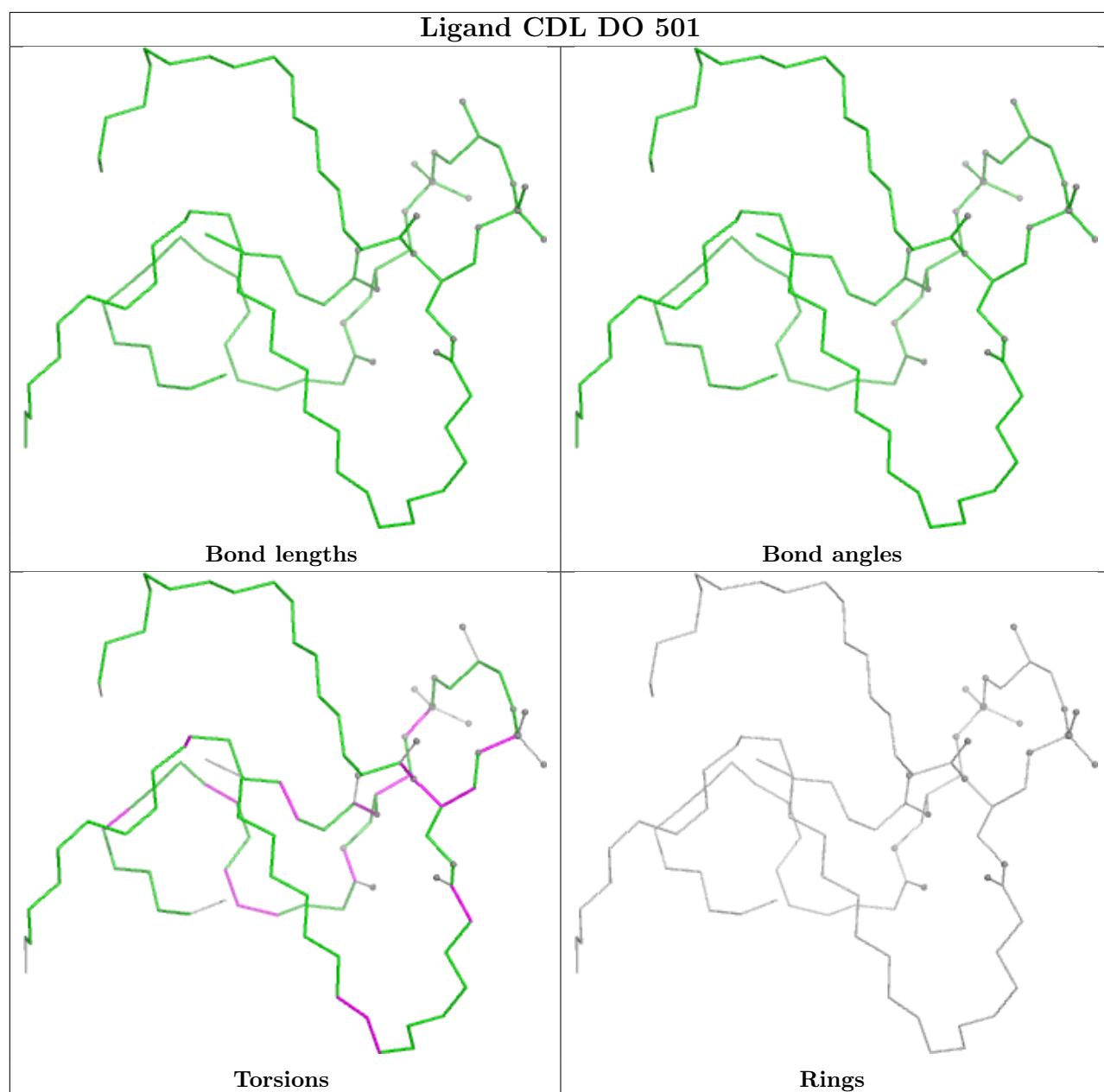


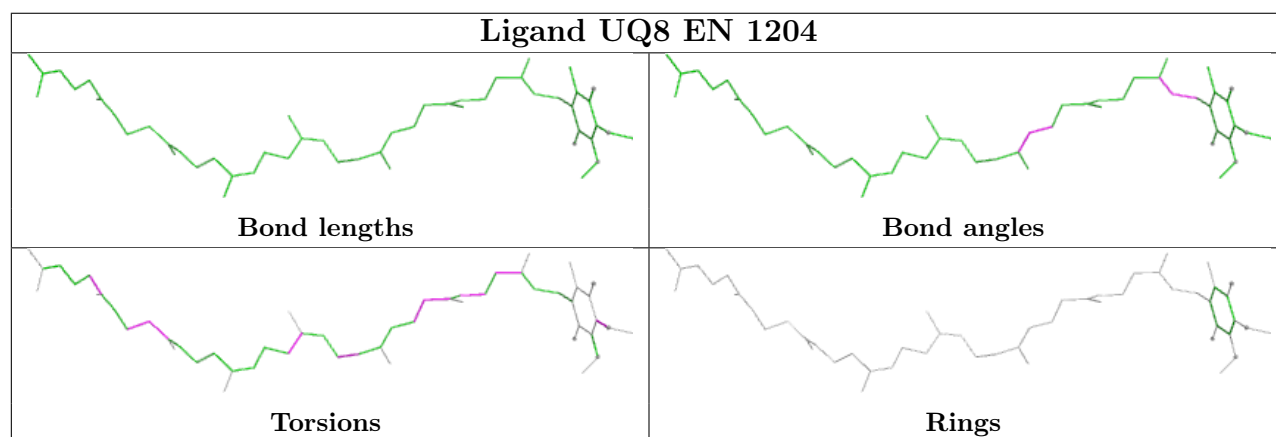
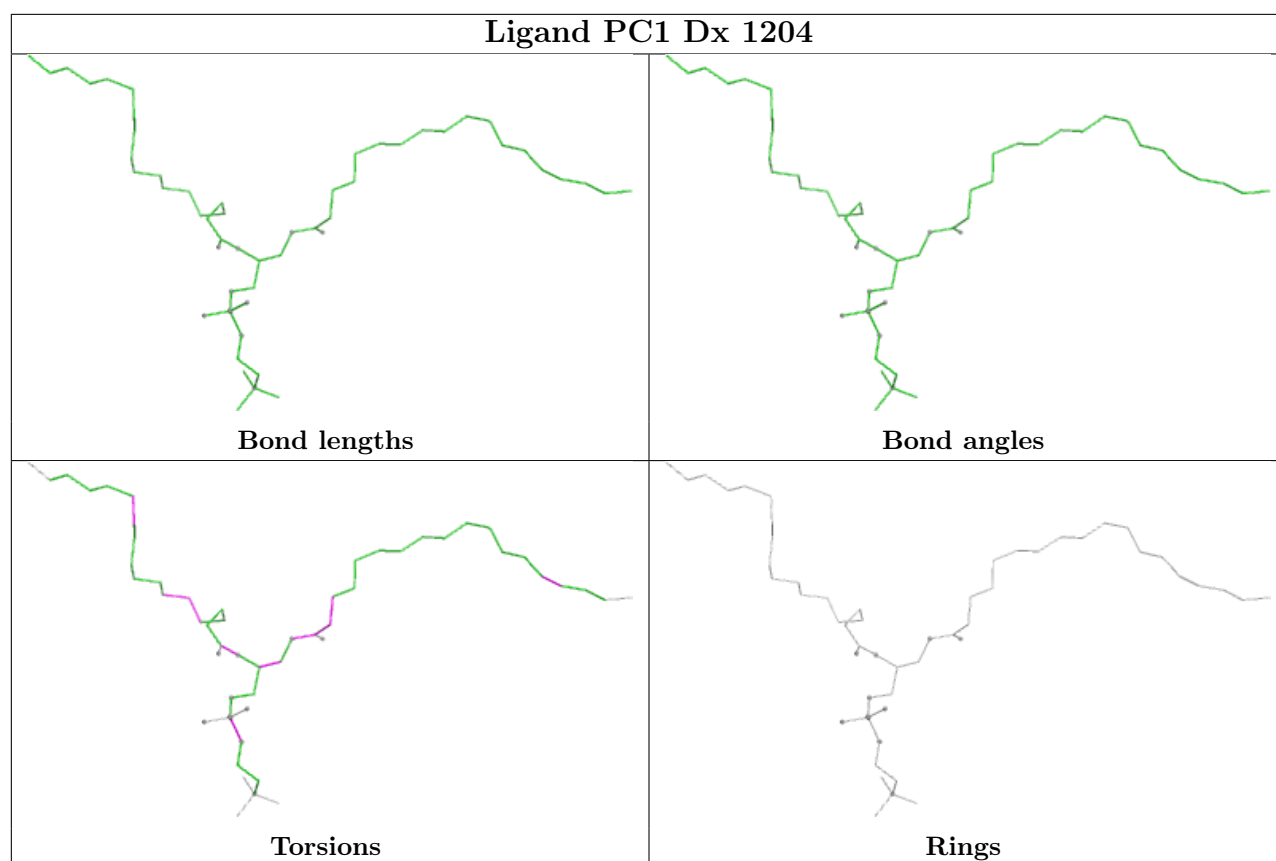


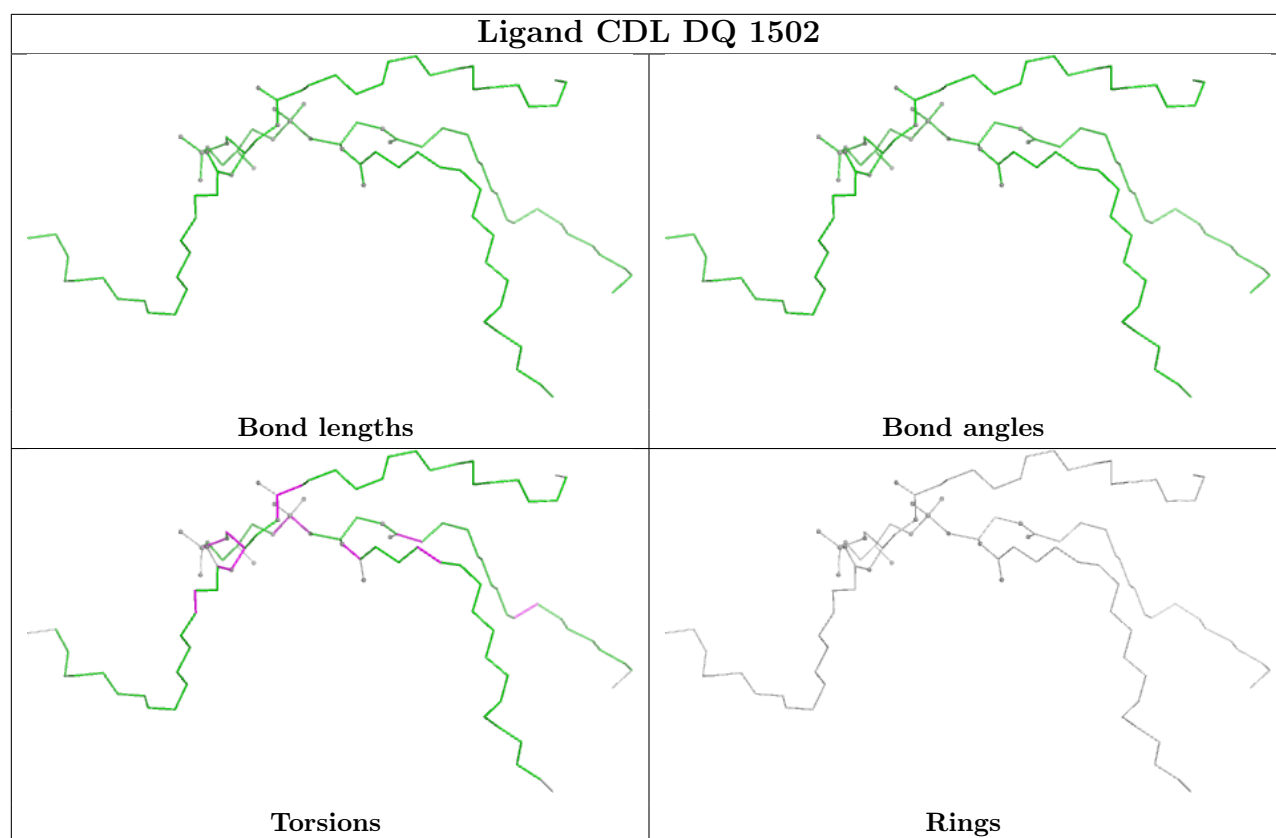


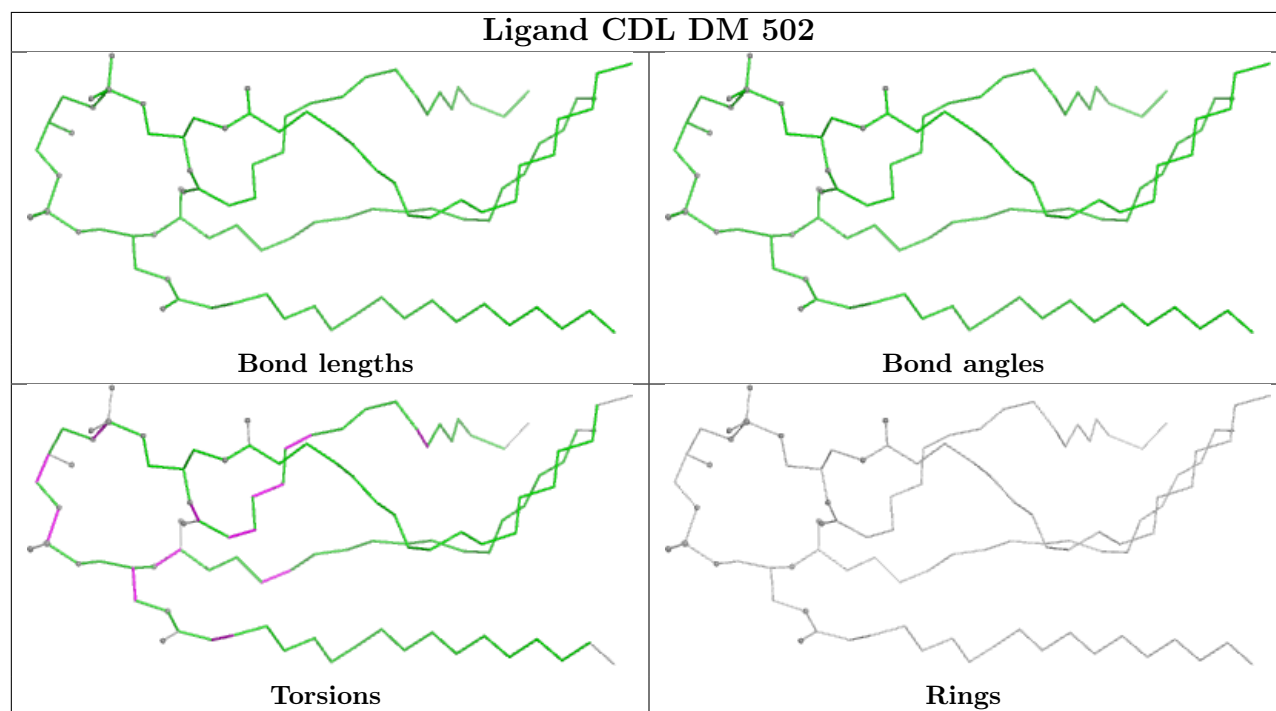
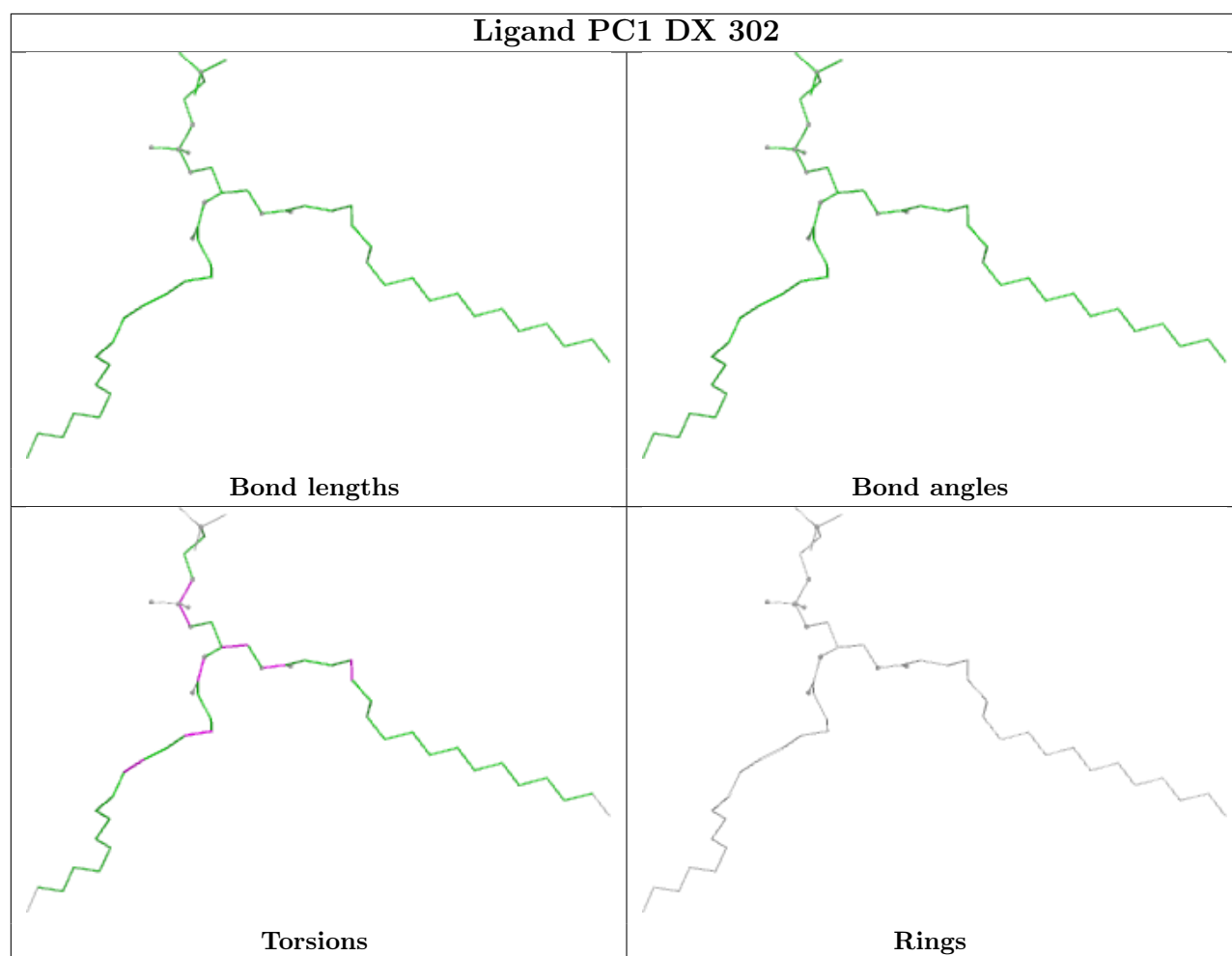


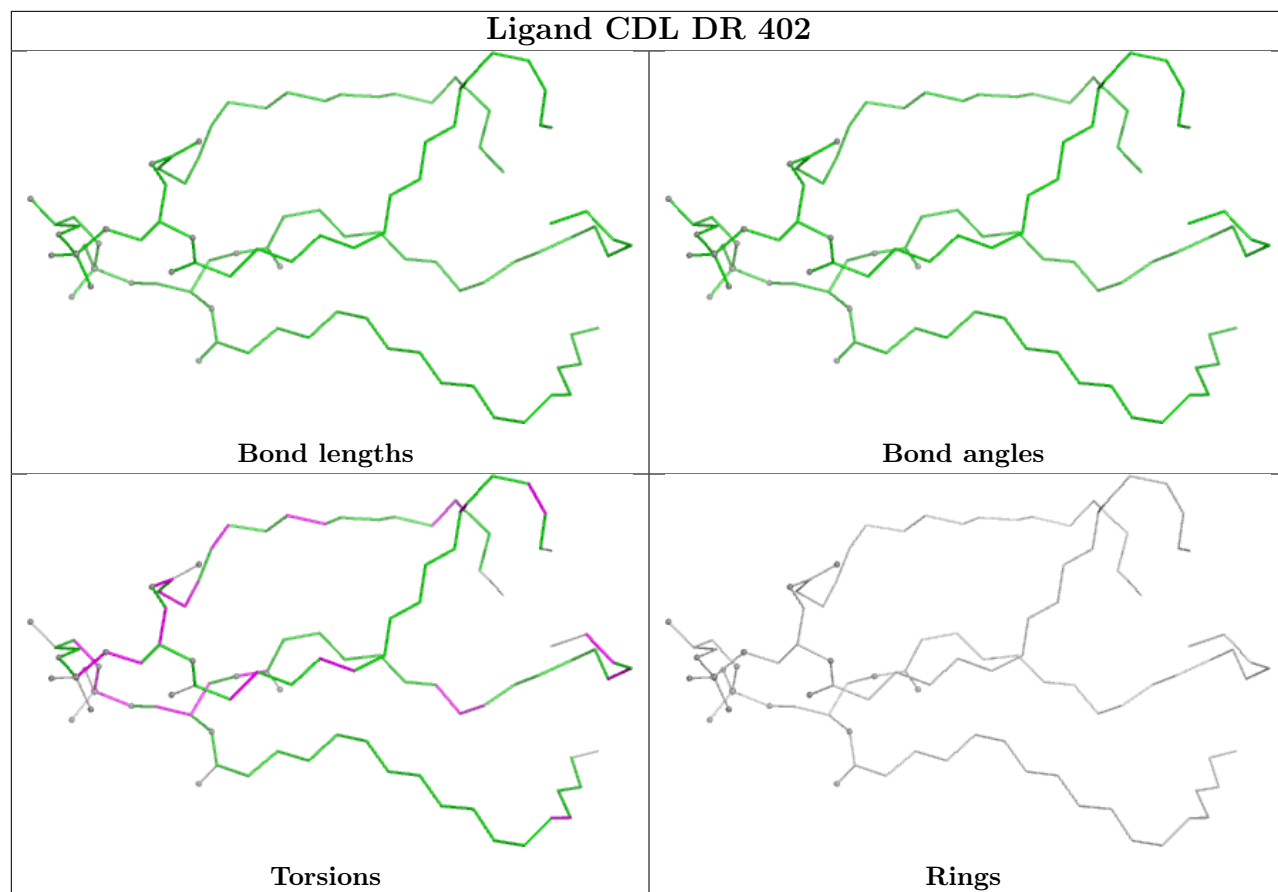


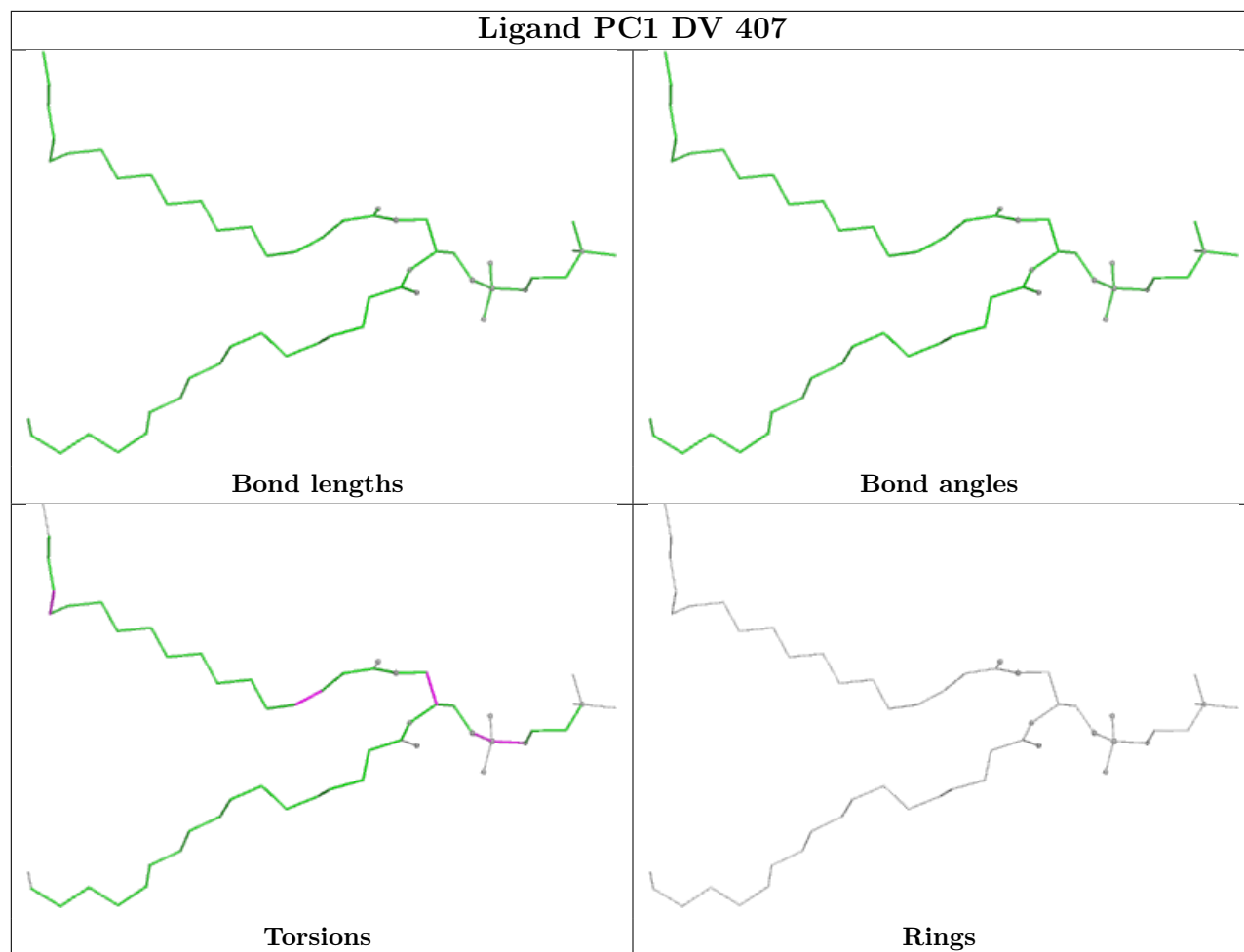


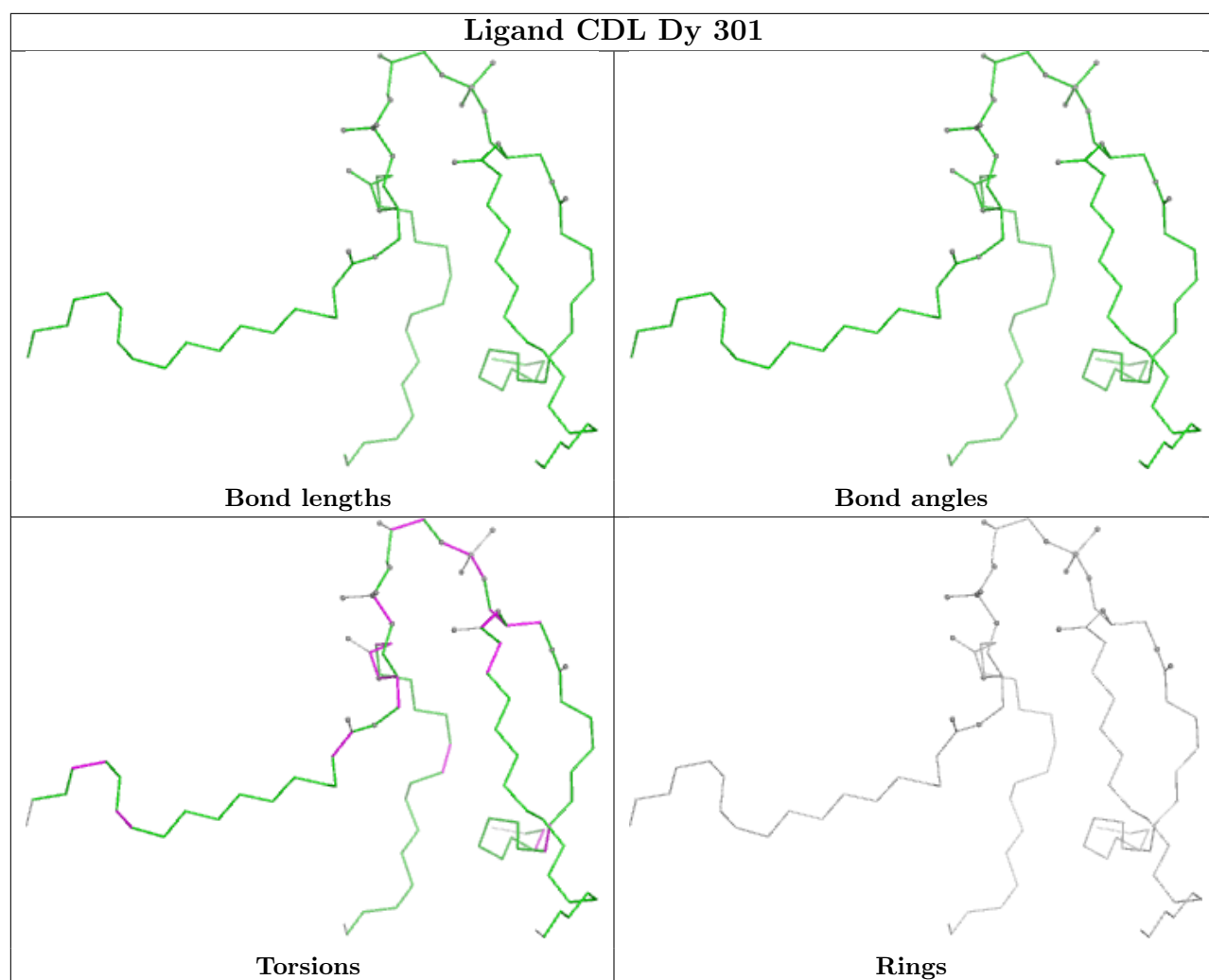


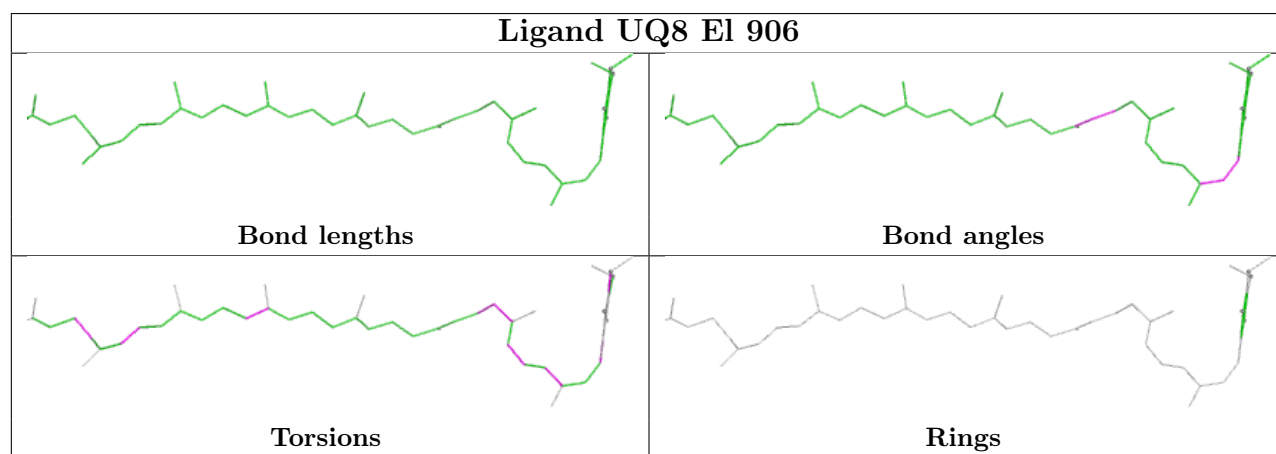
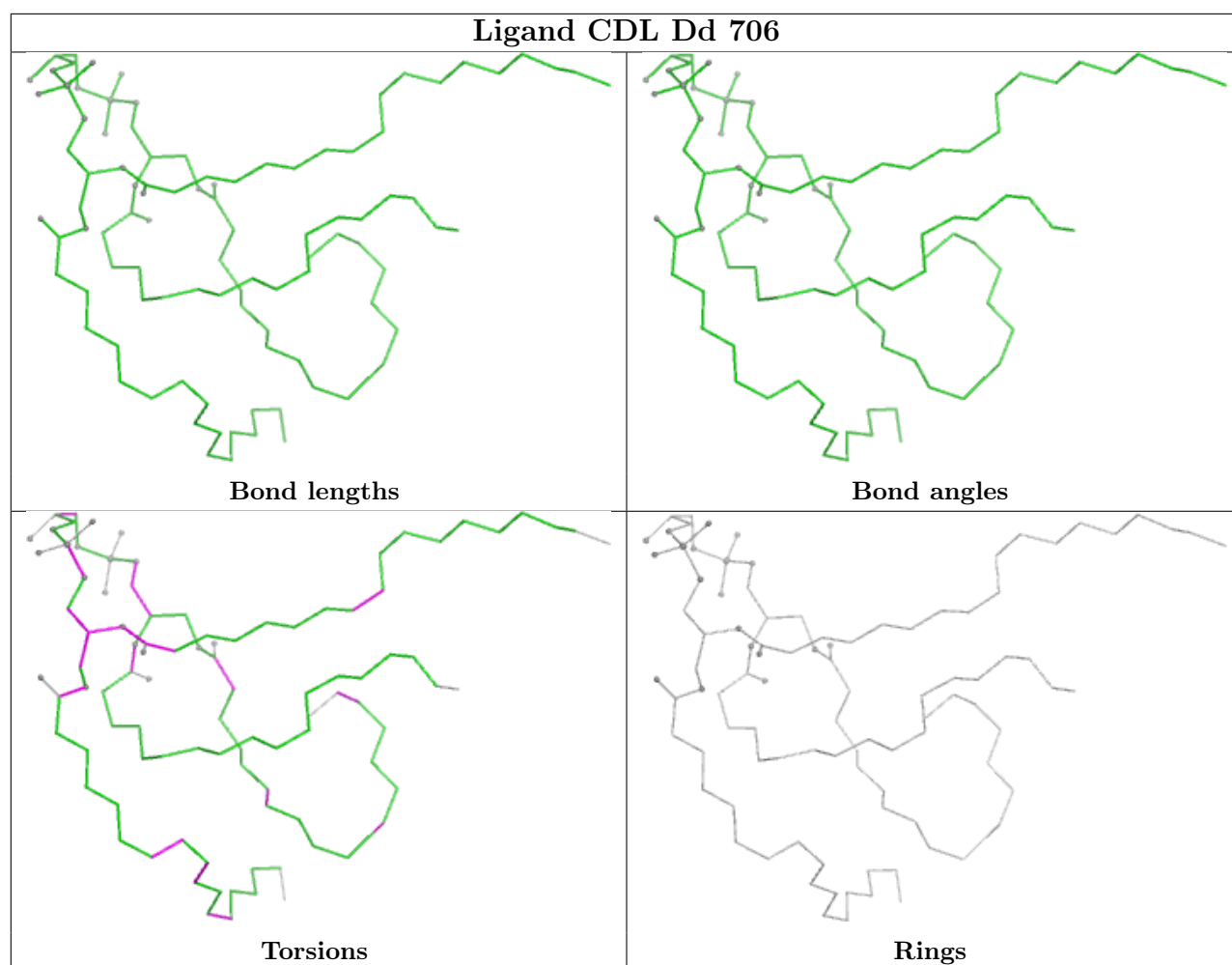


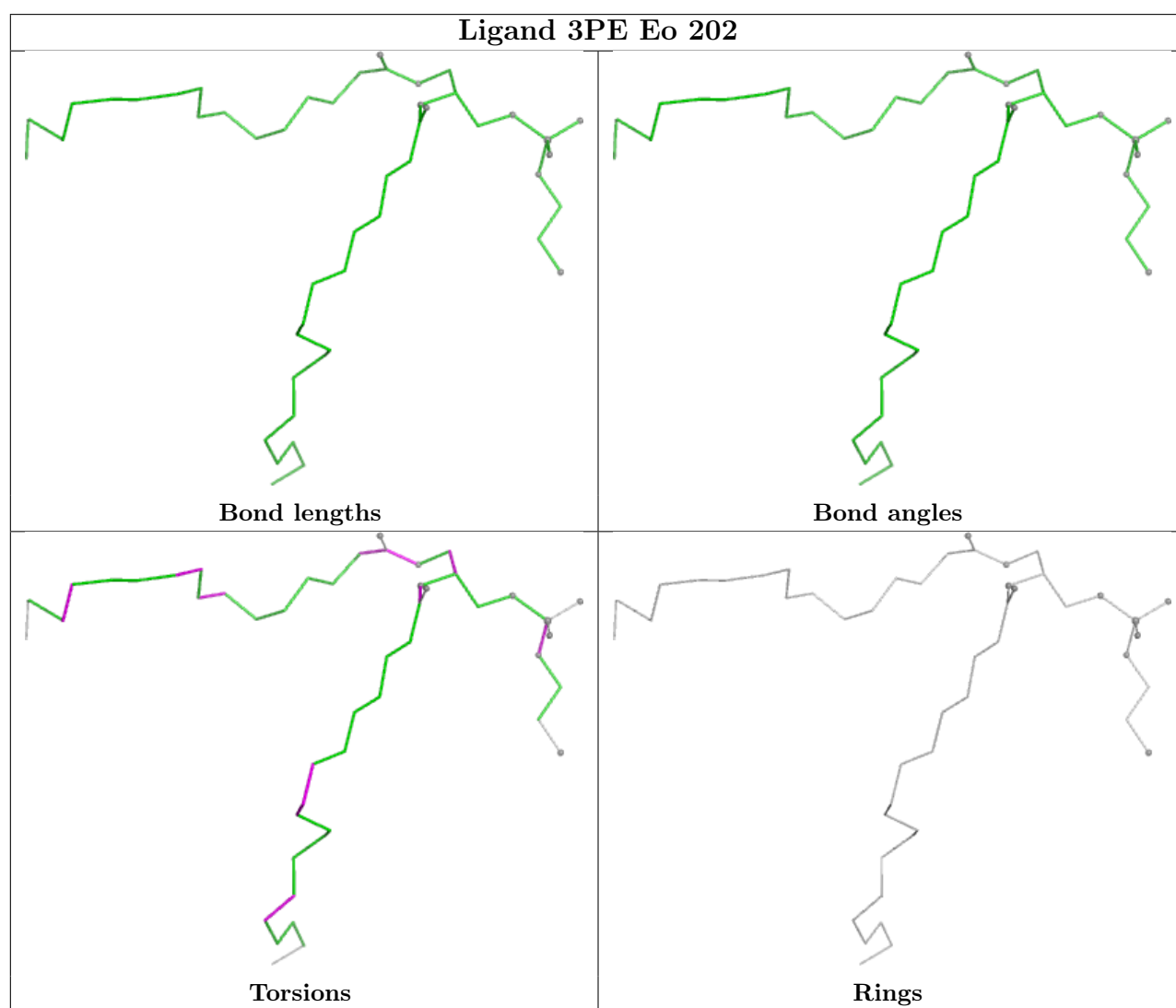
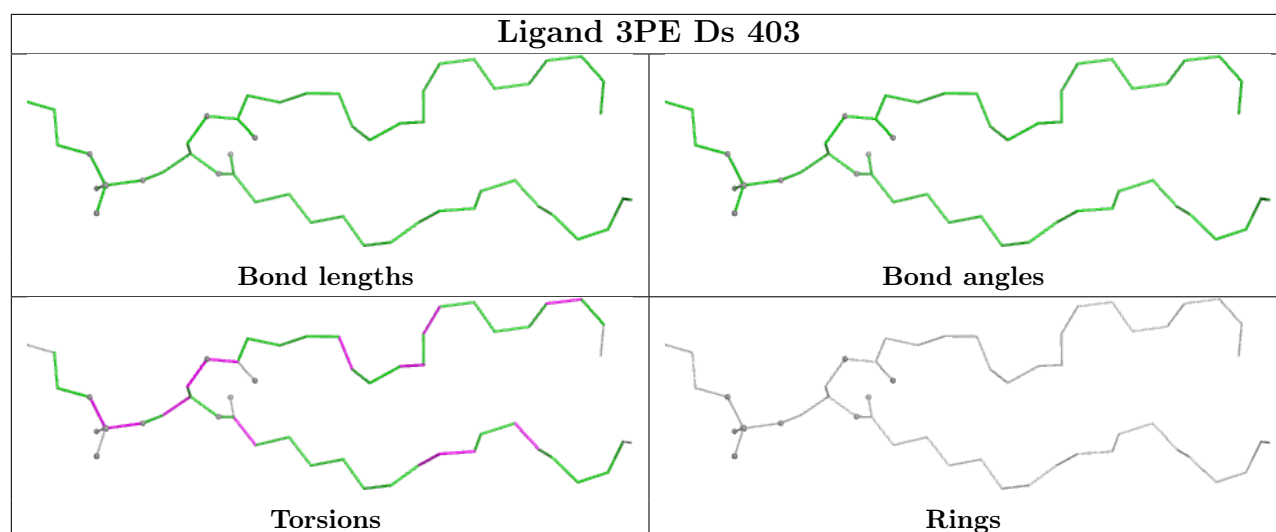


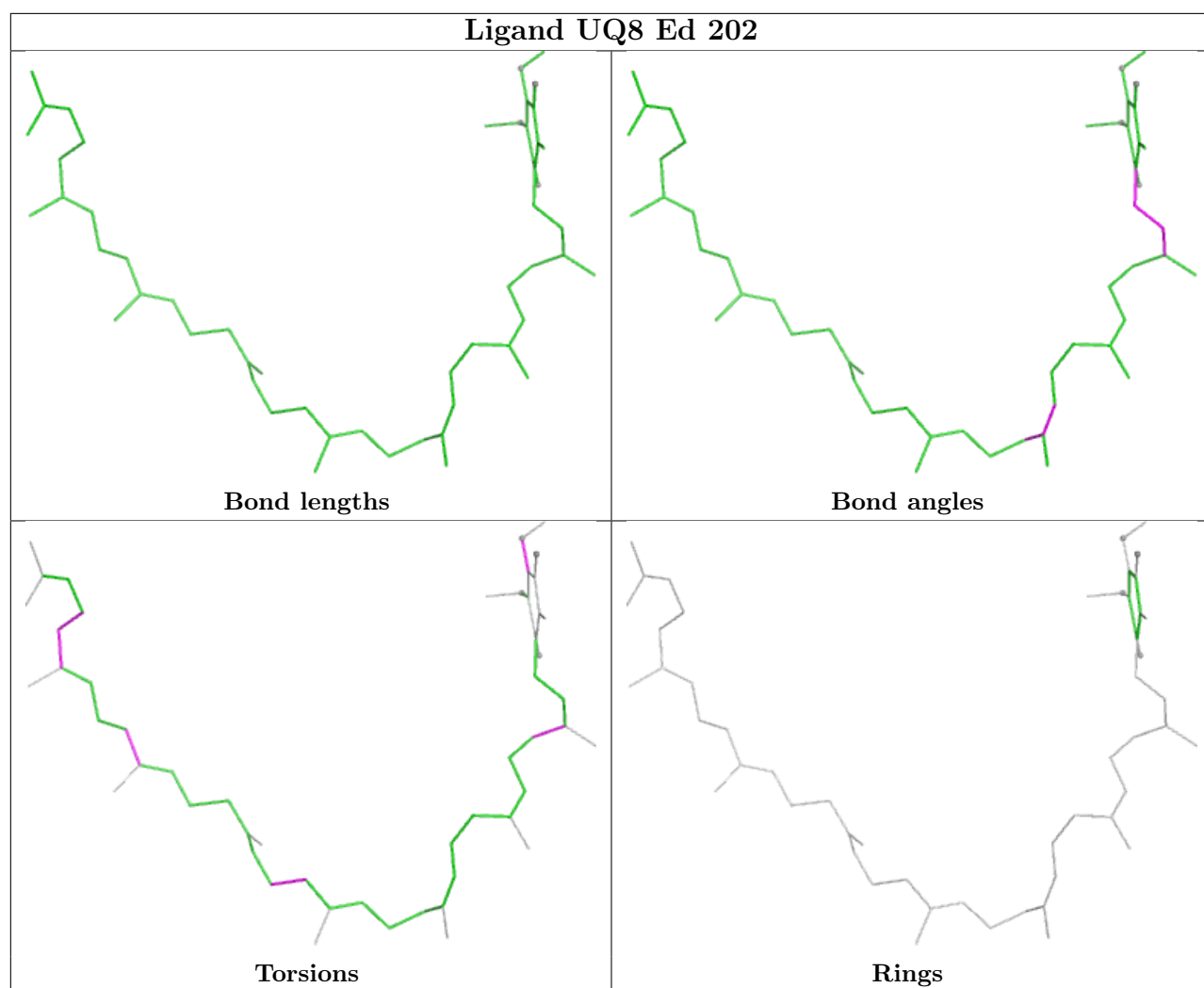


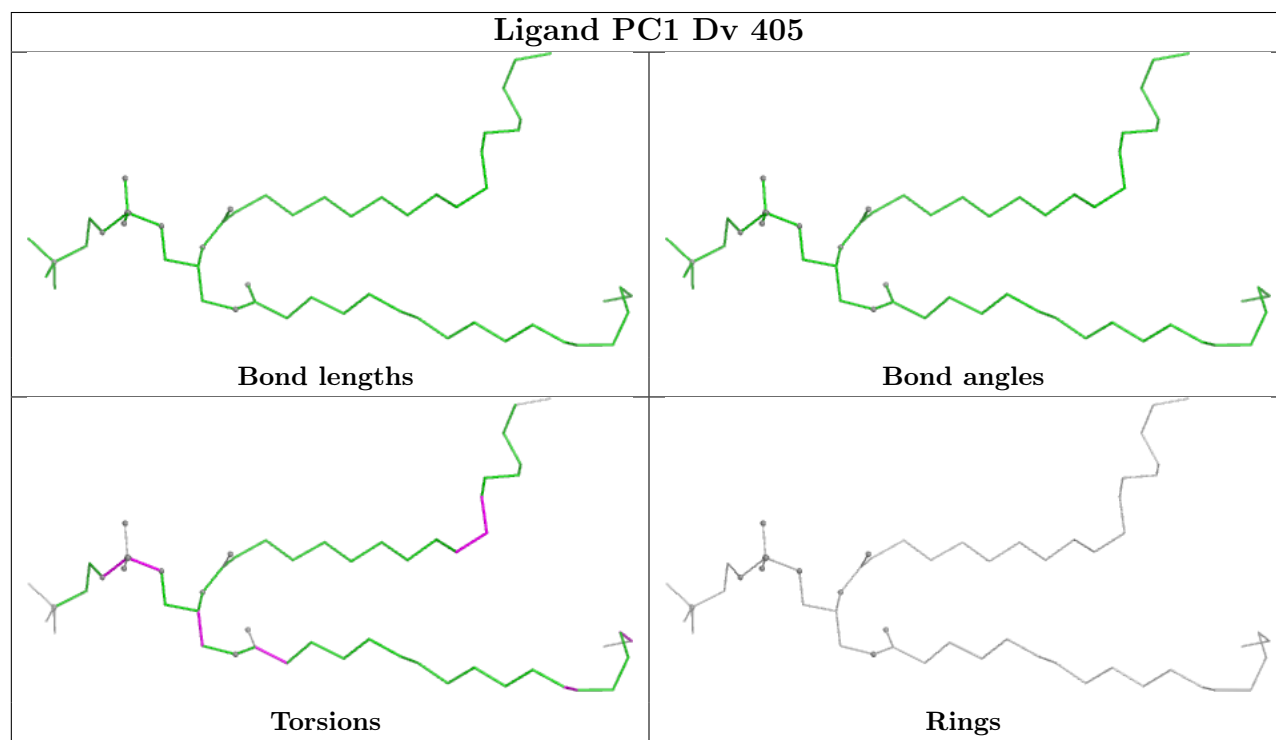
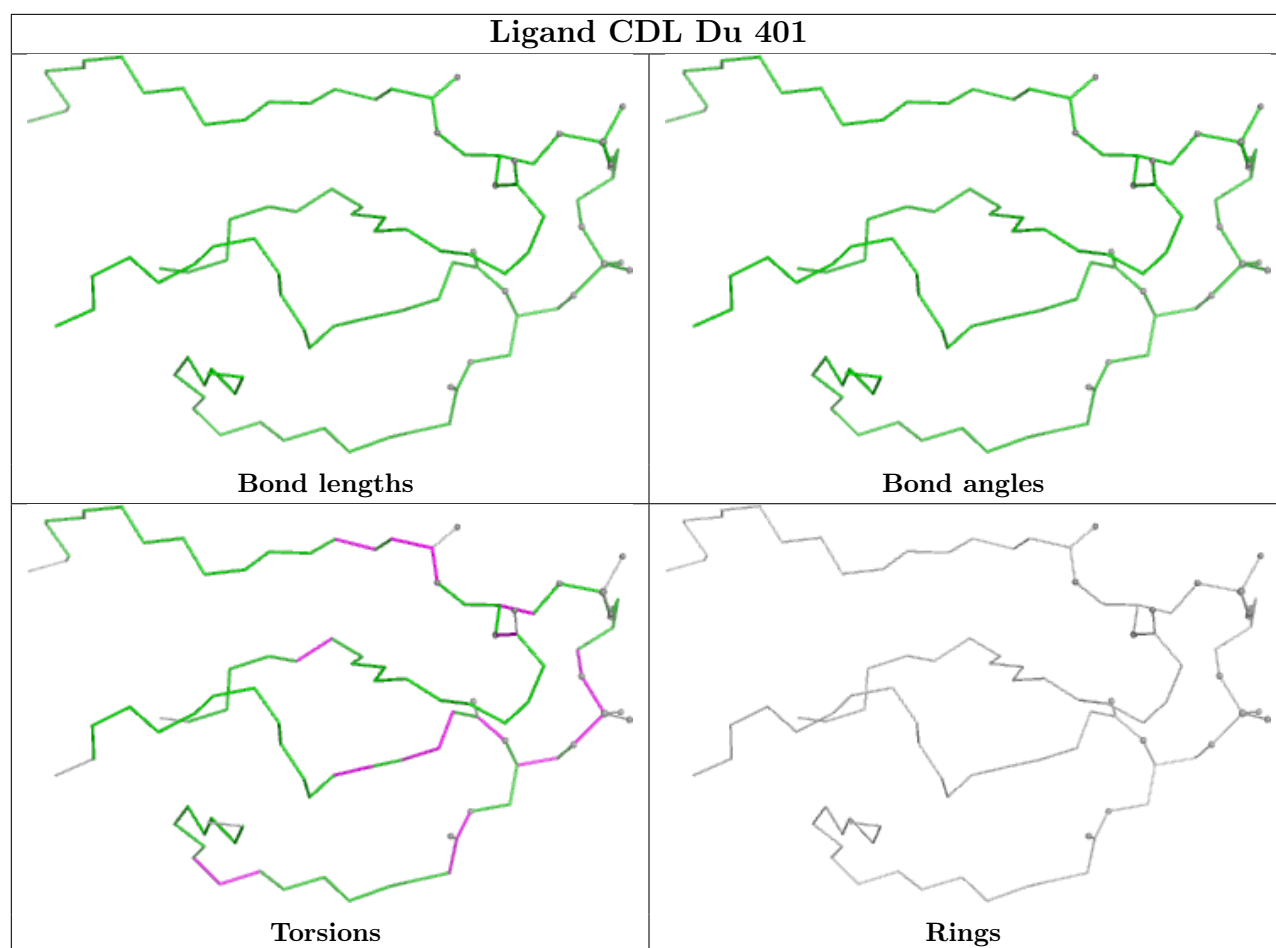


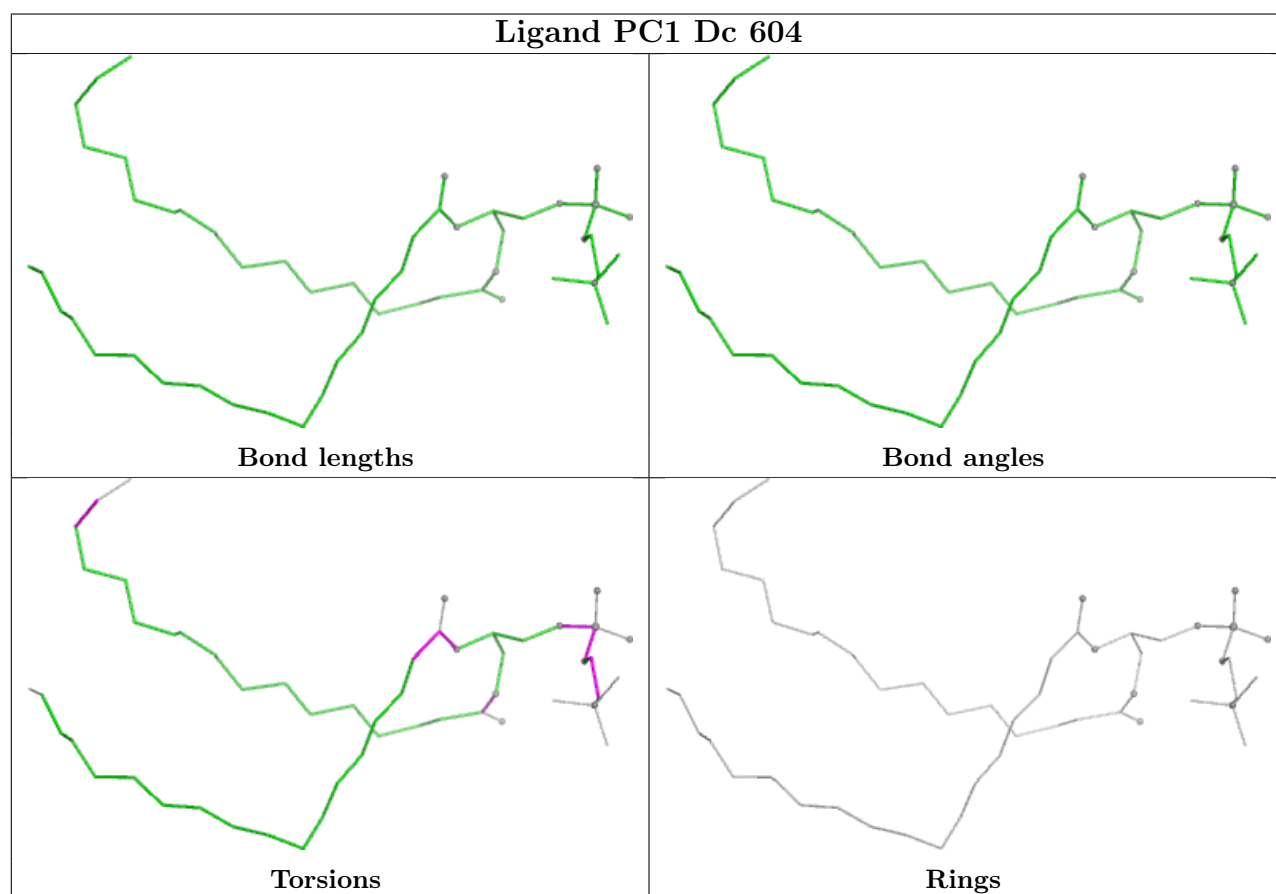
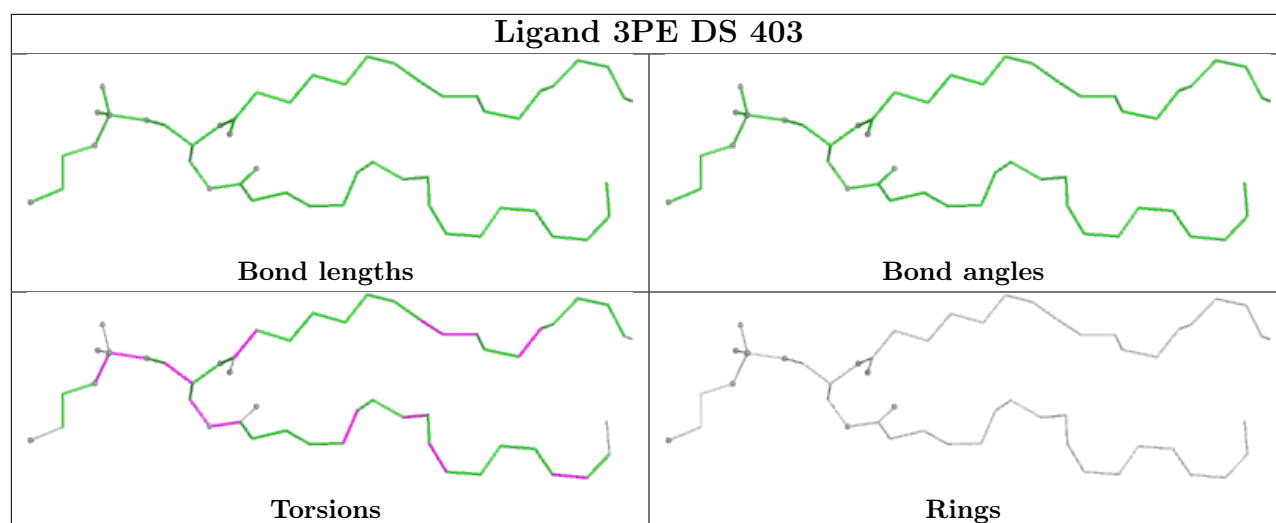


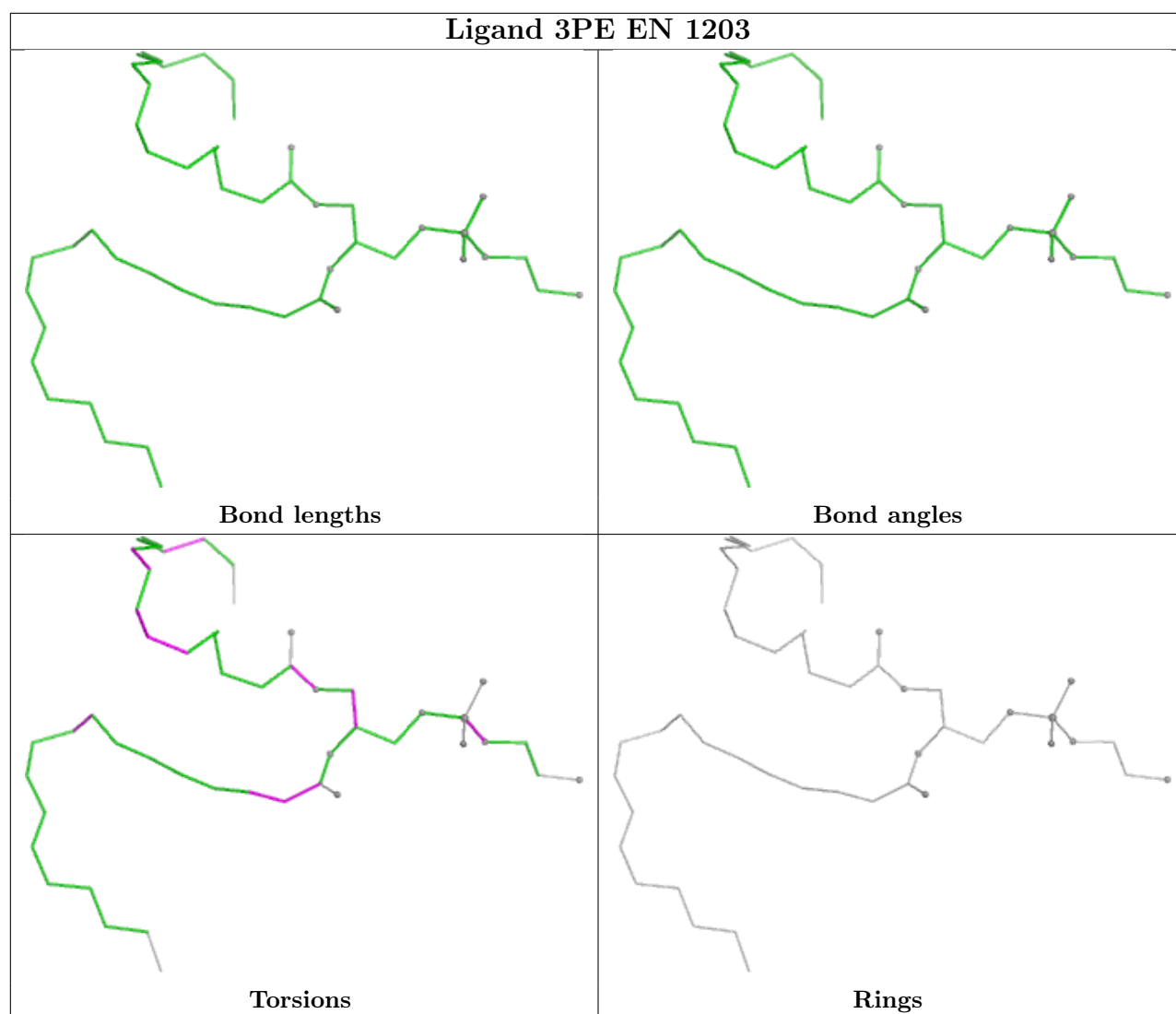


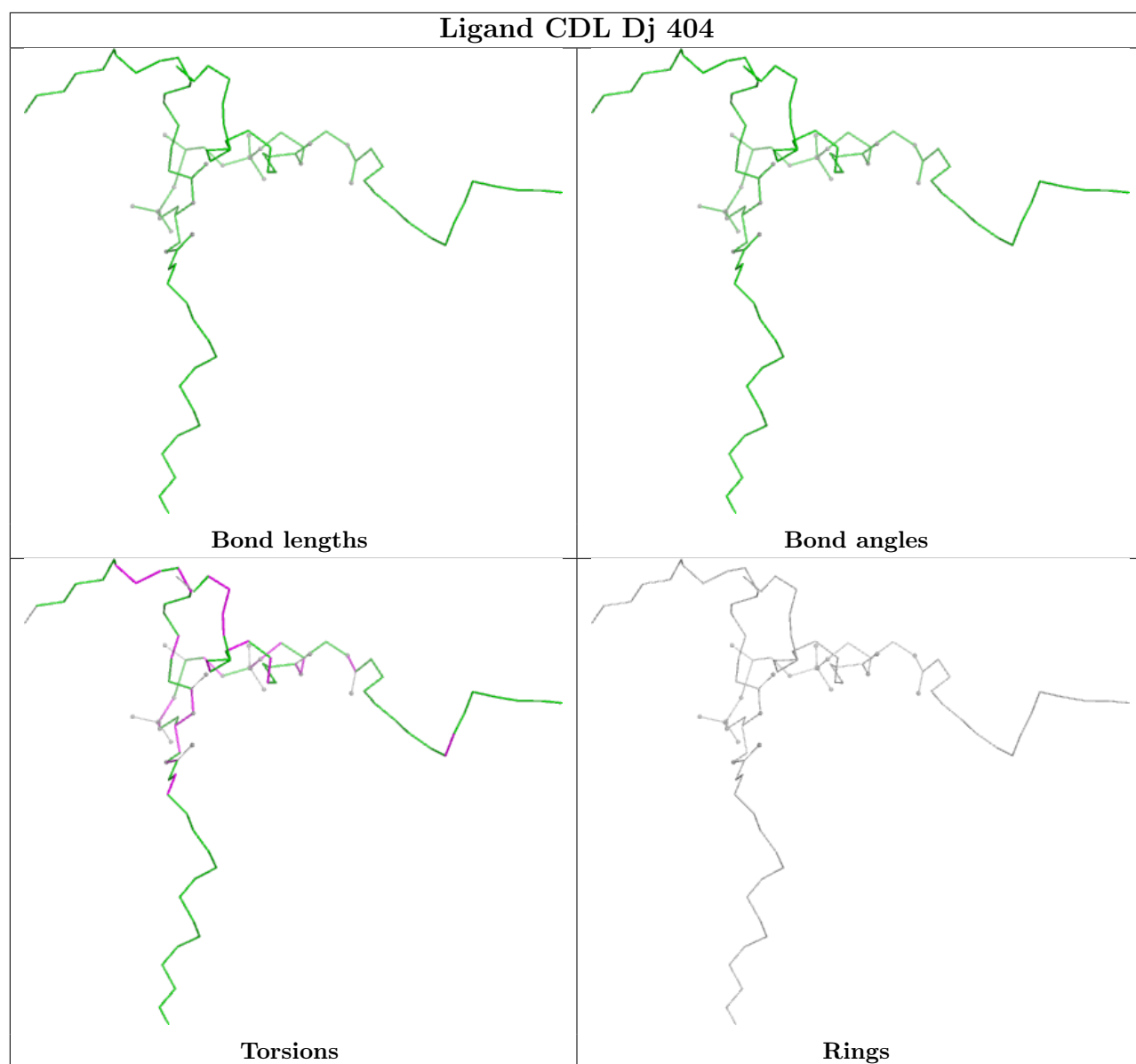


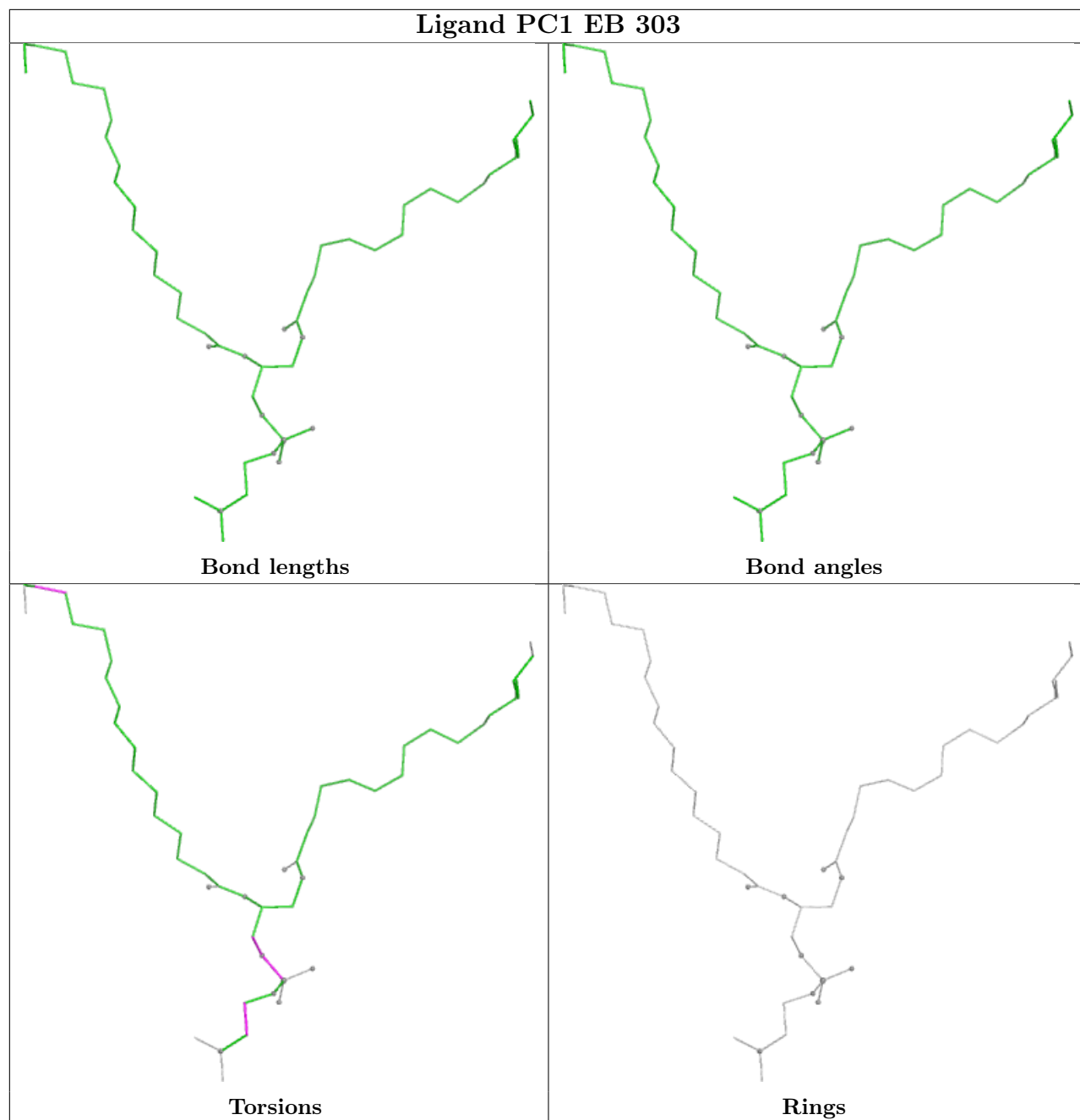


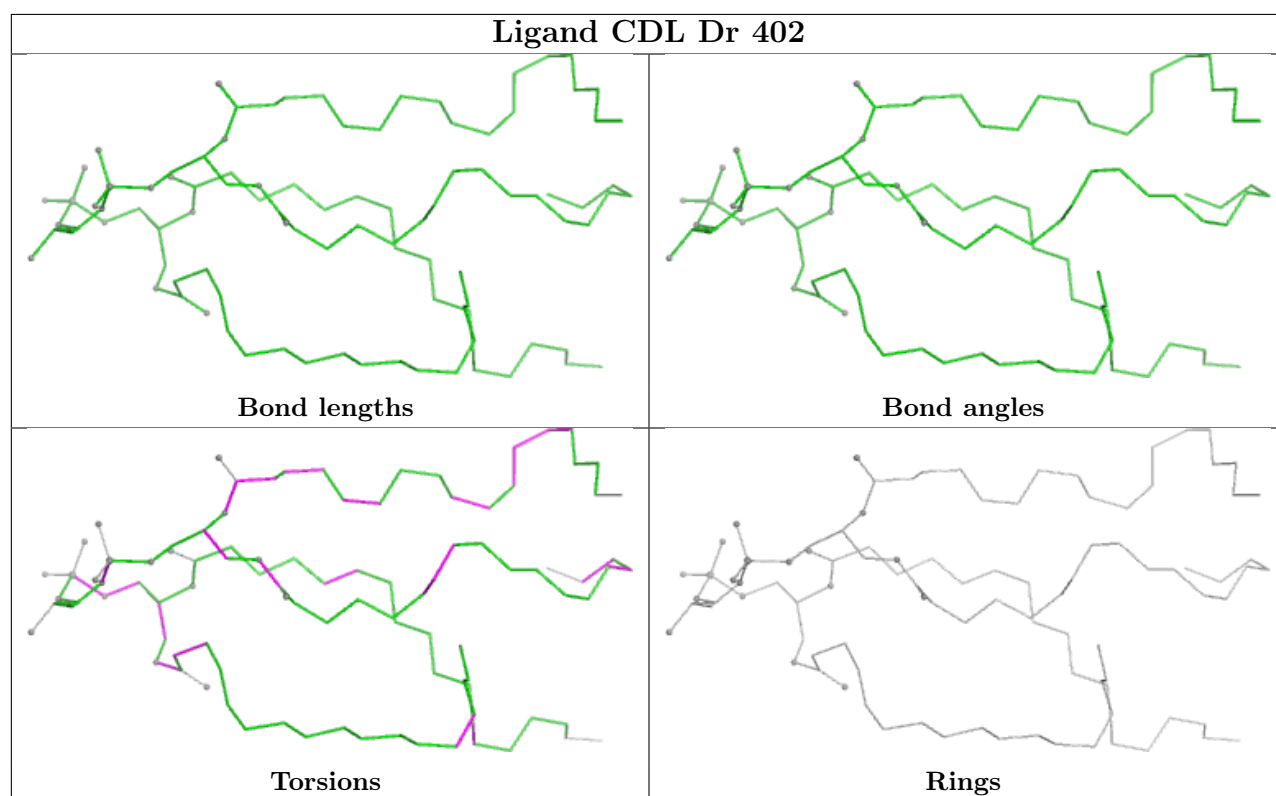
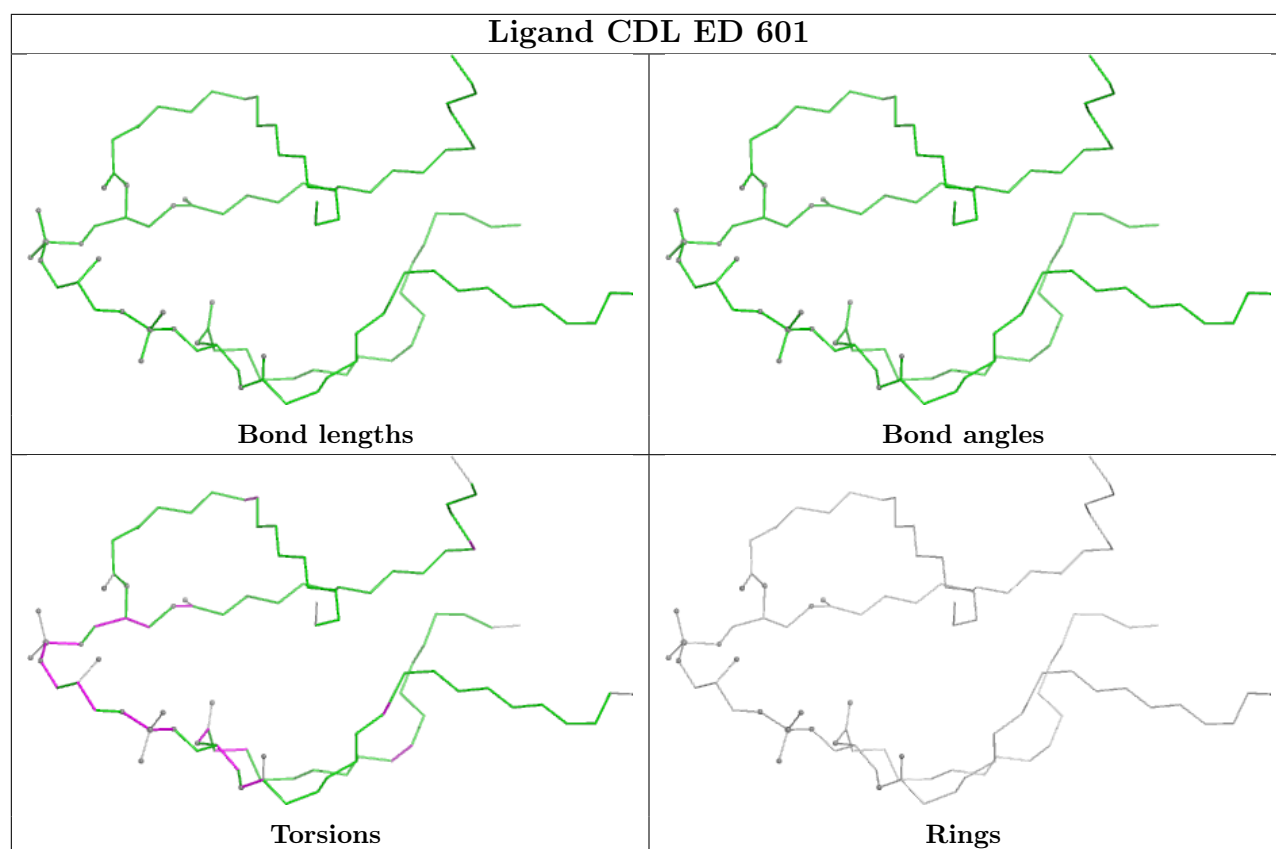


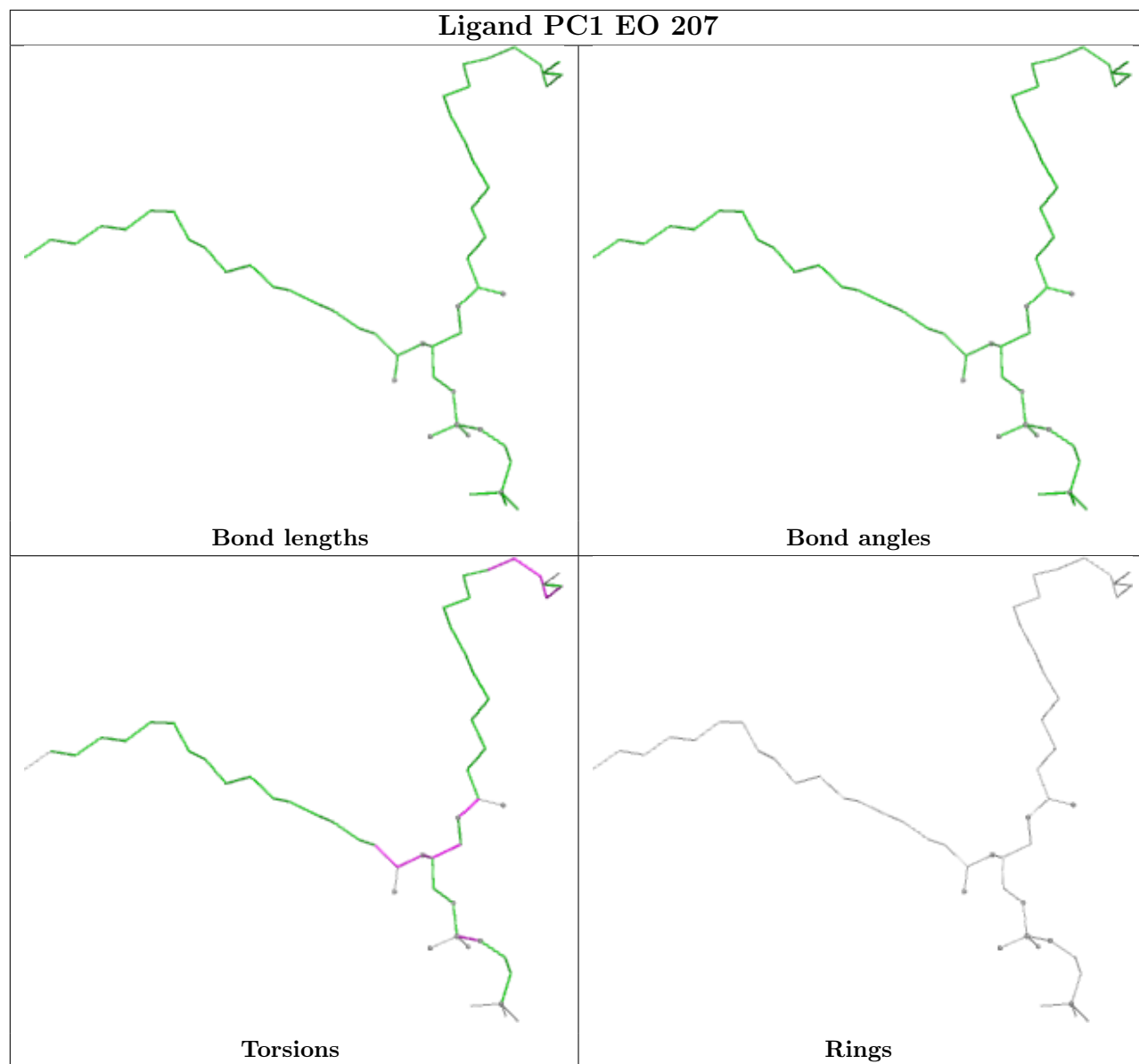


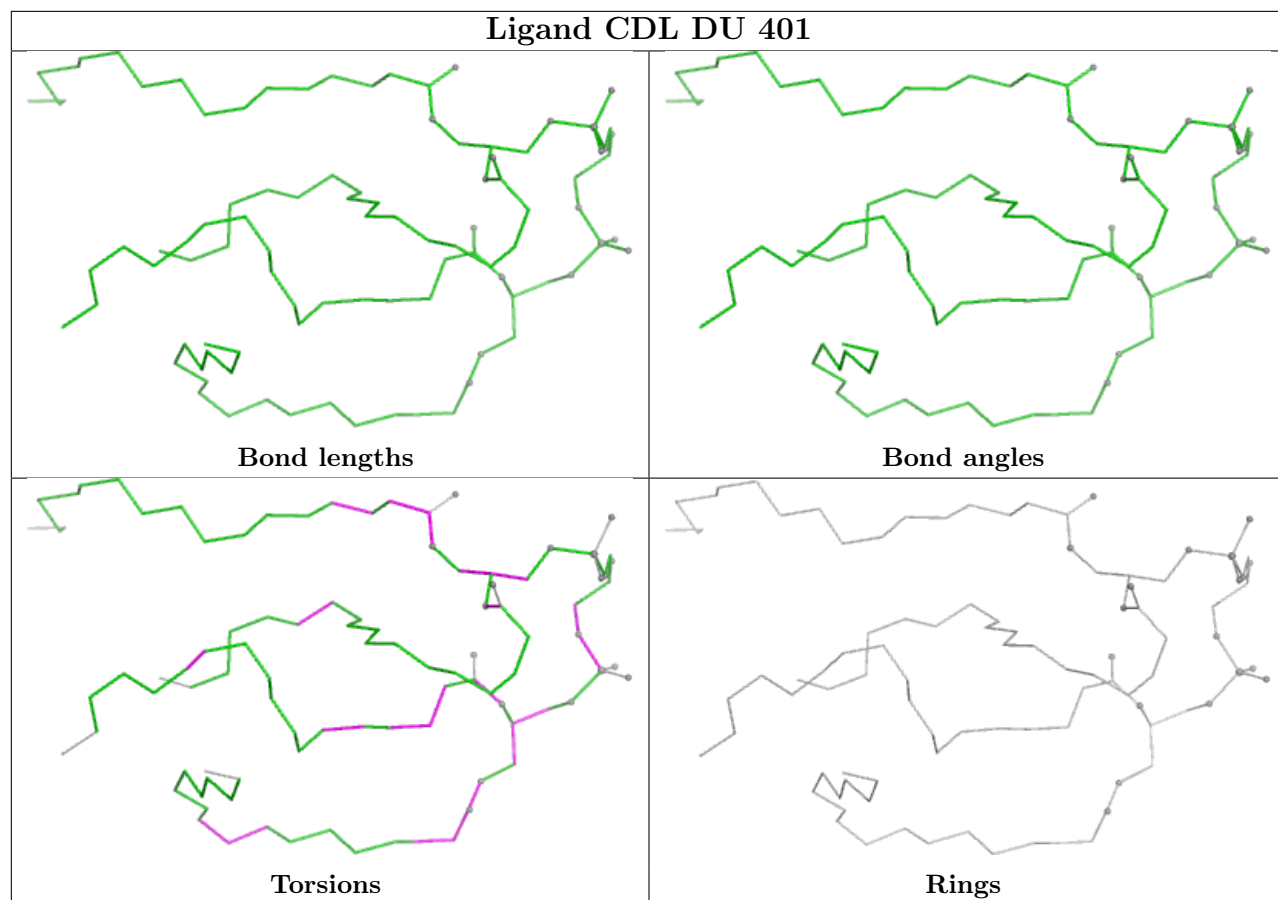


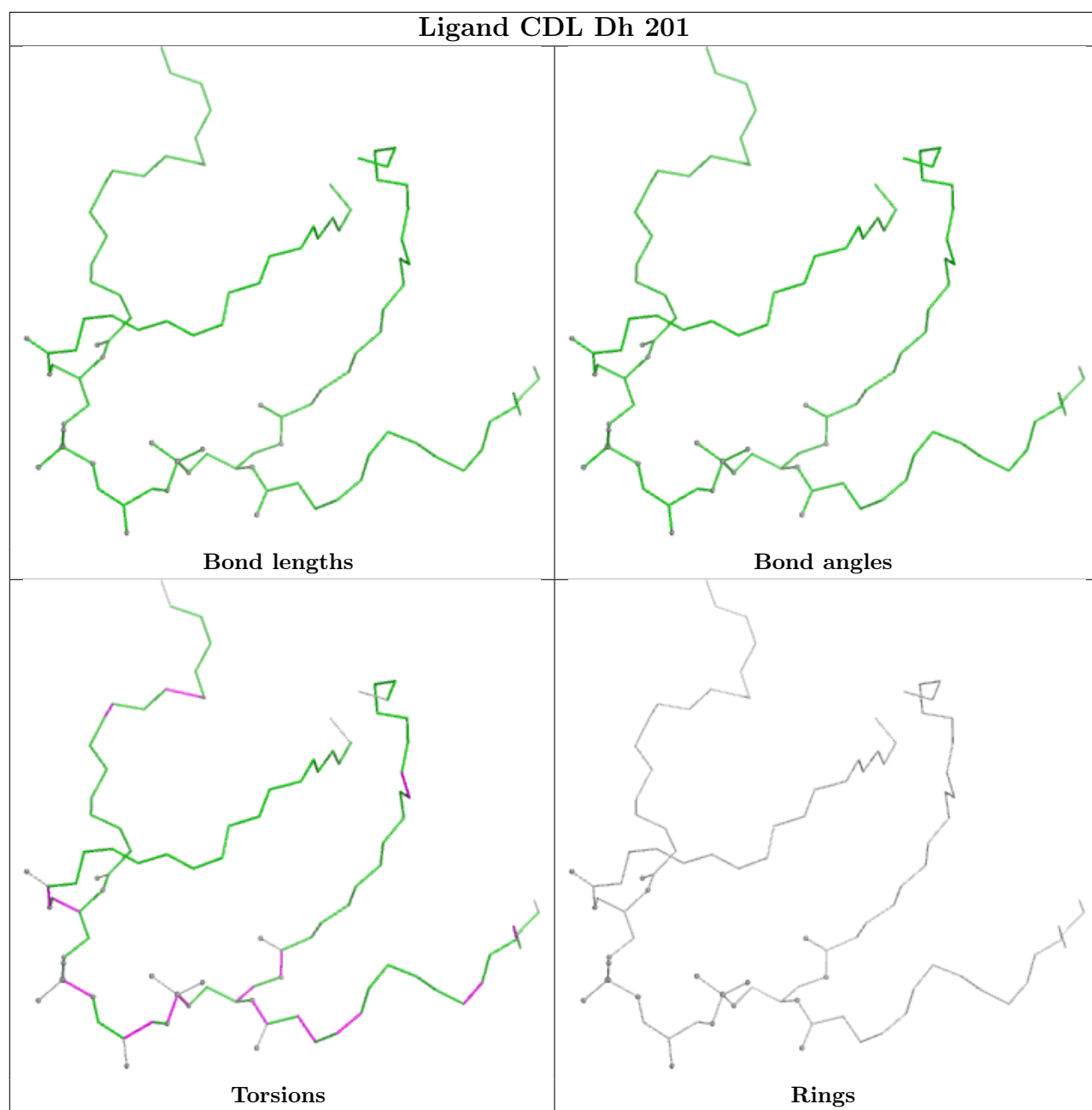


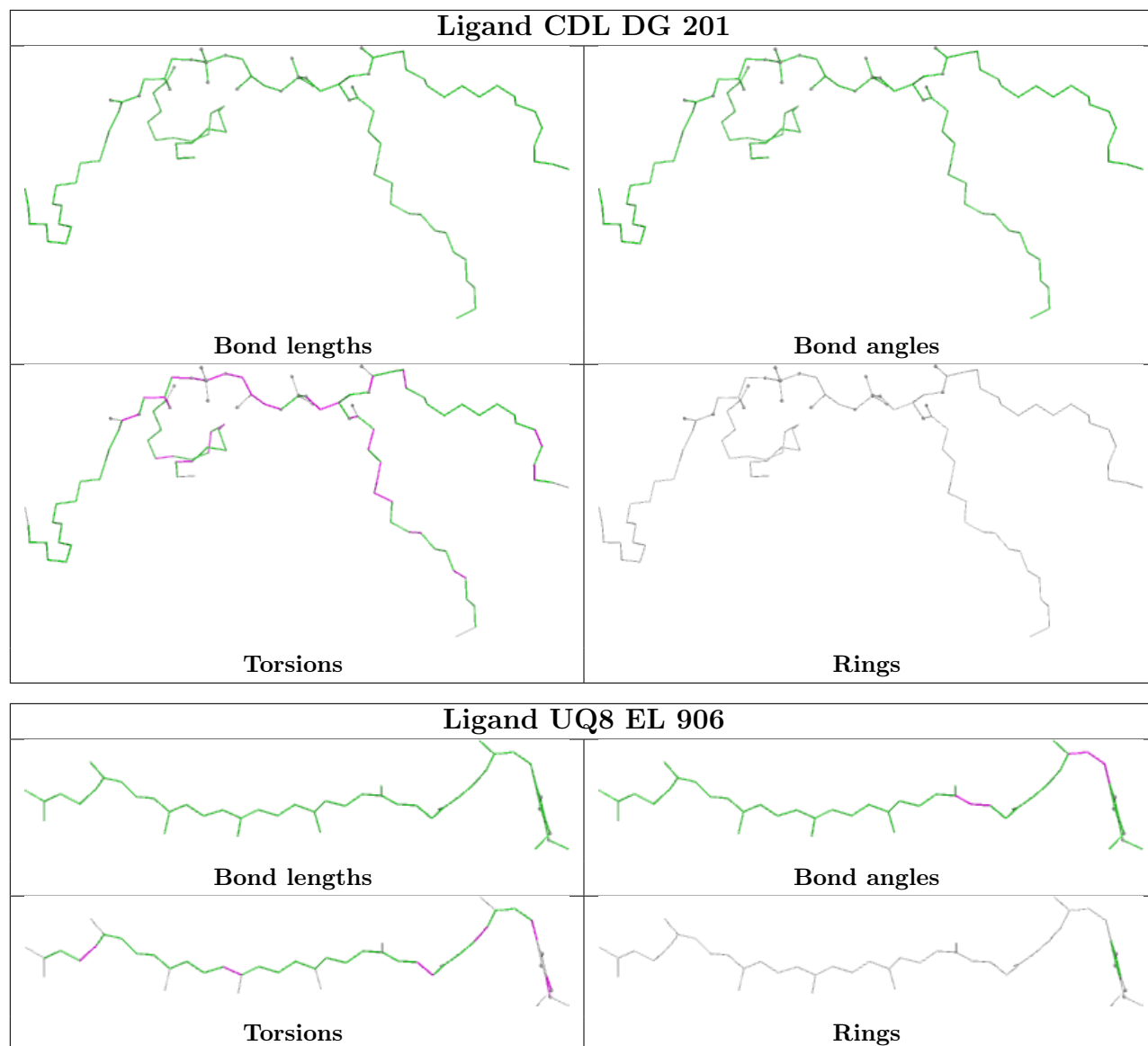


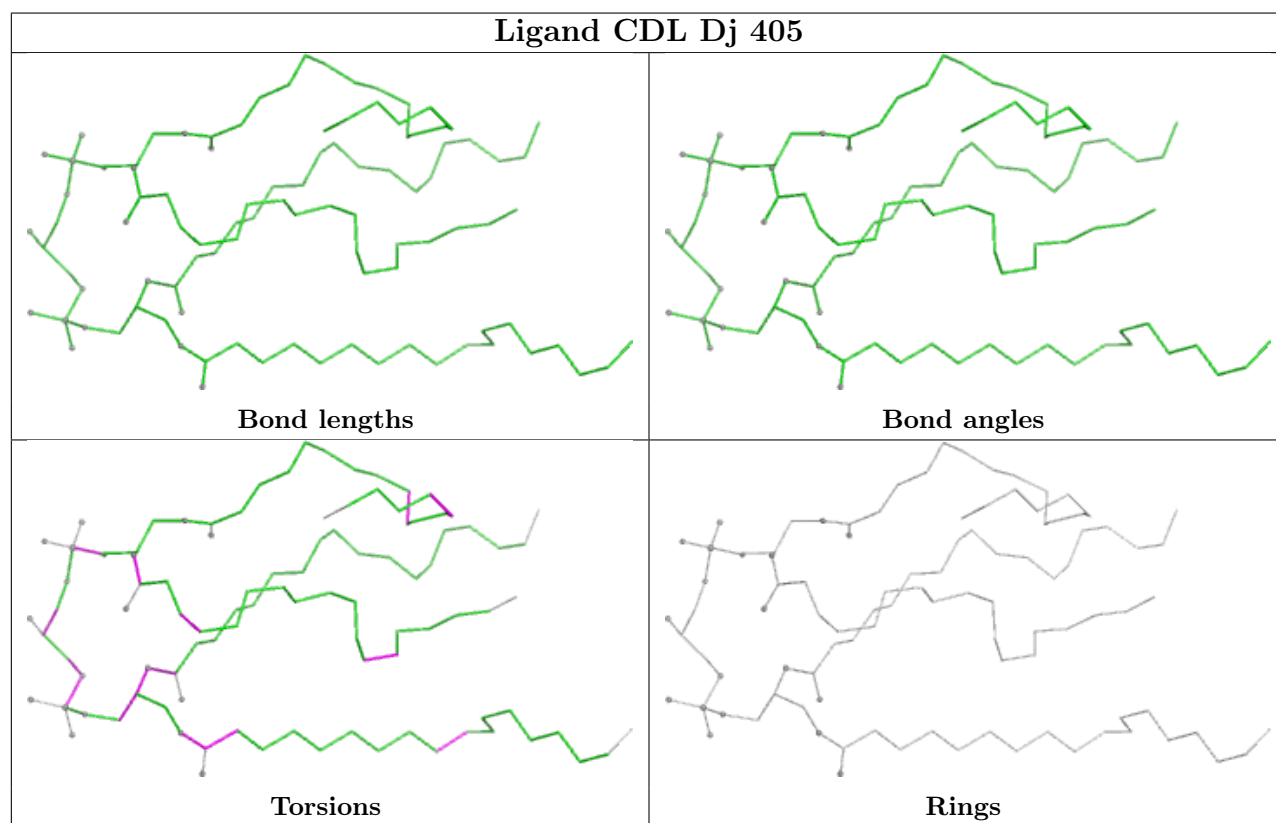
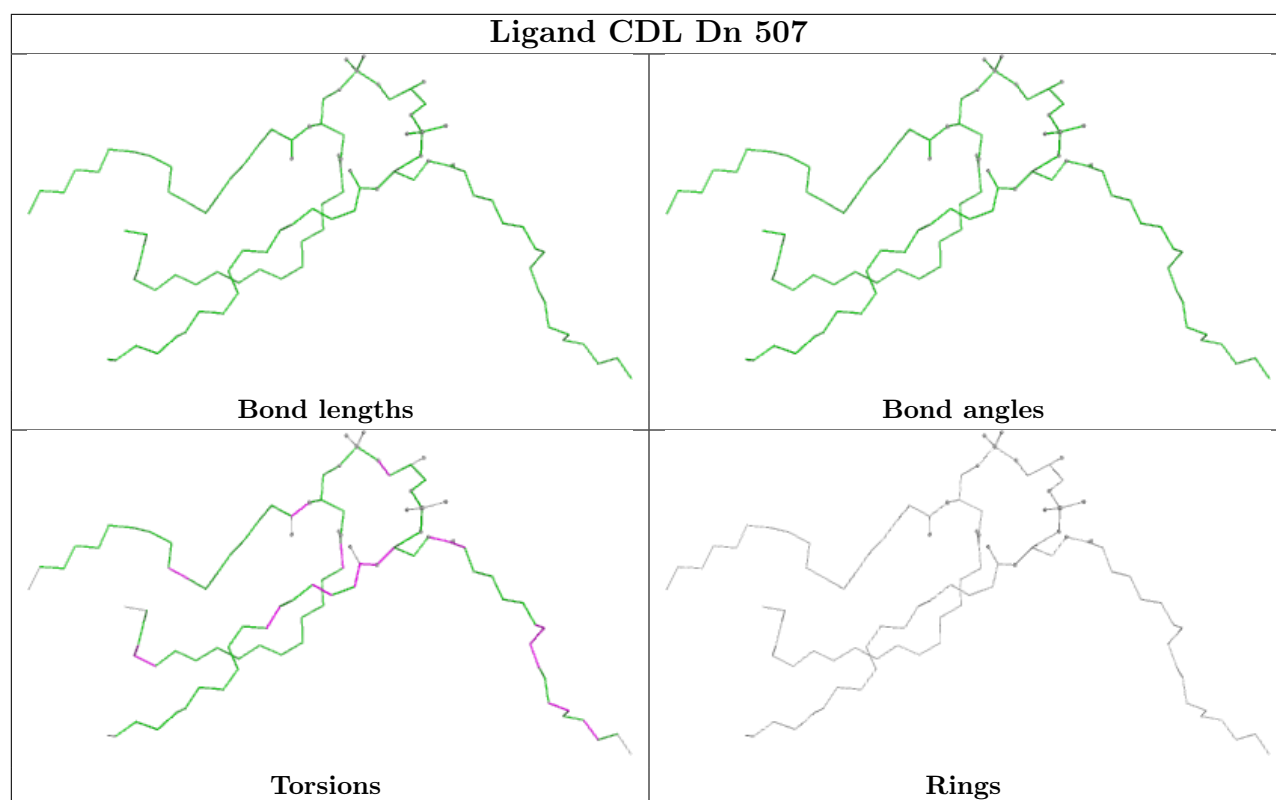


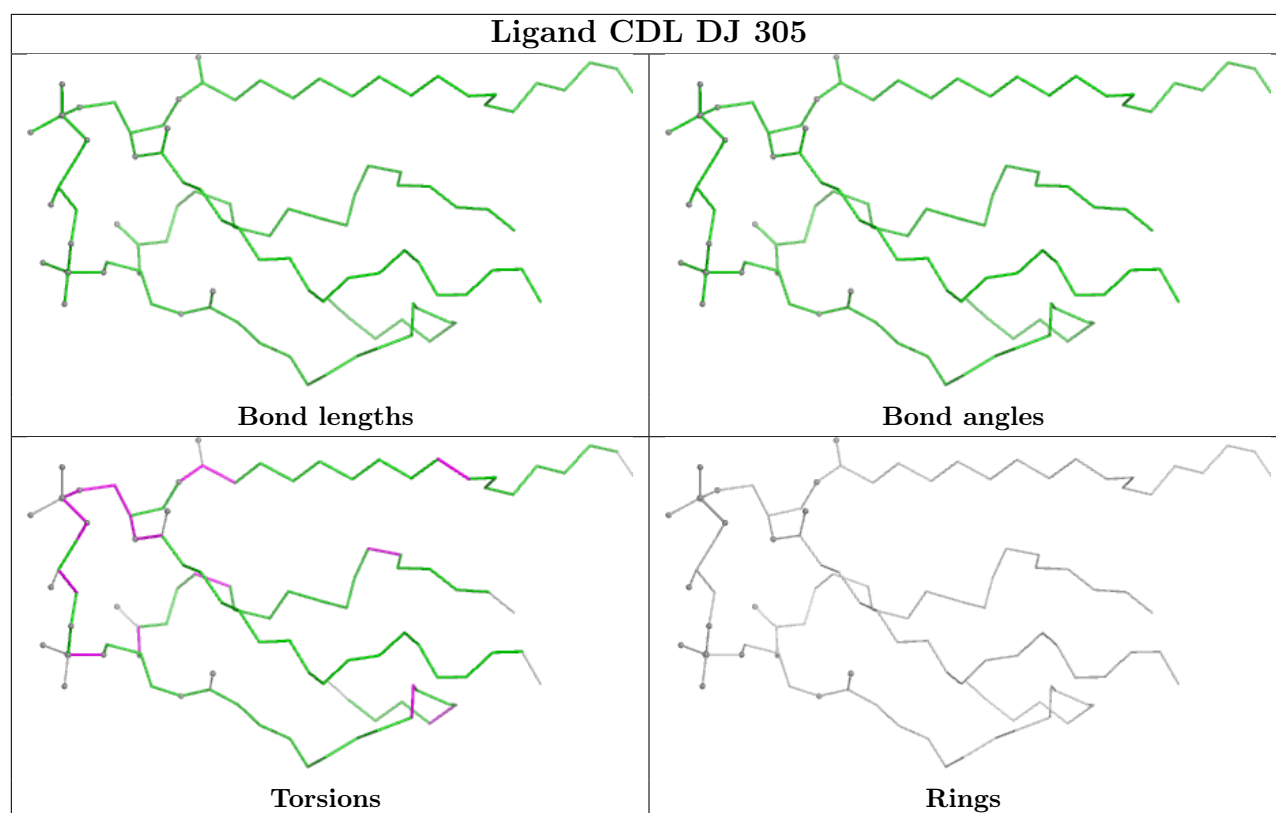
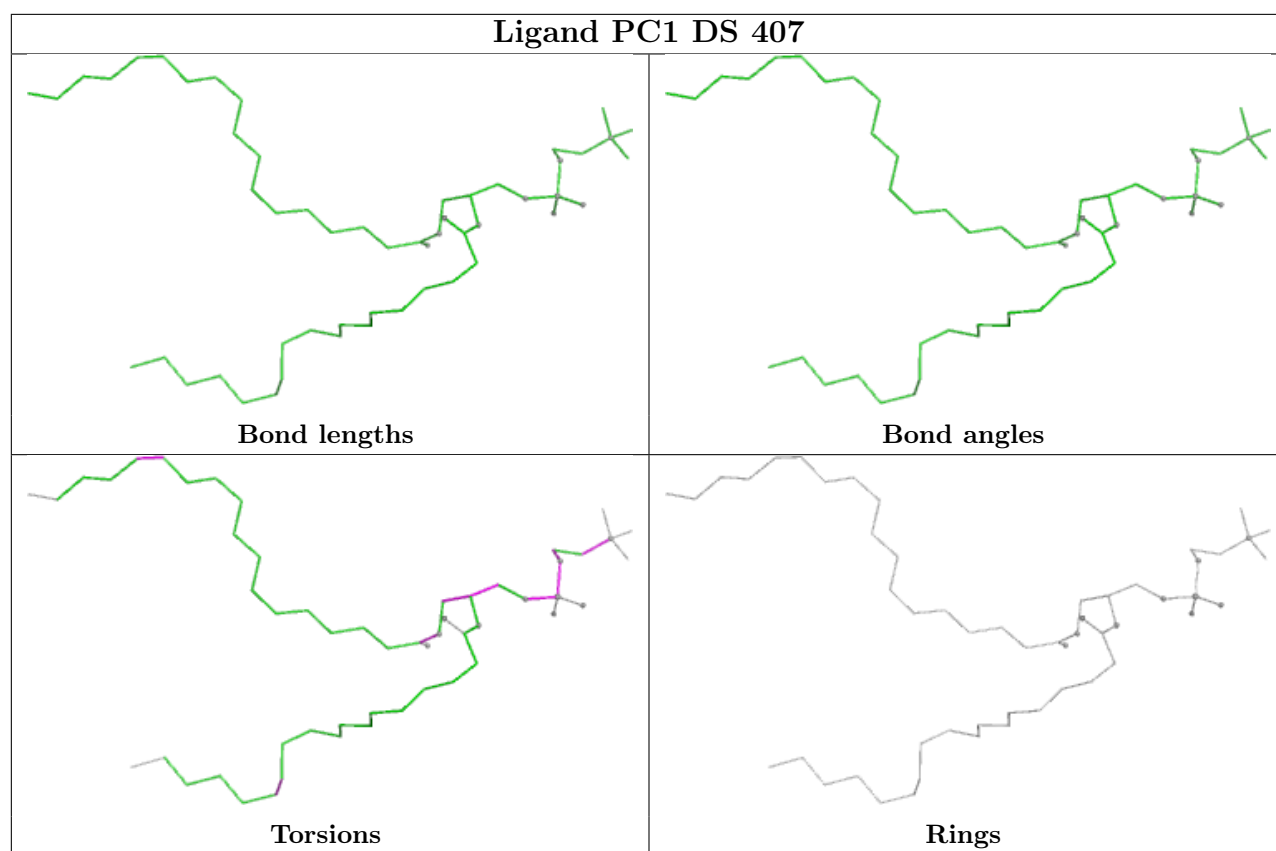


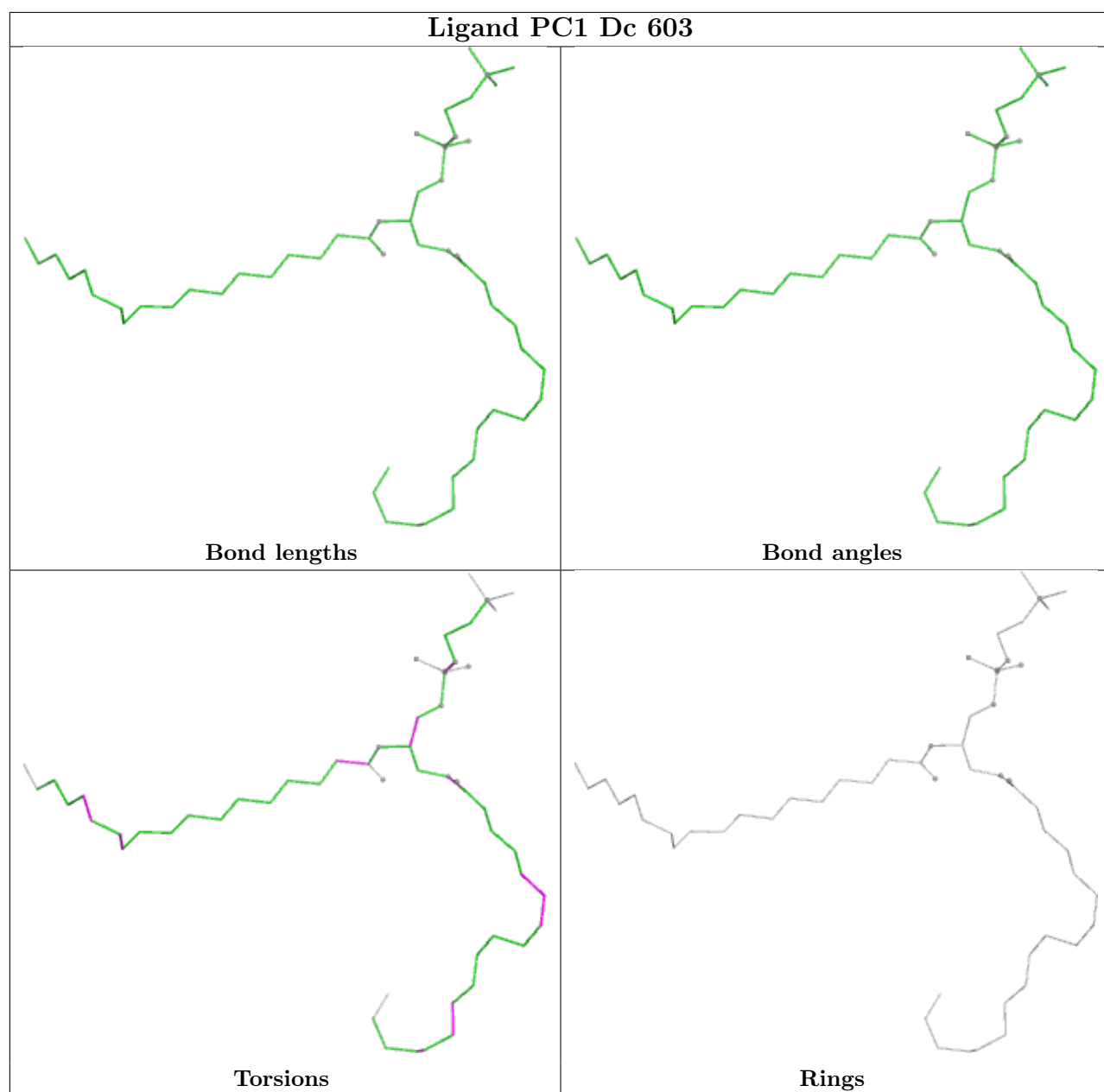


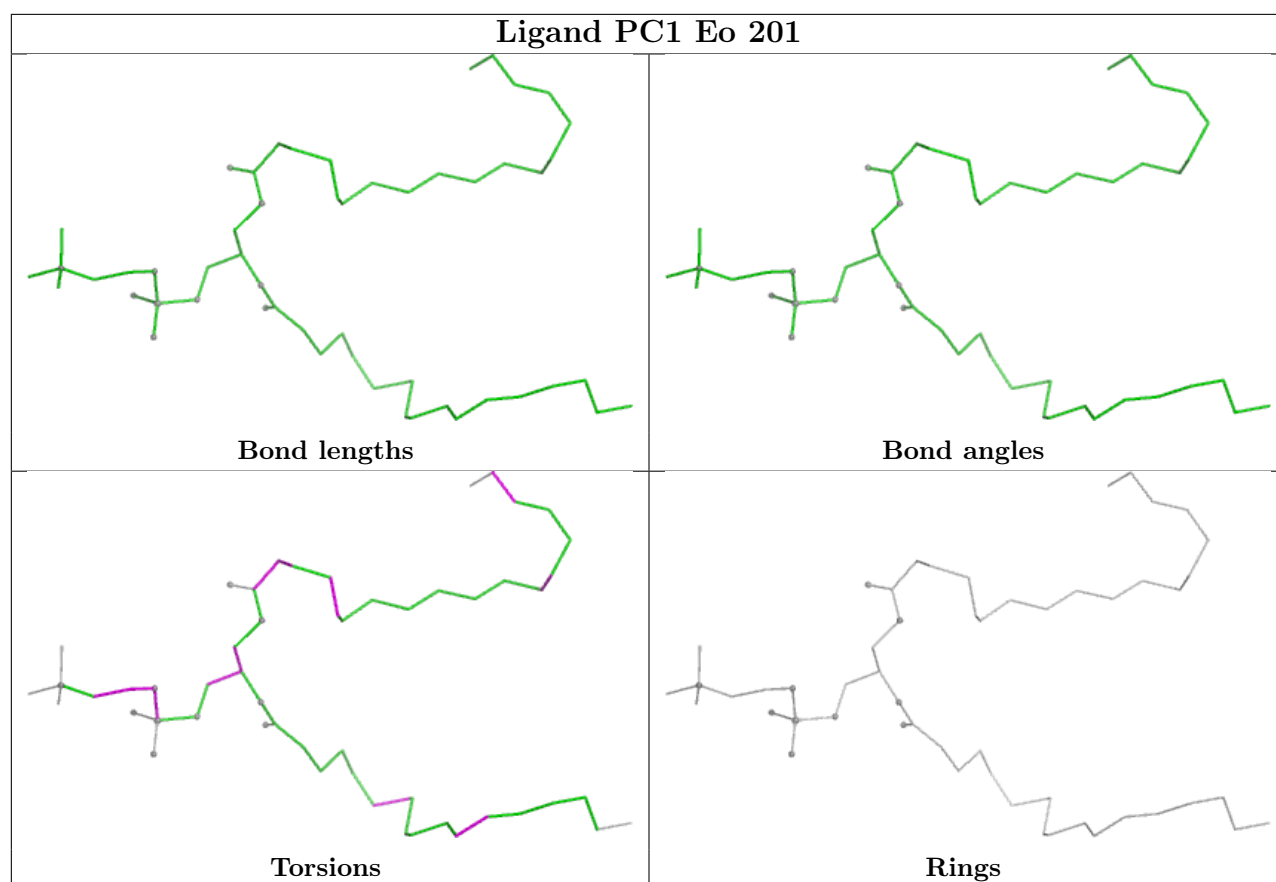


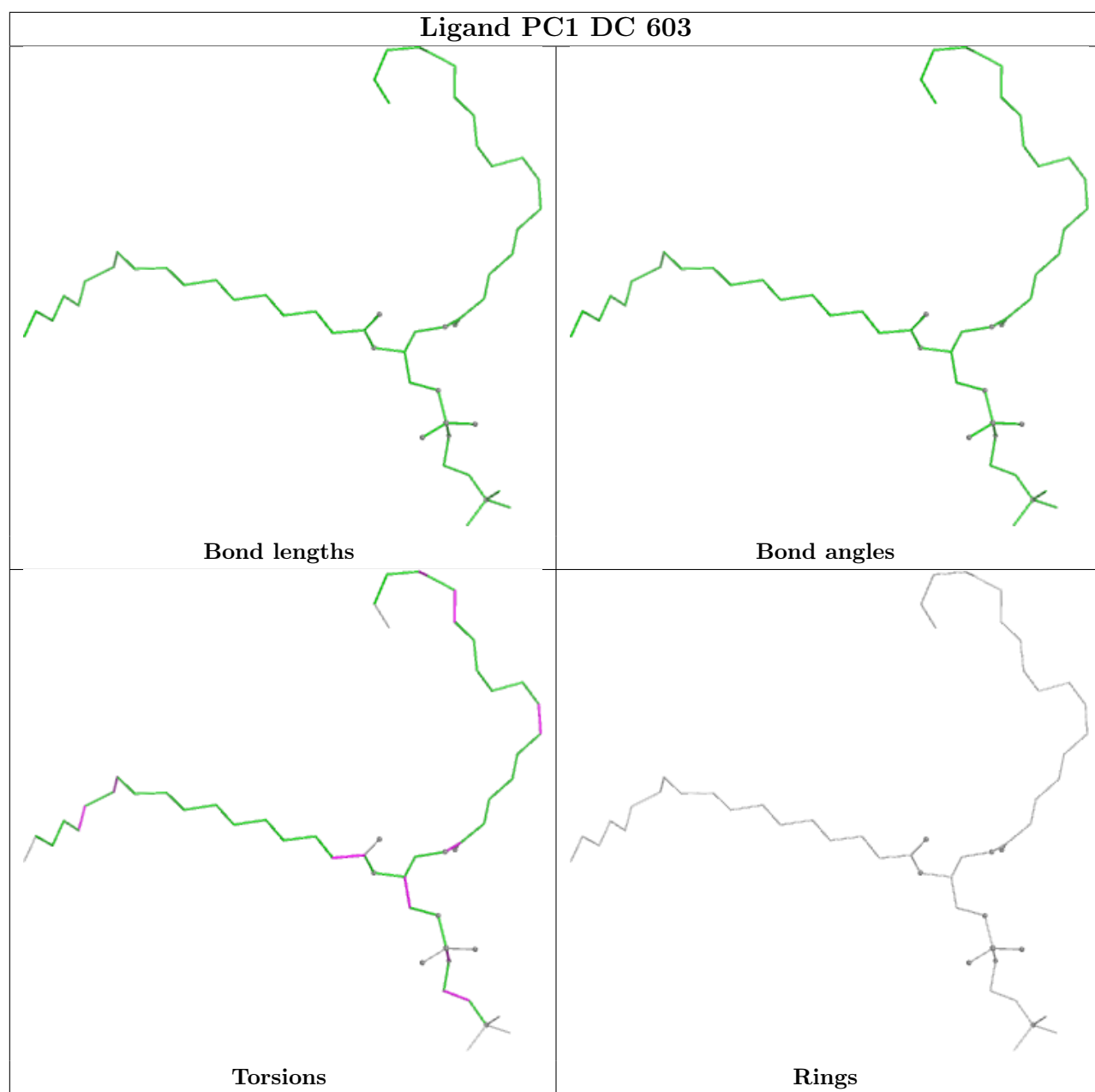


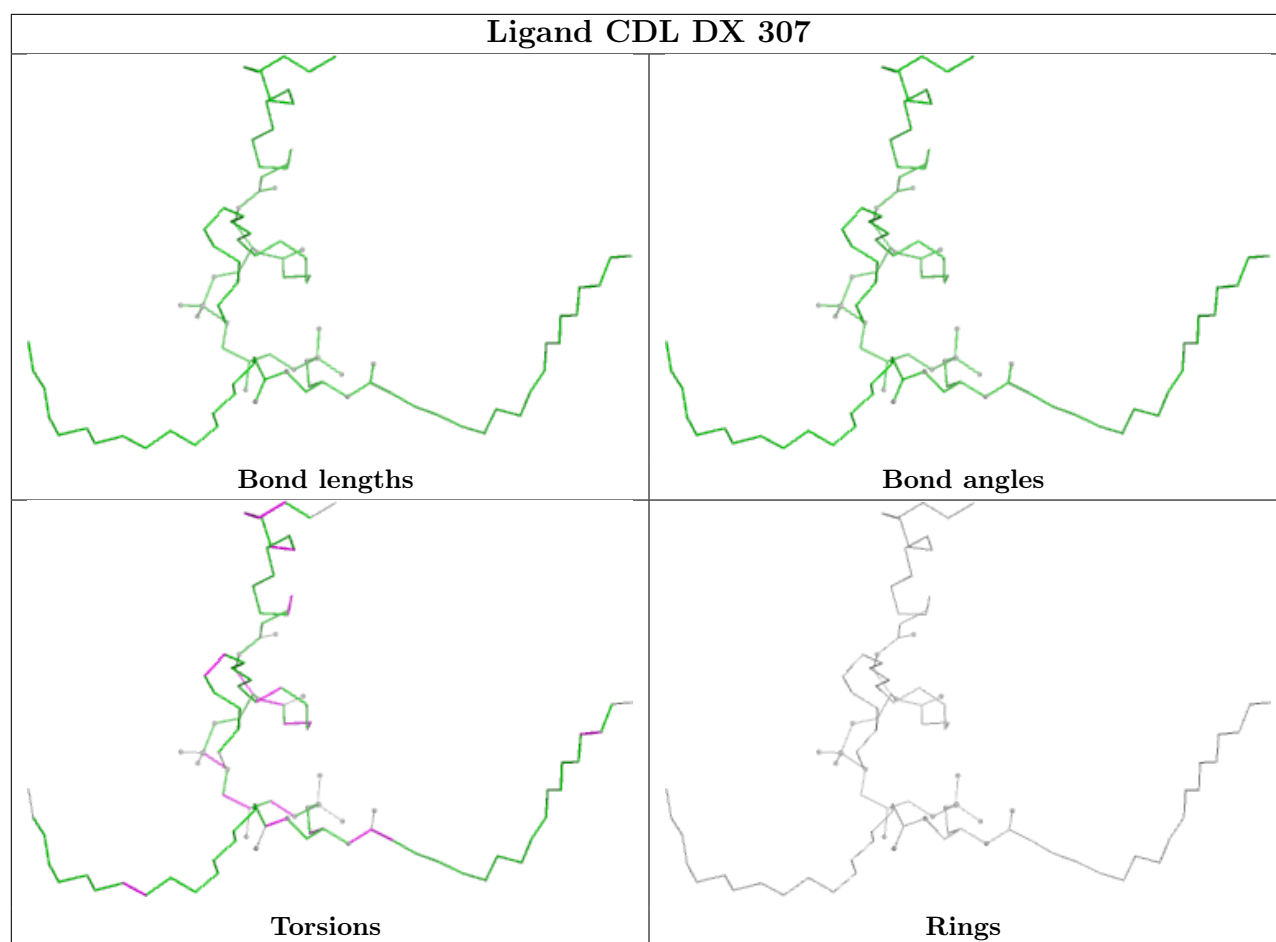


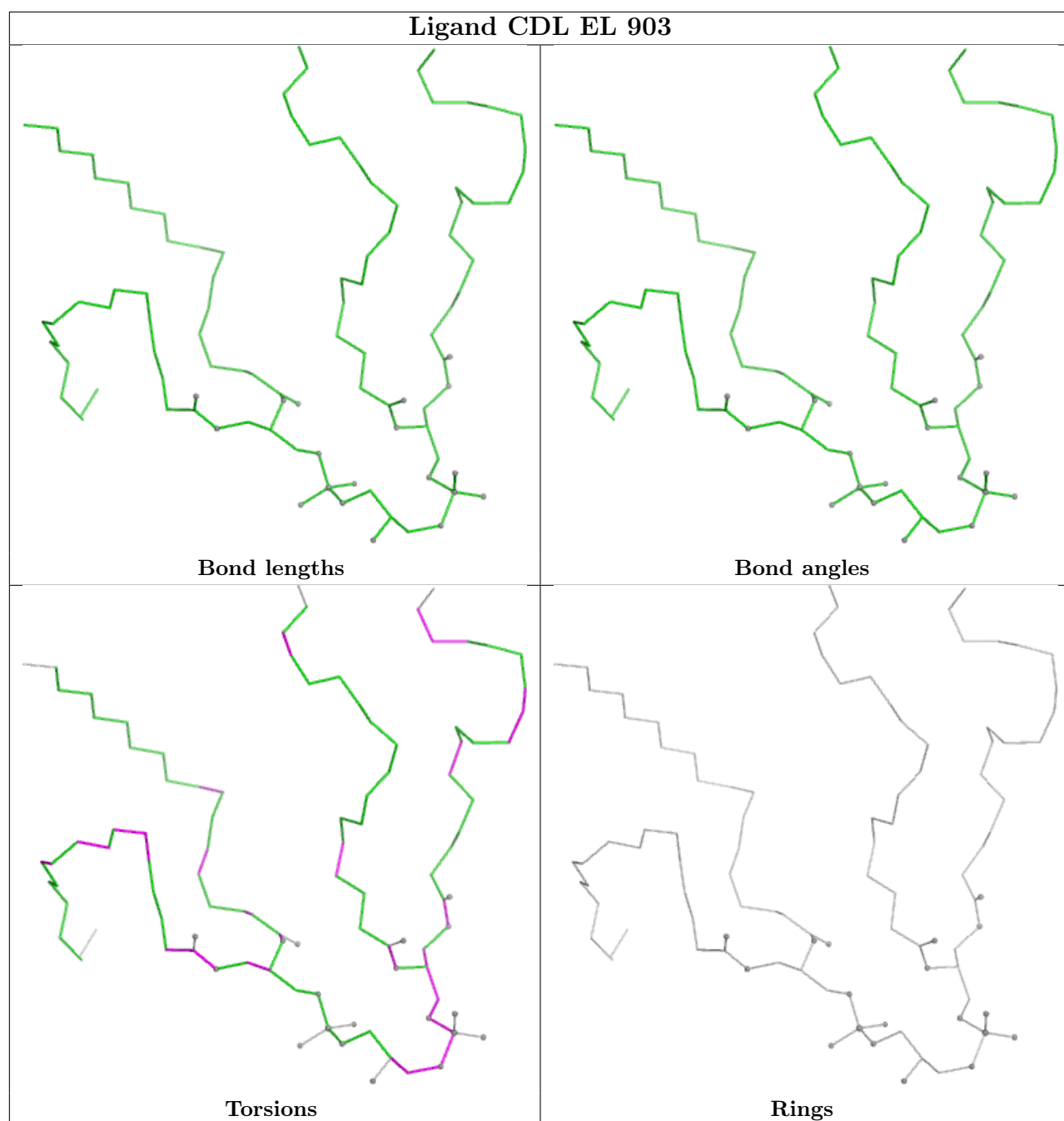


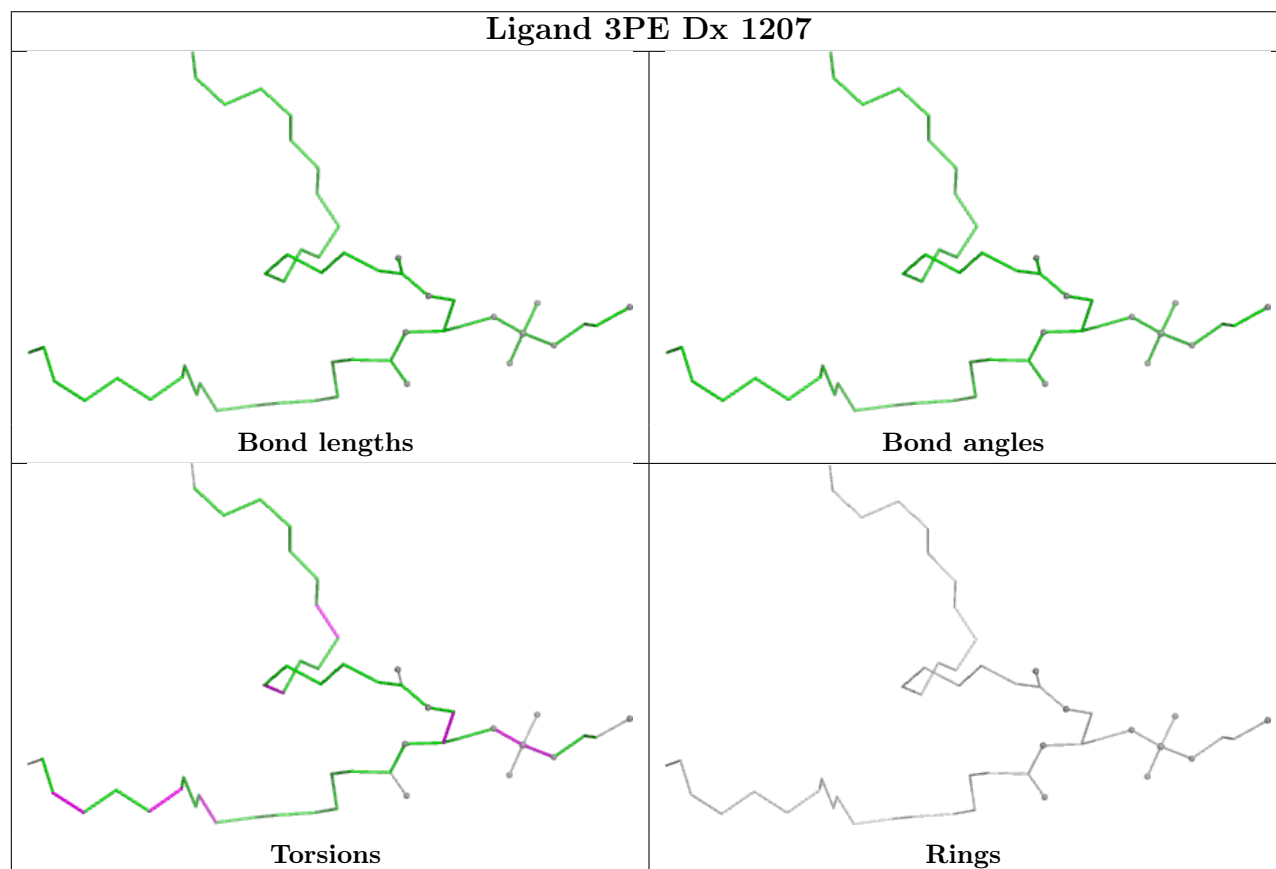
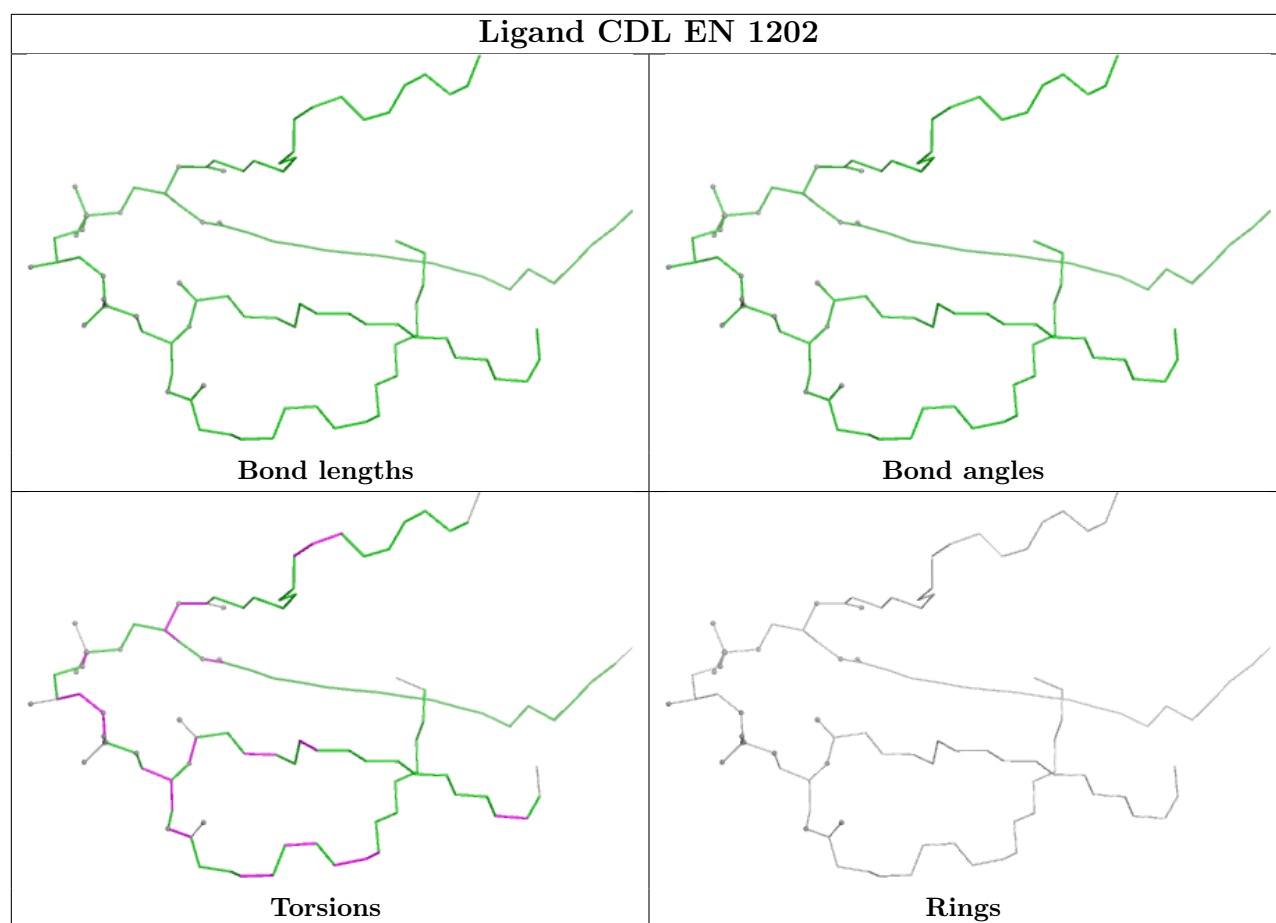


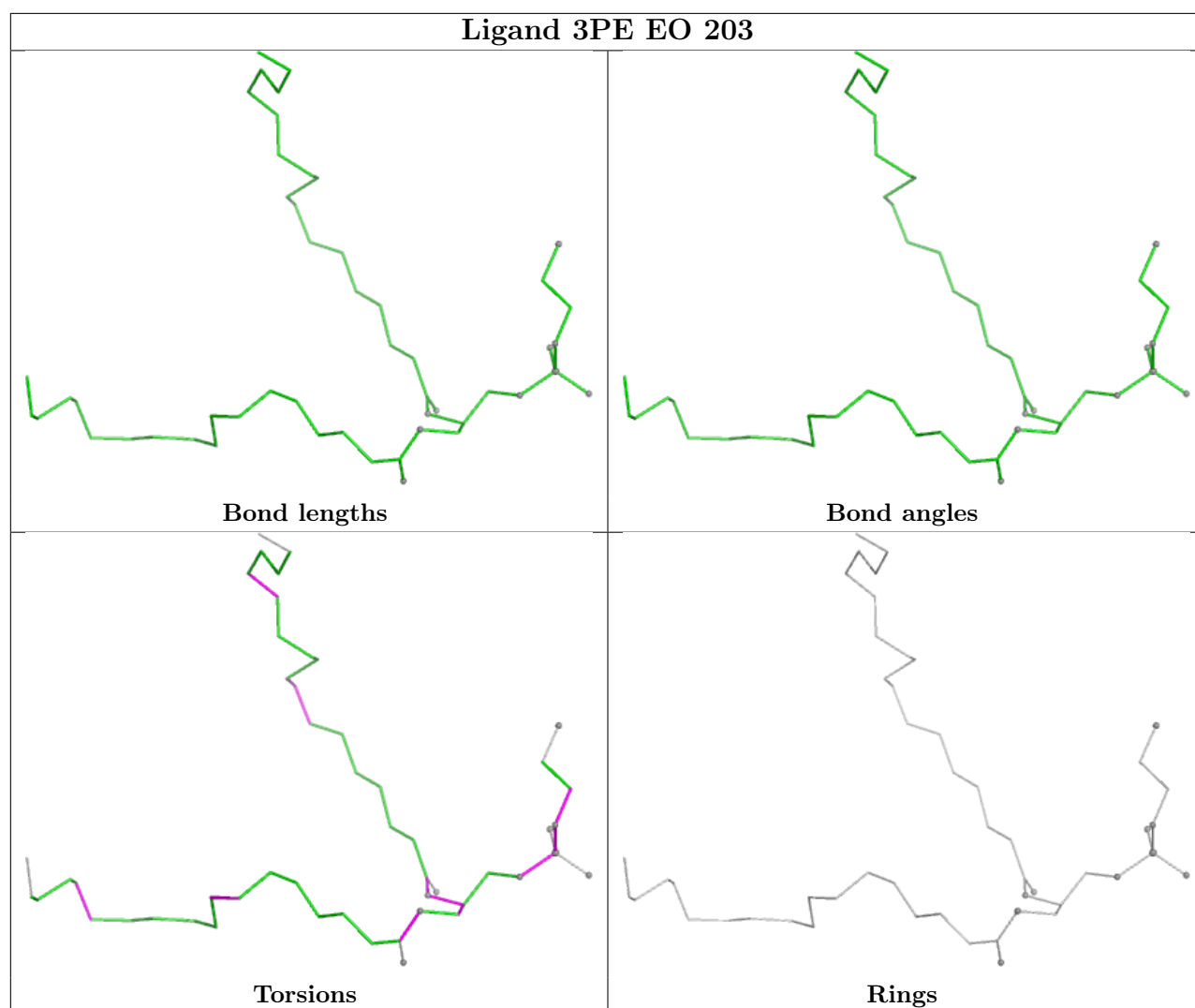


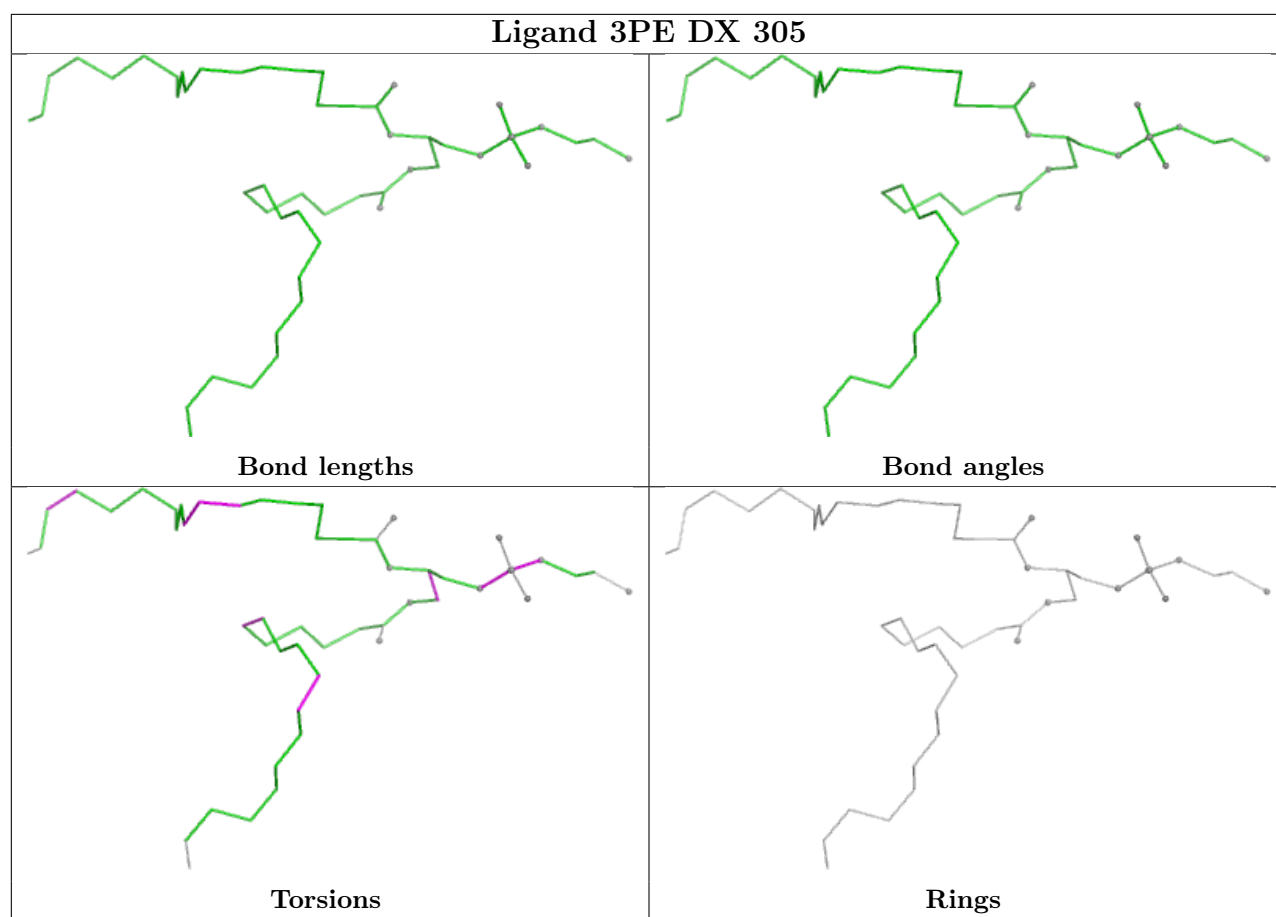


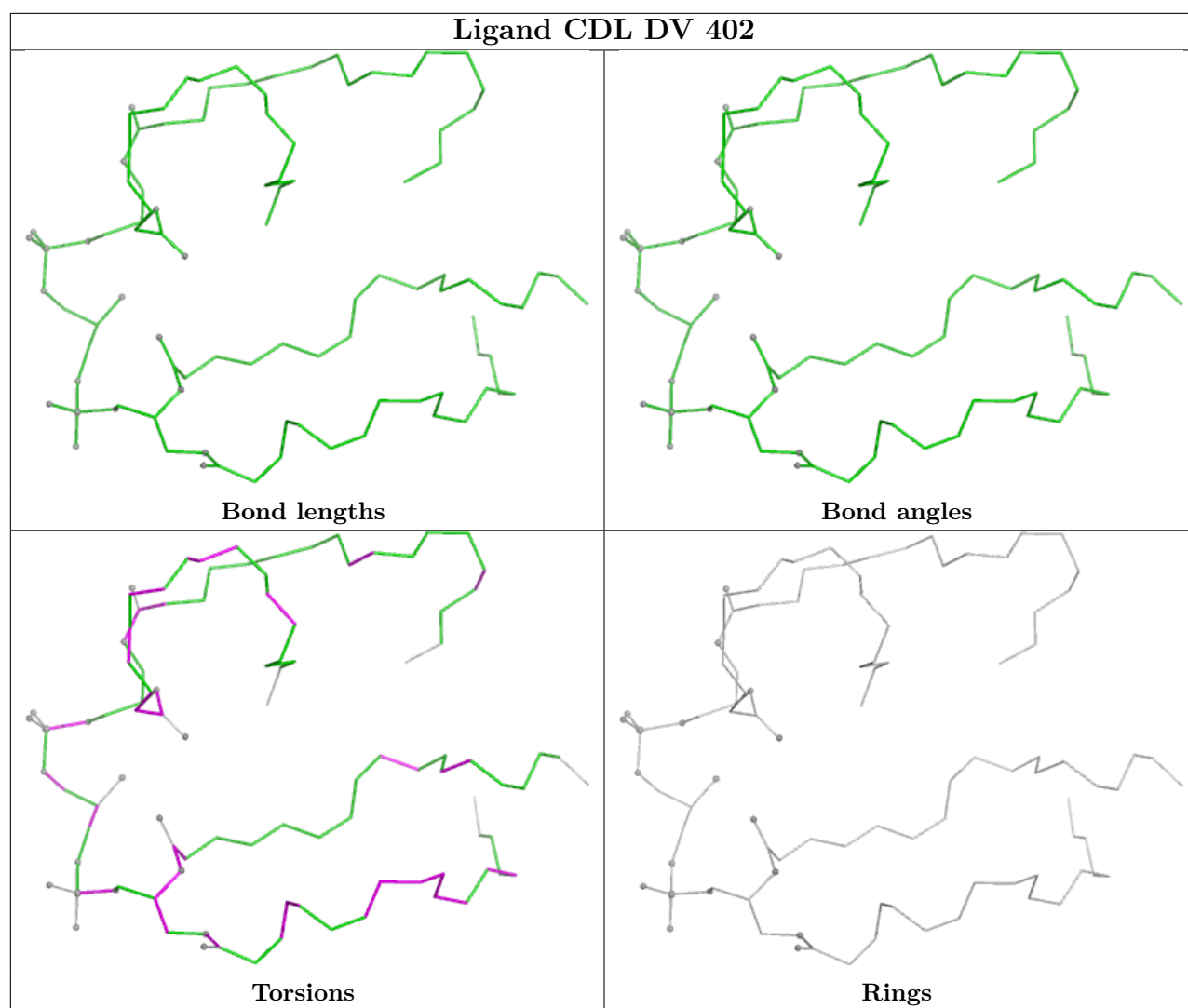


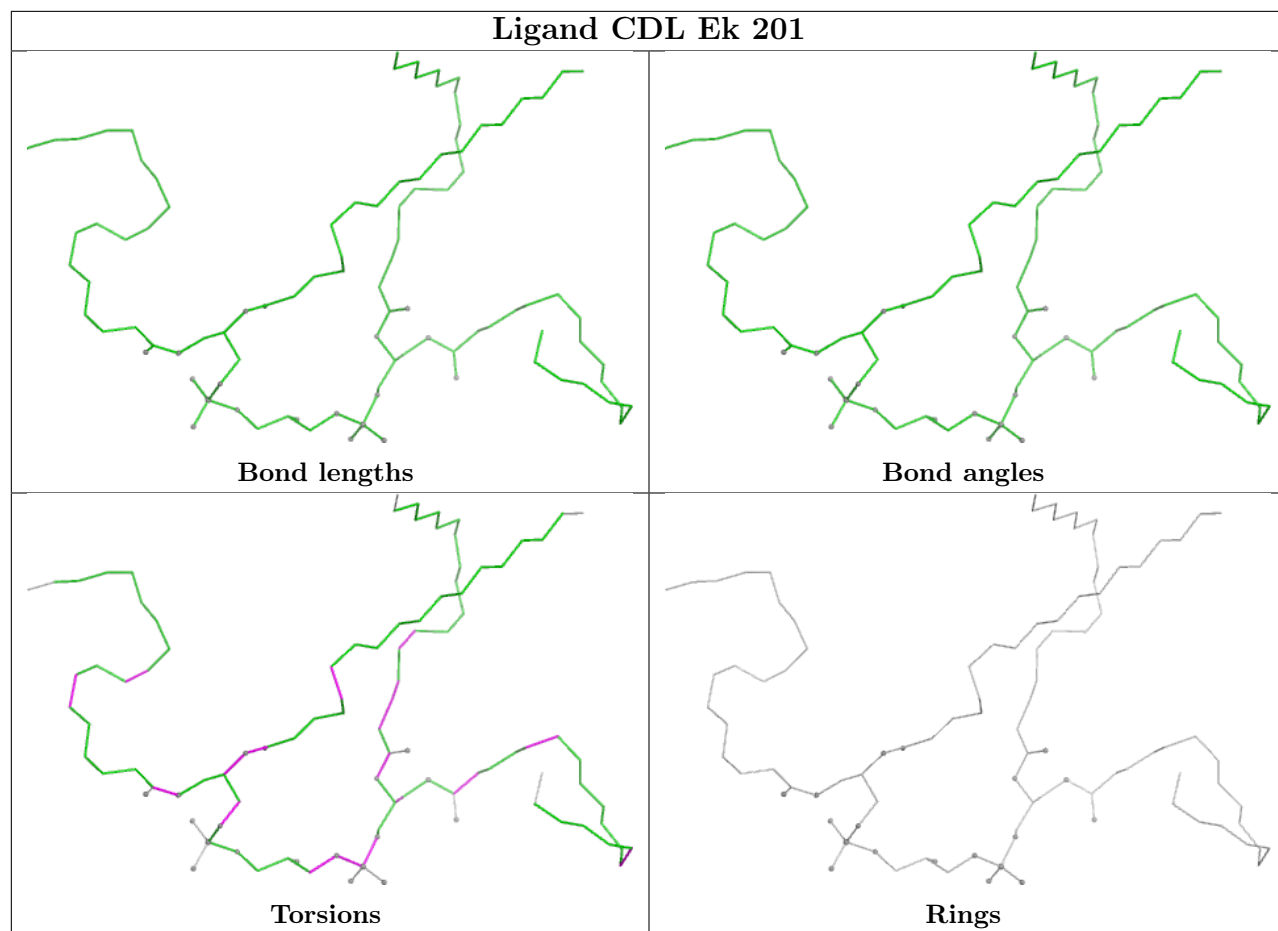


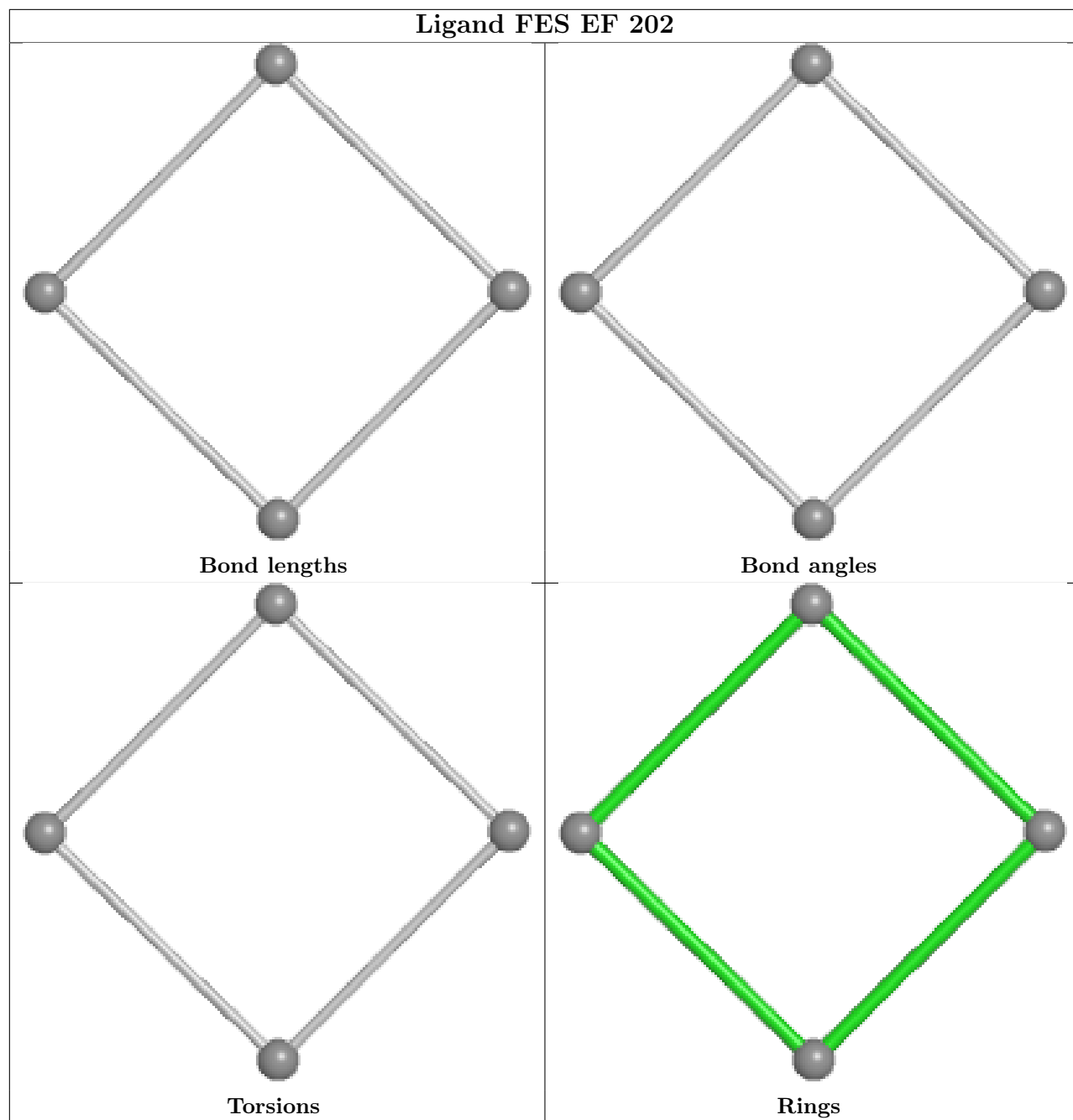


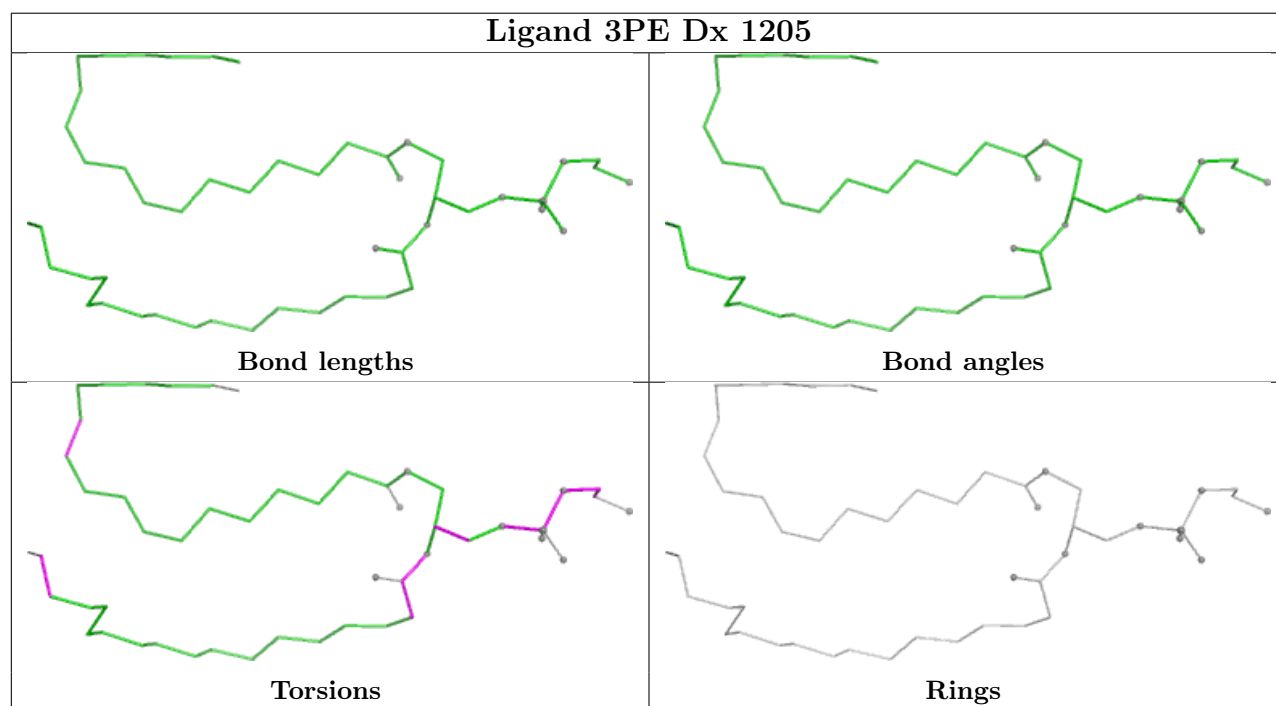
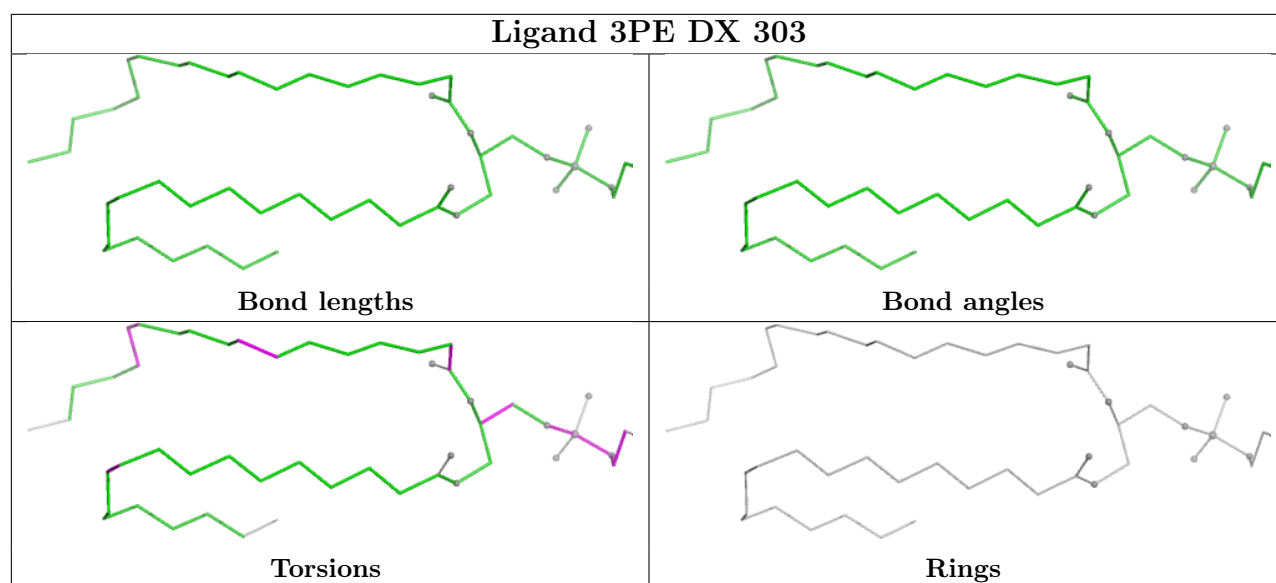


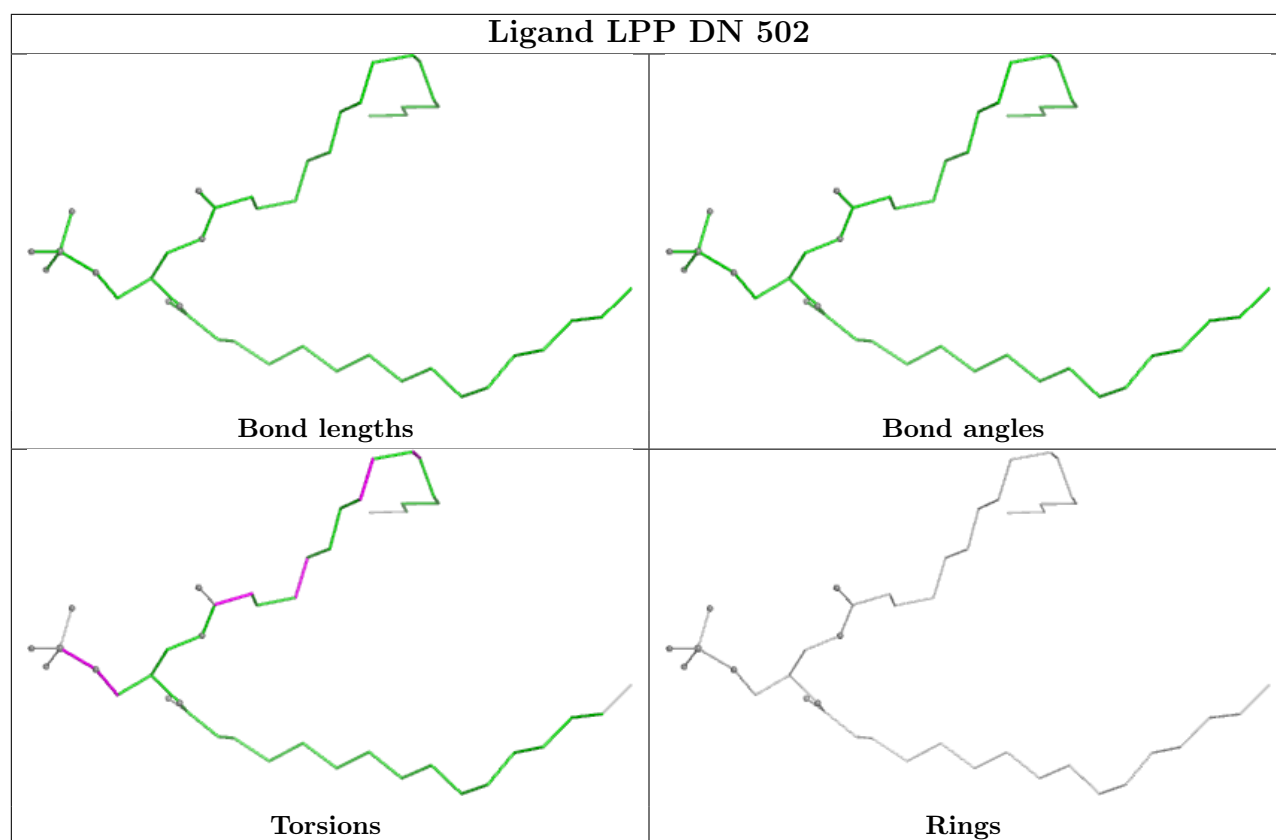


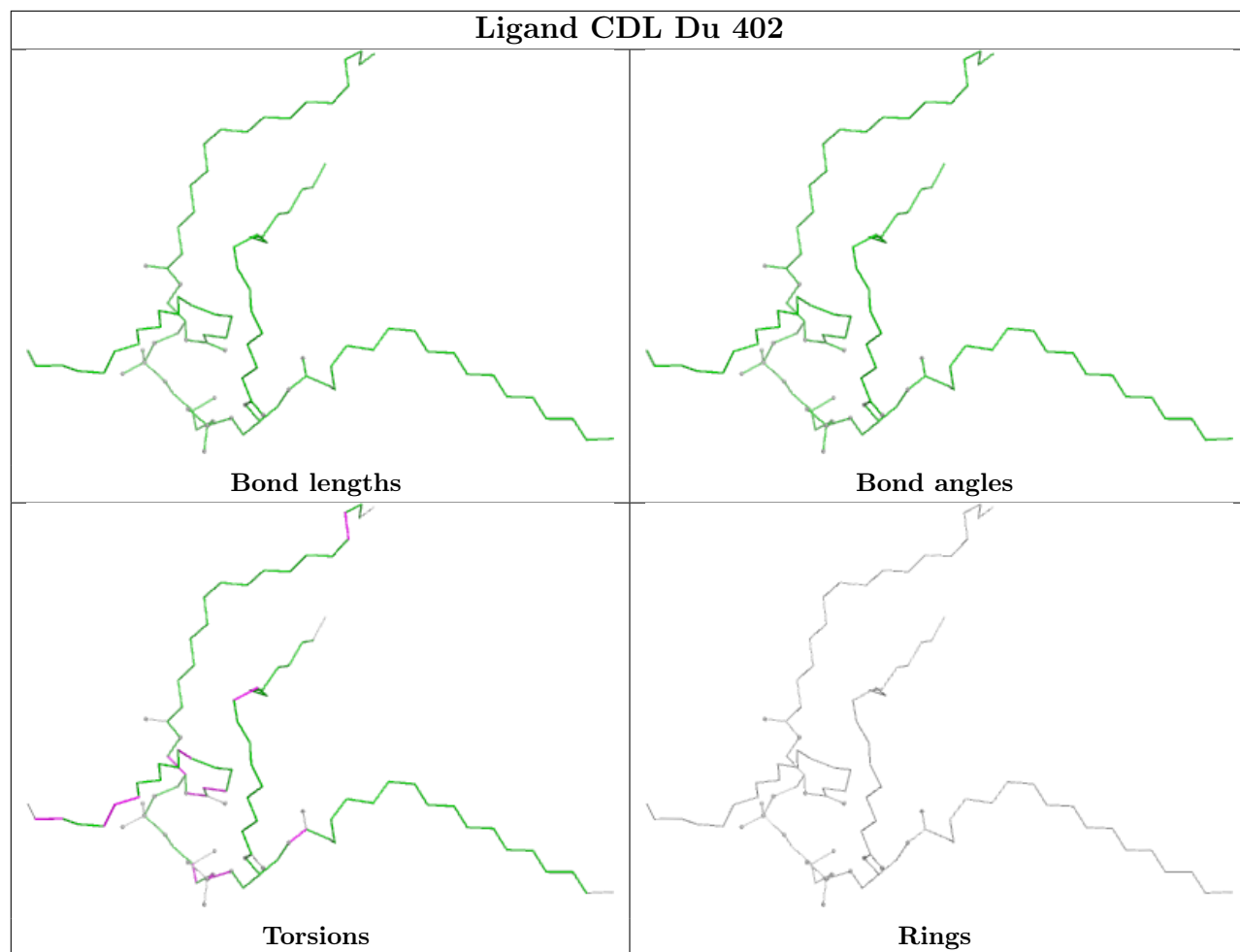


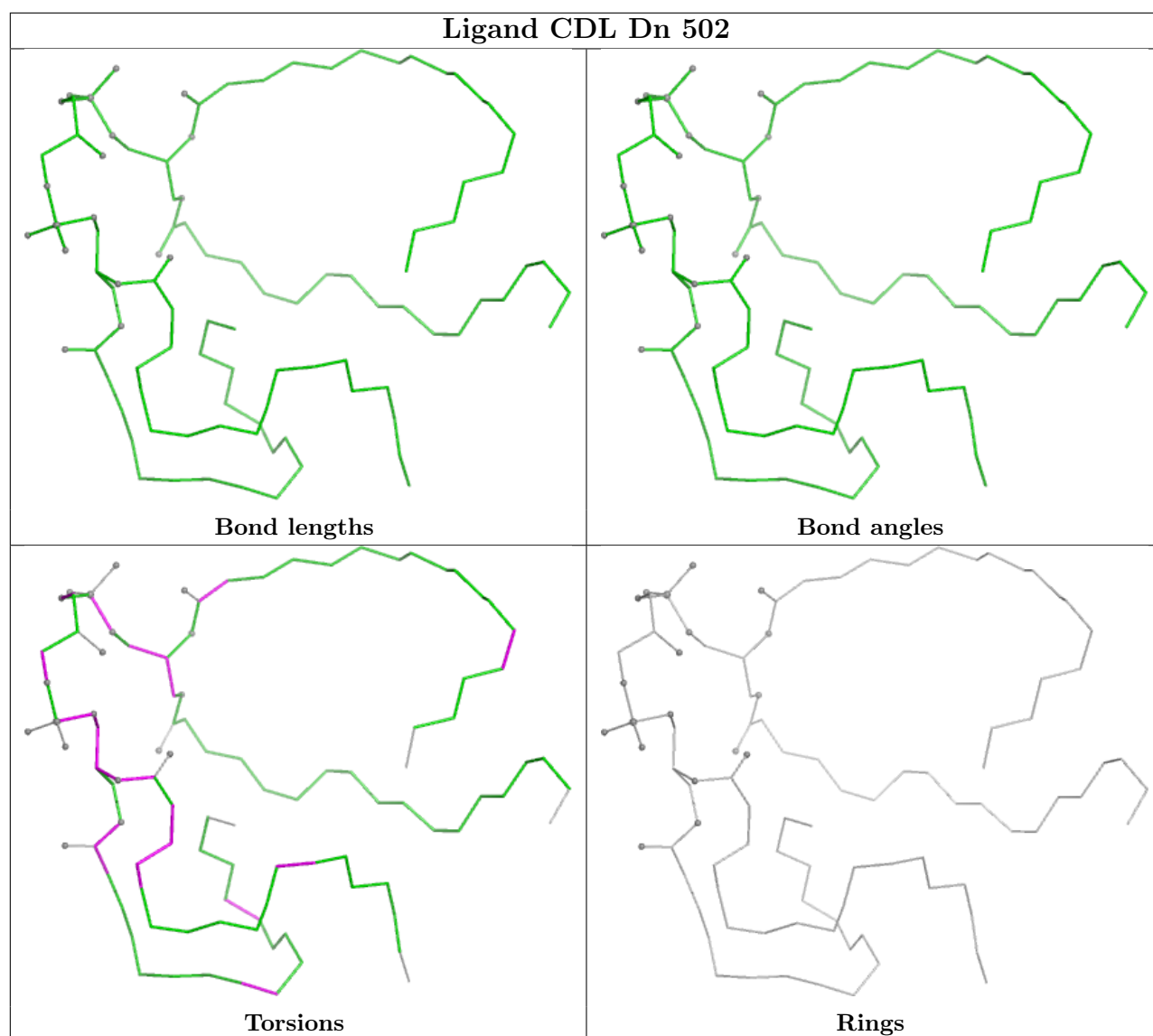


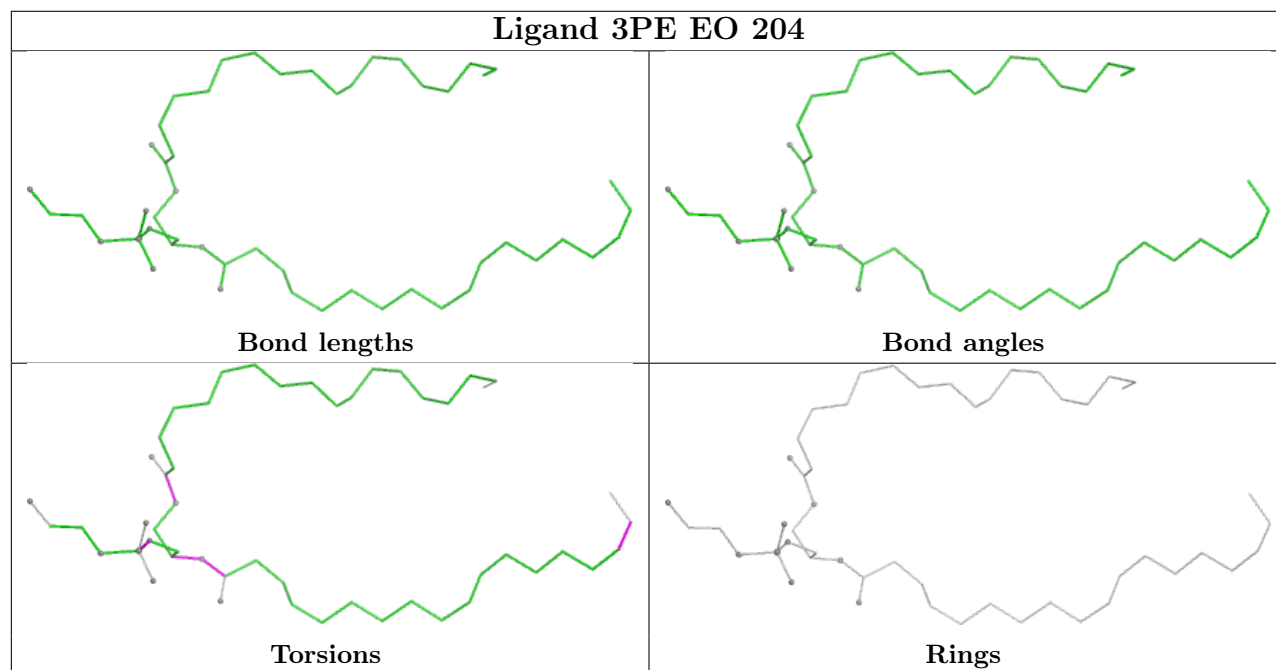
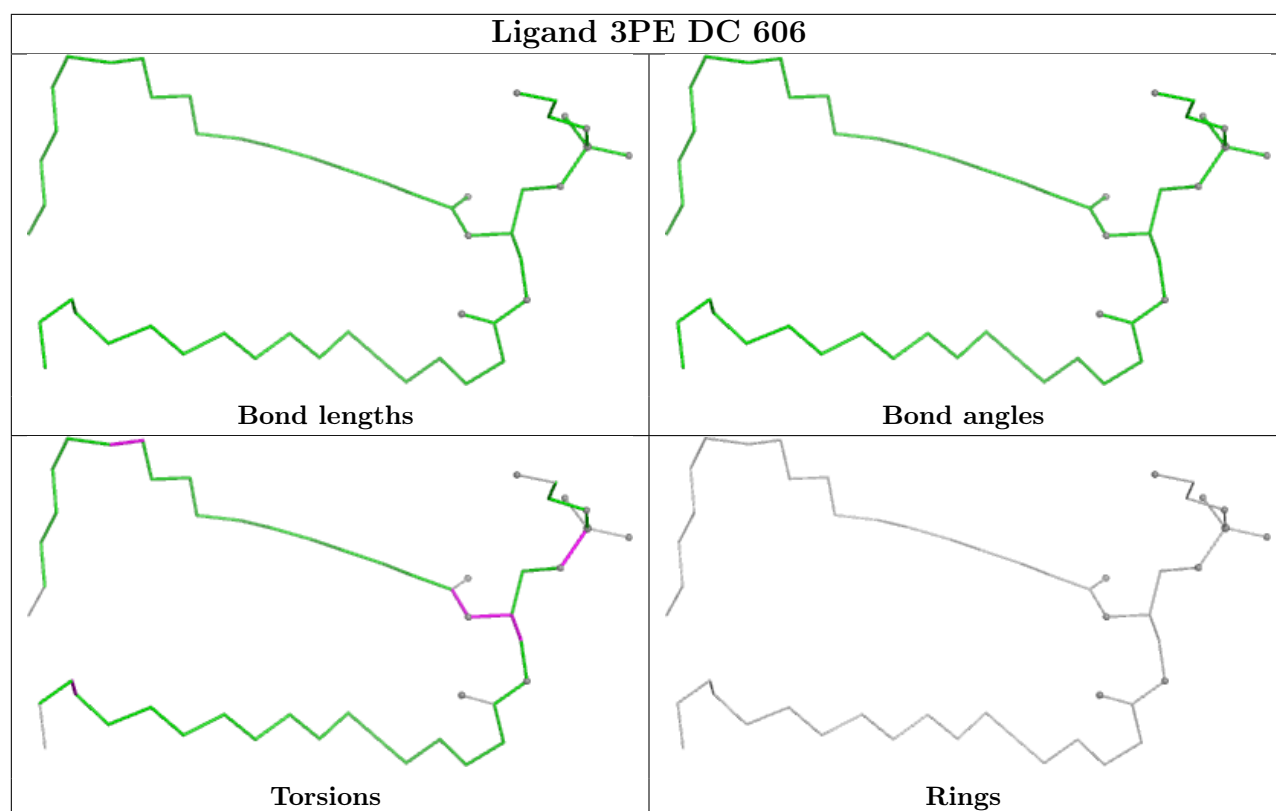


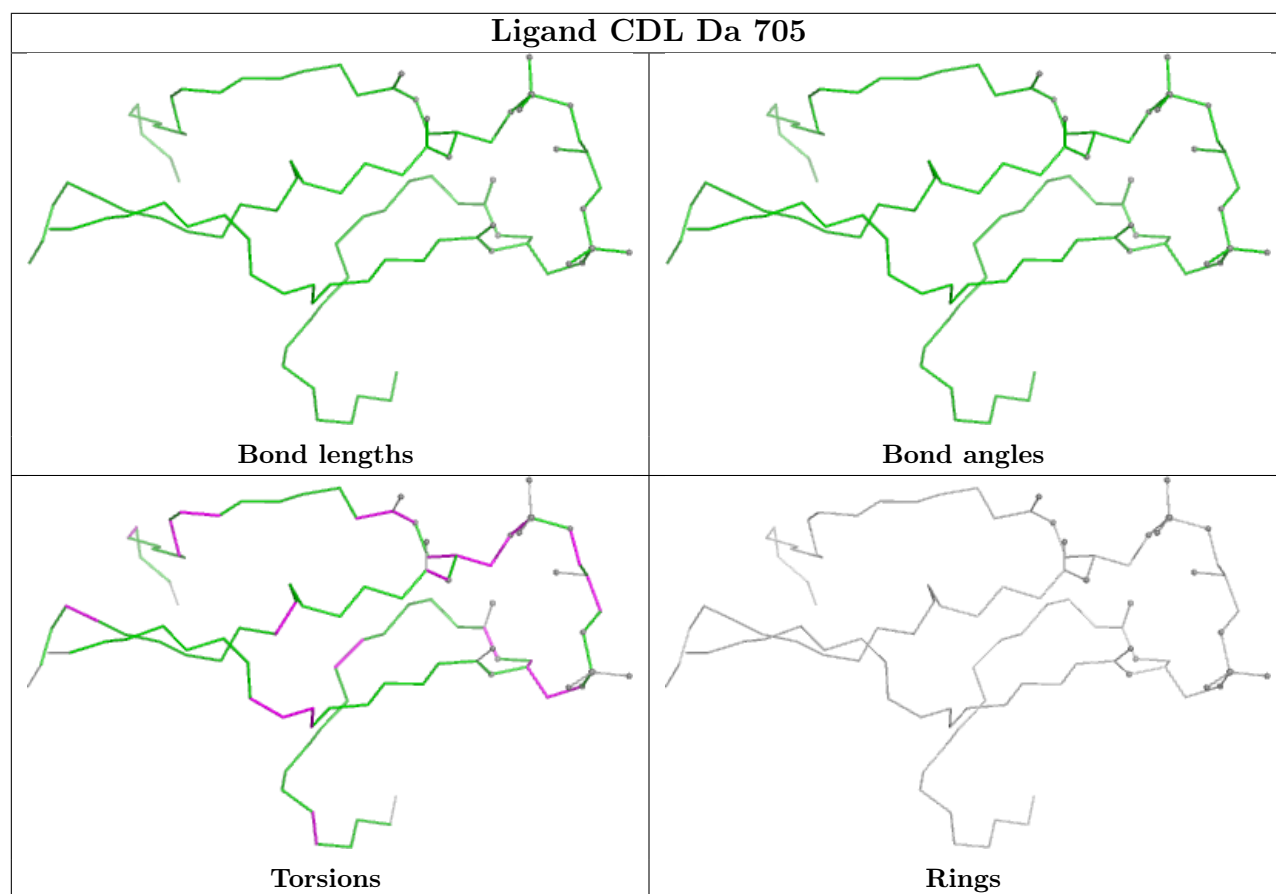
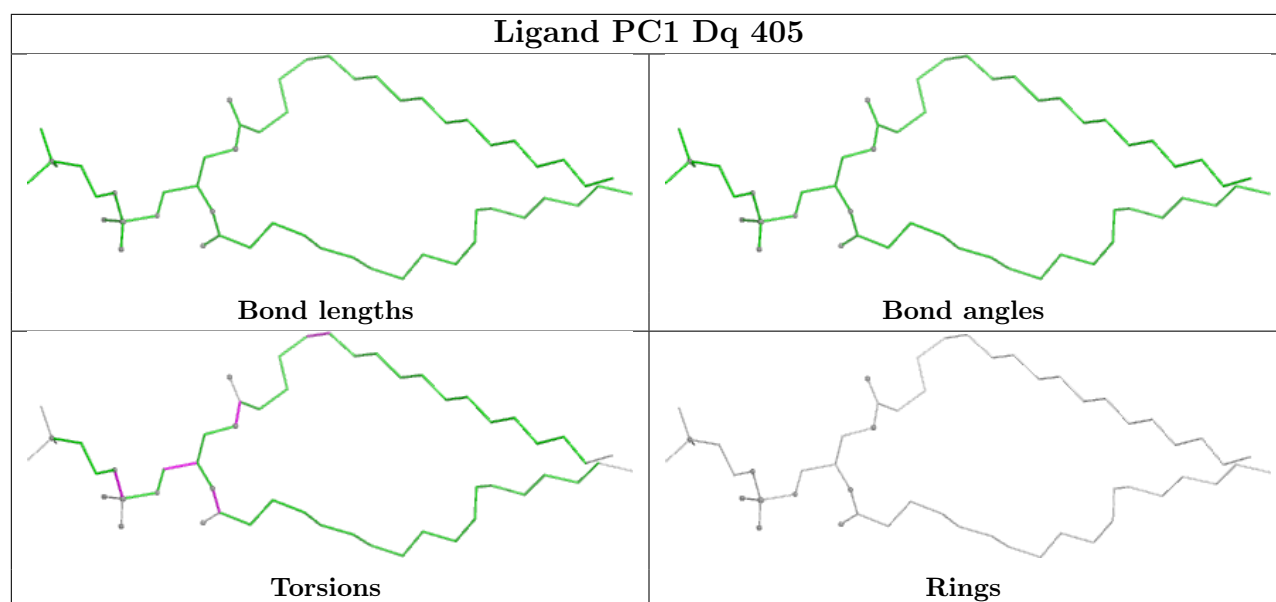


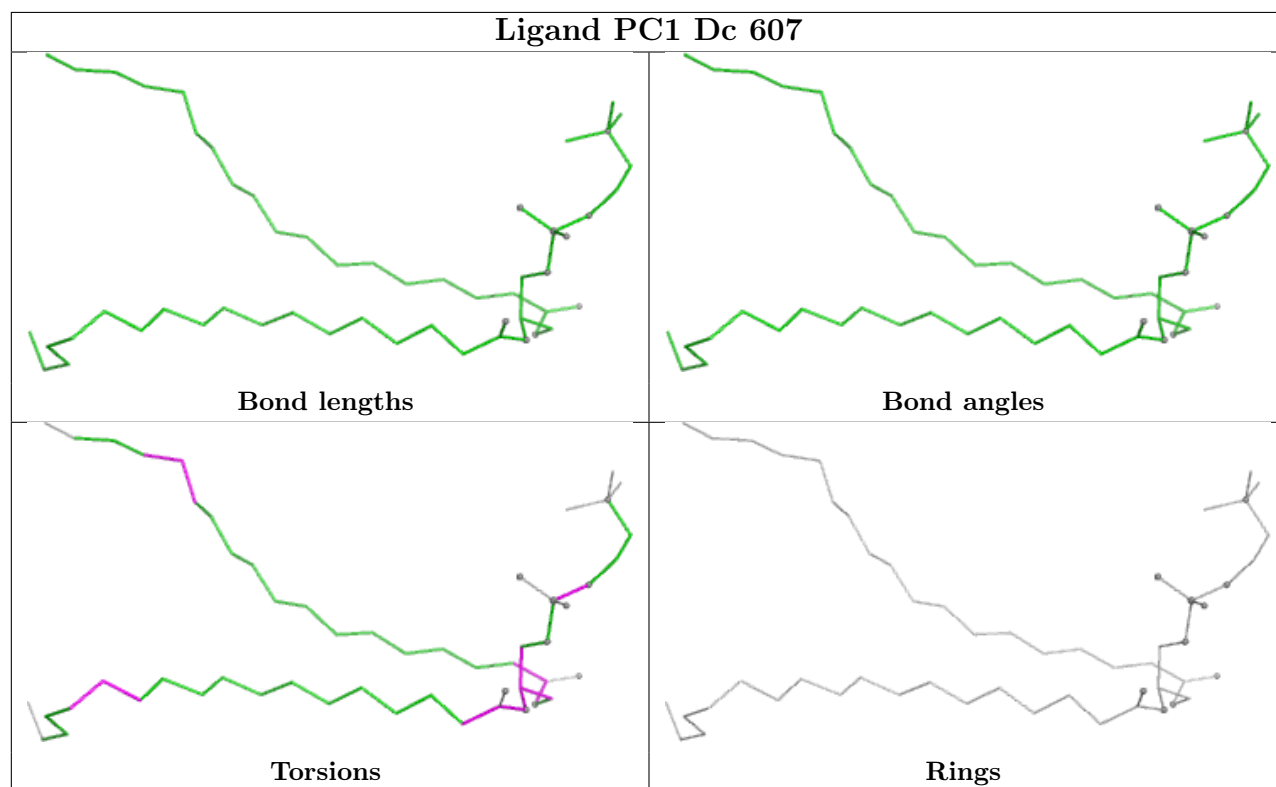
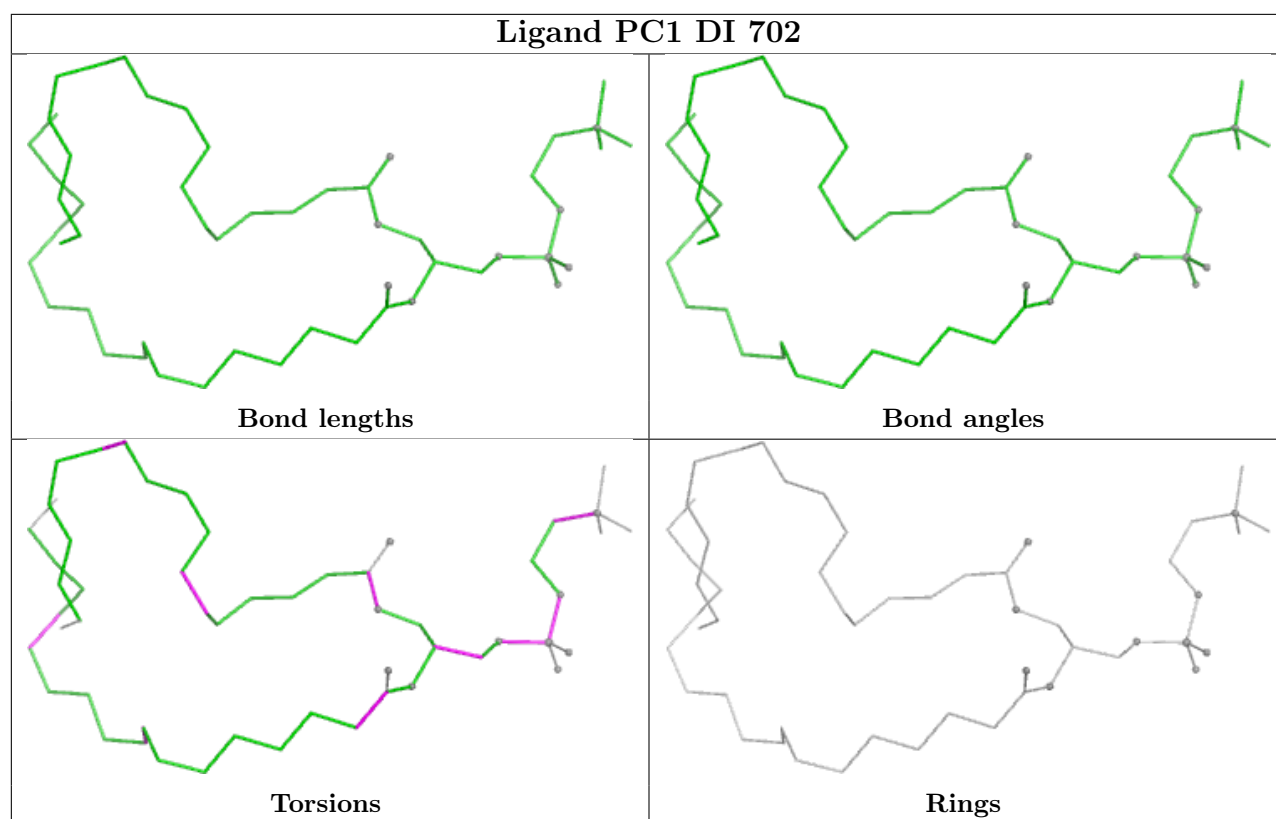


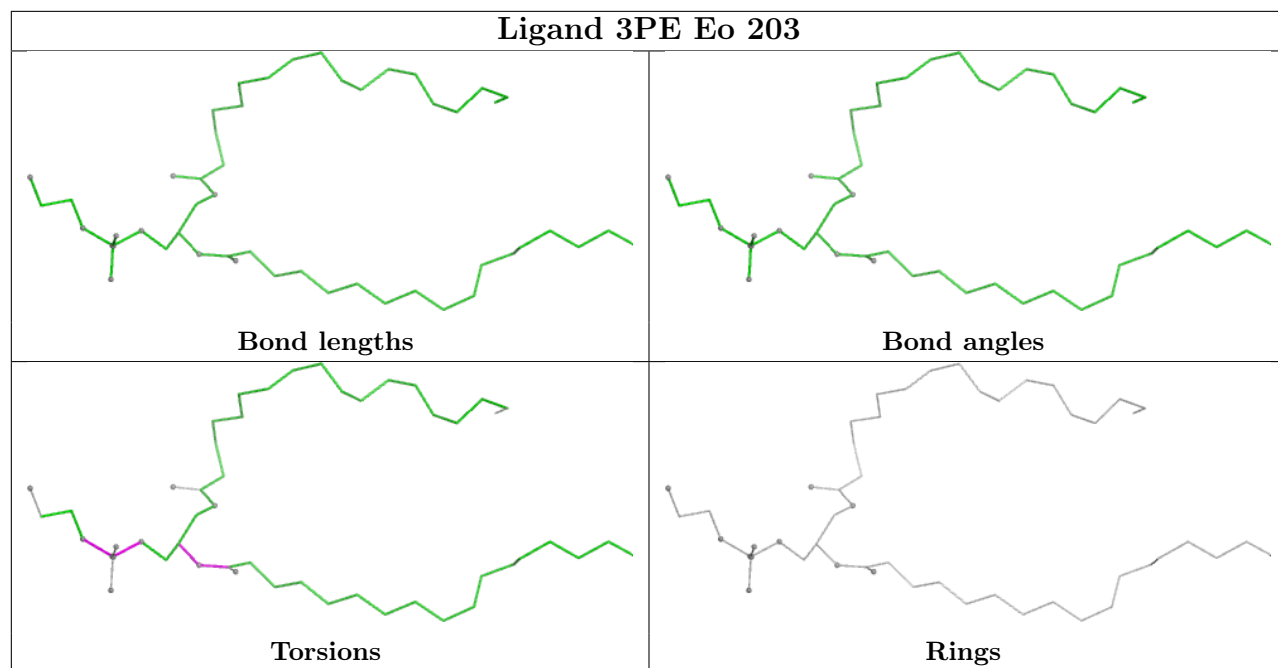


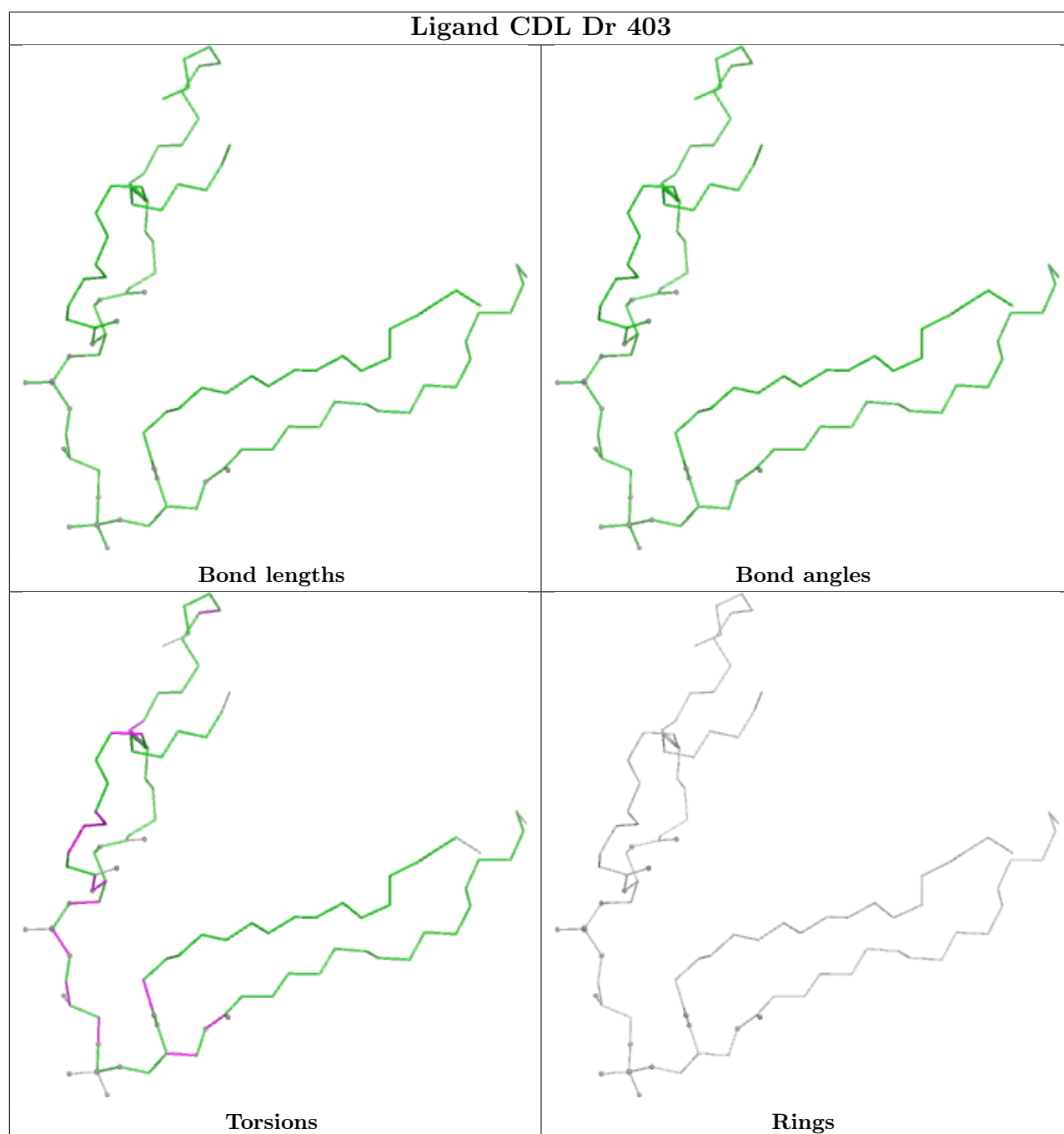


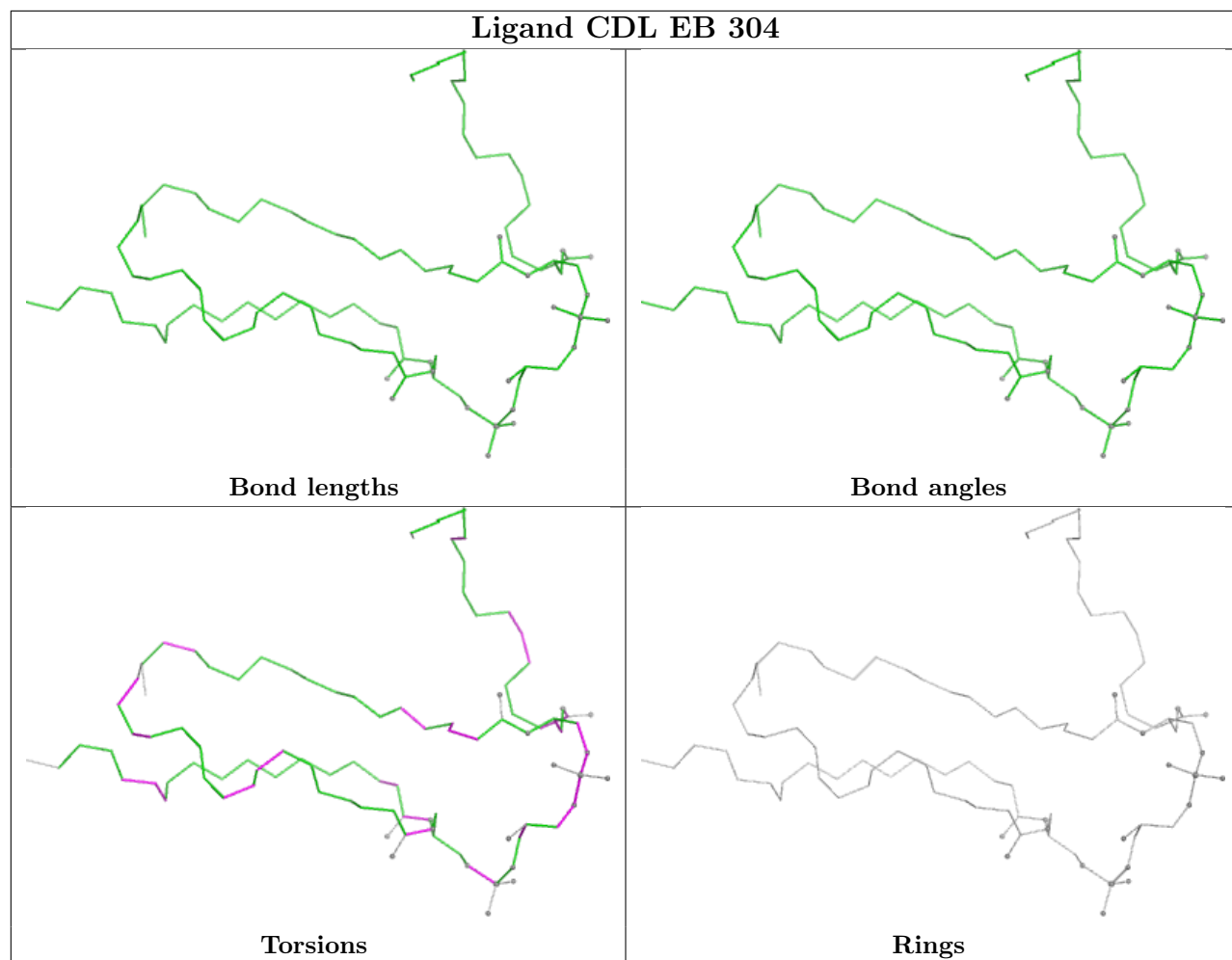


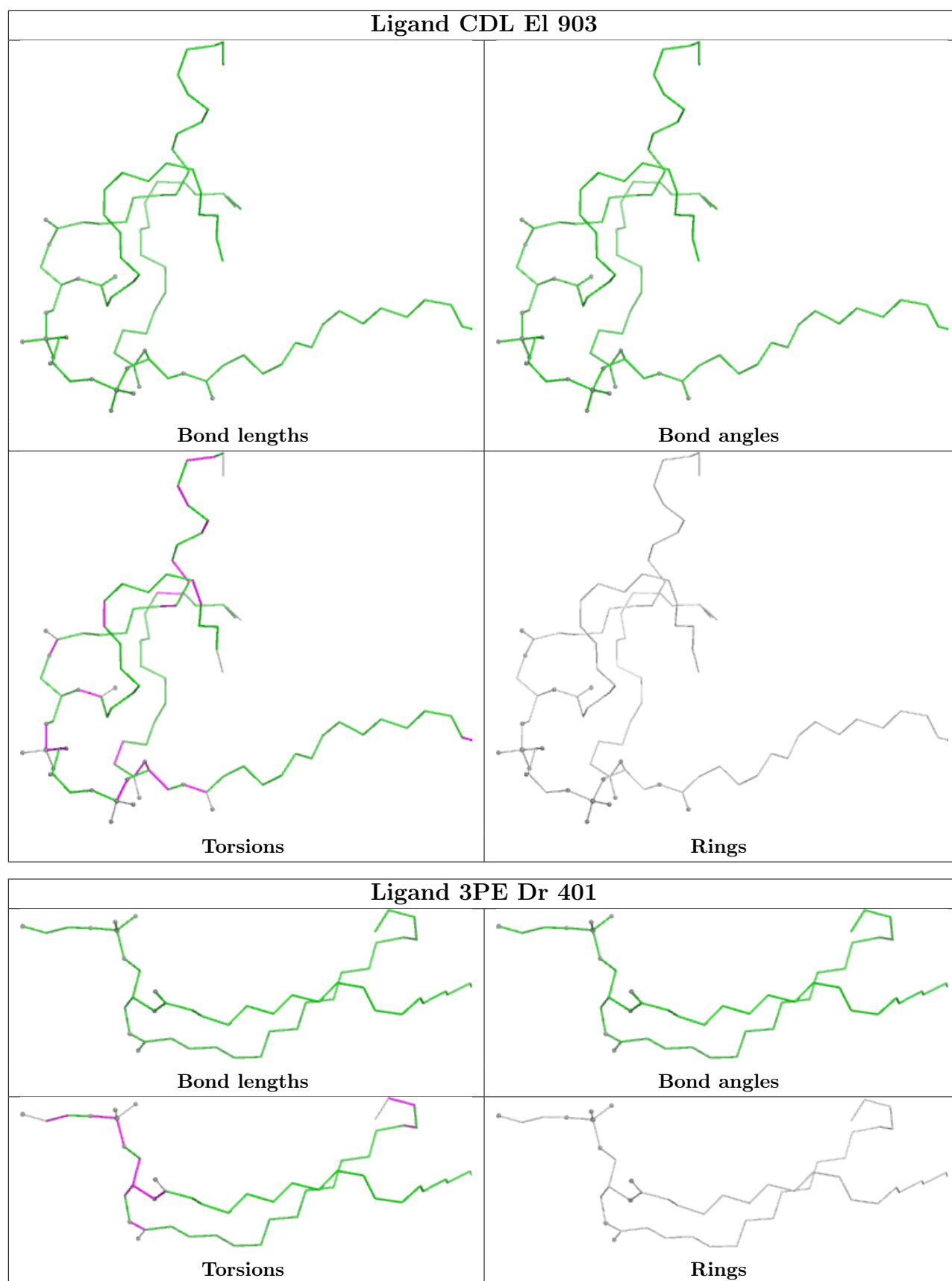


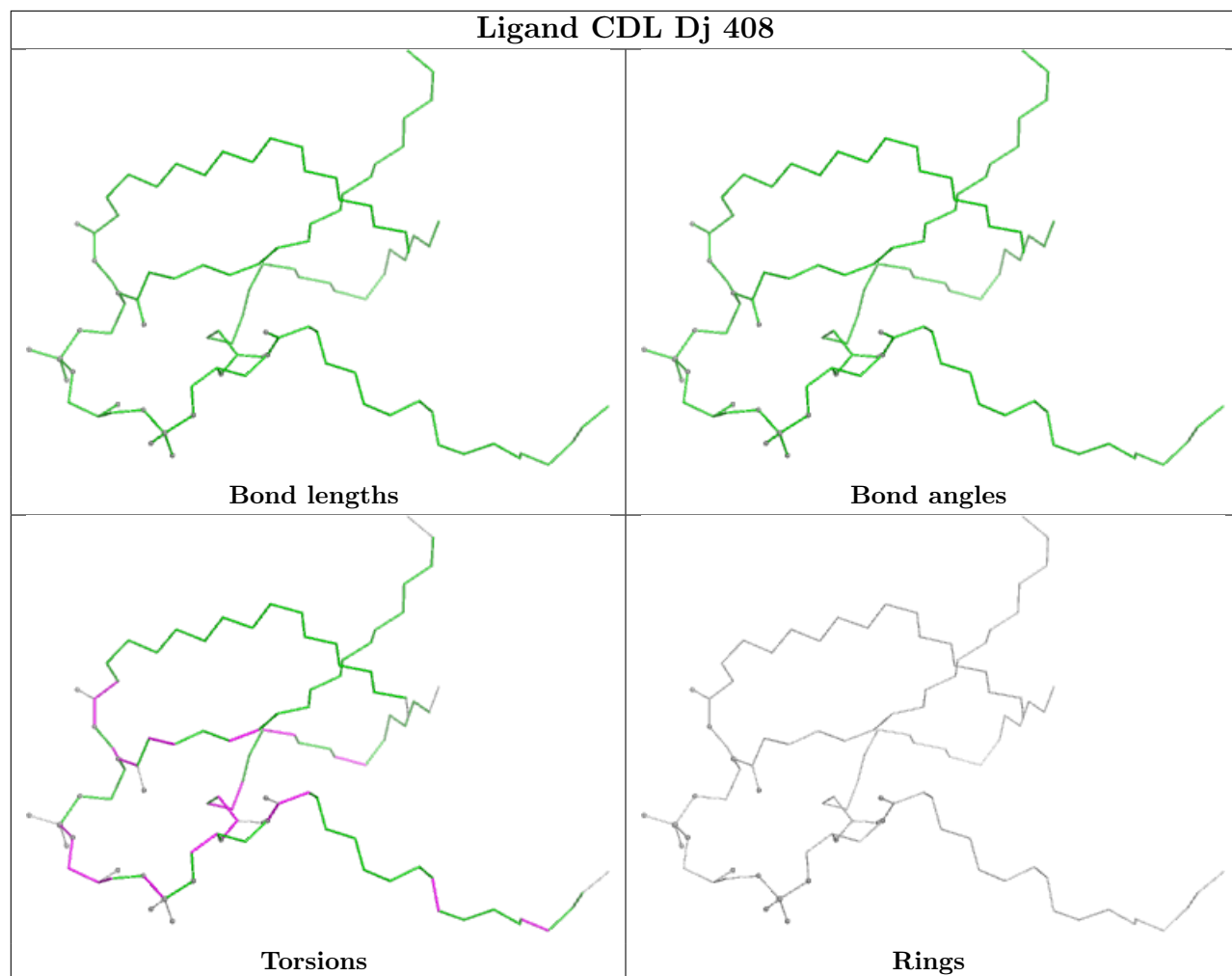


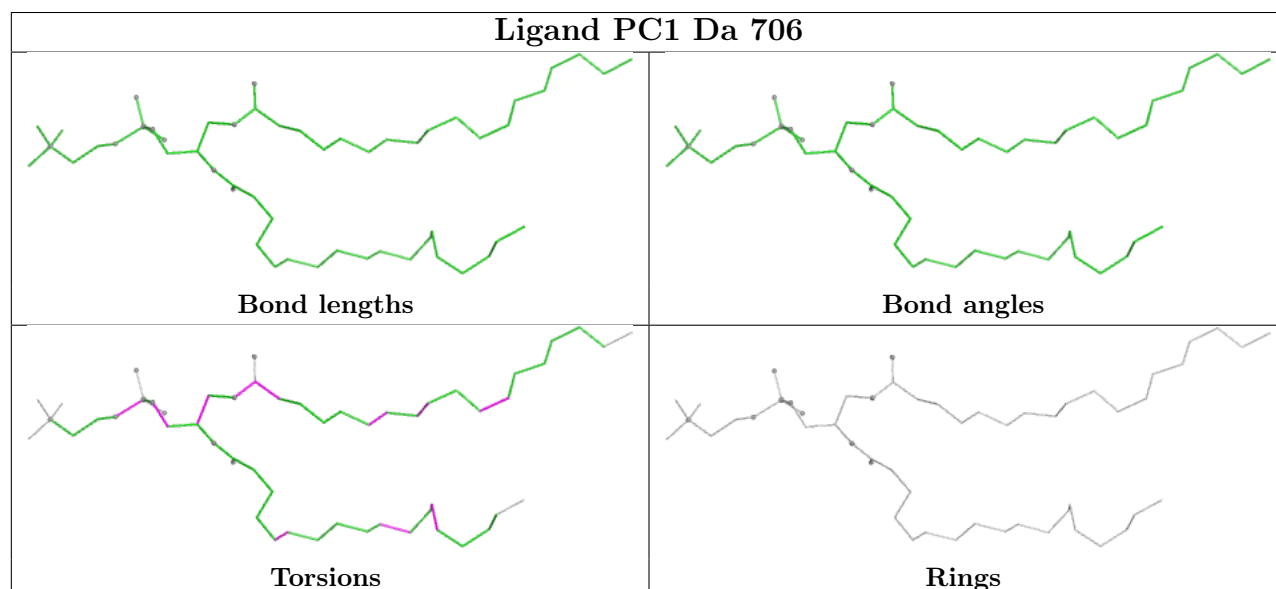
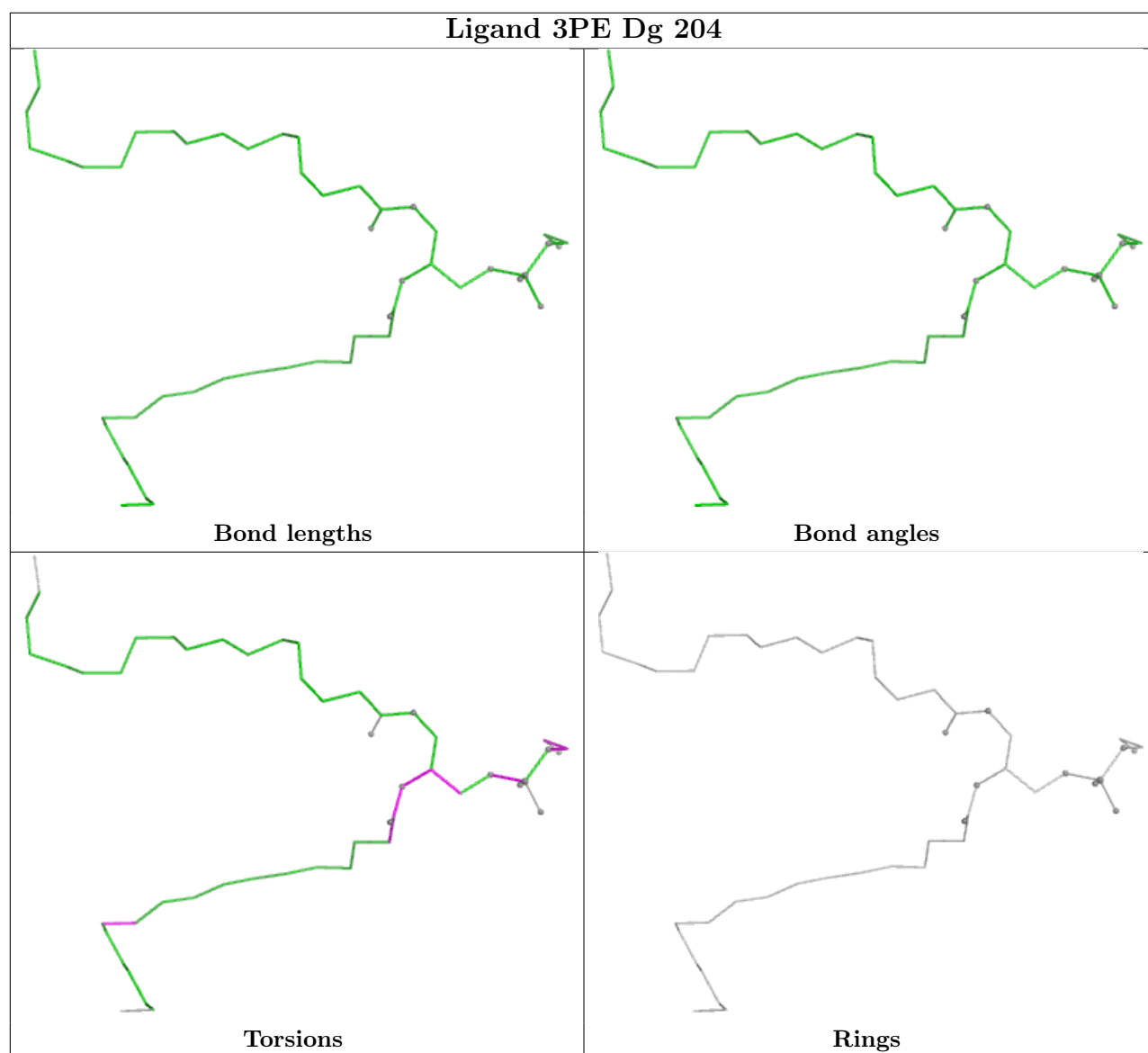


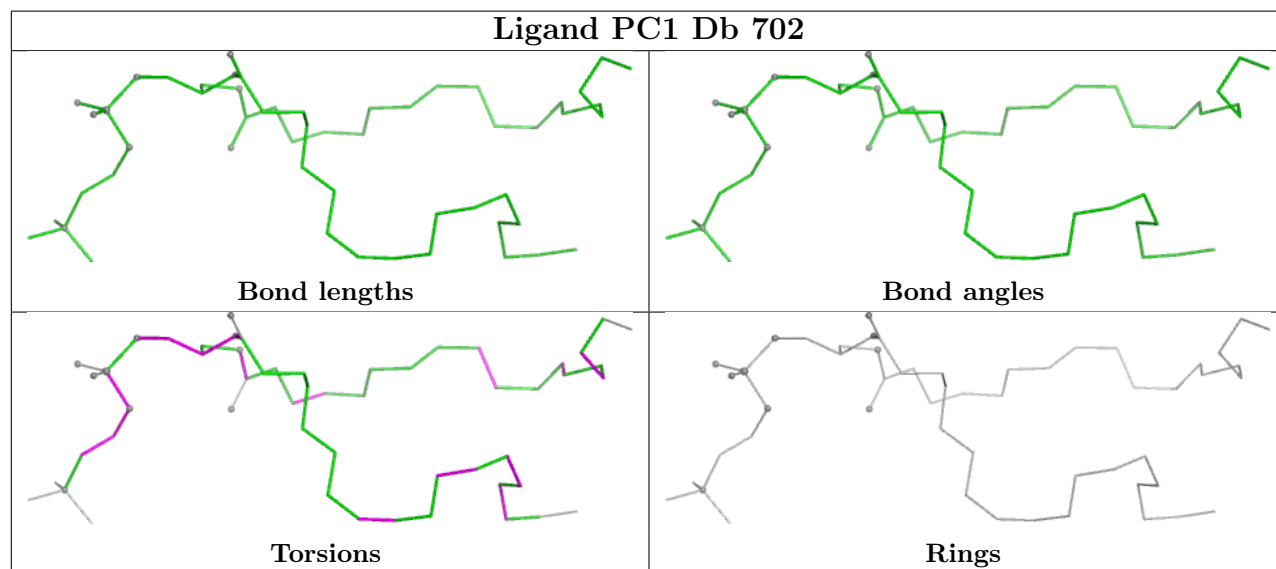
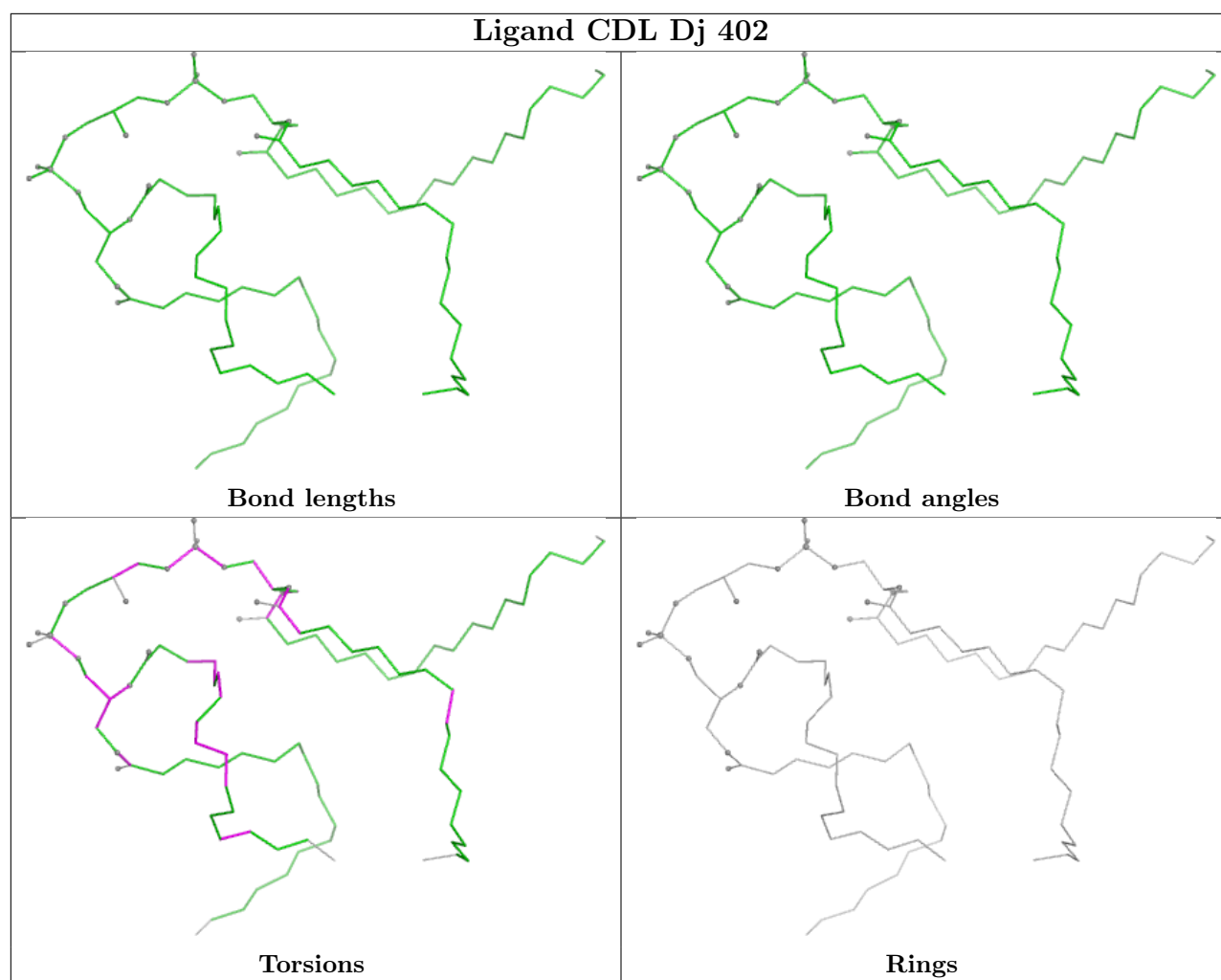


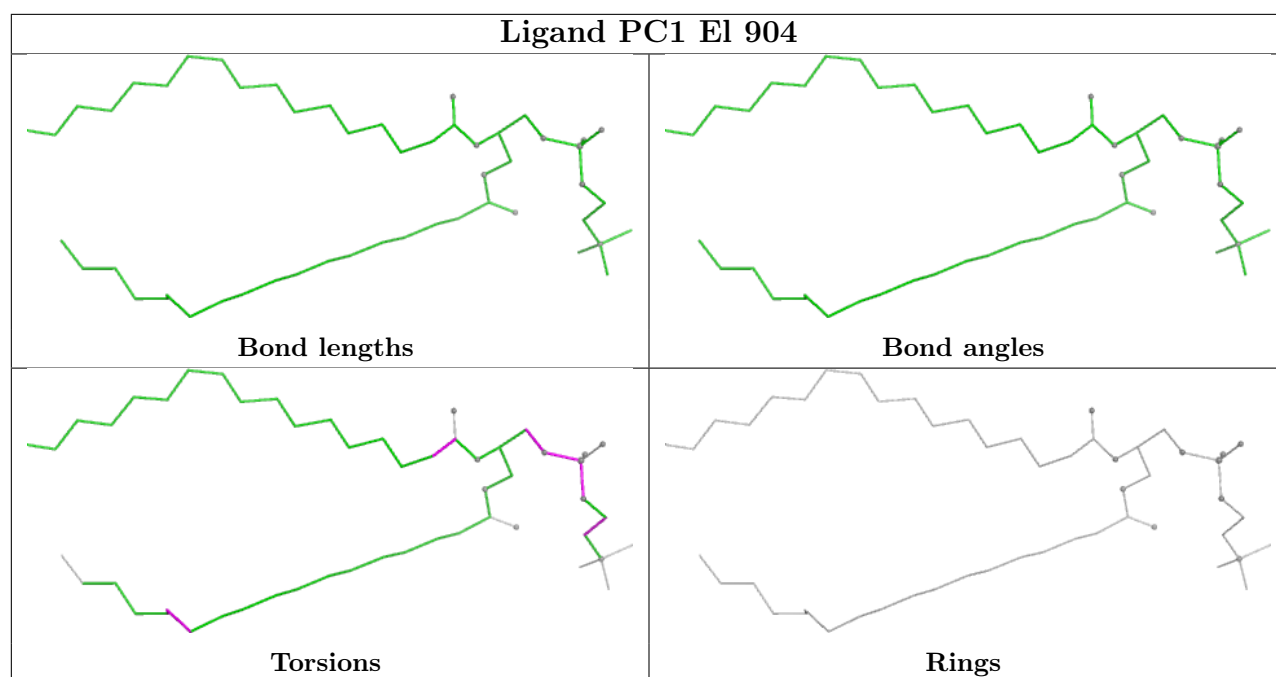


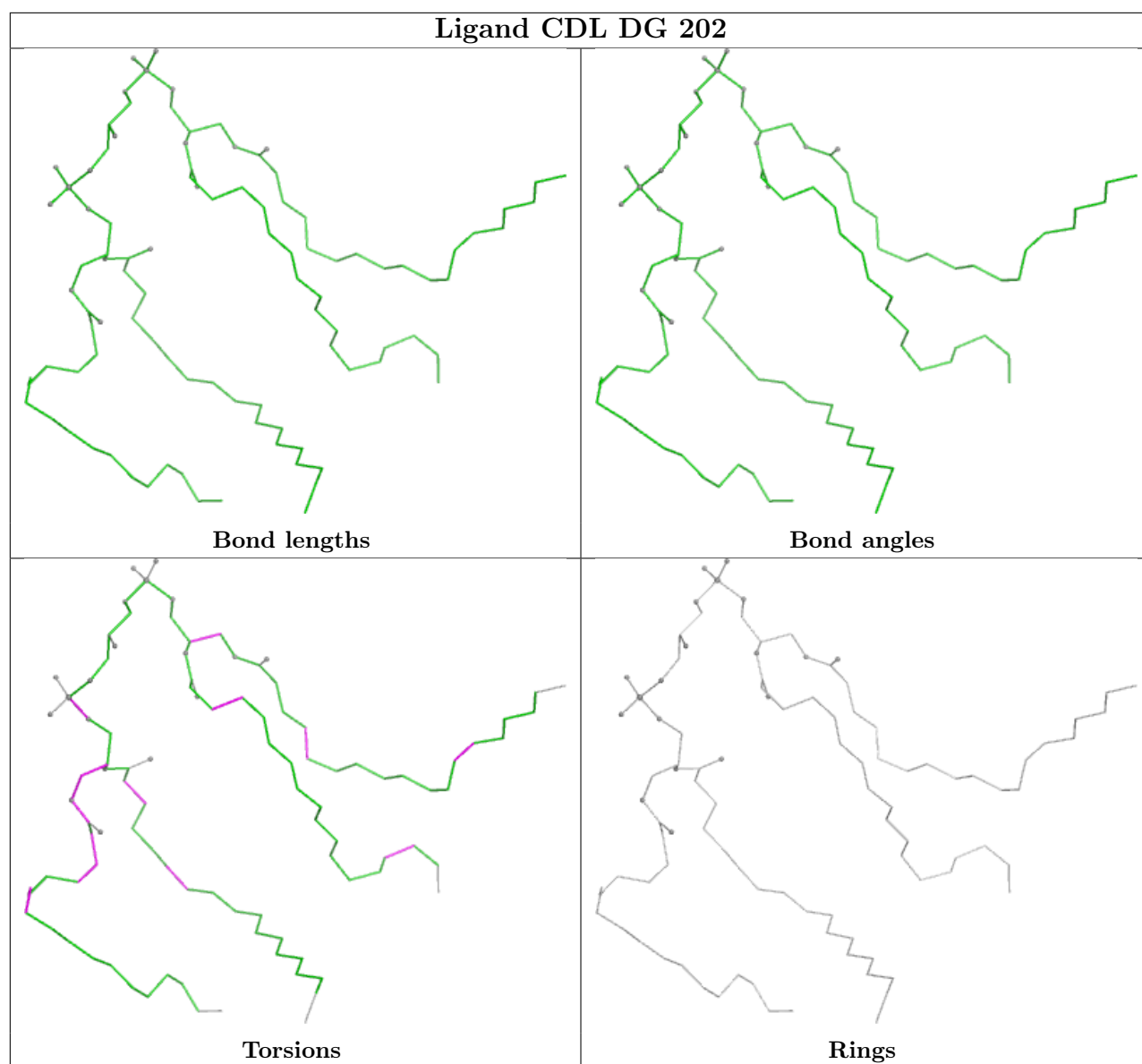


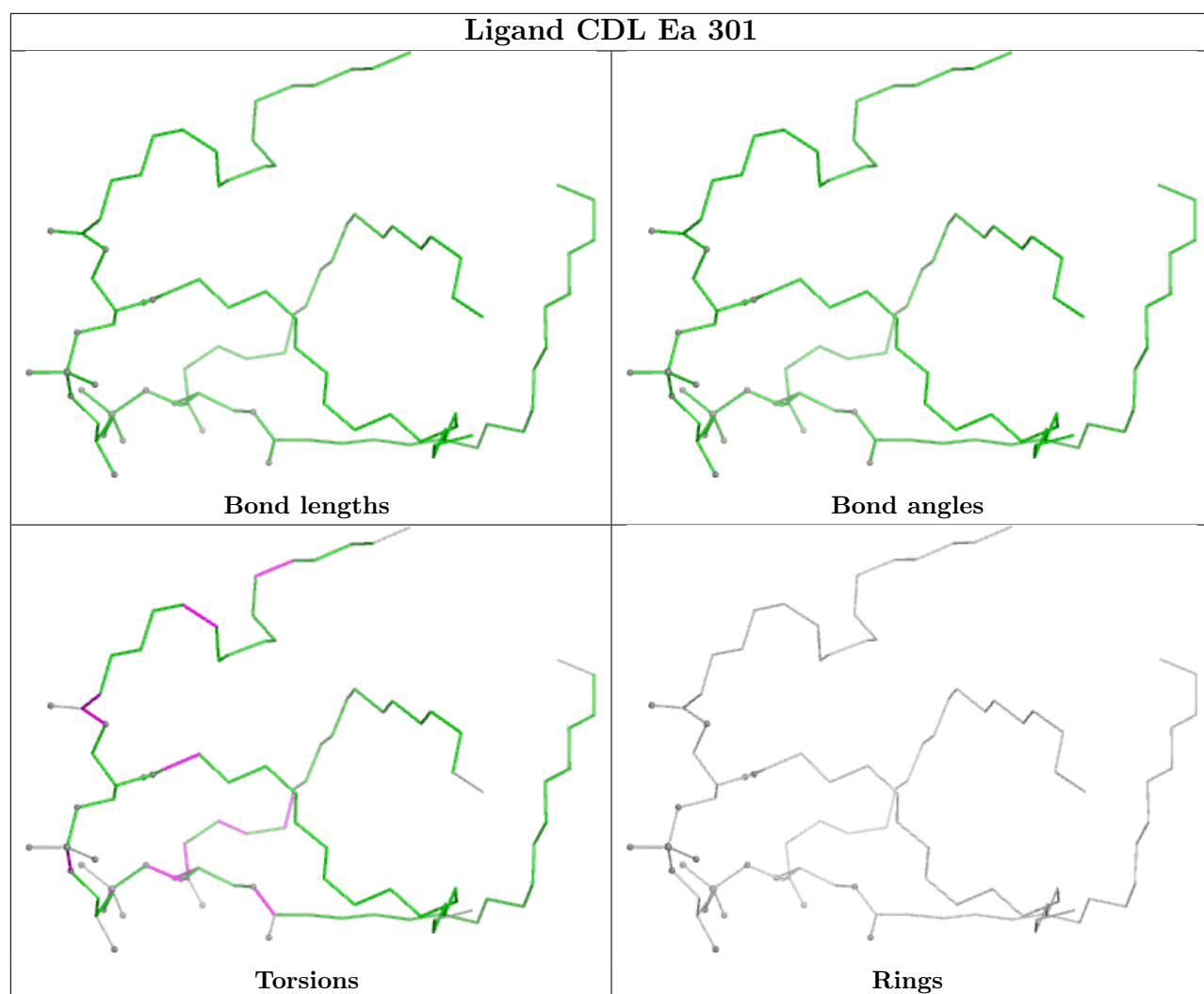


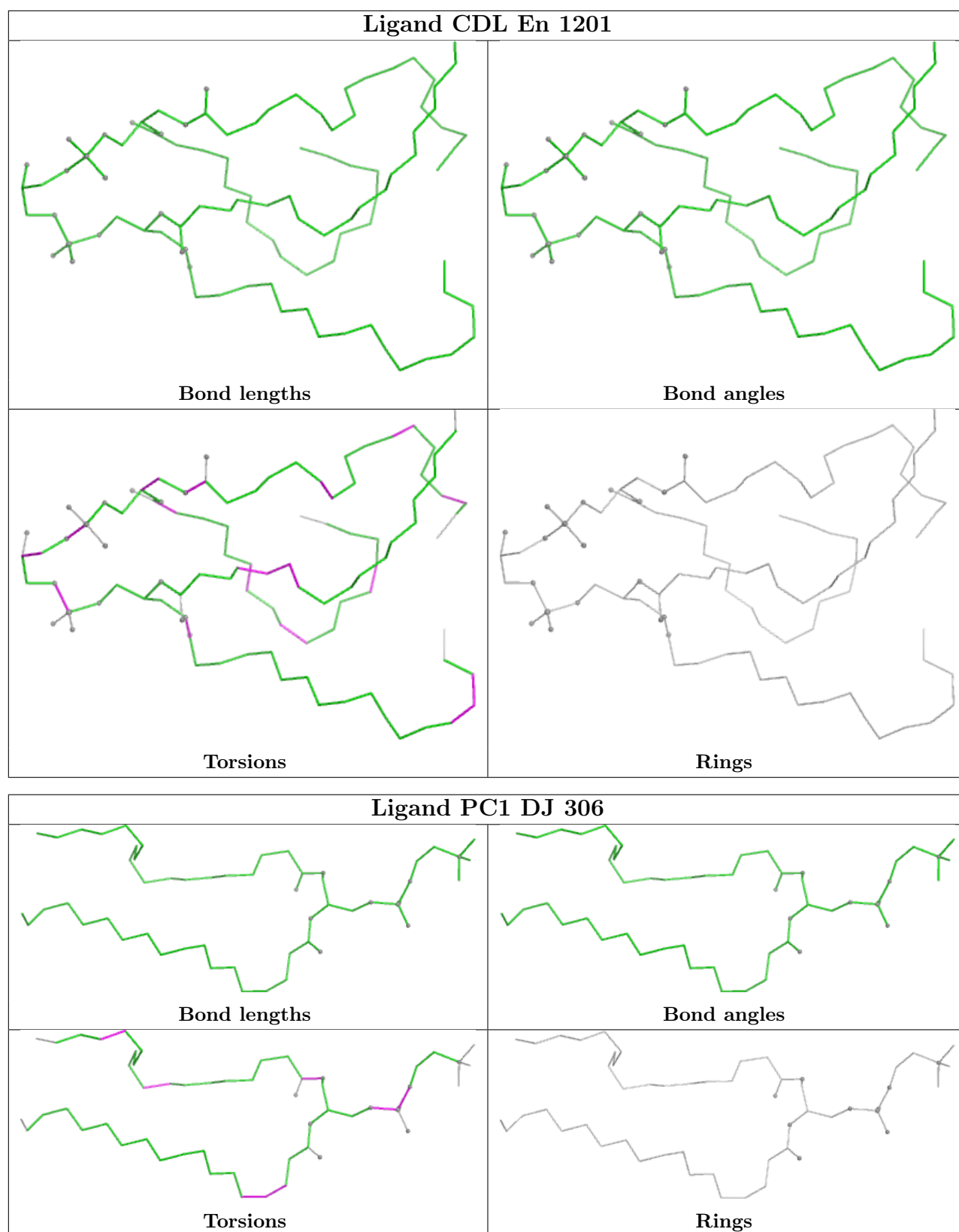


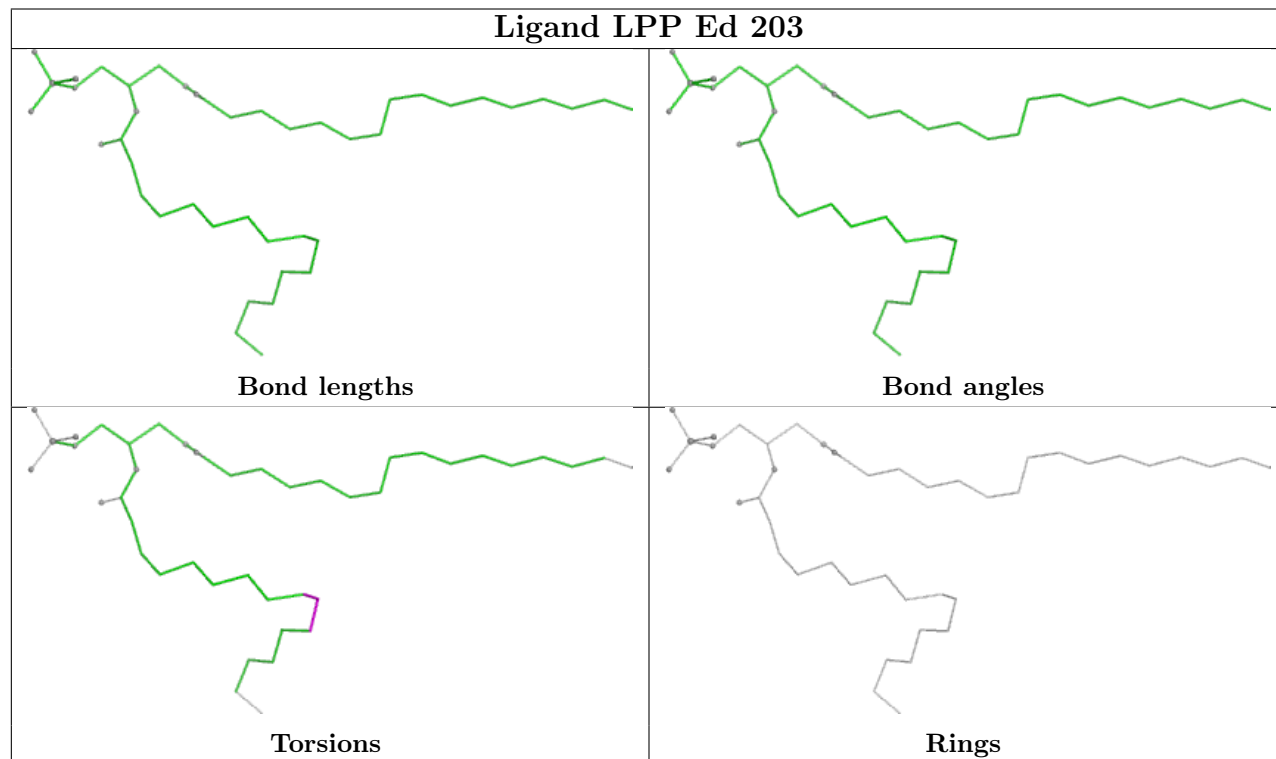
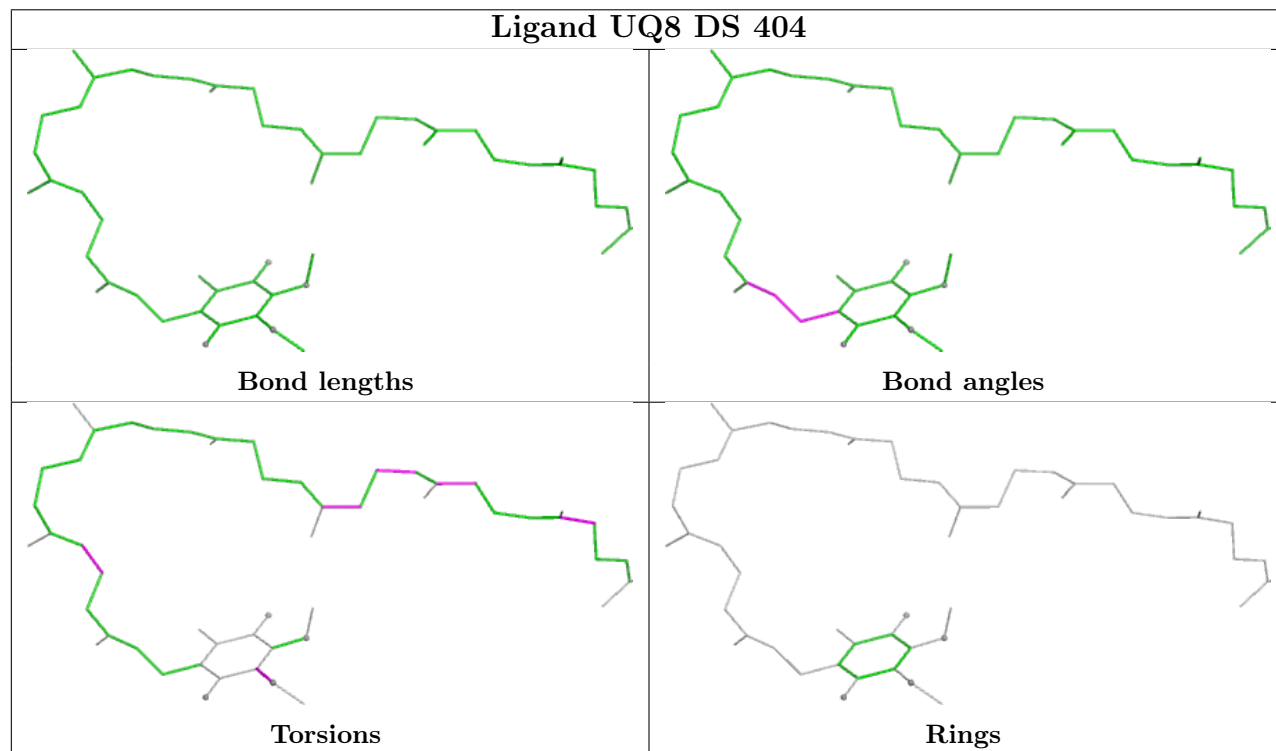
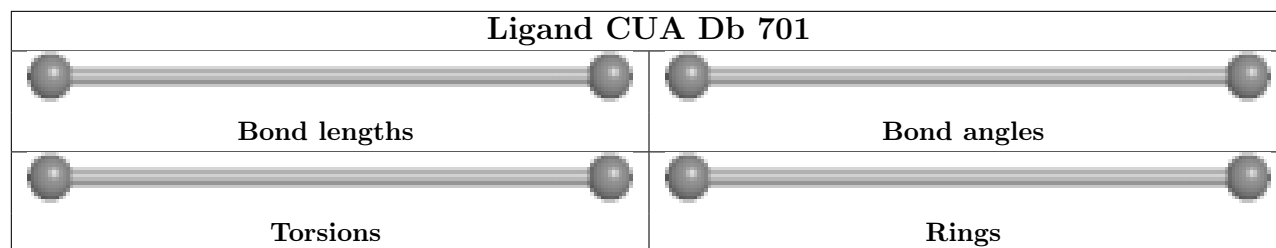


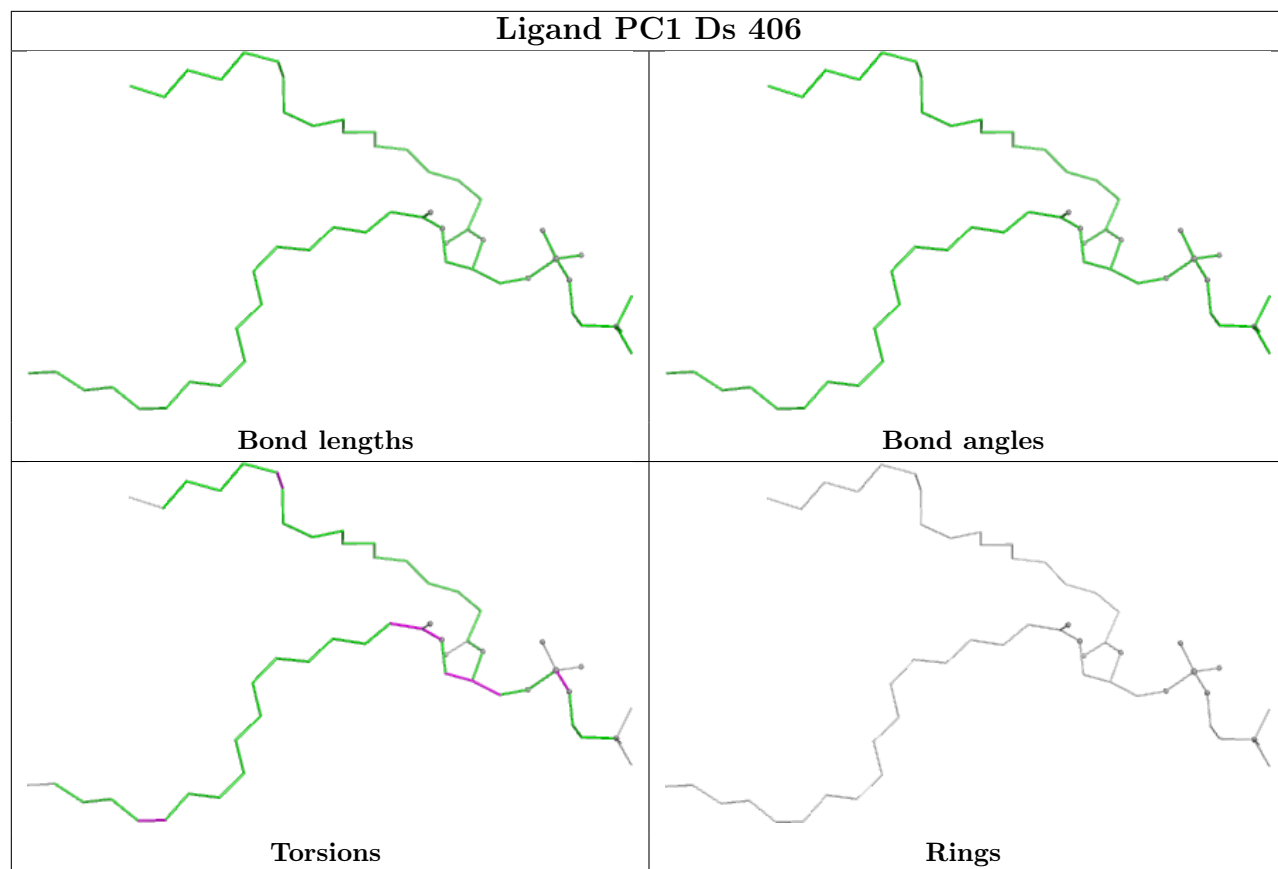


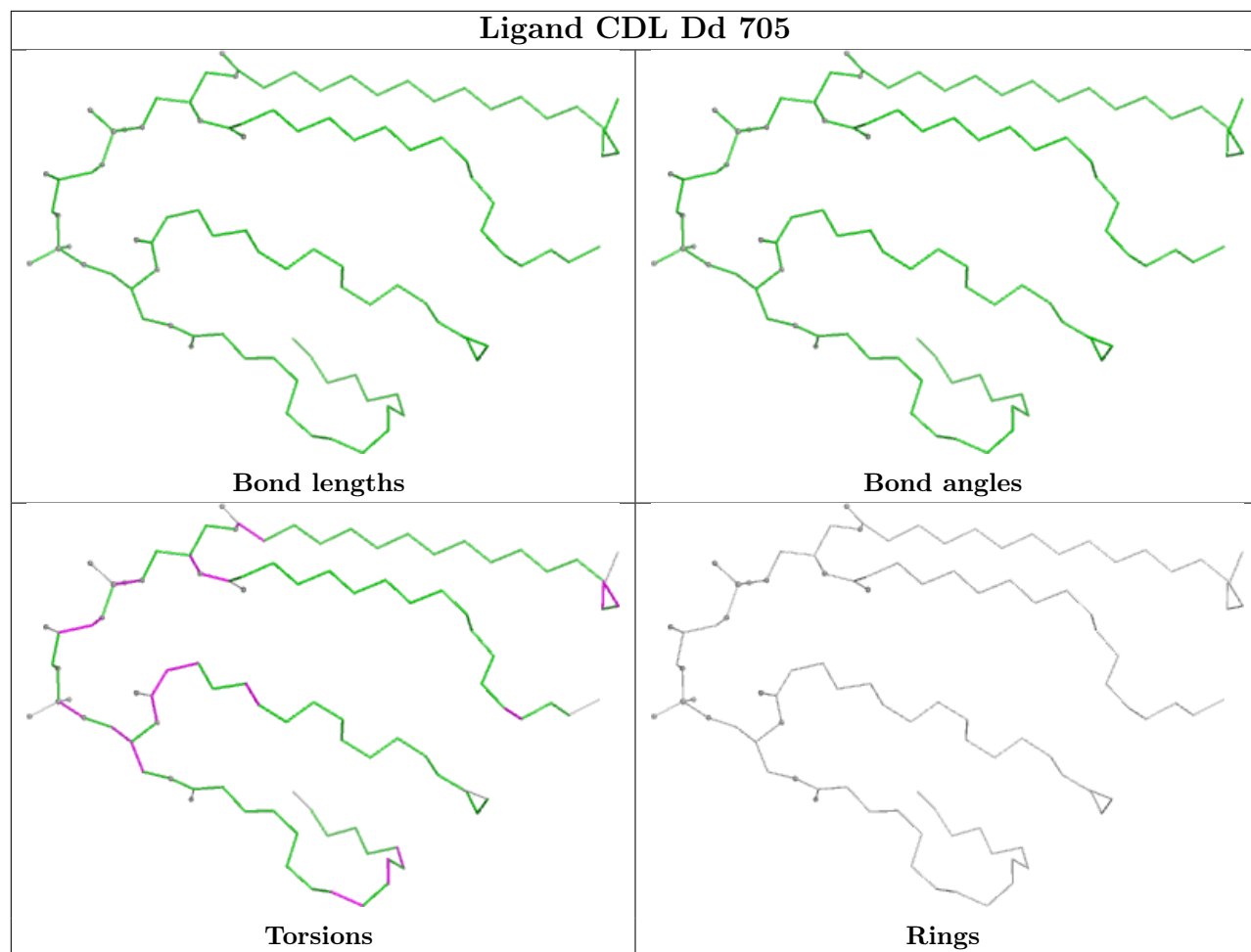


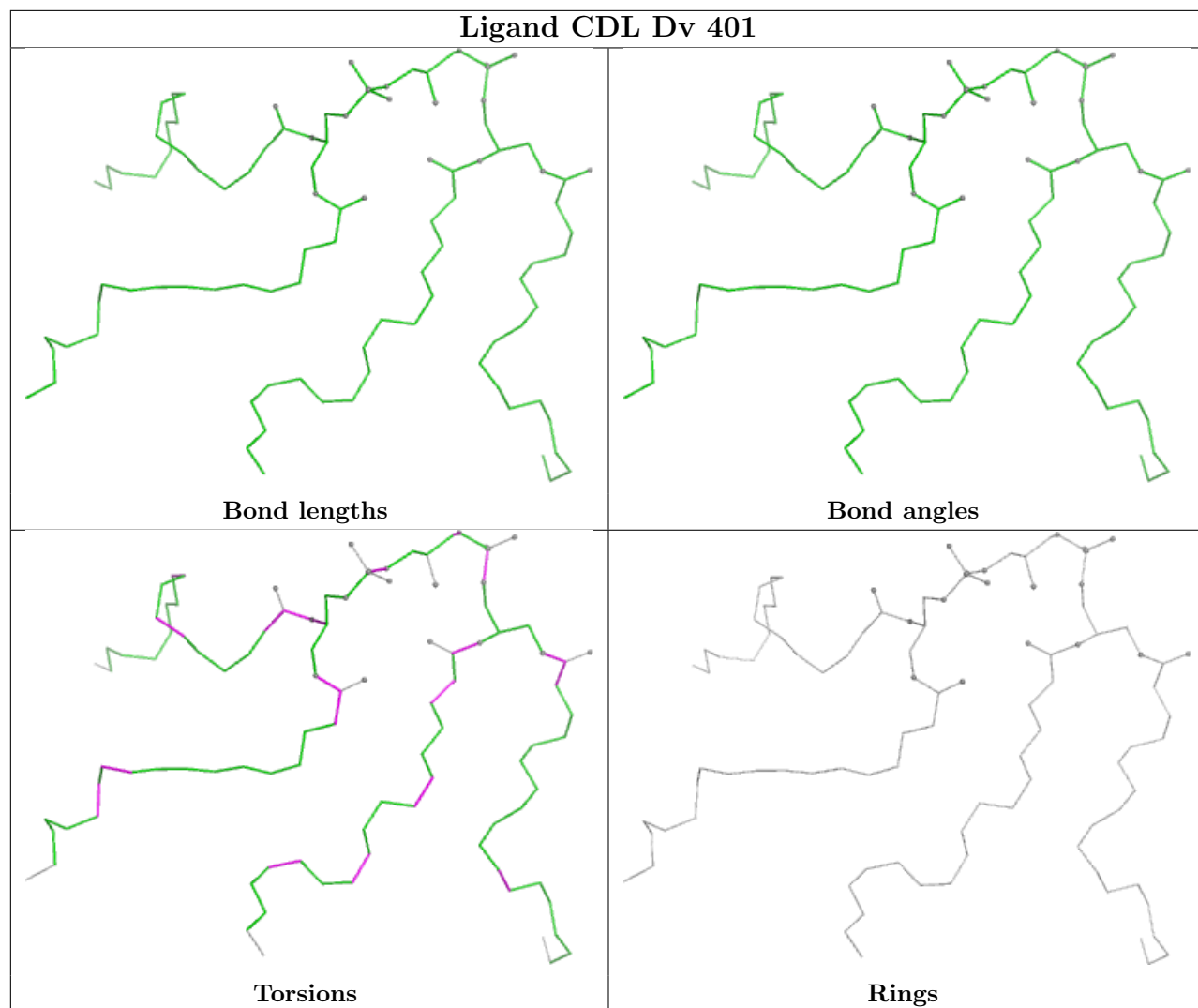


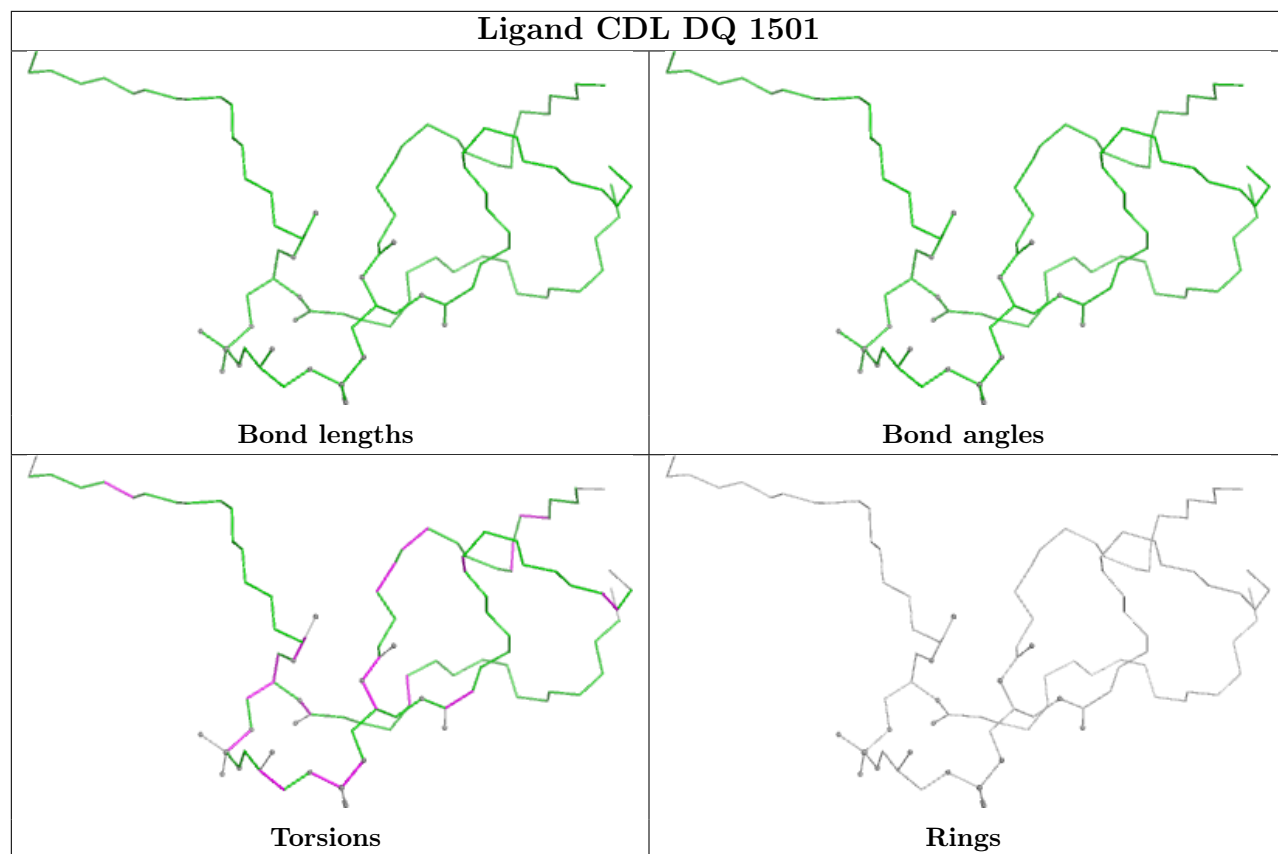


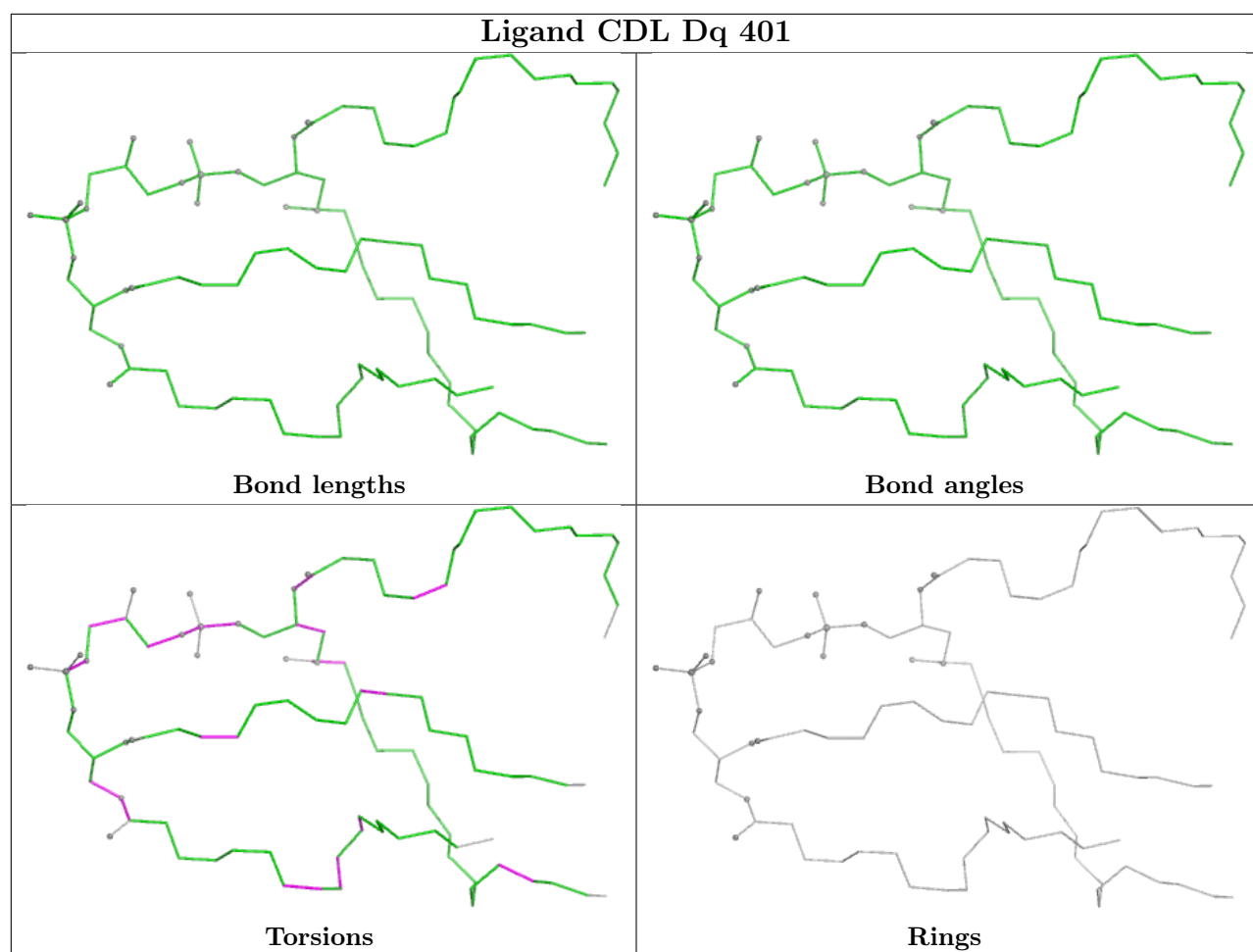


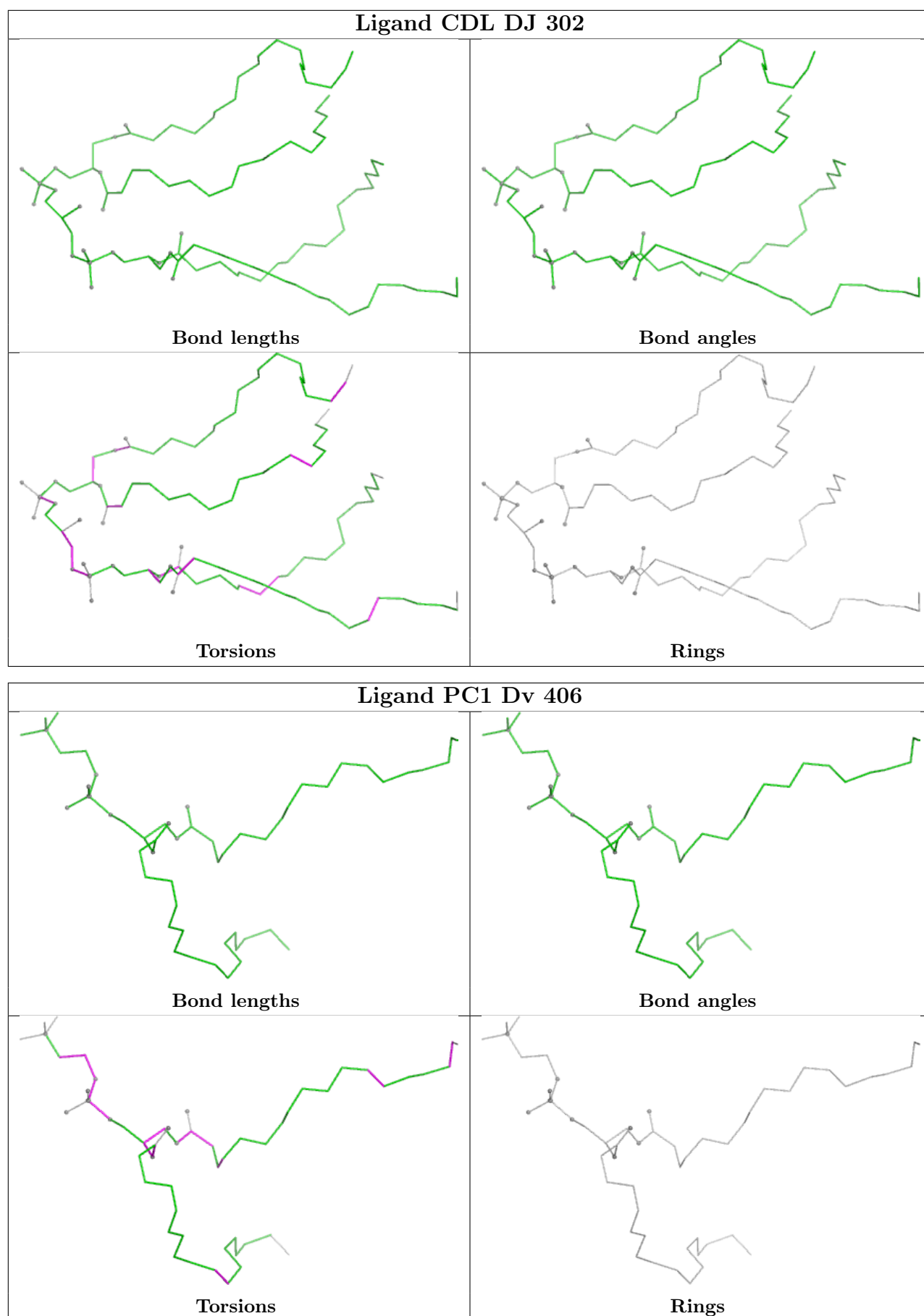


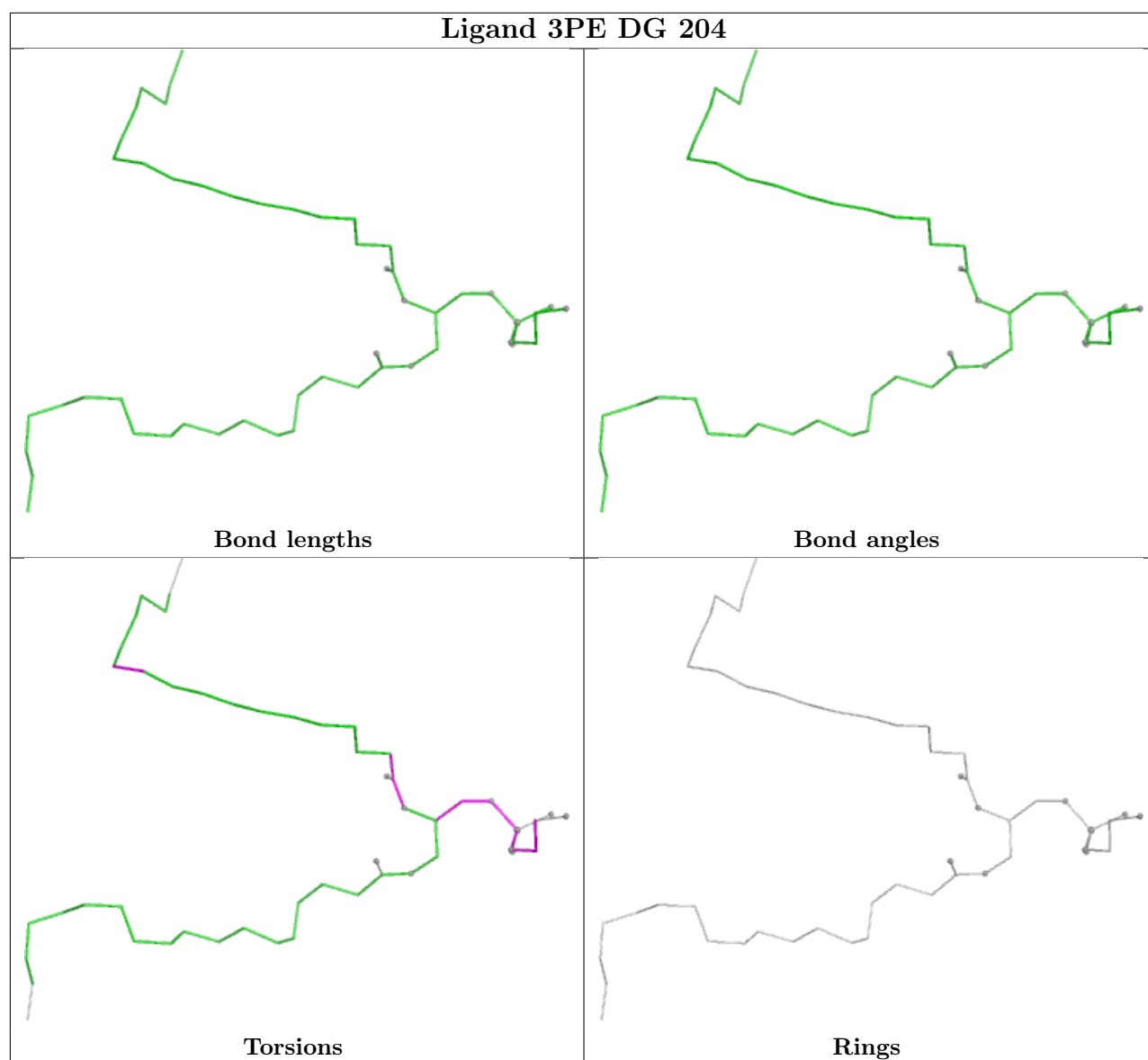


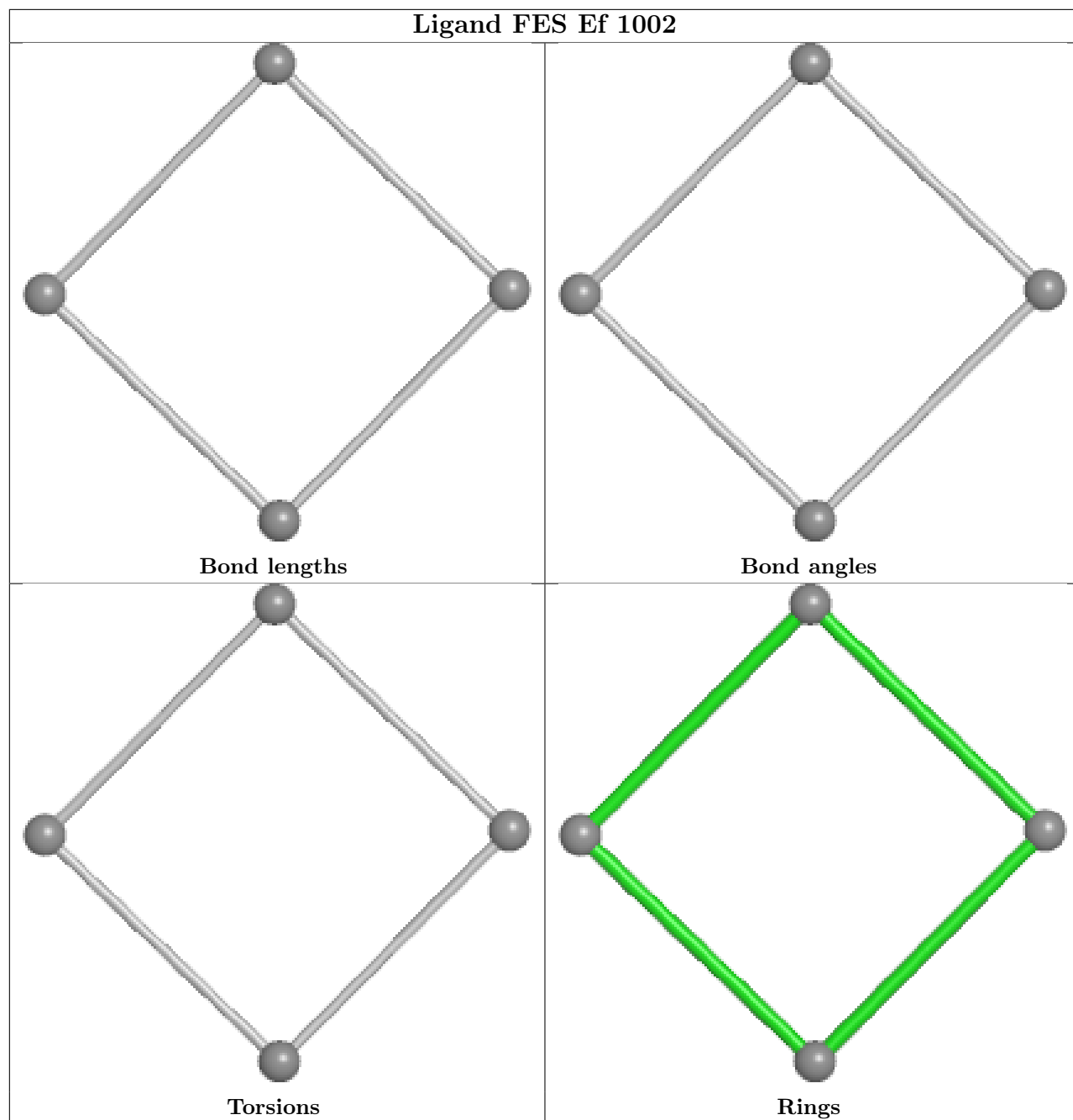


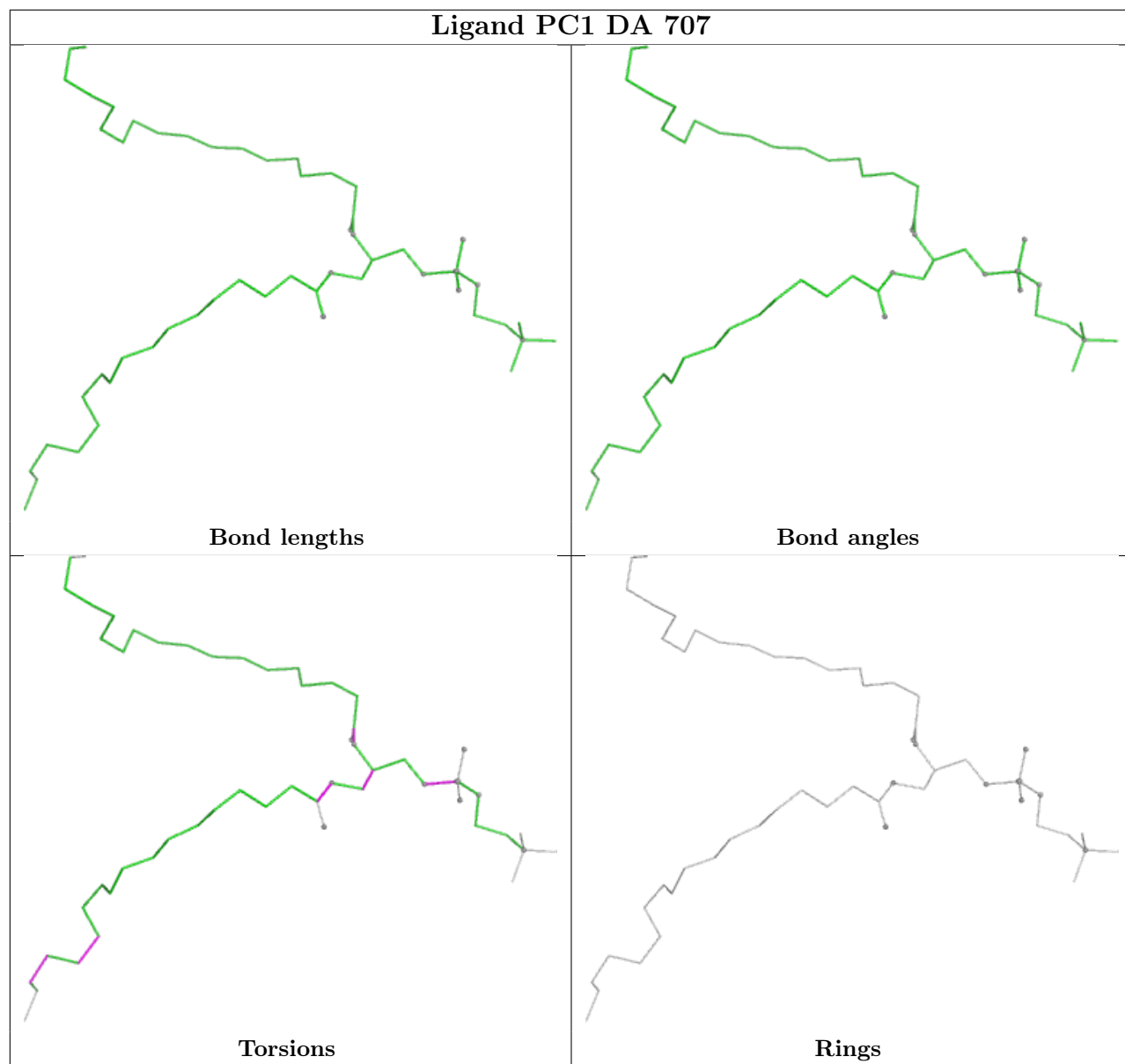


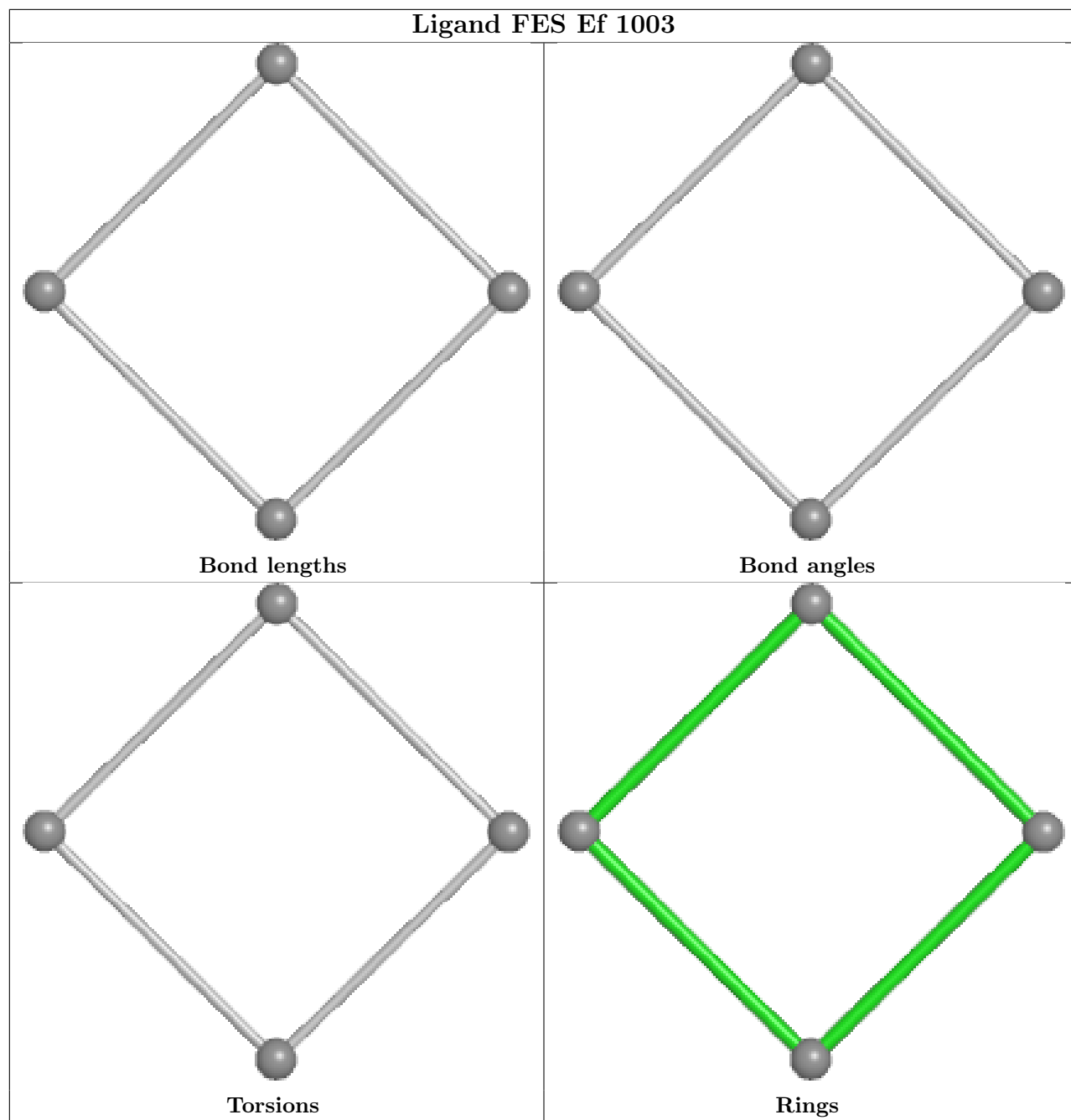


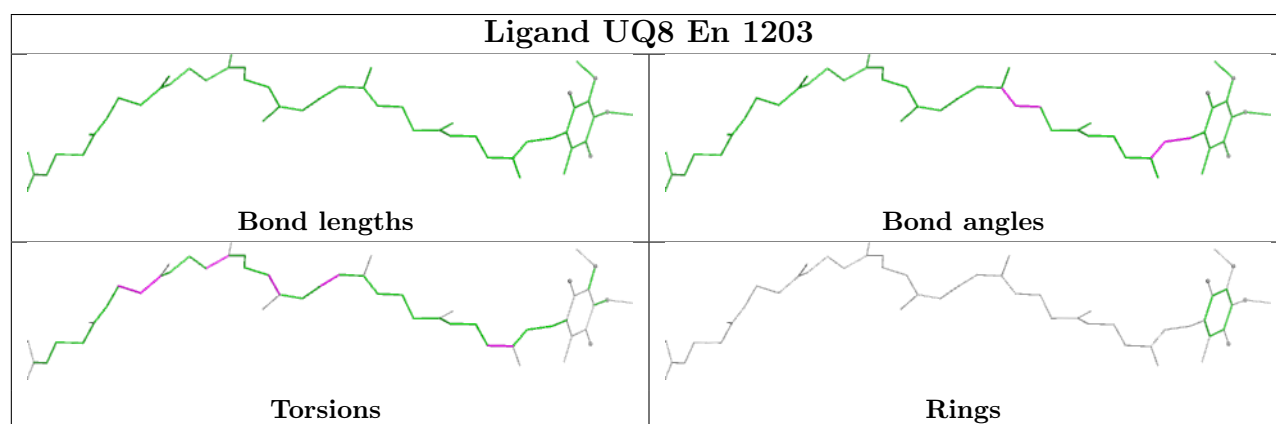
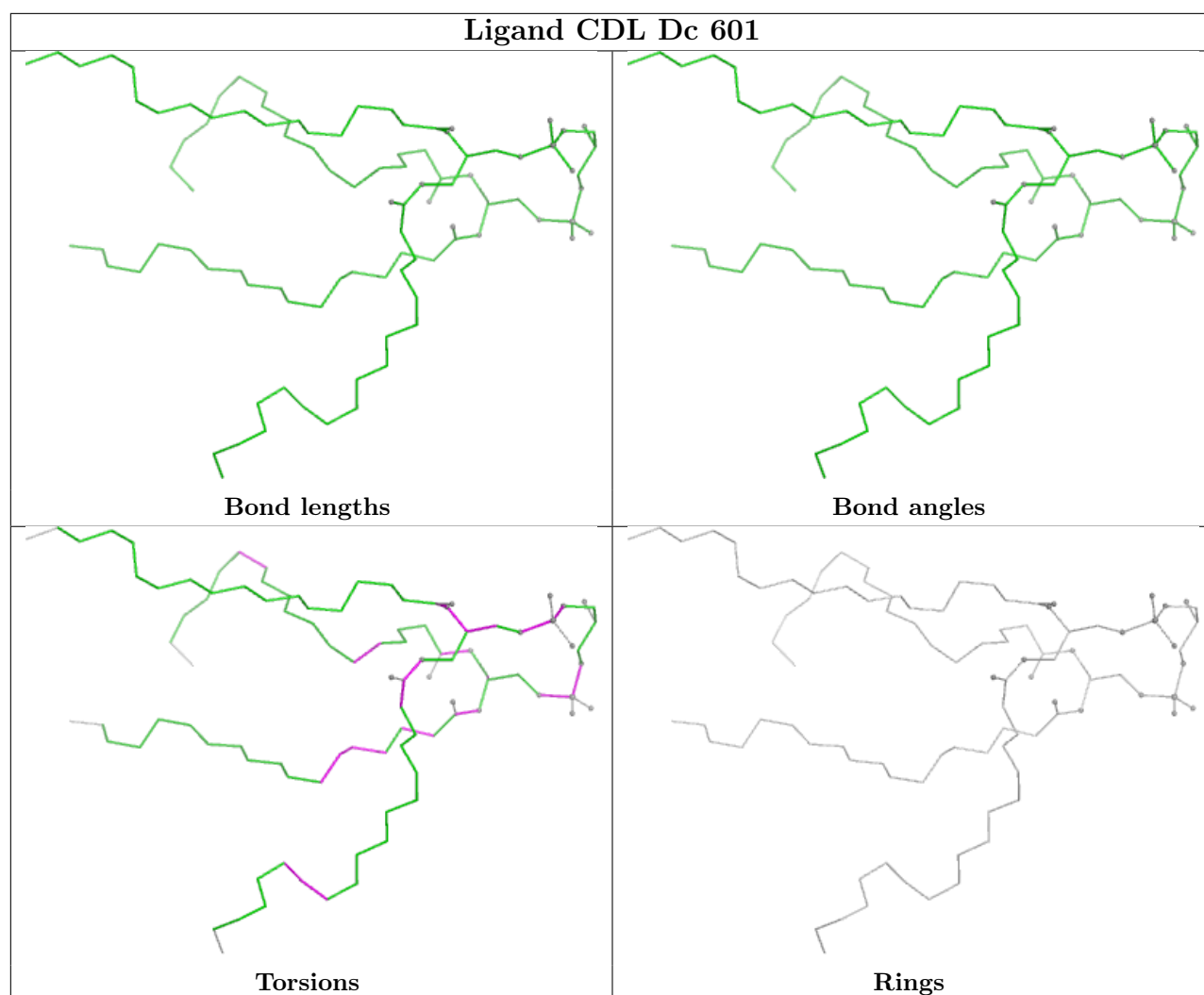


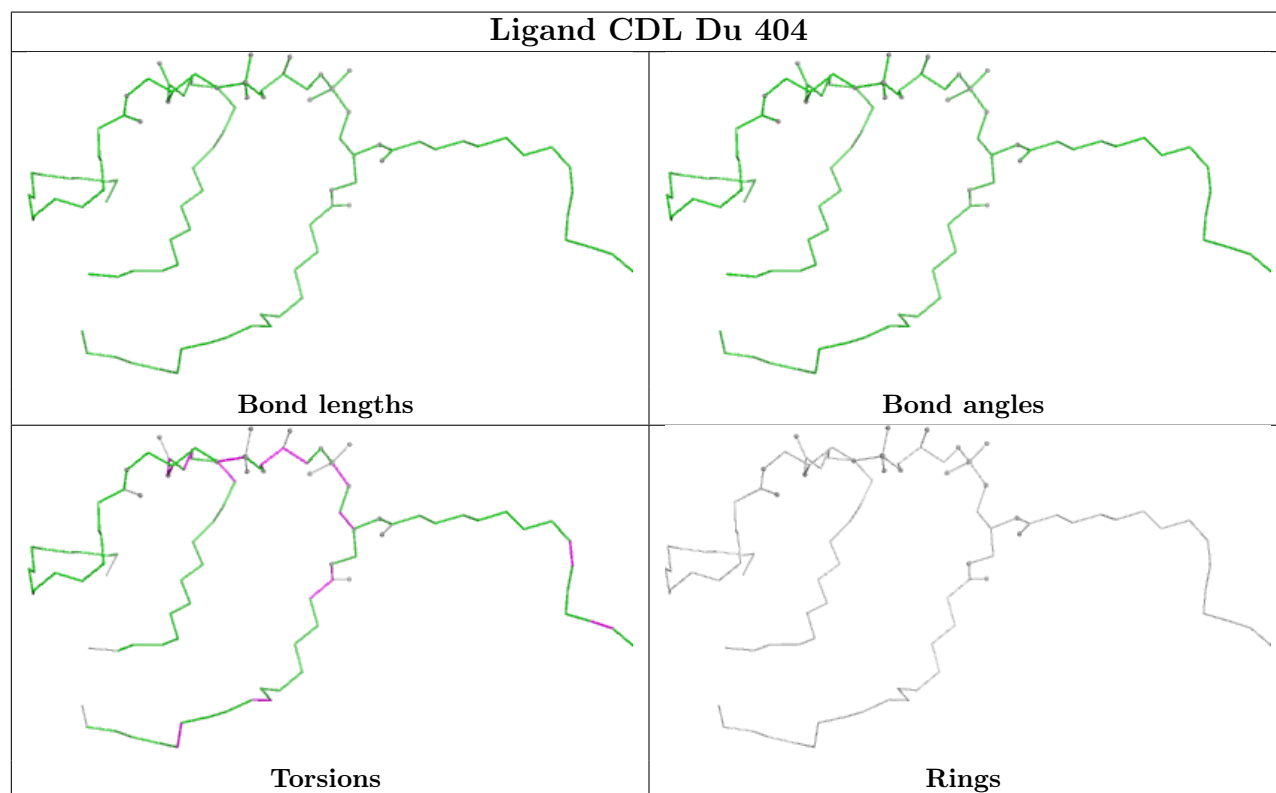
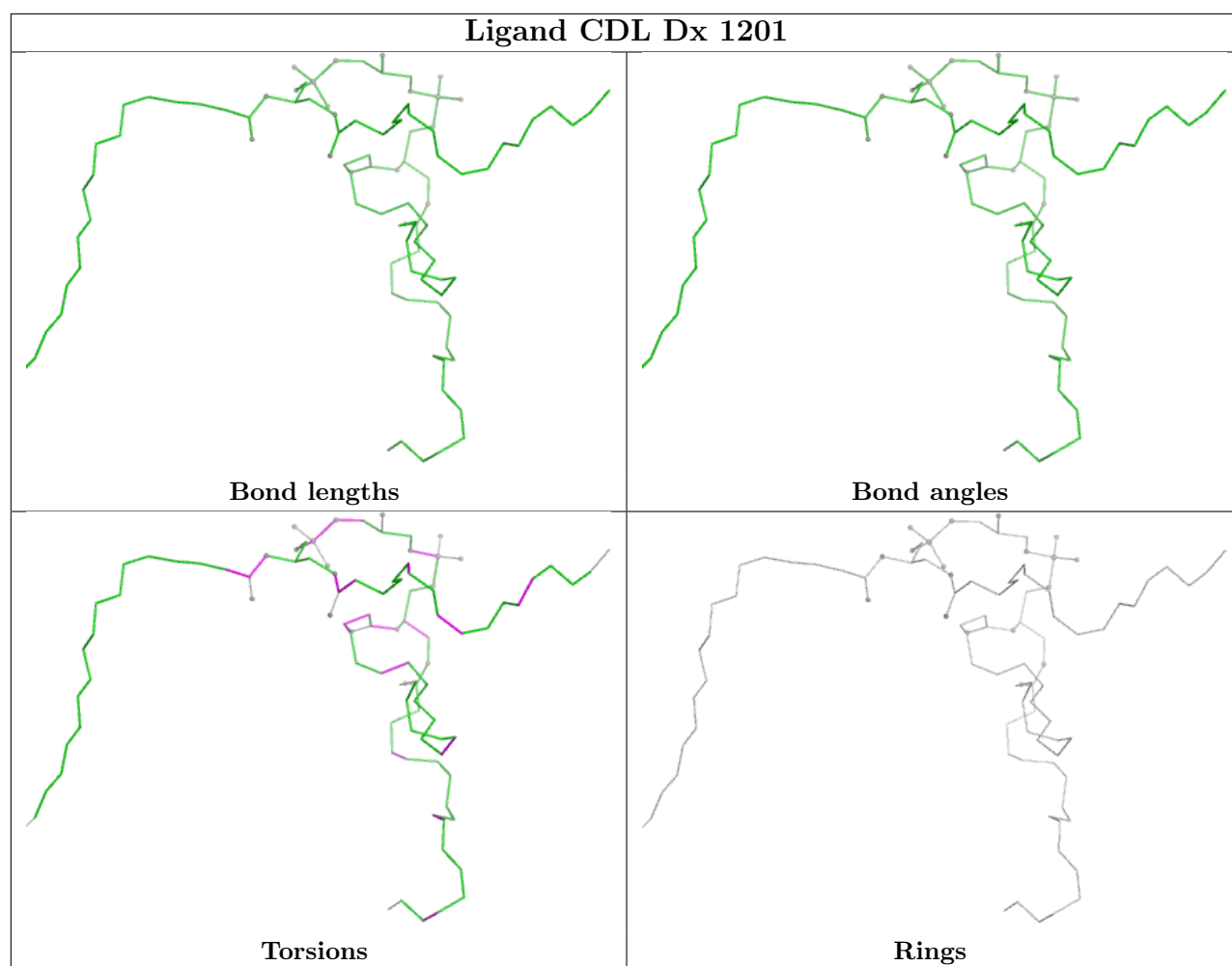


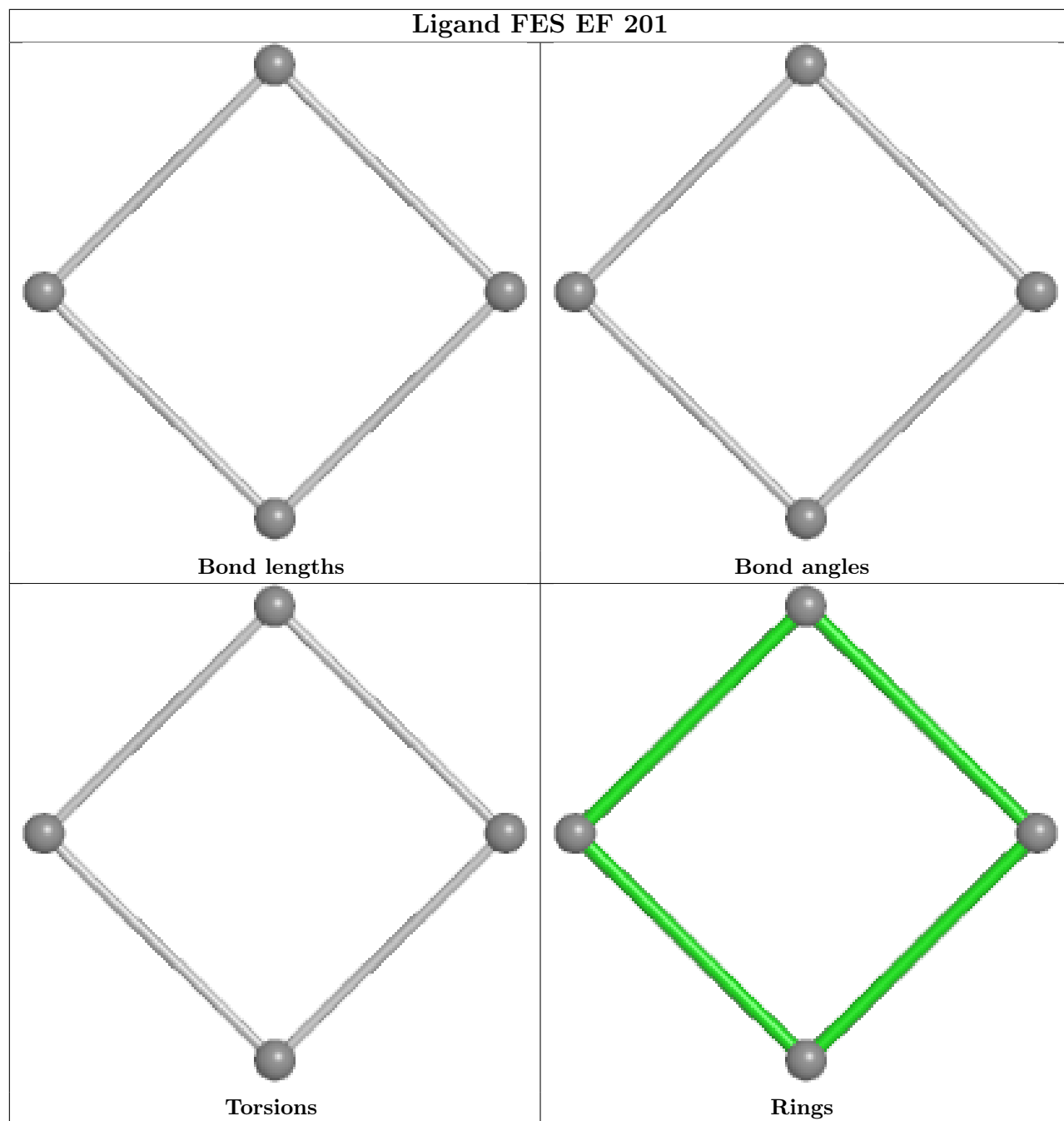


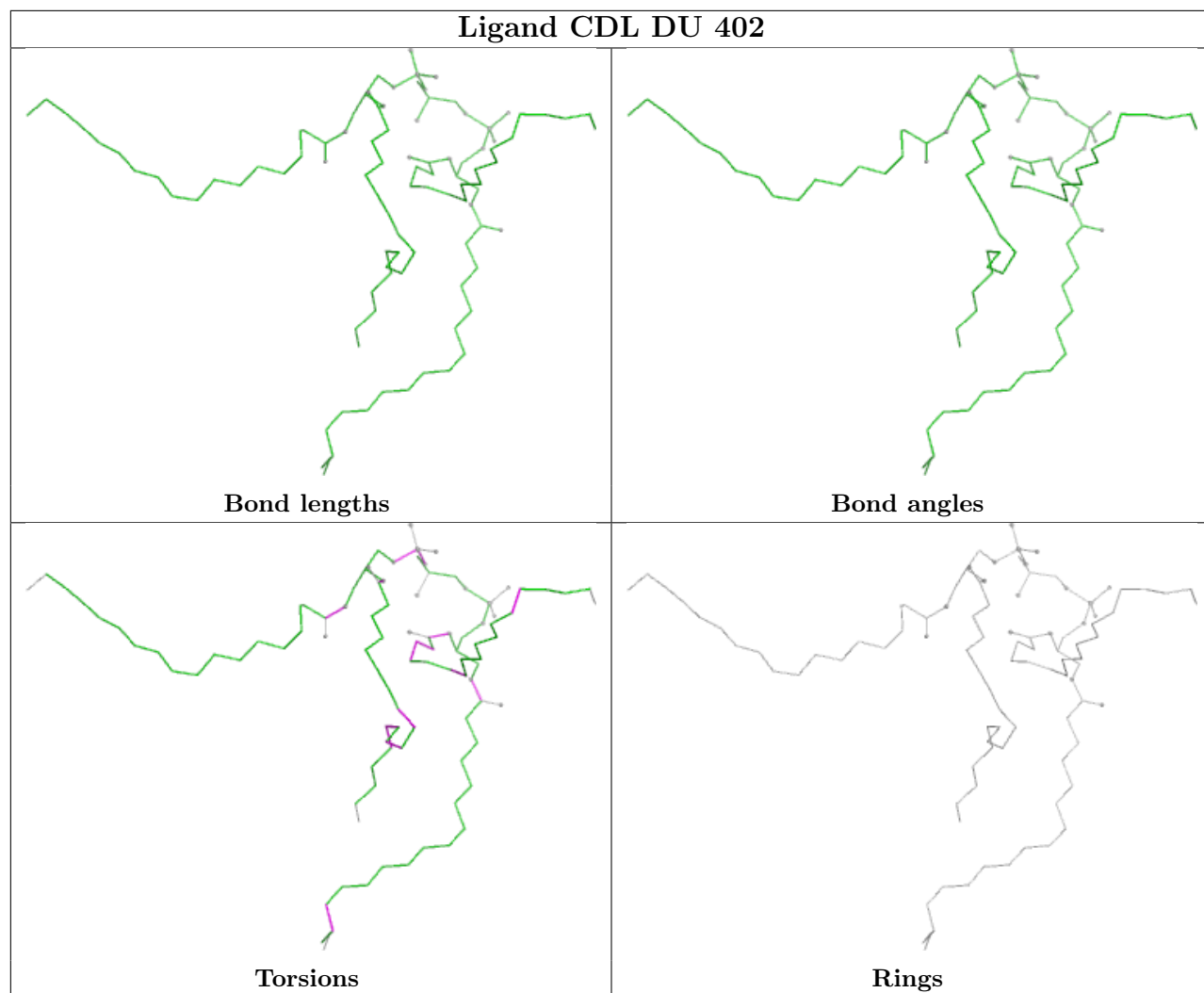


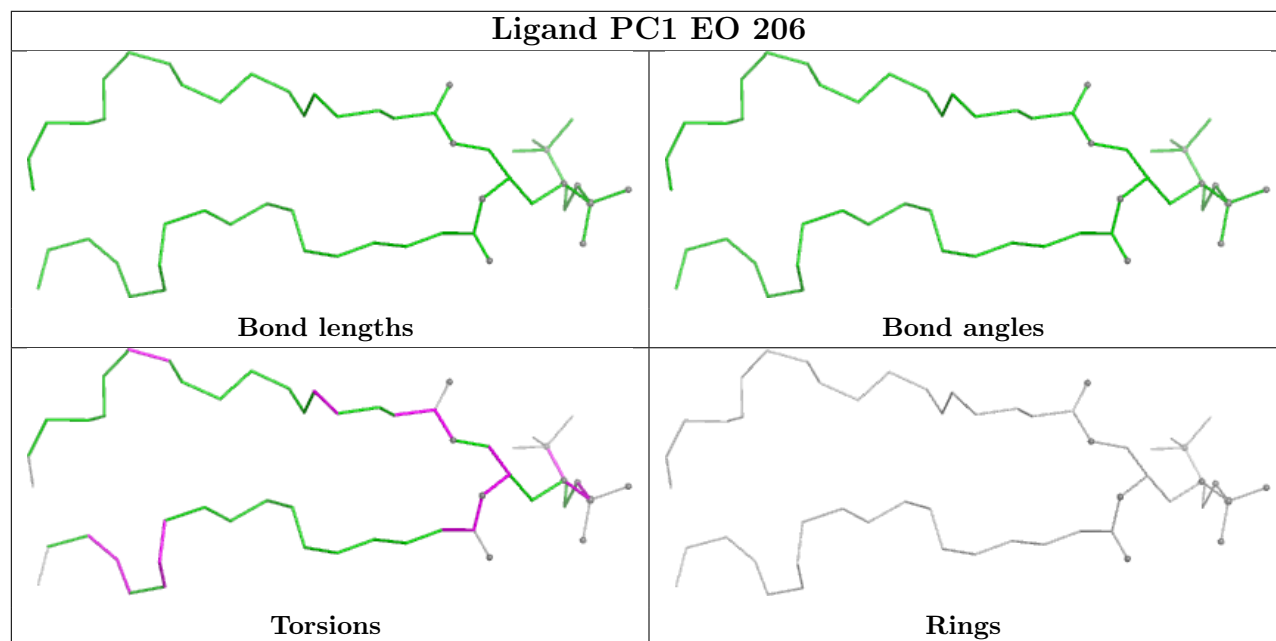
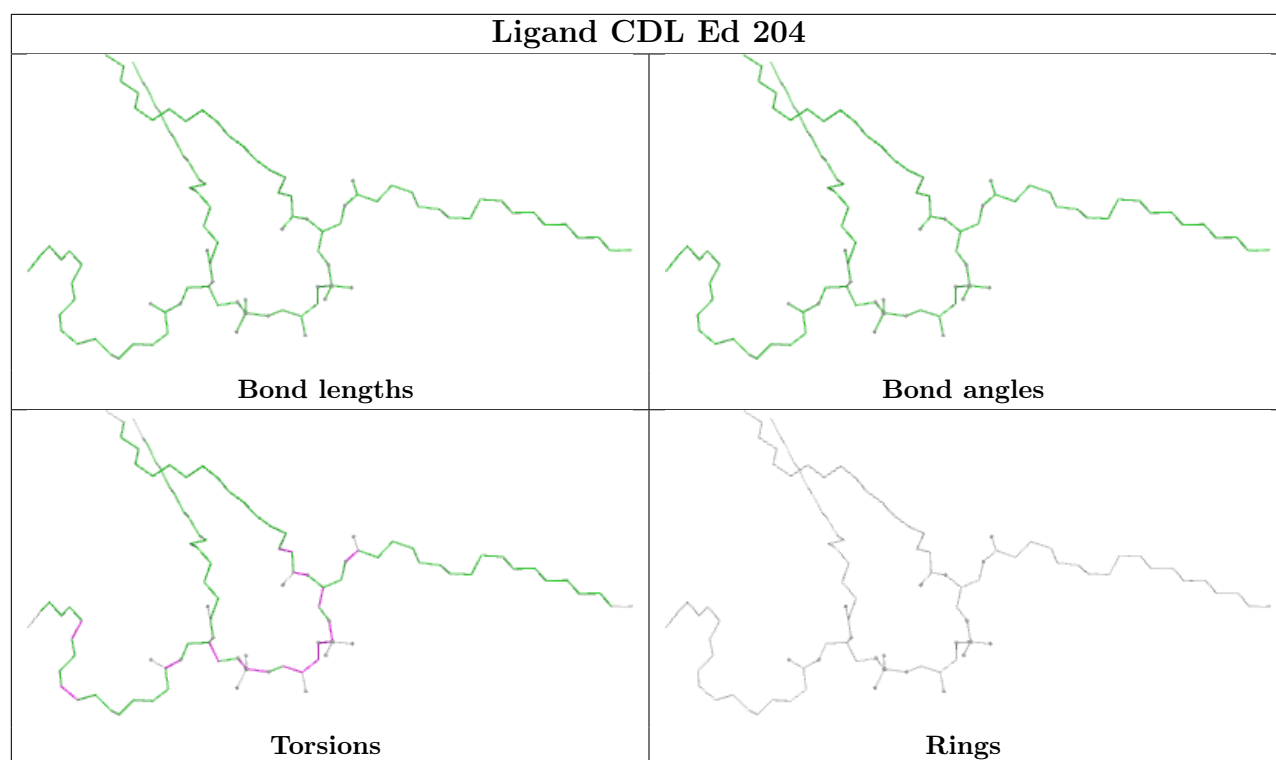


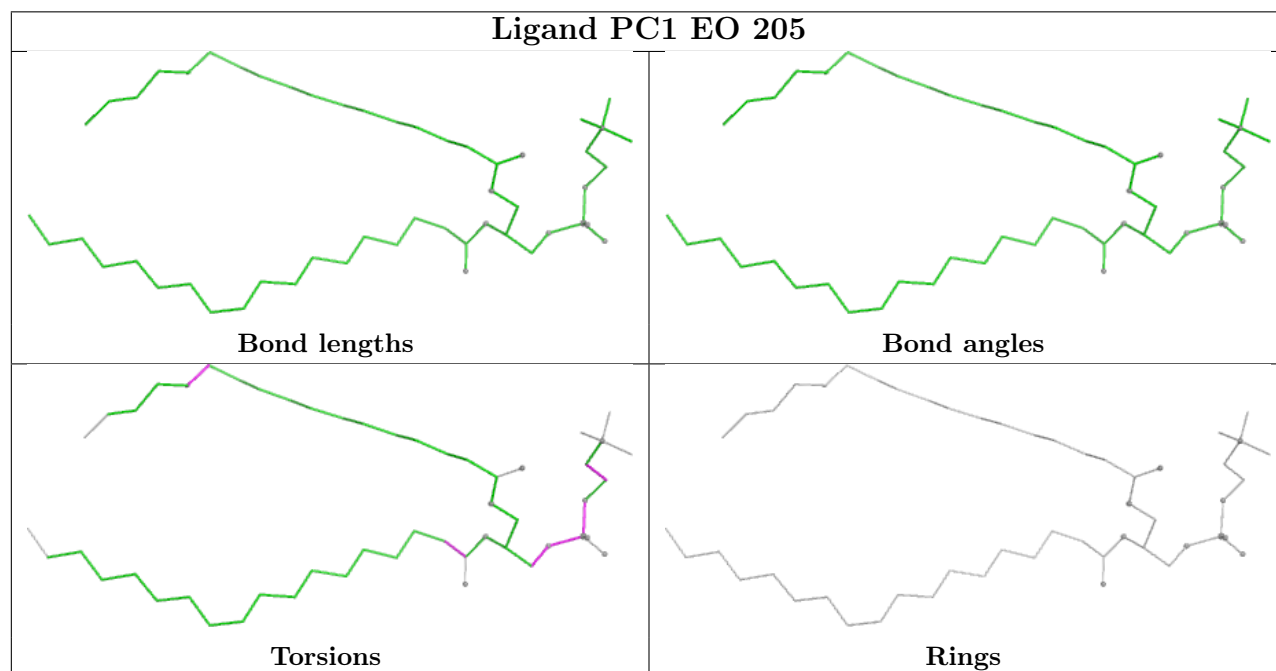
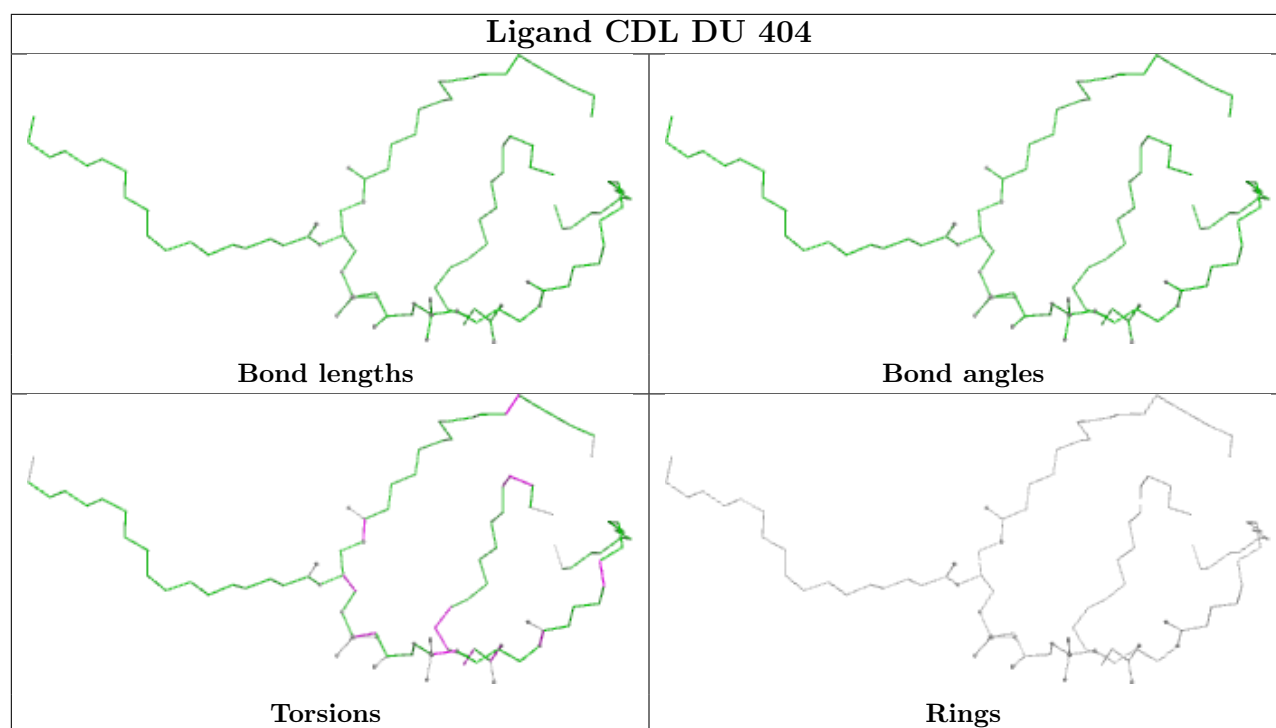


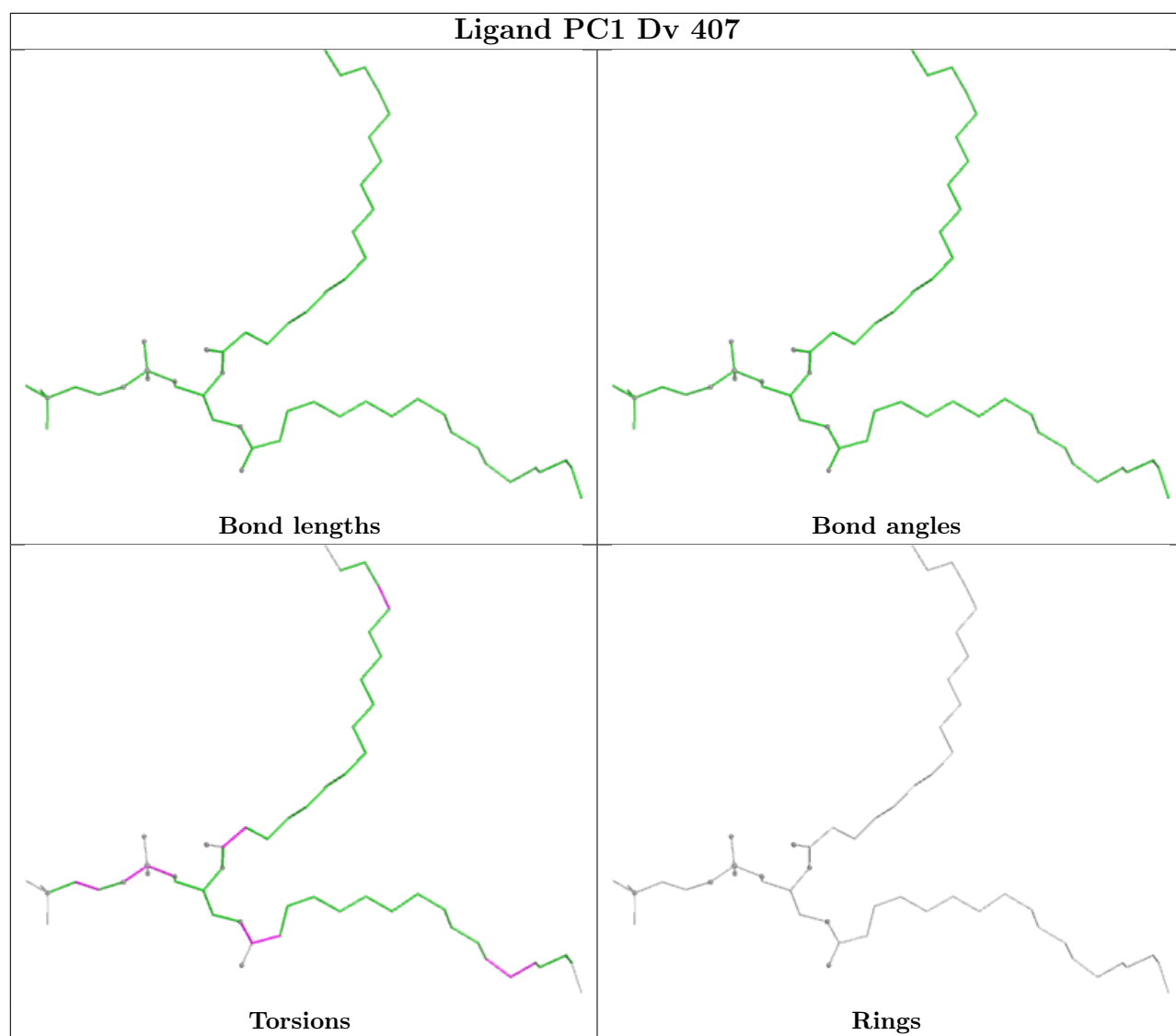


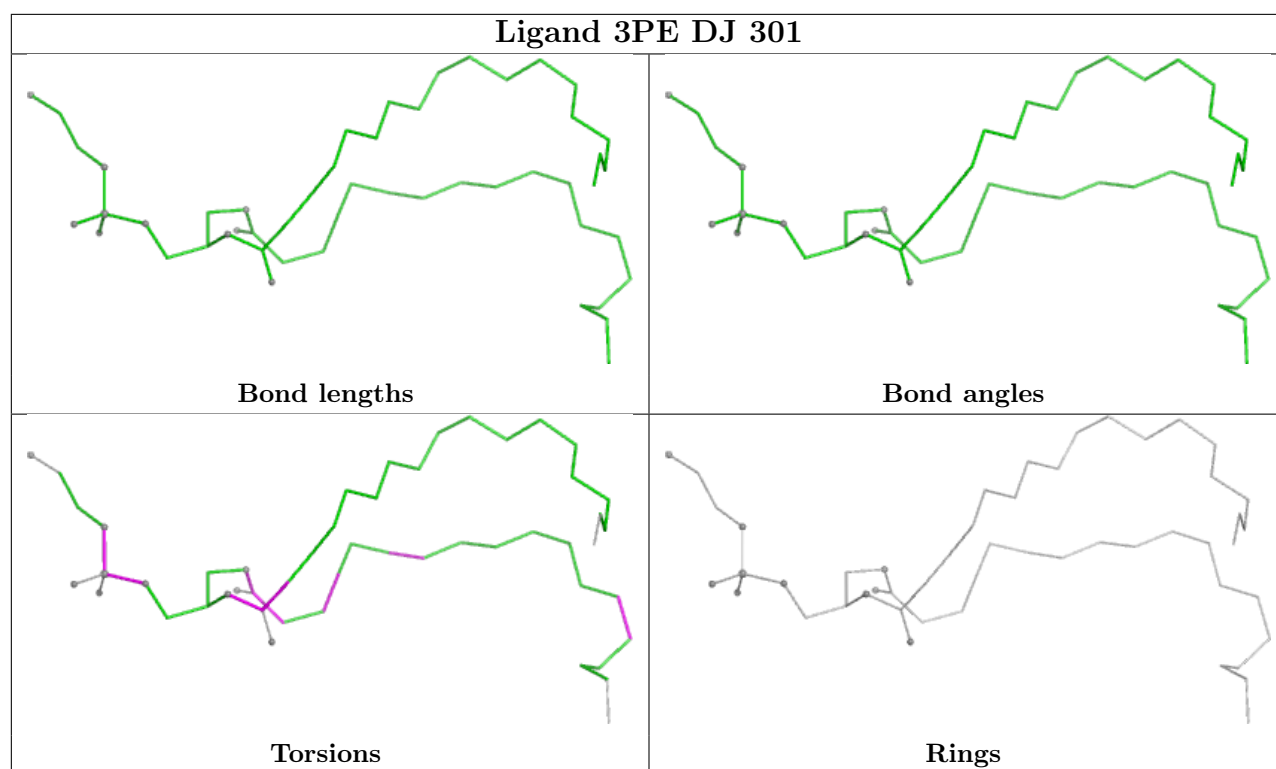


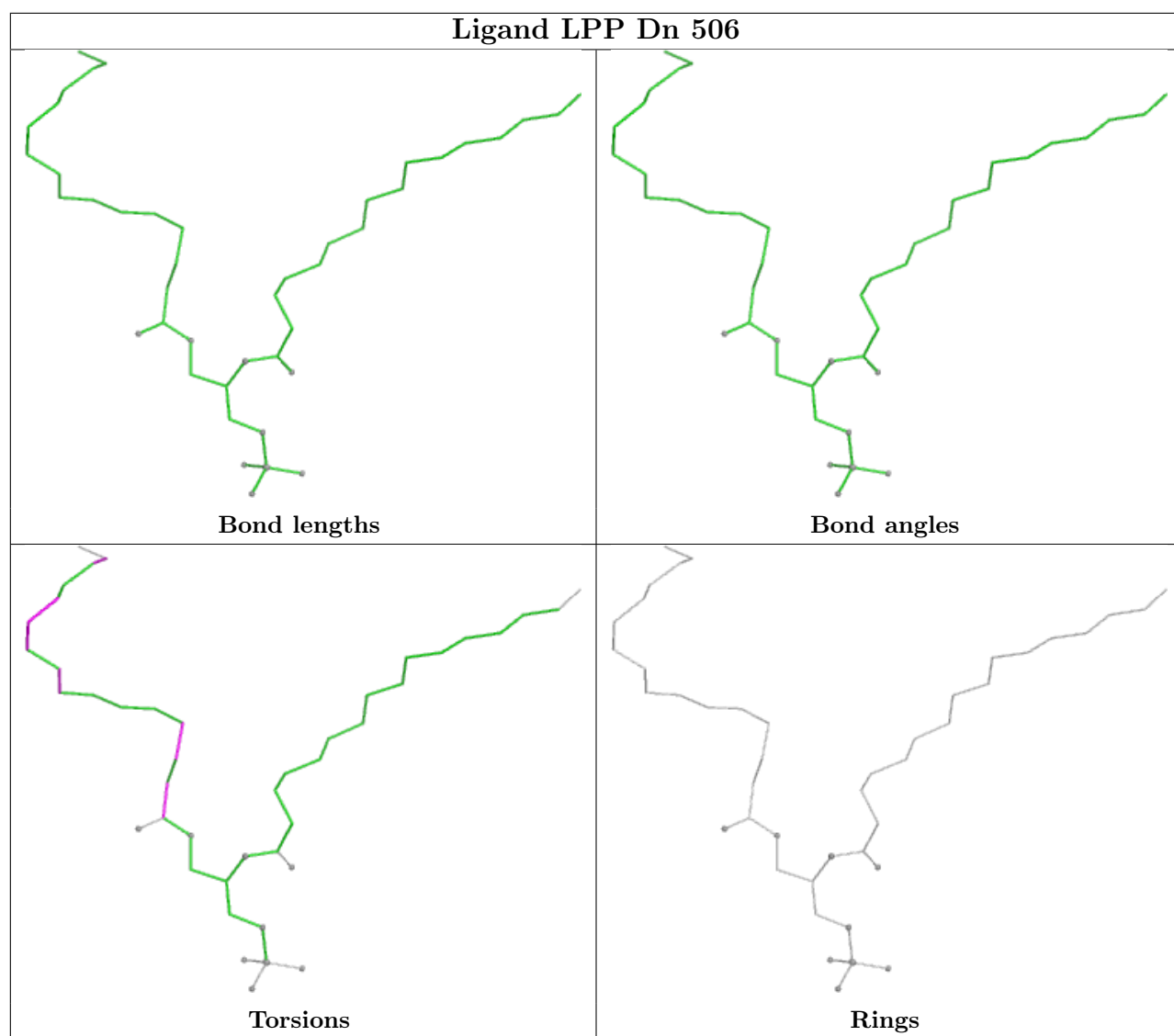


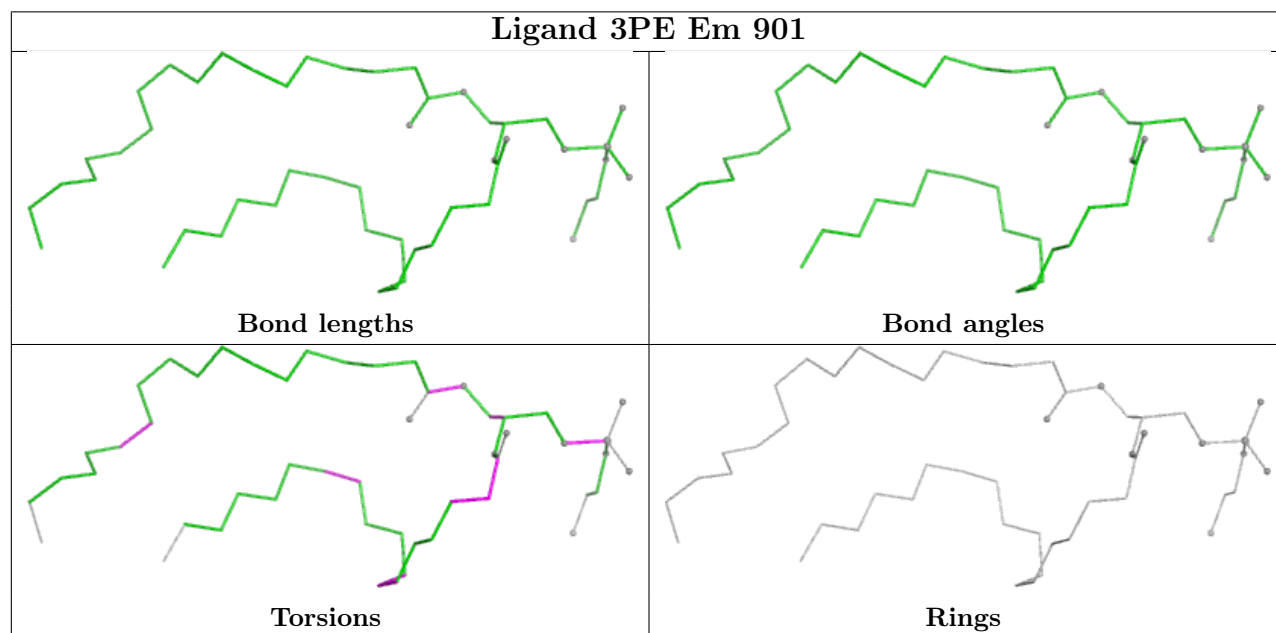
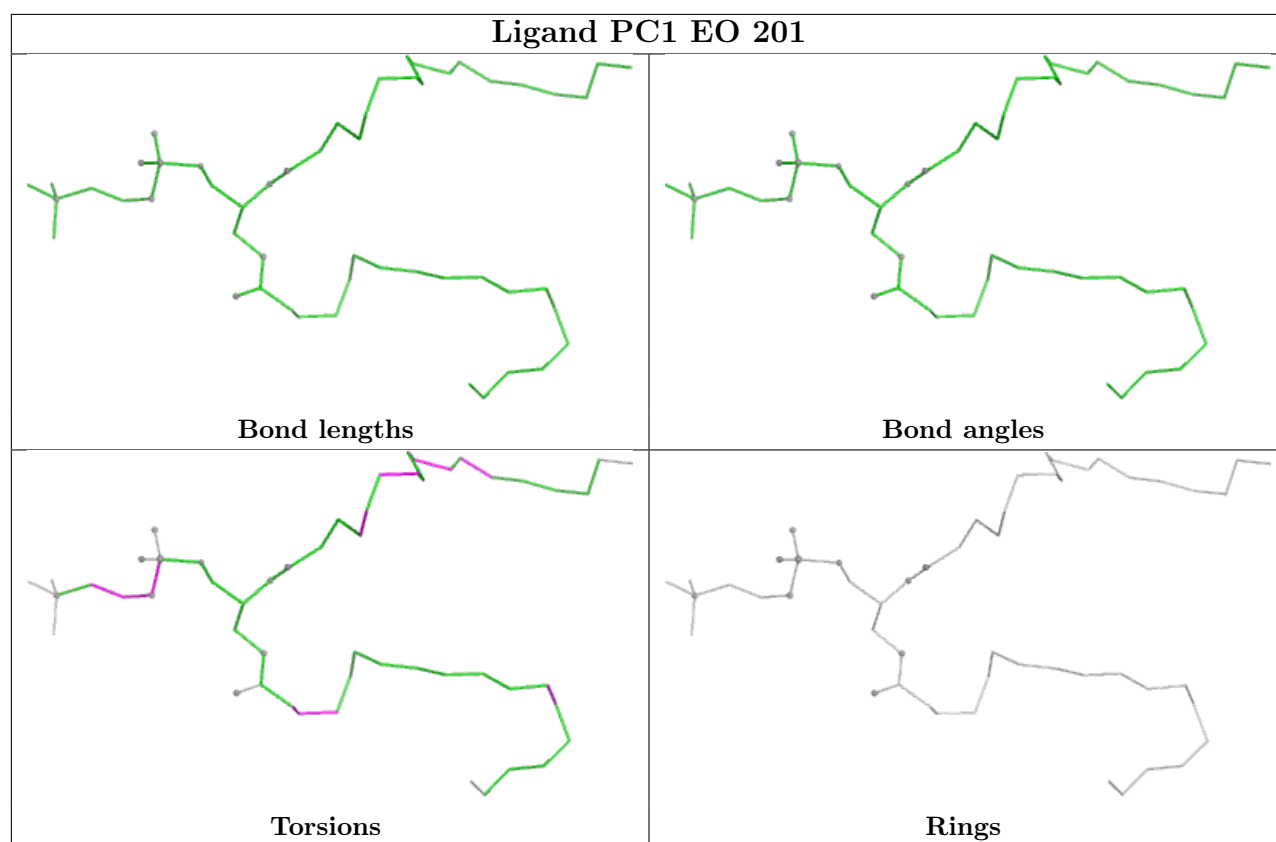


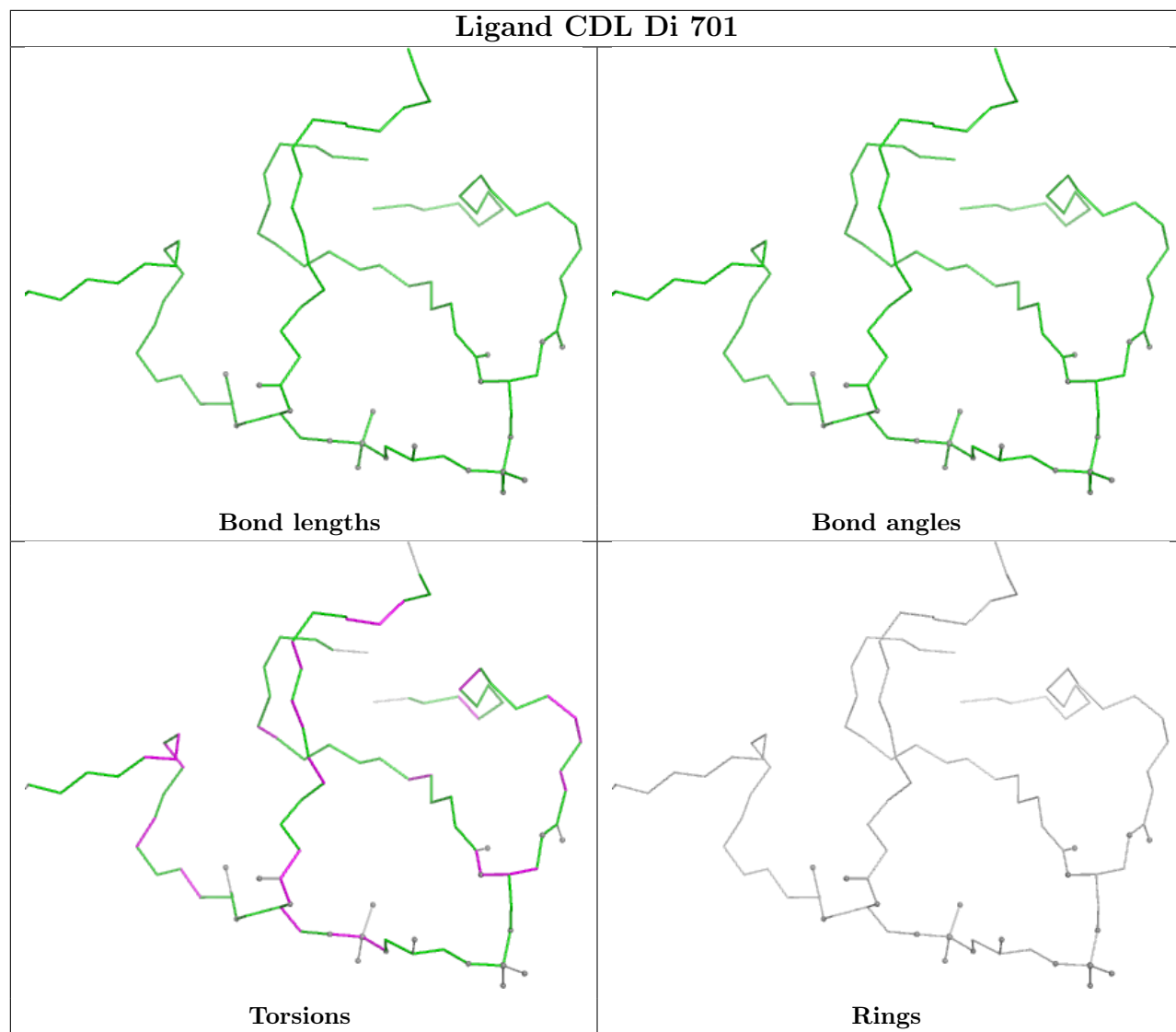


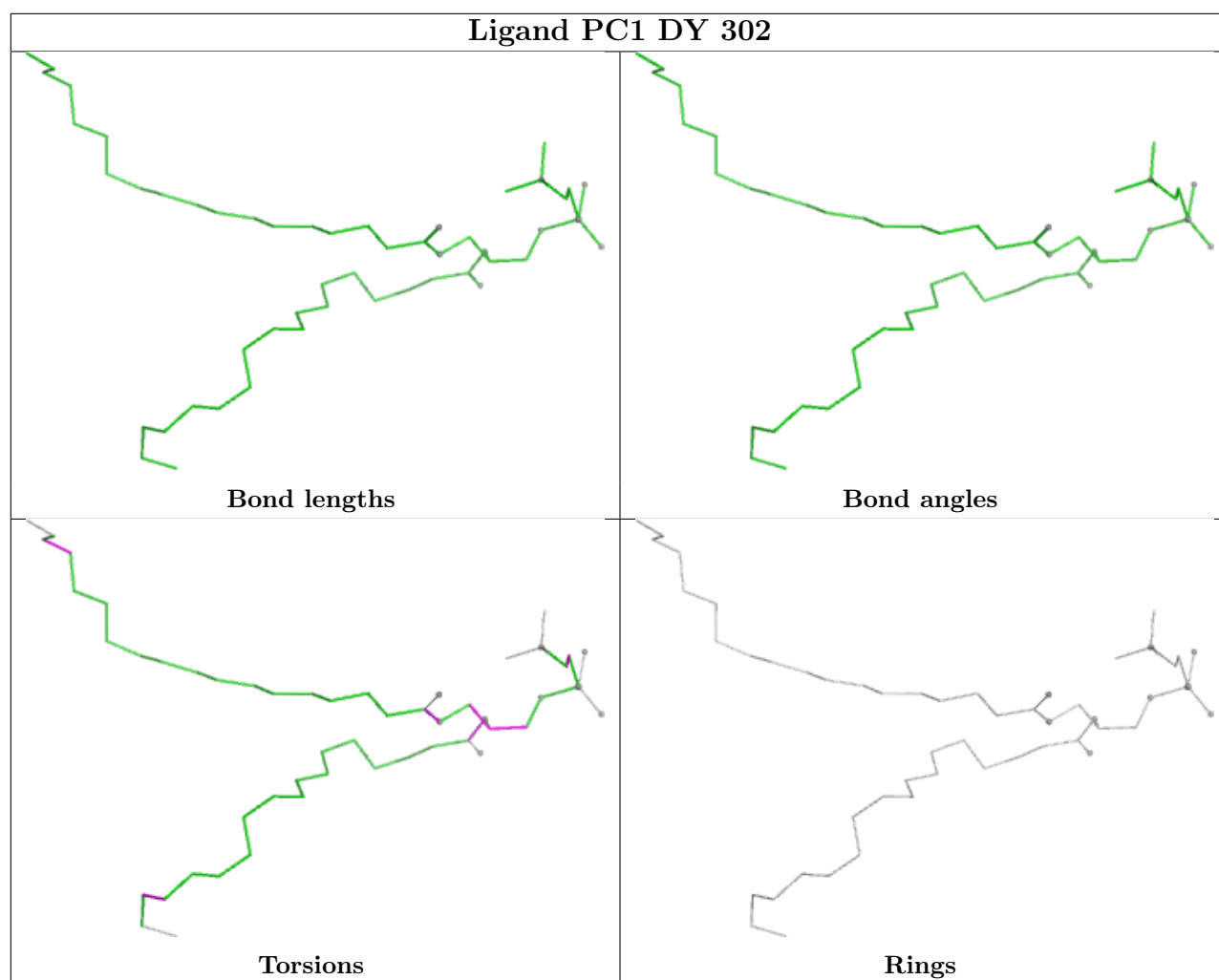


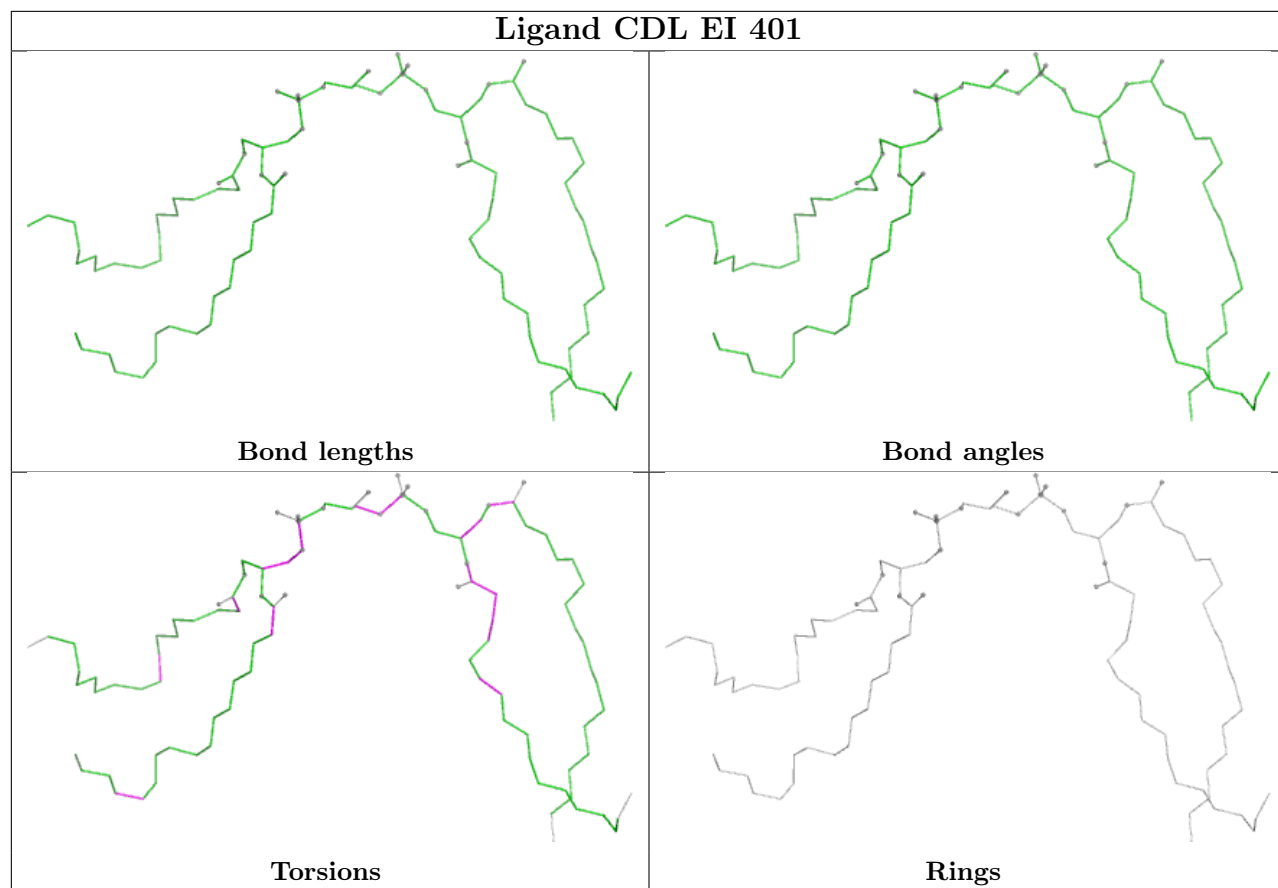


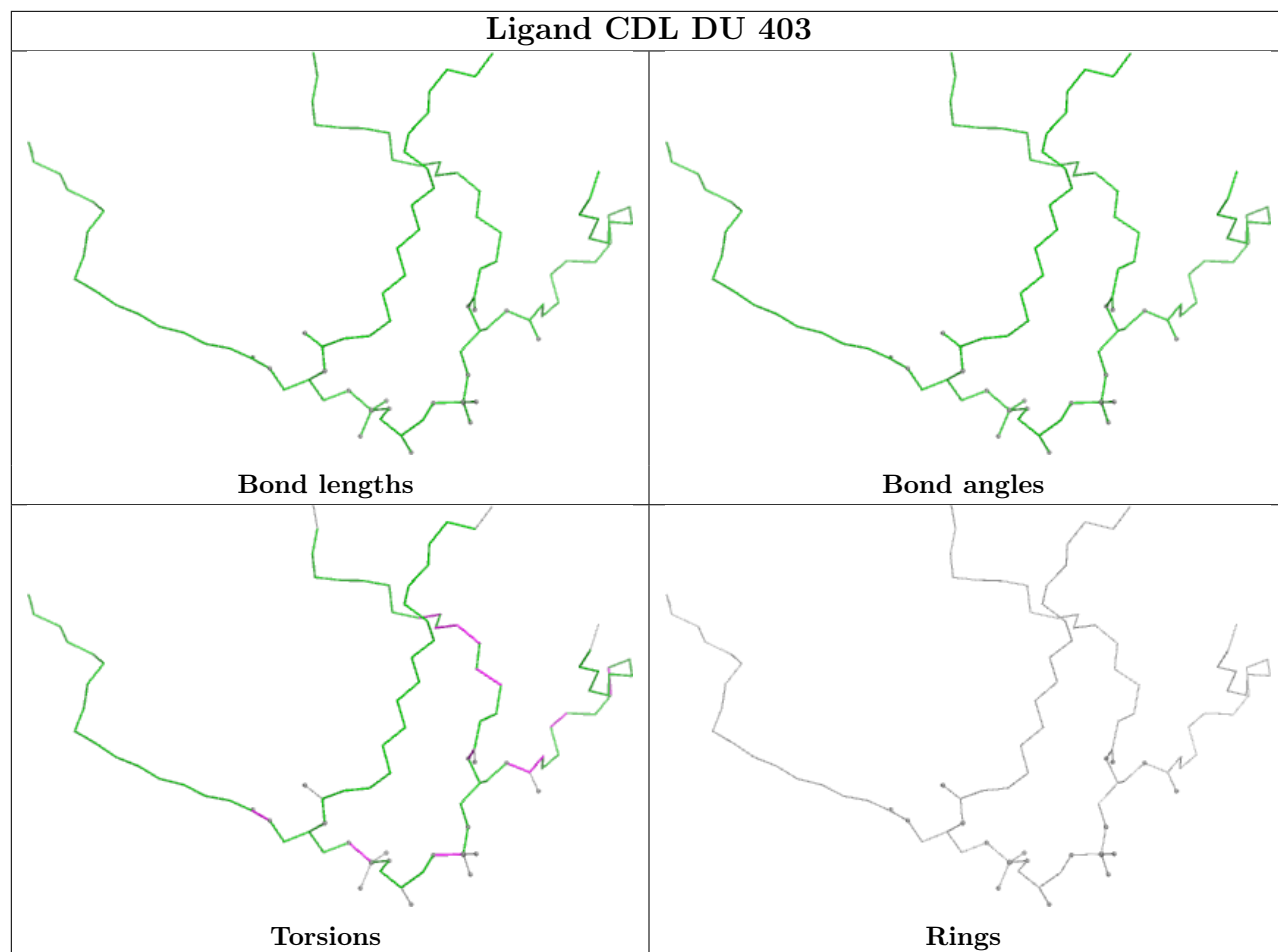


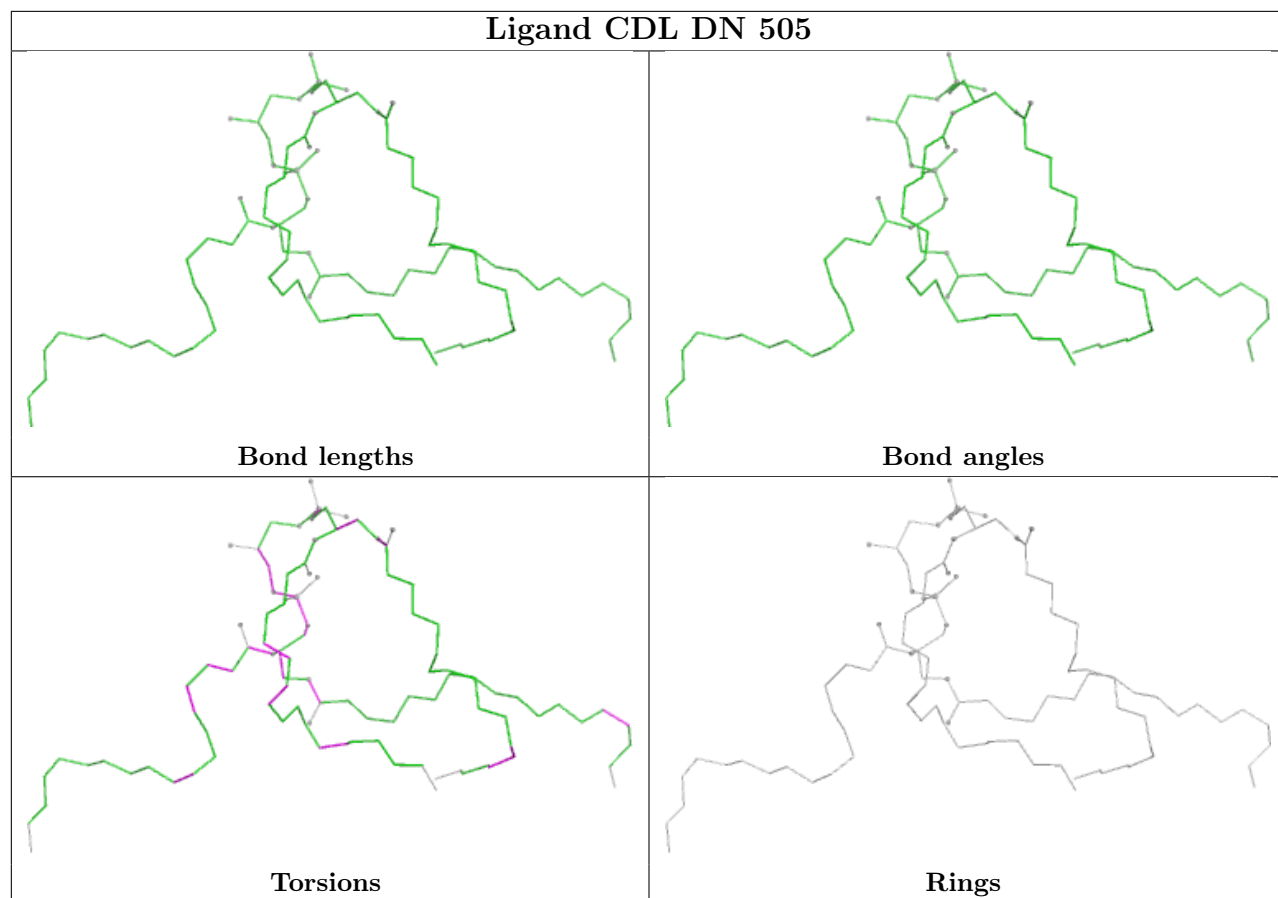


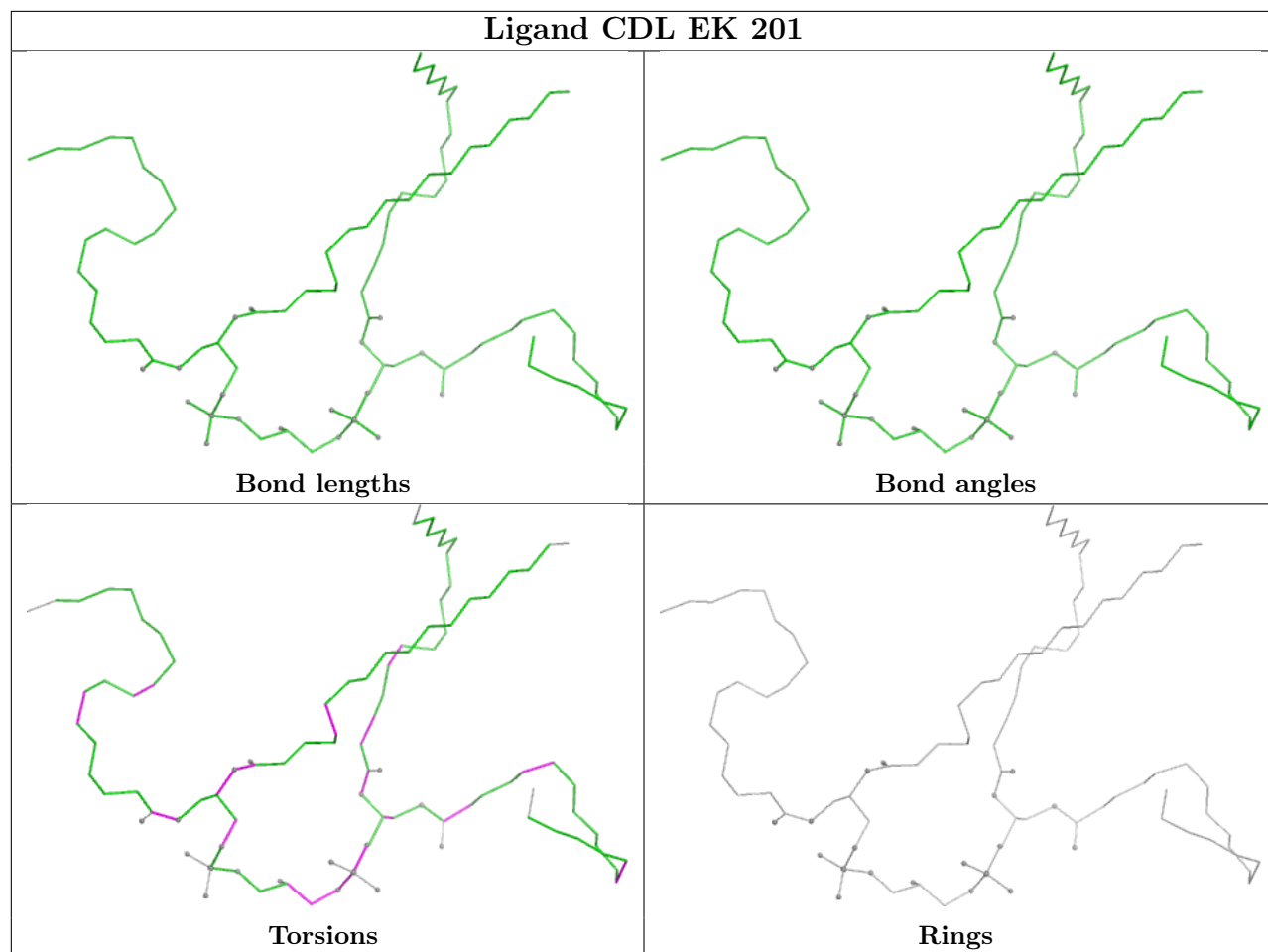


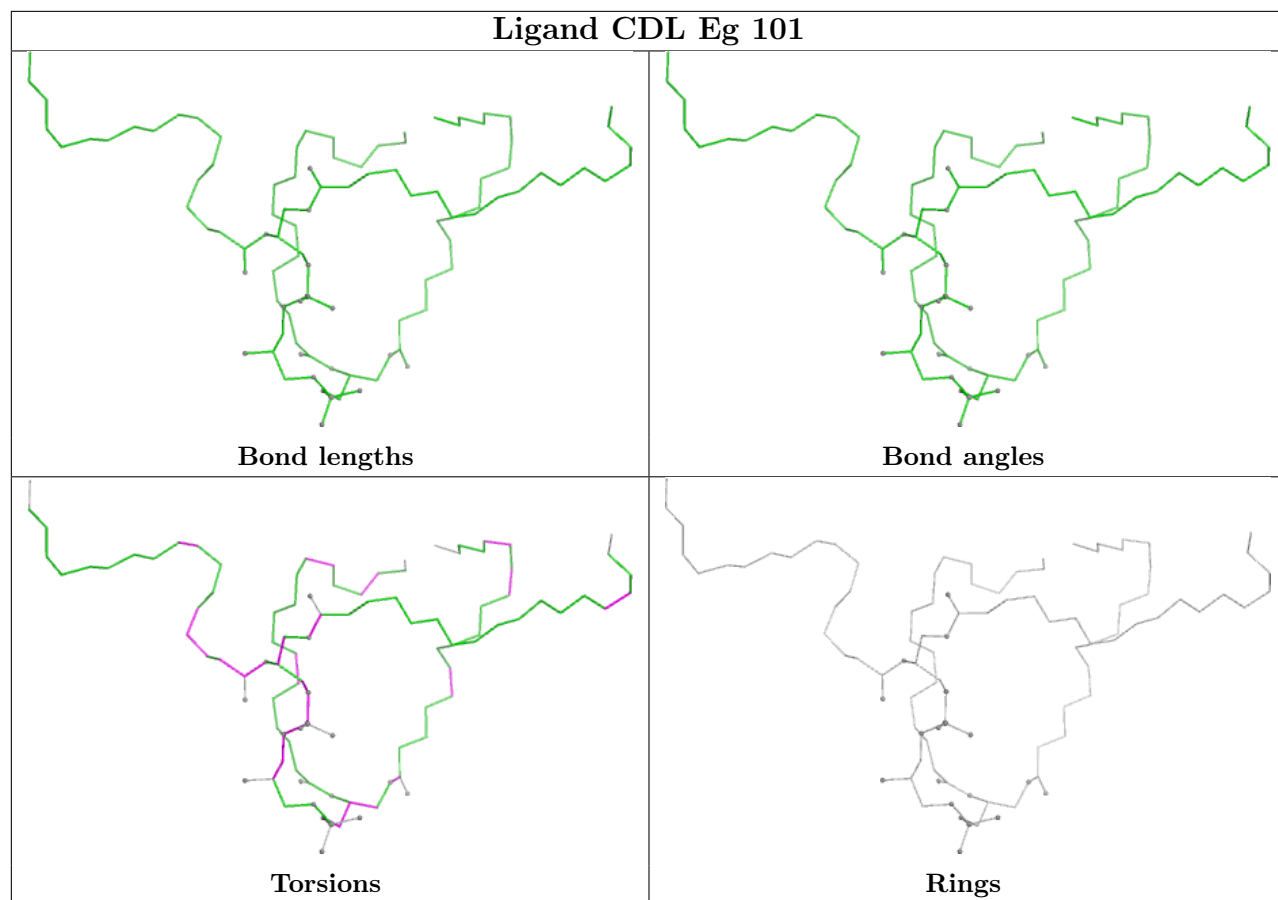




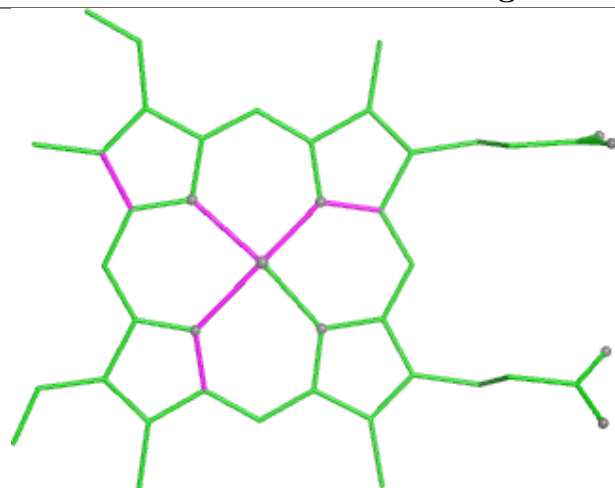




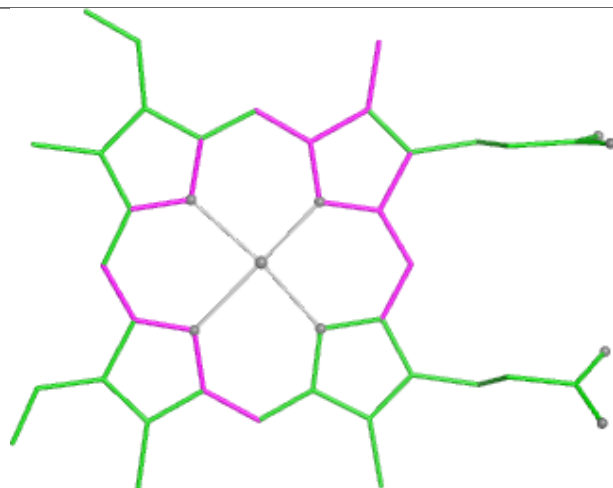




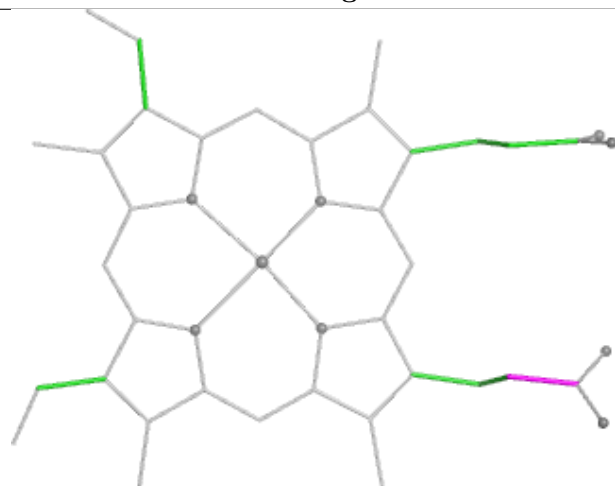
Ligand HEM ED 602



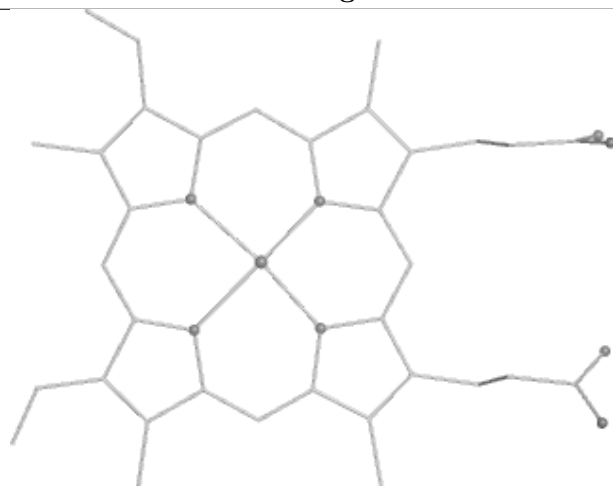
Bond lengths



Bond angles

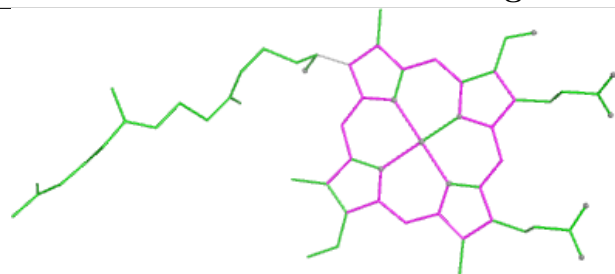


Torsions

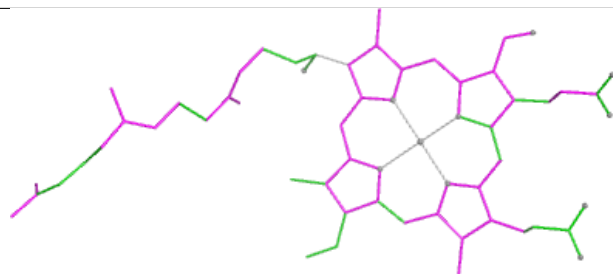


Rings

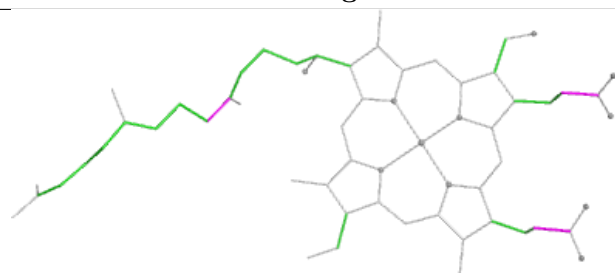
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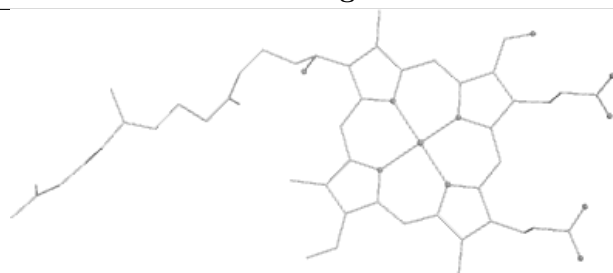
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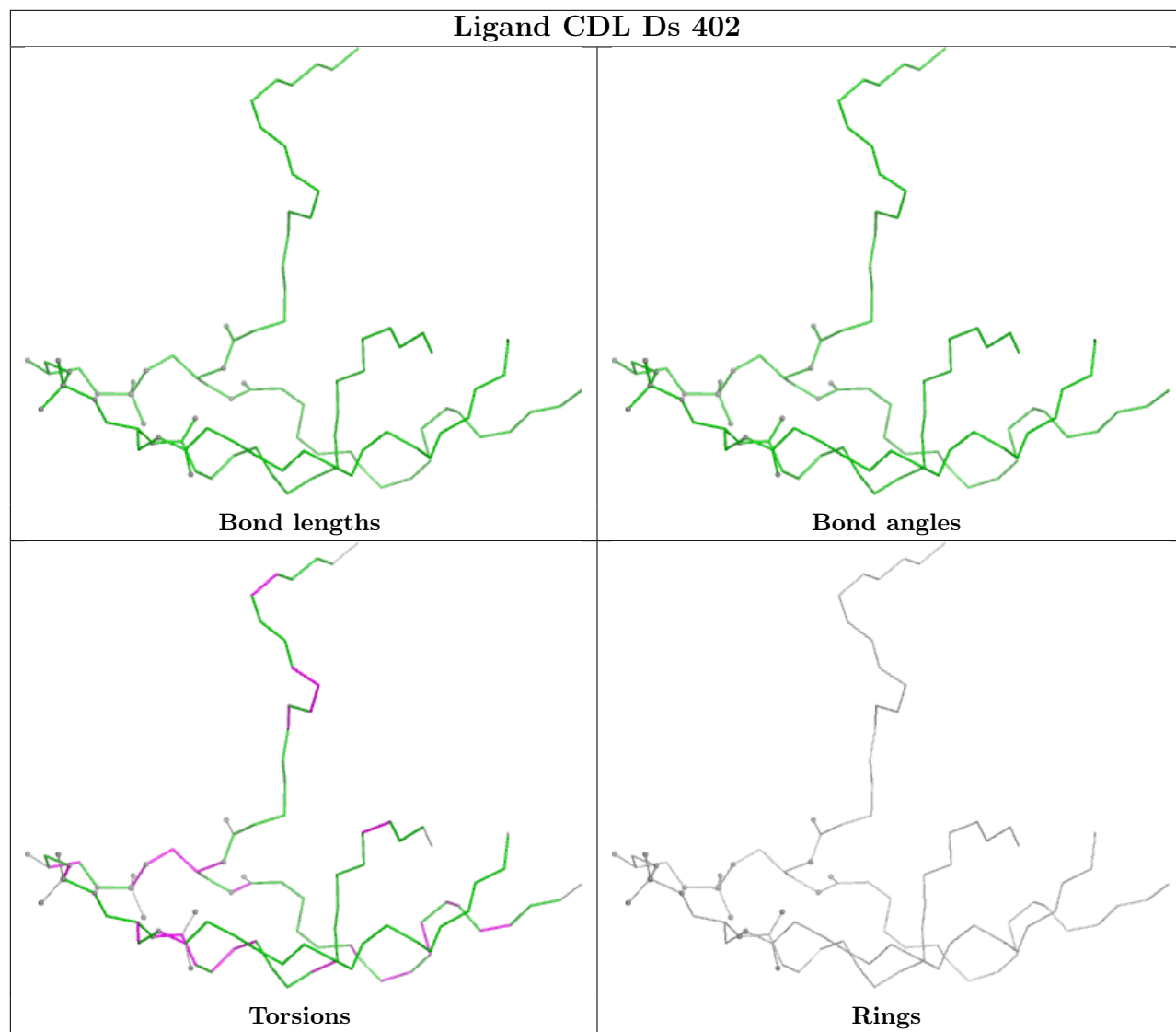
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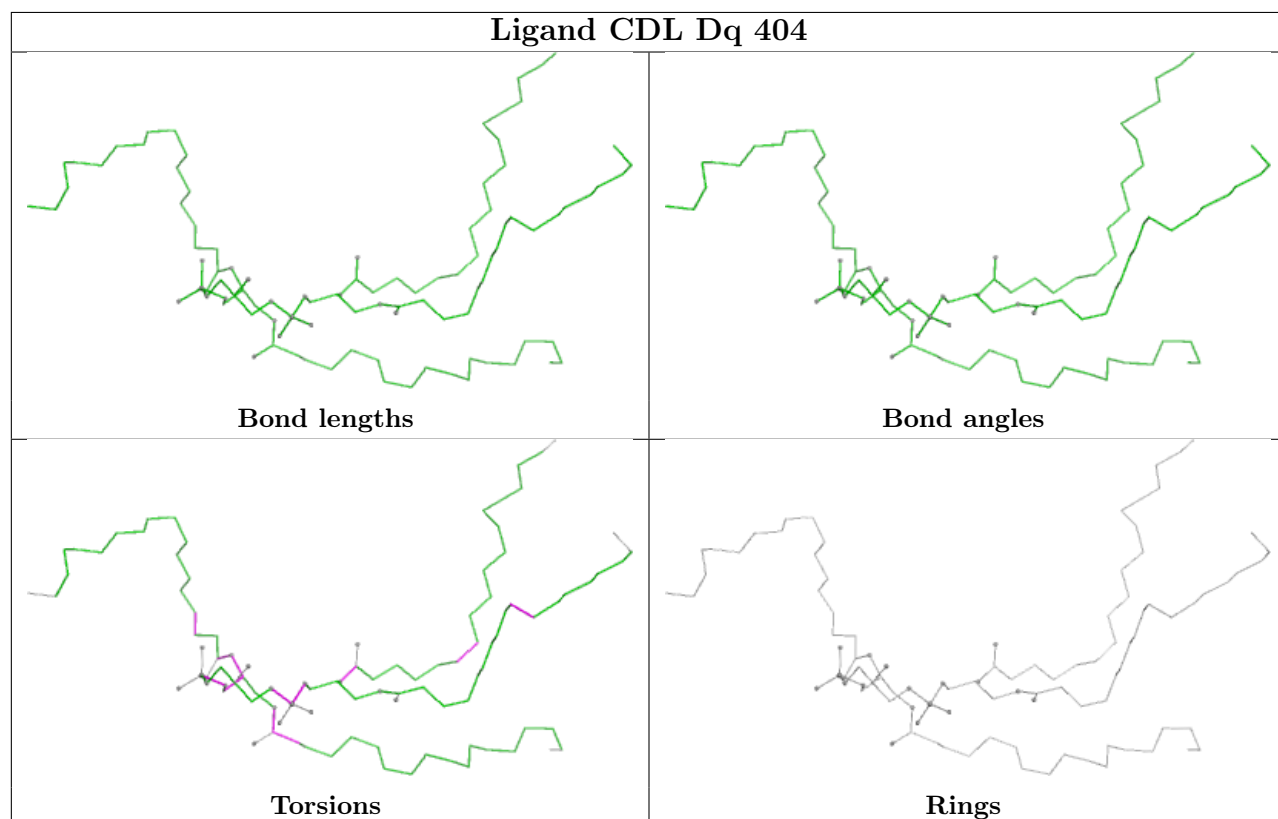
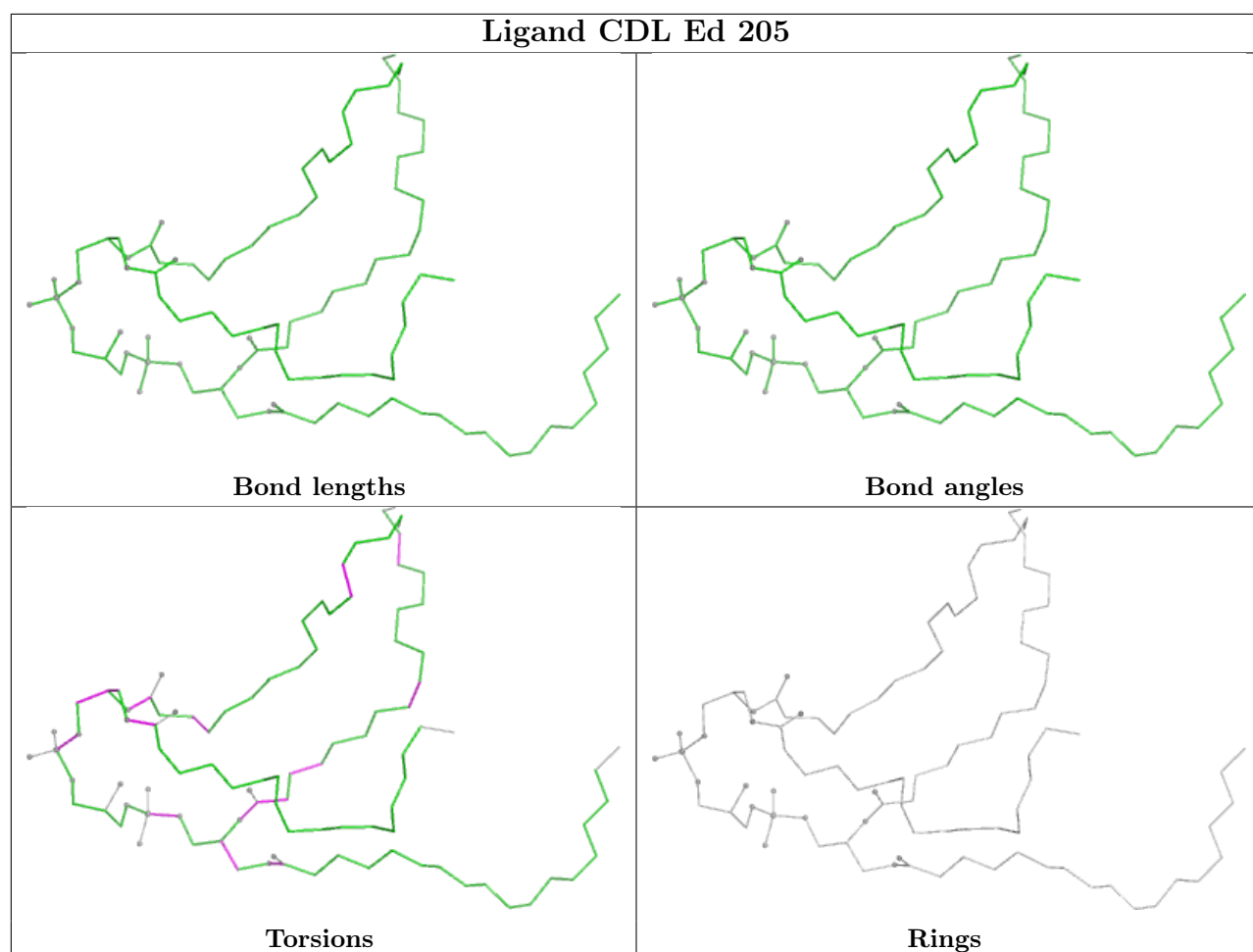


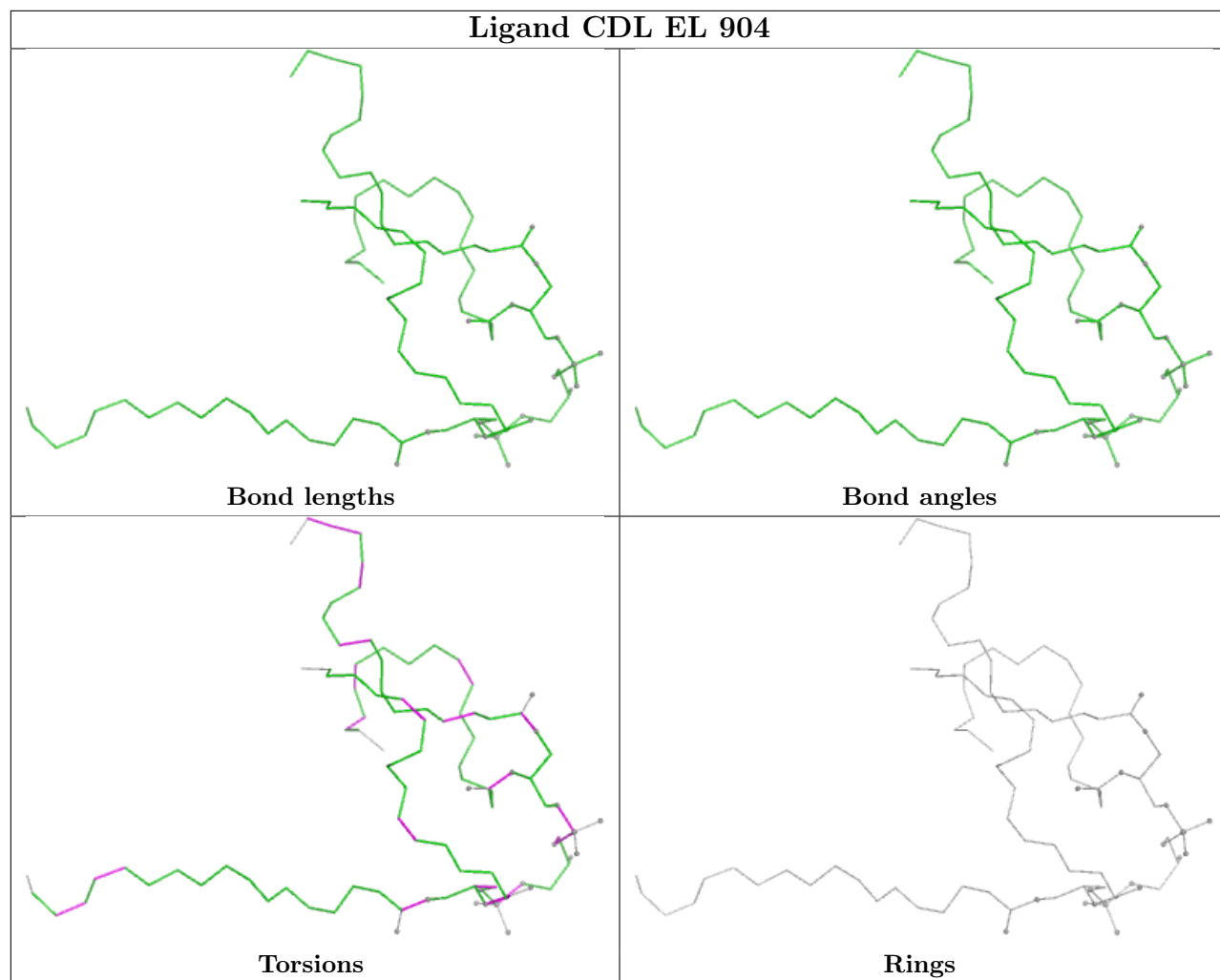
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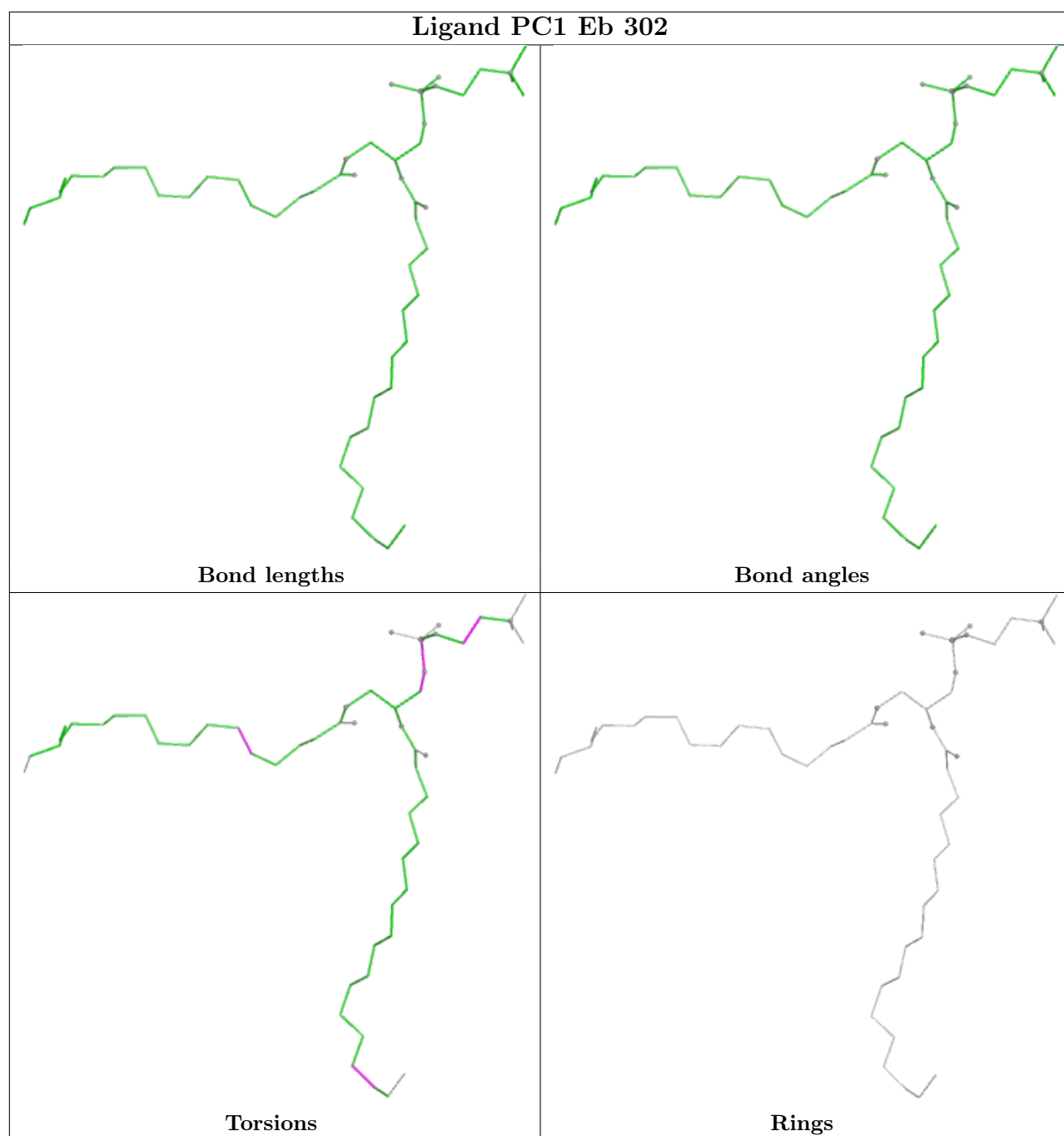


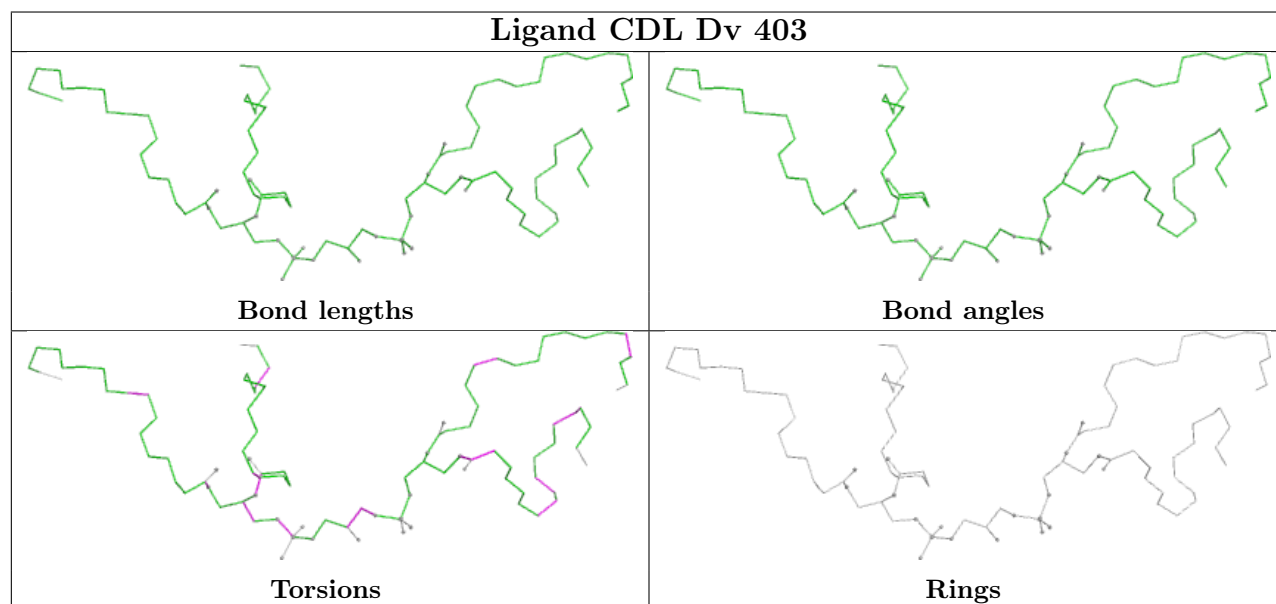
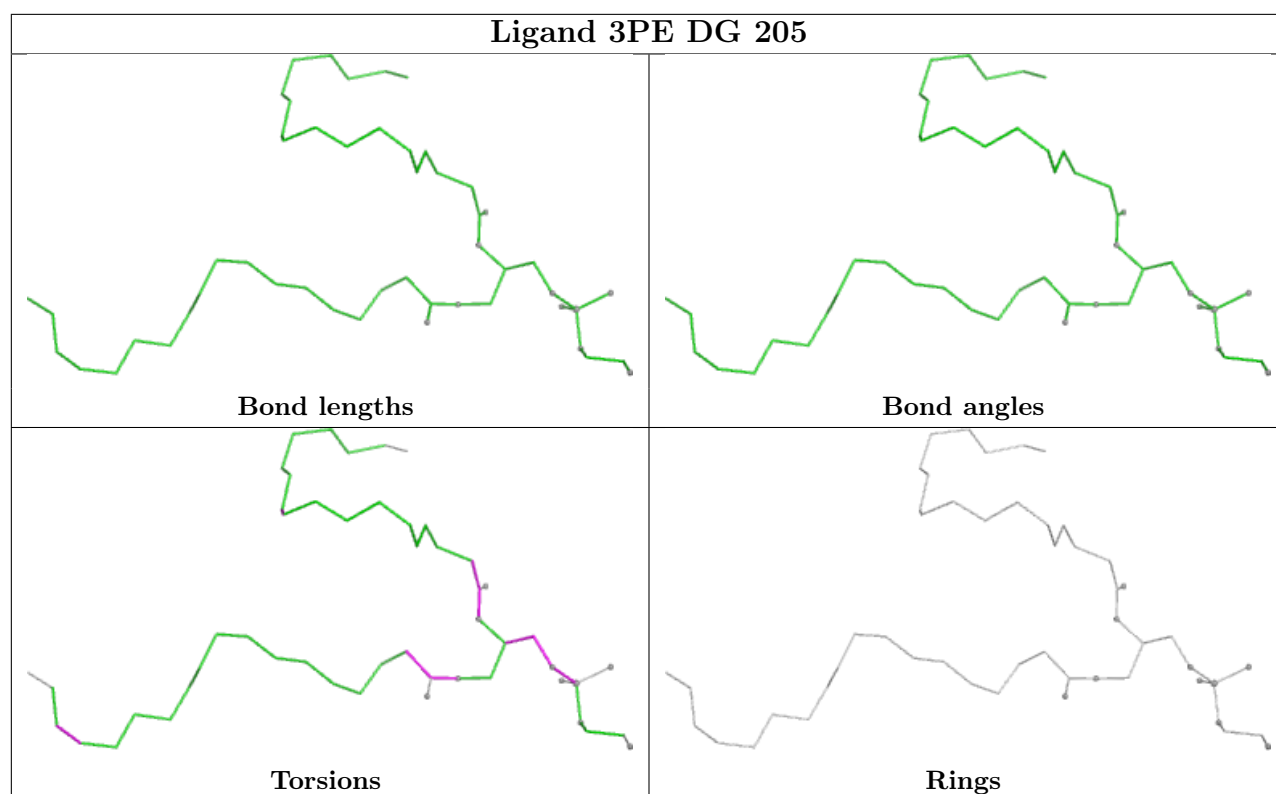
Rings

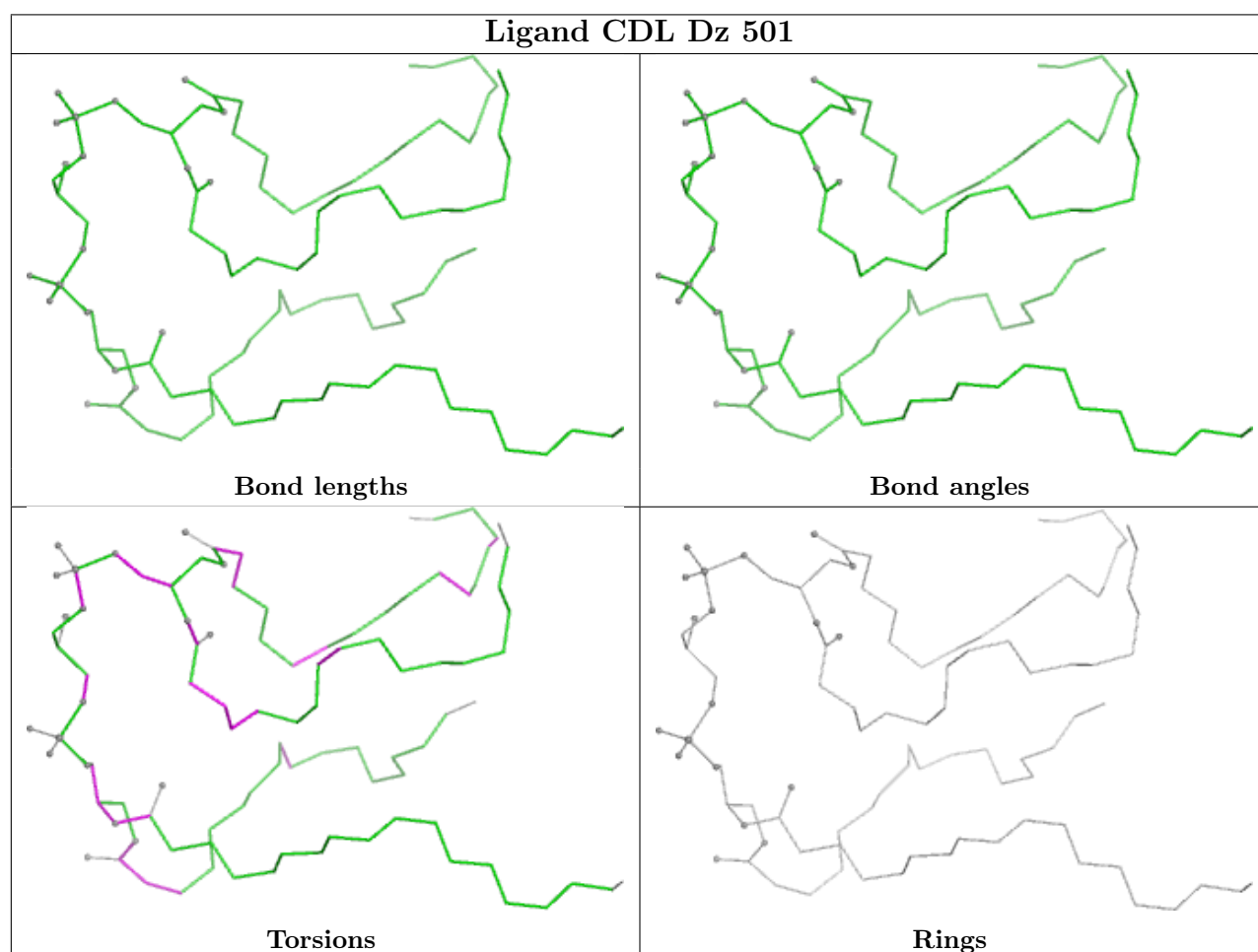
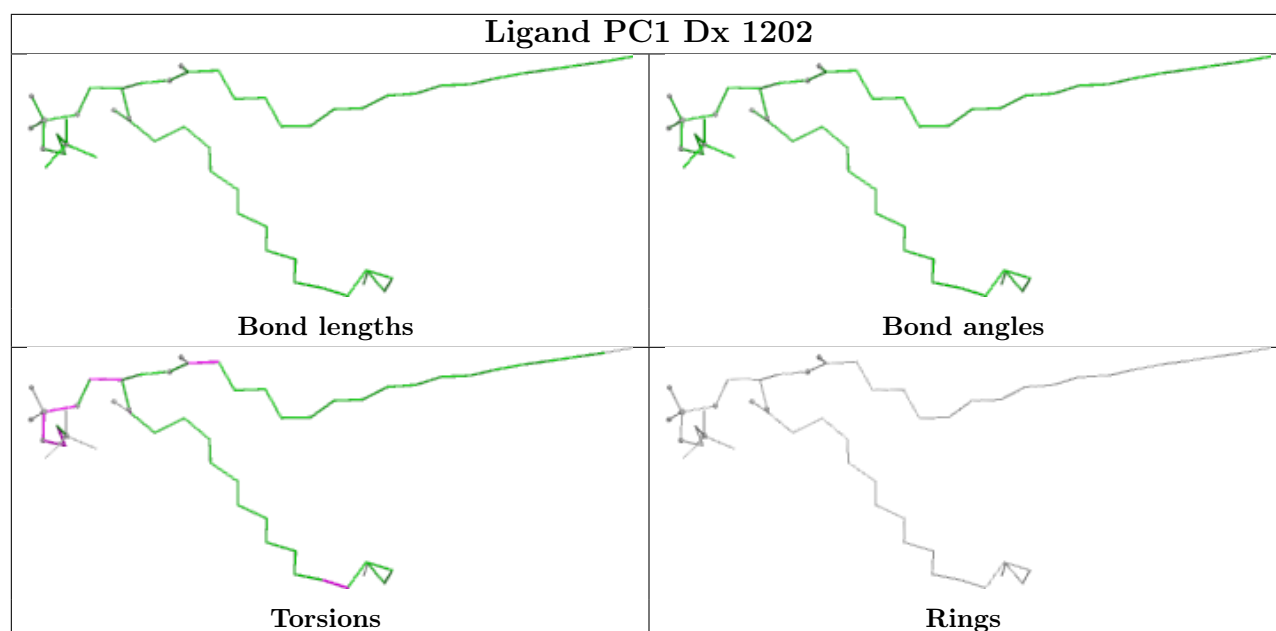


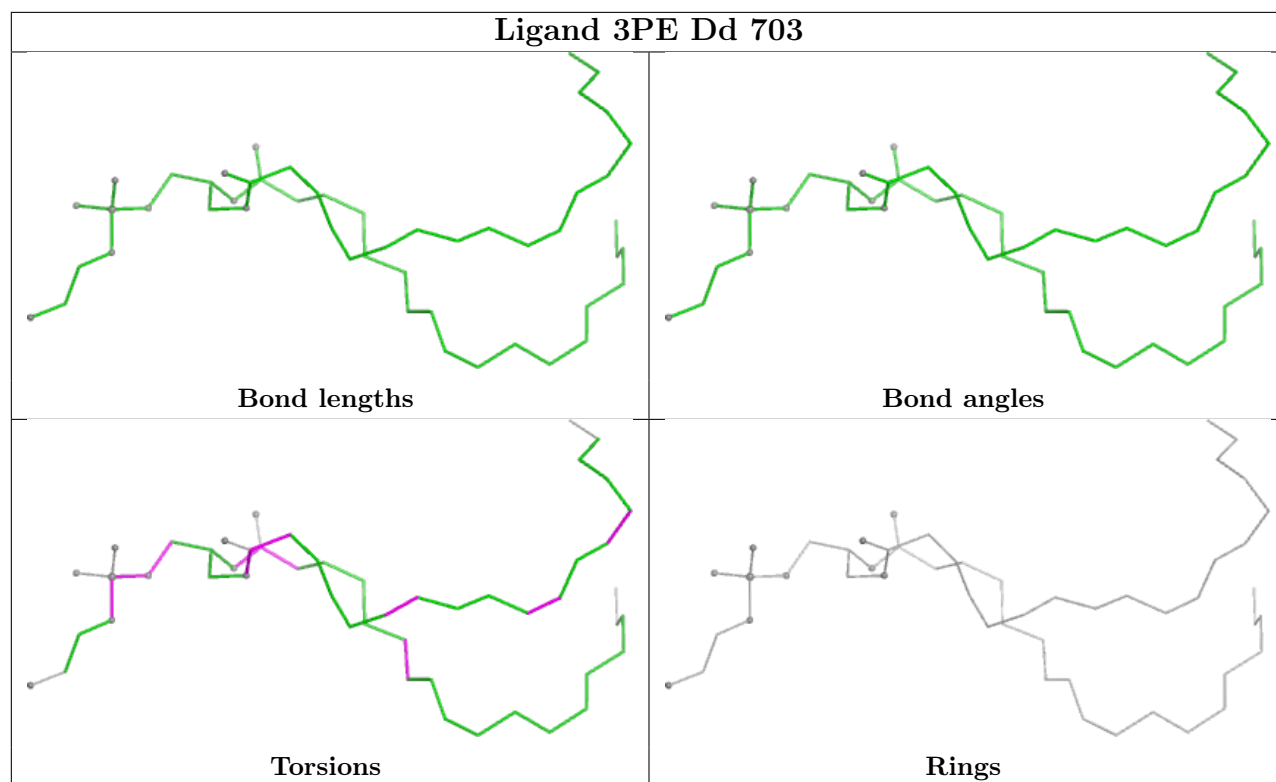
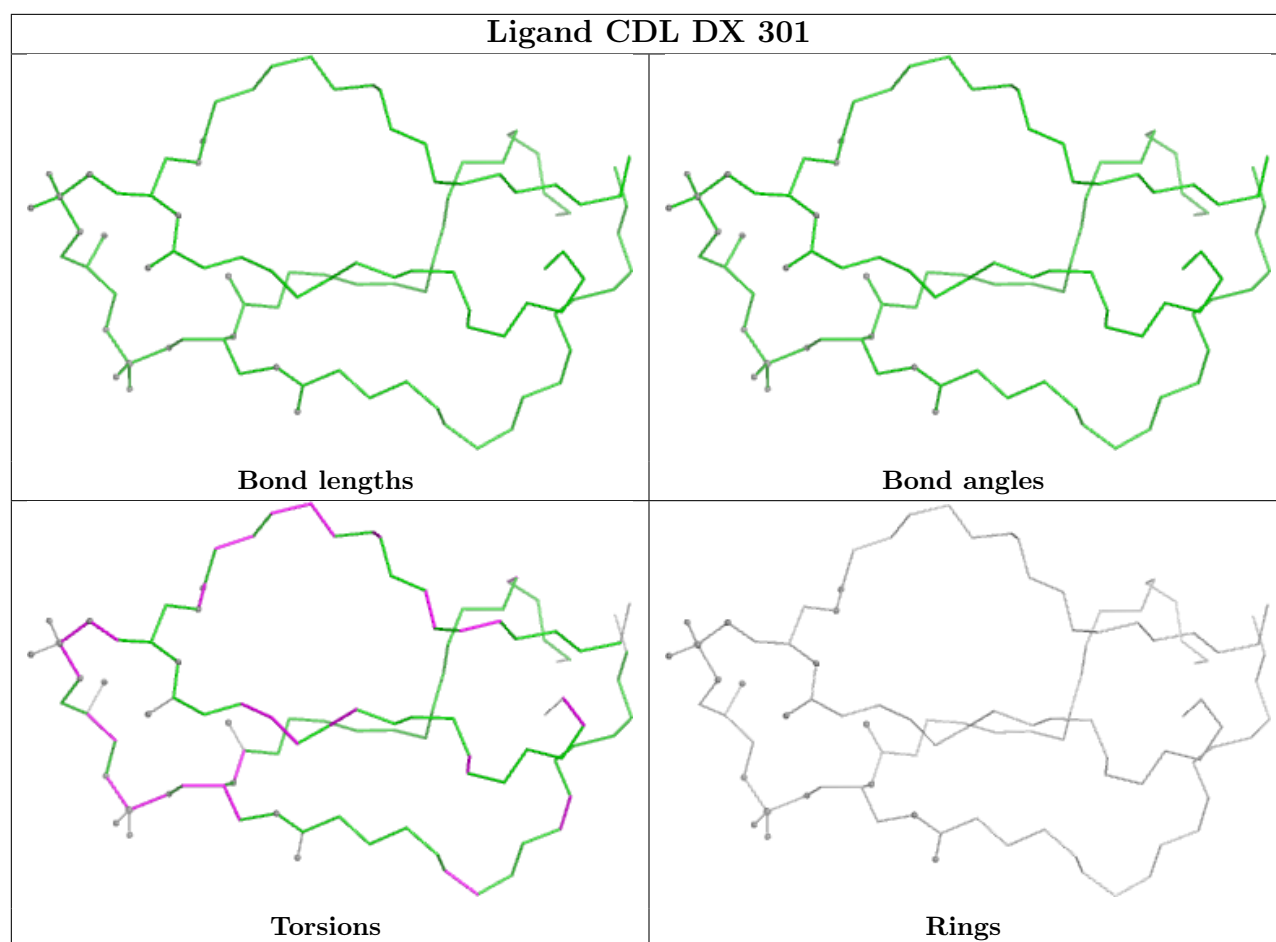


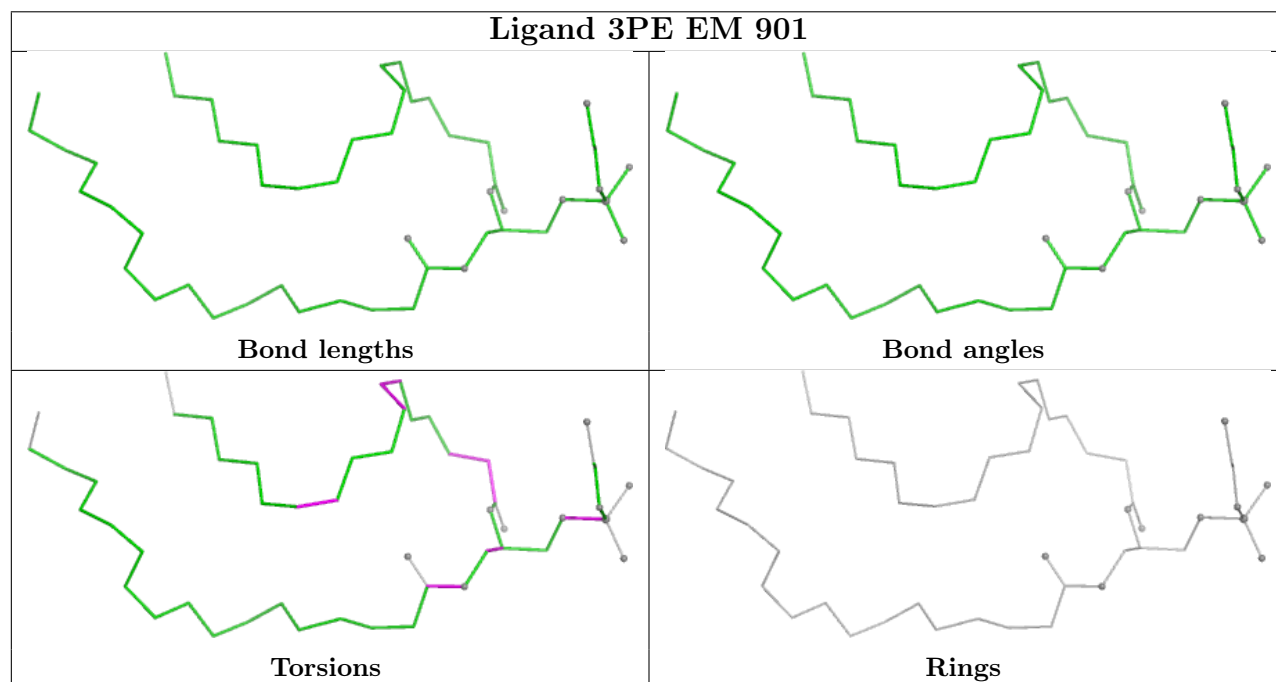
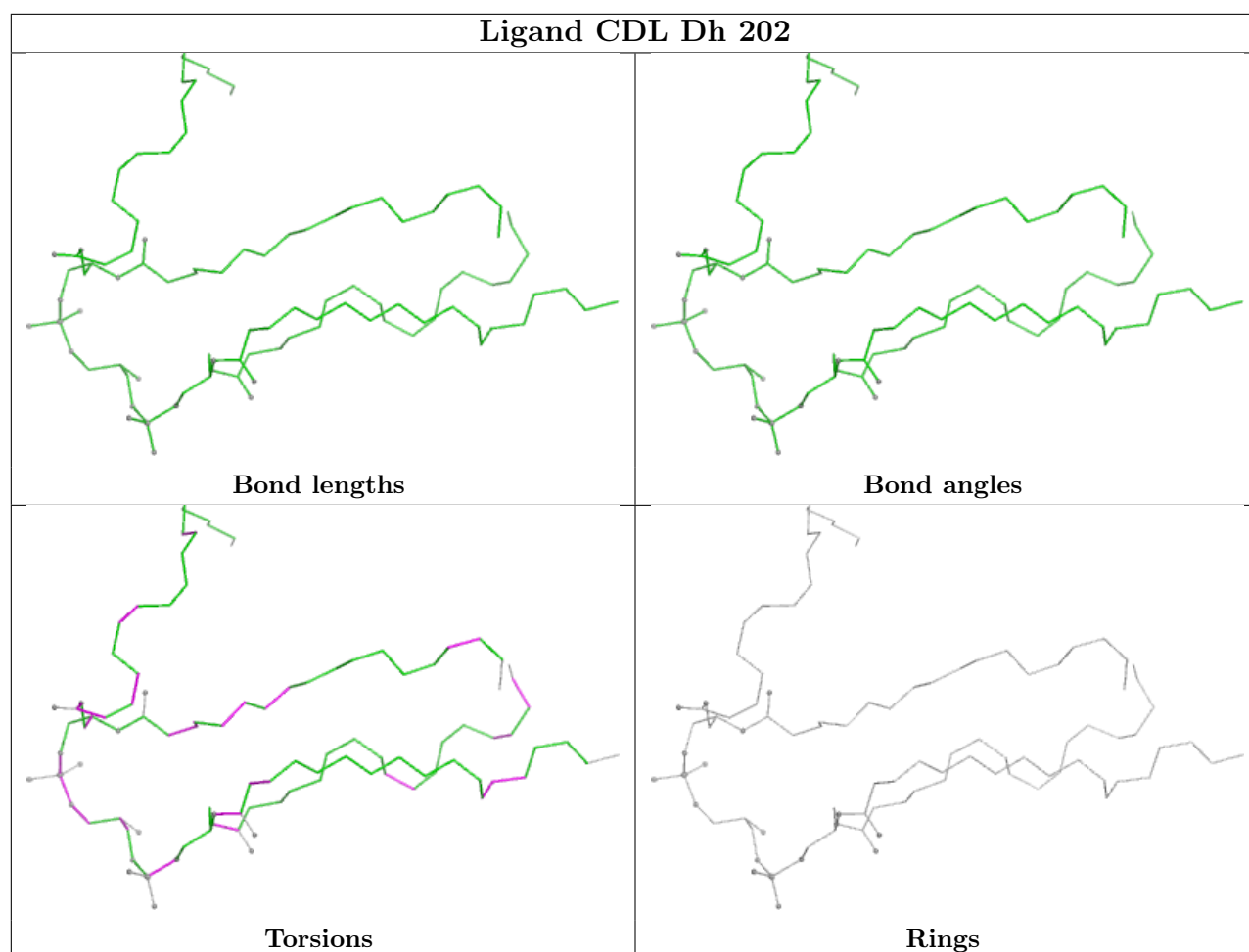


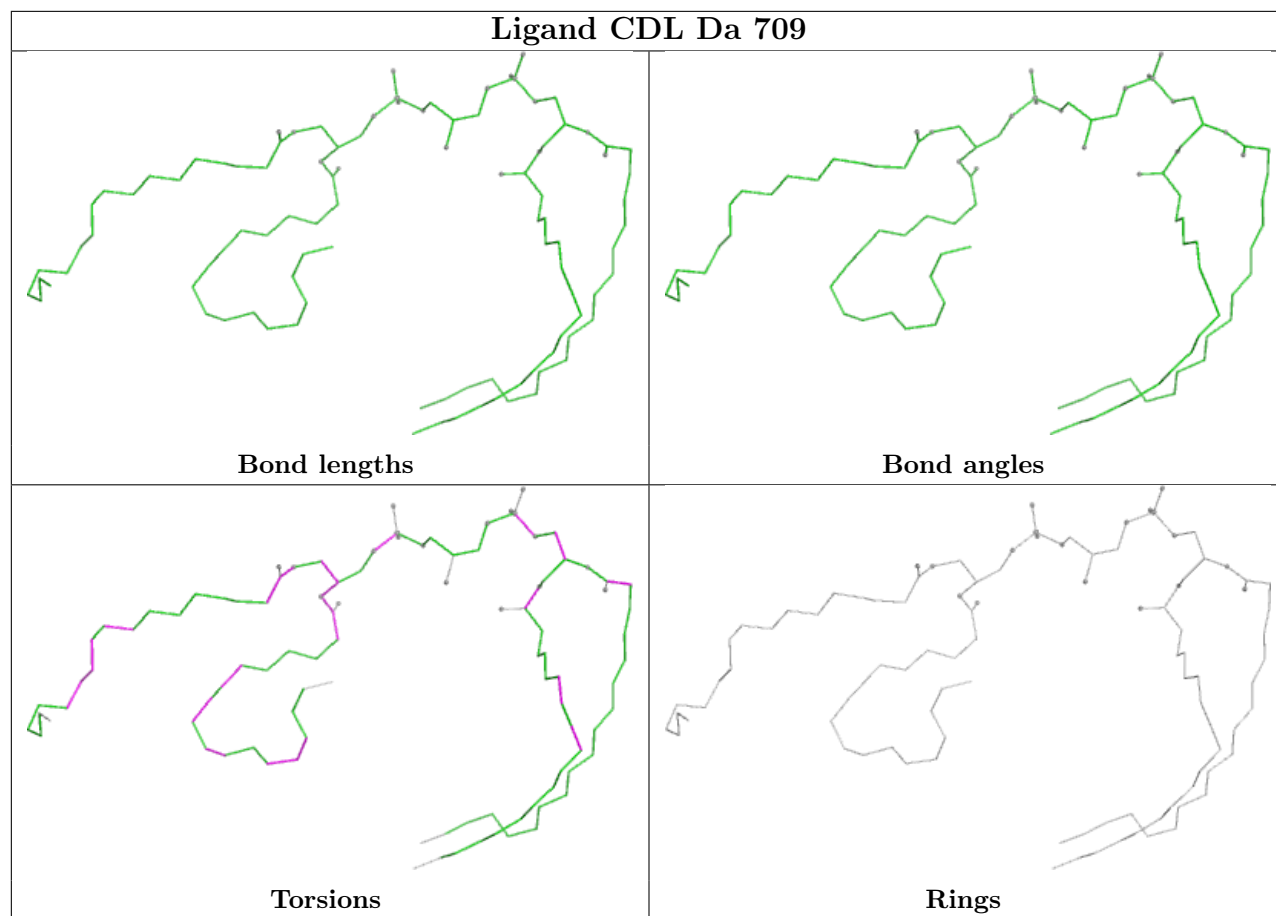


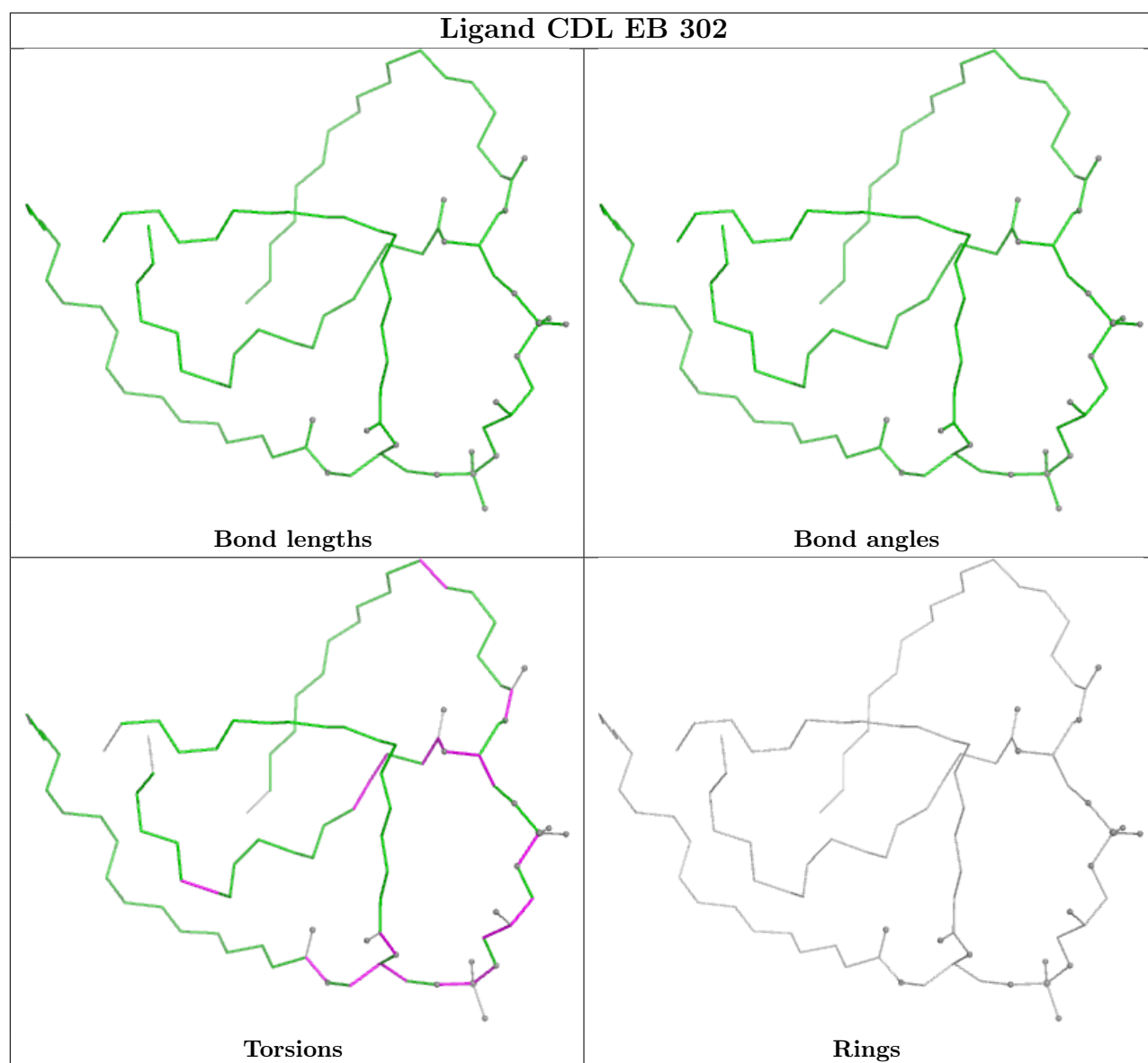


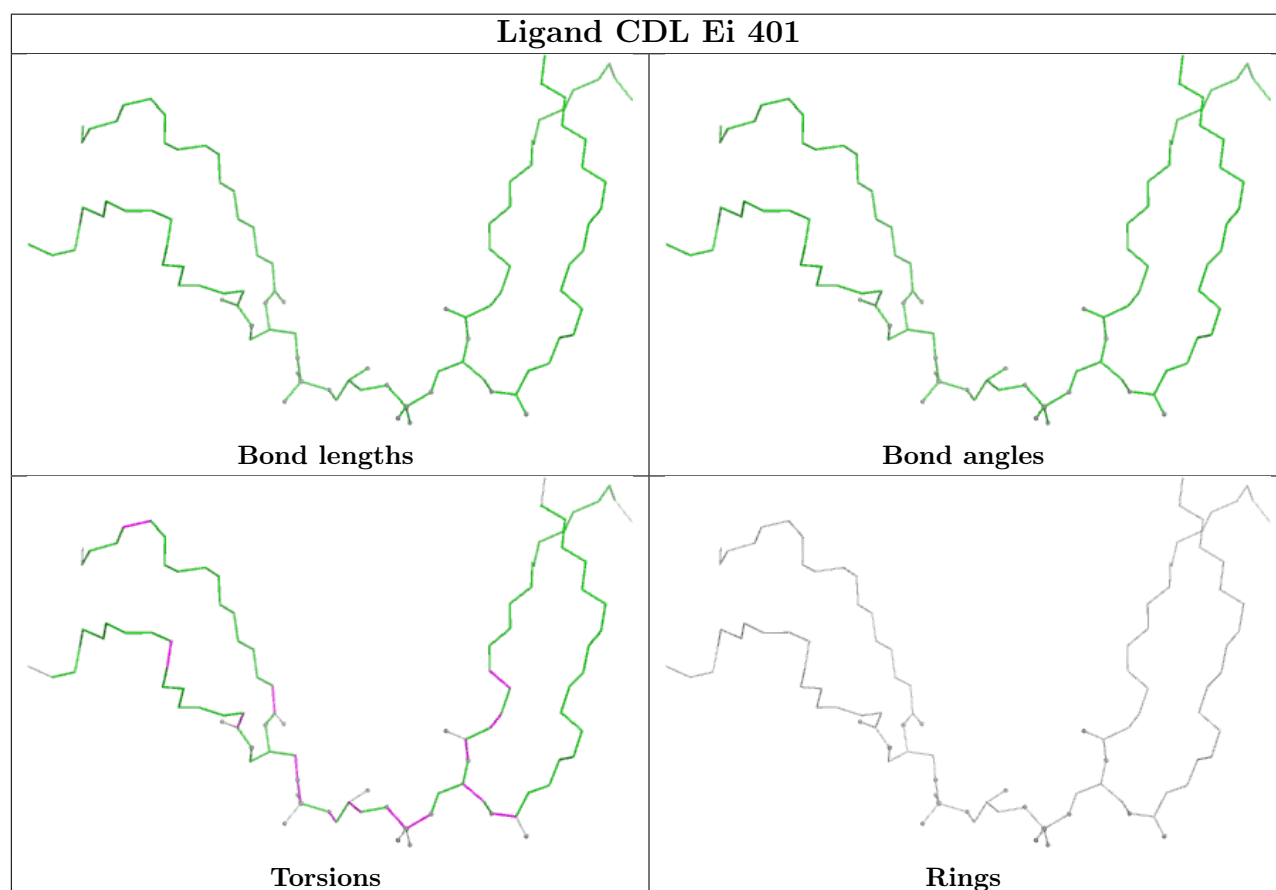
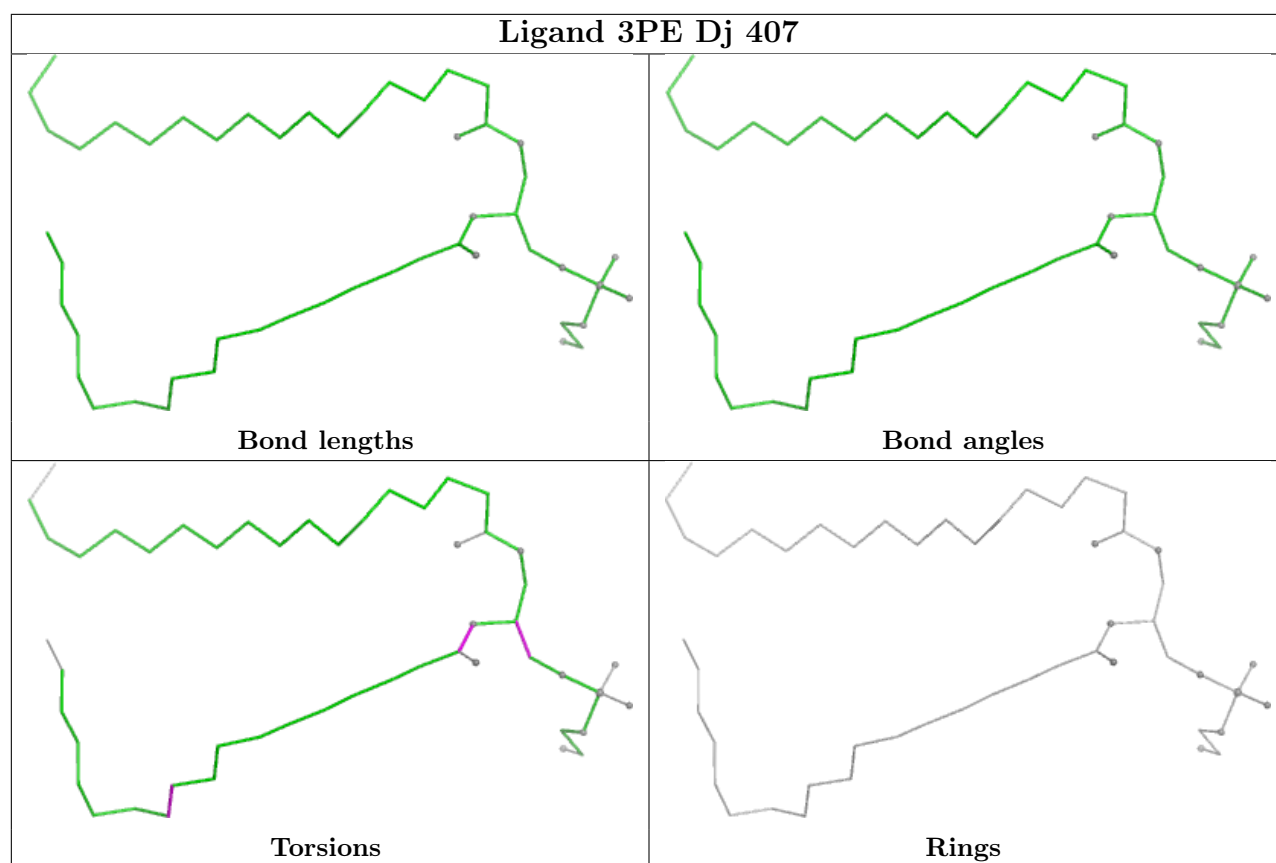


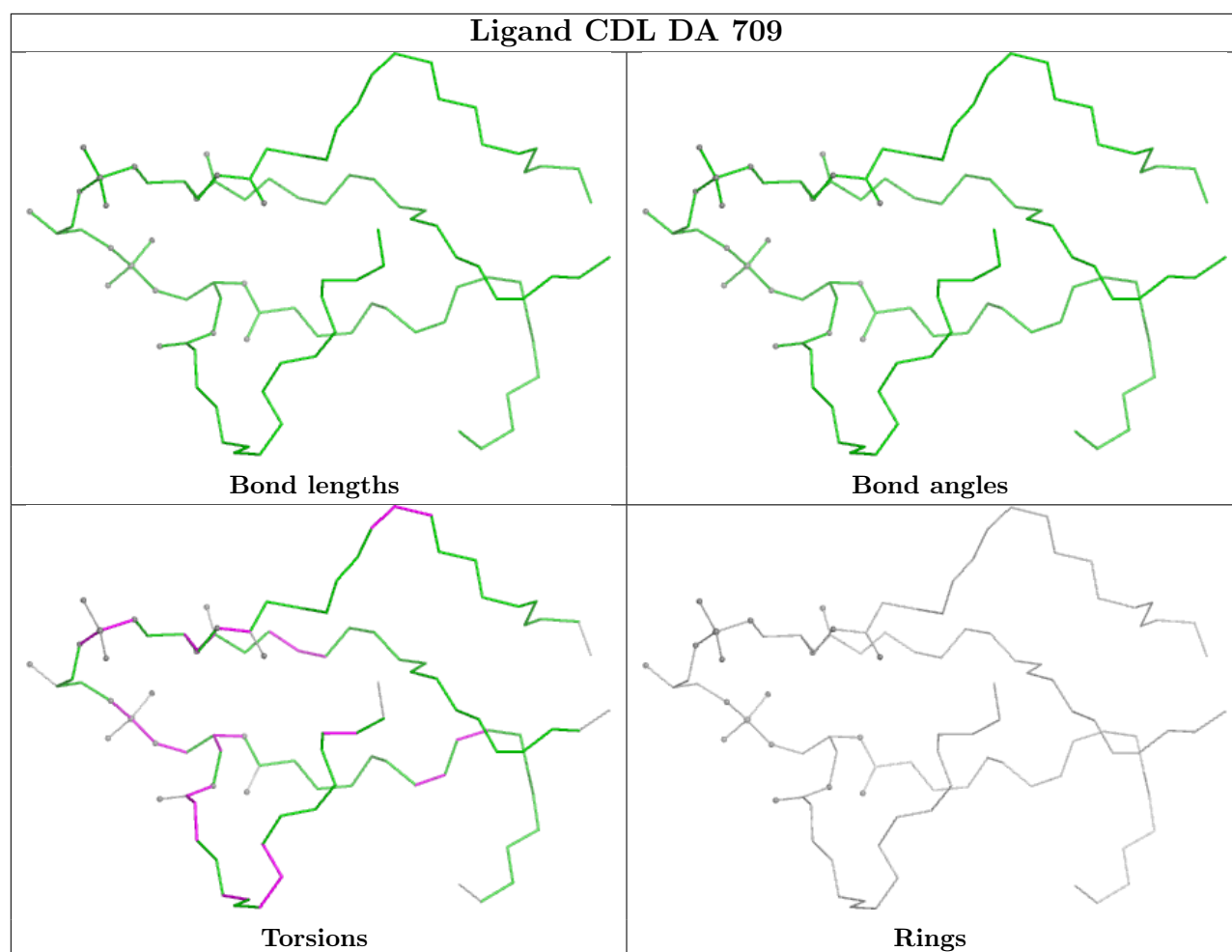


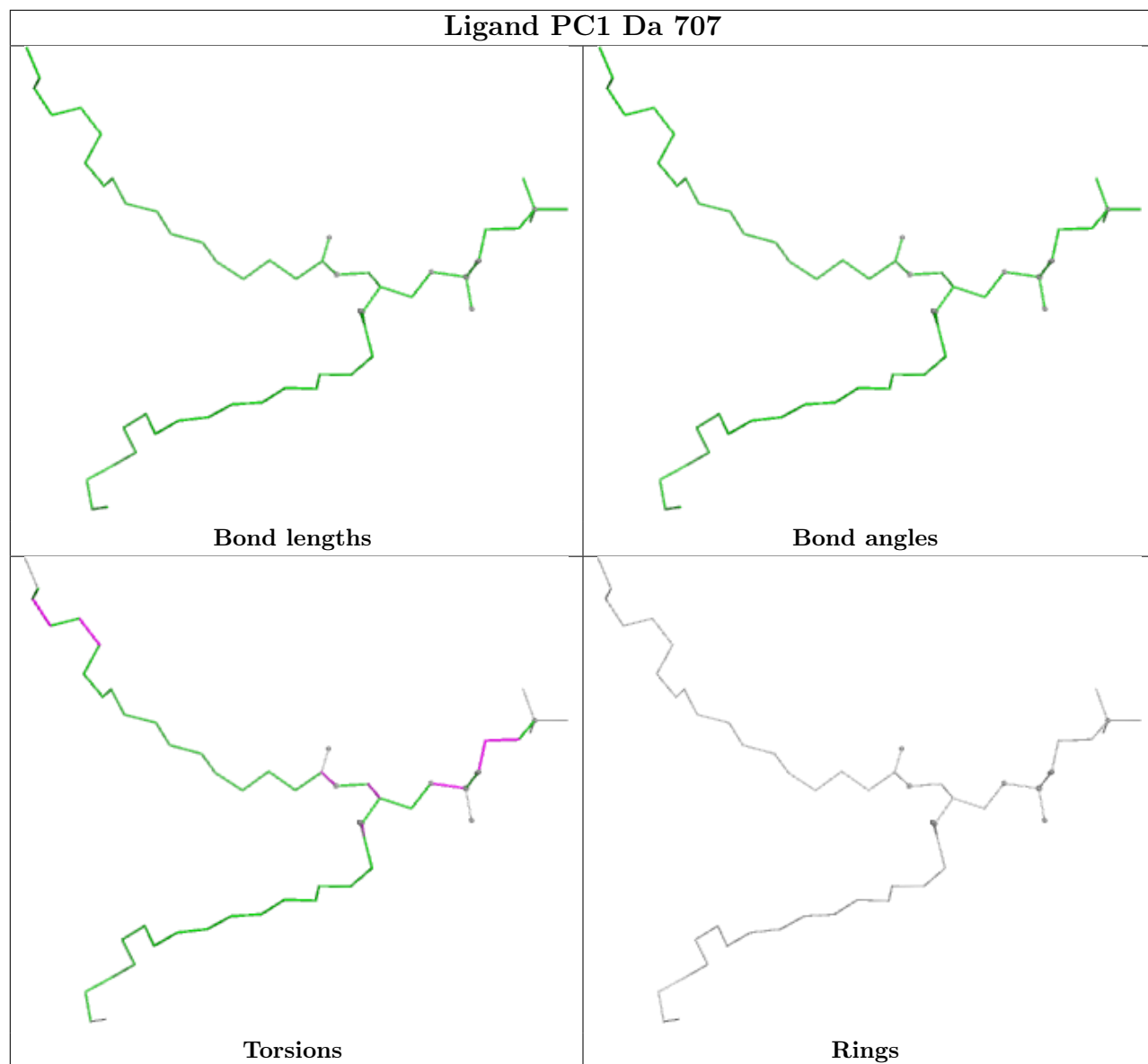


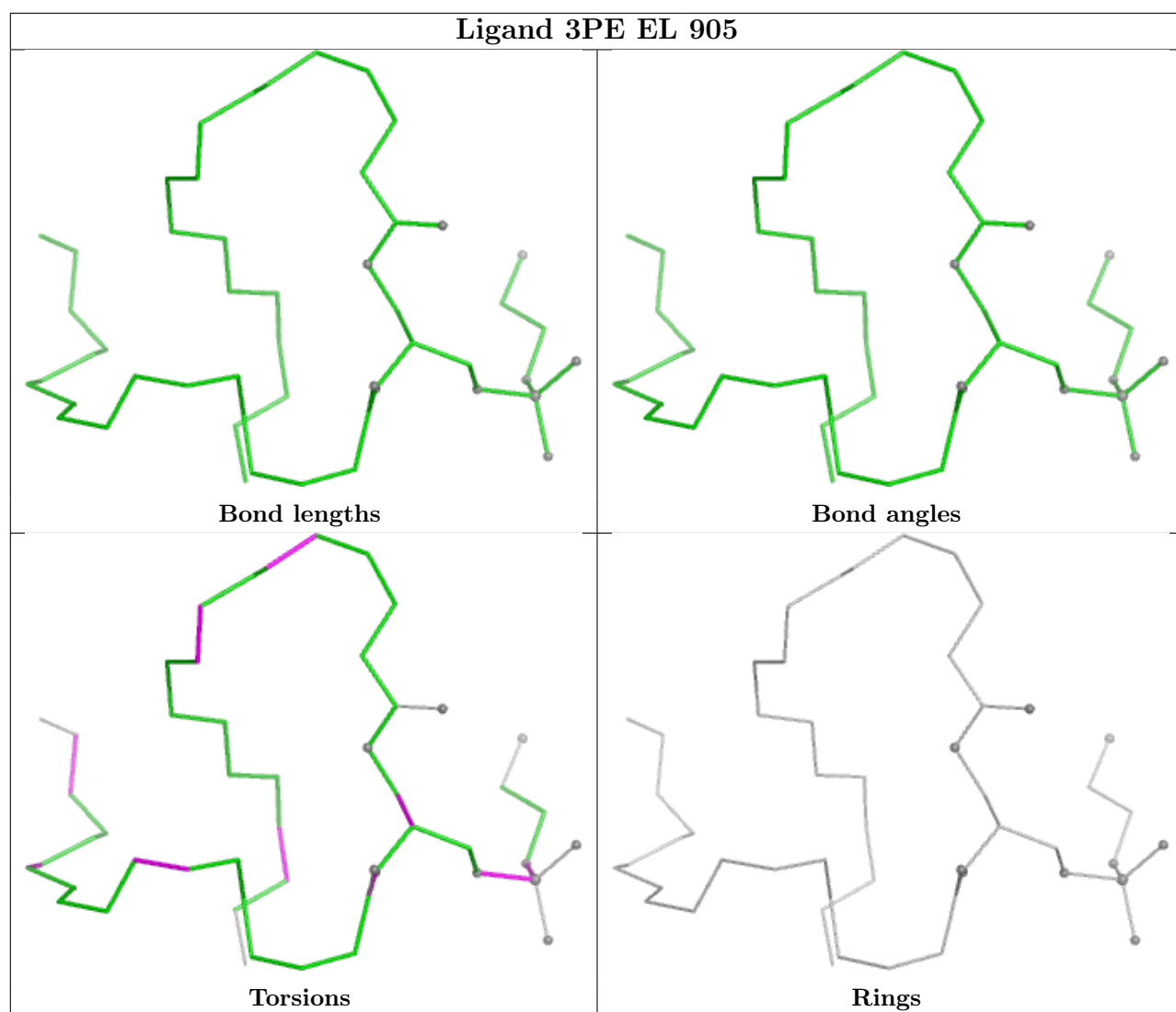


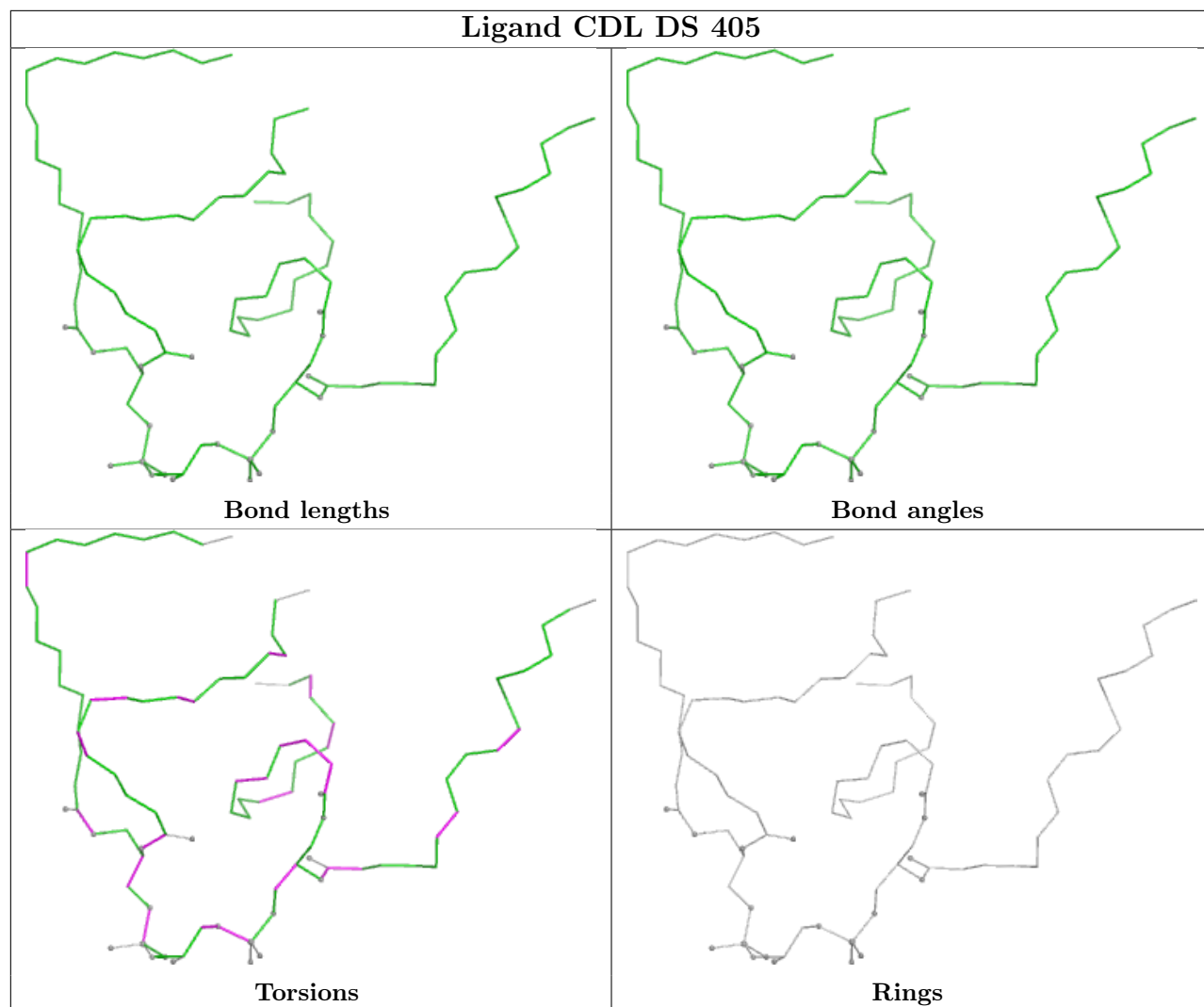


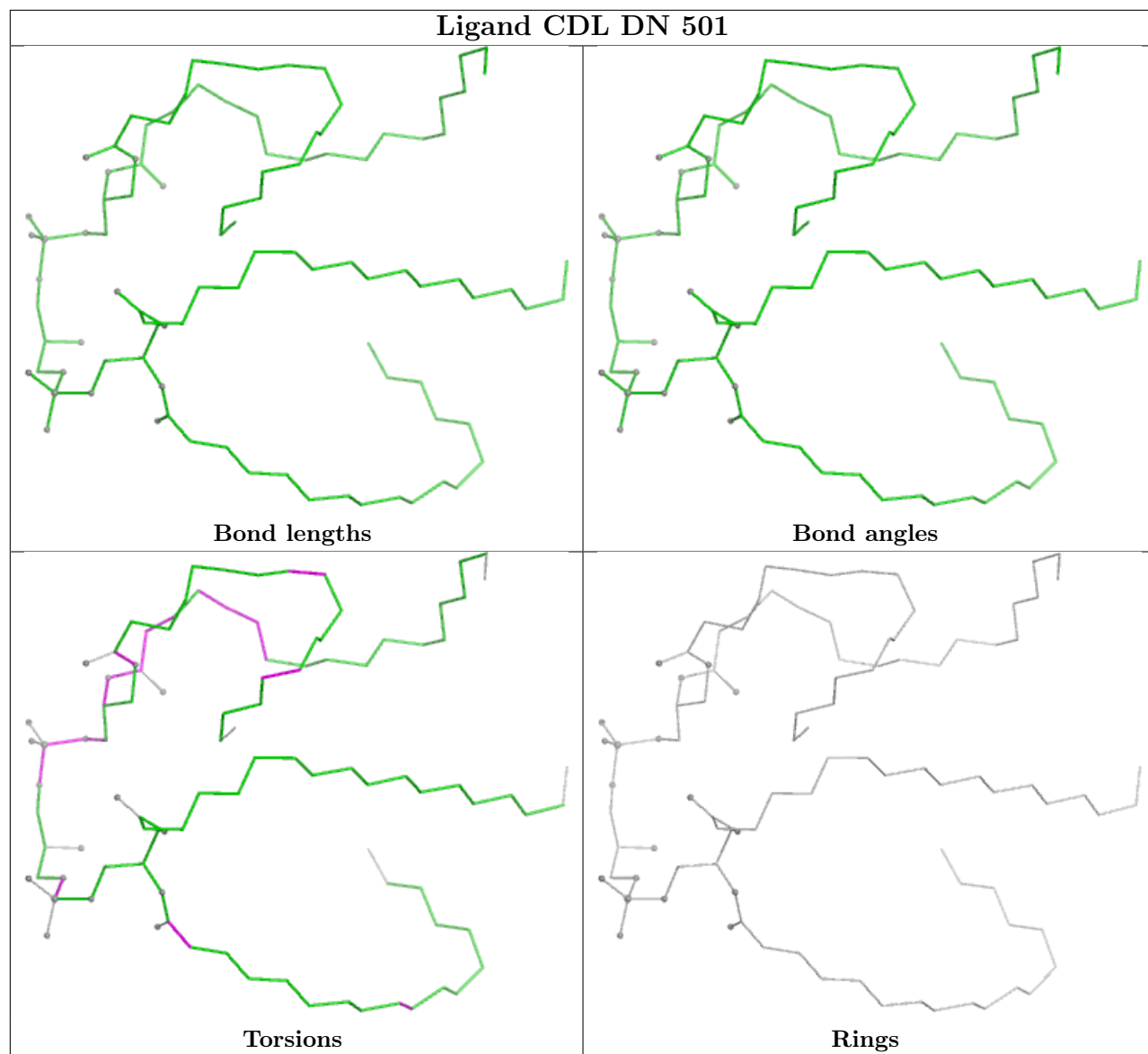


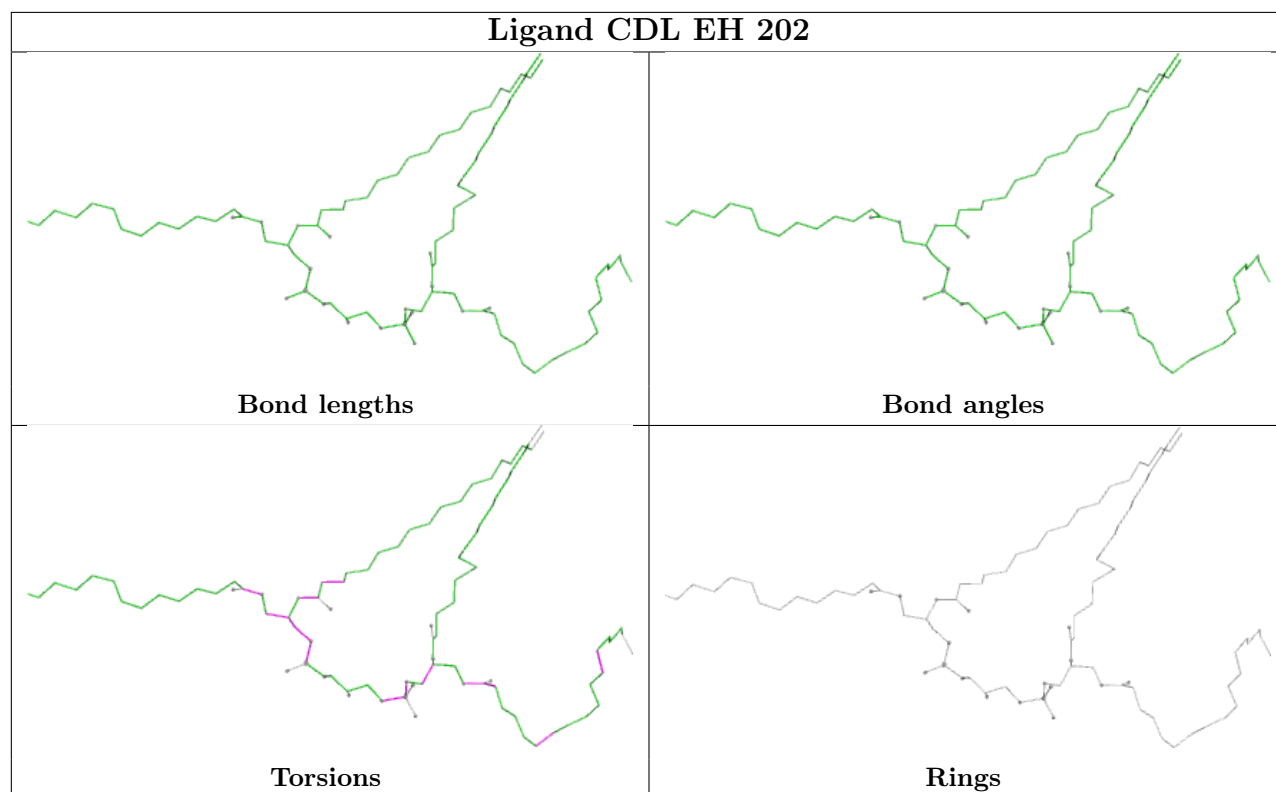
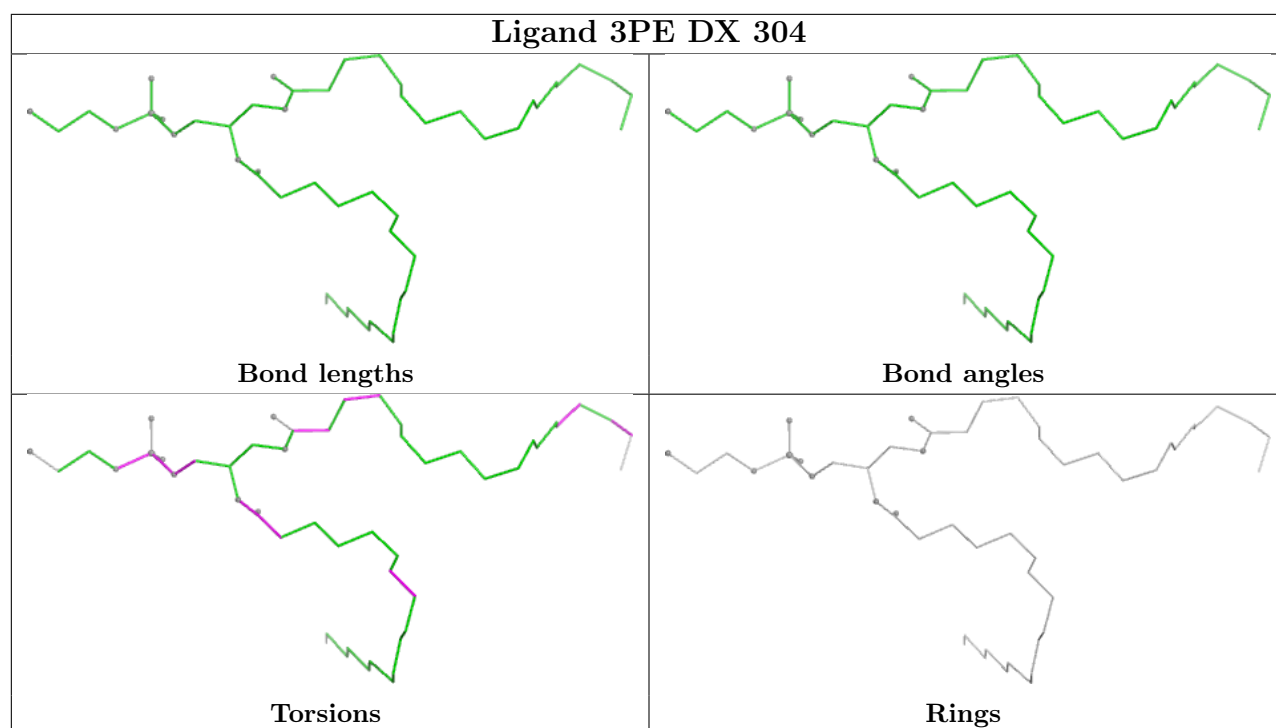


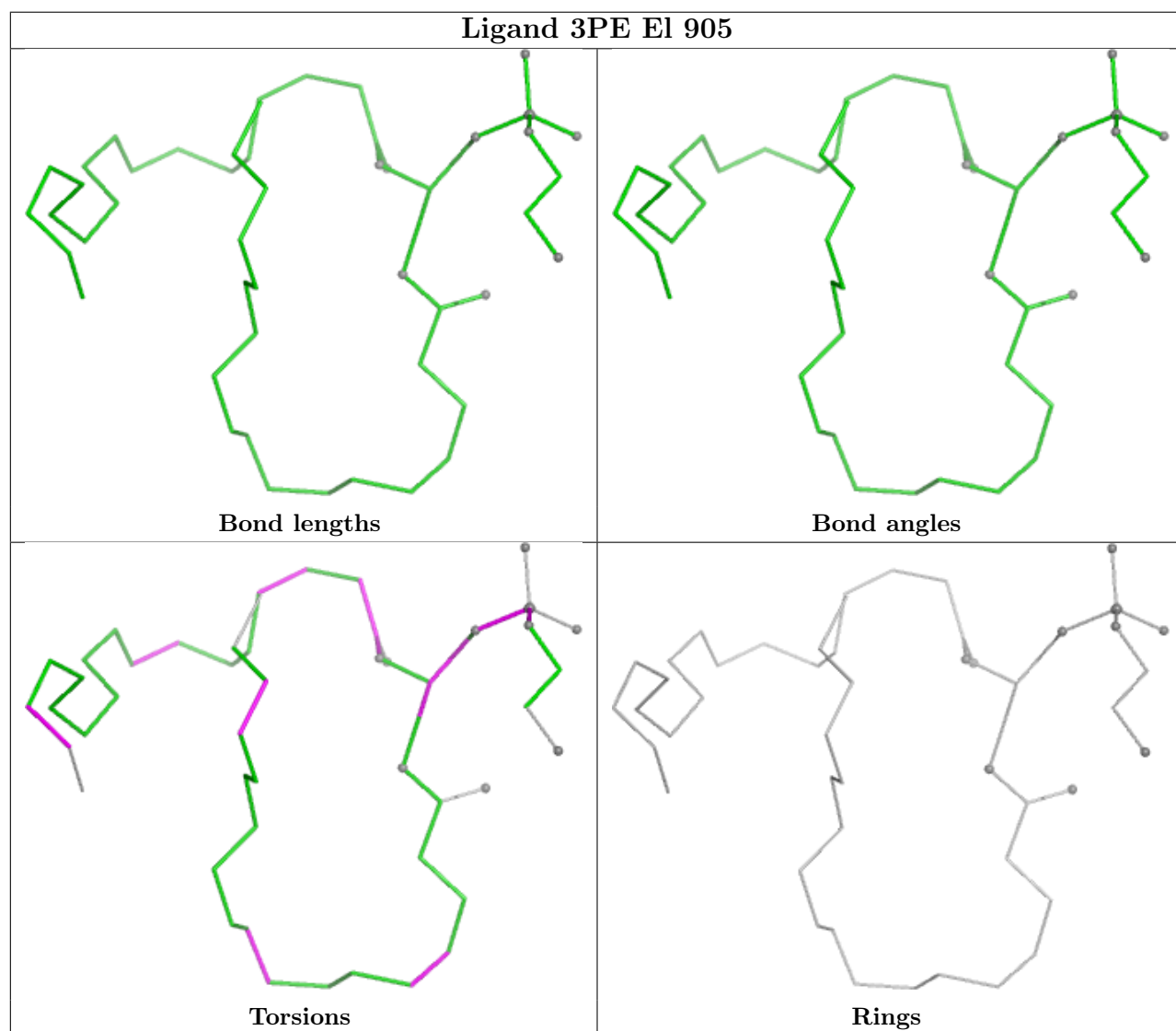
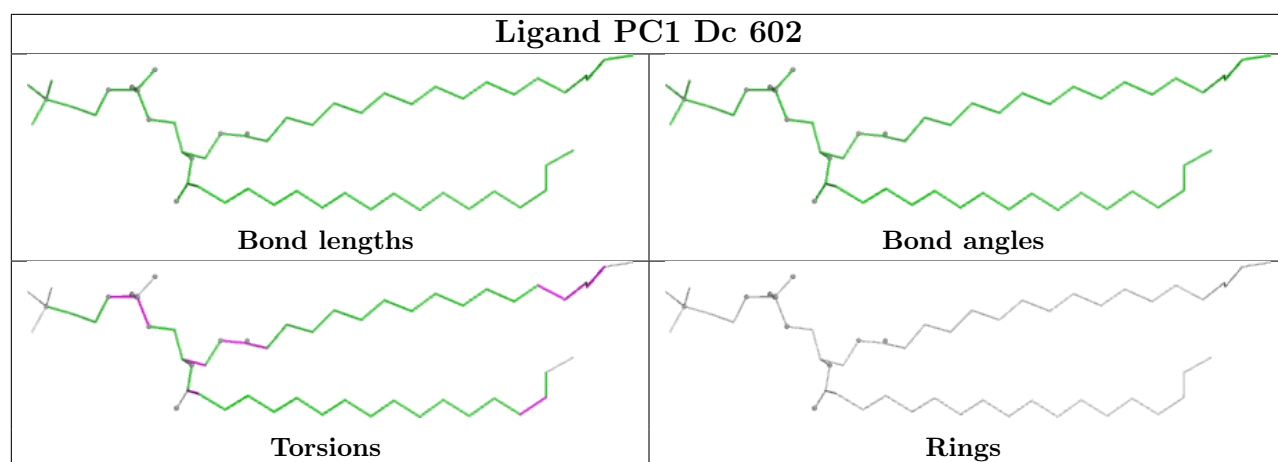


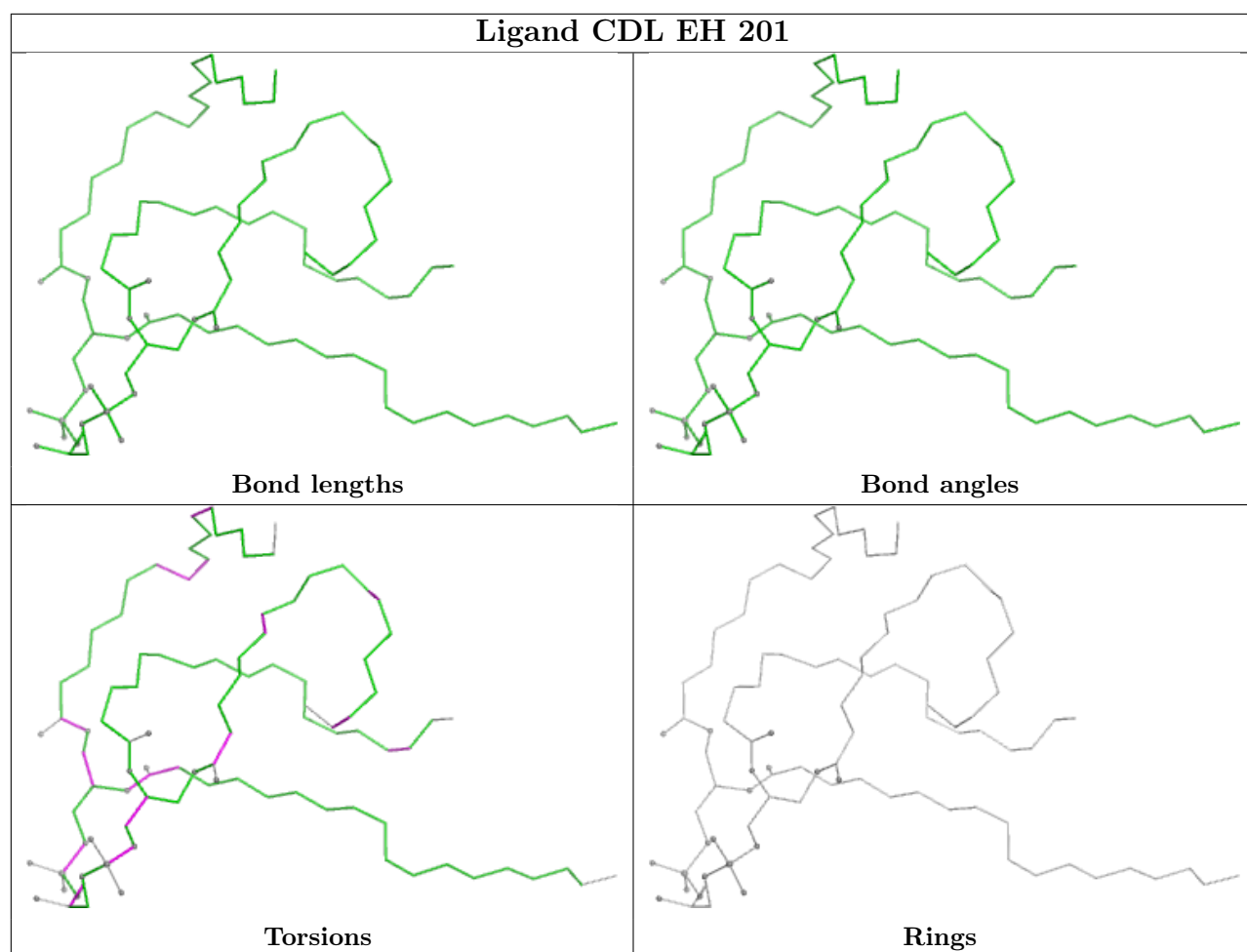


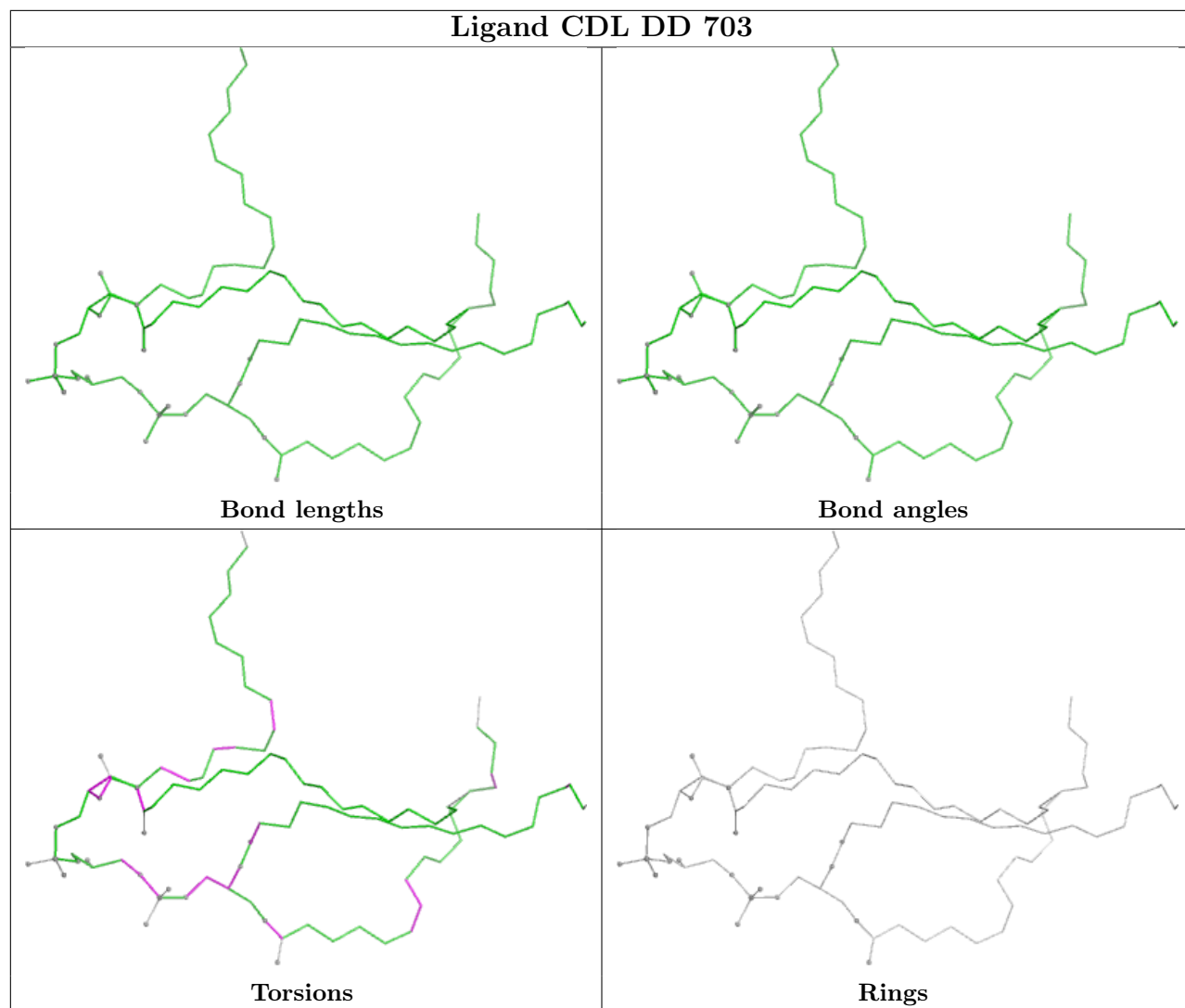


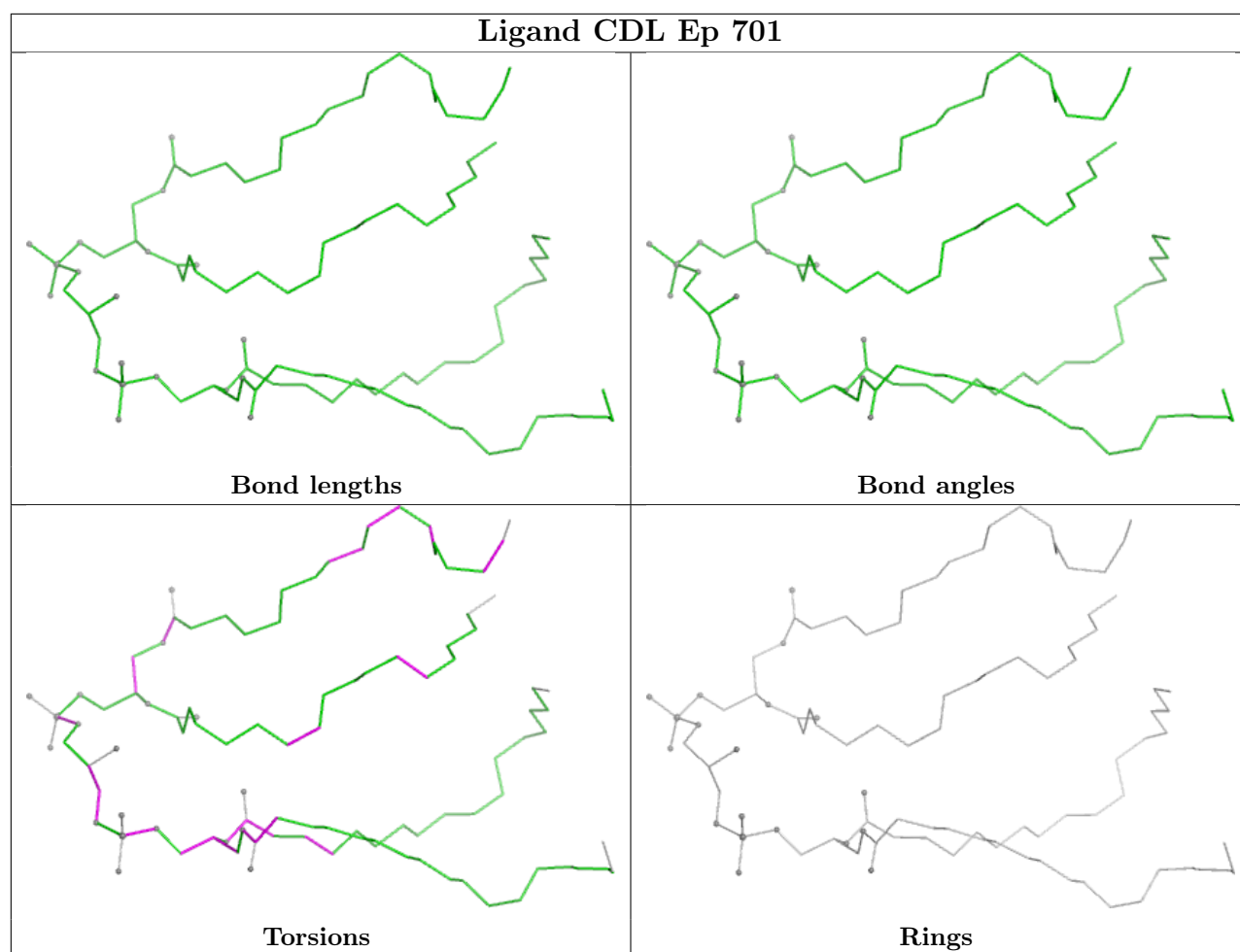


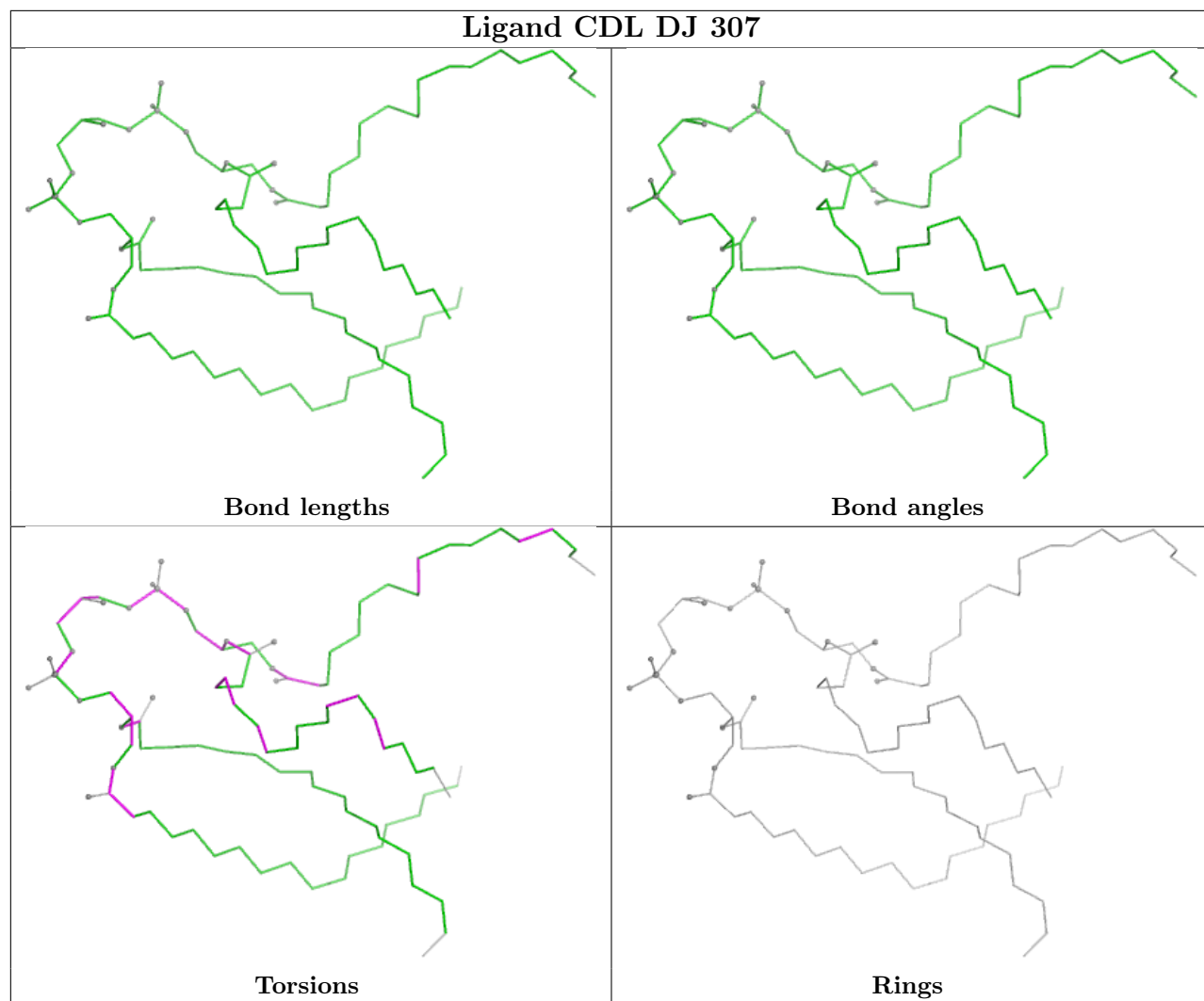


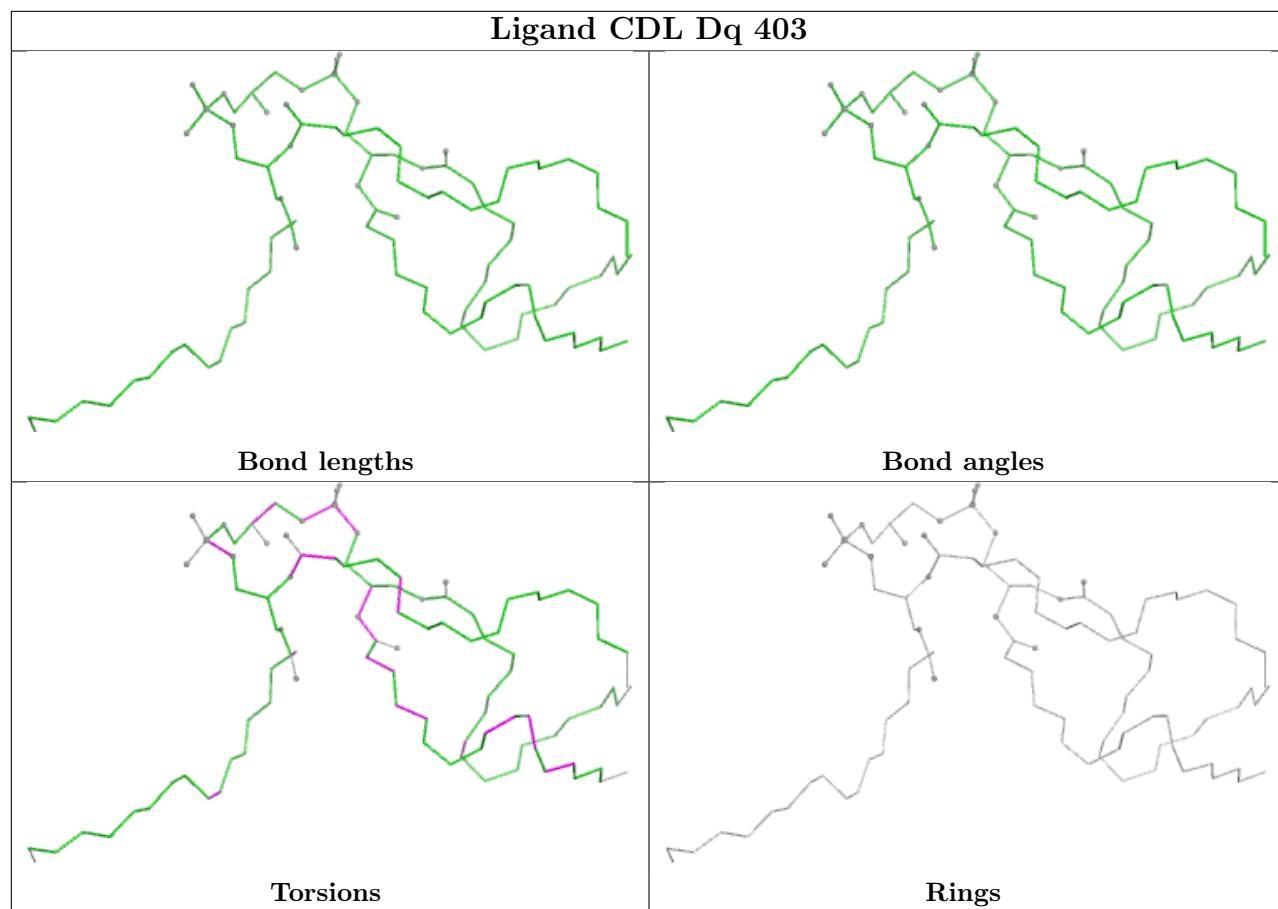


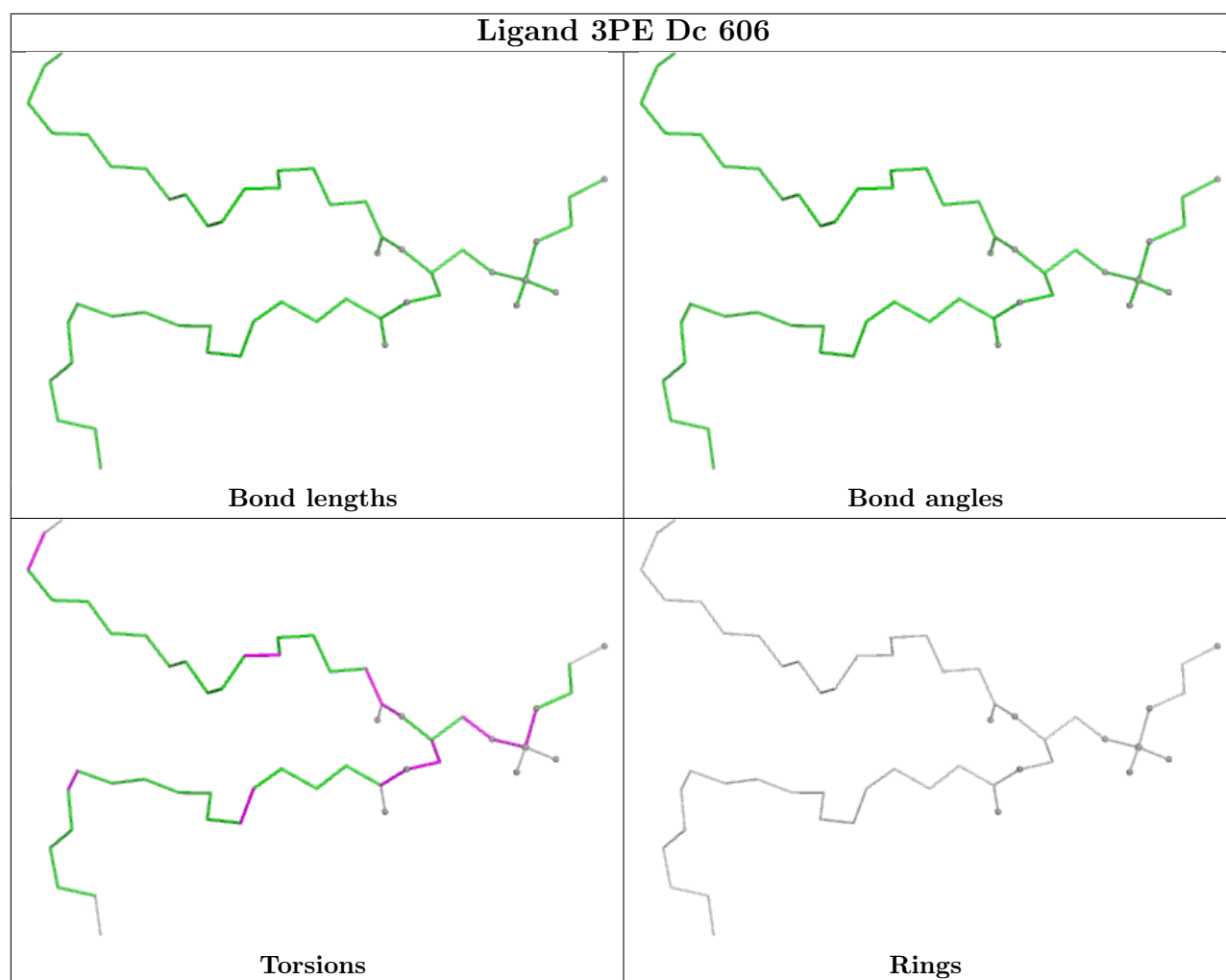


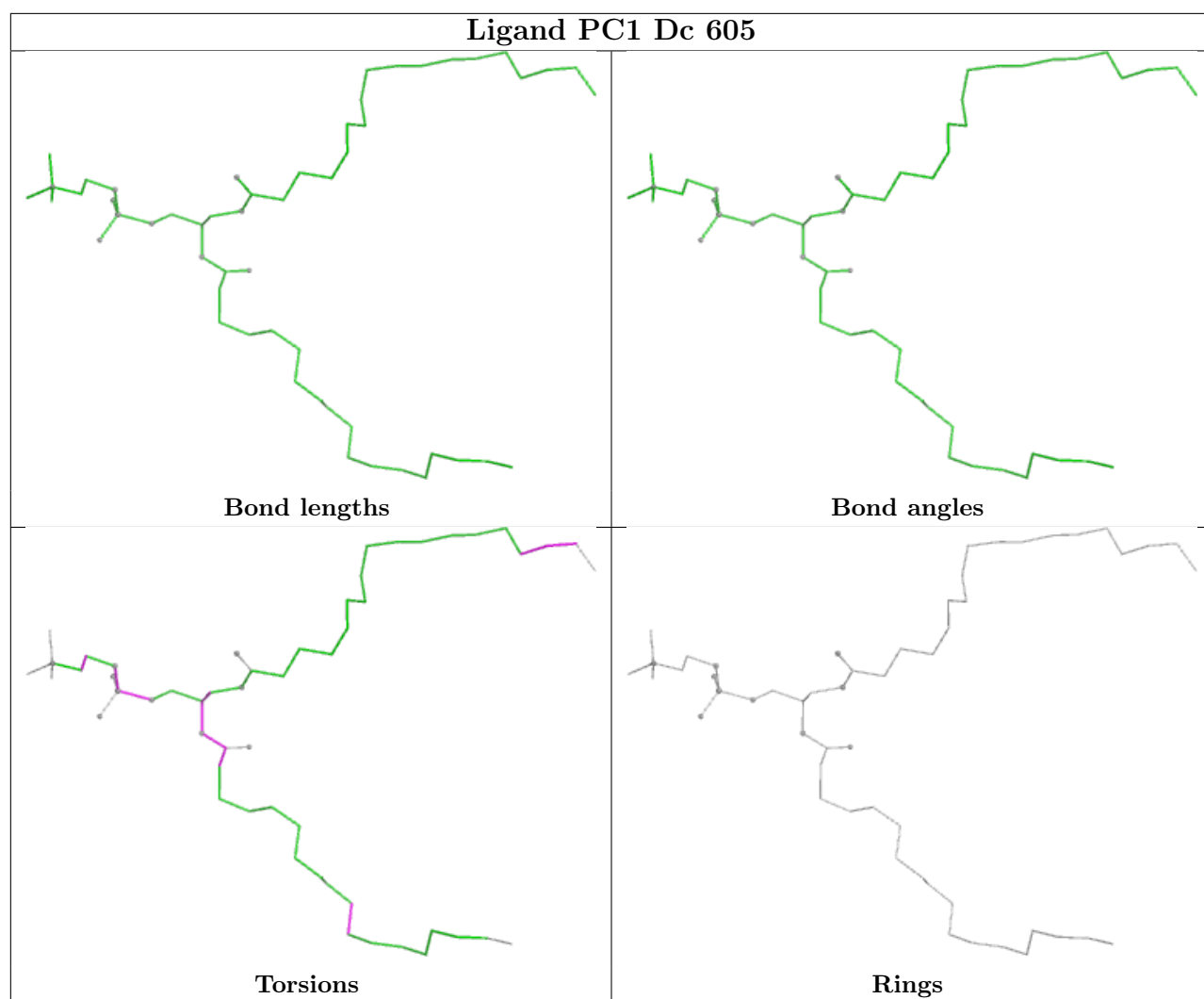


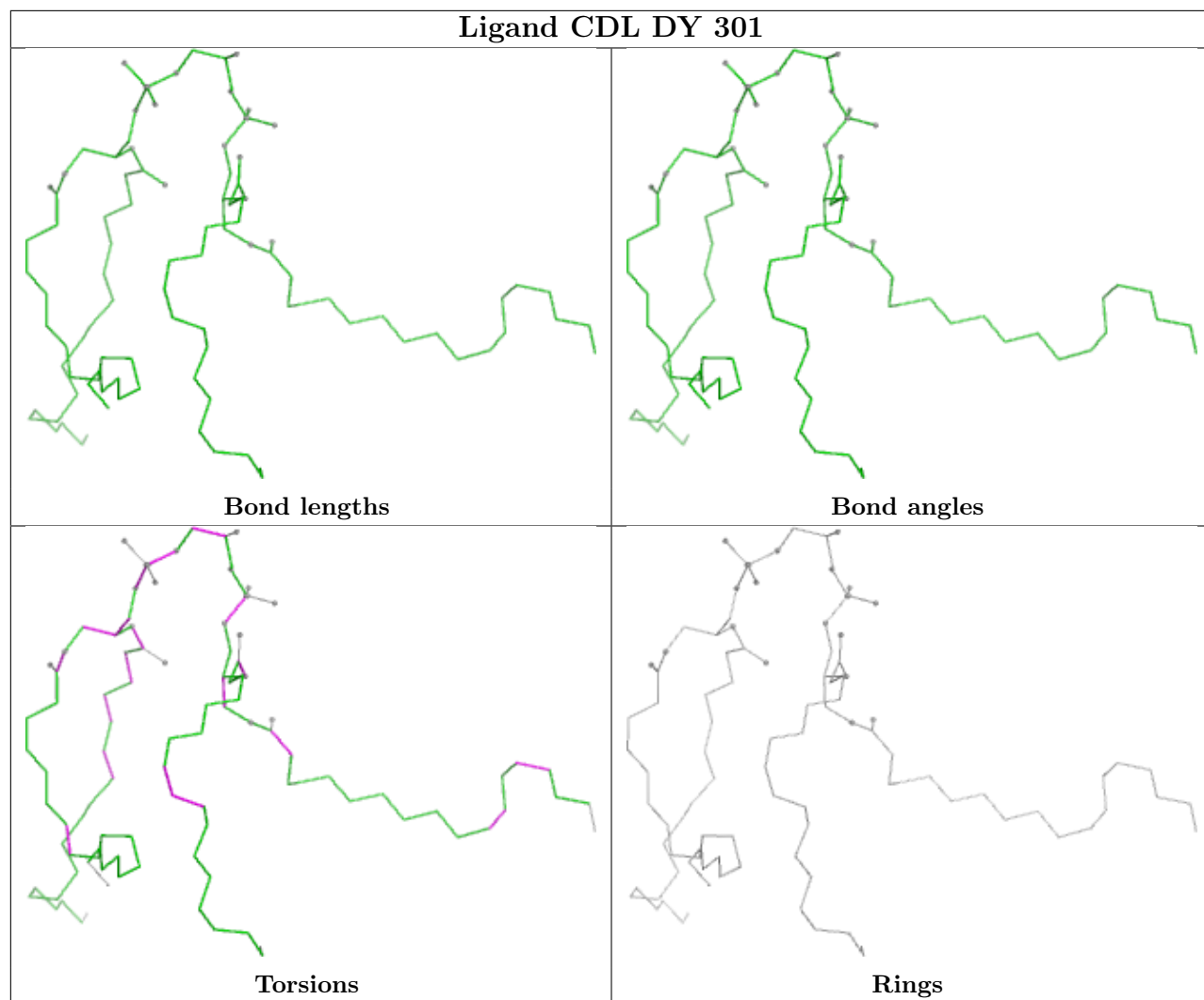


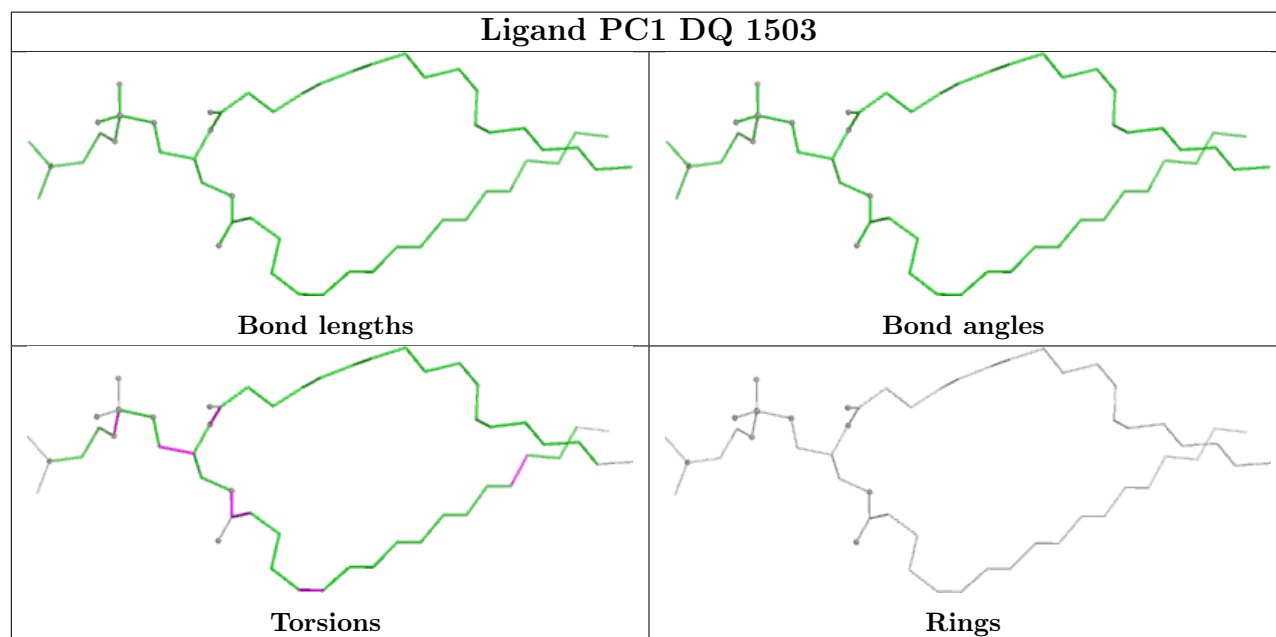
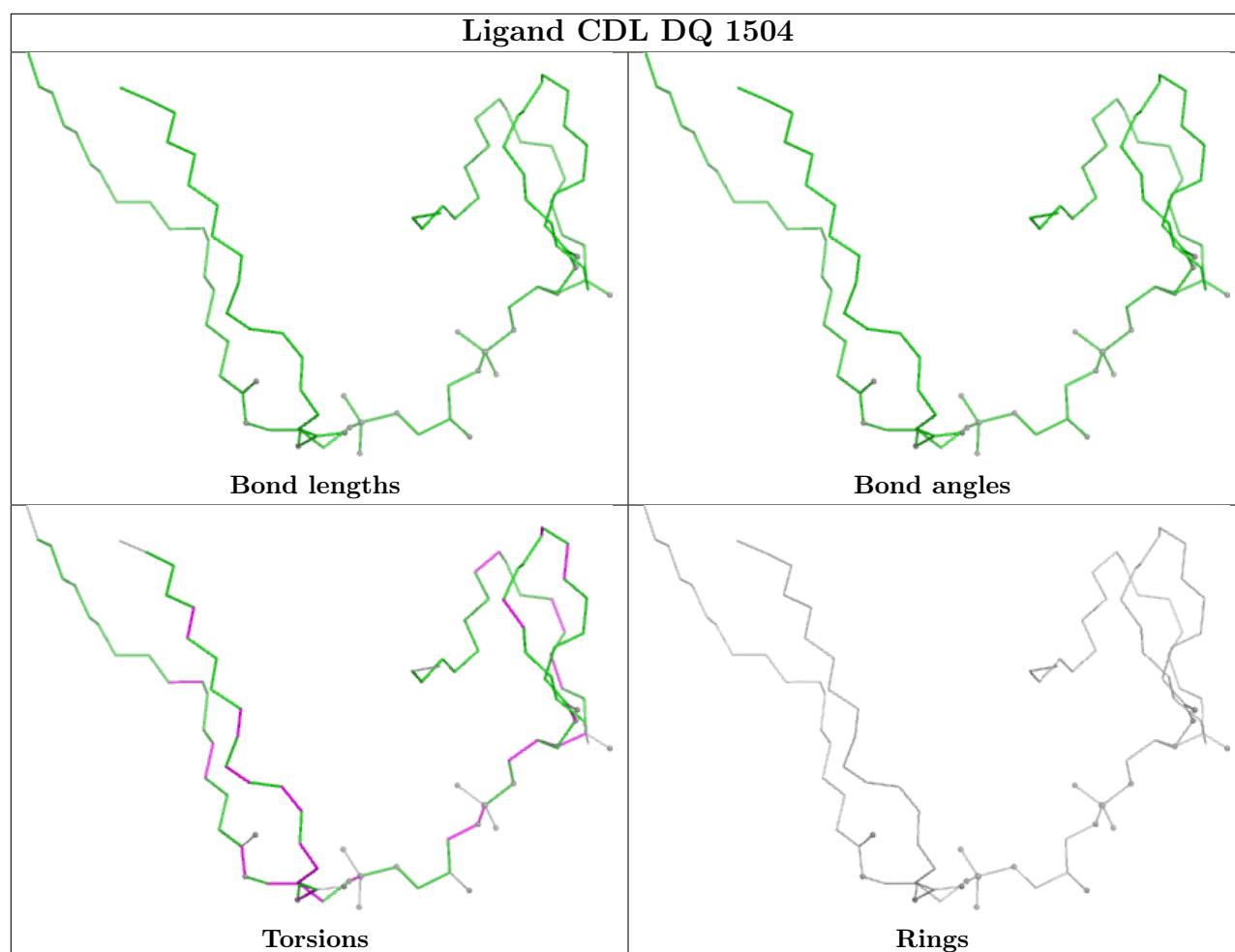


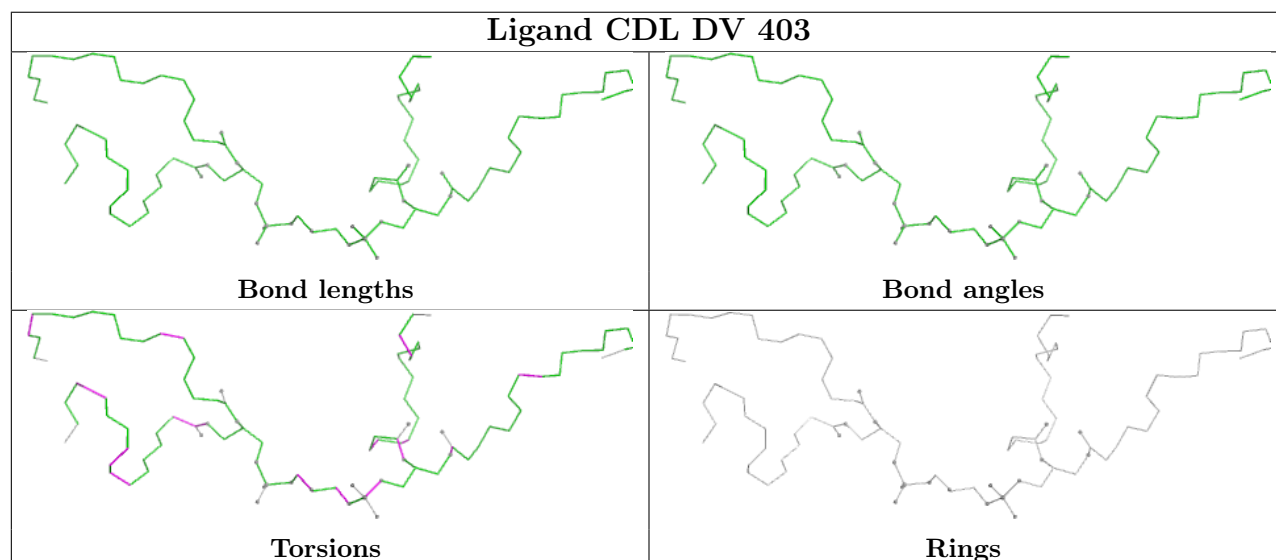
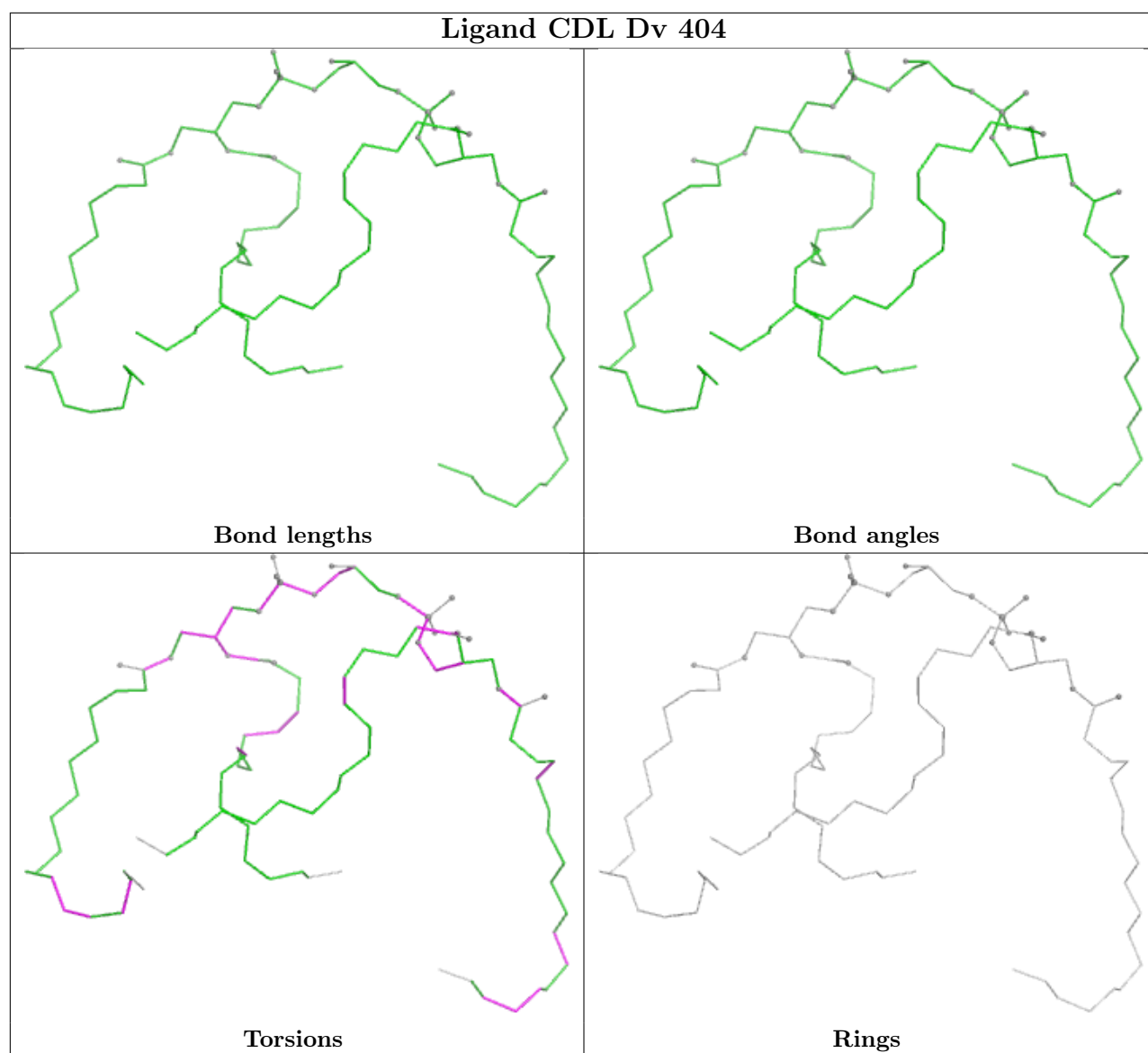


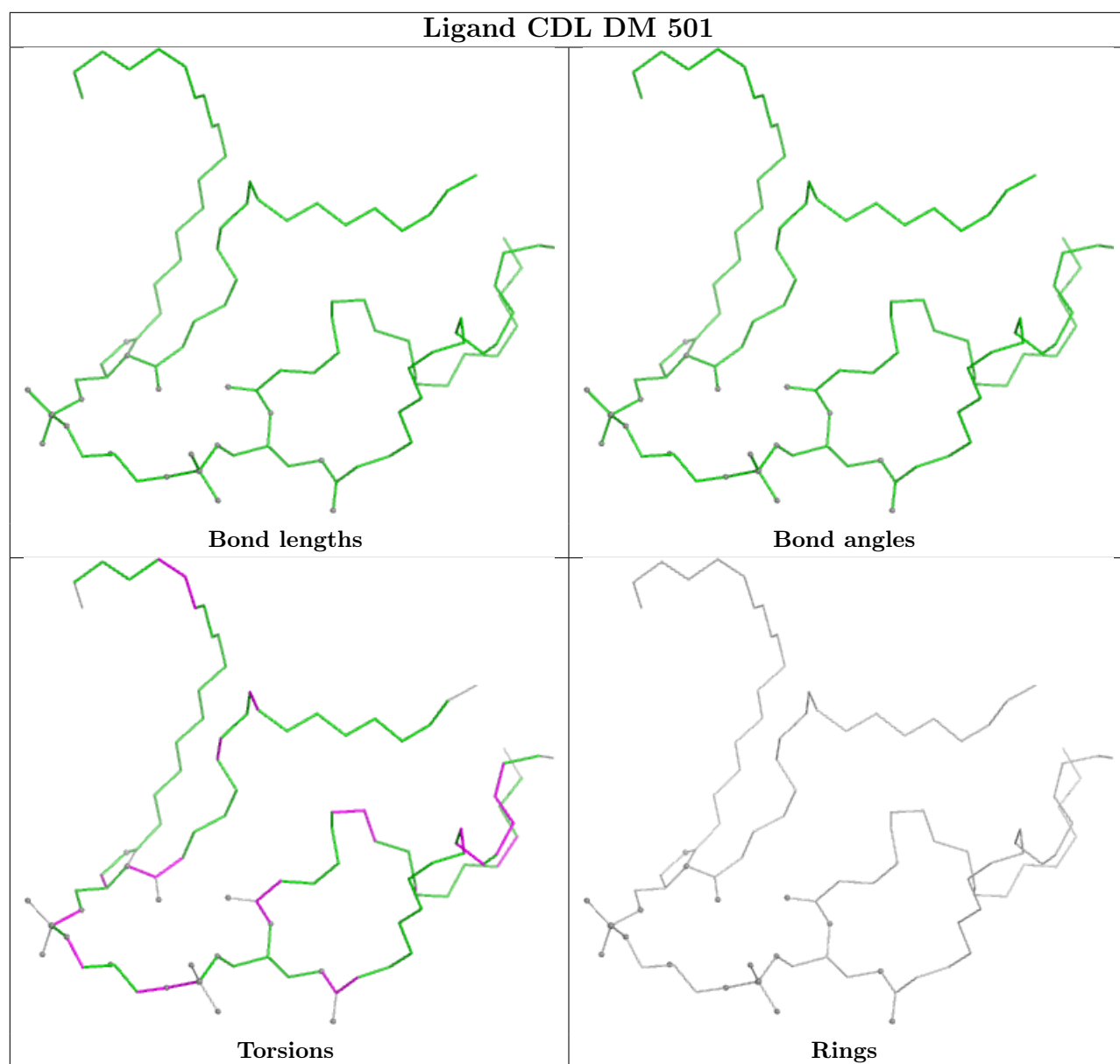


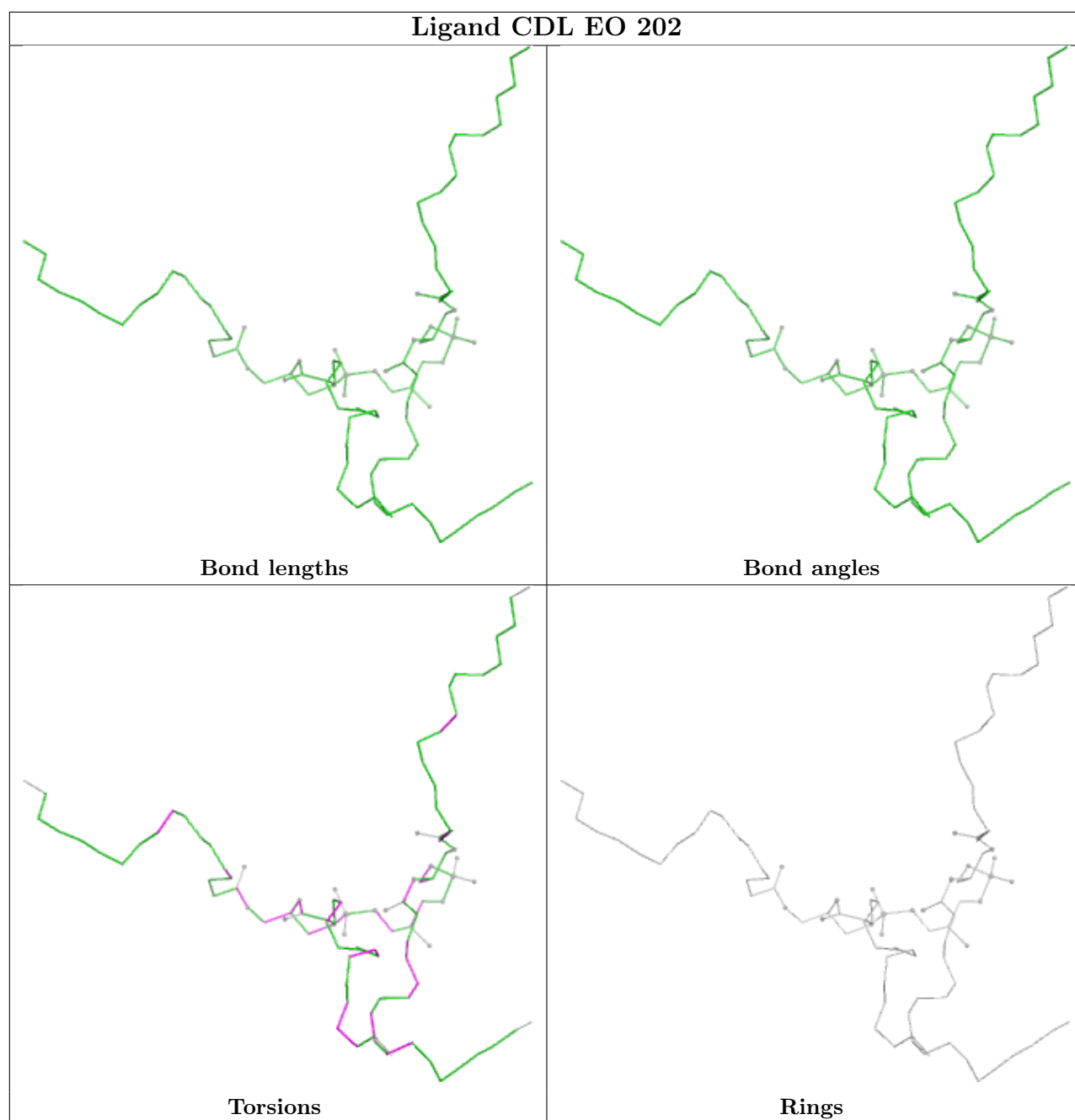


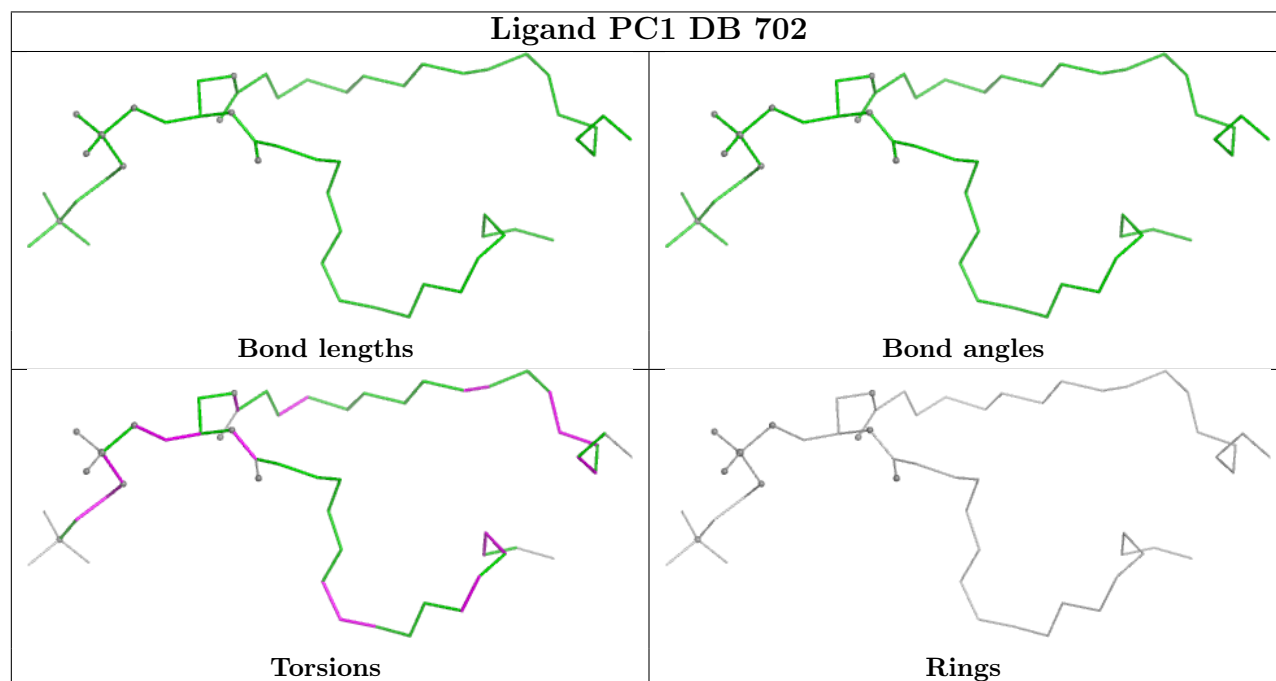
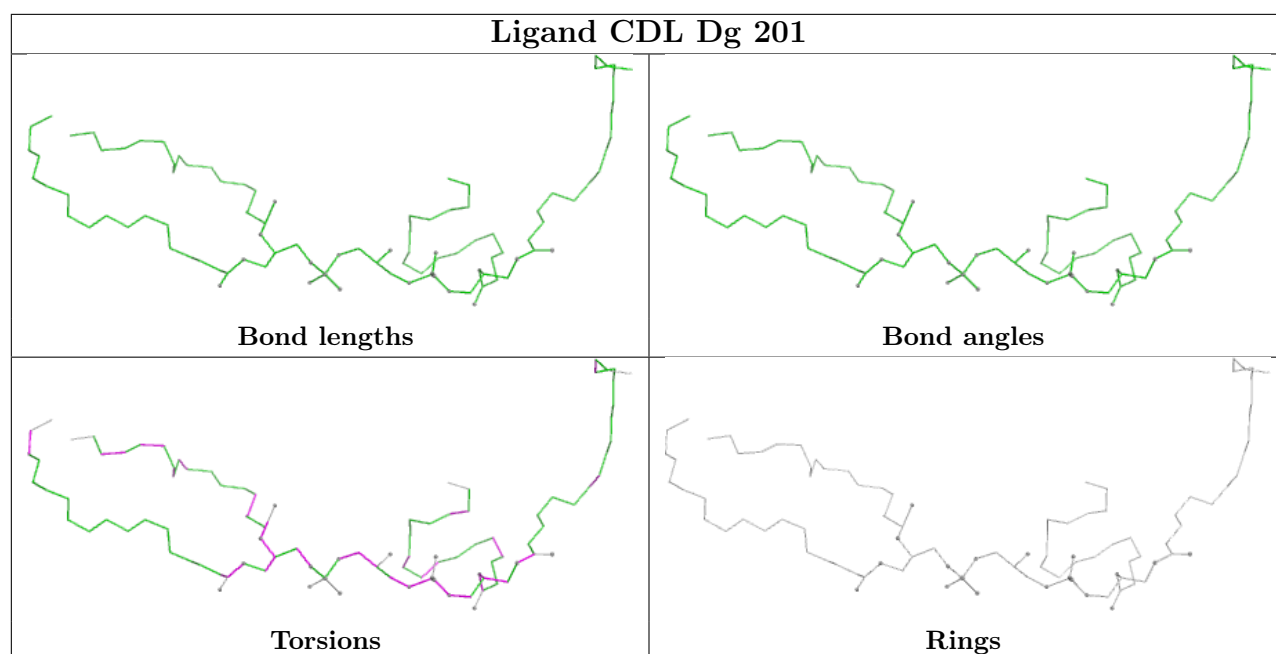


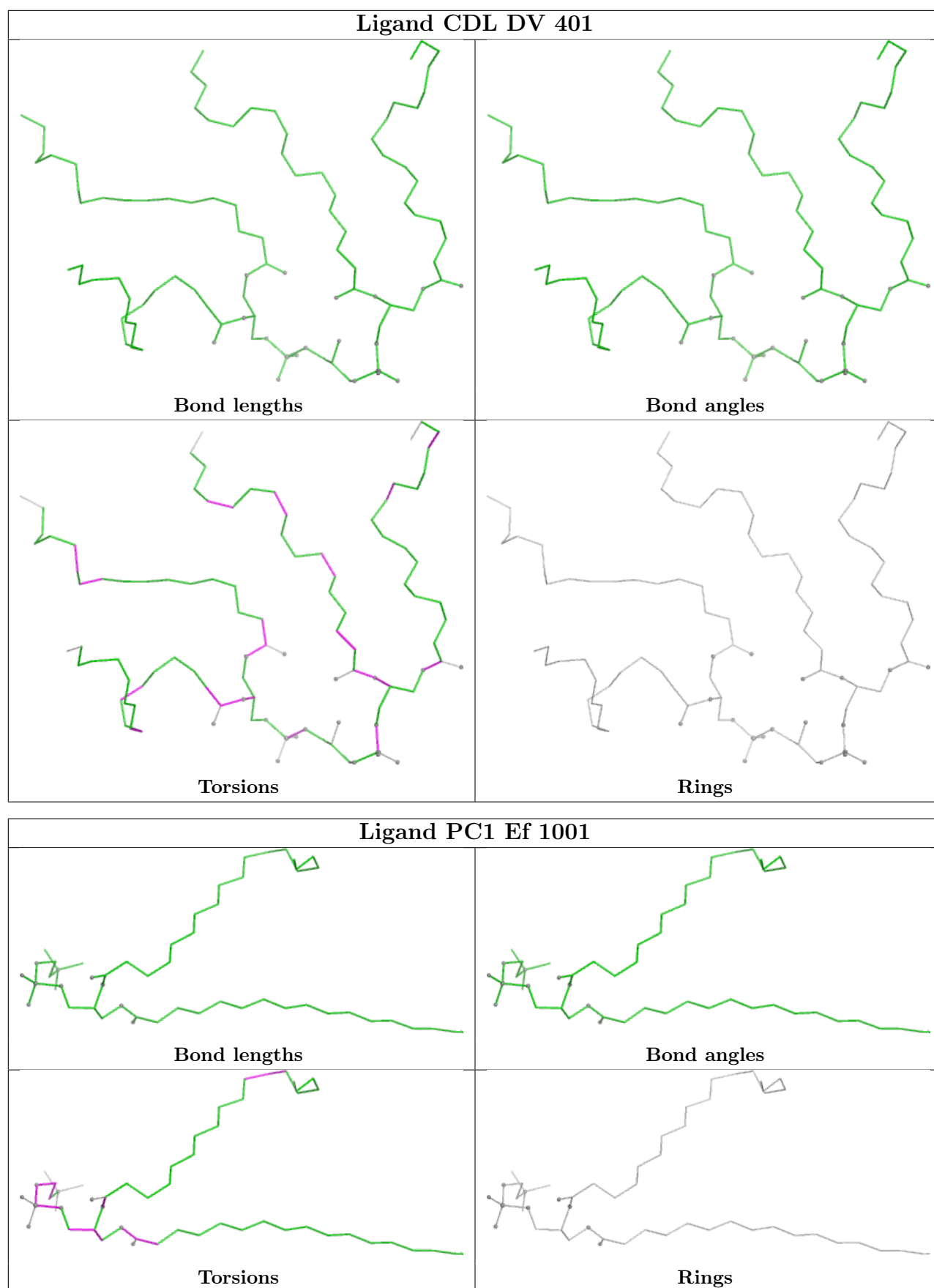


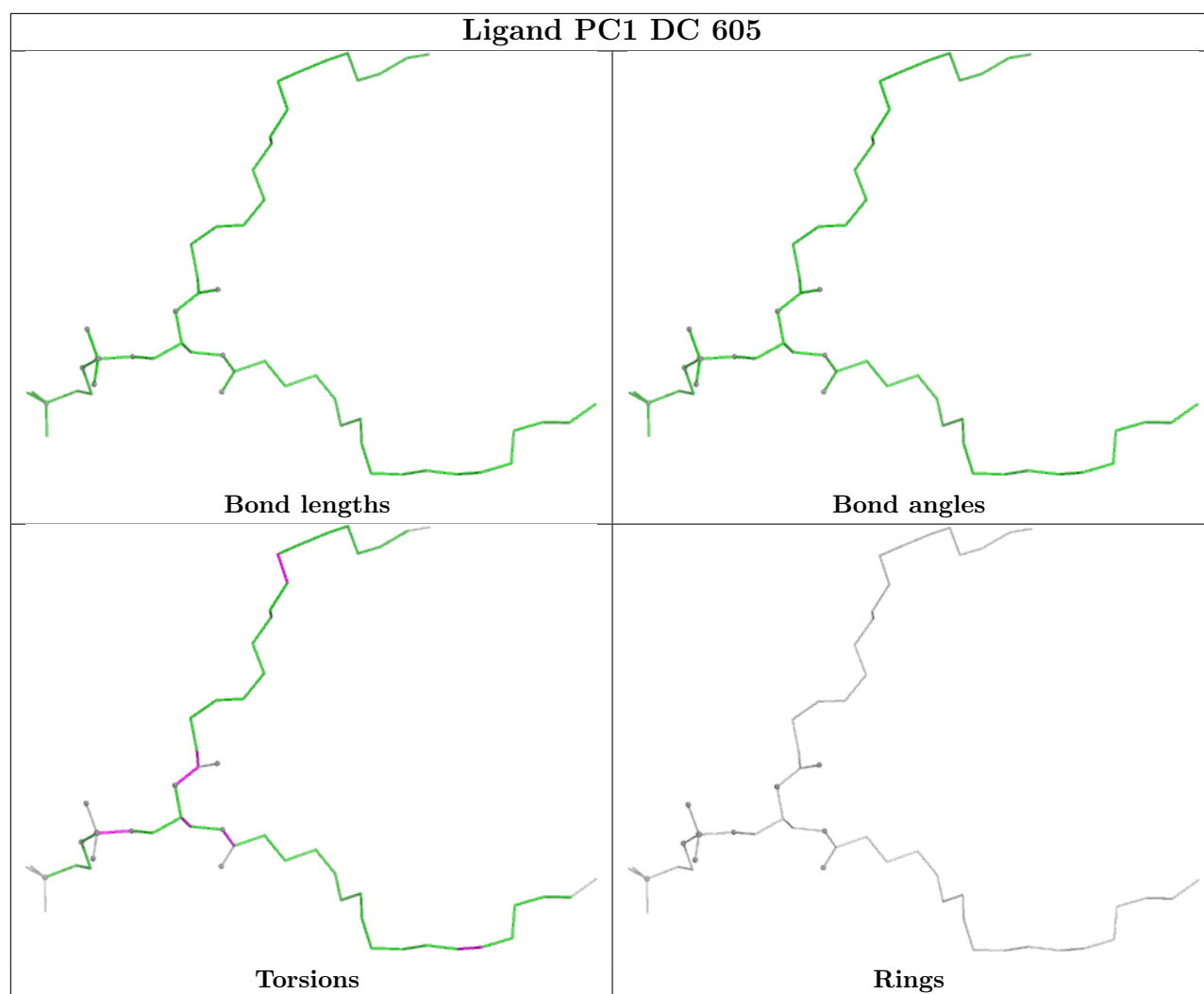


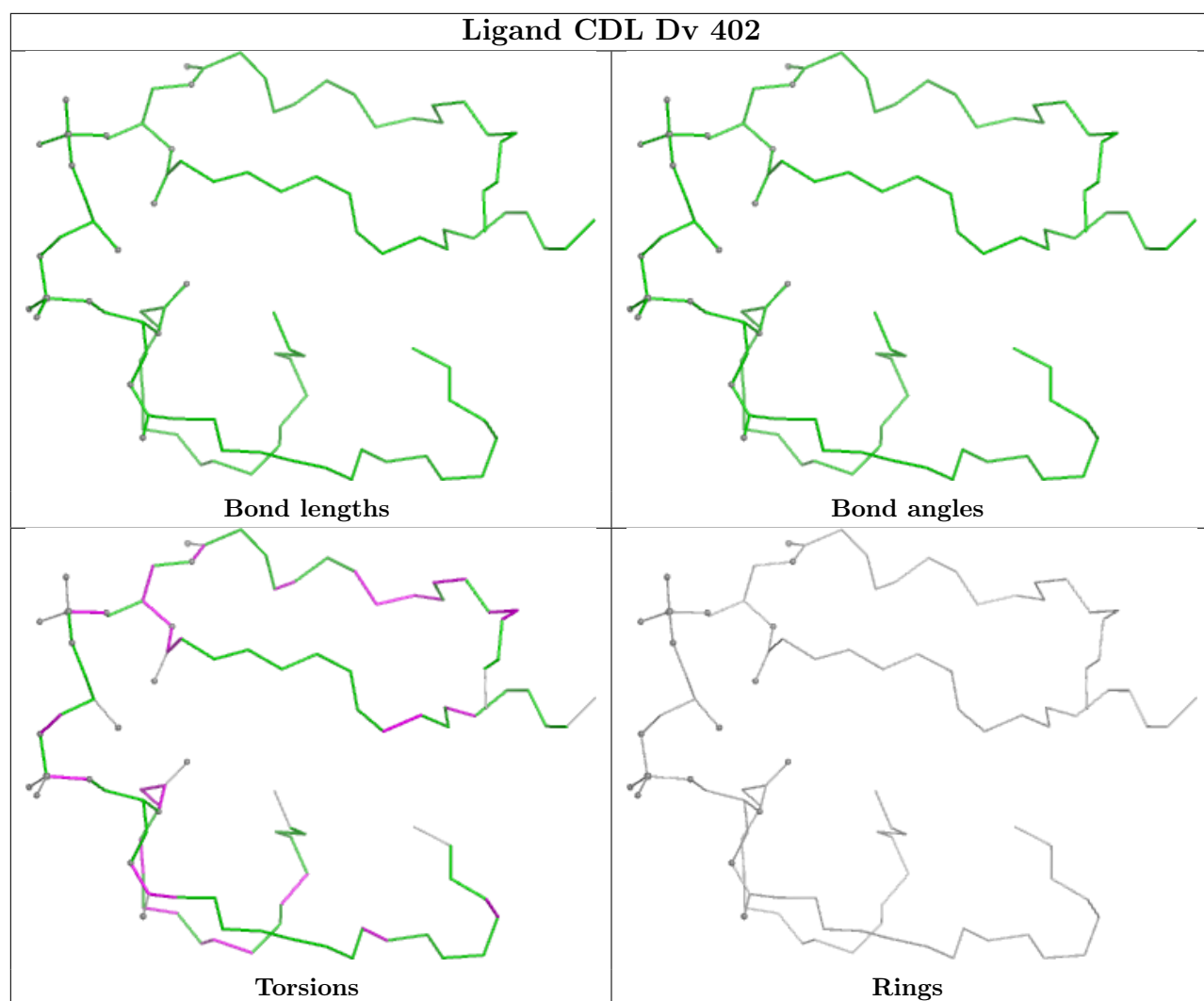


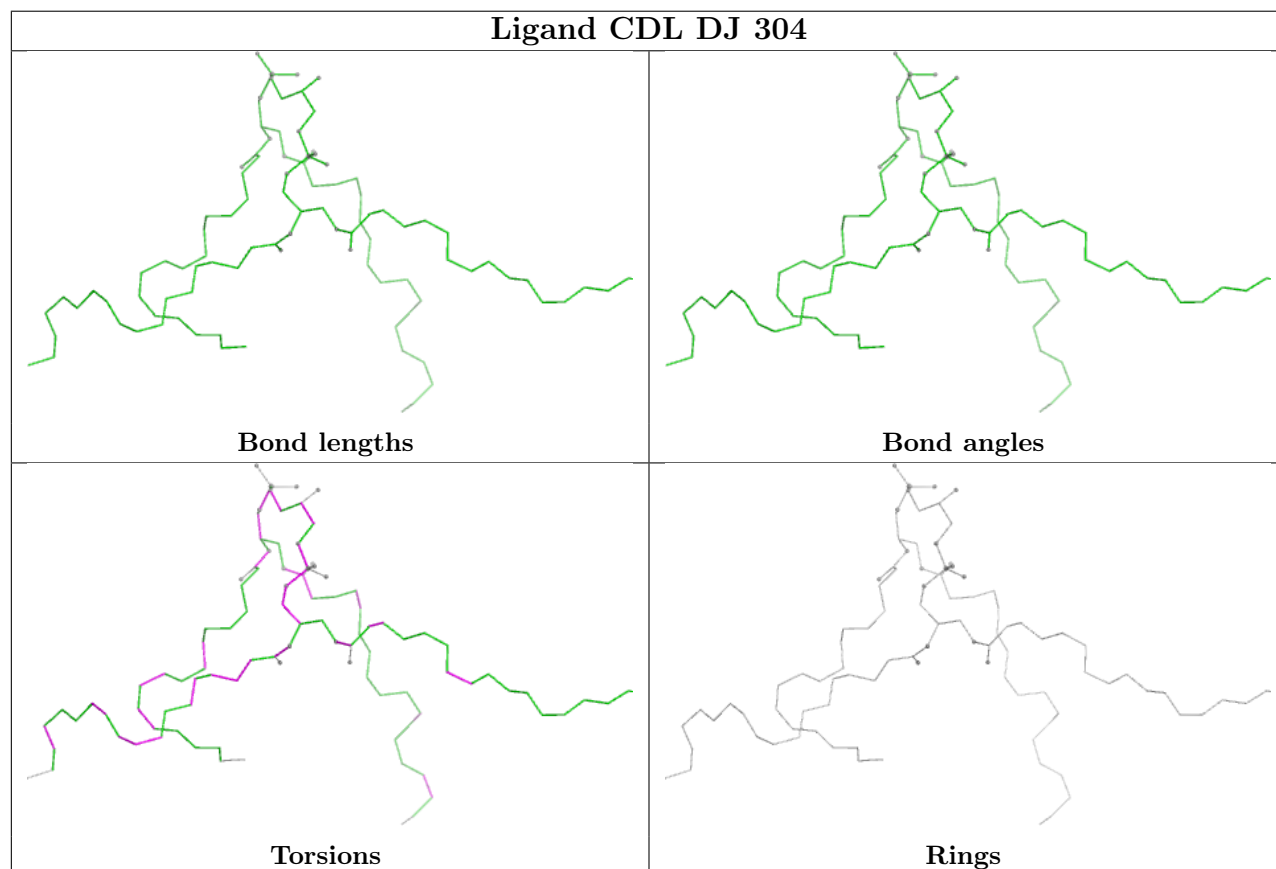
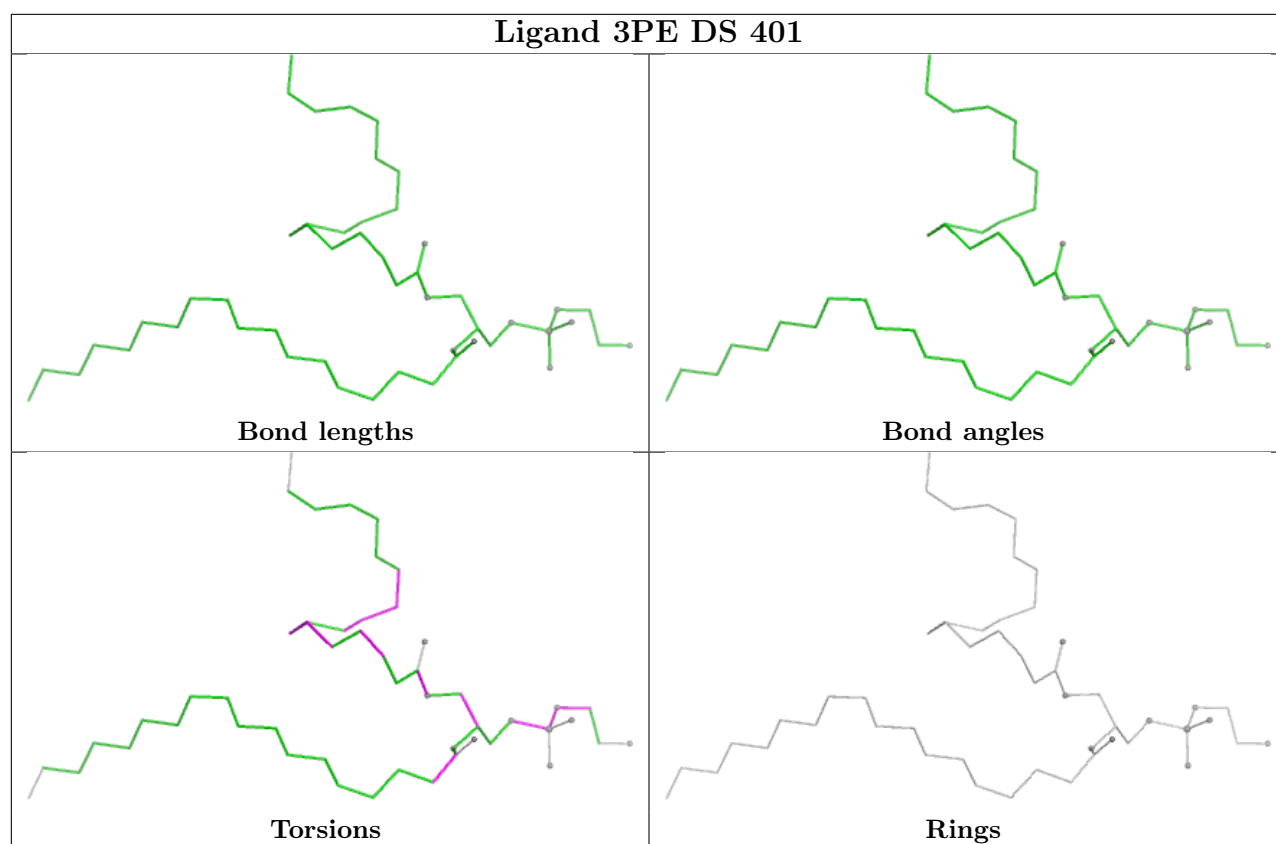


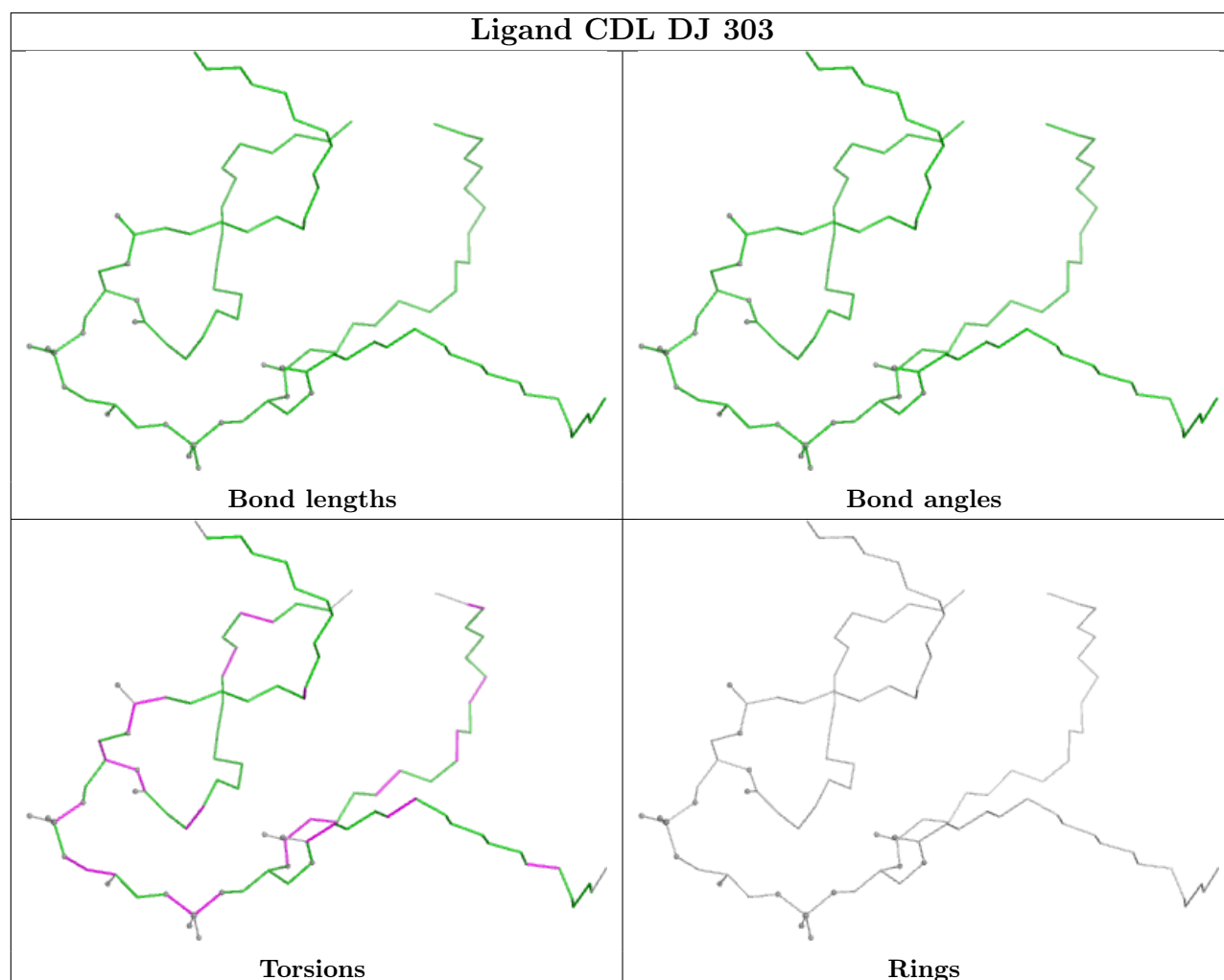
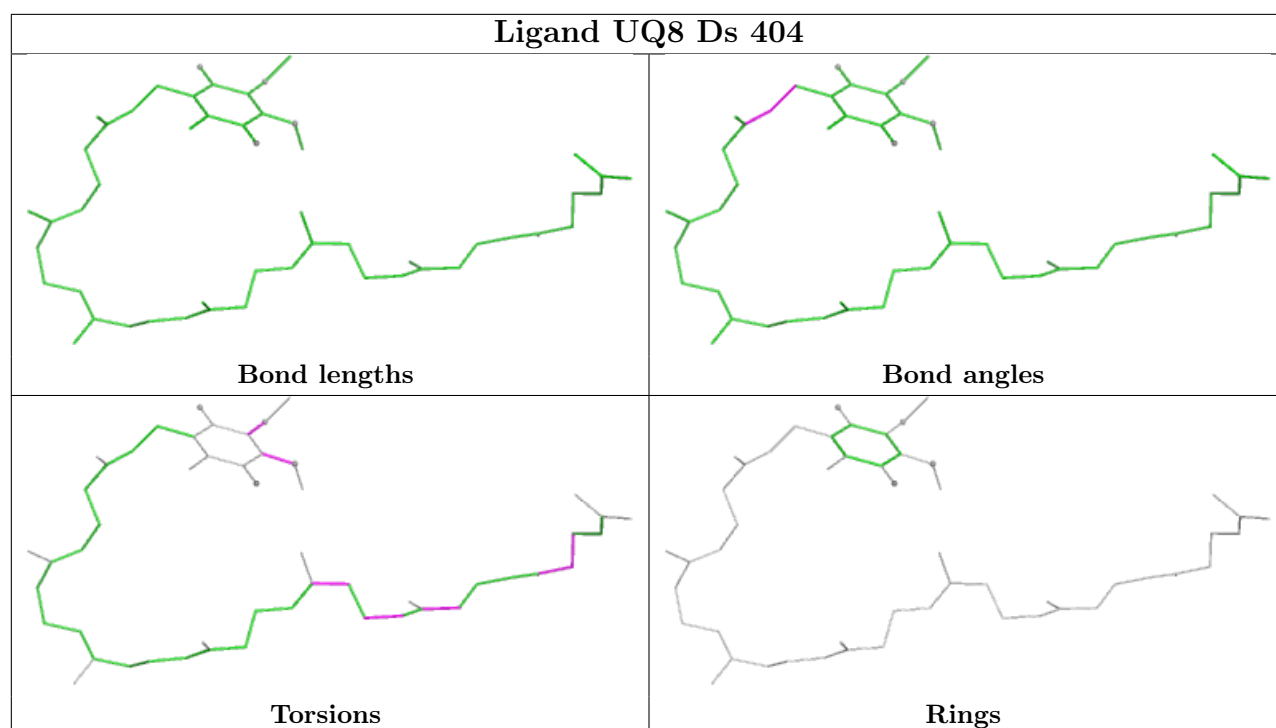


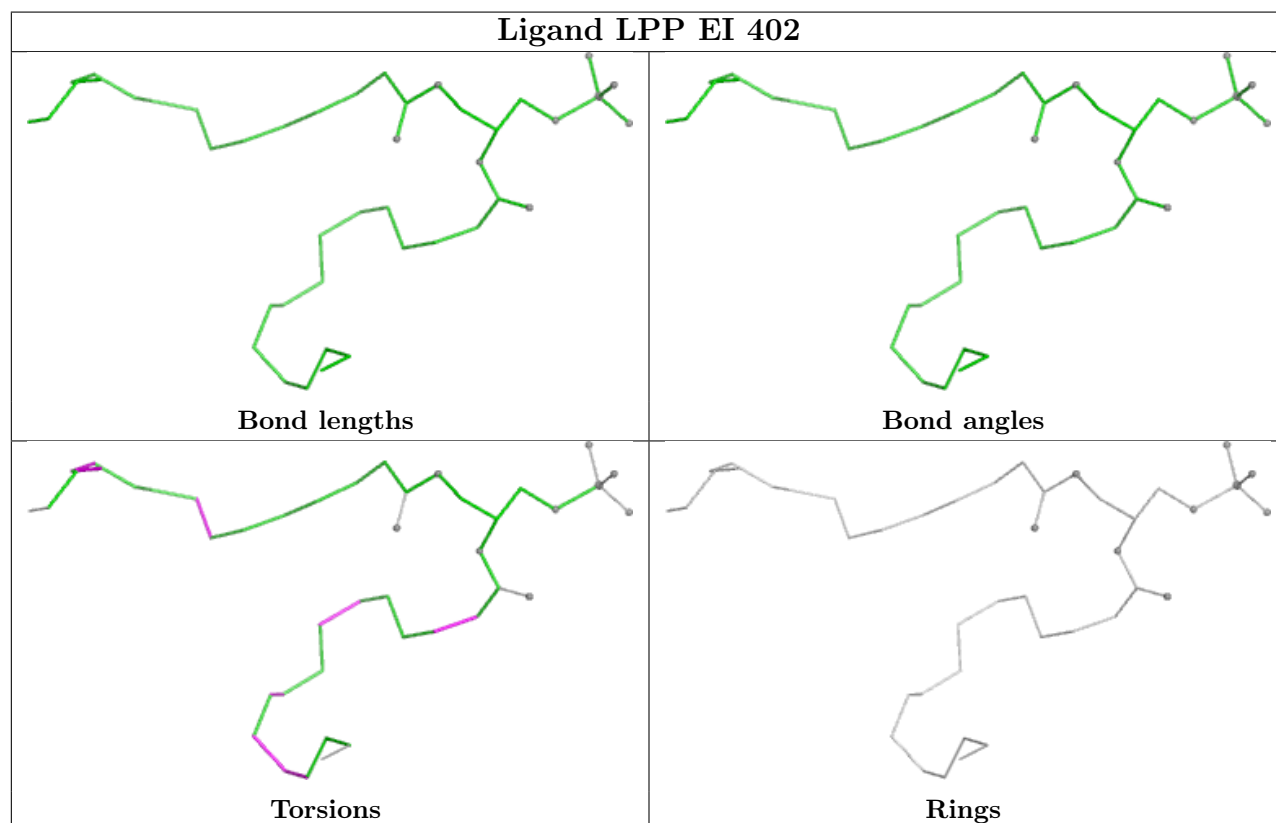
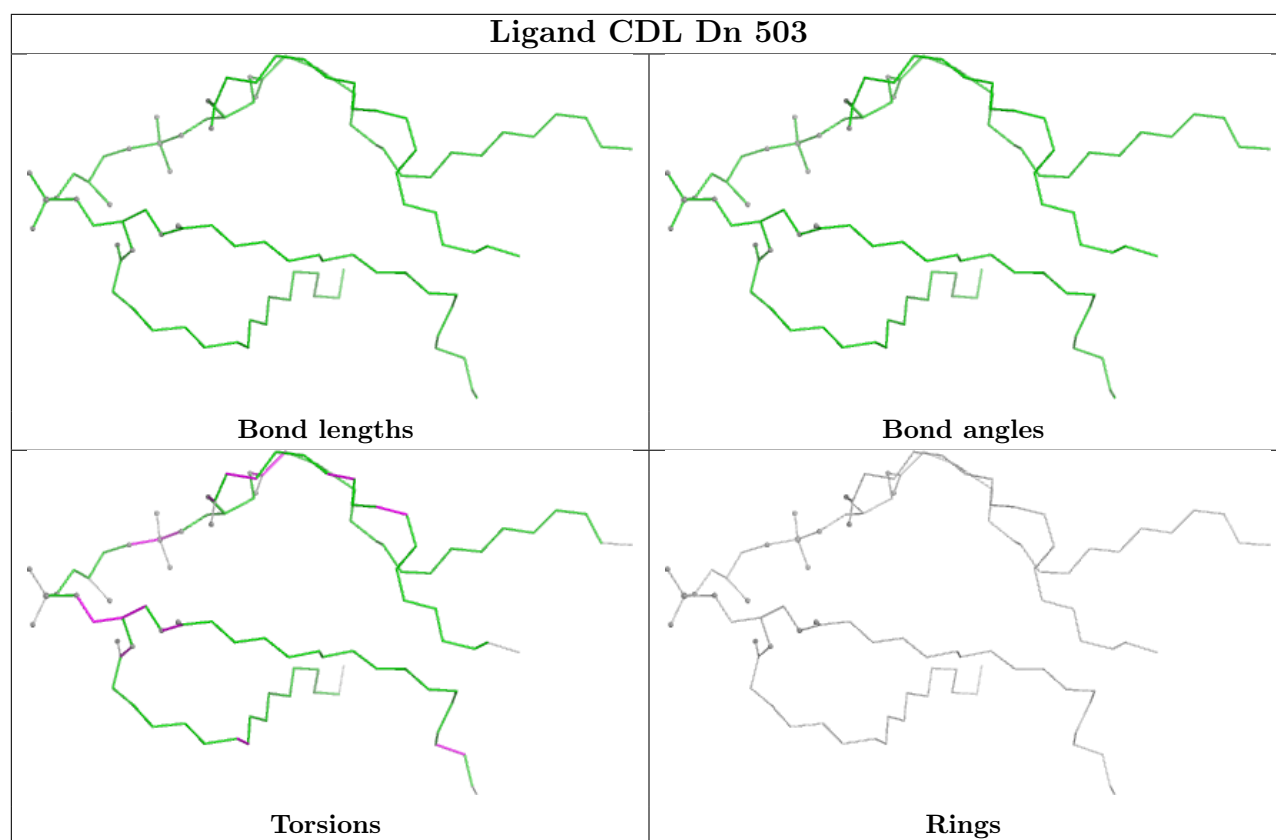


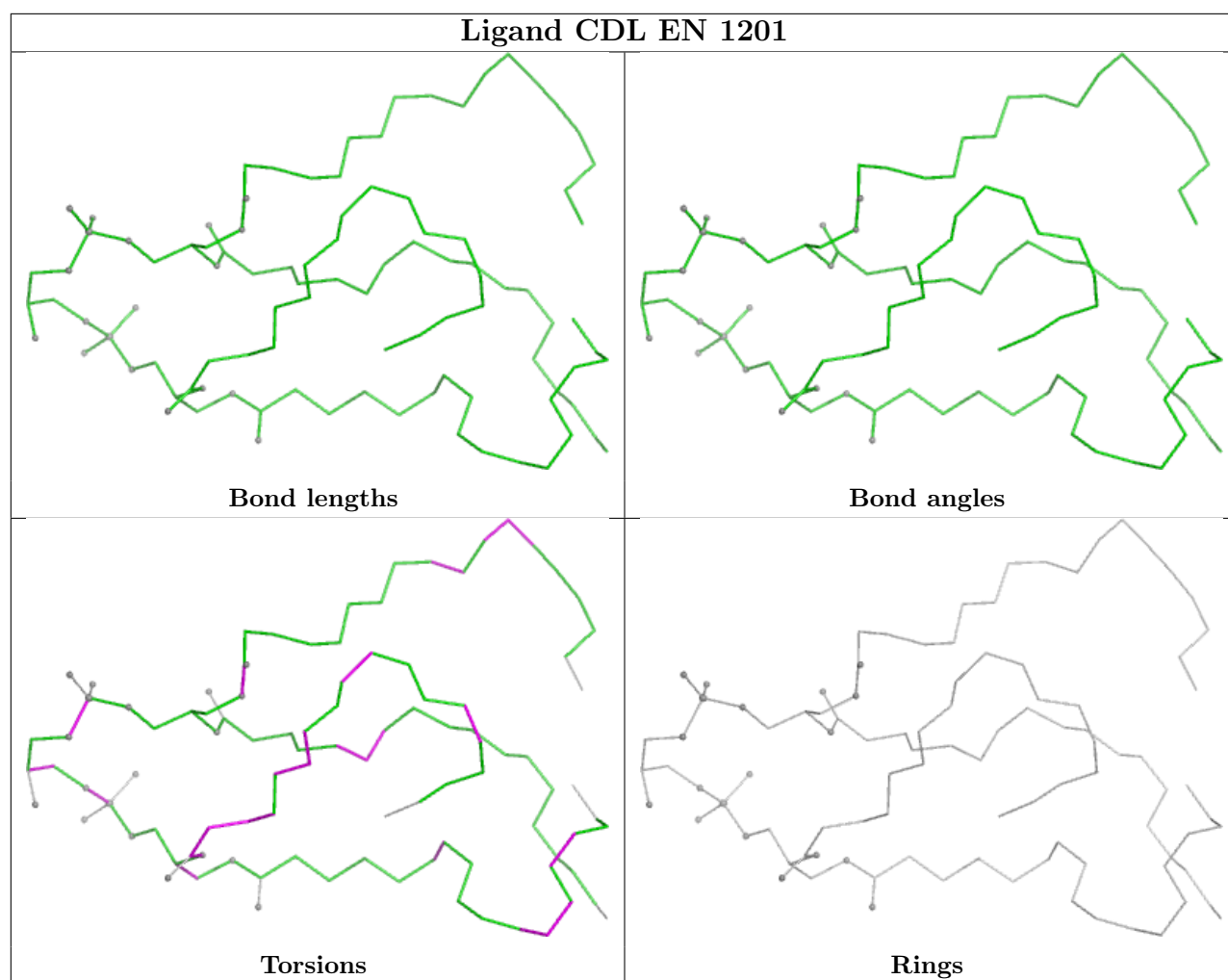


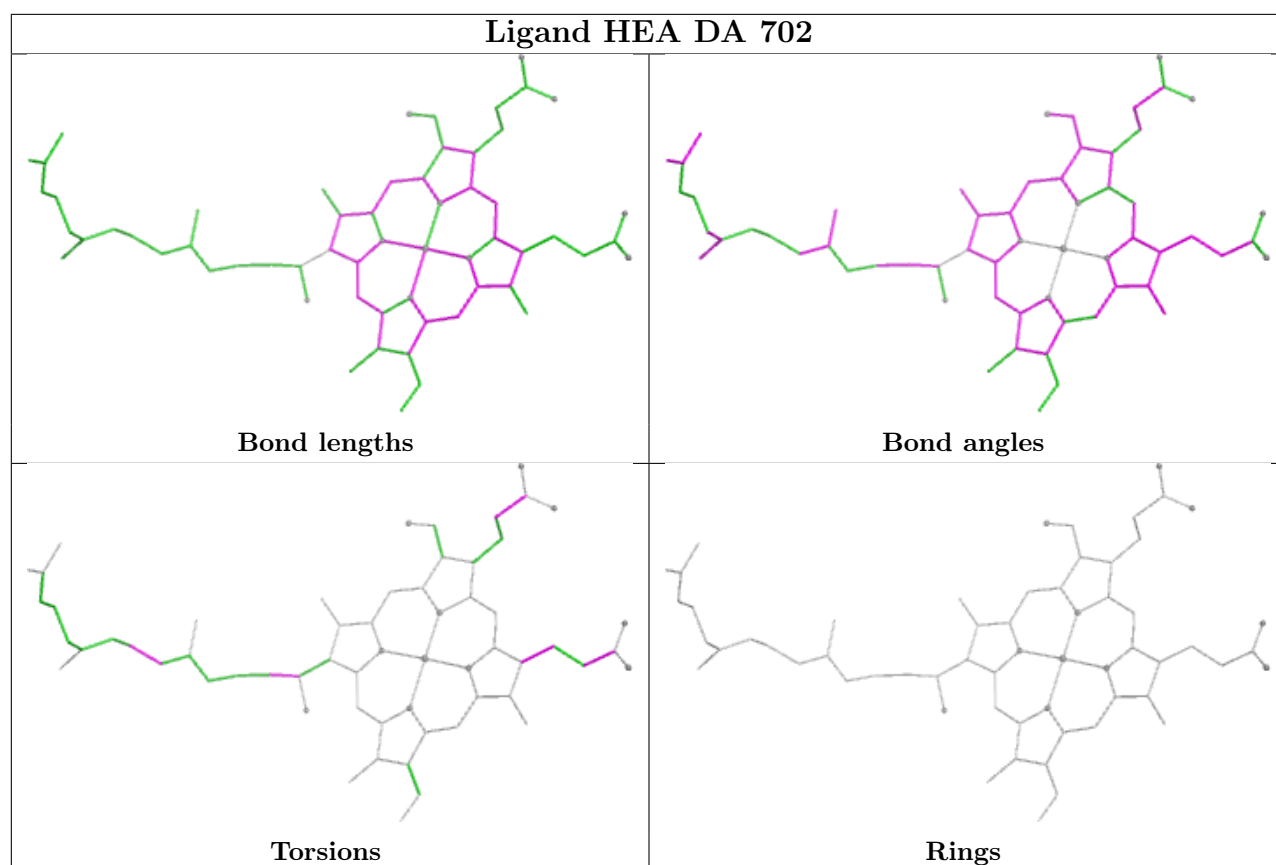












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

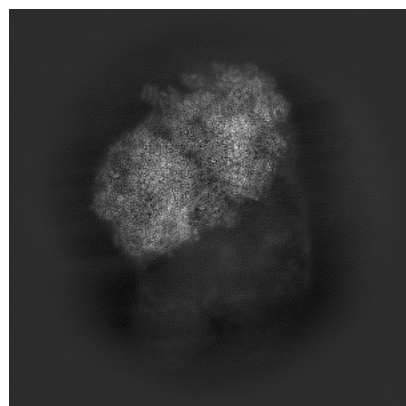
6 Map visualisation [i](#)

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.

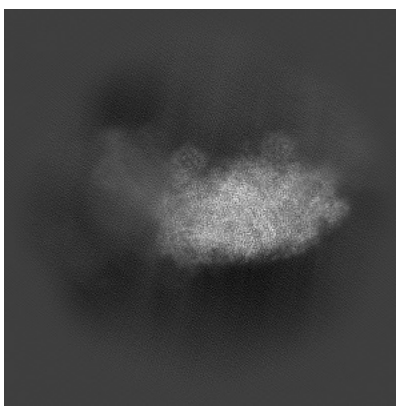
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

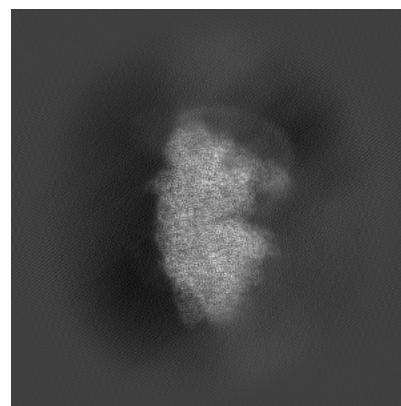
6.1.1 Primary map



X

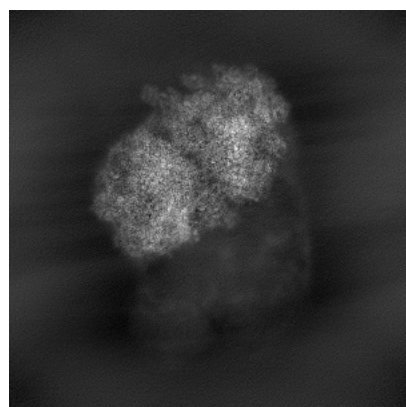


Y

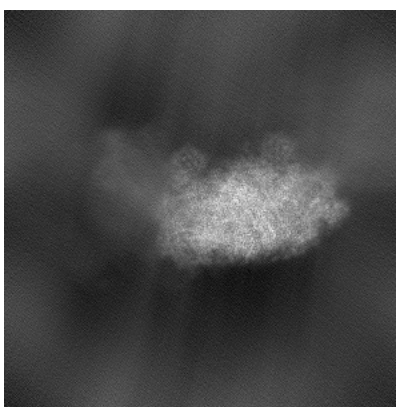


Z

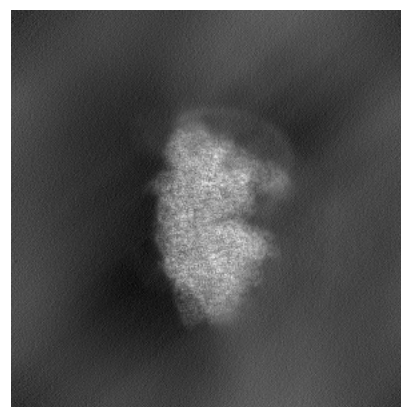
6.1.2 Raw map



X



Y

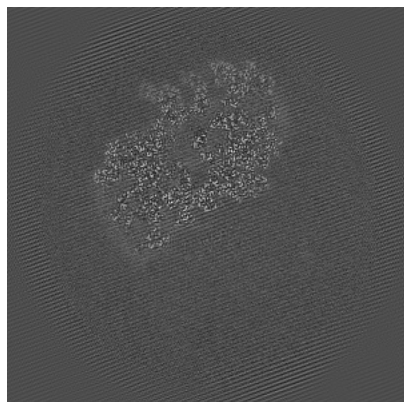


Z

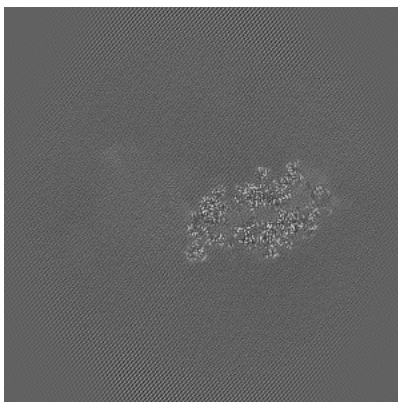
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

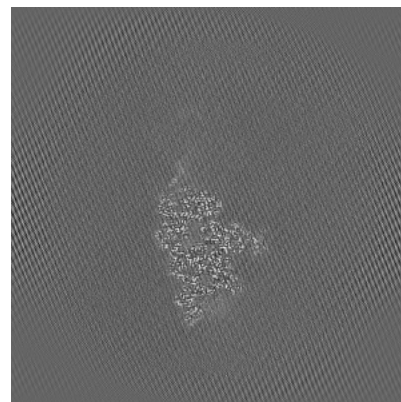
6.2.1 Primary map



X Index: 240

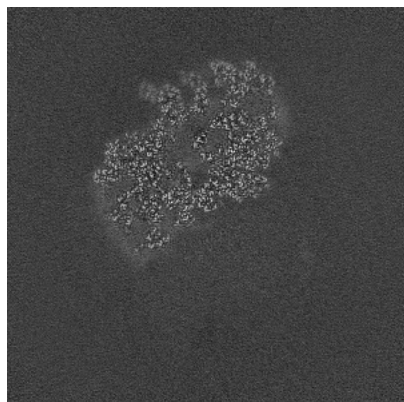


Y Index: 240

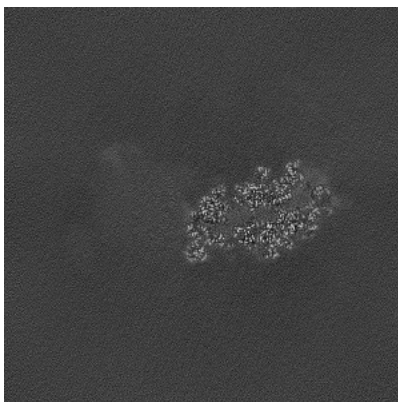


Z Index: 240

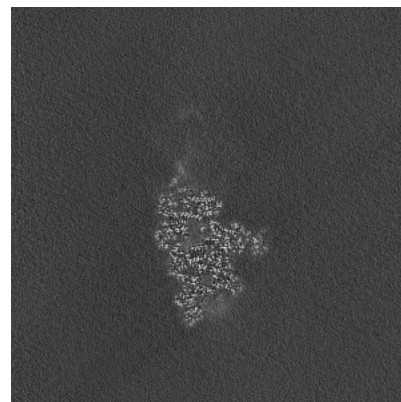
6.2.2 Raw map



X Index: 240



Y Index: 240

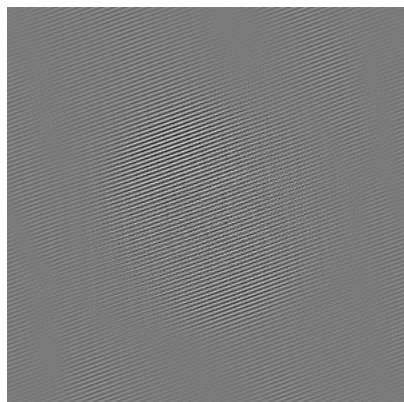


Z Index: 240

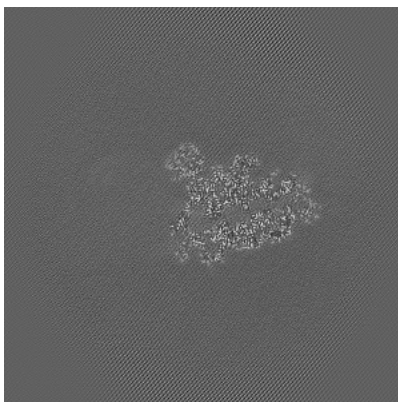
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

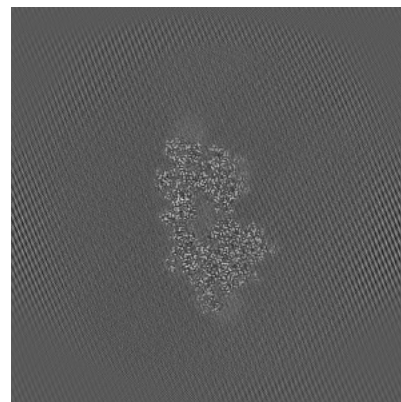
6.3.1 Primary map



X Index: 444

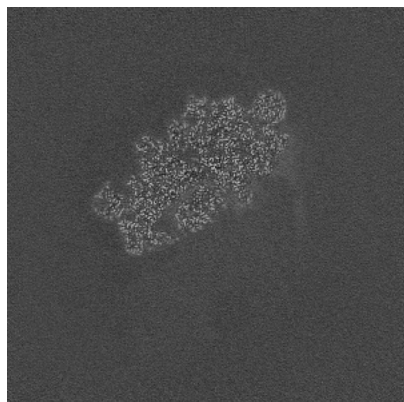


Y Index: 204

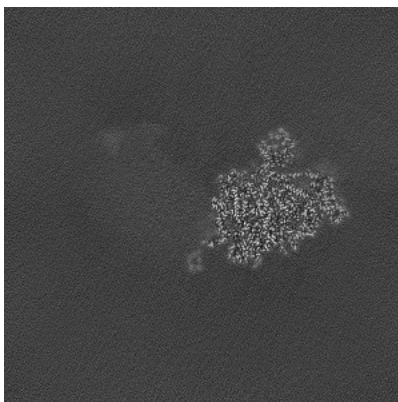


Z Index: 287

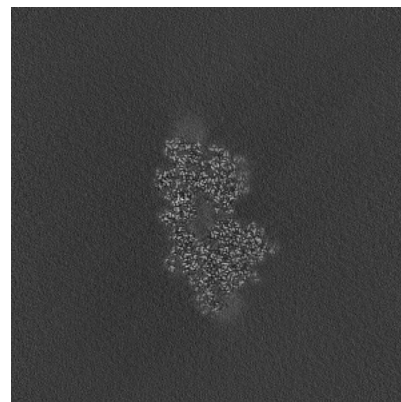
6.3.2 Raw map



X Index: 206



Y Index: 271

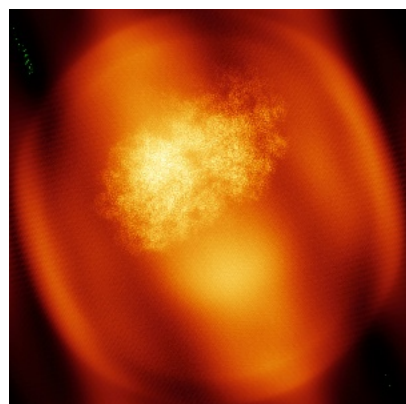


Z Index: 287

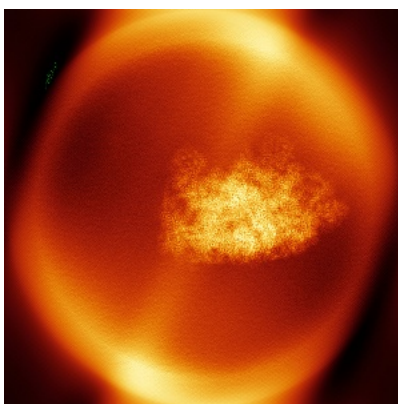
The images above show the largest variance slices of the map in three orthogonal directions.

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

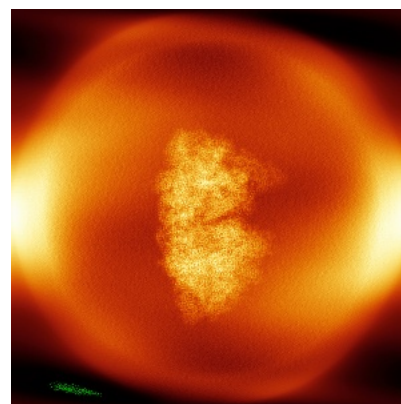
6.4.1 Primary map



X

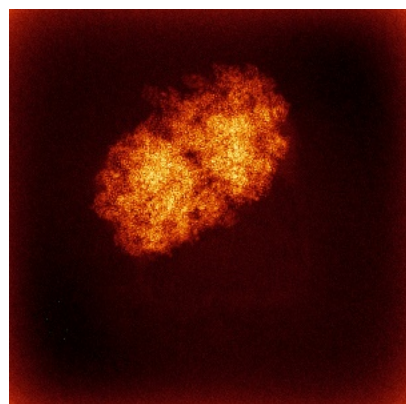


Y

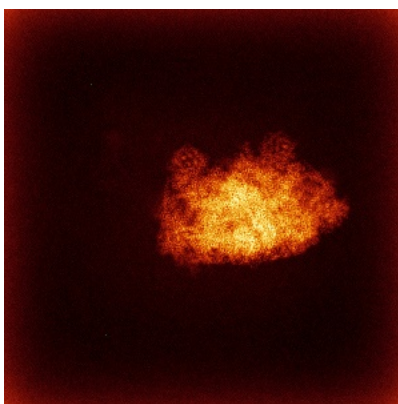


Z

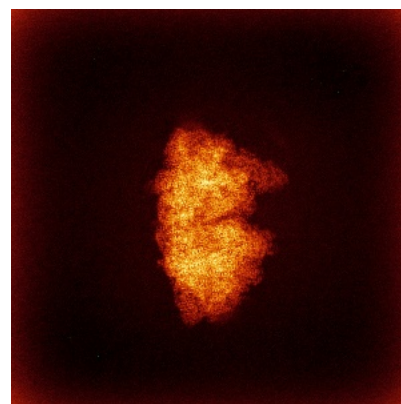
6.4.2 Raw map



X



Y

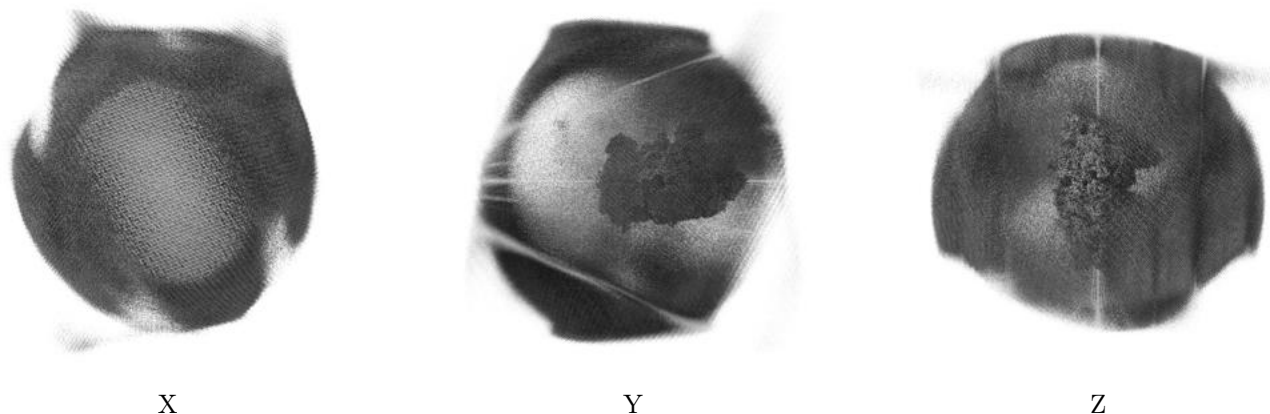


Z

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.

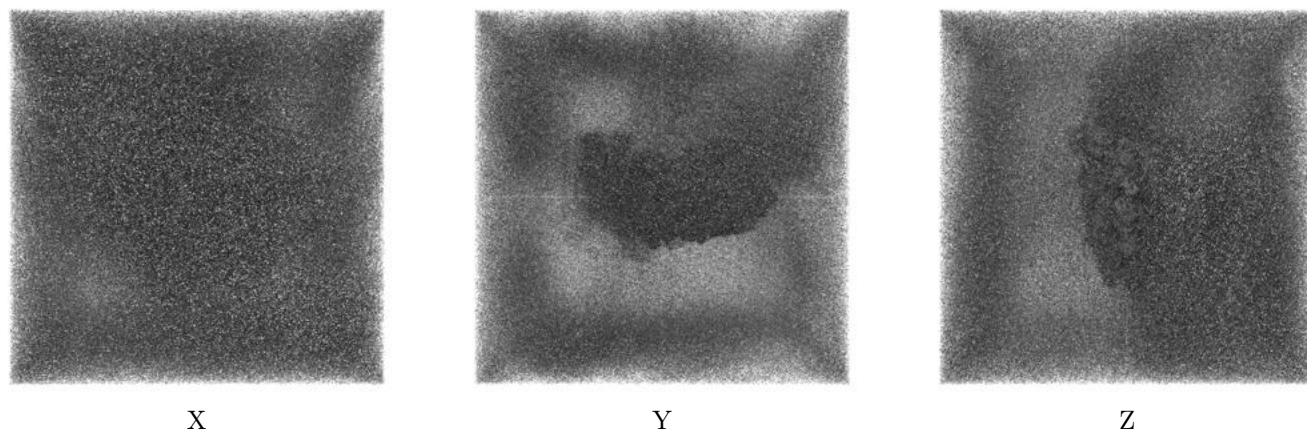
6.5 Orthogonal surface views [i](#)

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.

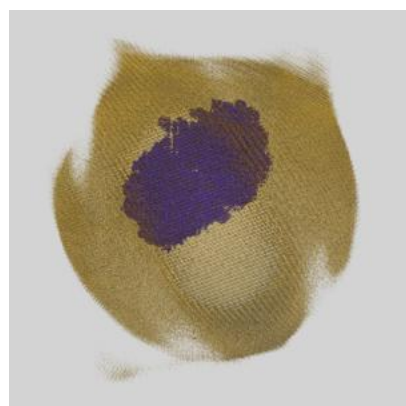
6.6 Mask visualisation [i](#)

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

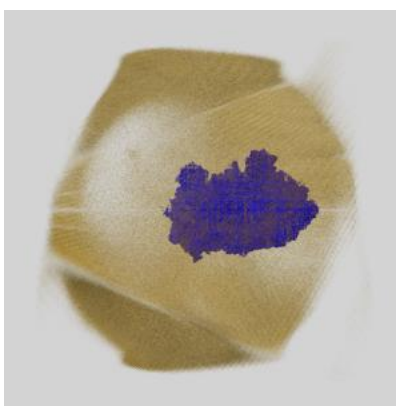
A mask typically either:

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

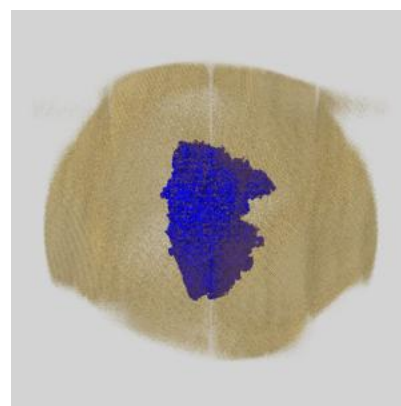
6.6.1 emd_15867_msk_1.map [i](#)



X



Y

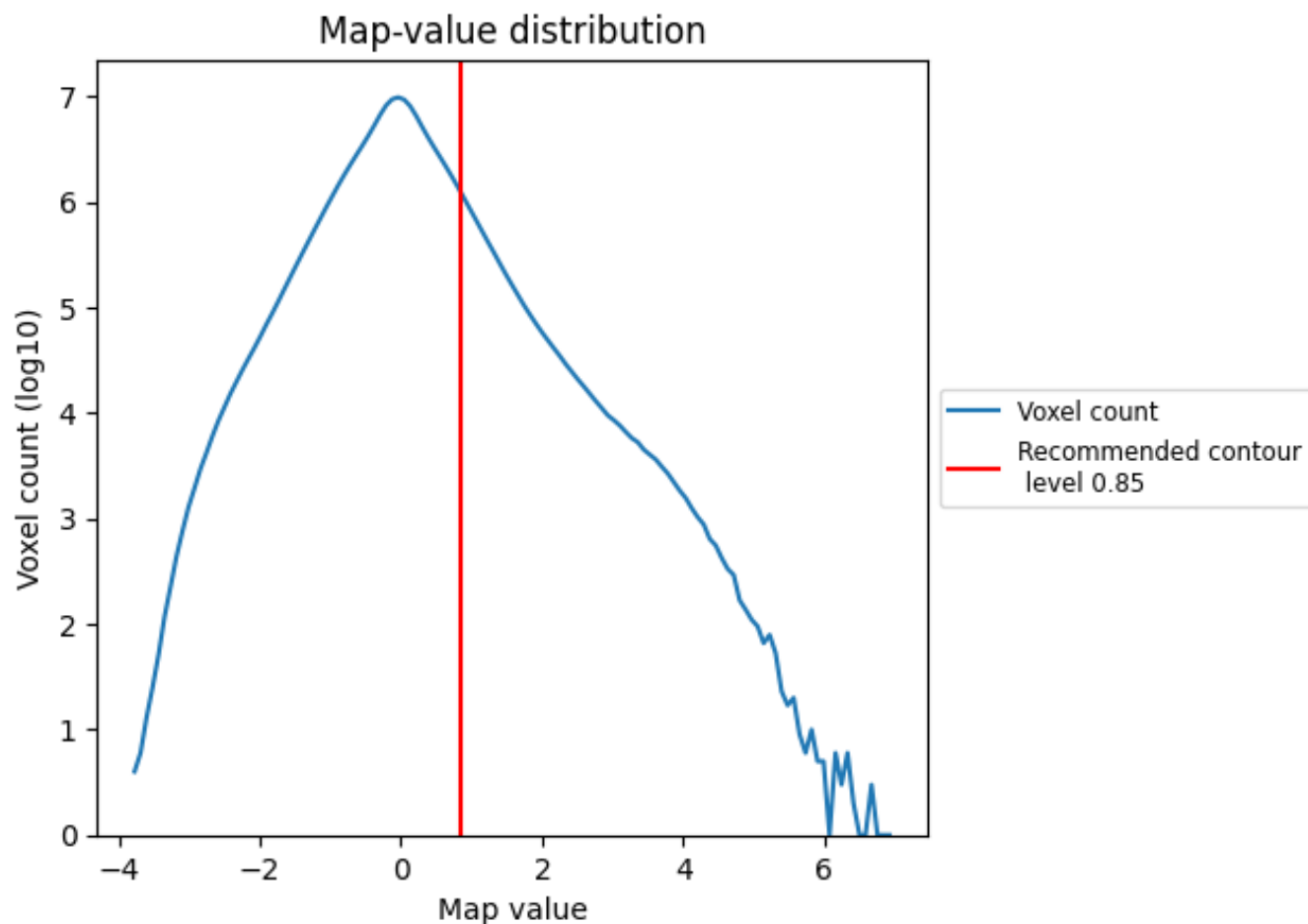


Z

7 Map analysis [i](#)

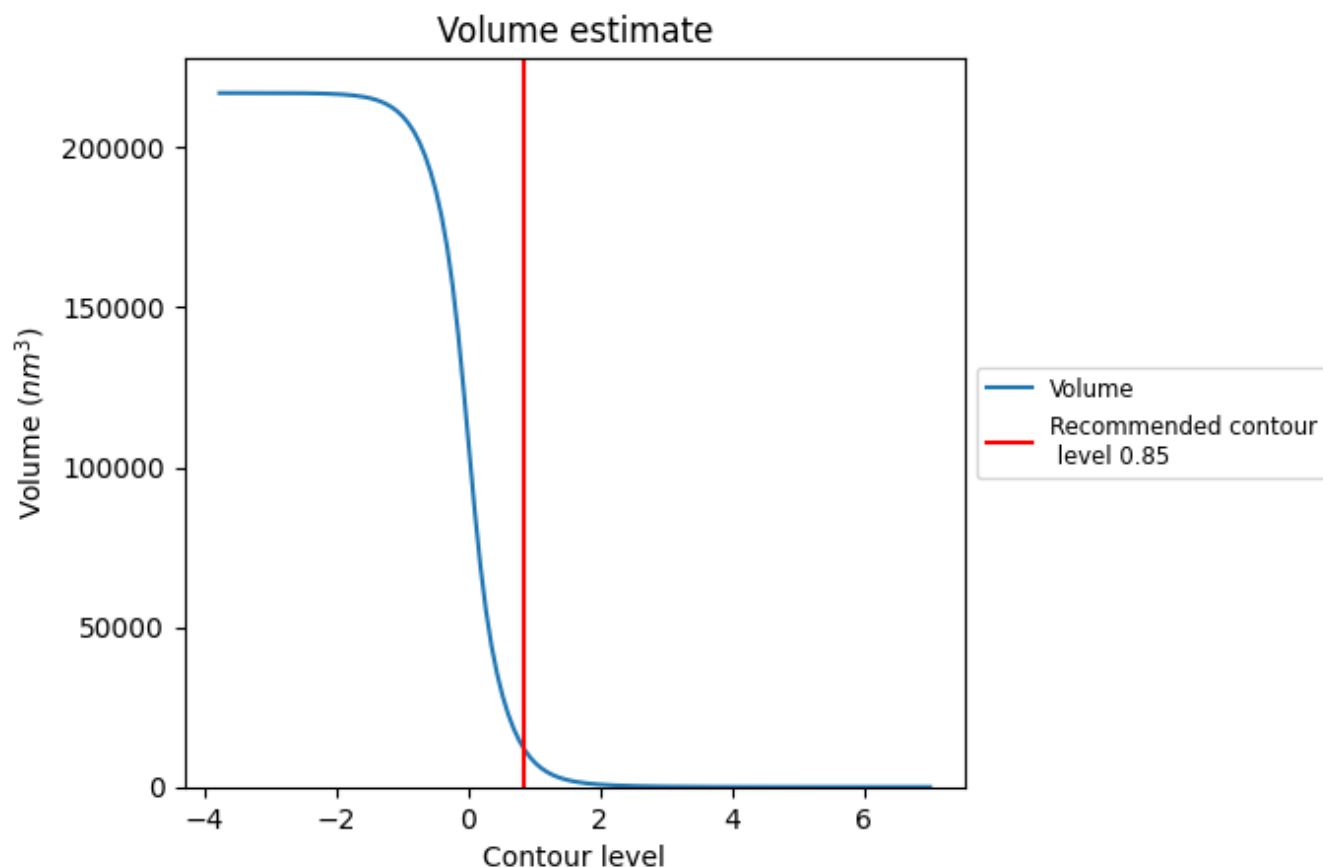
This section contains the results of statistical analysis of the map.

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.

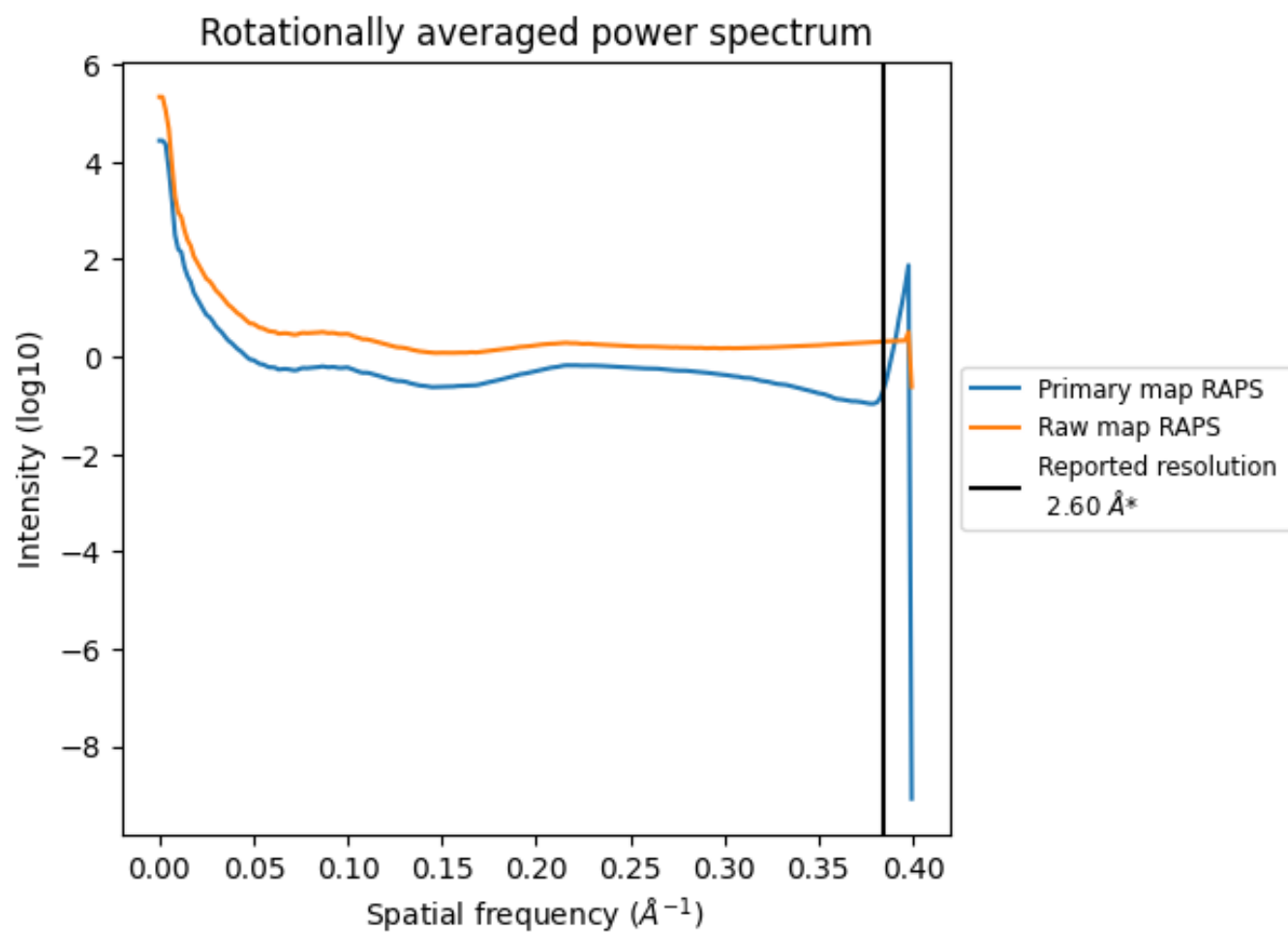
7.2 Volume estimate [i](#)



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 ⓘ

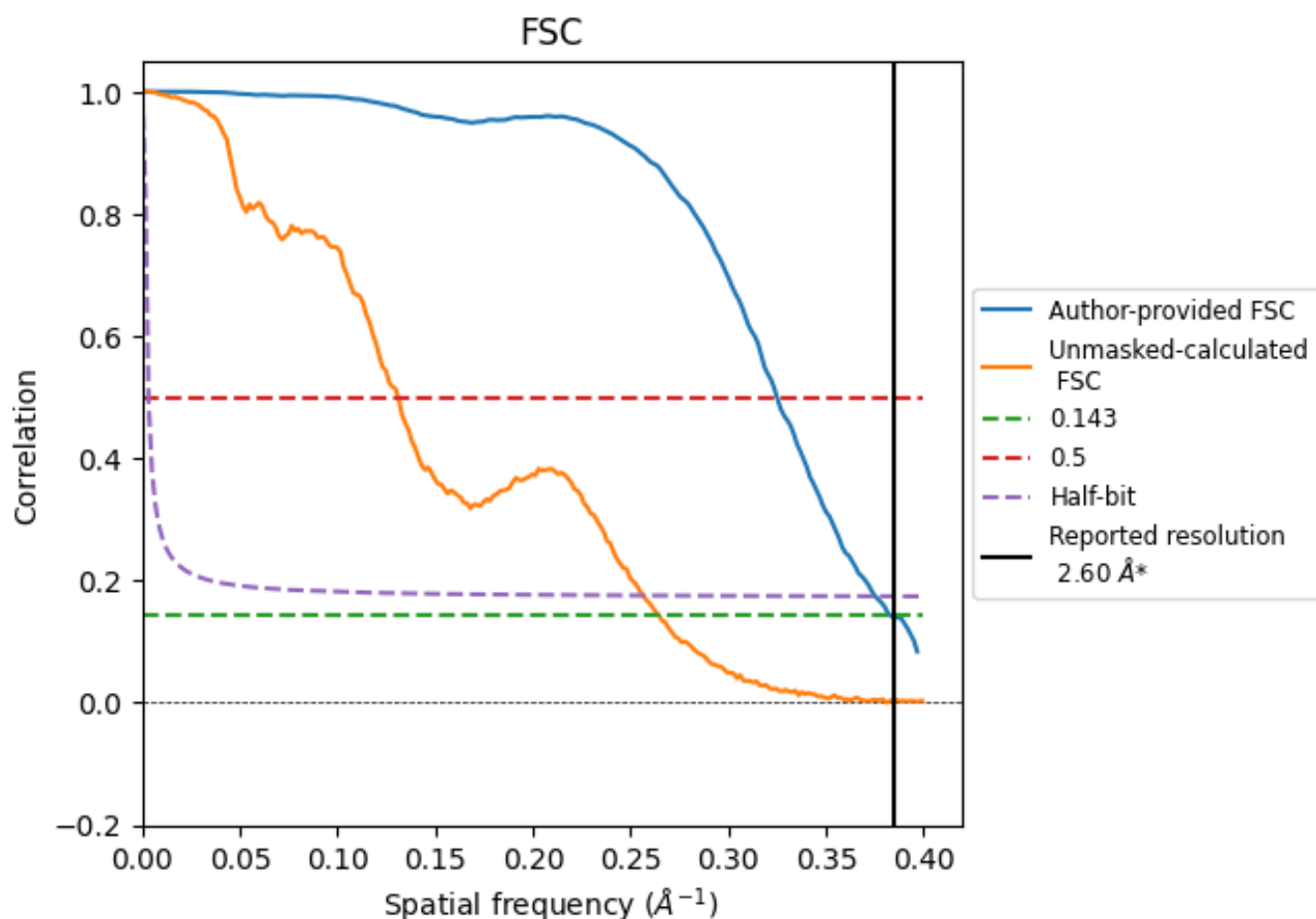


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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

8.2 Resolution estimates [i](#)

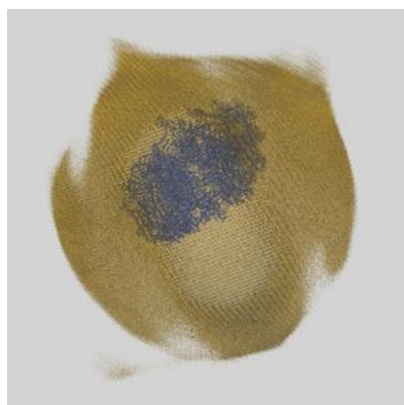
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	3.08	2.66
Unmasked-calculated*	3.78	7.63	3.90

*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 %

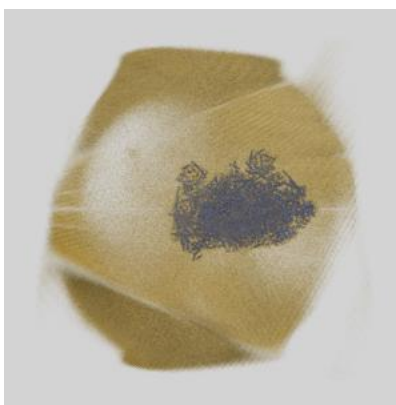
9 Map-model fit [i](#)

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 36](#).

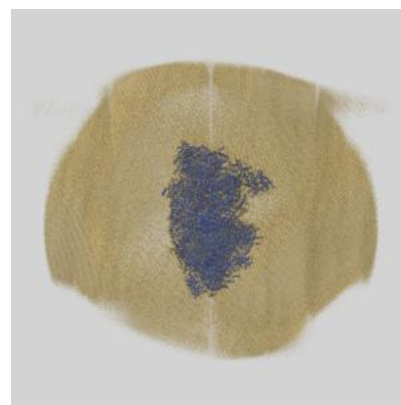
9.1 Map-model overlay [i](#)



X



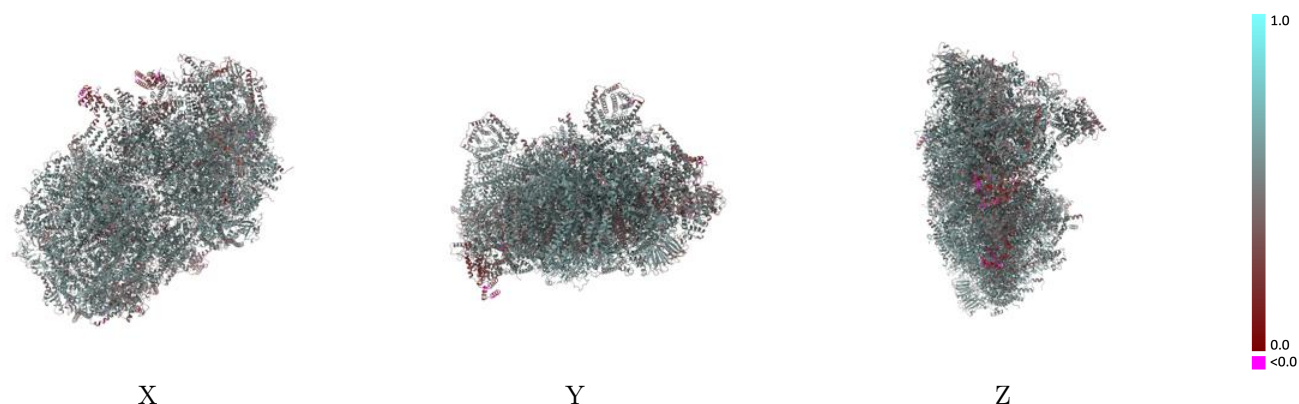
Y



Z

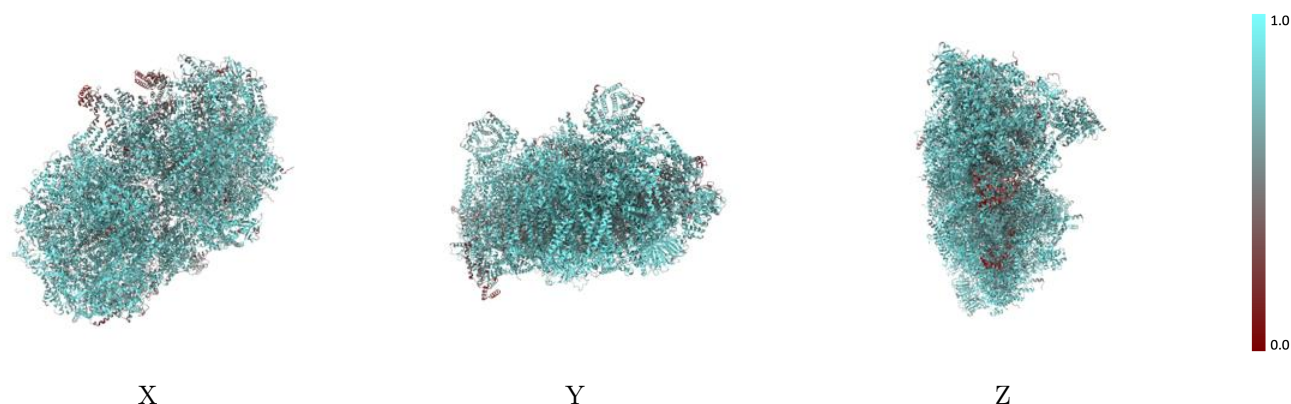
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



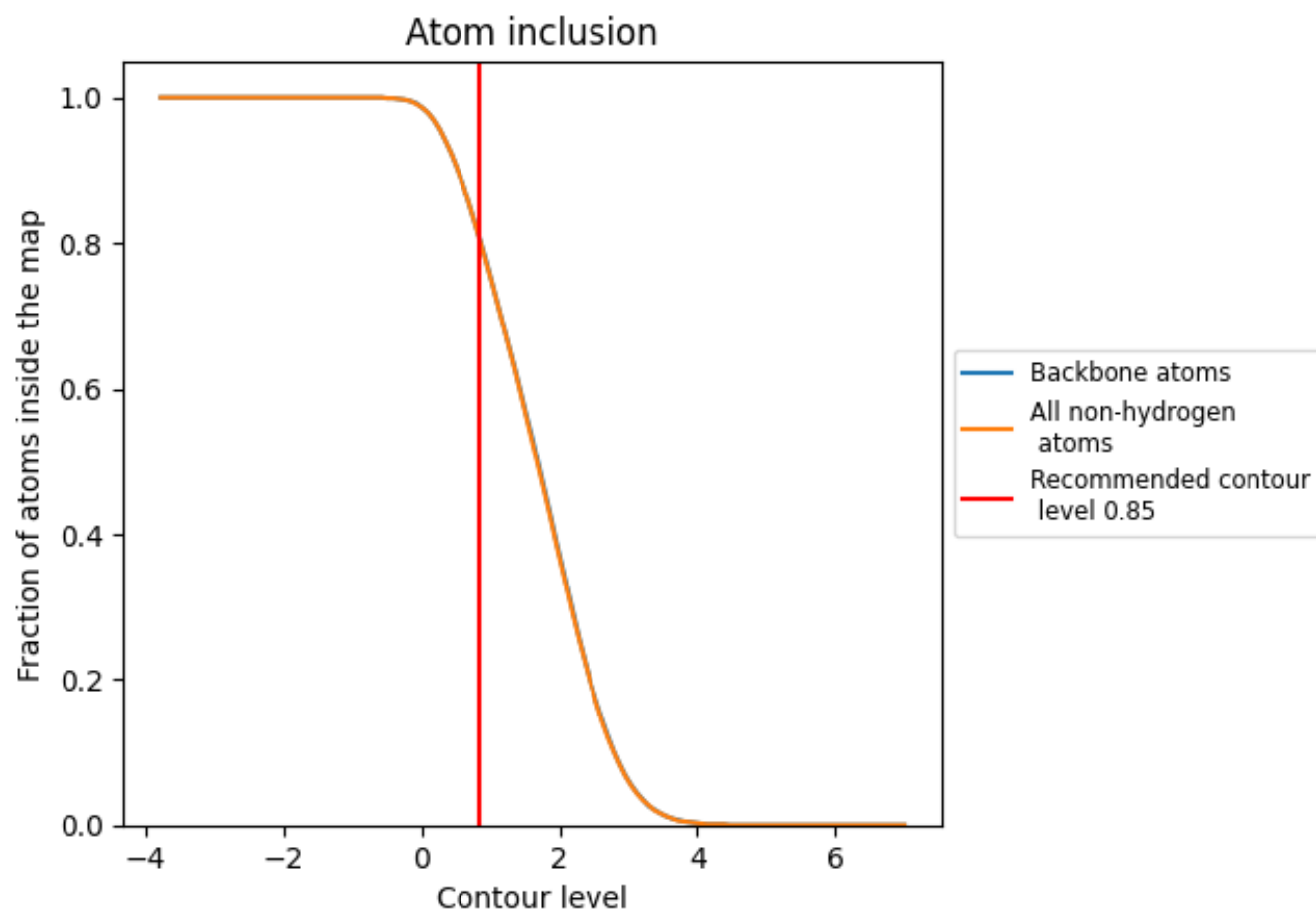
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

Continued from previous page...

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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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