



## wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 06:42 PM UTC

PDB ID : 8UGH / pdb\_00008ugh  
EMDB ID : EMD-42225  
Title : In-situ structure of typeA supercomplex with lipids in respiratory chain (composite)  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-05  
Resolution : 2.10 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](mailto: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>.

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

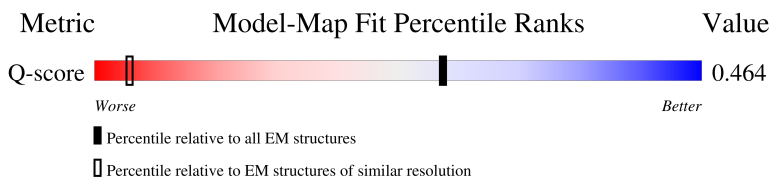
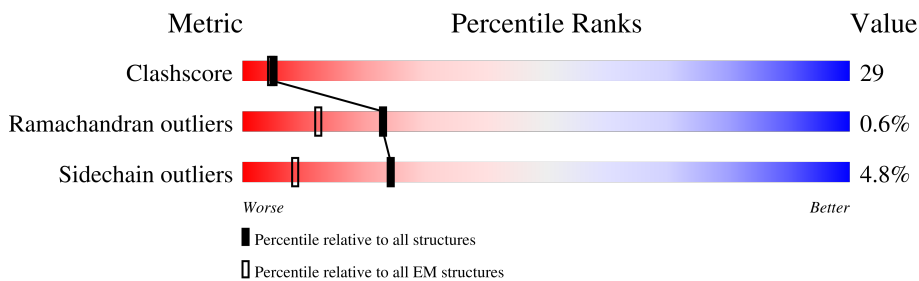
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.10 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	2317 ( 1.60 - 2.60 )

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  $\geq 3$ , 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	1A	115	52% 42% 5% .
2	1B	258	34% 23% . 40%
3	1C	264	62% 17% 21%
4	1D	466	59% 32% . 8%




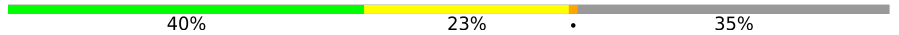





















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Mol	Chain	Length	Quality of chain
5	1E	249	53% 32% 14%
6	1F	464	57% 32% 7%
7	1G	727	64% 30% 6%
8	1H	318	53% 44% 3%
9	1I	239	43% 28% 26%
10	1J	175	51% 40% 7%
11	1K	98	53% 43% 4%
12	1L	606	61% 35% 4%
13	1M	459	61% 37% 2%
14	1N	347	59% 37% 4%
15	1O	357	55% 31% 10%
16	1P	377	60% 29% 9%
17	1Q	175	49% 22% 26%
18	1R	123	63% 15% 22%
19	1S	99	62% 23% 12%
20	1T	156	31% 23% 46%
20	1U	156	32% 23% 45%
21	1V	116	74% 22% 4%
22	1W	128	64% 25% 10%
23	1X	172	74% 23% 3%
24	1Y	141	45% 48% 5%
25	1Z	144	69% 26% 5%
26	1a	70	64% 34% 2%
27	1b	84	71% 25% 4%
28	1c	76	43% 20% 36%

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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	

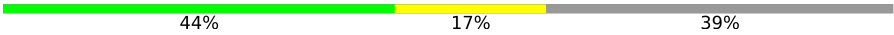

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Mol	Chain	Length	Quality of chain
49	3I	274	5% 9% . 83%
49	3R	274	23% 37% 12% 28%
49	3V	274	6% . . 89%
50	3F	111	51% 35% . . 12%
50	3S	111	61% 26% . 12%
51	3G	82	34% 50% 6% 10%
51	3T	82	41% 46% . 10%
52	3H	91	27% 40% . . 29%
52	3U	91	25% 36% 10% 29%
53	3J	64	39% 38% 5% 6% 12%
53	3W	64	42% 39% . 5% 12%
54	3X	56	34% 55% . 7%
54	3Y	56	36% 54% . 9%
55	4A	514	63% 36% .
56	4B	229	64% 34% .
57	4C	261	61% 37% . .
58	4D	169	53% 27% . 18%
59	4E	152	44% 25% 31%
60	4F	129	57% 17% . 25%
61	4G	97	49% 24% . 23%
62	4H	86	56% 37% . 5%
63	4I	75	64% 23% . 11%
64	4J	80	54% 19% 28%
65	4K	80	42% 18% . 39%
66	4L	63	52% 21% 27%

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Mol	Chain	Length	Quality of chain
67	4M	70	
68	4N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	FME	4A	1	-	-	X	-
69	3PE	1B	204	-	-	X	-
69	3PE	1B	205	-	-	X	-
69	3PE	1J	201	-	-	X	-
69	3PE	1L	703	-	-	X	-
69	3PE	1L	709	-	-	X	-
69	3PE	1N	401	-	-	X	-
69	3PE	1Y	201	-	-	X	-
69	3PE	1Y	208	-	-	X	-
69	3PE	1Y	209	-	-	X	-
69	3PE	1Y	213	-	-	X	-
69	3PE	1Y	214	-	-	X	-
69	3PE	1Y	215	-	-	X	-
69	3PE	1b	101	-	-	X	-
69	3PE	1d	201	-	-	X	-
69	3PE	1d	203	-	-	X	-
69	3PE	1d	206	-	-	X	-
69	3PE	1f	104	-	-	X	-
69	3PE	1g	202	-	-	X	-
69	3PE	1k	101	-	-	X	-
69	3PE	1m	202	-	-	X	-
69	3PE	1m	203	-	-	X	-
69	3PE	1m	205	-	-	X	-
69	3PE	1o	201	-	-	X	-
69	3PE	3A	502	-	-	X	-
69	3PE	3A	503	-	-	X	-
69	3PE	3C	507	-	-	X	-
69	3PE	3C	508	-	-	X	-
69	3PE	3C	509	-	-	X	-
69	3PE	3C	511	-	-	X	-
69	3PE	3C	512	-	-	X	-
69	3PE	3C	513	-	-	X	-
69	3PE	3C	515	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	3PE	3C	516	-	-	X	-
69	3PE	3G	109	-	-	X	-
69	3PE	3N	501	-	-	X	-
69	3PE	3N	503	-	-	X	-
69	3PE	3P	503	-	-	X	-
69	3PE	3P	507	-	-	X	-
69	3PE	3P	508	-	-	X	-
69	3PE	3P	511	-	-	X	-
69	3PE	3P	514	-	-	X	-
69	3PE	3P	517	-	-	X	-
69	3PE	3P	518	-	-	X	-
69	3PE	3P	519	-	-	X	-
69	3PE	3P	520	-	-	X	-
69	3PE	3R	305	-	-	X	-
69	3PE	3S	201	-	-	X	-
69	3PE	3T	103	-	-	X	-
69	3PE	3W	101	-	-	X	-
69	3PE	3W	102	-	-	X	-
69	3PE	3W	103	-	-	X	-
69	3PE	3X	101	-	-	X	-
69	3PE	3X	105	-	-	X	-
69	3PE	3X	107	-	-	X	-
69	3PE	3X	108	-	-	X	-
69	3PE	3Y	102	-	-	X	-
69	3PE	3Y	105	-	-	X	-
69	3PE	3Y	107	-	-	X	-
69	3PE	4G	104	-	-	X	-
70	PC1	1A	202	-	-	X	-
70	PC1	1B	202	-	-	X	-
70	PC1	1B	203	-	-	X	-
70	PC1	1H	403	-	-	X	-
70	PC1	1Y	206	-	-	X	-
70	PC1	1Y	207	-	-	X	-
70	PC1	1d	204	-	-	X	-
70	PC1	3T	102	-	-	X	-
71	SF4	1F	502	-	-	X	-
71	SF4	1G	802	-	-	X	-
71	SF4	1I	202	-	-	X	-
72	FES	1E	301	-	-	X	-
72	FES	1G	803	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	3R	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
75	CDL	1L	704	-	-	X	-
75	CDL	1N	402	-	-	X	-
75	CDL	1Y	217	-	-	X	-
75	CDL	1d	202	-	-	X	-
75	CDL	1d	205	-	-	X	-
75	CDL	1g	201	-	-	X	-
75	CDL	1i	201	-	-	X	-
75	CDL	1q	202	-	-	X	-
75	CDL	3A	501	-	-	X	-
75	CDL	3F	201	-	-	X	-
75	CDL	3N	502	-	-	X	-
75	CDL	3P	513	-	-	X	-
75	CDL	3X	103	-	-	X	-
75	CDL	3Y	106	-	-	X	-
75	CDL	4B	302	-	-	X	-
75	CDL	4C	307	-	-	X	-
76	AYA	1I	203	-	-	X	-
82	PGT	1Y	203	-	-	X	-
91	PGV	4A	609	-	-	X	-
93	PSC	4B	303	-	-	X	-

## 2 Entry composition [i](#)

There are 94 unique types of molecules in this entry. The entry contains 124052 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	115	916	616	134	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	155	1242	791	226	211	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1740	1125	297	316	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	429	3452	2207	593	628	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1E	214	1658	1058	278	312	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1F	432	3325	2100	592	613	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1G	699	5362	3360	933	1029	40	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1H	318	2504	1673	385	425	21	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	1I	176	1412	887	243	269	13	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	1J	174	1329	892	189	236	12	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1K	98	750	494	113	129	14	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1L	606	4818	3195	746	826	51	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1M	459	3632	2411	572	610	39	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	1N	347	2712	1783	420	463	46	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	1O	320	2590	1649	440	491	10	0	0

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	1P	342	2751	1783	481	478	9	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	1Q	129	1047	659	186	199	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	1R	96	741	452	140	146	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1Z	141	1168	752	202	205	9	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1a	70	562	361	101	94	6	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	1b	83	643	417	110	115	1	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	1c	49	417	276	71	70	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	1d	119	985	641	171	168	5	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	1e	99	816	519	151	140	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	1f	57	487	316	89	80	2	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
32	1g	100	835	535	138	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	1h	138	1151	754	195	199	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	1i	128	1100	723	194	181	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	1j	71	601	394	99	107	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	1k	81	649	422	110	116	1	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	1l	156	1310	847	213	242	8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	1m	128	1062	691	182	189	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	1n	172	1495	956	273	258	8	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	1o	122	1045	650	198	187	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	1p	173	1449	908	263	270	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	1q	145	1212	775	219	213	5	0	0

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	1r	94	759	478	143	135	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1s	45	382	238	70	73	1	0	0

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			464	305	82	77		
53	3W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	4A	514	4026	2693	625	676	32	0	0

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	4B	227	1828	1190	281	339	18	0	0

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	4C	259	2096	1399	336	351	10	0	0

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	4D	139	1163	757	190	212	4	0	0

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	4E	105	852	544	144	162	2	0	0

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	4F	97	734	455	130	143	6	0	0

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	4G	75	617	398	118	100	1	0	0

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

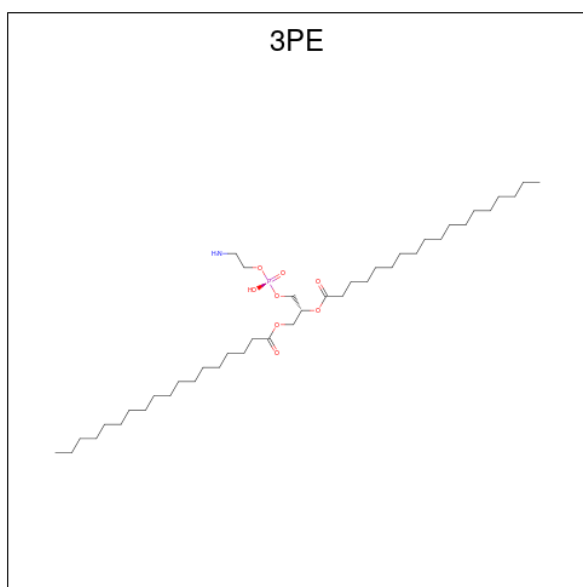
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1A	1	47	37	1	8	1	0
69	1A	1	41	31	1	8	1	0
69	1B	1	51	41	1	8	1	0
69	1B	1	51	41	1	8	1	0
69	1J	1	51	41	1	8	1	0
69	1J	1	44	34	1	8	1	0
69	1L	1	46	36	1	8	1	0
69	1L	1	45	35	1	8	1	0
69	1L	1	44	34	1	8	1	0
69	1L	1	49	39	1	8	1	0
69	1L	1	33	23	1	8	1	0
69	1L	1	42	32	1	8	1	0
69	1L	1	42	32	1	8	1	0
69	1L	1	42	32	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1L	1	Total 38	C 28	N 1	O 8	P 1	0
69	1L	1	Total 41	C 31	N 1	O 8	P 1	0
69	1L	1	Total 51	C 41	N 1	O 8	P 1	0
69	1M	1	Total 47	C 37	N 1	O 8	P 1	0
69	1N	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Y	1	Total 42	C 32	N 1	O 8	P 1	0
69	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
69	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	1Y	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Y	1	Total 42	C 32	N 1	O 8	P 1	0
69	1Y	1	Total 42	C 32	N 1	O 8	P 1	0
69	1Y	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Y	1	Total 44	C 34	N 1	O 8	P 1	0
69	1Y	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Y	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Y	1	Total 43	C 33	N 1	O 8	P 1	0
69	1Y	1	Total 51	C 41	N 1	O 8	P 1	0
69	1Z	1	Total 51	C 41	N 1	O 8	P 1	0
69	1b	1	Total 42	C 32	N 1	O 8	P 1	0
69	1d	1	Total 48	C 38	N 1	O 8	P 1	0
69	1d	1	Total 47	C 37	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1d	1	Total 51	41	1	8	1	0
69	1e	1	Total 51	41	1	8	1	0
69	1f	1	Total 45	35	1	8	1	0
69	1f	1	Total 43	33	1	8	1	0
69	1f	1	Total 45	35	1	8	1	0
69	1f	1	Total 48	38	1	8	1	0
69	1g	1	Total 51	41	1	8	1	0
69	1g	1	Total 33	23	1	8	1	0
69	1h	1	Total 47	37	1	8	1	0
69	1k	1	Total 46	36	1	8	1	0
69	1l	1	Total 42	32	1	8	1	0
69	1l	1	Total 33	23	1	8	1	0
69	1l	1	Total 51	41	1	8	1	0
69	1m	1	Total 50	40	1	8	1	0
69	1m	1	Total 42	32	1	8	1	0
69	1m	1	Total 42	32	1	8	1	0
69	1m	1	Total 51	41	1	8	1	0
69	1m	1	Total 51	41	1	8	1	0
69	1o	1	Total 51	41	1	8	1	0
69	3A	1	Total 51	41	1	8	1	0
69	3A	1	Total 51	41	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 46	C 36	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 47	C 37	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 48	C 38	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 35	C 25	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 51	C 41	N 1	O 8	P 1	0
69	3C	1	Total 35	C 25	N 1	O 8	P 1	0
69	3C	1	Total 48	C 38	N 1	O 8	P 1	0
69	3C	1	Total 43	C 33	N 1	O 8	P 1	0
69	3C	1	Total 32	C 22	N 1	O 8	P 1	0
69	3D	1	Total 41	C 31	N 1	O 8	P 1	0
69	3D	1	Total 45	C 35	N 1	O 8	P 1	0
69	3E	1	Total 51	C 41	N 1	O 8	P 1	0
69	3E	1	Total 49	C 39	N 1	O 8	P 1	0
69	3G	1	Total 51	C 41	N 1	O 8	P 1	0
69	3G	1	Total 33	C 23	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
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69	3G	1	Total 33	C 23	N 1	O 8	P 1	0
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69	3G	1	Total 33	C 23	N 1	O 8	P 1	0
69	3G	1	Total 33	C 23	N 1	O 8	P 1	0
69	3G	1	Total 51	C 41	N 1	O 8	P 1	0
69	3G	1	Total 43	C 33	N 1	O 8	P 1	0
69	3G	1	Total 48	C 38	N 1	O 8	P 1	0
69	3J	1	Total 47	C 37	N 1	O 8	P 1	0
69	3J	1	Total 38	C 28	N 1	O 8	P 1	0
69	3J	1	Total 51	C 41	N 1	O 8	P 1	0
69	3J	1	Total 51	C 41	N 1	O 8	P 1	0
69	3J	1	Total 51	C 41	N 1	O 8	P 1	0
69	3N	1	Total 51	C 41	N 1	O 8	P 1	0
69	3N	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 38	C 28	N 1	O 8	P 1	0
69	3P	1	Total 32	C 22	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0

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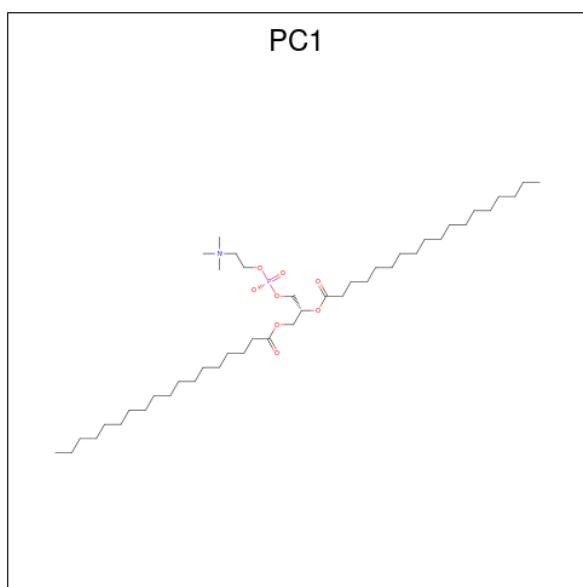
Mol	Chain	Residues	Atoms					AltConf
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69	3P	1	Total 45	C 35	N 1	O 8	P 1	0
69	3P	1	Total 48	C 38	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
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69	3P	1	Total 51	C 41	N 1	O 8	P 1	0
69	3Q	1	Total 41	C 31	N 1	O 8	P 1	0
69	3Q	1	Total 46	C 36	N 1	O 8	P 1	0
69	3Q	1	Total 46	C 36	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3R	1	Total 51	C 41	N 1	O 8	P 1	0
69	3S	1	Total 51	C 41	N 1	O 8	P 1	0
69	3T	1	Total 51	C 41	N 1	O 8	P 1	0
69	3W	1	Total 51	C 41	N 1	O 8	P 1	0
69	3W	1	Total 42	C 32	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	3W	1	51	41	1	8	1	0
69	3X	1	51	41	1	8	1	0
69	3X	1	51	41	1	8	1	0
69	3X	1	51	41	1	8	1	0
69	3X	1	51	41	1	8	1	0
69	3X	1	51	41	1	8	1	0
69	3Y	1	51	41	1	8	1	0
69	3Y	1	45	35	1	8	1	0
69	3Y	1	32	22	1	8	1	0
69	3Y	1	51	41	1	8	1	0
69	3Y	1	51	41	1	8	1	0
69	3Y	1	51	41	1	8	1	0
69	4G	1	32	22	1	8	1	0
69	4G	1	41	31	1	8	1	0

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



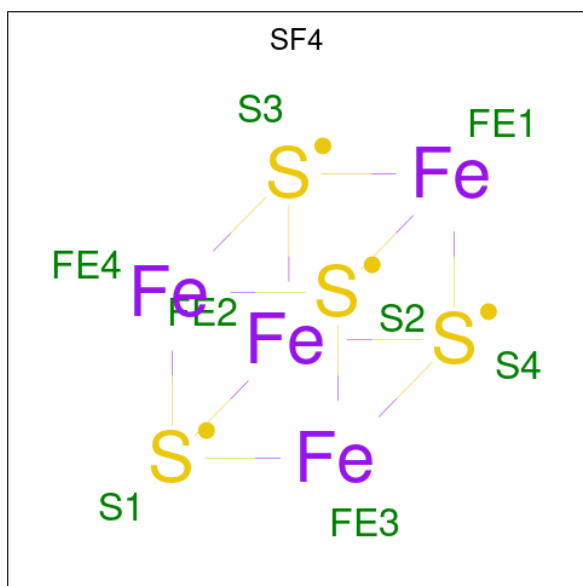
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
70	1A	1	35	25	1	8	1	0
70	1B	1	46	36	1	8	1	0
70	1B	1	48	38	1	8	1	0
70	1H	1	54	44	1	8	1	0
70	1H	1	48	38	1	8	1	0
70	1H	1	41	31	1	8	1	0
70	1J	1	35	25	1	8	1	0
70	1M	1	44	34	1	8	1	0
70	1P	1	33	23	1	8	1	0
70	1Y	1	35	25	1	8	1	0
70	1Y	1	46	36	1	8	1	0
70	1Y	1	54	44	1	8	1	0
70	1d	1	39	29	1	8	1	0
70	1h	1	47	37	1	8	1	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
70	1h	1	Total 46	C 36	N 1	O 8	P 1	0
70	3J	1	Total 54	C 44	N 1	O 8	P 1	0
70	3P	1	Total 54	C 44	N 1	O 8	P 1	0
70	3R	1	Total 54	C 44	N 1	O 8	P 1	0
70	3T	1	Total 54	C 44	N 1	O 8	P 1	0
70	3X	1	Total 54	C 44	N 1	O 8	P 1	0

- Molecule 71 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



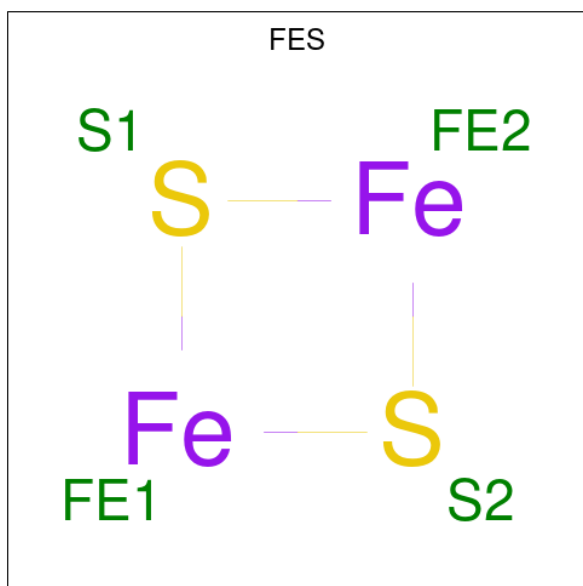
Mol	Chain	Residues	Atoms		AltConf	
			Total	Fe		S
71	1B	1	Total 8	Fe 4	S 4	0
71	1F	1	Total 8	Fe 4	S 4	0
71	1G	1	Total 8	Fe 4	S 4	0
71	1G	1	Total 8	Fe 4	S 4	0
71	1I	1	Total 8	Fe 4	S 4	0

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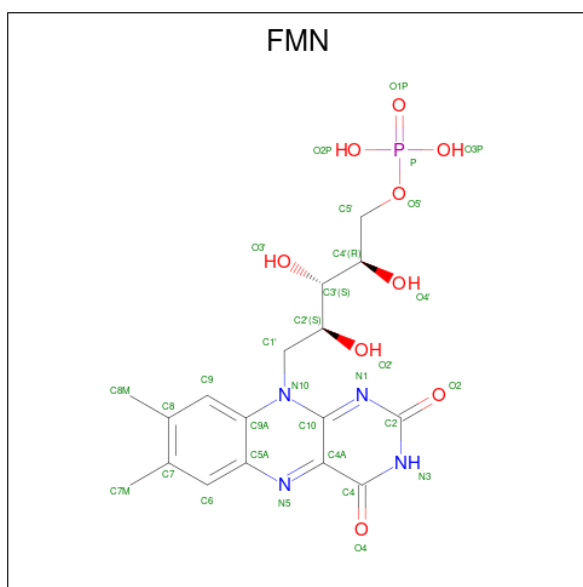
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
71	1I	1	8	4	4	0

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
72	1E	1	4	2	2	0
72	1G	1	4	2	2	0
72	3E	1	4	2	2	0
72	3R	1	4	2	2	0

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).

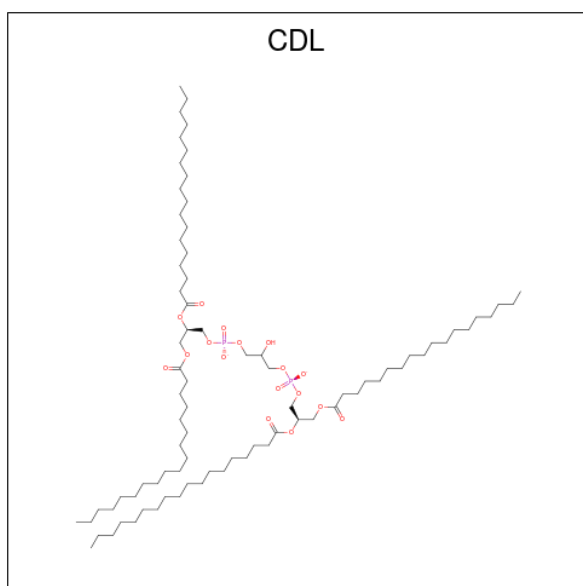


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

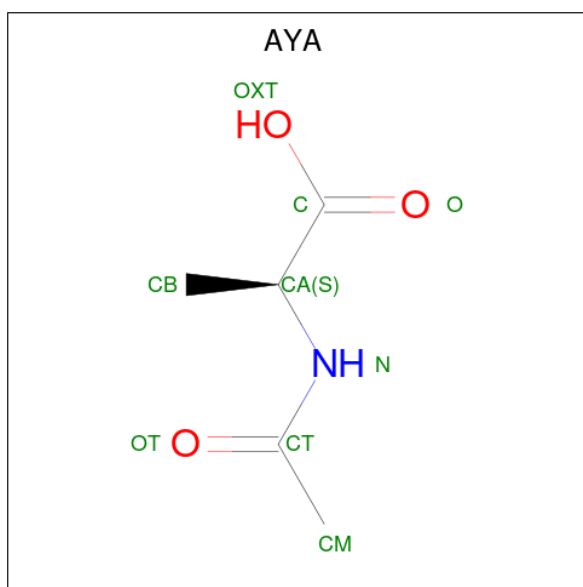
Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



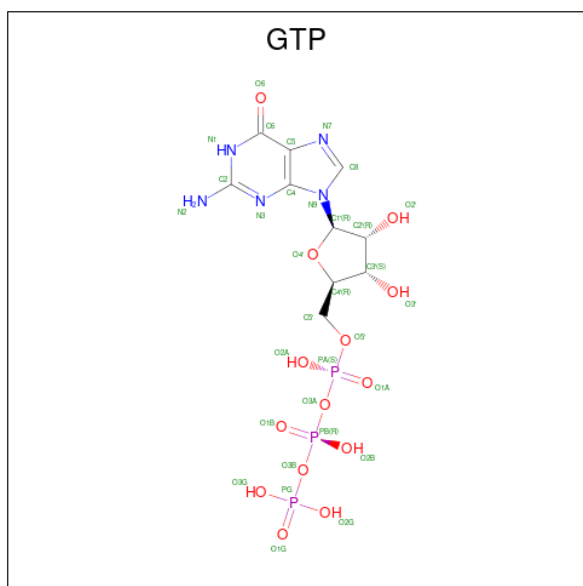
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			87	68	17	2	
75	1N	1	Total	C	O	P	0
			77	58	17	2	
75	1Y	1	Total	C	O	P	0
			100	81	17	2	
75	1d	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			93	74	17	2	
75	1g	1	Total	C	O	P	0
			100	81	17	2	
75	1i	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	1q	1	Total	C	O	P	0
			100	81	17	2	
75	3A	1	Total	C	O	P	0
			98	79	17	2	
75	3D	1	Total	C	O	P	0
			56	37	17	2	
75	3F	1	Total	C	O	P	0
			100	81	17	2	
75	3N	1	Total	C	O	P	0
			100	81	17	2	
75	3P	1	Total	C	O	P	0
			100	81	17	2	
75	3T	1	Total	C	O	P	0
			57	38	17	2	
75	3X	1	Total	C	O	P	0
			100	81	17	2	
75	3Y	1	Total	C	O	P	0
			100	81	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is N-ACETYLALANINE (CCD ID: AYA) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
76	1I	1	8	5	1	2	0

- Molecule 77 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

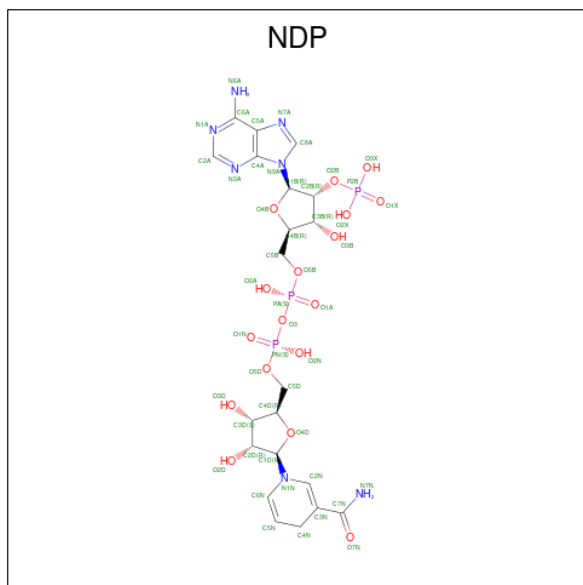


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
77	1O	1	32	10	5	14	3	0

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
78	1O	1	Total Mg 1 1	0
78	4A	1	Total Mg 1 1	0

- Molecule 79 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

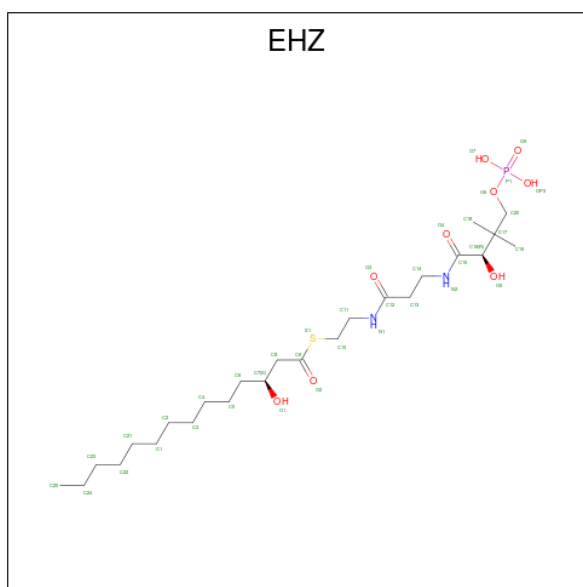


Mol	Chain	Residues	Atoms	AltConf
79	1P	1	Total C N O P 48 21 7 17 3	0

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

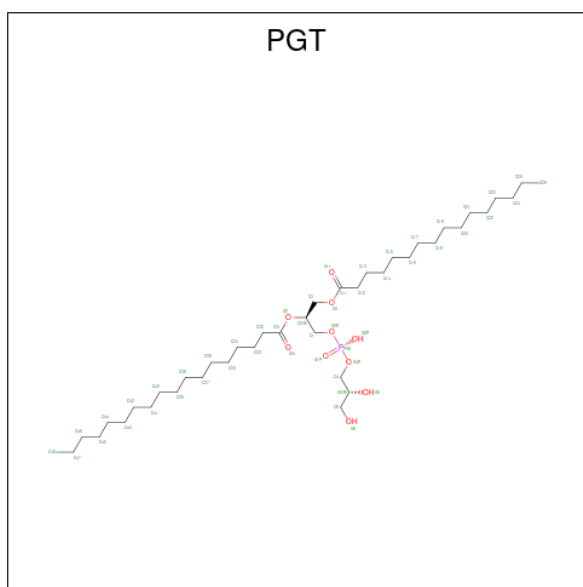
Mol	Chain	Residues	Atoms	AltConf
80	1R	1	Total Zn 1 1	0
80	4F	1	Total Zn 1 1	0

- Molecule 81 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).



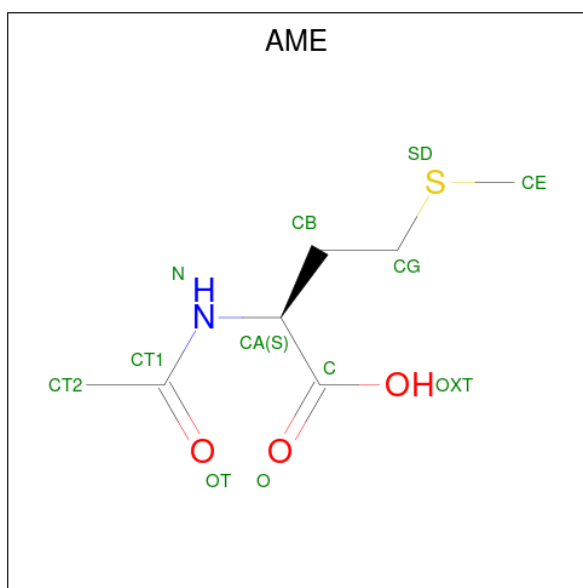
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
81	1T	1	37	25	2	8	1	1	0
81	1n	1	37	25	2	8	1	1	0

- Molecule 82 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



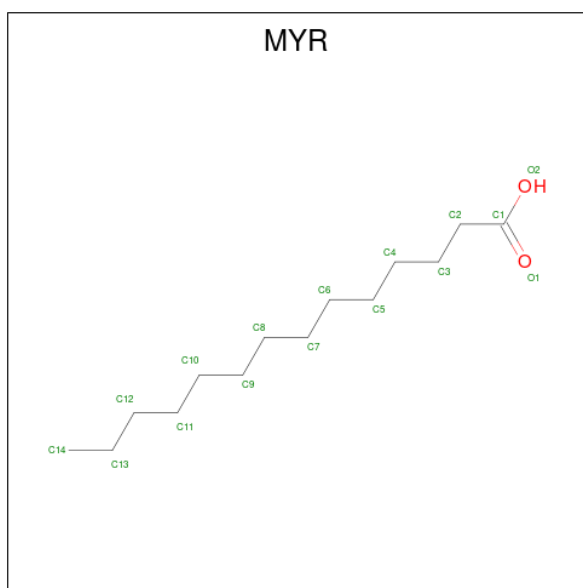
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
82	1Y	1	51	40	10	1	0

- Molecule 83 is N-ACETYL METHIONINE (CCD ID: AME) (formula:  $C_7H_{13}NO_3S$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
83	1h	1	11	7	1	2	1	0

- Molecule 84 is MYRISTIC ACID (CCD ID: MYR) (formula:  $C_{14}H_{28}O_2$ ).



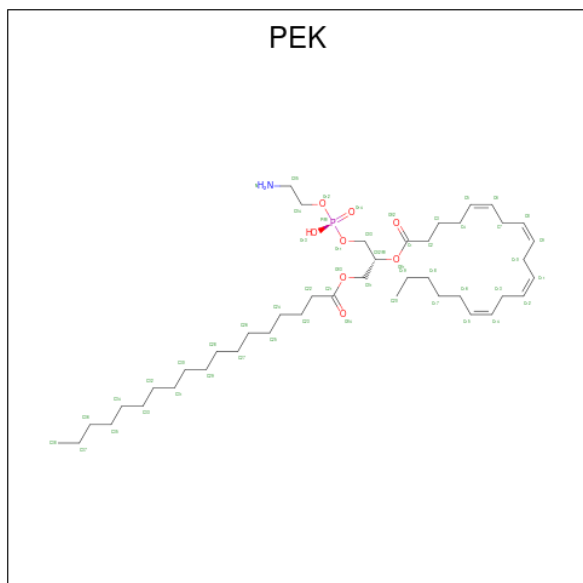
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
84	1l	1	15	14	1	0

- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:



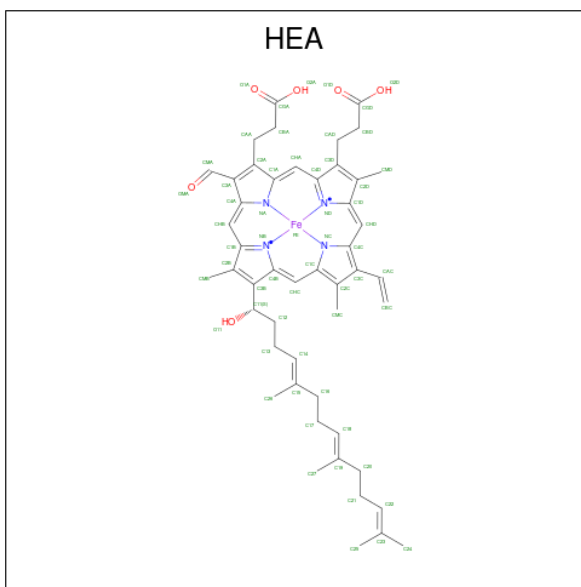
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
86	3D	1	42	34	1	4	3	0
86	3Q	1	43	34	1	4	4	0

- Molecule 87 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
87	3X	1	53	43	1	8	1	0
87	4G	1	52	42	1	8	1	0

- Molecule 88 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
88	4A	1	60	49	1	4	6	0
88	4A	1	60	49	1	4	6	0

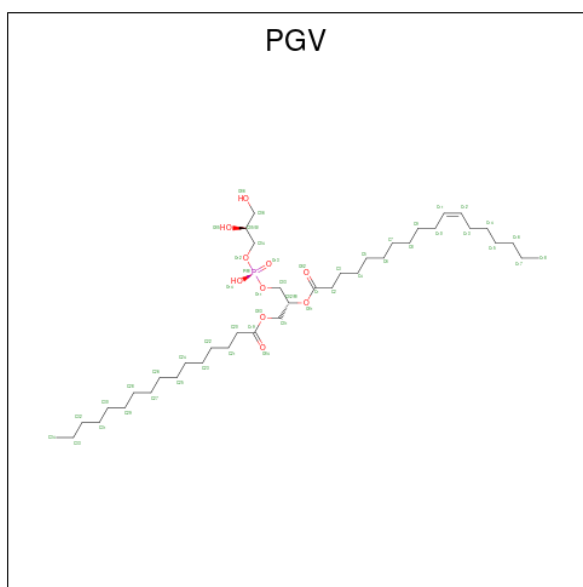
- Molecule 89 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
89	4A	1	1	1	0

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

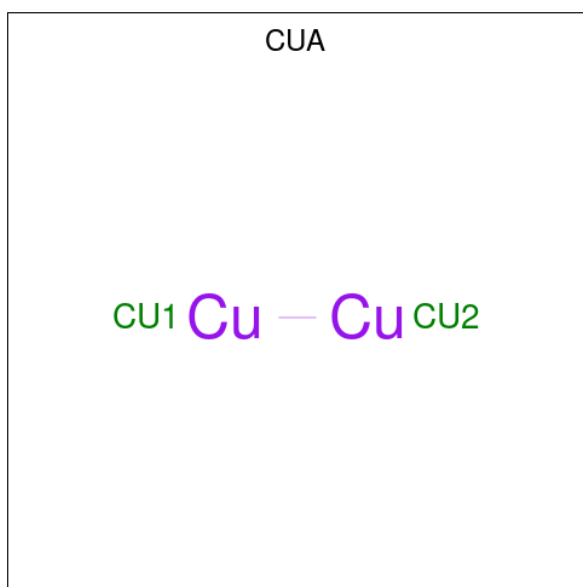
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
90	4A	1	1	1	0

- Molecule 91 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



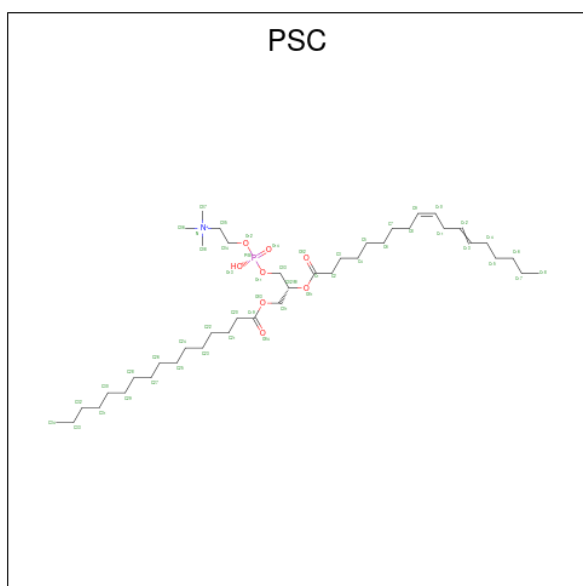
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
91	4A	1	51	40	10	1	0
91	4A	1	51	40	10	1	0
91	4A	1	51	40	10	1	0
91	4A	1	51	40	10	1	0
91	4C	1	51	40	10	1	0
91	4C	1	51	40	10	1	0
91	4C	1	51	40	10	1	0
91	4C	1	51	40	10	1	0
91	4C	1	51	40	10	1	0
91	4G	1	51	40	10	1	0
91	4J	1	42	31	10	1	0
91	4K	1	43	32	10	1	0
91	4N	1	51	40	10	1	0

- Molecule 92 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



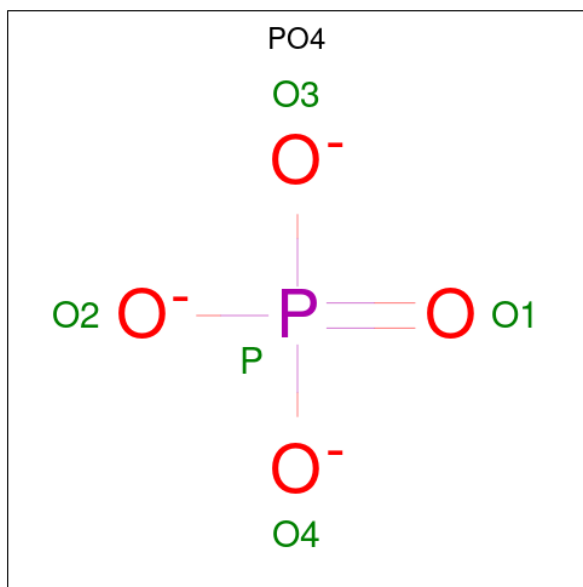
Mol	Chain	Residues	Atoms		AltConf
92	4B	1	Total	Cu	0
			2	2	

- Molecule 93 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



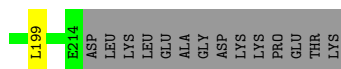
Mol	Chain	Residues	Atoms					AltConf
93	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 94 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).

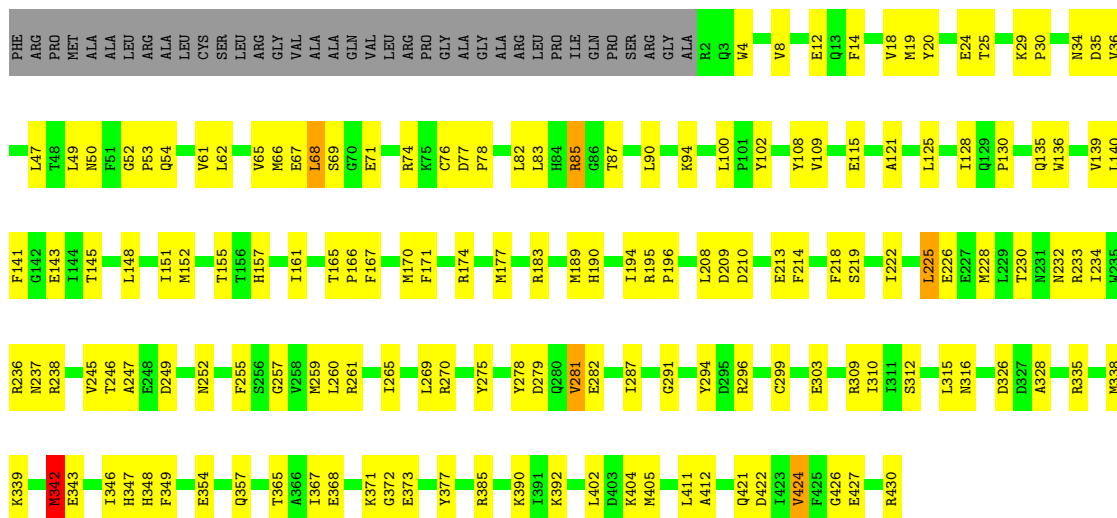


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
94	4H	1	5	4	1	0

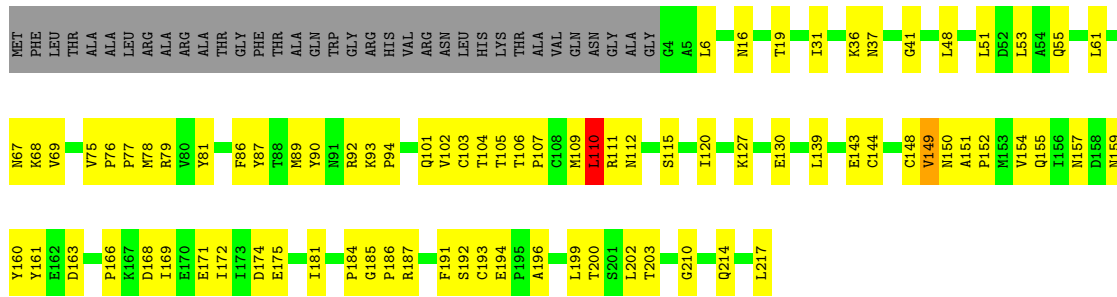




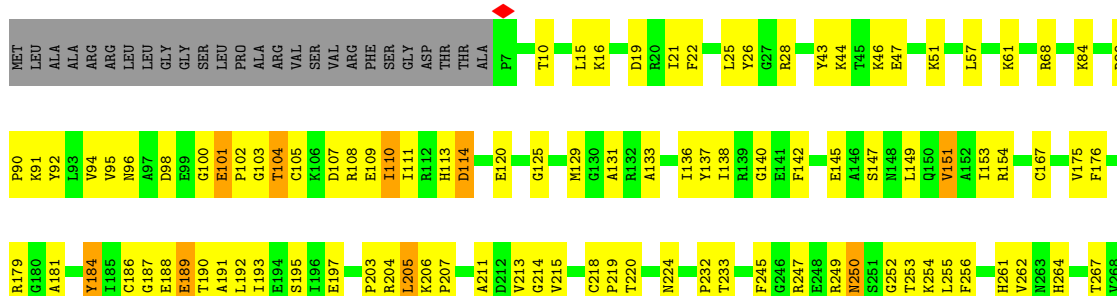
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

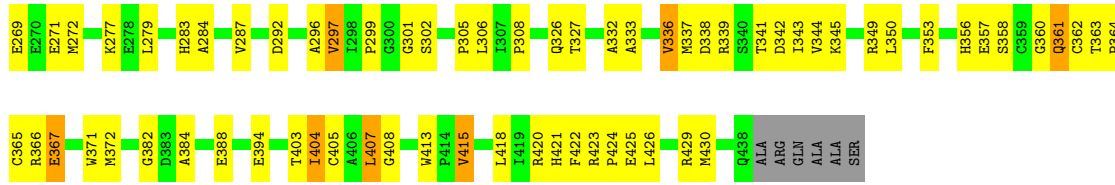


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



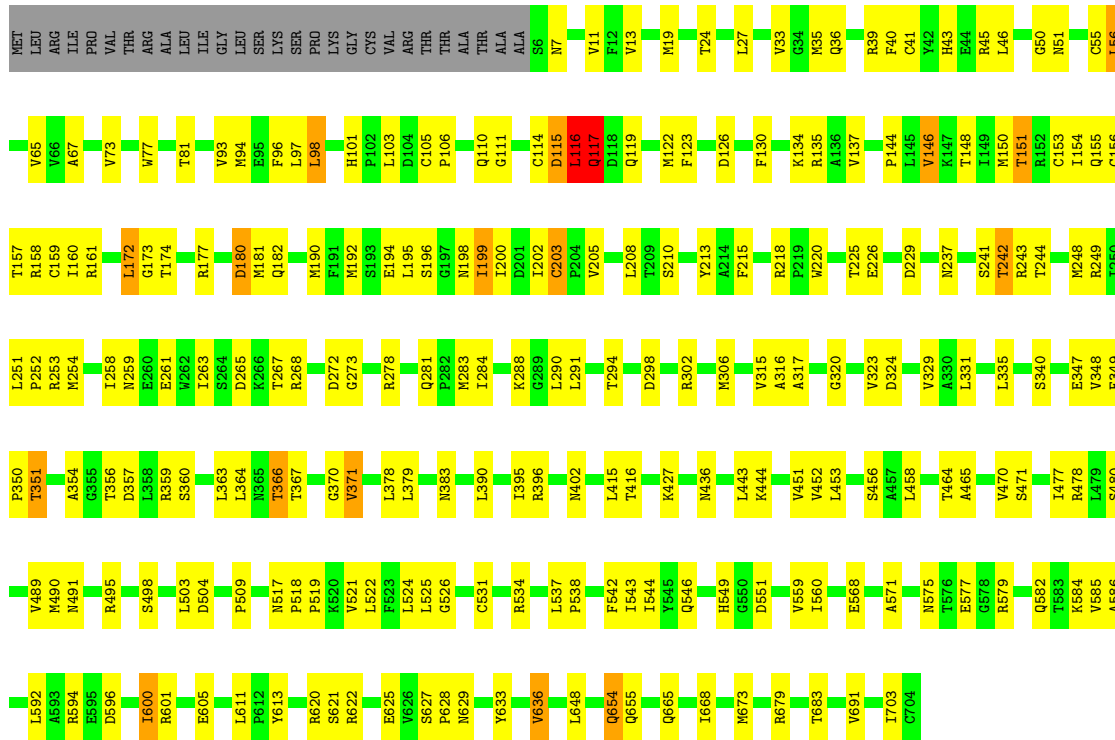
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





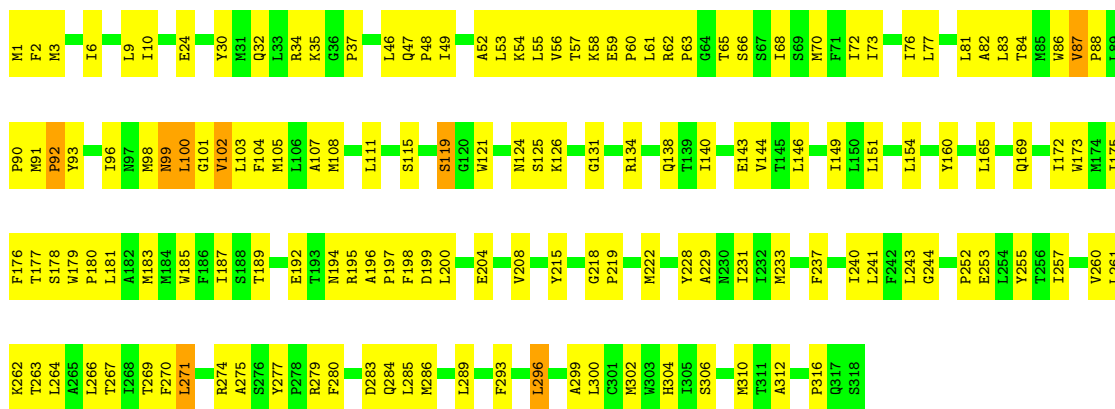
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G:



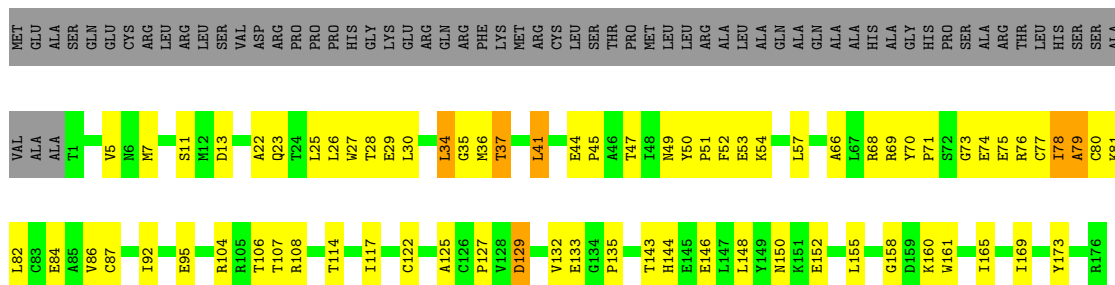
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:



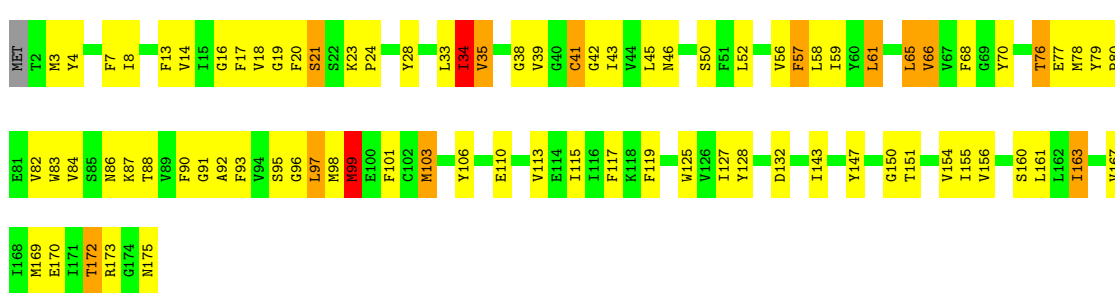
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 



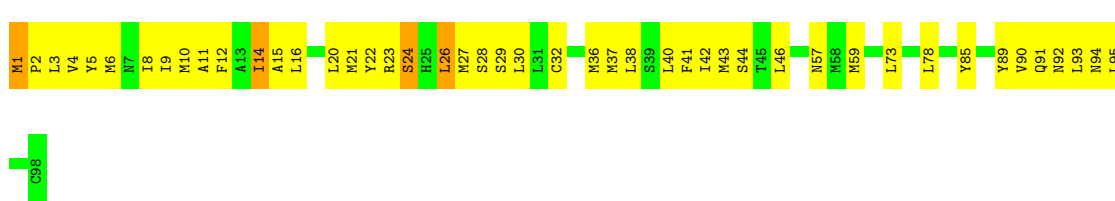
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J: 



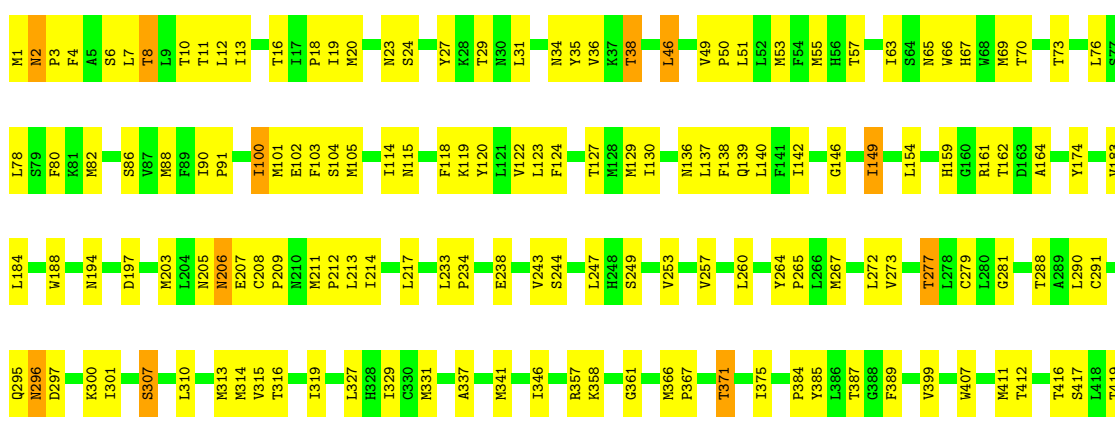
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K: 



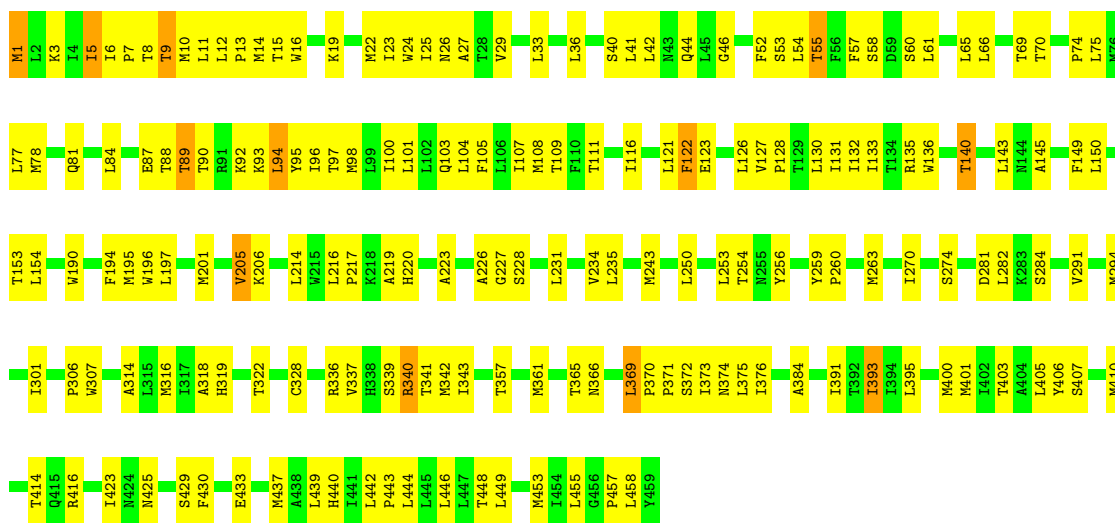
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L: 

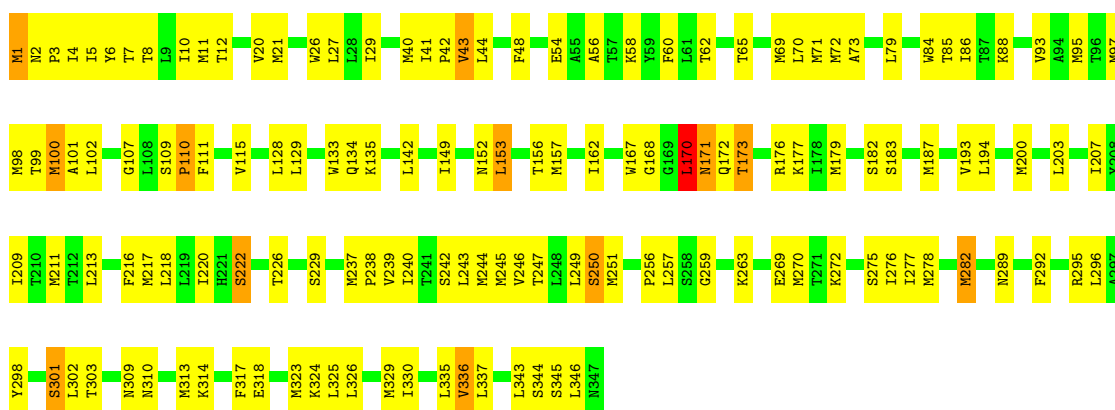




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

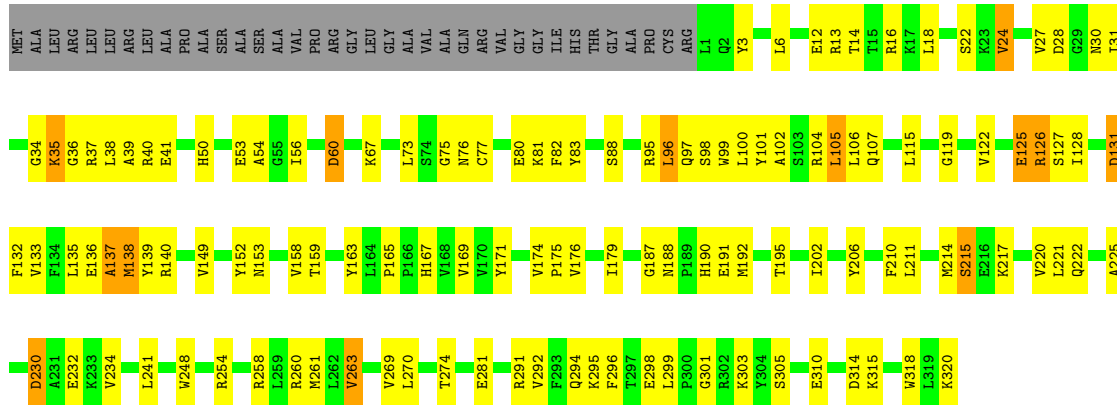


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

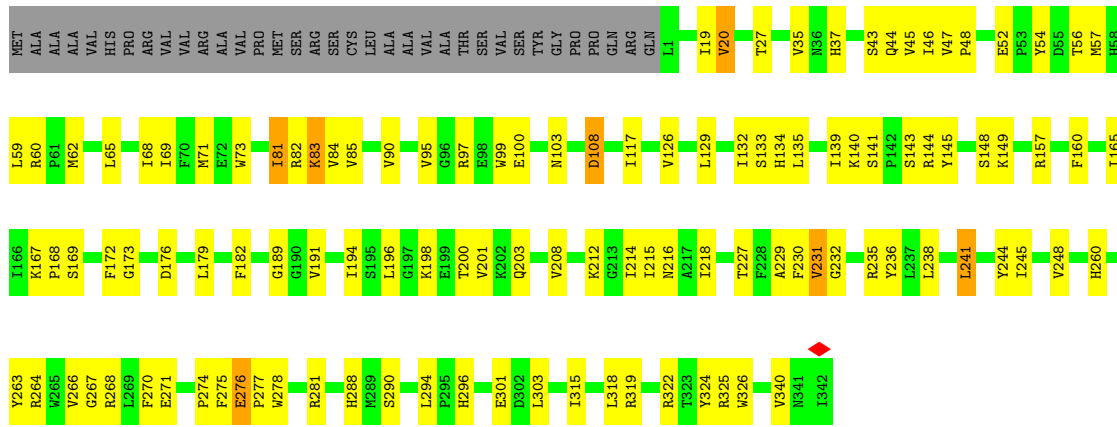


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

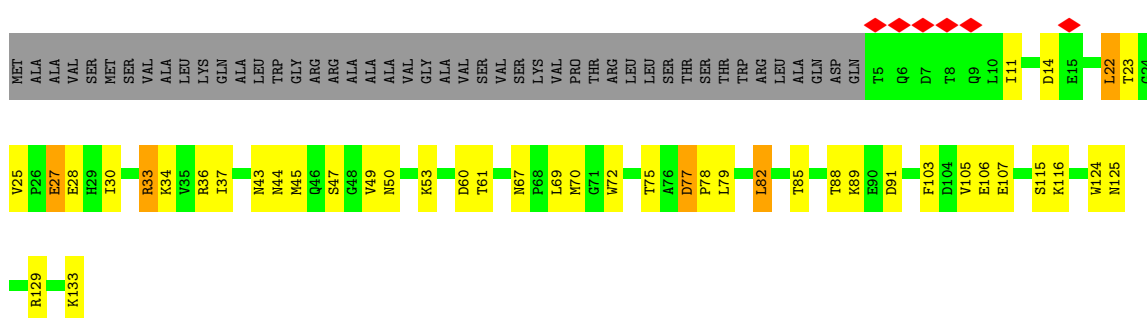




• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

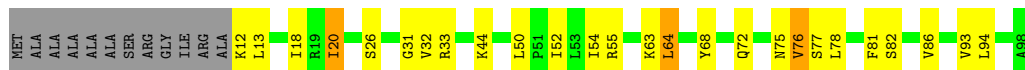


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

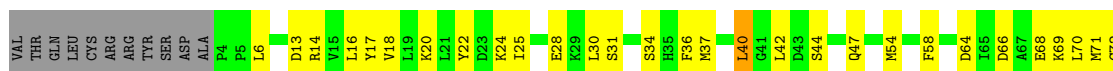
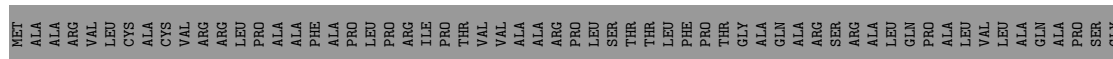
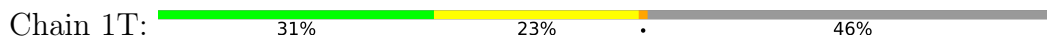




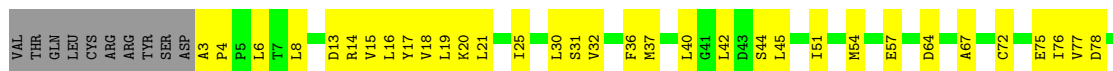
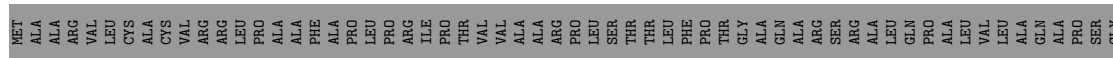
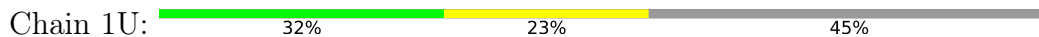
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



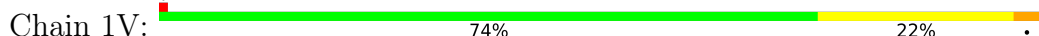
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6





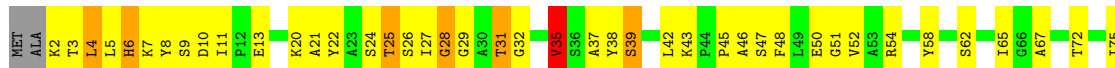
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X: 74% 23% ..



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: 45% 48% 5% ..



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z: 69% 26% ..



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a: 64% 34% ..



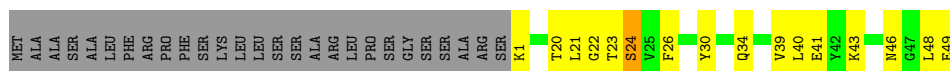
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b: 71% 25% ..



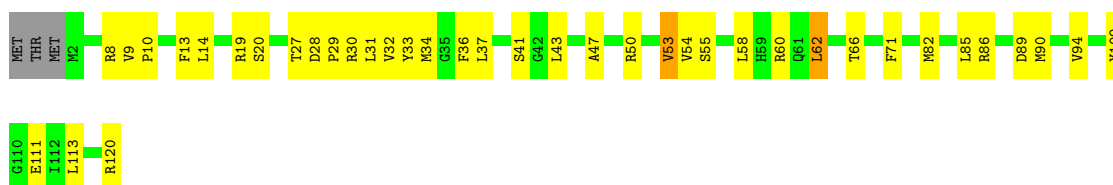
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c: 



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d: 



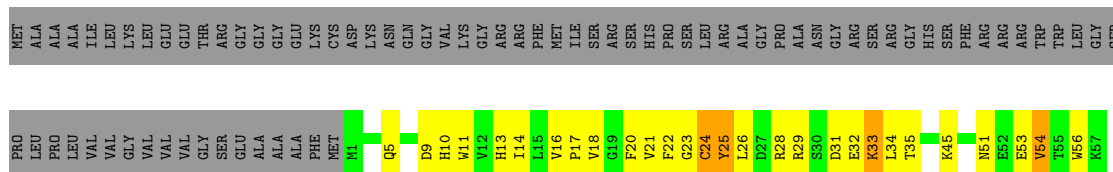
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e: 



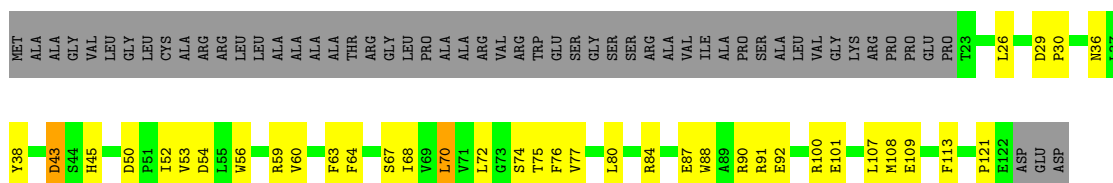
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f: 



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

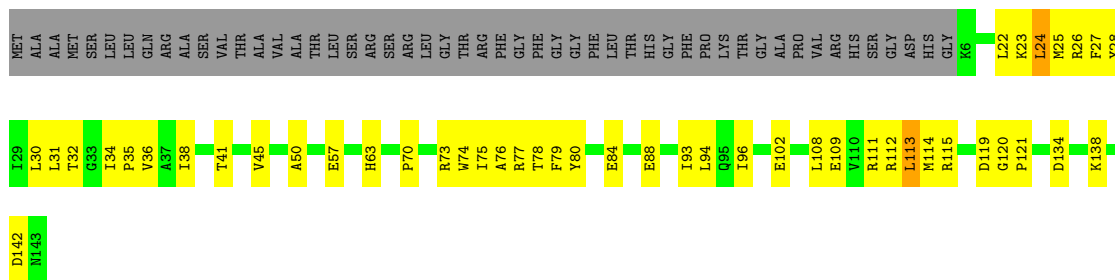
Chain 1g: 



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

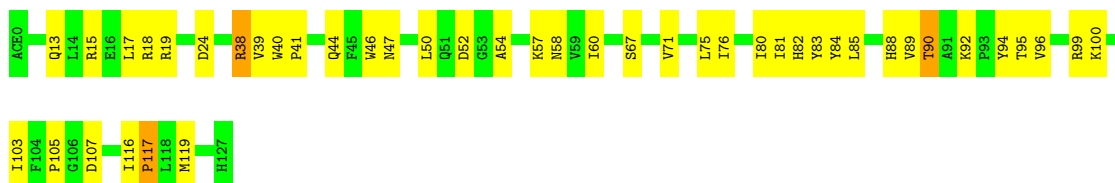
Chain 1h: 





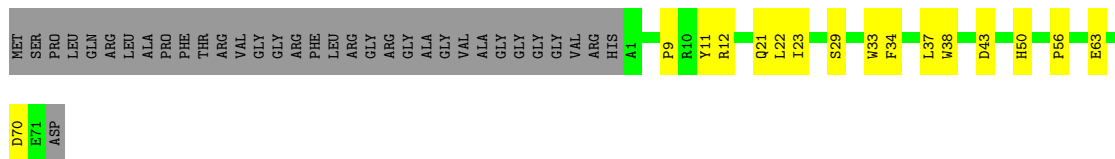
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i: 66% 32%



- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j: 52% 15% 32%



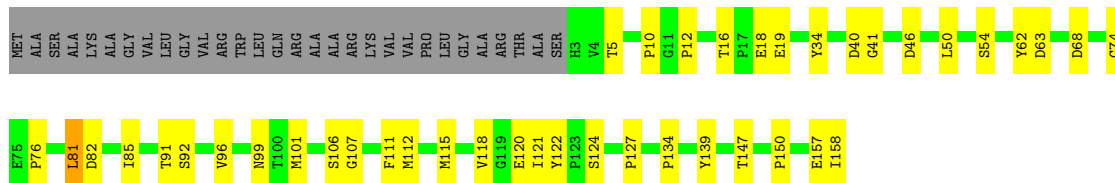
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k: 72% 10% 17%



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l: 61% 22% 16%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 65% 32%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



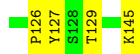
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

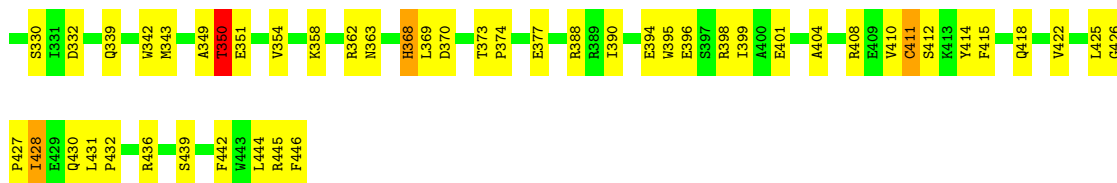


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

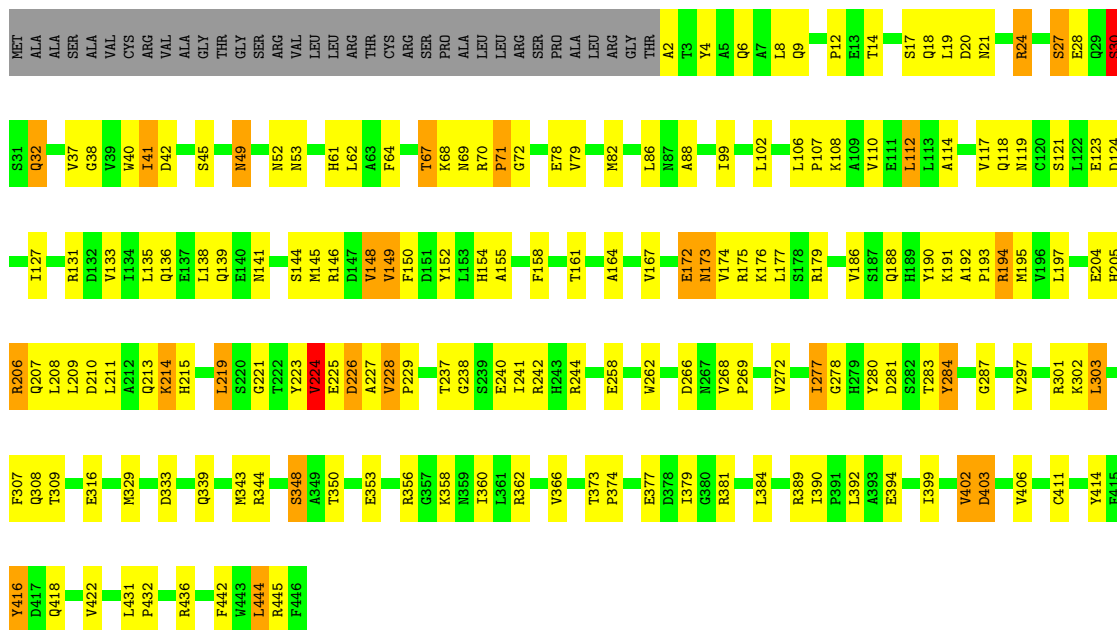


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

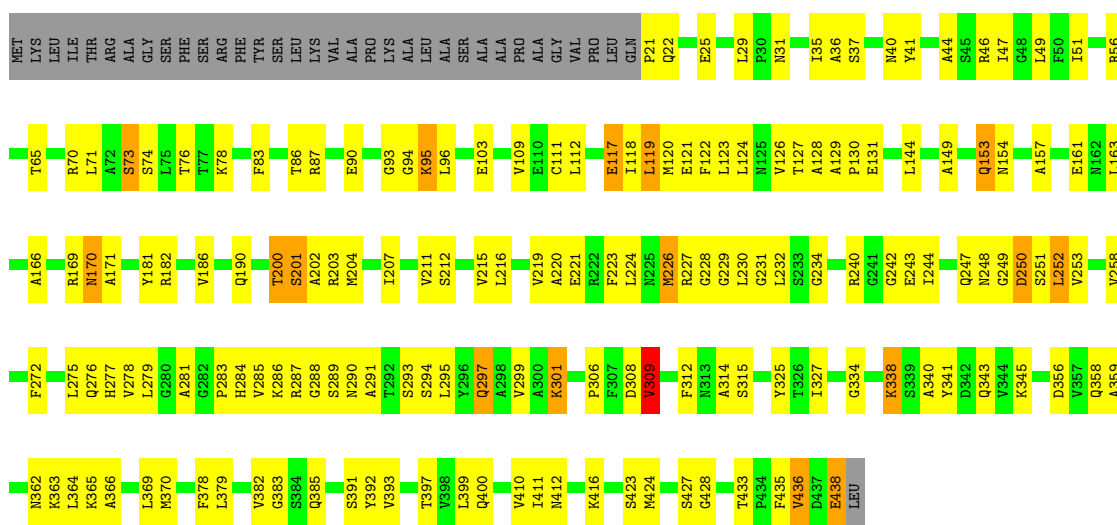




• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

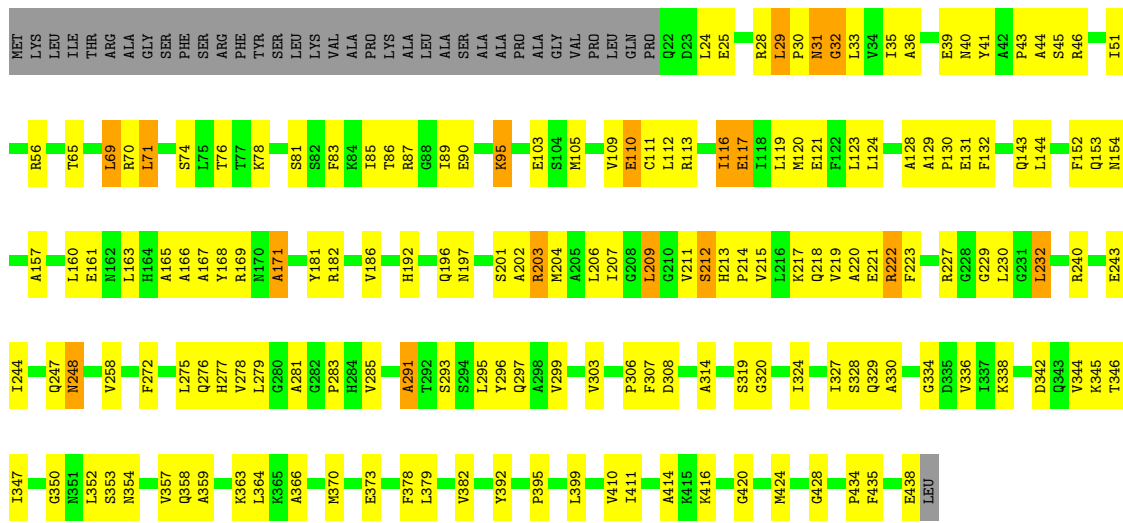


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



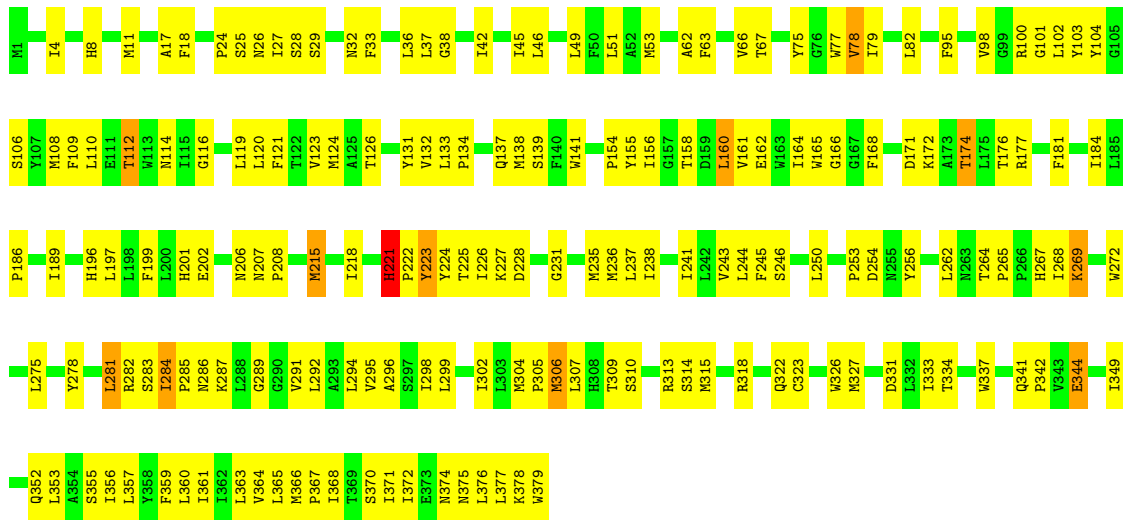
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 30: 55% 33% 8%



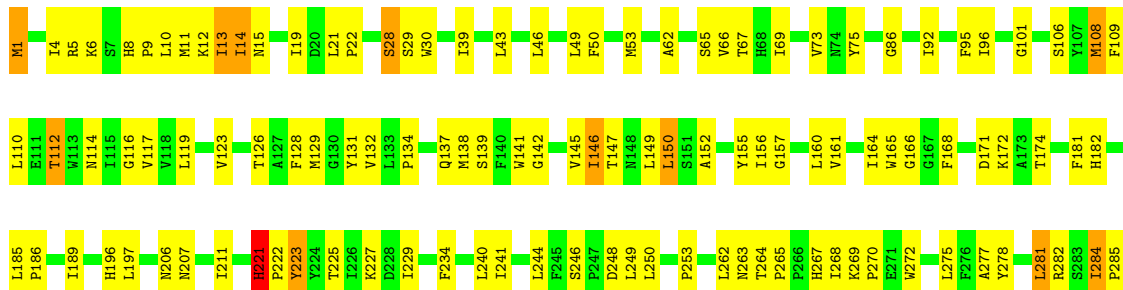
• Molecule 47: Cytochrome b

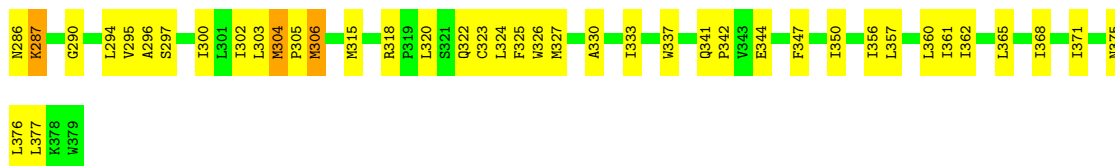
Chain 3C: 52% 45%



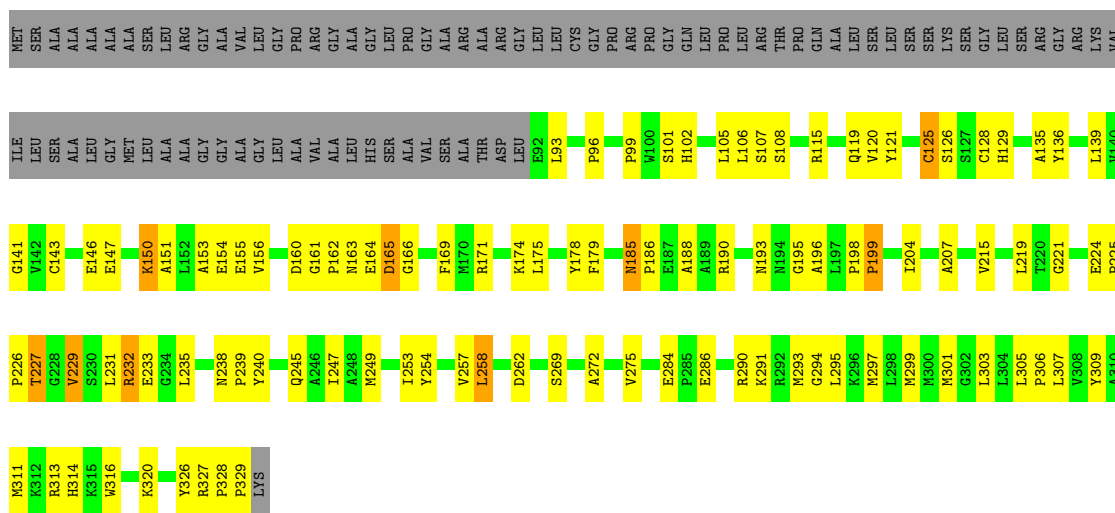
• Molecule 47: Cytochrome b

Chain 3P: 59% 37%

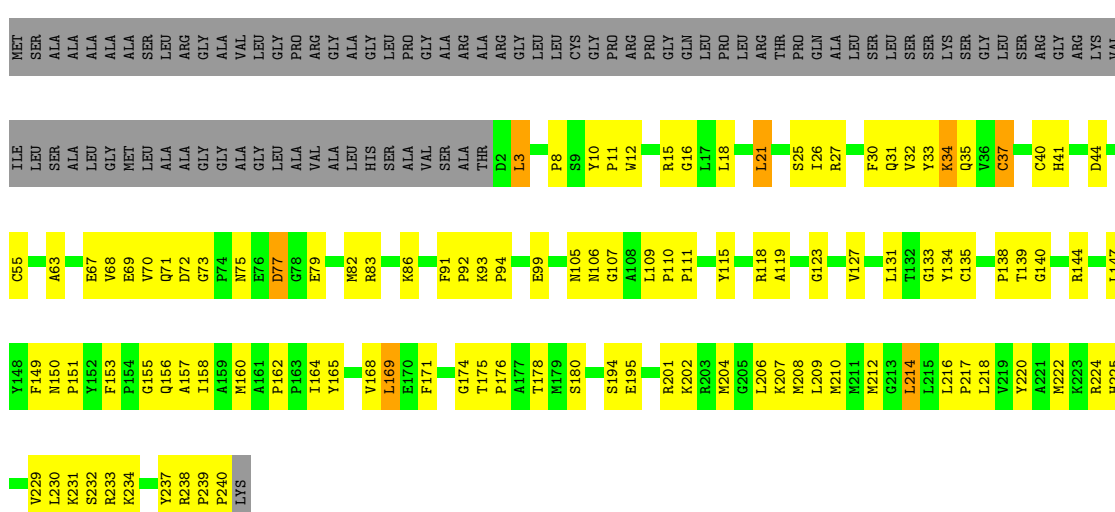




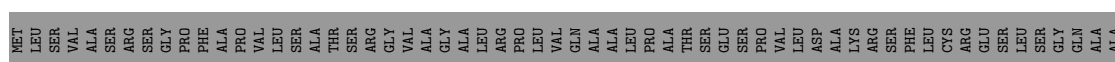
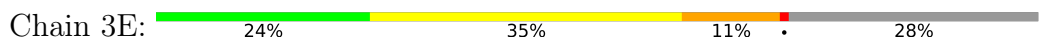
• Molecule 48: Cytochrome c1

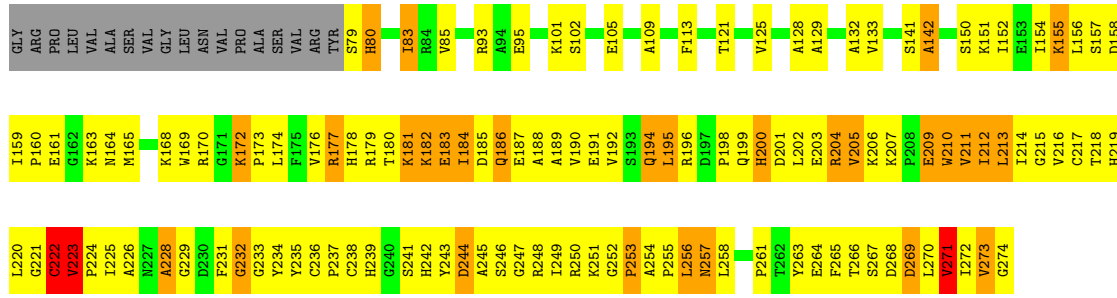


• Molecule 48: Cytochrome c1

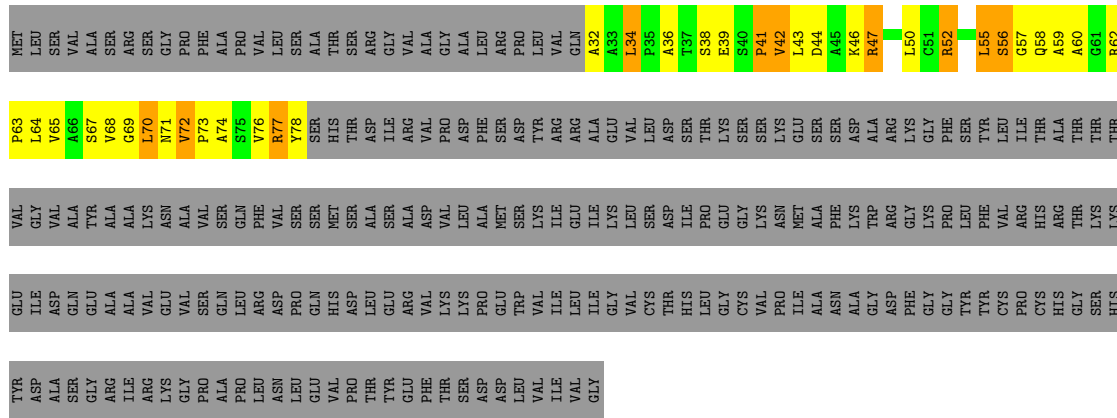


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

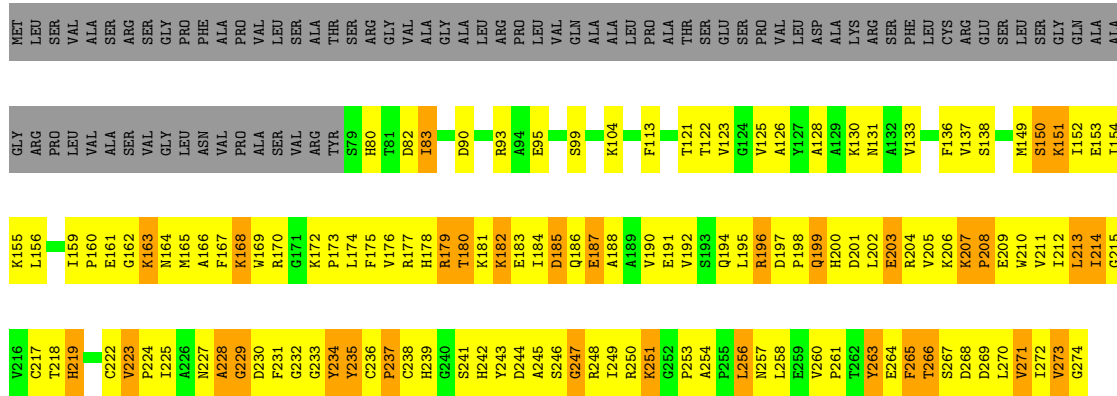
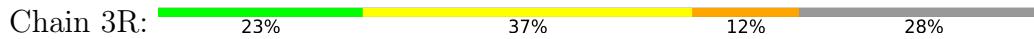




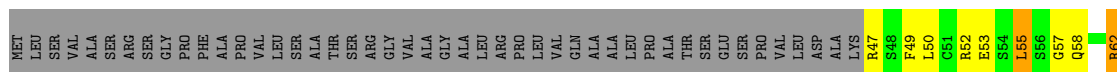
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



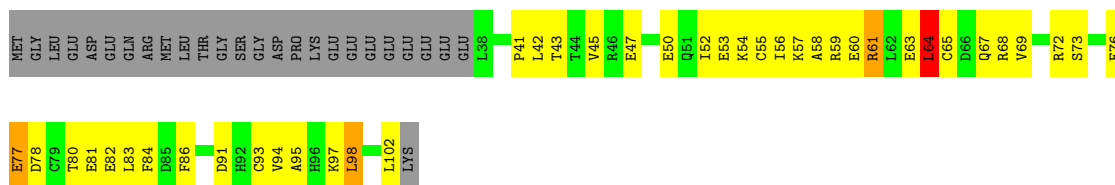
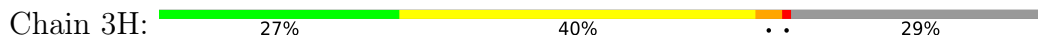
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



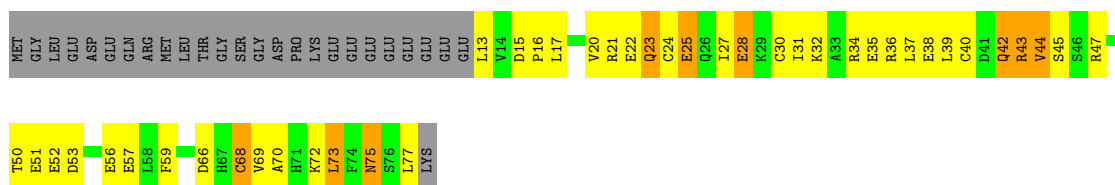
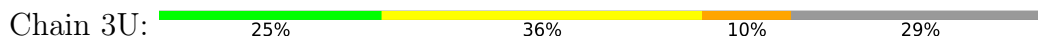
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial







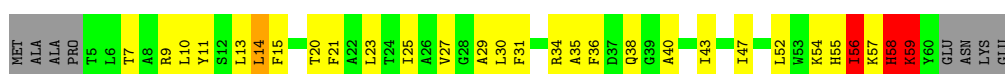
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



- Molecule 54: Cytochrome b-c1 complex subunit 10

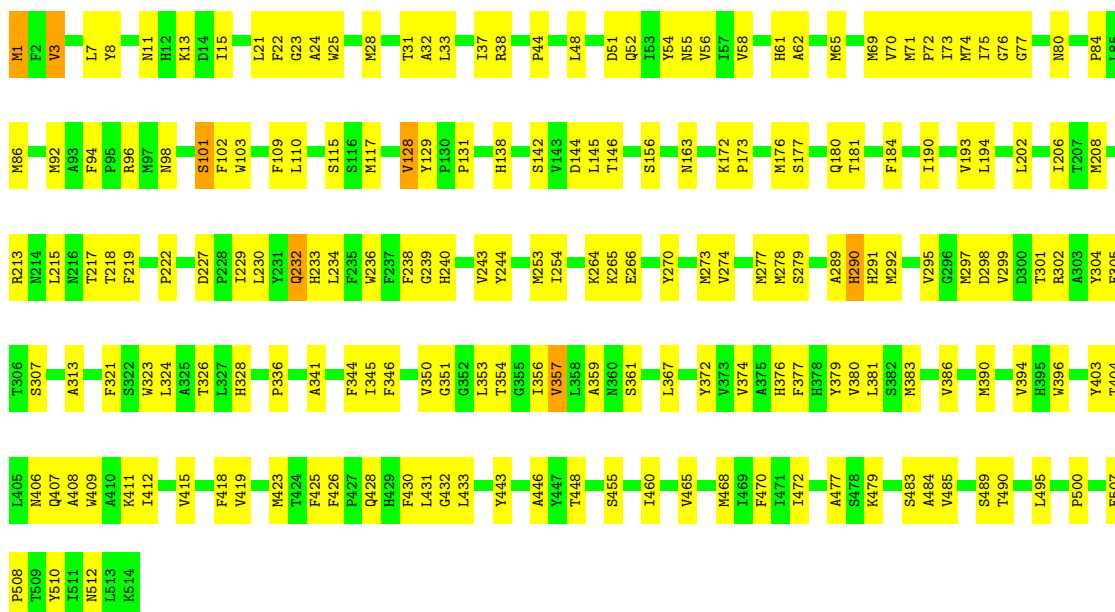


- Molecule 54: Cytochrome b-c1 complex subunit 10



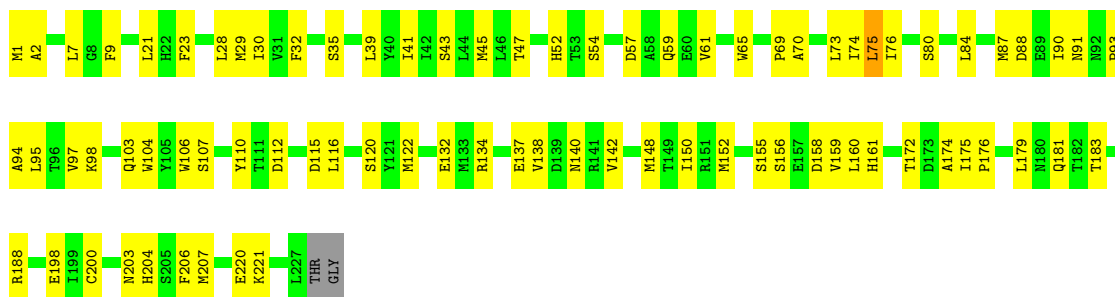
- Molecule 55: Cytochrome c oxidase subunit 1





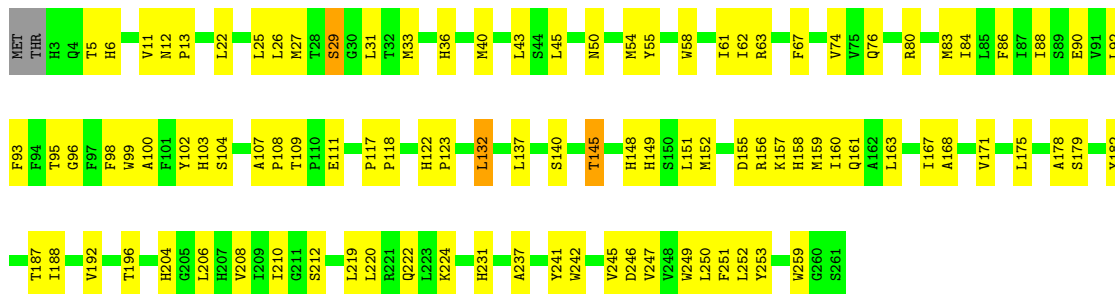
- Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 64% 34%



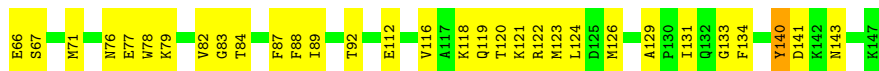
- Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C: 61% 37%

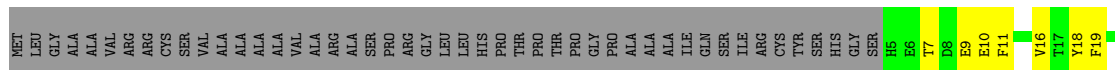


- Molecule 58: Cytochrome c oxidase subunit 4

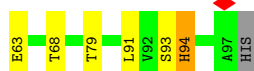
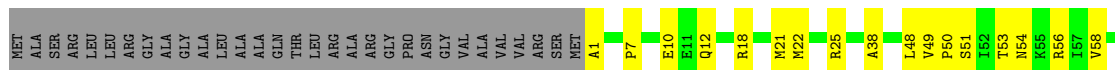
Chain 4D: 53% 27% 18%



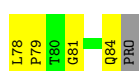
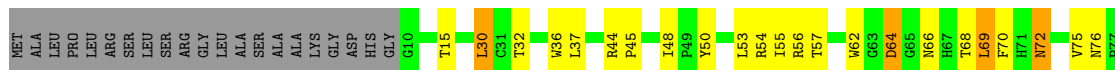
• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



• Molecule 61: Cytochrome c oxidase subunit 6A2



• Molecule 62: Cytochrome c oxidase subunit 6B1



• Molecule 63: Cytochrome c oxidase subunit 6C





- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 65: Cytochrome c oxidase subunit 7B



- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.404	Depositor
Minimum map value	-0.225	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, AME, PO4, ZN, PSC, AYA, CDL, PGT, MG, EHZ, PC1, PGV, 3PE, CU, K, FES, HEA, PEK, CUA, MYR, NDP, NA, GTP, HEM, FME, HEC, SF4, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.42	0/930	0.66	1/1271 (0.1%)
2	1B	0.62	0/1273	0.75	2/1722 (0.1%)
3	1C	0.12	0/1791	0.31	0/2439
4	1D	0.31	0/3545	0.42	2/4806 (0.0%)
5	1E	0.36	0/1698	0.56	2/2311 (0.1%)
6	1F	0.37	0/3401	0.54	11/4595 (0.2%)
7	1G	0.40	0/5451	0.54	9/7387 (0.1%)
8	1H	0.53	0/2566	0.67	9/3509 (0.3%)
9	1I	0.81	0/1443	0.91	9/1952 (0.5%)
10	1J	0.61	0/1364	0.88	7/1850 (0.4%)
11	1K	0.57	1/751 (0.1%)	0.70	4/1018 (0.4%)
12	1L	0.38	0/4939	0.46	5/6718 (0.1%)
13	1M	0.53	0/3713	0.57	3/5063 (0.1%)
14	1N	0.51	0/2765	0.62	5/3758 (0.1%)
15	1O	0.55	3/2650 (0.1%)	0.71	9/3588 (0.3%)
16	1P	0.25	0/2828	0.39	0/3834
17	1Q	0.20	0/1070	0.37	0/1446
18	1R	0.13	0/755	0.32	0/1018
19	1S	0.12	0/711	0.32	0/956
20	1T	0.15	0/701	0.43	0/946
20	1U	0.14	0/706	0.37	0/954
21	1V	0.11	0/946	0.30	0/1281
22	1W	0.12	0/995	0.31	0/1340
23	1X	0.17	0/1436	0.33	0/1938
24	1Y	1.01	0/1037	1.07	7/1404 (0.5%)
25	1Z	0.42	0/1199	0.58	4/1617 (0.2%)
26	1a	0.50	0/577	0.53	0/777
27	1b	0.12	0/664	0.33	0/912
28	1c	0.11	0/430	0.30	0/581
29	1d	0.42	0/1016	0.46	0/1374
30	1e	0.11	0/836	0.31	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	1f	0.57	1/499 (0.2%)	0.71	2/673 (0.3%)
32	1g	0.14	0/858	0.37	1/1165 (0.1%)
33	1h	0.12	0/1184	0.31	0/1603
34	1i	0.18	0/1138	0.43	1/1551 (0.1%)
35	1j	0.13	0/627	0.29	0/858
36	1k	0.12	0/668	0.31	0/903
37	1l	0.11	0/1365	0.32	0/1867
38	1m	0.27	0/1092	0.43	0/1481
39	1n	0.15	0/1549	0.35	0/2098
40	1o	0.11	0/1069	0.34	0/1430
41	1p	0.11	0/1481	0.31	0/1997
42	1q	0.56	0/1253	0.59	1/1704 (0.1%)
43	1r	0.45	0/777	0.53	0/1051
44	1s	0.18	0/394	0.45	0/533
45	3A	0.74	0/3481	0.94	14/4722 (0.3%)
45	3N	0.76	0/3496	0.97	15/4723 (0.3%)
46	3B	0.73	0/3190	0.90	7/4317 (0.2%)
46	3O	0.73	0/3175	0.94	8/4292 (0.2%)
47	3C	0.72	0/3123	0.89	10/4269 (0.2%)
47	3P	0.73	0/3122	0.93	12/4269 (0.3%)
48	3D	0.76	0/1946	0.91	2/2641 (0.1%)
48	3Q	0.70	0/1962	0.90	3/2663 (0.1%)
49	3E	0.58	0/1551	0.98	8/2098 (0.4%)
49	3I	0.84	0/342	1.14	2/465 (0.4%)
49	3R	0.63	0/1551	0.95	4/2098 (0.2%)
49	3V	0.67	0/225	0.97	1/303 (0.3%)
50	3F	0.78	0/888	0.99	4/1193 (0.3%)
50	3S	0.70	0/888	0.80	1/1193 (0.1%)
51	3G	0.81	0/648	0.99	2/874 (0.2%)
51	3T	0.69	0/649	0.91	0/878
52	3H	0.79	0/538	0.99	5/721 (0.7%)
52	3U	0.90	0/539	1.09	3/724 (0.4%)
53	3J	1.97	4/476 (0.8%)	3.94	14/641 (2.2%)
53	3W	2.04	3/475 (0.6%)	4.86	9/638 (1.4%)
54	3X	0.67	0/445	0.96	2/608 (0.3%)
54	3Y	0.67	0/437	0.86	0/598
55	4A	0.23	0/4156	0.40	1/5679 (0.0%)
56	4B	0.21	0/1865	0.44	0/2544
57	4C	0.31	0/2179	0.47	1/2981 (0.0%)
58	4D	0.19	0/1197	0.36	0/1617
59	4E	0.20	0/871	0.42	0/1182
60	4F	0.18	0/749	0.42	0/1016
61	4G	0.16	0/644	0.29	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
62	4H	0.26	0/708	0.52	1/956 (0.1%)
63	4I	0.18	0/563	0.34	0/748
64	4J	0.18	0/466	0.30	0/631
65	4K	0.16	0/396	0.34	0/543
66	4L	0.17	0/394	0.34	0/528
67	4M	0.18	0/349	0.29	0/477
68	4N	0.35	0/680	0.60	2/921 (0.2%)
All	All	0.53	12/116505 (0.0%)	0.77	225/158029 (0.1%)

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
6	1F	0	1
10	1J	0	1
12	1L	0	1
15	1O	0	1
26	1a	0	1
45	3N	0	2
49	3I	0	2
53	3J	0	3
53	3W	0	3
All	All	0	15

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	3J	59	LYS	C-N	32.71	1.79	1.33
53	3W	56	ILE	C-N	-30.29	0.94	1.33
53	3W	58	HIS	C-N	-22.00	1.02	1.33
53	3J	56	ILE	C-N	-18.58	1.07	1.33
53	3W	59	LYS	C-N	18.10	1.58	1.33

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	3W	59	LYS	CA-C-N	-58.59	16.25	121.70
53	3W	59	LYS	C-N-CA	-58.59	16.25	121.70
53	3W	56	ILE	CA-C-N	-55.49	32.31	122.21
53	3W	56	ILE	C-N-CA	-55.49	32.31	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	3J	57	LYS	O-C-N	-50.33	55.65	122.59

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
10	1J	86	ASN	Mainchain
12	1L	583	LEU	Mainchain
15	1O	301	GLY	Mainchain
26	1a	37	ARG	Mainchain

## 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	1A	916	0	950	103	0
2	1B	1242	0	1250	123	0
3	1C	1740	0	1691	30	0
4	1D	3452	0	3389	123	0
5	1E	1658	0	1664	75	0
6	1F	3325	0	3290	138	0
7	1G	5362	0	5391	174	0
8	1H	2504	0	2602	169	0
9	1I	1412	0	1368	71	0
10	1J	1329	0	1326	131	0
11	1K	750	0	798	62	0
12	1L	4818	0	4956	275	0
13	1M	3632	0	3836	184	0
14	1N	2712	0	2873	171	0
15	1O	2590	0	2556	114	0
16	1P	2751	0	2776	96	0
17	1Q	1047	0	1042	37	0
18	1R	741	0	704	13	0
19	1S	700	0	719	18	0
20	1T	689	0	687	30	0
20	1U	694	0	691	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	1V	927	0	972	20	0
22	1W	971	0	975	22	0
23	1X	1398	0	1378	34	0
24	1Y	1016	0	1012	232	0
25	1Z	1168	0	1161	47	0
26	1a	562	0	557	30	0
27	1b	643	0	645	44	0
28	1c	417	0	425	20	0
29	1d	985	0	978	67	0
30	1e	816	0	823	18	0
31	1f	487	0	493	74	0
32	1g	835	0	793	55	0
33	1h	1151	0	1164	87	0
34	1i	1100	0	1107	57	0
35	1j	601	0	546	27	0
36	1k	649	0	626	6	0
37	1l	1310	0	1204	41	0
38	1m	1062	0	1075	95	0
39	1n	1495	0	1431	54	0
40	1o	1045	0	1016	58	0
41	1p	1449	0	1416	42	0
42	1q	1212	0	1174	39	0
43	1r	759	0	783	29	0
44	1s	382	0	351	15	0
45	3A	3411	0	3309	138	0
45	3N	3424	0	3350	166	0
46	3B	3138	0	3116	143	0
46	3O	3124	0	3108	139	0
47	3C	3025	0	3090	236	0
47	3P	3024	0	3090	214	0
48	3D	1888	0	1834	110	0
48	3Q	1904	0	1849	131	0
49	3E	1518	0	1499	220	0
49	3I	337	0	347	41	0
49	3R	1518	0	1499	253	0
49	3V	223	0	233	21	0
50	3F	868	0	857	42	0
50	3S	868	0	857	30	0
51	3G	628	0	634	68	0
51	3T	628	0	634	63	0
52	3H	533	0	512	37	0
52	3U	533	0	513	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	3J	464	0	464	63	0
53	3W	464	0	462	37	0
54	3X	429	0	430	72	0
54	3Y	421	0	418	86	0
55	4A	4026	0	4005	203	0
56	4B	1828	0	1836	80	0
57	4C	2096	0	2027	109	0
58	4D	1163	0	1143	42	0
59	4E	852	0	845	27	0
60	4F	734	0	718	20	0
61	4G	617	0	585	34	0
62	4H	687	0	645	26	0
63	4I	550	0	560	26	0
64	4J	456	0	456	23	0
65	4K	383	0	366	16	0
66	4L	381	0	380	38	0
67	4M	338	0	345	11	0
68	4N	660	0	664	47	0
69	1A	88	0	127	33	0
69	1B	102	0	163	44	0
69	1J	95	0	144	51	0
69	1L	473	0	679	173	0
69	1M	47	0	71	13	0
69	1N	51	0	82	57	0
69	1Y	539	0	803	257	0
69	1Z	51	0	82	12	0
69	1b	42	0	61	31	0
69	1d	146	0	215	104	0
69	1e	51	0	82	15	0
69	1f	181	0	253	124	0
69	1g	84	0	122	43	0
69	1h	47	0	71	15	0
69	1k	46	0	67	32	0
69	1l	126	0	180	27	0
69	1m	236	0	357	91	0
69	1o	51	0	82	31	0
69	3A	102	0	164	61	0
69	3C	691	0	1046	267	0
69	3D	86	0	123	19	0
69	3E	100	0	157	27	0
69	3G	424	0	577	113	0
69	3J	238	0	363	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	3N	102	0	164	65	0
69	3P	772	0	1202	281	0
69	3Q	133	0	194	39	0
69	3R	153	0	246	59	0
69	3S	51	0	82	26	0
69	3T	51	0	82	26	0
69	3W	144	0	225	67	0
69	3X	255	0	410	121	0
69	3Y	281	0	433	109	0
69	4G	73	0	94	34	0
70	1A	35	0	44	28	0
70	1B	94	0	134	88	0
70	1H	143	0	220	58	0
70	1J	35	0	44	7	0
70	1M	44	0	65	12	0
70	1P	33	0	40	6	0
70	1Y	135	0	192	82	0
70	1d	39	0	52	24	0
70	1h	93	0	140	29	0
70	3J	54	0	88	13	0
70	3P	54	0	88	15	0
70	3R	54	0	88	16	0
70	3T	54	0	88	45	0
70	3X	54	0	88	17	0
71	1B	8	0	0	1	0
71	1F	8	0	0	8	0
71	1G	16	0	0	4	0
71	1I	16	0	0	3	0
72	1E	4	0	0	4	0
72	1G	4	0	0	4	0
72	3E	4	0	0	5	0
72	3R	4	0	0	4	0
73	1F	31	0	19	4	0
74	1G	1	0	0	0	0
75	1H	51	0	46	10	0
75	1L	87	0	124	38	0
75	1N	77	0	98	33	0
75	1Y	100	0	156	39	0
75	1d	179	0	264	60	0
75	1g	100	0	154	60	0
75	1i	80	0	104	35	0
75	1q	161	0	221	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	3A	98	0	149	45	0
75	3D	56	0	56	4	0
75	3F	100	0	156	26	0
75	3N	100	0	156	57	0
75	3P	100	0	156	60	0
75	3T	57	0	58	13	0
75	3X	100	0	156	31	0
75	3Y	100	0	156	31	0
75	4B	100	0	156	40	0
75	4C	200	0	312	41	0
76	1I	8	0	8	6	0
77	1O	32	0	12	7	0
78	1O	1	0	0	0	0
78	4A	1	0	0	0	0
79	1P	48	0	26	2	0
80	1R	1	0	0	0	0
80	4F	1	0	0	0	0
81	1T	37	0	0	0	0
81	1n	37	0	0	1	0
82	1Y	51	0	78	24	0
83	1h	11	0	12	2	0
84	1l	15	0	27	0	0
85	3C	86	0	60	8	0
85	3P	86	0	60	5	0
86	3D	42	0	32	6	0
86	3Q	43	0	32	10	0
87	3X	53	0	77	9	0
87	4G	52	0	72	13	0
88	4A	120	0	108	11	0
89	4A	1	0	0	0	0
90	4A	1	0	0	0	0
91	4A	204	0	304	104	0
91	4C	255	0	376	66	0
91	4G	51	0	76	10	0
91	4J	42	0	57	8	0
91	4K	43	0	59	7	0
91	4N	51	0	76	13	0
92	4B	2	0	0	0	0
93	4B	52	0	80	27	0
94	4H	5	0	0	0	0
All	All	124052	0	128247	7317	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 29.

The worst 5 of 7317 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)
69:3P:514:3PE:H121	54:3Y:2:LEU:CD1	1.30	1.61
69:1d:201:3PE:C2G	69:1d:201:3PE:C3C	1.74	1.60
37:1l:111:PHE:CD2	69:1l:203:3PE:H281	1.35	1.59
69:1d:201:3PE:C2G	69:1d:201:3PE:C3D	1.80	1.58
47:3P:306:MET:HE2	69:3P:514:3PE:C25	1.13	1.57

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	1A	113/115 (98%)	101 (89%)	9 (8%)	3 (3%)	4	1
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	198 (96%)	9 (4%)	0	100	100
4	1D	427/466 (92%)	411 (96%)	16 (4%)	0	100	100
5	1E	212/249 (85%)	198 (93%)	12 (6%)	2 (1%)	14	10
6	1F	430/464 (93%)	404 (94%)	22 (5%)	4 (1%)	14	10
7	1G	697/727 (96%)	667 (96%)	27 (4%)	3 (0%)	30	28
8	1H	316/318 (99%)	297 (94%)	17 (5%)	2 (1%)	21	18
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	160 (93%)	11 (6%)	1 (1%)	21	18
11	1K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
12	1L	604/606 (100%)	567 (94%)	33 (6%)	4 (1%)	18	15
13	1M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	36	36
15	1O	318/357 (89%)	296 (93%)	17 (5%)	5 (2%)	7	4
16	1P	340/377 (90%)	328 (96%)	11 (3%)	1 (0%)	36	36
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	18
24	1Y	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
25	1Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	53 (96%)	2 (4%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
33	1h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	1i	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	164 (96%)	6 (4%)	0	100	100
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	84 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
45	3A	436/480 (91%)	418 (96%)	13 (3%)	5 (1%)	11	8
45	3N	444/480 (92%)	426 (96%)	12 (3%)	6 (1%)	9	5
46	3B	414/453 (91%)	387 (94%)	21 (5%)	6 (1%)	9	5
46	3O	413/453 (91%)	393 (95%)	19 (5%)	1 (0%)	43	44
47	3C	377/379 (100%)	368 (98%)	8 (2%)	1 (0%)	36	36
47	3P	377/379 (100%)	367 (97%)	9 (2%)	1 (0%)	36	36
48	3D	235/326 (72%)	228 (97%)	6 (3%)	1 (0%)	30	28
48	3Q	237/326 (73%)	224 (94%)	12 (5%)	1 (0%)	30	28
49	3E	194/274 (71%)	166 (86%)	18 (9%)	10 (5%)	1	0
49	3I	45/274 (16%)	31 (69%)	12 (27%)	2 (4%)	2	0
49	3R	194/274 (71%)	163 (84%)	22 (11%)	9 (5%)	2	0
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	61/91 (67%)	60 (98%)	1 (2%)	0	100	100
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	50 (93%)	2 (4%)	2 (4%)	2	1
53	3W	52/64 (81%)	50 (96%)	1 (2%)	1 (2%)	6	3
54	3X	50/56 (89%)	46 (92%)	3 (6%)	1 (2%)	6	2
54	3Y	49/56 (88%)	45 (92%)	3 (6%)	1 (2%)	6	2
55	4A	512/514 (100%)	488 (95%)	21 (4%)	3 (1%)	21	18
56	4B	225/229 (98%)	211 (94%)	14 (6%)	0	100	100
57	4C	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	90 (95%)	5 (5%)	0	100	100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	72 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
All	All	14068/16999 (83%)	13360 (95%)	630 (4%)	78 (1%)	23	18

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	115	ASP
8	1H	92	PRO
10	1J	66	VAL
12	1L	562	LEU
15	1O	138	MET

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	92 (93%)	7 (7%)	13	11
2	1B	131/212 (62%)	121 (92%)	10 (8%)	12	9
3	1C	190/227 (84%)	186 (98%)	4 (2%)	47	54
4	1D	371/396 (94%)	357 (96%)	14 (4%)	29	32
5	1E	183/207 (88%)	177 (97%)	6 (3%)	33	37
6	1F	346/368 (94%)	332 (96%)	14 (4%)	28	29
7	1G	588/610 (96%)	556 (95%)	32 (5%)	20	18
8	1H	274/274 (100%)	267 (97%)	7 (3%)	40	46
9	1I	151/201 (75%)	143 (95%)	8 (5%)	20	19
10	1J	140/141 (99%)	126 (90%)	14 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1K	84/84 (100%)	80 (95%)	4 (5%)	23	23
12	1L	539/539 (100%)	510 (95%)	29 (5%)	20	18
13	1M	408/408 (100%)	388 (95%)	20 (5%)	22	22
14	1N	310/310 (100%)	294 (95%)	16 (5%)	21	20
15	1O	283/307 (92%)	266 (94%)	17 (6%)	17	15
16	1P	296/323 (92%)	280 (95%)	16 (5%)	20	18
17	1Q	117/152 (77%)	106 (91%)	11 (9%)	8	6
18	1R	79/97 (81%)	75 (95%)	4 (5%)	21	21
19	1S	77/82 (94%)	72 (94%)	5 (6%)	15	13
20	1T	79/133 (59%)	76 (96%)	3 (4%)	29	32
20	1U	79/133 (59%)	76 (96%)	3 (4%)	29	32
21	1V	100/101 (99%)	95 (95%)	5 (5%)	22	22
22	1W	107/112 (96%)	104 (97%)	3 (3%)	38	43
23	1X	153/154 (99%)	146 (95%)	7 (5%)	24	25
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	11	9
25	1Z	123/124 (99%)	120 (98%)	3 (2%)	43	49
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	35
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	11
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	12
29	1d	106/109 (97%)	100 (94%)	6 (6%)	18	17
30	1e	87/94 (93%)	83 (95%)	4 (5%)	24	25
31	1f	54/113 (48%)	49 (91%)	5 (9%)	8	6
32	1g	92/129 (71%)	90 (98%)	2 (2%)	45	53
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33	37
34	1i	120/120 (100%)	116 (97%)	4 (3%)	33	37
35	1j	62/84 (74%)	57 (92%)	5 (8%)	11	8
36	1k	63/76 (83%)	59 (94%)	4 (6%)	16	14
37	1l	141/161 (88%)	137 (97%)	4 (3%)	38	43
38	1m	113/114 (99%)	109 (96%)	4 (4%)	32	35
39	1n	156/160 (98%)	148 (95%)	8 (5%)	21	21
40	1o	110/119 (92%)	106 (96%)	4 (4%)	31	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1p	154/156 (99%)	152 (99%)	2 (1%)	61	69
42	1q	131/131 (100%)	128 (98%)	3 (2%)	44	51
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32	35
44	1s	44/351 (12%)	42 (96%)	2 (4%)	24	25
45	3A	367/397 (92%)	354 (96%)	13 (4%)	32	35
45	3N	372/397 (94%)	350 (94%)	22 (6%)	18	16
46	3B	328/355 (92%)	314 (96%)	14 (4%)	26	27
46	3O	327/355 (92%)	313 (96%)	14 (4%)	26	27
47	3C	332/332 (100%)	320 (96%)	12 (4%)	31	34
47	3P	332/332 (100%)	318 (96%)	14 (4%)	26	28
48	3D	202/259 (78%)	190 (94%)	12 (6%)	18	16
48	3Q	204/259 (79%)	195 (96%)	9 (4%)	25	26
49	3E	166/225 (74%)	146 (88%)	20 (12%)	5	3
49	3I	36/225 (16%)	27 (75%)	9 (25%)	0	0
49	3R	166/225 (74%)	144 (87%)	22 (13%)	4	2
49	3V	24/225 (11%)	21 (88%)	3 (12%)	4	2
50	3F	90/99 (91%)	89 (99%)	1 (1%)	65	74
50	3S	90/99 (91%)	89 (99%)	1 (1%)	65	74
51	3G	67/73 (92%)	63 (94%)	4 (6%)	17	15
51	3T	67/73 (92%)	63 (94%)	4 (6%)	17	15
52	3H	62/85 (73%)	59 (95%)	3 (5%)	23	23
52	3U	62/85 (73%)	55 (89%)	7 (11%)	5	3
53	3J	46/52 (88%)	45 (98%)	1 (2%)	45	53
53	3W	46/52 (88%)	44 (96%)	2 (4%)	26	27
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	43	49
55	4A	424/424 (100%)	417 (98%)	7 (2%)	53	62
56	4B	210/211 (100%)	201 (96%)	9 (4%)	26	27
57	4C	223/225 (99%)	216 (97%)	7 (3%)	35	39
58	4D	124/149 (83%)	119 (96%)	5 (4%)	28	29
59	4E	92/124 (74%)	90 (98%)	2 (2%)	45	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	4F	80/101 (79%)	76 (95%)	4 (5%)	22	22
61	4G	65/80 (81%)	59 (91%)	6 (9%)	8	6
62	4H	73/76 (96%)	71 (97%)	2 (3%)	39	45
63	4I	54/61 (88%)	50 (93%)	4 (7%)	13	10
64	4J	49/68 (72%)	49 (100%)	0	100	100
65	4K	38/66 (58%)	36 (95%)	2 (5%)	20	19
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	46
67	4M	37/57 (65%)	35 (95%)	2 (5%)	20	18
68	4N	70/70 (100%)	67 (96%)	3 (4%)	26	27
All	All	12266/14326 (86%)	11680 (95%)	586 (5%)	24	23

5 of 586 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	3O	117	GLU
62	4H	50	VAL
47	3P	174	THR
46	3O	116	ILE
52	3U	25	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
49	3E	186	GLN
48	3Q	105	ASN
52	3H	51	GLN
46	3O	290	ASN
50	3S	22	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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
56	FME	4B	1	56	8,9,10	0.54	0	8,9,11	0.89	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	0.84	1 (12%)
13	FME	1M	1	13	8,9,10	0.50	0	8,9,11	1.64	2 (25%)
1	FME	1A	1	1	8,9,10	0.50	0	8,9,11	1.10	1 (12%)
14	FME	1N	1	14	8,9,10	0.55	0	8,9,11	0.96	1 (12%)
55	FME	4A	1	55	8,9,10	0.55	0	8,9,11	1.73	2 (25%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.05	1 (12%)
11	FME	1K	1	11	8,9,10	0.57	0	8,9,11	0.97	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	4B	1	56	-	2/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
13	FME	1M	1	13	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-
8	FME	1H	1	8	-	2/7/9/11	-
11	FME	1K	1	11	-	2/7/9/11	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	4A	1	FME	CA-N-CN	3.85	128.74	122.82
13	1M	1	FME	O-C-CA	-2.98	117.11	124.77
13	1M	1	FME	CA-N-CN	-2.87	118.41	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1	FME	O-C-CA	-2.75	117.69	124.77
8	1H	1	FME	O-C-CA	-2.70	117.82	124.77

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O1-CN-N-CA
8	1H	1	FME	O1-CN-N-CA
13	1M	1	FME	C-CA-CB-CG
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1M	1	FME	5	0
1	1A	1	FME	1	0
14	1N	1	FME	1	0
55	4A	1	FME	7	0
11	1K	1	FME	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 226 ligands modelled in this entry, 7 are monoatomic - leaving 219 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
69	3PE	3P	507	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
69	3PE	3R	304	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	3 (5%)
69	3PE	3E	303	-	48,48,50	0.90	3 (6%)	51,53,55	1.17	4 (7%)
70	PC1	1Y	207	-	53,53,53	0.93	2 (3%)	59,61,61	1.16	3 (5%)
75	CDL	3X	103	-	99,99,99	0.91	4 (4%)	105,111,111	1.11	5 (4%)
69	3PE	1L	708	-	41,41,50	0.99	2 (4%)	44,46,55	1.27	4 (9%)
69	3PE	3G	107	-	32,32,50	1.14	2 (6%)	35,37,55	1.12	2 (5%)
69	3PE	3X	107	-	50,50,50	0.91	2 (4%)	53,55,55	0.96	3 (5%)
69	3PE	3C	511	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	3 (5%)
75	CDL	1H	401	-	50,50,99	1.28	4 (8%)	56,62,111	1.31	7 (12%)
75	CDL	3T	101	-	56,56,99	1.18	6 (10%)	62,68,111	1.41	8 (12%)
81	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.06	1 (2%)
91	PGV	4C	303	-	50,50,50	0.89	2 (4%)	53,56,56	0.93	2 (3%)
69	3PE	3W	102	-	41,41,50	0.99	2 (4%)	44,46,55	1.05	2 (4%)
69	3PE	3N	501	-	50,50,50	0.89	3 (6%)	53,55,55	1.13	3 (5%)
72	FES	1E	301	5	0,4,4	-	-	-	-	-
69	3PE	3C	506	-	46,46,50	0.93	2 (4%)	49,51,55	1.14	4 (8%)
69	3PE	3J	102	-	37,37,50	1.06	2 (5%)	40,42,55	1.27	4 (10%)
69	3PE	3P	508	-	50,50,50	0.90	4 (8%)	53,55,55	1.33	7 (13%)
69	3PE	3N	503	-	50,50,50	0.91	3 (6%)	53,55,55	1.14	4 (7%)
94	PO4	4H	101	-	4,4,4	0.98	0	6,6,6	0.47	0
69	3PE	3P	510	-	47,47,50	0.92	2 (4%)	50,52,55	1.09	5 (10%)
75	CDL	4C	306	-	99,99,99	0.91	4 (4%)	105,111,111	1.05	6 (5%)
69	3PE	1A	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.19	4 (9%)
69	3PE	1Y	211	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
91	PGV	4K	101	-	42,42,50	0.99	2 (4%)	45,48,56	1.11	3 (6%)
69	3PE	3G	103	-	32,32,50	1.12	2 (6%)	35,37,55	1.27	2 (5%)
69	3PE	1Y	208	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	3Q	502	-	40,40,50	1.02	2 (5%)	43,45,55	4.81	4 (9%)
71	SF4	1I	201	9	0,12,12	-	-	-	-	-
69	3PE	3E	302	-	50,50,50	0.87	2 (4%)	53,55,55	1.22	4 (7%)
70	PC1	1Y	206	-	45,45,53	1.00	2 (4%)	51,53,61	1.10	3 (5%)
69	3PE	3X	106	-	50,50,50	0.92	2 (4%)	53,55,55	0.97	2 (3%)
69	3PE	1Y	214	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	1Y	216	-	50,50,50	0.90	2 (4%)	53,55,55	1.15	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	AME	1h	201	-	9,10,11	0.53	0	9,11,13	0.99	1 (11%)
93	PSC	4B	303	-	51,51,51	0.95	2 (3%)	57,59,59	1.02	4 (7%)
91	PGV	4A	607	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	3X	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.06	4 (7%)
85	HEM	3C	502	-	50,50,50	1.60	9 (18%)	67,82,82	1.62	15 (22%)
69	3PE	3C	507	-	50,50,50	0.94	2 (4%)	53,55,55	1.06	2 (3%)
69	3PE	1L	712	-	50,50,50	0.93	2 (4%)	53,55,55	1.09	2 (3%)
69	3PE	1l	203	-	32,32,50	1.14	2 (6%)	35,37,55	1.16	2 (5%)
69	3PE	3C	510	-	34,34,50	1.16	3 (8%)	37,39,55	1.88	5 (13%)
69	3PE	3X	108	-	50,50,50	0.91	2 (4%)	53,55,55	1.00	2 (3%)
79	NDP	1P	501	-	51,52,52	0.51	0	71,80,80	0.82	2 (2%)
69	3PE	3P	517	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	1Y	205	-	39,39,50	1.05	2 (5%)	42,44,55	0.96	2 (4%)
69	3PE	1Y	201	-	41,41,50	1.00	2 (4%)	44,46,55	1.10	3 (6%)
84	MYR	1l	201	-	13,14,15	0.32	0	12,13,15	0.29	0
69	3PE	3S	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.02	2 (3%)
85	HEM	3P	502	47	50,50,50	1.61	9 (18%)	67,82,82	1.64	16 (23%)
69	3PE	3Q	503	-	45,45,50	0.99	2 (4%)	48,50,55	1.11	2 (4%)
76	AYA	1I	203	-	6,7,8	0.65	0	6,8,10	0.79	0
69	3PE	3C	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	4 (7%)
69	3PE	1L	705	-	48,48,50	0.91	2 (4%)	51,53,55	1.25	5 (9%)
75	CDL	3F	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.08	7 (6%)
86	HEC	3D	501	48	44,49,50	2.59	24 (54%)	56,80,82	2.10	18 (32%)
69	3PE	3P	516	-	50,50,50	0.91	2 (4%)	53,55,55	1.05	3 (5%)
69	3PE	3G	102	-	32,32,50	1.15	2 (6%)	35,37,55	1.08	2 (5%)
69	3PE	3R	302	-	50,50,50	0.87	3 (6%)	53,55,55	1.25	5 (9%)
69	3PE	1N	401	-	50,50,50	0.88	2 (4%)	53,55,55	1.24	5 (9%)
69	3PE	3C	514	-	34,34,50	1.05	2 (5%)	37,39,55	1.25	5 (13%)
81	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.11	1 (2%)
69	3PE	1l	204	-	50,50,50	0.93	2 (4%)	53,55,55	1.06	3 (5%)
69	3PE	3P	512	-	47,47,50	0.92	2 (4%)	50,52,55	1.10	3 (6%)
69	3PE	1L	706	-	32,32,50	1.16	2 (6%)	35,37,55	1.07	2 (5%)
70	PC1	1P	502	-	32,32,53	1.22	2 (6%)	38,40,61	1.11	4 (10%)
69	3PE	3G	110	-	42,42,50	0.97	2 (4%)	45,47,55	1.09	3 (6%)
69	3PE	1d	203	-	46,46,50	0.95	2 (4%)	49,51,55	1.12	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
69	3PE	1m	202	-	41,41,50	0.99	2 (4%)	44,46,55	1.17	3 (6%)
88	HEA	4A	601	55	67,67,67	2.40	23 (34%)	81,103,103	2.55	35 (43%)
69	3PE	3G	109	-	50,50,50	0.90	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	1m	201	-	49,49,50	0.92	2 (4%)	52,54,55	1.07	2 (3%)
69	3PE	3P	504	-	37,37,50	1.06	2 (5%)	40,42,55	1.16	2 (5%)
69	3PE	1f	102	-	42,42,50	0.99	2 (4%)	45,47,55	1.07	3 (6%)
88	HEA	4A	602	55	67,67,67	2.42	22 (32%)	81,103,103	2.50	36 (44%)
70	PC1	1H	404	-	40,40,53	1.12	3 (7%)	46,48,61	1.29	6 (13%)
69	3PE	1Y	215	-	42,42,50	0.96	2 (4%)	45,47,55	1.25	4 (8%)
69	3PE	3Y	104	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
69	3PE	1d	206	-	50,50,50	0.91	2 (4%)	53,55,55	0.93	3 (5%)
91	PGV	4A	606	-	50,50,50	0.90	2 (4%)	53,56,56	1.07	3 (5%)
75	CDL	1q	201	-	60,60,99	1.14	5 (8%)	66,72,111	1.39	9 (13%)
69	3PE	3P	506	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	3 (5%)
72	FES	3E	301	49	0,4,4	-	-	-	-	-
69	3PE	1L	703	-	43,43,50	0.98	2 (4%)	46,48,55	1.18	2 (4%)
69	3PE	1L	710	-	37,37,50	1.03	2 (5%)	40,42,55	5.05	5 (12%)
75	CDL	1d	205	-	92,92,99	0.93	4 (4%)	98,104,111	1.19	6 (6%)
69	3PE	1l	202	-	41,41,50	1.02	2 (4%)	44,46,55	1.21	4 (9%)
69	3PE	1g	203	-	32,32,50	1.15	2 (6%)	35,37,55	1.23	3 (8%)
87	PEK	4G	103	-	51,51,52	0.88	2 (3%)	54,56,57	1.11	4 (7%)
69	3PE	3P	519	-	50,50,50	0.87	2 (4%)	53,55,55	1.12	5 (9%)
69	3PE	1d	201	-	47,47,50	0.93	2 (4%)	50,52,55	1.04	2 (4%)
69	3PE	1f	104	-	47,47,50	0.94	2 (4%)	50,52,55	1.05	3 (6%)
70	PC1	3R	303	-	53,53,53	0.97	2 (3%)	59,61,61	1.15	4 (6%)
70	PC1	1B	202	-	45,45,53	6.15	8 (17%)	51,53,61	2.46	12 (23%)
70	PC1	3T	102	-	53,53,53	0.90	3 (5%)	59,61,61	1.07	4 (6%)
69	3PE	1o	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.29	5 (9%)
69	3PE	1Y	212	-	43,43,50	1.00	2 (4%)	46,48,55	1.04	2 (4%)
70	PC1	1B	203	-	47,47,53	0.97	2 (4%)	53,55,61	1.31	6 (11%)
75	CDL	4B	302	-	99,99,99	0.91	4 (4%)	105,111,111	1.05	7 (6%)
72	FES	1G	803	7	0,4,4	-	-	-	-	-
71	SF4	1B	201	2	0,12,12	-	-	-	-	-
85	HEM	3C	501	47	50,50,50	1.59	8 (16%)	67,82,82	1.64	12 (17%)
87	PEK	3X	102	-	52,52,52	0.90	2 (3%)	55,57,57	1.01	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
91	PGV	4N	101	-	50,50,50	0.90	2 (4%)	53,56,56	1.10	3 (5%)
91	PGV	4A	609	-	50,50,50	0.90	2 (4%)	53,56,56	1.13	4 (7%)
69	3PE	3A	503	-	50,50,50	0.87	2 (4%)	53,55,55	1.28	4 (7%)
69	3PE	3C	515	-	47,47,50	0.95	2 (4%)	50,52,55	1.11	2 (4%)
75	CDL	1q	202	-	99,99,99	0.90	4 (4%)	105,111,111	1.12	7 (6%)
69	3PE	1e	201	-	50,50,50	0.93	2 (4%)	53,55,55	1.12	4 (7%)
75	CDL	1L	704	-	86,86,99	0.96	5 (5%)	92,98,111	1.28	9 (9%)
69	3PE	3P	505	-	31,31,50	1.17	2 (6%)	34,36,55	1.24	3 (8%)
70	PC1	1d	204	-	38,38,53	1.11	2 (5%)	44,46,61	1.30	5 (11%)
73	FMN	1F	501	-	33,33,33	0.79	0	48,50,50	0.73	1 (2%)
69	3PE	3G	108	-	32,32,50	1.13	2 (6%)	35,37,55	1.19	2 (5%)
75	CDL	4C	307	-	99,99,99	0.92	4 (4%)	105,111,111	1.03	6 (5%)
69	3PE	3R	305	-	50,50,50	0.91	3 (6%)	53,55,55	1.13	3 (5%)
69	3PE	3P	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.17	4 (7%)
69	3PE	3P	518	-	50,50,50	0.92	2 (4%)	53,55,55	1.11	3 (5%)
69	3PE	3G	101	-	50,50,50	0.89	3 (6%)	53,55,55	1.33	6 (11%)
69	3PE	3P	515	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	3 (5%)
70	PC1	1M	501	-	43,43,53	1.03	2 (4%)	49,51,61	1.19	3 (6%)
92	CUA	4B	301	56	0,1,1	-	-	-	-	-
69	3PE	1b	101	-	41,41,50	0.99	2 (4%)	44,46,55	1.17	4 (9%)
69	3PE	3C	508	-	47,47,50	0.92	2 (4%)	50,52,55	1.13	4 (8%)
69	3PE	3G	105	-	32,32,50	1.12	2 (6%)	35,37,55	1.17	3 (8%)
69	3PE	1B	204	-	50,50,50	0.92	2 (4%)	53,55,55	1.12	4 (7%)
91	PGV	4G	102	-	50,50,50	0.92	2 (4%)	53,56,56	1.01	3 (5%)
69	3PE	3G	104	-	32,32,50	1.16	2 (6%)	35,37,55	1.24	3 (8%)
69	3PE	1B	205	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
69	3PE	1L	707	-	41,41,50	0.99	3 (7%)	44,46,55	1.26	5 (11%)
69	3PE	1m	204	-	50,50,50	0.91	2 (4%)	53,55,55	1.16	4 (7%)
69	3PE	1Y	210	-	41,41,50	0.98	2 (4%)	44,46,55	1.13	3 (6%)
69	3PE	3C	512	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	4 (7%)
69	3PE	3G	111	-	47,47,50	0.93	2 (4%)	50,52,55	1.07	2 (4%)
71	SF4	1G	802	7	0,12,12	-	-	-	-	-
86	HEC	3Q	501	48	46,50,50	2.58	23 (50%)	58,82,82	2.07	19 (32%)
69	3PE	1k	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.13	4 (8%)
69	3PE	3P	514	-	50,50,50	0.91	2 (4%)	53,55,55	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
69	3PE	3C	517	-	31,31,50	1.13	2 (6%)	34,36,55	1.15	3 (8%)
69	3PE	3C	509	-	50,50,50	0.89	2 (4%)	53,55,55	1.13	4 (7%)
69	3PE	1f	101	-	44,44,50	0.98	2 (4%)	47,49,55	1.02	2 (4%)
69	3PE	3C	504	-	45,45,50	0.29	0	48,50,55	0.34	0
71	SF4	1F	502	6	0,12,12	-	-	-	-	-
69	3PE	1L	701	-	45,45,50	0.96	3 (6%)	48,50,55	1.35	5 (10%)
69	3PE	1L	702	-	44,44,50	0.94	2 (4%)	47,49,55	1.16	5 (10%)
69	3PE	4G	101	-	31,31,50	1.16	2 (6%)	34,36,55	1.18	3 (8%)
72	FES	3R	301	-	0,4,4	-	-	-	-	-
69	3PE	1J	203	-	43,43,50	0.94	3 (6%)	46,48,55	1.19	4 (8%)
71	SF4	1G	801	7	0,12,12	-	-	-	-	-
75	CDL	3N	502	-	99,99,99	0.88	5 (5%)	105,111,111	1.09	6 (5%)
69	3PE	3Y	103	-	31,31,50	1.15	2 (6%)	34,36,55	1.25	4 (11%)
69	3PE	3Y	105	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	3 (5%)
70	PC1	1h	203	-	45,45,53	1.03	2 (4%)	51,53,61	1.17	4 (7%)
69	3PE	1L	709	-	41,41,50	0.99	2 (4%)	44,46,55	1.28	4 (9%)
69	3PE	3J	104	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	4 (7%)
91	PGV	4C	302	-	50,50,50	0.92	2 (4%)	53,56,56	1.03	3 (5%)
75	CDL	3D	504	-	55,55,99	1.21	6 (10%)	61,67,111	1.35	9 (14%)
91	PGV	4C	305	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	1M	502	-	46,46,50	0.93	2 (4%)	49,51,55	1.07	2 (4%)
69	3PE	3D	503	-	44,44,50	0.96	3 (6%)	47,49,55	1.23	4 (8%)
69	3PE	1Y	209	-	41,41,50	0.96	2 (4%)	44,46,55	1.17	4 (9%)
69	3PE	1m	205	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
82	PGT	1Y	203	-	50,50,50	0.92	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	3J	103	-	50,50,50	0.95	2 (4%)	53,55,55	0.99	2 (3%)
69	3PE	3J	105	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
69	3PE	1L	711	-	40,40,50	1.00	2 (5%)	43,45,55	1.05	2 (4%)
69	3PE	3P	511	-	44,44,50	0.95	2 (4%)	47,49,55	1.14	3 (6%)
69	3PE	3A	502	-	50,50,50	0.92	3 (6%)	53,55,55	1.17	4 (7%)
75	CDL	1d	202	-	85,85,99	0.95	5 (5%)	91,97,111	1.31	10 (10%)
69	3PE	1Y	204	-	30,30,50	1.17	2 (6%)	33,35,55	1.20	3 (9%)
69	3PE	3T	103	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	3G	106	-	32,32,50	1.11	2 (6%)	35,37,55	1.28	4 (11%)
70	PC1	3J	106	-	53,53,53	0.91	2 (3%)	59,61,61	2.70	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	PC1	1H	402	-	53,53,53	0.92	3 (5%)	59,61,61	1.10	3 (5%)
70	PC1	1A	202	-	34,34,53	1.16	2 (5%)	40,42,61	1.16	4 (10%)
70	PC1	1h	202	-	46,46,53	1.00	2 (4%)	52,54,61	1.13	3 (5%)
91	PGV	4C	301	-	50,50,50	0.90	2 (4%)	53,56,56	1.03	3 (5%)
69	3PE	3Y	107	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	3P	520	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	3 (5%)
75	CDL	1g	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.03	5 (4%)
70	PC1	3P	509	-	53,53,53	0.90	2 (3%)	59,61,61	1.20	6 (10%)
69	3PE	1h	204	-	46,46,50	0.97	2 (4%)	49,51,55	1.03	2 (4%)
69	3PE	3C	513	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	3Y	102	-	44,44,50	0.99	2 (4%)	47,49,55	1.04	3 (6%)
70	PC1	1J	202	-	34,34,53	1.15	2 (5%)	40,42,61	1.23	3 (7%)
69	3PE	3Q	504	-	45,45,50	0.98	2 (4%)	48,50,55	1.14	3 (6%)
75	CDL	3P	513	-	99,99,99	0.93	5 (5%)	105,111,111	1.28	11 (10%)
77	GTP	1O	401	78	33,34,34	1.14	2 (6%)	50,54,54	1.77	9 (18%)
75	CDL	3A	501	-	97,97,99	0.91	6 (6%)	103,109,111	1.17	8 (7%)
69	3PE	3J	101	-	46,46,50	0.94	2 (4%)	49,51,55	1.15	2 (4%)
91	PGV	4A	608	-	50,50,50	0.92	2 (4%)	53,56,56	1.02	3 (5%)
85	HEM	3P	501	47	50,50,50	1.59	8 (16%)	67,82,82	1.65	13 (19%)
70	PC1	1H	403	-	47,47,53	0.99	2 (4%)	53,55,61	0.97	3 (5%)
69	3PE	3W	101	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
69	3PE	3D	502	-	40,40,50	0.31	0	43,45,55	0.40	0
91	PGV	4J	101	-	41,41,50	1.00	2 (4%)	44,47,56	1.11	4 (9%)
69	3PE	1Z	201	-	50,50,50	0.90	2 (4%)	53,55,55	1.14	4 (7%)
69	3PE	1f	103	-	43,43,50	1.01	2 (4%)	45,47,55	1.15	3 (6%)
69	3PE	1g	202	-	50,50,50	0.88	2 (4%)	53,55,55	1.11	5 (9%)
70	PC1	1Y	202	-	34,34,53	1.16	2 (5%)	40,42,61	1.12	3 (7%)
69	3PE	4G	104	-	40,40,50	1.03	2 (5%)	43,45,55	1.15	4 (9%)
69	3PE	3W	103	-	50,50,50	0.93	2 (4%)	53,55,55	3.79	5 (9%)
91	PGV	4C	304	-	50,50,50	0.92	2 (4%)	53,56,56	1.04	4 (7%)
69	3PE	1Y	213	-	50,50,50	0.89	2 (4%)	53,55,55	1.11	3 (5%)
71	SF4	1I	202	9	0,12,12	-	-	-	-	-
69	3PE	3Y	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	2 (3%)
75	CDL	1Y	217	-	99,99,99	0.90	4 (4%)	105,111,111	1.03	5 (4%)
69	3PE	3X	105	-	50,50,50	0.92	2 (4%)	53,55,55	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
75	CDL	3Y	106	-	99,99,99	0.90	4 (4%)	105,111,111	1.10	5 (4%)
69	3PE	1A	201	-	46,46,50	0.93	2 (4%)	49,51,55	1.25	5 (10%)
69	3PE	1m	203	-	41,41,50	1.03	2 (4%)	44,46,55	1.13	3 (6%)
69	3PE	3C	505	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	4 (7%)
75	CDL	1N	402	-	76,76,99	1.01	4 (5%)	82,88,111	1.22	7 (8%)
75	CDL	1i	201	-	79,79,99	1.02	5 (6%)	85,91,111	1.31	10 (11%)
69	3PE	1J	201	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
70	PC1	3X	104	-	53,53,53	0.91	3 (5%)	59,61,61	1.12	5 (8%)
69	3PE	3C	516	-	42,42,50	0.98	2 (4%)	45,47,55	1.13	3 (6%)

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
69	3PE	3P	507	-	-	19/54/54/54	-
69	3PE	3R	304	-	-	18/54/54/54	-
69	3PE	3E	303	-	-	17/52/52/54	-
70	PC1	1Y	207	-	-	11/57/57/57	-
75	CDL	3X	103	-	-	44/110/110/110	-
69	3PE	1L	708	-	-	14/45/45/54	-
69	3PE	3G	107	-	-	8/36/36/54	-
69	3PE	3X	107	-	-	13/54/54/54	-
69	3PE	3C	511	-	-	15/54/54/54	-
75	CDL	1H	401	-	-	20/61/61/110	-
75	CDL	3T	101	-	-	21/67/67/110	-
81	EHZ	1n	201	-	-	5/42/44/45	-
91	PGV	4C	303	-	-	9/55/55/55	-
69	3PE	3W	102	-	-	16/45/45/54	-
69	3PE	3N	501	-	-	15/54/54/54	-
72	FES	1E	301	5	-	-	0/1/1/1
69	3PE	3C	506	-	-	16/50/50/54	-
69	3PE	3J	102	-	-	10/41/41/54	-
69	3PE	3P	508	-	-	16/54/54/54	-
69	3PE	3N	503	-	-	16/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3P	510	-	-	12/51/51/54	-
75	CDL	4C	306	-	-	39/110/110/110	-
69	3PE	1A	203	-	-	15/44/44/54	-
69	3PE	1Y	211	-	-	9/54/54/54	-
91	PGV	4K	101	-	-	10/47/47/55	-
69	3PE	3G	103	-	-	10/36/36/54	-
69	3PE	1Y	208	-	-	12/54/54/54	-
69	3PE	3Q	502	-	-	8/44/44/54	-
71	SF4	1I	201	9	-	-	0/6/5/5
69	3PE	3E	302	-	-	20/54/54/54	-
70	PC1	1Y	206	-	-	15/49/49/57	-
69	3PE	3X	106	-	-	14/54/54/54	-
69	3PE	1Y	214	-	-	14/54/54/54	-
69	3PE	1Y	216	-	-	14/54/54/54	-
83	AME	1h	201	-	-	2/9/10/12	-
93	PSC	4B	303	-	-	18/55/55/55	-
91	PGV	4A	607	-	-	15/55/55/55	-
69	3PE	3X	101	-	-	16/54/54/54	-
85	HEM	3C	502	-	-	6/14/54/54	-
69	3PE	3C	507	-	-	23/54/54/54	-
69	3PE	1L	712	-	-	20/54/54/54	-
69	3PE	1I	203	-	-	14/36/36/54	-
69	3PE	3C	510	-	-	14/38/38/54	-
69	3PE	3X	108	-	-	14/54/54/54	-
79	NDP	1P	501	-	-	3/34/77/77	0/5/5/5
69	3PE	3P	517	-	-	13/54/54/54	-
69	3PE	1Y	205	-	-	10/43/43/54	-
69	3PE	1Y	201	-	-	12/45/45/54	-
84	MYR	1I	201	-	-	2/12/12/13	-
69	3PE	3S	201	-	-	17/54/54/54	-
85	HEM	3P	502	47	-	8/14/54/54	-
69	3PE	3Q	503	-	-	17/49/49/54	-
76	AYA	1I	203	-	-	2/5/6/8	-
69	3PE	3C	503	-	-	13/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1L	705	-	-	14/52/52/54	-
75	CDL	3F	201	-	-	38/110/110/110	-
86	HEC	3D	501	48	-	4/13/53/54	-
69	3PE	3P	516	-	-	12/54/54/54	-
69	3PE	3G	102	-	-	13/36/36/54	-
69	3PE	3R	302	-	-	18/54/54/54	-
69	3PE	1N	401	-	-	17/54/54/54	-
69	3PE	3C	514	-	-	8/38/38/54	-
81	EHZ	1T	101	20	-	9/42/44/45	-
69	3PE	1l	204	-	-	19/54/54/54	-
69	3PE	3P	512	-	-	13/51/51/54	-
69	3PE	1L	706	-	-	9/36/36/54	-
70	PC1	1P	502	-	-	12/36/36/57	-
69	3PE	3G	110	-	-	10/46/46/54	-
69	3PE	1d	203	-	-	27/50/50/54	-
69	3PE	1m	202	-	-	10/45/45/54	-
88	HEA	4A	601	55	-	8/36/76/76	-
69	3PE	3G	109	-	-	15/54/54/54	-
69	3PE	1m	201	-	-	13/53/53/54	-
69	3PE	3P	504	-	-	8/41/41/54	-
69	3PE	1f	102	-	-	13/46/46/54	-
88	HEA	4A	602	55	-	8/36/76/76	-
70	PC1	1H	404	-	-	7/44/44/57	-
69	3PE	1Y	215	-	-	21/46/46/54	-
69	3PE	3Y	104	-	-	20/54/54/54	-
69	3PE	1d	206	-	-	12/54/54/54	-
91	PGV	4A	606	-	-	9/55/55/55	-
75	CDL	1q	201	-	-	15/71/71/110	-
69	3PE	3P	506	-	-	16/54/54/54	-
75	CDL	1d	205	-	-	41/103/103/110	-
69	3PE	1L	703	-	-	13/47/47/54	-
69	3PE	1L	710	-	-	16/41/41/54	-
72	FES	3E	301	49	-	-	0/1/1/1
69	3PE	1l	202	-	-	18/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1g	203	-	-	13/36/36/54	-
87	PEK	4G	103	-	-	12/55/55/56	-
69	3PE	3P	519	-	-	15/54/54/54	-
69	3PE	1d	201	-	-	33/51/51/54	-
69	3PE	1f	104	-	-	17/51/51/54	-
70	PC1	3R	303	-	-	17/57/57/57	-
70	PC1	1B	202	-	-	20/49/49/57	-
70	PC1	3T	102	-	-	18/57/57/57	-
69	3PE	1o	201	-	-	20/54/54/54	-
69	3PE	1Y	212	-	-	10/47/47/54	-
70	PC1	1B	203	-	-	21/51/51/57	-
75	CDL	4B	302	-	-	27/110/110/110	-
72	FES	1G	803	7	-	-	0/1/1/1
71	SF4	1B	201	2	-	-	0/6/5/5
85	HEM	3C	501	47	-	5/14/54/54	-
87	PEK	3X	102	-	-	19/56/56/56	-
91	PGV	4N	101	-	-	15/55/55/55	-
91	PGV	4A	609	-	-	13/55/55/55	-
69	3PE	3A	503	-	-	18/54/54/54	-
69	3PE	3C	515	-	-	16/51/51/54	-
75	CDL	1q	202	-	-	36/110/110/110	-
69	3PE	1e	201	-	-	13/54/54/54	-
75	CDL	1L	704	-	-	31/97/97/110	-
69	3PE	3P	505	-	-	11/35/35/54	-
70	PC1	1d	204	-	-	24/42/42/57	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
69	3PE	3G	108	-	-	8/36/36/54	-
75	CDL	4C	307	-	-	19/110/110/110	-
69	3PE	3R	305	-	-	15/54/54/54	-
69	3PE	3P	503	-	-	17/54/54/54	-
69	3PE	3P	518	-	-	16/54/54/54	-
69	3PE	3G	101	-	-	15/54/54/54	-
69	3PE	3P	515	-	-	20/54/54/54	-
70	PC1	1M	501	-	-	18/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1b	101	-	-	12/45/45/54	-
69	3PE	3C	508	-	-	14/51/51/54	-
69	3PE	3G	105	-	-	15/36/36/54	-
69	3PE	1B	204	-	-	15/54/54/54	-
91	PGV	4G	102	-	-	18/55/55/55	-
69	3PE	3G	104	-	-	14/36/36/54	-
69	3PE	1B	205	-	-	16/54/54/54	-
69	3PE	1L	707	-	-	5/45/45/54	-
69	3PE	1m	204	-	-	13/54/54/54	-
69	3PE	1Y	210	-	-	16/45/45/54	-
69	3PE	3C	512	-	-	16/54/54/54	-
69	3PE	3G	111	-	-	23/51/51/54	-
71	SF4	1G	802	7	-	-	0/6/5/5
86	HEC	3Q	501	48	-	2/14/54/54	-
69	3PE	1k	101	-	-	16/49/49/54	-
69	3PE	3P	514	-	-	15/54/54/54	-
69	3PE	3C	517	-	-	4/35/35/54	-
69	3PE	3C	509	-	-	16/54/54/54	-
69	3PE	1f	101	-	-	20/48/48/54	-
69	3PE	3C	504	-	-	10/49/49/54	-
71	SF4	1F	502	6	-	-	0/6/5/5
69	3PE	1L	701	-	-	16/49/49/54	-
69	3PE	1L	702	-	-	19/48/48/54	-
69	3PE	4G	101	-	-	15/35/35/54	-
72	FES	3R	301	-	-	-	0/1/1/1
69	3PE	1J	203	-	-	6/47/47/54	-
71	SF4	1G	801	7	-	-	0/6/5/5
75	CDL	3N	502	-	-	38/110/110/110	-
69	3PE	3Y	103	-	-	2/35/35/54	-
69	3PE	3Y	105	-	-	5/54/54/54	-
70	PC1	1h	203	-	-	17/49/49/57	-
69	3PE	1L	709	-	-	11/45/45/54	-
69	3PE	3J	104	-	-	14/54/54/54	-
91	PGV	4C	302	-	-	12/55/55/55	-
75	CDL	3D	504	-	-	20/66/66/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	PGV	4C	305	-	-	11/55/55/55	-
69	3PE	1M	502	-	-	17/50/50/54	-
69	3PE	3D	503	-	-	16/48/48/54	-
69	3PE	1Y	209	-	-	21/45/45/54	-
69	3PE	1m	205	-	-	11/54/54/54	-
82	PGT	1Y	203	-	-	26/55/55/55	-
69	3PE	3J	103	-	-	13/54/54/54	-
69	3PE	3J	105	-	-	12/54/54/54	-
69	3PE	1L	711	-	-	12/44/44/54	-
69	3PE	3P	511	-	-	7/48/48/54	-
69	3PE	3A	502	-	-	16/54/54/54	-
75	CDL	1d	202	-	-	31/96/96/110	-
69	3PE	1Y	204	-	-	5/34/34/54	-
69	3PE	3T	103	-	-	13/54/54/54	-
69	3PE	3G	106	-	-	11/36/36/54	-
70	PC1	3J	106	-	-	10/57/57/57	-
70	PC1	1H	402	-	-	14/57/57/57	-
70	PC1	1A	202	-	-	10/38/38/57	-
70	PC1	1h	202	-	-	13/50/50/57	-
91	PGV	4C	301	-	-	2/55/55/55	-
69	3PE	3Y	107	-	-	18/54/54/54	-
69	3PE	3P	520	-	-	14/54/54/54	-
75	CDL	1g	201	-	-	46/110/110/110	-
70	PC1	3P	509	-	-	17/57/57/57	-
69	3PE	1h	204	-	-	19/50/50/54	-
69	3PE	3C	513	-	-	14/54/54/54	-
69	3PE	3Y	102	-	-	9/48/48/54	-
70	PC1	1J	202	-	-	17/38/38/57	-
69	3PE	3Q	504	-	-	16/49/49/54	-
75	CDL	3P	513	-	-	15/110/110/110	-
77	GTP	1O	401	78	-	4/22/38/38	0/3/3/3
75	CDL	3A	501	-	-	29/108/108/110	-
69	3PE	3J	101	-	-	19/50/50/54	-
91	PGV	4A	608	-	-	4/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	HEM	3P	501	47	-	6/14/54/54	-
70	PC1	1H	403	-	-	12/51/51/57	-
69	3PE	3W	101	-	-	15/54/54/54	-
69	3PE	3D	502	-	-	16/44/44/54	-
91	PGV	4J	101	-	-	12/46/46/55	-
69	3PE	1Z	201	-	-	5/54/54/54	-
69	3PE	1f	103	-	-	10/46/46/54	-
69	3PE	1g	202	-	-	20/54/54/54	-
70	PC1	1Y	202	-	-	19/38/38/57	-
69	3PE	4G	104	-	-	6/44/44/54	-
69	3PE	3W	103	-	-	16/54/54/54	-
91	PGV	4C	304	-	-	6/55/55/55	-
69	3PE	1Y	213	-	-	35/54/54/54	-
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	3Y	101	-	-	22/54/54/54	-
75	CDL	1Y	217	-	-	39/110/110/110	-
69	3PE	3X	105	-	-	13/54/54/54	-
75	CDL	3Y	106	-	-	36/110/110/110	-
69	3PE	1A	201	-	-	11/50/50/54	-
69	3PE	1m	203	-	-	15/45/45/54	-
69	3PE	3C	505	-	-	17/54/54/54	-
75	CDL	1N	402	-	-	32/87/87/110	-
75	CDL	1i	201	-	-	12/90/90/110	-
69	3PE	1J	201	-	-	18/54/54/54	-
70	PC1	3X	104	-	-	20/57/57/57	-
69	3PE	3C	516	-	-	8/46/46/54	-

The worst 5 of 584 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1B	202	PC1	C24-C23	40.35	3.52	1.51
88	4A	601	HEA	FE-ND	5.59	2.12	1.94
88	4A	602	HEA	FE-ND	5.55	2.12	1.94
88	4A	601	HEA	FE-NB	5.55	2.12	1.94
88	4A	602	HEA	FE-NB	5.52	2.11	1.94

The worst 5 of 916 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1L	710	3PE	O21-C21-C22	22.31	159.74	111.48
69	3Q	502	3PE	O21-C21-C22	21.62	158.26	111.48
69	3Q	502	3PE	O21-C21-O22	-19.37	78.41	123.70
69	3W	103	3PE	O31-C31-O32	-19.03	76.02	123.63
69	1L	710	3PE	O21-C21-O22	-18.92	79.47	123.70

There are no chirality outliers.

5 of 3142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O11
69	1A	201	3PE	C11-O13-P-O12
69	1A	201	3PE	C11-O13-P-O14
69	1A	203	3PE	C11-O13-P-O11
69	1A	203	3PE	C11-O13-P-O12

There are no ring outliers.

214 monomers are involved in 3448 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	3P	507	3PE	21	0
69	3R	304	3PE	18	0
69	3E	303	3PE	13	0
70	1Y	207	PC1	34	0
75	3X	103	CDL	31	0
69	1L	708	3PE	10	0
69	3G	107	3PE	10	0
69	3X	107	3PE	26	0
69	3C	511	3PE	35	0
75	1H	401	CDL	10	0
75	3T	101	CDL	13	0
81	1n	201	EHZ	1	0
91	4C	303	PGV	19	0
69	3W	102	3PE	25	0
69	3N	501	3PE	38	0
72	1E	301	FES	4	0
69	3C	506	3PE	17	0
69	3J	102	3PE	1	0
69	3P	508	3PE	23	0
69	3N	503	3PE	28	0
69	3P	510	3PE	20	0
75	4C	306	CDL	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	1A	203	3PE	20	0
69	1Y	211	3PE	19	0
91	4K	101	PGV	7	0
69	3G	103	3PE	14	0
69	1Y	208	3PE	57	0
69	3Q	502	3PE	11	0
71	1I	201	SF4	1	0
69	3E	302	3PE	14	0
70	1Y	206	PC1	39	0
69	3X	106	3PE	9	0
69	1Y	214	3PE	35	0
69	1Y	216	3PE	14	0
83	1h	201	AME	2	0
93	4B	303	PSC	27	0
91	4A	607	PGV	11	0
69	3X	101	3PE	26	0
85	3C	502	HEM	4	0
69	3C	507	3PE	23	0
69	1L	712	3PE	17	0
69	1l	203	3PE	11	0
69	3C	510	3PE	9	0
69	3X	108	3PE	39	0
79	1P	501	NDP	2	0
69	3P	517	3PE	21	0
69	1Y	205	3PE	17	0
69	1Y	201	3PE	23	0
69	3S	201	3PE	26	0
85	3P	502	HEM	4	0
69	3Q	503	3PE	18	0
76	1I	203	AYA	6	0
69	3C	503	3PE	10	0
69	1L	705	3PE	15	0
75	3F	201	CDL	26	0
86	3D	501	HEC	6	0
69	3P	516	3PE	11	0
69	3G	102	3PE	9	0
69	3R	302	3PE	18	0
69	1N	401	3PE	57	0
69	3C	514	3PE	4	0
69	1l	204	3PE	12	0
69	3P	512	3PE	17	0
69	1L	706	3PE	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	1P	502	PC1	6	0
69	3G	110	3PE	18	0
69	1d	203	3PE	24	0
69	1m	202	3PE	23	0
88	4A	601	HEA	7	0
69	3G	109	3PE	21	0
69	1m	201	3PE	13	0
69	3P	504	3PE	12	0
69	1f	102	3PE	19	0
88	4A	602	HEA	4	0
70	1H	404	PC1	19	0
69	1Y	215	3PE	31	0
69	3Y	104	3PE	11	0
69	1d	206	3PE	32	0
91	4A	606	PGV	14	0
75	1q	201	CDL	11	0
69	3P	506	3PE	14	0
72	3E	301	FES	5	0
69	1L	703	3PE	29	0
69	1L	710	3PE	18	0
75	1d	205	CDL	28	0
69	1l	202	3PE	6	0
69	1g	203	3PE	13	0
87	4G	103	PEK	13	0
69	3P	519	3PE	24	0
69	1d	201	3PE	48	0
69	1f	104	3PE	77	0
70	3R	303	PC1	16	0
70	1B	202	PC1	66	0
70	3T	102	PC1	45	0
69	1o	201	3PE	31	0
69	1Y	212	3PE	20	0
70	1B	203	PC1	22	0
75	4B	302	CDL	40	0
72	1G	803	FES	4	0
71	1B	201	SF4	1	0
85	3C	501	HEM	4	0
87	3X	102	PEK	9	0
91	4N	101	PGV	13	0
91	4A	609	PGV	60	0
69	3A	503	3PE	27	0
69	3C	515	3PE	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	1q	202	CDL	29	0
69	1e	201	3PE	15	0
75	1L	704	CDL	38	0
69	3P	505	3PE	9	0
70	1d	204	PC1	24	0
73	1F	501	FMN	4	0
69	3G	108	3PE	10	0
75	4C	307	CDL	22	0
69	3R	305	3PE	23	0
69	3P	503	3PE	27	0
69	3P	518	3PE	24	0
69	3G	101	3PE	12	0
69	3P	515	3PE	11	0
70	1M	501	PC1	12	0
69	1b	101	3PE	31	0
69	3C	508	3PE	22	0
69	3G	105	3PE	13	0
69	1B	204	3PE	25	0
91	4G	102	PGV	10	0
69	3G	104	3PE	12	0
69	1B	205	3PE	26	0
69	1L	707	3PE	10	0
69	1m	204	3PE	5	0
69	1Y	210	3PE	9	0
69	3C	512	3PE	57	0
69	3G	111	3PE	8	0
71	1G	802	SF4	4	0
86	3Q	501	HEC	10	0
69	1k	101	3PE	32	0
69	3P	514	3PE	43	0
69	3C	517	3PE	16	0
69	3C	509	3PE	22	0
69	1f	101	3PE	14	0
69	3C	504	3PE	5	0
71	1F	502	SF4	8	0
69	1L	701	3PE	14	0
69	1L	702	3PE	9	0
69	4G	101	3PE	12	0
72	3R	301	FES	4	0
69	1J	203	3PE	17	0
75	3N	502	CDL	57	0
69	3Y	103	3PE	9	0

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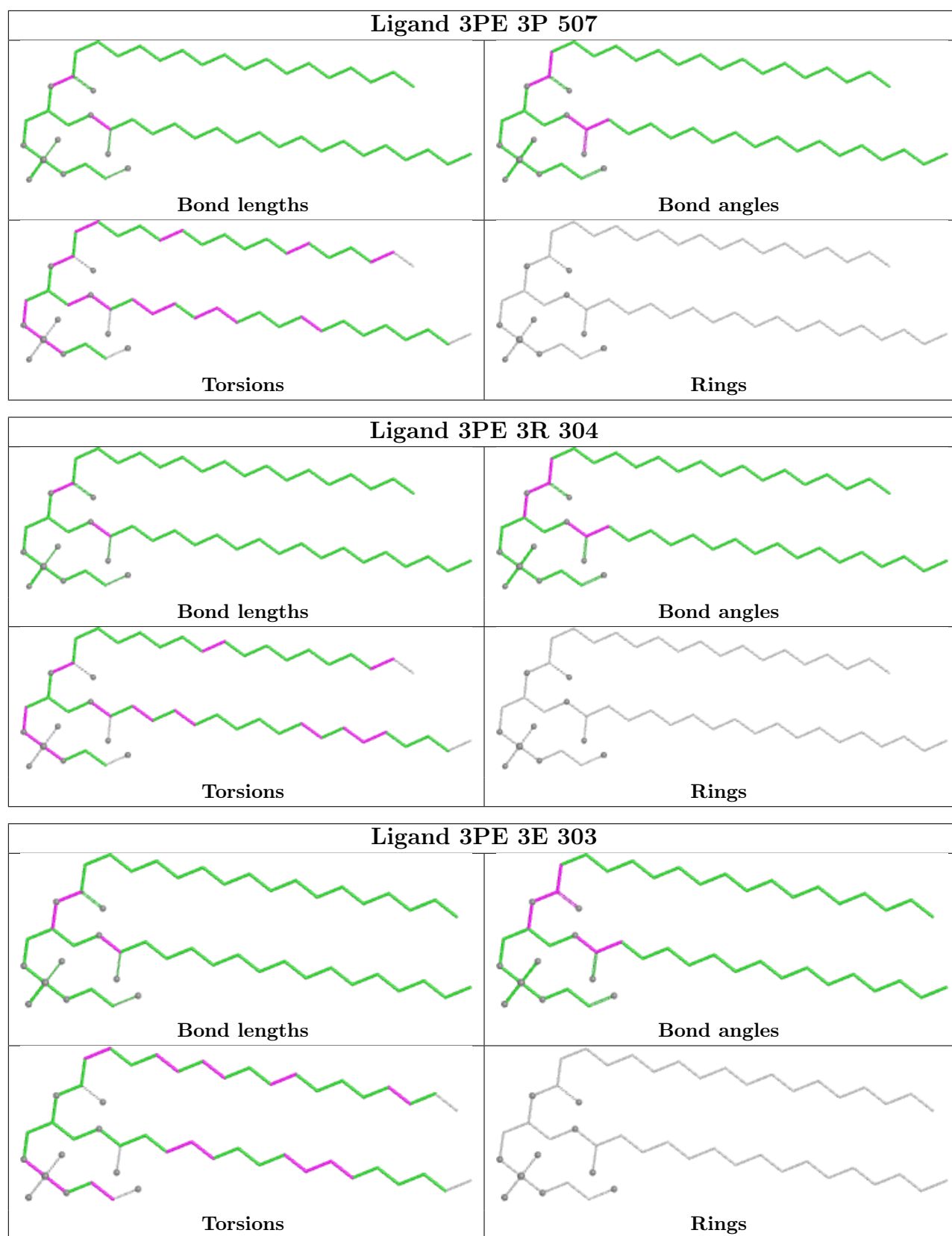
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70	1h	203	PC1	13	0
69	1L	709	3PE	24	0
69	3J	104	3PE	20	0
91	4C	302	PGV	19	0
75	3D	504	CDL	4	0
91	4C	305	PGV	14	0
69	1M	502	3PE	13	0
69	3D	503	3PE	13	0
69	1Y	209	3PE	25	0
69	1m	205	3PE	24	0
82	1Y	203	PGT	24	0
69	3J	103	3PE	20	0
69	3J	105	3PE	16	0
69	1L	711	3PE	14	0
69	3P	511	3PE	27	0
69	3A	502	3PE	34	0
75	1d	202	CDL	32	0
69	1Y	204	3PE	11	0
69	3T	103	3PE	26	0
69	3G	106	3PE	6	0
70	3J	106	PC1	13	0
70	1H	402	PC1	18	0
70	1A	202	PC1	28	0
70	1h	202	PC1	16	0
91	4C	301	PGV	5	0
69	3Y	107	3PE	28	0
69	3P	520	3PE	26	0
75	1g	201	CDL	60	0
70	3P	509	PC1	15	0
69	1h	204	3PE	15	0
69	3C	513	3PE	41	0
69	3Y	102	3PE	21	0
70	1J	202	PC1	7	0
69	3Q	504	3PE	14	0
75	3P	513	CDL	60	0
77	1O	401	GTP	7	0
75	3A	501	CDL	45	0
69	3J	101	3PE	11	0
91	4A	608	PGV	19	0
85	3P	501	HEM	1	0
70	1H	403	PC1	21	0

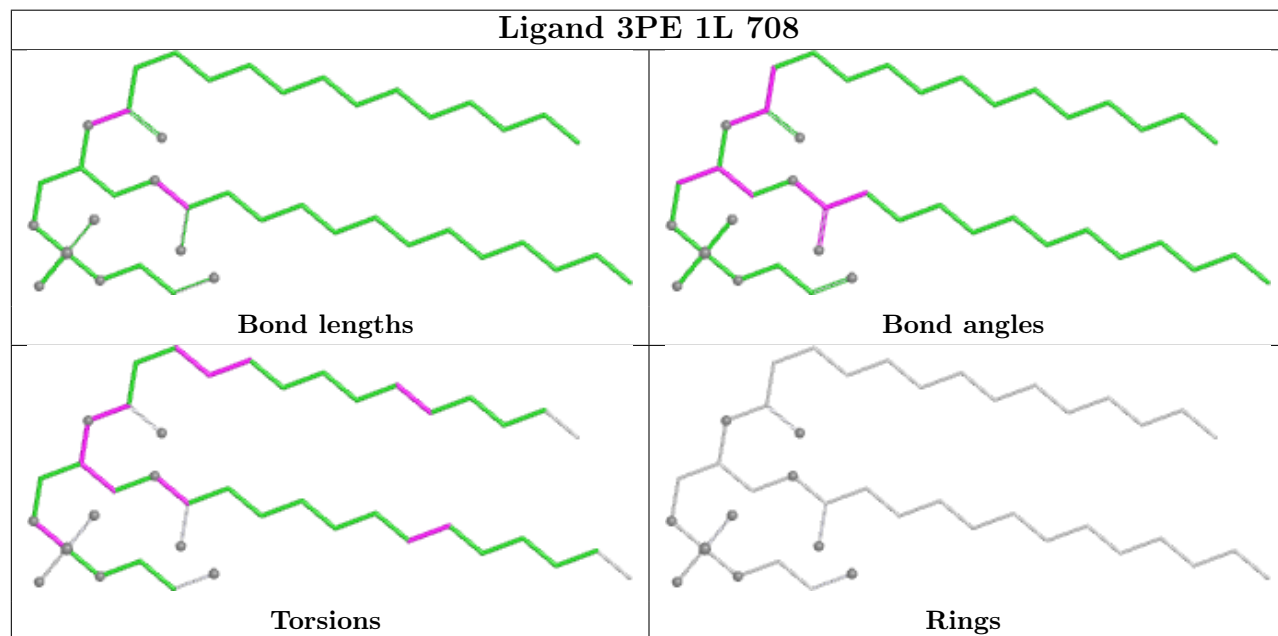
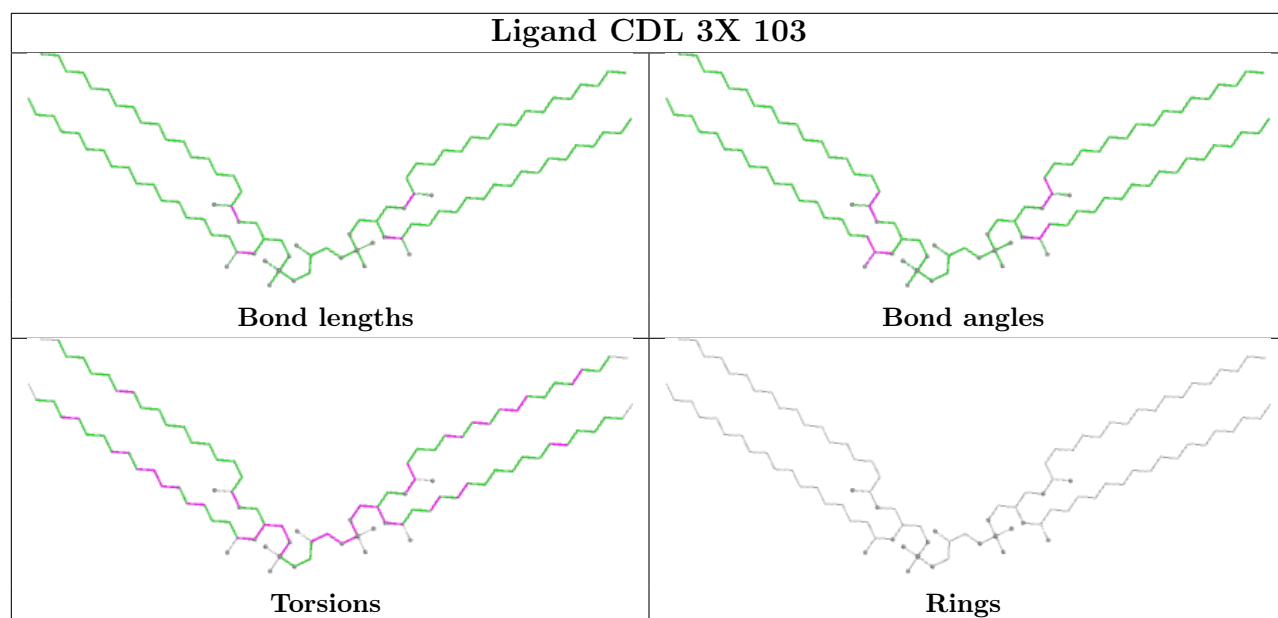
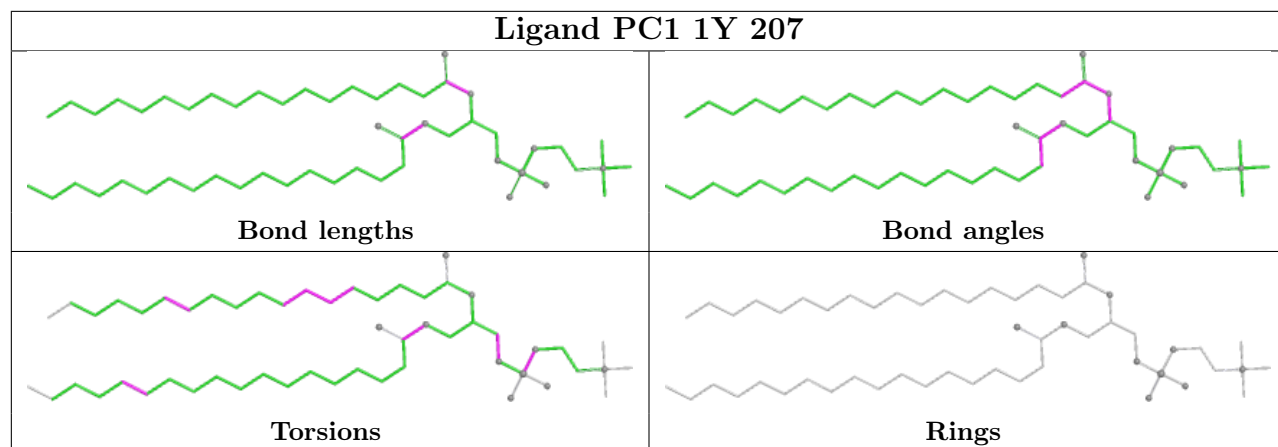
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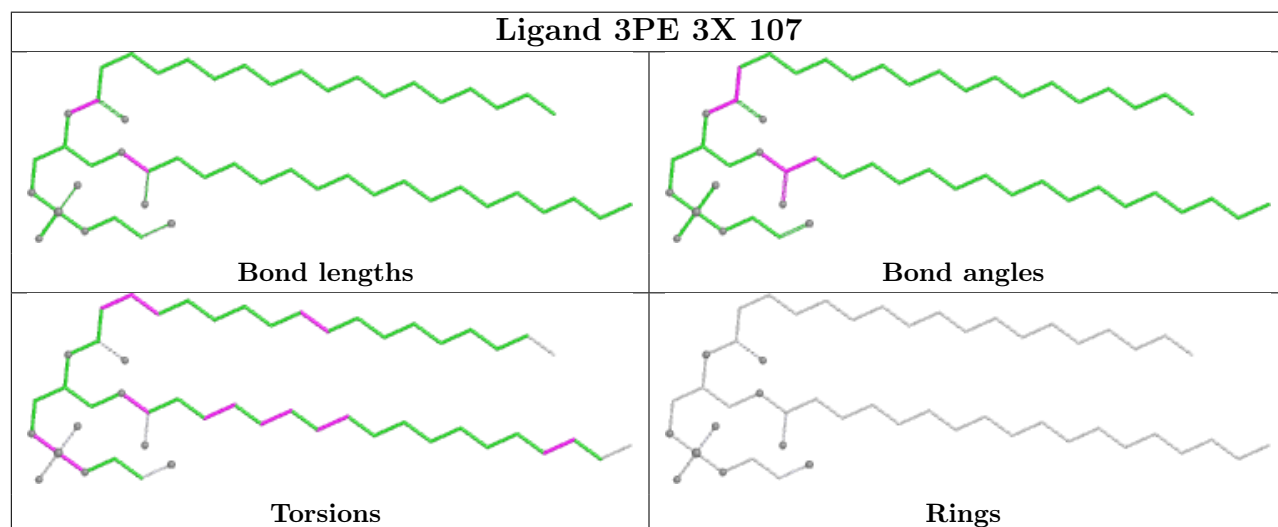
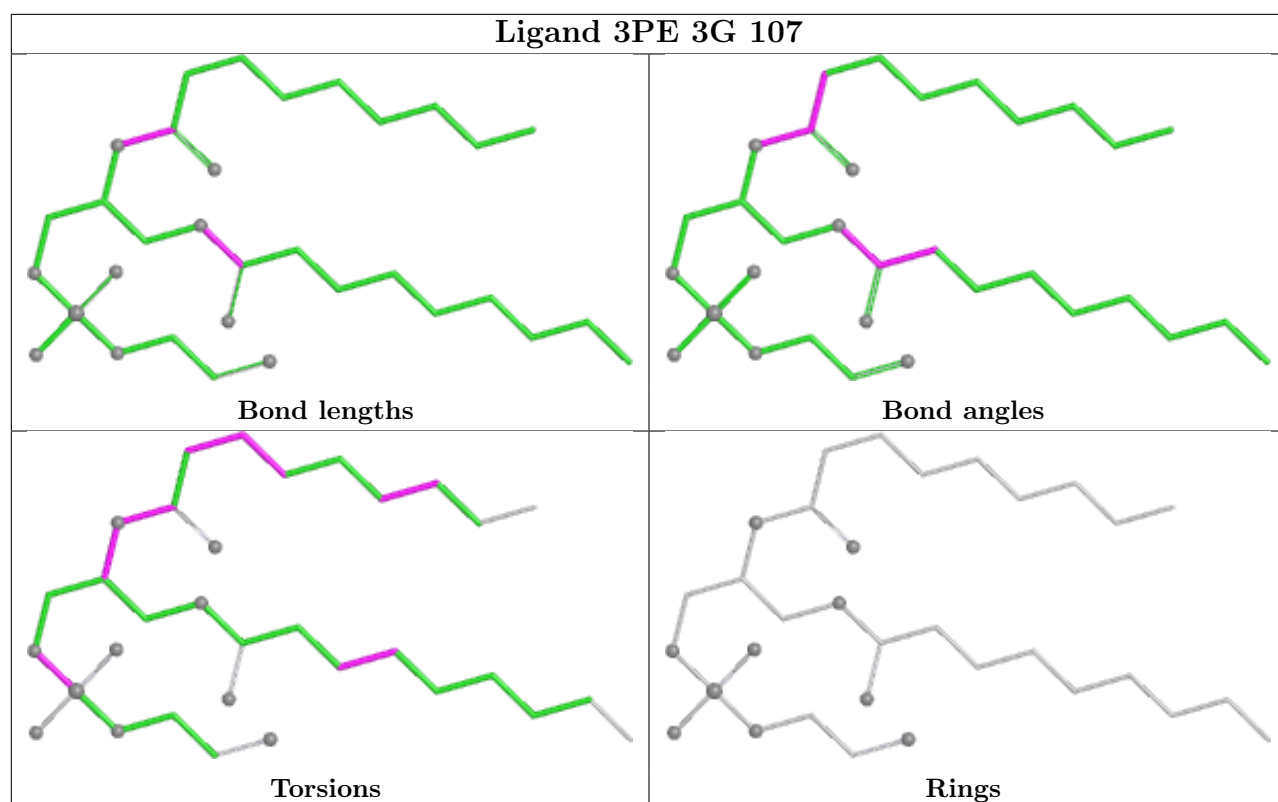
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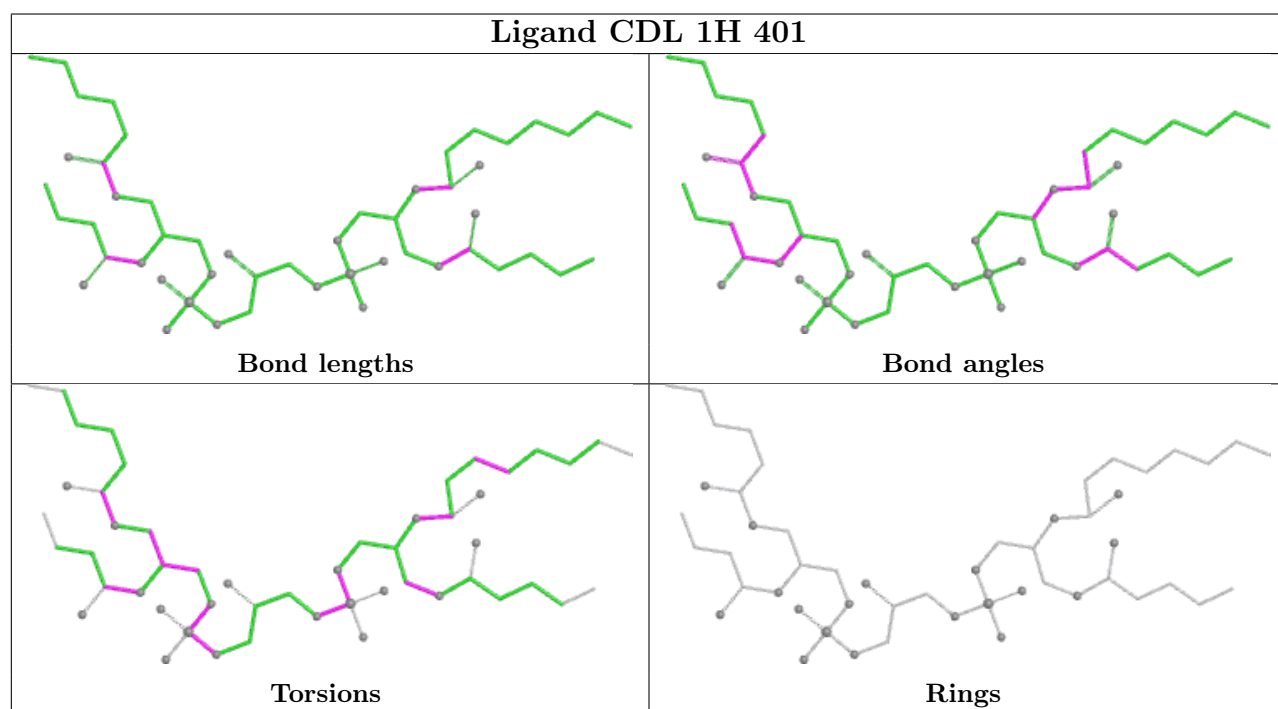
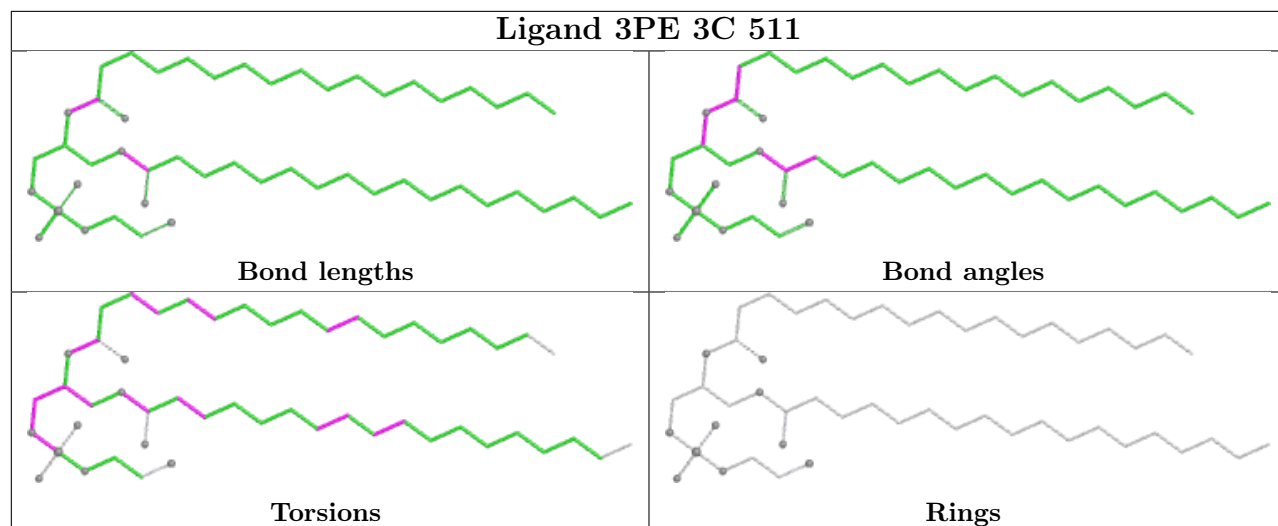
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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69	3D	502	3PE	6	0
91	4J	101	PGV	8	0
69	1Z	201	3PE	12	0
69	1f	103	3PE	16	0
69	1g	202	3PE	30	0
70	1Y	202	PC1	11	0
69	4G	104	3PE	25	0
69	3W	103	3PE	27	0
91	4C	304	PGV	9	0
69	1Y	213	3PE	21	0
71	1I	202	SF4	2	0
69	3Y	101	3PE	15	0
75	1Y	217	CDL	39	0
69	3X	105	3PE	24	0
75	3Y	106	CDL	31	0
69	1A	201	3PE	13	0
69	1m	203	3PE	34	0
69	3C	505	3PE	6	0
75	1N	402	CDL	33	0
75	1i	201	CDL	35	0
69	1J	201	3PE	37	0
70	3X	104	PC1	17	0
69	3C	516	3PE	24	0

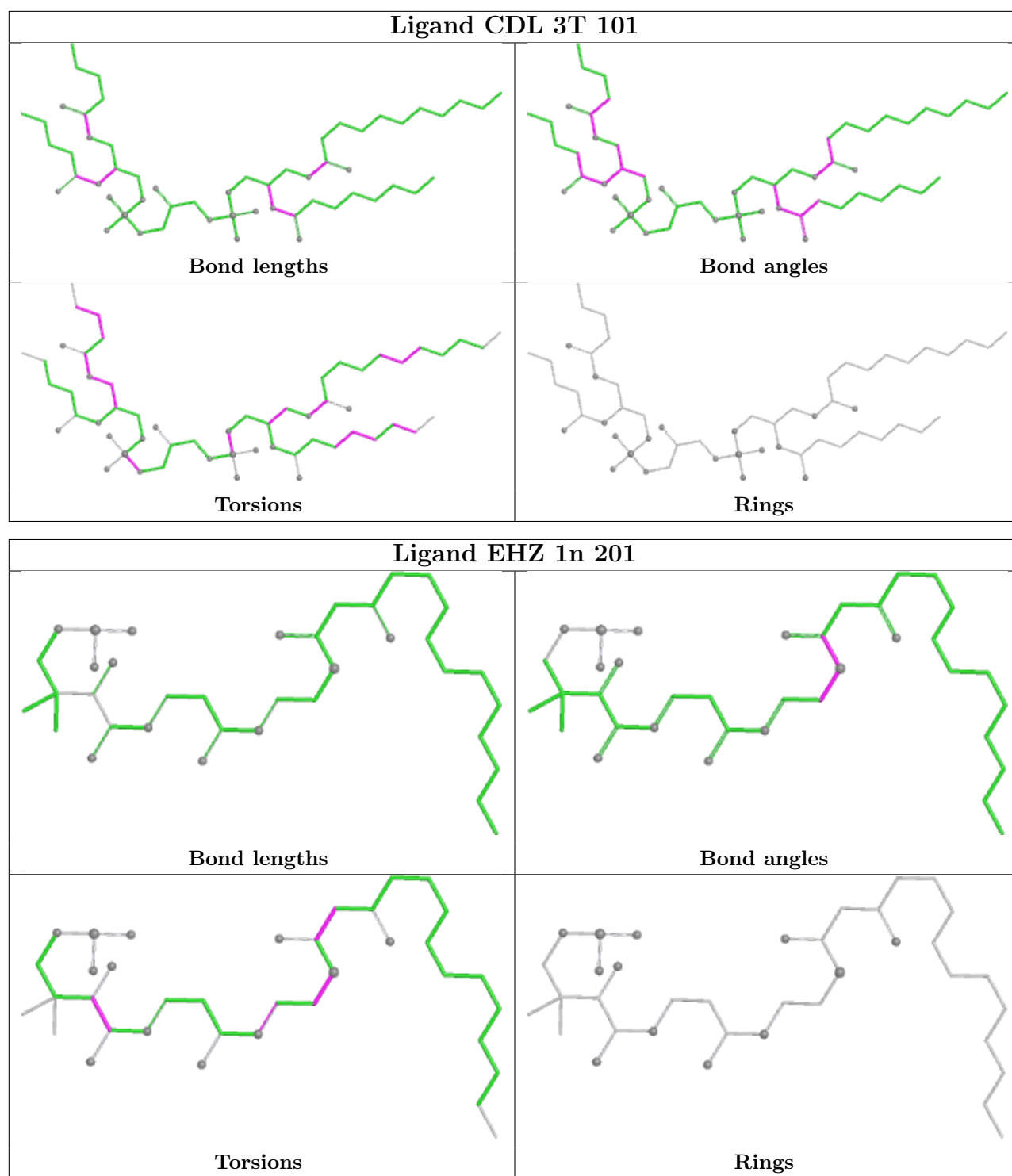
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

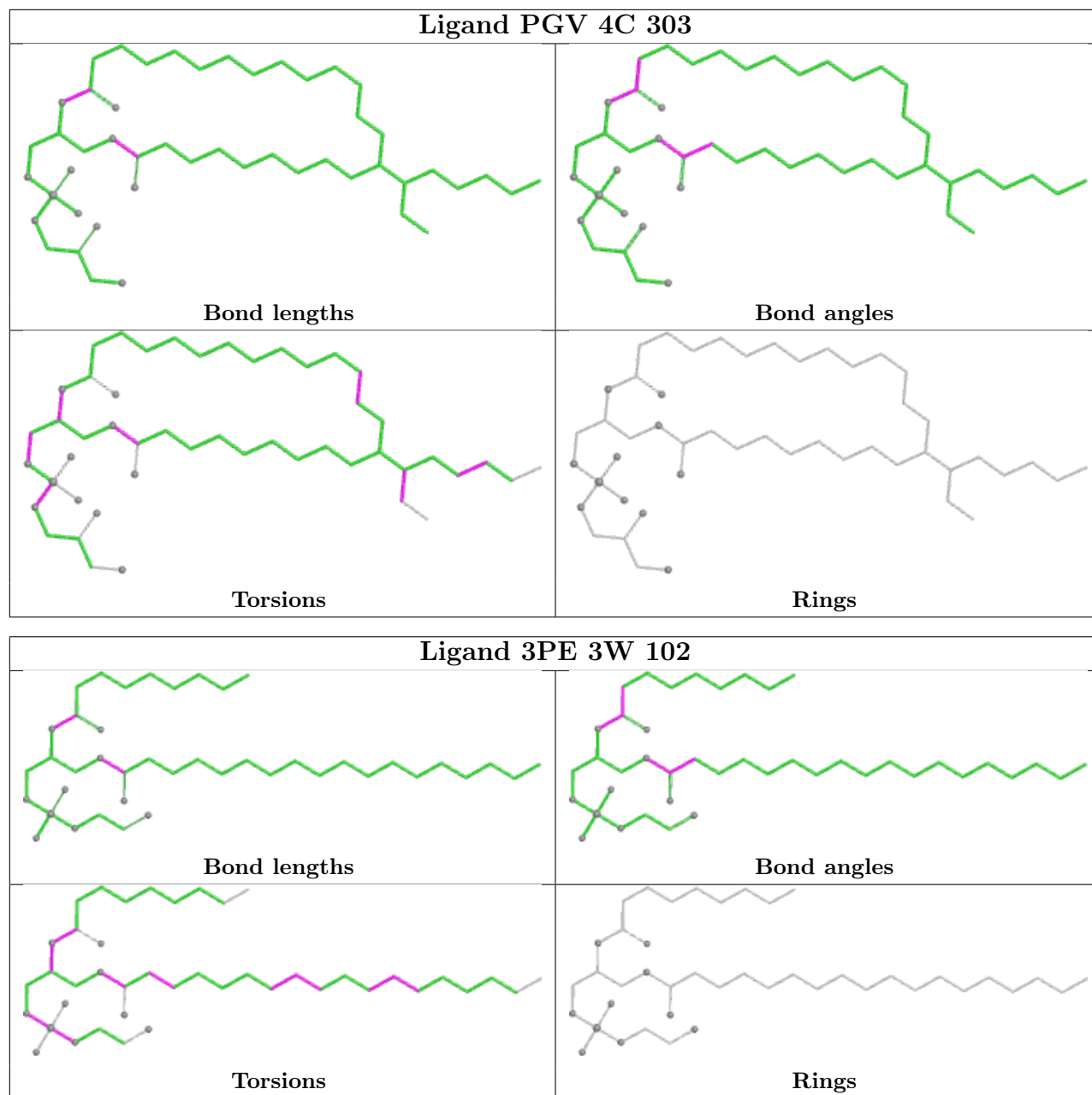


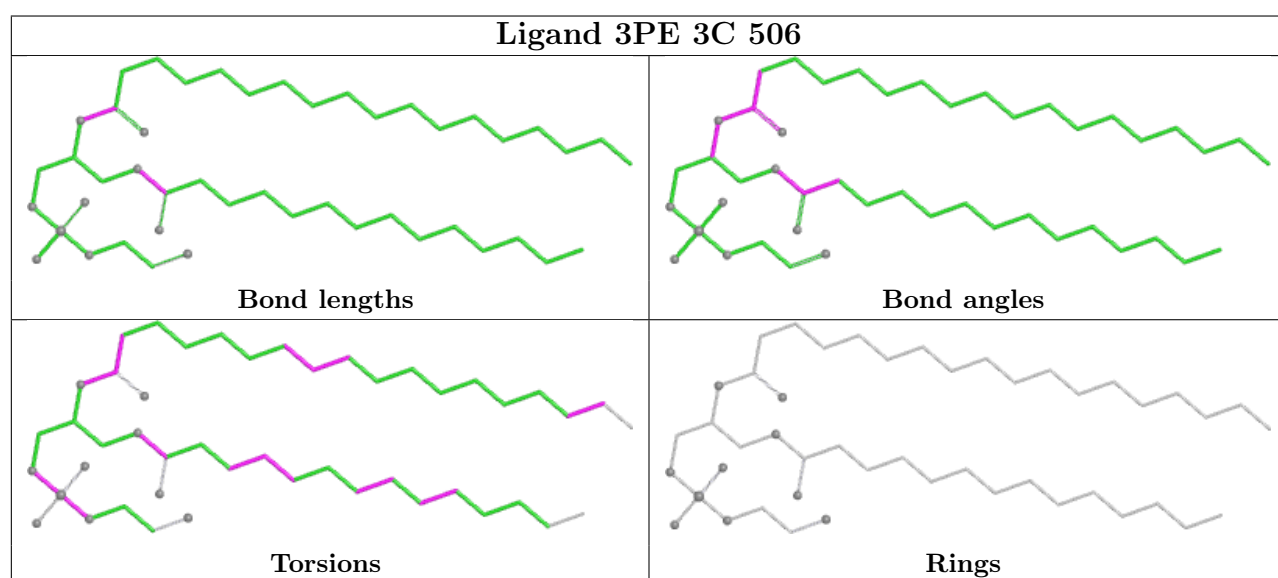
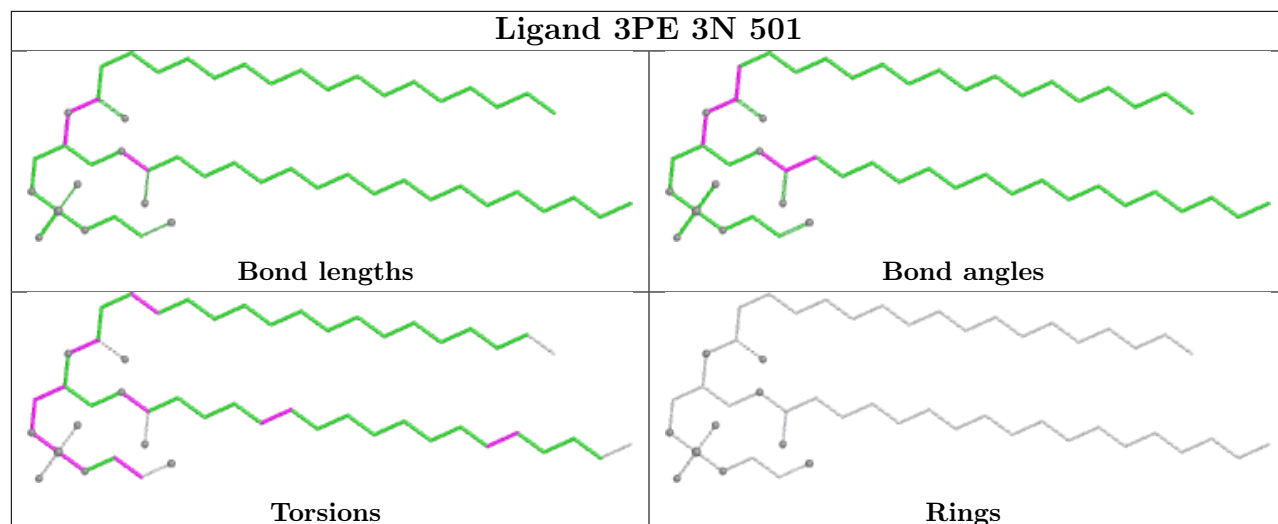


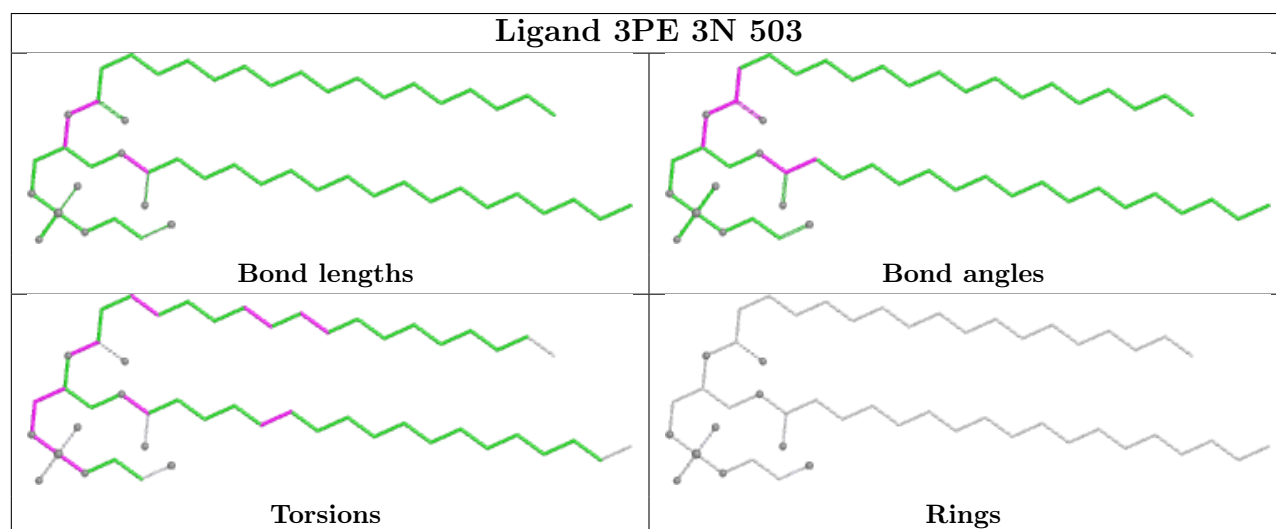
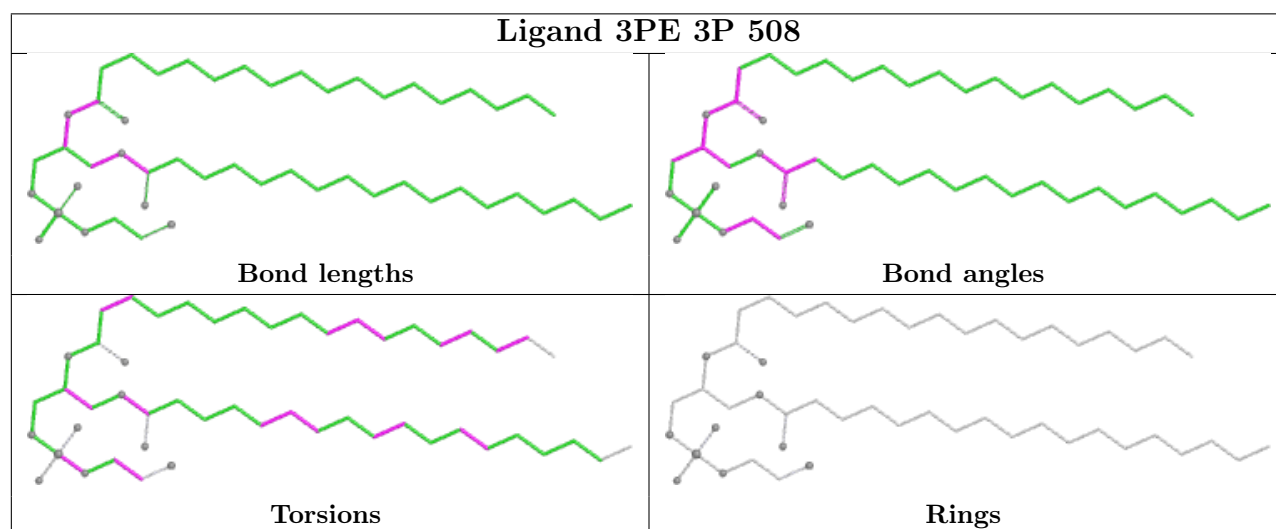
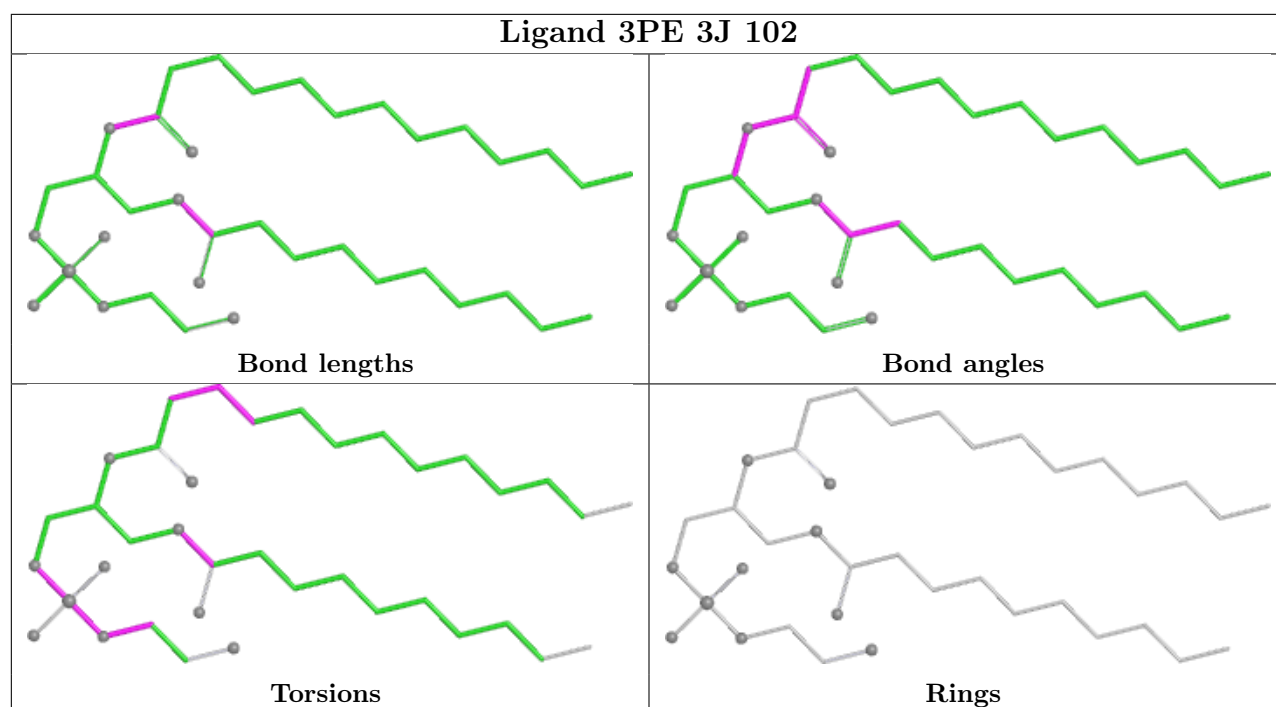


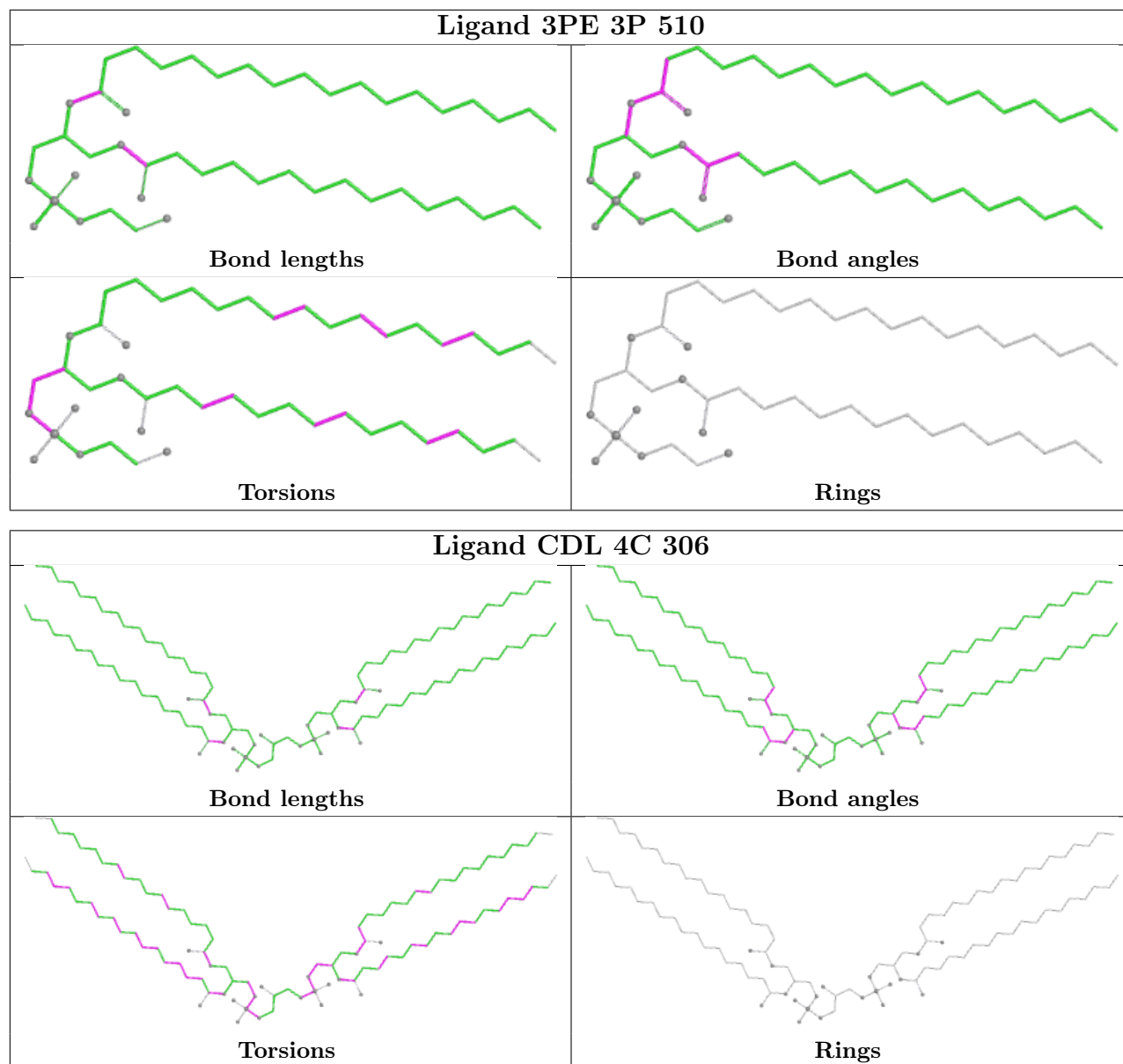


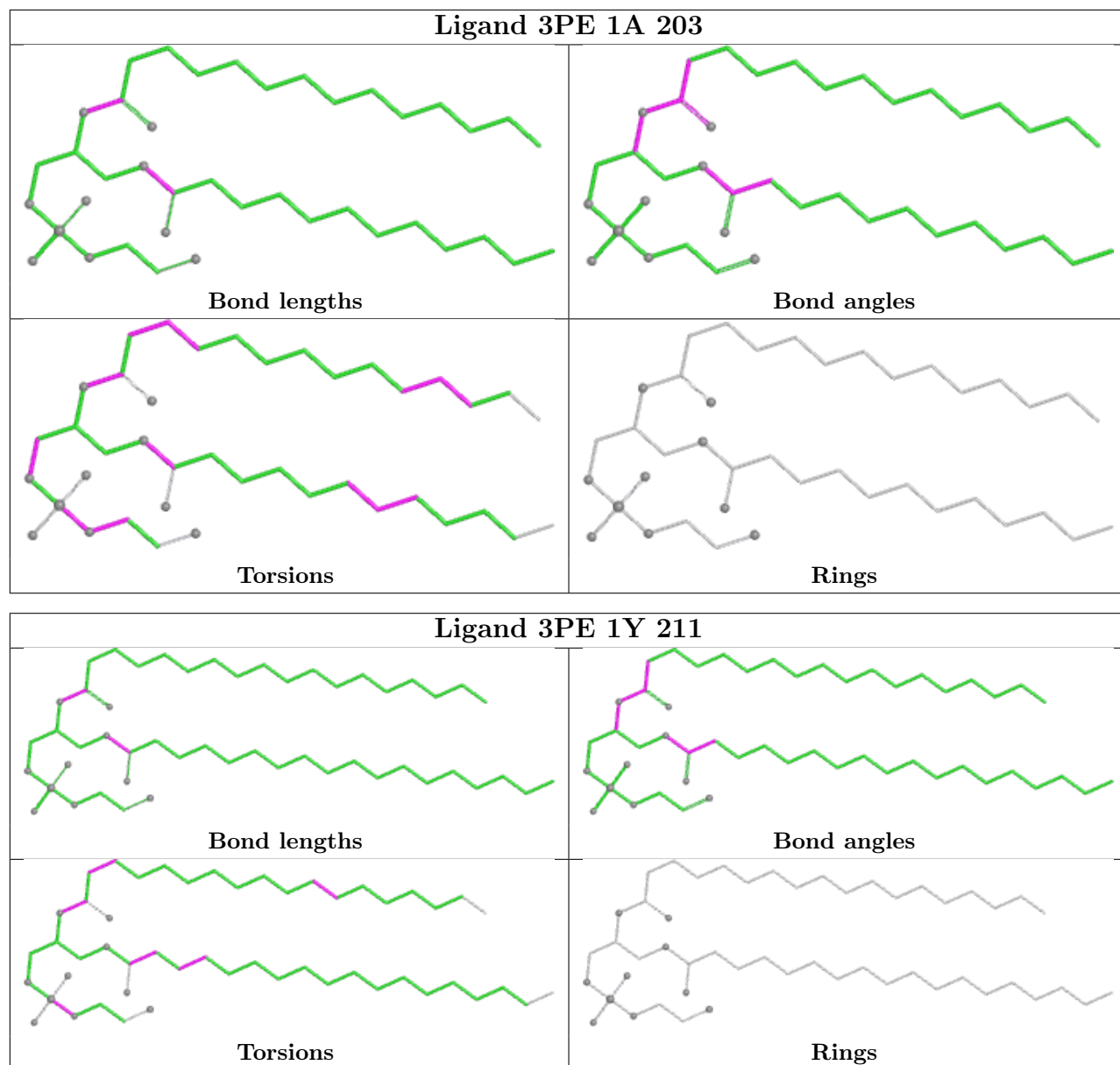


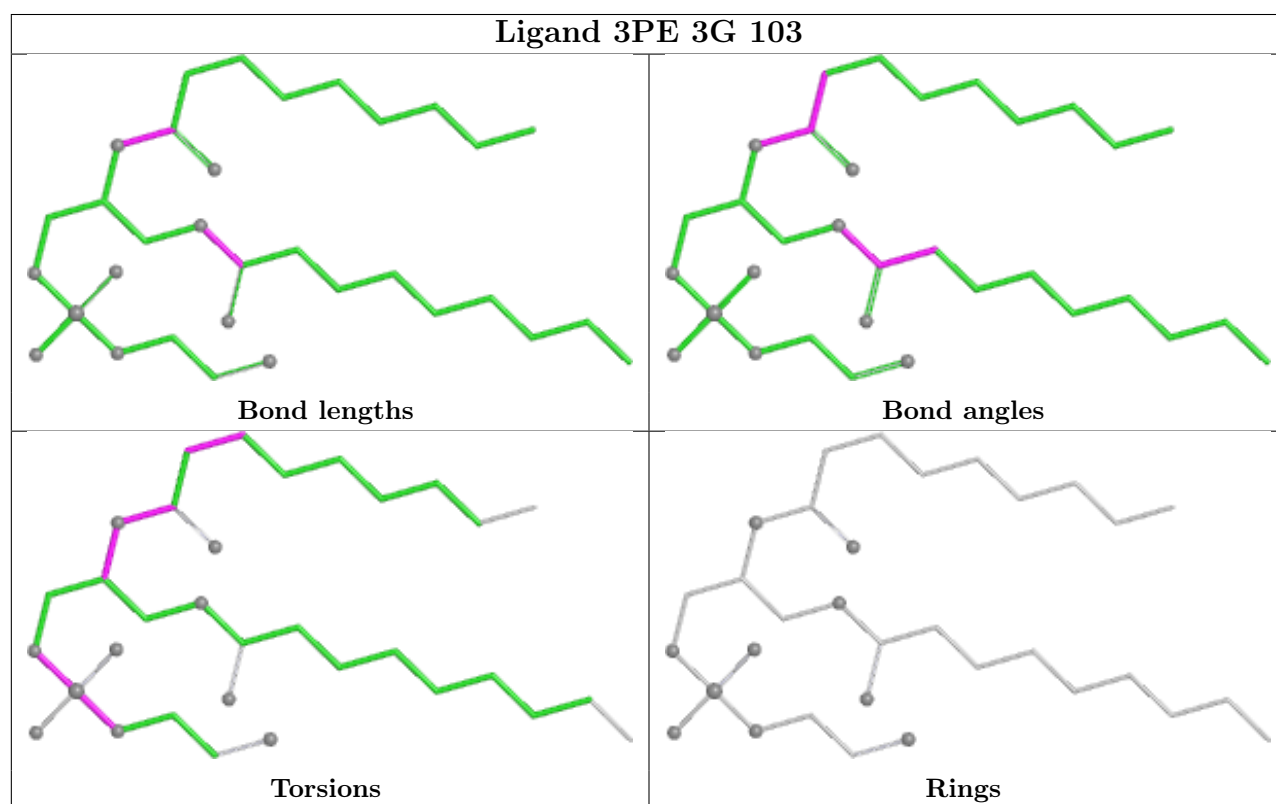
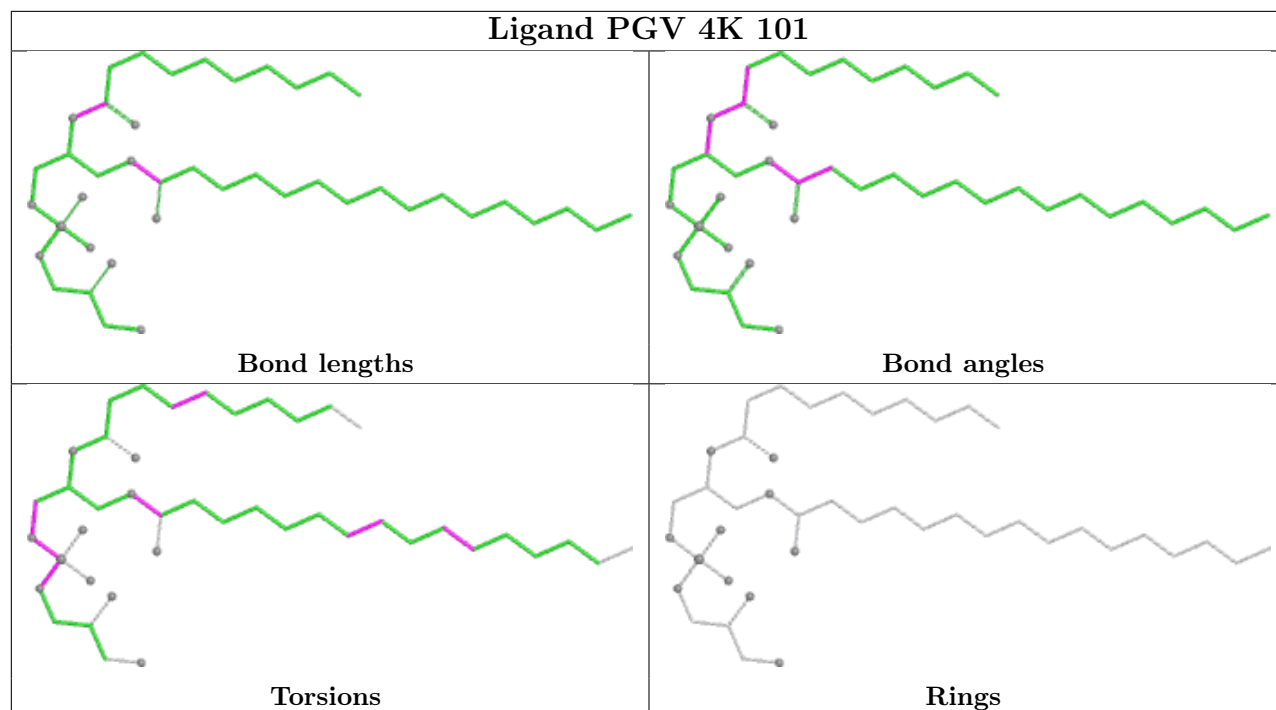


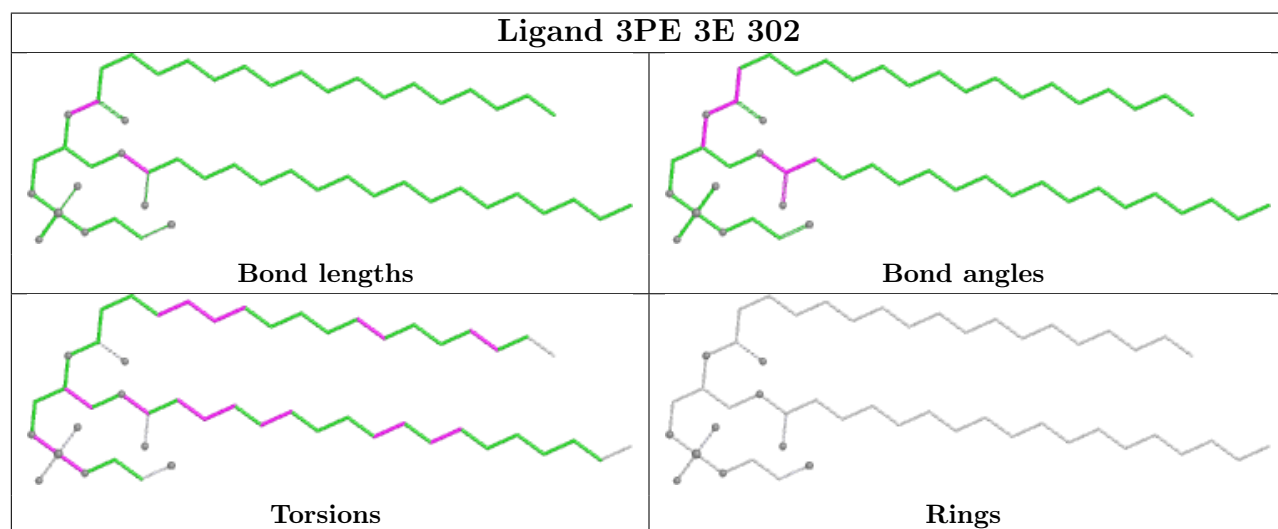
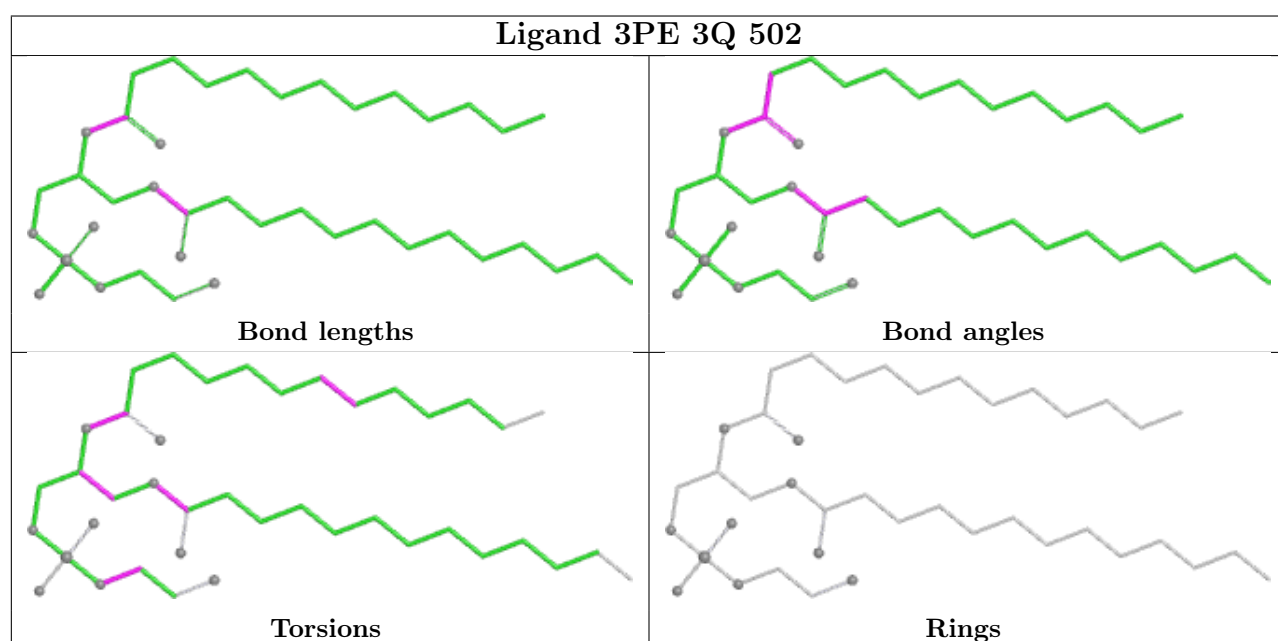
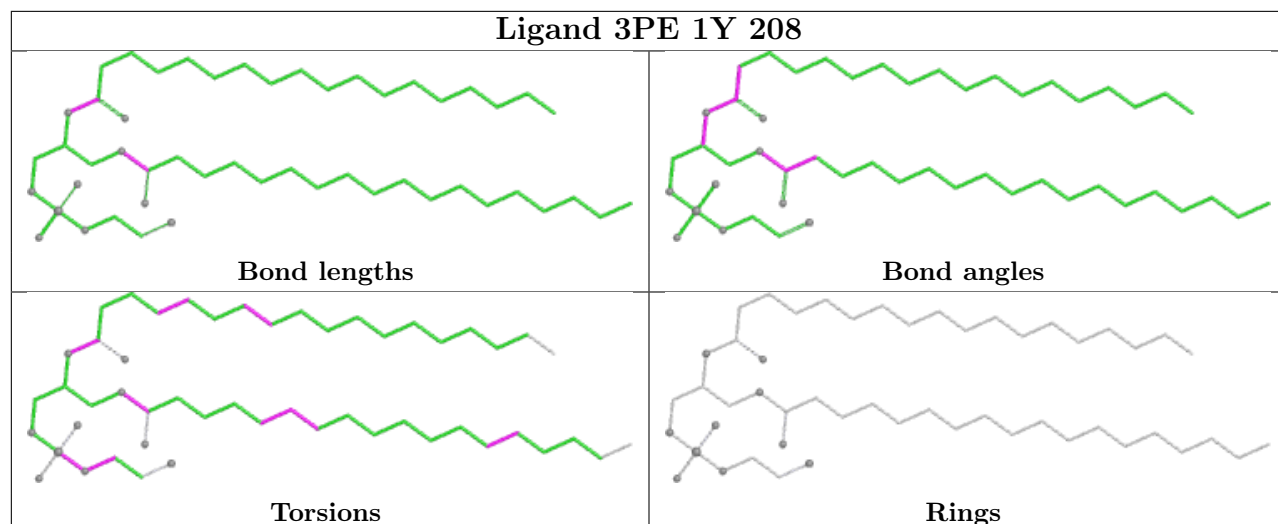


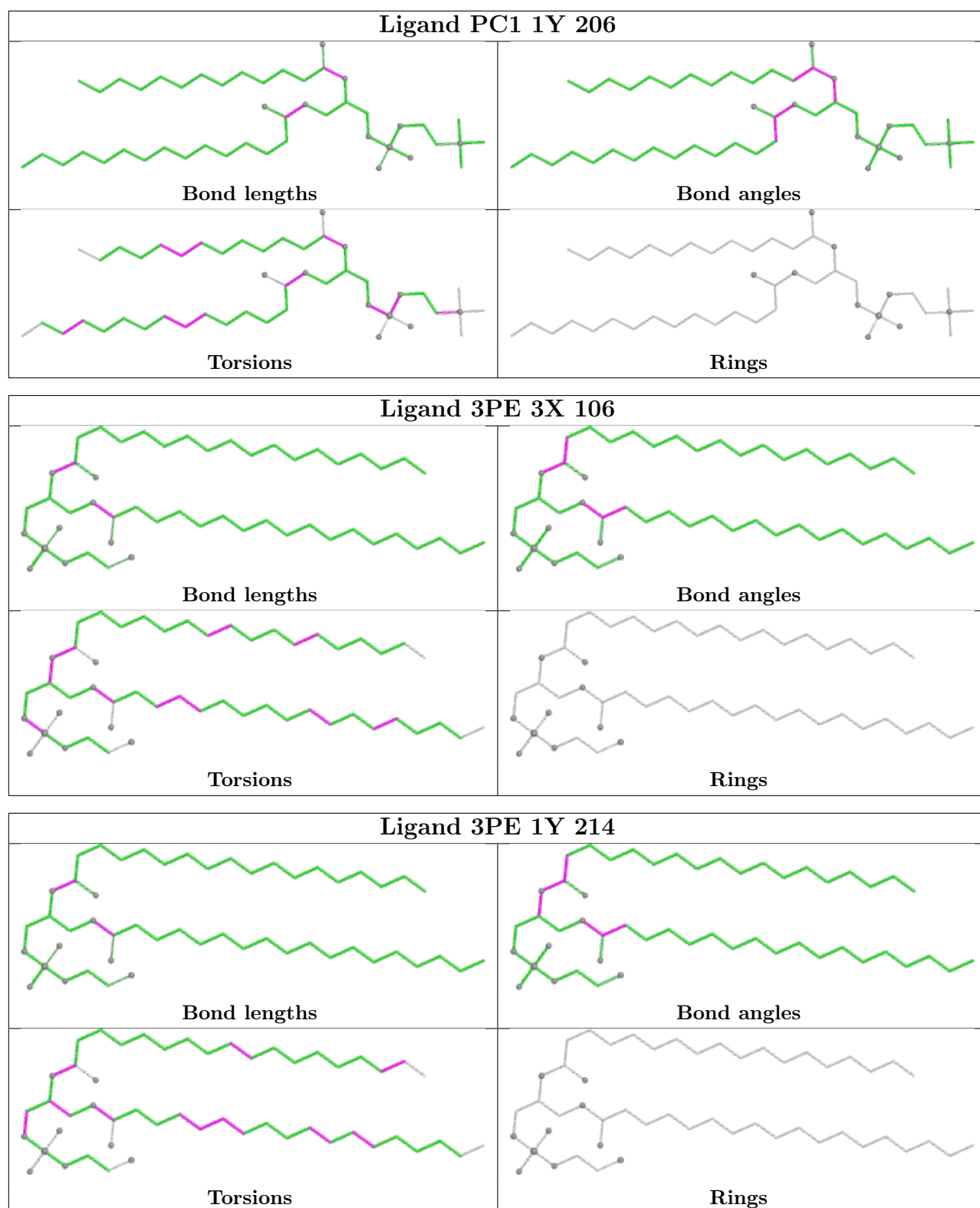


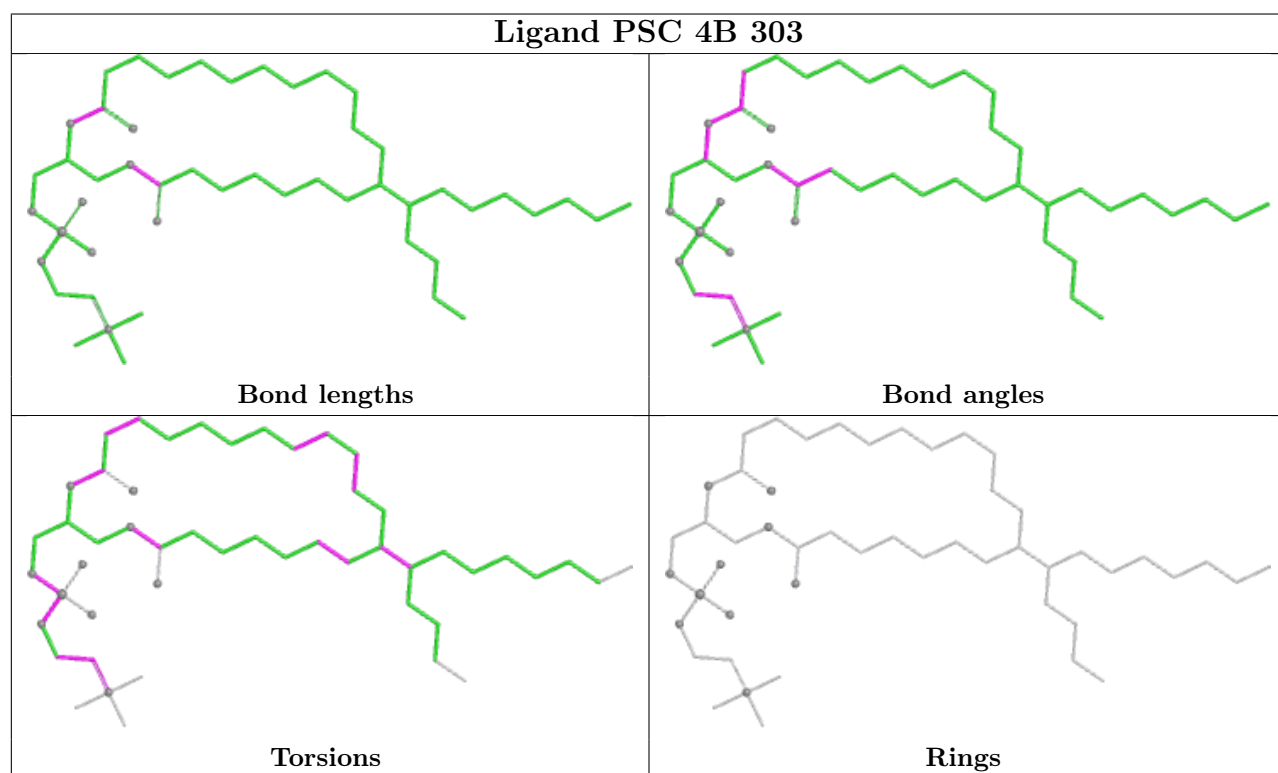
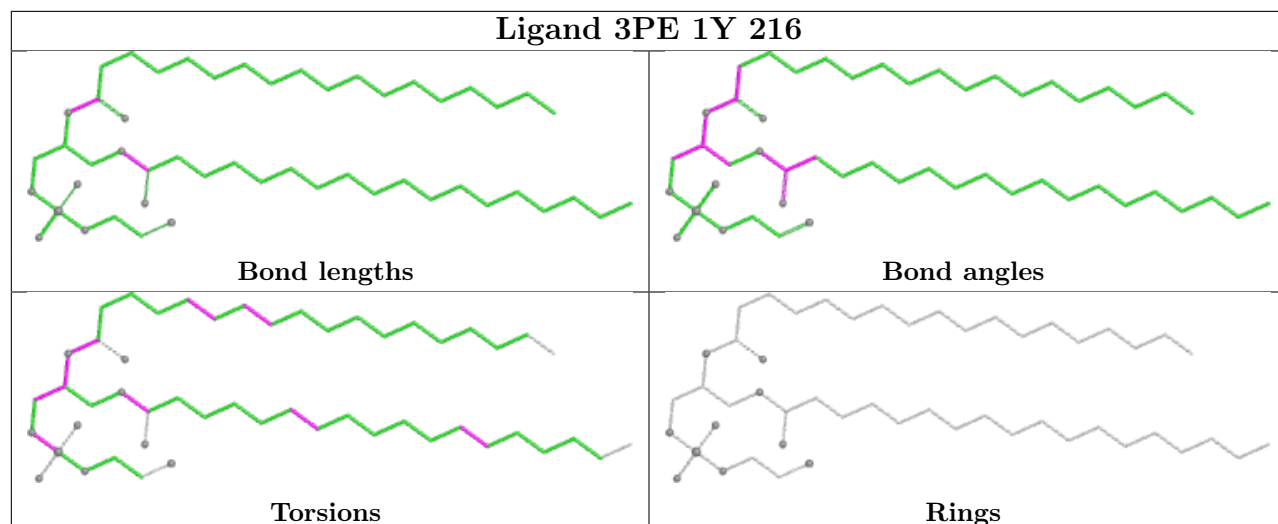


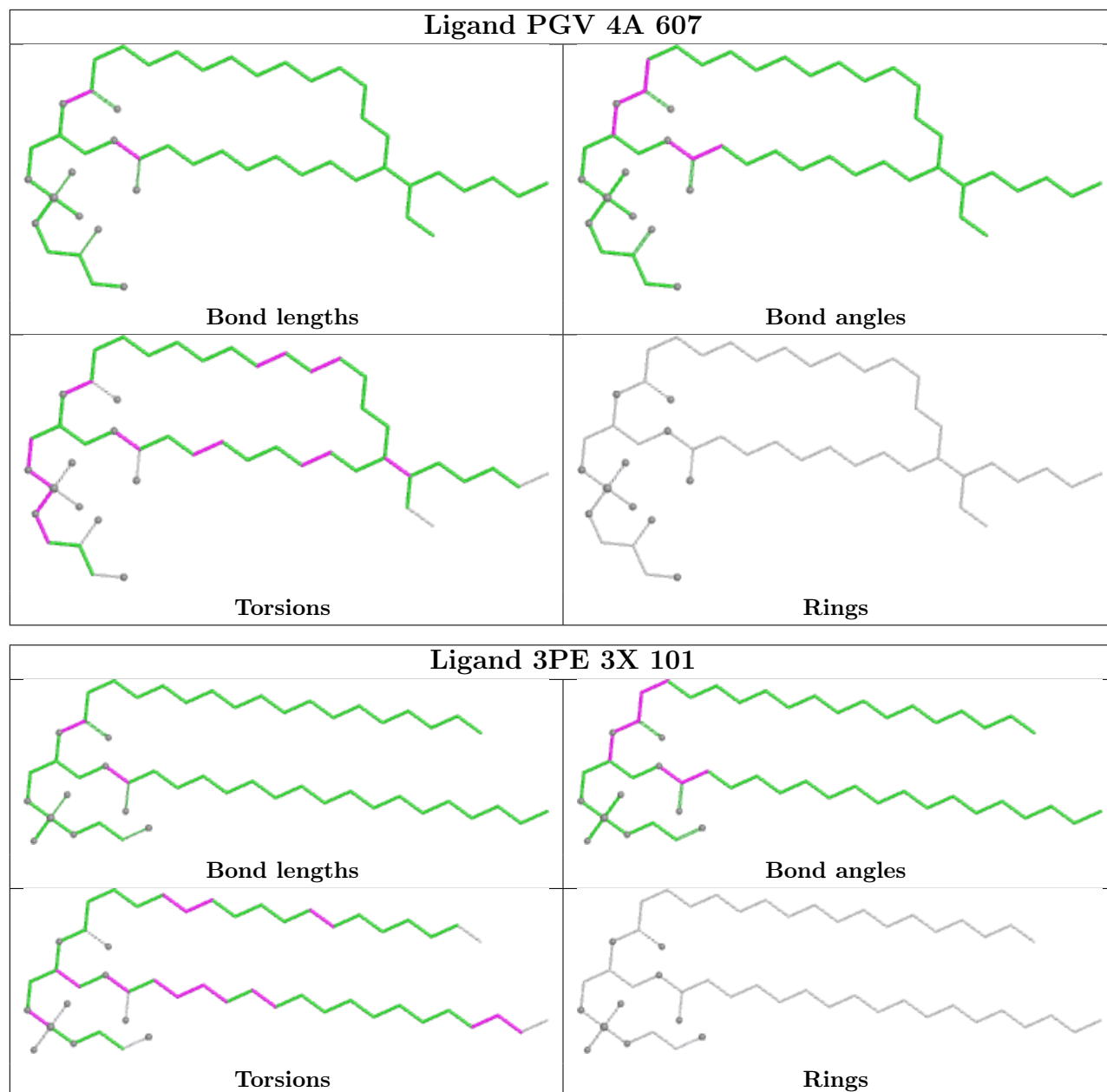


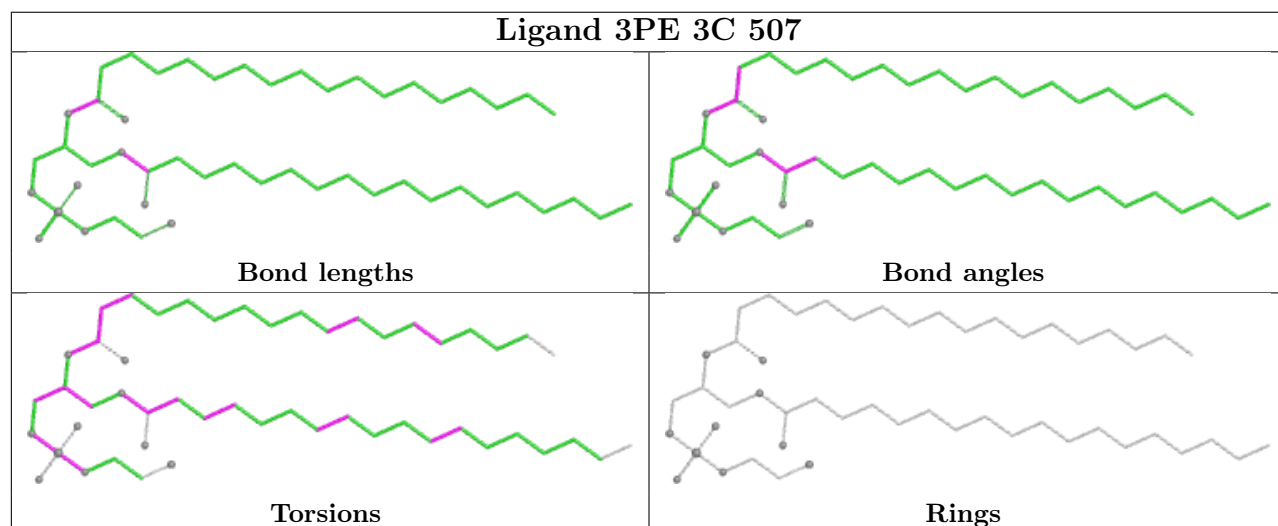
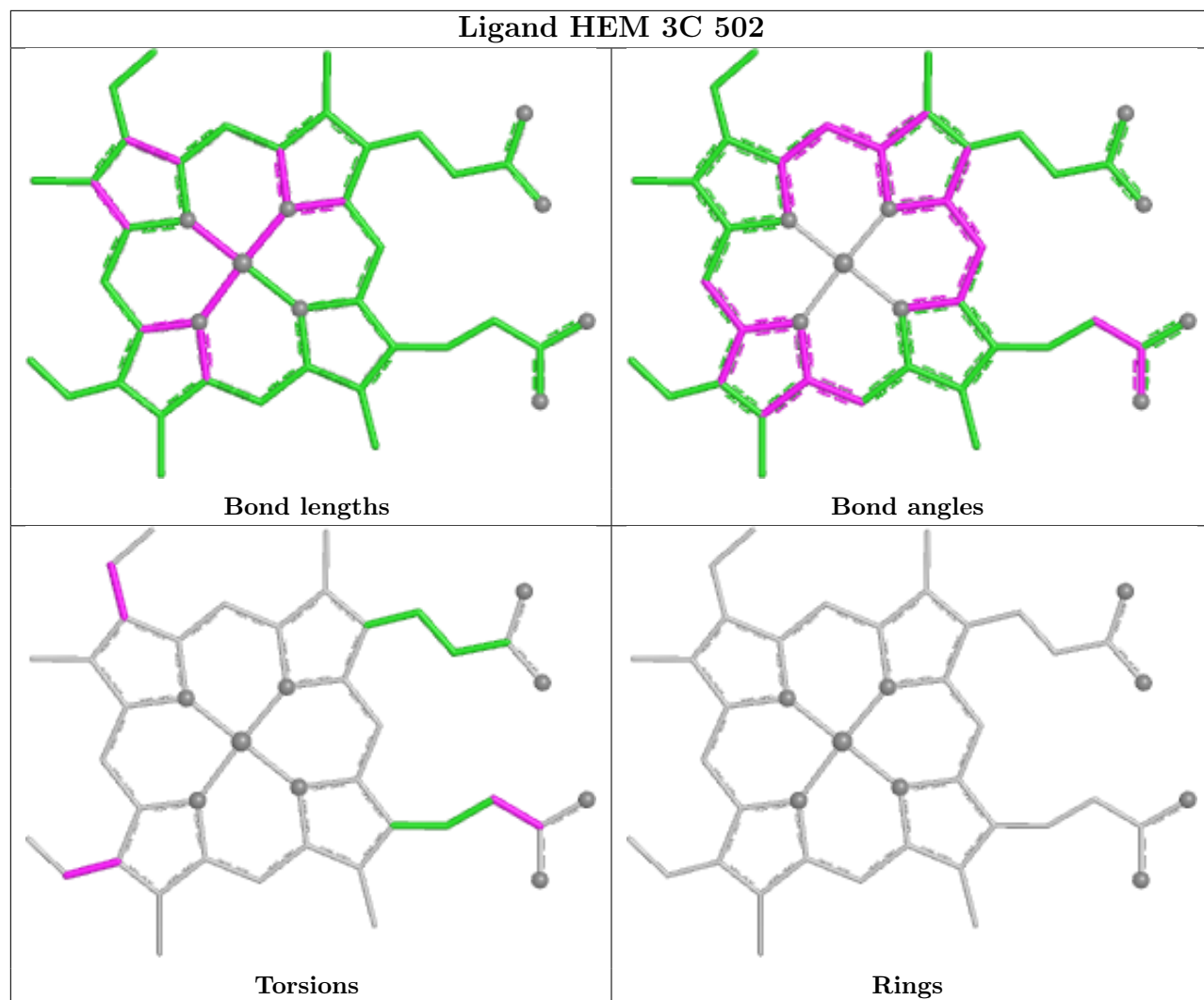


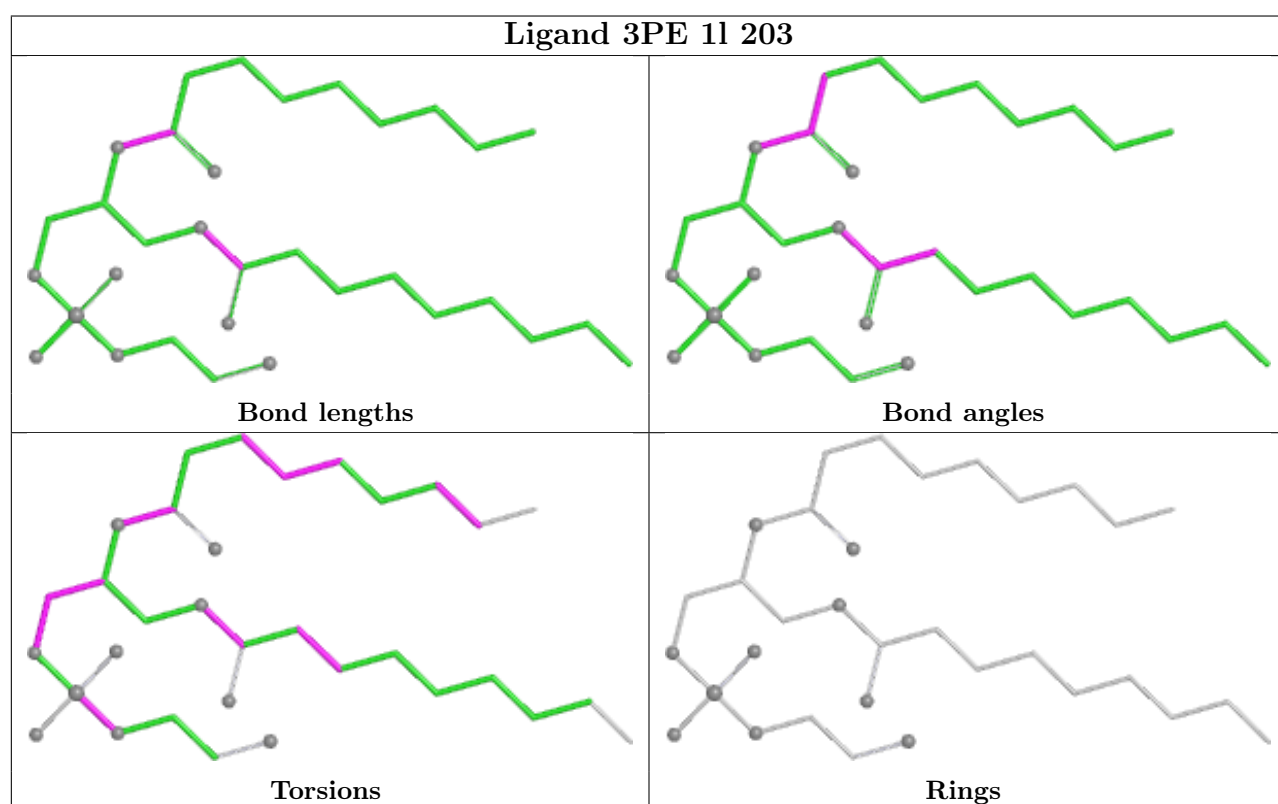
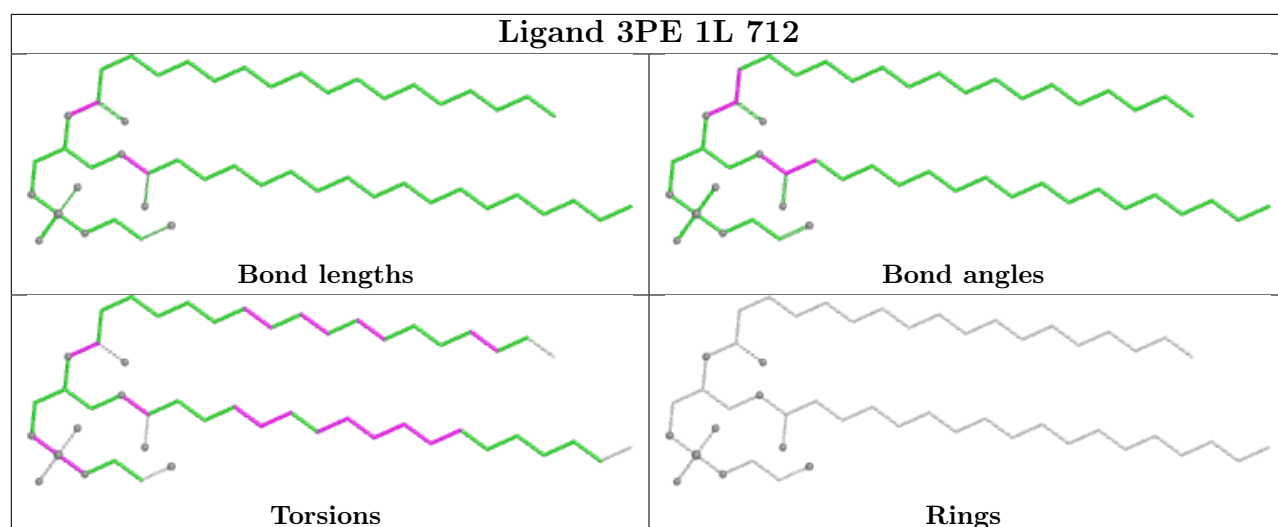


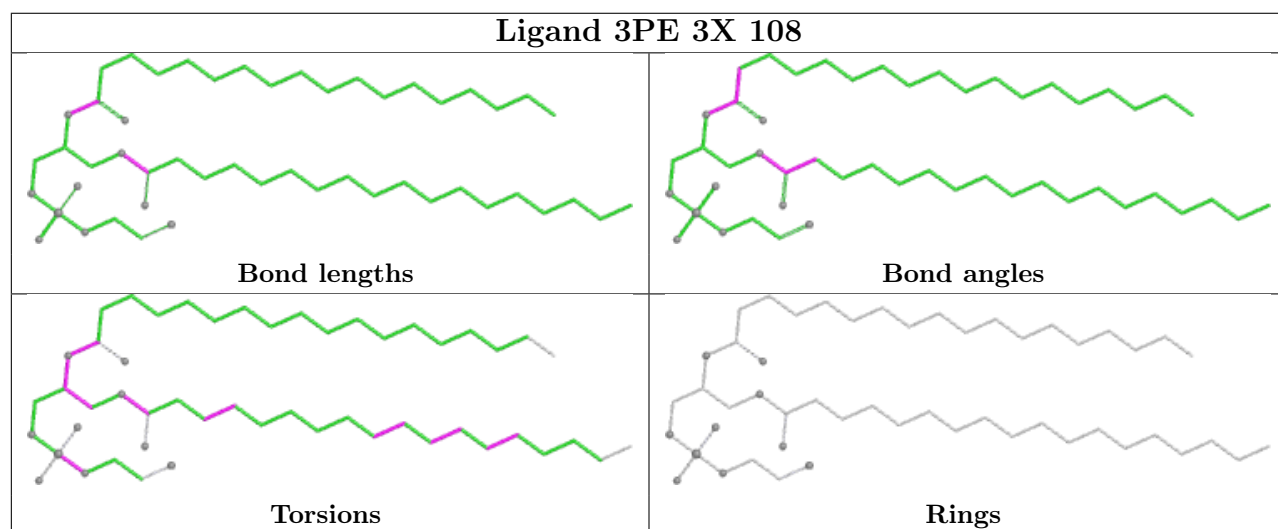
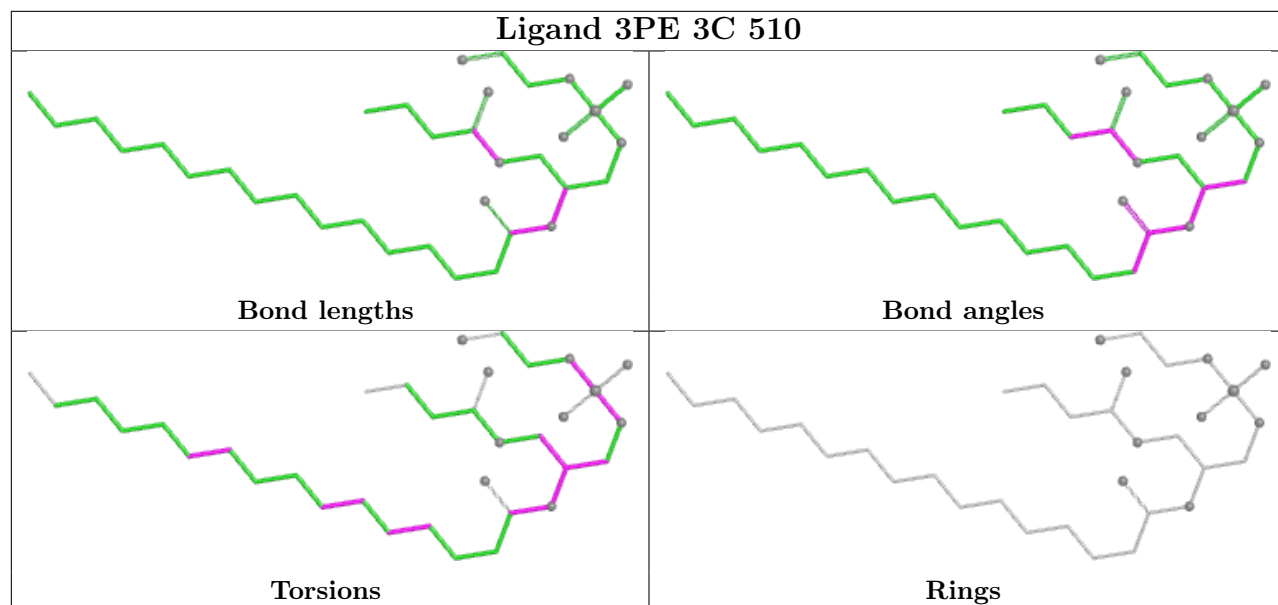


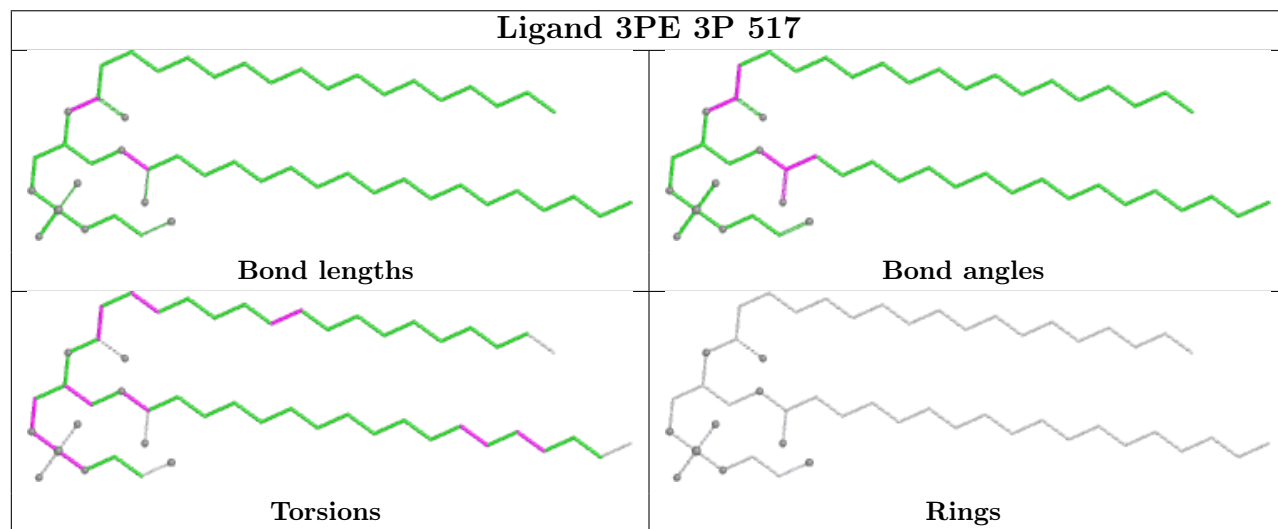
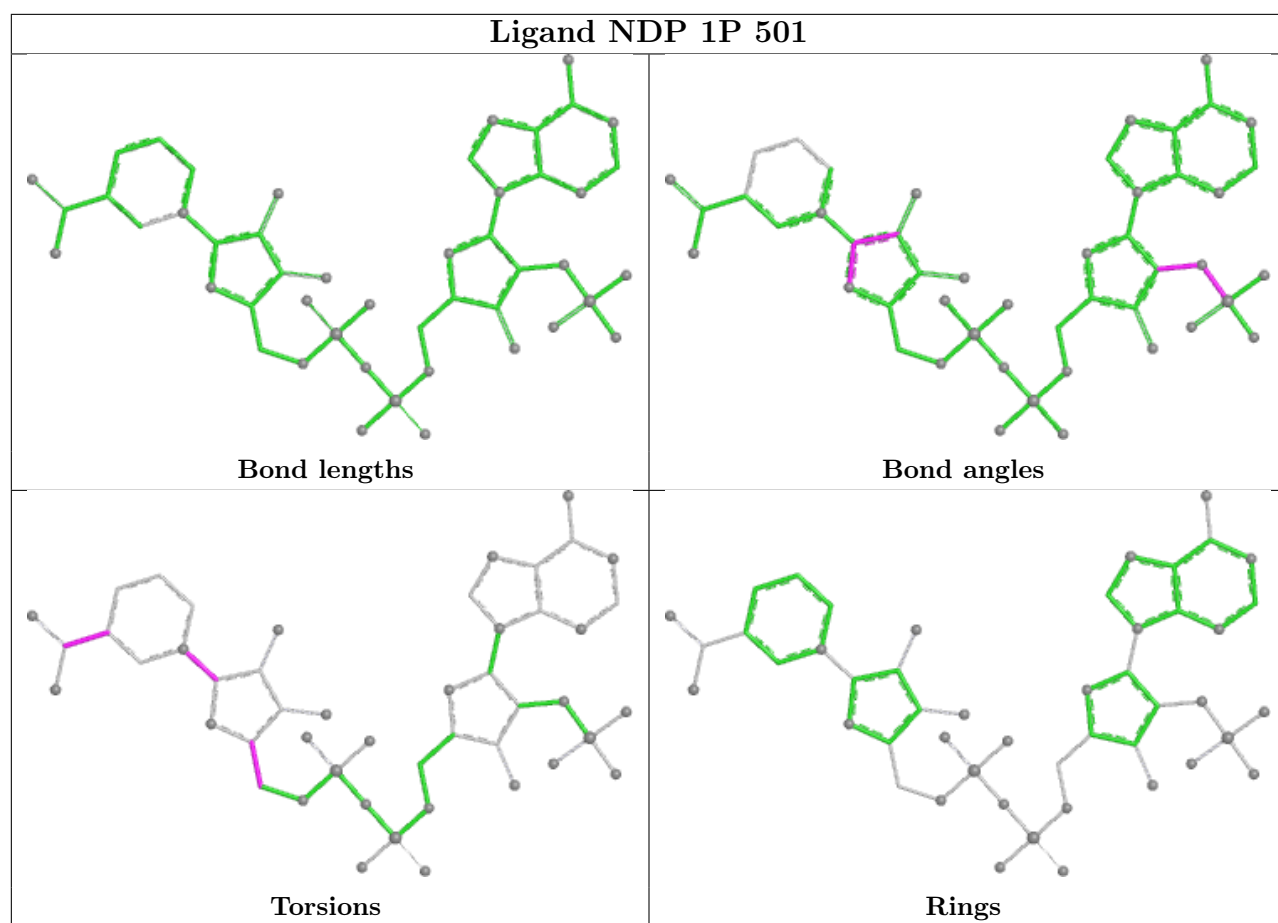


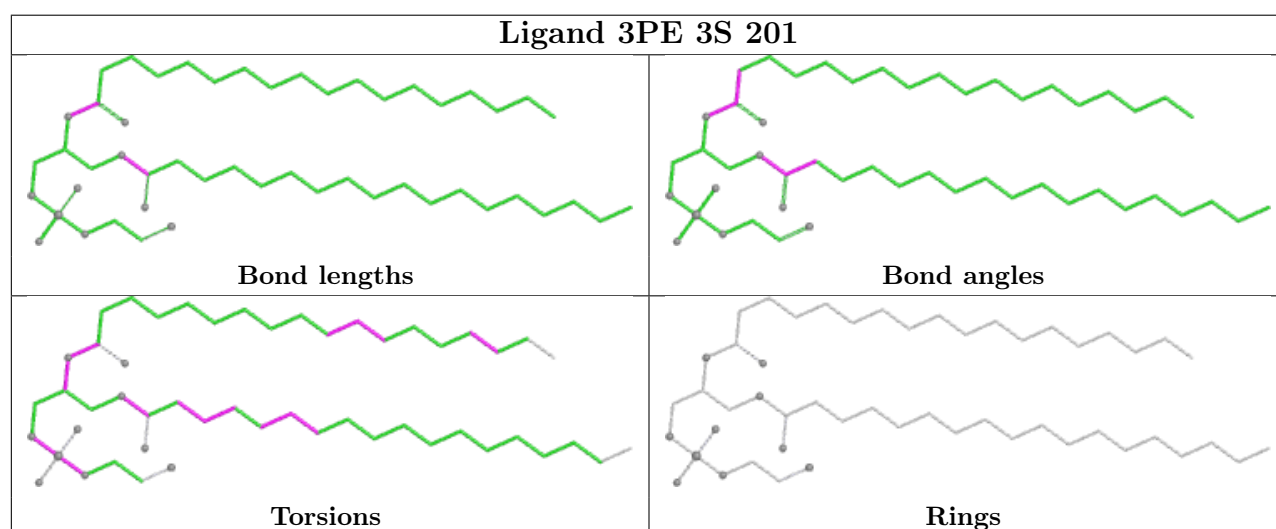
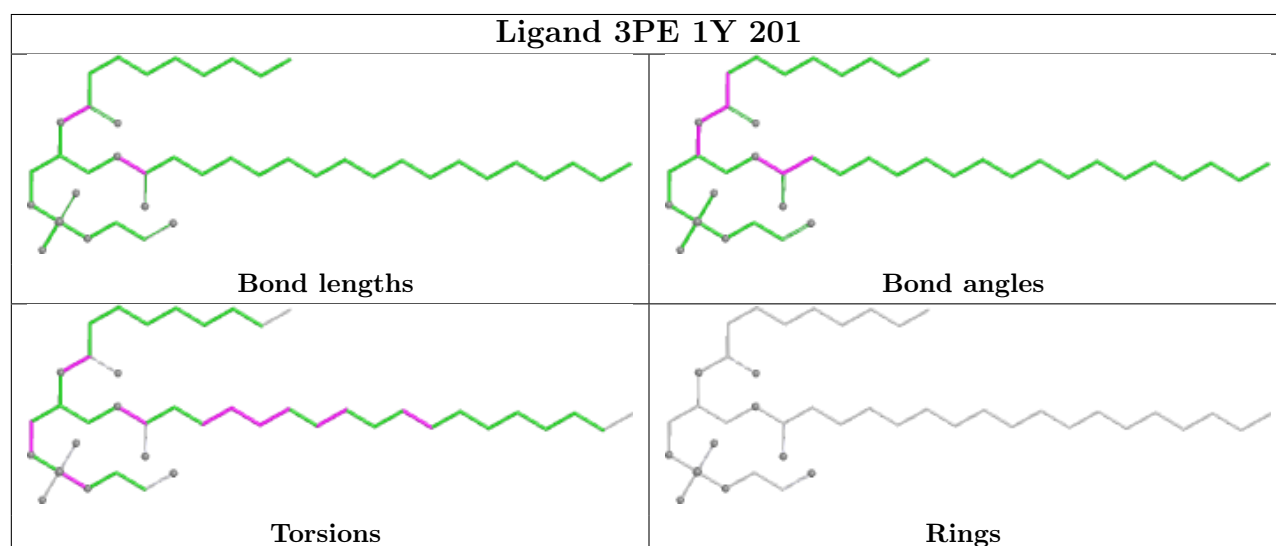
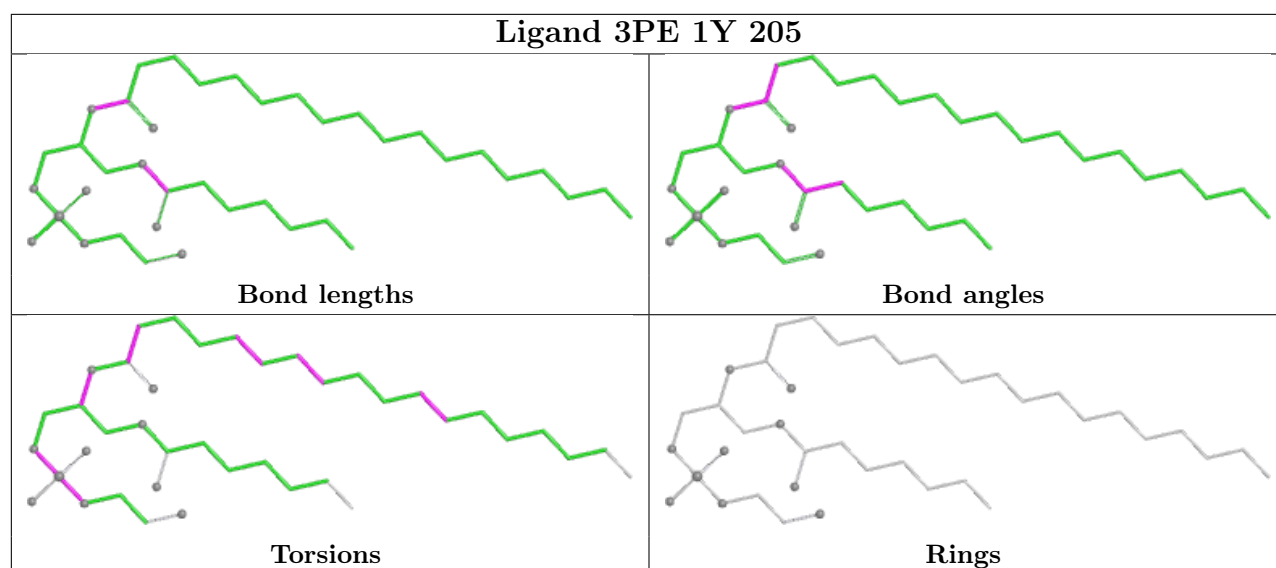


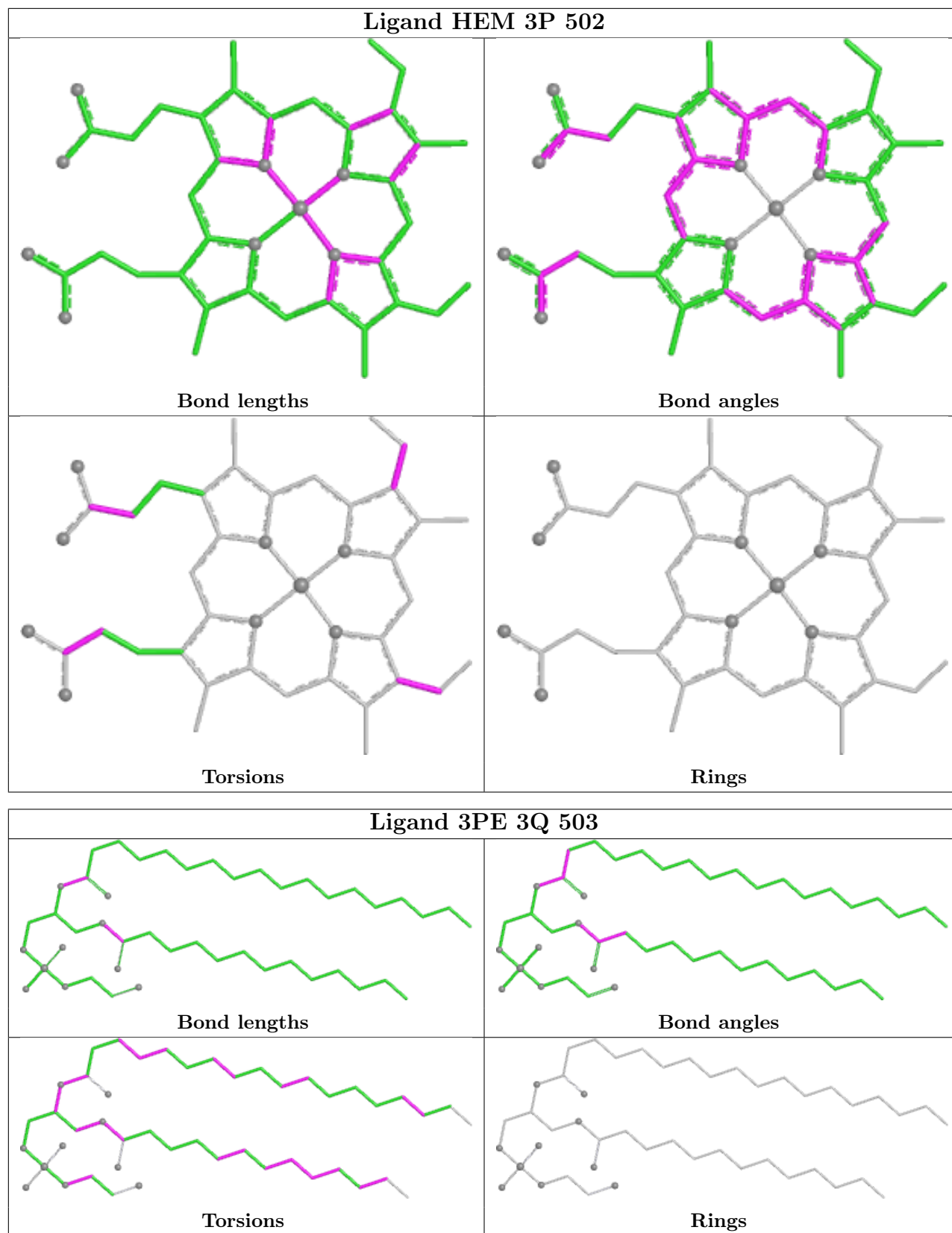


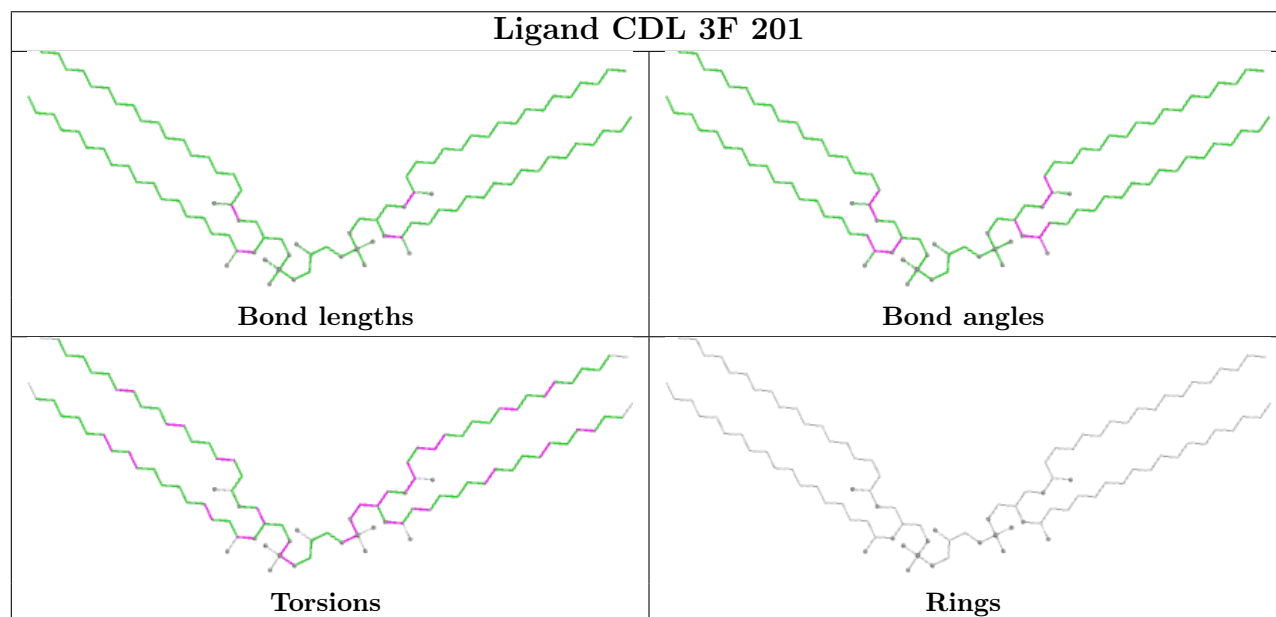
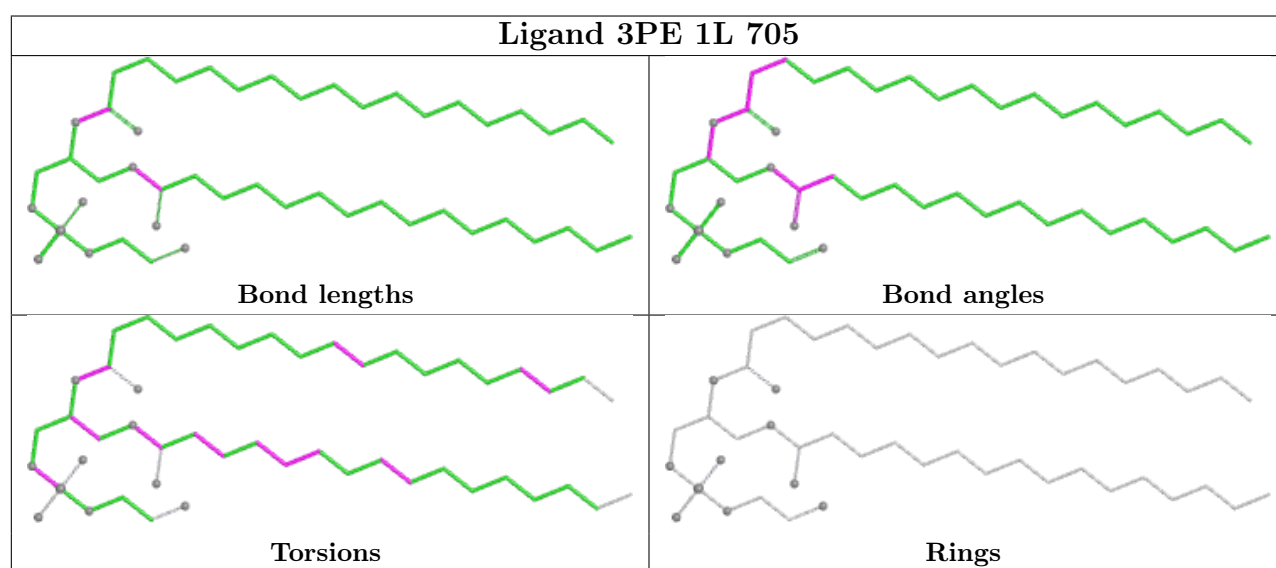
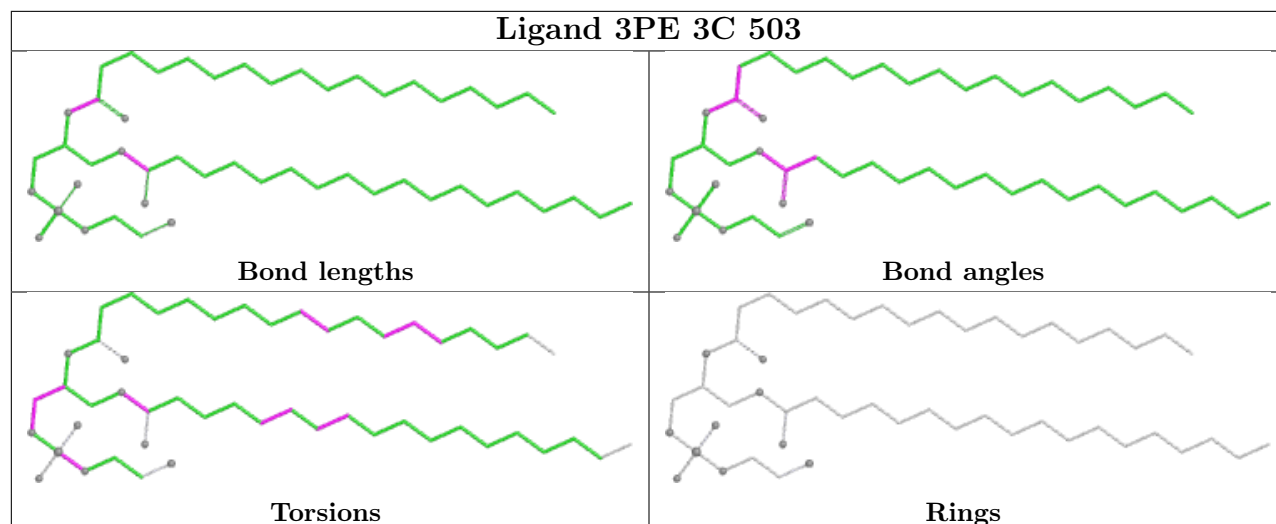


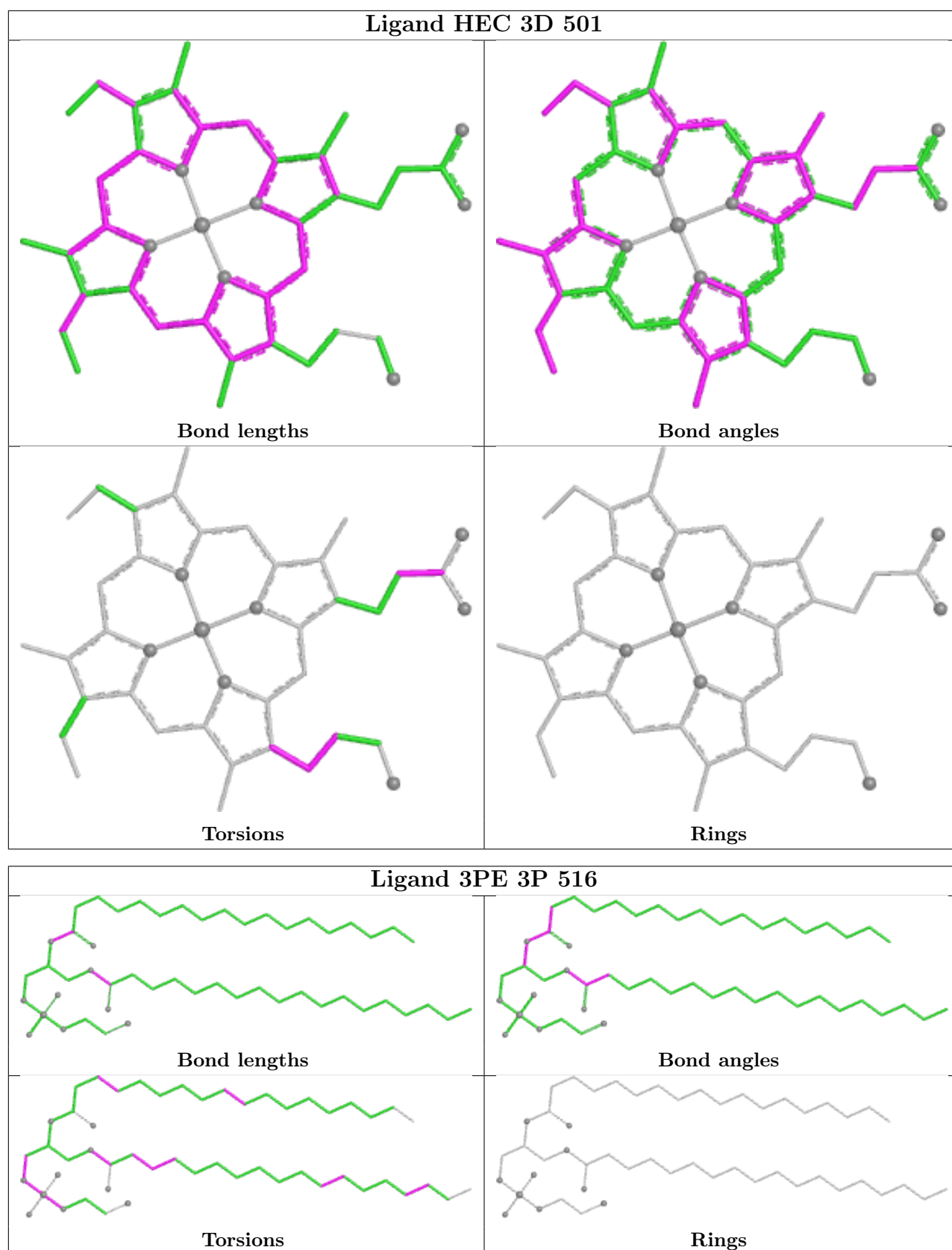


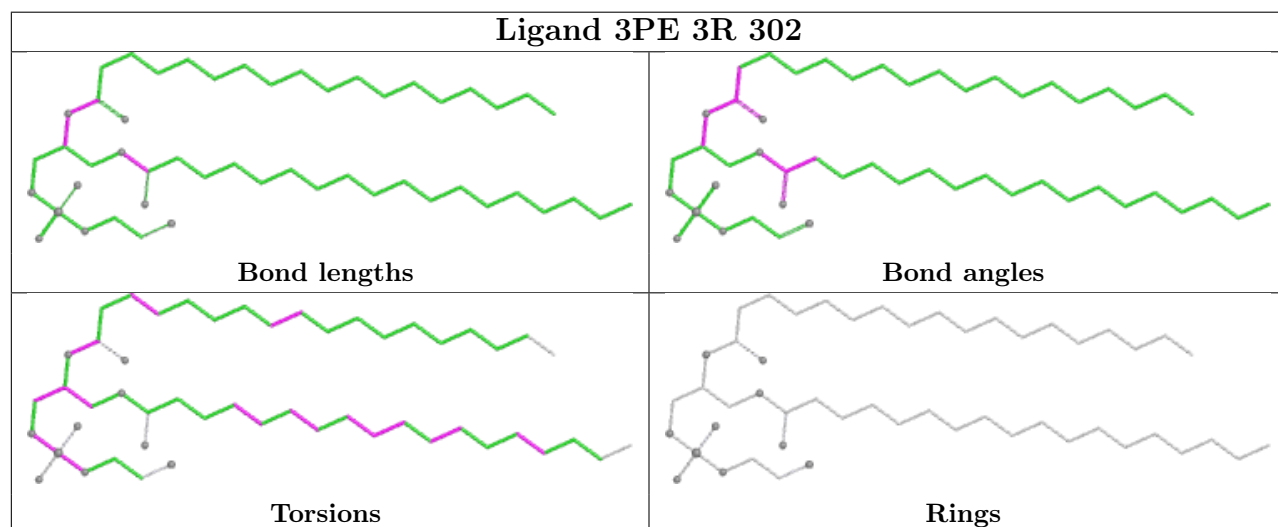
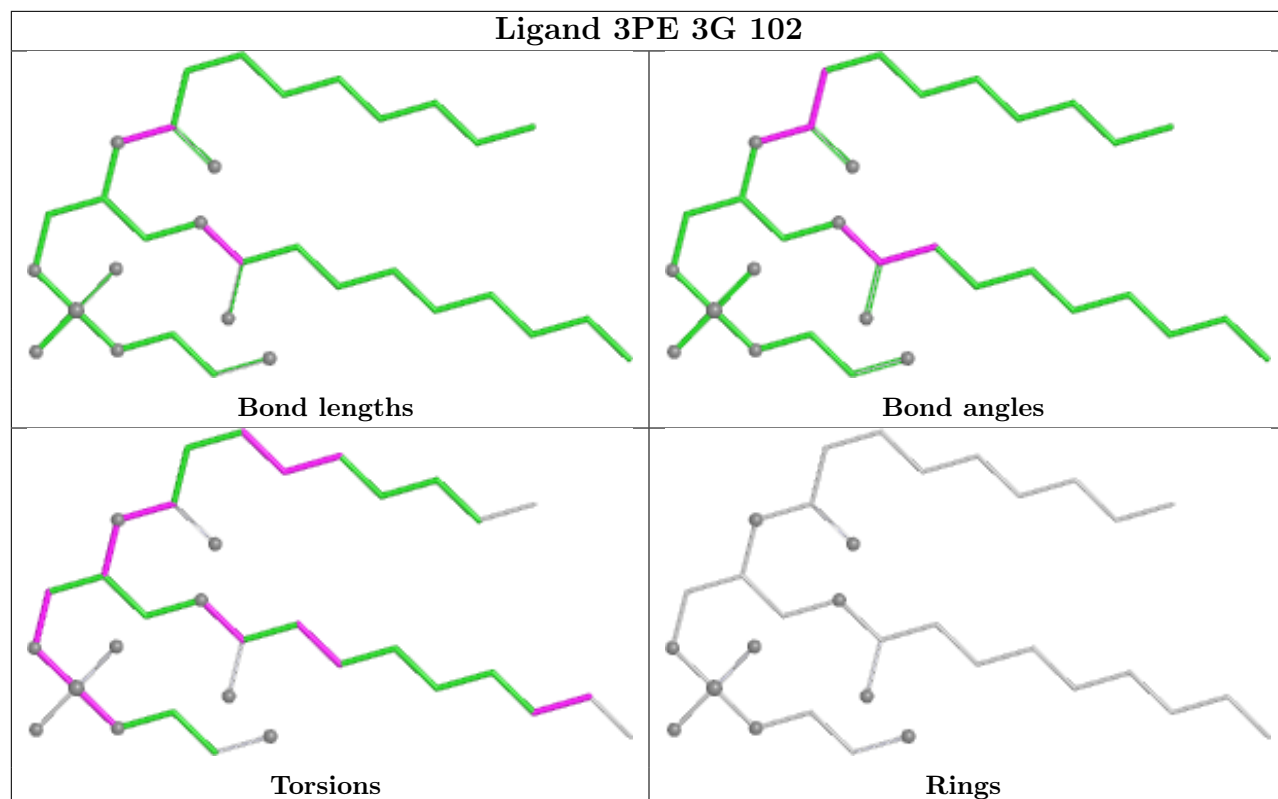


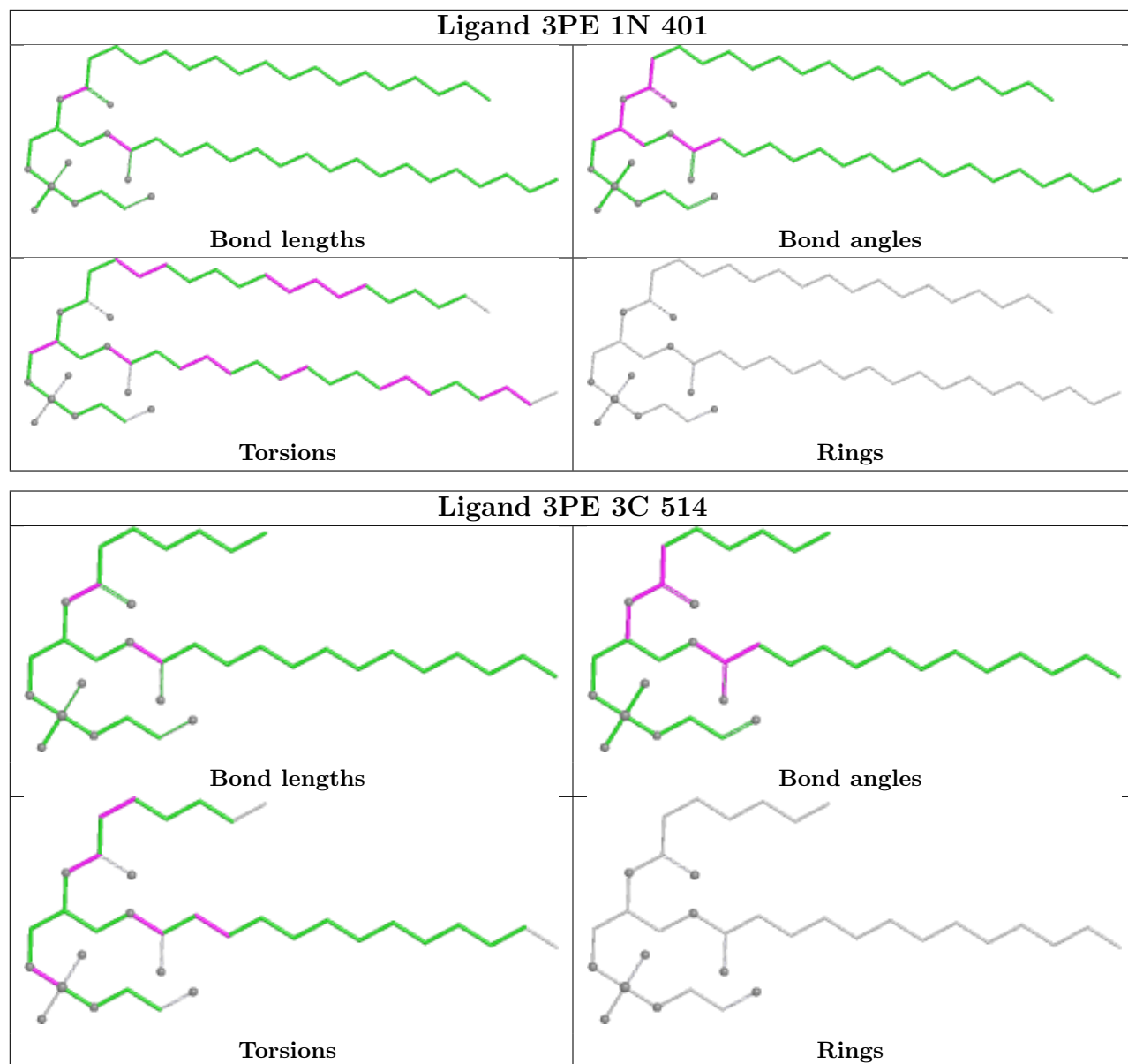


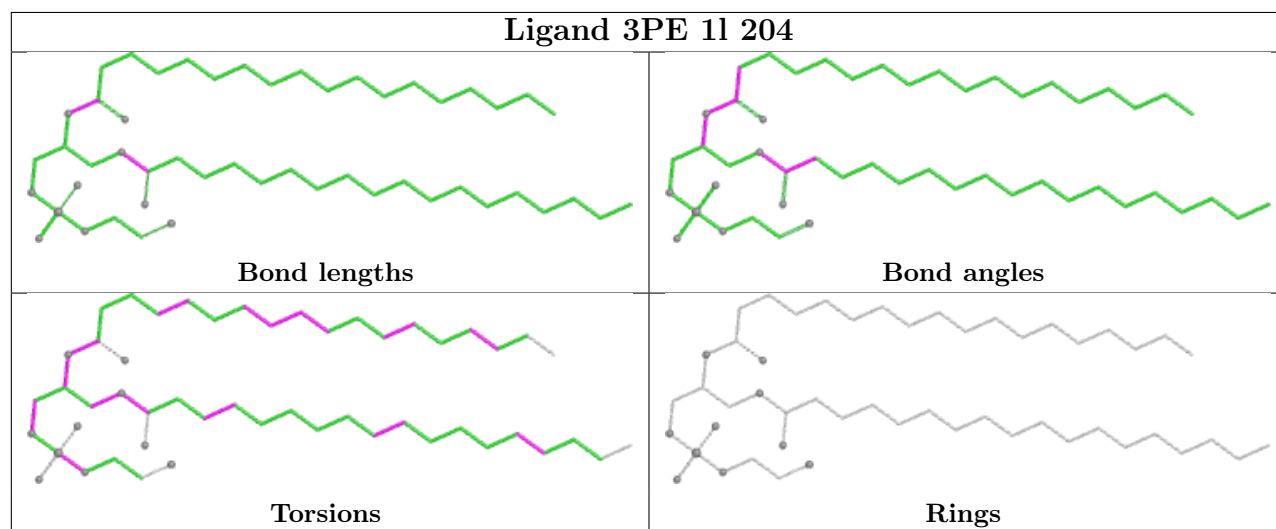
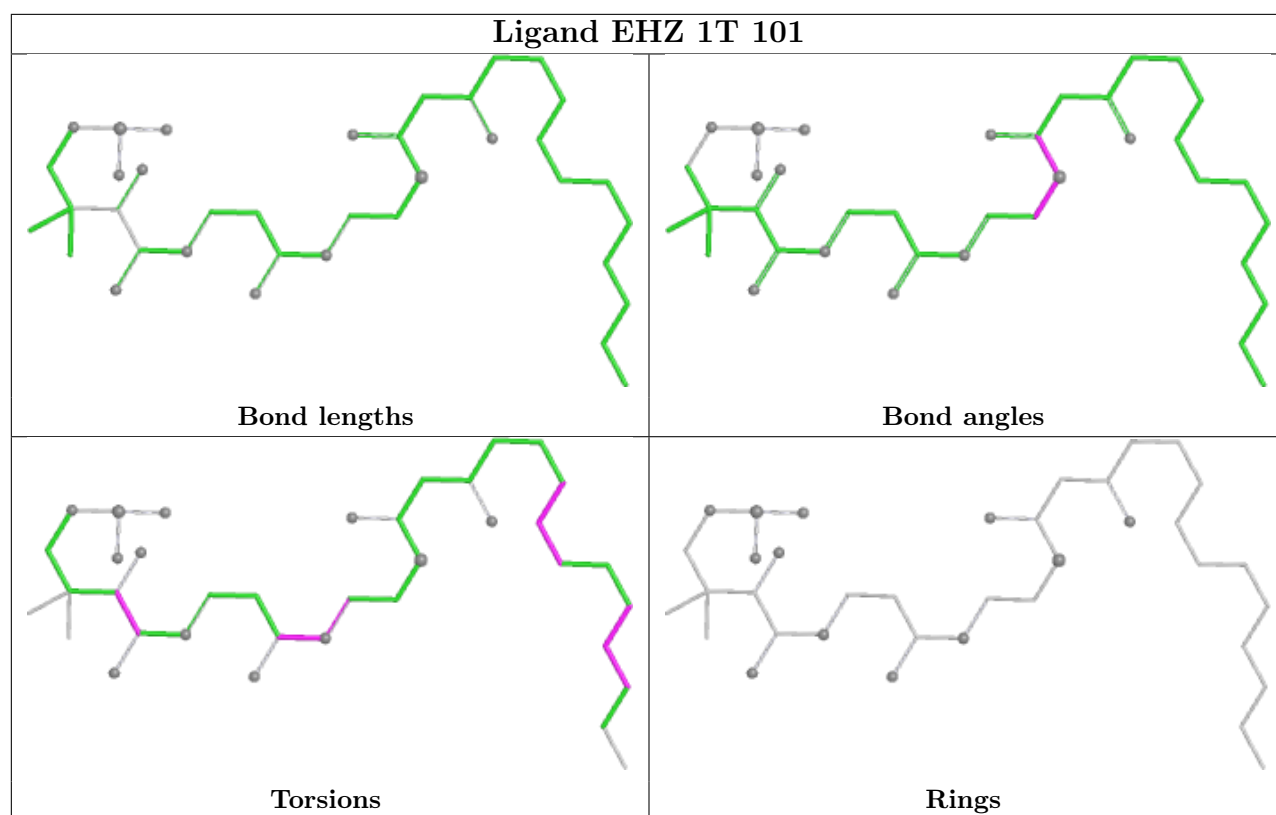


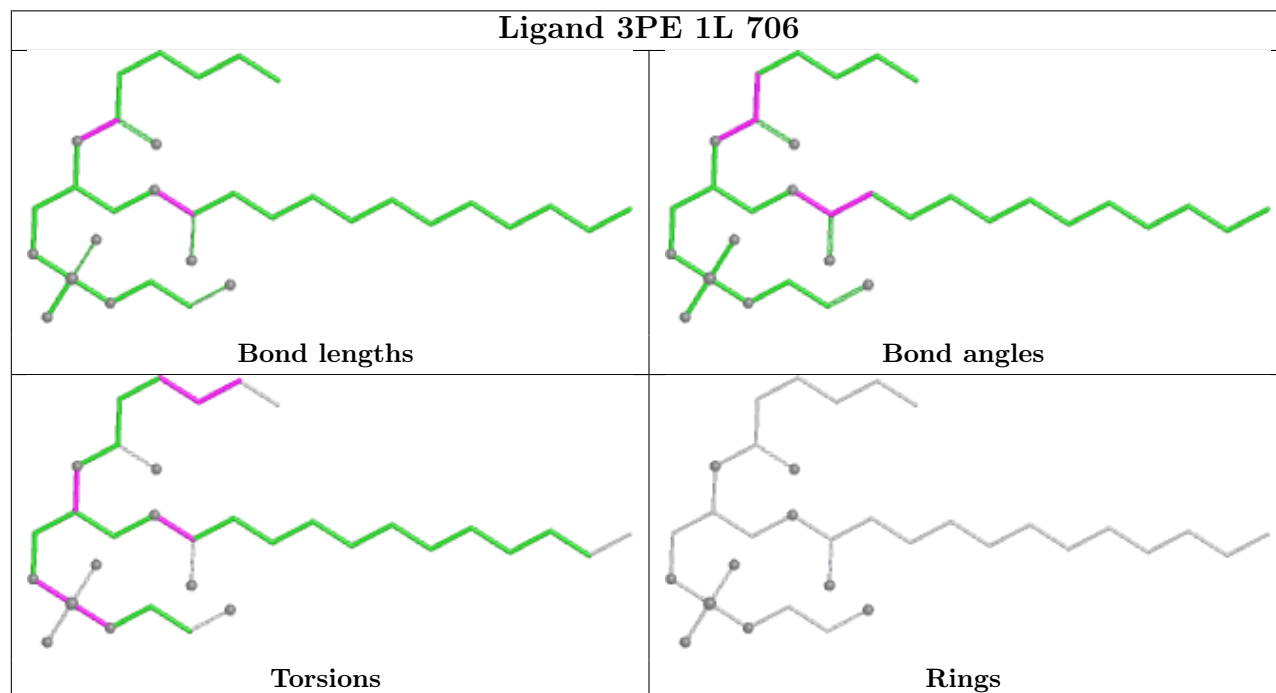
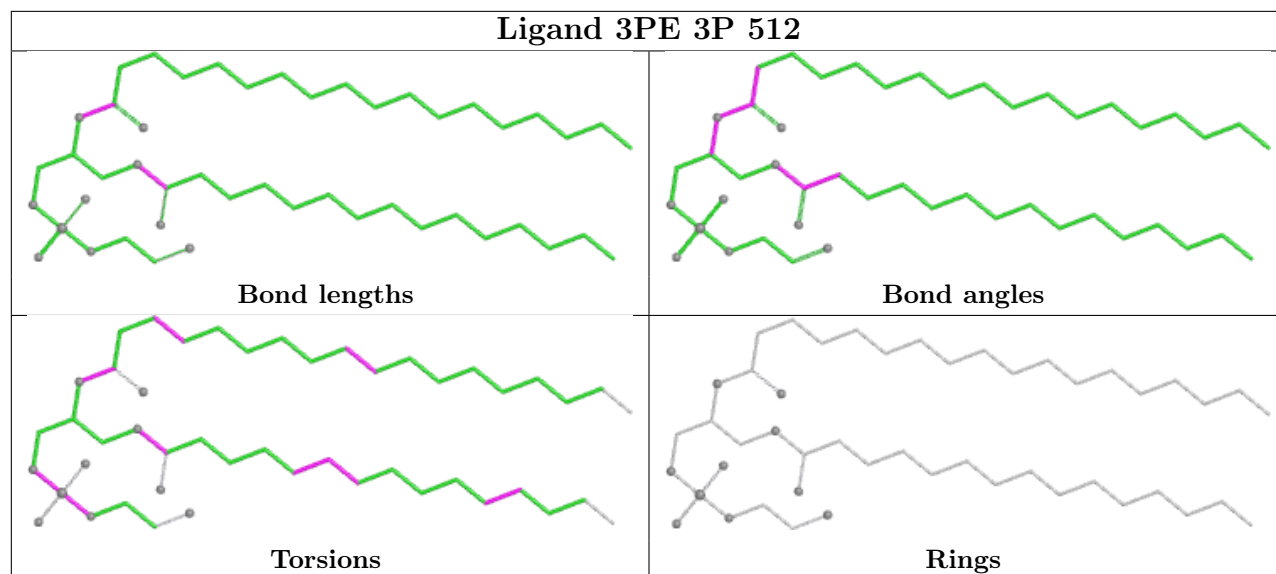


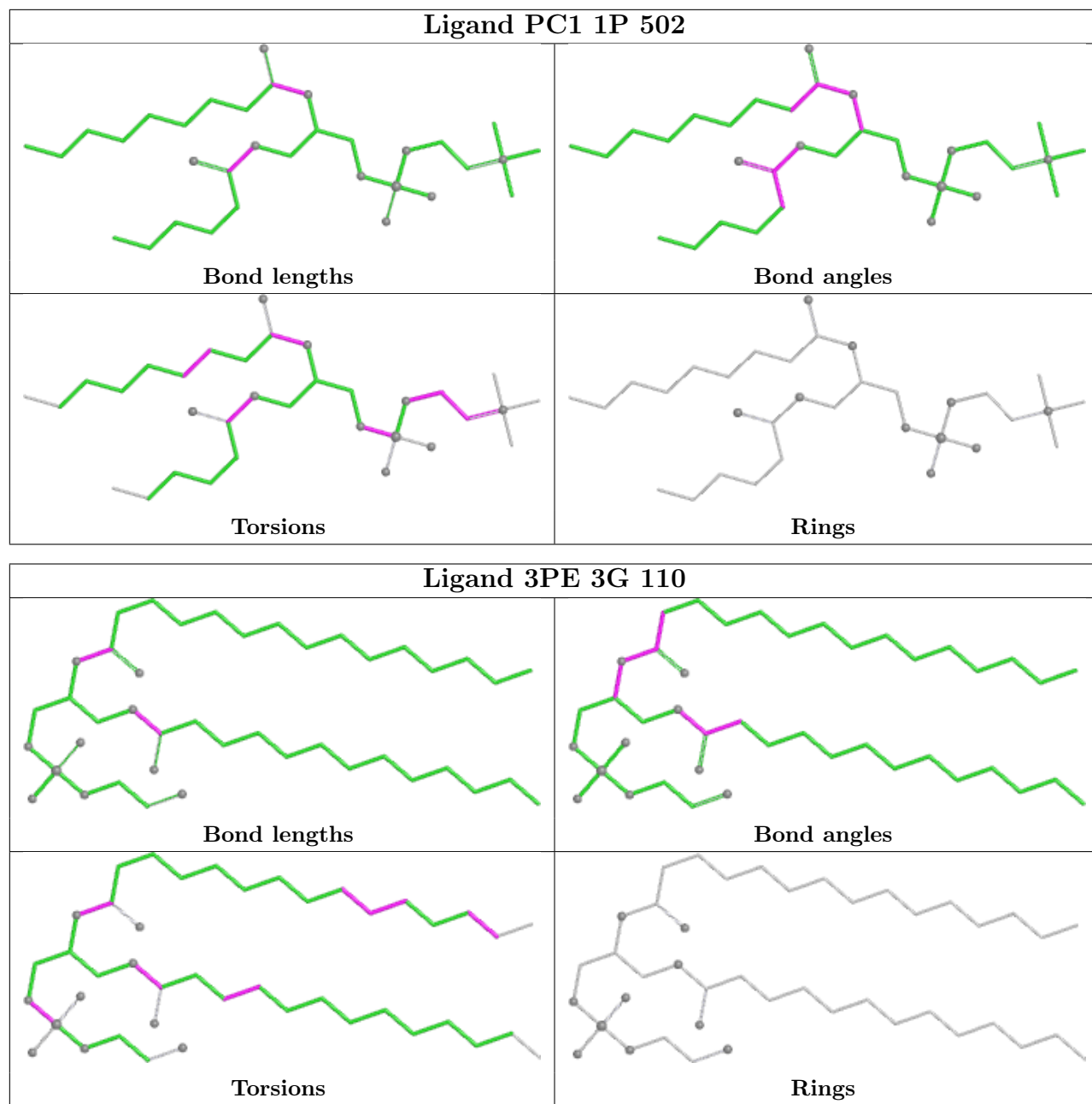


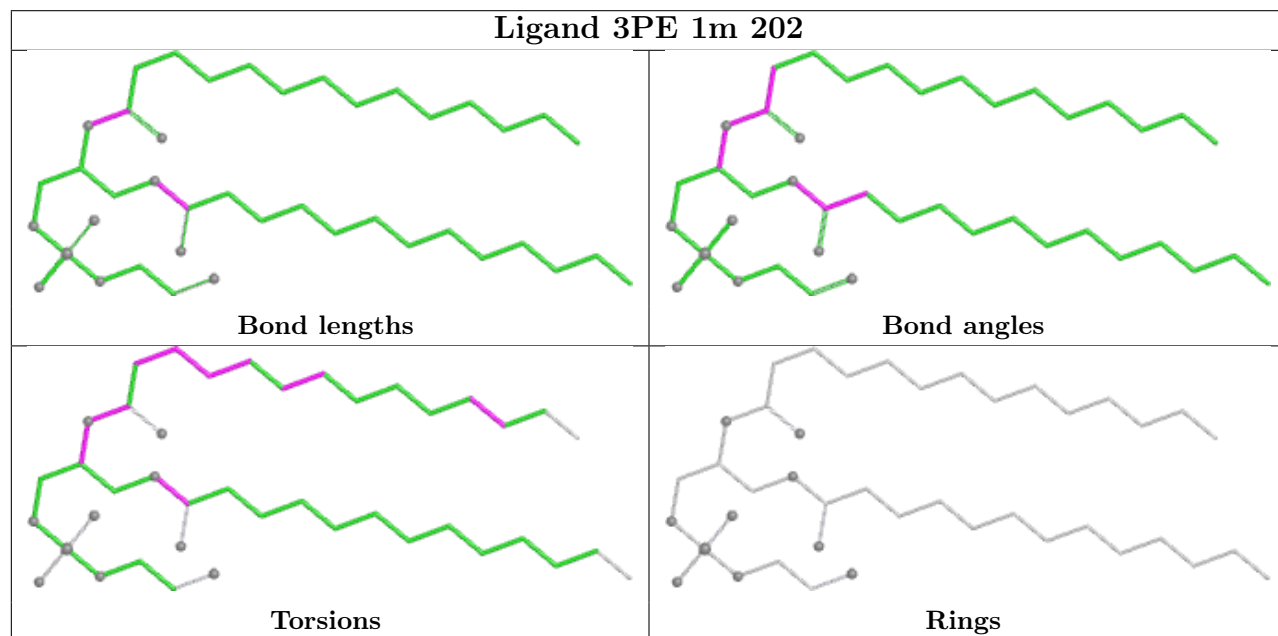
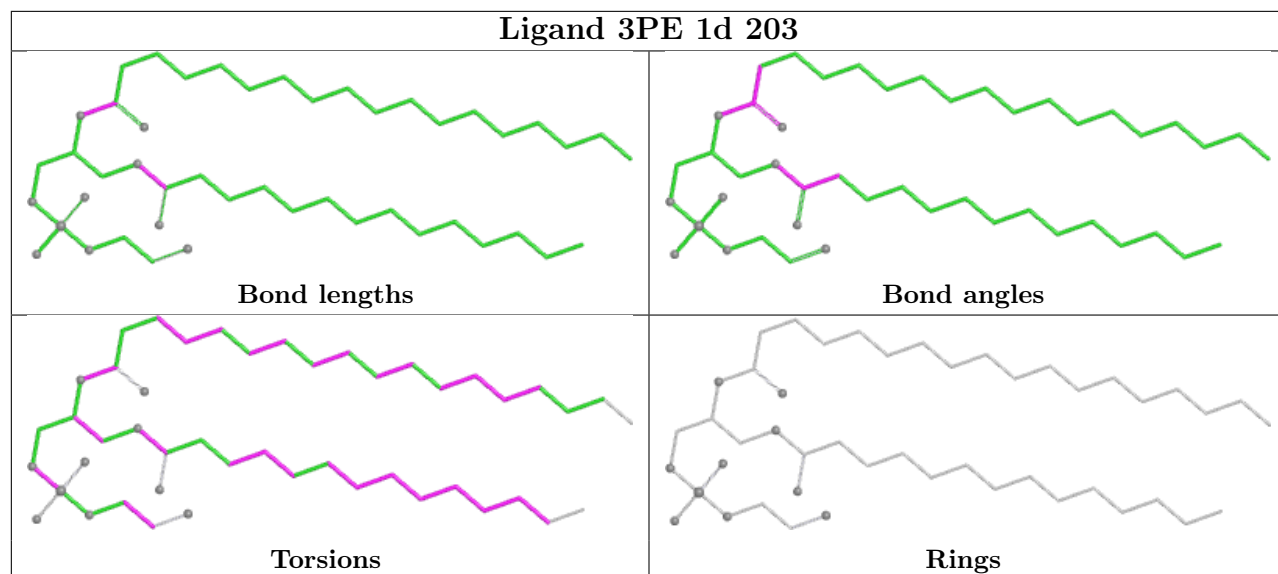


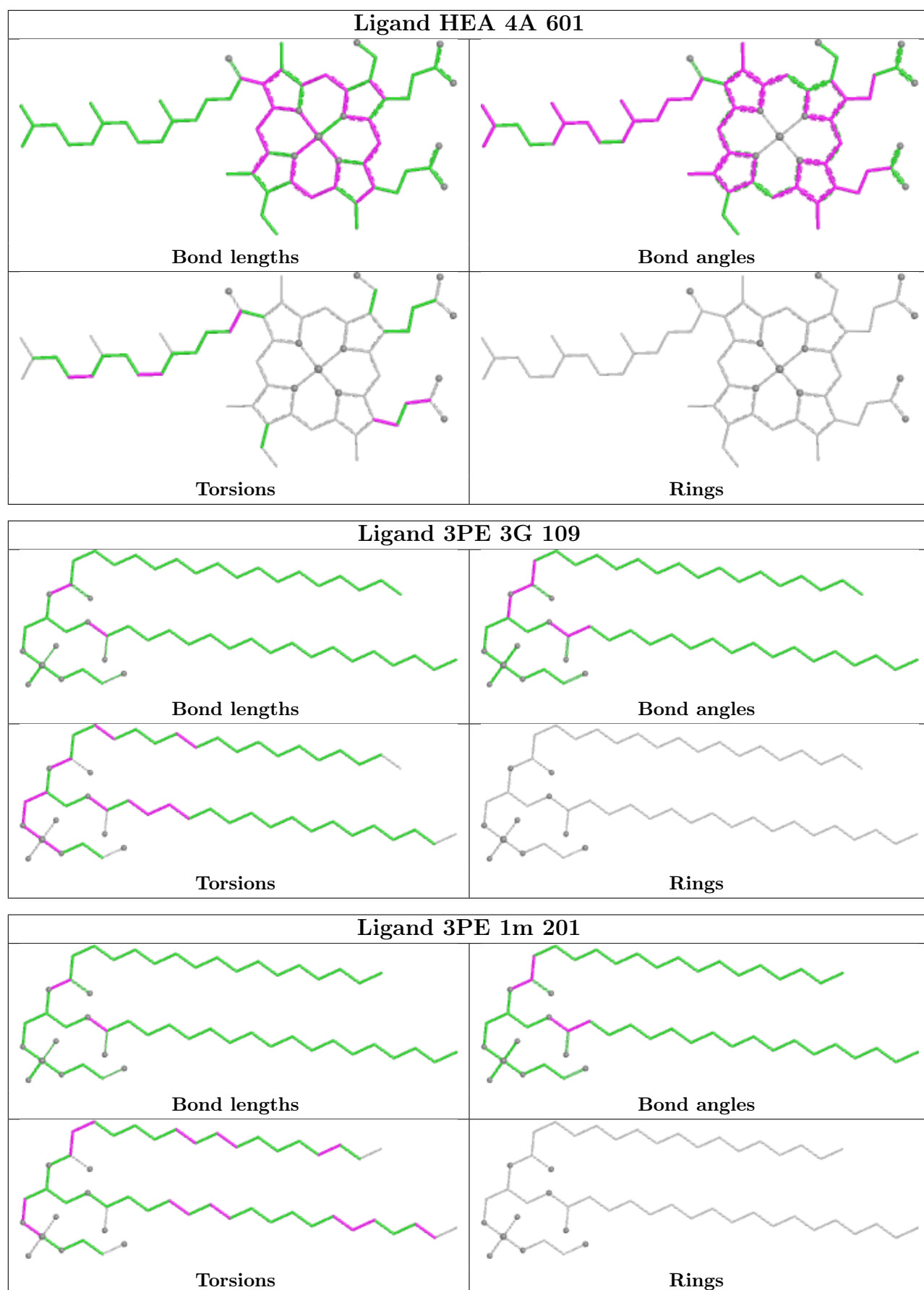


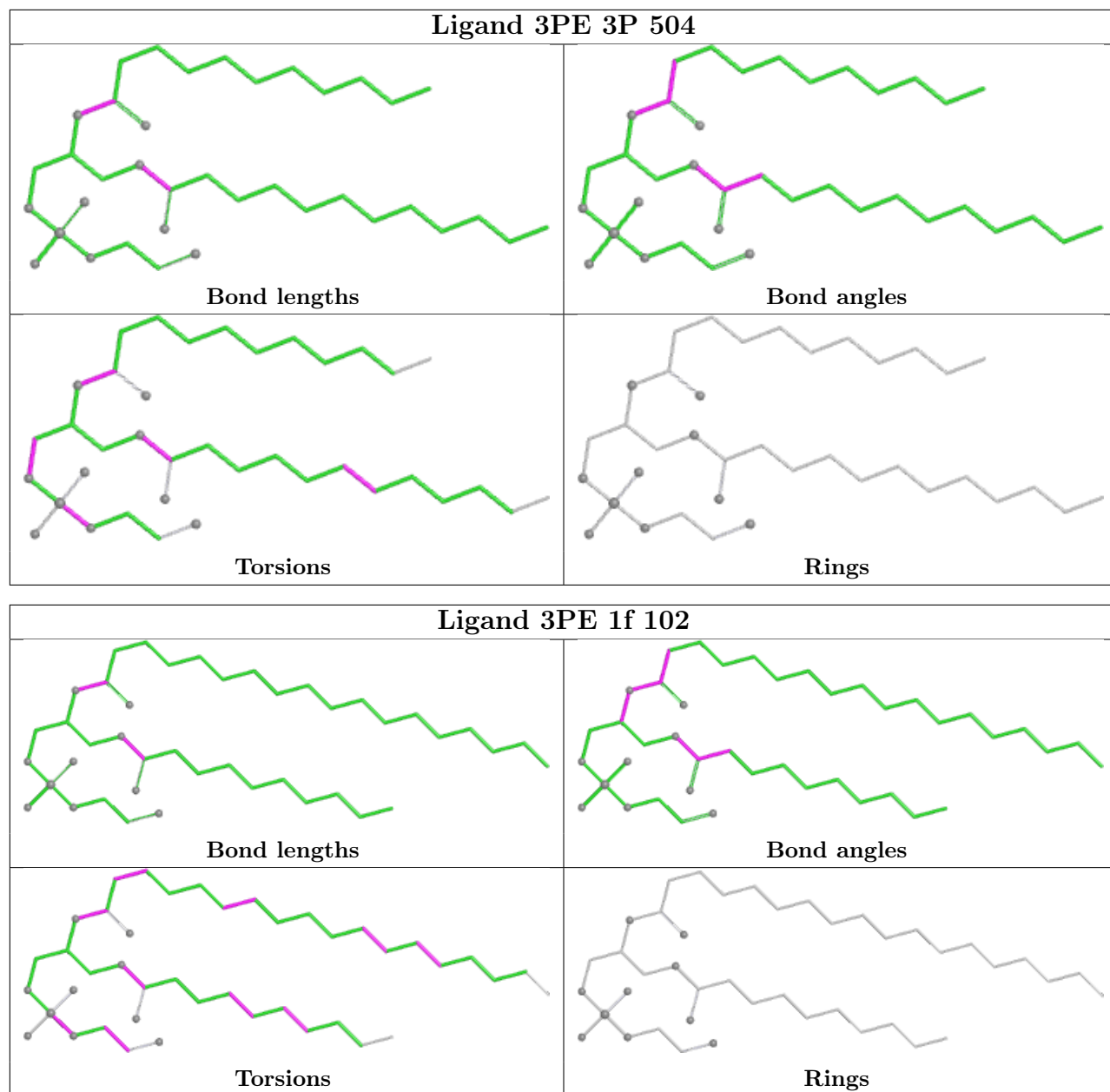


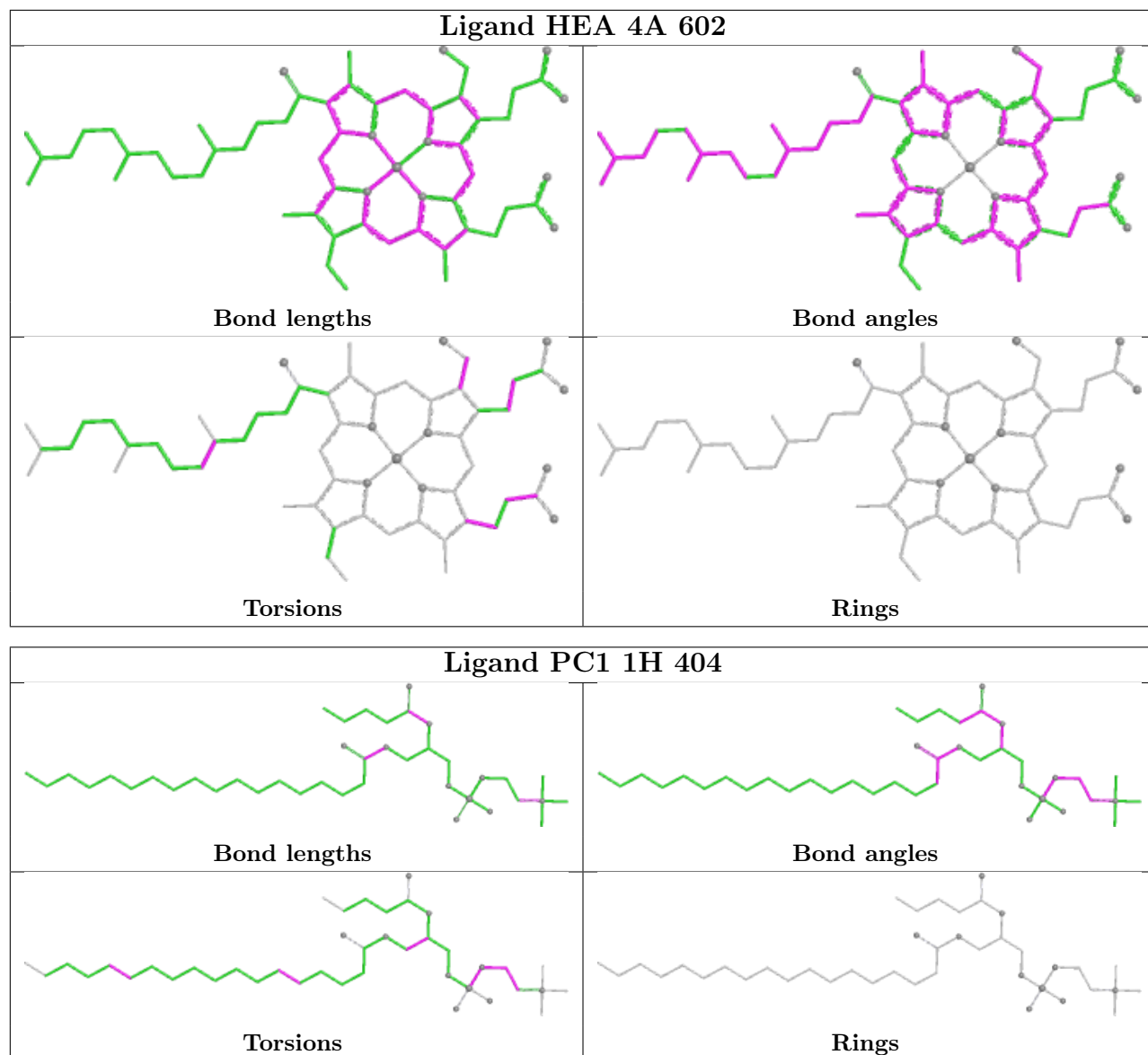


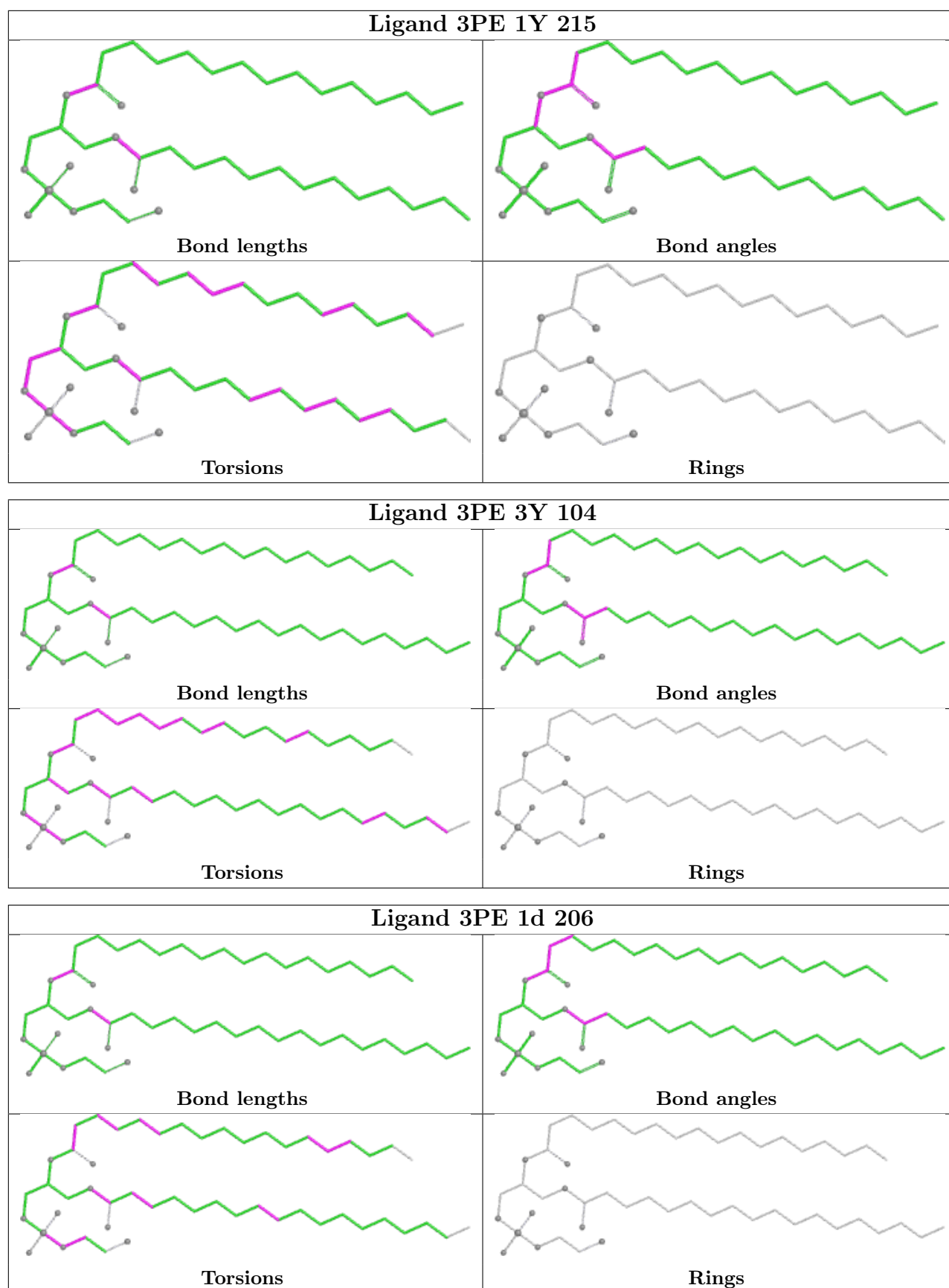


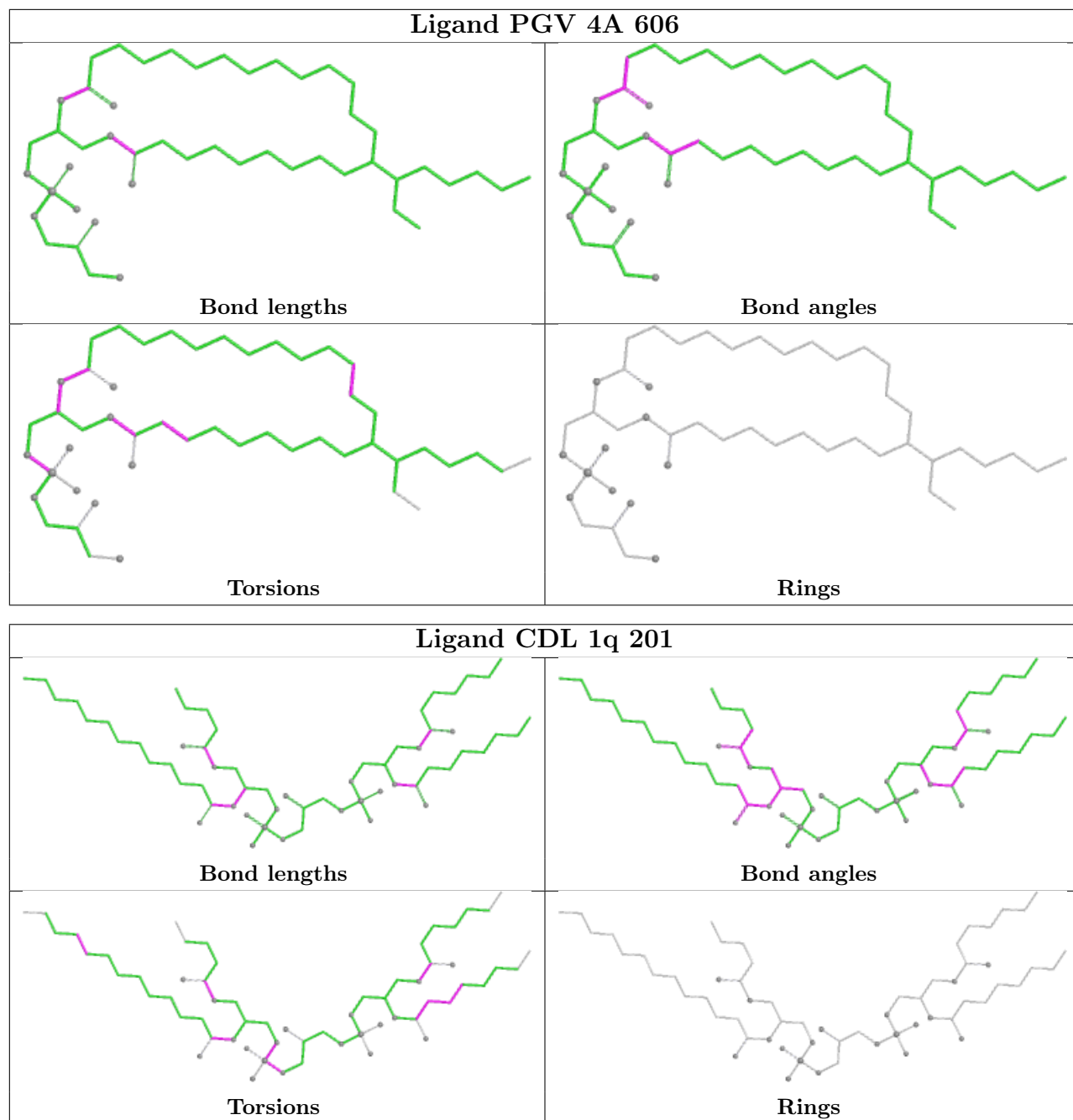


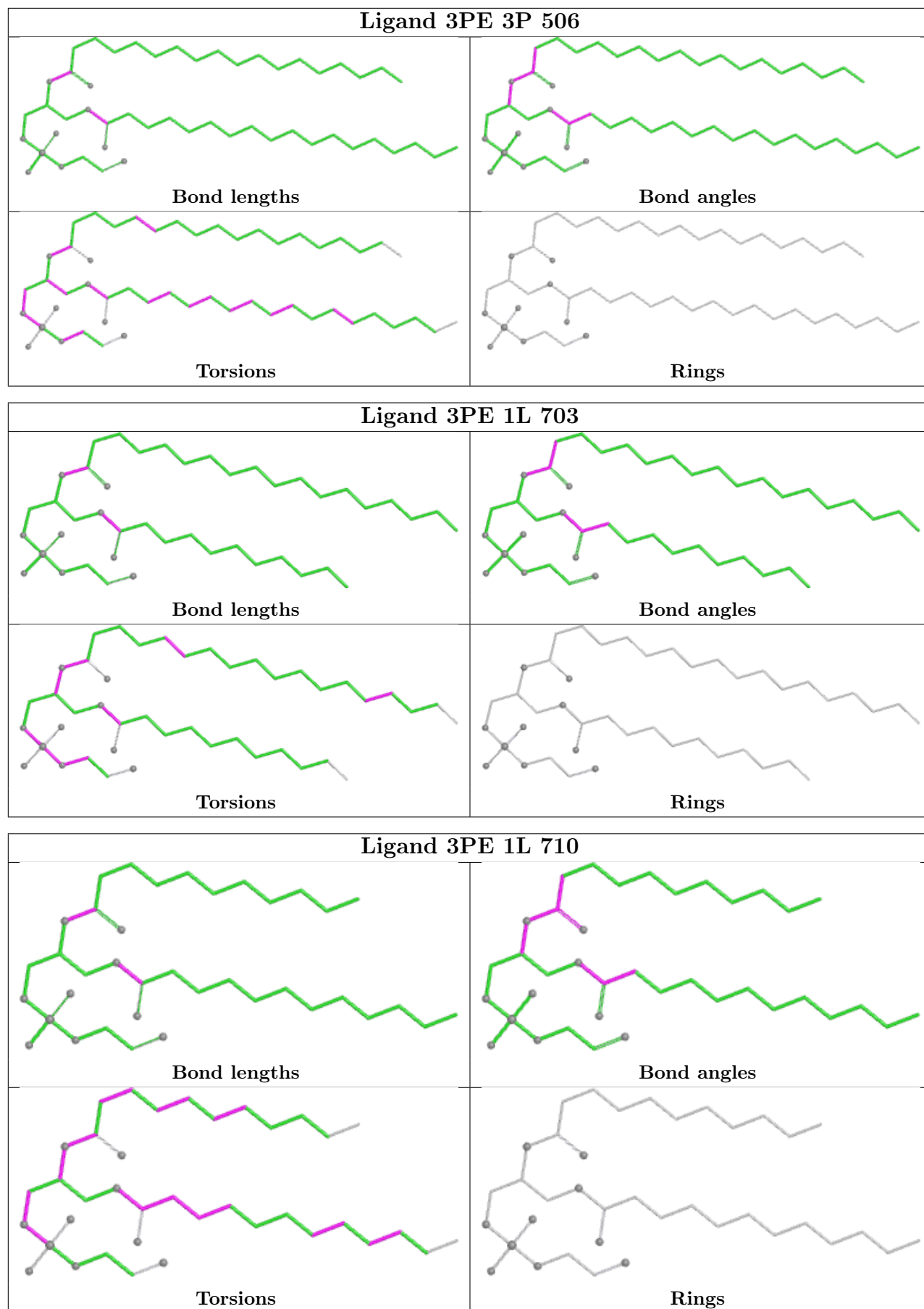


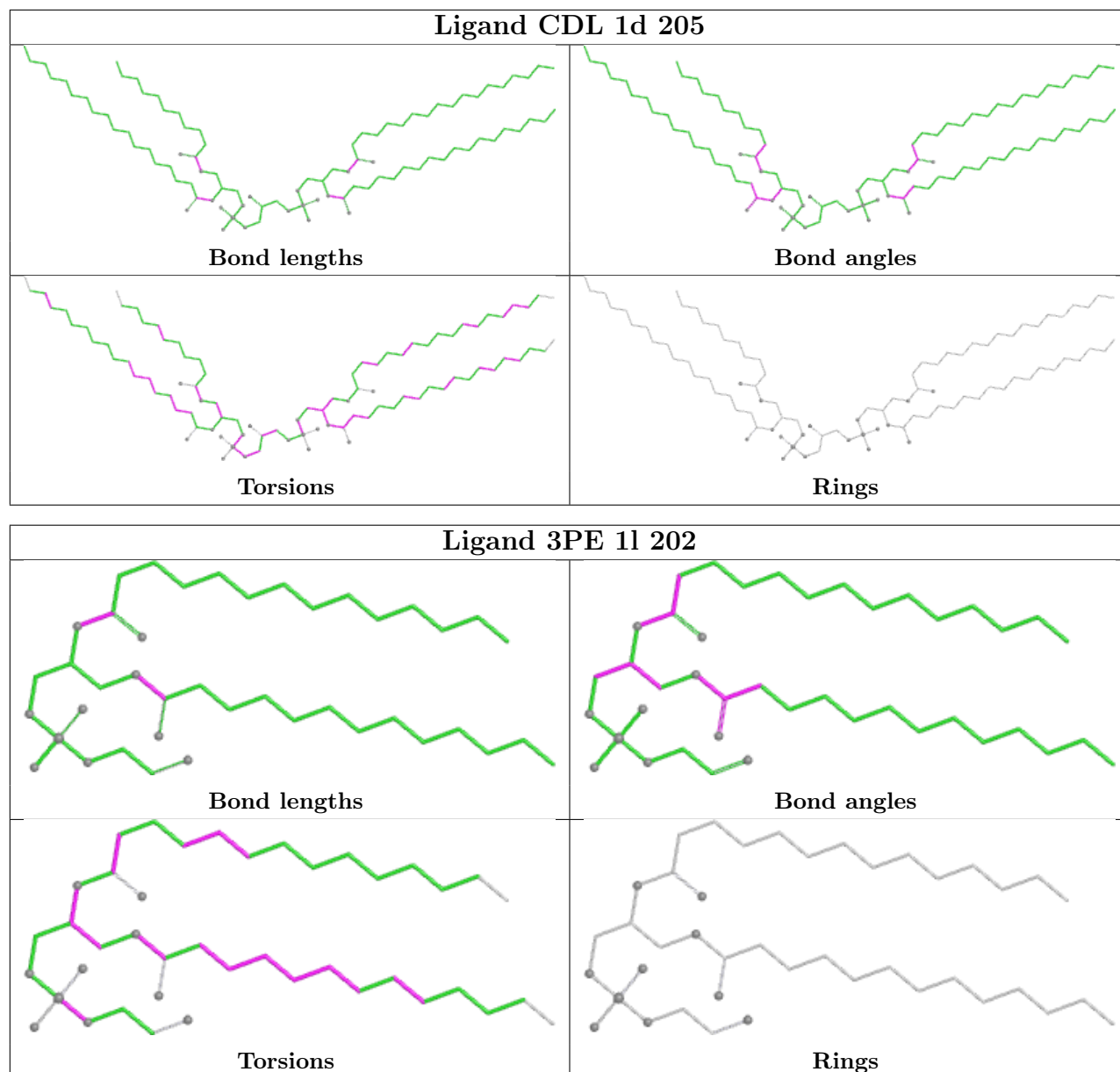


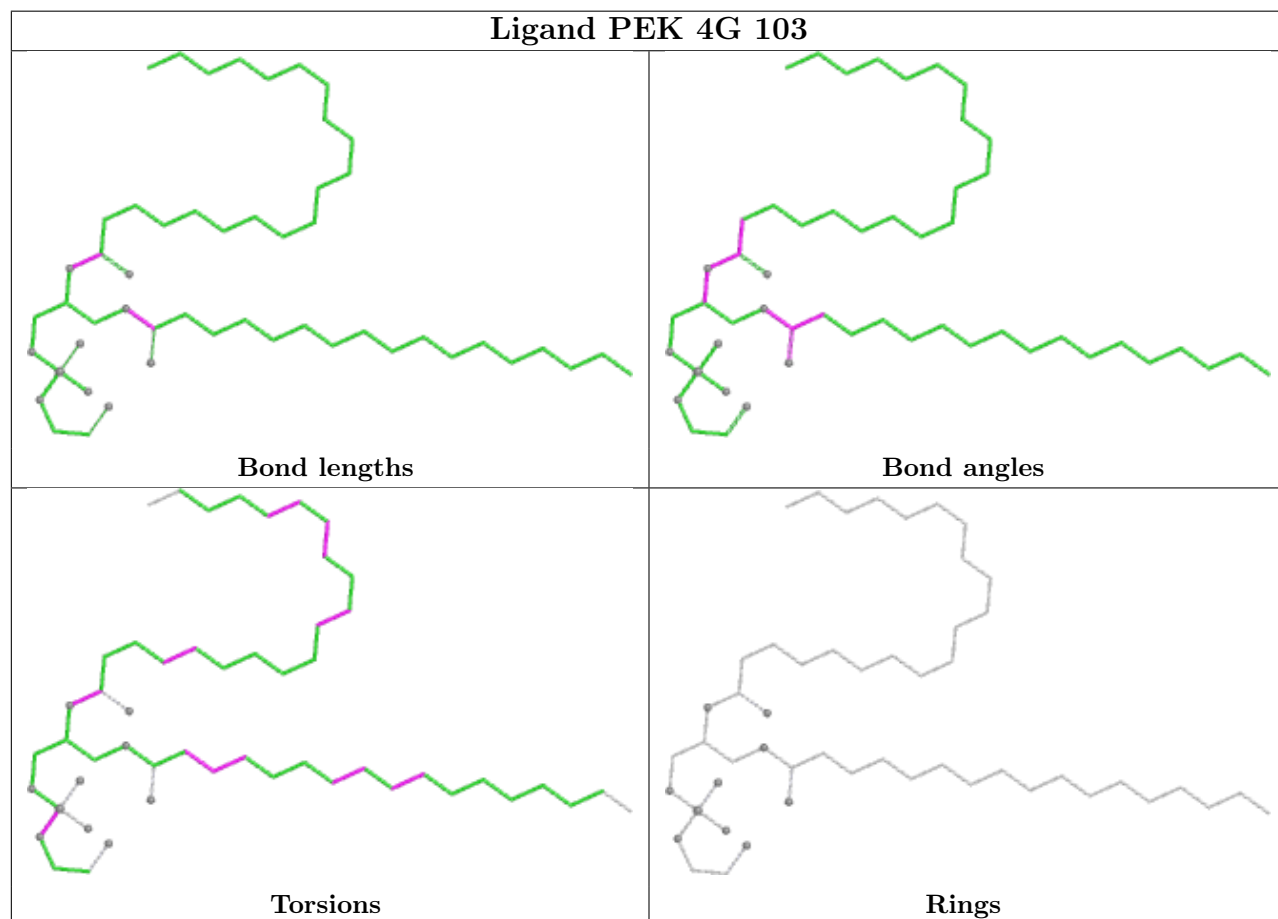
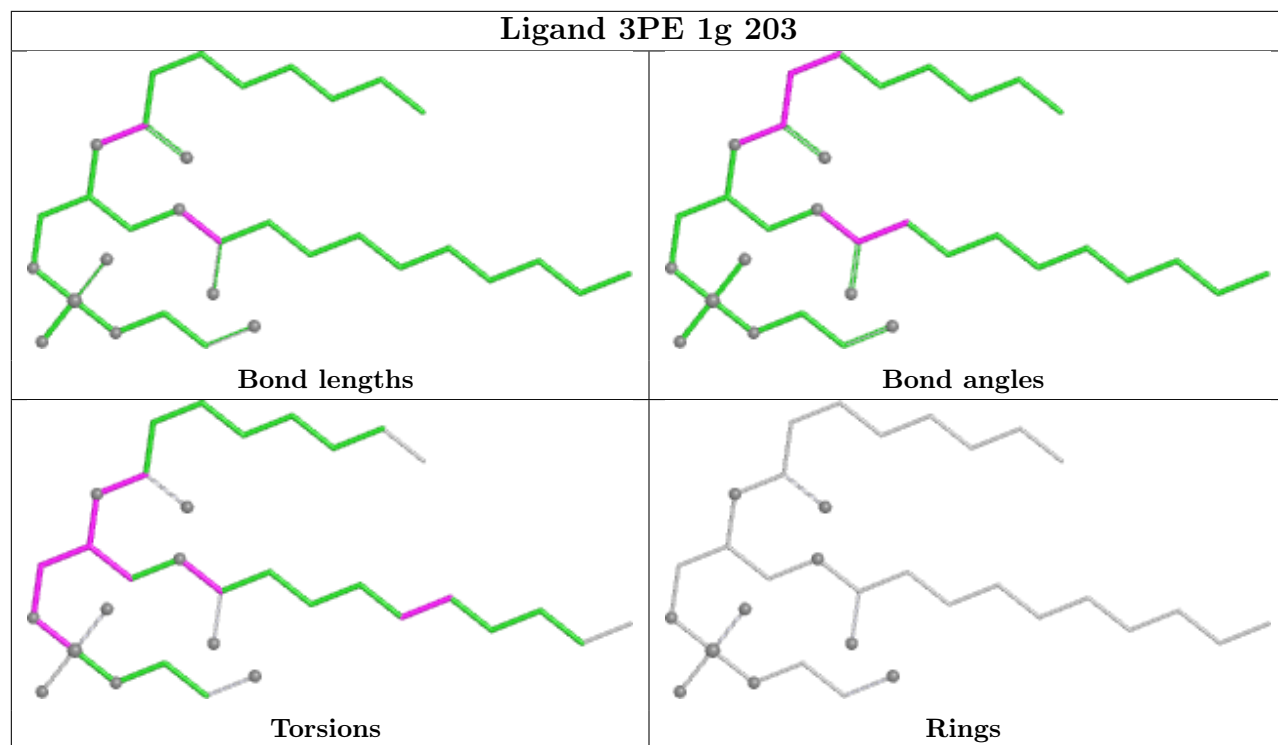


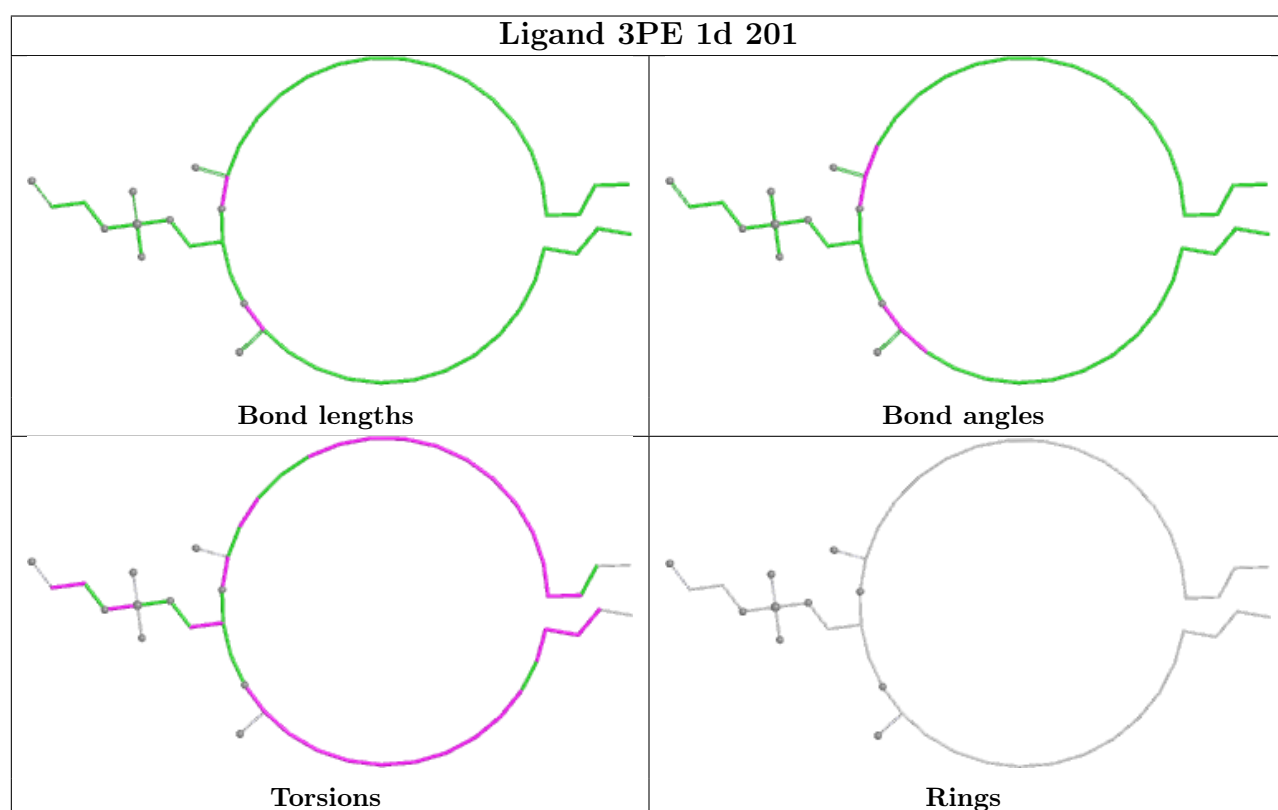
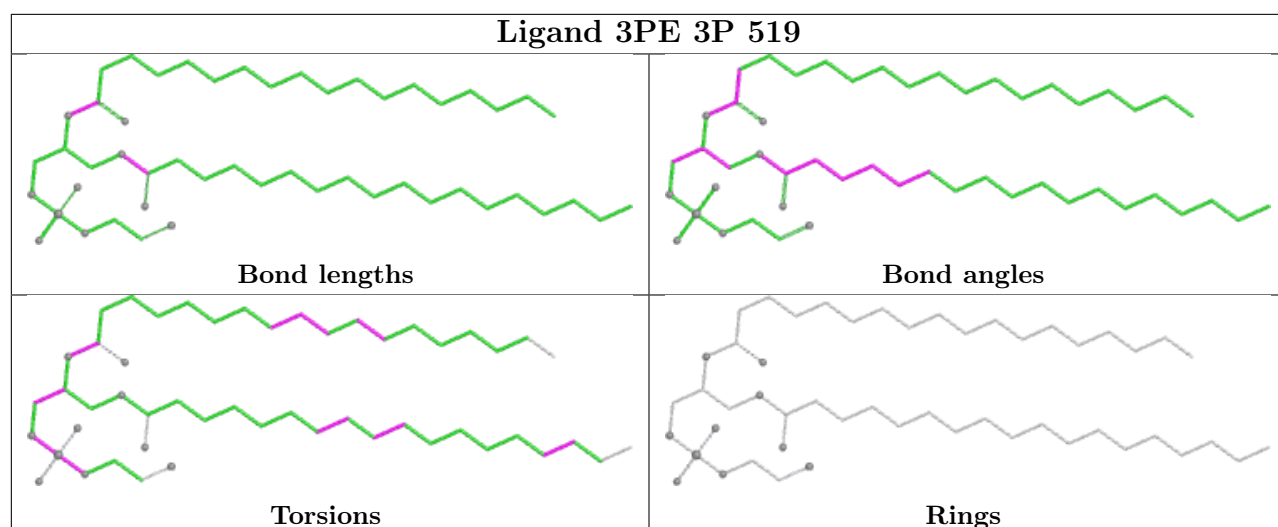


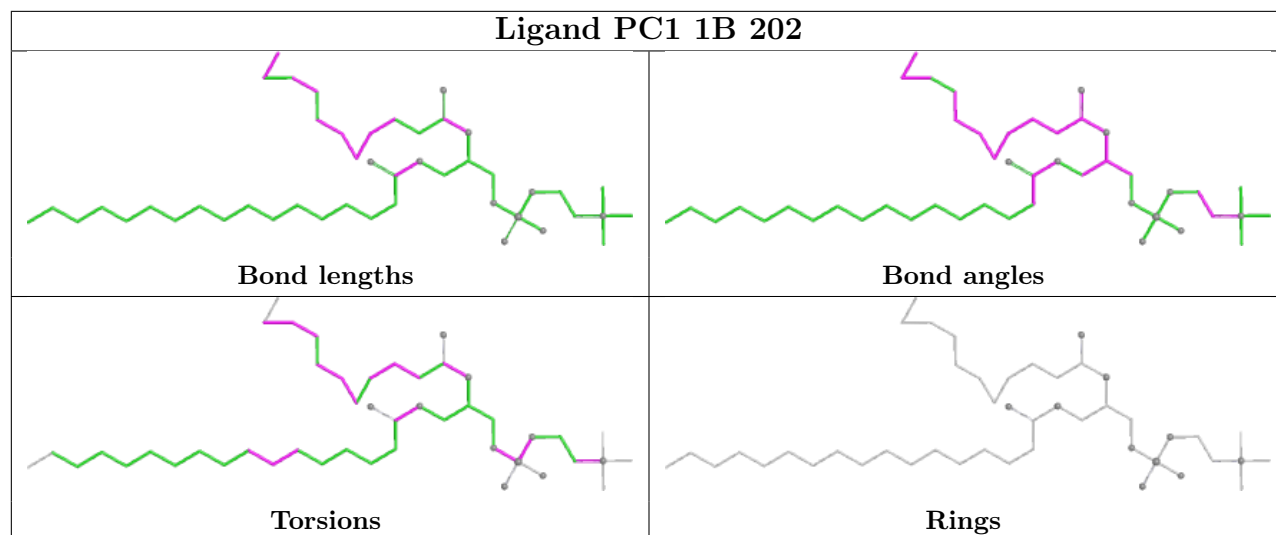
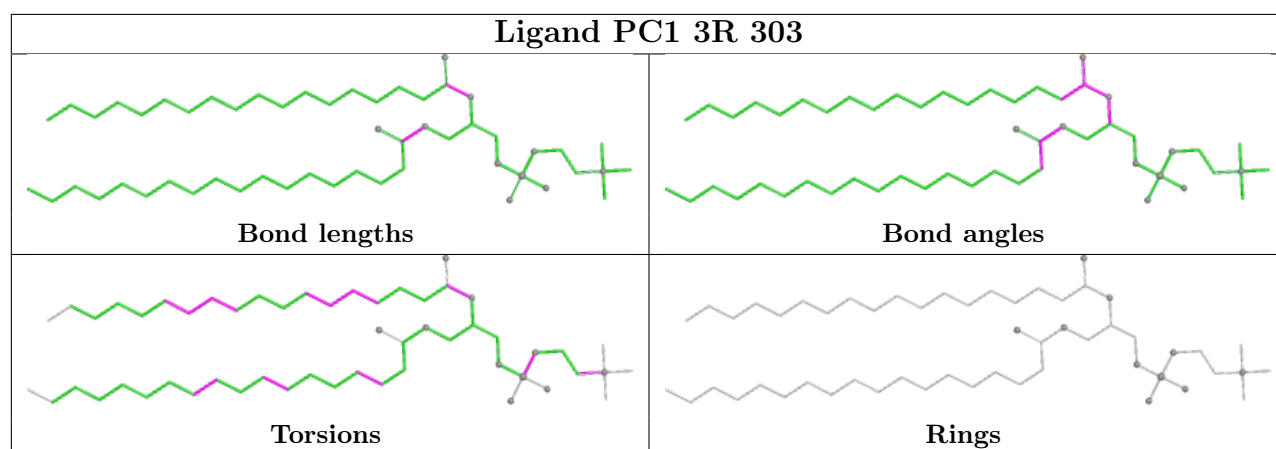
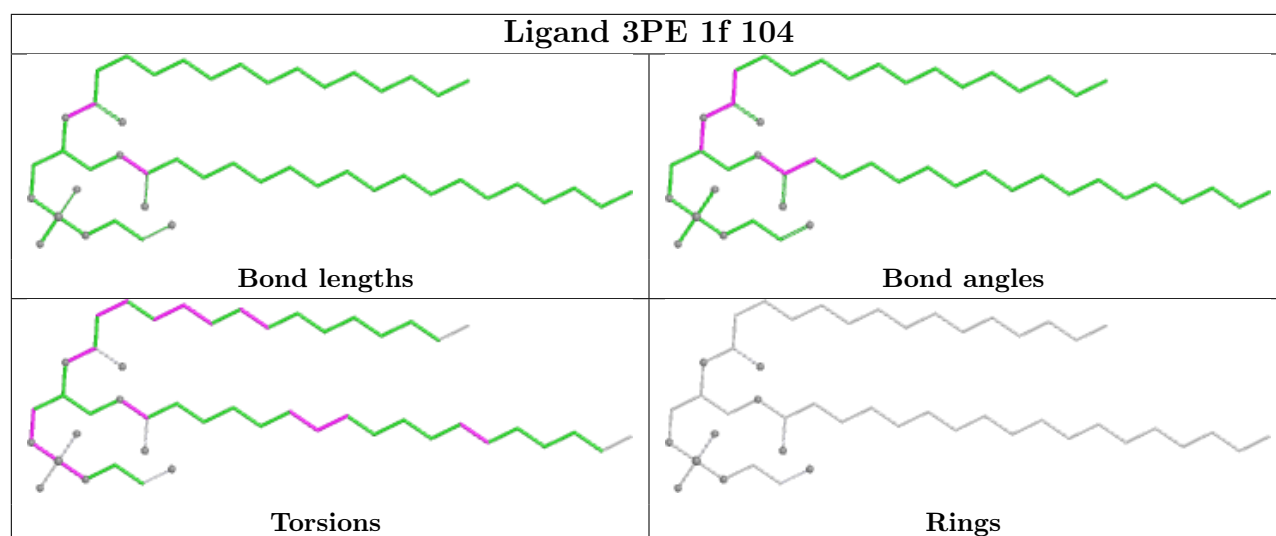


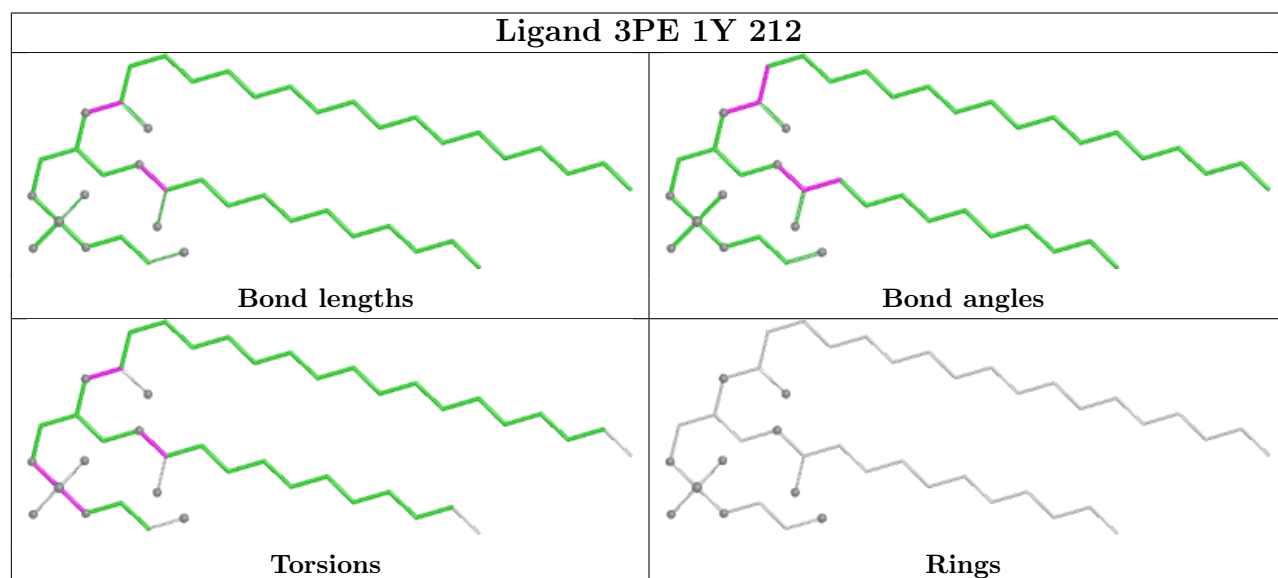
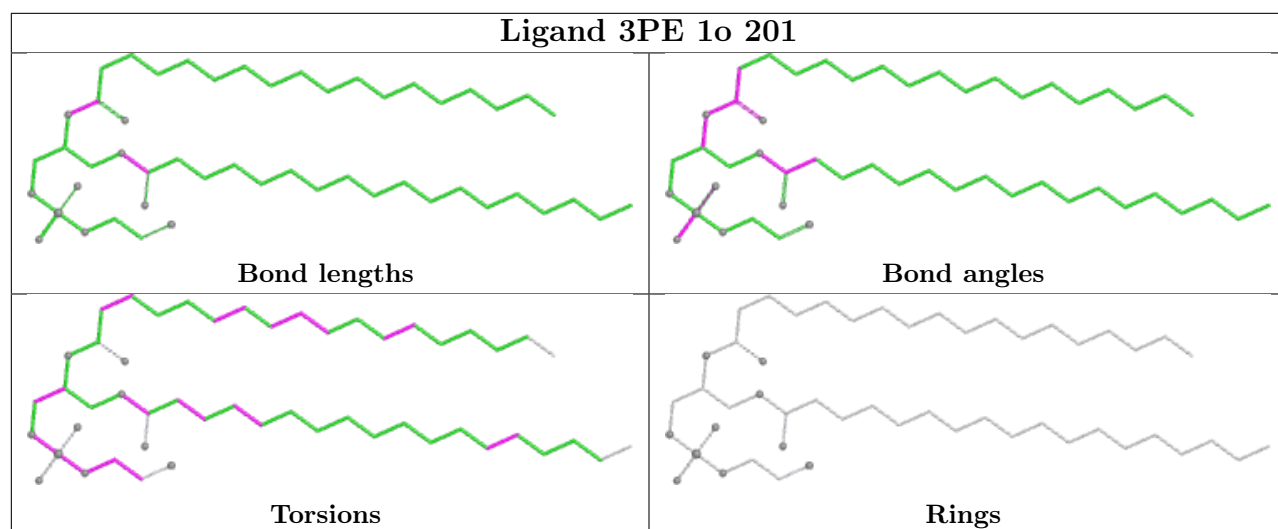
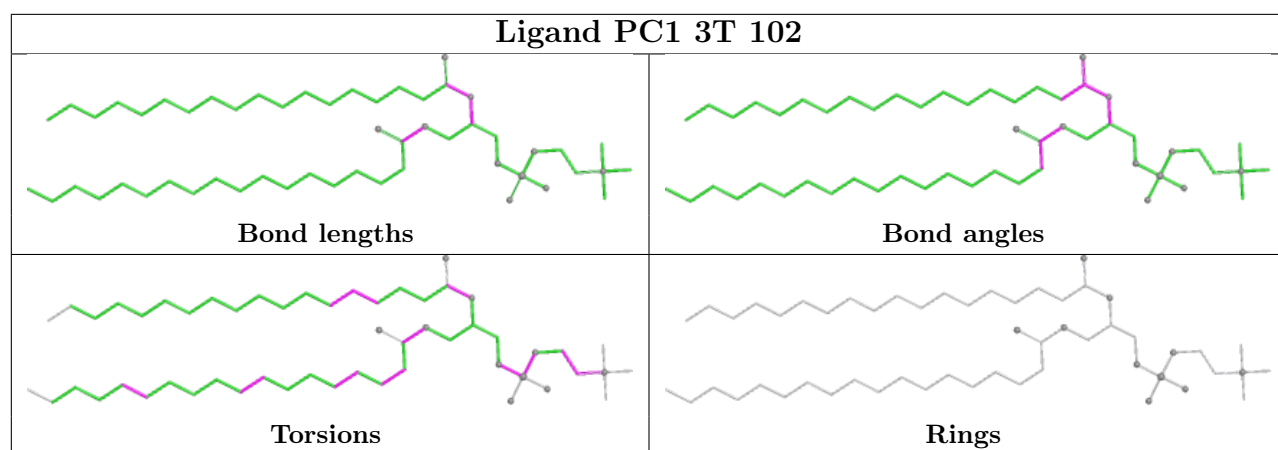


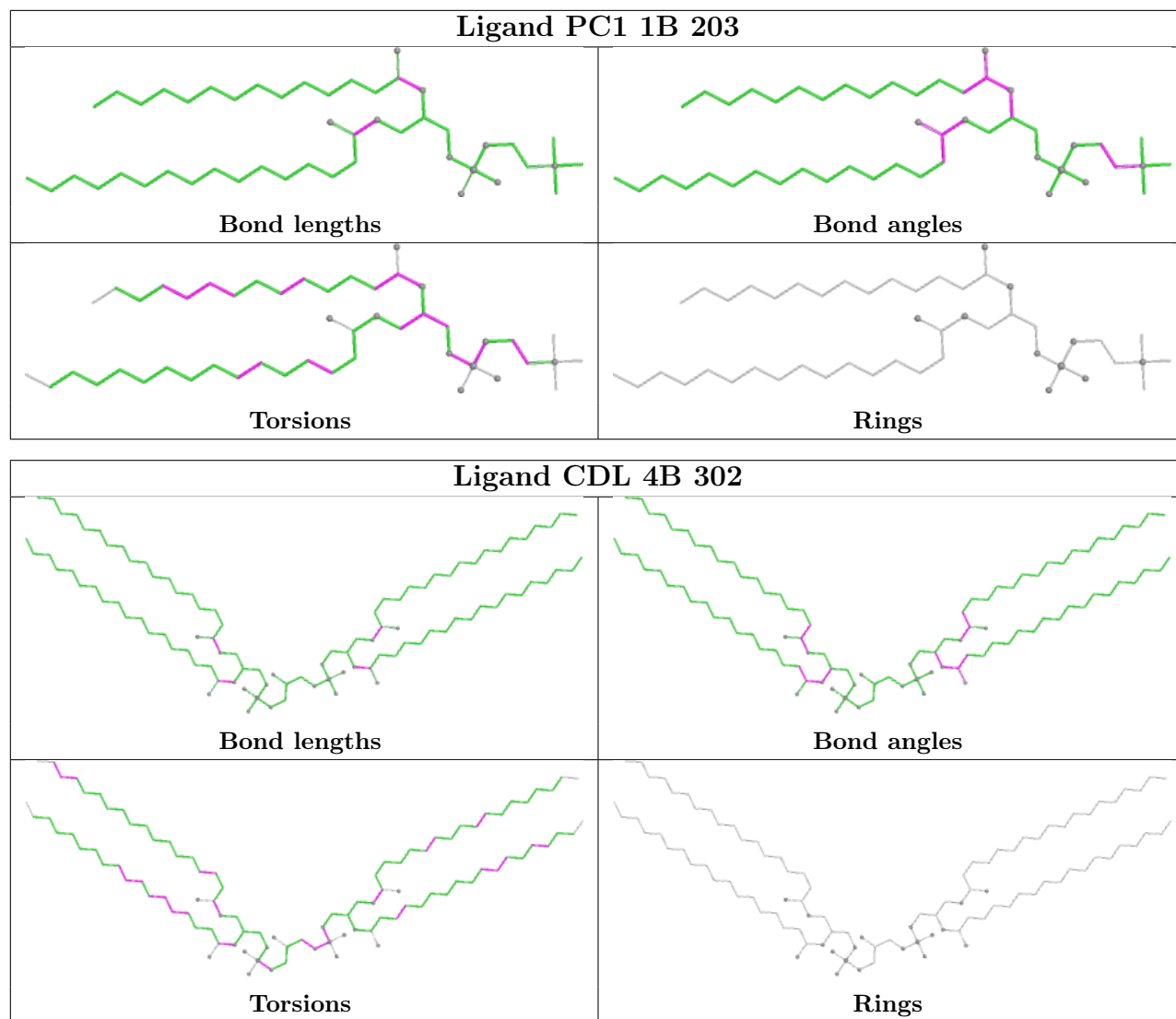


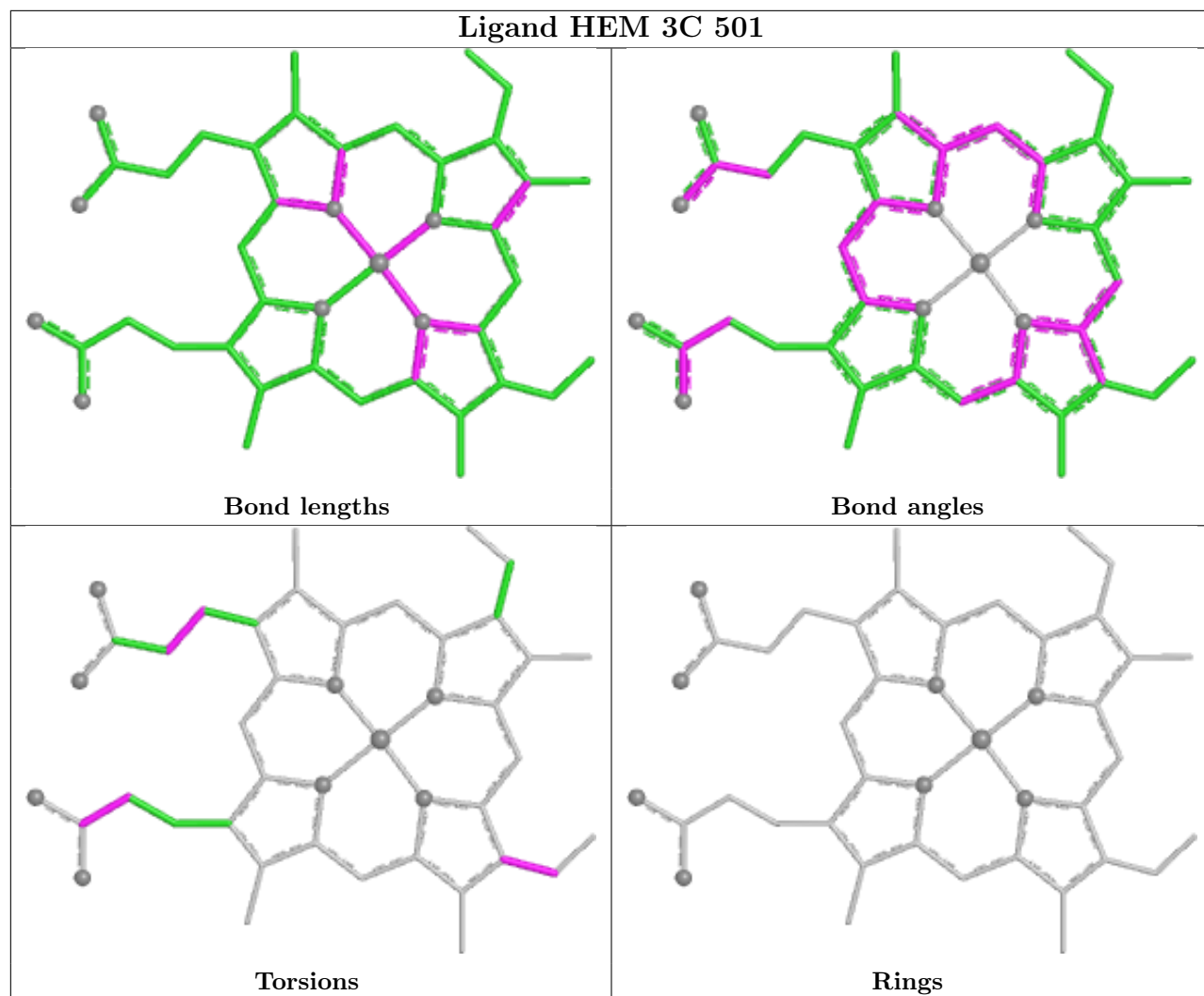


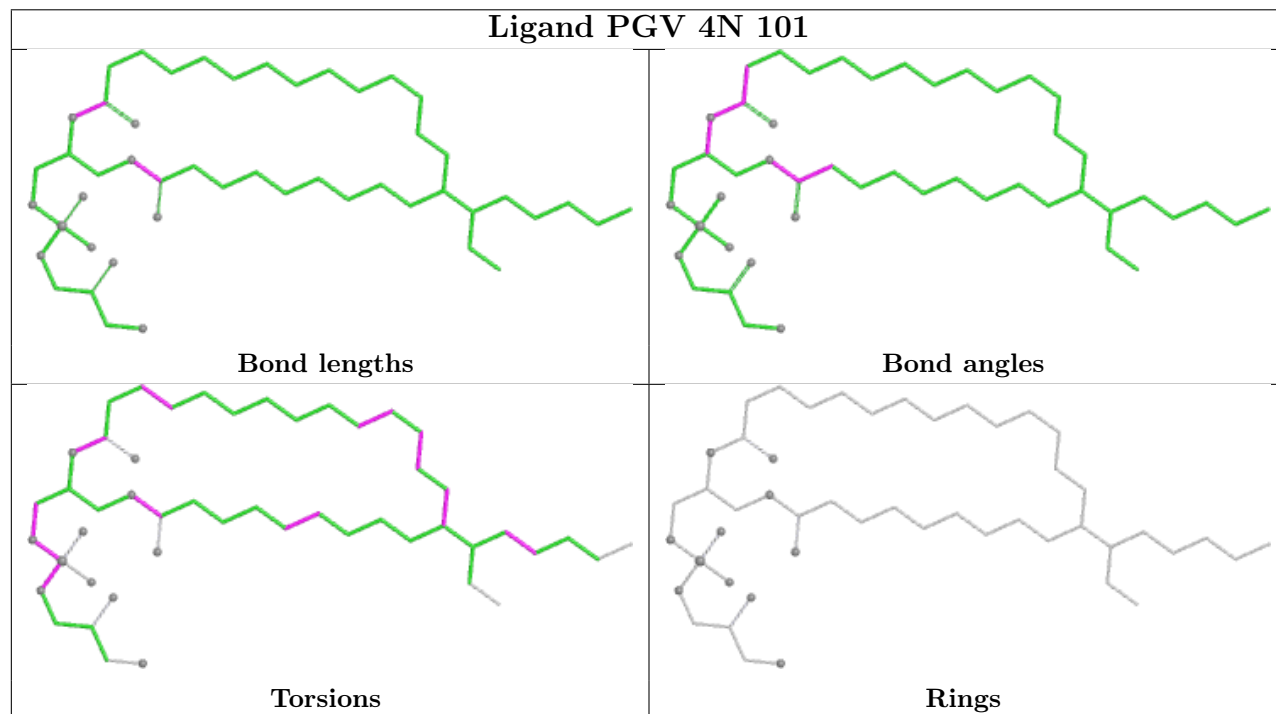
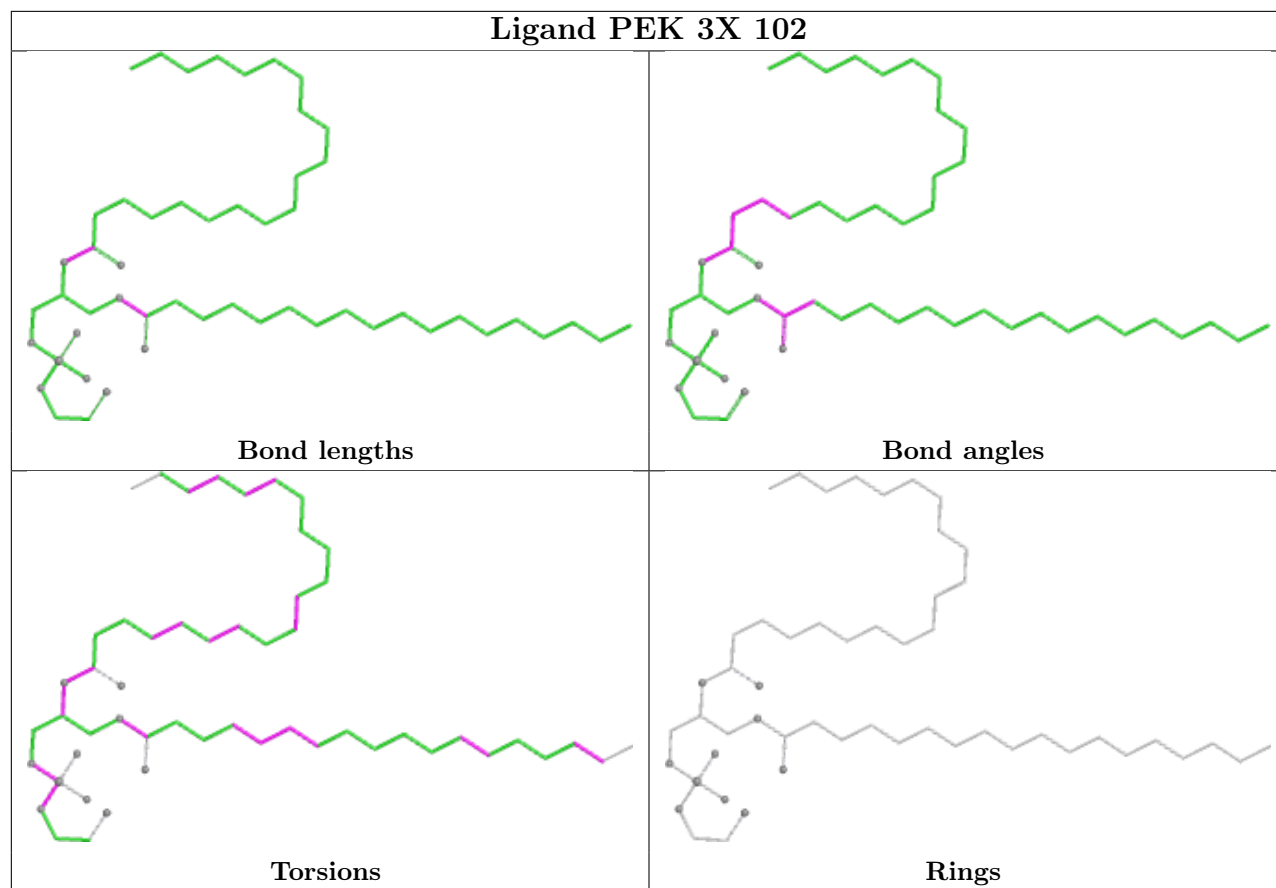


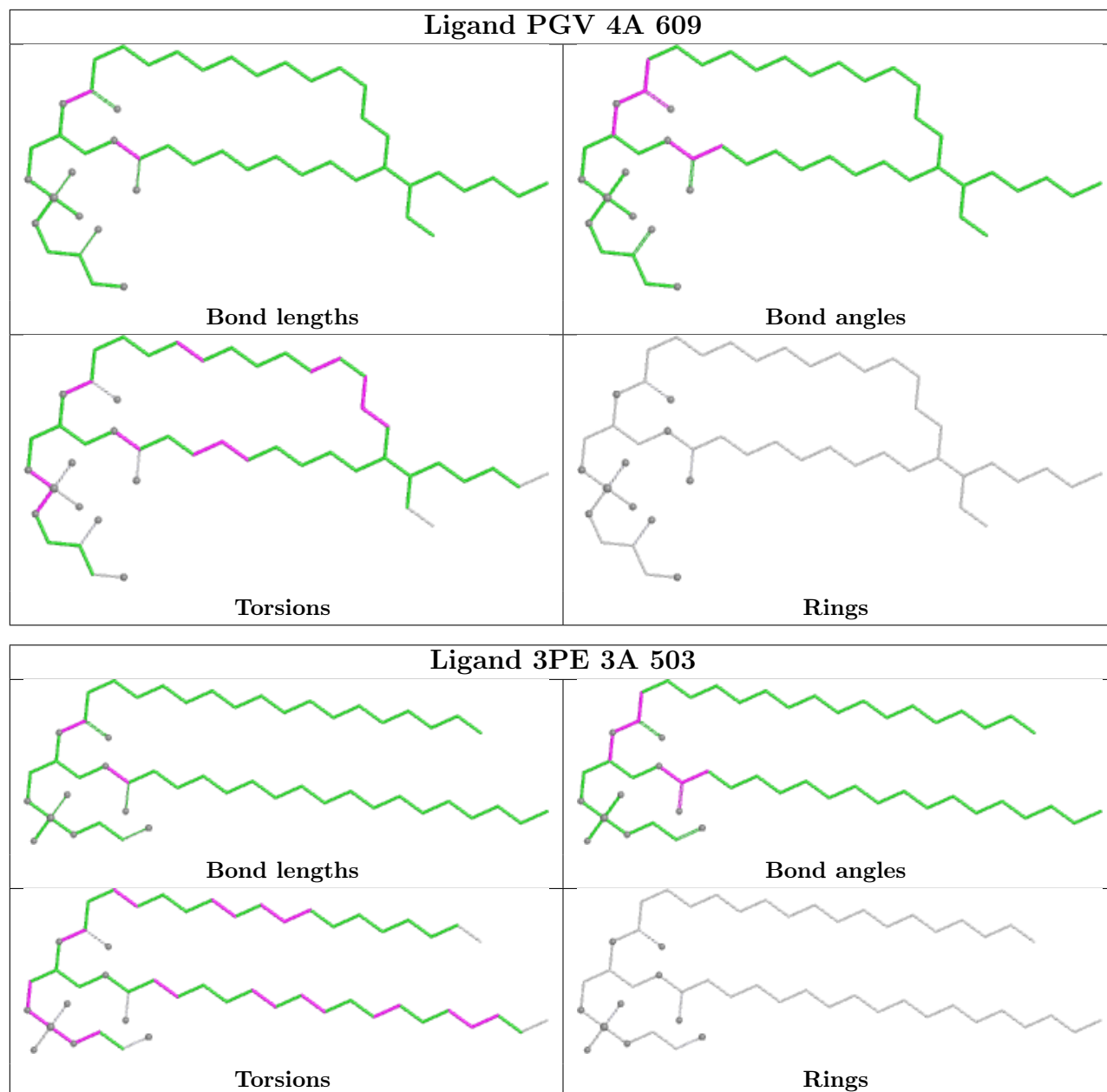


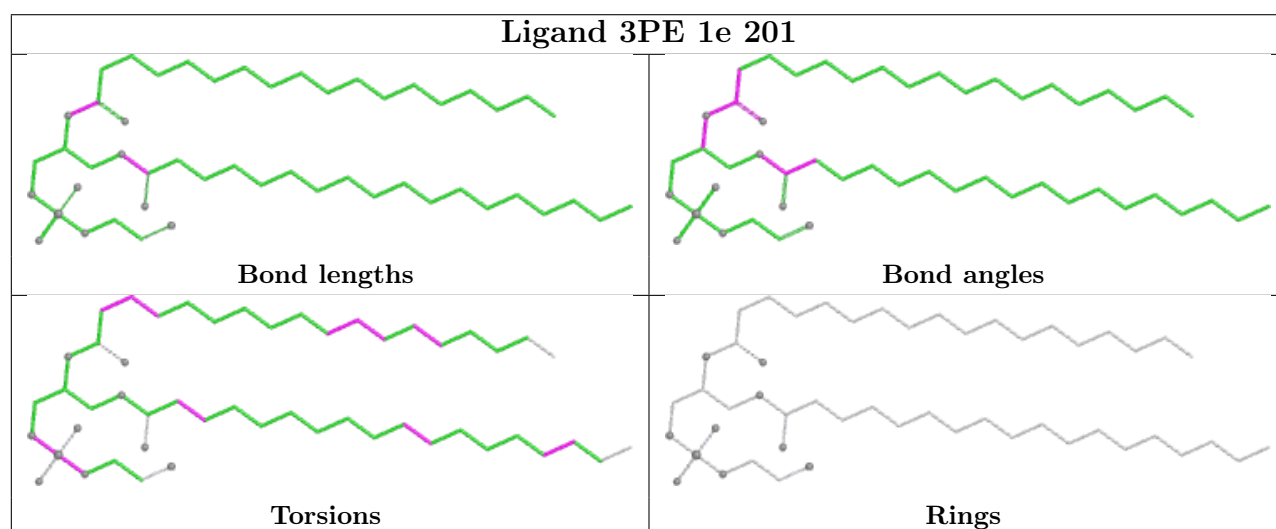
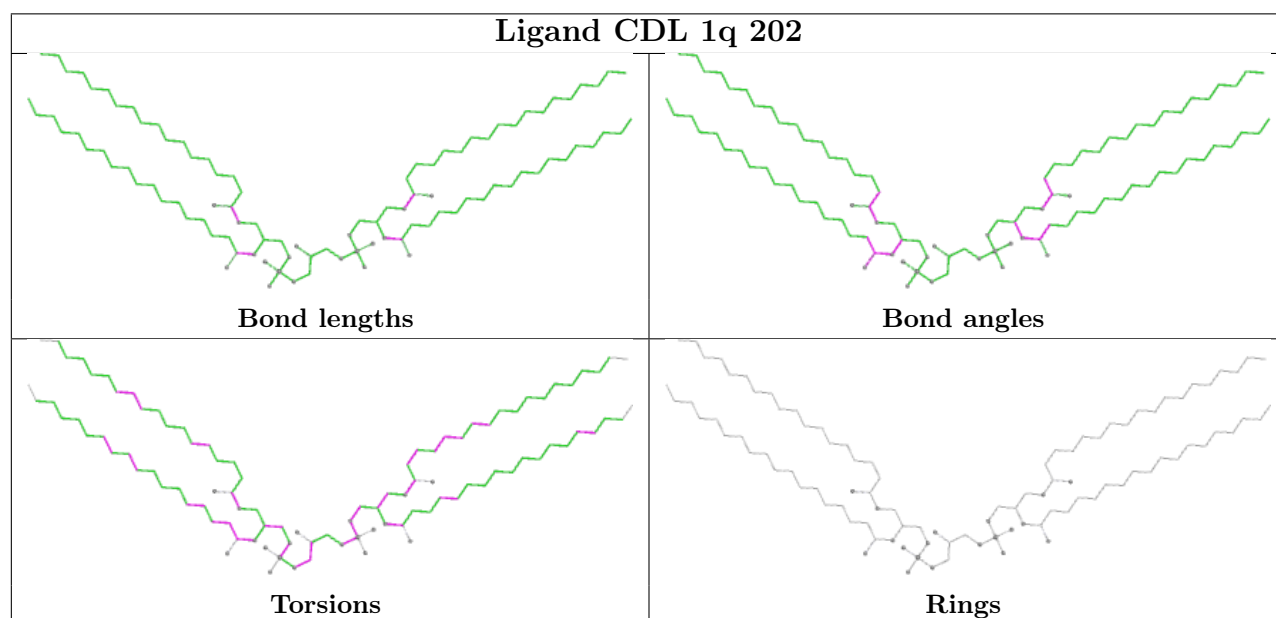
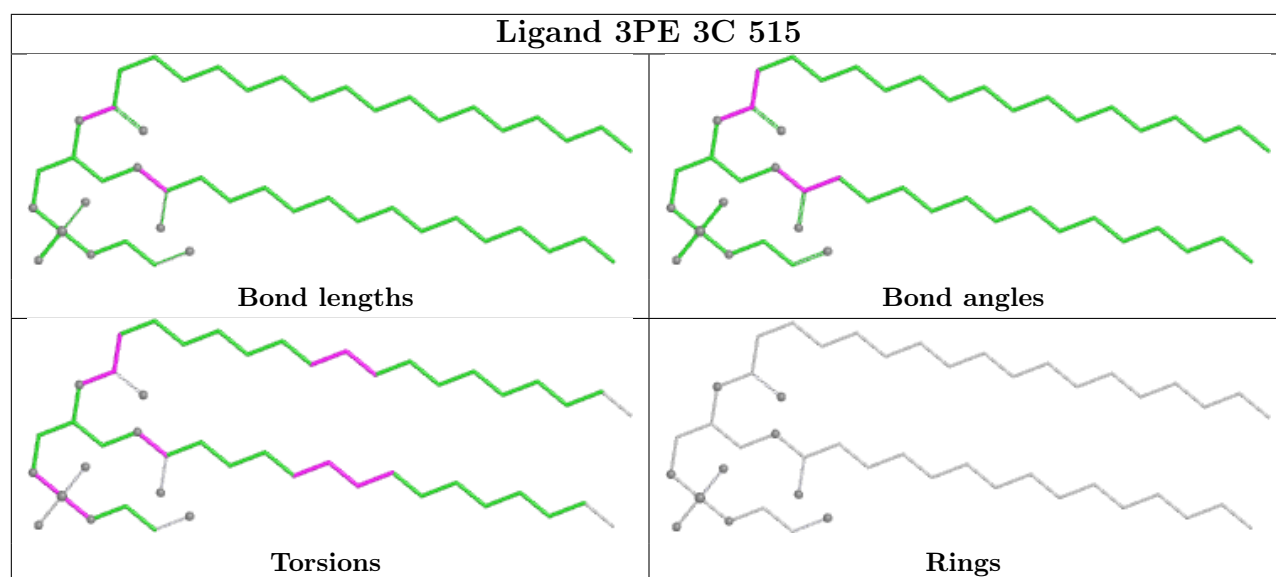


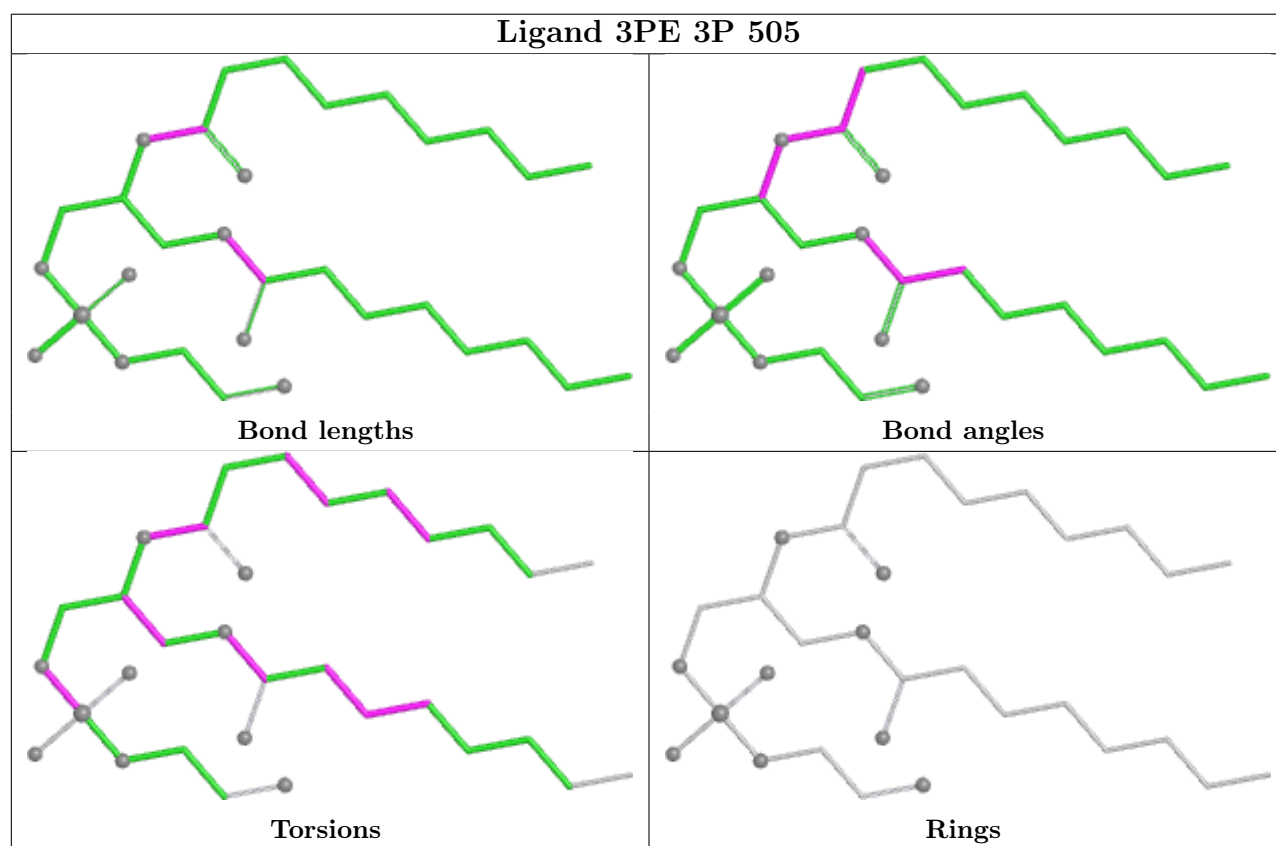
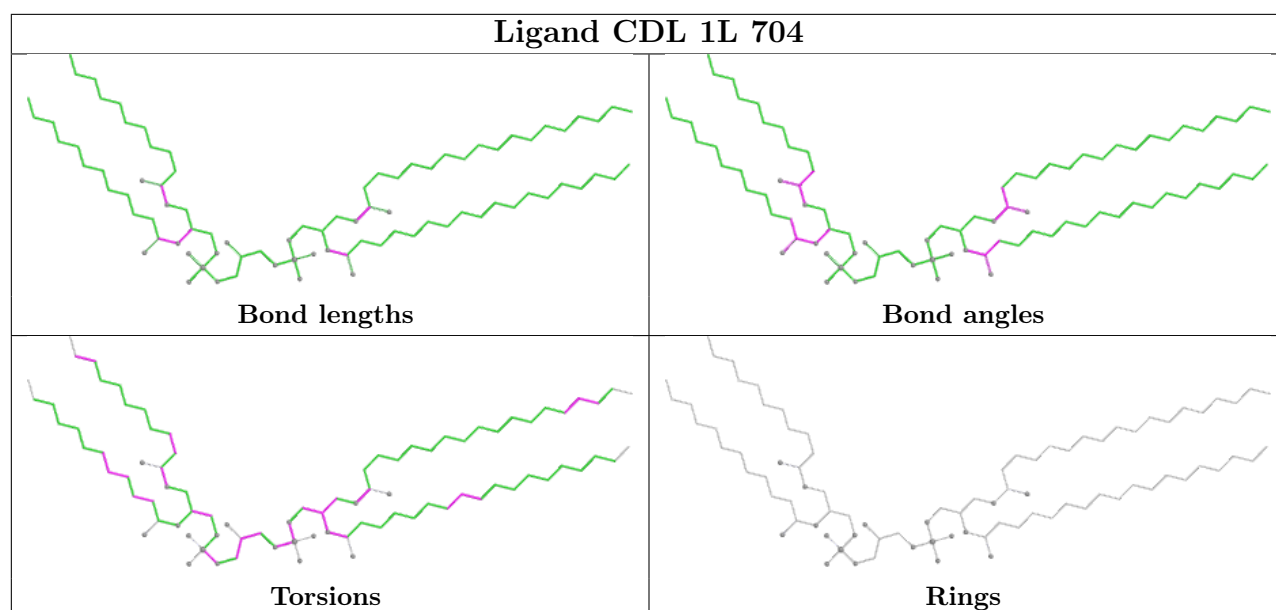


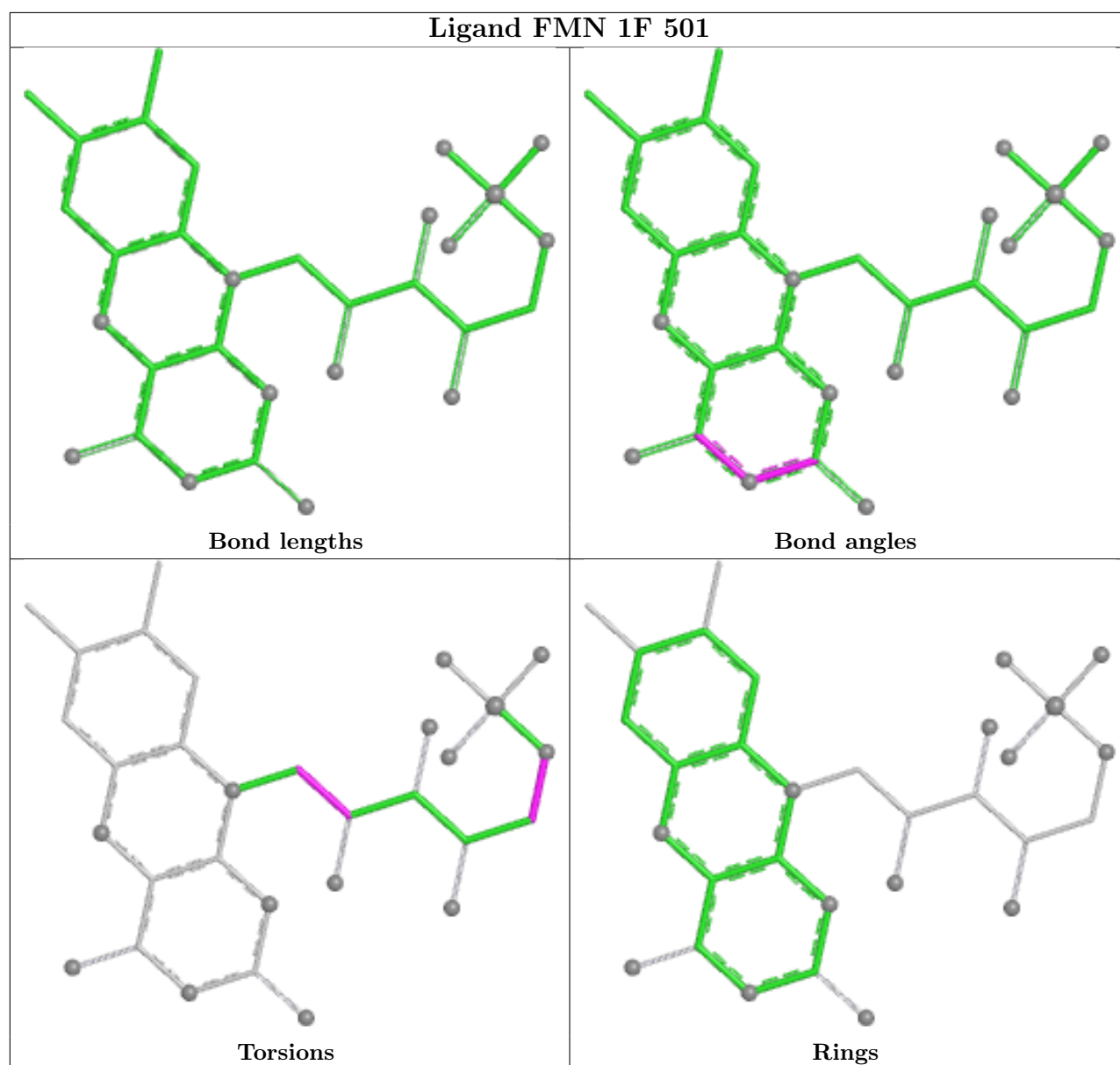
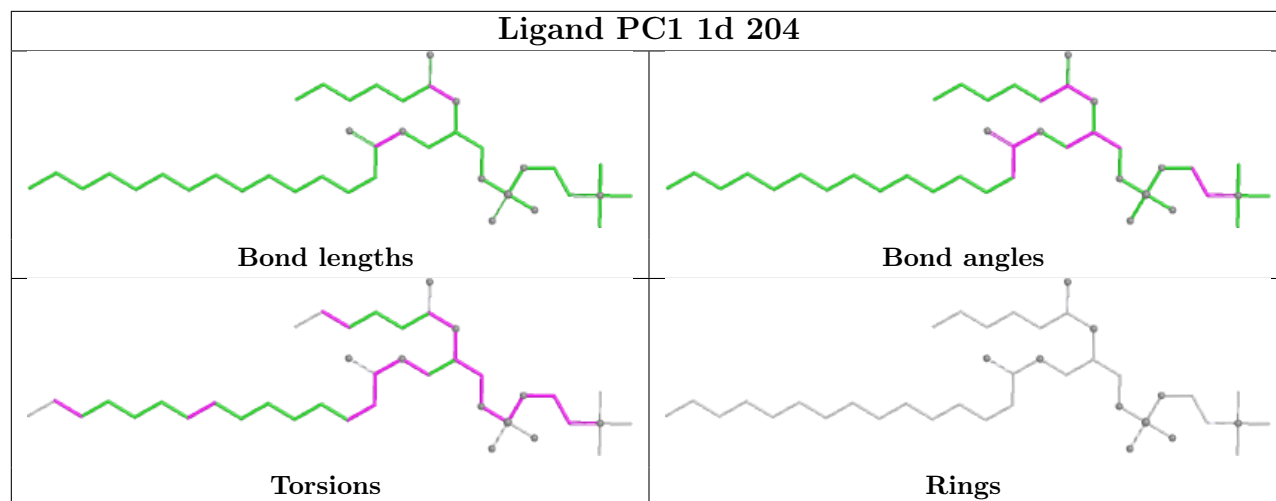


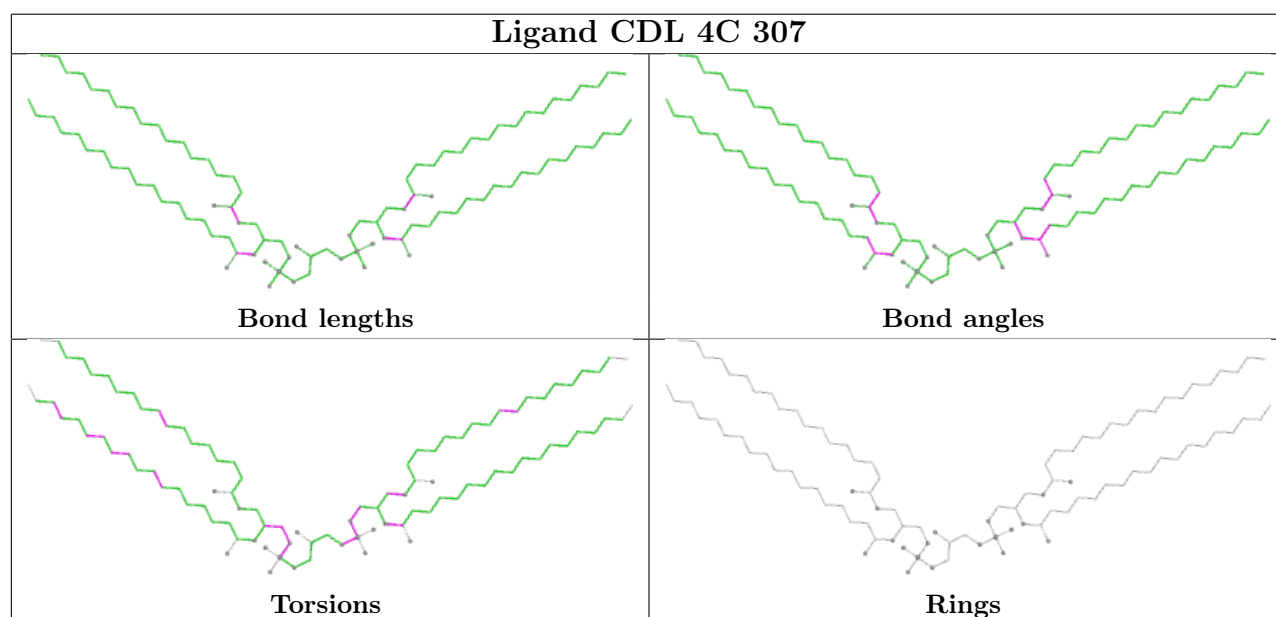
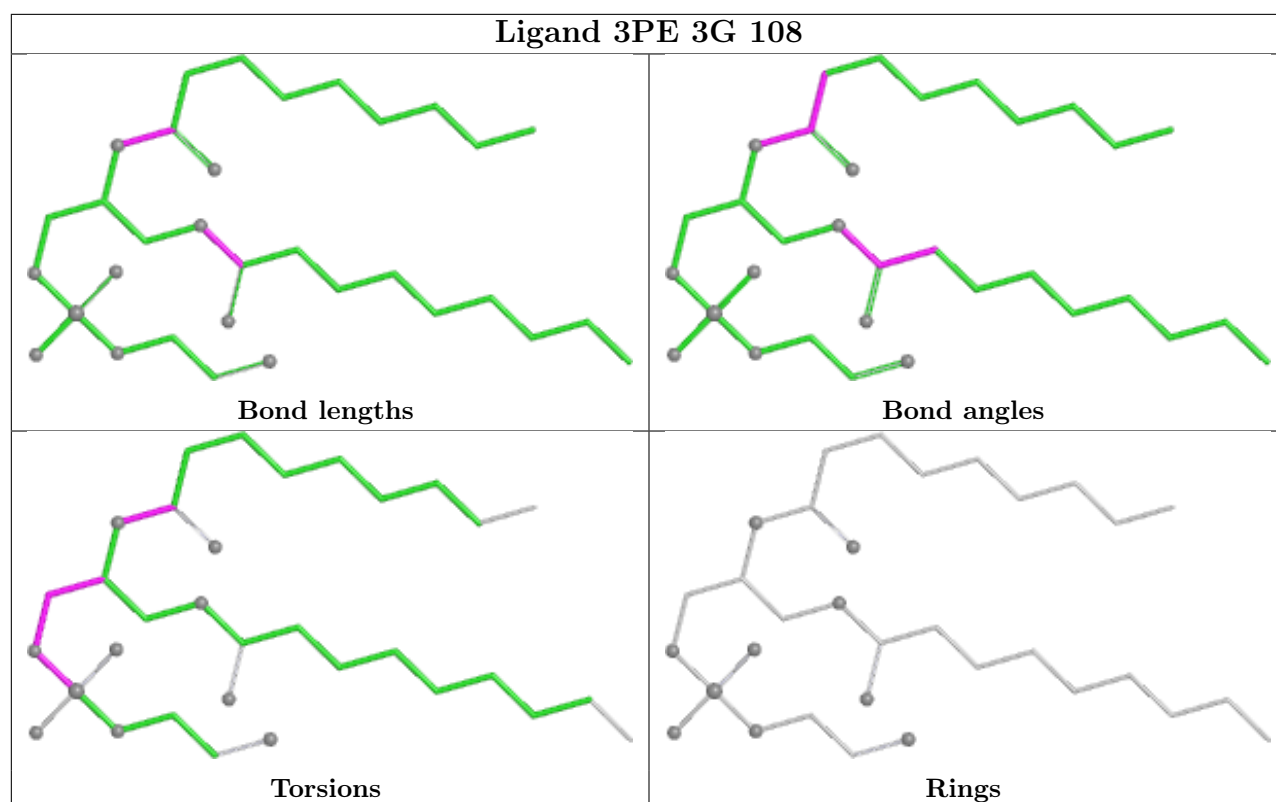


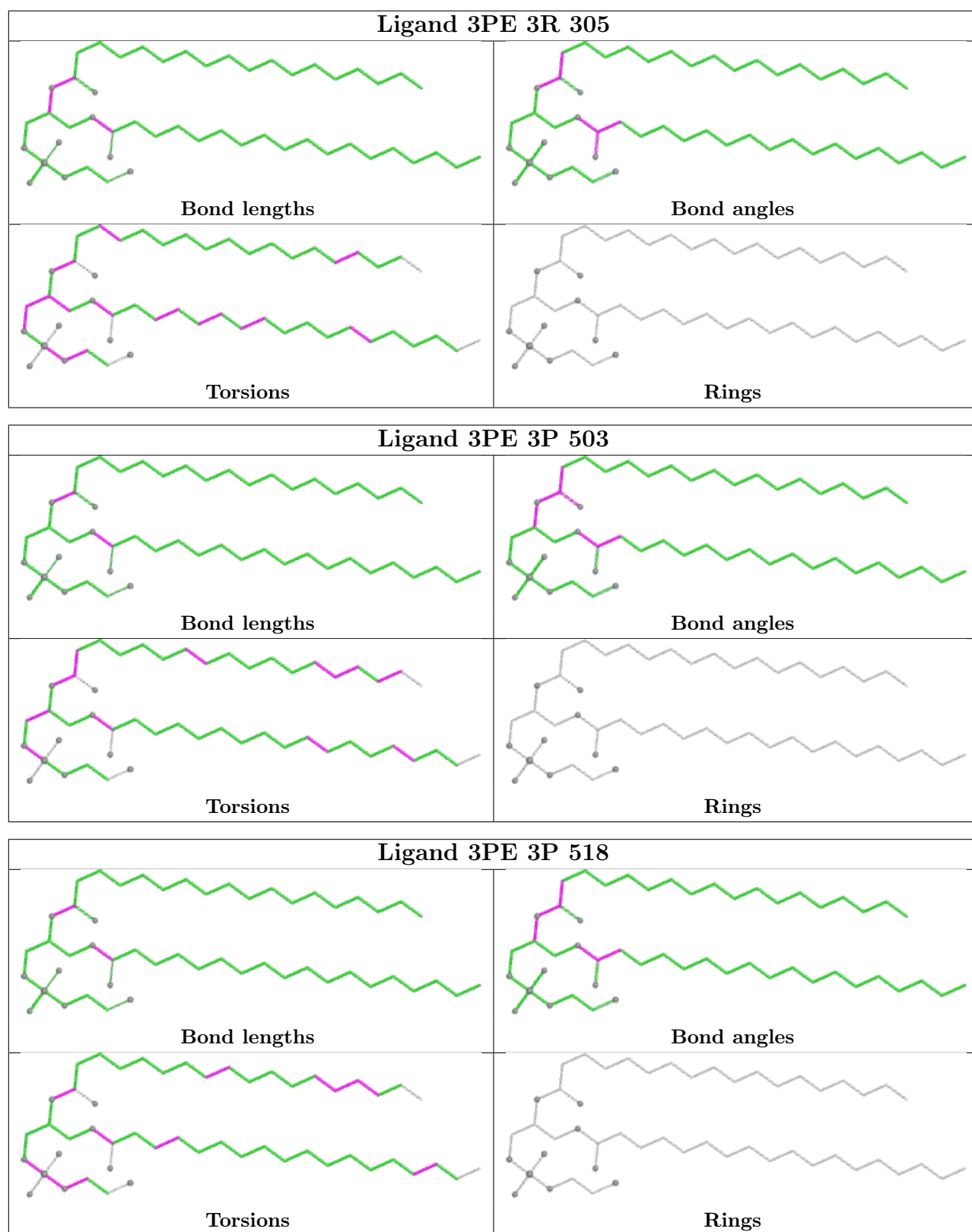


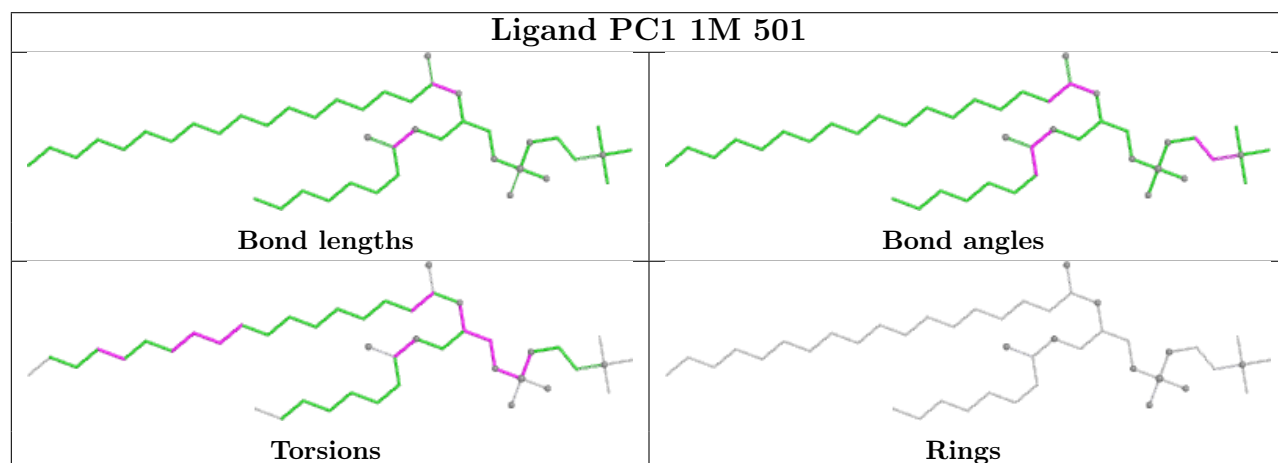
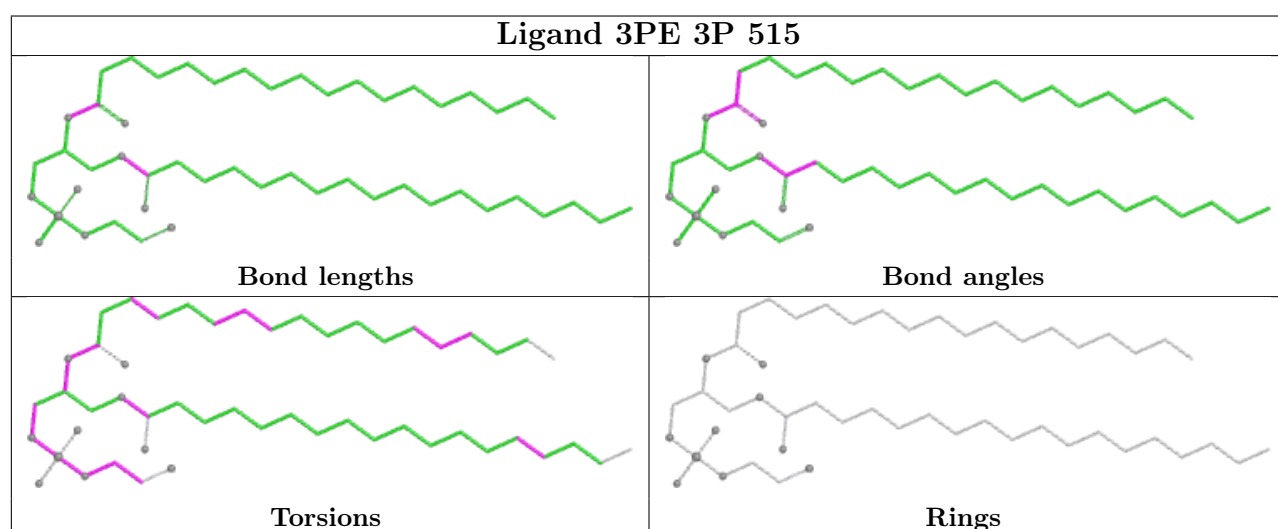
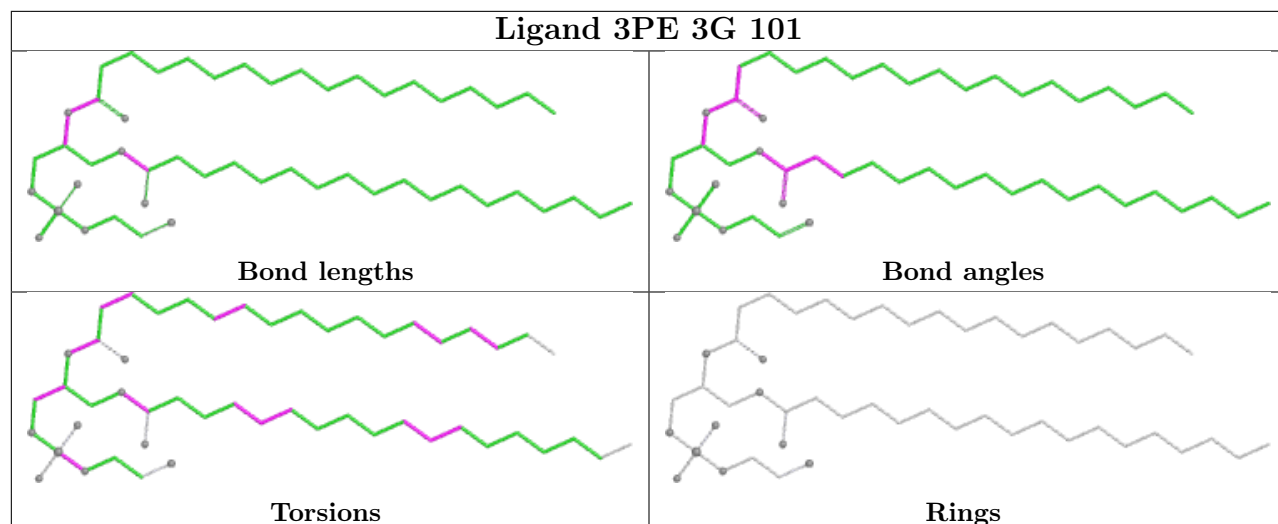


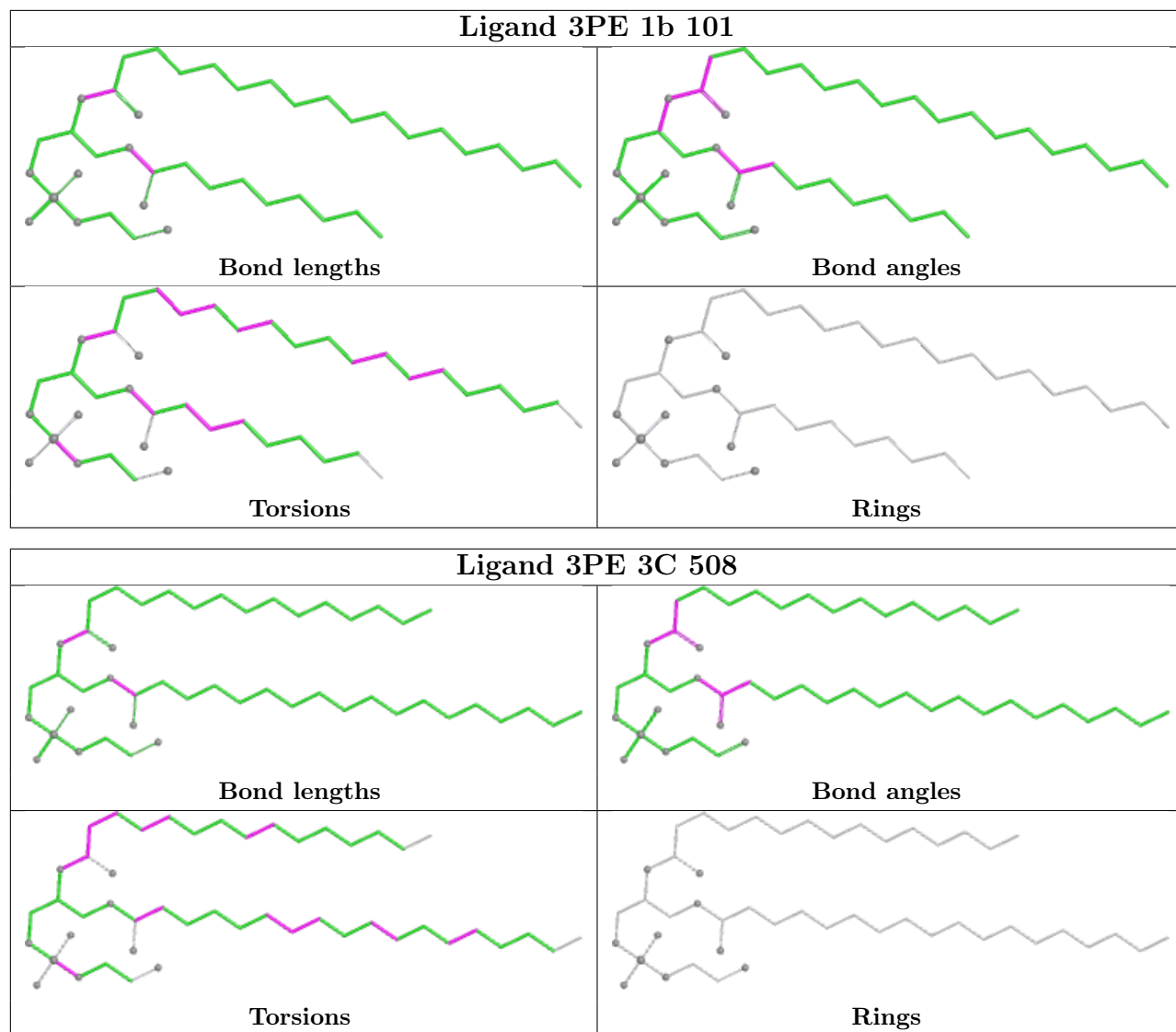


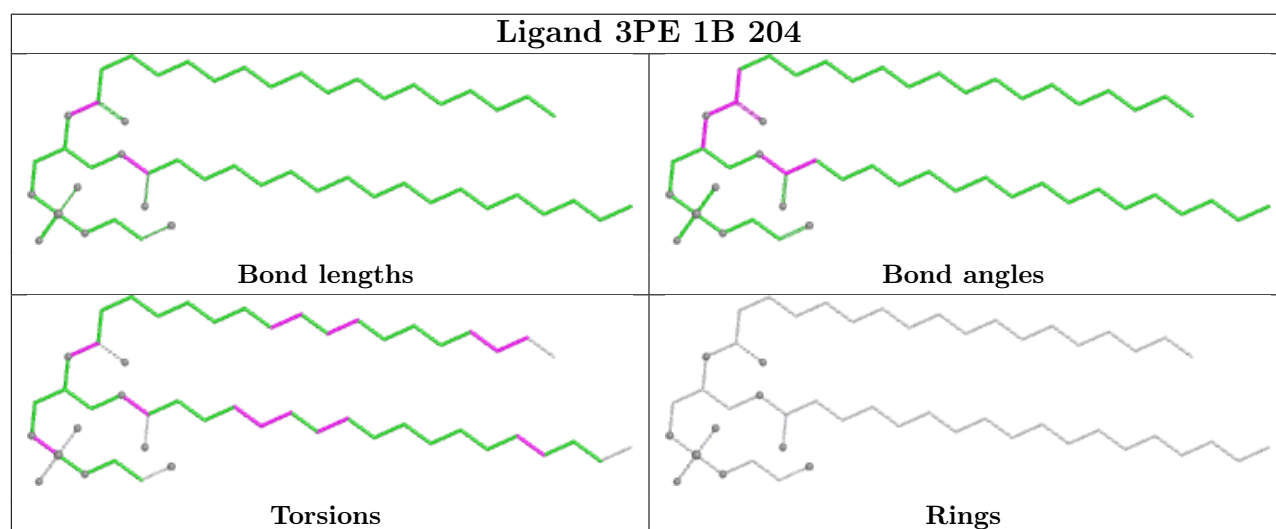
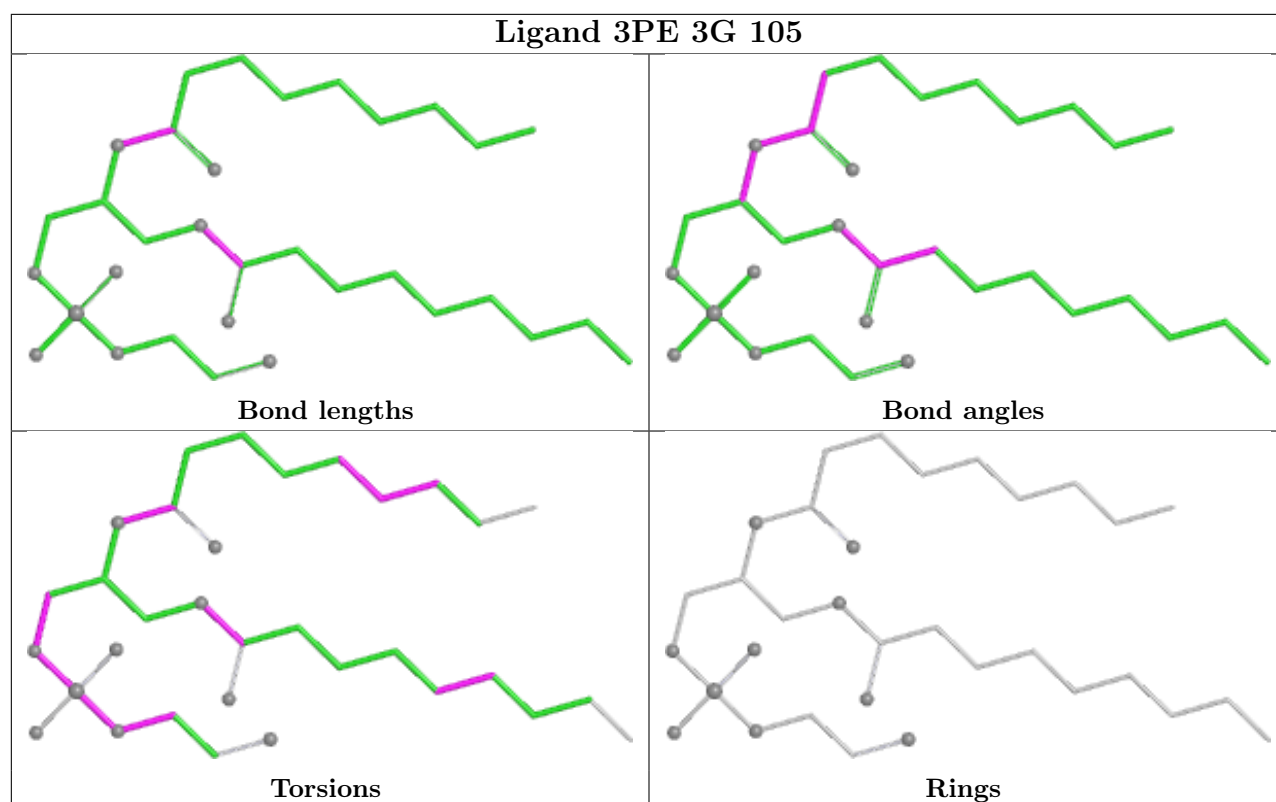


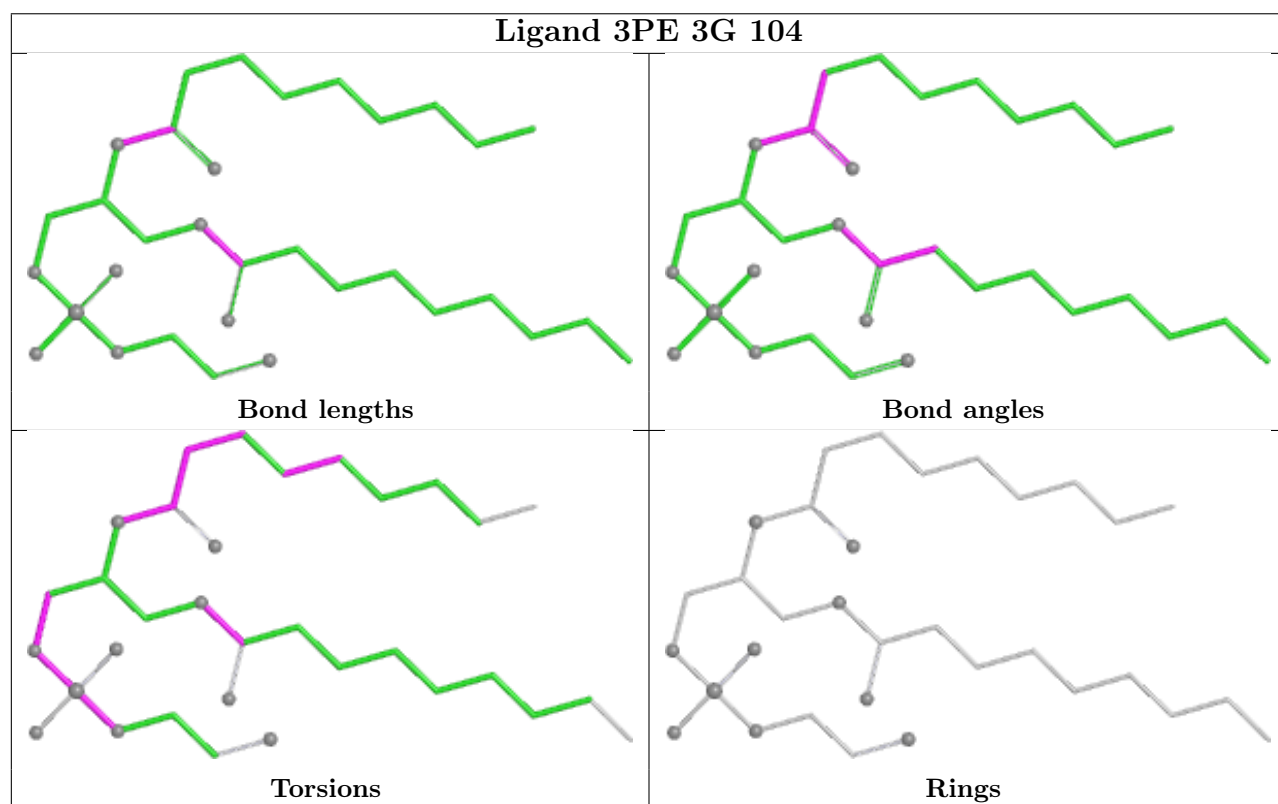
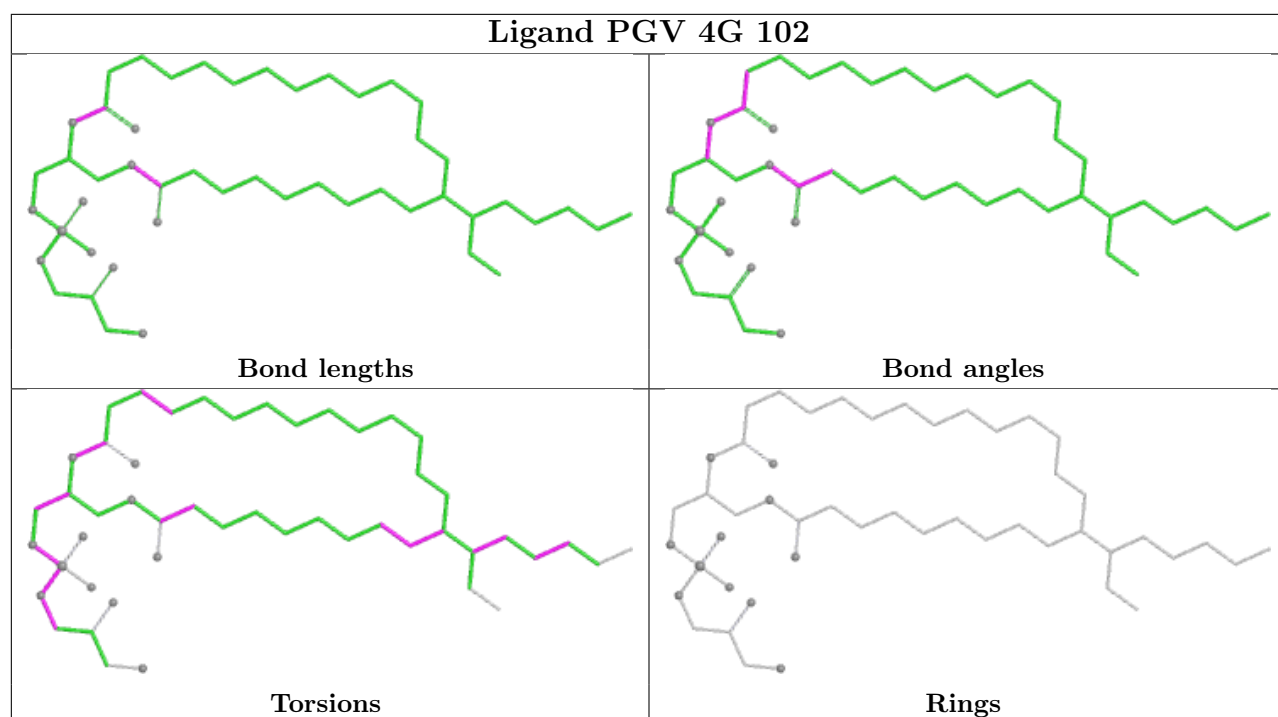


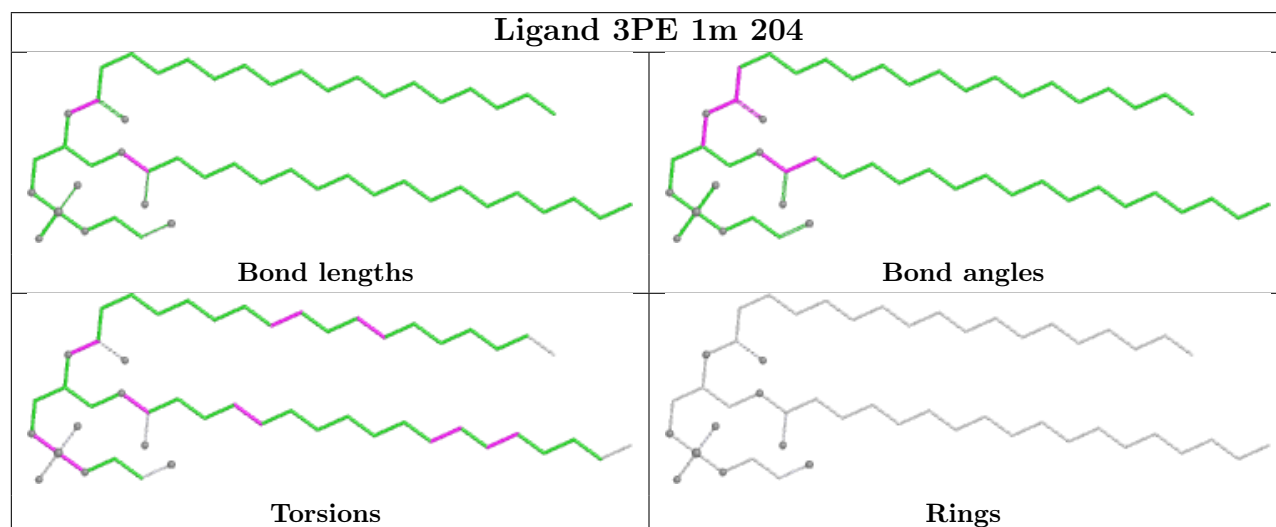
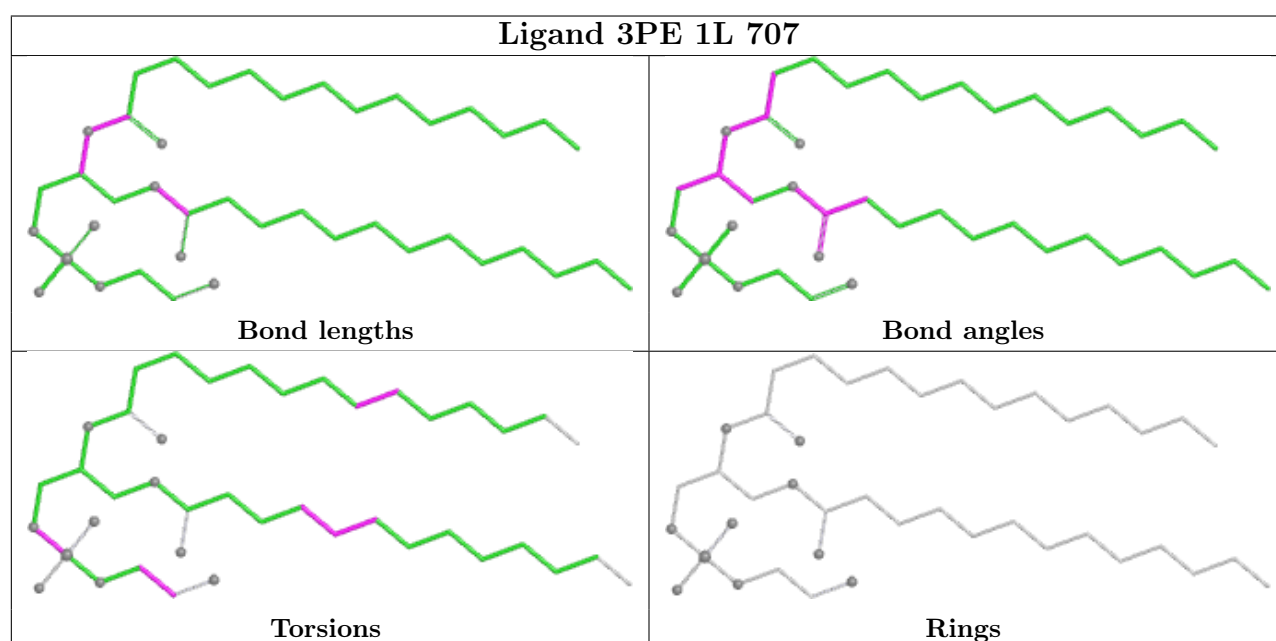
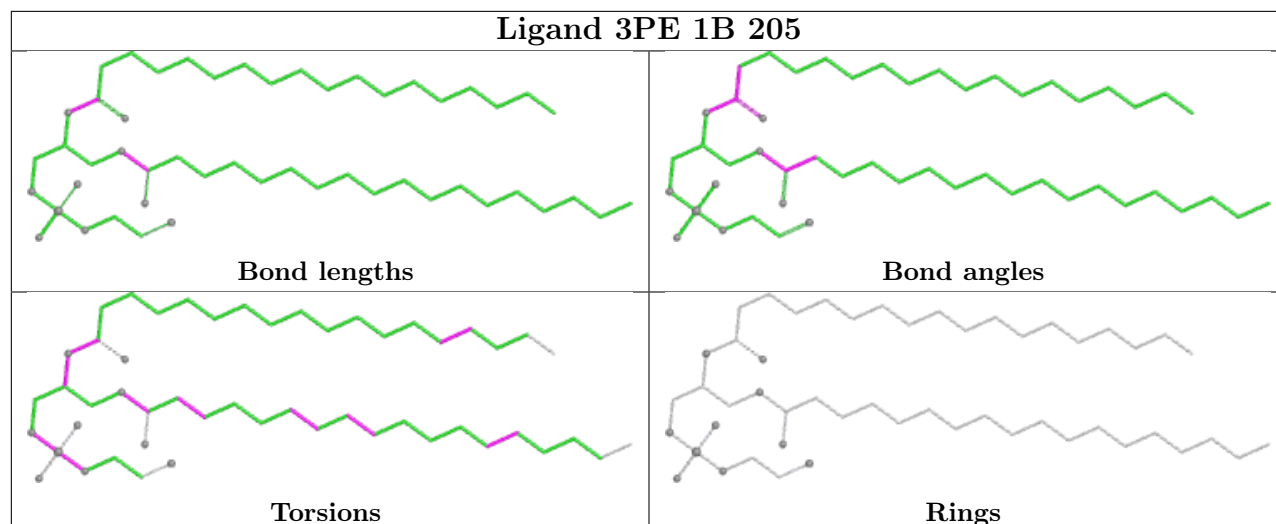


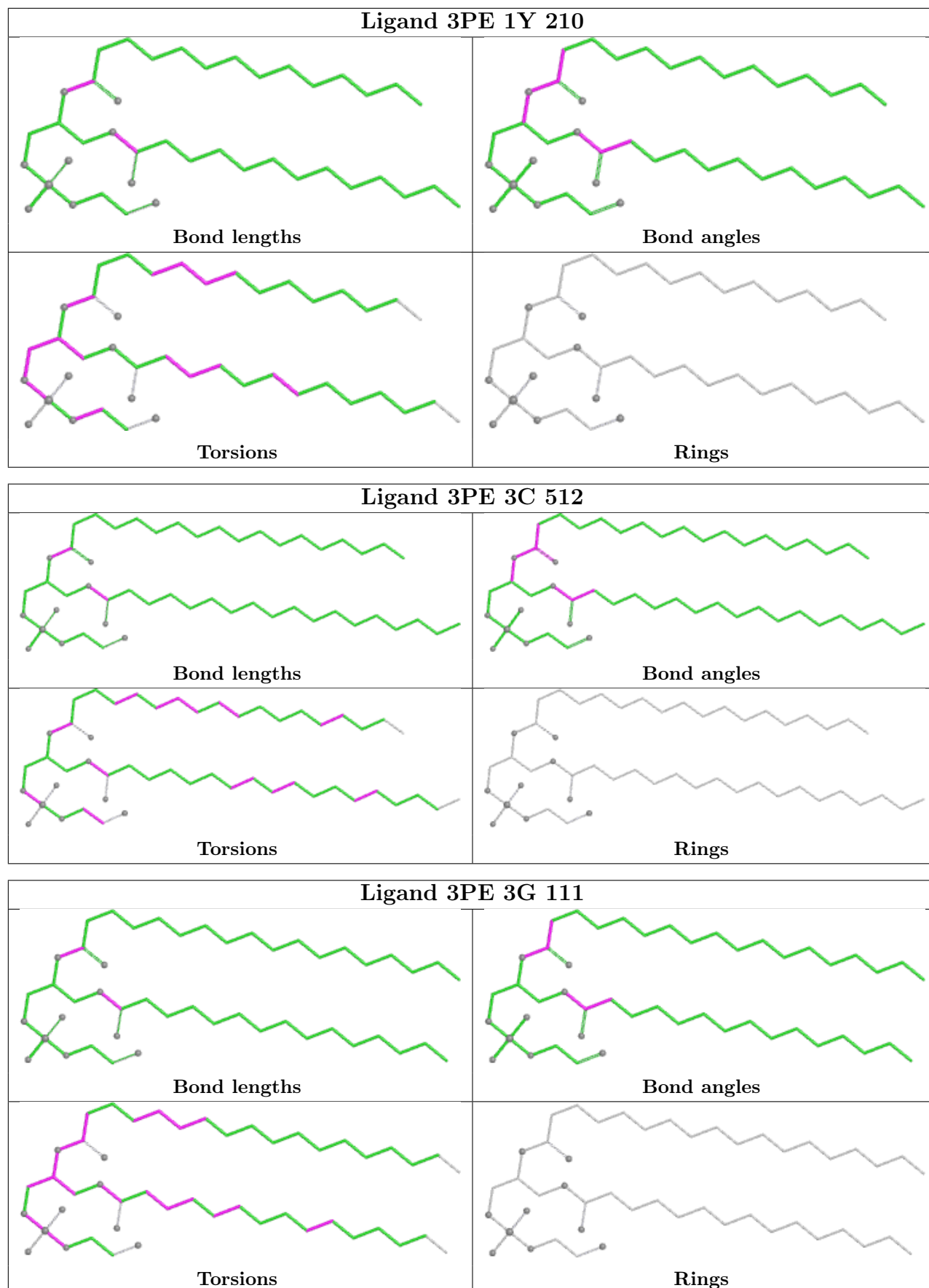


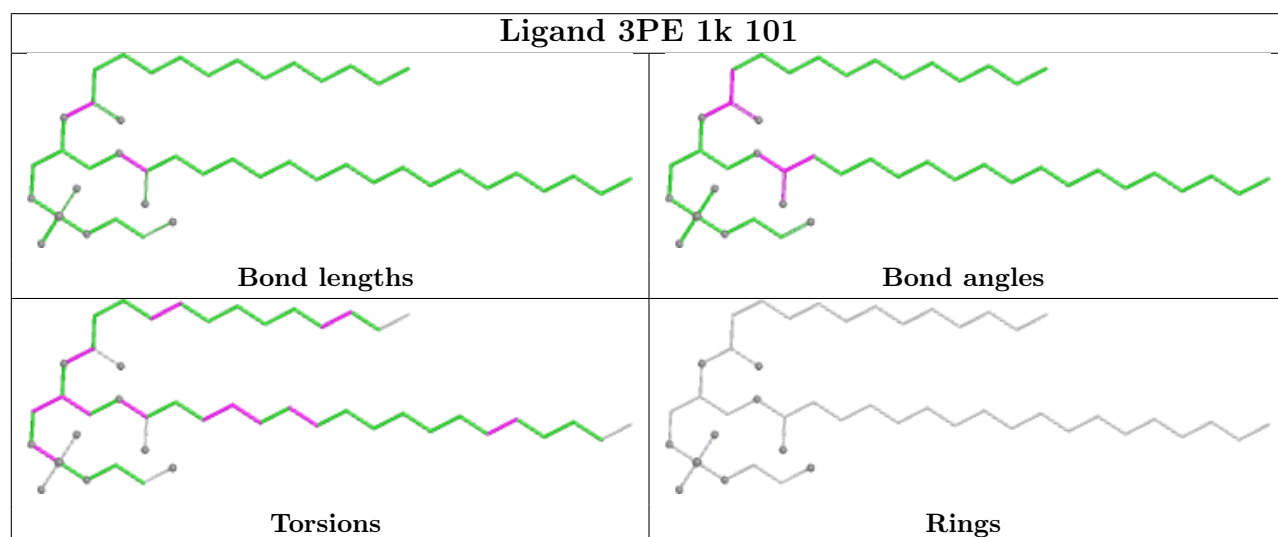
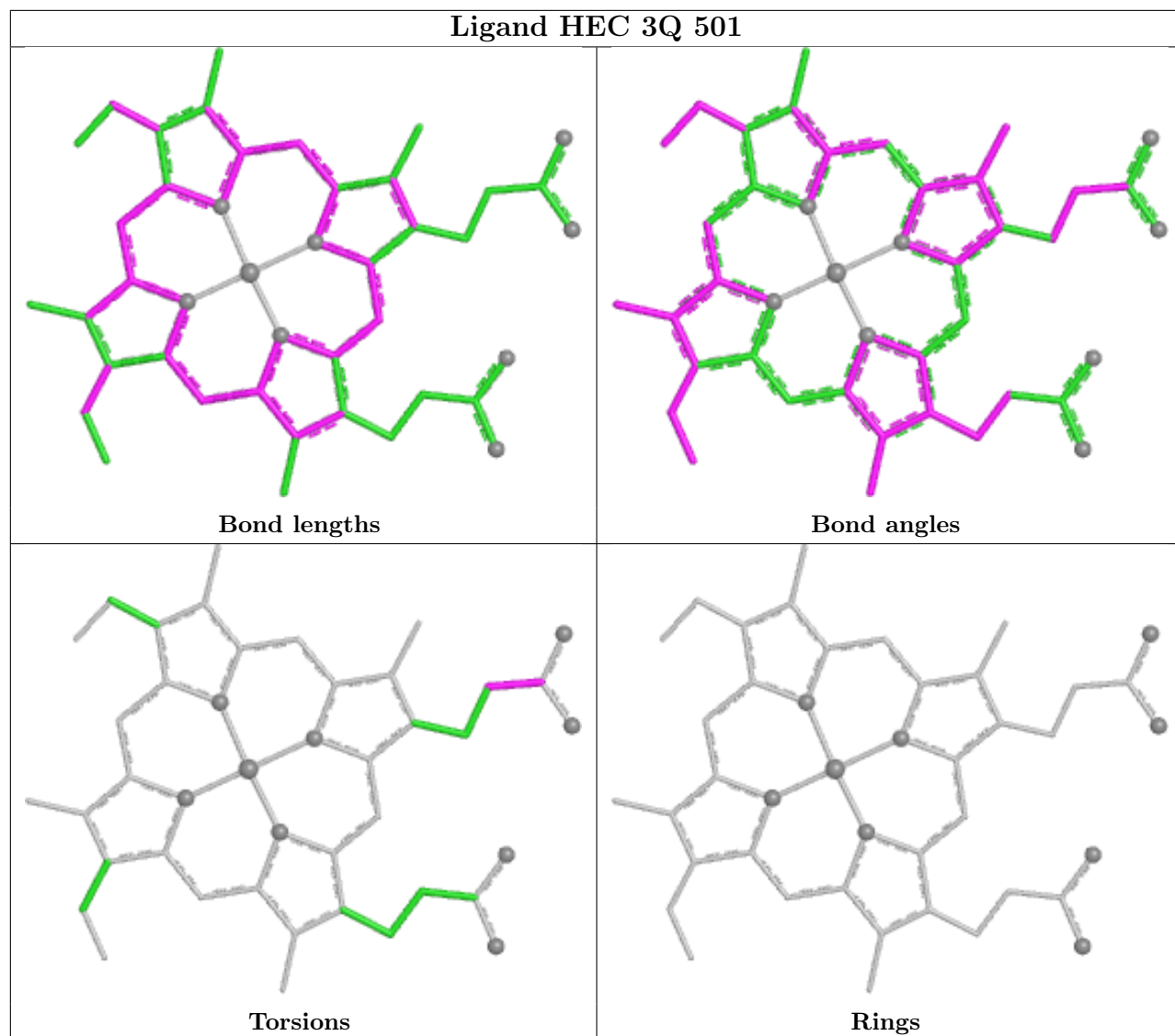


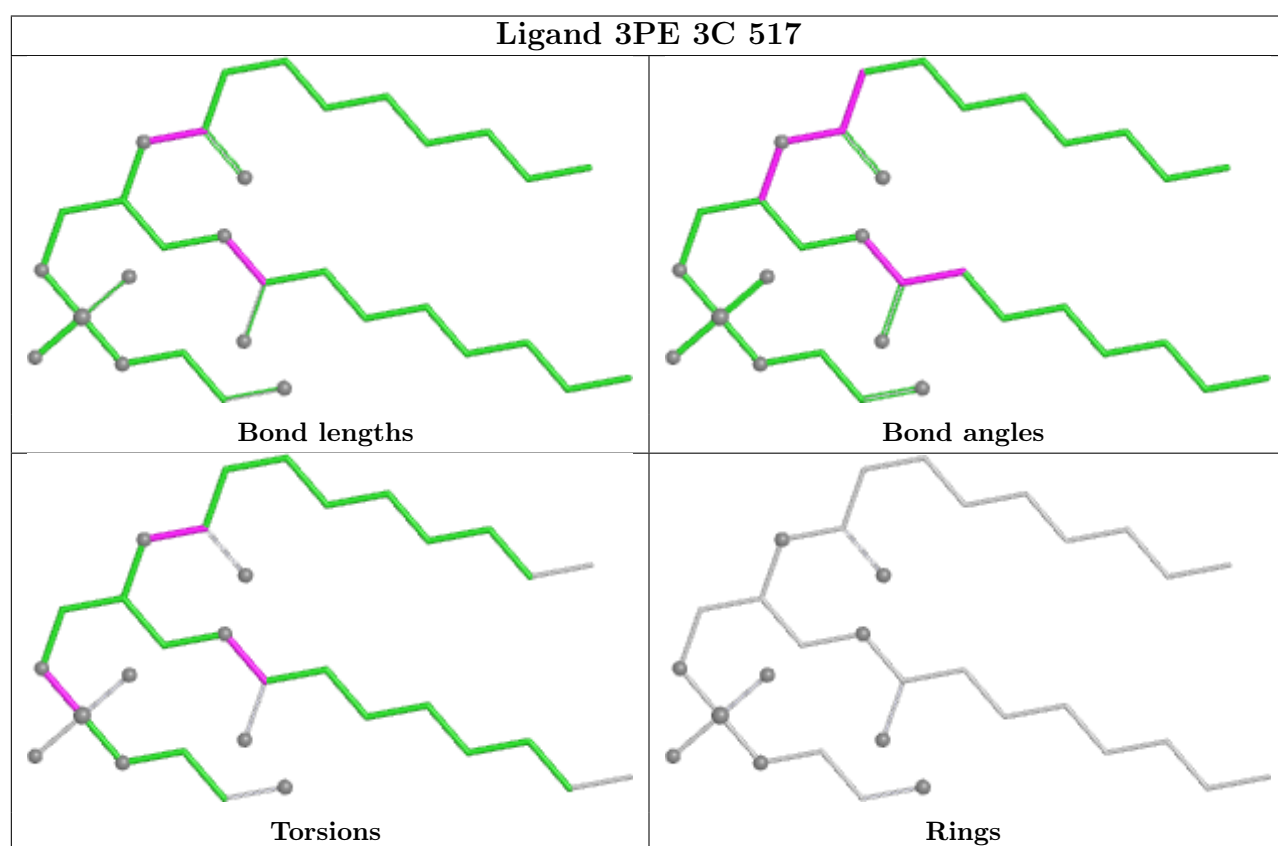
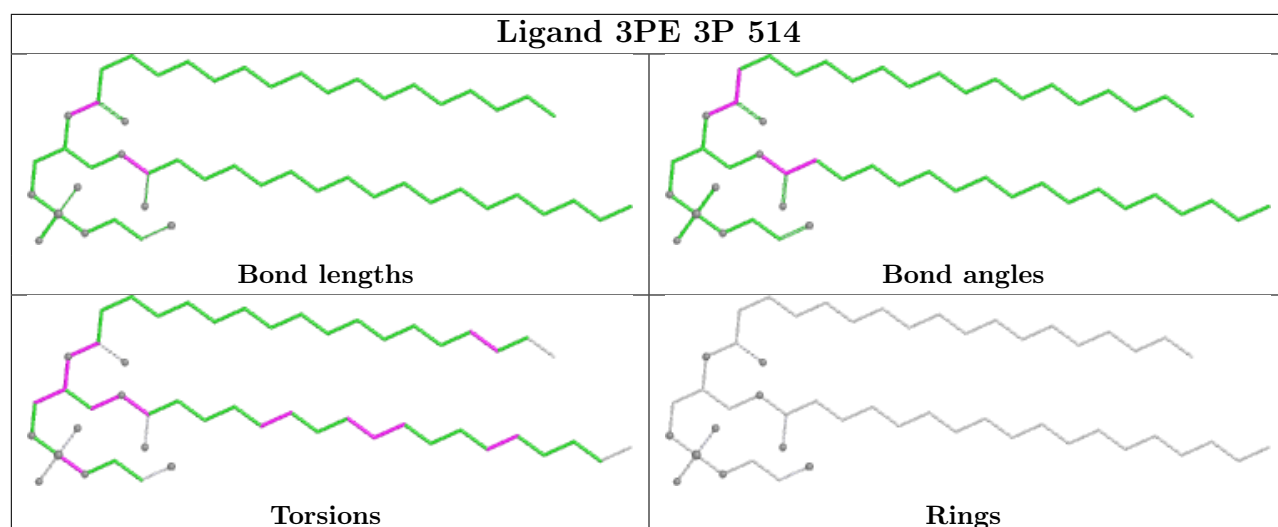


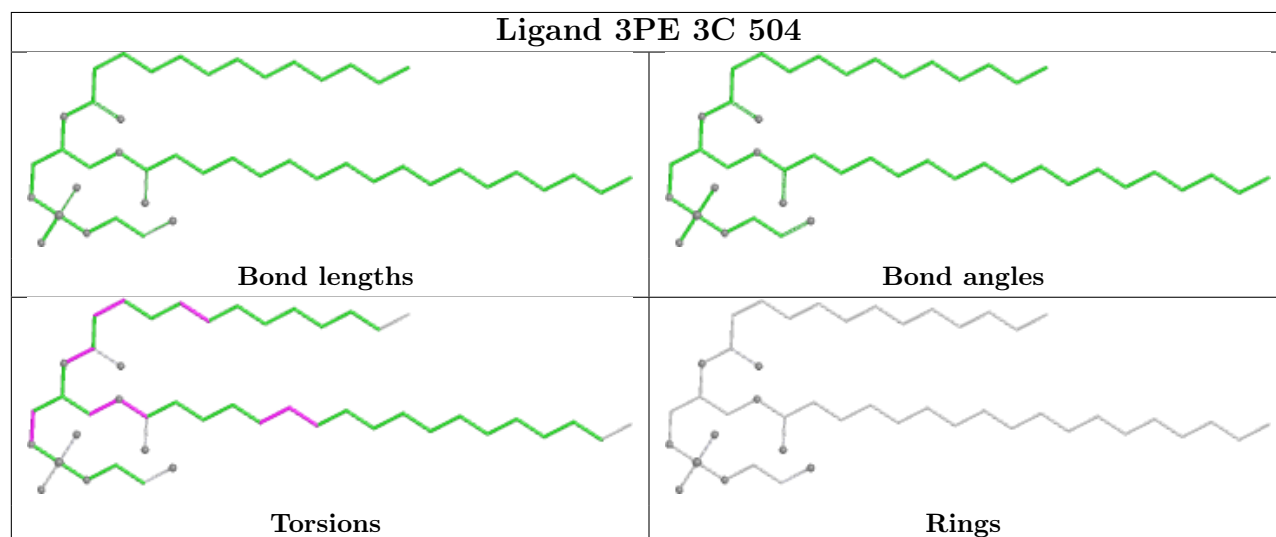
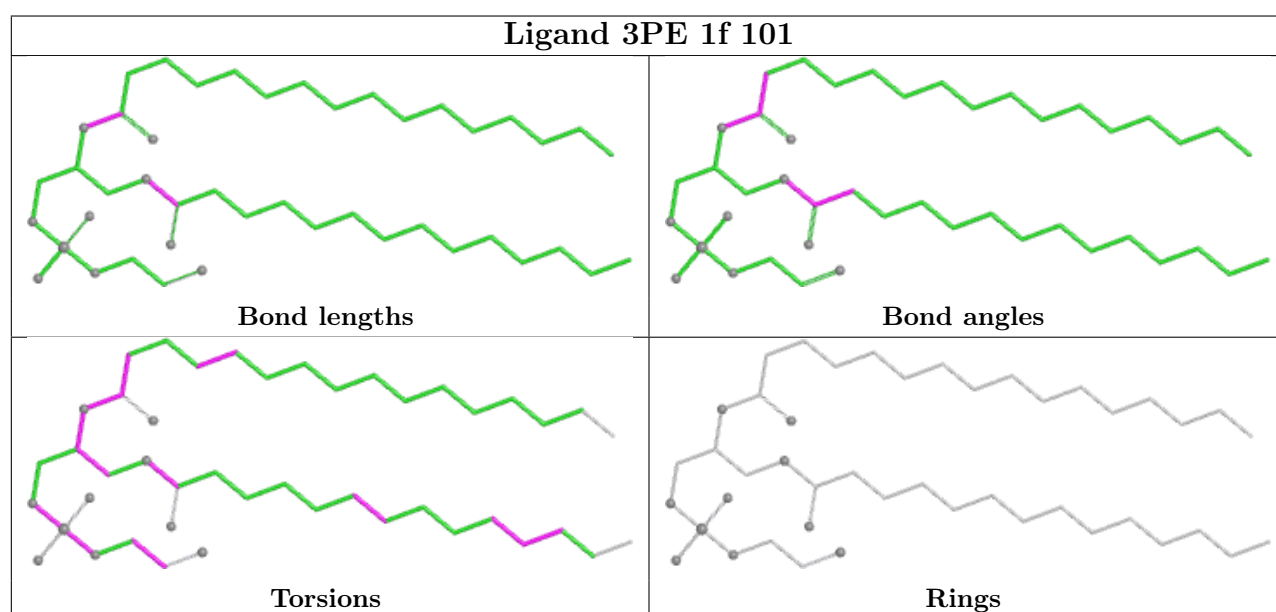
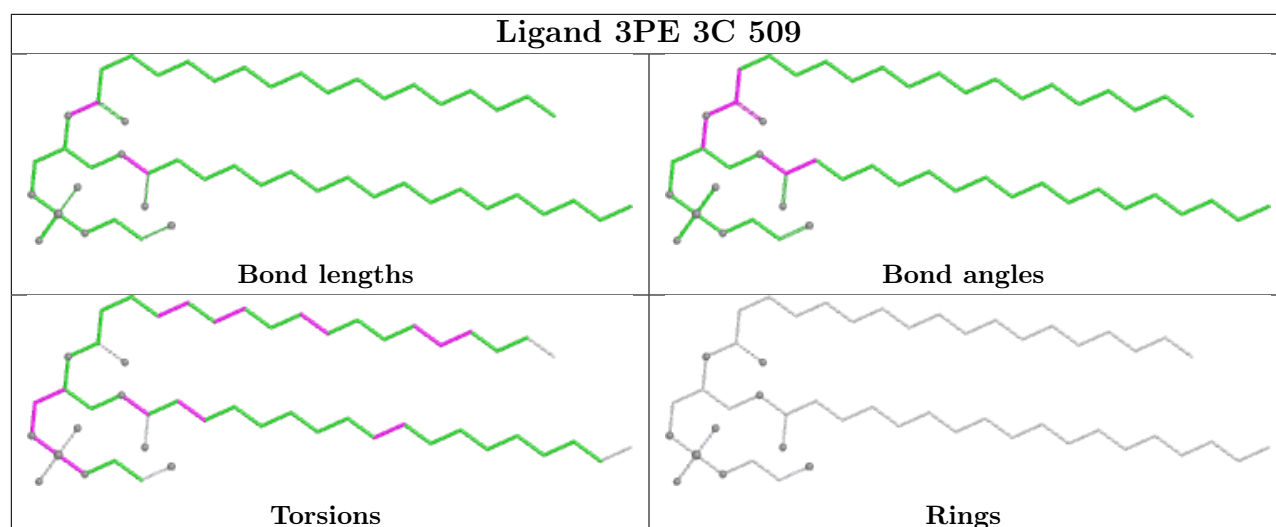


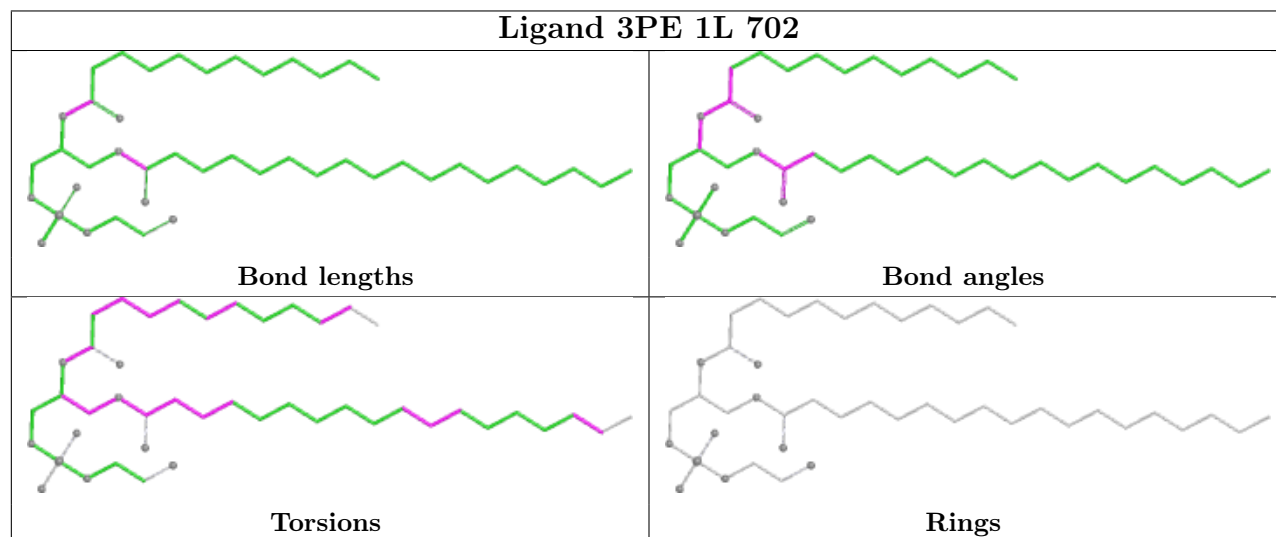
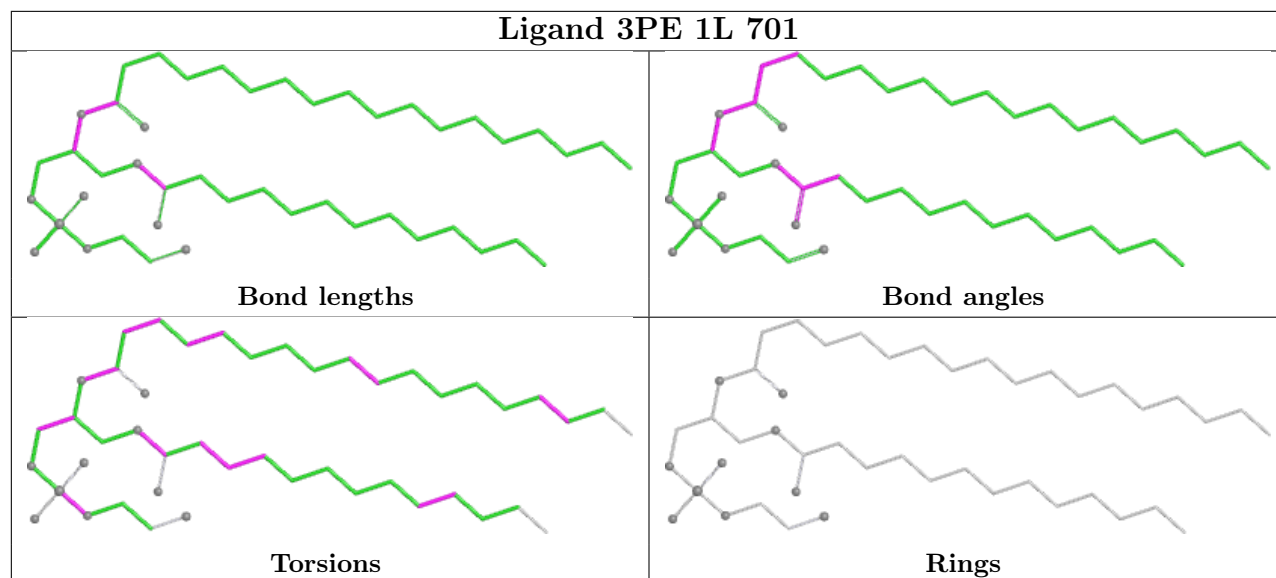


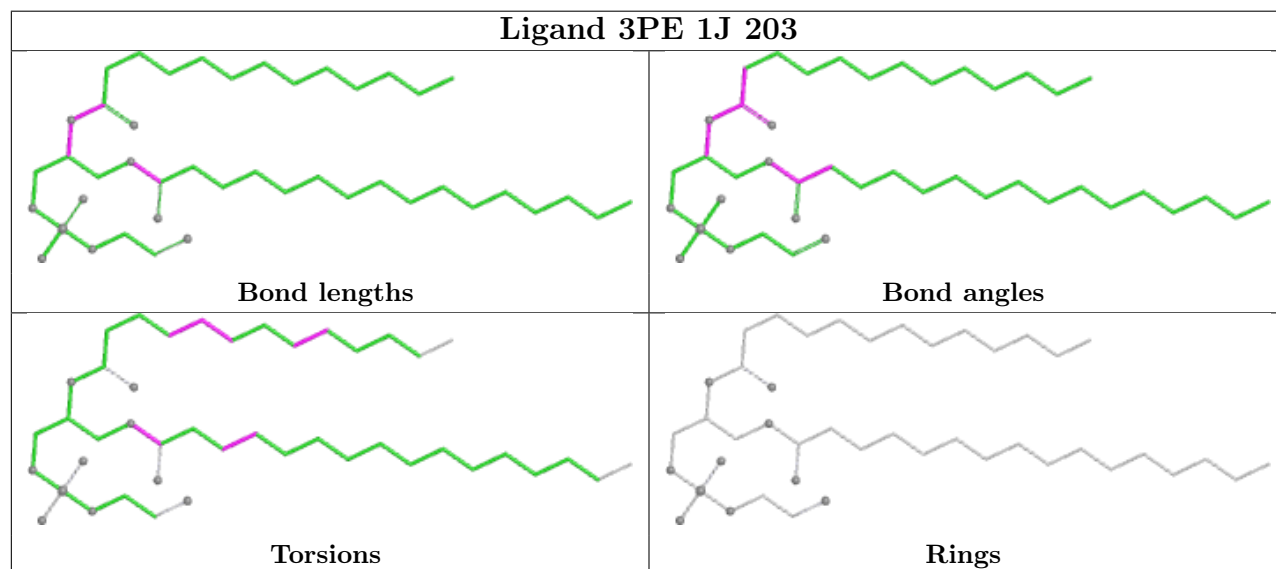
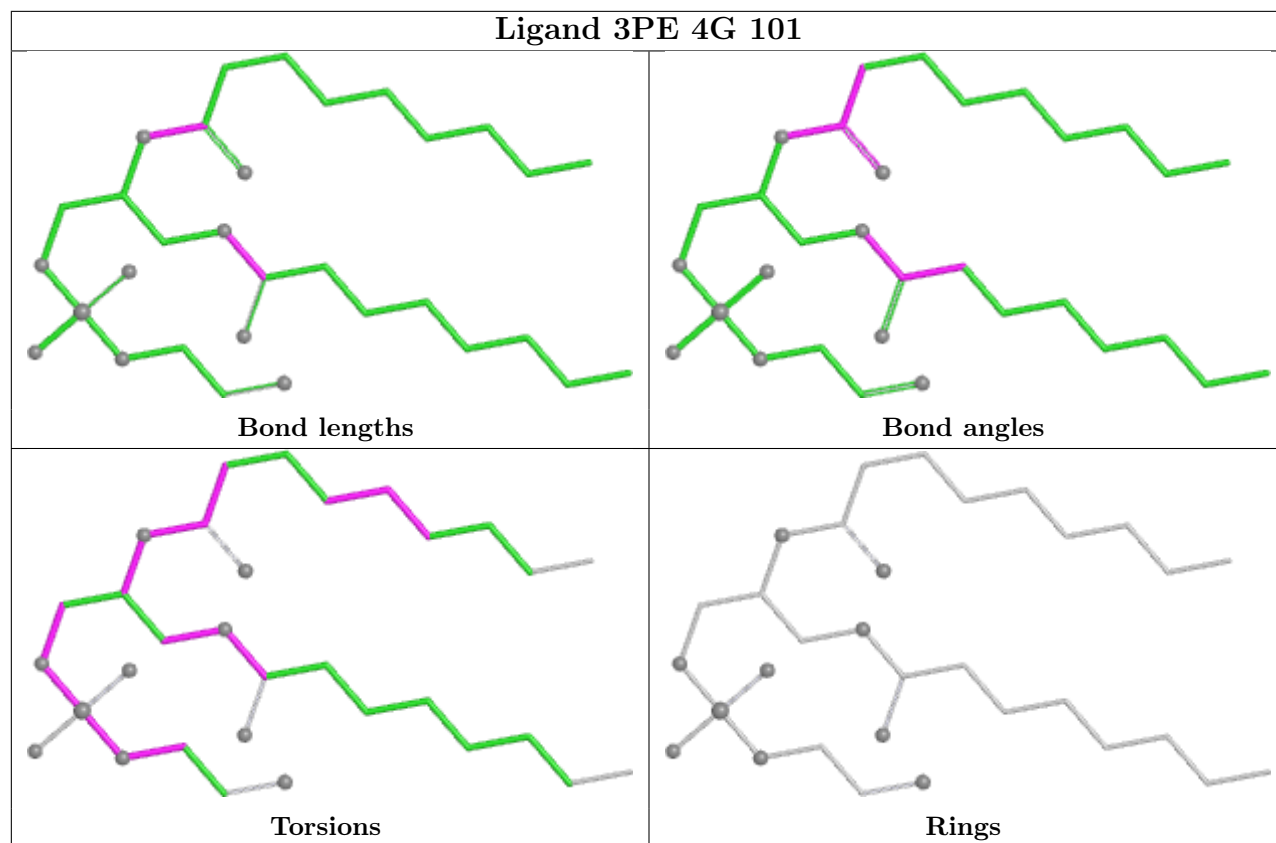


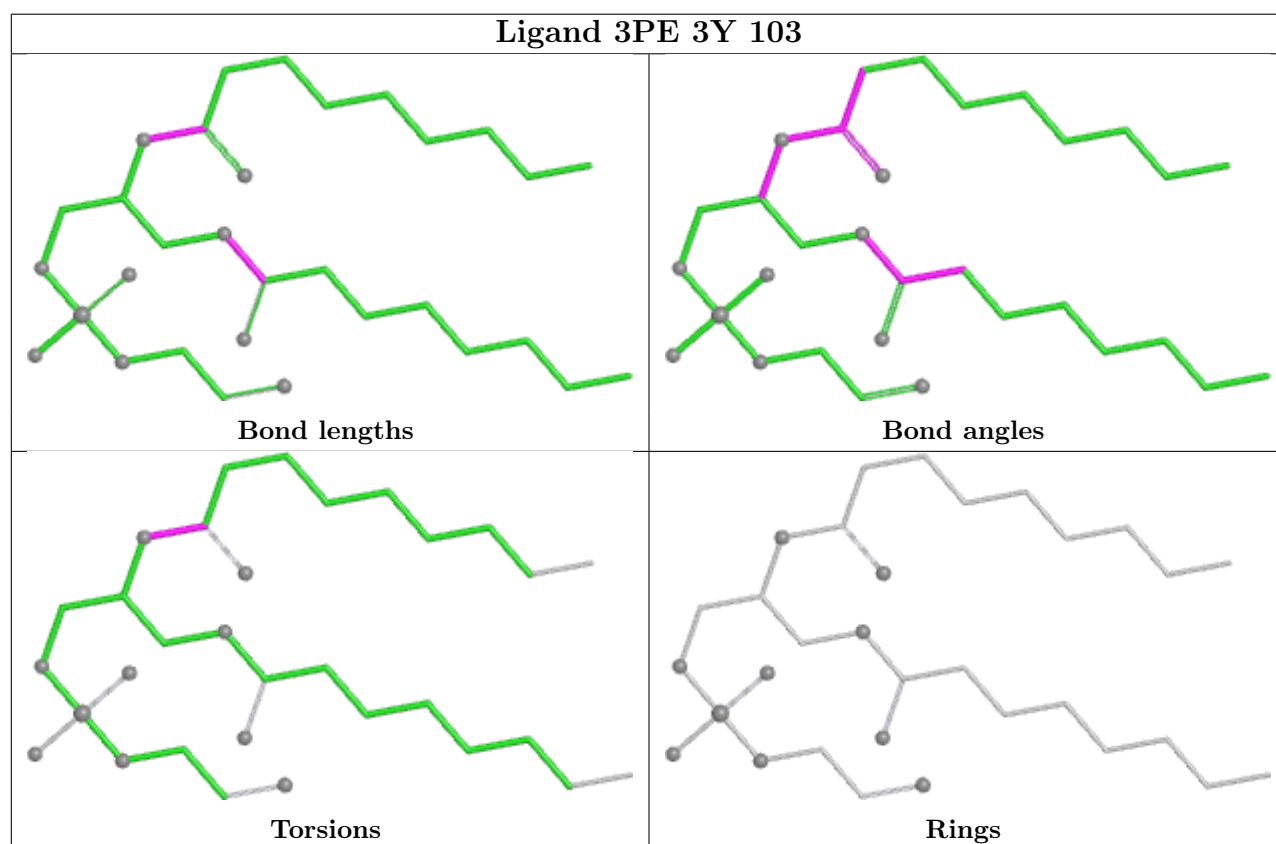
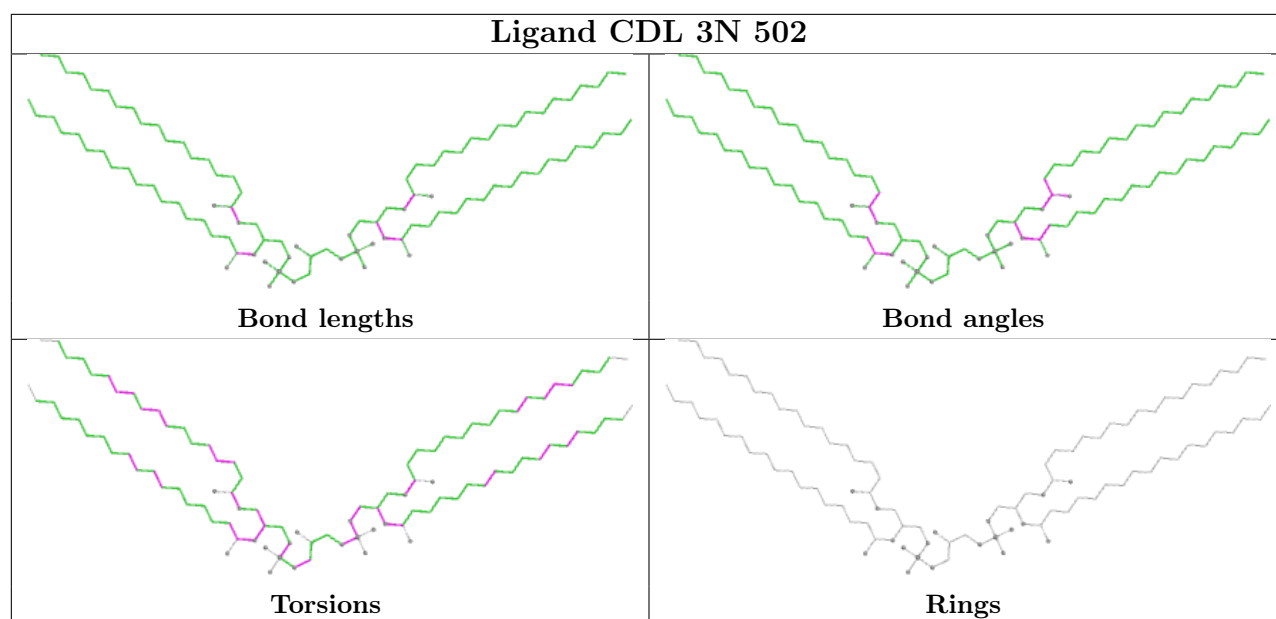


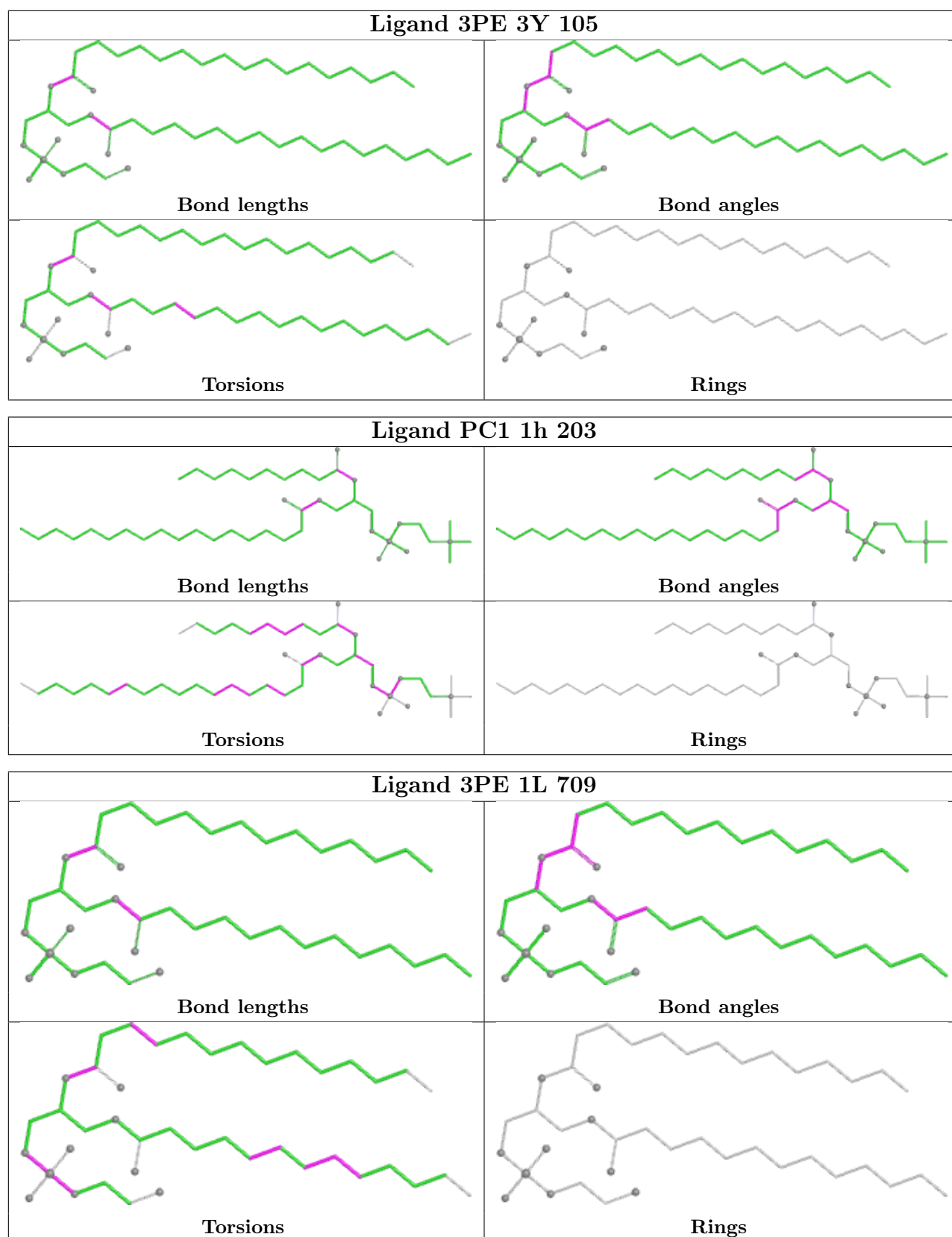


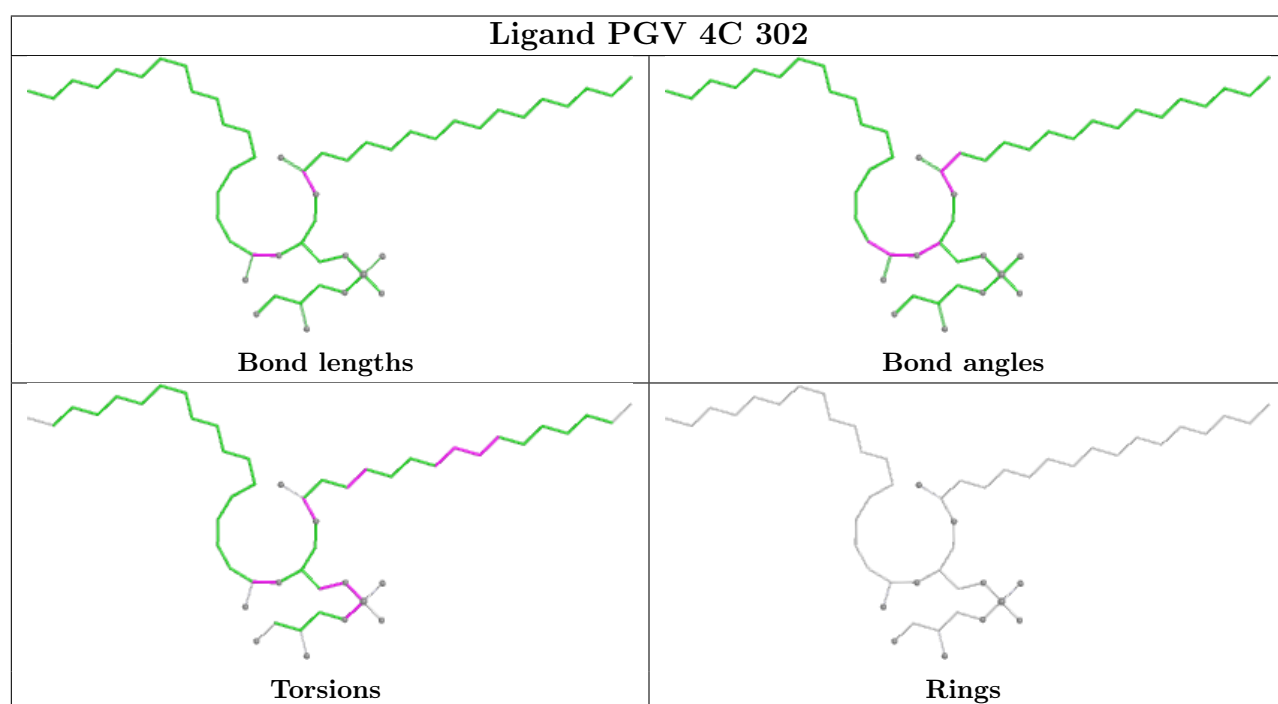
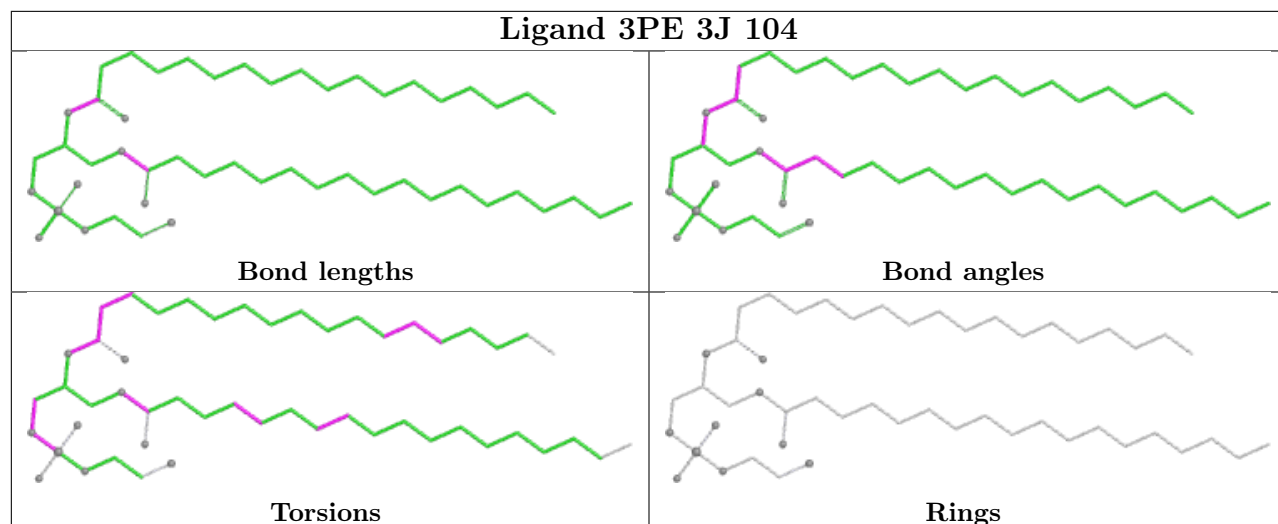


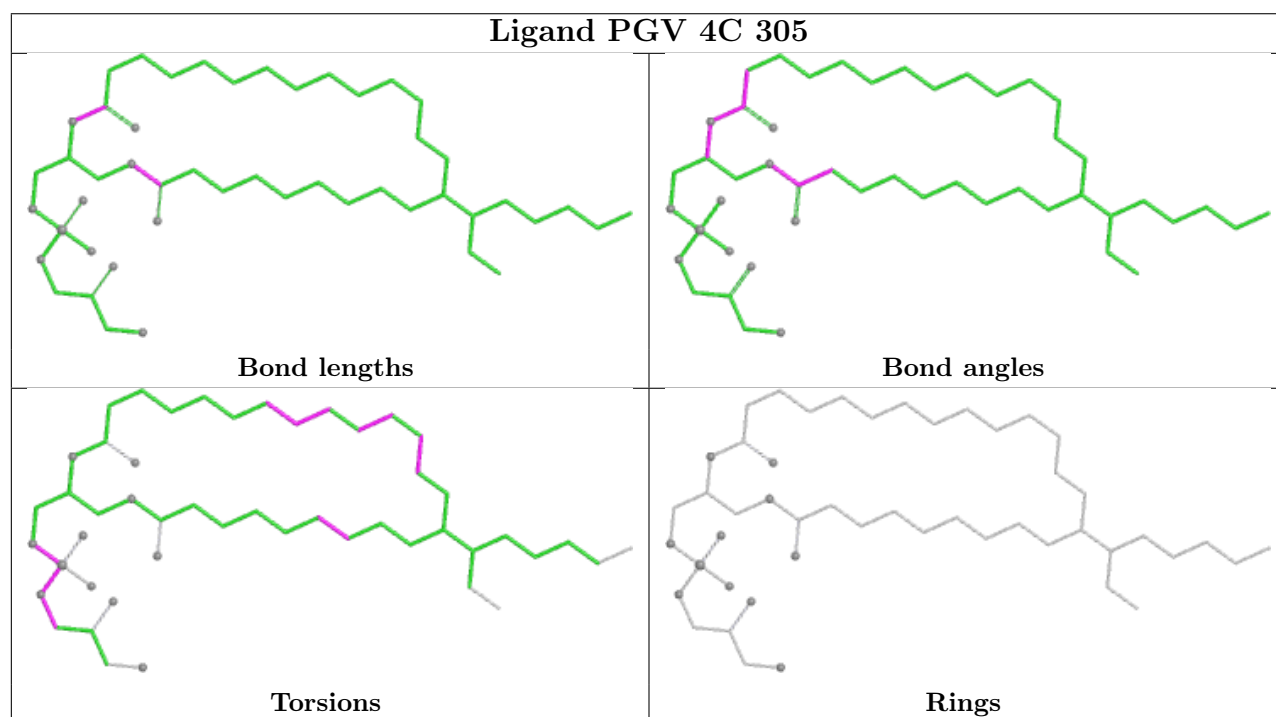
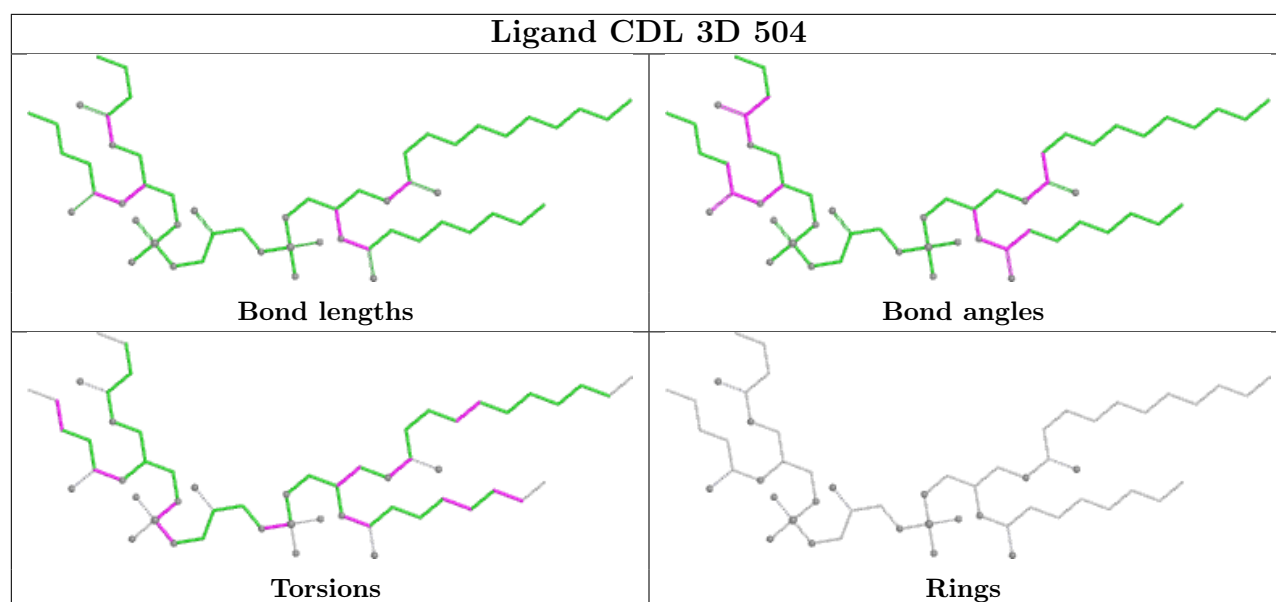


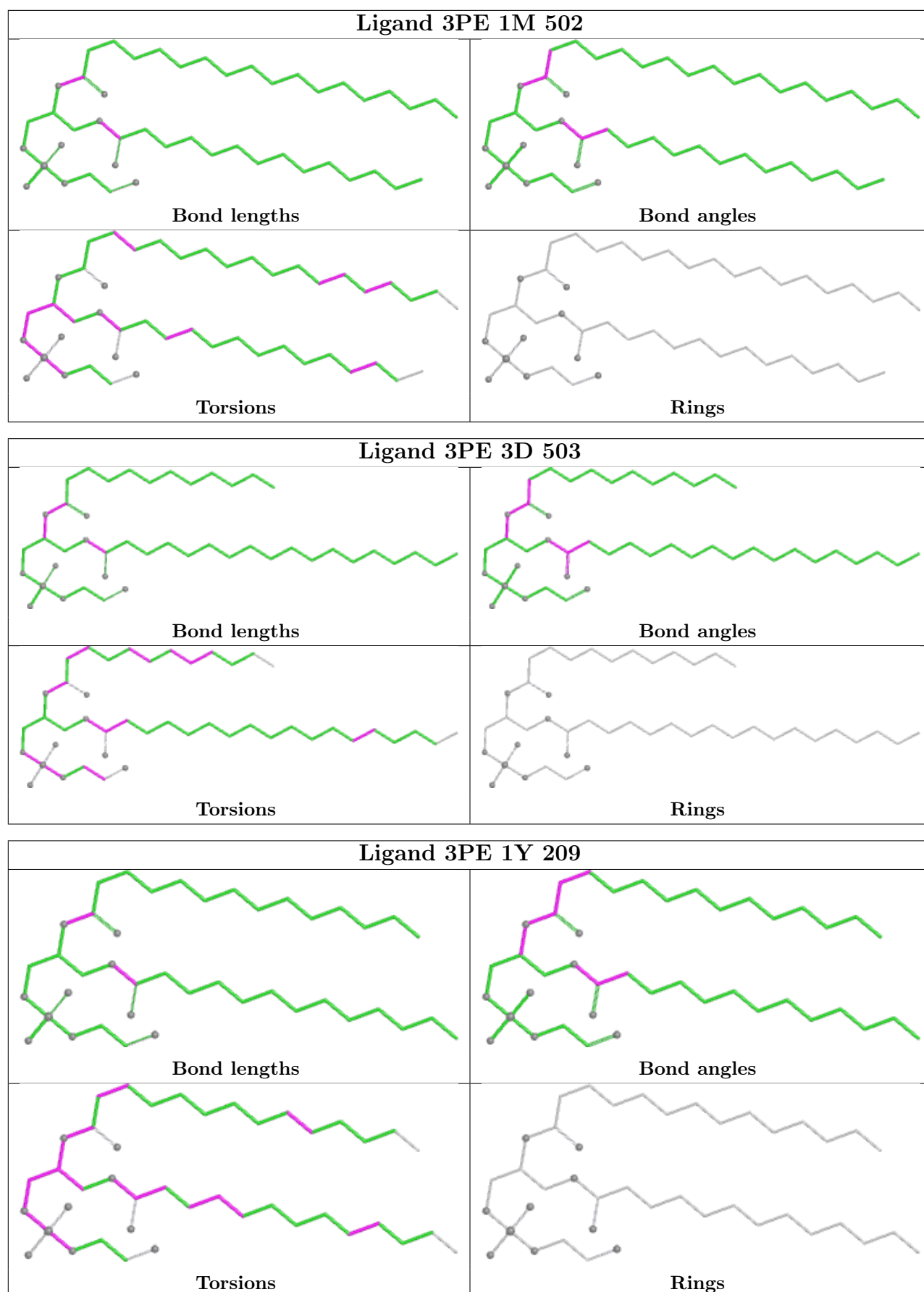


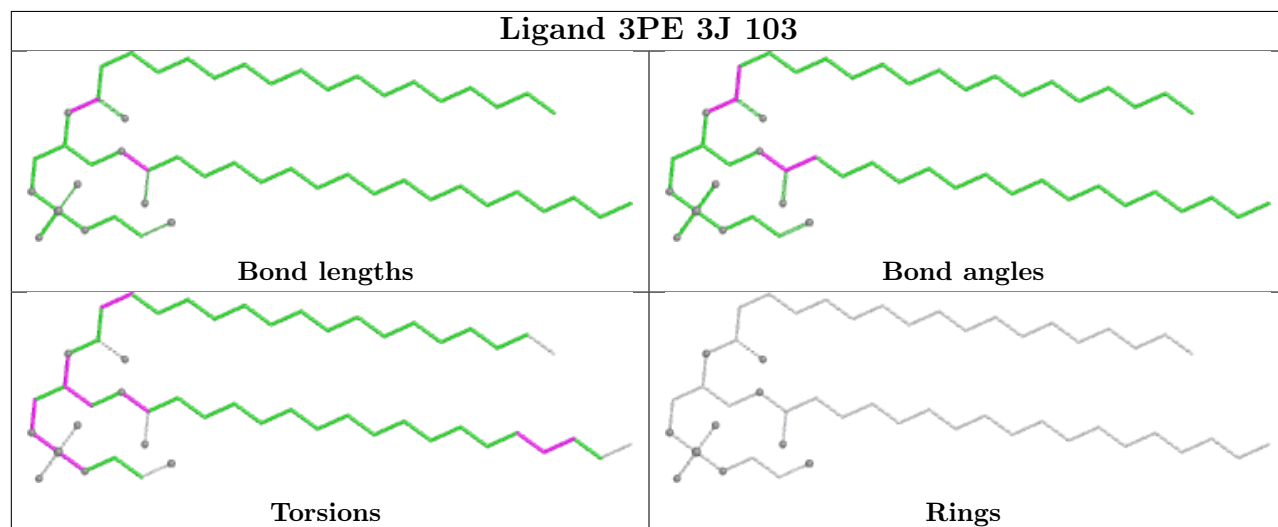
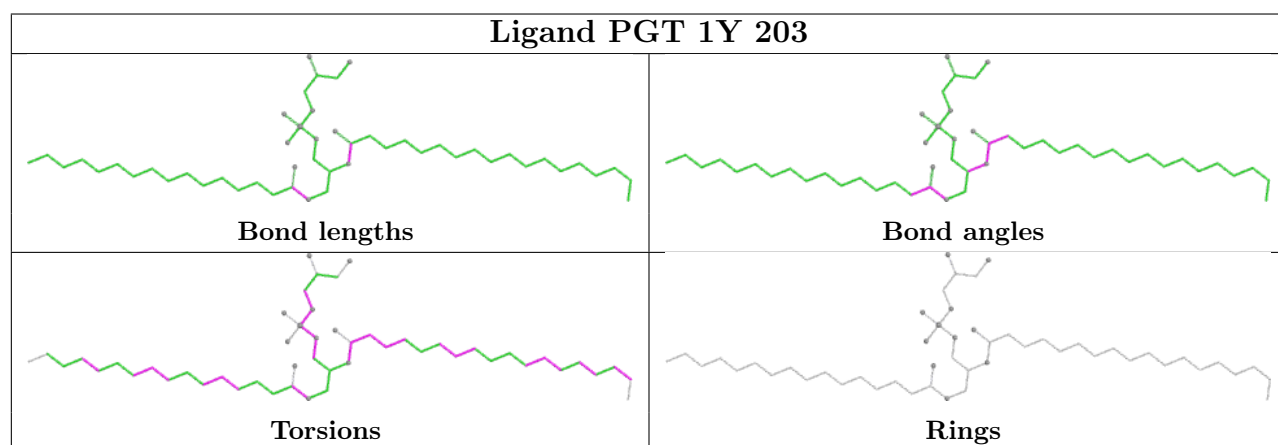
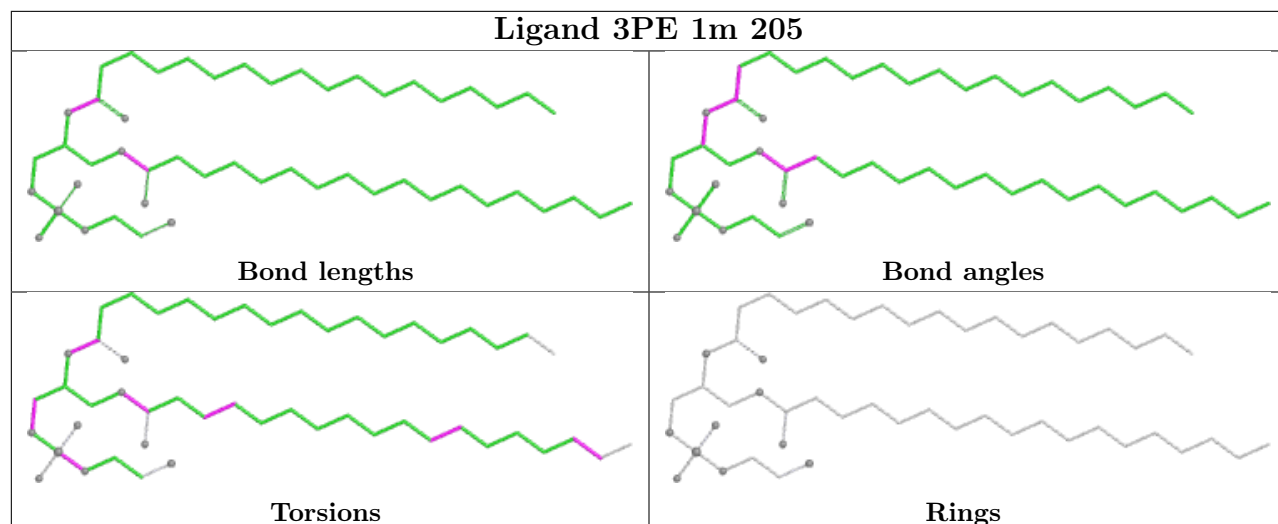


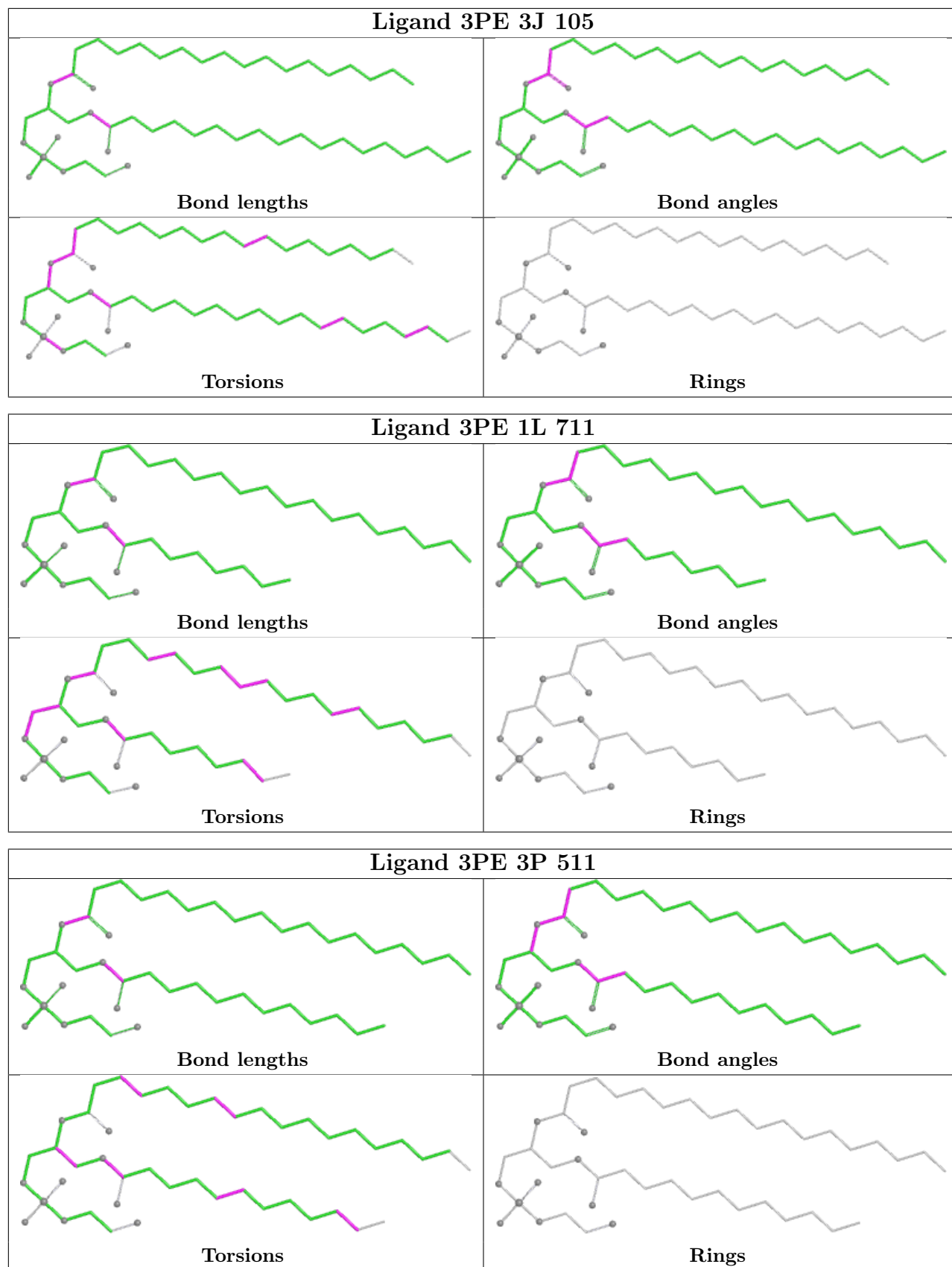


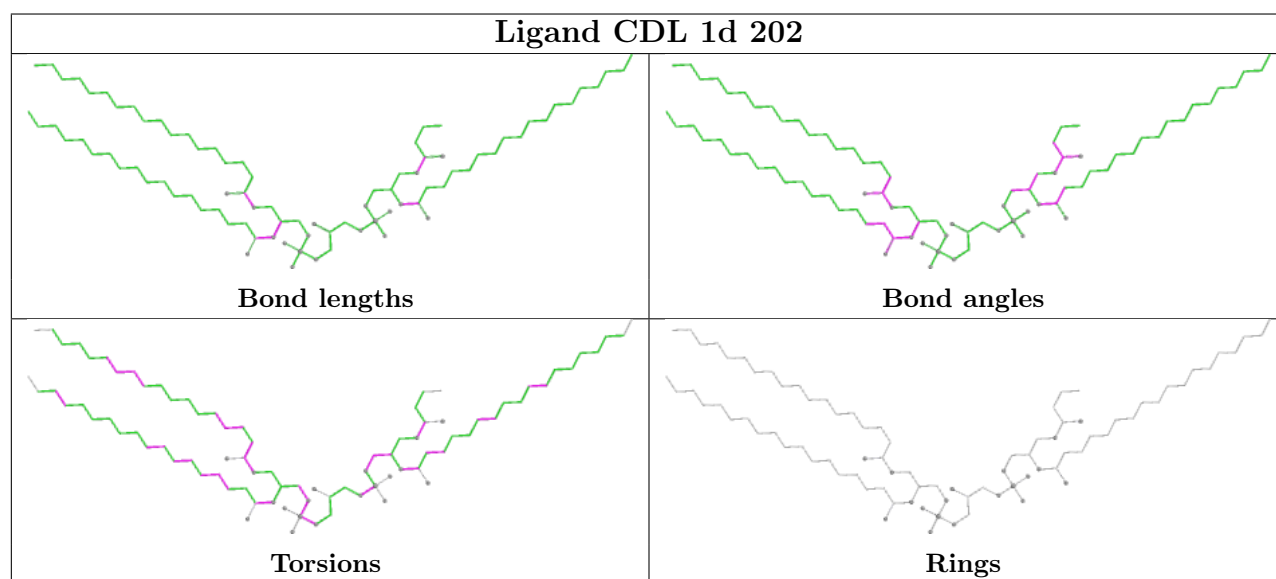
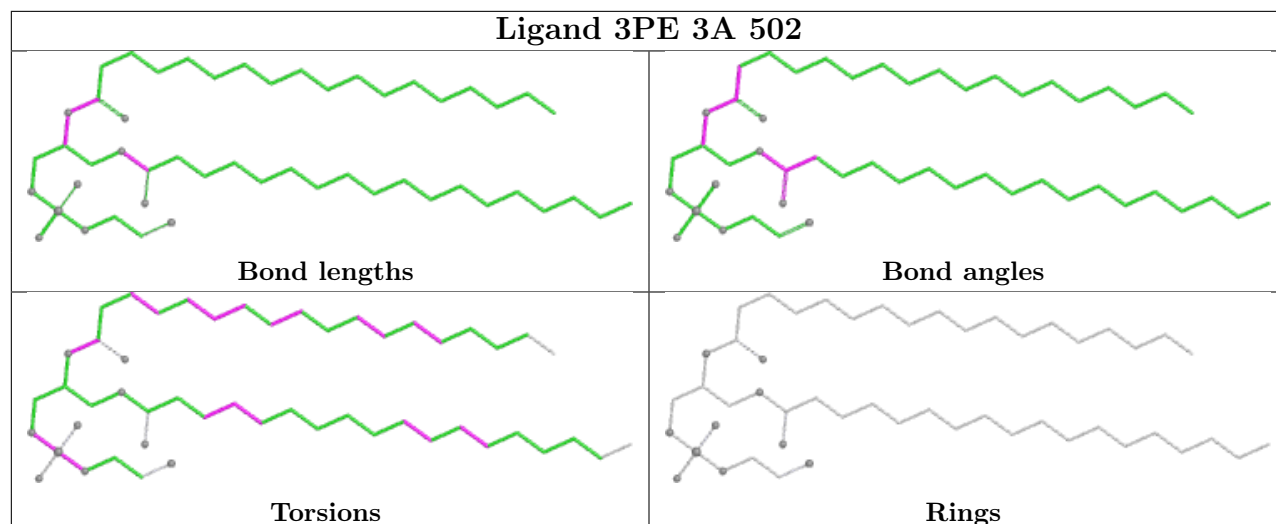


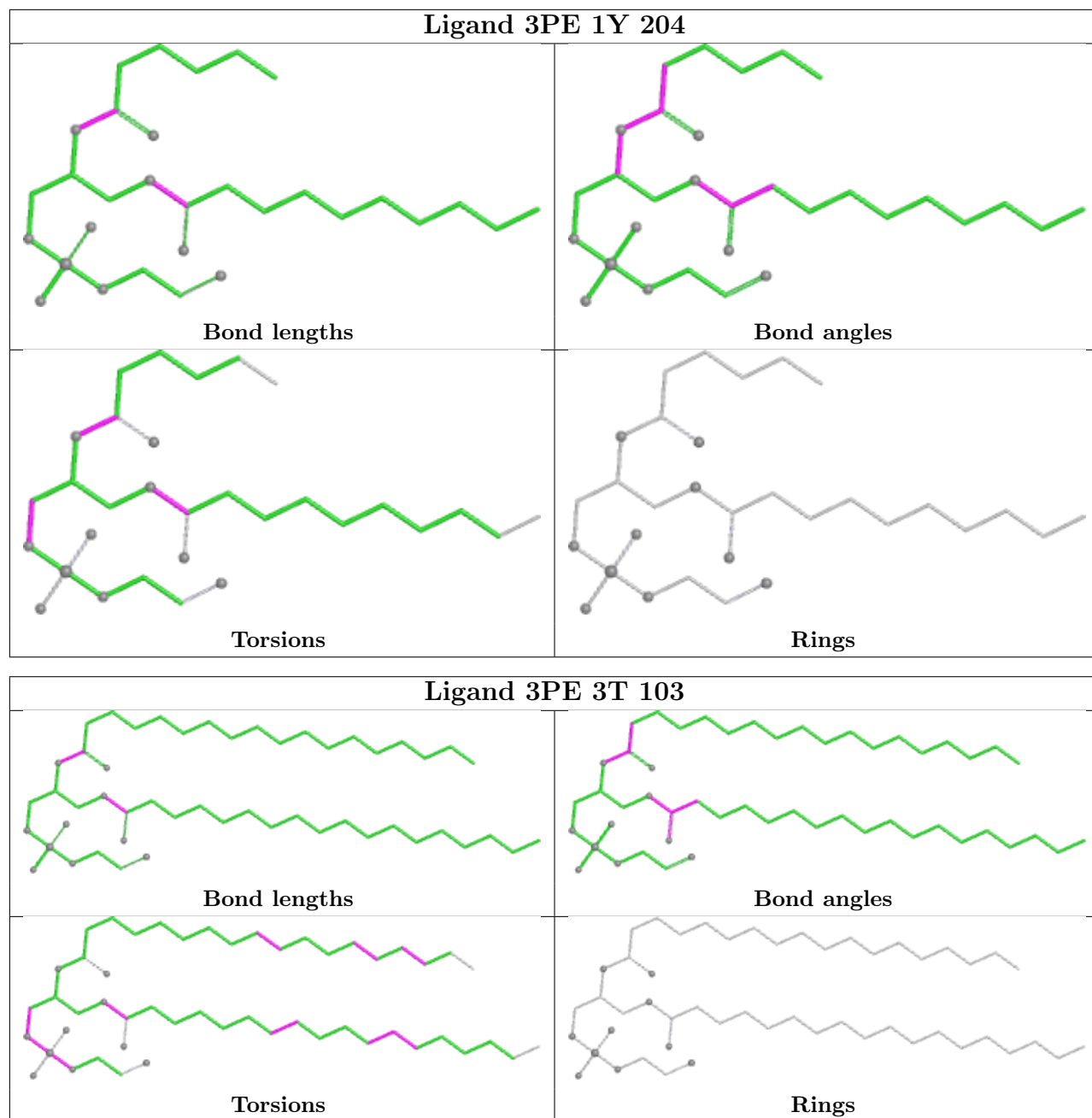


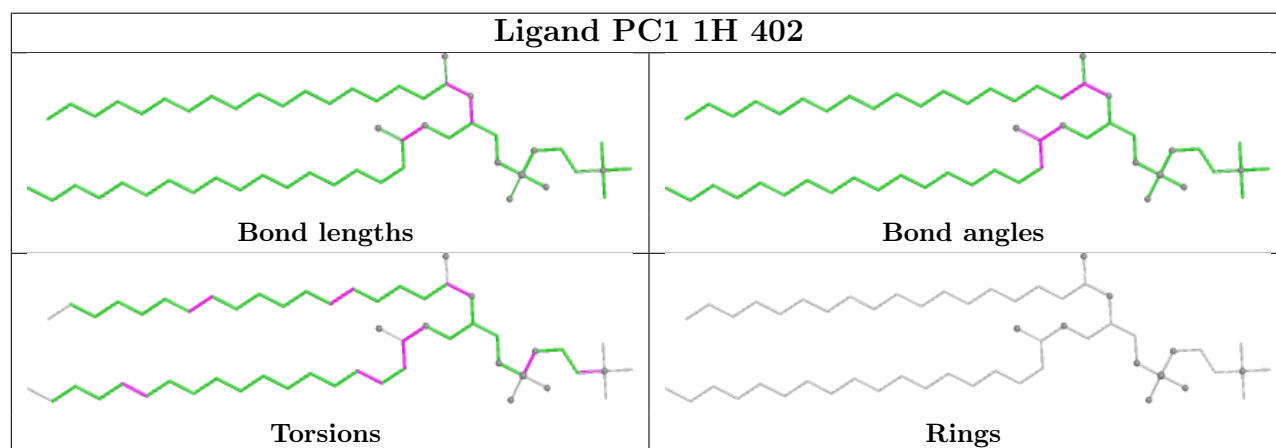
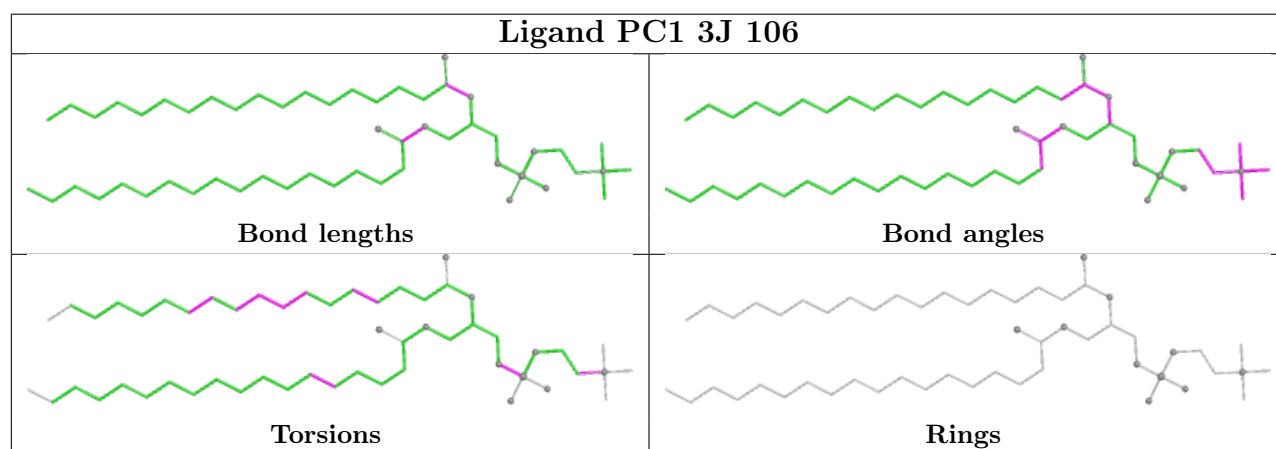
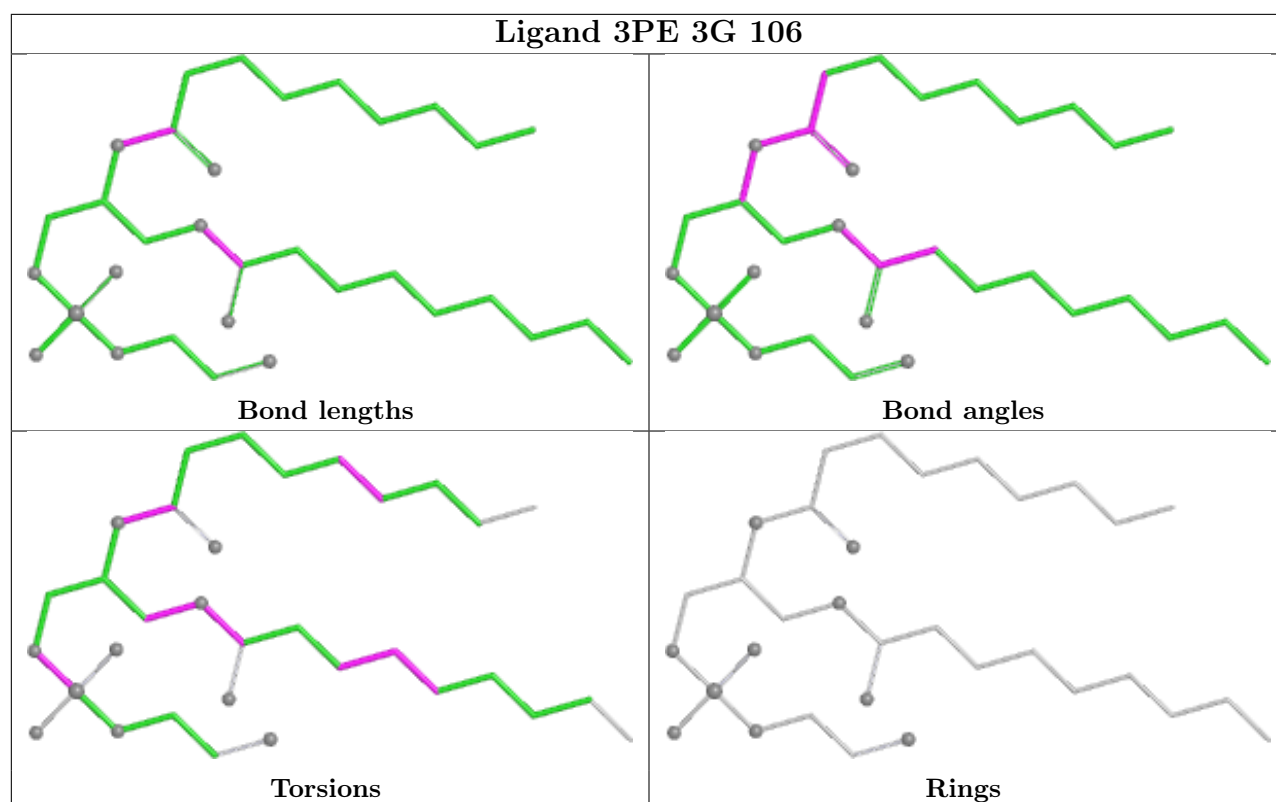


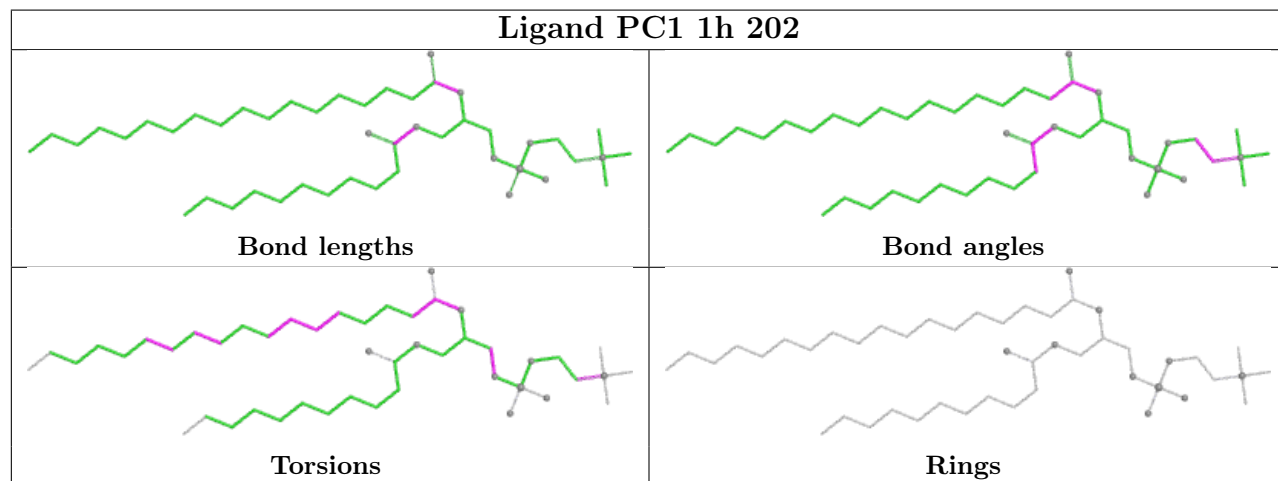
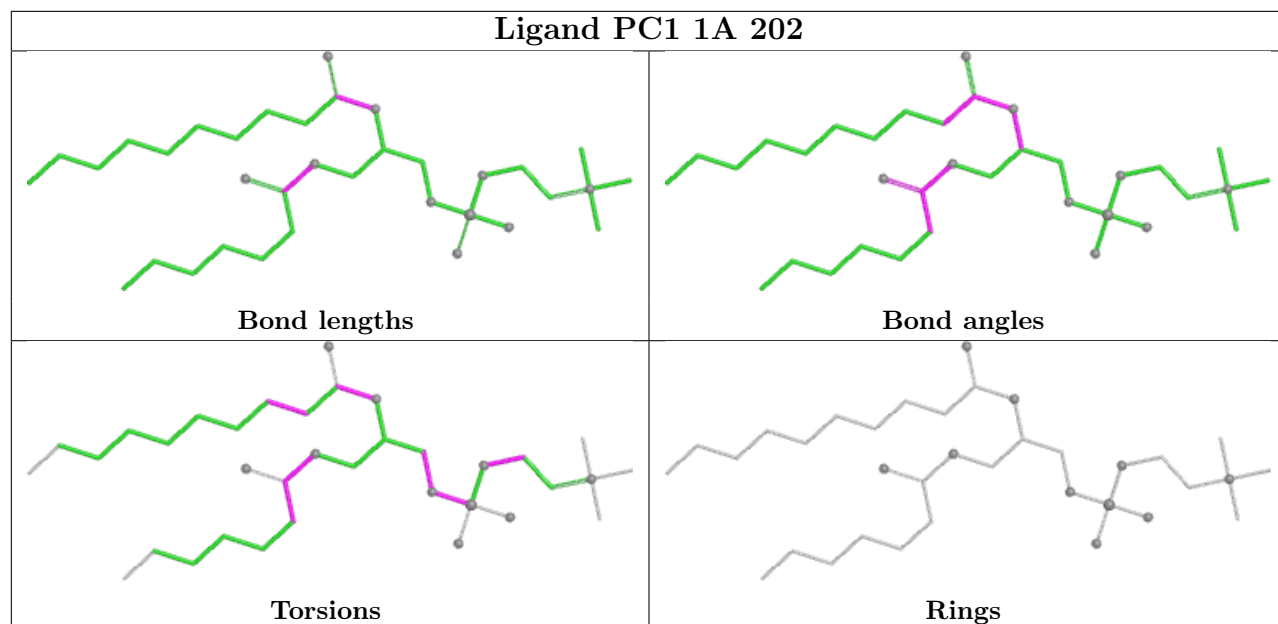


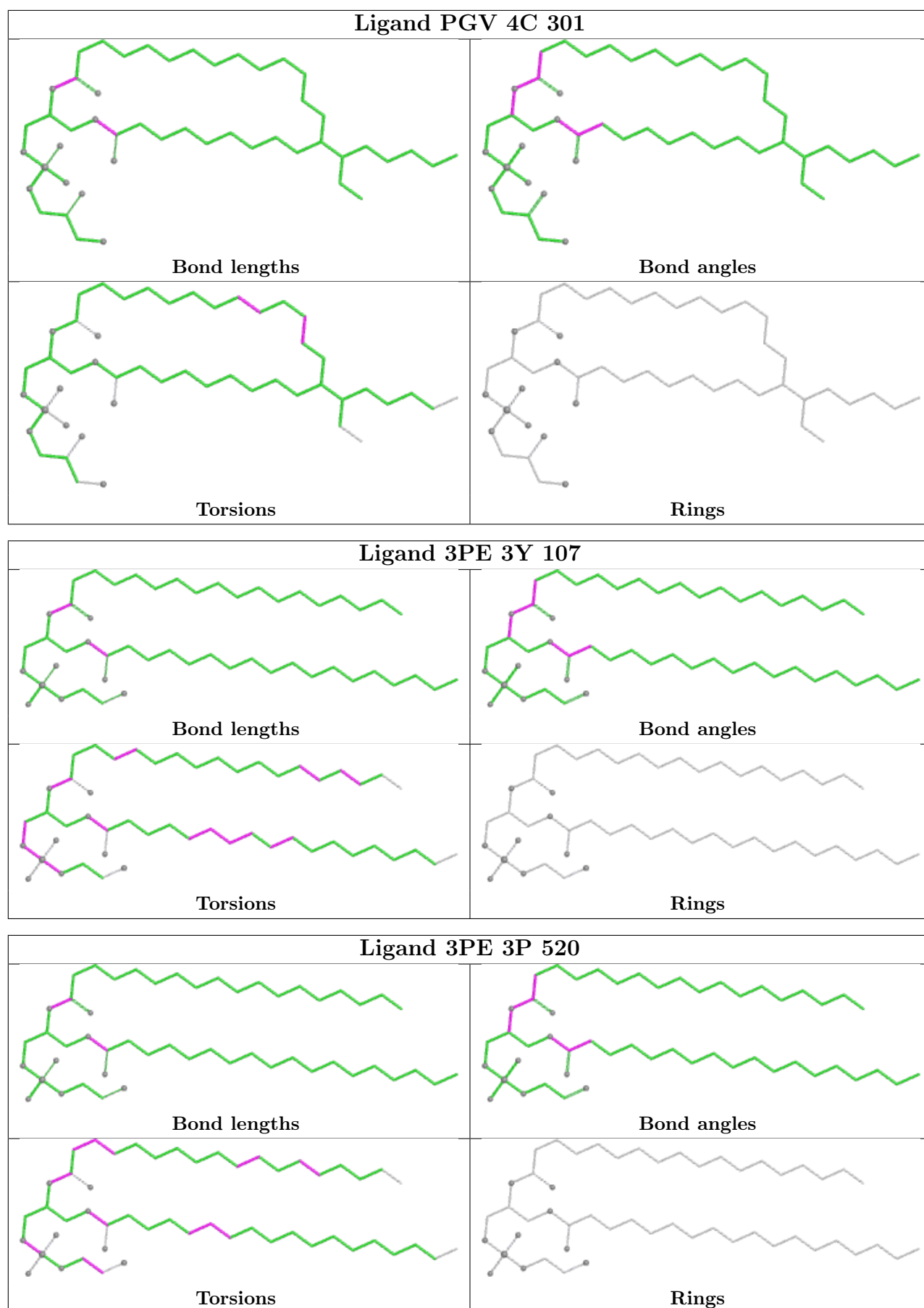


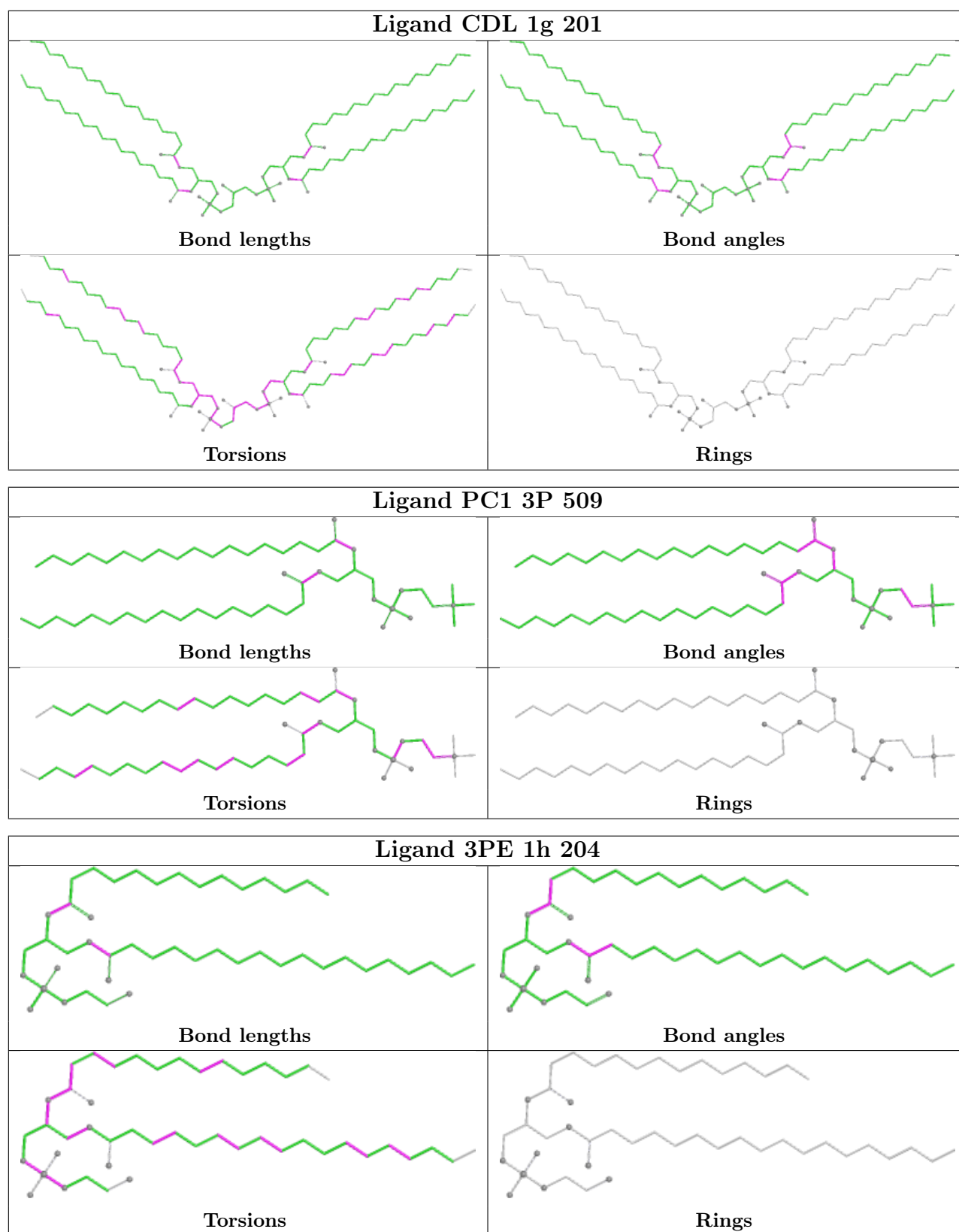


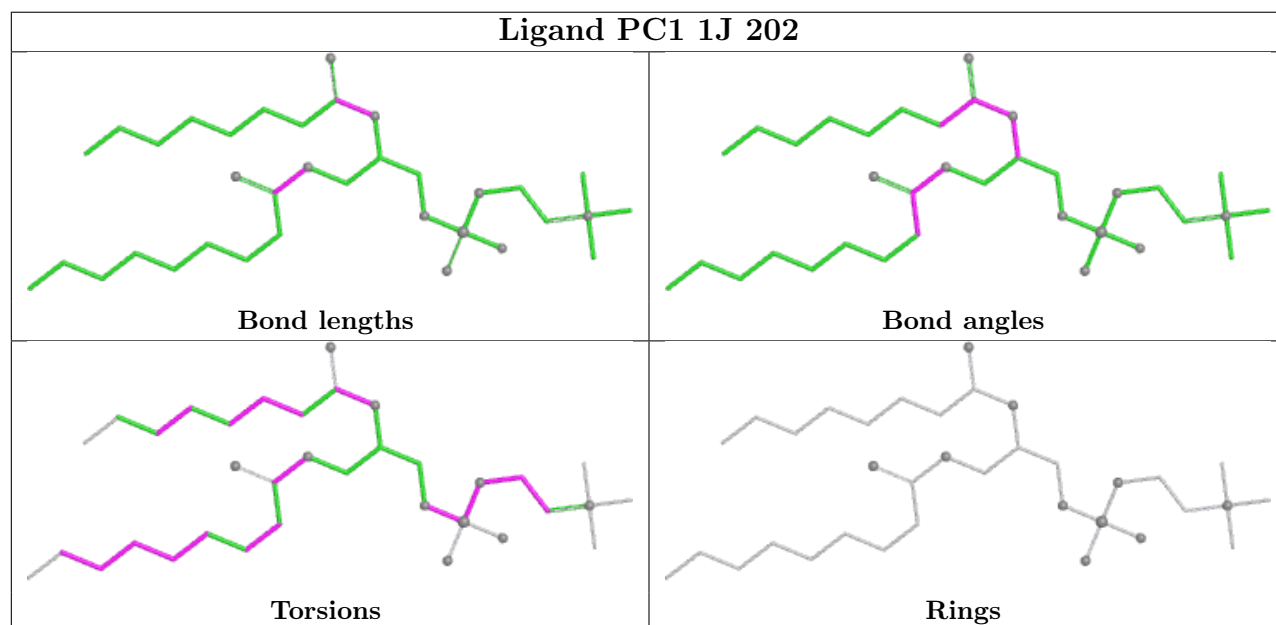
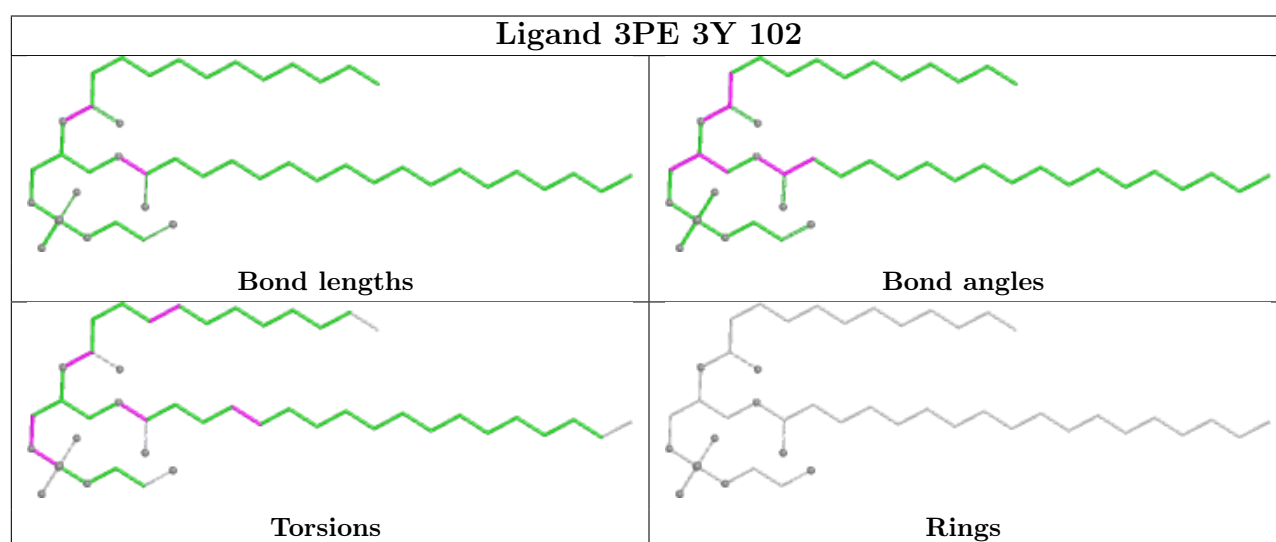
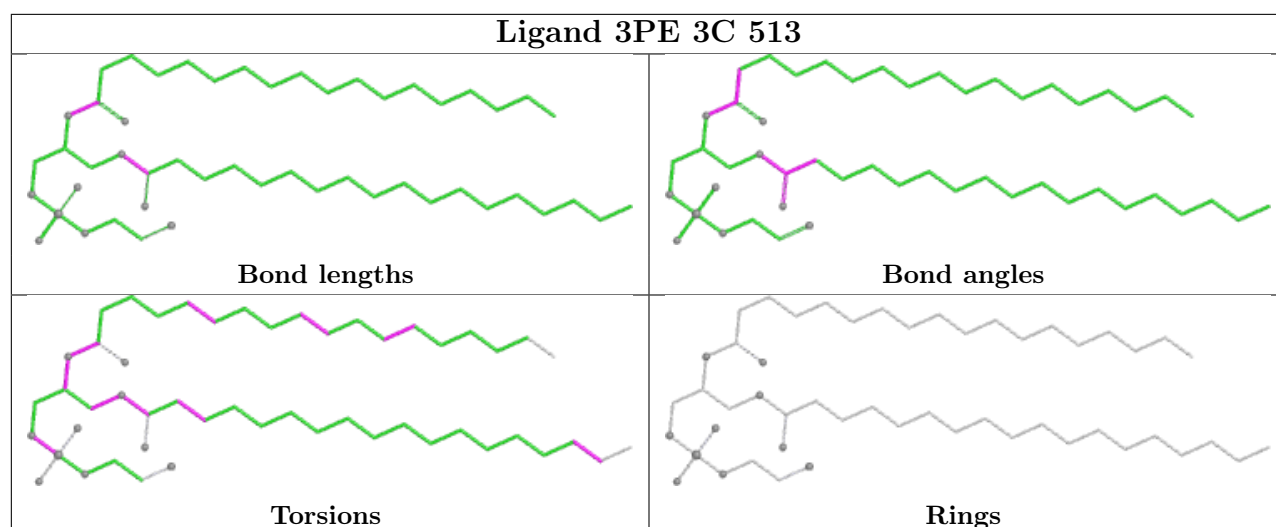


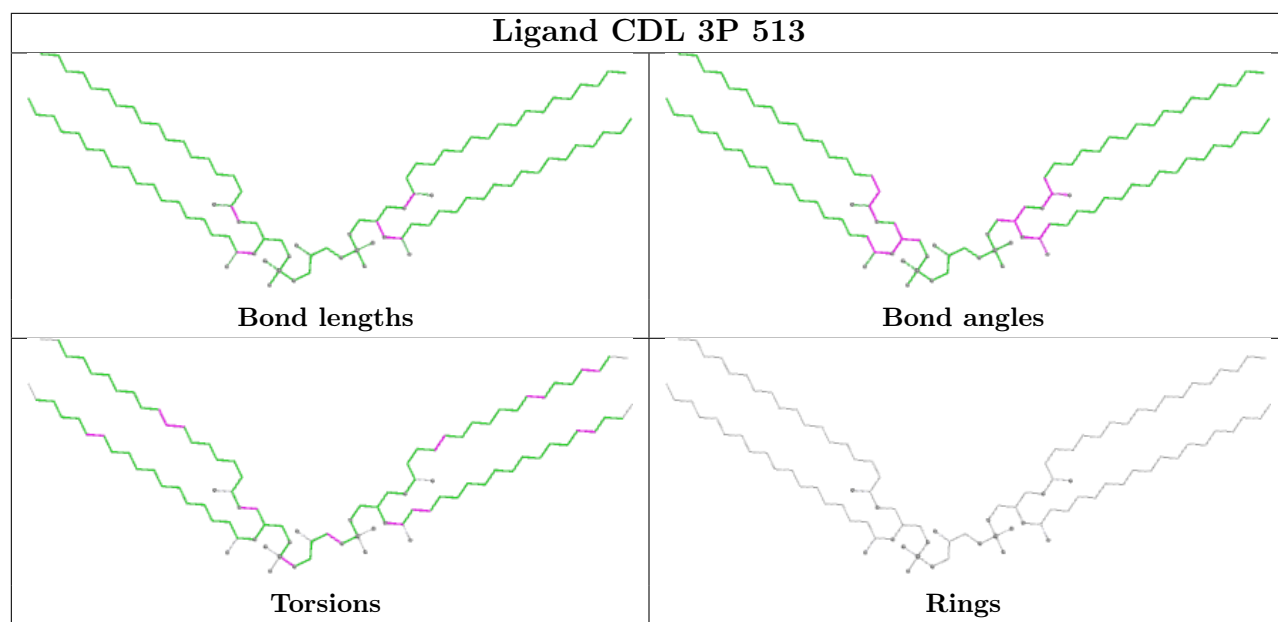
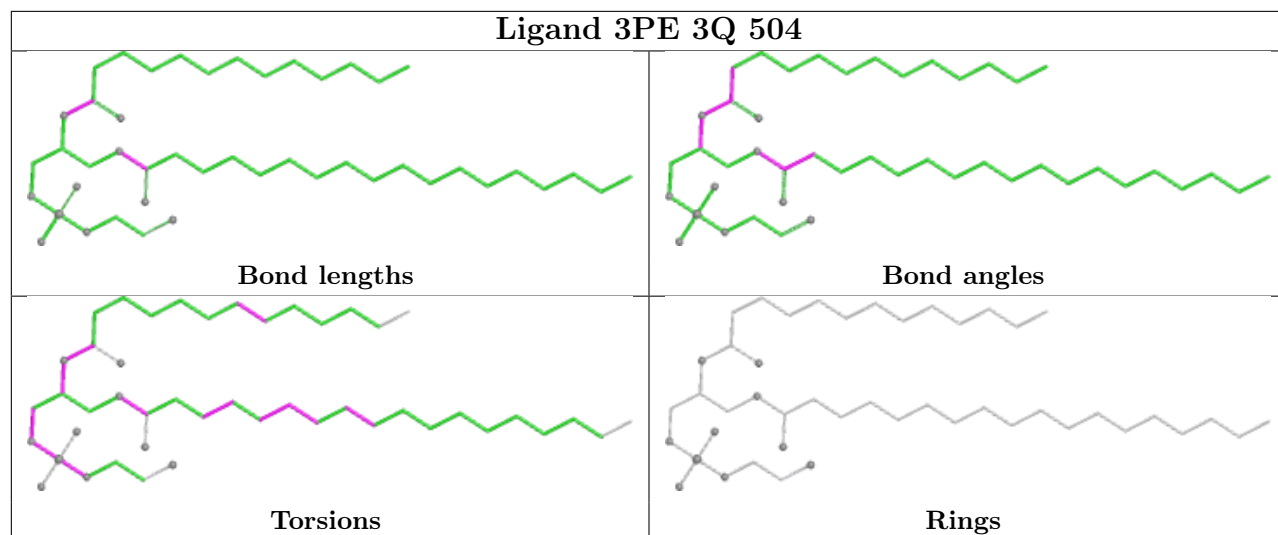


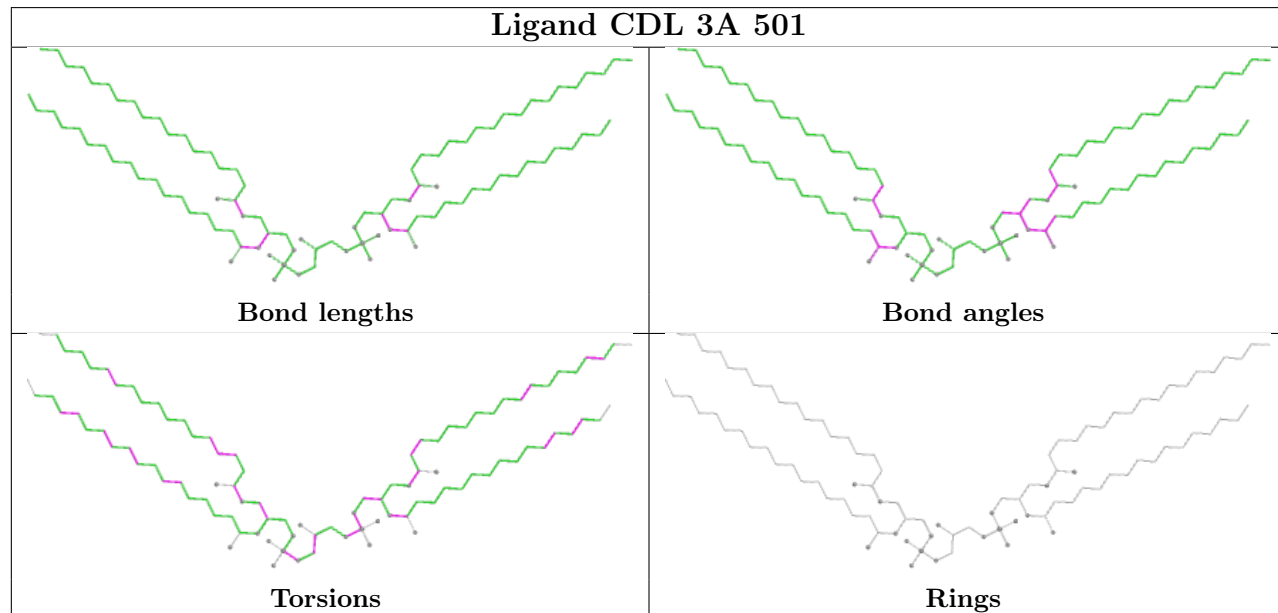
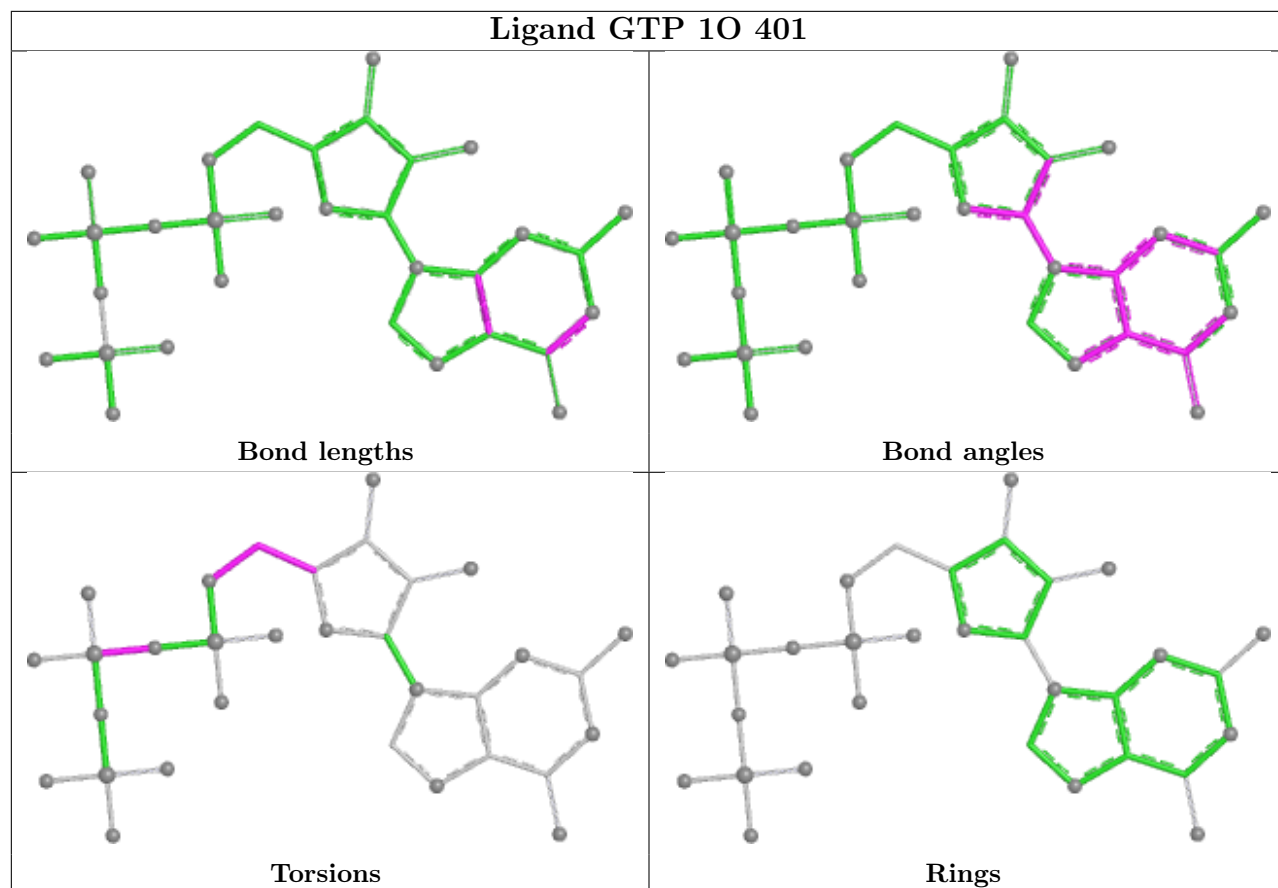


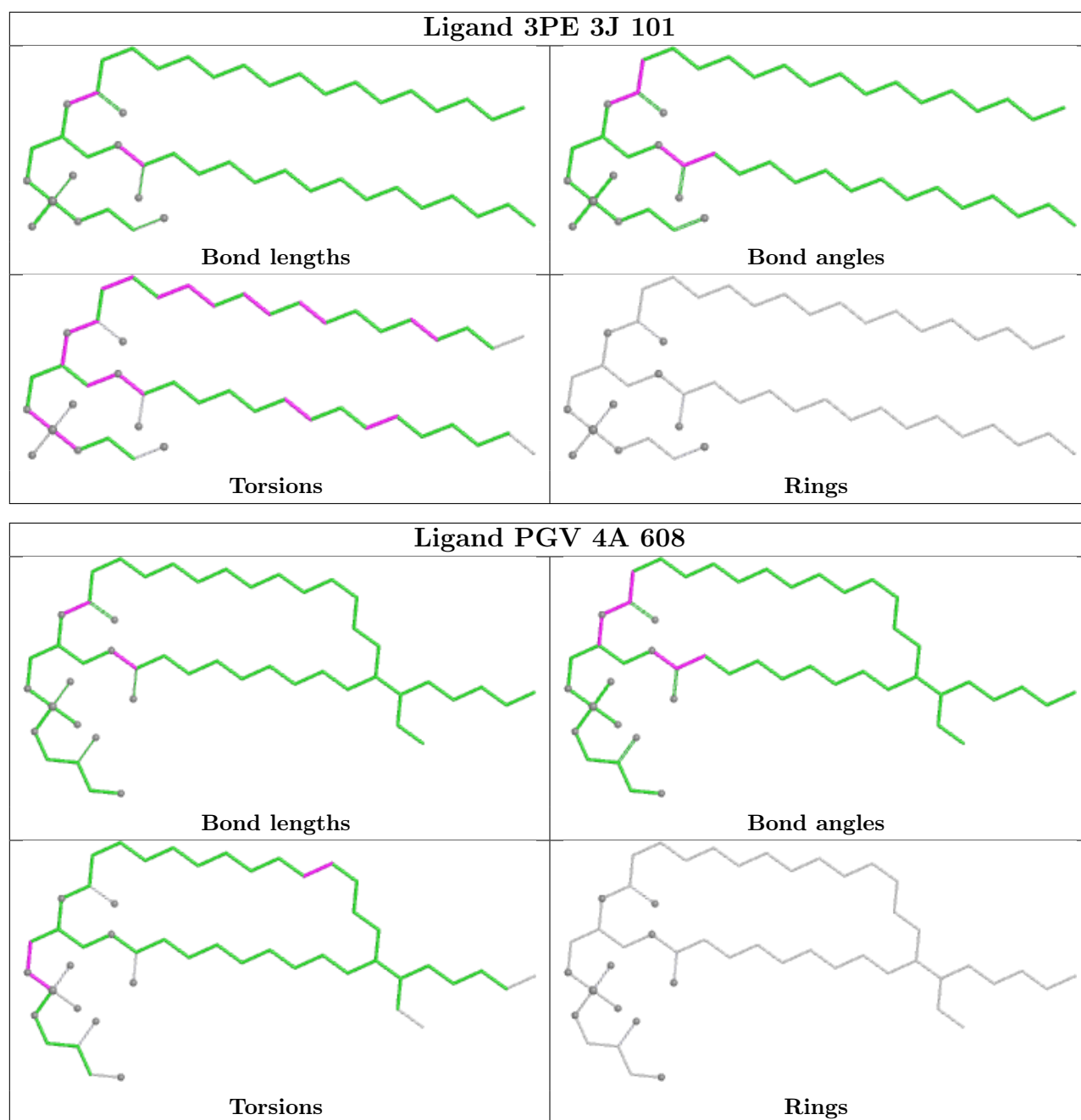


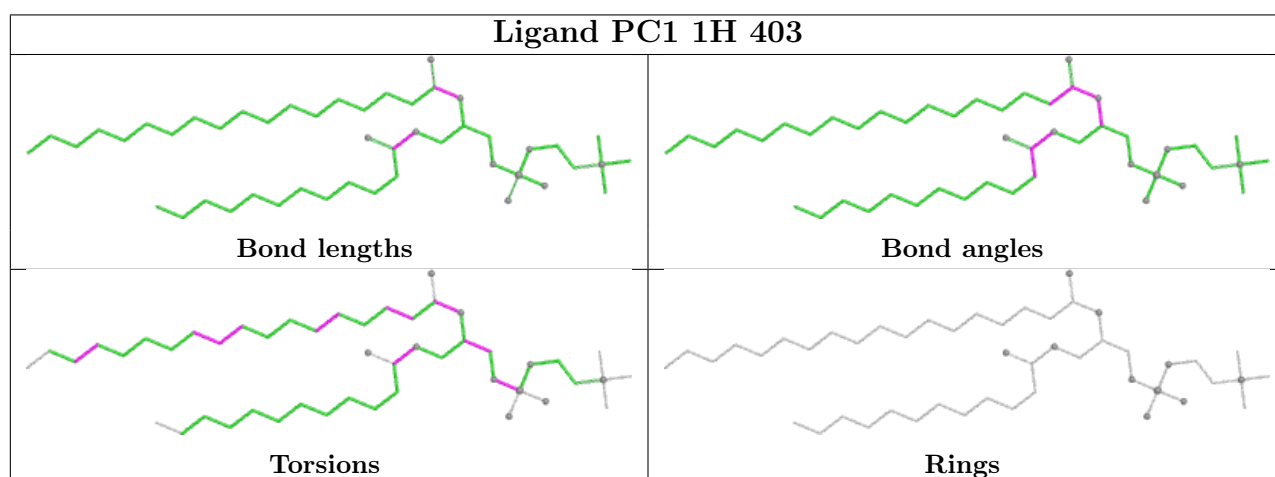
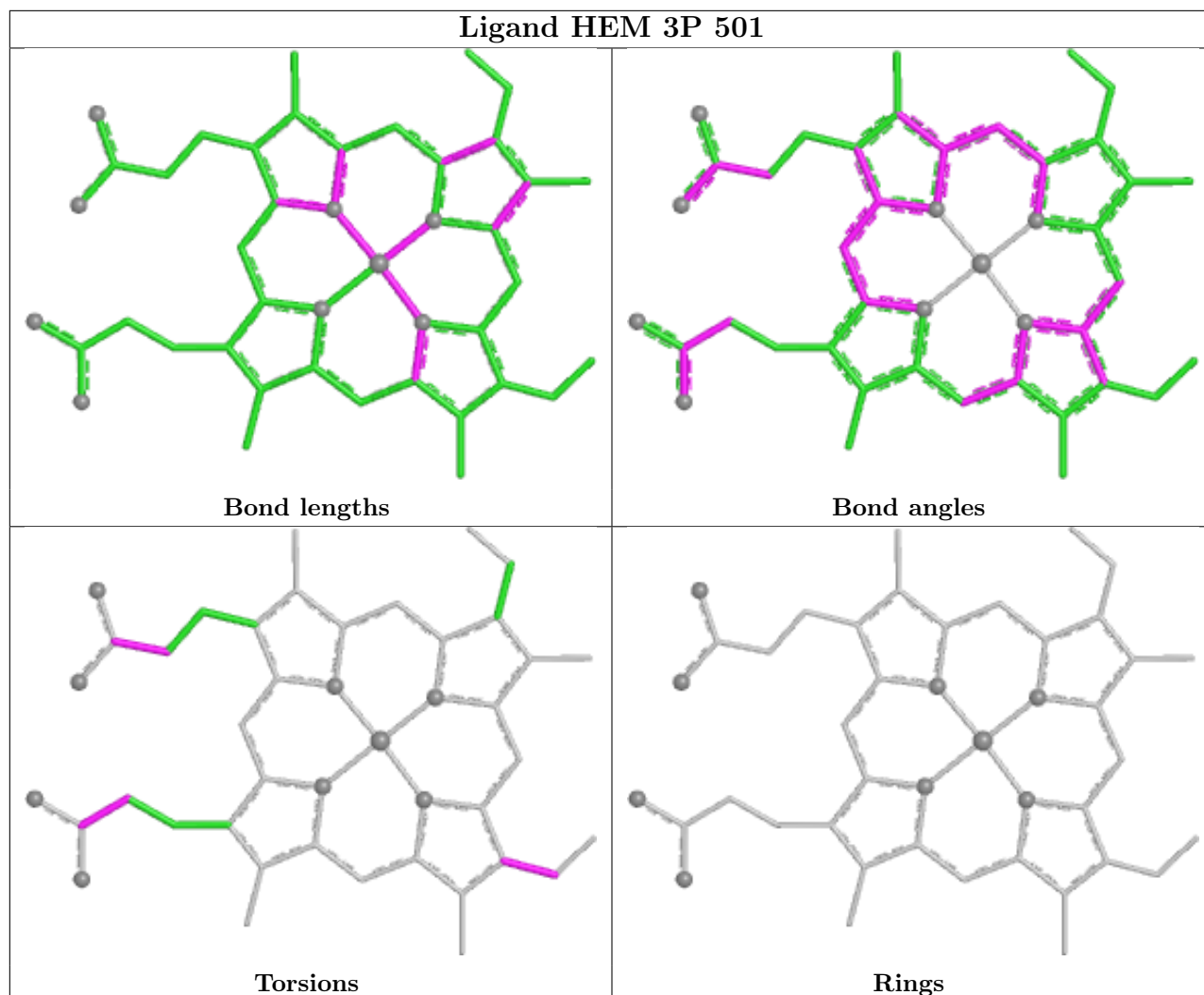


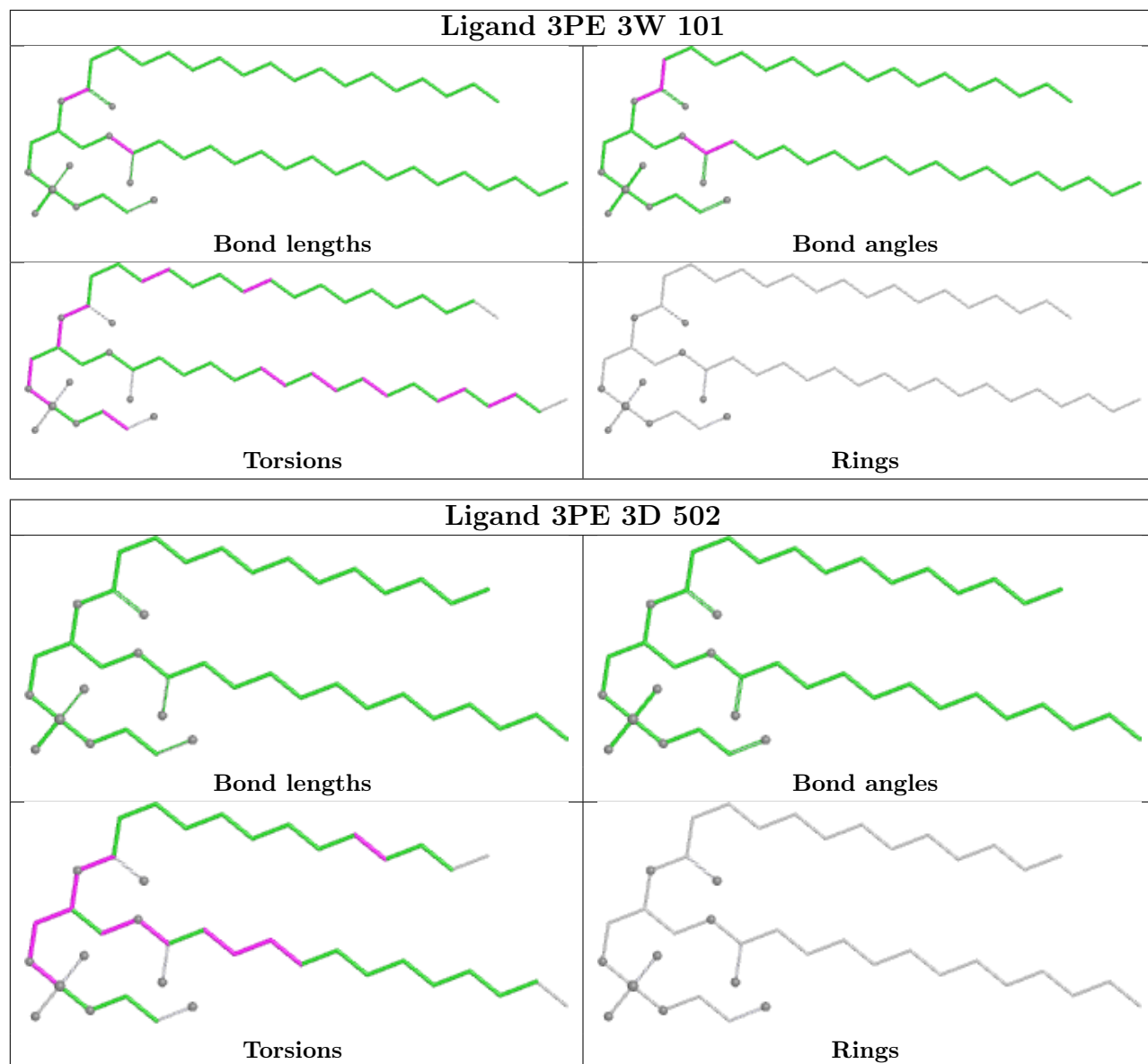


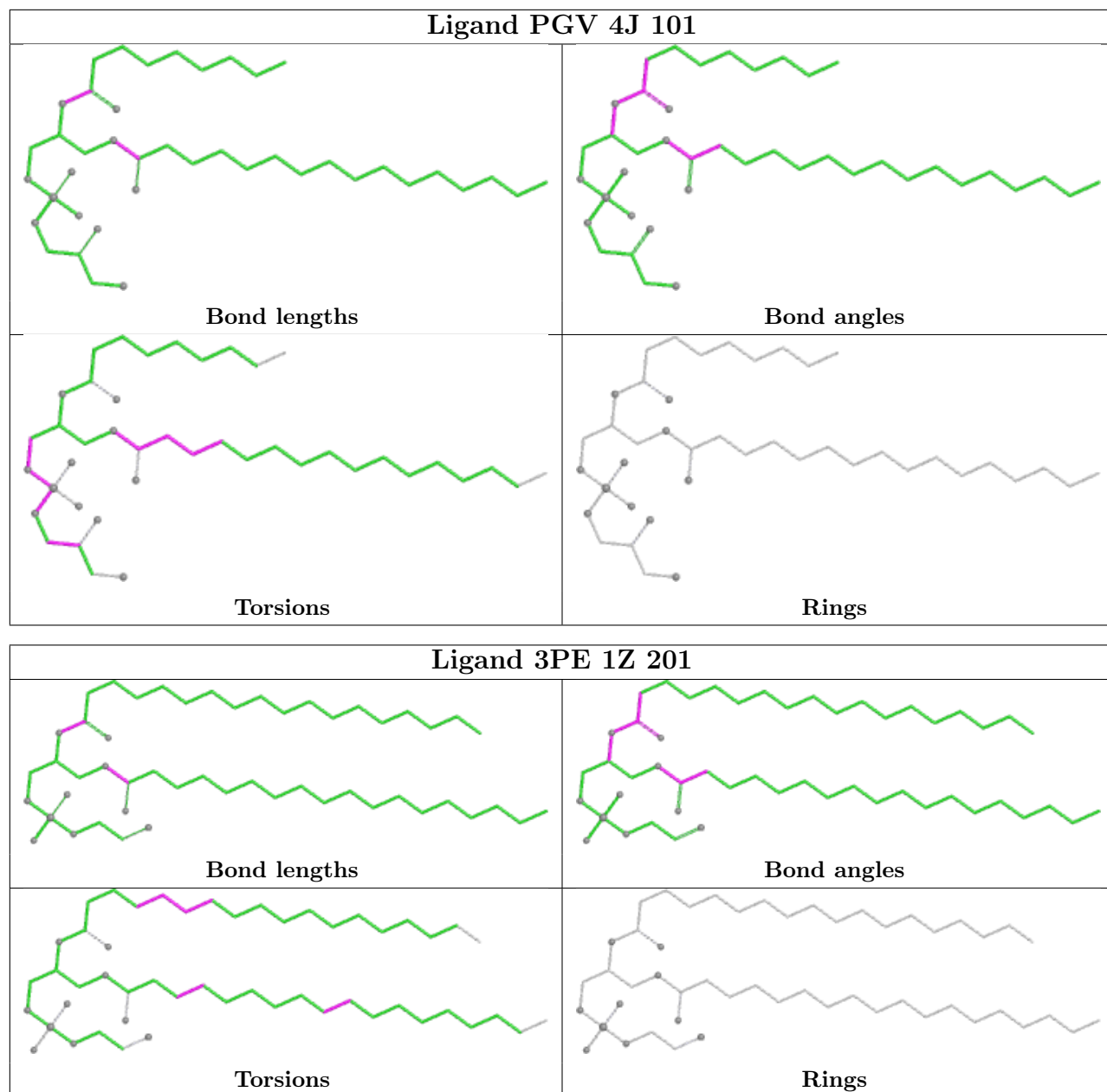


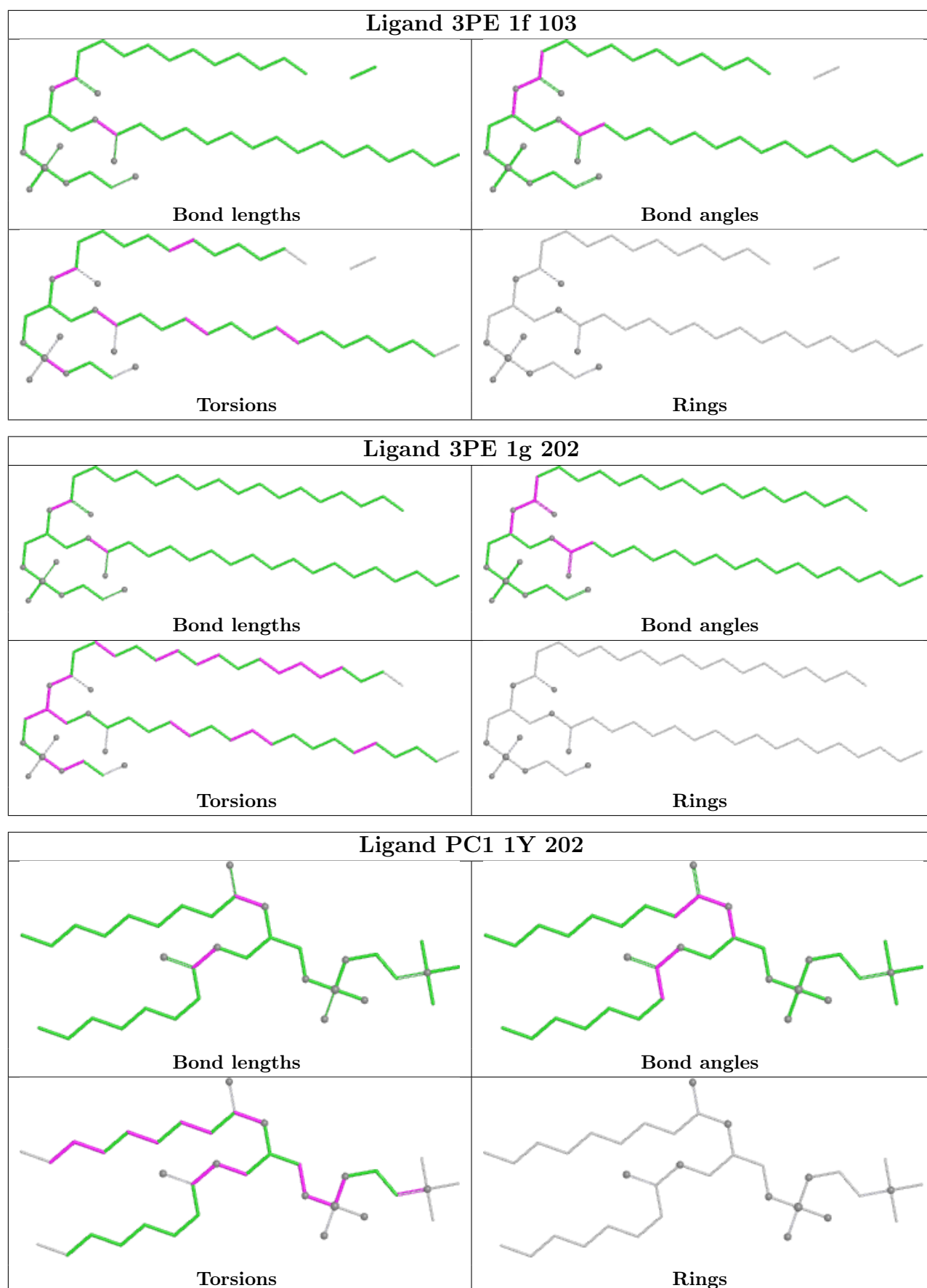


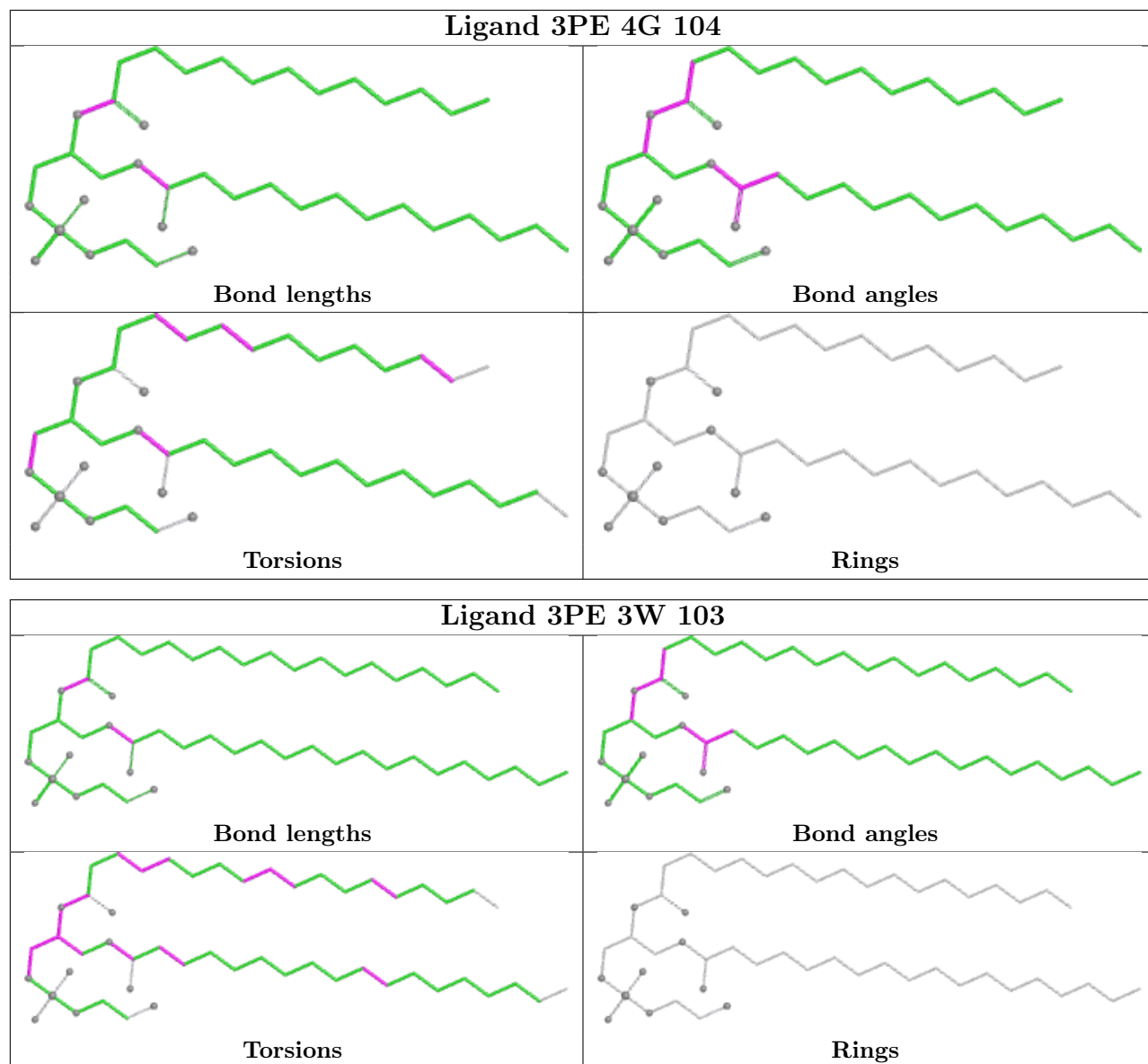


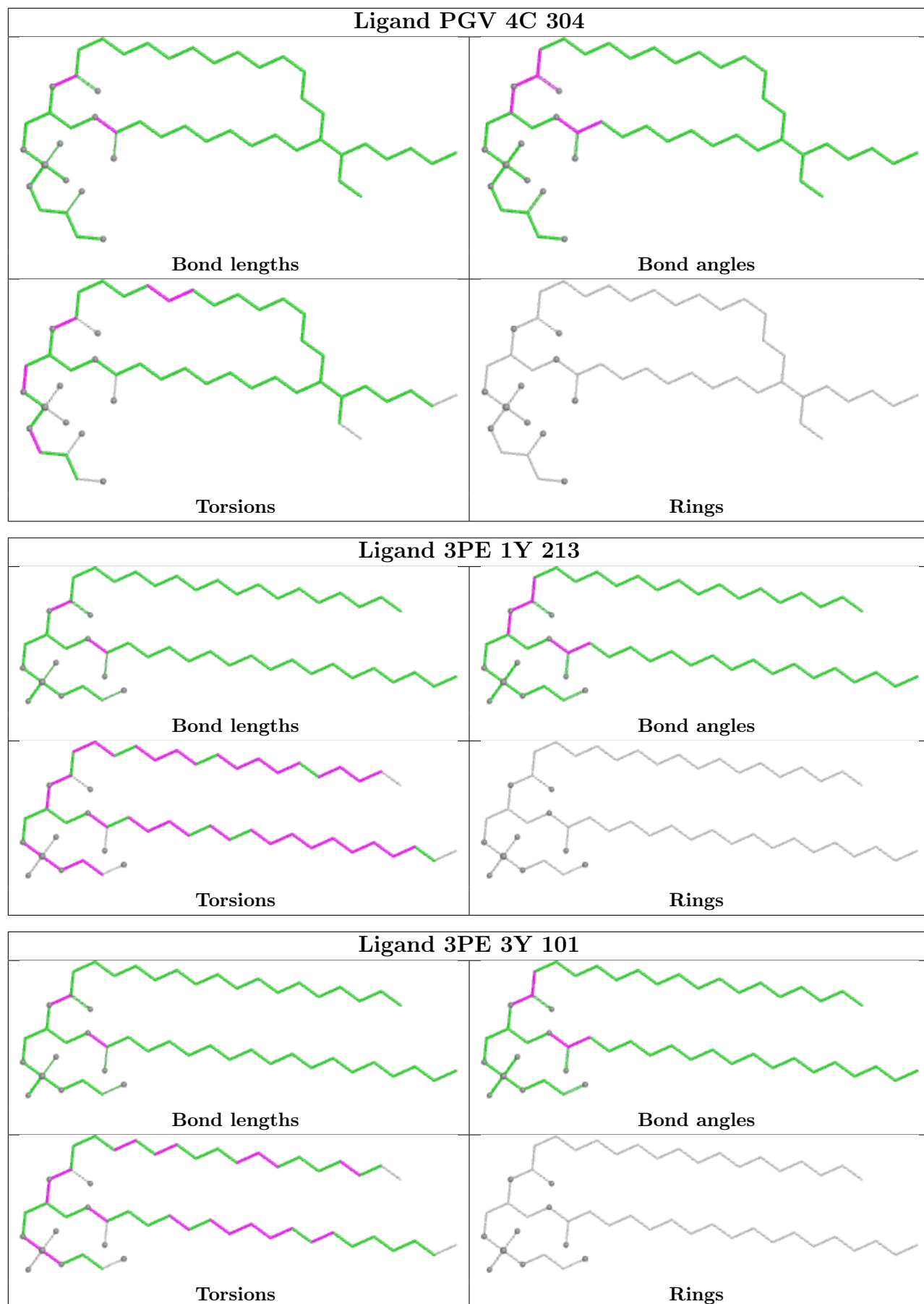


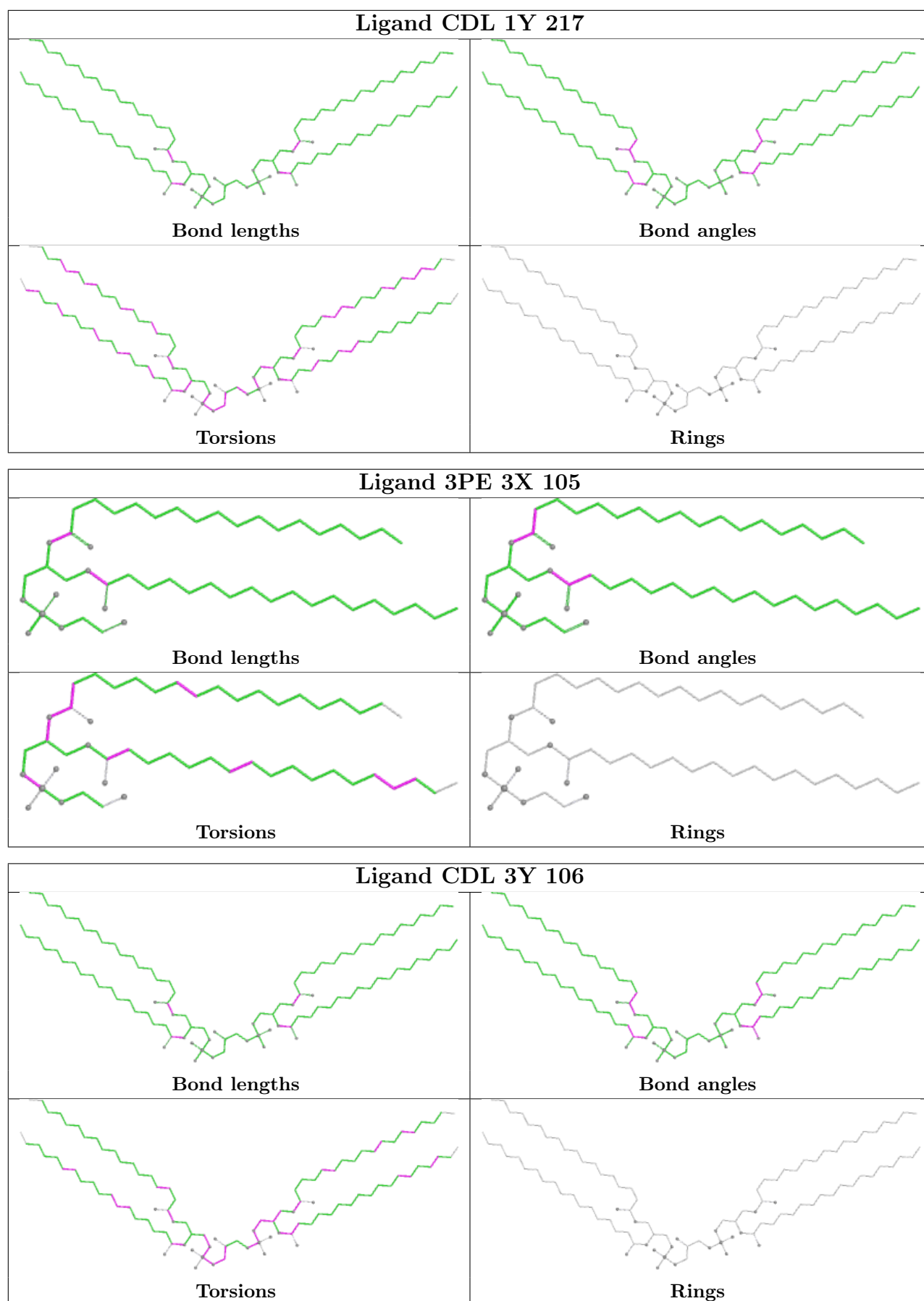


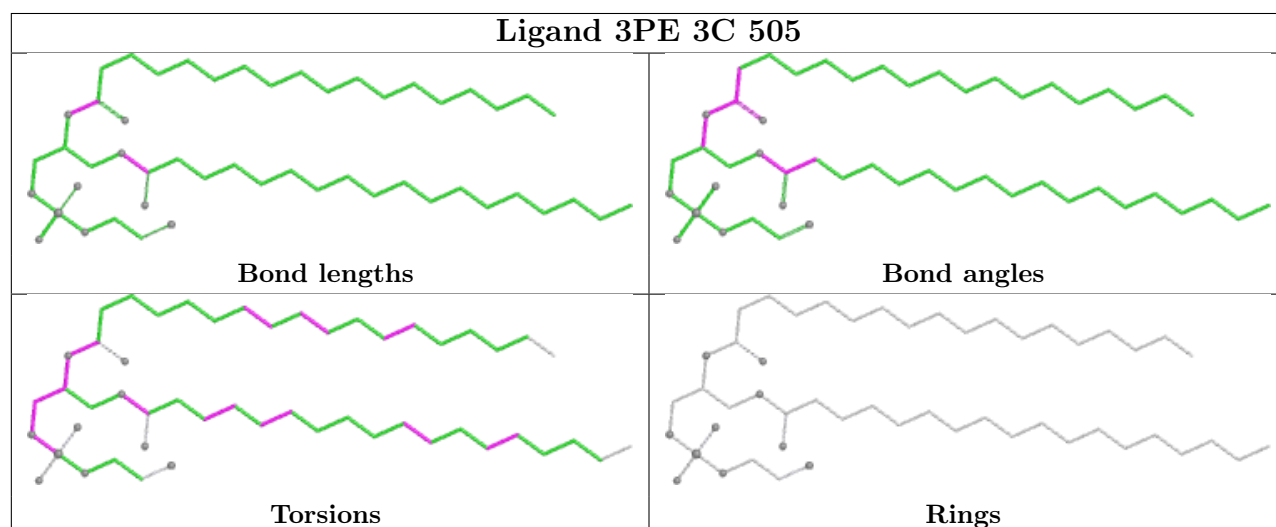
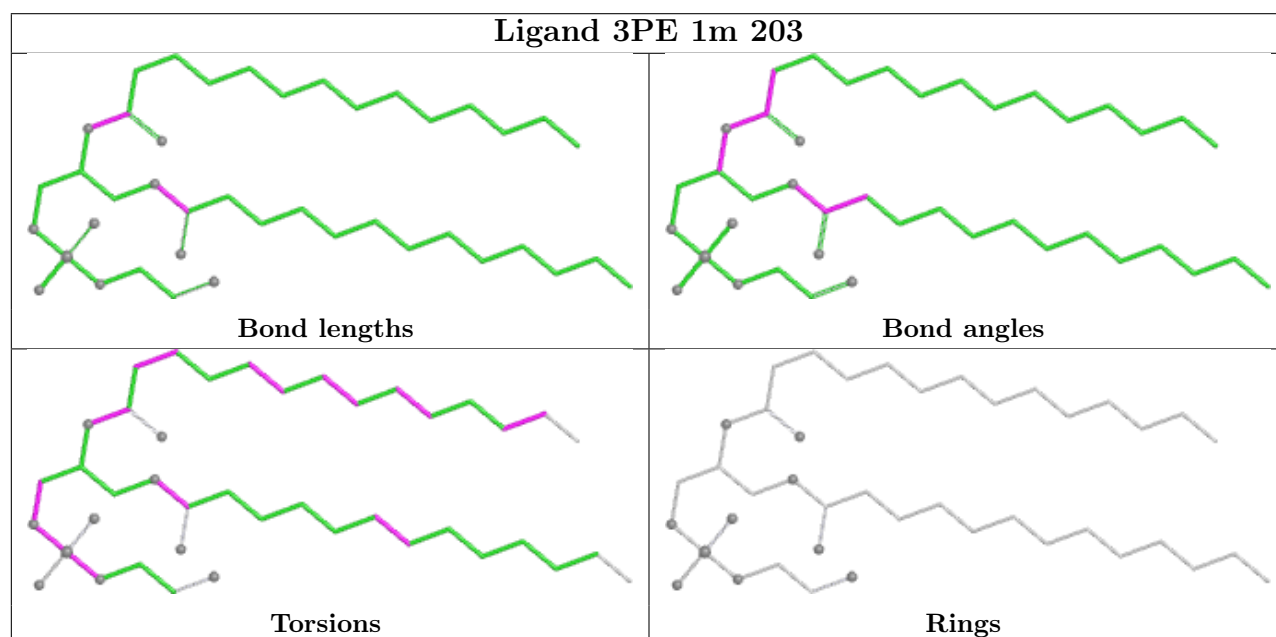
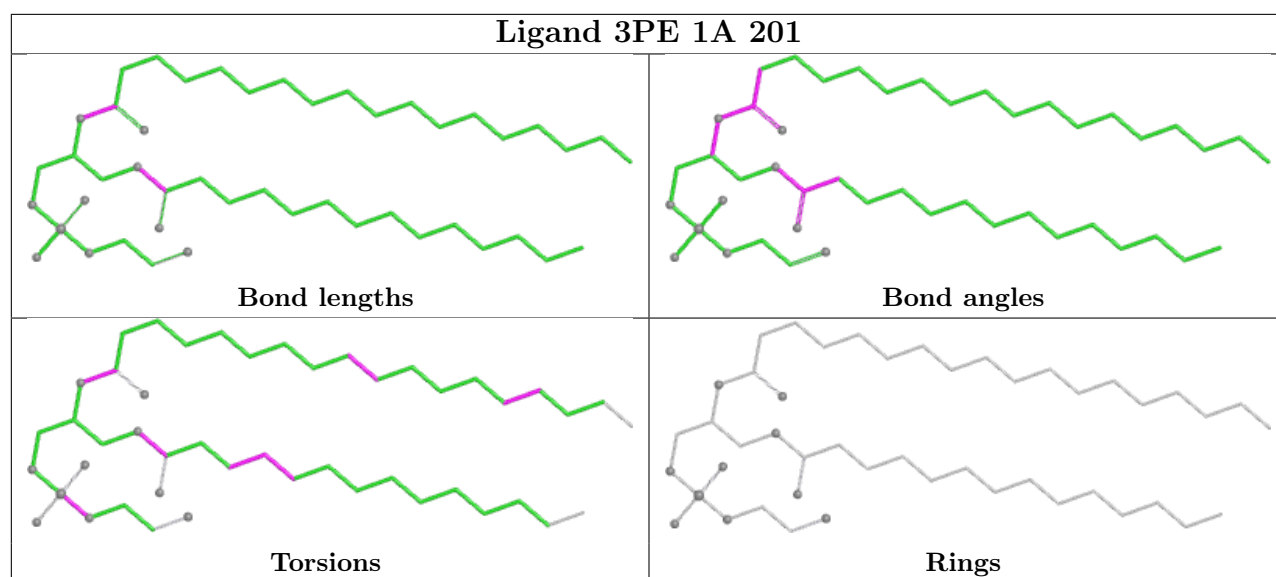


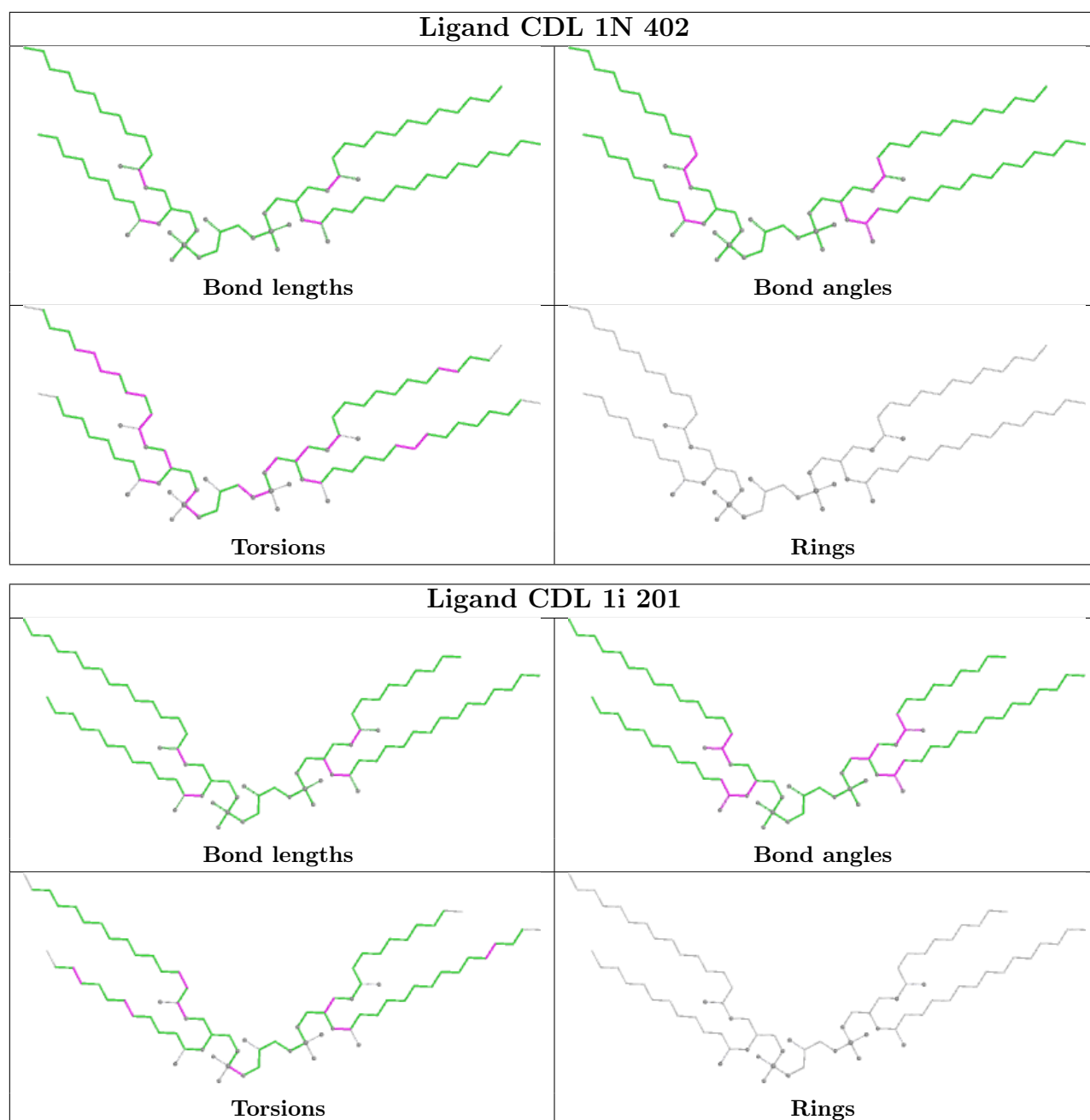


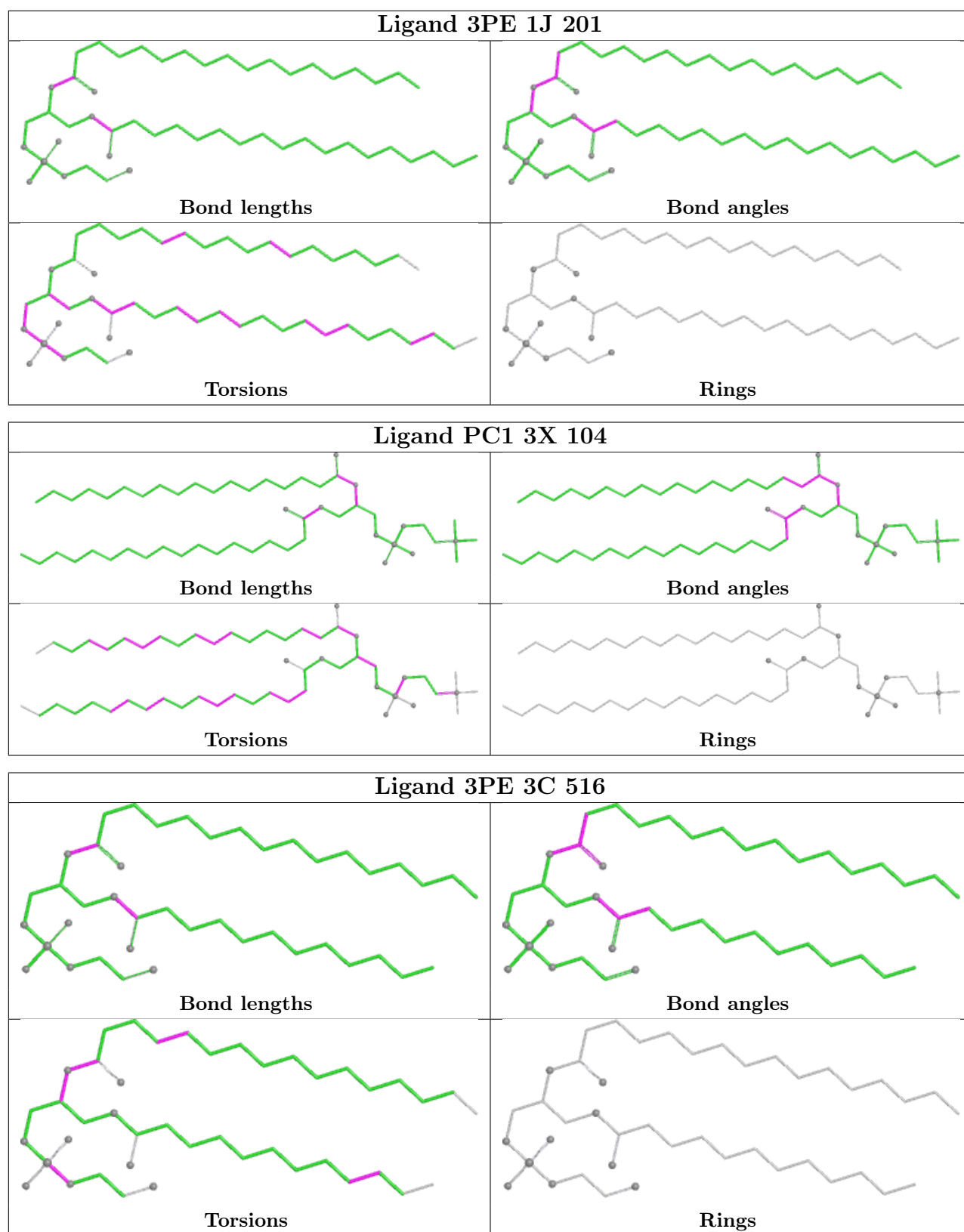












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	3W	3
53	3J	2
51	3G	1
52	3H	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	2.65
1	3H	77:GLU	C	78:ASP	N	2.52
1	3W	57:LYS	C	58:HIS	N	2.37
1	3J	59:LYS	C	60:TYR	N	1.79
1	3J	56:ILE	C	57:LYS	N	1.07

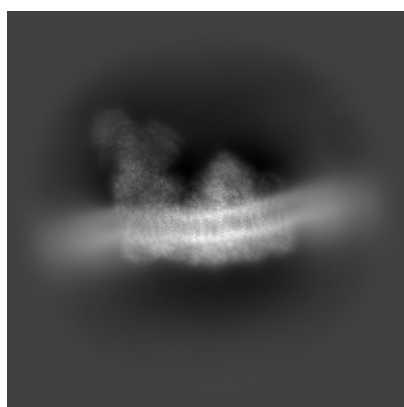
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42225. These allow visual inspection of the internal detail of the map and identification of artifacts.

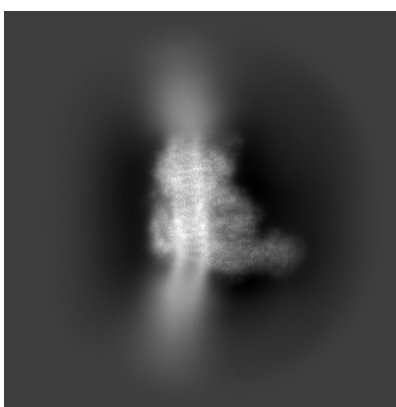
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

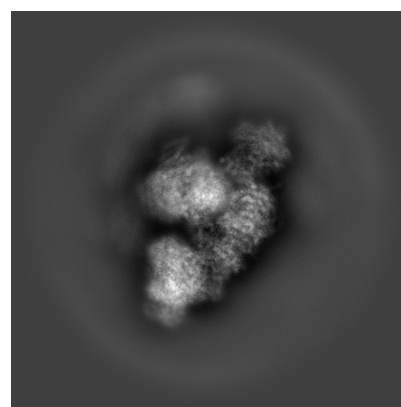
#### 6.1.1 Primary map



X



Y

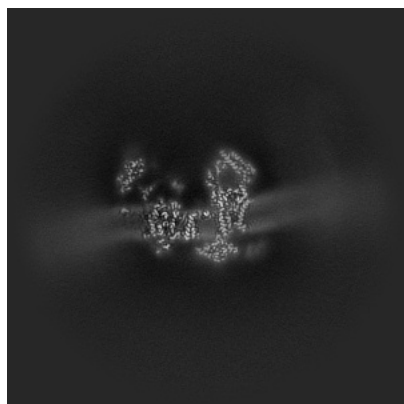


Z

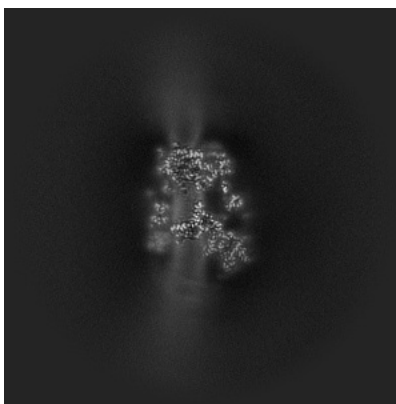
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

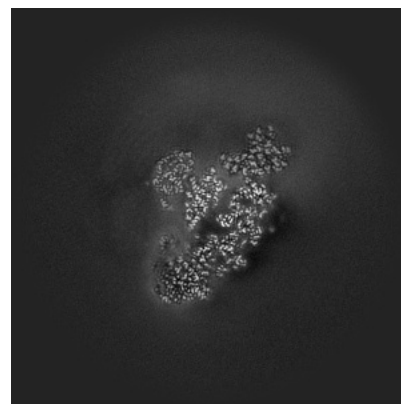
#### 6.2.1 Primary map



X Index: 320



Y Index: 320

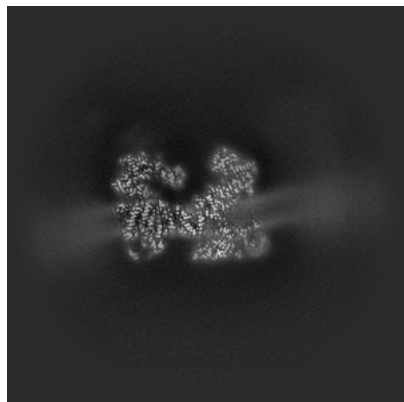


Z Index: 320

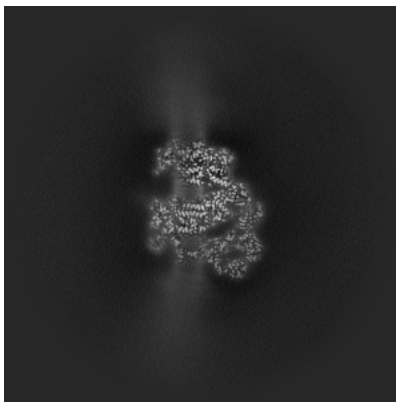
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

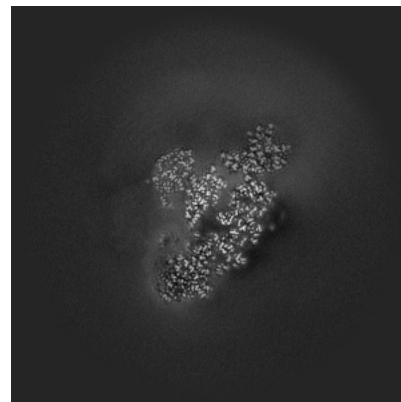
### 6.3.1 Primary map



X Index: 300



Y Index: 342

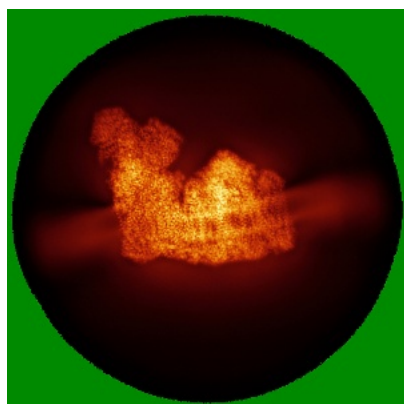


Z Index: 319

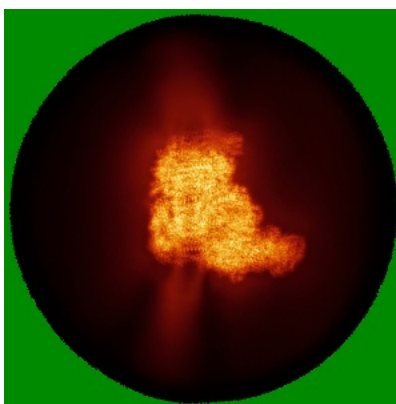
The images above show the largest variance slices of the map in three orthogonal directions.

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

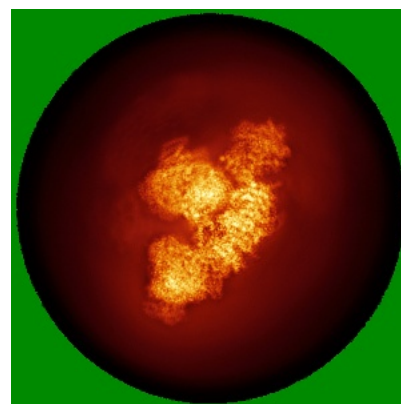
### 6.4.1 Primary map



X



Y

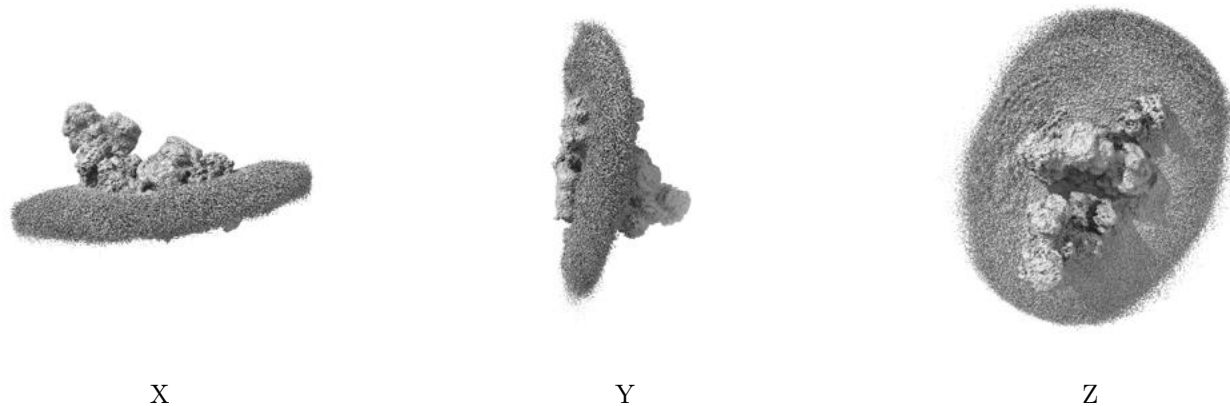


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

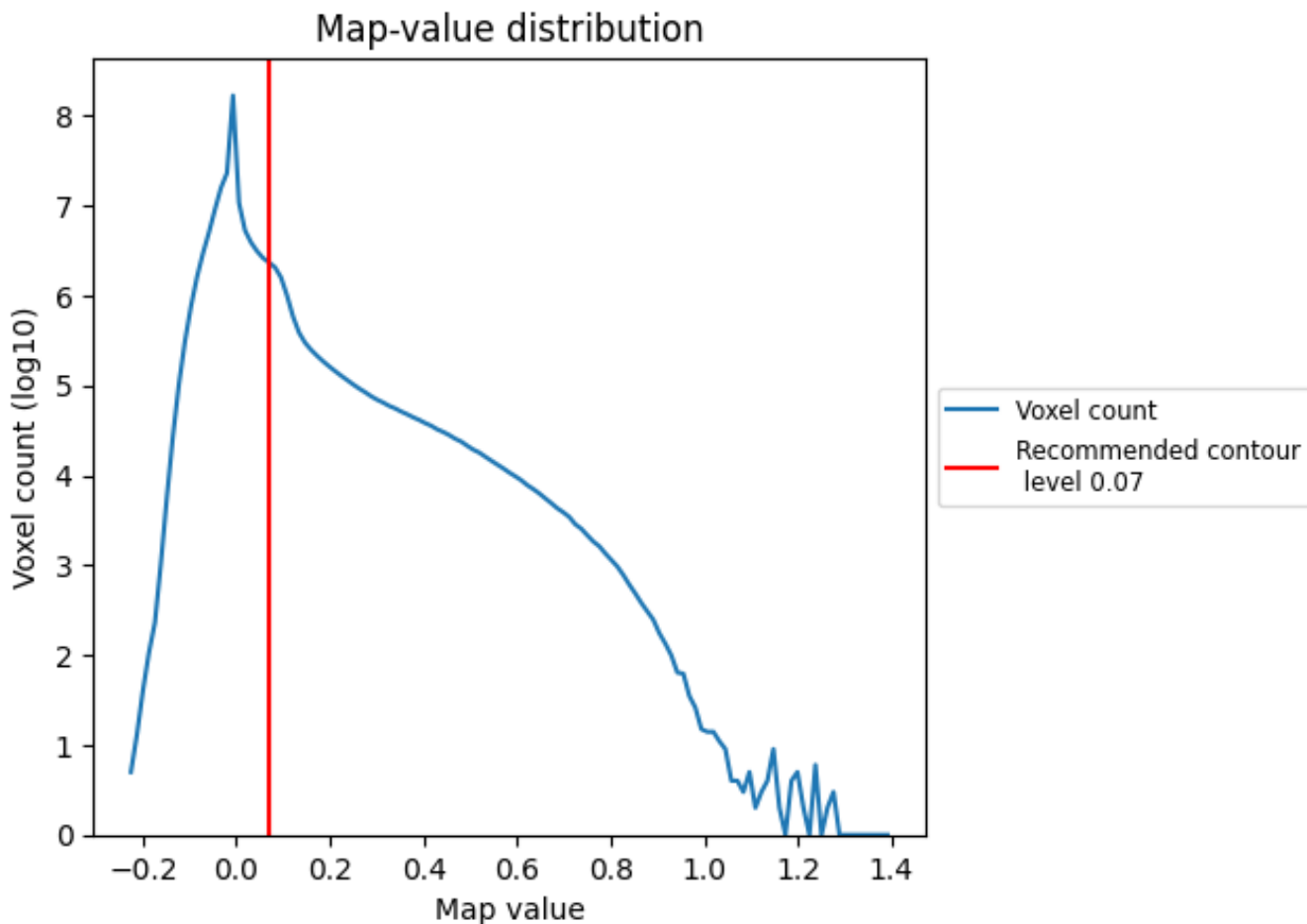
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

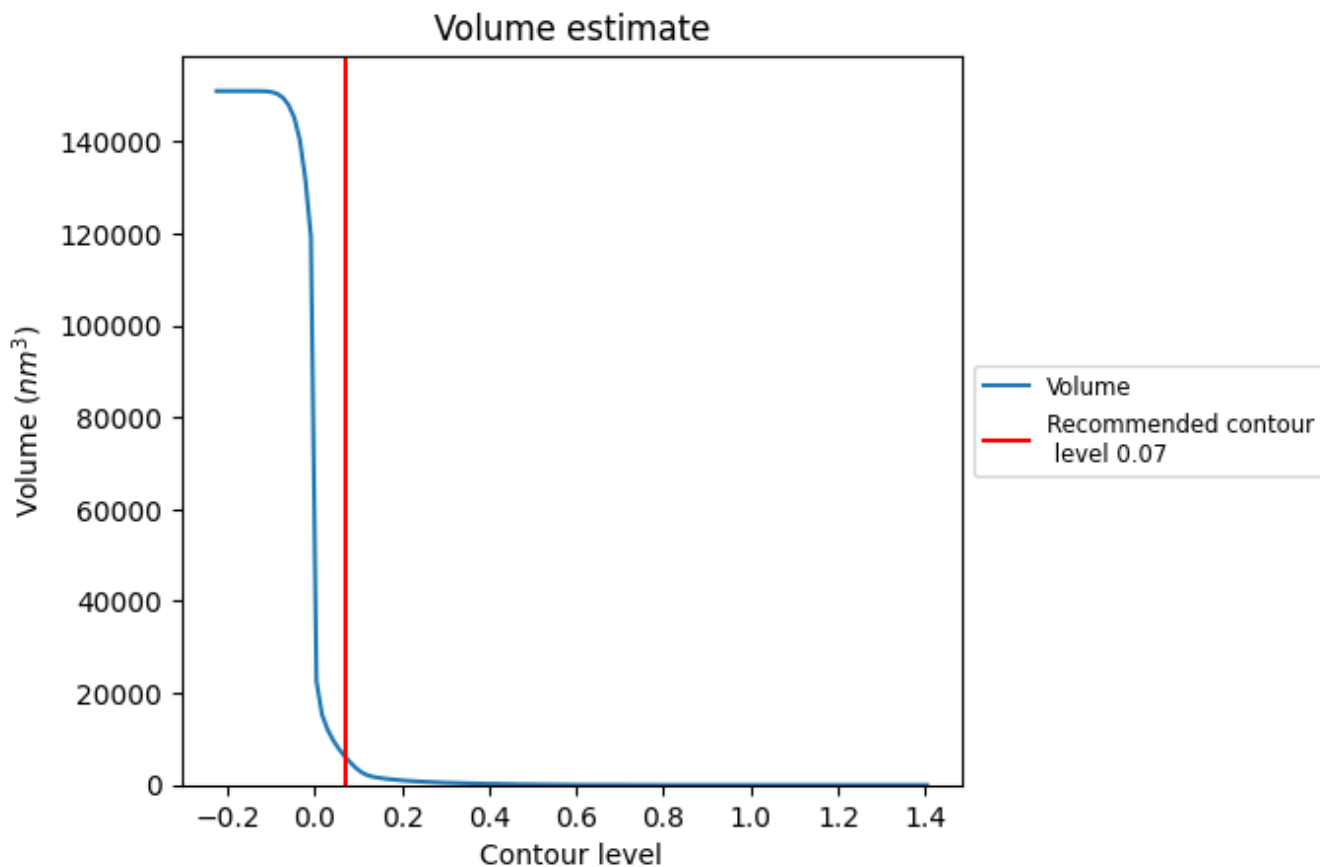
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

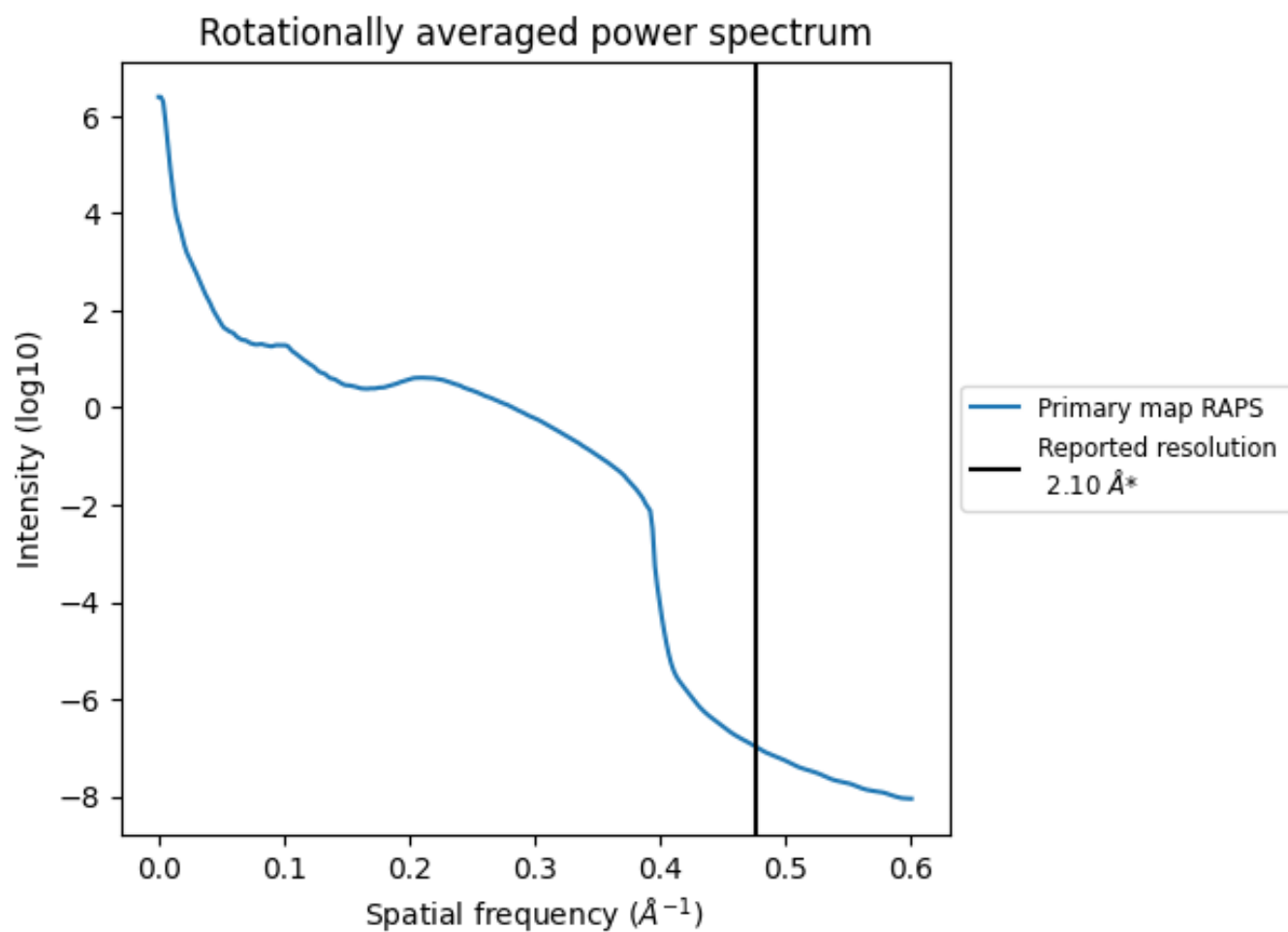
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $6122 \text{ nm}^3$ ; this corresponds to an approximate mass of 5530 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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.476 Å<sup>-1</sup>

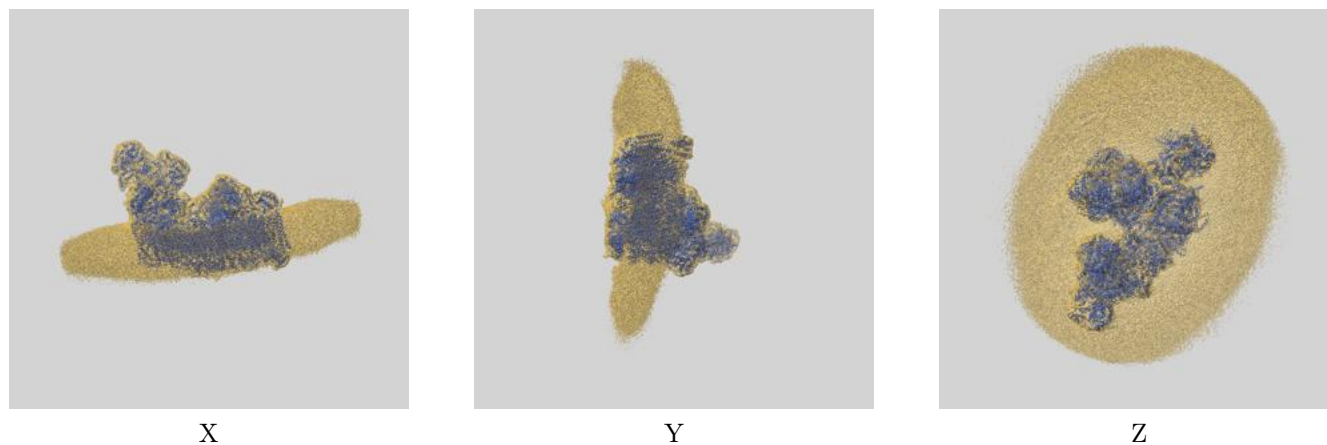
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

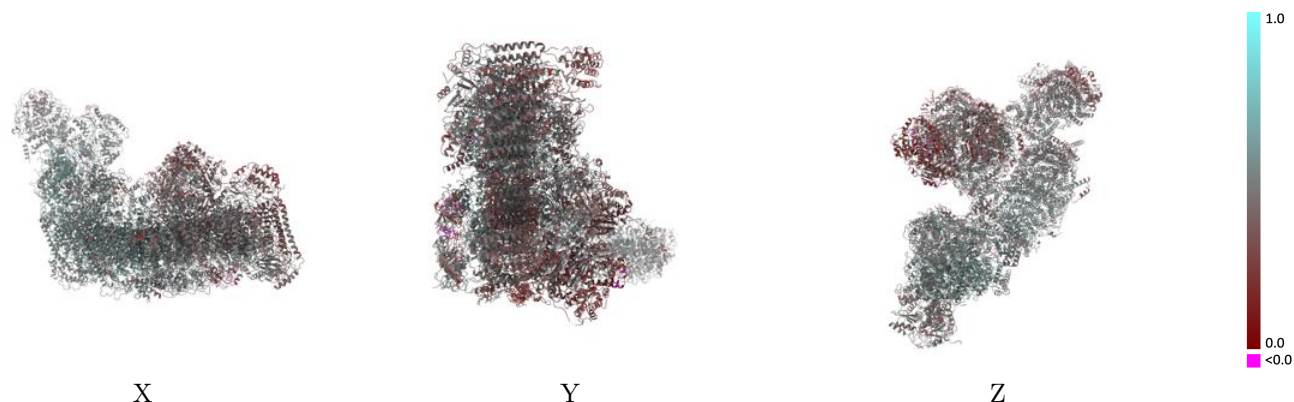
This section contains information regarding the fit between EMDB map EMD-42225 and PDB model 8UGH. Per-residue inclusion information can be found in section [3](#) on page [43](#).

### 9.1 Map-model overlay [i](#)



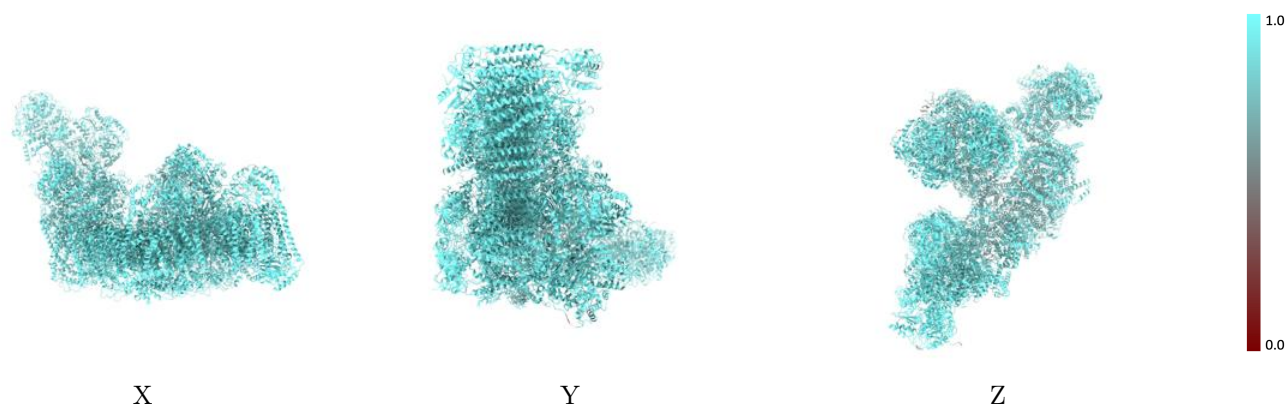
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



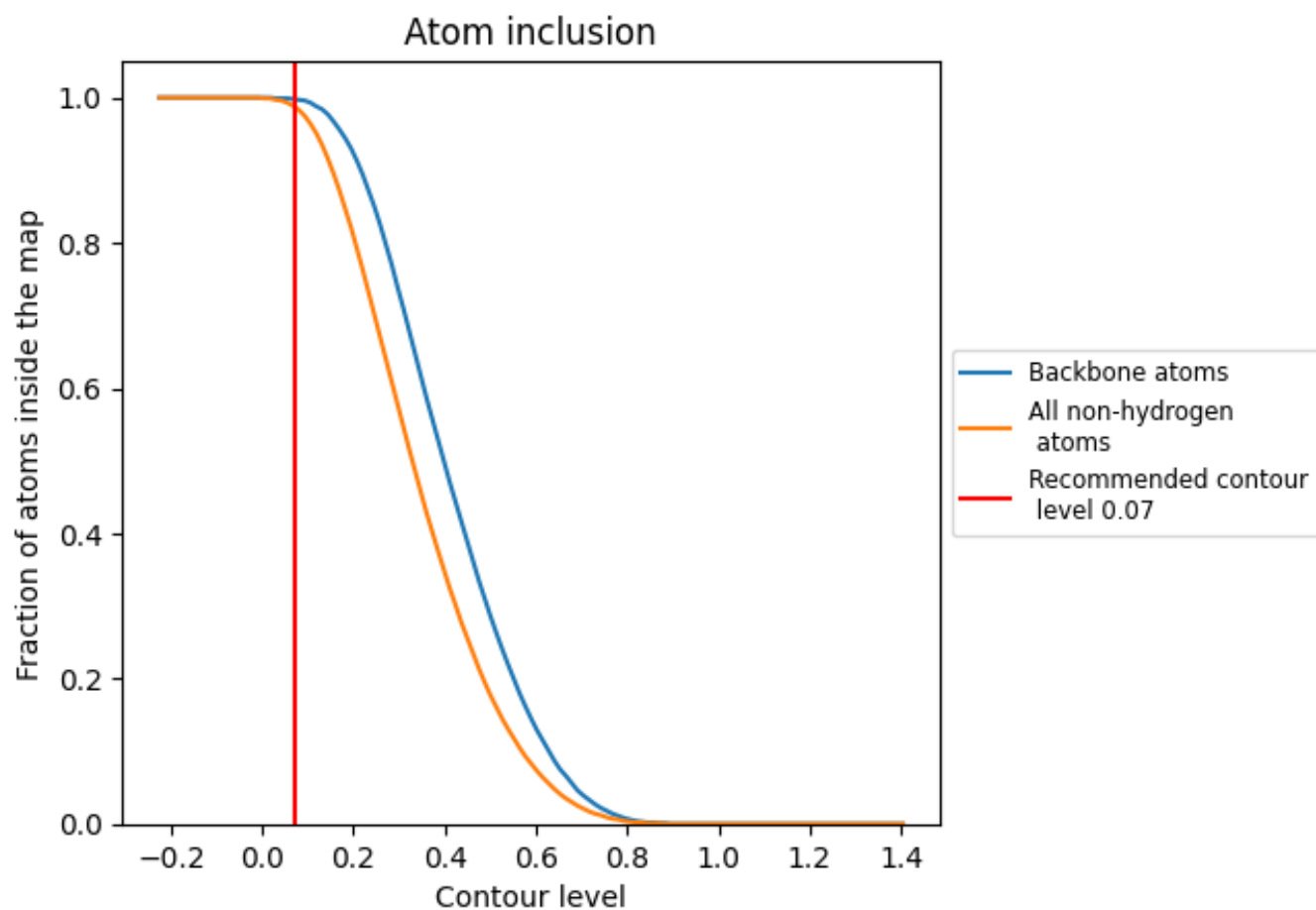
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.4640
1A	 0.9850	 0.4890
1B	 0.9970	 0.5530
1C	 0.9940	 0.5640
1D	 0.9930	 0.5690
1E	 0.9740	 0.4480
1F	 0.9800	 0.4530
1G	 0.9890	 0.4920
1H	 0.9960	 0.5470
1I	 0.9970	 0.5700
1J	 0.9970	 0.4700
1K	 0.9960	 0.5340
1L	 0.9980	 0.5100
1M	 1.0000	 0.5660
1N	 0.9990	 0.5680
1O	 0.9810	 0.5080
1P	 0.9820	 0.5060
1Q	 0.9330	 0.4950
1R	 0.9810	 0.5220
1S	 0.9720	 0.4570
1T	 0.9580	 0.3790
1U	 0.9910	 0.4370
1V	 0.9630	 0.5190
1W	 0.9640	 0.5210
1X	 0.9960	 0.5020
1Y	 0.9960	 0.4570
1Z	 0.9950	 0.5150
1a	 0.9980	 0.5440
1b	 0.9820	 0.4920
1c	 0.9850	 0.4660
1d	 0.9970	 0.5400
1e	 0.9940	 0.5000
1f	 0.9800	 0.4660
1g	 0.9920	 0.4970
1h	 0.9980	 0.5310













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Chain	Atom inclusion	Q-score
1i	 0.9930	 0.4440
1j	 0.9930	 0.4170
1k	 0.9840	 0.3990
1l	 0.9940	 0.4960
1m	 0.9990	 0.4860
1n	 0.9970	 0.4730
1o	 0.9980	 0.4490
1p	 1.0000	 0.5200
1q	 0.9960	 0.5390
1r	 0.9930	 0.5460
1s	 0.9380	 0.4160
3A	 0.9670	 0.3190
3B	 0.9820	 0.3030
3C	 0.9940	 0.4390
3D	 0.9960	 0.4890
3E	 0.9910	 0.3270
3F	 0.9540	 0.3590
3G	 0.9070	 0.3240
3H	 0.9710	 0.4230
3I	 0.9970	 0.3670
3J	 0.9960	 0.4200
3N	 1.0000	 0.4360
3O	 0.9970	 0.3550
3P	 1.0000	 0.4720
3Q	 1.0000	 0.5100
3R	 0.9890	 0.3080
3S	 1.0000	 0.4180
3T	 0.9970	 0.4580
3U	 1.0000	 0.4590
3V	 0.9910	 0.3240
3W	 1.0000	 0.4340
3X	 1.0000	 0.3610
3Y	 0.9940	 0.3390
4A	 0.9900	 0.4630
4B	 0.9900	 0.4110
4C	 0.9900	 0.4560
4D	 0.9470	 0.3920
4E	 0.9400	 0.3040
4F	 0.9290	 0.4000
4G	 0.9940	 0.4080
4H	 0.9700	 0.4090
4I	 0.9870	 0.3920

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Chain	Atom inclusion	Q-score
4J	 0.9940	 0.4810
4K	 0.9980	 0.4330
4L	 0.9650	 0.4530
4M	 0.9850	 0.4420
4N	 0.9710	 0.3780