



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 10:19 PM EDT

PDB ID : 8UGN  
EMDB ID : EMD-42230  
Title : In-situ structure of typeO supercomplex in respiratory chain (composite)  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-05  
Resolution : 2.70 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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:

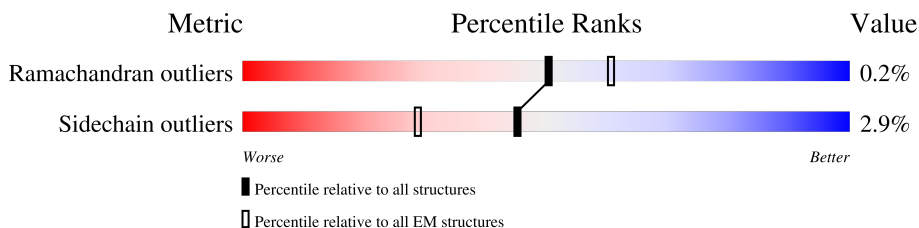
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 2.70 Å.

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






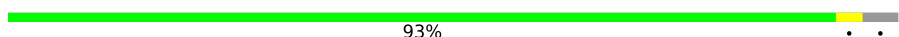

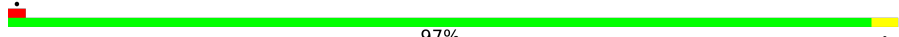




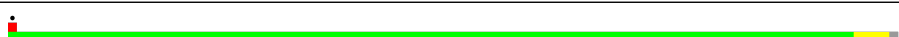


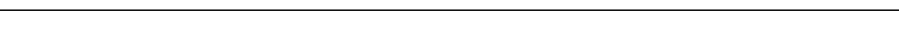
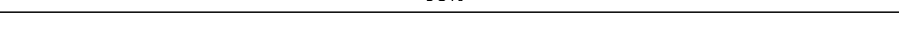
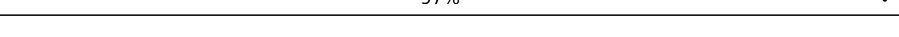
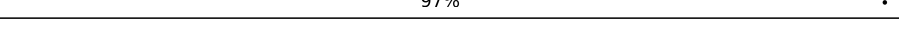
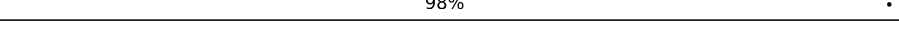
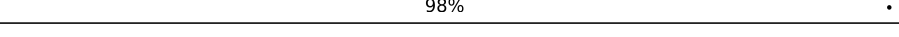
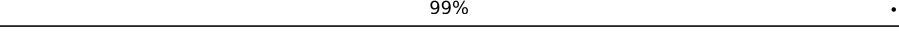





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	96%
1	5A	115	97%
2	1B	258	58% 40%
2	5B	258	59% 40%
3	1C	264	78% 21%
3	5C	264	78% 21%
4	1D	476	88% 10%
4	5D	476	89% 10%
5	1E	249	83% 14%




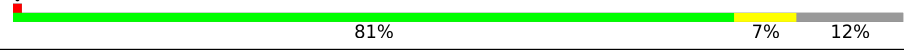
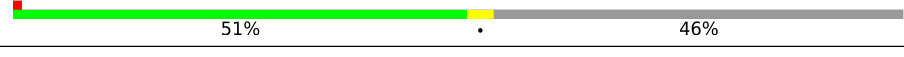



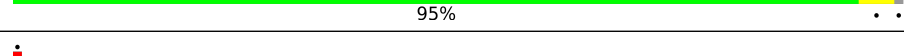
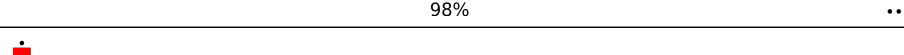
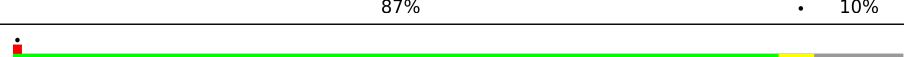
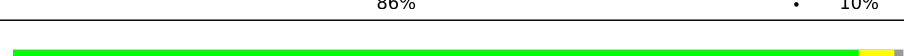
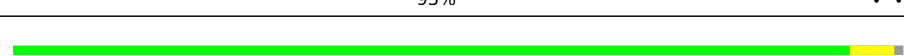
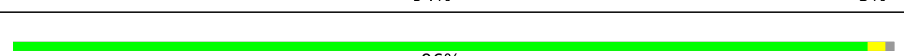
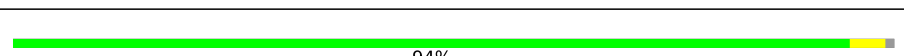
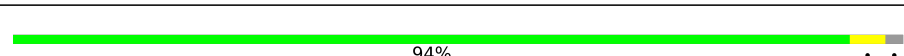
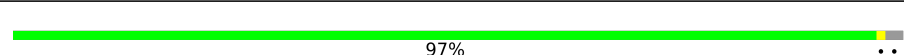
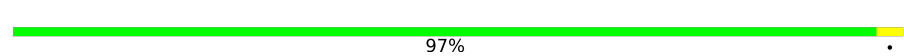

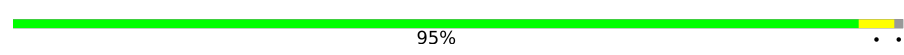
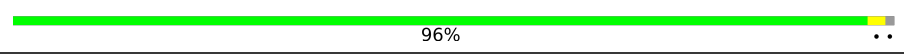
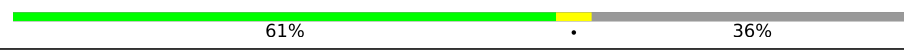

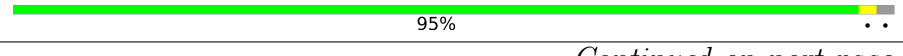

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Mol	Chain	Length	Quality of chain
5	5E	249	 83% 14%
6	1F	464	 91% 7%
6	5F	464	 91% 7%
7	1G	727	 93%
7	5G	727	 93%
8	1H	318	 97%
8	5H	318	 97%
9	1I	239	 73% 26%
9	5I	239	 73% 26%
10	1J	175	 95% 5%
10	5J	175	 95%
11	1K	98	 98%
11	5K	98	 96%
12	1L	606	 98%
12	5L	606	 97%
13	1M	459	 97%
13	5M	459	 98%
14	1N	347	 98%
14	5N	347	 99%
15	1O	357	 88% 10%
15	5O	357	 87% 10%
16	1P	377	 88% 9%
16	5P	377	 88% 9%
17	1Q	175	 68% 6% 26%
17	5Q	175	 71% 26%

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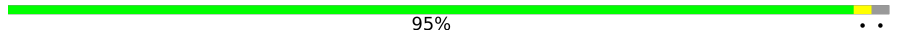







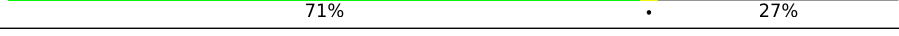
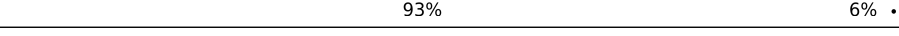
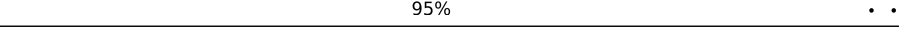
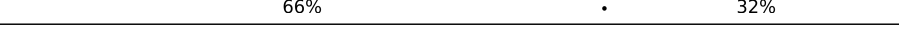

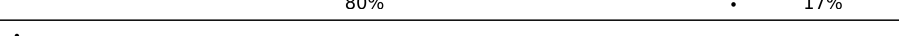


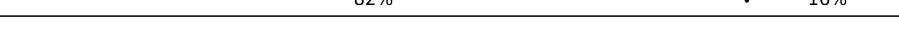
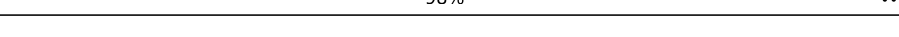
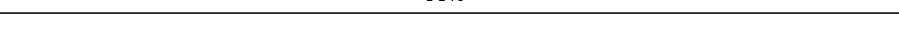






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Mol	Chain	Length	Quality of chain
18	1R	123	 74% 22%
18	5R	123	 74% 22%
19	1S	99	 81% 7% 12%
19	5S	99	 81% 7% 12%
20	1T	156	 51% 46%
20	1U	156	 53% 45%
20	5T	156	 51% 46%
20	5U	156	 51% 45%
21	1V	116	 95%
21	5V	116	 98%
22	1W	128	 87% 10%
22	5W	128	 86% 10%
23	1X	172	 95%
23	5X	172	 94% 5%
24	1Y	141	 96%
24	5Y	141	 94%
25	1Z	144	 94%
25	5Z	144	 97%
26	1a	70	 97%
26	5a	70	 100%
27	1b	84	 95%
27	5b	84	 96%
28	1c	76	 61% 36%
28	5c	76	 64% 36%
29	1d	122	 95%

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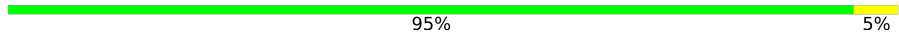
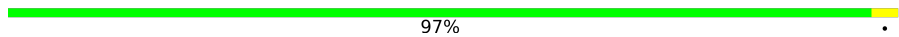








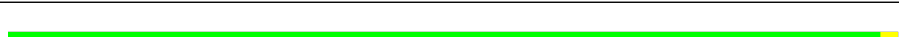


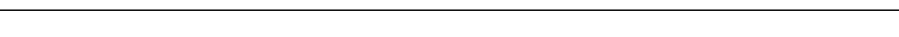
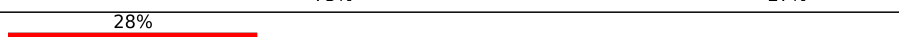
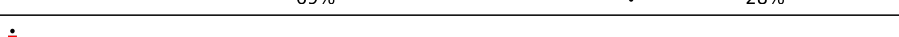



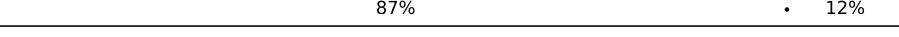







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Mol	Chain	Length	Quality of chain
29	5d	122	 95%
30	1e	106	 89% 5% 7%
30	5e	106	 91% 7%
31	1f	135	 40% 58%
31	5f	135	 41% 58%
32	1g	154	 62% 35%
32	5g	154	 63% 35%
33	1h	189	 71% 27%
33	5h	189	 71% 27%
34	1i	128	 93% 6%
34	5i	128	 95%
35	1j	105	 66% 32%
35	5j	105	 64% 32%
36	1k	98	 80% 17%
36	5k	98	 82% 17%
37	1l	186	 82% 16%
37	5l	186	 82% 16%
38	1m	129	 98%
38	5m	129	 98%
39	1n	179	 95%
39	5n	179	 93%
40	1o	137	 87% 11%
40	5o	137	 84% 5% 11%
41	1p	176	 97%
41	5p	176	 95%

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Mol	Chain	Length	Quality of chain
42	1q	145	 95% 5%
42	5q	145	 97%
43	1r	113	 83% 17%
43	5r	113	 80% 17%
44	1s	471	 9% 90%
44	5s	471	 9% 90%
45	3A	480	 90% 8%
45	3N	480	 91% 7%
46	3B	453	 91% 8%
46	3O	453	 90% 8%
47	3C	379	 98%
47	3P	379	 98%
48	3D	326	 71% 27%
48	3Q	326	 73% 27%
49	3E	274	 28% 69% 28%
49	3I	274	 17% 83%
49	3R	274	 26% 68% 28%
49	3V	274	 9% 89%
50	3F	111	 87% 12%
50	3S	111	 87% 12%
51	3G	82	 90% 10%
51	3T	82	 89% 10%
52	3H	91	 68% 29%
52	3U	91	 67% 29%
53	3J	64	 86% 12%



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Mol	Chain	Length	Quality of chain
53	3W	64	80% 8% 12%
54	3X	56	91% 7%
54	3Y	56	89% 9%
55	4A	514	97%
55	8A	514	98%
56	4B	229	96%
56	8B	229	96%
57	4C	261	95%
57	8C	261	98%
58	4D	169	79% 18%
58	8D	169	80% 18%
59	4E	152	68% 31%
59	8E	152	67% 31%
60	4F	128	73% 24%
60	8F	128	73% 24%
61	4G	97	74% 23%
61	8G	97	74% 23%
62	4H	86	90% 6% 5%
62	8H	86	93% 5%
63	4I	75	85% 11%
63	8I	75	89% 11%
64	4J	80	71% 28%
64	8J	80	69% 28%
65	4K	80	60% 39%
65	8K	80	60% 39%

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Mol	Chain	Length	Quality of chain
66	4L	63	
66	8L	63	
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

## 2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 202910 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
1	5A	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
2	5B	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
3	5C	209	1740	1125	297	316	2	0	0

There are 4 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
5C	104	GLN	ARG	conflict	UNP A0A286ZNN4
5C	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
4	5D	429	3452	2207	593	628	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68
5D	0	GLY	GLU	conflict	UNP A0A8D0QM68

- 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
5	5E	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
6	5F	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
7	5G	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	5H	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
9	5I	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
10	5J	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
11	5K	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
12	5L	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	5M	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
14	5N	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
15	5O	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
16	5P	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
17	5Q	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
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		
18	5R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		
19	5S	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		
20	5T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	5U	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		
21	5V	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		
22	5W	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
			Total	C	N	O	S		
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		
23	5X	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
			Total	C	N	O	S		
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		
24	5Y	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	Total	C	N	O	S	0	0
			1168	752	202	205	9		
25	5Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- 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	Total	C	N	O	S	0	0
			562	361	101	94	6		
26	5a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- 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	Total	C	N	O	S	0	0
			643	417	110	115	1		
27	5b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

drial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		
28	5c	49	Total	C	N	O	0	0
			417	276	71	70		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		
30	5e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		
31	5f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 58 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
5f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
5f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
5f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-67	THR	-	expression tag	UNP A0A8D1IZ33
5f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
5f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
5f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-57	ASN	-	expression tag	UNP A0A8D1IZ33

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Chain	Residue	Modelled	Actual	Comment	Reference
5f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
5f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
5f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-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
32	5g	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
33	5h	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	127	1100	723	194	181	2	0	0
34	5i	127	1100	723	194	181	2	0	0

- 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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	5j	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
36	5k	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
37	5l	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
38	5m	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
39	5n	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
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1
5o	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
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		
41	5p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		
43	5r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		
44	5s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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
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
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
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
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	3I	47	Total	C	N	O	S	0	0
			340	211	65	63	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
			224	136	48	39	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3E	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3E	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3E	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3E	56	ARG	SER	conflict	UNP A0A4X1TWD8
3I	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3I	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3I	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3I	56	ARG	SER	conflict	UNP A0A4X1TWD8
3R	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3R	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3R	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3R	56	ARG	SER	conflict	UNP A0A4X1TWD8
3V	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3V	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3V	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3V	56	ARG	SER	conflict	UNP A0A4X1TWD8

- 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
			Total	C	N	O	S		
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 53 complex iii.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	3J	56	Total	C	N	O	0	0
			454	295	81	78		
53	3W	56	Total	C	N	O	0	0
			454	295	81	78		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3J	60	ASN	LYS	conflict	UNP Q2EN79
3J	61	GLN	HIS	conflict	UNP Q2EN79
3J	62	GLY	LYS	conflict	UNP Q2EN79
3J	63	LYS	TYR	conflict	UNP Q2EN79
3W	56	ASN	LYS	conflict	UNP Q2EN79
3W	57	GLN	HIS	conflict	UNP Q2EN79
3W	58	GLY	LYS	conflict	UNP Q2EN79
3W	59	LYS	TYR	conflict	UNP Q2EN79

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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	Total	C	N	O	S	0	0
			4026	2693	625	676	32		
55	8A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- 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	Total	C	N	O	S	0	0
			1828	1190	281	339	18		
56	8B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- 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	Total	C	N	O	S	0	0
			2096	1399	336	351	10		
57	8C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- 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	Total	C	N	O	S	0	0
			1163	757	190	212	4		
58	8D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- 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	Total	C	N	O	S	0	0
			852	544	144	162	2		
59	8E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- 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	Total	C	N	O	S	0	0
			734	455	130	143	6		
60	8F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		
61	8G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- 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		
62	8H	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		
63	8I	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		
64	8J	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		
65	8K	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	8L	46	381	254	64	61	2	0	0

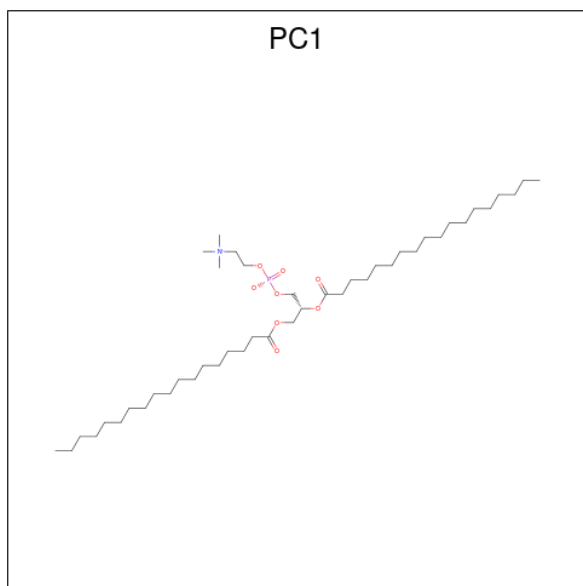
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
67	4M	43	338	222	57	59	0	0
67	8M	43	338	222	57	59	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	4N	82	660	432	112	114	2	0	0
68	8N	82	660	432	112	114	2	0	0

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: 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	
69	1A	1	35	25	1	8	1	0

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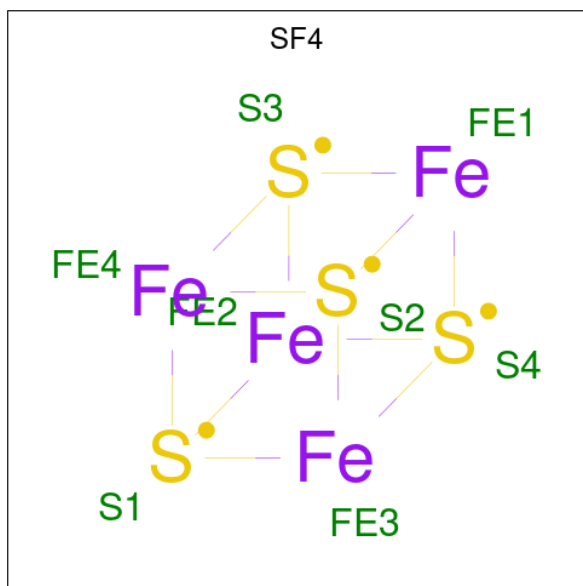
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1A	1	Total 35	C 25	N 1	O 8	P 1	0
69	1A	1	Total 33	C 23	N 1	O 8	P 1	0
69	1B	1	Total 46	C 36	N 1	O 8	P 1	0
69	1B	1	Total 48	C 38	N 1	O 8	P 1	0
69	1H	1	Total 48	C 38	N 1	O 8	P 1	0
69	1I	1	Total 54	C 44	N 1	O 8	P 1	0
69	1I	1	Total 44	C 34	N 1	O 8	P 1	0
69	1L	1	Total 46	C 36	N 1	O 8	P 1	0
69	1M	1	Total 35	C 25	N 1	O 8	P 1	0
69	1M	1	Total 44	C 34	N 1	O 8	P 1	0
69	1d	1	Total 39	C 29	N 1	O 8	P 1	0
69	1h	1	Total 47	C 37	N 1	O 8	P 1	0
69	1q	1	Total 49	C 39	N 1	O 8	P 1	0
69	3J	1	Total 47	C 37	N 1	O 8	P 1	0
69	3R	1	Total 45	C 35	N 1	O 8	P 1	0
69	3X	1	Total 29	C 19	N 1	O 8	P 1	0
69	5A	1	Total 35	C 25	N 1	O 8	P 1	0
69	5A	1	Total 35	C 25	N 1	O 8	P 1	0
69	5B	1	Total 46	C 36	N 1	O 8	P 1	0
69	5B	1	Total 48	C 38	N 1	O 8	P 1	0
69	5H	1	Total 48	C 38	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	5I	1	Total 54	C 44	N 1	O 8	P 1	0
69	5I	1	Total 44	C 34	N 1	O 8	P 1	0
69	5L	1	Total 46	C 36	N 1	O 8	P 1	0
69	5M	1	Total 35	C 25	N 1	O 8	P 1	0
69	5M	1	Total 44	C 34	N 1	O 8	P 1	0
69	5P	1	Total 33	C 23	N 1	O 8	P 1	0
69	5d	1	Total 39	C 29	N 1	O 8	P 1	0
69	5h	1	Total 47	C 37	N 1	O 8	P 1	0
69	5q	1	Total 49	C 39	N 1	O 8	P 1	0

- Molecule 70 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



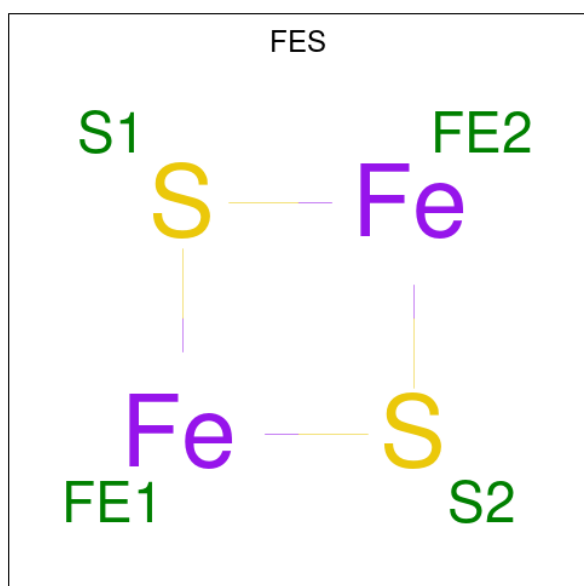
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
70	1B	1	Total 8	Fe 4	S 4	0
70	1F	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
70	1G	1	Total 8	Fe 4	S 4	0
70	1G	1	Total 8	Fe 4	S 4	0
70	1I	1	Total 8	Fe 4	S 4	0
70	1I	1	Total 8	Fe 4	S 4	0
70	5B	1	Total 8	Fe 4	S 4	0
70	5F	1	Total 8	Fe 4	S 4	0
70	5G	1	Total 8	Fe 4	S 4	0
70	5G	1	Total 8	Fe 4	S 4	0
70	5I	1	Total 8	Fe 4	S 4	0
70	5I	1	Total 8	Fe 4	S 4	0

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
71	1E	1	Total 4	Fe 2	S 2	0

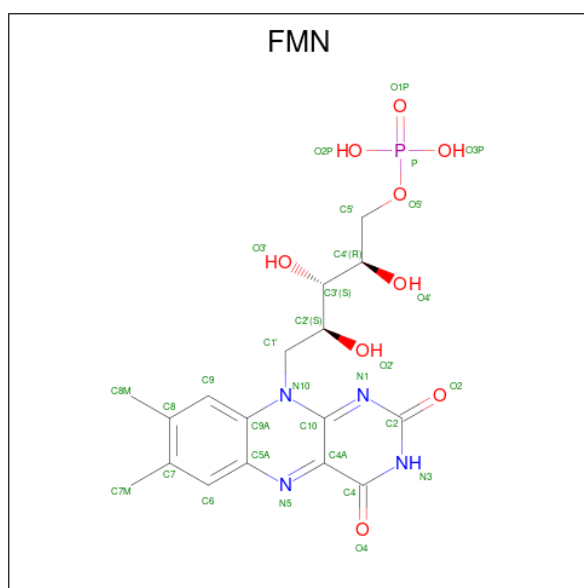
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Mol	Chain	Residues	Atoms			AltConf
71	1G	1	Total	Fe	S	0
			4	2	2	
71	3E	1	Total	Fe	S	0
			4	2	2	
71	3R	1	Total	Fe	S	0
			4	2	2	
71	5E	1	Total	Fe	S	0
			4	2	2	
71	5G	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).

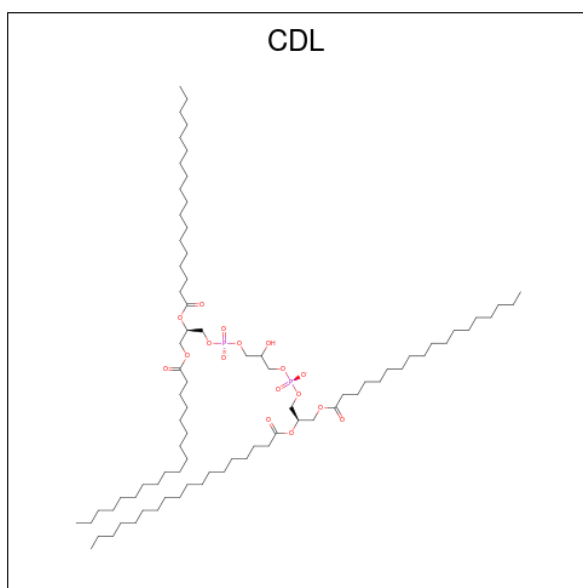


Mol	Chain	Residues	Atoms					AltConf
72	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	
72	5F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 73 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
73	1G	1	Total	K	0
			1	1	
73	5G	1	Total	K	0
			1	1	

- Molecule 74 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



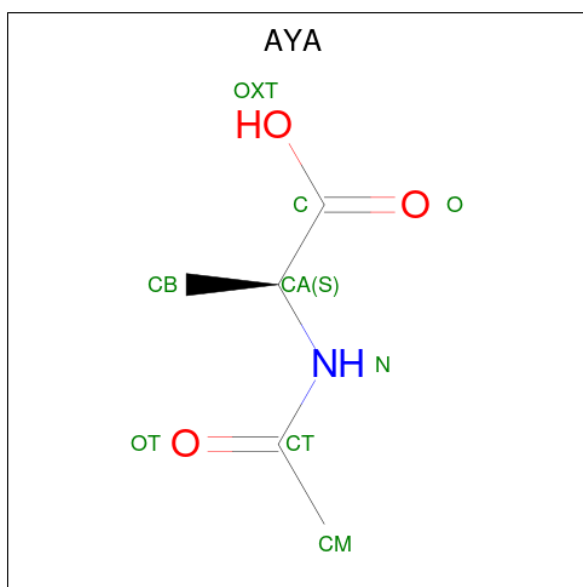
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
74	1H	1	51	32	17	2	0
74	1L	1	76	57	17	2	0
74	1N	1	62	43	17	2	0
74	1X	1	86	67	17	2	0
74	1d	1	65	46	17	2	0
74	1h	1	80	61	17	2	0
74	1q	1	61	42	17	2	0
74	3A	1	58	39	17	2	0
74	3C	1	52	33	17	2	0
74	3G	1	56	37	17	2	0
74	3N	1	43	24	17	2	0
74	3P	1	56	37	17	2	0
74	3T	1	57	38	17	2	0

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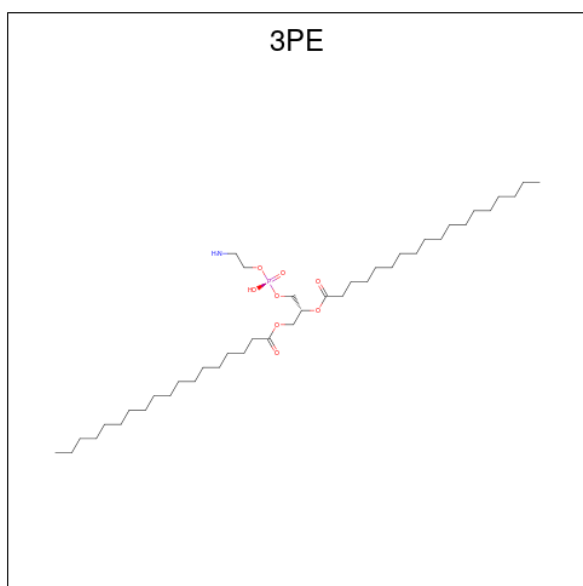
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
74	4B	1	100	81	17	2	0
74	4C	1	100	81	17	2	0
74	4D	1	100	81	17	2	0
74	5H	1	51	32	17	2	0
74	5L	1	76	57	17	2	0
74	5N	1	62	43	17	2	0
74	5X	1	86	67	17	2	0
74	5d	1	65	46	17	2	0
74	5h	1	80	61	17	2	0
74	5q	1	61	42	17	2	0
74	8B	1	100	81	17	2	0
74	8C	1	100	81	17	2	0
74	8D	1	100	81	17	2	0

- Molecule 75 is N-ACETYLLALANINE (three-letter code: AYA) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
75	1I	1	8	5	1	2	0
75	5q	1	8	5	1	2	0

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	1K	1	44	34	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	1L	1	Total 46	C 36	N 1	O 8	P 1	0
76	1L	1	Total 45	C 35	N 1	O 8	P 1	0
76	1M	1	Total 49	C 39	N 1	O 8	P 1	0
76	1M	1	Total 45	C 35	N 1	O 8	P 1	0
76	1M	1	Total 48	C 38	N 1	O 8	P 1	0
76	1M	1	Total 50	C 40	N 1	O 8	P 1	0
76	1O	1	Total 51	C 41	N 1	O 8	P 1	0
76	1P	1	Total 35	C 25	N 1	O 8	P 1	0
76	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
76	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
76	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
76	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
76	1Y	1	Total 41	C 31	N 1	O 8	P 1	0
76	1b	1	Total 47	C 37	N 1	O 8	P 1	0
76	1d	1	Total 49	C 39	N 1	O 8	P 1	0
76	1j	1	Total 44	C 34	N 1	O 8	P 1	0
76	3A	1	Total 27	C 17	N 1	O 8	P 1	0
76	3A	1	Total 32	C 22	N 1	O 8	P 1	0
76	3C	1	Total 35	C 25	N 1	O 8	P 1	0
76	3C	1	Total 34	C 24	N 1	O 8	P 1	0

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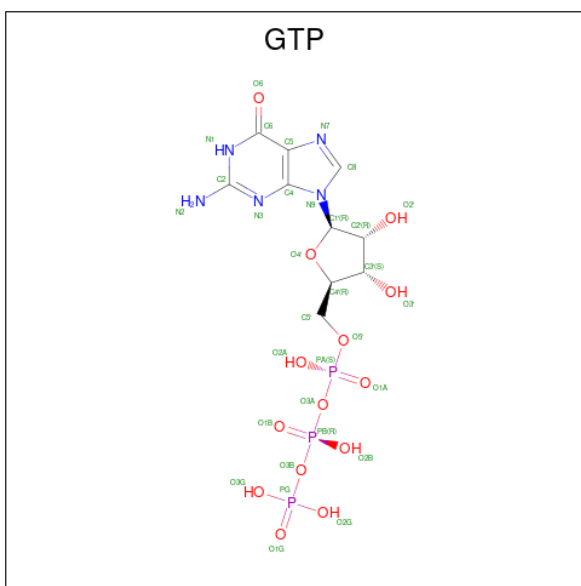
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	3D	1	Total 33	C 23	N 1	O 8	P 1	0
76	3G	1	Total 29	C 19	N 1	O 8	P 1	0
76	3N	1	Total 33	C 23	N 1	O 8	P 1	0
76	3N	1	Total 25	C 15	N 1	O 8	P 1	0
76	3P	1	Total 33	C 23	N 1	O 8	P 1	0
76	3Q	1	Total 47	C 37	N 1	O 8	P 1	0
76	3Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	5A	1	Total 47	C 37	N 1	O 8	P 1	0
76	5K	1	Total 44	C 34	N 1	O 8	P 1	0
76	5L	1	Total 46	C 36	N 1	O 8	P 1	0
76	5L	1	Total 45	C 35	N 1	O 8	P 1	0
76	5L	1	Total 49	C 39	N 1	O 8	P 1	0
76	5M	1	Total 45	C 35	N 1	O 8	P 1	0
76	5M	1	Total 48	C 38	N 1	O 8	P 1	0
76	5M	1	Total 51	C 41	N 1	O 8	P 1	0
76	5M	1	Total 50	C 40	N 1	O 8	P 1	0
76	5P	1	Total 35	C 25	N 1	O 8	P 1	0
76	5Y	1	Total 31	C 21	N 1	O 8	P 1	0
76	5Y	1	Total 40	C 30	N 1	O 8	P 1	0
76	5Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	5Y	1	Total 33	C 23	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	5Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
76	5Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	5d	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	5j	1	Total	C	N	O	P	0
			44	34	1	8	1	

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



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

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

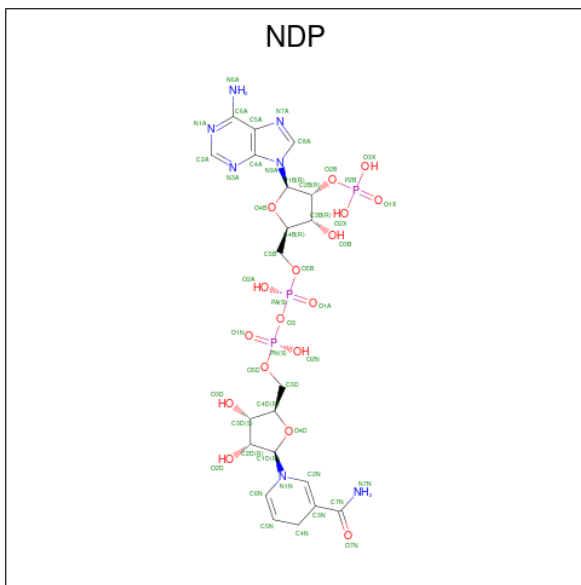
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
78	1O	1	Total	Mg	0
			1	1	
78	4A	1	Total	Mg	0
			1	1	
78	5O	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
78	8A	1	1	1	0

- Molecule 79 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



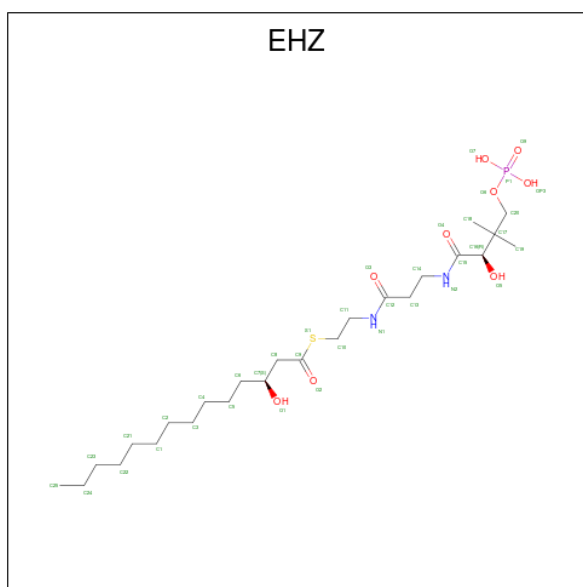
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
79	1P	1	48	21	7	17	3	0
79	5P	1	48	21	7	17	3	0

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	1R	1	1	1	0
80	4F	1	1	1	0
80	5R	1	1	1	0
80	8F	1	1	1	0

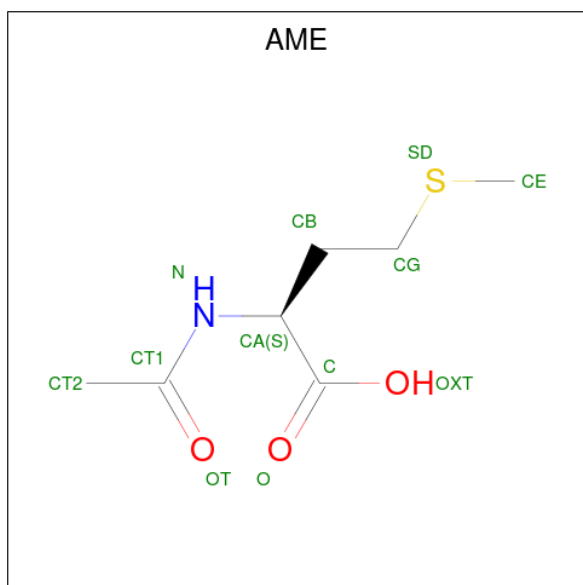
- Molecule 81 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula:  $C_{25}H_{49}N_2O_9PS$ ).





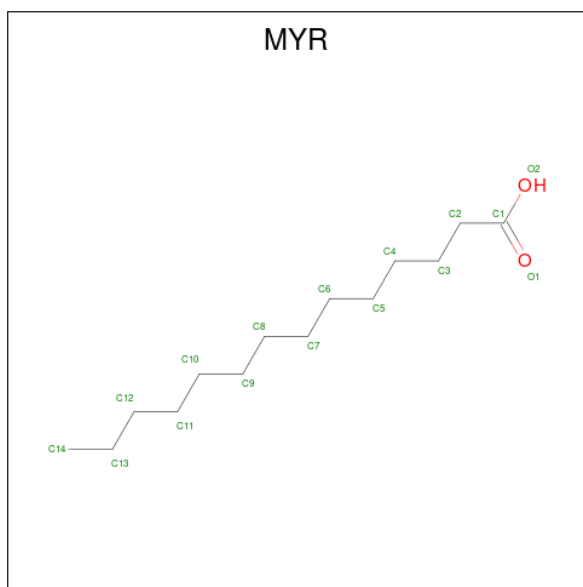
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
81	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 82 is N-ACETYL METHIONINE (three-letter code: AME) (formula:  $C_7H_{13}NO_3S$ ).



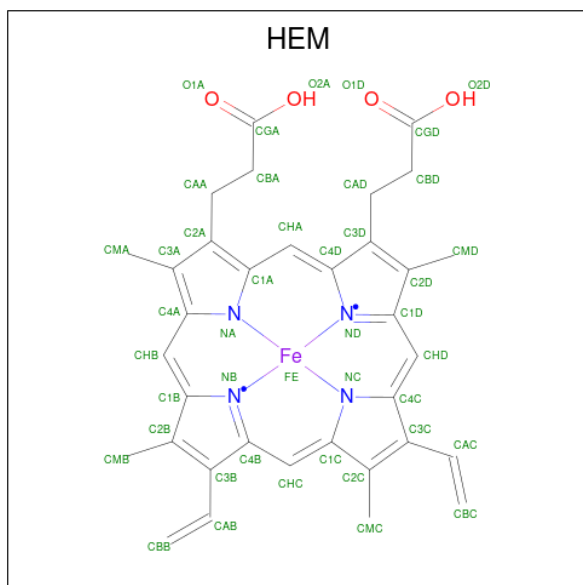
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
82	5h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 83 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



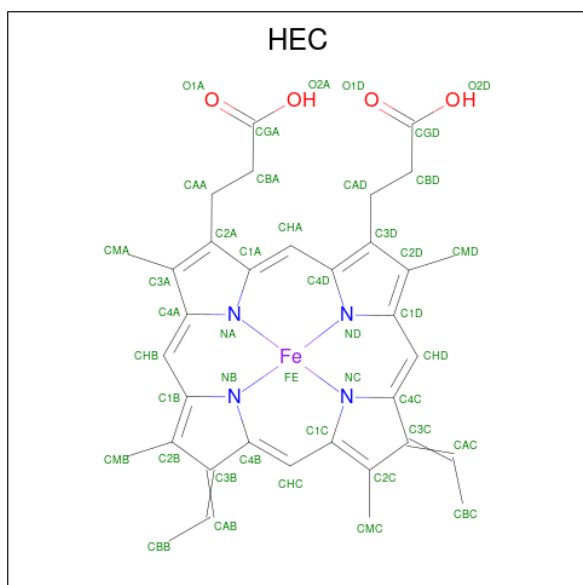
Mol	Chain	Residues	Atoms			AltConf
83	1o	1	Total	C	O	0
			15	14	1	
83	5o	1	Total	C	O	0
			15	14	1	

- Molecule 84 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



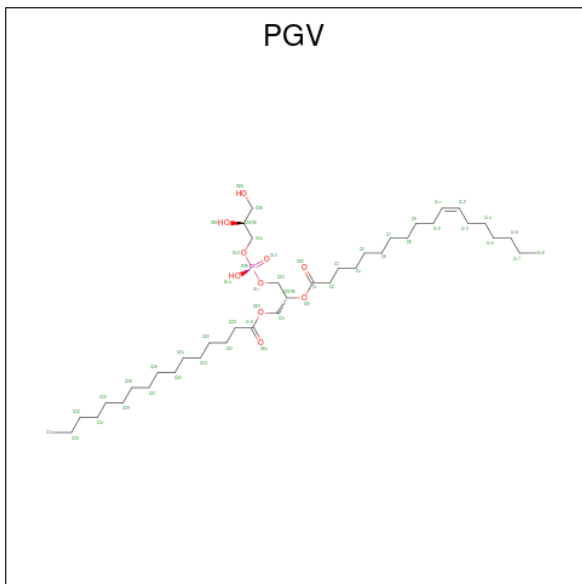
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
84	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 85 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
85	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
85	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 86 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



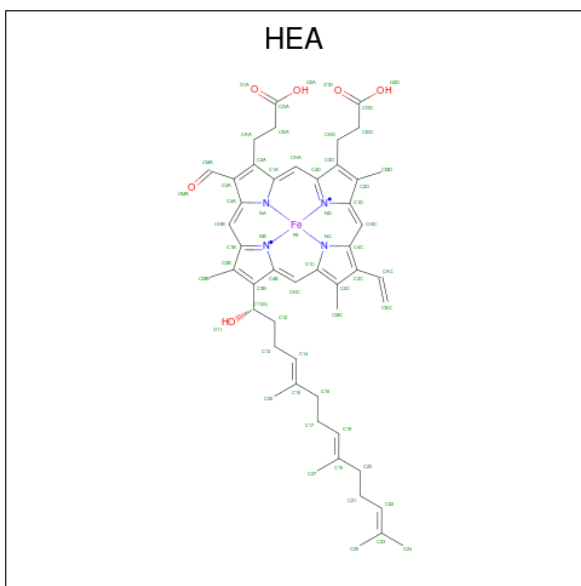
Mol	Chain	Residues	Atoms			AltConf	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4B	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
86	4C	1	51	40	10	1	0
86	4G	1	51	40	10	1	0
86	4J	1	51	40	10	1	0
86	4K	1	51	40	10	1	0
86	4L	1	51	40	10	1	0
86	4M	1	51	40	10	1	0
86	8A	1	51	40	10	1	0
86	8A	1	51	40	10	1	0
86	8B	1	51	40	10	1	0
86	8B	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8C	1	51	40	10	1	0
86	8G	1	51	40	10	1	0
86	8J	1	51	40	10	1	0
86	8K	1	51	40	10	1	0
86	8L	1	51	40	10	1	0
86	8M	1	51	40	10	1	0

- Molecule 87 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



Mol	Chain	Residues	Atoms				AltConf	
87	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
87	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
87	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
87	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 88 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

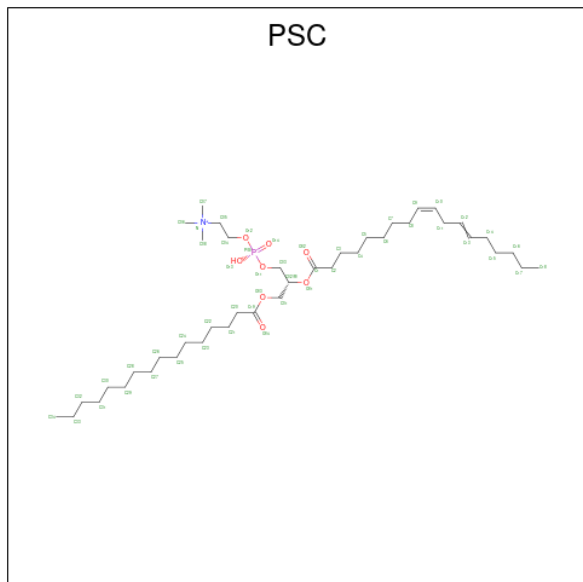
Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Cu	0
			1	1	
88	8A	1	Total	Cu	0
			1	1	

- Molecule 89 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Na	0
			1	1	
89	8A	1	Total	Na	0
			1	1	

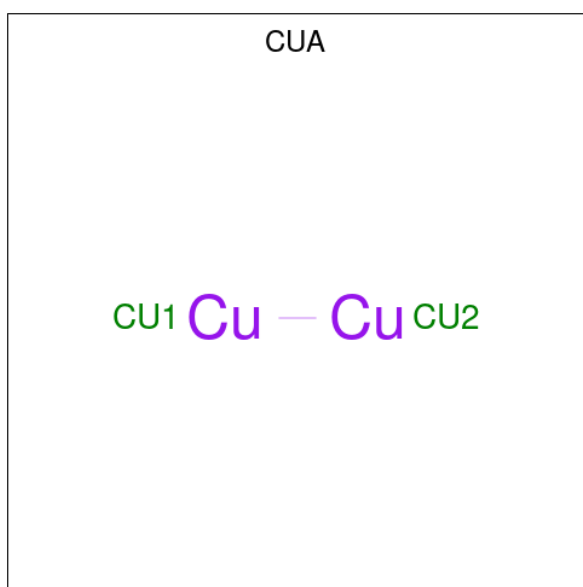
- Molecule 90 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO

YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM  
4-OXIDE (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).



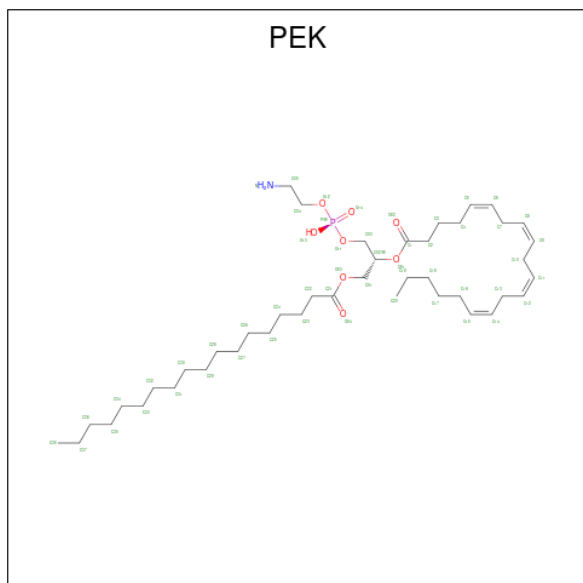
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
90	4A	1	52	42	1	8	1	0
90	8I	1	52	42	1	8	1	0

- Molecule 91 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



Mol	Chain	Residues	Atoms	AltConf
91	4B	1	Total Cu 2 2	0
91	8B	1	Total Cu 2 2	0

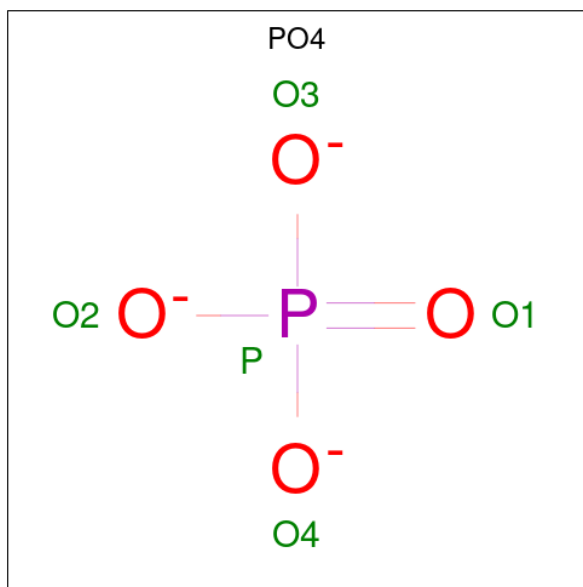
- Molecule 92 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	AltConf
92	4C	1	Total C N O P 52 42 1 8 1	0
92	4G	1	Total C N O P 53 43 1 8 1	0
92	8C	1	Total C N O P 52 42 1 8 1	0
92	8G	1	Total C N O P 53 43 1 8 1	0

- Molecule 93 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



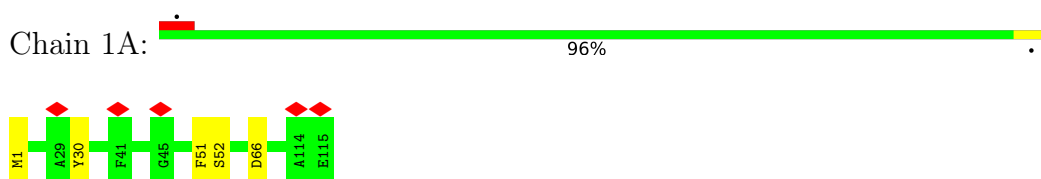


Mol	Chain	Residues	Atoms			AltConf
93	4H	1	Total	O	P	0
			5	4	1	
93	8H	1	Total	O	P	0
			5	4	1	

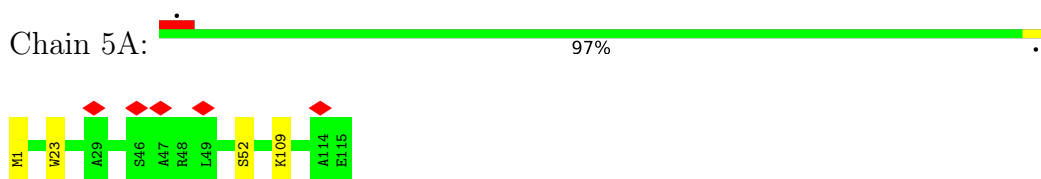
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

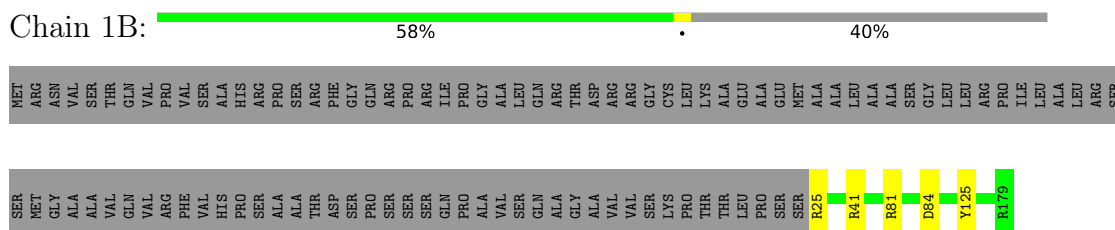
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



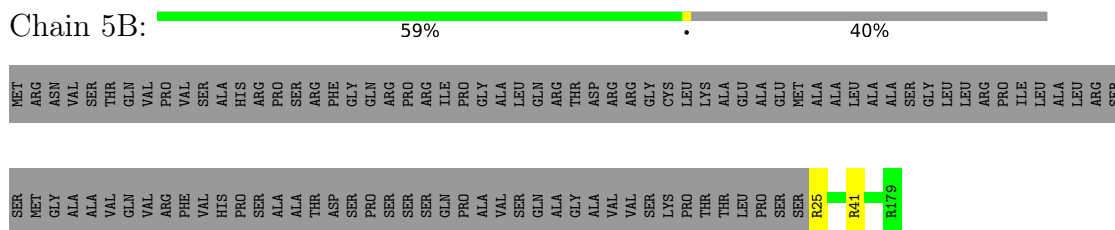
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



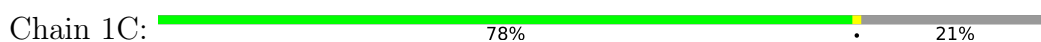
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

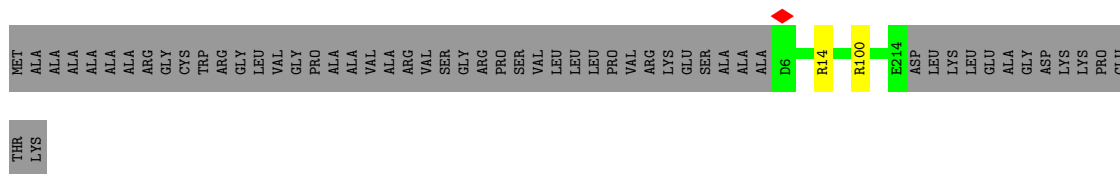


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

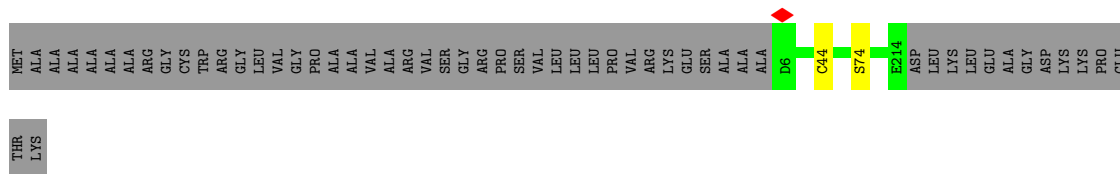
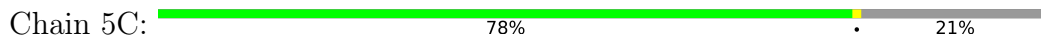


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

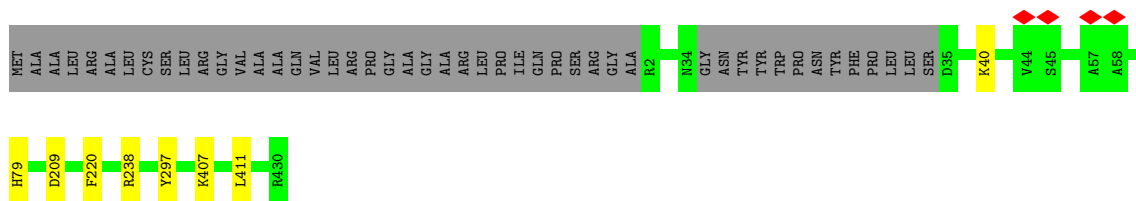
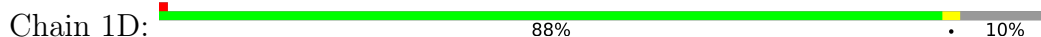




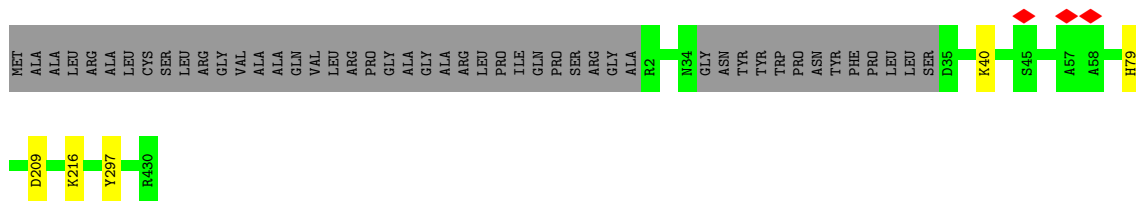
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



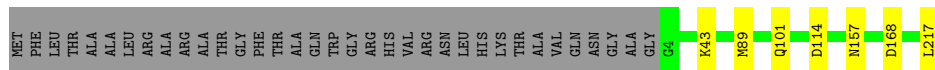
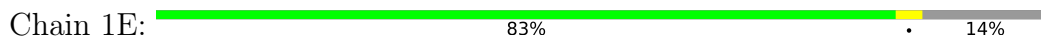
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



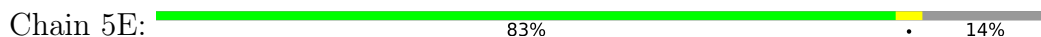
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

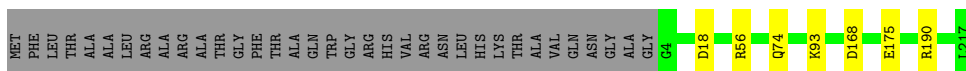


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

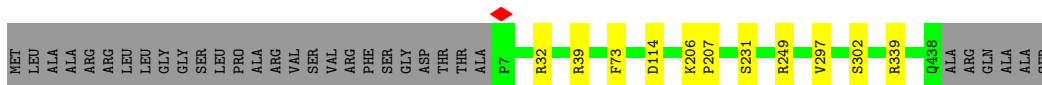


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

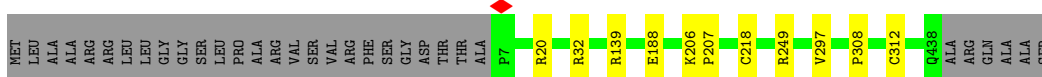




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



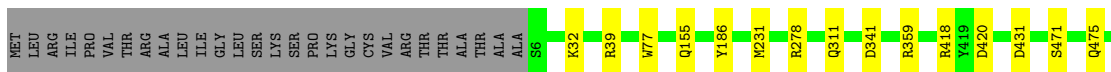
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



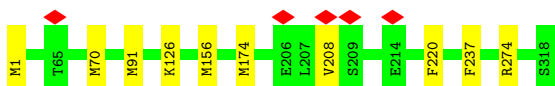
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



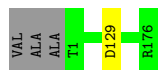
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1





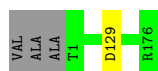
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 73% 26%



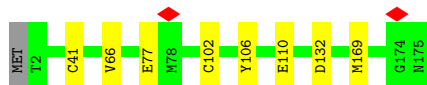
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 5I: 73% 26%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J: 95% 5%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 5J: 95% 5%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K: 98%



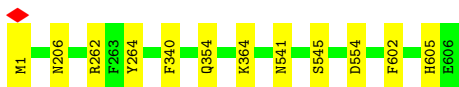
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 5K: 96%



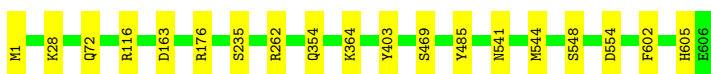
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L: 98%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 5L: 97%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M: 97%



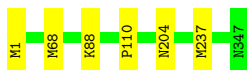
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 5M: 98%



- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N: 98%



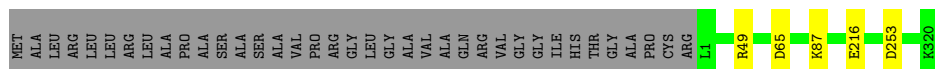
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 5N: 99%



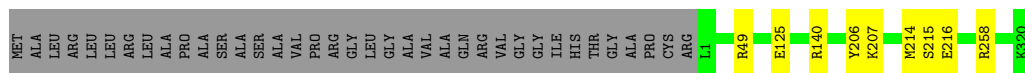
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 10: 88% 10%



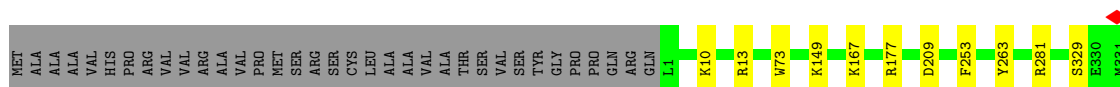
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 5O: 87% 10%



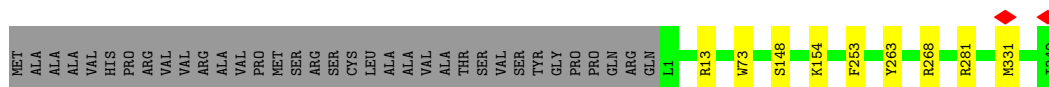
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P: 88% 9%



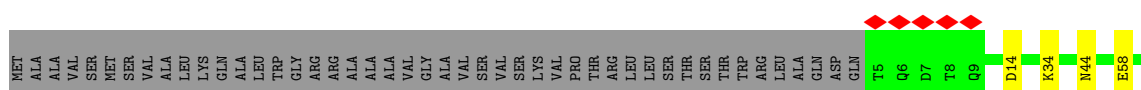
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P: 88% 9%



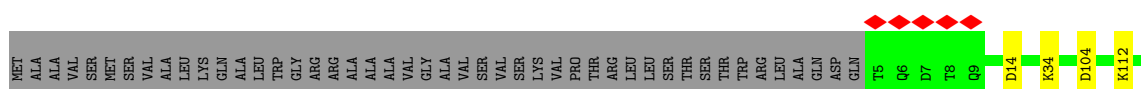
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q: 68% 6% 26%



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

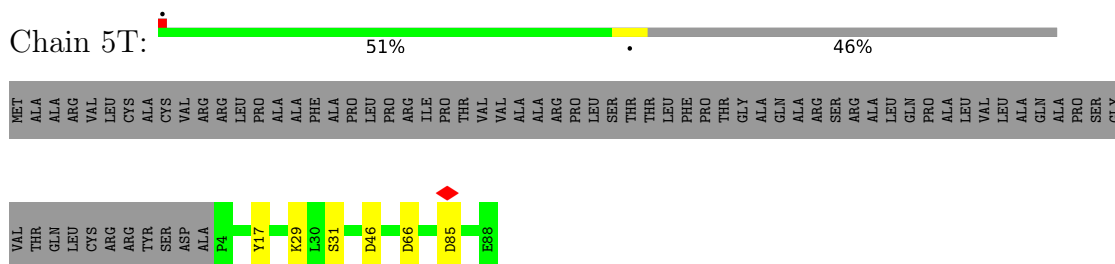
Chain 5Q: 71% 26%



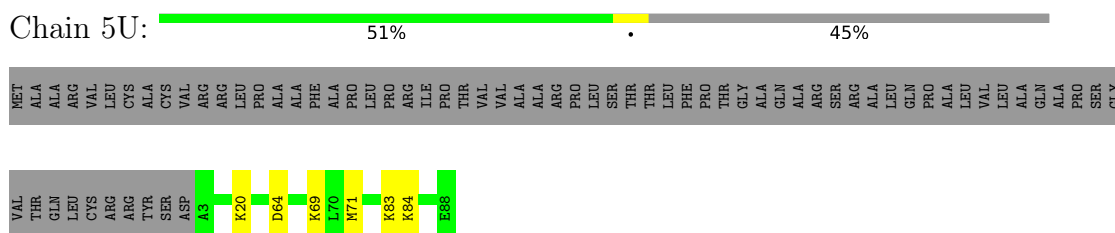




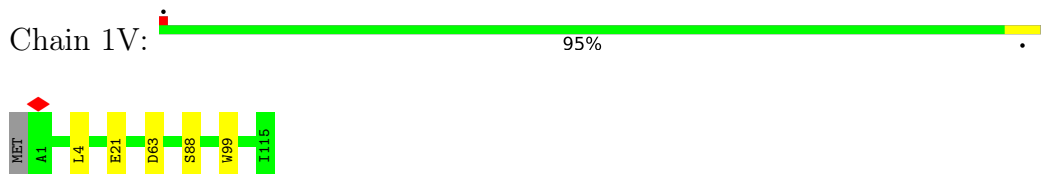
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



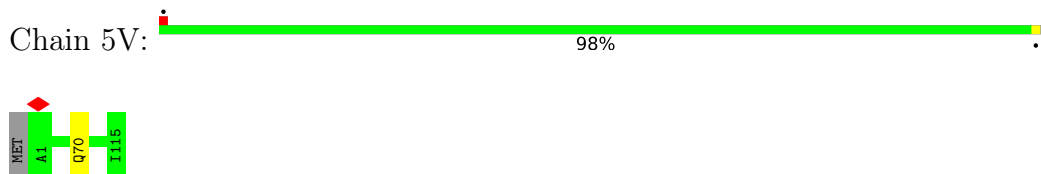
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



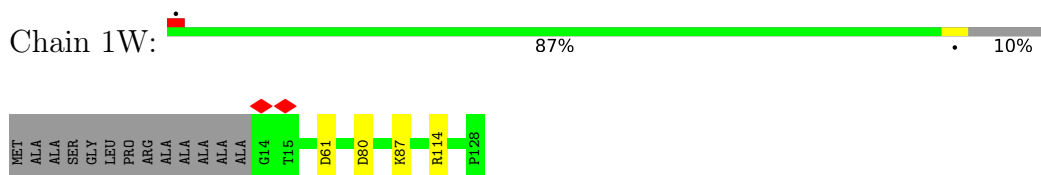
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



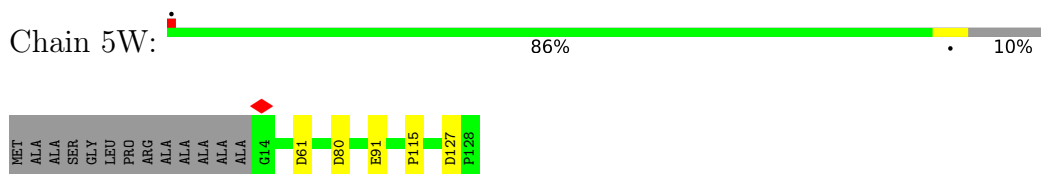
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



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



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



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

Chain 1X:  95% ..



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

Chain 5X:  94% 5% ..



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

Chain 1Y:  96% ..



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

Chain 5Y:  94% ..



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:  94% ..



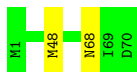
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 5Z:  97% ..



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

Chain 1a:  97% .



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

Chain 5a:  100%

There are no outlier residues recorded for this chain.

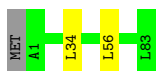
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b:  95%



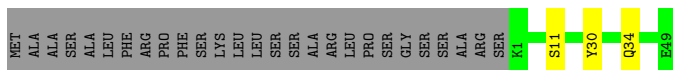
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 5b:  96%



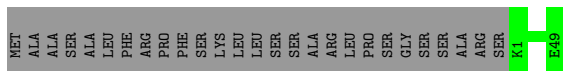
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c:  61%



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

Chain 5c:  64%



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

Chain 1d:  95%




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

Chain 5d:  95%



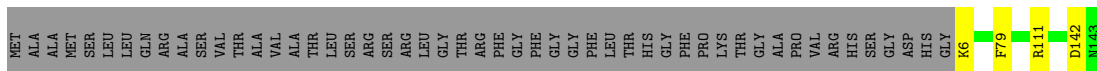
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:  89%



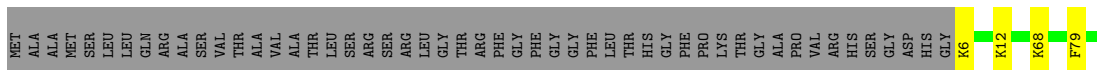
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:  71% 27%



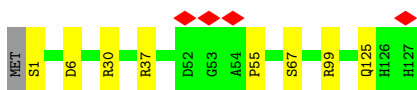
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 5h:  71% 27%



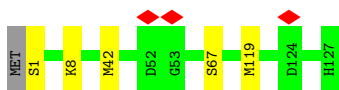
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:  93% 6%



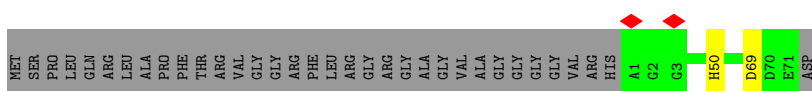
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 5i:  95%



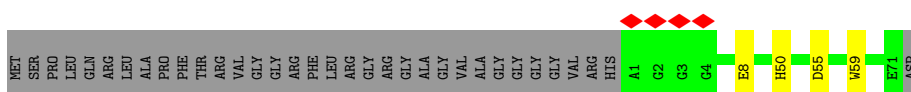
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:  66% 32%




- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 5j:  64% 32%

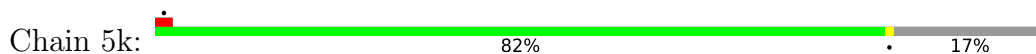


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

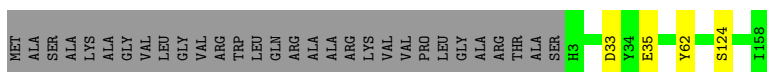
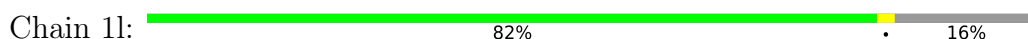
Chain 1k:  80% 17%



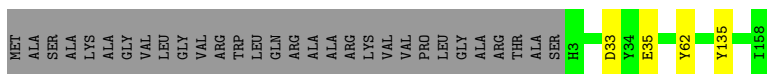
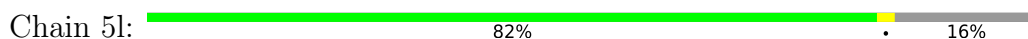
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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



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



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



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



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




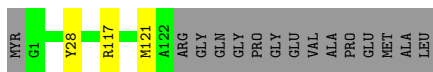
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 5n:  93%




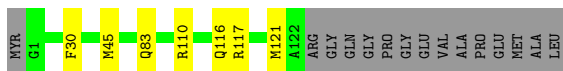
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:  87%



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

Chain 5o:  84%



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

Chain 1p:  97%



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

Chain 5p:  95%



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

Chain 1q:  95%



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

Chain 5q:  97%



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

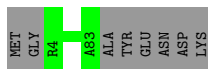








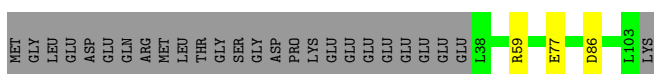




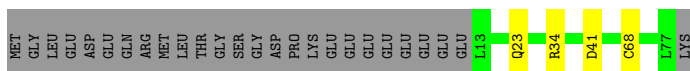
- Molecule 51: Cytochrome b-c1 complex subunit 8



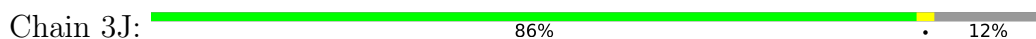
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



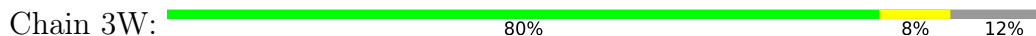
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



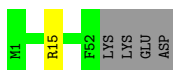
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein 53 complex iii



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

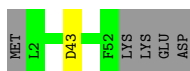


- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 54: Cytochrome b-c1 complex subunit 10





- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A: 97%



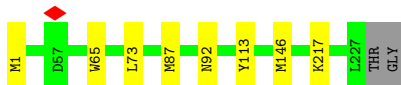
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 8A: 98%



- Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 96%



- Molecule 56: Cytochrome c oxidase subunit 2

Chain 8B: 96%



- Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C: 95%



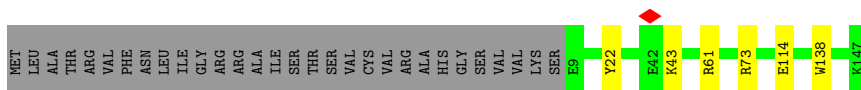
- Molecule 57: Cytochrome c oxidase subunit 3

Chain 8C: 98%

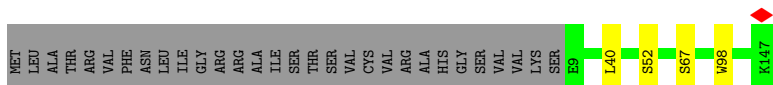
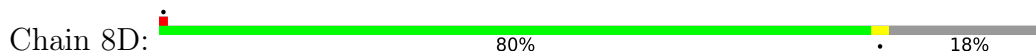


- Molecule 58: Cytochrome c oxidase subunit 4

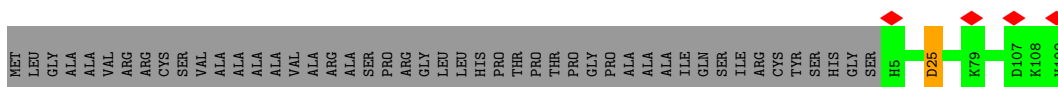
Chain 4D: 79% 18%



- Molecule 58: Cytochrome c oxidase subunit 4



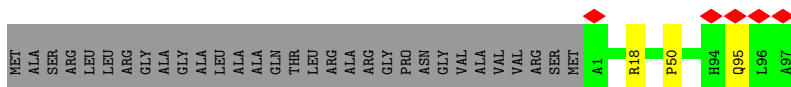
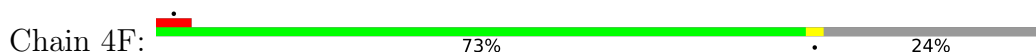
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



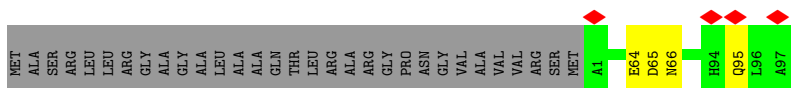
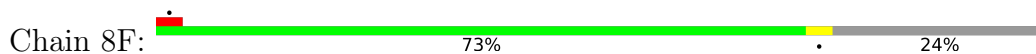
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



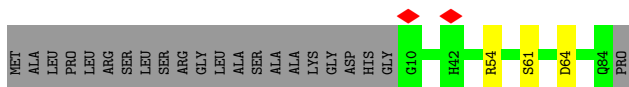
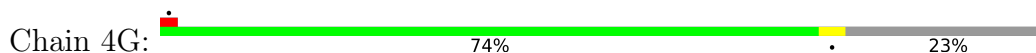
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



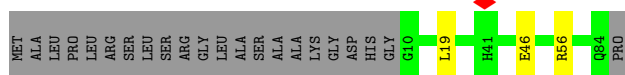
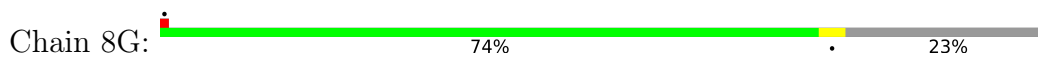
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



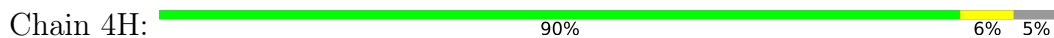
- Molecule 61: Cytochrome c oxidase subunit 6A2



- Molecule 61: Cytochrome c oxidase subunit 6A2



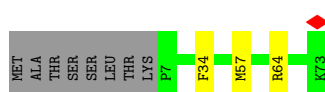
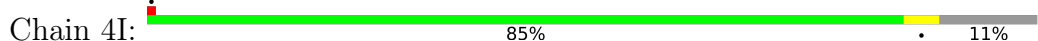
• Molecule 62: Cytochrome c oxidase subunit 6B1



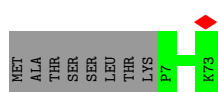
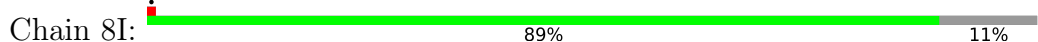
• Molecule 62: Cytochrome c oxidase subunit 6B1



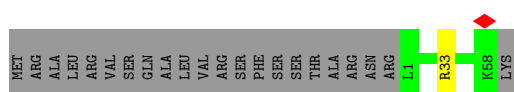
• Molecule 63: Cytochrome c oxidase subunit 6C



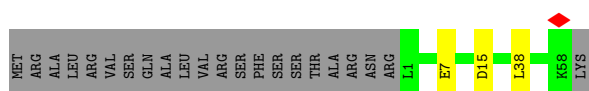
• Molecule 63: Cytochrome c oxidase subunit 6C



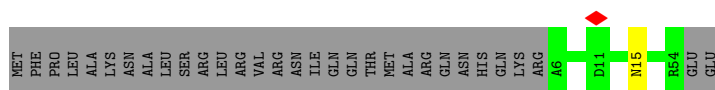
• Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



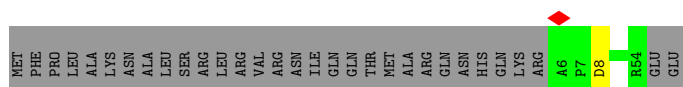
• Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



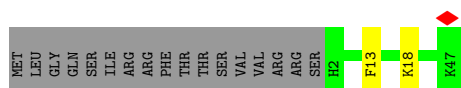
• Molecule 65: Cytochrome c oxidase subunit 7B



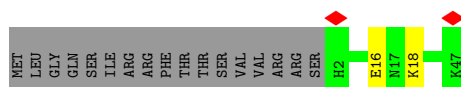
• Molecule 65: Cytochrome c oxidase subunit 7B



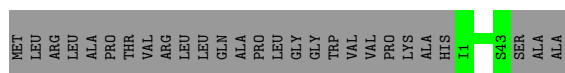
• Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



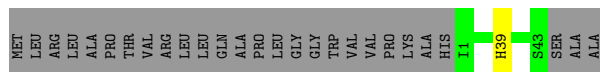
• Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



• Molecule 67: Cytochrome c oxidase subunit 8



• Molecule 67: Cytochrome c oxidase subunit 8



• Molecule 68: Cytochrome c oxidase subunit NDUF4A







- 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	80000	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	1.531	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.09	Depositor
Map size ( $\text{\AA}$ )	643.50006, 643.50006, 643.50006	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1700001, 1.1700001, 1.1700001	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.26	0/930	0.46	0/1271
1	5A	0.26	0/930	0.48	0/1271
2	1B	0.29	0/1273	0.56	0/1722
2	5B	0.28	0/1273	0.53	0/1722
3	1C	0.26	0/1791	0.48	0/2439
3	5C	0.27	0/1791	0.48	0/2439
4	1D	0.26	0/3545	0.48	0/4806
4	5D	0.27	0/3545	0.48	0/4806
5	1E	0.26	0/1698	0.46	0/2311
5	5E	0.26	0/1698	0.47	0/2311
6	1F	0.26	0/3401	0.48	0/4595
6	5F	0.27	0/3401	0.51	1/4595 (0.0%)
7	1G	0.26	0/5451	0.50	0/7387
7	5G	0.26	0/5451	0.50	0/7387
8	1H	0.26	0/2566	0.45	0/3509
8	5H	0.26	0/2566	0.45	0/3509
9	1I	0.27	0/1443	0.50	0/1952
9	5I	0.28	0/1443	0.49	0/1952
10	1J	0.27	0/1364	0.45	0/1850
10	5J	0.28	0/1364	0.47	0/1850
11	1K	0.25	0/751	0.45	0/1018
11	5K	0.25	0/751	0.46	0/1018
12	1L	0.25	0/4939	0.42	0/6718
12	5L	0.26	0/4939	0.43	0/6718
13	1M	0.24	0/3713	0.43	0/5063
13	5M	0.24	0/3713	0.42	0/5063
14	1N	0.25	0/2765	0.42	0/3758
14	5N	0.25	0/2765	0.42	0/3758
15	1O	0.25	0/2650	0.45	0/3588
15	5O	0.25	0/2650	0.45	0/3588
16	1P	0.25	0/2828	0.47	0/3834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	5P	0.25	0/2828	0.48	0/3834
17	1Q	0.26	0/1070	0.52	0/1446
17	5Q	0.26	0/1070	0.52	0/1446
18	1R	0.27	0/755	0.54	0/1018
18	5R	0.27	0/755	0.51	0/1018
19	1S	0.26	0/711	0.57	0/956
19	5S	0.25	0/711	0.53	0/956
20	1T	0.27	0/701	0.54	1/946 (0.1%)
20	1U	0.30	0/706	0.53	1/954 (0.1%)
20	5T	0.27	0/701	0.51	0/946
20	5U	0.28	0/706	0.47	0/954
21	1V	0.25	0/946	0.43	0/1281
21	5V	0.25	0/946	0.42	0/1281
22	1W	0.25	0/995	0.51	0/1340
22	5W	0.27	0/995	0.60	1/1340 (0.1%)
23	1X	0.24	0/1436	0.46	0/1938
23	5X	0.24	0/1436	0.47	0/1938
24	1Y	0.28	0/1037	0.48	0/1404
24	5Y	0.27	0/1037	0.47	0/1404
25	1Z	0.28	0/1199	0.58	1/1617 (0.1%)
25	5Z	0.26	0/1199	0.50	0/1617
26	1a	0.25	0/577	0.46	0/777
26	5a	0.25	0/577	0.45	0/777
27	1b	0.27	0/664	0.52	0/912
27	5b	0.26	0/664	0.52	1/912 (0.1%)
28	1c	0.28	0/430	0.53	0/581
28	5c	0.27	0/430	0.50	0/581
29	1d	0.27	0/1016	0.48	0/1374
29	5d	0.28	0/1016	0.49	0/1374
30	1e	0.25	0/836	0.48	0/1118
30	5e	0.25	0/836	0.48	0/1118
31	1f	0.24	0/499	0.52	0/673
31	5f	0.24	0/499	0.57	1/673 (0.1%)
32	1g	0.27	0/858	0.54	0/1165
32	5g	0.27	0/858	0.51	0/1165
33	1h	0.25	0/1184	0.47	0/1603
33	5h	0.26	0/1184	0.47	0/1603
34	1i	0.28	0/1131	0.54	1/1541 (0.1%)
34	5i	0.25	0/1131	0.48	0/1541
35	1j	0.25	0/627	0.45	0/858
35	5j	0.26	0/627	0.48	0/858
36	1k	0.28	0/668	0.53	1/903 (0.1%)
36	5k	0.28	0/668	0.49	0/903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	1l	0.27	0/1365	0.47	0/1867
37	5l	0.26	0/1365	0.46	0/1867
38	1m	0.26	0/1092	0.54	1/1481 (0.1%)
38	5m	0.26	0/1092	0.53	0/1481
39	1n	0.26	0/1549	0.52	0/2098
39	5n	0.31	1/1549 (0.1%)	0.59	2/2098 (0.1%)
40	1o	0.26	0/1069	0.55	0/1430
40	5o	0.25	0/1069	0.56	0/1430
41	1p	0.25	0/1481	0.50	0/1997
41	5p	0.25	0/1481	0.51	1/1997 (0.1%)
42	1q	0.26	0/1253	0.50	0/1704
42	5q	0.26	0/1253	0.50	0/1704
43	1r	0.27	0/777	0.51	0/1051
43	5r	0.27	0/777	0.54	0/1051
44	1s	0.28	0/394	0.54	0/533
44	5s	0.28	0/394	0.53	0/533
45	3A	0.25	0/3481	0.47	0/4722
45	3N	0.26	0/3496	0.49	0/4723
46	3B	0.25	0/3190	0.46	0/4317
46	3O	0.27	0/3175	0.47	0/4292
47	3C	0.25	0/3123	0.42	0/4269
47	3P	0.26	0/3122	0.42	0/4269
48	3D	0.27	0/1946	0.46	0/2641
48	3Q	0.27	0/1962	0.47	0/2663
49	3E	0.27	0/1551	0.50	0/2098
49	3I	0.26	0/344	0.60	0/468
49	3R	0.29	0/1551	0.54	1/2098 (0.0%)
49	3V	0.48	0/225	0.64	0/303
50	3F	0.25	0/888	0.47	0/1193
50	3S	0.25	0/888	0.47	0/1193
51	3G	0.26	0/649	0.51	0/878
51	3T	0.26	0/649	0.51	0/878
52	3H	0.25	0/539	0.57	1/724 (0.1%)
52	3U	0.26	0/539	0.51	0/724
53	3J	0.26	0/464	0.46	0/625
53	3W	0.31	0/464	0.51	0/625
54	3X	0.24	0/445	0.47	0/608
54	3Y	0.26	0/437	0.57	1/598 (0.2%)
55	4A	0.27	0/4156	0.44	0/5679
55	8A	0.27	0/4156	0.43	0/5679
56	4B	0.25	0/1865	0.48	0/2544
56	8B	0.26	0/1865	0.46	0/2544
57	4C	0.25	0/2179	0.40	0/2981

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
57	8C	0.26	0/2179	0.40	0/2981
58	4D	0.25	0/1197	0.44	0/1617
58	8D	0.26	0/1197	0.44	0/1617
59	4E	0.26	0/871	0.57	1/1182 (0.1%)
59	8E	0.27	0/871	0.53	0/1182
60	4F	0.25	0/749	0.50	0/1016
60	8F	0.26	0/749	0.51	0/1016
61	4G	0.25	0/644	0.52	0/881
61	8G	0.25	0/644	0.51	0/881
62	4H	0.27	0/708	0.48	0/956
62	8H	0.27	0/708	0.49	0/956
63	4I	0.27	0/563	0.47	0/748
63	8I	0.26	0/563	0.46	0/748
64	4J	0.26	0/466	0.52	0/631
64	8J	0.26	0/466	0.49	0/631
65	4K	0.29	0/396	0.52	0/543
65	8K	0.24	0/396	0.50	0/543
66	4L	0.27	0/394	0.45	0/528
66	8L	0.26	0/394	0.40	0/528
67	4M	0.25	0/349	0.48	0/477
67	8M	0.24	0/349	0.44	0/477
68	4N	0.26	0/680	0.44	0/921
68	8N	0.26	0/680	0.48	0/921
All	All	0.26	1/199830 (0.0%)	0.48	17/271091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1F	0	1
6	5F	0	1
8	1H	0	1
8	5H	0	1
46	3O	0	1
49	3V	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5n	145	PRO	CG-CD	-5.67	1.31	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5W	115	PRO	CA-N-CD	-10.33	97.04	111.50
25	1Z	18	PRO	CA-N-CD	-9.82	97.75	111.50
39	5n	145	PRO	N-CD-CG	-9.20	89.40	103.20
34	1i	55	PRO	CA-N-CD	-8.08	100.19	111.50
39	5n	145	PRO	CA-CB-CG	-8.04	88.73	104.00
49	3R	222	CYS	CA-CB-SG	7.35	127.22	114.00
52	3H	77	GLU	C-N-CA	7.32	140.01	121.70
20	1U	4	PRO	CA-N-CD	-7.29	101.29	111.50
6	5F	308	PRO	CA-N-CD	-6.82	101.95	111.50
38	1m	23	ASP	CB-CG-OD1	6.47	124.12	118.30
36	1k	42	ASP	CB-CG-OD1	6.15	123.84	118.30
54	3Y	43	ASP	CB-CG-OD1	5.74	123.46	118.30
27	5b	34	LEU	CA-CB-CG	5.53	128.03	115.30
20	1T	19	LEU	CA-CB-CG	5.51	127.97	115.30
31	5f	31	ASP	CB-CG-OD1	5.23	123.01	118.30
41	5p	38	LEU	CA-CB-CG	5.05	126.92	115.30
59	4E	25	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
8	1H	91	MET	Peptide
46	3O	287	ARG	Sidechain
49	3V	47	ARG	Sidechain
49	3V	52	ARG	Sidechain
49	3V	56	ARG	Sidechain
6	5F	206	LYS	Peptide
8	5H	91	MET	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	100 (88%)	12 (11%)	1 (1%)	17	40
1	5A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	8	21
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
2	5B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
3	5C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
4	1D	427/476 (90%)	411 (96%)	16 (4%)	0	100	100
4	5D	427/476 (90%)	408 (96%)	19 (4%)	0	100	100
5	1E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	29	54
5	5E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
6	1F	430/464 (93%)	409 (95%)	18 (4%)	3 (1%)	22	46
6	5F	430/464 (93%)	403 (94%)	24 (6%)	3 (1%)	22	46
7	1G	697/727 (96%)	666 (96%)	29 (4%)	2 (0%)	41	66
7	5G	697/727 (96%)	669 (96%)	25 (4%)	3 (0%)	34	60
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	41	66
8	5H	316/318 (99%)	300 (95%)	14 (4%)	2 (1%)	25	50
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
9	5I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	25	50
10	5J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	25	50
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
11	5K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	15	37
12	1L	604/606 (100%)	562 (93%)	42 (7%)	0	100	100
12	5L	604/606 (100%)	562 (93%)	41 (7%)	1 (0%)	47	73
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	1N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	41	66
14	5N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	41	66
15	1O	318/357 (89%)	307 (96%)	11 (4%)	0	100	100
15	5O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
16	5P	340/377 (90%)	330 (97%)	10 (3%)	0	100	100
17	1Q	127/175 (73%)	116 (91%)	11 (9%)	0	100	100
17	5Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
18	5R	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
19	1S	85/99 (86%)	78 (92%)	7 (8%)	0	100	100
19	5S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	80 (95%)	4 (5%)	0	100	100
20	5T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	5U	84/156 (54%)	82 (98%)	2 (2%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
21	5V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
22	5W	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	50
23	5X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	50
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
24	5Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
25	1Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
25	5Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
26	5a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
27	5b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
28	5c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
29	5d	117/122 (96%)	115 (98%)	2 (2%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/135 (41%)	52 (94%)	3 (6%)	0	100	100
32	1g	98/154 (64%)	89 (91%)	9 (9%)	0	100	100
32	5g	98/154 (64%)	91 (93%)	7 (7%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
33	5h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	1i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
34	5i	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
35	5j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100
37	5l	154/186 (83%)	144 (94%)	10 (6%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
38	5m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
39	5n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	25	50
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
40	5o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
41	5p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
42	5q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	5r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
44	5s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
45	3A	436/480 (91%)	429 (98%)	5 (1%)	2 (0%)	29	54
45	3N	444/480 (92%)	425 (96%)	18 (4%)	1 (0%)	47	73
46	3B	414/453 (91%)	405 (98%)	9 (2%)	0	100	100
46	3O	413/453 (91%)	406 (98%)	7 (2%)	0	100	100
47	3C	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
47	3P	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	230 (97%)	7 (3%)	0	100	100
49	3E	194/274 (71%)	176 (91%)	17 (9%)	1 (0%)	29	54
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	175 (90%)	16 (8%)	3 (2%)	10	26
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	96 (100%)	0	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	63/91 (69%)	61 (97%)	2 (3%)	0	100	100
52	3U	63/91 (69%)	63 (100%)	0	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	8	20
53	3W	54/64 (84%)	54 (100%)	0	0	100	100
54	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
55	4A	512/514 (100%)	492 (96%)	18 (4%)	2 (0%)	34	60
55	8A	512/514 (100%)	489 (96%)	21 (4%)	2 (0%)	34	60
56	4B	225/229 (98%)	219 (97%)	6 (3%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	4D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
58	8D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	100 (97%)	3 (3%)	0	100	100
60	4F	95/128 (74%)	91 (96%)	3 (3%)	1 (1%)	14	34
60	8F	95/128 (74%)	89 (94%)	5 (5%)	1 (1%)	14	34
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	71 (97%)	2 (3%)	0	100	100
62	4H	80/86 (93%)	76 (95%)	4 (5%)	0	100	100
62	8H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
63	4I	65/75 (87%)	65 (100%)	0	0	100	100
63	8I	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
64	4J	56/80 (70%)	52 (93%)	4 (7%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	47 (100%)	0	0	100	100
65	8K	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
66	8L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	30
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	30
All	All	24082/28836 (84%)	23087 (96%)	952 (4%)	43 (0%)	50	73

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	208	VAL
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	224	VAL
8	5H	92	PRO

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Mol	Chain	Res	Type
10	5J	66	VAL
23	5X	28	ALA
49	3R	150	SER
49	3R	273	VAL
6	5F	297	VAL
8	5H	208	VAL
5	1E	157	ASN
6	1F	249	ARG
6	1F	297	VAL
49	3R	228	ALA
12	5L	72	GLN
7	1G	654	GLN
1	5A	52	SER
6	5F	249	ARG
7	5G	654	GLN
68	8N	33	VAL
1	1A	52	SER
14	1N	110	PRO
45	3A	231	PHE
45	3A	350	THR
60	4F	95	GLN
7	5G	155	GLN
14	5N	110	PRO
6	1F	207	PRO
7	1G	155	GLN
68	4N	33	VAL
1	5A	109	LYS
6	5F	207	PRO
7	5G	186	TYR
60	8F	95	GLN
55	4A	3	VAL
11	5K	2	PRO
55	8A	3	VAL
55	8A	128	VAL
55	4A	128	VAL
39	5n	31	VAL

### 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%)	96 (97%)	3 (3%)	41	70
1	5A	99/99 (100%)	98 (99%)	1 (1%)	76	91
2	1B	131/212 (62%)	126 (96%)	5 (4%)	33	62
2	5B	131/212 (62%)	129 (98%)	2 (2%)	65	86
3	1C	190/227 (84%)	188 (99%)	2 (1%)	73	90
3	5C	190/227 (84%)	188 (99%)	2 (1%)	73	90
4	1D	371/405 (92%)	363 (98%)	8 (2%)	52	79
4	5D	371/405 (92%)	366 (99%)	5 (1%)	69	87
5	1E	183/207 (88%)	177 (97%)	6 (3%)	38	67
5	5E	183/207 (88%)	176 (96%)	7 (4%)	33	62
6	1F	346/368 (94%)	339 (98%)	7 (2%)	55	81
6	5F	346/368 (94%)	340 (98%)	6 (2%)	60	84
7	1G	588/610 (96%)	566 (96%)	22 (4%)	34	63
7	5G	588/610 (96%)	565 (96%)	23 (4%)	32	61
8	1H	274/274 (100%)	267 (97%)	7 (3%)	46	75
8	5H	274/274 (100%)	267 (97%)	7 (3%)	46	75
9	1I	151/201 (75%)	150 (99%)	1 (1%)	84	94
9	5I	151/201 (75%)	150 (99%)	1 (1%)	84	94
10	1J	140/141 (99%)	133 (95%)	7 (5%)	24	51
10	5J	140/141 (99%)	134 (96%)	6 (4%)	29	57
11	1K	84/84 (100%)	83 (99%)	1 (1%)	71	88
11	5K	84/84 (100%)	82 (98%)	2 (2%)	49	77
12	1L	539/539 (100%)	528 (98%)	11 (2%)	55	81
12	5L	539/539 (100%)	522 (97%)	17 (3%)	39	68
13	1M	408/408 (100%)	397 (97%)	11 (3%)	44	74
13	5M	408/408 (100%)	402 (98%)	6 (2%)	65	86
14	1N	310/310 (100%)	306 (99%)	4 (1%)	69	87
14	5N	310/310 (100%)	307 (99%)	3 (1%)	76	91
15	1O	283/307 (92%)	278 (98%)	5 (2%)	59	83
15	5O	283/307 (92%)	274 (97%)	9 (3%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1P	296/323 (92%)	284 (96%)	12 (4%)	30	59
16	5P	296/323 (92%)	287 (97%)	9 (3%)	41	70
17	1Q	117/152 (77%)	107 (92%)	10 (8%)	10	24
17	5Q	117/152 (77%)	112 (96%)	5 (4%)	29	57
18	1R	79/97 (81%)	74 (94%)	5 (6%)	18	40
18	5R	79/97 (81%)	74 (94%)	5 (6%)	18	40
19	1S	77/82 (94%)	70 (91%)	7 (9%)	9	21
19	5S	77/82 (94%)	70 (91%)	7 (9%)	9	21
20	1T	79/133 (59%)	75 (95%)	4 (5%)	24	50
20	1U	79/133 (59%)	77 (98%)	2 (2%)	47	76
20	5T	79/133 (59%)	73 (92%)	6 (8%)	13	30
20	5U	79/133 (59%)	73 (92%)	6 (8%)	13	30
21	1V	100/101 (99%)	95 (95%)	5 (5%)	24	51
21	5V	100/101 (99%)	99 (99%)	1 (1%)	76	91
22	1W	107/112 (96%)	103 (96%)	4 (4%)	34	63
22	5W	107/112 (96%)	103 (96%)	4 (4%)	34	63
23	1X	153/154 (99%)	147 (96%)	6 (4%)	32	61
23	5X	153/154 (99%)	145 (95%)	8 (5%)	23	49
24	1Y	101/102 (99%)	98 (97%)	3 (3%)	41	70
24	5Y	101/102 (99%)	95 (94%)	6 (6%)	19	43
25	1Z	123/124 (99%)	118 (96%)	5 (4%)	30	59
25	5Z	123/124 (99%)	121 (98%)	2 (2%)	62	85
26	1a	58/58 (100%)	56 (97%)	2 (3%)	37	66
26	5a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	57
27	5b	69/70 (99%)	68 (99%)	1 (1%)	67	86
28	1c	45/66 (68%)	42 (93%)	3 (7%)	16	37
28	5c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	103 (97%)	3 (3%)	43	73
29	5d	106/109 (97%)	103 (97%)	3 (3%)	43	73
30	1e	87/94 (93%)	82 (94%)	5 (6%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	5e	87/94 (93%)	84 (97%)	3 (3%)	37	66
31	1f	54/113 (48%)	51 (94%)	3 (6%)	21	45
31	5f	54/113 (48%)	53 (98%)	1 (2%)	57	82
32	1g	92/129 (71%)	87 (95%)	5 (5%)	22	47
32	5g	92/129 (71%)	89 (97%)	3 (3%)	38	67
33	1h	121/158 (77%)	117 (97%)	4 (3%)	38	67
33	5h	121/158 (77%)	117 (97%)	4 (3%)	38	67
34	1i	119/120 (99%)	113 (95%)	6 (5%)	24	51
34	5i	119/120 (99%)	115 (97%)	4 (3%)	37	66
35	1j	62/84 (74%)	60 (97%)	2 (3%)	39	68
35	5j	62/84 (74%)	58 (94%)	4 (6%)	17	38
36	1k	63/76 (83%)	61 (97%)	2 (3%)	39	68
36	5k	63/76 (83%)	62 (98%)	1 (2%)	62	85
37	1l	141/161 (88%)	137 (97%)	4 (3%)	43	73
37	5l	141/161 (88%)	137 (97%)	4 (3%)	43	73
38	1m	113/114 (99%)	111 (98%)	2 (2%)	59	83
38	5m	113/114 (99%)	112 (99%)	1 (1%)	78	92
39	1n	156/160 (98%)	154 (99%)	2 (1%)	69	87
39	5n	156/160 (98%)	152 (97%)	4 (3%)	46	75
40	1o	110/119 (92%)	107 (97%)	3 (3%)	44	74
40	5o	110/119 (92%)	103 (94%)	7 (6%)	17	39
41	1p	154/156 (99%)	151 (98%)	3 (2%)	57	82
41	5p	154/156 (99%)	150 (97%)	4 (3%)	46	75
42	1q	131/131 (100%)	124 (95%)	7 (5%)	22	48
42	5q	131/131 (100%)	127 (97%)	4 (3%)	40	69
43	1r	85/98 (87%)	85 (100%)	0	100	100
43	5r	85/98 (87%)	81 (95%)	4 (5%)	26	54
44	1s	44/351 (12%)	41 (93%)	3 (7%)	16	36
44	5s	44/351 (12%)	41 (93%)	3 (7%)	16	36
45	3A	367/397 (92%)	362 (99%)	5 (1%)	67	86
45	3N	372/397 (94%)	364 (98%)	8 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	3B	328/355 (92%)	323 (98%)	5 (2%)	65	86
46	3O	327/355 (92%)	320 (98%)	7 (2%)	53	80
47	3C	332/332 (100%)	325 (98%)	7 (2%)	53	80
47	3P	332/332 (100%)	324 (98%)	8 (2%)	49	77
48	3D	202/259 (78%)	198 (98%)	4 (2%)	55	81
48	3Q	204/259 (79%)	202 (99%)	2 (1%)	76	91
49	3E	166/226 (74%)	161 (97%)	5 (3%)	41	70
49	3I	37/226 (16%)	36 (97%)	1 (3%)	44	74
49	3R	166/226 (74%)	159 (96%)	7 (4%)	30	58
49	3V	24/226 (11%)	18 (75%)	6 (25%)	0	1
50	3F	90/99 (91%)	89 (99%)	1 (1%)	73	90
50	3S	90/99 (91%)	89 (99%)	1 (1%)	73	90
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	66 (98%)	1 (2%)	65	86
52	3H	62/85 (73%)	60 (97%)	2 (3%)	39	68
52	3U	62/85 (73%)	58 (94%)	4 (6%)	17	38
53	3J	45/51 (88%)	45 (100%)	0	100	100
53	3W	45/51 (88%)	40 (89%)	5 (11%)	6	14
54	3X	42/46 (91%)	41 (98%)	1 (2%)	49	77
54	3Y	41/46 (89%)	41 (100%)	0	100	100
55	4A	424/424 (100%)	411 (97%)	13 (3%)	40	69
55	8A	424/424 (100%)	416 (98%)	8 (2%)	57	82
56	4B	210/211 (100%)	203 (97%)	7 (3%)	38	67
56	8B	210/211 (100%)	204 (97%)	6 (3%)	42	71
57	4C	223/225 (99%)	213 (96%)	10 (4%)	27	55
57	8C	223/225 (99%)	219 (98%)	4 (2%)	59	83
58	4D	124/149 (83%)	118 (95%)	6 (5%)	25	53
58	8D	124/149 (83%)	120 (97%)	4 (3%)	39	68
59	4E	92/124 (74%)	91 (99%)	1 (1%)	73	90
59	8E	92/124 (74%)	89 (97%)	3 (3%)	38	67
60	4F	80/100 (80%)	78 (98%)	2 (2%)	47	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	8F	80/100 (80%)	77 (96%)	3 (4%)	33	62
61	4G	65/80 (81%)	62 (95%)	3 (5%)	27	54
61	8G	65/80 (81%)	62 (95%)	3 (5%)	27	54
62	4H	73/76 (96%)	68 (93%)	5 (7%)	16	36
62	8H	73/76 (96%)	71 (97%)	2 (3%)	44	74
63	4I	54/61 (88%)	51 (94%)	3 (6%)	21	45
63	8I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	48 (98%)	1 (2%)	55	81
64	8J	49/68 (72%)	46 (94%)	3 (6%)	18	41
65	4K	38/66 (58%)	37 (97%)	1 (3%)	46	75
65	8K	38/66 (58%)	37 (97%)	1 (3%)	46	75
66	4L	39/55 (71%)	37 (95%)	2 (5%)	24	50
66	8L	39/55 (71%)	37 (95%)	2 (5%)	24	50
67	4M	37/57 (65%)	37 (100%)	0	100	100
67	8M	37/57 (65%)	36 (97%)	1 (3%)	44	74
68	4N	70/70 (100%)	67 (96%)	3 (4%)	29	57
68	8N	70/70 (100%)	67 (96%)	3 (4%)	29	57
All	All	21060/24374 (86%)	20444 (97%)	616 (3%)	45	71

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	30	TYR
1	1A	51	PHE
1	1A	66	ASP
2	1B	25	ARG
2	1B	41	ARG
2	1B	81	ARG
2	1B	84	ASP
2	1B	125	TYR
3	1C	14	ARG
3	1C	100	ARG
4	1D	40	LYS
4	1D	79	HIS
4	1D	209	ASP
4	1D	220	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	1D	238	ARG
4	1D	297	TYR
4	1D	407	LYS
4	1D	411	LEU
5	1E	43	LYS
5	1E	89	MET
5	1E	101	GLN
5	1E	114	ASP
5	1E	168	ASP
5	1E	217	LEU
6	1F	32	ARG
6	1F	39	ARG
6	1F	73	PHE
6	1F	114	ASP
6	1F	231	SER
6	1F	302	SER
6	1F	339	ARG
7	1G	39	ARG
7	1G	64	LYS
7	1G	77	TRP
7	1G	109	ASP
7	1G	110	GLN
7	1G	153	CYS
7	1G	210	SER
7	1G	302	ARG
7	1G	337	ARG
7	1G	359	ARG
7	1G	420	ASP
7	1G	486	ASP
7	1G	520	LYS
7	1G	594	ARG
7	1G	596	ASP
7	1G	613	TYR
7	1G	655	GLN
7	1G	661	LEU
7	1G	675	ASP
7	1G	681	SER
7	1G	689	LYS
7	1G	700	GLU
8	1H	70	MET
8	1H	126	LYS
8	1H	156	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1H	174	MET
8	1H	220	PHE
8	1H	237	PHE
8	1H	274	ARG
9	1I	129	ASP
10	1J	41	CYS
10	1J	77	GLU
10	1J	102	CYS
10	1J	106	TYR
10	1J	110	GLU
10	1J	132	ASP
10	1J	169	MET
11	1K	53	PHE
12	1L	206	ASN
12	1L	262	ARG
12	1L	264	TYR
12	1L	340	PHE
12	1L	354	GLN
12	1L	364	LYS
12	1L	541	ASN
12	1L	545	SER
12	1L	554	ASP
12	1L	602	PHE
12	1L	605	HIS
13	1M	57	PHE
13	1M	135	ARG
13	1M	152	TYR
13	1M	263	MET
13	1M	304	GLN
13	1M	307	TRP
13	1M	400	MET
13	1M	410	MET
13	1M	416	ARG
13	1M	425	ASN
13	1M	427	LYS
14	1N	68	MET
14	1N	88	LYS
14	1N	204	ASN
14	1N	237	MET
15	1O	49	ARG
15	1O	65	ASP
15	1O	87	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	1O	216	GLU
15	1O	253	ASP
16	1P	10	LYS
16	1P	13	ARG
16	1P	73	TRP
16	1P	149	LYS
16	1P	167	LYS
16	1P	177	ARG
16	1P	209	ASP
16	1P	253	PHE
16	1P	263	TYR
16	1P	281	ARG
16	1P	329	SER
16	1P	338	LYS
17	1Q	14	ASP
17	1Q	34	LYS
17	1Q	44	ASN
17	1Q	58	GLU
17	1Q	62	ARG
17	1Q	91	ASP
17	1Q	102	SER
17	1Q	112	LYS
17	1Q	123	SER
17	1Q	133	LYS
18	1R	10	LYS
18	1R	22	ASP
18	1R	25	ARG
18	1R	92	ARG
18	1R	96	HIS
19	1S	12	LYS
19	1S	16	ARG
19	1S	24	GLN
19	1S	34	ASP
19	1S	72	GLN
19	1S	78	LEU
19	1S	84	ASP
20	1T	17	TYR
20	1T	20	LYS
20	1T	39	ASP
20	1T	46	ASP
20	1U	24	LYS
20	1U	61	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	1V	4	LEU
21	1V	21	GLU
21	1V	63	ASP
21	1V	88	SER
21	1V	99	TRP
22	1W	61	ASP
22	1W	80	ASP
22	1W	87	LYS
22	1W	114	ARG
23	1X	11	ASP
23	1X	47	TRP
23	1X	65	CYS
23	1X	118	ARG
23	1X	120	ASP
23	1X	156	ASP
24	1Y	9	SER
24	1Y	76	SER
24	1Y	114	CYS
25	1Z	10	MET
25	1Z	85	GLN
25	1Z	112	HIS
25	1Z	120	MET
25	1Z	135	SER
26	1a	48	MET
26	1a	68	ASN
27	1b	39	ASN
27	1b	56	LEU
27	1b	82	ASN
28	1c	11	SER
28	1c	30	TYR
28	1c	34	GLN
29	1d	19	ARG
29	1d	20	SER
29	1d	64	TYR
30	1e	8	ARG
30	1e	12	ASP
30	1e	73	LYS
30	1e	84	LYS
30	1e	97	HIS
31	1f	1	MET
31	1f	9	ASP
31	1f	33	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1g	40	LYS
32	1g	48	ASP
32	1g	57	ASN
32	1g	59	ARG
32	1g	107	LEU
33	1h	6	LYS
33	1h	79	PHE
33	1h	111	ARG
33	1h	142	ASP
34	1i	6	ASP
34	1i	30	ARG
34	1i	37	ARG
34	1i	67	SER
34	1i	99	ARG
34	1i	125	GLN
35	1j	50	HIS
35	1j	69	ASP
36	1k	20	GLN
36	1k	21	TRP
37	1l	33	ASP
37	1l	35	GLU
37	1l	62	TYR
37	1l	124	SER
38	1m	22	TYR
38	1m	23	ASP
39	1n	157	ARG
39	1n	176	ARG
40	1o	28	TYR
40	1o	117	ARG
40	1o	121	MET
41	1p	24	SER
41	1p	42	ARG
41	1p	59	ARG
42	1q	21	ARG
42	1q	43	LYS
42	1q	55	PHE
42	1q	95	ASP
42	1q	131	ARG
42	1q	144	TYR
42	1q	145	LYS
44	1s	35	ASN
44	1s	38	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	1s	61	PHE
45	3A	42	ASP
45	3A	58	PHE
45	3A	75	LEU
45	3A	124	ASP
45	3A	132	ASP
46	3B	189	ASP
46	3B	225	ASN
46	3B	301	LYS
46	3B	319	SER
46	3B	338	LYS
47	3C	7	SER
47	3C	80	ARG
47	3C	90	PHE
47	3C	183	PHE
47	3C	215	MET
47	3C	267	HIS
47	3C	379	TRP
48	3D	122	LYS
48	3D	170	MET
48	3D	232	ARG
48	3D	280	ARG
49	3E	90	ASP
49	3E	155	LYS
49	3E	161	GLU
49	3E	197	ASP
49	3E	256	LEU
50	3F	30	LYS
52	3H	59	ARG
52	3H	86	ASP
49	3I	47	ARG
45	3N	42	ASP
45	3N	51	LYS
45	3N	58	PHE
45	3N	112	LEU
45	3N	124	ASP
45	3N	172	GLU
45	3N	218	SER
45	3N	307	PHE
46	3O	74	SER
46	3O	180	ASP
46	3O	217	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	3O	222	ARG
46	3O	223	PHE
46	3O	296	TYR
46	3O	400	GLN
47	3P	12	LYS
47	3P	43	LEU
47	3P	80	ARG
47	3P	215	MET
47	3P	228	ASP
47	3P	234	PHE
47	3P	345	HIS
47	3P	379	TRP
48	3Q	43	MET
48	3Q	97	ASN
49	3R	90	ASP
49	3R	149	MET
49	3R	151	LYS
49	3R	169	TRP
49	3R	178	HIS
49	3R	222	CYS
49	3R	263	TYR
50	3S	12	TRP
51	3T	6	HIS
52	3U	23	GLN
52	3U	34	ARG
52	3U	41	ASP
52	3U	68	CYS
49	3V	47	ARG
49	3V	49	VAL
49	3V	50	LEU
49	3V	51	CYS
49	3V	52	ARG
49	3V	62	ARG
53	3W	16	ARG
53	3W	53	LYS
53	3W	56	ASN
53	3W	57	GLN
53	3W	59	LYS
54	3X	15	ARG
55	4A	19	TYR
55	4A	69	MET
55	4A	81	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	4A	97	MET
55	4A	109	PHE
55	4A	136	LEU
55	4A	138	HIS
55	4A	176	MET
55	4A	219	PHE
55	4A	290	HIS
55	4A	292	MET
55	4A	335	SER
55	4A	514	LYS
56	4B	65	TRP
56	4B	73	LEU
56	4B	87	MET
56	4B	92	ASN
56	4B	113	TYR
56	4B	146	MET
56	4B	217	LYS
57	4C	40	MET
57	4C	50	ASN
57	4C	55	TYR
57	4C	143	SER
57	4C	159	MET
57	4C	182	TYR
57	4C	203	PHE
57	4C	214	PHE
57	4C	235	PHE
57	4C	261	SER
58	4D	22	TYR
58	4D	43	LYS
58	4D	61	ARG
58	4D	73	ARG
58	4D	114	GLU
58	4D	138	TRP
59	4E	25	ASP
60	4F	18	ARG
60	4F	50	PRO
61	4G	54	ARG
61	4G	61	SER
61	4G	64	ASP
62	4H	7	LYS
62	4H	29	CYS
62	4H	60	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
62	4H	67	SER
62	4H	70	SER
63	4I	34	PHE
63	4I	57	MET
63	4I	64	ARG
64	4J	33	ARG
65	4K	15	ASN
66	4L	13	PHE
66	4L	18	LYS
68	4N	49	ASN
68	4N	50	ASN
68	4N	55	ASN
1	5A	23	TRP
2	5B	25	ARG
2	5B	41	ARG
3	5C	44	CYS
3	5C	74	SER
4	5D	40	LYS
4	5D	79	HIS
4	5D	209	ASP
4	5D	216	LYS
4	5D	297	TYR
5	5E	18	ASP
5	5E	56	ARG
5	5E	74	GLN
5	5E	93	LYS
5	5E	168	ASP
5	5E	175	GLU
5	5E	190	ARG
6	5F	20	ARG
6	5F	32	ARG
6	5F	139	ARG
6	5F	188	GLU
6	5F	218	CYS
6	5F	312	CYS
7	5G	32	LYS
7	5G	39	ARG
7	5G	77	TRP
7	5G	231	MET
7	5G	278	ARG
7	5G	311	GLN
7	5G	341	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	5G	359	ARG
7	5G	418	ARG
7	5G	420	ASP
7	5G	431	ASP
7	5G	471	SER
7	5G	475	GLN
7	5G	517	ASN
7	5G	520	LYS
7	5G	528	ASP
7	5G	539	LYS
7	5G	594	ARG
7	5G	596	ASP
7	5G	613	TYR
7	5G	614	ASP
7	5G	632	ARG
7	5G	669	LYS
8	5H	5	ASN
8	5H	69	SER
8	5H	98	MET
8	5H	121	TRP
8	5H	237	PHE
8	5H	274	ARG
8	5H	317	GLN
9	5I	129	ASP
10	5J	25	SER
10	5J	70	TYR
10	5J	76	THR
10	5J	77	GLU
10	5J	101	PHE
10	5J	135	PHE
11	5K	53	PHE
11	5K	91	GLN
12	5L	28	LYS
12	5L	116	ARG
12	5L	163	ASP
12	5L	176	ARG
12	5L	235	SER
12	5L	262	ARG
12	5L	354	GLN
12	5L	364	LYS
12	5L	403	TYR
12	5L	469	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	5L	485	TYR
12	5L	541	ASN
12	5L	544	MET
12	5L	548	SER
12	5L	554	ASP
12	5L	602	PHE
12	5L	605	HIS
13	5M	57	PHE
13	5M	122	PHE
13	5M	152	TYR
13	5M	307	TRP
13	5M	410	MET
13	5M	425	ASN
14	5N	98	MET
14	5N	109	SER
14	5N	216	PHE
15	5O	49	ARG
15	5O	125	GLU
15	5O	140	ARG
15	5O	206	TYR
15	5O	207	LYS
15	5O	214	MET
15	5O	215	SER
15	5O	216	GLU
15	5O	258	ARG
16	5P	13	ARG
16	5P	73	TRP
16	5P	148	SER
16	5P	154	LYS
16	5P	253	PHE
16	5P	263	TYR
16	5P	268	ARG
16	5P	281	ARG
16	5P	331	MET
17	5Q	14	ASP
17	5Q	34	LYS
17	5Q	104	ASP
17	5Q	112	LYS
17	5Q	133	LYS
18	5R	10	LYS
18	5R	25	ARG
18	5R	50	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	5R	70	ARG
18	5R	80	LYS
19	5S	39	ARG
19	5S	42	GLU
19	5S	61	GLN
19	5S	72	GLN
19	5S	84	ASP
19	5S	88	ARG
19	5S	97	LYS
20	5T	17	TYR
20	5T	29	LYS
20	5T	31	SER
20	5T	46	ASP
20	5T	66	ASP
20	5T	85	ASP
20	5U	20	LYS
20	5U	64	ASP
20	5U	69	LYS
20	5U	71	MET
20	5U	83	LYS
20	5U	84	LYS
21	5V	70	GLN
22	5W	61	ASP
22	5W	80	ASP
22	5W	91	GLU
22	5W	127	ASP
23	5X	1	PRO
23	5X	11	ASP
23	5X	13	LYS
23	5X	47	TRP
23	5X	111	LEU
23	5X	118	ARG
23	5X	120	ASP
23	5X	156	ASP
24	5Y	2	LYS
24	5Y	9	SER
24	5Y	10	ASP
24	5Y	19	ARG
24	5Y	106	SER
24	5Y	137	GLU
25	5Z	13	PRO
25	5Z	28	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	5b	56	LEU
29	5d	17	GLU
29	5d	28	ASP
29	5d	64	TYR
30	5e	8	ARG
30	5e	12	ASP
30	5e	97	HIS
31	5f	31	ASP
32	5g	39	GLU
32	5g	57	ASN
32	5g	83	TYR
33	5h	6	LYS
33	5h	12	LYS
33	5h	68	LYS
33	5h	79	PHE
34	5i	8	LYS
34	5i	42	MET
34	5i	67	SER
34	5i	119	MET
35	5j	8	GLU
35	5j	50	HIS
35	5j	55	ASP
35	5j	59	TRP
36	5k	21	TRP
37	5l	33	ASP
37	5l	35	GLU
37	5l	62	TYR
37	5l	135	TYR
38	5m	43	LYS
39	5n	44	ARG
39	5n	157	ARG
39	5n	159	GLU
39	5n	176	ARG
40	5o	30	PHE
40	5o	45	MET
40	5o	83	GLN
40	5o	110	ARG
40	5o	116	GLN
40	5o	117	ARG
40	5o	121	MET
41	5p	34	LYS
41	5p	96	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	5p	126	LYS
41	5p	141	ARG
42	5q	55	PHE
42	5q	107	LYS
42	5q	133	LYS
42	5q	145	LYS
43	5r	26	ARG
43	5r	60	ARG
43	5r	69	MET
43	5r	107	LYS
44	5s	35	ASN
44	5s	39	ARG
44	5s	67	SER
55	8A	19	TYR
55	8A	109	PHE
55	8A	115	SER
55	8A	238	PHE
55	8A	290	HIS
55	8A	298	ASP
55	8A	379	TYR
55	8A	390	MET
56	8B	35	SER
56	8B	65	TRP
56	8B	86	MET
56	8B	146	MET
56	8B	163	TRP
56	8B	226	MET
57	8C	155	ASP
57	8C	212	SER
57	8C	214	PHE
57	8C	244	PHE
58	8D	40	LEU
58	8D	52	SER
58	8D	67	SER
58	8D	98	TRP
59	8E	21	LYS
59	8E	84	TYR
59	8E	88	GLU
60	8F	64	GLU
60	8F	65	ASP
60	8F	66	ASN
61	8G	19	LEU

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Mol	Chain	Res	Type
61	8G	46	GLU
61	8G	56	ARG
62	8H	12	GLN
62	8H	27	ARG
64	8J	7	GLU
64	8J	15	ASP
64	8J	38	LEU
65	8K	8	ASP
66	8L	16	GLU
66	8L	18	LYS
67	8M	39	HIS
68	8N	3	ARG
68	8N	69	ASN
68	8N	73	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
5	1E	16	ASN
7	1G	101	HIS
7	1G	255	HIS
7	1G	629	ASN
12	1L	23	ASN
12	1L	194	ASN
13	1M	220	HIS
13	1M	304	GLN
21	1V	110	GLN
22	1W	70	ASN
23	1X	76	HIS
26	1a	68	ASN
29	1d	46	ASN
29	1d	61	GLN
29	1d	97	HIS
33	1h	143	ASN
34	1i	47	ASN
37	1l	126	GLN
41	1p	106	GLN
41	1p	148	HIS
43	1r	12	ASN
43	1r	35	GLN
43	1r	46	HIS
43	1r	109	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	1s	43	HIS
44	1s	65	GLN
49	3E	135	GLN
49	3E	257	ASN
45	3N	9	GLN
45	3N	339	GLN
49	3R	135	GLN
49	3R	199	GLN
49	3R	239	HIS
53	3W	57	GLN
57	4C	76	GLN
2	5B	82	GLN
4	5D	34	ASN
5	5E	57	GLN
6	5F	148	ASN
6	5F	150	GLN
6	5F	200	GLN
7	5G	101	HIS
12	5L	2	ASN
12	5L	23	ASN
12	5L	194	ASN
13	5M	220	HIS
13	5M	440	HIS
16	5P	136	ASN
29	5d	46	ASN
33	5h	143	ASN
34	5i	13	GLN
37	5l	56	GLN
39	5n	61	GLN
41	5p	58	ASN
41	5p	106	GLN
42	5q	87	HIS
43	5r	12	ASN
43	5r	35	GLN
43	5r	46	HIS
43	5r	72	GLN
43	5r	109	GLN
44	5s	43	HIS
44	5s	44	HIS
55	8A	291	HIS
55	8A	428	GLN
56	8B	52	HIS

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Mol	Chain	Res	Type
56	8B	161	HIS
57	8C	76	GLN
62	8H	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

18 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
12	FME	1L	1	12	8,9,10	0.52	0	7,9,11	0.90	1 (14%)
8	FME	5H	1	8	8,9,10	0.51	0	7,9,11	1.09	1 (14%)
14	FME	1N	1	14	8,9,10	0.50	0	7,9,11	1.02	1 (14%)
34	SAC	1i	1	34	7,8,9	0.54	0	8,9,11	0.88	1 (12%)
1	FME	1A	1	1	8,9,10	0.50	0	7,9,11	1.13	1 (14%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
12	FME	5L	1	12	8,9,10	0.51	0	7,9,11	0.91	1 (14%)
55	FME	4A	1	55	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
34	SAC	5i	1	34	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
13	FME	5M	1	13	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
56	FME	8B	1	56	8,9,10	0.52	0	7,9,11	1.09	1 (14%)
56	FME	4B	1	56	8,9,10	0.53	0	7,9,11	1.00	1 (14%)
14	FME	5N	1	14	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
1	FME	5A	1	1	8,9,10	0.50	0	7,9,11	1.10	1 (14%)
55	FME	8A	1	55	8,9,10	0.51	0	7,9,11	1.03	1 (14%)
13	FME	1M	1	13	8,9,10	0.50	0	7,9,11	1.02	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	FME	1K	1	11	8,9,10	0.50	0	7,9,11	1.01	1 (14%)
11	FME	5K	1	11	8,9,10	0.51	0	7,9,11	1.04	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	1L	1	12	-	0/7/9/11	-
8	FME	5H	1	8	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
1	FME	1A	1	1	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
55	FME	4A	1	55	-	3/7/9/11	-
34	SAC	5i	1	34	-	0/7/8/10	-
13	FME	5M	1	13	-	0/7/9/11	-
56	FME	8B	1	56	-	2/7/9/11	-
56	FME	4B	1	56	-	3/7/9/11	-
14	FME	5N	1	14	-	1/7/9/11	-
1	FME	5A	1	1	-	1/7/9/11	-
55	FME	8A	1	55	-	1/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
11	FME	5K	1	11	-	3/7/9/11	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5H	1	FME	O-C-CA	-2.64	117.86	124.78
8	1H	1	FME	O-C-CA	-2.63	117.90	124.78
11	1K	1	FME	O-C-CA	-2.62	117.92	124.78
1	1A	1	FME	O-C-CA	-2.58	118.02	124.78
11	5K	1	FME	O-C-CA	-2.57	118.05	124.78
13	5M	1	FME	O-C-CA	-2.53	118.16	124.78
56	8B	1	FME	O-C-CA	-2.51	118.19	124.78
13	1M	1	FME	O-C-CA	-2.51	118.19	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	4B	1	FME	O-C-CA	-2.47	118.30	124.78
14	1N	1	FME	O-C-CA	-2.47	118.31	124.78
1	5A	1	FME	O-C-CA	-2.47	118.31	124.78
14	5N	1	FME	O-C-CA	-2.46	118.32	124.78
55	8A	1	FME	O-C-CA	-2.42	118.44	124.78
55	4A	1	FME	O-C-CA	-2.40	118.49	124.78
34	1i	1	SAC	O-C-CA	-2.34	118.65	124.78
12	5L	1	FME	O-C-CA	-2.34	118.65	124.78
34	5i	1	SAC	O-C-CA	-2.31	118.73	124.78
12	1L	1	FME	O-C-CA	-2.23	118.93	124.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
56	4B	1	FME	O-C-CA-CB
8	5H	1	FME	O1-CN-N-CA
14	5N	1	FME	O1-CN-N-CA
56	8B	1	FME	O1-CN-N-CA
56	8B	1	FME	O-C-CA-CB
55	4A	1	FME	CA-CB-CG-SD
55	8A	1	FME	CA-CB-CG-SD
1	5A	1	FME	CB-CG-SD-CE
11	5K	1	FME	CB-CG-SD-CE
55	4A	1	FME	C-CA-CB-CG
11	5K	1	FME	C-CA-CB-CG
11	5K	1	FME	N-CA-CB-CG
55	4A	1	FME	N-CA-CB-CG
11	1K	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 202 ligands modelled in this entry, 14 are monoatomic - leaving 188 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
70	SF4	1G	801	7	0,12,12	-	-	-		
74	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.39	0
74	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.42	0
69	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
86	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.39	0
76	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.38	0
76	3PE	5Y	805	-	26,26,50	0.34	0	29,31,55	0.54	0
76	3PE	5M	506	-	49,49,50	0.27	0	52,54,55	0.33	0
87	HEA	4A	604	55	57,67,67	2.08	17 (29%)	61,103,103	2.51	27 (44%)
69	PC1	5M	503	-	34,34,53	0.32	0	40,42,61	0.47	0
69	PC1	5A	203	-	34,34,53	0.33	0	40,42,61	0.38	0
74	CDL	3C	503	-	51,51,99	0.35	0	57,63,111	0.53	1 (1%)
76	3PE	1Y	805	-	26,26,50	0.34	0	29,31,55	0.54	0
76	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.41	0
76	3PE	1b	201	-	46,46,50	0.28	0	49,51,55	0.36	0
69	PC1	5d	202	-	38,38,53	0.30	0	44,46,61	0.48	1 (2%)
76	3PE	5P	403	-	34,34,50	0.31	0	37,39,55	0.37	0
86	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
86	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.35	0
92	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
70	SF4	5I	202	9	0,12,12	-	-	-		
93	PO4	8H	101	-	4,4,4	0.91	0	6,6,6	0.45	0
74	CDL	5X	201	-	85,85,99	0.28	0	91,97,111	0.38	0
72	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.67	1 (2%)
74	CDL	3T	101	-	56,56,99	0.34	0	62,68,111	0.43	0
91	CUA	4B	303	56	0,1,1	-	-	-		
86	PGV	8M	101	-	50,50,50	0.29	0	53,56,56	0.30	0
83	MYR	5o	201	-	14,14,15	0.35	0	13,13,15	0.38	0
86	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
86	PGV	8A	601	-	50,50,50	0.28	0	53,56,56	0.41	0
69	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
74	CDL	1d	203	-	64,64,99	0.31	0	70,76,111	0.42	0
76	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.45	0
76	3PE	1Y	803	-	29,29,50	0.34	0	32,34,55	0.79	1 (3%)
71	FES	3R	301	49	0,4,4	-	-	-	-	-
76	3PE	1Y	802	-	39,39,50	0.31	0	42,44,55	0.44	0
69	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.36	0
74	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.40	0
69	PC1	5I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
75	AYA	5q	202	-	6,7,8	0.65	0	5,8,10	0.43	0
76	3PE	5A	201	-	46,46,50	0.27	0	49,51,55	0.35	0
69	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
69	PC1	5B	203	-	47,47,53	0.29	0	53,55,61	0.44	0
76	3PE	1Y	806	-	40,40,50	0.29	0	43,45,55	0.40	0
69	PC1	5I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
69	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
76	3PE	1M	902	-	44,44,50	0.29	0	47,49,55	0.35	0
74	CDL	5h	202	-	79,79,99	0.30	0	85,91,111	0.40	0
87	HEA	8A	603	55	57,67,67	2.07	16 (28%)	61,103,103	2.53	28 (45%)
71	FES	5E	301	5	0,4,4	-	-	-	-	-
70	SF4	5F	502	6	0,12,12	-	-	-	-	-
82	AME	5h	201	-	9,10,11	0.49	0	9,11,13	0.98	1 (11%)
76	3PE	5Y	804	-	32,32,50	0.33	0	35,37,55	0.49	0
86	PGV	8G	101	-	50,50,50	0.28	0	53,56,56	0.46	1 (1%)
87	HEA	8A	604	55	57,67,67	2.07	17 (29%)	61,103,103	2.49	27 (44%)
74	CDL	5L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
75	AYA	1I	205	-	6,7,8	0.64	0	5,8,10	0.42	0
86	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.32	0
90	PSC	8I	101	-	51,51,51	0.30	0	57,59,59	0.47	1 (1%)
69	PC1	5q	201	-	48,48,53	0.27	0	54,56,61	0.33	0
76	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.50	0
76	3PE	3Q	502	-	46,46,50	0.28	0	49,51,55	0.38	0
92	PEK	4C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
84	HEM	3C	502	-	41,50,50	1.33	4 (9%)	45,82,82	1.75	8 (17%)
69	PC1	3R	302	-	44,44,53	0.29	0	50,52,61	0.36	0
86	PGV	4C	305	-	50,50,50	0.29	0	53,56,56	0.49	1 (1%)
70	SF4	5G	801	7	0,12,12	-	-	-	-	-
74	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
86	PGV	4J	101	-	50,50,50	0.28	0	53,56,56	0.38	0
71	FES	5G	803	7	0,4,4	-	-	-	-	-
71	FES	3E	301	49	0,4,4	-	-	-	-	-
84	HEM	3P	502	47	41,50,50	1.32	4 (9%)	45,82,82	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
76	3PE	5M	504	-	50,50,50	0.28	0	53,55,55	0.46	0
76	3PE	5M	502	-	47,47,50	0.27	0	50,52,55	0.34	0
86	PGV	8L	101	-	50,50,50	0.29	0	53,56,56	0.37	0
70	SF4	1I	202	9	0,12,12	-	-	-	-	-
76	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.31	0
87	HEA	4A	605	55	57,67,67	2.08	17 (29%)	61,103,103	2.45	27 (44%)
76	3PE	5Y	806	-	40,40,50	0.29	0	43,45,55	0.40	0
69	PC1	5B	202	-	45,45,53	0.28	0	51,53,61	0.36	0
76	3PE	1P	502	-	34,34,50	0.31	0	37,39,55	0.37	0
74	CDL	4D	201	-	99,99,99	0.26	0	105,111,111	0.42	0
70	SF4	1B	201	2	0,12,12	-	-	-	-	-
76	3PE	5Y	803	-	29,29,50	0.34	0	32,34,55	0.76	1 (3%)
69	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.43	0
70	SF4	1G	802	7	0,12,12	-	-	-	-	-
85	HEC	3D	501	48	31,49,50	2.36	12 (38%)	22,80,82	2.40	5 (22%)
70	SF4	5B	201	2	0,12,12	-	-	-	-	-
76	3PE	3C	504	-	34,34,50	0.32	0	37,39,55	0.46	0
74	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.60	1 (1%)
76	3PE	5L	703	-	44,44,50	0.28	0	47,49,55	0.33	0
76	3PE	3C	505	-	33,33,50	0.33	0	36,38,55	0.40	0
91	CUA	8B	304	56	0,1,1	-	-	-	-	-
69	PC1	1M	905	-	43,43,53	0.30	0	49,51,61	0.37	0
69	PC1	5h	203	-	46,46,53	0.28	0	52,54,61	0.29	0
76	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.66	1 (3%)
69	PC1	5L	705	-	45,45,53	0.30	0	51,53,61	0.36	0
76	3PE	1M	903	-	47,47,50	0.27	0	50,52,55	0.34	0
74	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.40	1 (0%)
69	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
77	GTP	5O	401	78	26,34,34	0.95	2 (7%)	32,54,54	0.80	0
74	CDL	3P	504	-	55,55,99	0.36	0	61,67,111	0.52	0
86	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.70	1 (1%)
86	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.31	0
74	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
76	3PE	1K	101	-	43,43,50	0.29	0	46,48,55	0.34	0
69	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.36	0
74	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.42	0
69	PC1	1H	402	-	47,47,53	0.28	0	53,55,61	0.34	0
74	CDL	5q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
83	MYR	1o	201	-	14,14,15	0.35	0	13,13,15	0.39	0
86	PGV	8C	304	-	50,50,50	0.28	0	53,56,56	0.38	0
86	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.33	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
71	FES	1G	803	7	0,4,4	-	-	-		
76	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.61	0
74	CDL	5N	401	-	61,61,99	0.31	0	67,73,111	0.60	1 (1%)
74	CDL	8B	303	-	99,99,99	0.26	0	105,111,111	0.31	0
86	PGV	8B	302	-	50,50,50	0.28	0	53,56,56	0.36	0
86	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.42	0
70	SF4	5I	203	9	0,12,12	-	-	-		
76	3PE	5L	701	-	45,45,50	0.28	0	48,50,55	0.31	0
81	EHZ	5n	201	-	29,36,37	0.15	0	35,44,47	1.05	1 (2%)
86	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.31	0
71	FES	1E	301	5	0,4,4	-	-	-		
90	PSC	4A	609	-	51,51,51	0.29	0	57,59,59	0.45	1 (1%)
86	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
76	3PE	5L	704	-	48,48,50	0.27	0	51,53,55	0.36	0
84	HEM	3C	501	47	41,50,50	1.31	5 (12%)	45,82,82	1.80	8 (17%)
70	SF4	1I	203	9	0,12,12	-	-	-		
79	NDP	5P	402	-	45,52,52	0.61	0	53,80,80	0.73	2 (3%)
86	PGV	4C	304	-	50,50,50	0.28	0	53,56,56	0.38	0
86	PGV	8B	301	-	50,50,50	0.27	0	53,56,56	0.32	0
76	3PE	1L	703	-	44,44,50	0.28	0	47,49,55	0.34	0
76	3PE	1Y	801	-	30,30,50	0.33	0	33,35,55	0.50	0
77	GTP	1O	402	78	26,34,34	0.95	2 (7%)	32,54,54	0.81	1 (3%)
76	3PE	3A	503	-	31,31,50	0.33	0	34,36,55	0.38	0
69	PC1	1L	704	-	45,45,53	0.29	0	51,53,61	0.37	0
76	3PE	3P	503	-	32,32,50	0.34	0	35,37,55	0.37	0
84	HEM	3P	501	47	41,50,50	1.32	4 (9%)	45,82,82	1.82	9 (20%)
93	PO4	4H	101	-	4,4,4	0.91	0	6,6,6	0.44	0
69	PC1	1d	202	-	38,38,53	0.30	0	44,46,61	0.47	0
76	3PE	5K	101	-	43,43,50	0.29	0	46,48,55	0.34	0
76	3PE	5M	501	-	44,44,50	0.29	0	47,49,55	0.35	0
69	PC1	1q	201	-	48,48,53	0.27	0	54,56,61	0.33	0
76	3PE	1M	906	-	49,49,50	0.27	0	52,54,55	0.33	0
76	3PE	5Y	801	-	30,30,50	0.32	0	33,35,55	0.49	0
86	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.42	0
86	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.37	0
81	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.02	1 (2%)
76	3PE	5Y	802	-	39,39,50	0.31	0	42,44,55	0.46	0
69	PC1	3J	101	-	46,46,53	0.28	0	52,54,61	0.33	0
69	PC1	5M	505	-	43,43,53	0.30	0	49,51,61	0.38	0
69	PC1	5H	402	-	47,47,53	0.28	0	53,55,61	0.33	0
86	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
69	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.41	0
74	CDL	5d	203	-	64,64,99	0.31	0	70,76,111	0.42	0
72	FMN	5F	501	-	33,33,33	0.59	0	48,50,50	0.67	1 (2%)
74	CDL	4B	302	-	99,99,99	0.26	0	105,111,111	0.30	0
76	3PE	1O	401	-	50,50,50	0.27	0	53,55,55	0.46	0
76	3PE	1j	101	-	43,43,50	0.28	0	46,48,55	0.45	0
76	3PE	5j	101	-	43,43,50	0.29	0	46,48,55	0.46	0
86	PGV	4L	101	-	50,50,50	0.29	0	53,56,56	0.38	0
86	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.69	1 (1%)
86	PGV	8C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
79	NDP	1P	501	-	45,52,52	0.60	0	53,80,80	0.74	2 (3%)
74	CDL	3G	102	-	55,55,99	0.34	0	61,67,111	0.47	0
85	HEC	3Q	501	48	32,50,50	2.37	12 (37%)	24,82,82	2.39	7 (29%)
92	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
86	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.36	0
70	SF4	5G	802	7	0,12,12	-	-	-	-	-
69	PC1	1A	203	-	32,32,53	0.34	0	38,40,61	0.35	0
69	PC1	1A	201	-	34,34,53	0.32	0	40,42,61	0.38	0
76	3PE	1M	901	-	48,48,50	0.27	0	51,53,55	0.35	0
74	CDL	3N	502	-	42,42,99	0.37	0	48,54,111	0.51	0
92	PEK	4G	102	-	52,52,52	0.26	0	55,57,57	0.41	0
76	3PE	5d	201	-	48,48,50	0.26	0	51,53,55	0.33	0
82	AME	1h	201	-	9,10,11	0.47	0	9,11,13	0.96	1 (11%)
70	SF4	1F	502	6	0,12,12	-	-	-	-	-
81	EHZ	5T	101	20	29,36,37	0.17	0	35,44,47	1.02	1 (2%)
86	PGV	8C	307	-	50,50,50	0.28	0	53,56,56	0.38	0
69	PC1	1M	904	-	34,34,53	0.33	0	40,42,61	0.46	0
74	CDL	1N	401	-	61,61,99	0.31	0	67,73,111	0.61	1 (1%)
86	PGV	4A	603	-	50,50,50	0.27	0	53,56,56	0.32	0
81	EHZ	1T	101	20	29,36,37	0.16	0	35,44,47	1.03	1 (2%)
76	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.32	0
76	3PE	1Y	804	-	32,32,50	0.33	0	35,37,55	0.48	0
74	CDL	5H	401	-	50,50,99	0.36	0	56,62,111	0.60	1 (1%)
74	CDL	8D	201	-	99,99,99	0.26	0	105,111,111	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SF4	1G	801	7	-	-	0/6/5/5
74	CDL	1X	201	-	-	19/96/96/110	-
74	CDL	1q	202	-	-	7/71/71/110	-
69	PC1	1h	203	-	-	13/50/50/57	-
86	PGV	8J	101	-	-	6/55/55/55	-
76	3PE	3G	101	-	-	6/32/32/54	-
76	3PE	5Y	805	-	-	7/30/30/54	-
76	3PE	5M	506	-	-	8/53/53/54	-
87	HEA	4A	604	55	-	7/32/76/76	-
69	PC1	5M	503	-	-	7/38/38/57	-
69	PC1	5A	203	-	-	3/38/38/57	-
74	CDL	3C	503	-	-	9/62/62/110	-
76	3PE	1Y	805	-	-	8/30/30/54	-
76	3PE	3Y	101	-	-	6/33/33/54	-
76	3PE	1b	201	-	-	9/50/50/54	-
69	PC1	5d	202	-	-	8/42/42/57	-
76	3PE	5P	403	-	-	2/38/38/54	-
86	PGV	8C	305	-	-	7/55/55/55	-
86	PGV	4A	602	-	-	6/55/55/55	-
92	PEK	8G	102	-	-	7/56/56/56	-
70	SF4	5I	202	9	-	-	0/6/5/5
74	CDL	5X	201	-	-	19/96/96/110	-
72	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
74	CDL	3T	101	-	-	9/67/67/110	-
86	PGV	8M	101	-	-	5/55/55/55	-
83	MYR	5o	201	-	-	0/11/12/13	-
86	PGV	4K	101	-	-	12/55/55/55	-
86	PGV	8A	601	-	-	15/55/55/55	-
69	PC1	3X	101	-	-	3/32/32/57	-
74	CDL	1d	203	-	-	14/75/75/110	-
76	3PE	3N	501	-	-	10/35/35/54	-
76	3PE	1Y	803	-	-	10/33/33/54	-
71	FES	3R	301	49	-	-	0/1/1/1
76	3PE	1Y	802	-	-	16/43/43/54	-
69	PC1	5P	401	-	-	3/36/36/57	-
74	CDL	1h	202	-	-	18/90/90/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	PC1	5I	204	-	-	5/47/47/57	-
75	AYA	5q	202	-	-	0/4/6/8	-
76	3PE	5A	201	-	-	7/50/50/54	-
69	PC1	1I	204	-	-	4/47/47/57	-
69	PC1	5B	203	-	-	10/51/51/57	-
76	3PE	1Y	806	-	-	11/44/44/54	-
69	PC1	5I	201	-	-	6/57/57/57	-
69	PC1	1I	201	-	-	5/57/57/57	-
76	3PE	1M	902	-	-	10/48/48/54	-
74	CDL	5h	202	-	-	18/90/90/110	-
87	HEA	8A	603	55	-	10/32/76/76	-
71	FES	5E	301	5	-	-	0/1/1/1
82	AME	5h	201	-	-	1/9/10/12	-
70	SF4	5F	502	6	-	-	0/6/5/5
76	3PE	5Y	804	-	-	6/36/36/54	-
86	PGV	8G	101	-	-	11/55/55/55	-
87	HEA	8A	604	55	-	6/32/76/76	-
74	CDL	5L	702	-	-	15/86/86/110	-
75	AYA	1I	205	-	-	0/4/6/8	-
86	PGV	4M	101	-	-	4/55/55/55	-
90	PSC	8I	101	-	-	13/55/55/55	-
69	PC1	5q	201	-	-	3/52/52/57	-
76	3PE	3D	502	-	-	2/36/36/54	-
76	3PE	3Q	502	-	-	4/50/50/54	-
92	PEK	4C	308	-	-	4/55/55/56	-
84	HEM	3C	502	-	-	4/12/54/54	-
69	PC1	3R	302	-	-	4/48/48/57	-
86	PGV	4C	305	-	-	7/55/55/55	-
70	SF4	5G	801	7	-	-	0/6/5/5
74	CDL	8C	306	-	-	22/110/110/110	-
86	PGV	4J	101	-	-	5/55/55/55	-
84	HEM	3P	502	47	-	6/12/54/54	-
71	FES	3E	301	49	-	-	0/1/1/1
71	FES	5G	803	7	-	-	0/1/1/1
76	3PE	5M	504	-	-	11/54/54/54	-
76	3PE	5M	502	-	-	17/51/51/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PGV	8L	101	-	-	7/55/55/55	-
70	SF4	1I	202	9	-	-	0/6/5/5
76	3PE	1L	701	-	-	6/49/49/54	-
87	HEA	4A	605	55	-	4/32/76/76	-
76	3PE	5Y	806	-	-	11/44/44/54	-
69	PC1	5B	202	-	-	4/49/49/57	-
76	3PE	1P	502	-	-	1/38/38/54	-
74	CDL	4D	201	-	-	19/110/110/110	-
70	SF4	1B	201	2	-	-	0/6/5/5
76	3PE	5Y	803	-	-	10/33/33/54	-
69	PC1	1B	203	-	-	11/51/51/57	-
70	SF4	1G	802	7	-	-	0/6/5/5
85	HEC	3D	501	48	-	3/8/53/54	-
70	SF4	5B	201	2	-	-	0/6/5/5
76	3PE	3C	504	-	-	11/38/38/54	-
74	CDL	1H	401	-	-	4/61/61/110	-
76	3PE	5L	703	-	-	6/48/48/54	-
76	3PE	3C	505	-	-	5/37/37/54	-
69	PC1	1M	905	-	-	15/47/47/57	-
69	PC1	5h	203	-	-	13/50/50/57	-
76	3PE	3A	502	-	-	7/30/30/54	-
69	PC1	5L	705	-	-	6/49/49/57	-
76	3PE	1M	903	-	-	18/51/51/54	-
74	CDL	4C	306	-	-	22/110/110/110	-
69	PC1	1A	202	-	-	3/38/38/57	-
77	GTP	5O	401	78	-	2/18/38/38	0/3/3/3
74	CDL	3P	504	-	-	16/66/66/110	-
86	PGV	8C	302	-	-	10/55/55/55	-
86	PGV	8C	303	-	-	14/55/55/55	-
74	CDL	1L	702	-	-	18/86/86/110	-
76	3PE	1K	101	-	-	8/47/47/54	-
69	PC1	1B	202	-	-	5/49/49/57	-
74	CDL	3A	501	-	-	3/68/68/110	-
69	PC1	1H	402	-	-	3/51/51/57	-
74	CDL	5q	203	-	-	8/71/71/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	MYR	1o	201	-	-	0/11/12/13	-
86	PGV	8C	304	-	-	9/55/55/55	-
86	PGV	4B	301	-	-	4/55/55/55	-
76	3PE	3N	503	-	-	9/28/28/54	-
71	FES	1G	803	7	-	-	0/1/1/1
74	CDL	5N	401	-	-	17/71/71/110	-
74	CDL	8B	303	-	-	15/110/110/110	-
86	PGV	8B	302	-	-	5/55/55/55	-
86	PGV	4A	601	-	-	14/55/55/55	-
76	3PE	5L	701	-	-	5/49/49/54	-
81	EHZ	5n	201	-	-	2/42/44/45	-
86	PGV	4C	303	-	-	11/55/55/55	-
70	SF4	5I	203	9	-	-	0/6/5/5
71	FES	1E	301	5	-	-	0/1/1/1
90	PSC	4A	609	-	-	11/55/55/55	-
86	PGV	8K	101	-	-	13/55/55/55	-
76	3PE	5L	704	-	-	12/52/52/54	-
84	HEM	3C	501	47	-	5/12/54/54	-
79	NDP	5P	402	-	-	3/30/77/77	0/5/5/5
86	PGV	4C	304	-	-	10/55/55/55	-
70	SF4	1I	203	9	-	-	0/6/5/5
86	PGV	8B	301	-	-	4/55/55/55	-
76	3PE	1L	703	-	-	6/48/48/54	-
76	3PE	1Y	801	-	-	9/34/34/54	-
77	GTP	1O	402	78	-	3/18/38/38	0/3/3/3
76	3PE	3A	503	-	-	6/35/35/54	-
69	PC1	1L	704	-	-	6/49/49/57	-
76	3PE	3P	503	-	-	6/36/36/54	-
84	HEM	3P	501	47	-	7/12/54/54	-
69	PC1	1d	202	-	-	8/42/42/57	-
76	3PE	5K	101	-	-	9/47/47/54	-
76	3PE	5M	501	-	-	11/48/48/54	-
69	PC1	1q	201	-	-	3/52/52/57	-
76	3PE	1M	906	-	-	9/53/53/54	-
76	3PE	5Y	801	-	-	11/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PGV	4G	101	-	-	10/55/55/55	-
86	PGV	4C	307	-	-	2/55/55/55	-
81	EHZ	1n	201	-	-	3/42/44/45	-
76	3PE	5Y	802	-	-	14/43/43/54	-
69	PC1	3J	101	-	-	1/50/50/57	-
69	PC1	5M	505	-	-	12/47/47/57	-
69	PC1	5H	402	-	-	2/51/51/57	-
86	PGV	4C	301	-	-	1/55/55/55	-
76	3PE	1O	401	-	-	10/54/54/54	-
69	PC1	5A	202	-	-	4/38/38/57	-
72	FMN	5F	501	-	-	1/18/18/18	0/3/3/3
74	CDL	4B	302	-	-	15/110/110/110	-
74	CDL	5d	203	-	-	14/75/75/110	-
76	3PE	1j	101	-	-	7/47/47/54	-
76	3PE	5j	101	-	-	8/47/47/54	-
86	PGV	4L	101	-	-	7/55/55/55	-
86	PGV	4C	302	-	-	13/55/55/55	-
86	PGV	8C	301	-	-	2/55/55/55	-
79	NDP	1P	501	-	-	3/30/77/77	0/5/5/5
74	CDL	3G	102	-	-	10/66/66/110	-
85	HEC	3Q	501	48	-	2/10/54/54	-
92	PEK	8C	308	-	-	4/55/55/56	-
86	PGV	8A	602	-	-	5/55/55/55	-
70	SF4	5G	802	7	-	-	0/6/5/5
69	PC1	1A	203	-	-	3/36/36/57	-
69	PC1	1A	201	-	-	8/38/38/57	-
76	3PE	1M	901	-	-	14/52/52/54	-
74	CDL	3N	502	-	-	5/53/53/110	-
92	PEK	4G	102	-	-	7/56/56/56	-
76	3PE	5d	201	-	-	4/52/52/54	-
82	AME	1h	201	-	-	2/9/10/12	-
86	PGV	8C	307	-	-	2/55/55/55	-
81	EHZ	5T	101	20	-	10/42/44/45	-
70	SF4	1F	502	6	-	-	0/6/5/5
69	PC1	1M	904	-	-	6/38/38/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	CDL	1N	401	-	-	20/71/71/110	-
86	PGV	4A	603	-	-	3/55/55/55	-
81	EHZ	1T	101	20	-	9/42/44/45	-
76	3PE	1d	201	-	-	3/52/52/54	-
76	3PE	1Y	804	-	-	6/36/36/54	-
74	CDL	5H	401	-	-	6/61/61/110	-
74	CDL	8D	201	-	-	19/110/110/110	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	3Q	501	HEC	C2B-C3B	6.95	1.48	1.40
85	3Q	501	HEC	C3C-C2C	6.78	1.47	1.40
85	3D	501	HEC	C3C-C2C	6.75	1.47	1.40
85	3D	501	HEC	C2B-C3B	6.73	1.47	1.40
87	4A	604	HEA	C3B-C2B	5.54	1.47	1.34
87	4A	605	HEA	C3B-C2B	5.53	1.47	1.34
87	8A	604	HEA	C3B-C2B	5.49	1.47	1.34
87	8A	603	HEA	C3B-C2B	5.48	1.47	1.34
87	4A	604	HEA	C3A-C2A	5.30	1.47	1.40
87	4A	605	HEA	C3A-C2A	5.20	1.47	1.40
87	8A	603	HEA	C3A-C2A	5.17	1.47	1.40
87	8A	604	HEA	C3A-C2A	5.11	1.47	1.40
87	4A	605	HEA	C3D-C2D	4.91	1.47	1.36
87	8A	604	HEA	C3D-C2D	4.89	1.47	1.36
87	8A	603	HEA	C3D-C2D	4.88	1.47	1.36
87	4A	604	HEA	C3D-C2D	4.85	1.47	1.36
87	4A	605	HEA	CHD-C1D	4.82	1.47	1.35
87	4A	605	HEA	CHC-C4B	4.82	1.47	1.35
87	4A	604	HEA	CHC-C4B	4.79	1.47	1.35
87	8A	604	HEA	CHD-C1D	4.77	1.47	1.35
87	8A	603	HEA	CHC-C4B	4.76	1.47	1.35
87	8A	604	HEA	C3C-C2C	4.74	1.47	1.40
87	8A	603	HEA	CHD-C1D	4.73	1.47	1.35
87	8A	604	HEA	CHC-C4B	4.71	1.47	1.35
87	4A	604	HEA	CHD-C1D	4.71	1.47	1.35
87	4A	605	HEA	C3C-C2C	4.60	1.46	1.40
87	8A	603	HEA	C3C-C2C	4.53	1.46	1.40
87	4A	604	HEA	C3C-C2C	4.42	1.46	1.40
84	3C	502	HEM	C1B-NB	-3.50	1.34	1.40
84	3P	502	HEM	C1B-NB	-3.38	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	3P	501	HEM	C1B-NB	-3.33	1.34	1.40
84	3C	501	HEM	C1B-NB	-3.29	1.34	1.40
85	3Q	501	HEC	C3D-C2D	3.29	1.47	1.37
85	3D	501	HEC	C3D-C2D	3.27	1.47	1.37
85	3D	501	HEC	C2A-C3A	3.26	1.47	1.37
85	3Q	501	HEC	C2A-C3A	3.26	1.47	1.37
84	3P	501	HEM	C4D-ND	-3.26	1.34	1.40
84	3C	502	HEM	C4D-ND	-3.26	1.34	1.40
84	3P	502	HEM	C4D-ND	-3.25	1.34	1.40
84	3C	501	HEM	C4D-ND	-3.22	1.34	1.40
87	4A	604	HEA	FE-ND	3.11	2.12	1.96
87	4A	604	HEA	FE-NB	3.10	2.12	1.96
87	8A	603	HEA	FE-NB	3.10	2.12	1.96
87	8A	603	HEA	FE-ND	3.08	2.12	1.96
87	4A	605	HEA	FE-ND	3.06	2.12	1.96
87	8A	604	HEA	FE-ND	3.04	2.11	1.96
87	8A	604	HEA	FE-NB	3.04	2.11	1.96
87	8A	603	HEA	C4B-C3B	3.02	1.49	1.44
87	4A	605	HEA	FE-NB	3.00	2.11	1.96
85	3D	501	HEC	C3C-C4C	3.00	1.48	1.43
87	4A	604	HEA	C4B-C3B	2.96	1.49	1.44
85	3Q	501	HEC	C3C-C4C	2.91	1.48	1.43
84	3C	501	HEM	FE-NB	2.91	2.11	1.96
84	3P	501	HEM	FE-NB	2.90	2.11	1.96
84	3C	502	HEM	FE-NB	2.84	2.10	1.96
84	3P	502	HEM	FE-NB	2.83	2.10	1.96
87	4A	604	HEA	C2A-C1A	2.83	1.49	1.42
85	3D	501	HEC	C3A-C4A	2.83	1.49	1.42
87	8A	604	HEA	C4B-NB	-2.80	1.35	1.40
85	3Q	501	HEC	C2A-C1A	2.80	1.48	1.42
87	4A	605	HEA	C1D-ND	-2.79	1.35	1.40
87	4A	604	HEA	C1D-ND	-2.79	1.35	1.40
85	3Q	501	HEC	C4B-C3B	2.78	1.48	1.43
87	8A	603	HEA	C1D-ND	-2.76	1.35	1.40
87	8A	603	HEA	C2A-C1A	2.74	1.48	1.42
87	4A	605	HEA	C4B-NB	-2.74	1.35	1.40
87	4A	605	HEA	C4B-C3B	2.74	1.49	1.44
87	8A	603	HEA	C4B-NB	-2.73	1.35	1.40
87	8A	604	HEA	C1D-ND	-2.72	1.35	1.40
87	8A	604	HEA	C2A-C1A	2.72	1.48	1.42
87	4A	605	HEA	C2A-C1A	2.71	1.48	1.42
87	4A	604	HEA	C4B-NB	-2.66	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	3D	501	HEC	C4B-C3B	2.66	1.47	1.43
85	3D	501	HEC	C2A-C1A	2.65	1.48	1.42
87	8A	604	HEA	C4B-C3B	2.62	1.49	1.44
77	1O	402	GTP	C5-C6	-2.61	1.42	1.47
77	5O	401	GTP	C5-C6	-2.60	1.42	1.47
85	3Q	501	HEC	C3A-C4A	2.58	1.48	1.42
87	4A	604	HEA	C4D-C3D	2.56	1.49	1.45
85	3Q	501	HEC	C4D-CHA	2.51	1.48	1.41
87	8A	603	HEA	C4D-C3D	2.43	1.49	1.45
85	3D	501	HEC	C4D-CHA	2.43	1.47	1.41
85	3D	501	HEC	C1B-CHB	2.40	1.47	1.41
85	3D	501	HEC	C1D-CHD	2.40	1.47	1.41
85	3Q	501	HEC	C1C-CHC	2.38	1.47	1.41
85	3Q	501	HEC	C1D-CHD	2.36	1.47	1.41
85	3Q	501	HEC	C1B-CHB	2.36	1.47	1.41
85	3D	501	HEC	C1C-CHC	2.33	1.47	1.41
87	4A	605	HEA	C4C-CHD	2.30	1.47	1.41
87	8A	604	HEA	C1D-C2D	2.30	1.49	1.44
87	8A	604	HEA	C4C-CHD	2.26	1.47	1.41
87	4A	605	HEA	C4D-C3D	2.26	1.48	1.45
87	4A	605	HEA	C1D-C2D	2.24	1.48	1.44
87	4A	605	HEA	C1C-CHC	2.23	1.47	1.41
87	4A	604	HEA	C1C-CHC	2.22	1.47	1.41
87	8A	604	HEA	C1C-CHC	2.21	1.47	1.41
87	8A	603	HEA	C1D-C2D	2.20	1.48	1.44
87	8A	603	HEA	C1C-CHC	2.18	1.47	1.41
87	8A	603	HEA	C4C-CHD	2.18	1.47	1.41
87	4A	604	HEA	C4C-CHD	2.13	1.46	1.41
87	8A	604	HEA	C4D-C3D	2.08	1.48	1.45
87	4A	604	HEA	C1B-C2B	2.08	1.48	1.44
87	4A	604	HEA	C1D-C2D	2.08	1.48	1.44
87	8A	604	HEA	C1B-C2B	2.07	1.48	1.44
77	5O	401	GTP	C8-N7	-2.07	1.31	1.35
87	4A	605	HEA	C1B-C2B	2.06	1.48	1.44
84	3C	501	HEM	CHB-C1B	2.06	1.40	1.35
77	1O	402	GTP	C8-N7	-2.05	1.31	1.35
84	3P	501	HEM	CHB-C1B	2.03	1.40	1.35
84	3C	501	HEM	C1D-ND	-2.03	1.34	1.38
84	3P	502	HEM	C1D-ND	-2.02	1.34	1.38
84	3C	502	HEM	C1D-ND	-2.01	1.34	1.38

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	604	HEA	C3D-C4D-ND	6.63	116.77	110.36
87	8A	603	HEA	C3D-C4D-ND	6.59	116.74	110.36
87	4A	605	HEA	C3D-C4D-ND	6.48	116.63	110.36
87	4A	604	HEA	C3D-C4D-ND	6.43	116.59	110.36
85	3Q	501	HEC	C1D-C2D-C3D	-6.26	102.64	107.00
85	3D	501	HEC	C1D-C2D-C3D	-5.98	102.83	107.00
87	8A	603	HEA	C2B-C1B-NB	5.66	116.67	109.88
81	5n	201	EHZ	C10-S1-C9	5.66	119.50	101.87
87	4A	604	HEA	C2B-C1B-NB	5.62	116.61	109.88
87	8A	604	HEA	C2B-C1B-NB	5.61	116.60	109.88
81	1T	101	EHZ	C10-S1-C9	5.56	119.17	101.87
81	1n	201	EHZ	C10-S1-C9	5.51	119.03	101.87
87	4A	604	HEA	C2D-C1D-ND	5.49	116.35	109.84
87	4A	604	HEA	C3B-C4B-NB	5.47	116.33	109.84
87	4A	605	HEA	C2D-C1D-ND	5.45	116.29	109.84
87	8A	604	HEA	C2D-C1D-ND	5.45	116.29	109.84
87	4A	605	HEA	C2B-C1B-NB	5.44	116.40	109.88
87	8A	603	HEA	C3B-C4B-NB	5.44	116.28	109.84
81	5T	101	EHZ	C10-S1-C9	5.43	118.78	101.87
87	8A	604	HEA	C3B-C4B-NB	5.40	116.24	109.84
85	3D	501	HEC	CMC-C2C-C3C	5.40	132.17	125.82
87	8A	603	HEA	C2D-C1D-ND	5.36	116.19	109.84
85	3Q	501	HEC	CMB-C2B-C3B	5.25	132.00	125.82
85	3D	501	HEC	CMB-C2B-C3B	5.20	131.93	125.82
87	4A	605	HEA	C3B-C4B-NB	5.16	115.95	109.84
84	3C	501	HEM	CHC-C4B-NB	5.09	129.96	124.43
85	3Q	501	HEC	CMC-C2C-C3C	5.08	131.80	125.82
84	3P	501	HEM	CHC-C4B-NB	5.08	129.95	124.43
84	3C	502	HEM	CHC-C4B-NB	4.81	129.66	124.43
84	3P	502	HEM	CHC-C4B-NB	4.75	129.59	124.43
87	4A	604	HEA	CHA-C4D-ND	-4.61	119.42	124.43
84	3P	501	HEM	CHD-C1D-ND	4.41	129.22	124.43
84	3C	501	HEM	CHD-C1D-ND	4.29	129.09	124.43
87	8A	603	HEA	CHA-C4D-ND	-4.24	119.82	124.43
87	8A	604	HEA	C1D-C2D-C3D	-4.24	102.50	106.96
84	3P	502	HEM	CHD-C1D-ND	4.22	129.02	124.43
87	4A	605	HEA	C1D-C2D-C3D	-4.16	102.59	106.96
84	3C	502	HEM	CHD-C1D-ND	4.14	128.93	124.43
87	8A	604	HEA	C3C-C4C-NC	4.01	114.39	109.21
87	4A	604	HEA	C3C-C4C-NC	3.96	114.33	109.21
84	3P	502	HEM	C1B-NB-C4B	3.95	109.16	105.07
87	8A	603	HEA	C3C-C4C-NC	3.90	114.25	109.21
84	3C	502	HEM	C1B-NB-C4B	3.89	109.09	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	CAD-C3D-C4D	3.86	131.40	124.66
87	8A	603	HEA	C1D-C2D-C3D	-3.85	102.90	106.96
87	4A	604	HEA	C1D-C2D-C3D	-3.84	102.92	106.96
87	8A	603	HEA	CBA-CAA-C2A	-3.84	106.14	112.60
87	4A	605	HEA	C3C-C4C-NC	3.83	114.16	109.21
87	8A	604	HEA	C13-C12-C11	-3.83	108.59	114.35
84	3P	501	HEM	C1B-NB-C4B	3.82	109.02	105.07
87	4A	605	HEA	C13-C12-C11	-3.81	108.63	114.35
84	3C	501	HEM	C1B-NB-C4B	3.80	109.00	105.07
87	8A	604	HEA	C1B-C2B-C3B	-3.73	102.34	106.80
87	4A	605	HEA	C1B-C2B-C3B	-3.63	102.46	106.80
87	8A	604	HEA	CBA-CAA-C2A	-3.60	106.53	112.60
87	8A	603	HEA	C13-C14-C15	-3.58	119.05	127.66
87	4A	605	HEA	CHA-C4D-ND	-3.57	120.55	124.43
86	8C	302	PGV	O01-C1-C2	3.54	119.13	111.50
84	3C	501	HEM	CHA-C4D-ND	3.53	128.75	124.38
84	3P	501	HEM	CHA-C4D-ND	3.50	128.71	124.38
87	4A	604	HEA	C1B-C2B-C3B	-3.47	102.65	106.80
87	8A	603	HEA	C4D-C3D-C2D	-3.45	101.86	106.90
87	4A	604	HEA	C4D-C3D-C2D	-3.45	101.87	106.90
87	8A	603	HEA	C1B-C2B-C3B	-3.44	102.68	106.80
87	8A	603	HEA	CAD-C3D-C4D	3.44	130.67	124.66
87	4A	604	HEA	CBA-CAA-C2A	-3.44	106.81	112.60
84	3P	502	HEM	CHA-C4D-ND	3.44	128.63	124.38
74	1N	401	CDL	OB6-CB5-C51	3.43	117.40	111.09
84	3C	502	HEM	CHA-C4D-ND	3.38	128.55	124.38
87	4A	605	HEA	CBA-CAA-C2A	-3.37	106.92	112.60
86	4C	302	PGV	O01-C1-C2	3.37	118.77	111.50
84	3P	501	HEM	CHB-C1B-NB	3.36	128.53	124.38
74	5N	401	CDL	OB6-CB5-C51	3.35	117.26	111.09
84	3P	502	HEM	CHB-C1B-NB	3.35	128.51	124.38
84	3C	501	HEM	CHB-C1B-NB	3.34	128.50	124.38
87	8A	604	HEA	CMC-C2C-C3C	3.31	130.86	124.68
87	4A	605	HEA	C4D-C3D-C2D	-3.26	102.15	106.90
87	8A	604	HEA	C4D-C3D-C2D	-3.21	102.22	106.90
87	8A	604	HEA	C13-C14-C15	-3.15	120.08	127.66
84	3C	502	HEM	CHB-C1B-NB	3.15	128.27	124.38
87	8A	603	HEA	C4B-C3B-C2B	-3.14	102.04	107.41
87	4A	605	HEA	C13-C14-C15	-3.14	120.10	127.66
76	1Y	803	3PE	O21-C21-C22	3.14	118.27	111.50
87	4A	604	HEA	C4B-C3B-C2B	-3.12	102.08	107.41
87	8A	603	HEA	C13-C12-C11	-3.11	109.67	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	C26-C15-C16	3.07	120.43	115.27
87	4A	604	HEA	C13-C14-C15	-3.04	120.34	127.66
87	8A	603	HEA	CMC-C2C-C3C	3.04	130.36	124.68
87	8A	603	HEA	C26-C15-C16	3.02	120.35	115.27
87	4A	604	HEA	CHB-C1B-NB	-3.00	121.18	124.43
87	8A	604	HEA	CHA-C4D-ND	-2.99	121.18	124.43
76	5Y	803	3PE	O21-C21-C22	2.97	117.91	111.50
87	4A	605	HEA	CMC-C2C-C3C	2.94	130.17	124.68
87	4A	605	HEA	C26-C15-C16	2.92	120.19	115.27
87	8A	604	HEA	C4B-C3B-C2B	-2.90	102.46	107.41
87	4A	605	HEA	C4B-C3B-C2B	-2.86	102.52	107.41
87	8A	604	HEA	C26-C15-C16	2.85	120.06	115.27
87	4A	604	HEA	CAD-CBD-CGD	-2.84	107.50	113.60
87	8A	604	HEA	C27-C19-C20	2.81	119.99	115.27
87	4A	604	HEA	CMC-C2C-C3C	2.80	129.91	124.68
82	5h	201	AME	O-C-CA	-2.79	117.45	124.78
87	8A	604	HEA	C1D-ND-C4D	-2.78	102.21	105.07
87	4A	605	HEA	C27-C19-C20	2.77	119.92	115.27
82	1h	201	AME	O-C-CA	-2.76	117.55	124.78
84	3P	501	HEM	CHD-C1D-C2D	-2.75	120.69	124.98
84	3C	501	HEM	CHD-C1D-C2D	-2.73	120.71	124.98
87	4A	604	HEA	C1D-ND-C4D	-2.72	102.27	105.07
85	3D	501	HEC	CAA-CBA-CGA	-2.71	106.15	113.76
87	8A	603	HEA	C17-C18-C19	-2.69	121.19	127.66
87	8A	603	HEA	C1D-ND-C4D	-2.68	102.30	105.07
87	8A	603	HEA	CHB-C1B-NB	-2.68	121.52	124.43
84	3P	501	HEM	CBA-CAA-C2A	-2.68	108.06	112.62
87	8A	603	HEA	C4B-NB-C1B	-2.67	102.32	105.07
87	4A	604	HEA	C4B-NB-C1B	-2.65	102.33	105.07
87	8A	603	HEA	C27-C19-C20	2.64	119.72	115.27
87	4A	605	HEA	C1D-ND-C4D	-2.64	102.35	105.07
87	8A	604	HEA	C4B-NB-C1B	-2.63	102.35	105.07
87	8A	603	HEA	CAD-CBD-CGD	-2.63	107.95	113.60
79	1P	501	NDP	O4D-C1D-C2D	-2.62	100.93	106.64
87	4A	604	HEA	C27-C19-C20	2.57	119.59	115.27
85	3Q	501	HEC	CAA-CBA-CGA	-2.56	106.57	113.76
87	4A	605	HEA	C17-C18-C19	-2.55	121.52	127.66
79	5P	402	NDP	O4D-C1D-C2D	-2.53	101.14	106.64
84	3P	502	HEM	C4D-ND-C1D	2.51	107.66	105.07
84	3C	502	HEM	C4D-ND-C1D	2.50	107.66	105.07
87	8A	604	HEA	CHB-C1B-NB	-2.46	121.75	124.43
87	8A	604	HEA	C25-C23-C24	2.46	120.04	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	604	HEA	C17-C18-C19	-2.46	121.74	127.66
85	3Q	501	HEC	CMA-C3A-C2A	2.45	129.57	124.94
87	4A	605	HEA	CAD-C3D-C4D	2.44	128.92	124.66
87	4A	604	HEA	C17-C18-C19	-2.44	121.79	127.66
84	3P	502	HEM	CHD-C1D-C2D	-2.42	121.19	124.98
84	3C	502	HEM	CHD-C1D-C2D	-2.42	121.19	124.98
87	4A	605	HEA	C25-C23-C24	2.42	119.95	114.60
87	4A	605	HEA	CHB-C1B-NB	-2.41	121.81	124.43
76	3A	502	3PE	O21-C21-C22	2.41	116.69	111.50
87	8A	604	HEA	CMB-C2B-C1B	2.39	128.68	125.04
87	4A	605	HEA	CMB-C2B-C1B	2.38	128.66	125.04
87	4A	604	HEA	CHD-C1D-C2D	-2.35	120.21	126.72
86	4C	305	PGV	O01-C1-C2	2.35	116.57	111.50
90	8I	101	PSC	O01-C1-C2	2.35	116.56	111.50
85	3Q	501	HEC	CBD-CAD-C3D	-2.35	108.61	112.62
87	4A	605	HEA	C4B-NB-C1B	-2.33	102.67	105.07
87	4A	604	HEA	C25-C23-C24	2.33	119.74	114.60
87	8A	603	HEA	C25-C23-C24	2.31	119.71	114.60
86	8G	101	PGV	O01-C1-C2	2.30	116.46	111.50
87	8A	604	HEA	CMD-C2D-C1D	2.30	128.54	125.04
87	8A	603	HEA	CMD-C2D-C1D	2.30	128.54	125.04
87	4A	604	HEA	CMB-C2B-C1B	2.29	128.53	125.04
87	8A	604	HEA	CAD-CBD-CGD	-2.29	108.67	113.60
87	8A	603	HEA	CHD-C1D-C2D	-2.29	120.40	126.72
87	8A	604	HEA	CAD-C3D-C4D	2.26	128.61	124.66
87	4A	604	HEA	CMD-C2D-C1D	2.26	128.48	125.04
87	8A	603	HEA	CMB-C2B-C1B	2.25	128.47	125.04
87	4A	605	HEA	CMD-C2D-C1D	2.24	128.46	125.04
79	1P	501	NDP	C5A-C6A-N6A	2.23	123.74	120.35
79	5P	402	NDP	C5A-C6A-N6A	2.22	123.73	120.35
84	3C	501	HEM	CHA-C4D-C3D	-2.19	121.21	125.33
74	1H	401	CDL	OB6-CB5-C51	2.19	116.22	111.50
87	4A	605	HEA	CHD-C1D-C2D	-2.19	120.67	126.72
87	8A	604	HEA	CHD-C1D-C2D	-2.18	120.69	126.72
84	3P	501	HEM	C4D-ND-C1D	2.16	107.30	105.07
87	8A	604	HEA	CHB-C1B-C2B	-2.14	121.64	124.98
74	5H	401	CDL	OB6-CB5-C51	2.13	116.10	111.50
84	3P	501	HEM	CHA-C4D-C3D	-2.13	121.34	125.33
90	4A	609	PSC	O01-C1-C2	2.12	116.08	111.50
74	3C	503	CDL	OA6-CA5-C11	2.11	116.06	111.50
84	3C	502	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
87	8A	603	HEA	CHC-C4B-NB	-2.08	121.81	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	605	HEA	C21-C22-C23	-2.08	120.65	127.75
87	4A	604	HEA	C21-C22-C23	-2.06	120.69	127.75
87	4A	604	HEA	CHC-C4B-NB	-2.06	121.83	124.38
85	3Q	501	HEC	CMD-C2D-C3D	2.06	128.82	124.94
72	1F	501	FMN	C4-N3-C2	-2.05	121.85	125.64
87	4A	605	HEA	CHB-C1B-C2B	-2.05	121.78	124.98
84	3C	501	HEM	C4D-ND-C1D	2.04	107.19	105.07
86	8C	305	PGV	O01-C1-C2	2.03	115.88	111.50
72	5F	501	FMN	C4-N3-C2	-2.03	121.89	125.64
87	8A	603	HEA	CHB-C1B-C2B	-2.03	121.81	124.98
77	1O	402	GTP	O6-C6-C5	2.03	128.33	124.37
74	4C	306	CDL	OB6-CB5-C51	2.02	115.86	111.50
85	3D	501	HEC	CMD-C2D-C3D	2.01	128.74	124.94
69	5d	202	PC1	O21-C21-C22	2.00	115.82	111.50

There are no chirality outliers.

All (1305) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1B	203	PC1	O22-C21-O21-C2
69	1B	203	PC1	C22-C21-O21-C2
69	1I	204	PC1	C1-O11-P-O14
69	1M	904	PC1	O22-C21-O21-C2
69	1M	904	PC1	C22-C21-O21-C2
69	1d	202	PC1	O22-C21-O21-C2
69	1d	202	PC1	C22-C21-O21-C2
69	1h	203	PC1	C11-O13-P-O14
69	1h	203	PC1	O32-C31-O31-C3
69	1h	203	PC1	C32-C31-O31-C3
69	3R	302	PC1	O32-C31-O31-C3
69	3R	302	PC1	C32-C31-O31-C3
69	3X	101	PC1	C1-O11-P-O14
69	5B	203	PC1	O22-C21-O21-C2
69	5B	203	PC1	C22-C21-O21-C2
69	5I	204	PC1	C1-O11-P-O14
69	5I	204	PC1	C1-O11-P-O13
69	5M	503	PC1	O22-C21-O21-C2
69	5M	503	PC1	C22-C21-O21-C2
69	5d	202	PC1	O22-C21-O21-C2
69	5d	202	PC1	C22-C21-O21-C2
69	5h	203	PC1	C11-O13-P-O14
69	5h	203	PC1	O32-C31-O31-C3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
69	5h	203	PC1	C32-C31-O31-C3
74	1H	401	CDL	CA4-CA3-OA5-PA1
74	1H	401	CDL	OB7-CB5-OB6-CB4
74	1H	401	CDL	C51-CB5-OB6-CB4
74	1L	702	CDL	OA6-CA4-CA6-OA8
74	1N	401	CDL	CB3-OB5-PB2-OB3
74	1X	201	CDL	C1-CA2-OA2-PA1
74	1X	201	CDL	C1-CB2-OB2-PB2
74	1d	203	CDL	CB2-OB2-PB2-OB3
74	1h	202	CDL	CA2-OA2-PA1-OA5
74	1h	202	CDL	C1-CB2-OB2-PB2
74	1h	202	CDL	CB2-OB2-PB2-OB3
74	1h	202	CDL	OB7-CB5-OB6-CB4
74	1h	202	CDL	C51-CB5-OB6-CB4
74	1h	202	CDL	OB9-CB7-OB8-CB6
74	1h	202	CDL	C71-CB7-OB8-CB6
74	3C	503	CDL	CB2-OB2-PB2-OB3
74	3G	102	CDL	CB2-OB2-PB2-OB5
74	3P	504	CDL	OB9-CB7-OB8-CB6
74	3P	504	CDL	C71-CB7-OB8-CB6
74	3T	101	CDL	OB9-CB7-OB8-CB6
74	3T	101	CDL	C71-CB7-OB8-CB6
74	4B	302	CDL	OA9-CA7-OA8-CA6
74	4B	302	CDL	C31-CA7-OA8-CA6
74	4B	302	CDL	CB3-OB5-PB2-OB3
74	4C	306	CDL	C1-CA2-OA2-PA1
74	4C	306	CDL	OB7-CB5-OB6-CB4
74	4C	306	CDL	C51-CB5-OB6-CB4
74	4C	306	CDL	OB9-CB7-OB8-CB6
74	4C	306	CDL	C71-CB7-OB8-CB6
74	4D	201	CDL	C1-CA2-OA2-PA1
74	4D	201	CDL	CA3-OA5-PA1-OA3
74	4D	201	CDL	CB3-OB5-PB2-OB3
74	4D	201	CDL	OB7-CB5-OB6-CB4
74	4D	201	CDL	C51-CB5-OB6-CB4
74	4D	201	CDL	OB9-CB7-OB8-CB6
74	4D	201	CDL	C71-CB7-OB8-CB6
74	5H	401	CDL	CA3-OA5-PA1-OA4
74	5H	401	CDL	CA4-CA3-OA5-PA1
74	5H	401	CDL	OB7-CB5-OB6-CB4
74	5H	401	CDL	C51-CB5-OB6-CB4
74	5L	702	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
74	5N	401	CDL	CB3-OB5-PB2-OB3
74	5X	201	CDL	C1-CA2-OA2-PA1
74	5X	201	CDL	C1-CB2-OB2-PB2
74	5d	203	CDL	CB2-OB2-PB2-OB3
74	5h	202	CDL	CA2-OA2-PA1-OA5
74	5h	202	CDL	C1-CB2-OB2-PB2
74	5h	202	CDL	CB2-OB2-PB2-OB3
74	5h	202	CDL	OB7-CB5-OB6-CB4
74	5h	202	CDL	C51-CB5-OB6-CB4
74	5h	202	CDL	OB9-CB7-OB8-CB6
74	5h	202	CDL	C71-CB7-OB8-CB6
74	8B	303	CDL	OA9-CA7-OA8-CA6
74	8B	303	CDL	C31-CA7-OA8-CA6
74	8B	303	CDL	CB3-OB5-PB2-OB3
74	8C	306	CDL	C1-CA2-OA2-PA1
74	8C	306	CDL	OB7-CB5-OB6-CB4
74	8C	306	CDL	C51-CB5-OB6-CB4
74	8C	306	CDL	OB9-CB7-OB8-CB6
74	8C	306	CDL	C71-CB7-OB8-CB6
74	8D	201	CDL	C1-CA2-OA2-PA1
74	8D	201	CDL	CA3-OA5-PA1-OA3
74	8D	201	CDL	CB3-OB5-PB2-OB3
74	8D	201	CDL	OB7-CB5-OB6-CB4
74	8D	201	CDL	C51-CB5-OB6-CB4
74	8D	201	CDL	OB9-CB7-OB8-CB6
74	8D	201	CDL	C71-CB7-OB8-CB6
76	1K	101	3PE	C1-O11-P-O14
76	1L	701	3PE	O32-C31-O31-C3
76	1L	701	3PE	C32-C31-O31-C3
76	1L	703	3PE	C2-C1-O11-P
76	1M	901	3PE	C1-O11-P-O12
76	1M	901	3PE	C1-O11-P-O14
76	1M	903	3PE	C1-O11-P-O12
76	1M	903	3PE	C1-O11-P-O14
76	1M	903	3PE	C2-C1-O11-P
76	1M	903	3PE	O32-C31-O31-C3
76	1M	903	3PE	C32-C31-O31-C3
76	1M	906	3PE	C1-O11-P-O14
76	1O	401	3PE	C2-C1-O11-P
76	1Y	802	3PE	C1-O11-P-O13
76	1Y	802	3PE	C1-O11-P-O14
76	1Y	802	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
76	1Y	802	3PE	O22-C21-O21-C2
76	1Y	802	3PE	C22-C21-O21-C2
76	1Y	803	3PE	O22-C21-O21-C2
76	1Y	803	3PE	C22-C21-O21-C2
76	1Y	805	3PE	C11-O13-P-O14
76	1Y	806	3PE	O32-C31-O31-C3
76	1Y	806	3PE	C32-C31-O31-C3
76	1b	201	3PE	C11-O13-P-O12
76	1j	101	3PE	O22-C21-O21-C2
76	1j	101	3PE	C22-C21-O21-C2
76	3A	502	3PE	O32-C31-O31-C3
76	3A	502	3PE	C32-C31-O31-C3
76	3A	502	3PE	O22-C21-O21-C2
76	3A	502	3PE	C22-C21-O21-C2
76	3A	503	3PE	C2-C1-O11-P
76	3C	504	3PE	C11-O13-P-O11
76	3C	504	3PE	C11-O13-P-O12
76	3C	504	3PE	C11-O13-P-O14
76	3C	505	3PE	O21-C2-C3-O31
76	3G	101	3PE	O32-C31-O31-C3
76	3G	101	3PE	C32-C31-O31-C3
76	3N	501	3PE	C1-O11-P-O14
76	3N	503	3PE	O22-C21-O21-C2
76	3N	503	3PE	C22-C21-O21-C2
76	3P	503	3PE	C11-O13-P-O11
76	3P	503	3PE	C11-O13-P-O12
76	3P	503	3PE	C11-O13-P-O14
76	5A	201	3PE	C11-O13-P-O12
76	5K	101	3PE	C1-O11-P-O14
76	5L	701	3PE	O32-C31-O31-C3
76	5L	701	3PE	C32-C31-O31-C3
76	5L	703	3PE	C2-C1-O11-P
76	5L	704	3PE	C1-O11-P-O12
76	5L	704	3PE	C1-O11-P-O14
76	5M	502	3PE	C1-O11-P-O12
76	5M	502	3PE	C2-C1-O11-P
76	5M	502	3PE	O32-C31-O31-C3
76	5M	502	3PE	C32-C31-O31-C3
76	5M	504	3PE	C2-C1-O11-P
76	5M	506	3PE	C1-O11-P-O14
76	5Y	801	3PE	C2-C1-O11-P
76	5Y	802	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
76	5Y	802	3PE	C1-O11-P-O14
76	5Y	802	3PE	C2-C1-O11-P
76	5Y	802	3PE	O22-C21-O21-C2
76	5Y	802	3PE	C22-C21-O21-C2
76	5Y	803	3PE	O22-C21-O21-C2
76	5Y	803	3PE	C22-C21-O21-C2
76	5Y	805	3PE	C11-O13-P-O14
76	5Y	805	3PE	C12-C11-O13-P
76	5Y	806	3PE	O32-C31-O31-C3
76	5Y	806	3PE	C32-C31-O31-C3
76	5j	101	3PE	C1-O11-P-O14
76	5j	101	3PE	C11-O13-P-O14
76	5j	101	3PE	O22-C21-O21-C2
76	5j	101	3PE	C22-C21-O21-C2
77	5O	401	GTP	PB-O3A-PA-O5'
81	1T	101	EHZ	N2-C15-C16-O5
81	1n	201	EHZ	C7-C8-C9-O2
81	5T	101	EHZ	N2-C15-C16-O5
81	5n	201	EHZ	C7-C8-C9-O2
84	3C	501	HEM	C2B-C3B-CAB-CBB
84	3C	502	HEM	C2B-C3B-CAB-CBB
84	3P	501	HEM	C2B-C3B-CAB-CBB
84	3P	502	HEM	C2B-C3B-CAB-CBB
86	4A	601	PGV	O04-C19-O03-C01
86	4A	601	PGV	C20-C19-O03-C01
86	4A	602	PGV	C02-C03-O11-P
86	4C	302	PGV	C05-C04-O12-P
86	4C	302	PGV	O02-C1-O01-C02
86	4C	302	PGV	C2-C1-O01-C02
86	4C	303	PGV	O04-C19-O03-C01
86	4C	303	PGV	C20-C19-O03-C01
86	4C	304	PGV	C03-O11-P-O13
86	4C	305	PGV	O02-C1-O01-C02
86	4C	305	PGV	C2-C1-O01-C02
86	4G	101	PGV	O02-C1-O01-C02
86	4G	101	PGV	C2-C1-O01-C02
86	4G	101	PGV	O04-C19-O03-C01
86	4G	101	PGV	C20-C19-O03-C01
86	4K	101	PGV	O04-C19-O03-C01
86	4K	101	PGV	C20-C19-O03-C01
86	8A	601	PGV	O04-C19-O03-C01
86	8A	601	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
86	8A	602	PGV	C02-C03-O11-P
86	8C	302	PGV	C05-C04-O12-P
86	8C	302	PGV	O02-C1-O01-C02
86	8C	302	PGV	C2-C1-O01-C02
86	8C	303	PGV	O04-C19-O03-C01
86	8C	303	PGV	C20-C19-O03-C01
86	8C	304	PGV	C03-O11-P-O13
86	8C	305	PGV	O02-C1-O01-C02
86	8C	305	PGV	C2-C1-O01-C02
86	8G	101	PGV	O02-C1-O01-C02
86	8G	101	PGV	C2-C1-O01-C02
86	8G	101	PGV	O04-C19-O03-C01
86	8G	101	PGV	C20-C19-O03-C01
86	8K	101	PGV	C03-O11-P-O14
86	8K	101	PGV	O04-C19-O03-C01
86	8K	101	PGV	C20-C19-O03-C01
87	8A	603	HEA	C3B-C11-C12-C13
87	8A	603	HEA	O11-C11-C12-C13
90	4A	609	PSC	O02-C1-O01-C02
90	4A	609	PSC	C2-C1-O01-C02
90	8I	101	PSC	C03-O11-P-O12
90	8I	101	PSC	O02-C1-O01-C02
90	8I	101	PSC	C2-C1-O01-C02
81	1T	101	EHZ	C13-C12-N1-C11
81	5T	101	EHZ	C13-C12-N1-C11
74	1N	401	CDL	C51-CB5-OB6-CB4
74	5N	401	CDL	C51-CB5-OB6-CB4
74	4D	201	CDL	O1-C1-CB2-OB2
74	8C	306	CDL	O1-C1-CA2-OA2
74	8D	201	CDL	O1-C1-CB2-OB2
74	1N	401	CDL	OB7-CB5-OB6-CB4
74	5N	401	CDL	OB7-CB5-OB6-CB4
69	1L	704	PC1	C2-C1-O11-P
69	5L	705	PC1	C2-C1-O11-P
76	1Y	801	3PE	C2-C1-O11-P
76	3Y	101	3PE	C2-C1-O11-P
90	8I	101	PSC	C02-C03-O11-P
87	8A	603	HEA	C19-C20-C21-C22
81	1T	101	EHZ	O3-C12-N1-C11
81	5T	101	EHZ	O3-C12-N1-C11
74	8C	306	CDL	CB2-C1-CA2-OA2
74	5X	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
69	1L	704	PC1	C24-C25-C26-C27
74	4C	306	CDL	O1-C1-CA2-OA2
76	1O	401	3PE	C31-C32-C33-C34
74	5N	401	CDL	OA6-CA4-CA6-OA8
86	8J	101	PGV	C19-C20-C21-C22
76	1Y	806	3PE	C31-C32-C33-C34
86	8B	302	PGV	C1-C2-C3-C4
86	4C	307	PGV	C02-C03-O11-P
90	4A	609	PSC	C02-C03-O11-P
69	5q	201	PC1	C31-C32-C33-C34
76	3C	504	3PE	C21-C22-C23-C24
76	3Q	502	3PE	C21-C22-C23-C24
69	1M	905	PC1	C11-O13-P-O11
74	1h	202	CDL	CB2-OB2-PB2-OB5
74	3C	503	CDL	CB2-OB2-PB2-OB5
74	3N	502	CDL	CB3-OB5-PB2-OB2
74	4B	302	CDL	CB3-OB5-PB2-OB2
74	8B	303	CDL	CB3-OB5-PB2-OB2
76	1K	101	3PE	C1-O11-P-O13
76	1M	901	3PE	C1-O11-P-O13
76	1M	903	3PE	C1-O11-P-O13
76	5K	101	3PE	C1-O11-P-O13
76	5L	704	3PE	C1-O11-P-O13
76	5M	502	3PE	C1-O11-P-O13
86	8K	101	PGV	C03-O11-P-O12
90	4A	609	PSC	C03-O11-P-O12
69	5L	705	PC1	C24-C25-C26-C27
79	1P	501	NDP	O4D-C1D-N1N-C6N
76	1M	901	3PE	C32-C33-C34-C35
86	4A	603	PGV	C22-C23-C24-C25
74	5d	203	CDL	C32-C33-C34-C35
69	1h	203	PC1	C2-C1-O11-P
69	5h	203	PC1	C2-C1-O11-P
72	5F	501	FMN	C4'-C5'-O5'-P
74	5N	401	CDL	C1-CA2-OA2-PA1
76	3C	505	3PE	C2-C1-O11-P
86	8C	307	PGV	C02-C03-O11-P
76	5L	703	3PE	C39-C3A-C3B-C3C
76	5d	201	3PE	C3C-C3D-C3E-C3F
74	5N	401	CDL	O1-C1-CB2-OB2
76	3Q	502	3PE	C35-C36-C37-C38
76	5Y	806	3PE	C31-C32-C33-C34

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
86	4J	101	PGV	C19-C20-C21-C22
74	1N	401	CDL	OA6-CA4-CA6-OA8
74	8B	303	CDL	C59-C60-C61-C62
86	8B	301	PGV	C22-C23-C24-C25
76	1L	703	3PE	C39-C3A-C3B-C3C
74	1d	203	CDL	CA5-C11-C12-C13
74	5d	203	CDL	CA5-C11-C12-C13
76	1M	902	3PE	C21-C22-C23-C24
74	8C	306	CDL	C79-C80-C81-C82
76	3A	503	3PE	C32-C33-C34-C35
74	1d	203	CDL	C32-C33-C34-C35
74	1q	202	CDL	C16-C17-C18-C19
76	5L	704	3PE	C32-C33-C34-C35
69	1q	201	PC1	C2A-C2B-C2C-C2D
74	4C	306	CDL	C79-C80-C81-C82
69	5M	505	PC1	C23-C24-C25-C26
74	4B	302	CDL	C59-C60-C61-C62
76	3Q	502	3PE	C27-C28-C29-C2A
87	8A	604	HEA	C2A-CAA-CBA-CGA
76	5Y	803	3PE	C23-C24-C25-C26
76	5M	504	3PE	C31-C32-C33-C34
86	4C	302	PGV	C26-C27-C28-C29
74	5L	702	CDL	O1-C1-CB2-OB2
74	4C	306	CDL	CB2-C1-CA2-OA2
76	1Y	803	3PE	C23-C24-C25-C26
74	5h	202	CDL	C60-C61-C62-C63
69	5q	201	PC1	C2A-C2B-C2C-C2D
69	1q	201	PC1	C31-C32-C33-C34
86	4B	301	PGV	C1-C2-C3-C4
86	8C	302	PGV	C28-C29-C30-C31
74	1h	202	CDL	C60-C61-C62-C63
86	4C	302	PGV	C7-C8-C9-C10
74	5q	203	CDL	C16-C17-C18-C19
86	4K	101	PGV	C22-C23-C24-C25
69	1h	203	PC1	C2B-C2C-C2D-C2E
86	4C	302	PGV	C27-C28-C29-C30
76	1Y	802	3PE	C22-C23-C24-C25
76	1b	201	3PE	C36-C37-C38-C39
76	5Y	802	3PE	C22-C23-C24-C25
76	1M	903	3PE	C22-C23-C24-C25
74	4C	306	CDL	C36-C37-C38-C39
74	5X	201	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
76	5M	502	3PE	C3B-C3C-C3D-C3E
74	5L	702	CDL	C58-C59-C60-C61
74	8C	306	CDL	C36-C37-C38-C39
76	1M	906	3PE	C23-C24-C25-C26
76	3Y	101	3PE	C31-C32-C33-C34
74	5L	702	CDL	C37-C38-C39-C40
76	5M	502	3PE	C22-C23-C24-C25
84	3C	501	HEM	C4B-C3B-CAB-CBB
84	3C	502	HEM	C4B-C3B-CAB-CBB
84	3P	501	HEM	C4B-C3B-CAB-CBB
84	3P	502	HEM	C4B-C3B-CAB-CBB
76	5M	504	3PE	C38-C39-C3A-C3B
76	3D	502	3PE	C31-C32-C33-C34
69	1M	905	PC1	C32-C33-C34-C35
69	5M	505	PC1	C32-C33-C34-C35
76	1M	903	3PE	C3B-C3C-C3D-C3E
86	4B	301	PGV	C24-C25-C26-C27
74	5d	203	CDL	C42-C43-C44-C45
76	5L	704	3PE	C2E-C2F-C2G-C2H
86	4K	101	PGV	C2-C3-C4-C5
86	4L	101	PGV	C6-C7-C8-C9
74	1X	201	CDL	C36-C37-C38-C39
76	1M	902	3PE	C26-C27-C28-C29
86	4C	303	PGV	C5-C6-C7-C8
76	1M	901	3PE	C2E-C2F-C2G-C2H
86	4J	101	PGV	C21-C22-C23-C24
76	1L	703	3PE	C33-C34-C35-C36
69	1I	204	PC1	C1-O11-P-O13
69	5M	503	PC1	C11-O13-P-O11
69	5M	505	PC1	C1-O11-P-O13
74	1X	201	CDL	CA2-OA2-PA1-OA5
74	3T	101	CDL	CA3-OA5-PA1-OA2
74	5h	202	CDL	CB2-OB2-PB2-OB5
76	3G	101	3PE	C1-O11-P-O13
76	5Y	801	3PE	C1-O11-P-O13
79	5P	402	NDP	O4D-C1D-N1N-C6N
86	8C	303	PGV	C03-O11-P-O12
72	1F	501	FMN	C4'-C5'-O5'-P
74	1N	401	CDL	C1-CA2-OA2-PA1
76	3N	501	3PE	C2-C1-O11-P
74	5N	401	CDL	C12-C13-C14-C15
74	1d	203	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
74	5d	203	CDL	OA5-CA3-CA4-CA6
92	4C	308	PEK	C21-C22-C23-C24
92	8C	308	PEK	C21-C22-C23-C24
69	1h	203	PC1	C32-C33-C34-C35
74	1L	702	CDL	C33-C34-C35-C36
86	8L	101	PGV	C6-C7-C8-C9
87	4A	605	HEA	C2A-CAA-CBA-CGA
74	1N	401	CDL	C12-C13-C14-C15
76	5A	201	3PE	C36-C37-C38-C39
69	1B	203	PC1	C28-C29-C2A-C2B
74	1L	702	CDL	CA3-CA4-CA6-OA8
74	5L	702	CDL	CA3-CA4-CA6-OA8
74	8B	303	CDL	CB3-CB4-CB6-OB8
76	1L	703	3PE	C1-C2-C3-O31
76	1Y	803	3PE	C1-C2-C3-O31
76	3P	503	3PE	C1-C2-C3-O31
76	5L	703	3PE	C1-C2-C3-O31
76	5M	501	3PE	C1-C2-C3-O31
76	5Y	801	3PE	C1-C2-C3-O31
76	5Y	803	3PE	C1-C2-C3-O31
86	4J	101	PGV	O03-C01-C02-C03
87	4A	604	HEA	C4D-C3D-CAD-CBD
76	1M	906	3PE	C27-C28-C29-C2A
76	1O	401	3PE	C38-C39-C3A-C3B
74	1h	202	CDL	C34-C35-C36-C37
76	1M	903	3PE	C34-C35-C36-C37
76	5L	703	3PE	C33-C34-C35-C36
81	1T	101	EHZ	O4-C15-C16-O5
81	5T	101	EHZ	O4-C15-C16-O5
86	8C	302	PGV	C7-C8-C9-C10
76	5M	502	3PE	C34-C35-C36-C37
90	8I	101	PSC	C25-C26-C27-C28
69	1d	202	PC1	C37-C38-C39-C3A
74	3C	503	CDL	C72-C71-CB7-OB8
76	5M	506	3PE	C25-C26-C27-C28
74	1d	203	CDL	C71-C72-C73-C74
74	5L	702	CDL	C33-C34-C35-C36
74	1d	203	CDL	C1-CA2-OA2-PA1
76	5L	704	3PE	C2-C1-O11-P
76	1Y	801	3PE	C33-C34-C35-C36
69	1I	201	PC1	O11-C1-C2-O21
69	5I	201	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
74	1L	702	CDL	OA5-CA3-CA4-OA6
74	3T	101	CDL	OA5-CA3-CA4-OA6
74	5L	702	CDL	OA5-CA3-CA4-OA6
76	3N	501	3PE	O21-C21-C22-C23
86	8B	302	PGV	C24-C25-C26-C27
90	4A	609	PSC	C25-C26-C27-C28
76	5M	501	3PE	C21-C22-C23-C24
76	1Y	803	3PE	O31-C31-C32-C33
76	5Y	803	3PE	O31-C31-C32-C33
69	1M	905	PC1	O21-C2-C3-O31
74	8B	303	CDL	OB6-CB4-CB6-OB8
69	5h	203	PC1	C32-C33-C34-C35
74	1L	702	CDL	C37-C38-C39-C40
74	1X	201	CDL	C61-C62-C63-C64
74	4C	306	CDL	C75-C76-C77-C78
69	1M	905	PC1	C2A-C2B-C2C-C2D
69	5B	203	PC1	C28-C29-C2A-C2B
86	8L	101	PGV	C21-C22-C23-C24
74	1N	401	CDL	C32-C31-CA7-OA8
74	3P	504	CDL	C31-C32-C33-C34
74	5N	401	CDL	CA2-C1-CB2-OB2
74	8D	201	CDL	CA2-C1-CB2-OB2
74	8C	306	CDL	C75-C76-C77-C78
69	5d	202	PC1	C37-C38-C39-C3A
69	1M	905	PC1	O11-C1-C2-C3
74	1L	702	CDL	OA5-CA3-CA4-CA6
74	3P	504	CDL	OB5-CB3-CB4-CB6
74	3T	101	CDL	OA5-CA3-CA4-CA6
74	5L	702	CDL	OA5-CA3-CA4-CA6
76	1M	901	3PE	O11-C1-C2-C3
76	1O	401	3PE	O11-C1-C2-C3
76	5L	704	3PE	O11-C1-C2-C3
74	5h	202	CDL	C34-C35-C36-C37
92	8G	102	PEK	C21-C22-C23-C24
74	8D	201	CDL	C59-C60-C61-C62
74	5q	203	CDL	C52-C51-CB5-OB6
86	8L	101	PGV	C3-C4-C5-C6
76	1M	906	3PE	C21-C22-C23-C24
74	1N	401	CDL	O1-C1-CB2-OB2
74	5d	203	CDL	C71-C72-C73-C74
76	5M	501	3PE	C26-C27-C28-C29
76	5M	506	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
76	5M	506	3PE	C27-C28-C29-C2A
74	4B	302	CDL	C1-CA2-OA2-PA1
74	5d	203	CDL	C1-CA2-OA2-PA1
74	8B	303	CDL	C1-CA2-OA2-PA1
76	1M	901	3PE	C2-C1-O11-P
86	4C	305	PGV	C02-C03-O11-P
86	4K	101	PGV	C02-C03-O11-P
86	8C	305	PGV	C02-C03-O11-P
86	8K	101	PGV	C02-C03-O11-P
86	8K	101	PGV	C05-C04-O12-P
81	5T	101	EHZ	S1-C10-C11-N1
74	4D	201	CDL	C59-C60-C61-C62
74	4D	201	CDL	C62-C63-C64-C65
86	8A	601	PGV	C21-C22-C23-C24
86	4C	302	PGV	C1-C2-C3-C4
69	5M	505	PC1	C2A-C2B-C2C-C2D
86	4L	101	PGV	C3-C4-C5-C6
84	3C	501	HEM	C3D-CAD-CBD-CGD
84	3P	501	HEM	C3D-CAD-CBD-CGD
76	1d	201	3PE	C28-C29-C2A-C2B
76	3C	504	3PE	C29-C2A-C2B-C2C
69	1h	203	PC1	C1-C2-C3-O31
74	1N	401	CDL	CA3-CA4-CA6-OA8
74	4B	302	CDL	CB3-CB4-CB6-OB8
76	1M	902	3PE	C1-C2-C3-O31
76	1M	903	3PE	C1-C2-C3-O31
76	3C	505	3PE	C1-C2-C3-O31
76	5M	502	3PE	C1-C2-C3-O31
86	8J	101	PGV	O03-C01-C02-C03
74	1X	201	CDL	C58-C59-C60-C61
69	1H	402	PC1	C39-C3A-C3B-C3C
87	4A	604	HEA	C2D-C3D-CAD-CBD
69	1M	905	PC1	C23-C24-C25-C26
86	8C	303	PGV	C5-C6-C7-C8
69	5H	402	PC1	C39-C3A-C3B-C3C
74	1X	201	CDL	C23-C24-C25-C26
69	1M	904	PC1	C11-O13-P-O11
69	5M	505	PC1	C11-O13-P-O11
74	3A	501	CDL	CB2-OB2-PB2-OB5
86	4C	303	PGV	C03-O11-P-O12
90	4A	609	PSC	C9-C10-C11-C12
90	4A	609	PSC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
90	8I	101	PSC	C9-C10-C11-C12
90	8I	101	PSC	C10-C11-C12-C13
92	4G	102	PEK	C5-C6-C7-C8
92	4G	102	PEK	C9-C10-C11-C12
92	8G	102	PEK	C5-C6-C7-C8
92	8G	102	PEK	C9-C10-C11-C12
74	5X	201	CDL	C32-C31-CA7-OA8
74	1d	203	CDL	OA5-CA3-CA4-OA6
76	3A	502	3PE	O11-C1-C2-O21
86	8C	303	PGV	O01-C02-C03-O11
74	1L	702	CDL	CA7-C31-C32-C33
74	1q	202	CDL	C52-C51-CB5-OB6
74	3C	503	CDL	C12-C11-CA5-OA6
74	5N	401	CDL	C32-C31-CA7-OA8
76	1b	201	3PE	O21-C21-C22-C23
76	3G	101	3PE	O21-C21-C22-C23
76	5A	201	3PE	O21-C21-C22-C23
74	1L	702	CDL	O1-C1-CB2-OB2
76	1Y	801	3PE	C32-C33-C34-C35
86	8B	302	PGV	C20-C21-C22-C23
74	3N	502	CDL	OA6-CA4-CA6-OA8
74	3P	504	CDL	OB6-CB4-CB6-OB8
76	1M	901	3PE	O21-C2-C3-O31
76	1Y	803	3PE	O21-C2-C3-O31
76	5L	704	3PE	O21-C2-C3-O31
76	5M	502	3PE	O21-C2-C3-O31
76	5Y	803	3PE	O21-C2-C3-O31
86	4C	304	PGV	O03-C01-C02-O01
86	8C	304	PGV	O03-C01-C02-O01
92	4G	102	PEK	O03-C21-C22-C23
74	1L	702	CDL	C58-C59-C60-C61
86	4A	602	PGV	C14-C15-C16-C17
74	4D	201	CDL	CA2-C1-CB2-OB2
74	8C	306	CDL	C59-C60-C61-C62
69	5B	202	PC1	C36-C37-C38-C39
69	1I	201	PC1	C2-C1-O11-P
69	5M	505	PC1	C2-C1-O11-P
74	1h	202	CDL	CB4-CB3-OB5-PB2
74	3T	101	CDL	CA4-CA3-OA5-PA1
74	5L	702	CDL	CA4-CA3-OA5-PA1
76	5Y	803	3PE	C2-C1-O11-P
86	4K	101	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
86	8C	304	PGV	C02-C03-O11-P
69	5I	204	PC1	C37-C38-C39-C3A
69	5h	203	PC1	C2A-C2B-C2C-C2D
69	5h	203	PC1	C2B-C2C-C2D-C2E
74	4C	306	CDL	C59-C60-C61-C62
92	8G	102	PEK	O03-C21-C22-C23
74	3P	504	CDL	C13-C14-C15-C16
74	5L	702	CDL	CA7-C31-C32-C33
92	4G	102	PEK	C21-C22-C23-C24
76	1P	502	3PE	C37-C38-C39-C3A
77	1O	402	GTP	PB-O3A-PA-O5'
86	4C	304	PGV	C5-C6-C7-C8
69	5I	201	PC1	O11-C1-C2-C3
74	8B	303	CDL	OA5-CA3-CA4-CA6
76	3A	503	3PE	O11-C1-C2-C3
76	5M	504	3PE	O11-C1-C2-C3
76	5Y	801	3PE	O11-C1-C2-C3
69	1B	203	PC1	C35-C36-C37-C38
74	8C	306	CDL	C52-C53-C54-C55
69	5A	202	PC1	C22-C23-C24-C25
81	5T	101	EHZ	C21-C22-C23-C24
86	4L	101	PGV	C21-C22-C23-C24
86	8C	302	PGV	C6-C7-C8-C9
74	5X	201	CDL	C58-C59-C60-C61
74	1h	202	CDL	C76-C77-C78-C79
69	1A	201	PC1	C1-C2-C3-O31
69	1B	203	PC1	C1-C2-C3-O31
69	5B	203	PC1	C1-C2-C3-O31
69	5I	201	PC1	C2-C1-O11-P
69	5I	201	PC1	C1-C2-C3-O31
74	1L	702	CDL	CA4-CA3-OA5-PA1
74	1N	401	CDL	C1-CB2-OB2-PB2
74	3P	504	CDL	CB3-CB4-CB6-OB8
74	5N	401	CDL	CA3-CA4-CA6-OA8
74	5N	401	CDL	C1-CB2-OB2-PB2
74	5d	203	CDL	C1-CB2-OB2-PB2
74	5h	202	CDL	CB4-CB3-OB5-PB2
76	3N	501	3PE	C1-C2-C3-O31
76	3N	503	3PE	C1-C2-C3-O31
86	4G	101	PGV	C02-C03-O11-P
69	1M	905	PC1	O11-C1-C2-O21
74	1X	201	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
74	3P	504	CDL	OB5-CB3-CB4-OB6
74	8B	303	CDL	OA5-CA3-CA4-OA6
76	1Y	802	3PE	O11-C1-C2-O21
76	5L	704	3PE	O11-C1-C2-O21
76	5Y	802	3PE	O11-C1-C2-O21
76	5Y	806	3PE	O11-C1-C2-O21
86	4C	303	PGV	O01-C02-C03-O11
69	5B	203	PC1	C35-C36-C37-C38
74	4C	306	CDL	C16-C17-C18-C19
74	1N	401	CDL	CA2-C1-CB2-OB2
81	1n	201	EHZ	O1-C7-C8-C9
74	1L	702	CDL	C57-C58-C59-C60
69	5B	203	PC1	O21-C2-C3-O31
74	4B	302	CDL	OB6-CB4-CB6-OB8
76	1M	902	3PE	O21-C2-C3-O31
76	1M	903	3PE	O21-C2-C3-O31
76	5M	501	3PE	O21-C2-C3-O31
76	5Y	801	3PE	O21-C2-C3-O31
74	4D	201	CDL	C71-C72-C73-C74
74	5X	201	CDL	C23-C24-C25-C26
74	4C	306	CDL	C52-C53-C54-C55
86	4C	304	PGV	C24-C25-C26-C27
90	8I	101	PSC	C19-C20-C21-C22
76	5M	502	3PE	C24-C25-C26-C27
74	5L	702	CDL	C57-C58-C59-C60
74	8D	201	CDL	C71-C72-C73-C74
76	1M	903	3PE	C24-C25-C26-C27
86	8C	304	PGV	C24-C25-C26-C27
69	1I	204	PC1	C37-C38-C39-C3A
74	8C	306	CDL	C16-C17-C18-C19
86	8C	304	PGV	C5-C6-C7-C8
82	1h	201	AME	C-CA-N-CT1
74	8B	303	CDL	C38-C39-C40-C41
69	3X	101	PC1	C1-O11-P-O13
74	1N	401	CDL	CB3-OB5-PB2-OB2
74	1X	201	CDL	CB3-OB5-PB2-OB2
74	1h	202	CDL	CB3-OB5-PB2-OB2
74	4D	201	CDL	CB3-OB5-PB2-OB2
74	5L	702	CDL	CA2-OA2-PA1-OA5
74	5N	401	CDL	CB3-OB5-PB2-OB2
74	5X	201	CDL	CA2-OA2-PA1-OA5
74	5X	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
74	5h	202	CDL	CB3-OB5-PB2-OB2
74	8B	303	CDL	CA3-OA5-PA1-OA2
74	8D	201	CDL	CB3-OB5-PB2-OB2
76	1Y	805	3PE	C11-O13-P-O11
76	5M	506	3PE	C1-O11-P-O13
76	5Y	805	3PE	C11-O13-P-O11
86	4A	602	PGV	C03-O11-P-O12
86	4A	602	PGV	C04-O12-P-O11
86	4C	305	PGV	C03-O11-P-O12
86	4K	101	PGV	C03-O11-P-O12
86	8A	602	PGV	C04-O12-P-O11
86	8C	304	PGV	C03-O11-P-O12
86	8C	305	PGV	C03-O11-P-O12
86	4C	302	PGV	C3-C4-C5-C6
86	8K	101	PGV	C2-C3-C4-C5
69	1M	905	PC1	C2-C1-O11-P
74	1d	203	CDL	C1-CB2-OB2-PB2
86	4A	601	PGV	C02-C03-O11-P
86	8A	601	PGV	C02-C03-O11-P
86	8G	101	PGV	C02-C03-O11-P
74	4C	306	CDL	C51-C52-C53-C54
69	1M	905	PC1	C11-O13-P-O12
74	1h	202	CDL	CA2-OA2-PA1-OA4
74	1h	202	CDL	CB2-OB2-PB2-OB4
74	3C	503	CDL	CB2-OB2-PB2-OB4
74	3G	102	CDL	CB2-OB2-PB2-OB4
74	3N	502	CDL	CB3-OB5-PB2-OB3
74	4B	302	CDL	CB3-OB5-PB2-OB4
74	5h	202	CDL	CA2-OA2-PA1-OA4
74	8B	303	CDL	CB3-OB5-PB2-OB4
76	1K	101	3PE	C1-O11-P-O12
76	5K	101	3PE	C1-O11-P-O12
76	5M	502	3PE	C1-O11-P-O14
86	4C	304	PGV	C03-O11-P-O14
86	8C	303	PGV	C03-O11-P-O14
86	8C	304	PGV	C03-O11-P-O14
86	8C	305	PGV	C03-O11-P-O14
90	4A	609	PSC	C03-O11-P-O13
90	8I	101	PSC	C03-O11-P-O13
69	1I	201	PC1	O11-C1-C2-C3
69	5H	402	PC1	O11-C1-C2-C3
69	5M	505	PC1	O11-C1-C2-C3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
74	4B	302	CDL	OA5-CA3-CA4-CA6
74	8C	306	CDL	OB5-CB3-CB4-CB6
86	4A	601	PGV	C01-C02-C03-O11
86	8A	601	PGV	C01-C02-C03-O11
74	1X	201	CDL	C35-C36-C37-C38
87	4A	604	HEA	O11-C11-C12-C13
86	8K	101	PGV	C22-C23-C24-C25
74	4C	306	CDL	C11-C12-C13-C14
69	1A	202	PC1	C12-C11-O13-P
69	1A	203	PC1	C12-C11-O13-P
69	1B	203	PC1	C12-C11-O13-P
69	5A	203	PC1	C12-C11-O13-P
69	5B	203	PC1	C12-C11-O13-P
69	5P	401	PC1	C12-C11-O13-P
76	1K	101	3PE	C12-C11-O13-P
76	1L	701	3PE	C12-C11-O13-P
76	1M	902	3PE	C12-C11-O13-P
76	1O	401	3PE	C12-C11-O13-P
76	1Y	802	3PE	C12-C11-O13-P
76	1Y	804	3PE	C12-C11-O13-P
76	1Y	805	3PE	C12-C11-O13-P
76	1Y	806	3PE	C12-C11-O13-P
76	1j	101	3PE	C12-C11-O13-P
76	3C	504	3PE	C12-C11-O13-P
76	3C	505	3PE	C12-C11-O13-P
76	3P	503	3PE	C12-C11-O13-P
76	5K	101	3PE	C12-C11-O13-P
76	5L	701	3PE	C12-C11-O13-P
76	5M	504	3PE	C12-C11-O13-P
76	5Y	802	3PE	C12-C11-O13-P
76	5Y	804	3PE	C12-C11-O13-P
76	5j	101	3PE	C12-C11-O13-P
92	4C	308	PEK	C05-C04-O12-P
92	4G	102	PEK	C05-C04-O12-P
92	8C	308	PEK	C05-C04-O12-P
92	8G	102	PEK	C05-C04-O12-P
74	4B	302	CDL	C38-C39-C40-C41
74	3G	102	CDL	C52-C53-C54-C55
69	5M	505	PC1	O11-C1-C2-O21
74	4B	302	CDL	OA5-CA3-CA4-OA6
74	5d	203	CDL	OA5-CA3-CA4-OA6
76	1M	901	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
81	1T	101	EHZ	S1-C10-C11-N1
86	4A	601	PGV	O01-C02-C03-O11
86	8A	601	PGV	O01-C02-C03-O11
85	3D	501	HEC	C3D-CAD-CBD-CGD
69	1L	704	PC1	O31-C31-C32-C33
86	4C	302	PGV	C6-C7-C8-C9
81	1T	101	EHZ	C10-C11-N1-C12
81	1n	201	EHZ	C10-C11-N1-C12
81	5T	101	EHZ	C10-C11-N1-C12
74	1X	201	CDL	C55-C56-C57-C58
74	5h	202	CDL	C76-C77-C78-C79
69	1M	905	PC1	C21-C22-C23-C24
69	1A	201	PC1	O13-C11-C12-N
69	1A	203	PC1	O13-C11-C12-N
69	1B	203	PC1	O13-C11-C12-N
69	1L	704	PC1	O13-C11-C12-N
69	1h	203	PC1	O13-C11-C12-N
69	5A	202	PC1	O13-C11-C12-N
69	5B	203	PC1	O13-C11-C12-N
69	5L	705	PC1	O13-C11-C12-N
69	5P	401	PC1	O13-C11-C12-N
69	5h	203	PC1	O13-C11-C12-N
69	1B	203	PC1	O21-C2-C3-O31
76	1L	703	3PE	O21-C2-C3-O31
76	3N	501	3PE	O21-C2-C3-O31
76	3N	503	3PE	O21-C2-C3-O31
76	5L	703	3PE	O21-C2-C3-O31
86	4J	101	PGV	O03-C01-C02-O01
86	8J	101	PGV	O03-C01-C02-O01
92	4C	308	PEK	O03-C01-C02-O01
81	1T	101	EHZ	C21-C22-C23-C24
74	8C	306	CDL	C51-C52-C53-C54
69	5L	705	PC1	O31-C31-C32-C33
76	1K	101	3PE	O21-C21-C22-C23
76	1Y	803	3PE	C2-C1-O11-P
86	4C	304	PGV	C02-C03-O11-P
69	5B	202	PC1	C3D-C3E-C3F-C3G
74	5X	201	CDL	C35-C36-C37-C38
76	5K	101	3PE	O21-C21-C22-C23
76	1M	901	3PE	C33-C34-C35-C36
74	8C	306	CDL	C11-C12-C13-C14
76	1M	906	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
76	5A	201	3PE	C2A-C2B-C2C-C2D
69	5L	705	PC1	C23-C24-C25-C26
86	8C	303	PGV	C9-C10-C11-C12
76	5Y	802	3PE	C27-C28-C29-C2A
76	1Y	806	3PE	O21-C21-C22-C23
74	1H	401	CDL	CA3-CA4-OA6-CA5
74	5H	401	CDL	CA3-CA4-OA6-CA5
74	5X	201	CDL	CB2-C1-CA2-OA2
87	8A	603	HEA	C11-C12-C13-C14
69	1M	905	PC1	C2D-C2E-C2F-C2G
74	8D	201	CDL	C62-C63-C64-C65
76	5Y	806	3PE	O21-C21-C22-C23
69	1L	704	PC1	C3A-C3B-C3C-C3D
86	8C	303	PGV	C26-C27-C28-C29
76	1O	401	3PE	O11-C1-C2-O21
76	5M	504	3PE	O11-C1-C2-O21
86	8L	101	PGV	C9-C10-C11-C12
76	3P	503	3PE	O21-C2-C3-O31
69	5M	505	PC1	C2D-C2E-C2F-C2G
69	1A	202	PC1	C1-O11-P-O13
69	1B	202	PC1	C11-O13-P-O11
69	1M	904	PC1	C1-O11-P-O13
69	1d	202	PC1	C1-O11-P-O13
69	1h	203	PC1	C11-O13-P-O11
69	1q	201	PC1	C1-O11-P-O13
69	3R	302	PC1	C1-O11-P-O13
69	5A	203	PC1	C1-O11-P-O13
69	5B	202	PC1	C11-O13-P-O11
69	5M	503	PC1	C1-O11-P-O13
69	5d	202	PC1	C1-O11-P-O13
69	5h	203	PC1	C11-O13-P-O11
69	5q	201	PC1	C1-O11-P-O13
74	1L	702	CDL	CA2-OA2-PA1-OA5
74	1N	401	CDL	CA3-OA5-PA1-OA2
74	1d	203	CDL	CB2-OB2-PB2-OB5
74	1q	202	CDL	CA3-OA5-PA1-OA2
74	1q	202	CDL	CB2-OB2-PB2-OB5
74	3G	102	CDL	CA2-OA2-PA1-OA5
74	3P	504	CDL	CA3-OA5-PA1-OA2
74	3P	504	CDL	CB3-OB5-PB2-OB2
74	3T	101	CDL	CA2-OA2-PA1-OA5
74	4B	302	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
74	4C	306	CDL	CA3-OA5-PA1-OA2
74	4C	306	CDL	CB2-OB2-PB2-OB5
74	4C	306	CDL	CB3-OB5-PB2-OB2
74	4D	201	CDL	CA3-OA5-PA1-OA2
74	4D	201	CDL	CB2-OB2-PB2-OB5
74	5N	401	CDL	CA3-OA5-PA1-OA2
74	5d	203	CDL	CB2-OB2-PB2-OB5
74	5q	203	CDL	CA3-OA5-PA1-OA2
74	5q	203	CDL	CB2-OB2-PB2-OB5
74	8C	306	CDL	CA3-OA5-PA1-OA2
74	8C	306	CDL	CB2-OB2-PB2-OB5
74	8C	306	CDL	CB3-OB5-PB2-OB2
74	8D	201	CDL	CA3-OA5-PA1-OA2
74	8D	201	CDL	CB2-OB2-PB2-OB5
76	1L	701	3PE	C11-O13-P-O11
76	1M	902	3PE	C11-O13-P-O11
76	1M	903	3PE	C11-O13-P-O11
76	1M	906	3PE	C1-O11-P-O13
76	1M	906	3PE	C11-O13-P-O11
76	1O	401	3PE	C1-O11-P-O13
76	1O	401	3PE	C11-O13-P-O11
76	1Y	801	3PE	C1-O11-P-O13
76	1Y	801	3PE	C11-O13-P-O11
76	1Y	804	3PE	C1-O11-P-O13
76	1Y	806	3PE	C11-O13-P-O11
76	1b	201	3PE	C11-O13-P-O11
76	1d	201	3PE	C11-O13-P-O11
76	1j	101	3PE	C1-O11-P-O13
76	1j	101	3PE	C11-O13-P-O11
76	3N	501	3PE	C1-O11-P-O13
76	3N	501	3PE	C11-O13-P-O11
76	3N	503	3PE	C11-O13-P-O11
76	3Y	101	3PE	C1-O11-P-O13
76	5L	701	3PE	C11-O13-P-O11
76	5M	501	3PE	C11-O13-P-O11
76	5M	502	3PE	C11-O13-P-O11
76	5M	504	3PE	C1-O11-P-O13
76	5M	504	3PE	C11-O13-P-O11
76	5M	506	3PE	C11-O13-P-O11
76	5Y	801	3PE	C11-O13-P-O11
76	5Y	804	3PE	C1-O11-P-O13
76	5Y	806	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
76	5d	201	3PE	C11-O13-P-O11
76	5j	101	3PE	C1-O11-P-O13
76	5j	101	3PE	C11-O13-P-O11
86	4A	601	PGV	C04-O12-P-O11
86	4A	603	PGV	C04-O12-P-O11
86	4C	304	PGV	C03-O11-P-O12
86	4G	101	PGV	C04-O12-P-O11
86	4K	101	PGV	C04-O12-P-O11
86	4L	101	PGV	C03-O11-P-O12
86	4L	101	PGV	C04-O12-P-O11
86	8A	601	PGV	C04-O12-P-O11
86	8A	602	PGV	C03-O11-P-O12
86	8B	301	PGV	C04-O12-P-O11
86	8G	101	PGV	C04-O12-P-O11
86	8K	101	PGV	C04-O12-P-O11
86	8L	101	PGV	C03-O11-P-O12
86	8L	101	PGV	C04-O12-P-O11
69	1M	905	PC1	C1-C2-C3-O31
74	1N	401	CDL	CB3-CB4-CB6-OB8
76	1M	901	3PE	C1-C2-C3-O31
76	5j	101	3PE	C1-C2-C3-O31
86	8C	302	PGV	C1-C2-C3-C4
86	4C	303	PGV	C9-C10-C11-C12
86	4L	101	PGV	C9-C10-C11-C12
86	8C	305	PGV	C9-C10-C11-C12
90	8I	101	PSC	C12-C13-C14-C15
86	4A	601	PGV	C29-C30-C31-C32
76	5M	504	3PE	C24-C25-C26-C27
92	4C	308	PEK	C02-C03-O11-P
74	1X	201	CDL	C31-C32-C33-C34
76	5d	201	3PE	C28-C29-C2A-C2B
86	4A	603	PGV	C1-C2-C3-C4
86	4C	302	PGV	C11-C12-C13-C14
86	4M	101	PGV	C11-C12-C13-C14
86	8M	101	PGV	C9-C10-C11-C12
90	4A	609	PSC	C12-C13-C14-C15
74	1h	202	CDL	CB7-C71-C72-C73
74	3C	503	CDL	C11-C12-C13-C14
84	3P	501	HEM	CAA-CBA-CGA-O2A
69	5I	204	PC1	C24-C25-C26-C27
76	1M	901	3PE	C23-C24-C25-C26
76	1Y	802	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
86	4B	301	PGV	C20-C21-C22-C23
86	8K	101	PGV	C9-C10-C11-C12
84	3C	501	HEM	CAA-CBA-CGA-O2A
76	1Y	801	3PE	O11-C1-C2-C3
76	3C	505	3PE	O11-C1-C2-C3
76	3Y	101	3PE	O11-C1-C2-C3
74	5X	201	CDL	OB5-CB3-CB4-OB6
76	1Y	806	3PE	O11-C1-C2-O21
86	4K	101	PGV	C19-C20-C21-C22
69	1A	201	PC1	C23-C24-C25-C26
69	5M	503	PC1	C22-C23-C24-C25
74	1X	201	CDL	C34-C35-C36-C37
86	4M	101	PGV	C3-C4-C5-C6
76	5M	501	3PE	C25-C26-C27-C28
86	8A	602	PGV	C11-C12-C13-C14
74	3A	501	CDL	O1-C1-CA2-OA2
69	5L	705	PC1	C3A-C3B-C3C-C3D
69	3X	101	PC1	O21-C21-C22-C23
76	1L	703	3PE	C29-C2A-C2B-C2C
69	1B	202	PC1	C36-C37-C38-C39
76	1M	902	3PE	C23-C24-C25-C26
69	1h	203	PC1	O21-C2-C3-O31
74	3G	102	CDL	OB6-CB4-CB6-OB8
74	5q	203	CDL	OB6-CB4-CB6-OB8
86	4B	301	PGV	C27-C28-C29-C30
86	8M	101	PGV	C3-C4-C5-C6
69	1A	203	PC1	C24-C25-C26-C27
74	4B	302	CDL	C13-C14-C15-C16
84	3C	502	HEM	CAA-CBA-CGA-O1A
84	3P	501	HEM	CAD-CBD-CGD-O1D
84	3P	502	HEM	CAD-CBD-CGD-O1D
86	4K	101	PGV	C9-C10-C11-C12
86	8M	101	PGV	C11-C12-C13-C14
69	5M	505	PC1	C28-C29-C2A-C2B
86	8A	601	PGV	C22-C23-C24-C25
86	8B	302	PGV	C27-C28-C29-C30
84	3C	501	HEM	CAA-CBA-CGA-O1A
90	4A	609	PSC	C19-C20-C21-C22
74	5X	201	CDL	C36-C37-C38-C39
76	1Y	806	3PE	C23-C24-C25-C26
81	5n	201	EHZ	C10-C11-N1-C12
69	1H	402	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
76	5K	101	3PE	C26-C27-C28-C29
69	5h	203	PC1	C1-C2-C3-O31
76	5L	704	3PE	C1-C2-C3-O31
87	8A	603	HEA	CAD-CBD-CGD-O1D
76	5Y	804	3PE	C33-C34-C35-C36
87	8A	603	HEA	C4D-C3D-CAD-CBD
87	4A	605	HEA	CAD-CBD-CGD-O1D
87	8A	604	HEA	CAD-CBD-CGD-O1D
87	8A	603	HEA	C2D-C3D-CAD-CBD
84	3P	502	HEM	CAA-CBA-CGA-O1A
76	1O	401	3PE	C1-C2-O21-C21
76	1Y	804	3PE	C1-C2-O21-C21
76	3C	504	3PE	C1-C2-O21-C21
76	5M	504	3PE	C1-C2-O21-C21
76	5Y	805	3PE	C3-C2-O21-C21
86	4C	304	PGV	C01-C02-O01-C1
76	1K	101	3PE	C26-C27-C28-C29
86	4C	305	PGV	C9-C10-C11-C12
86	4M	101	PGV	C9-C10-C11-C12
86	8C	304	PGV	C9-C10-C11-C12
76	5A	201	3PE	C11-O13-P-O11
76	1O	401	3PE	C24-C25-C26-C27
76	3D	502	3PE	C24-C25-C26-C27
76	1d	201	3PE	C2-C1-O11-P
74	5d	203	CDL	OB5-CB3-CB4-OB6
74	5h	202	CDL	OB5-CB3-CB4-OB6
84	3C	502	HEM	CAA-CBA-CGA-O2A
69	1H	402	PC1	O11-C1-C2-C3
74	4C	306	CDL	OB5-CB3-CB4-CB6
86	8M	101	PGV	C01-C02-C03-O11
86	4C	301	PGV	C11-C12-C13-C14
74	5X	201	CDL	C55-C56-C57-C58
84	3P	502	HEM	CAD-CBD-CGD-O2D
74	8B	303	CDL	C13-C14-C15-C16
86	4G	101	PGV	C1-C2-C3-C4
86	8B	301	PGV	C1-C2-C3-C4
81	1T	101	EHZ	C11-C10-S1-C9
81	5T	101	EHZ	C11-C10-S1-C9
87	4A	605	HEA	CAD-CBD-CGD-O2D
69	5I	201	PC1	O21-C2-C3-O31
74	1N	401	CDL	OB6-CB4-CB6-OB8
76	3Y	101	3PE	O21-C2-C3-O31

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
92	8C	308	PEK	O03-C01-C02-O01
76	1M	903	3PE	C2A-C2B-C2C-C2D
84	3P	502	HEM	CAA-CBA-CGA-O2A
74	3C	503	CDL	C12-C13-C14-C15
76	5L	703	3PE	C29-C2A-C2B-C2C
92	4G	102	PEK	O04-C21-C22-C23
69	1I	204	PC1	C24-C25-C26-C27
84	3P	501	HEM	CAA-CBA-CGA-O1A
86	8J	101	PGV	C9-C10-C11-C12
87	8A	603	HEA	CAD-CBD-CGD-O2D
87	8A	604	HEA	CAD-CBD-CGD-O2D
74	3C	503	CDL	C72-C71-CB7-OB9
74	5q	203	CDL	CA5-C11-C12-C13
74	1N	401	CDL	C32-C31-CA7-OA9
86	4C	304	PGV	C9-C10-C11-C12
86	8L	101	PGV	C11-C12-C13-C14
69	1I	201	PC1	C1-C2-C3-O31
76	3Q	502	3PE	C34-C35-C36-C37
87	4A	605	HEA	C26-C15-C16-C17
76	3C	504	3PE	C2C-C2D-C2E-C2F
84	3P	501	HEM	CAD-CBD-CGD-O2D
69	1B	202	PC1	C3D-C3E-C3F-C3G
76	5L	704	3PE	C23-C24-C25-C26
76	5P	403	3PE	C36-C37-C38-C39
74	8C	306	CDL	C71-C72-C73-C74
86	4A	601	PGV	C11-C12-C13-C14
86	4C	307	PGV	C11-C12-C13-C14
86	4J	101	PGV	C9-C10-C11-C12
86	8A	601	PGV	C9-C10-C11-C12
86	8C	302	PGV	C9-C10-C11-C12
74	1d	203	CDL	OB5-CB3-CB4-OB6
74	1h	202	CDL	OB5-CB3-CB4-OB6
76	1Y	805	3PE	O11-C1-C2-O21
76	3A	503	3PE	O11-C1-C2-O21
90	8I	101	PSC	O01-C02-C03-O11
74	1d	203	CDL	C72-C73-C74-C75
76	5Y	803	3PE	O32-C31-C32-C33
69	1B	202	PC1	C3C-C3D-C3E-C3F
76	5M	506	3PE	C23-C24-C25-C26
81	5T	101	EHZ	C1-C21-C22-C23
74	1X	201	CDL	OB5-CB3-CB4-CB6
74	1h	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
74	5h	202	CDL	OB5-CB3-CB4-CB6
76	1Y	802	3PE	O11-C1-C2-C3
76	1Y	806	3PE	O11-C1-C2-C3
76	3A	502	3PE	O11-C1-C2-C3
76	5Y	802	3PE	O11-C1-C2-C3
76	5Y	806	3PE	O11-C1-C2-C3
86	8C	303	PGV	C01-C02-C03-O11
74	4C	306	CDL	C72-C73-C74-C75
76	5L	701	3PE	C28-C29-C2A-C2B
86	8A	601	PGV	C29-C30-C31-C32
87	4A	604	HEA	CAD-CBD-CGD-O2D
86	4A	602	PGV	C11-C12-C13-C14
76	1Y	803	3PE	O32-C31-C32-C33
76	5d	201	3PE	C2-C1-O11-P
86	8A	601	PGV	C11-C10-C9-C8
74	4D	201	CDL	OB6-CB4-CB6-OB8
76	3A	502	3PE	O21-C2-C3-O31
76	5Y	805	3PE	O21-C2-C3-O31
74	5d	203	CDL	C72-C73-C74-C75
92	8G	102	PEK	O04-C21-C22-C23
76	5K	101	3PE	C24-C25-C26-C27
76	1Y	804	3PE	C33-C34-C35-C36
86	4A	601	PGV	C24-C25-C26-C27
86	8A	602	PGV	C6-C7-C8-C9
81	1T	101	EHZ	C1-C21-C22-C23
81	5T	101	EHZ	C1-C2-C3-C4
87	4A	604	HEA	CAD-CBD-CGD-O1D
69	1M	905	PC1	C1-O11-P-O13
74	3G	102	CDL	CB3-OB5-PB2-OB2
86	8C	305	PGV	C7-C8-C9-C10
76	1b	201	3PE	C2B-C2C-C2D-C2E
74	5X	201	CDL	C31-C32-C33-C34
74	5h	202	CDL	C74-C75-C76-C77
76	5M	502	3PE	C2A-C2B-C2C-C2D
74	1L	702	CDL	C11-C12-C13-C14
86	8A	601	PGV	C11-C12-C13-C14
86	8C	301	PGV	C11-C12-C13-C14
86	8C	307	PGV	C11-C12-C13-C14
69	1M	904	PC1	C22-C23-C24-C25
76	1Y	801	3PE	C1-C2-O21-C21
76	1Y	805	3PE	C3-C2-O21-C21
76	5Y	801	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
76	5Y	804	3PE	C1-C2-O21-C21
86	8C	304	PGV	C01-C02-O01-C1
69	5I	201	PC1	C36-C37-C38-C39
76	1M	903	3PE	C29-C2A-C2B-C2C
76	5M	501	3PE	C22-C23-C24-C25
76	3N	501	3PE	O22-C21-C22-C23
76	1M	902	3PE	C25-C26-C27-C28
76	5M	501	3PE	C29-C2A-C2B-C2C
74	4C	306	CDL	C71-C72-C73-C74
87	8A	603	HEA	CAA-CBA-CGA-O2A
86	4C	302	PGV	C20-C21-C22-C23
86	4A	601	PGV	O03-C19-C20-C21
74	5L	702	CDL	C11-C12-C13-C14
86	4C	302	PGV	C9-C10-C11-C12
86	4G	101	PGV	C9-C10-C11-C12
86	4K	101	PGV	C11-C12-C13-C14
86	4L	101	PGV	C11-C12-C13-C14
86	8G	101	PGV	C9-C10-C11-C12
86	8K	101	PGV	C11-C12-C13-C14
87	8A	603	HEA	CAA-CBA-CGA-O1A
76	1b	201	3PE	C27-C28-C29-C2A
74	5X	201	CDL	C32-C31-CA7-OA9
76	5K	101	3PE	C34-C35-C36-C37
86	8C	303	PGV	C2-C3-C4-C5
69	1B	203	PC1	O11-C1-C2-O21
74	3T	101	CDL	OB5-CB3-CB4-OB6
76	3C	504	3PE	O11-C1-C2-O21
74	3C	503	CDL	C12-C11-CA5-OA7
76	5M	502	3PE	C29-C2A-C2B-C2C
69	1L	704	PC1	C28-C29-C2A-C2B
74	1X	201	CDL	CA7-C31-C32-C33
76	5Y	806	3PE	C23-C24-C25-C26
86	8G	101	PGV	C27-C28-C29-C30
86	8J	101	PGV	C21-C22-C23-C24
87	8A	604	HEA	C26-C15-C16-C17
86	8C	302	PGV	C3-C4-C5-C6
69	1B	203	PC1	O11-C1-C2-C3
69	5B	203	PC1	O11-C1-C2-C3
74	5X	201	CDL	OB5-CB3-CB4-CB6
86	4C	303	PGV	C01-C02-C03-O11
69	1d	202	PC1	O21-C21-C22-C23
74	5d	203	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
74	1q	202	CDL	OB6-CB4-CB6-OB8
76	1Y	805	3PE	O21-C2-C3-O31
69	1h	203	PC1	C22-C23-C24-C25
76	5Y	802	3PE	C2D-C2E-C2F-C2G
92	8G	102	PEK	C22-C23-C24-C25
69	5d	202	PC1	O21-C21-C22-C23
74	1d	203	CDL	C32-C31-CA7-OA8
74	3P	504	CDL	C32-C31-CA7-OA8
69	1A	201	PC1	C22-C23-C24-C25
87	8A	604	HEA	CAA-CBA-CGA-O1A
69	1A	201	PC1	O31-C31-C32-C33
76	1Y	804	3PE	C21-C22-C23-C24
92	8C	308	PEK	C02-C03-O11-P
86	4C	303	PGV	C2-C3-C4-C5
86	4A	601	PGV	C9-C10-C11-C12
69	3R	302	PC1	C27-C28-C29-C2A
74	5N	401	CDL	C32-C31-CA7-OA9
77	5O	401	GTP	O4'-C4'-C5'-O5'
79	1P	501	NDP	O4B-C4B-C5B-O5B
79	5P	402	NDP	O4B-C4B-C5B-O5B
85	3D	501	HEC	CAA-CBA-CGA-O2A
74	5q	203	CDL	C52-C51-CB5-OB7
76	1M	906	3PE	C25-C26-C27-C28
69	5I	204	PC1	C25-C26-C27-C28
76	1Y	802	3PE	C34-C35-C36-C37
87	4A	604	HEA	CAA-CBA-CGA-O1A
76	1Y	805	3PE	O21-C21-C22-C23
76	5M	501	3PE	C23-C24-C25-C26
86	8K	101	PGV	C3-C4-C5-C6
74	1q	202	CDL	CA5-C11-C12-C13
76	5Y	801	3PE	O11-C1-C2-O21
69	5h	203	PC1	C22-C23-C24-C25
86	4G	101	PGV	C7-C8-C9-C10
74	1X	201	CDL	CB2-C1-CA2-OA2
82	5h	201	AME	C-CA-N-CT1
74	4D	201	CDL	C37-C38-C39-C40
86	4M	101	PGV	C15-C16-C17-C18
76	5L	704	3PE	C33-C34-C35-C36
74	1d	203	CDL	C38-C39-C40-C41
74	8C	306	CDL	C72-C73-C74-C75
76	5Y	804	3PE	C21-C22-C23-C24
69	1M	905	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	5d	202	PC1	O22-C21-C22-C23
74	3N	502	CDL	CA4-CA6-OA8-CA7
86	4C	305	PGV	C3-C4-C5-C6
69	1A	201	PC1	O32-C31-C32-C33
69	1A	202	PC1	C1-O11-P-O14
69	1B	202	PC1	C11-O13-P-O14
69	1M	904	PC1	C11-O13-P-O14
69	1d	202	PC1	C1-O11-P-O14
69	5A	203	PC1	C1-O11-P-O14
69	5B	202	PC1	C11-O13-P-O14
69	5M	503	PC1	C11-O13-P-O14
69	5M	503	PC1	C1-O11-P-O14
69	5M	505	PC1	C1-O11-P-O14
69	5d	202	PC1	C1-O11-P-O14
74	1L	702	CDL	CB3-OB5-PB2-OB3
74	1L	702	CDL	CB3-OB5-PB2-OB4
74	1N	401	CDL	CA3-OA5-PA1-OA3
74	1X	201	CDL	CA2-OA2-PA1-OA4
74	1X	201	CDL	CB2-OB2-PB2-OB3
74	3G	102	CDL	CA2-OA2-PA1-OA3
74	3G	102	CDL	CB3-OB5-PB2-OB3
74	3P	504	CDL	CA3-OA5-PA1-OA3
74	3T	101	CDL	CA3-OA5-PA1-OA3
74	4D	201	CDL	CB2-OB2-PB2-OB3
74	5H	401	CDL	CA3-OA5-PA1-OA3
74	5N	401	CDL	CA3-OA5-PA1-OA3
74	5X	201	CDL	CB2-OB2-PB2-OB3
74	5h	202	CDL	CB2-OB2-PB2-OB4
74	8D	201	CDL	CB2-OB2-PB2-OB3
76	1K	101	3PE	C11-O13-P-O14
76	1M	902	3PE	C11-O13-P-O14
76	1M	906	3PE	C11-O13-P-O14
76	1Y	801	3PE	C11-O13-P-O14
76	1Y	802	3PE	C11-O13-P-O14
76	1Y	804	3PE	C1-O11-P-O14
76	1Y	806	3PE	C11-O13-P-O14
76	1b	201	3PE	C11-O13-P-O14
76	1j	101	3PE	C1-O11-P-O14
76	1j	101	3PE	C11-O13-P-O14
76	3C	504	3PE	C1-O11-P-O14
76	3G	101	3PE	C1-O11-P-O12
76	3N	501	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
76	3N	503	3PE	C11-O13-P-O14
76	5A	201	3PE	C11-O13-P-O14
76	5K	101	3PE	C11-O13-P-O14
76	5M	501	3PE	C11-O13-P-O14
76	5M	506	3PE	C11-O13-P-O14
76	5Y	801	3PE	C1-O11-P-O14
76	5Y	801	3PE	C11-O13-P-O14
76	5Y	802	3PE	C11-O13-P-O14
76	5Y	804	3PE	C1-O11-P-O14
76	5Y	806	3PE	C11-O13-P-O14
77	1O	402	GTP	C5'-O5'-PA-O1A
79	1P	501	NDP	C2N-C3N-C7N-N7N
79	5P	402	NDP	C2N-C3N-C7N-N7N
86	4A	601	PGV	C04-O12-P-O13
86	4C	303	PGV	C03-O11-P-O14
86	4C	305	PGV	C03-O11-P-O14
86	4G	101	PGV	C04-O12-P-O13
86	4K	101	PGV	C04-O12-P-O13
86	8A	601	PGV	C04-O12-P-O13
86	8B	301	PGV	C04-O12-P-O13
86	8G	101	PGV	C04-O12-P-O13
86	8K	101	PGV	C04-O12-P-O13
77	1O	402	GTP	O4'-C4'-C5'-O5'
74	1L	702	CDL	C38-C39-C40-C41
76	5M	504	3PE	C33-C34-C35-C36
86	4C	303	PGV	C6-C7-C8-C9
76	3G	101	3PE	O22-C21-C22-C23
76	5Y	802	3PE	O21-C21-C22-C23
86	8M	101	PGV	O01-C1-C2-C3
76	1M	903	3PE	C2D-C2E-C2F-C2G
76	3A	503	3PE	C34-C35-C36-C37
69	1d	202	PC1	O22-C21-C22-C23
74	5d	203	CDL	C32-C31-CA7-OA9
86	4A	601	PGV	O04-C19-C20-C21
86	8C	303	PGV	C3-C4-C5-C6
74	5q	203	CDL	C12-C11-CA5-OA6
76	5Y	803	3PE	O21-C21-C22-C23
76	1b	201	3PE	C2A-C2B-C2C-C2D
85	3Q	501	HEC	CAD-CBD-CGD-O2D
76	3Y	101	3PE	C2-C3-O31-C31
86	4A	601	PGV	C11-C10-C9-C8
86	8B	302	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
76	1Y	802	3PE	C2D-C2E-C2F-C2G
86	4C	304	PGV	C13-C14-C15-C16
76	1Y	802	3PE	C33-C34-C35-C36
69	1B	203	PC1	O21-C21-C22-C23
74	8D	201	CDL	C32-C31-CA7-OA8
76	1M	903	3PE	O21-C21-C22-C23
76	1Y	806	3PE	O31-C31-C32-C33
76	5M	502	3PE	O31-C31-C32-C33
76	5M	502	3PE	O21-C21-C22-C23
74	3P	504	CDL	C32-C31-CA7-OA9
76	1K	101	3PE	C24-C25-C26-C27
76	3C	504	3PE	C23-C24-C25-C26
69	1A	201	PC1	C12-C11-O13-P
69	5A	202	PC1	C12-C11-O13-P
74	3N	502	CDL	CB6-CB4-OB6-CB5
76	1Y	801	3PE	C3-C2-O21-C21
76	3A	503	3PE	C12-C11-O13-P
76	5M	501	3PE	C12-C11-O13-P
76	5Y	801	3PE	C3-C2-O21-C21
76	5Y	806	3PE	C12-C11-O13-P
82	1h	201	AME	CB-CA-N-CT1
74	1L	702	CDL	C52-C51-CB5-OB7
76	1Y	805	3PE	O22-C21-C22-C23
76	1b	201	3PE	O22-C21-C22-C23
76	5A	201	3PE	O22-C21-C22-C23
74	1N	401	CDL	C32-C33-C34-C35
74	5N	401	CDL	C32-C33-C34-C35
86	4A	602	PGV	C6-C7-C8-C9
86	8C	301	PGV	C26-C27-C28-C29
86	8G	101	PGV	C7-C8-C9-C10
69	1h	203	PC1	O31-C31-C32-C33
76	5Y	806	3PE	O31-C31-C32-C33
76	1M	902	3PE	C22-C23-C24-C25
69	5M	505	PC1	O21-C21-C22-C23
74	3G	102	CDL	C12-C11-CA5-OA6
74	3G	102	CDL	C52-C51-CB5-OB6
74	3P	504	CDL	C72-C71-CB7-OB8
76	1Y	802	3PE	O21-C21-C22-C23
76	3N	503	3PE	O31-C31-C32-C33
76	5Y	805	3PE	O21-C21-C22-C23
86	8C	302	PGV	O03-C19-C20-C21
74	1X	201	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
87	8A	604	HEA	CAA-CBA-CGA-O2A
69	3J	101	PC1	C22-C23-C24-C25
69	1M	905	PC1	O21-C21-C22-C23
69	5d	202	PC1	O31-C31-C32-C33
74	3P	504	CDL	C52-C51-CB5-OB6
74	5L	702	CDL	C52-C51-CB5-OB6
74	5N	401	CDL	C12-C11-CA5-OA6
76	5Y	802	3PE	O31-C31-C32-C33
86	4C	302	PGV	O03-C19-C20-C21
86	4C	303	PGV	O03-C19-C20-C21
86	8A	601	PGV	O03-C19-C20-C21
76	1M	901	3PE	C38-C39-C3A-C3B
76	3N	501	3PE	C22-C23-C24-C25
74	1d	203	CDL	C32-C31-CA7-OA9
74	5L	702	CDL	C52-C51-CB5-OB7
74	5X	201	CDL	C63-C64-C65-C66
86	8C	303	PGV	C6-C7-C8-C9
72	1F	501	FMN	N10-C1'-C2'-O2'
74	4B	302	CDL	CB5-C51-C52-C53
86	8A	601	PGV	O04-C19-C20-C21
69	5P	401	PC1	C24-C25-C26-C27
74	3A	501	CDL	C31-C32-C33-C34
69	1A	201	PC1	O21-C21-C22-C23
74	1L	702	CDL	C52-C51-CB5-OB6
74	4D	201	CDL	C32-C31-CA7-OA8
76	1M	903	3PE	O31-C31-C32-C33
76	3N	503	3PE	O21-C21-C22-C23
76	1L	701	3PE	C28-C29-C2A-C2B
90	8I	101	PSC	C2-C3-C4-C5
69	5h	203	PC1	O32-C31-C32-C33
76	1Y	802	3PE	O22-C21-C22-C23
76	5Y	805	3PE	O22-C21-C22-C23
85	3D	501	HEC	CAA-CBA-CGA-O1A
69	5A	202	PC1	O21-C21-C22-C23
69	5h	203	PC1	O31-C31-C32-C33
74	1N	401	CDL	C12-C11-CA5-OA6
74	1q	202	CDL	C12-C11-CA5-OA6
74	8D	201	CDL	C52-C51-CB5-OB6
76	1Y	803	3PE	O21-C21-C22-C23
86	8C	303	PGV	O03-C19-C20-C21
76	1M	901	3PE	C35-C36-C37-C38
74	8B	303	CDL	CB5-C51-C52-C53

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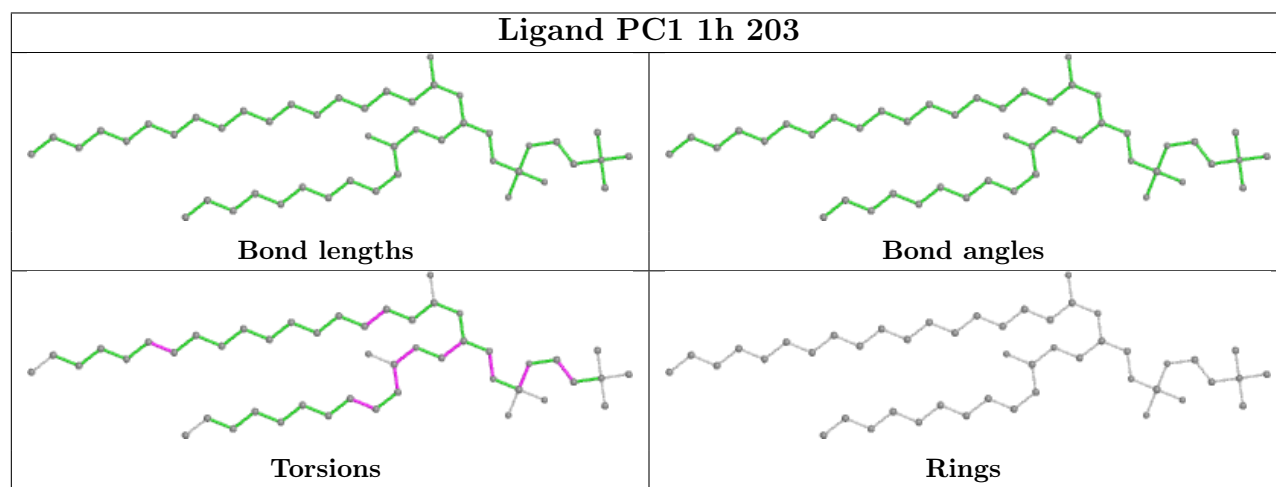
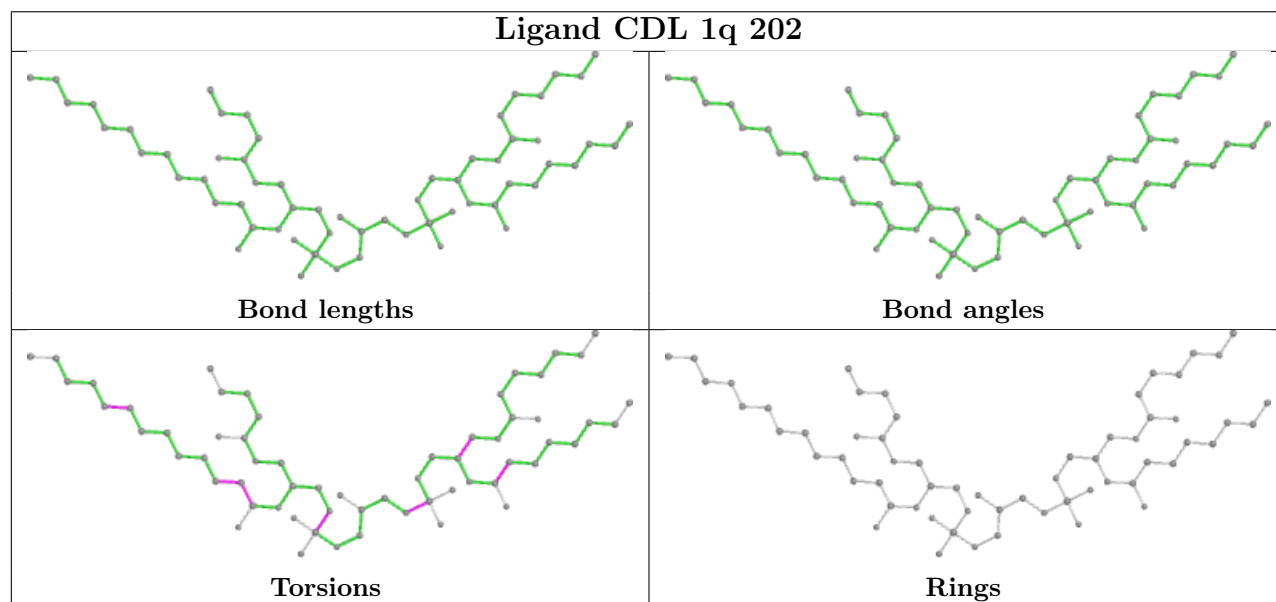
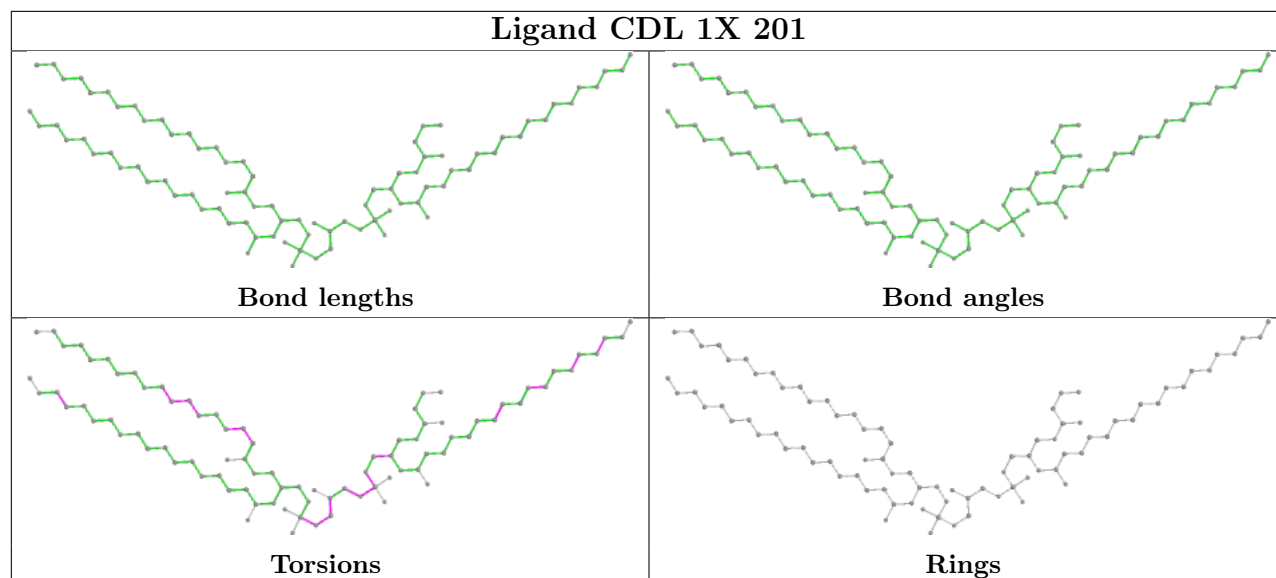
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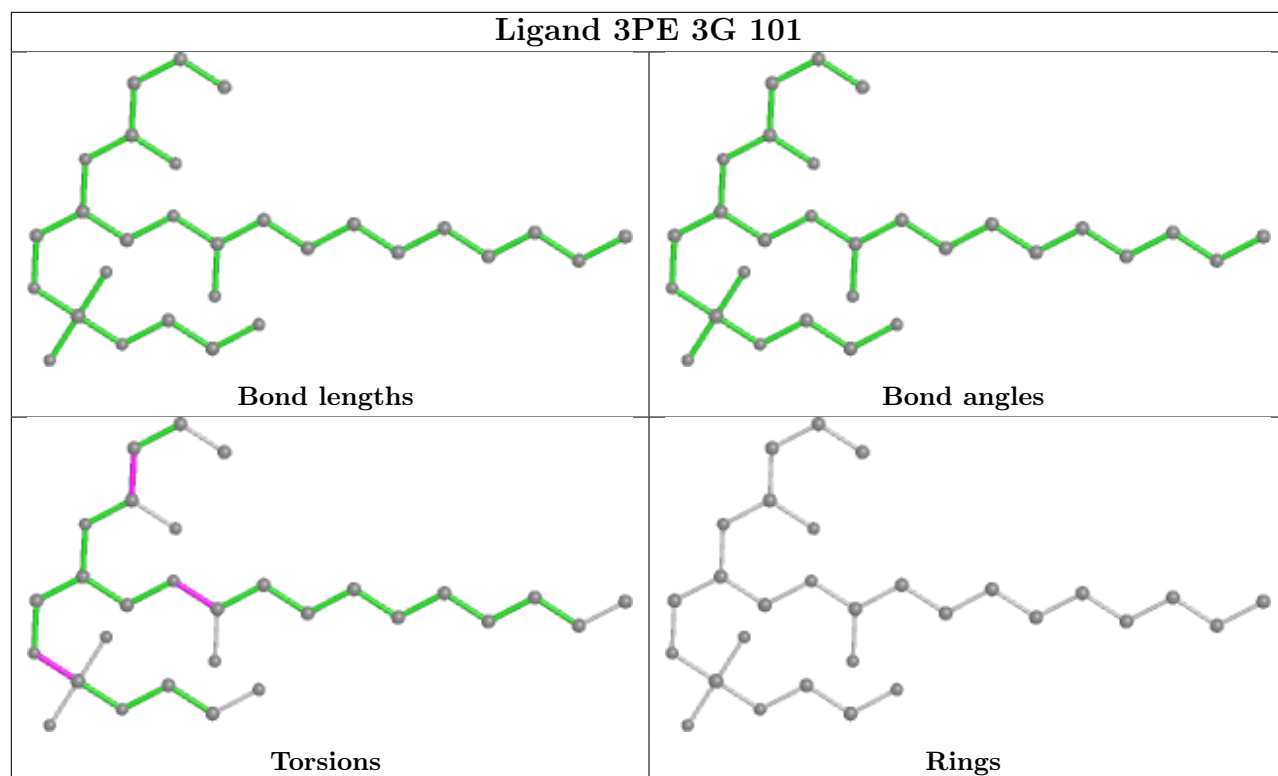
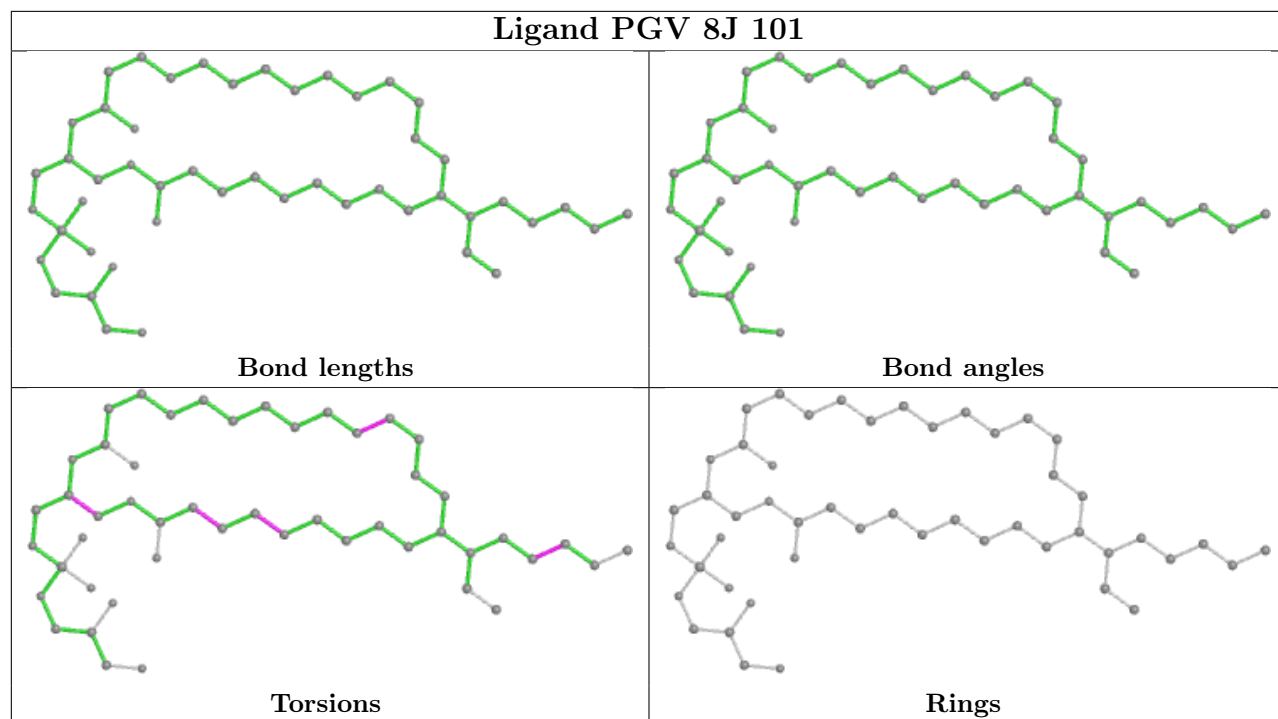
Mol	Chain	Res	Type	Atoms
76	1Y	803	3PE	O22-C21-C22-C23
76	3N	503	3PE	O22-C21-C22-C23
85	3Q	501	HEC	CAA-CBA-CGA-O2A
87	4A	604	HEA	CAA-CBA-CGA-O2A
69	1I	201	PC1	C36-C37-C38-C39
76	5P	403	3PE	C37-C38-C39-C3A
86	8C	303	PGV	C30-C31-C32-C33
69	1d	202	PC1	O31-C31-C32-C33
69	5B	203	PC1	O21-C21-C22-C23
74	4C	306	CDL	C32-C31-CA7-OA8
92	4G	102	PEK	C22-C23-C24-C25
74	8D	201	CDL	C32-C31-CA7-OA9
74	8C	306	CDL	C18-C19-C20-C21
69	1h	203	PC1	O32-C31-C32-C33
74	1N	401	CDL	C12-C11-CA5-OA7
74	3P	504	CDL	C72-C71-CB7-OB9
76	5Y	803	3PE	O22-C21-C22-C23
76	1L	701	3PE	C2A-C2B-C2C-C2D
86	8J	101	PGV	C30-C31-C32-C33
86	8G	101	PGV	O03-C19-C20-C21
90	4A	609	PSC	O03-C19-C20-C21
90	8I	101	PSC	O03-C19-C20-C21

There are no ring outliers.

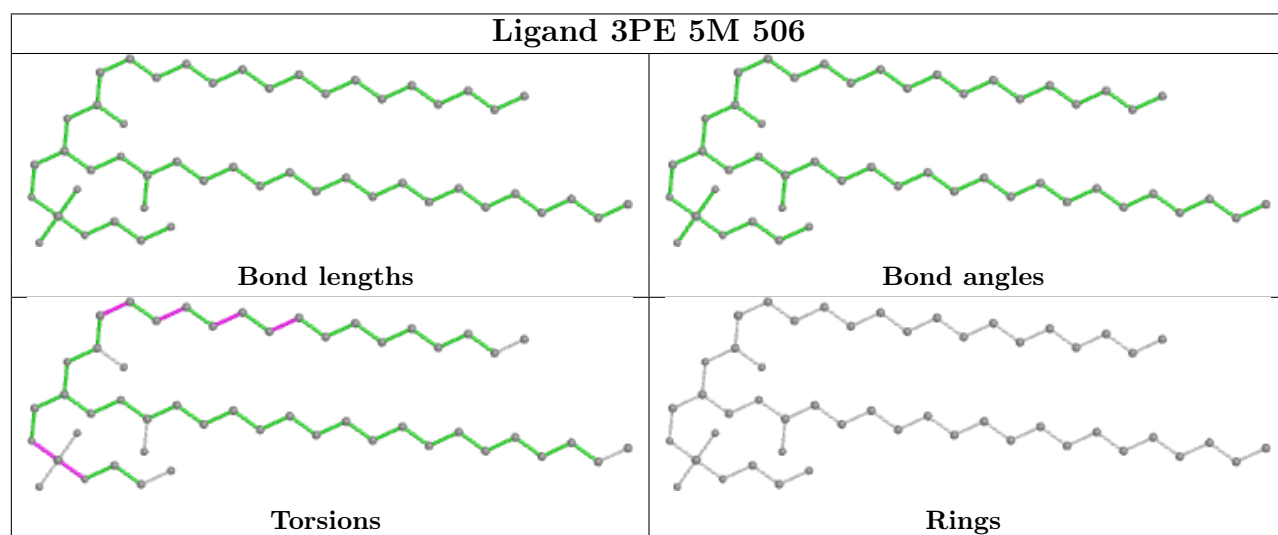
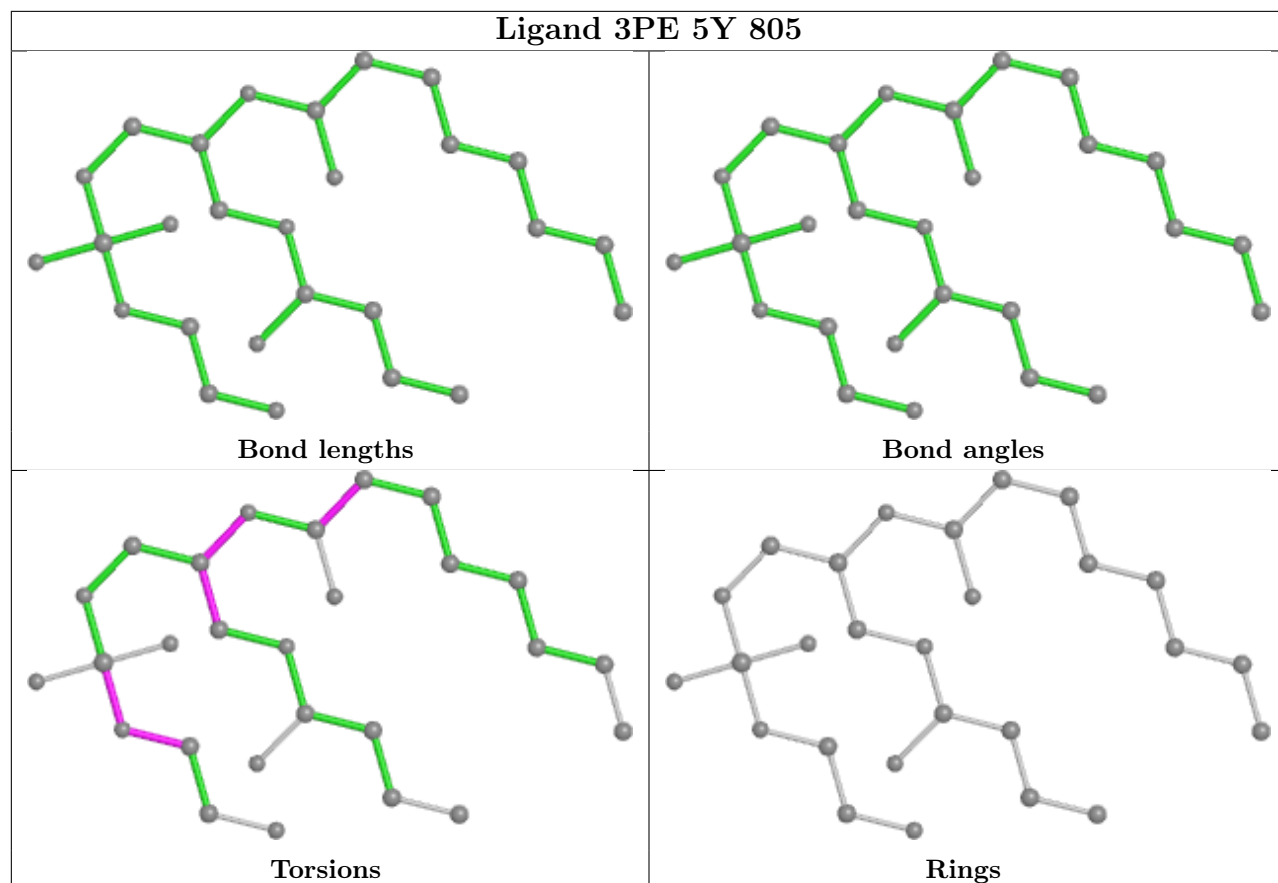
No monomer is involved in short contacts.

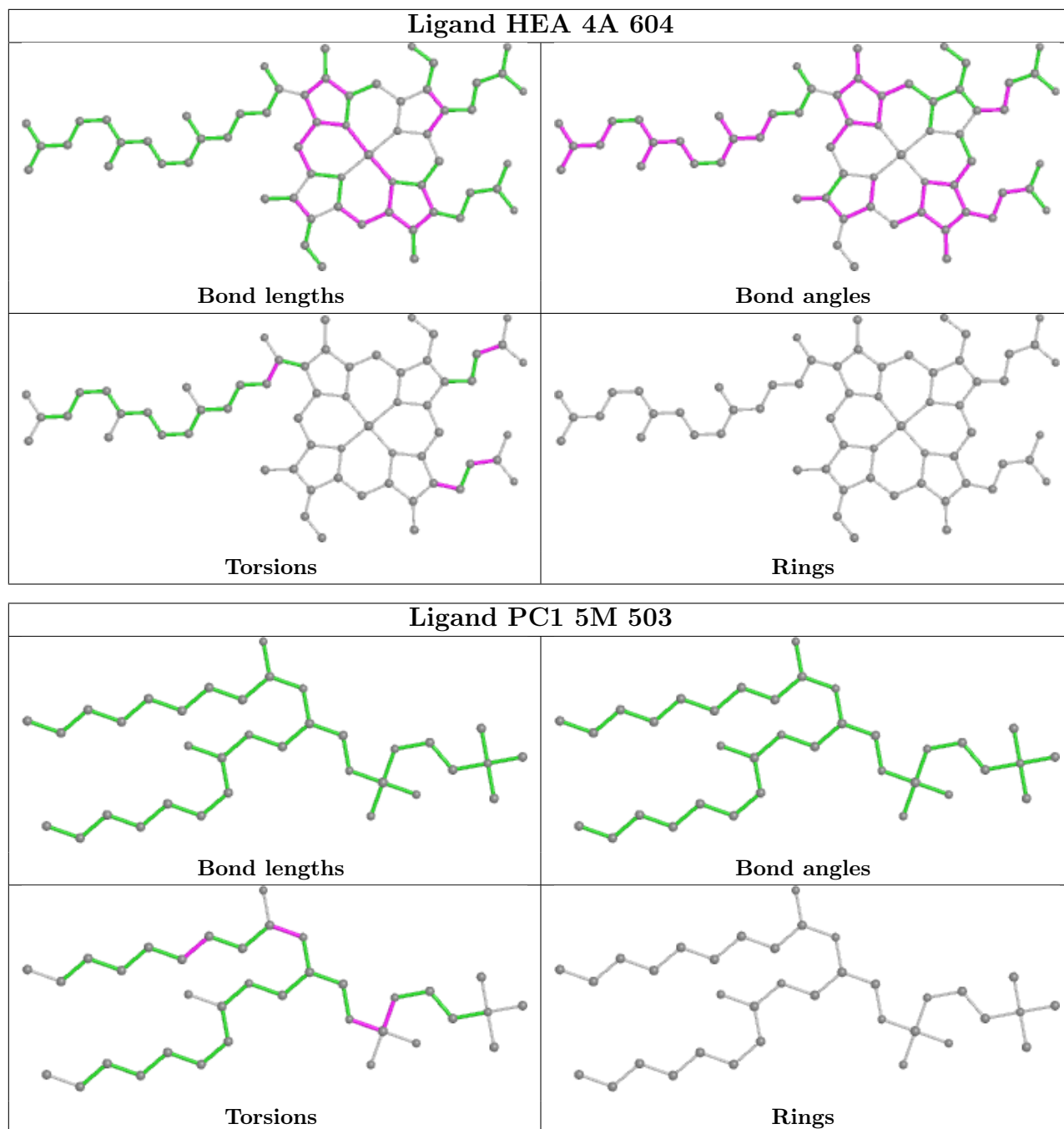
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

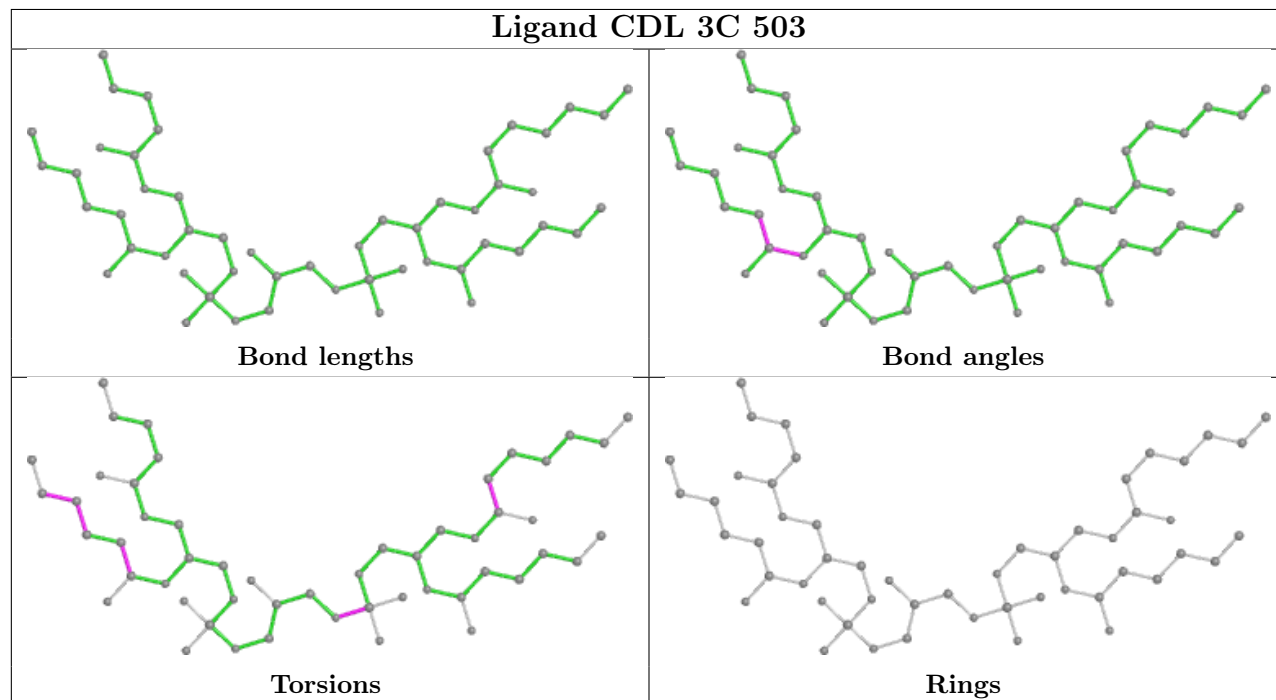
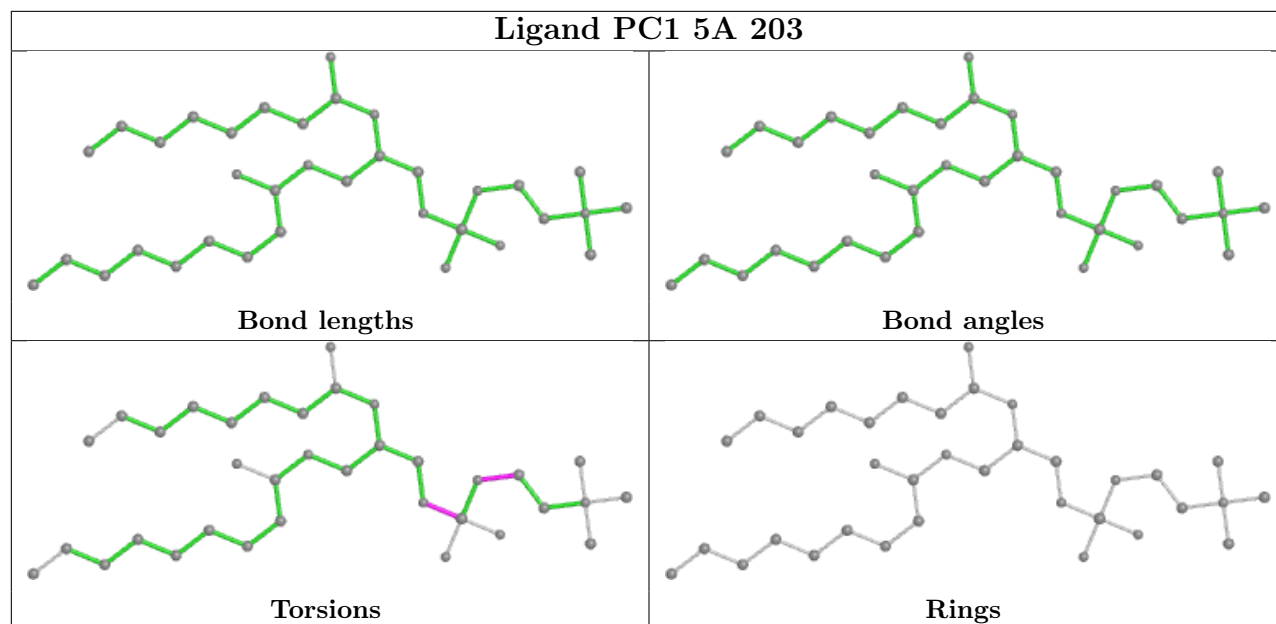


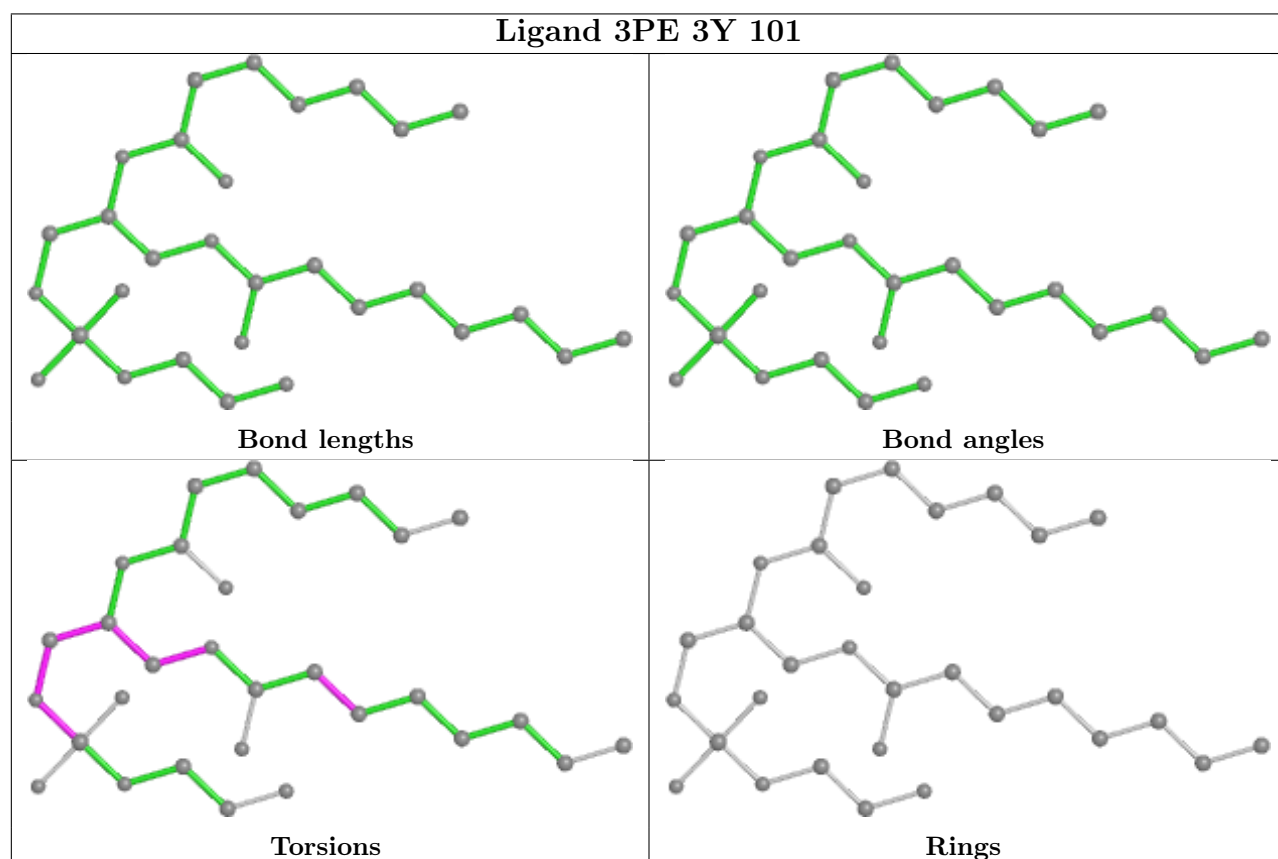
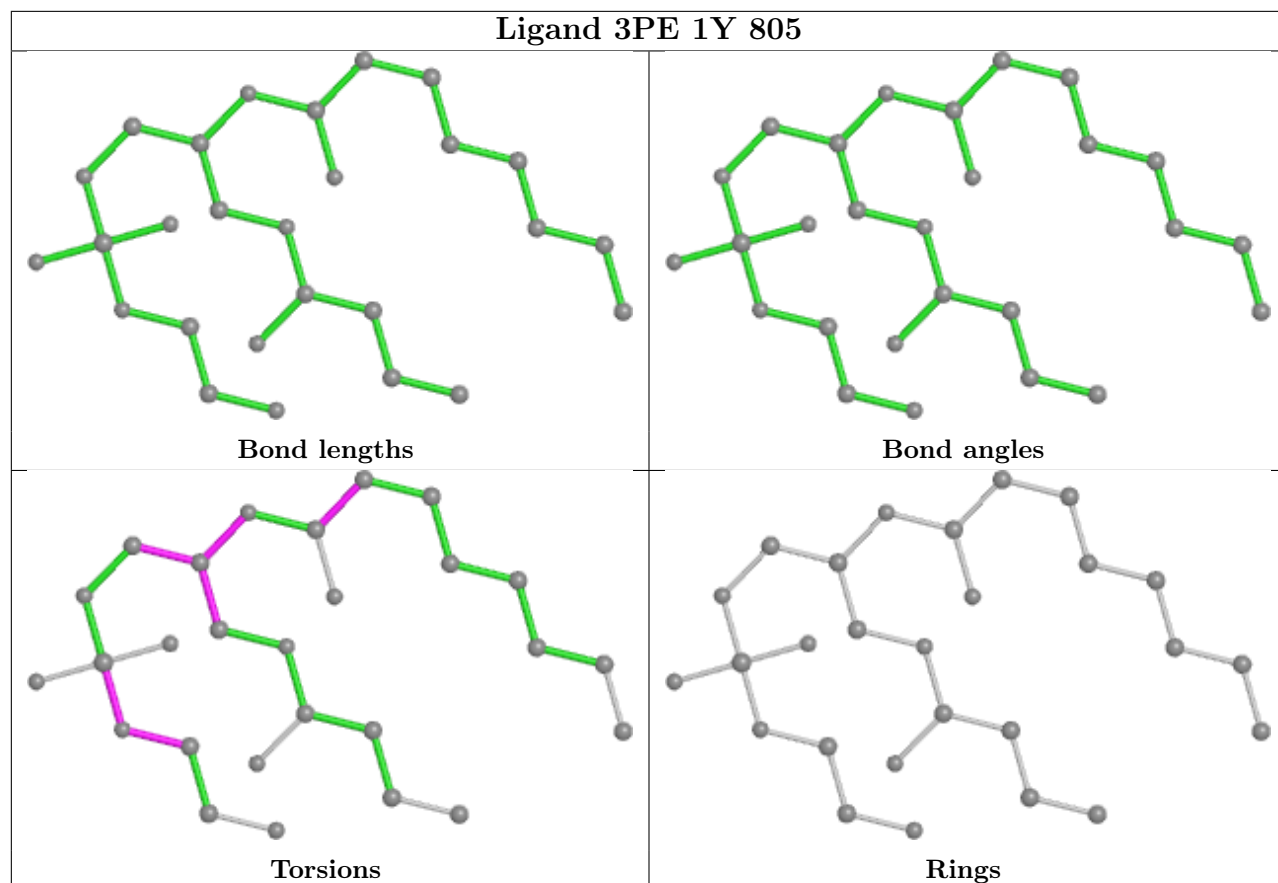


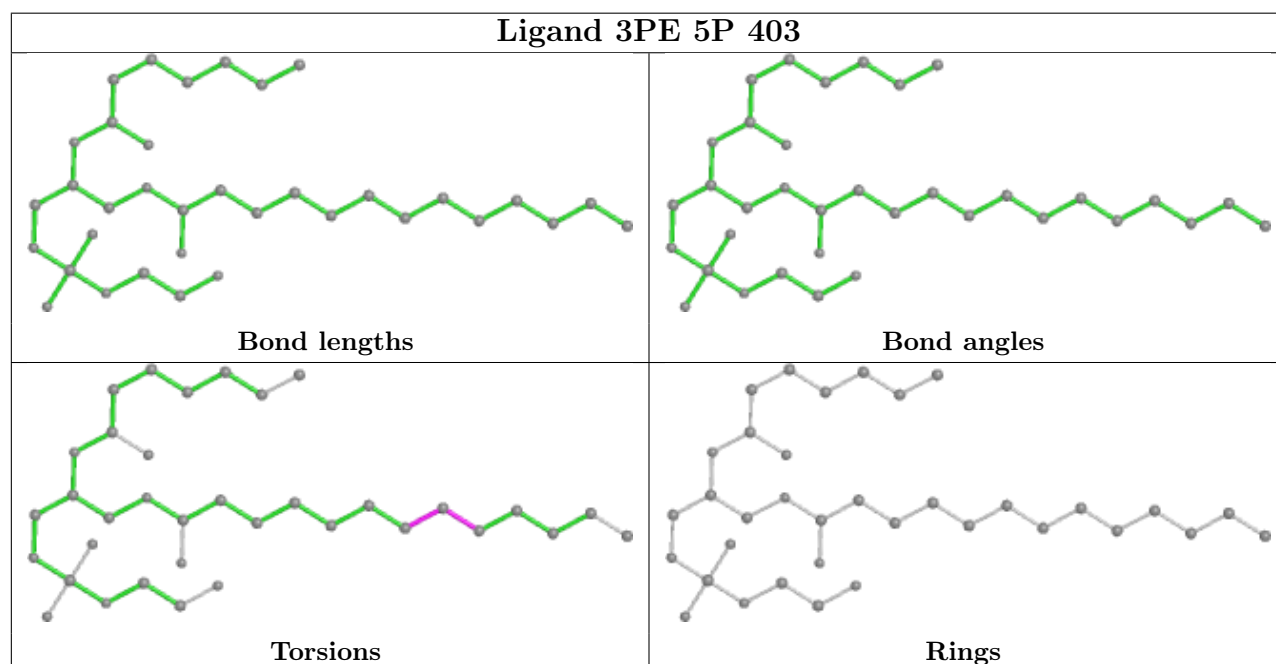
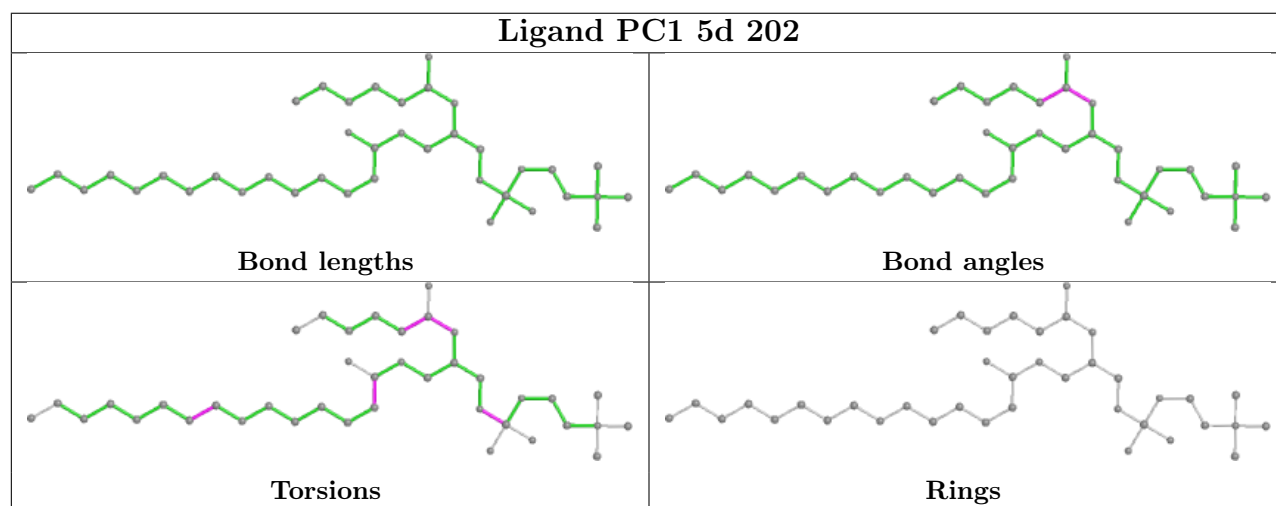
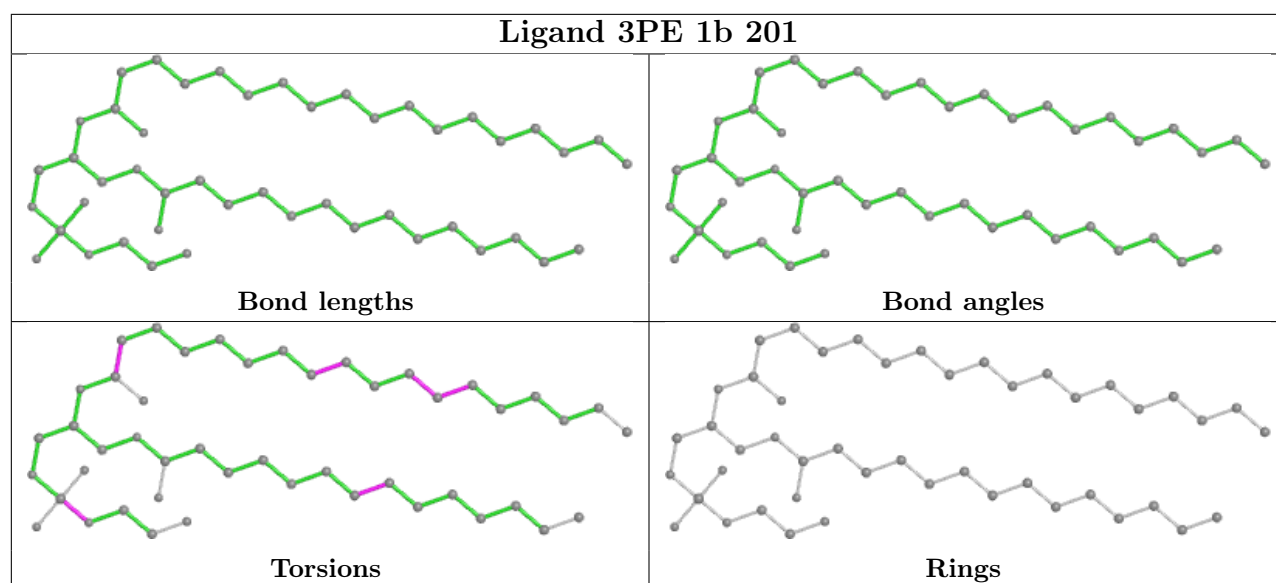


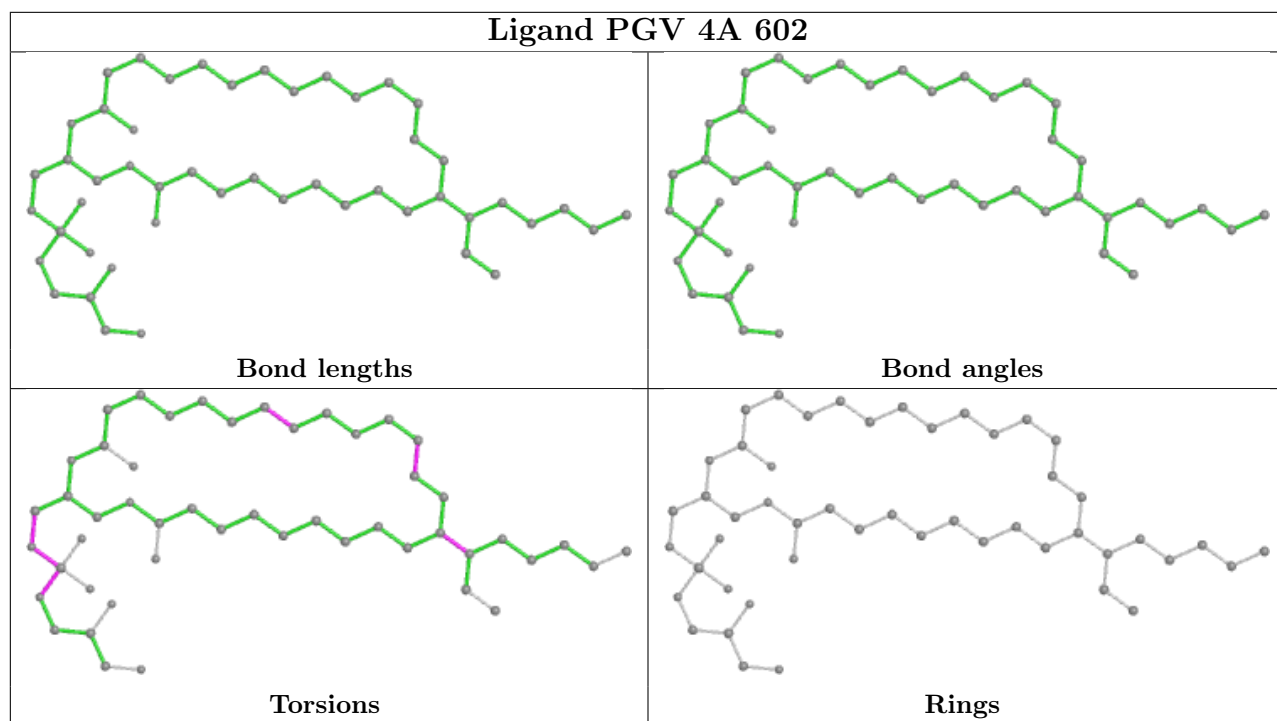
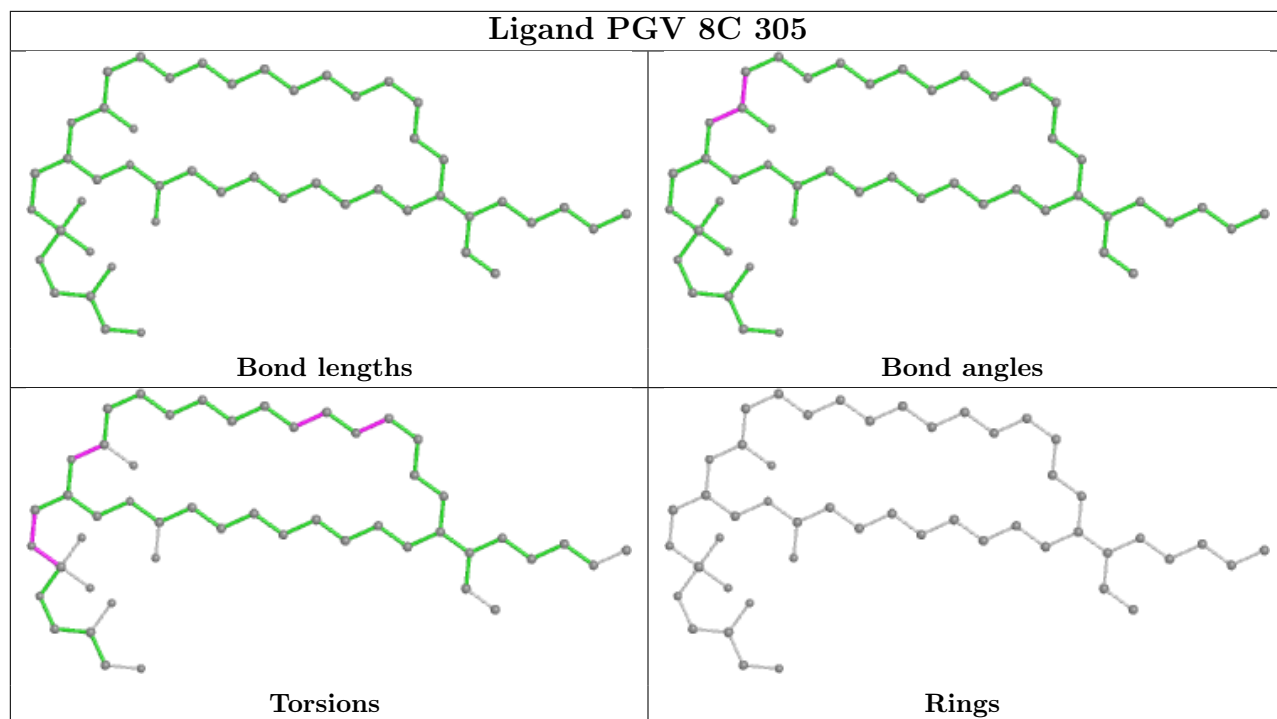


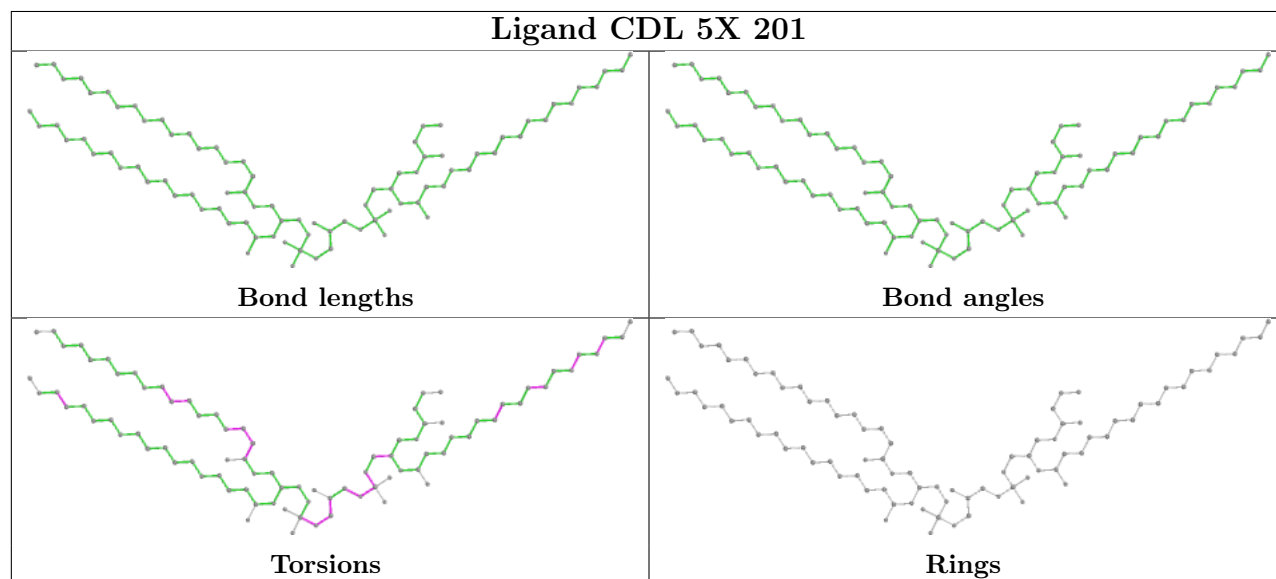
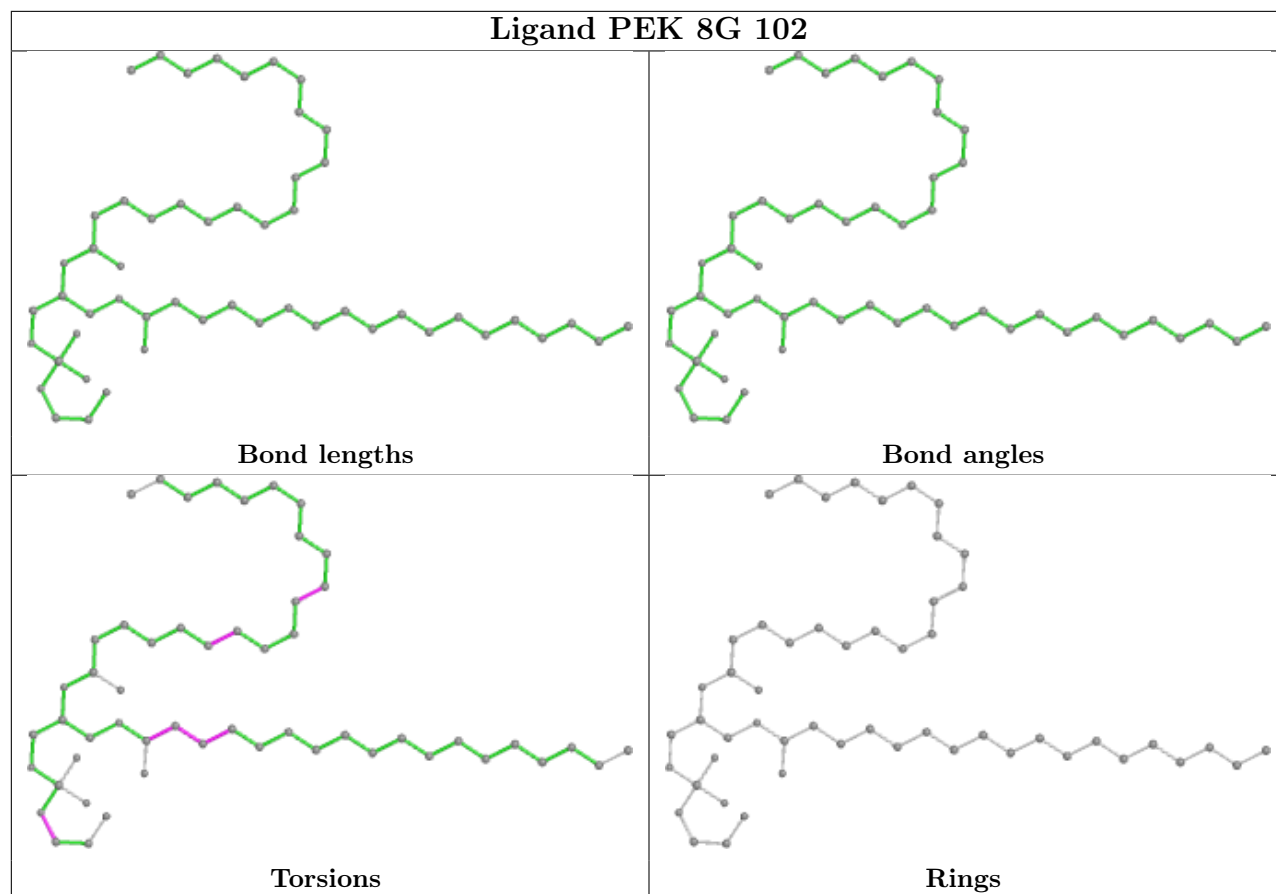


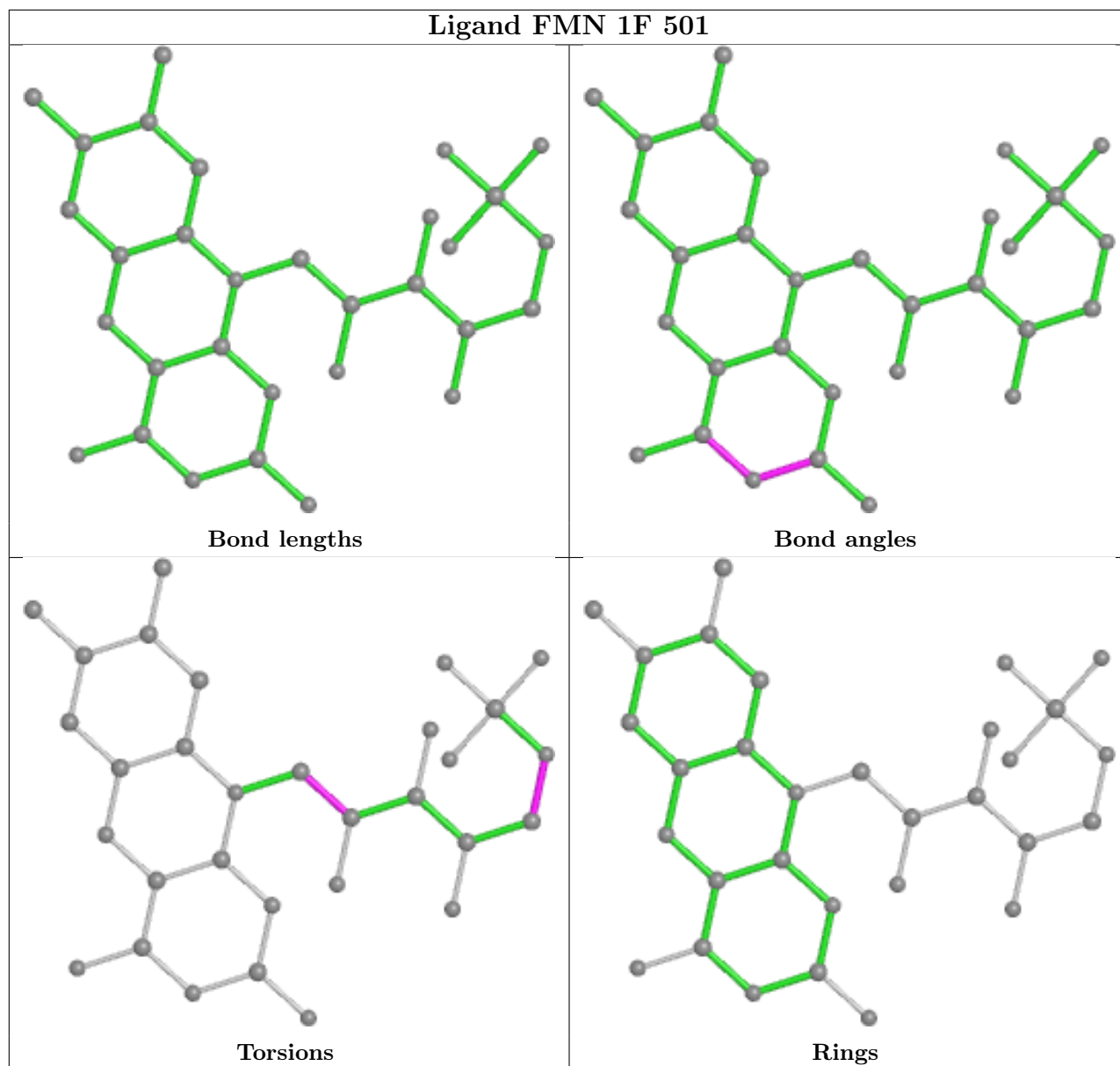




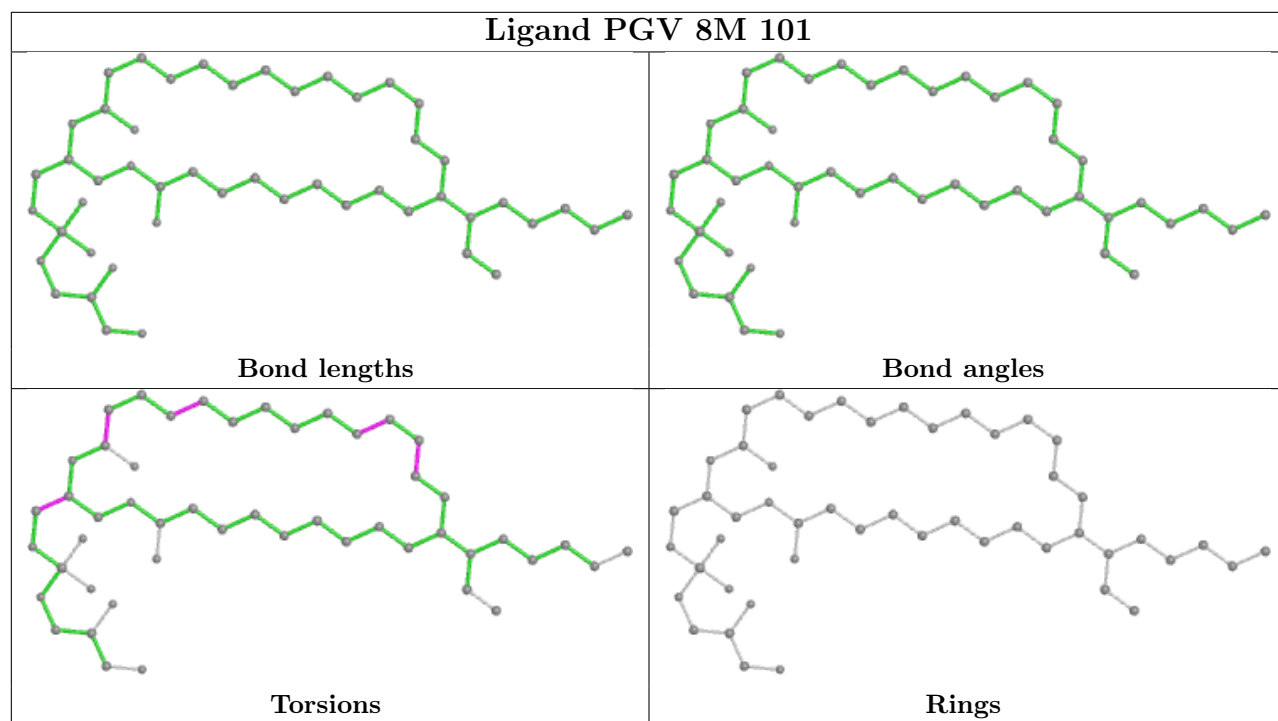
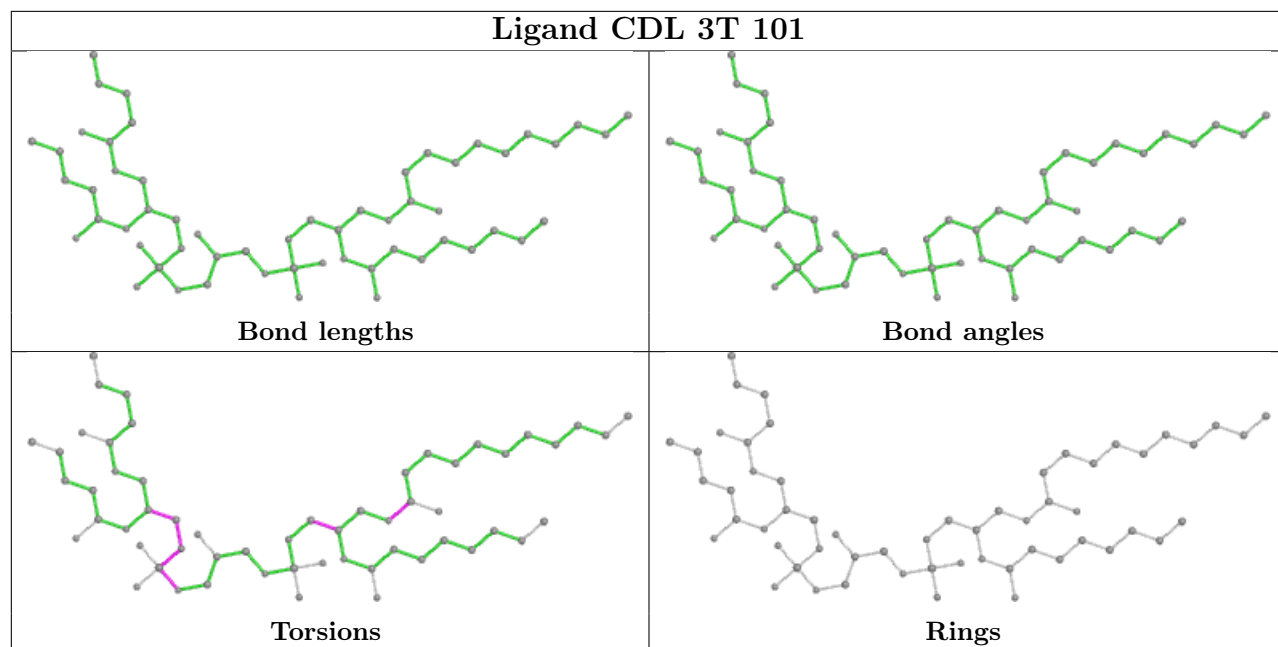


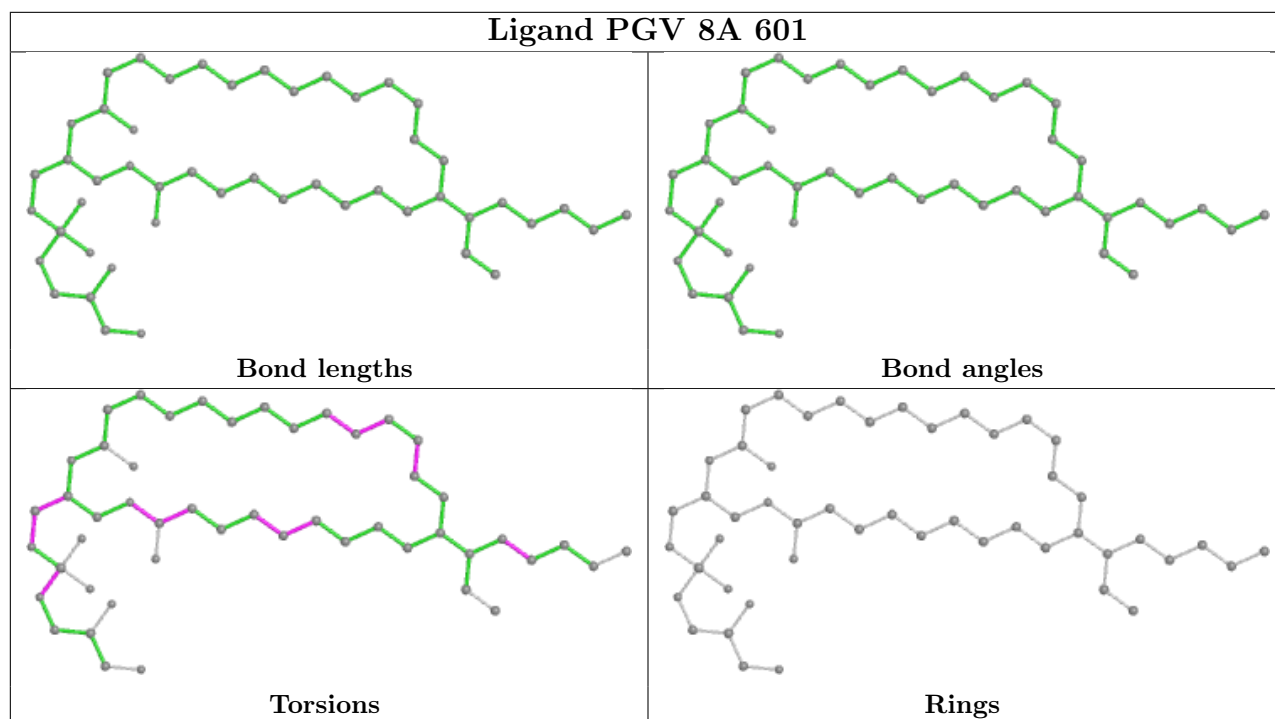
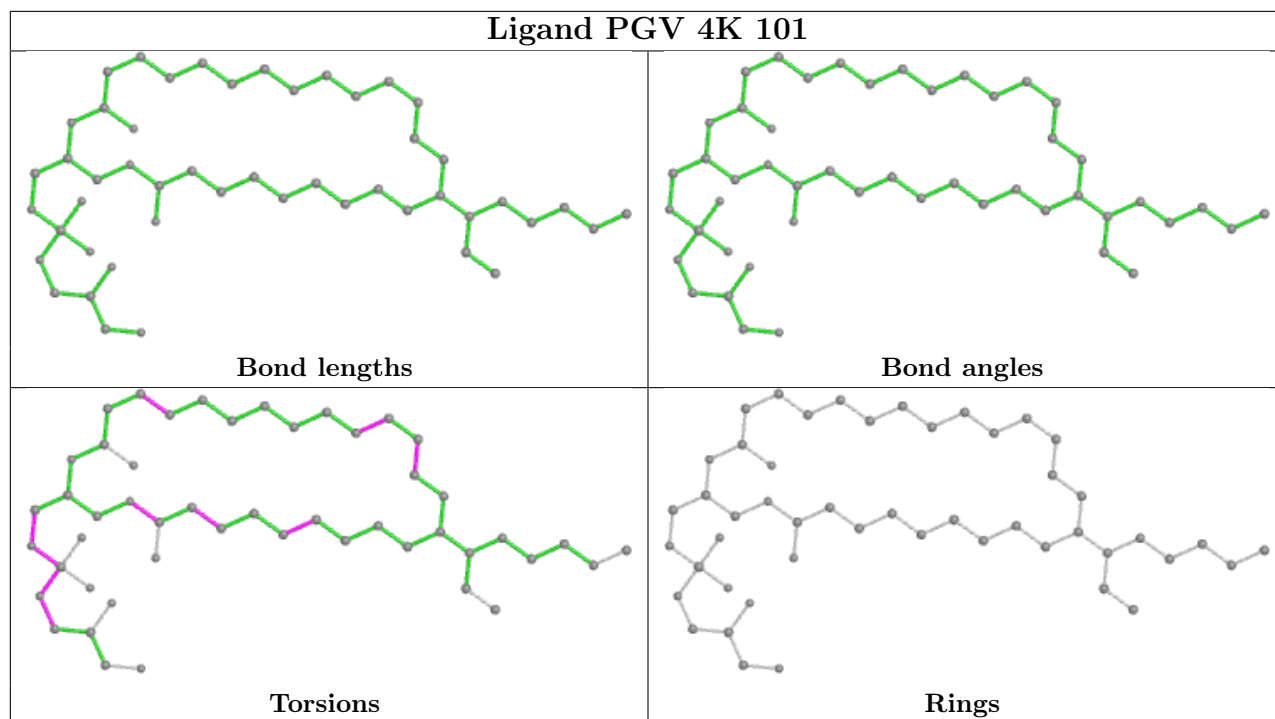


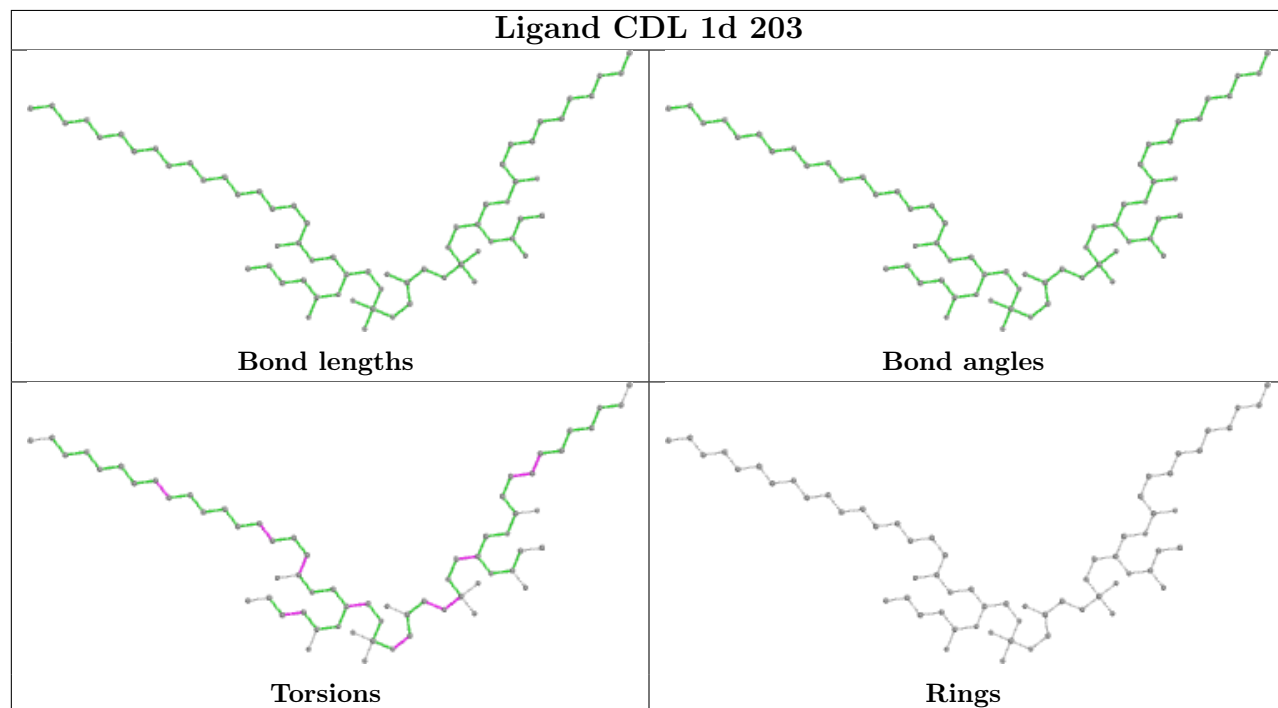
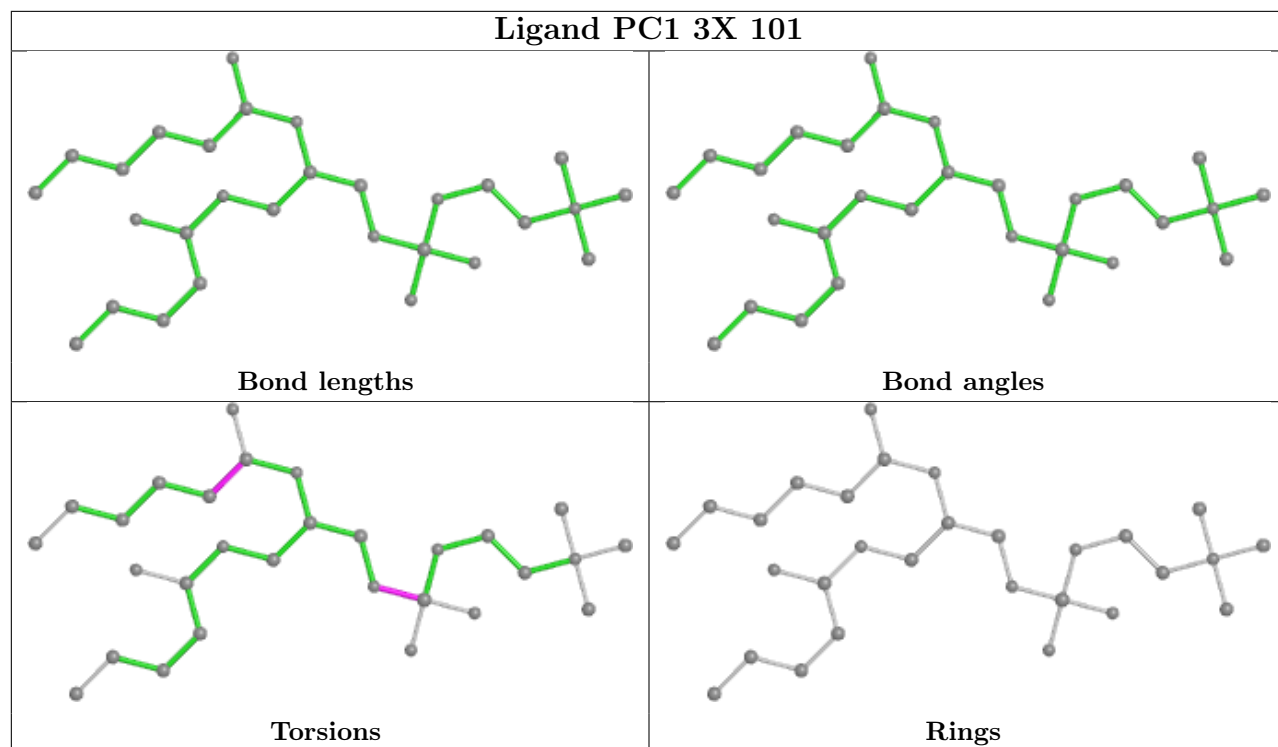


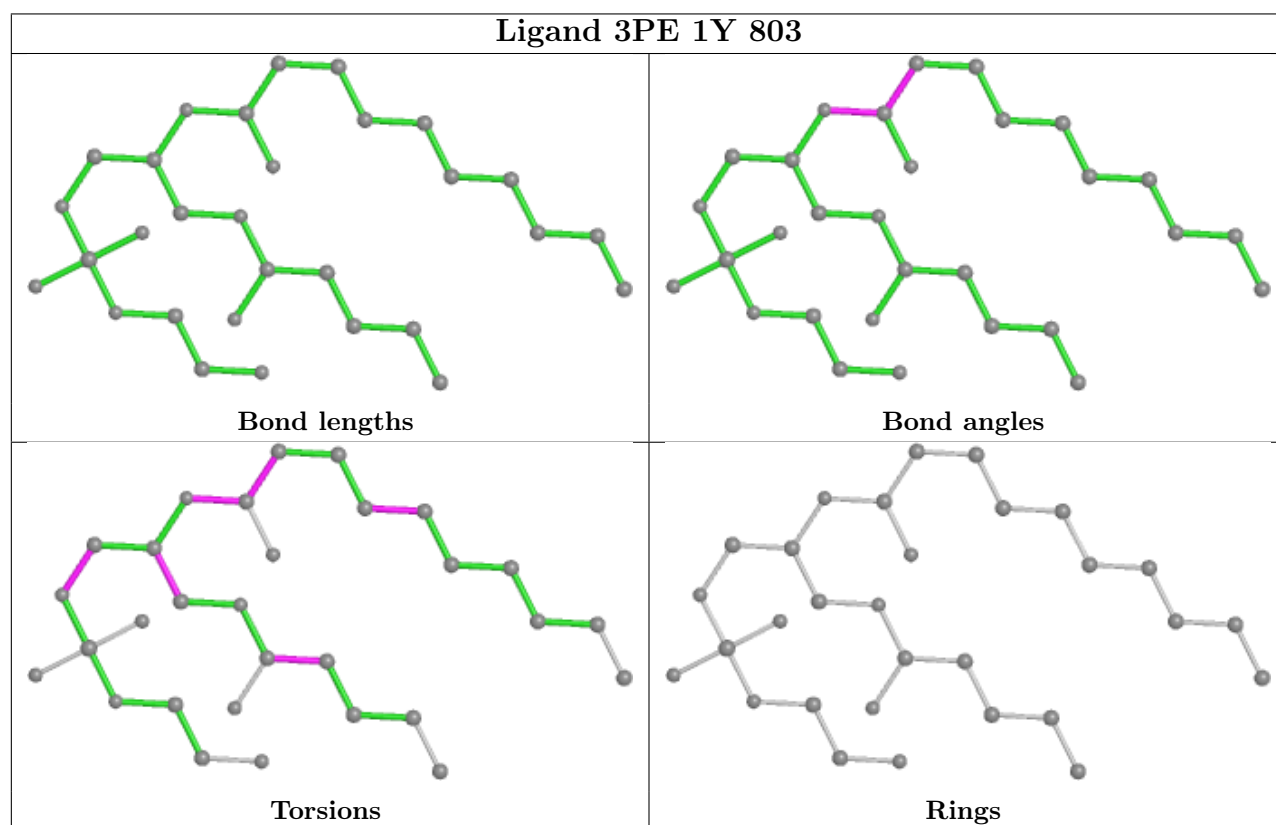
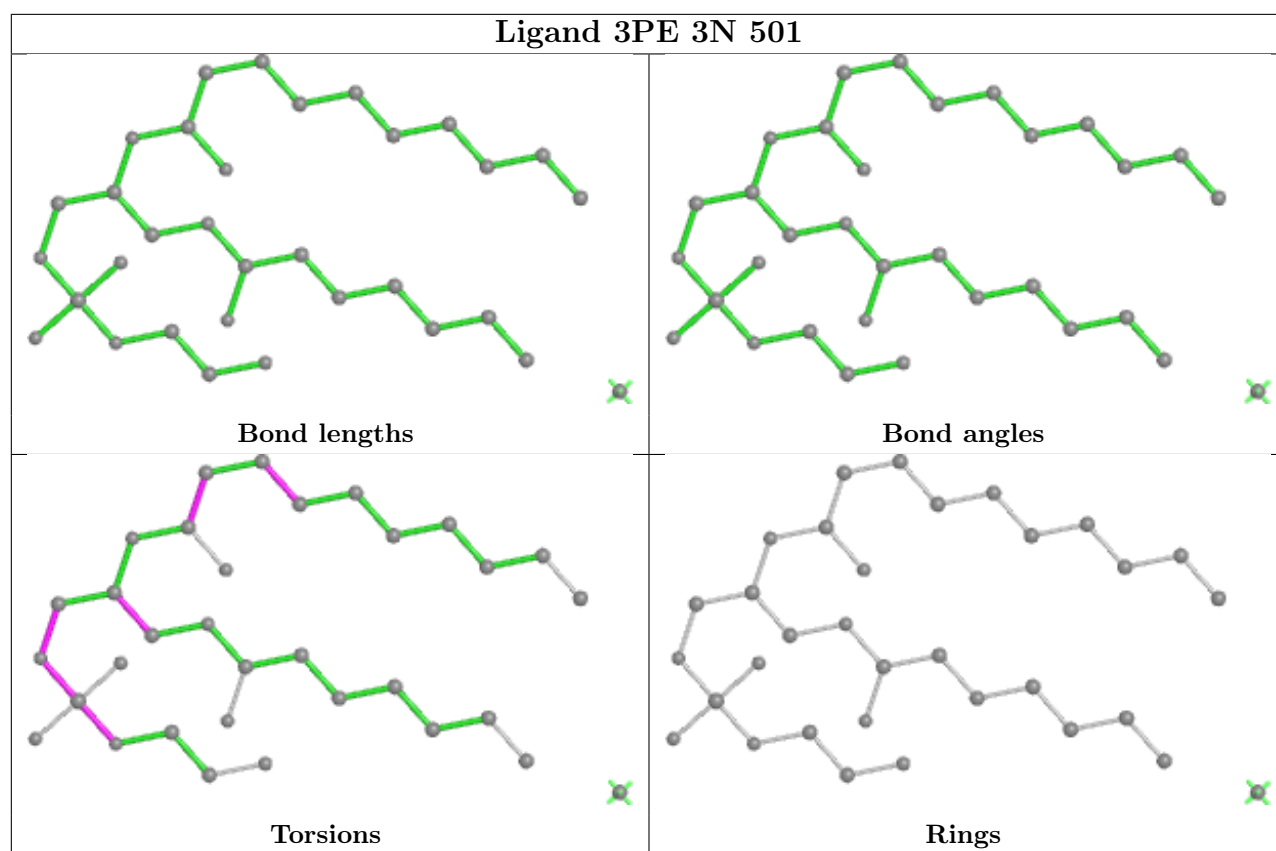


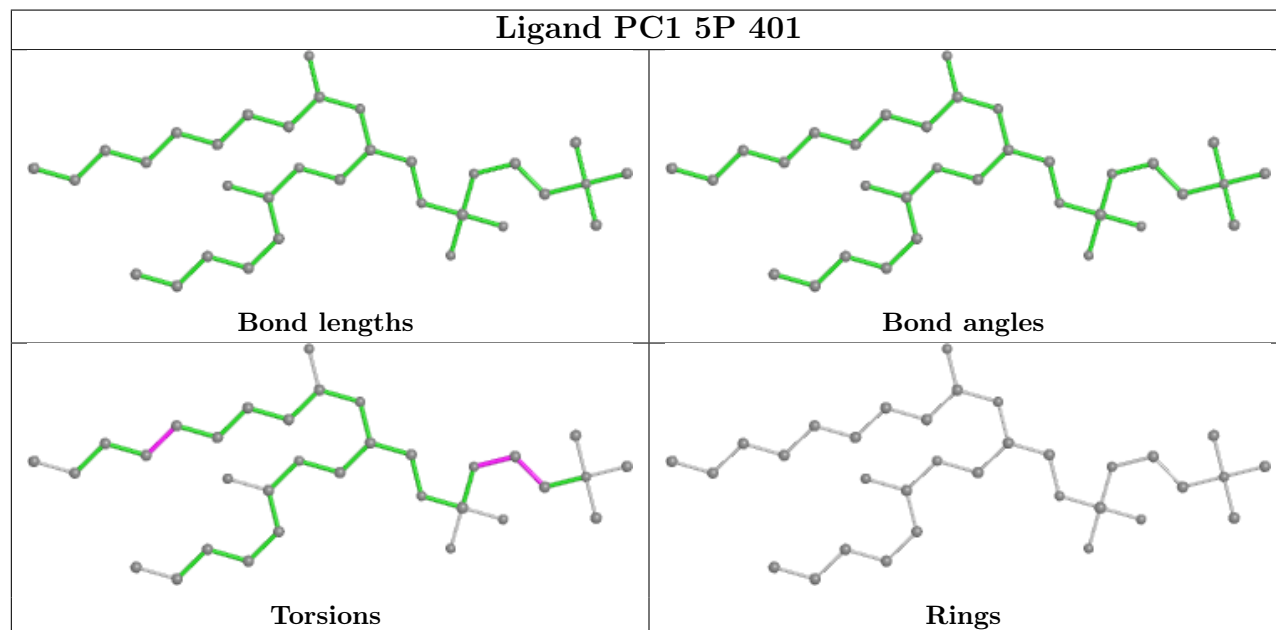
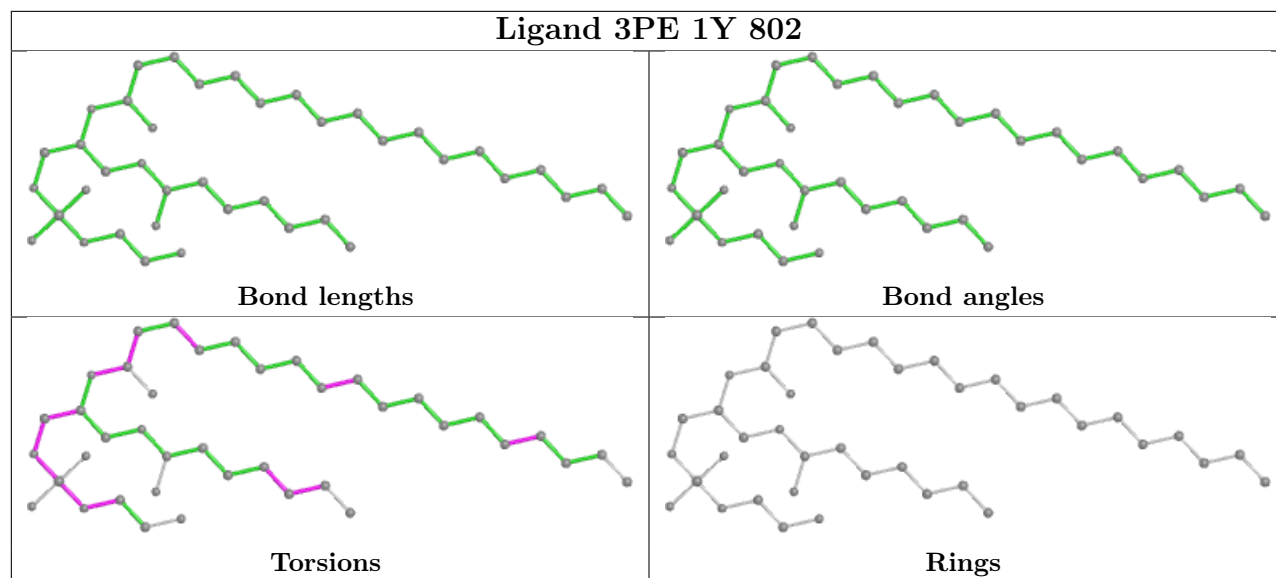


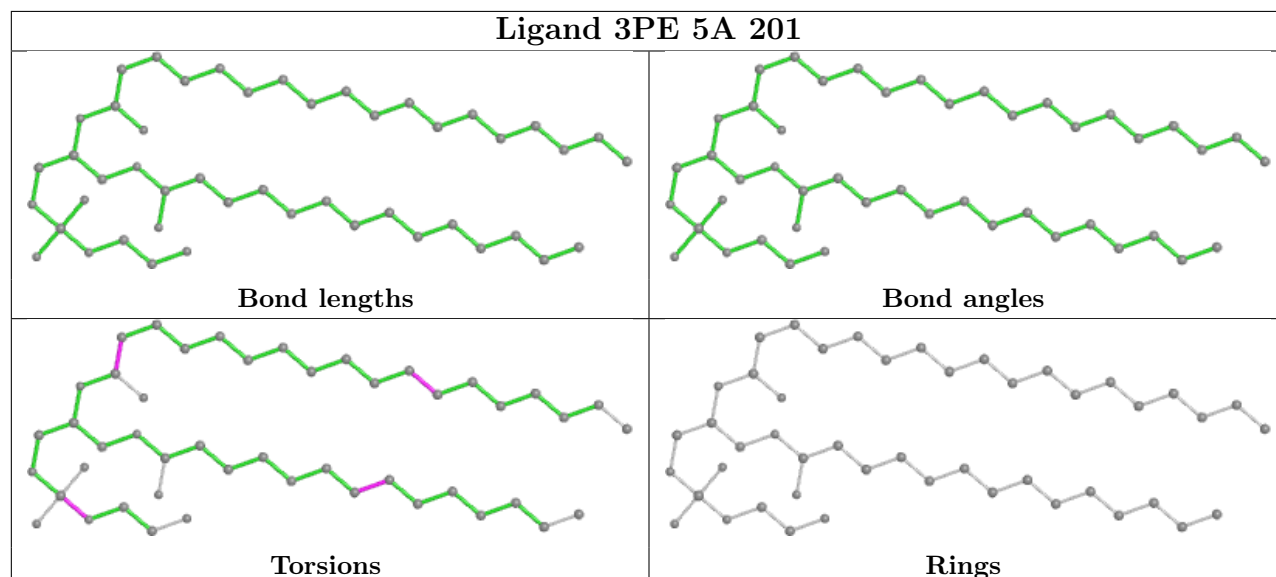
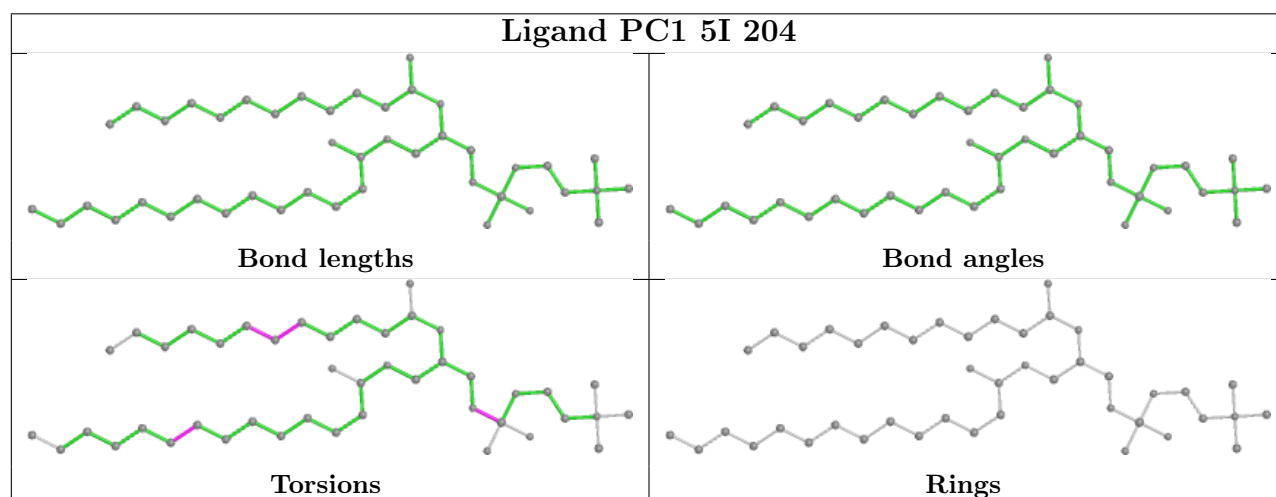
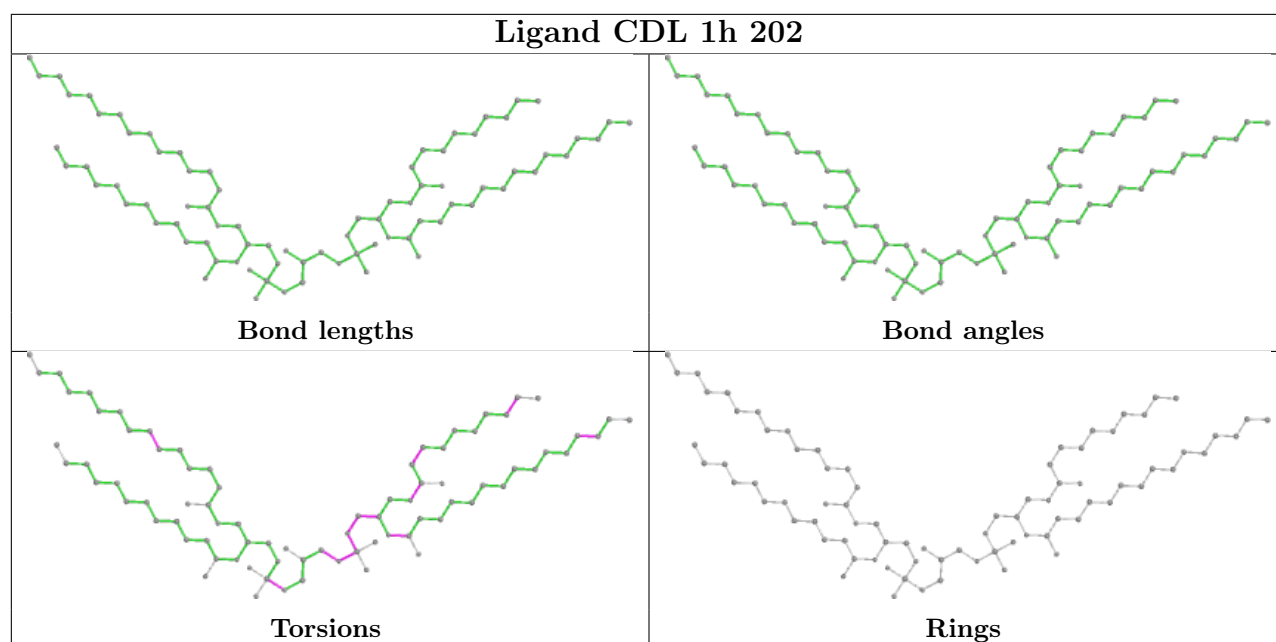


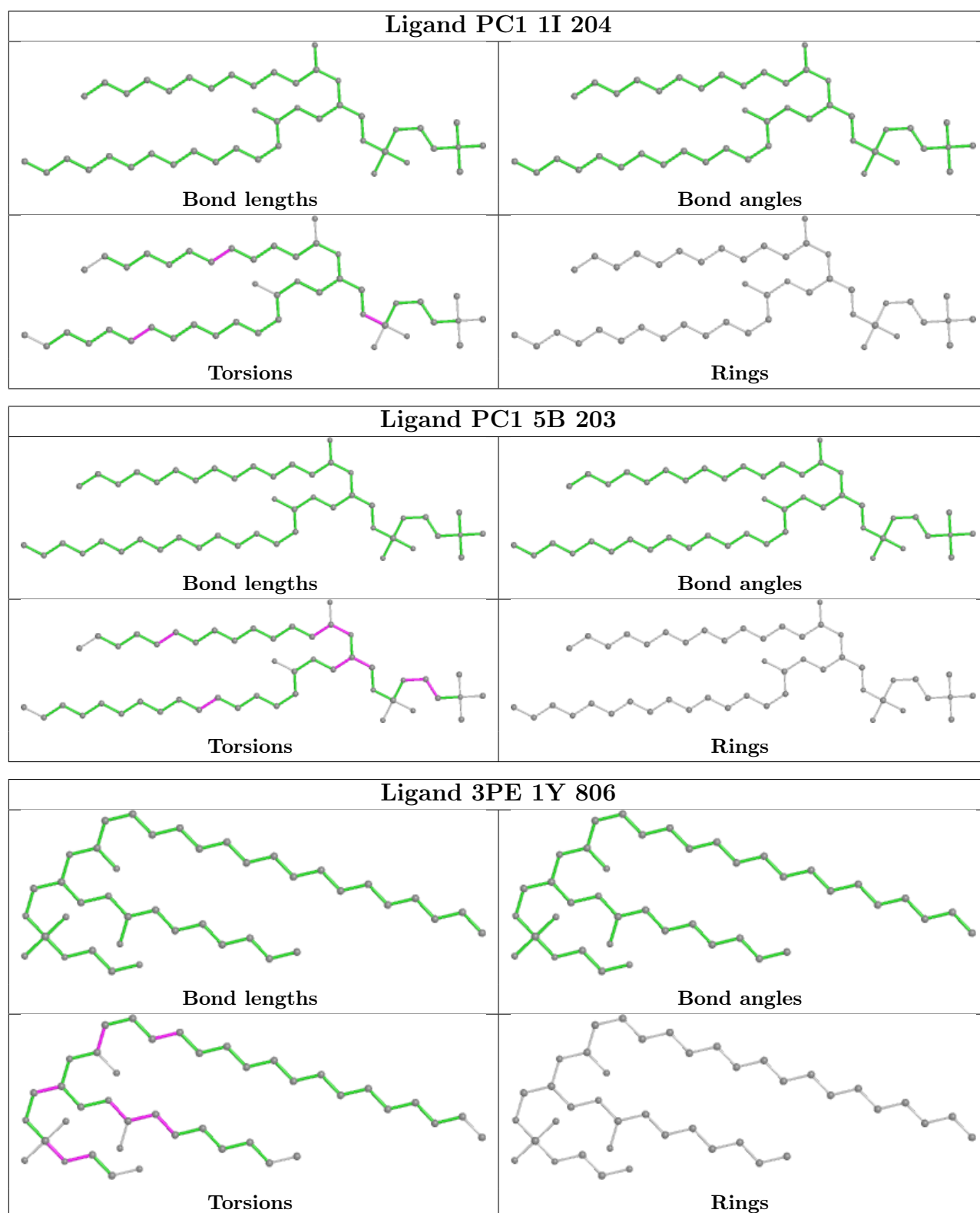


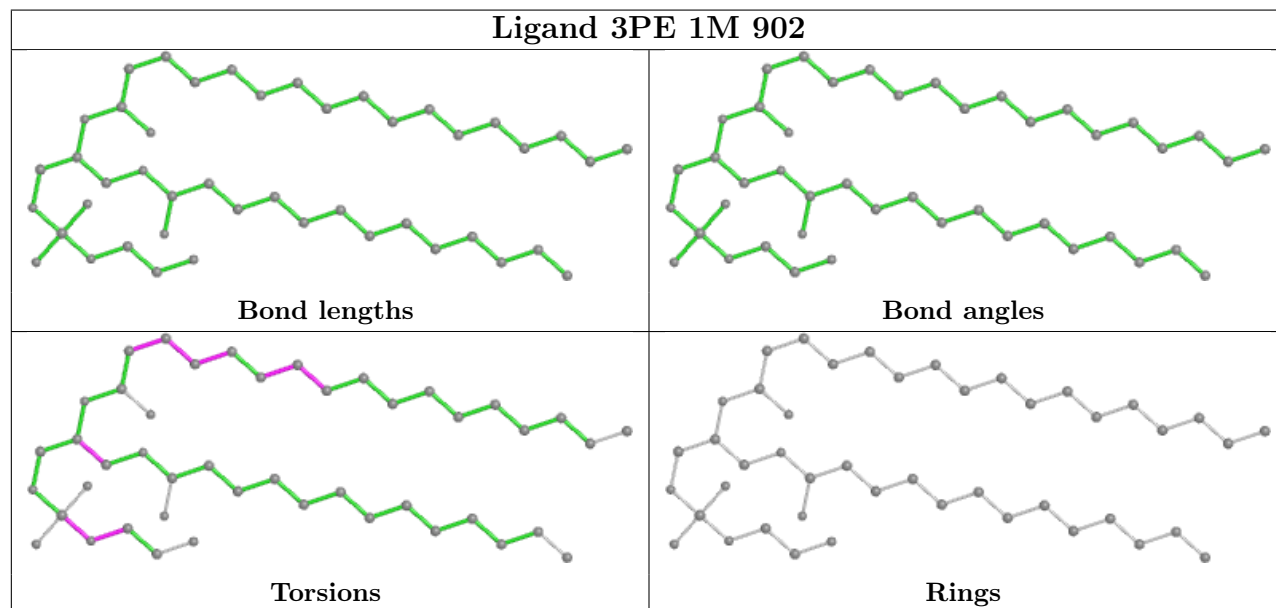
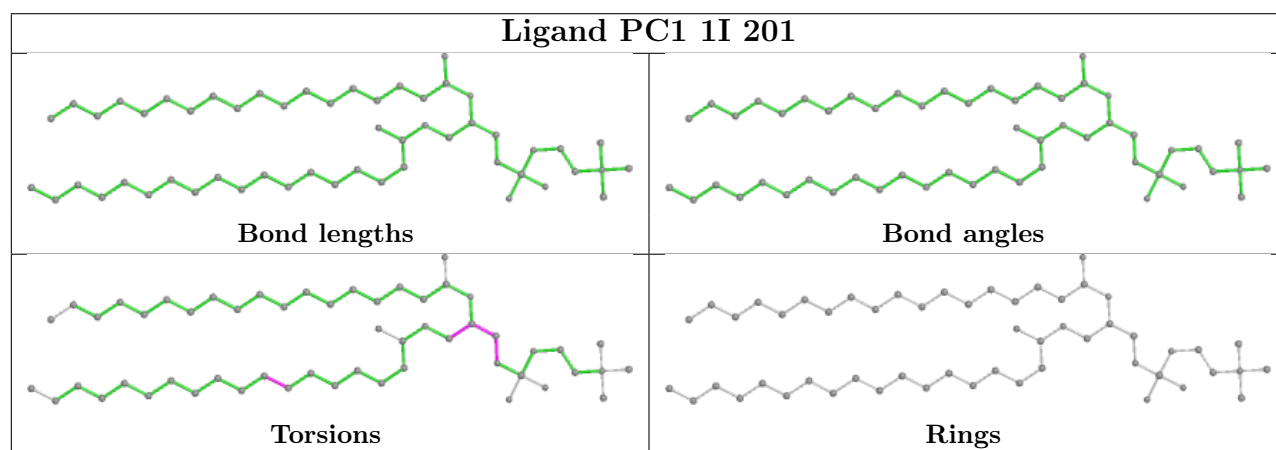
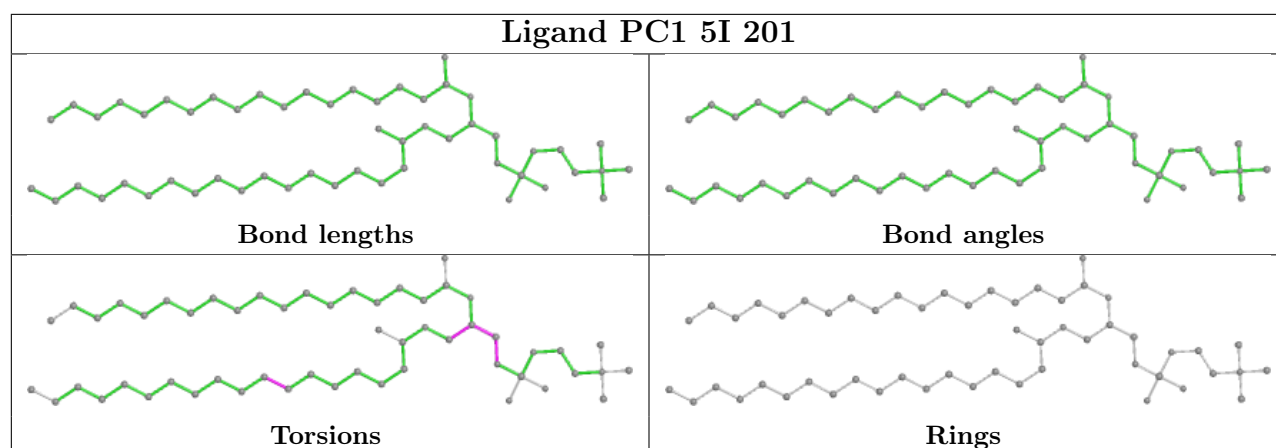




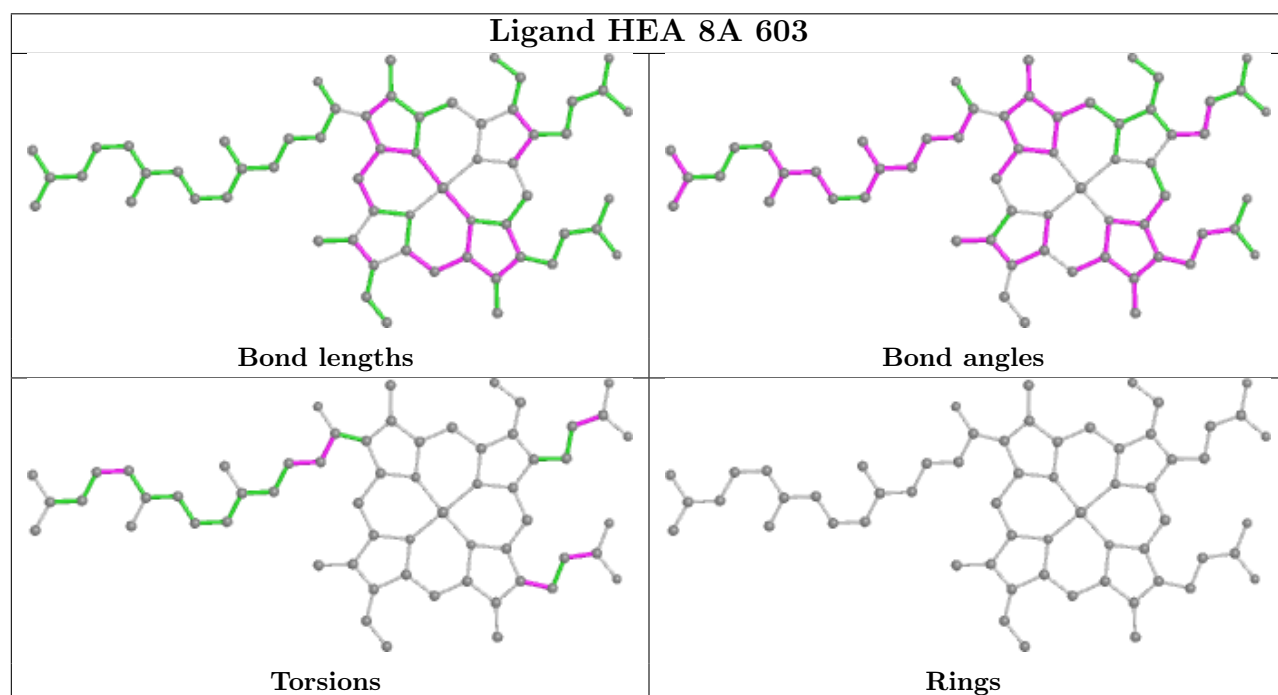
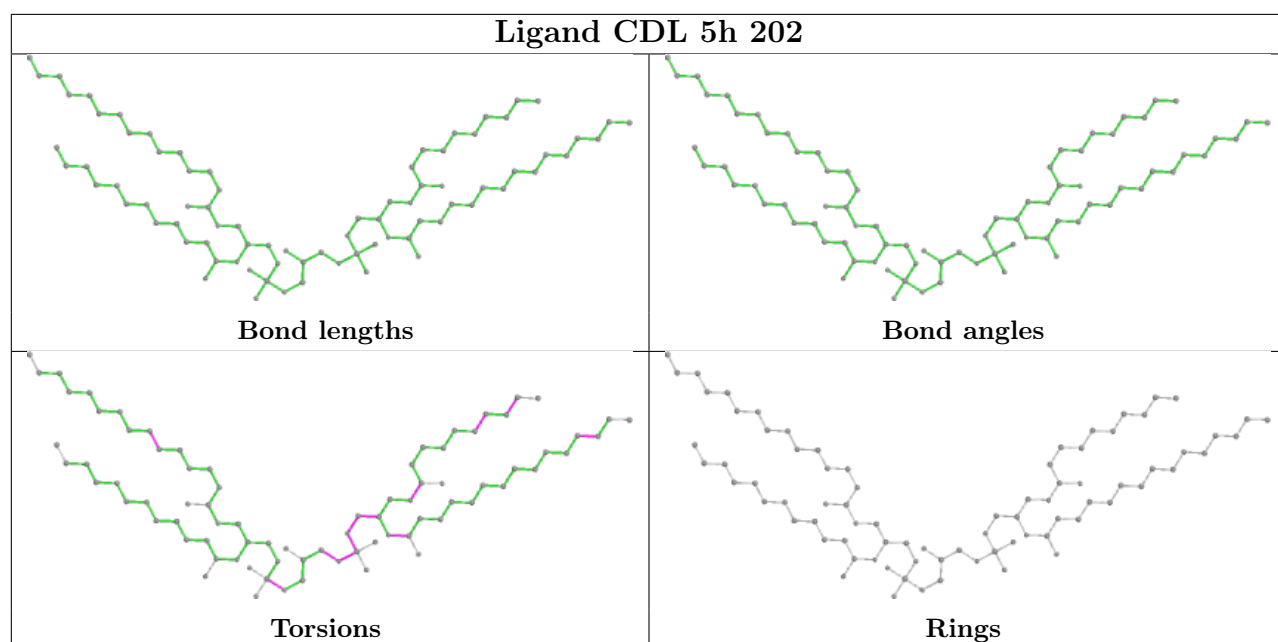


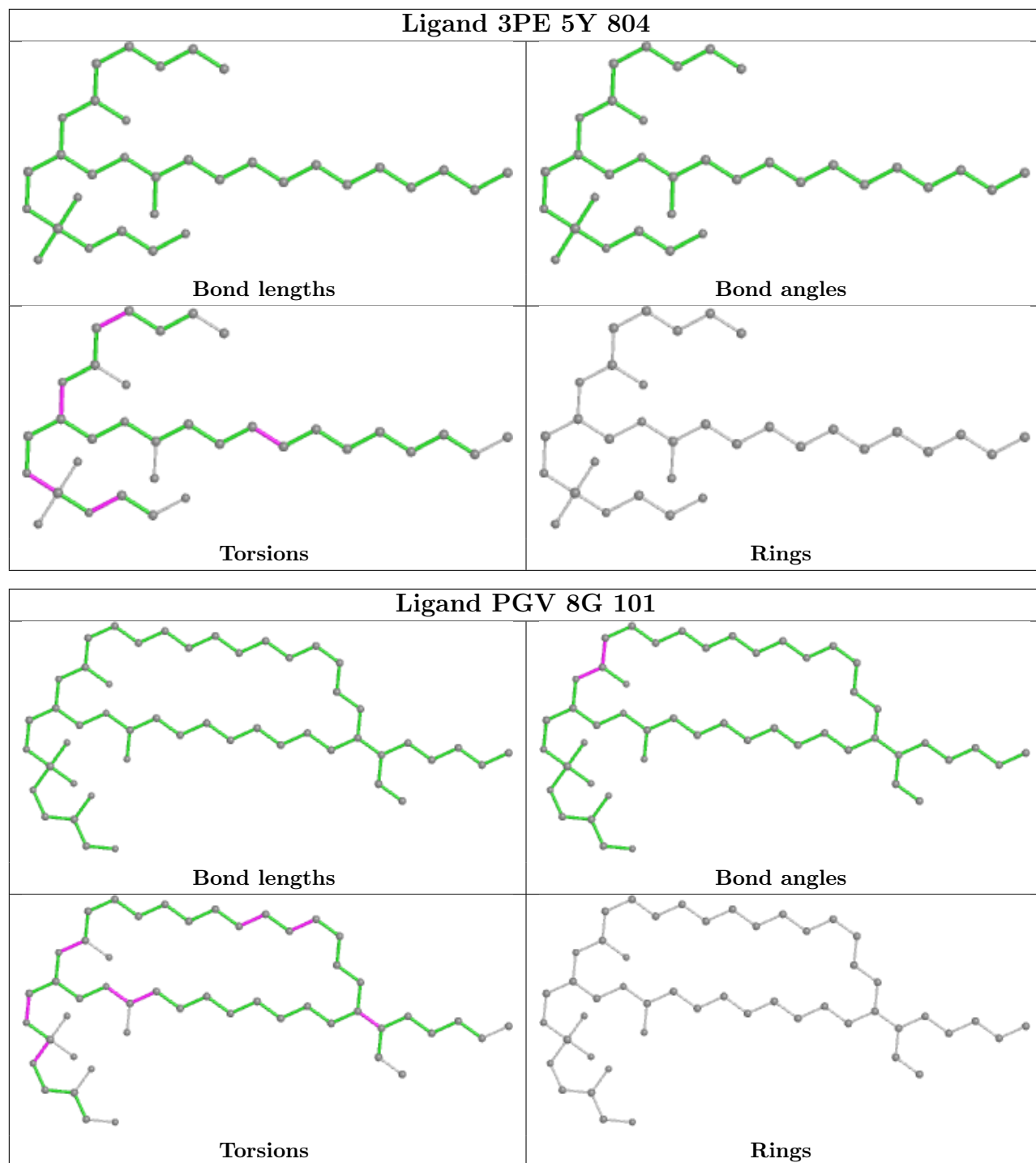


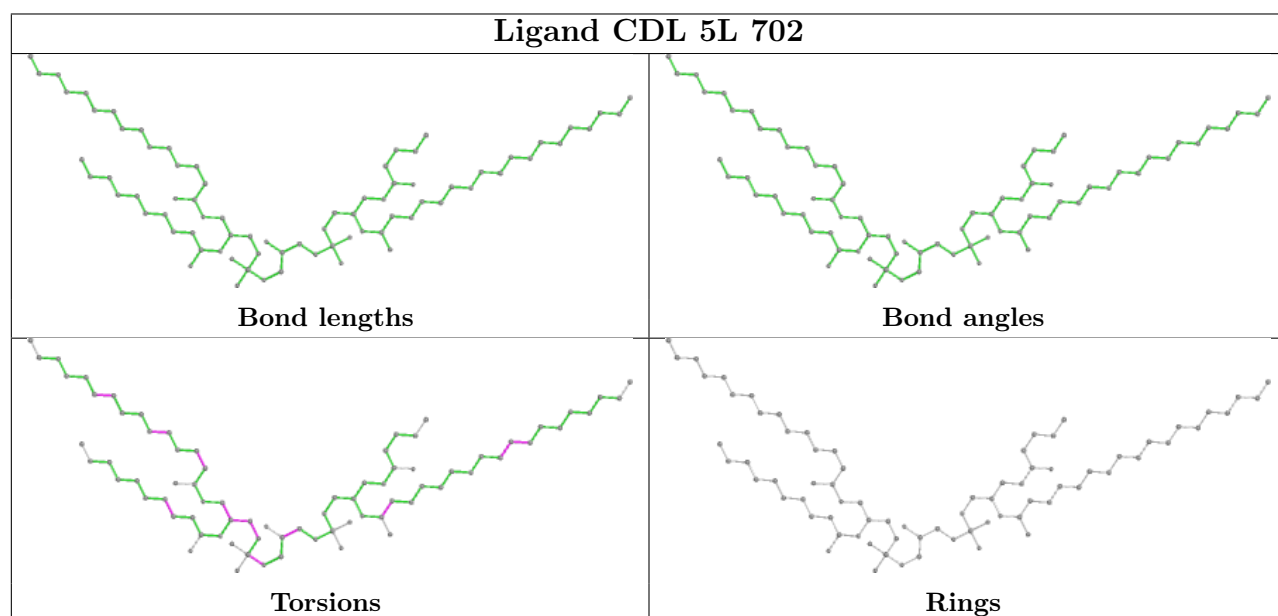
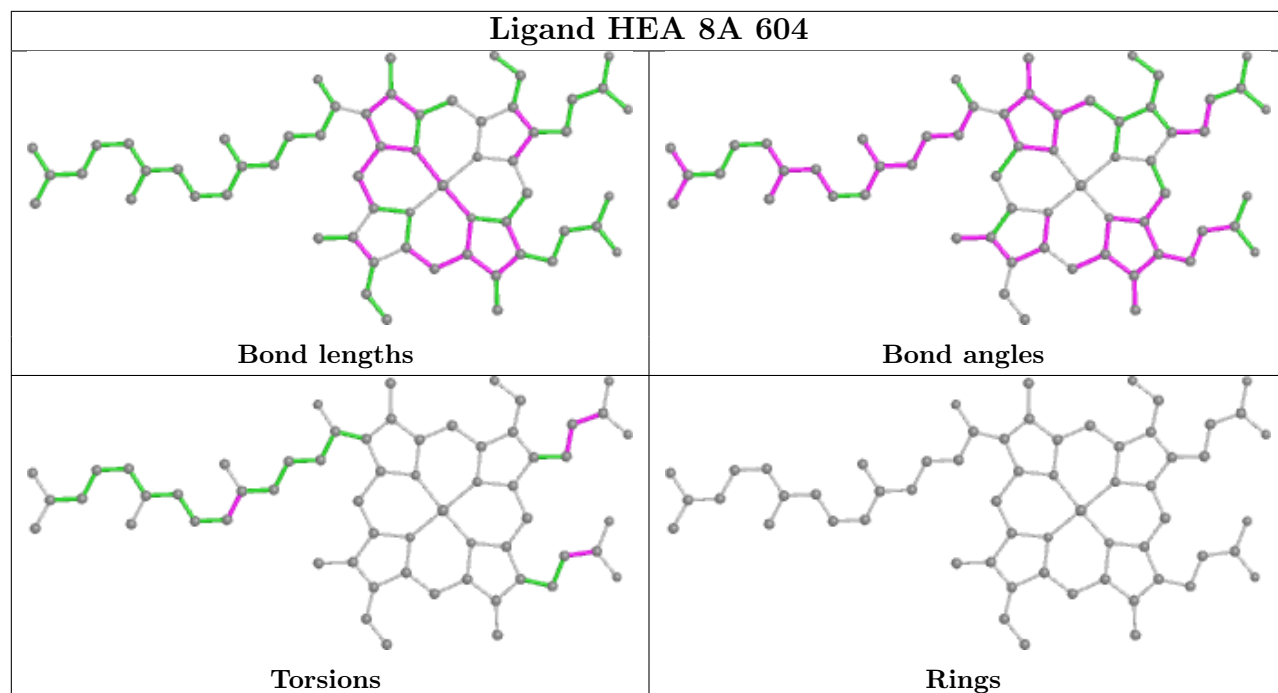


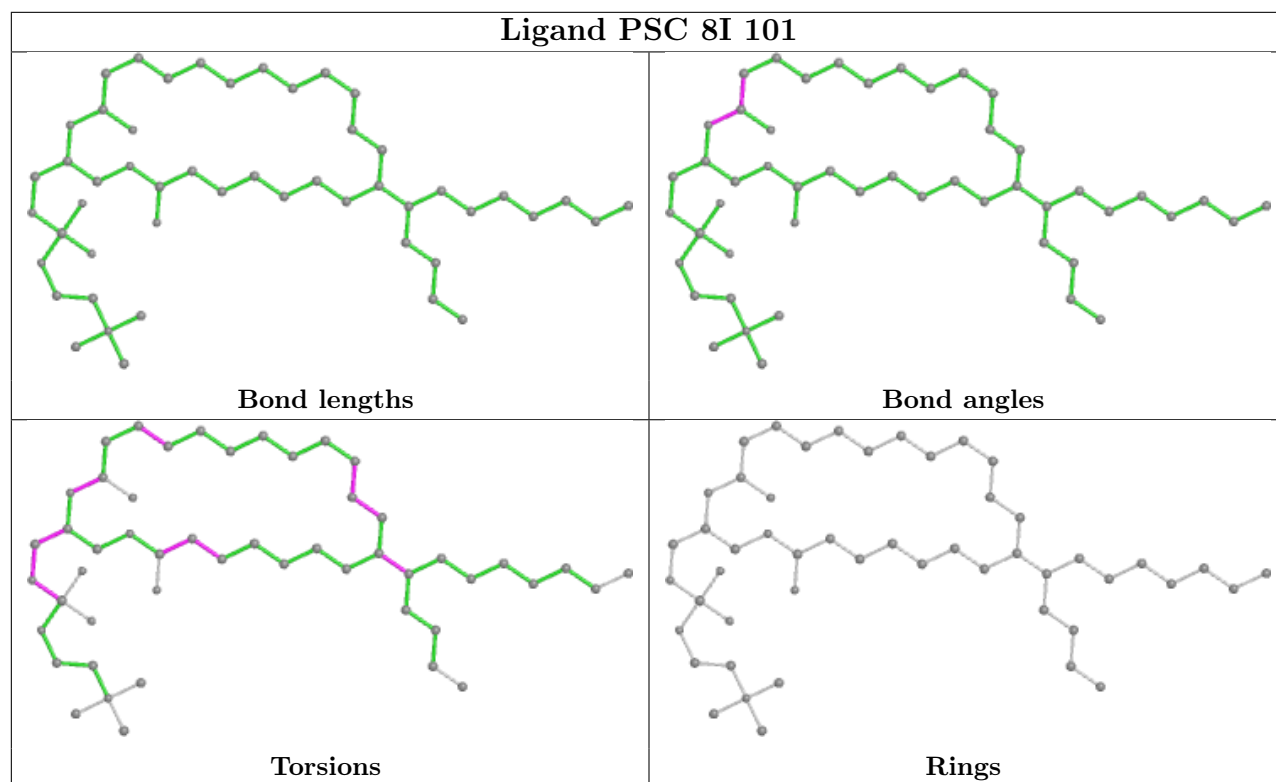
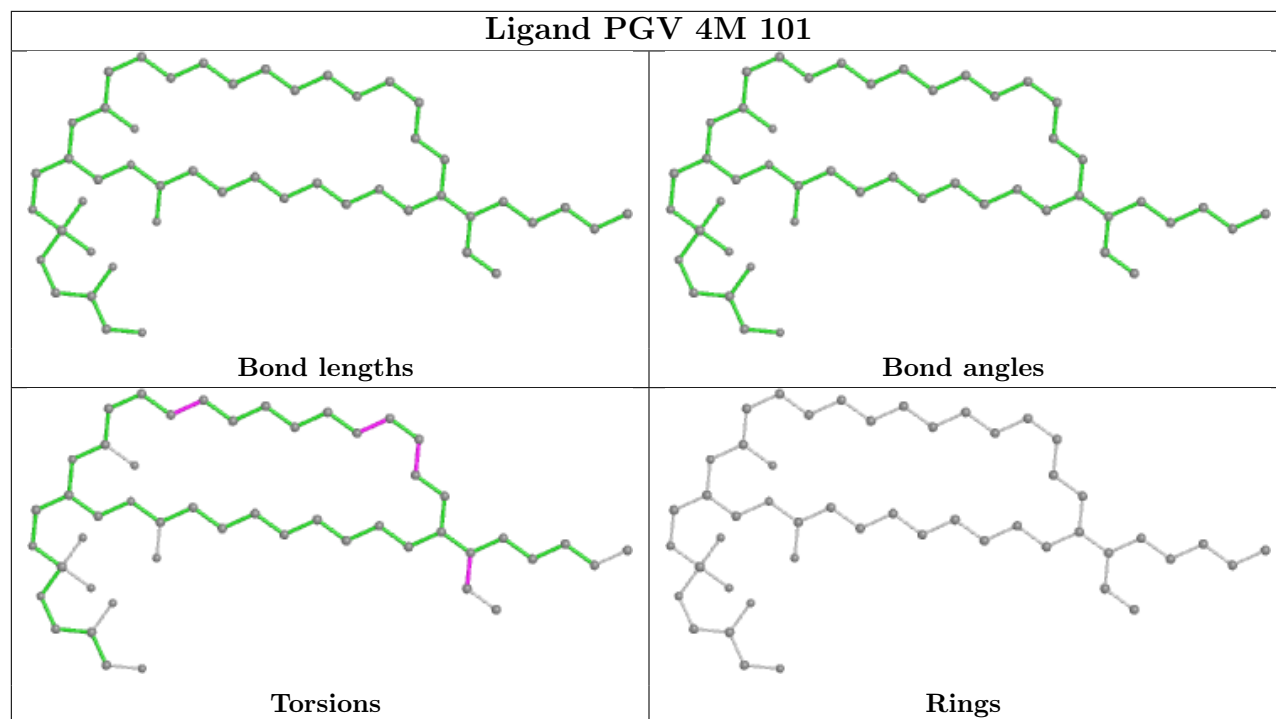


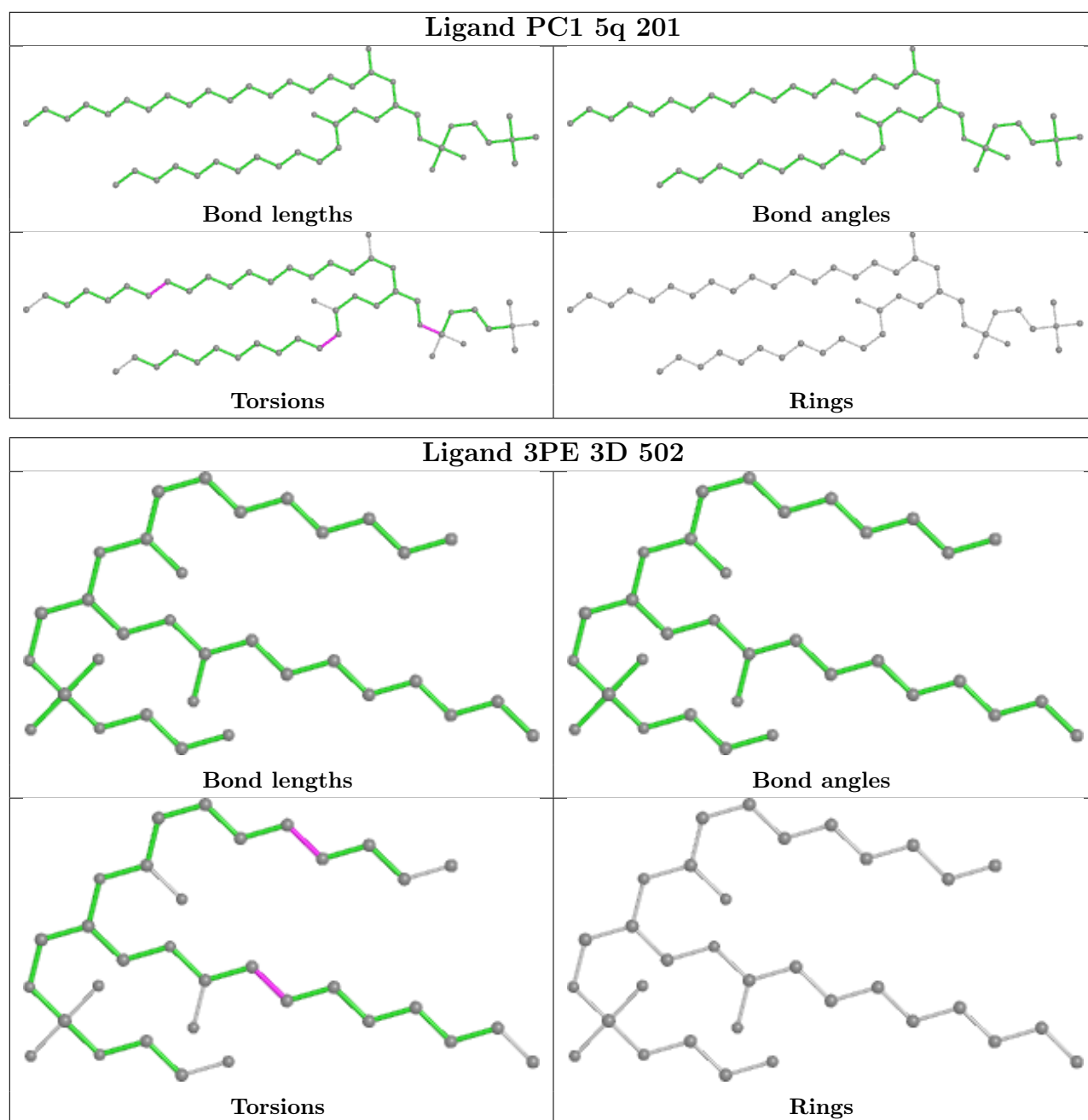


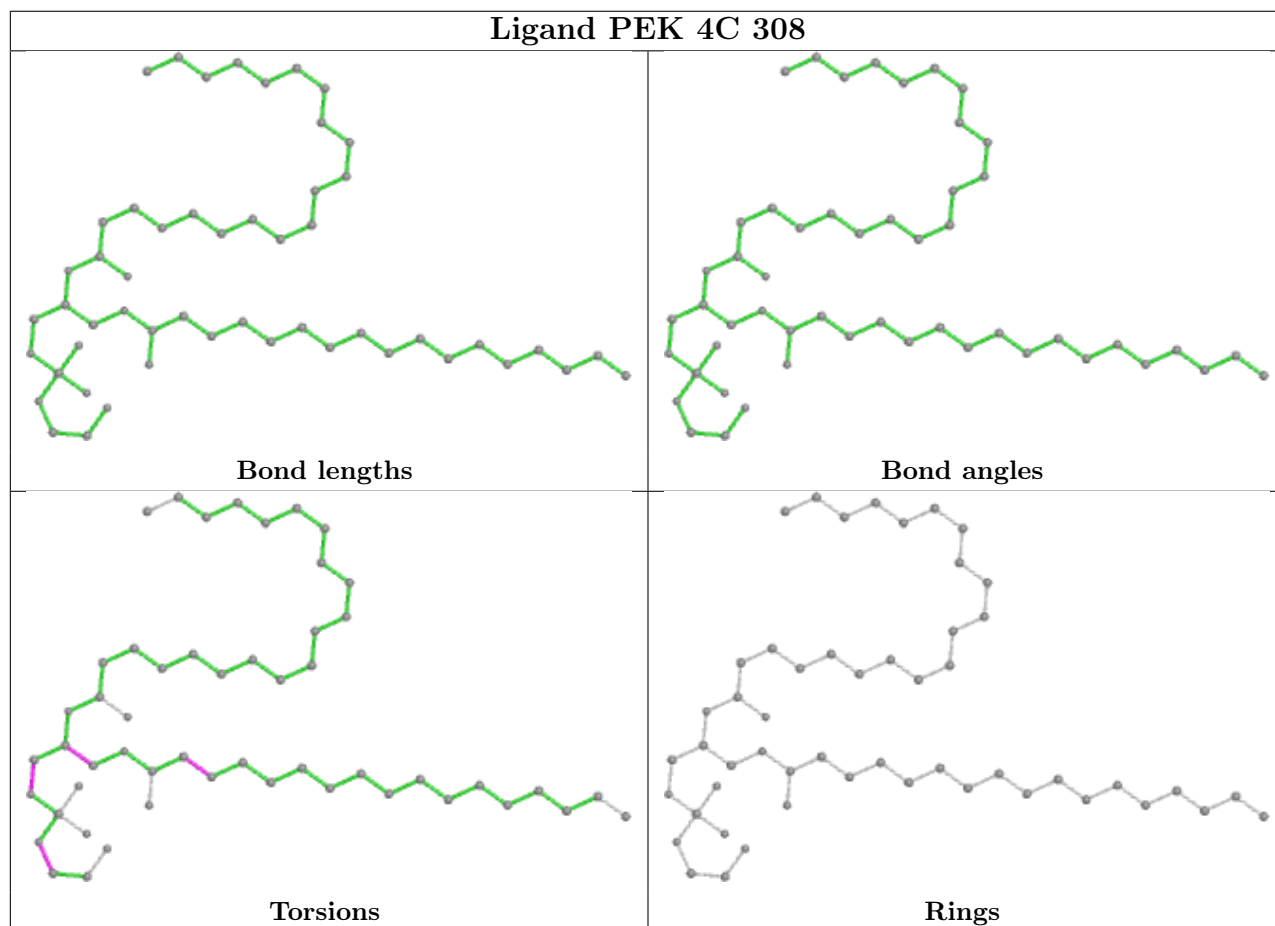
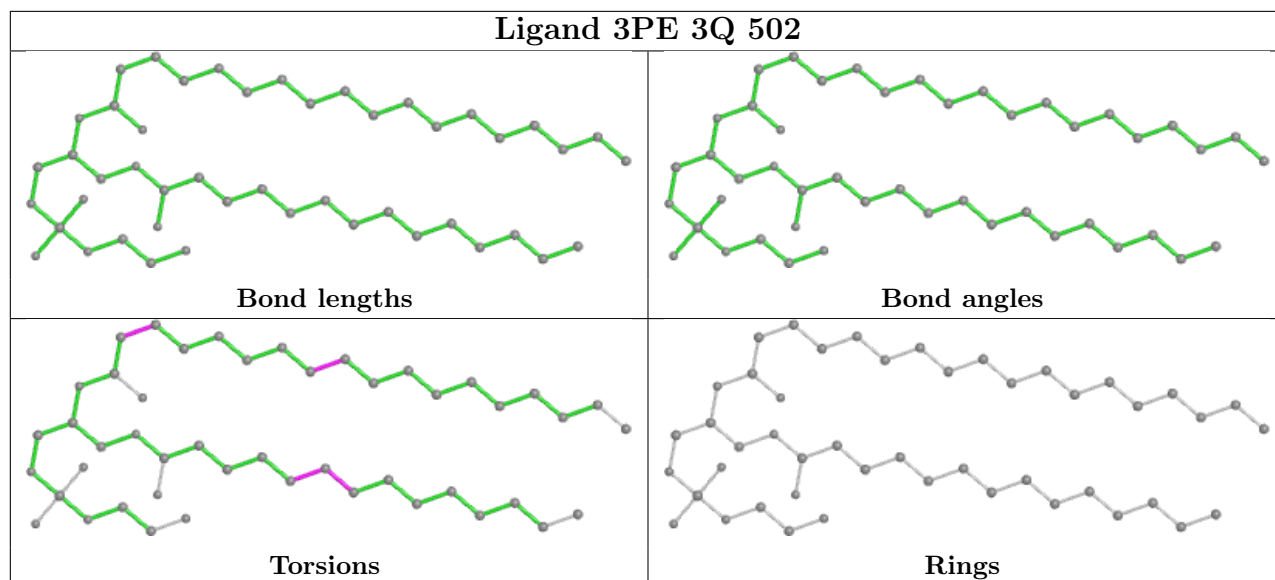


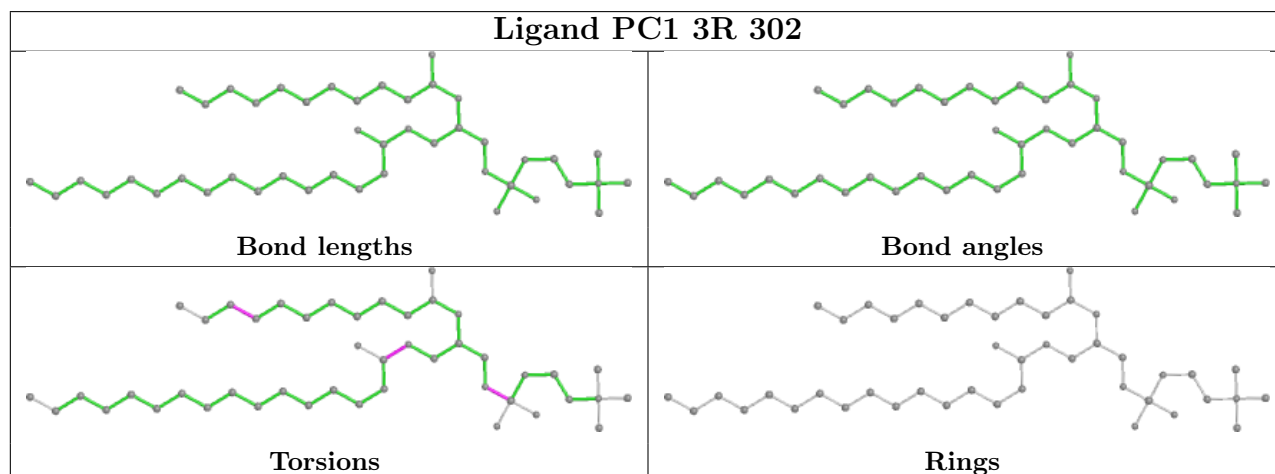
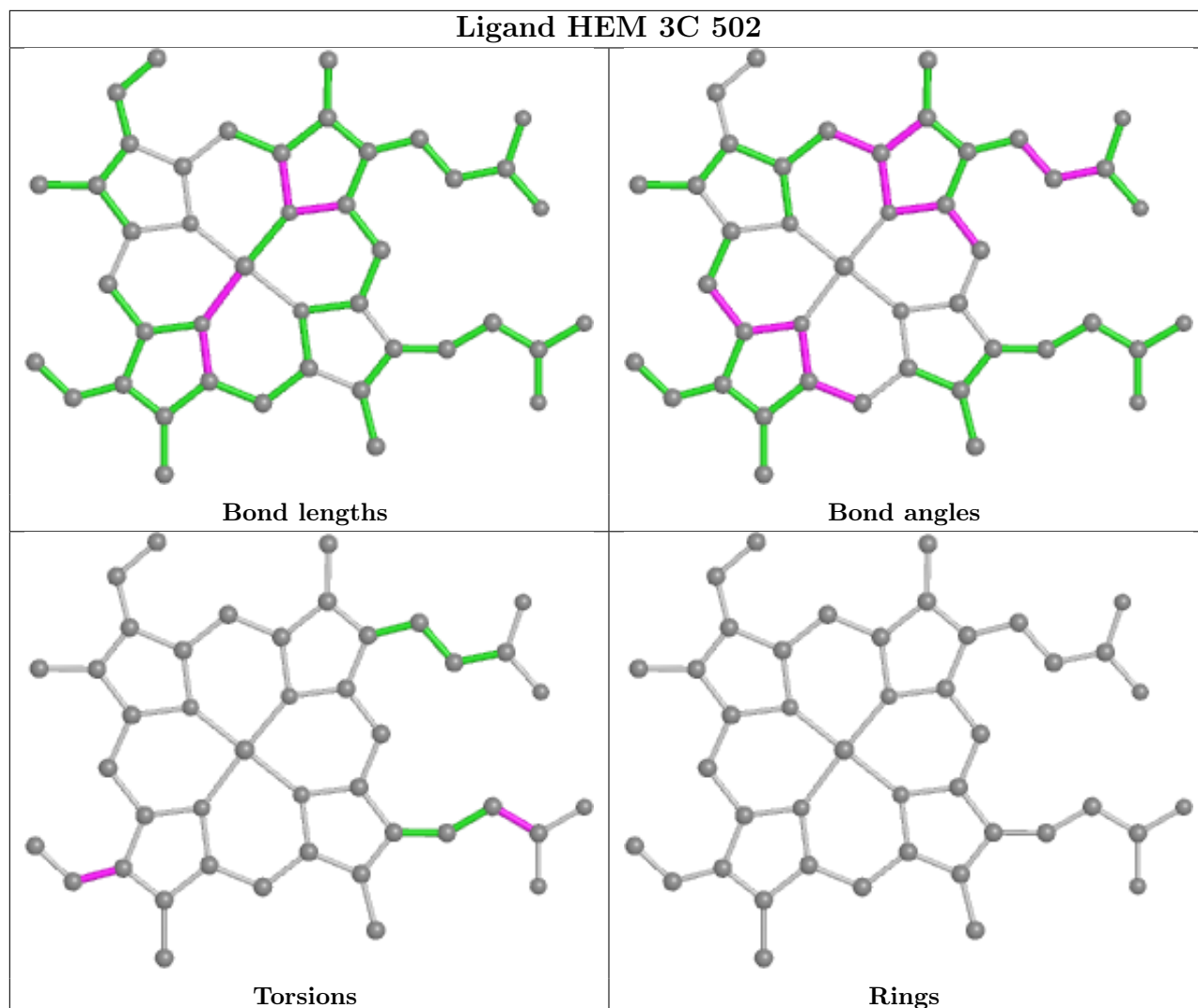


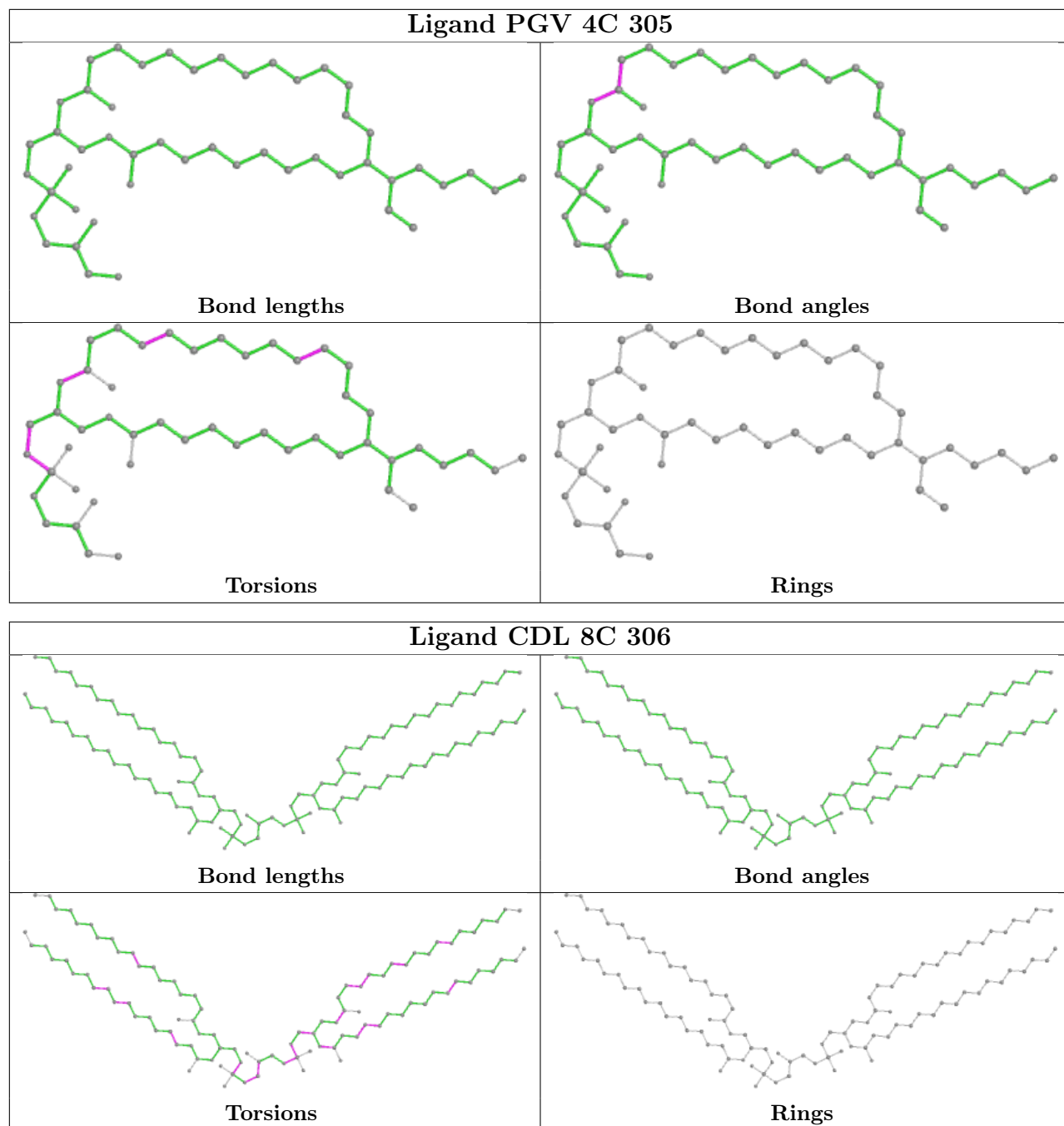




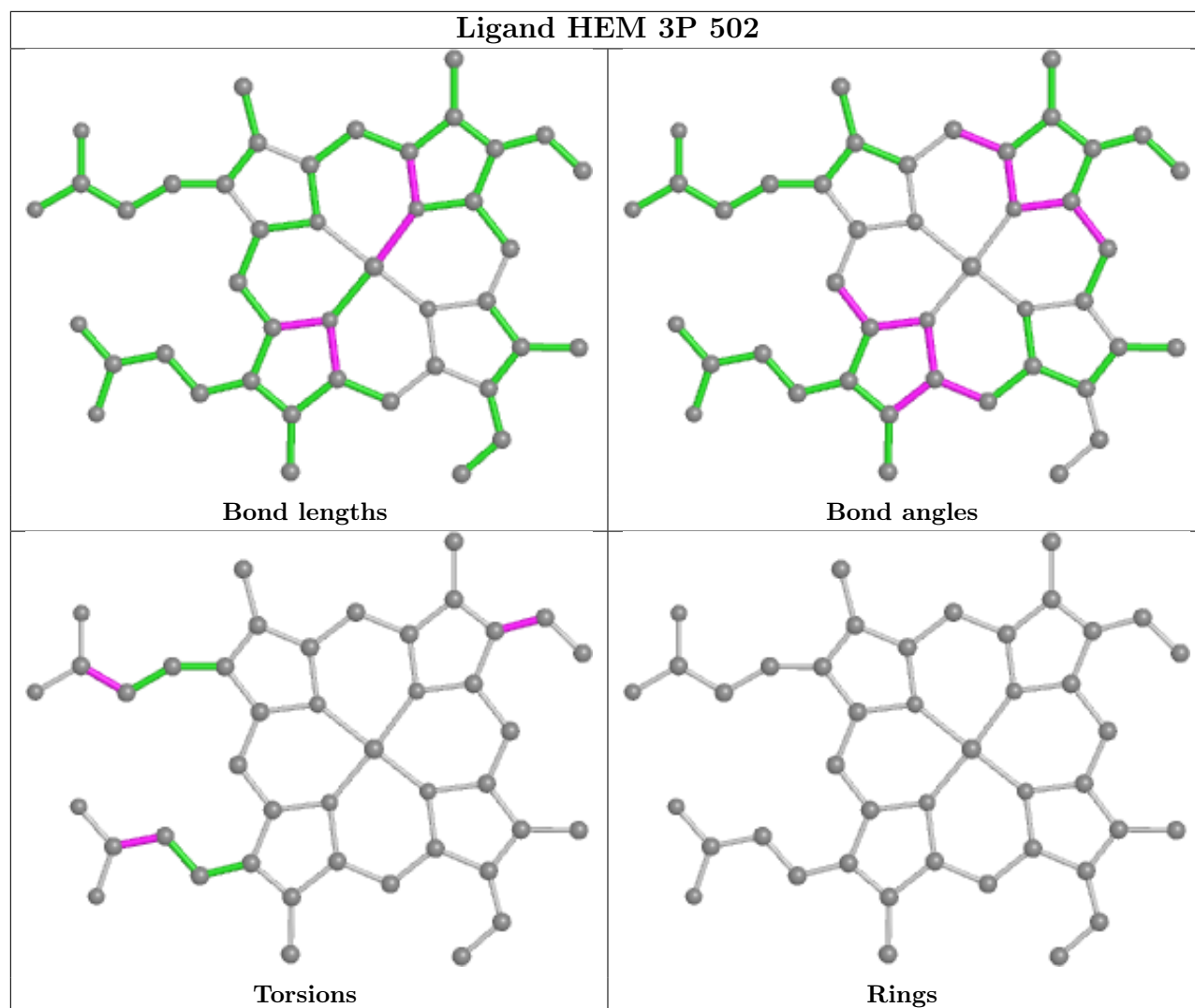
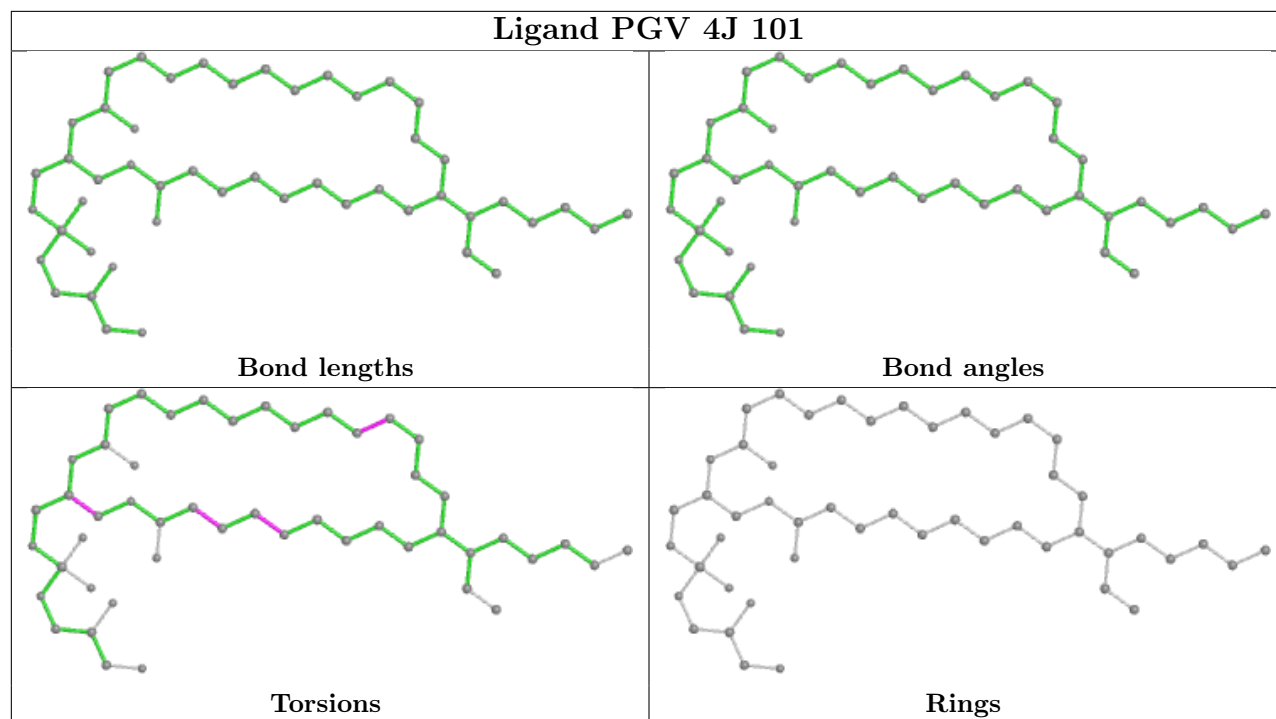


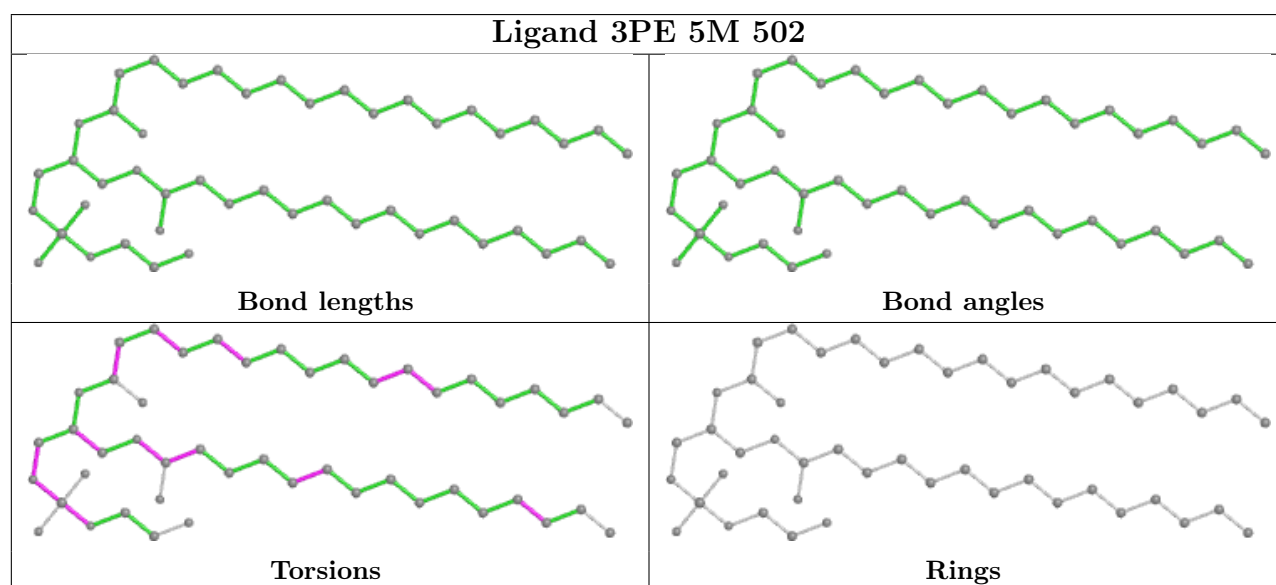
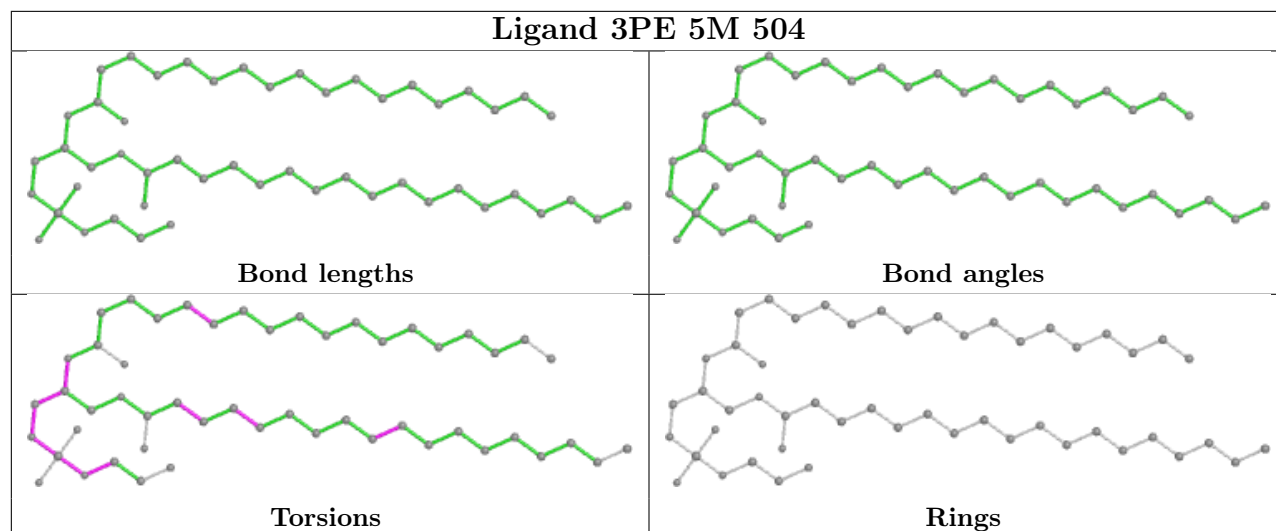


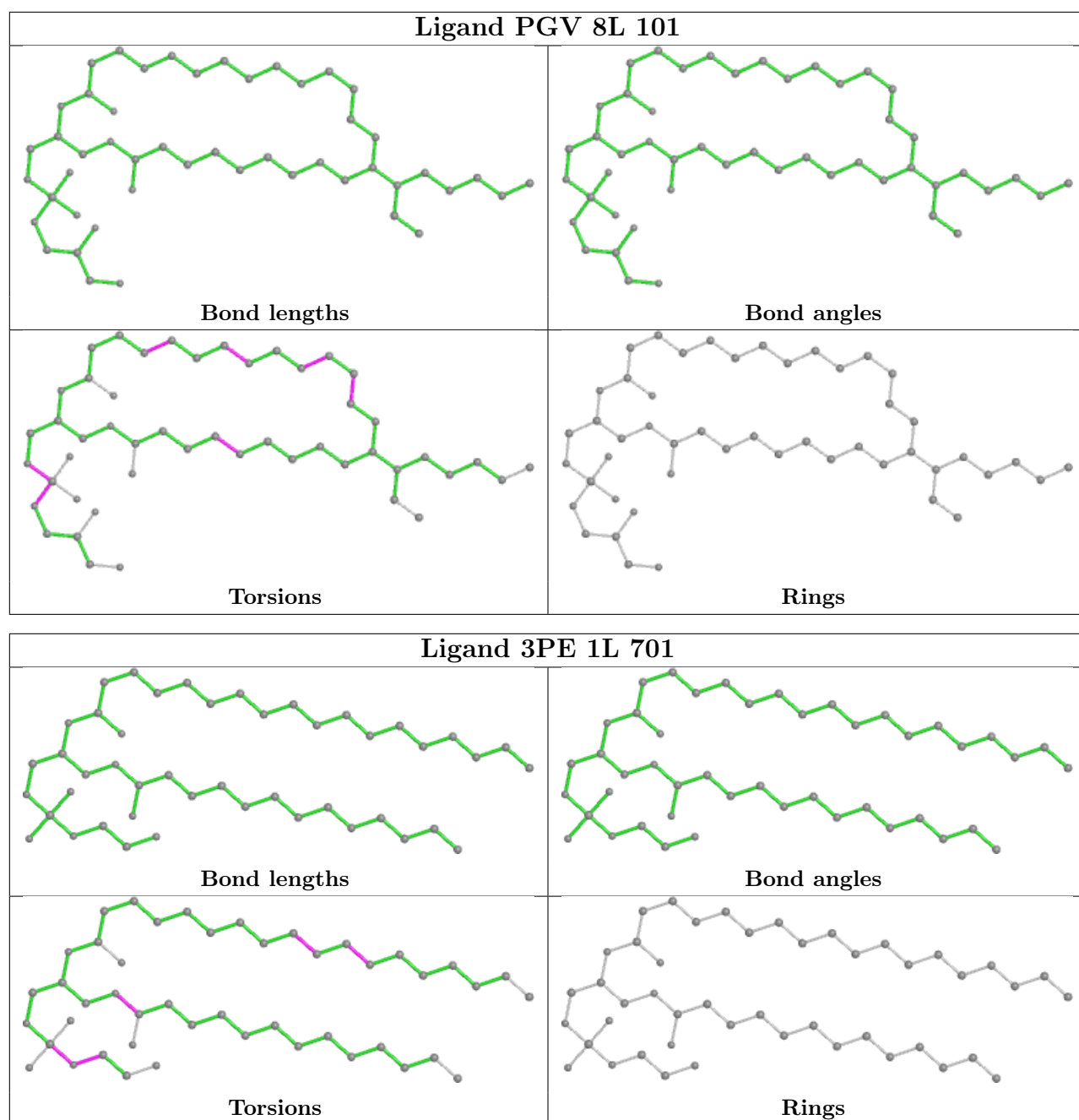


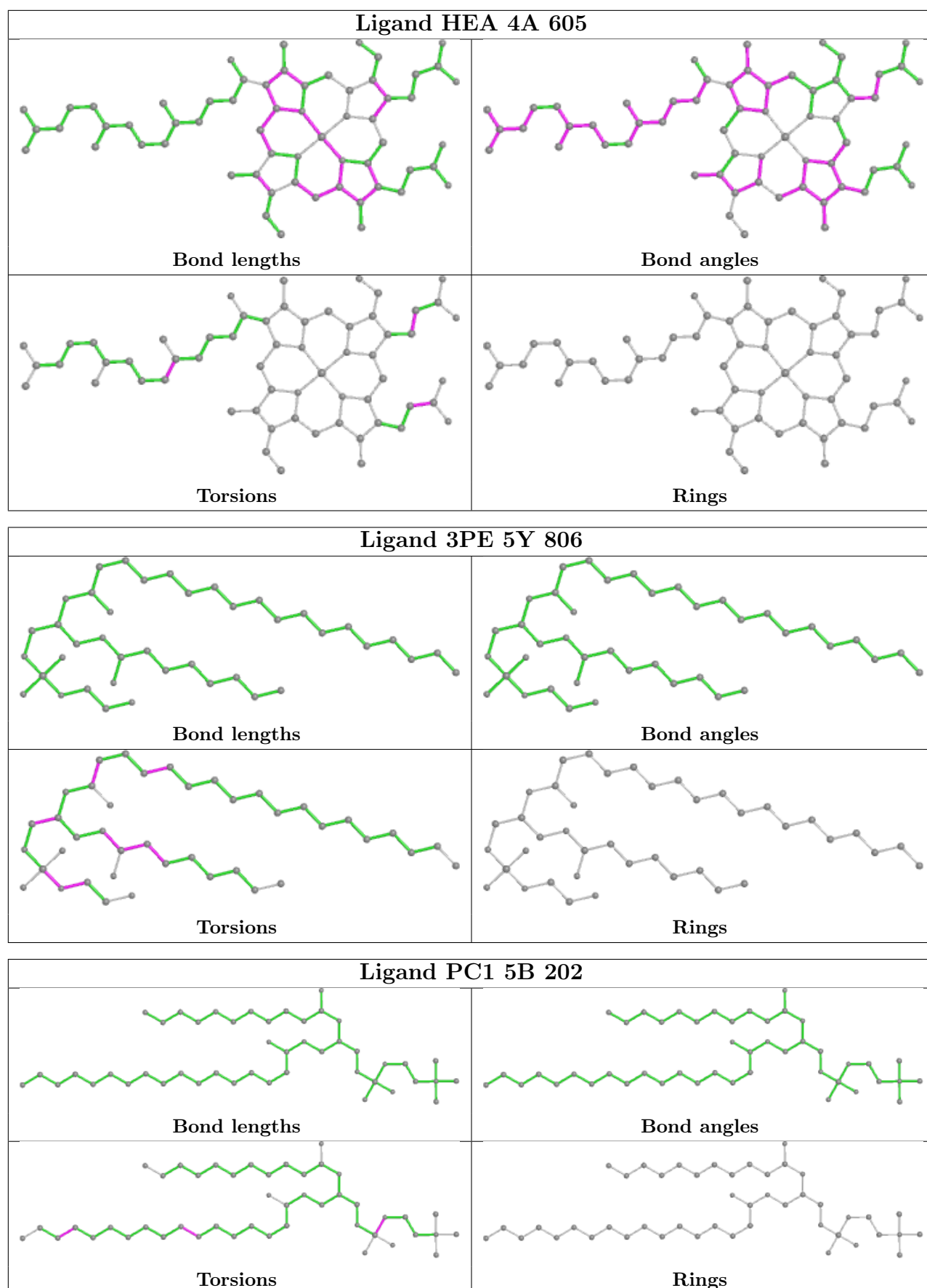


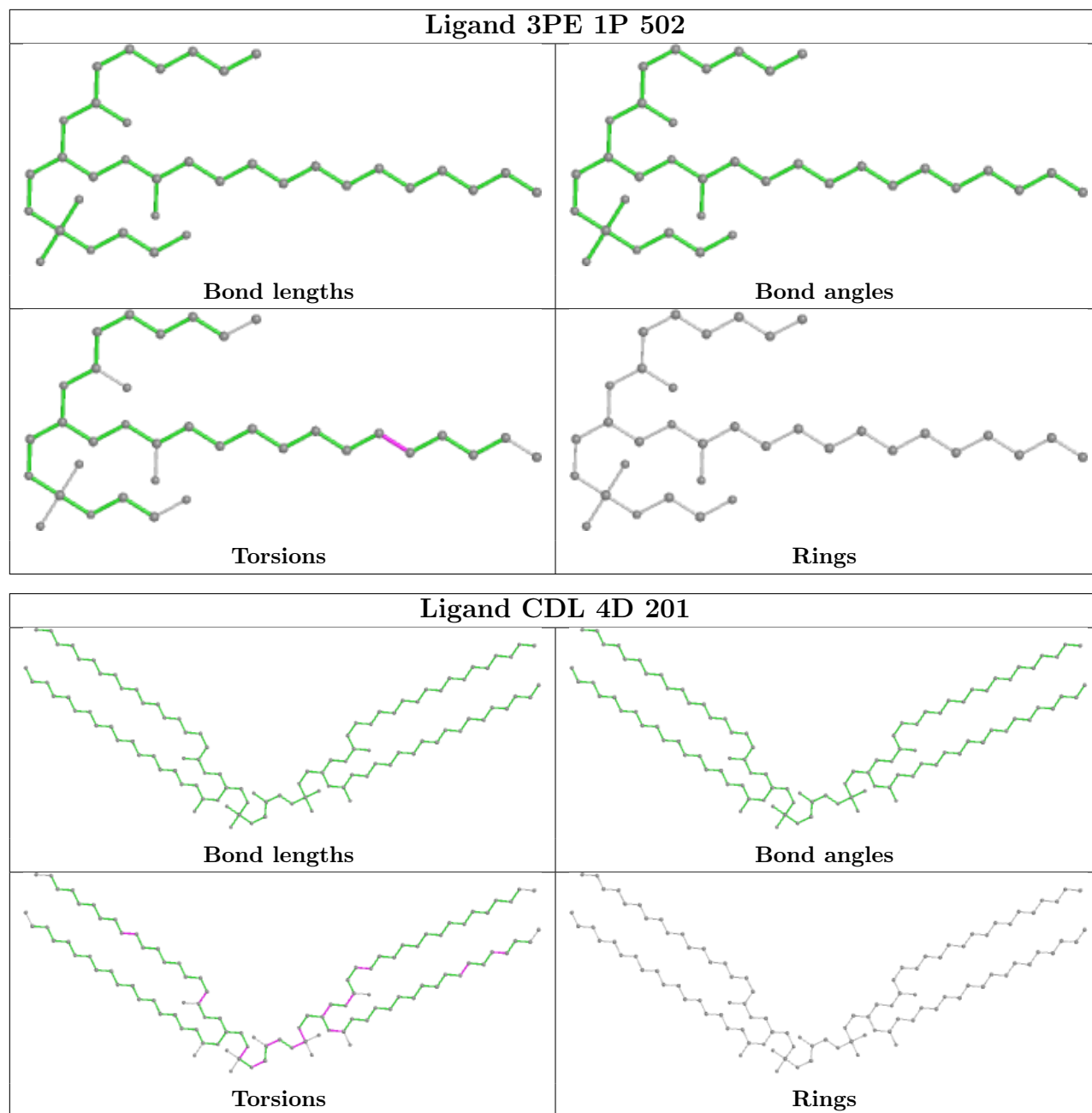


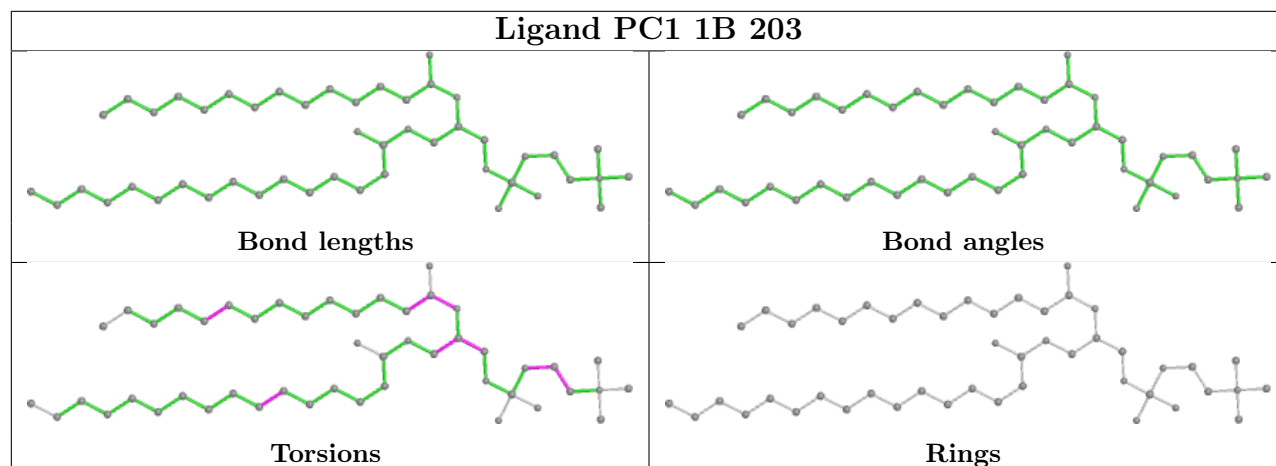
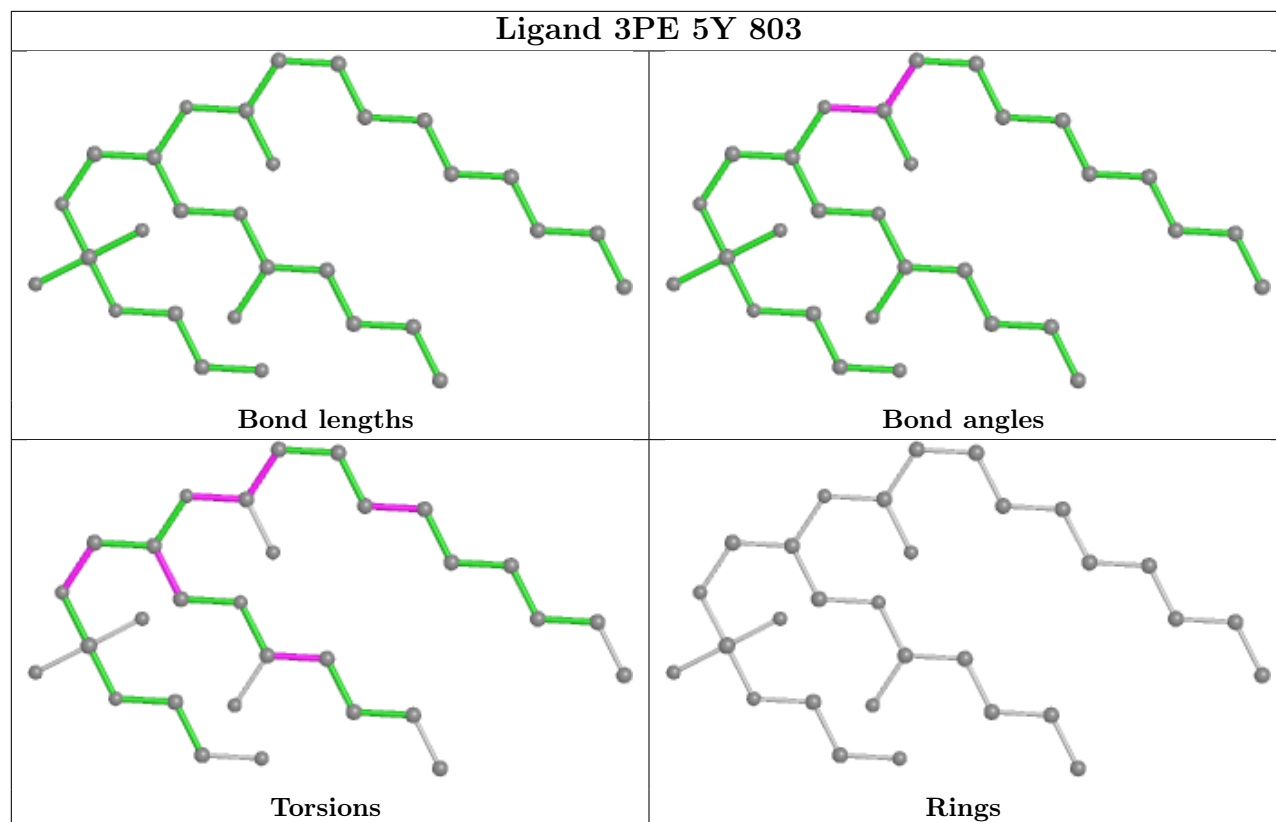


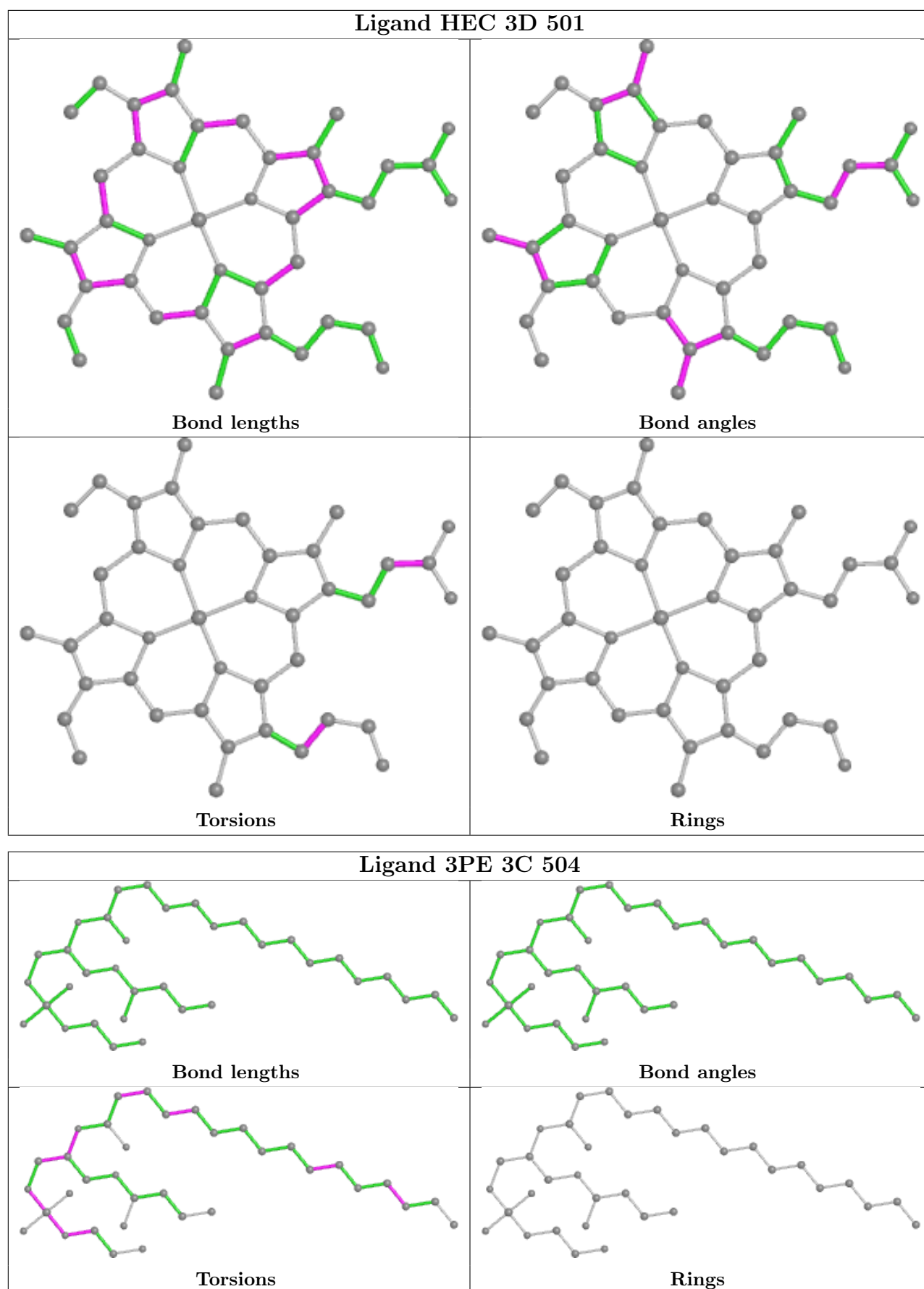


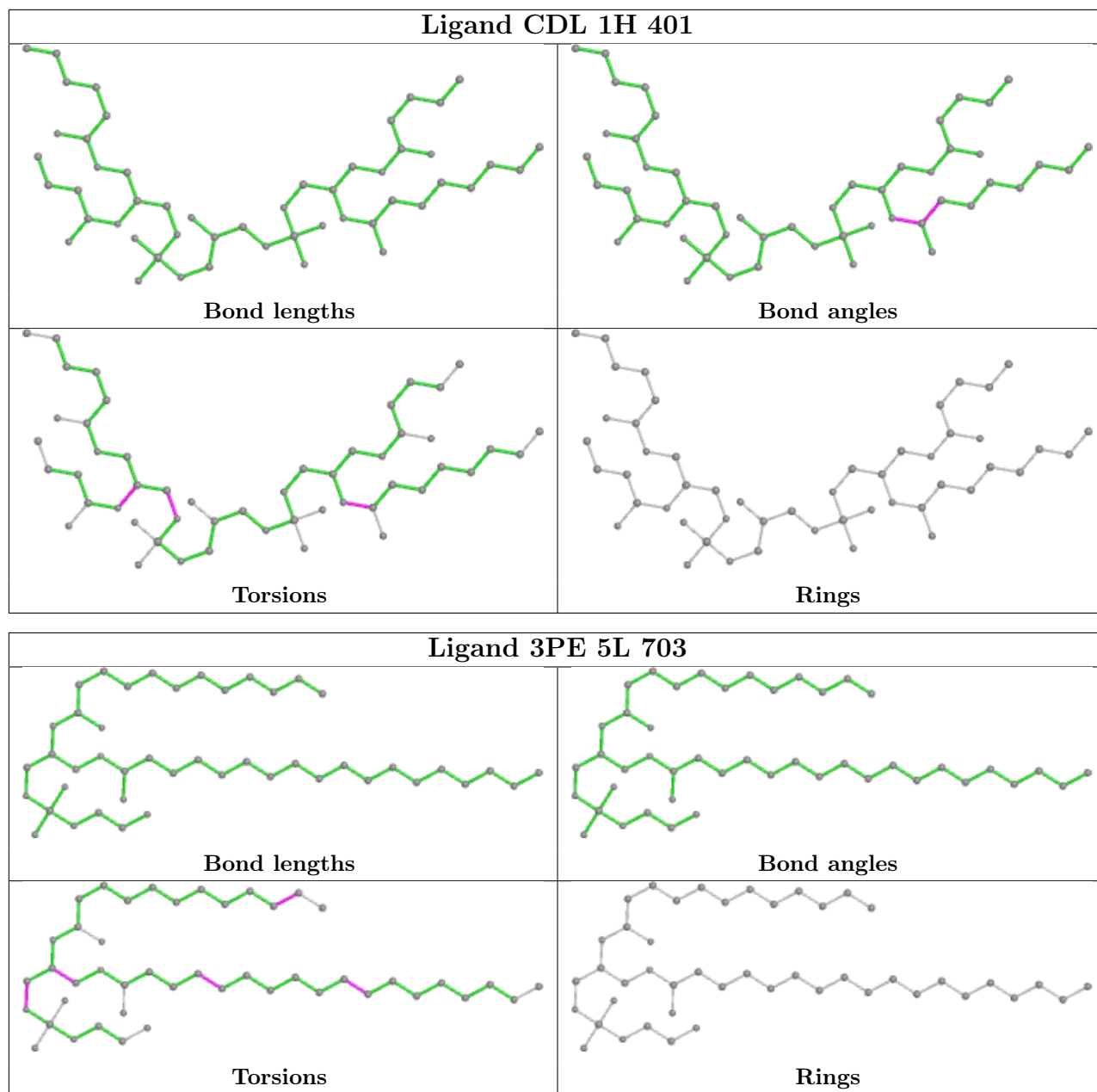




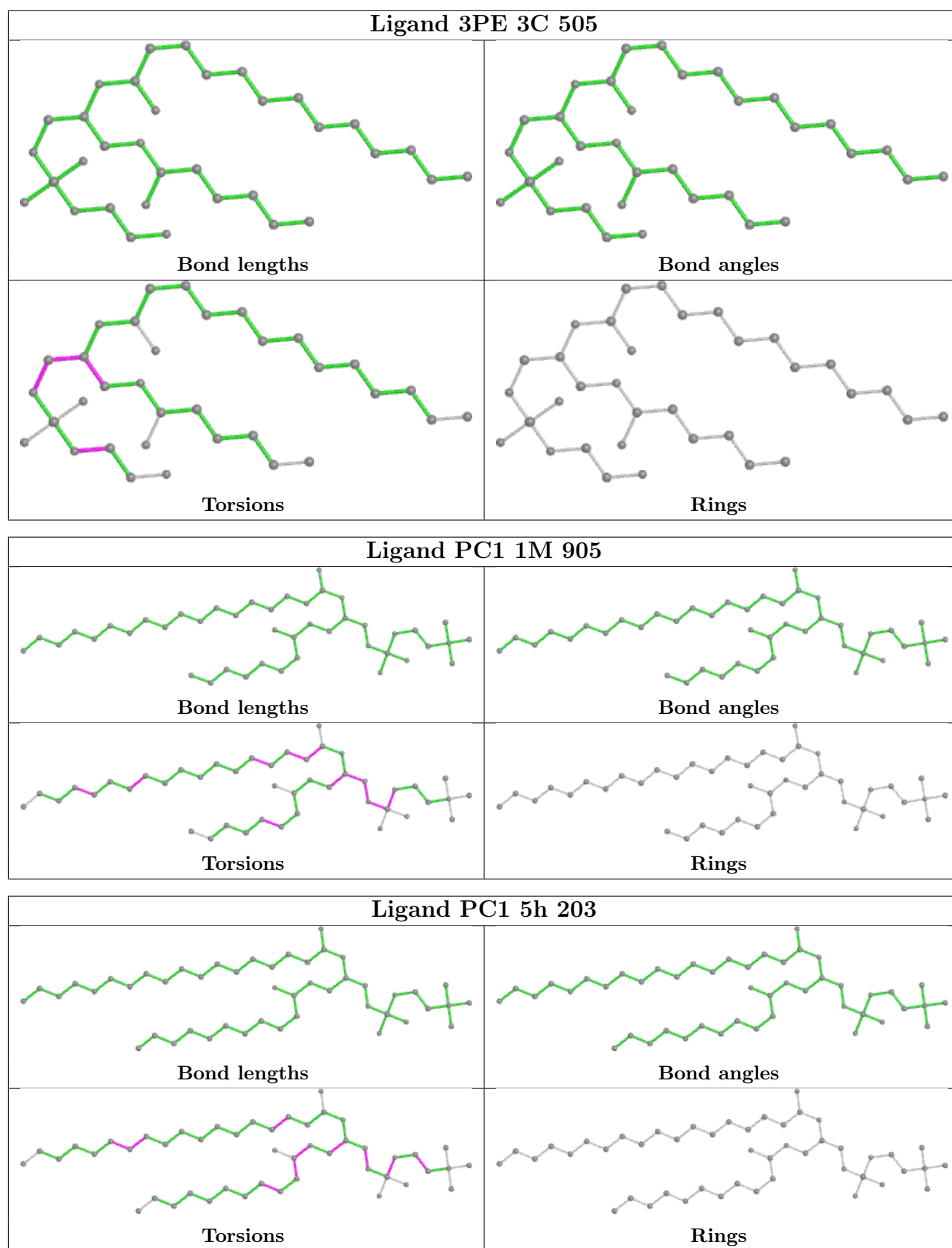


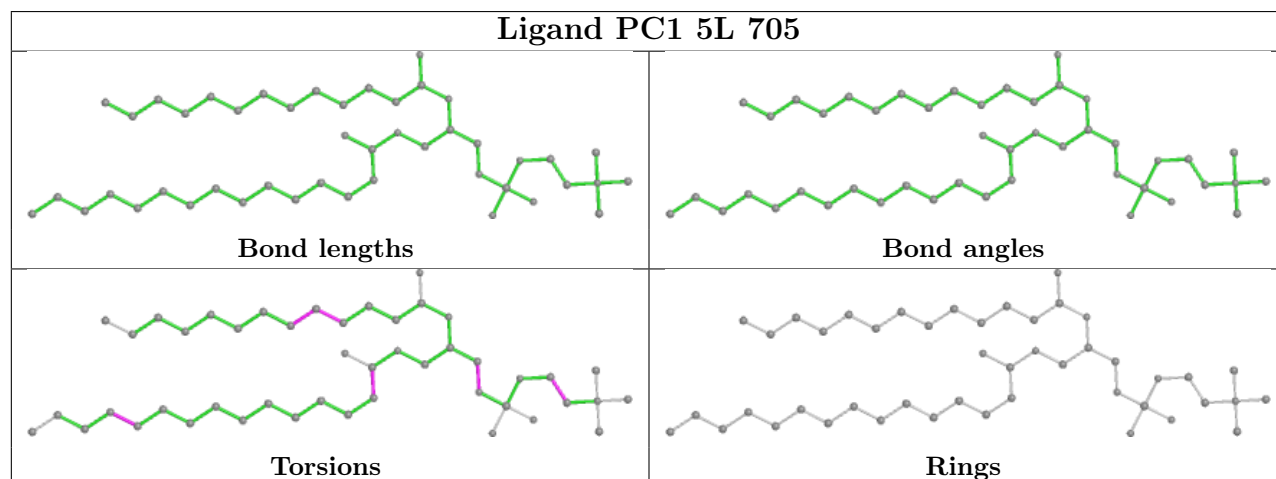
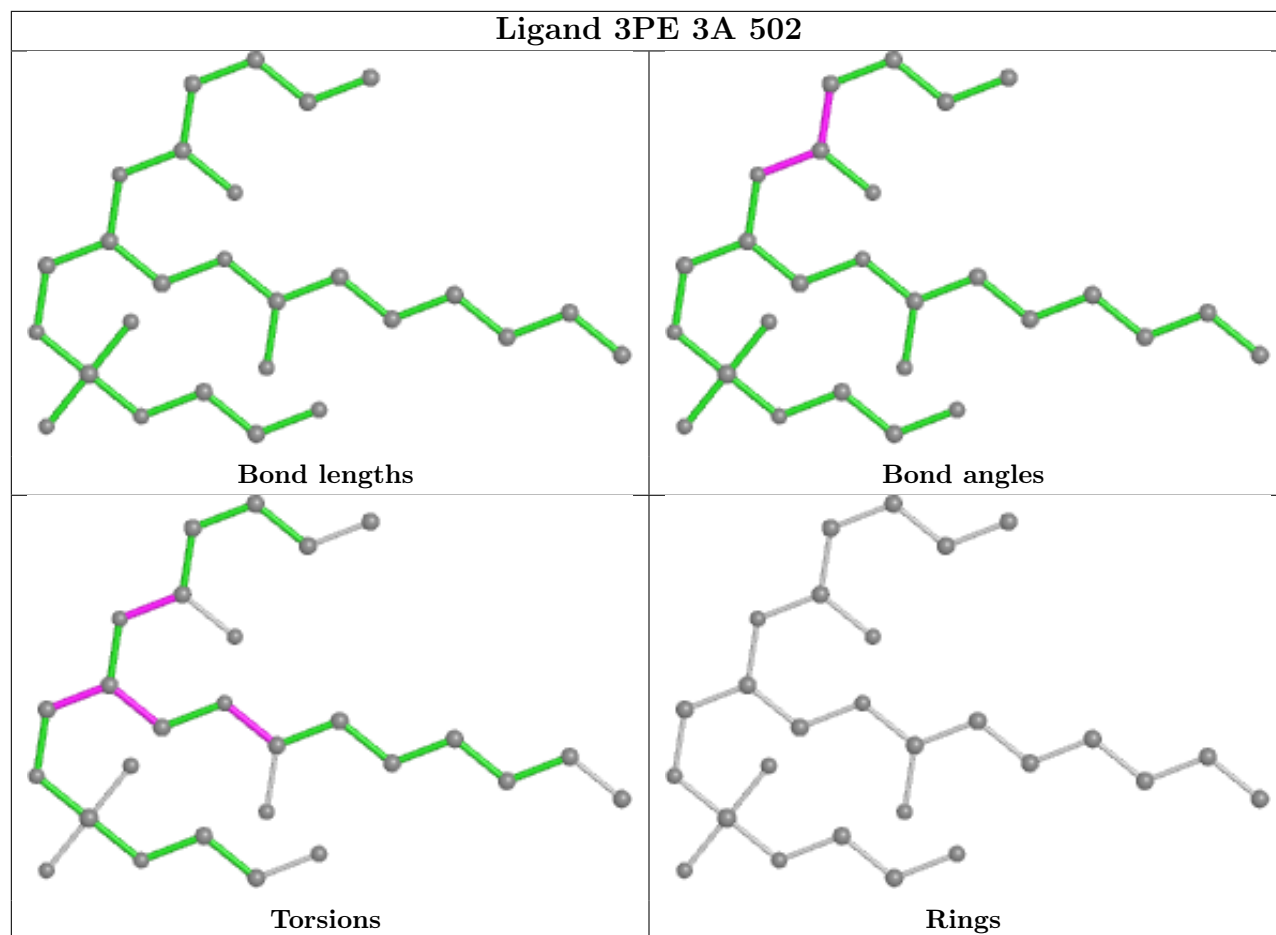


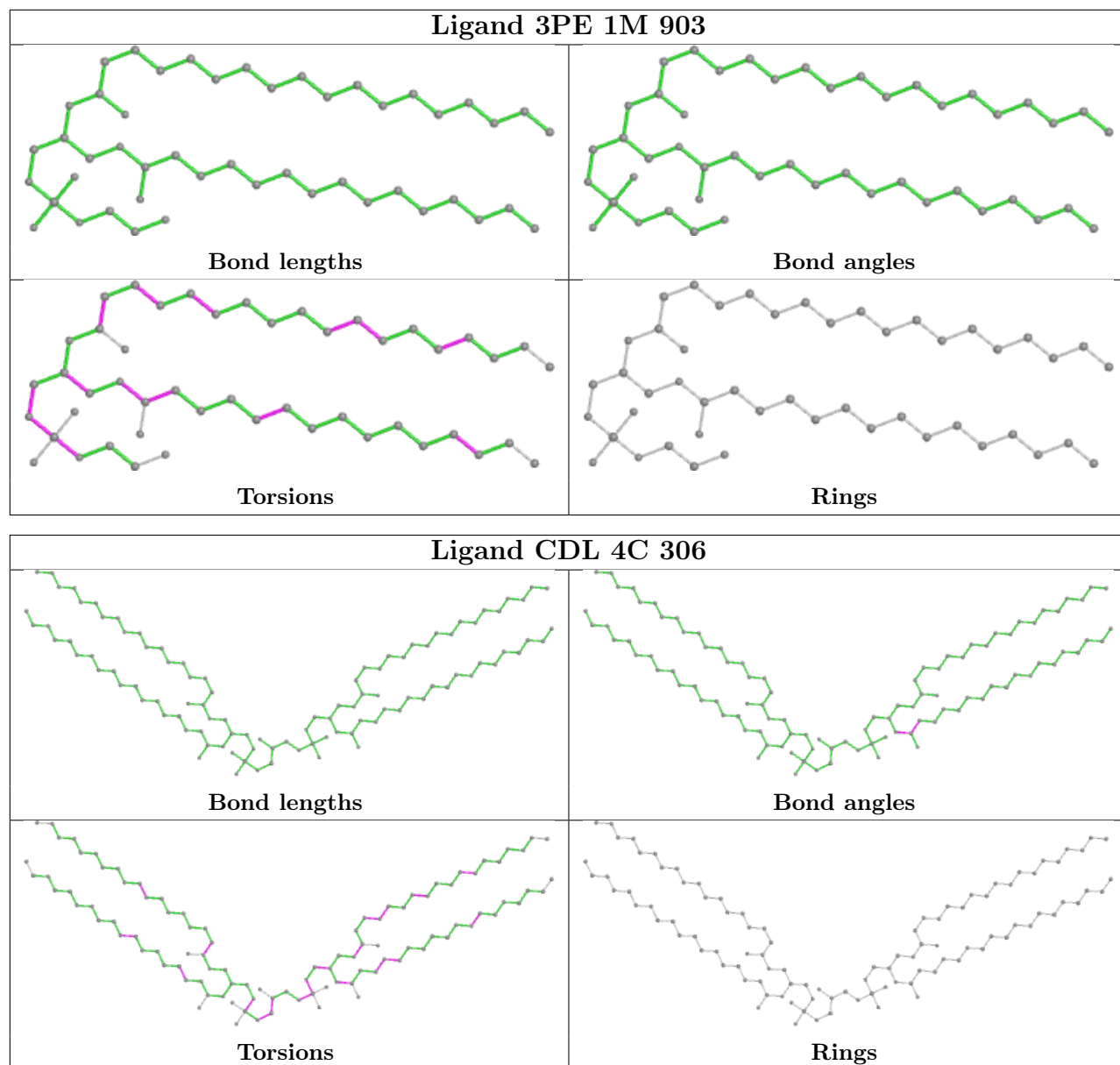


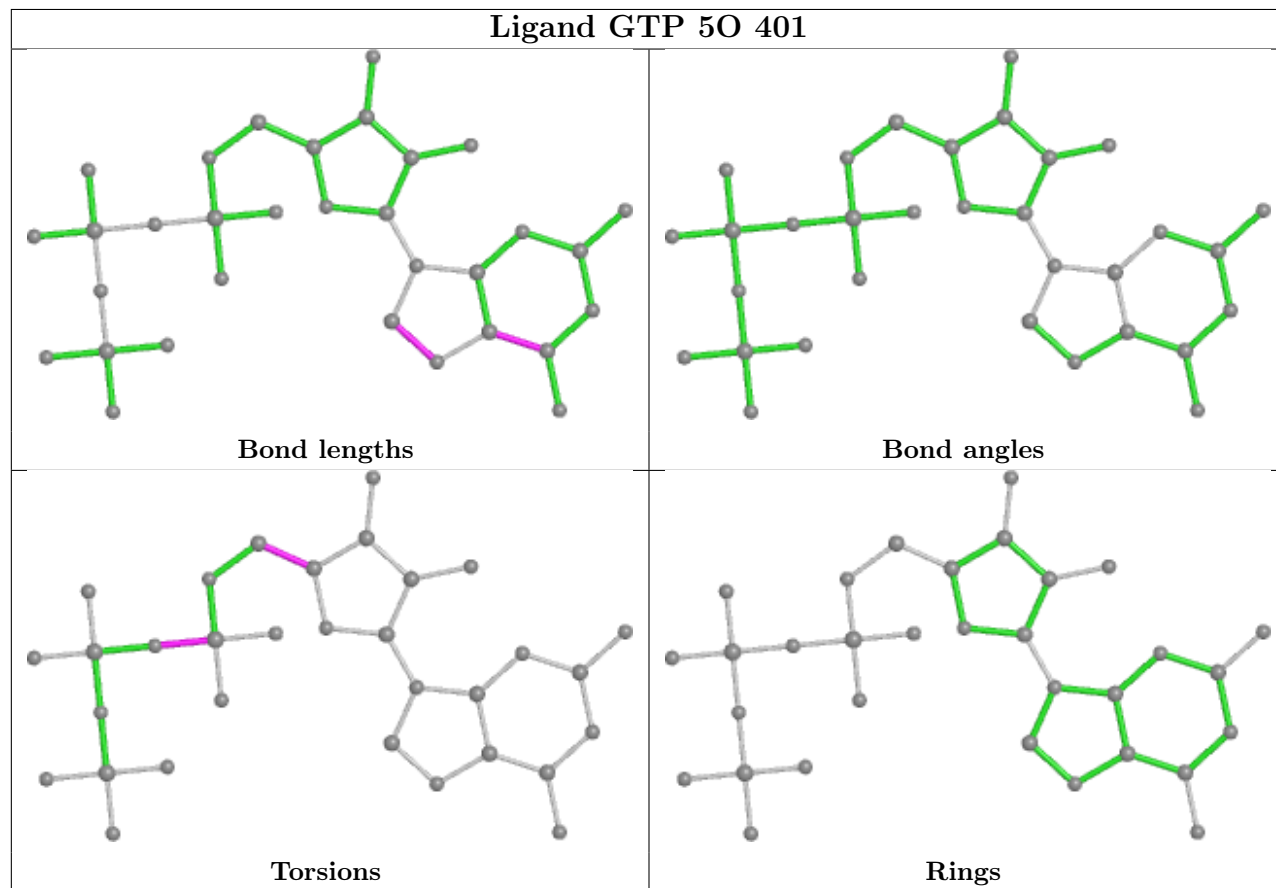
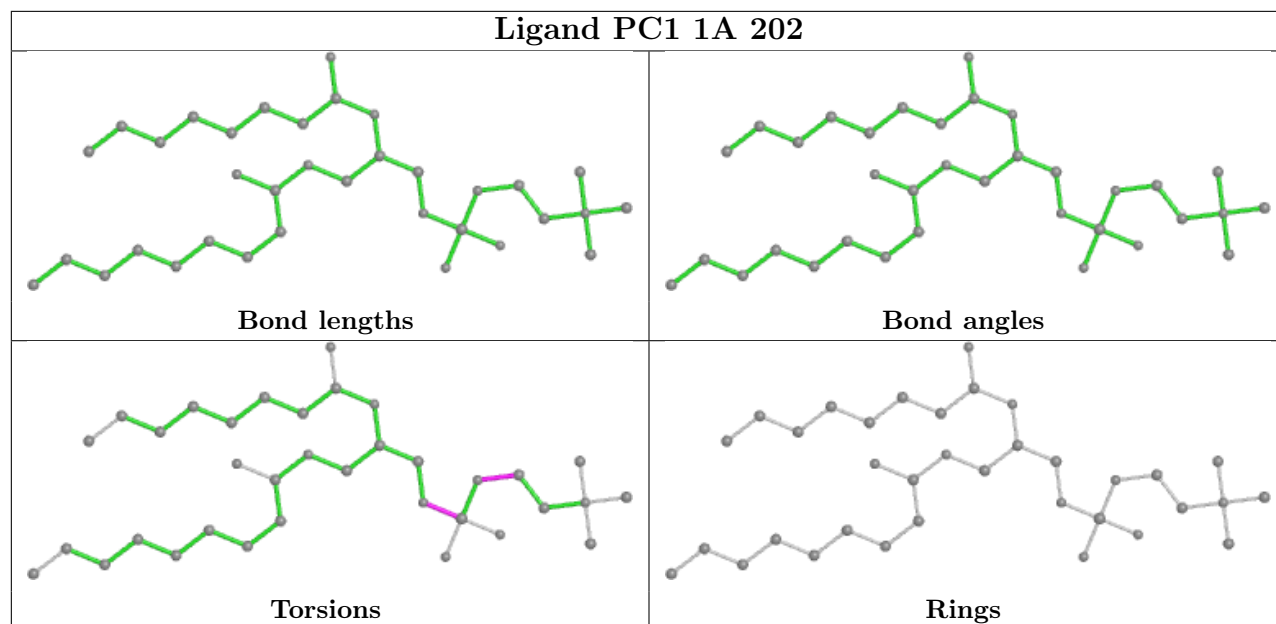


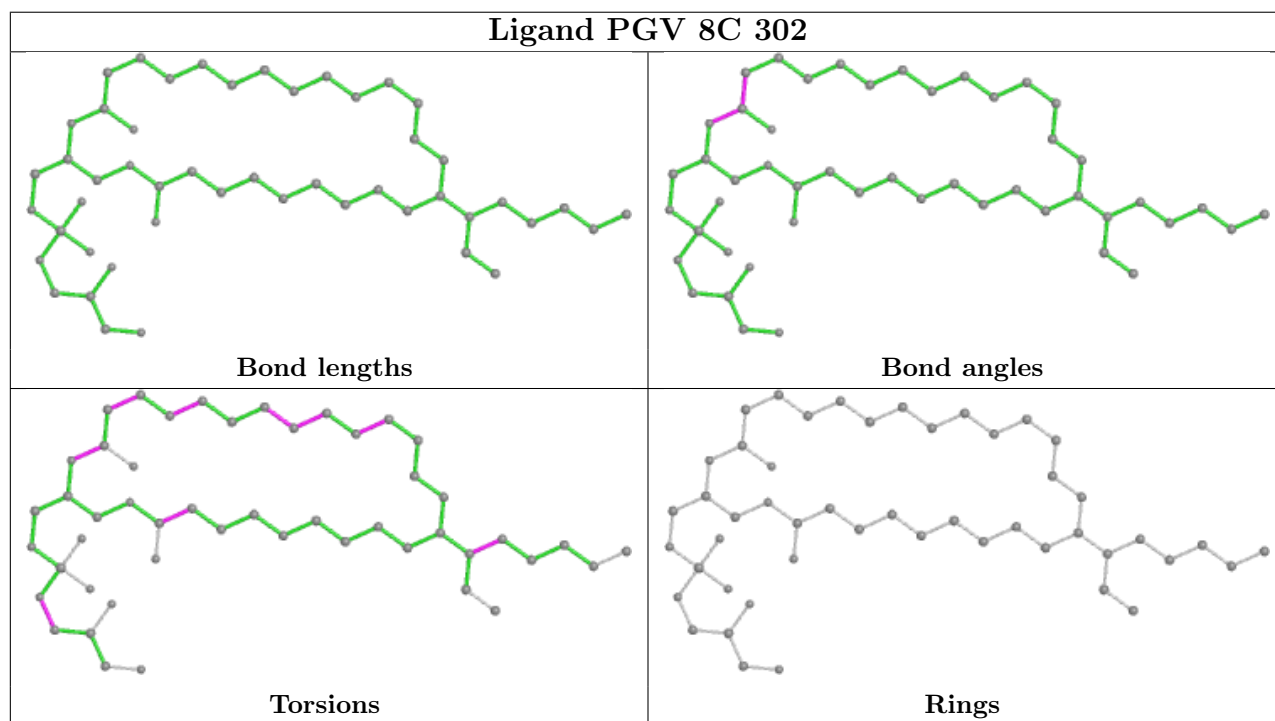
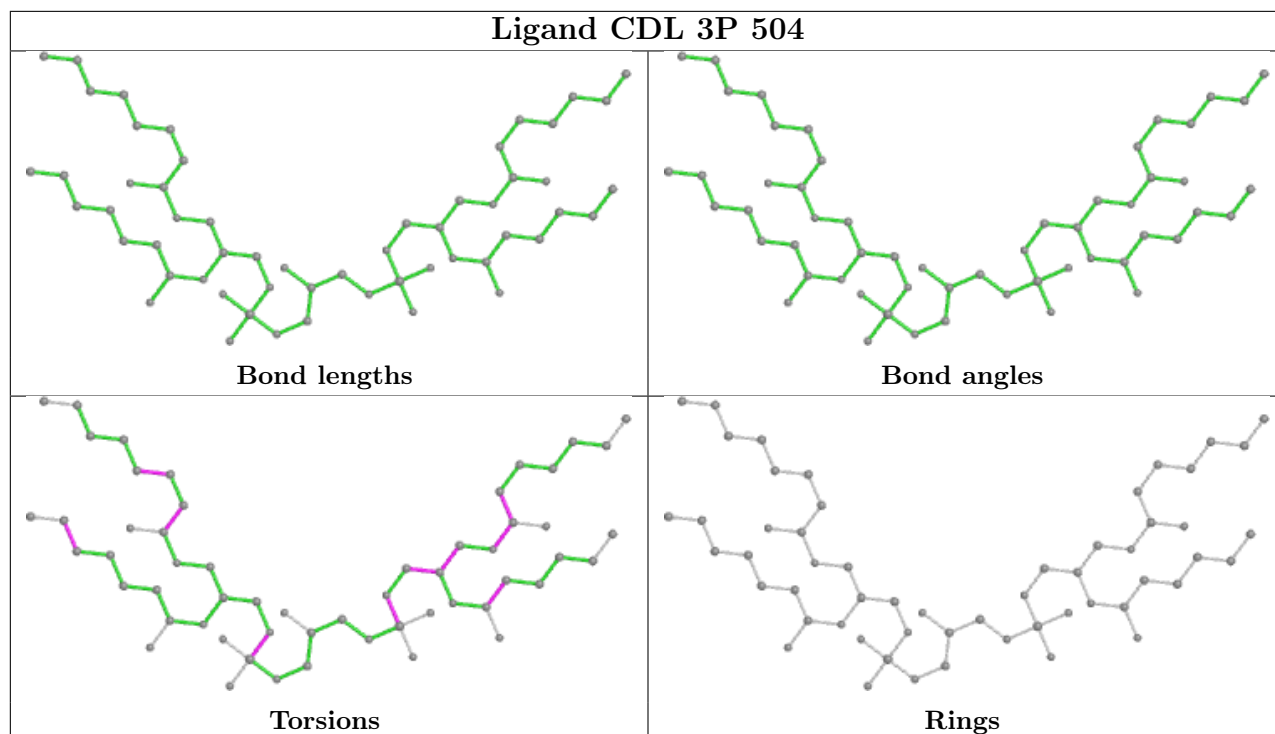


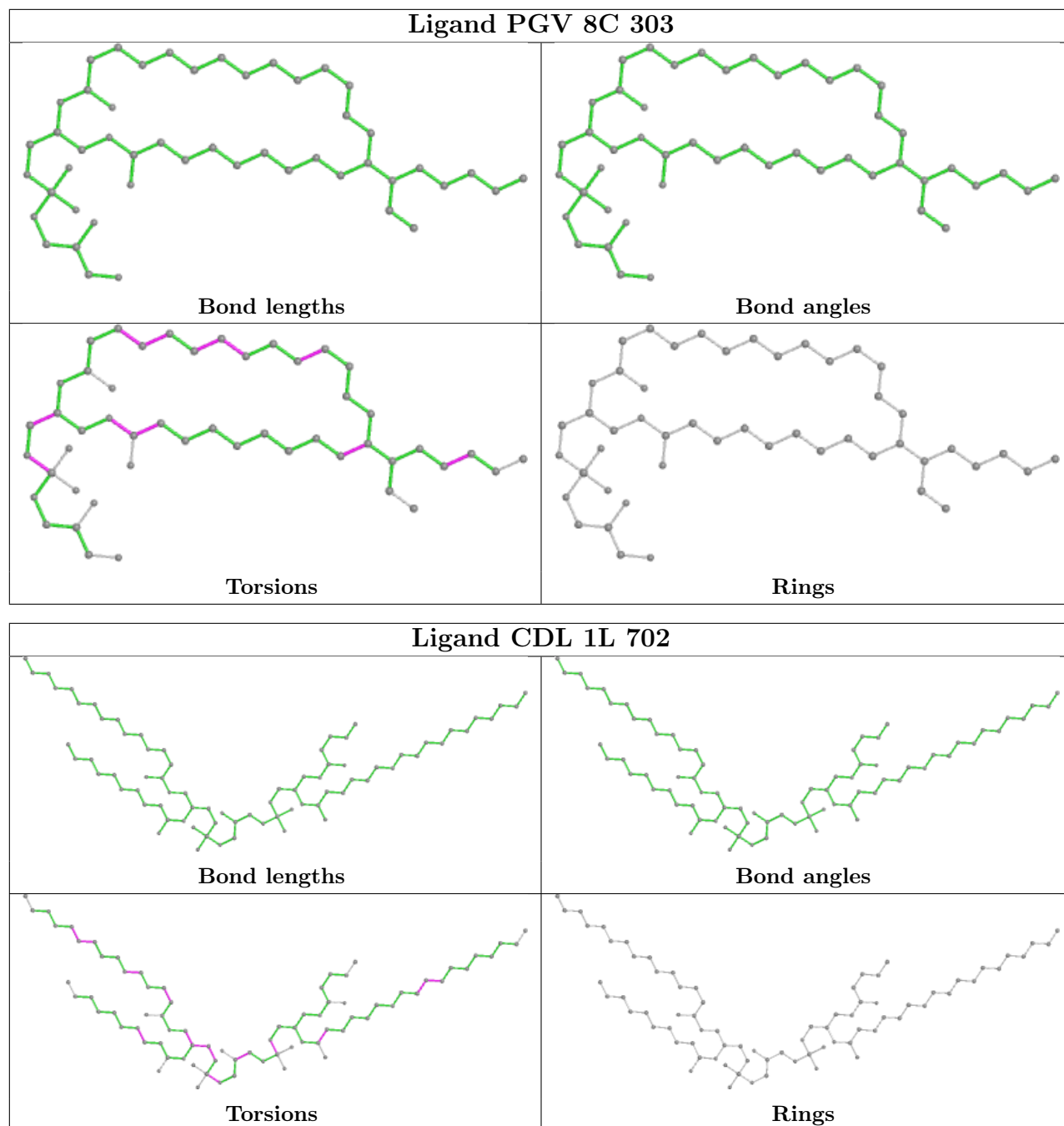


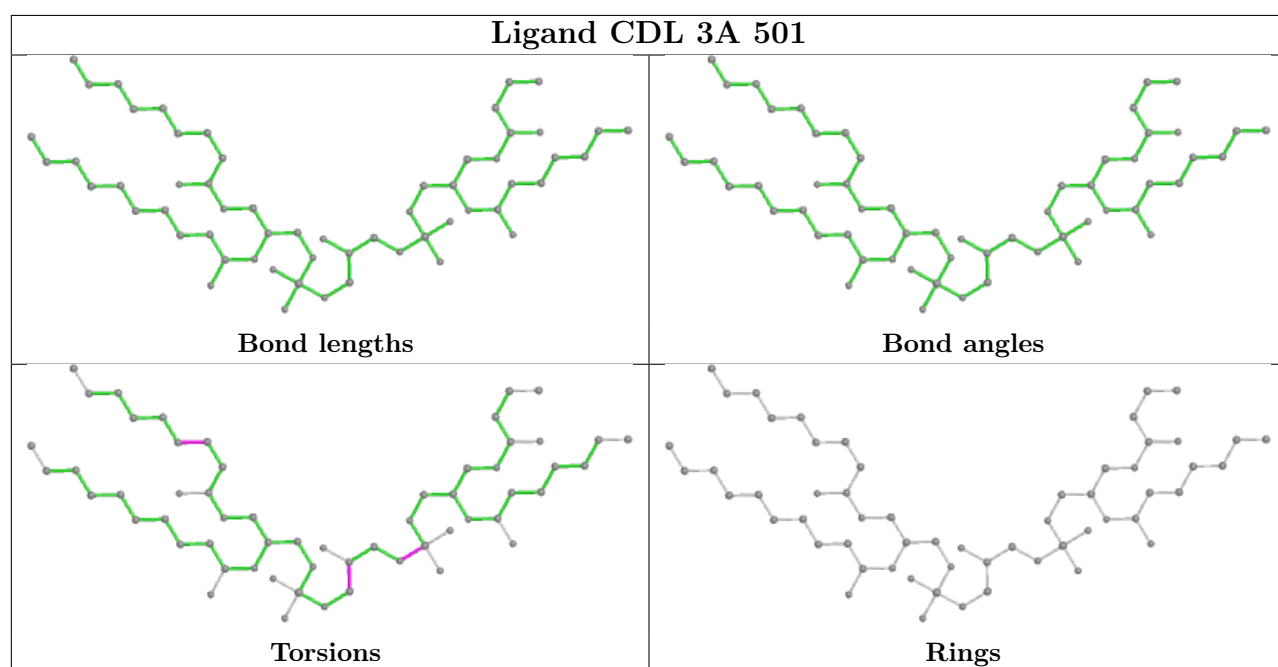
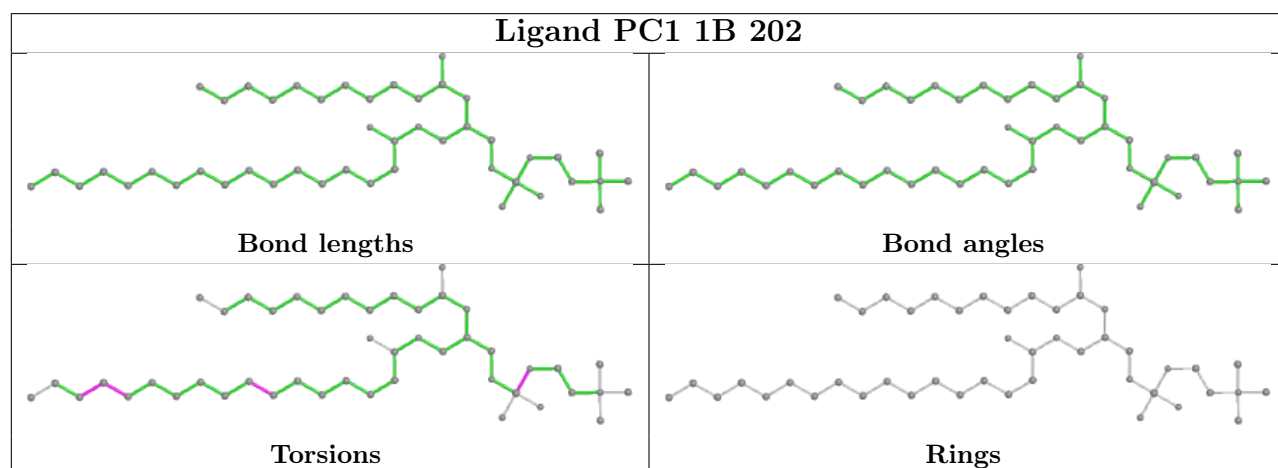
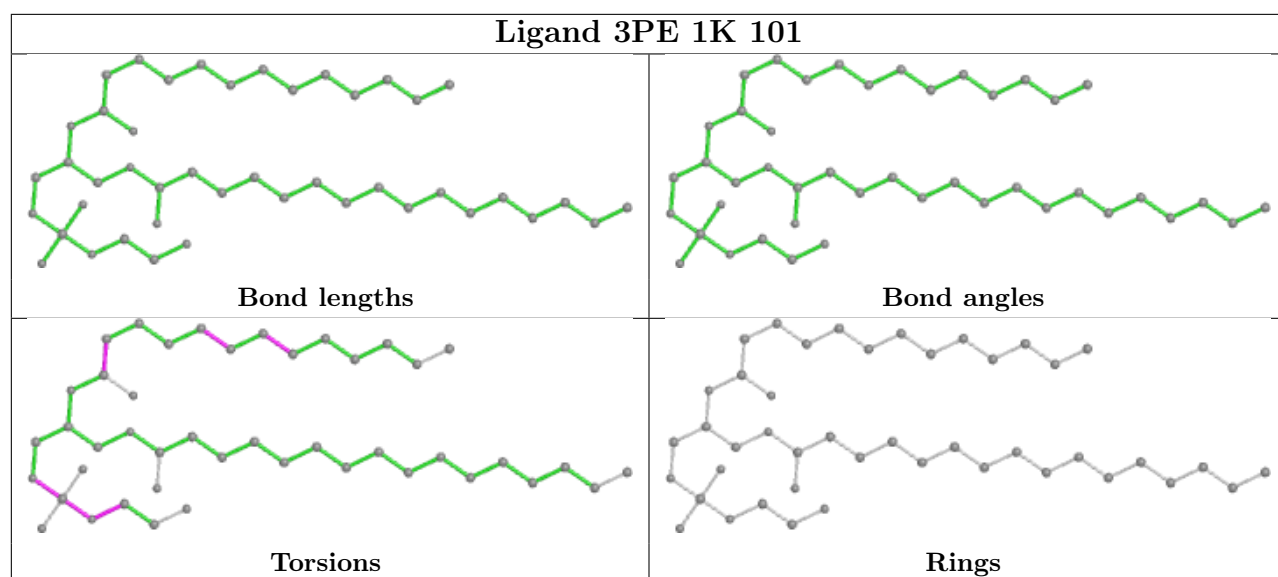


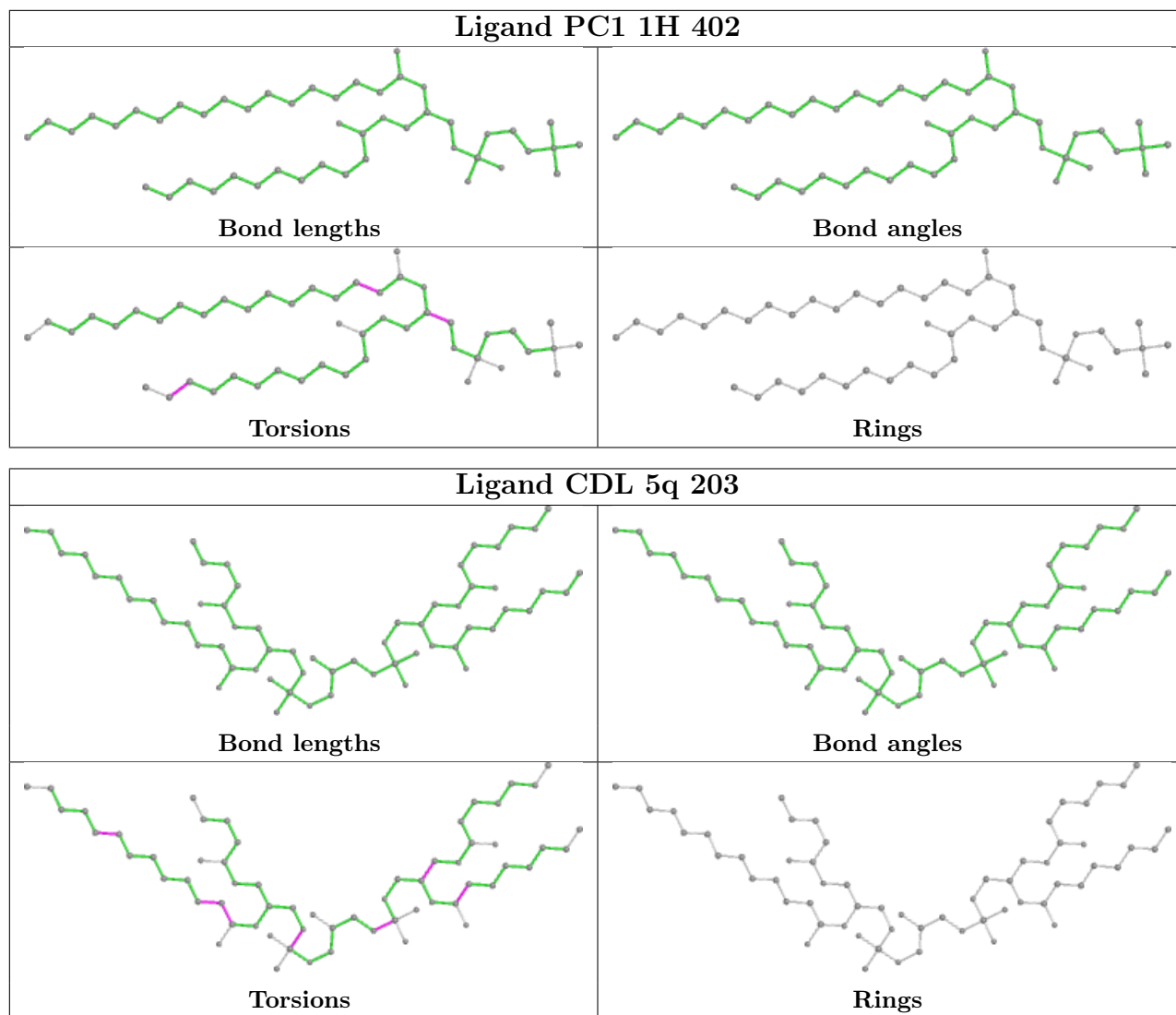




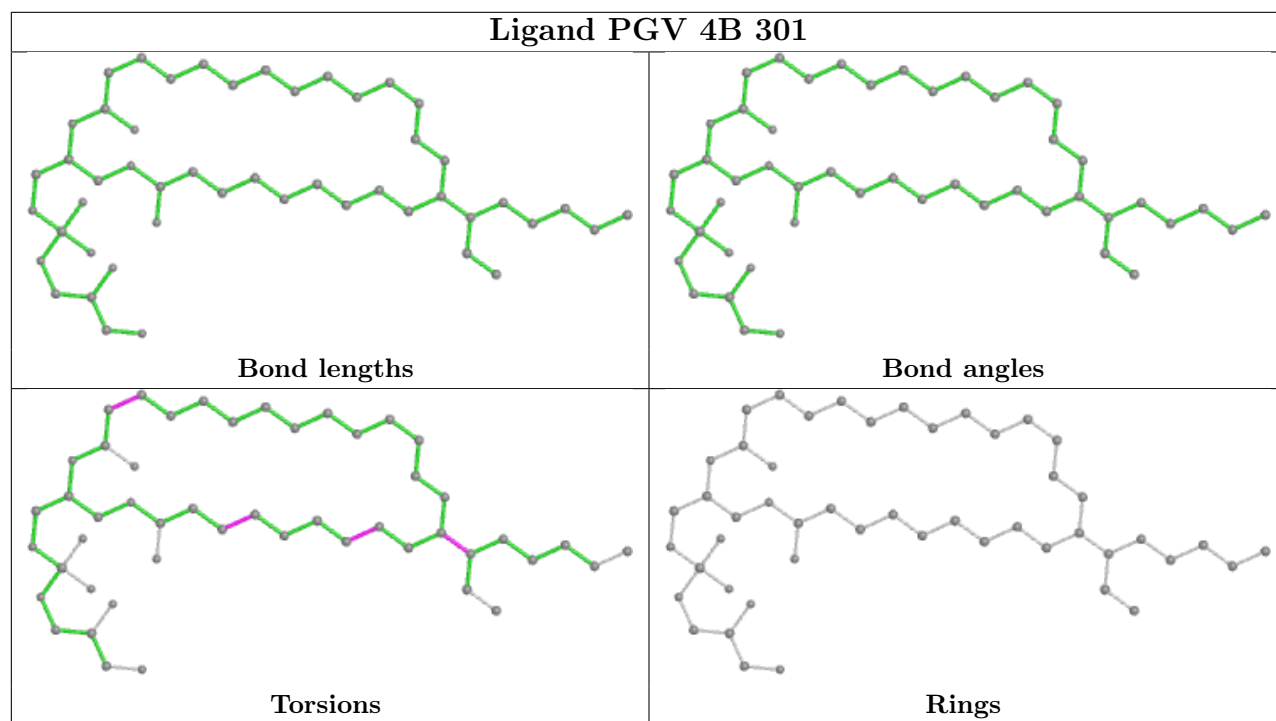
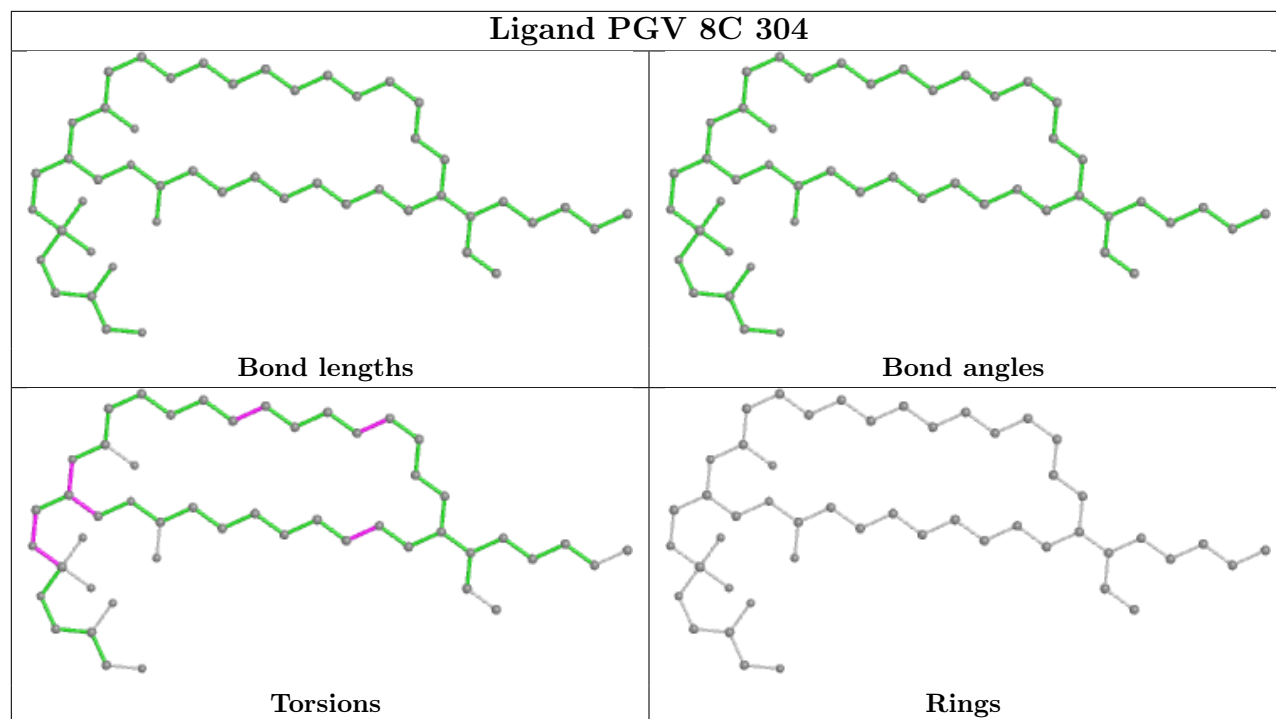


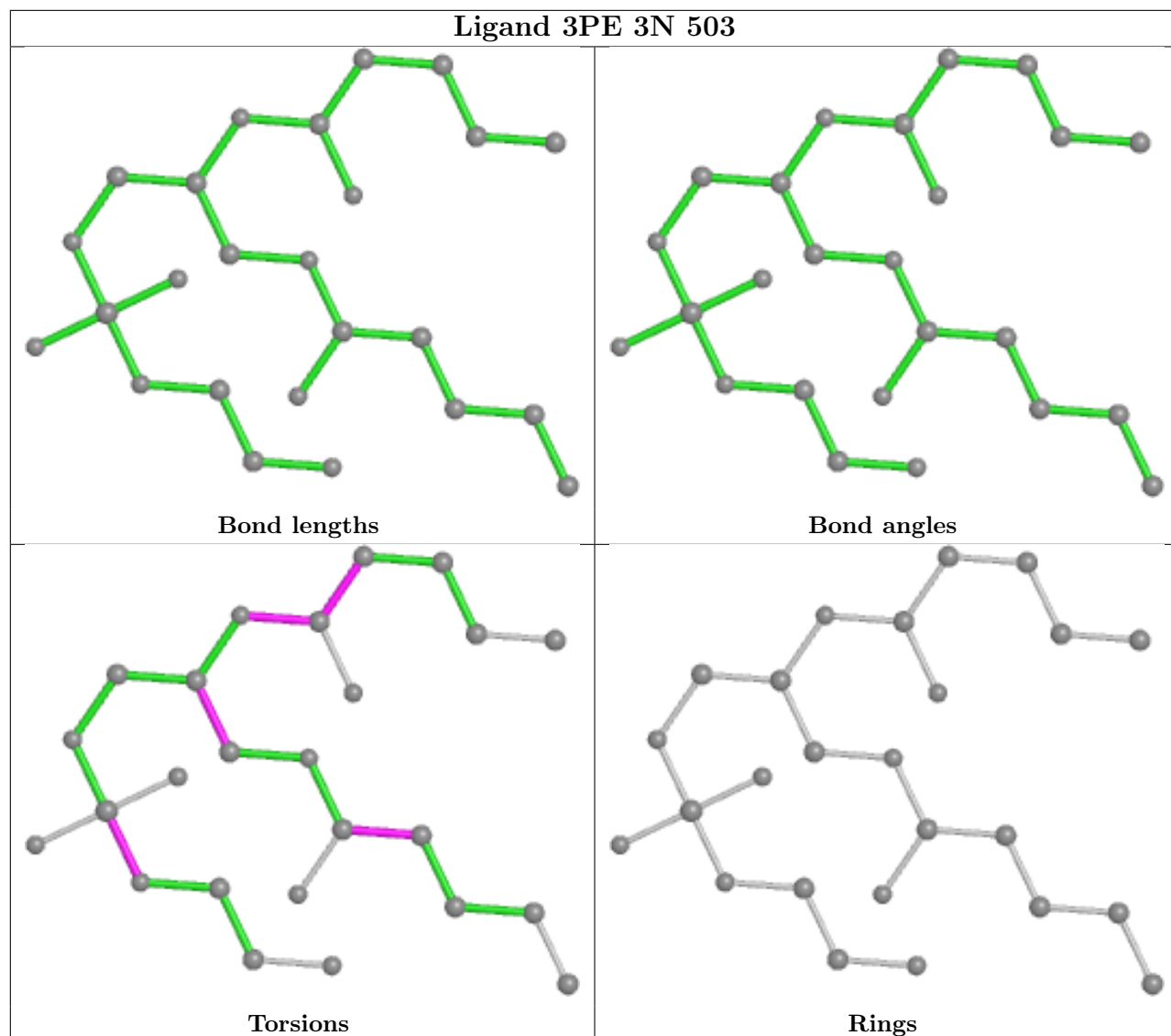


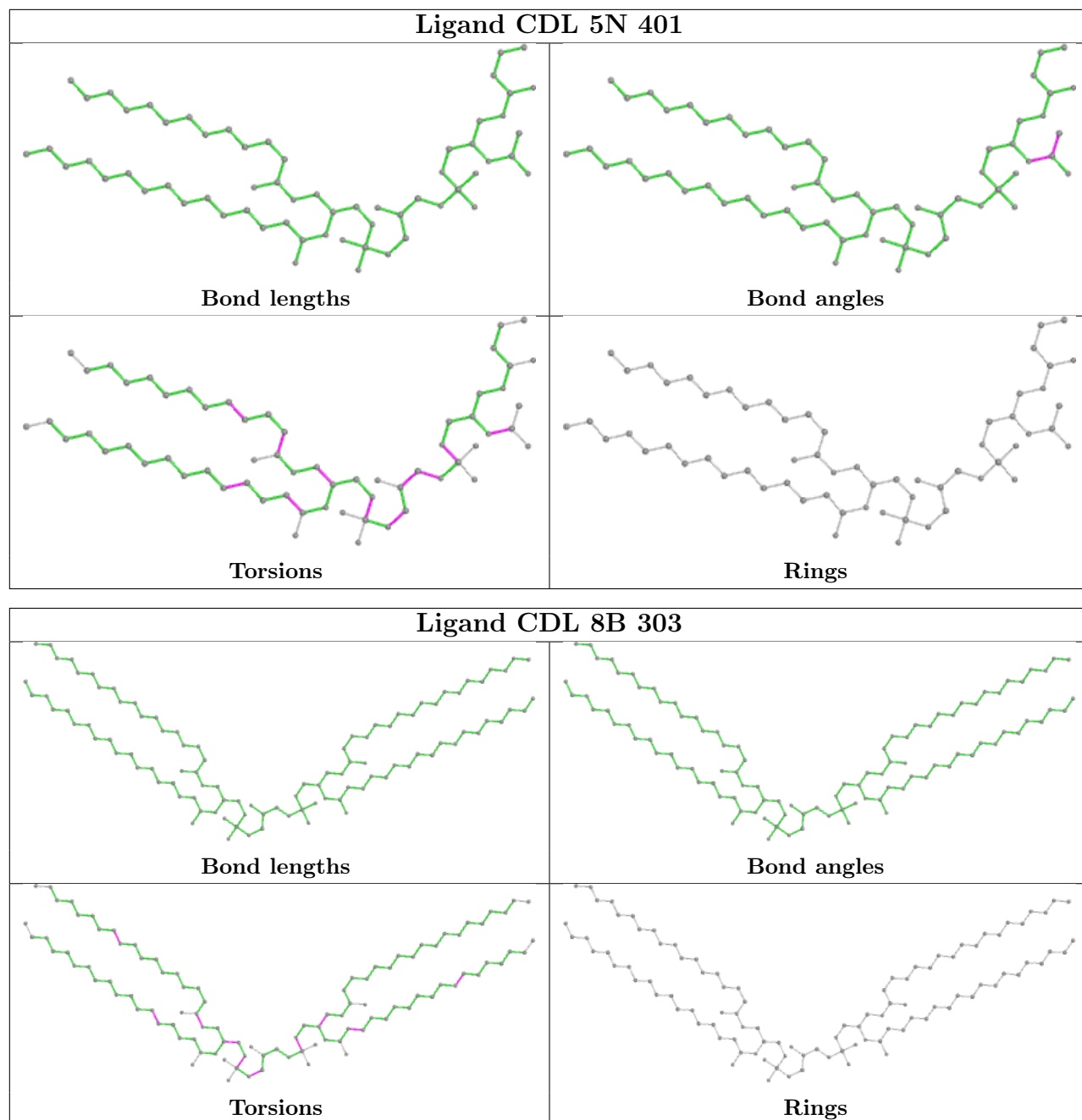


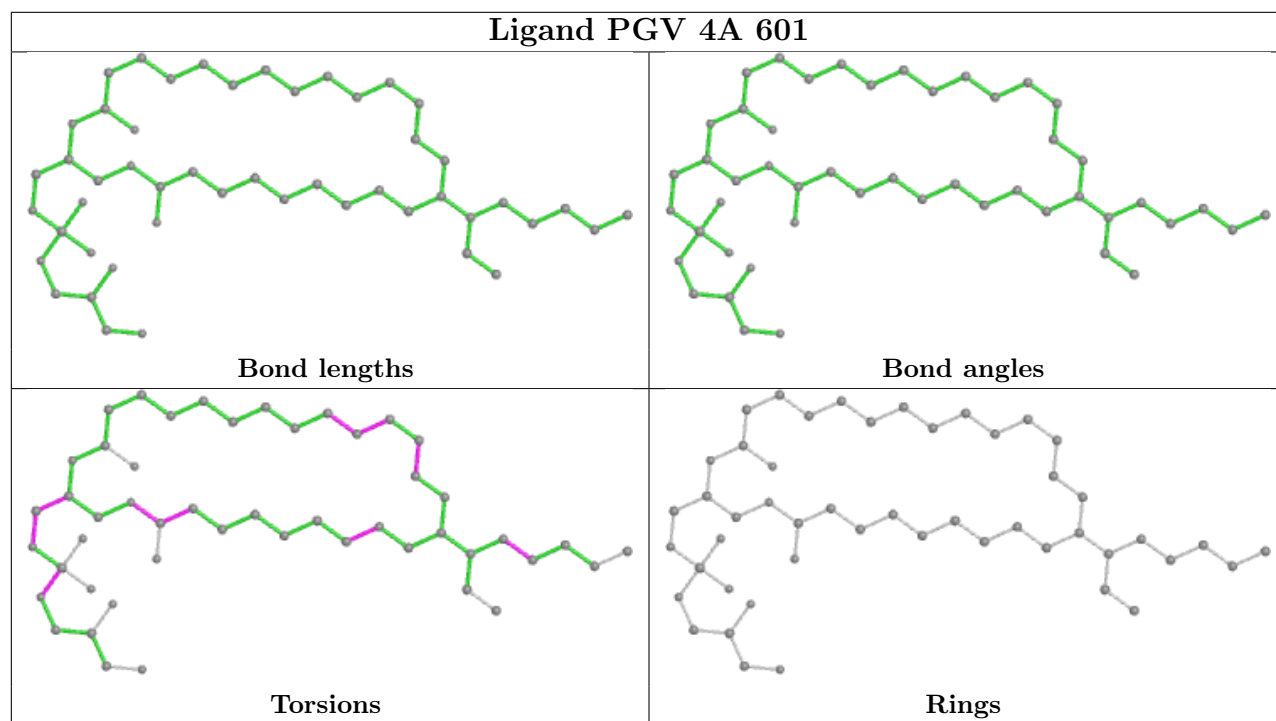
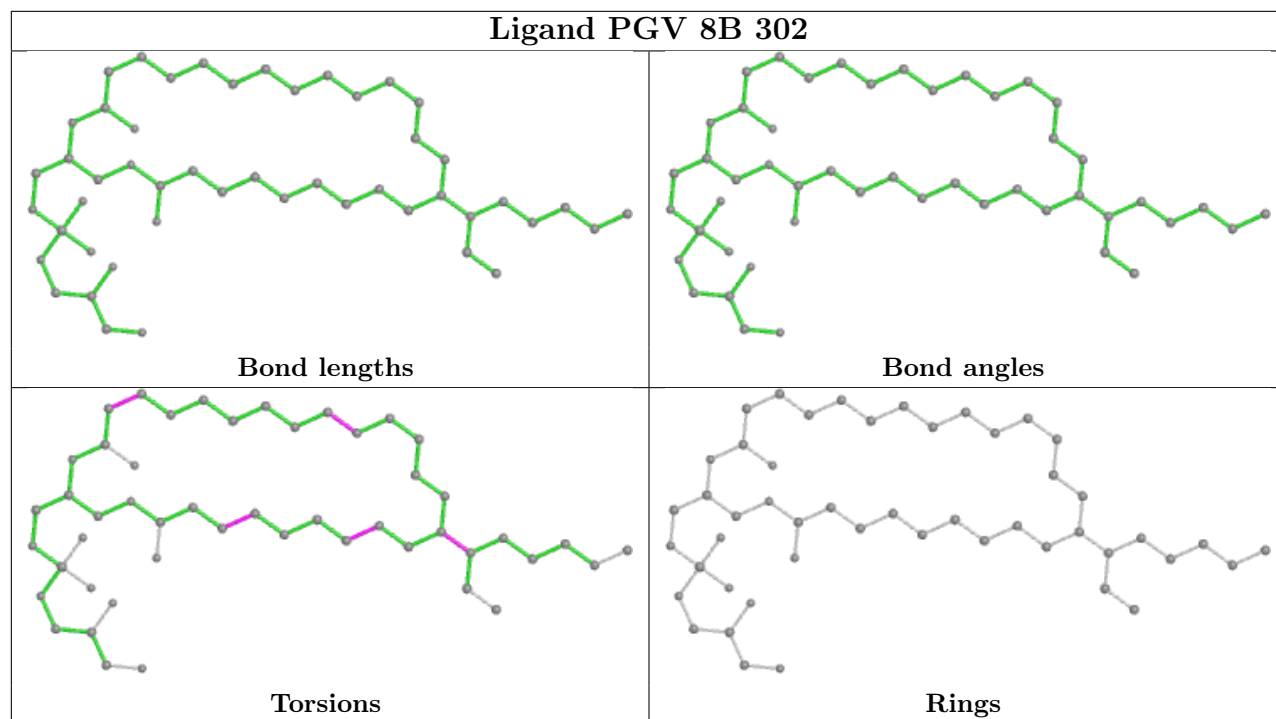


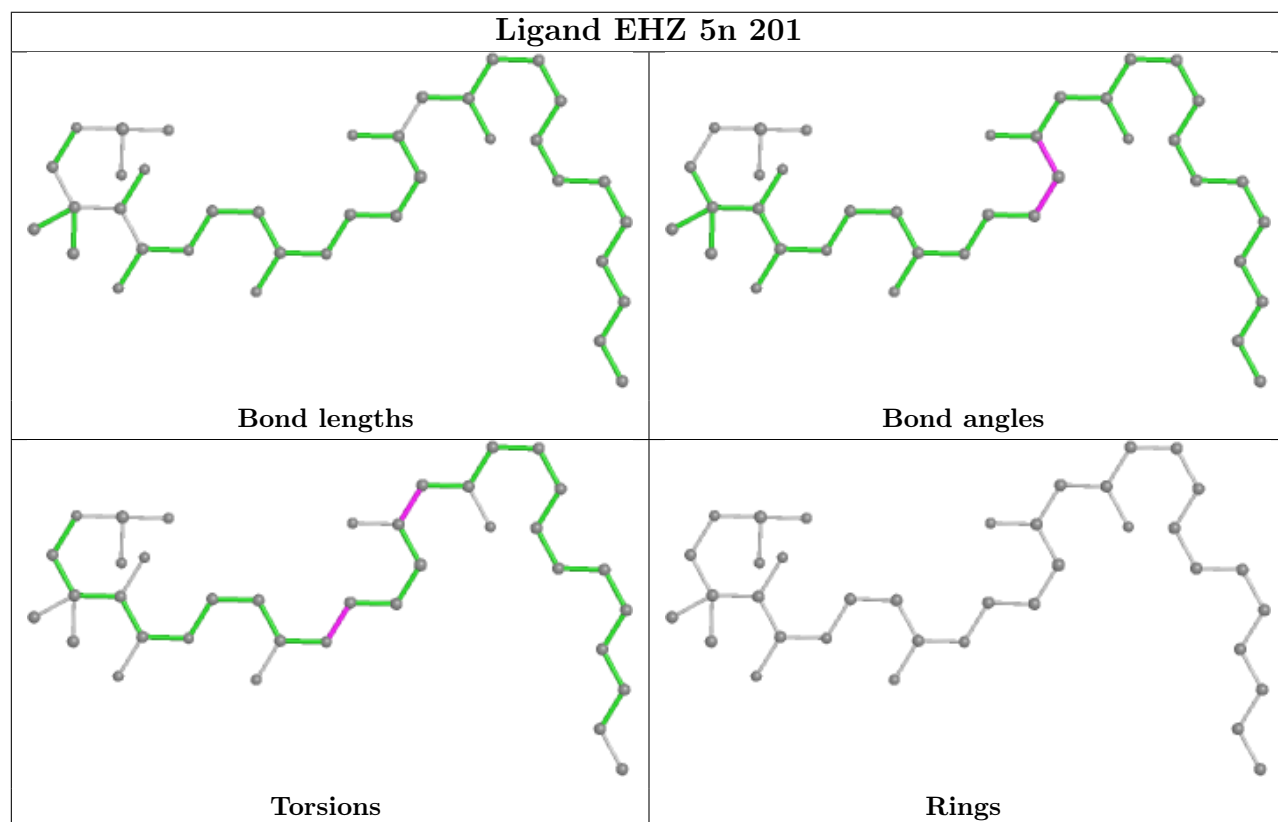
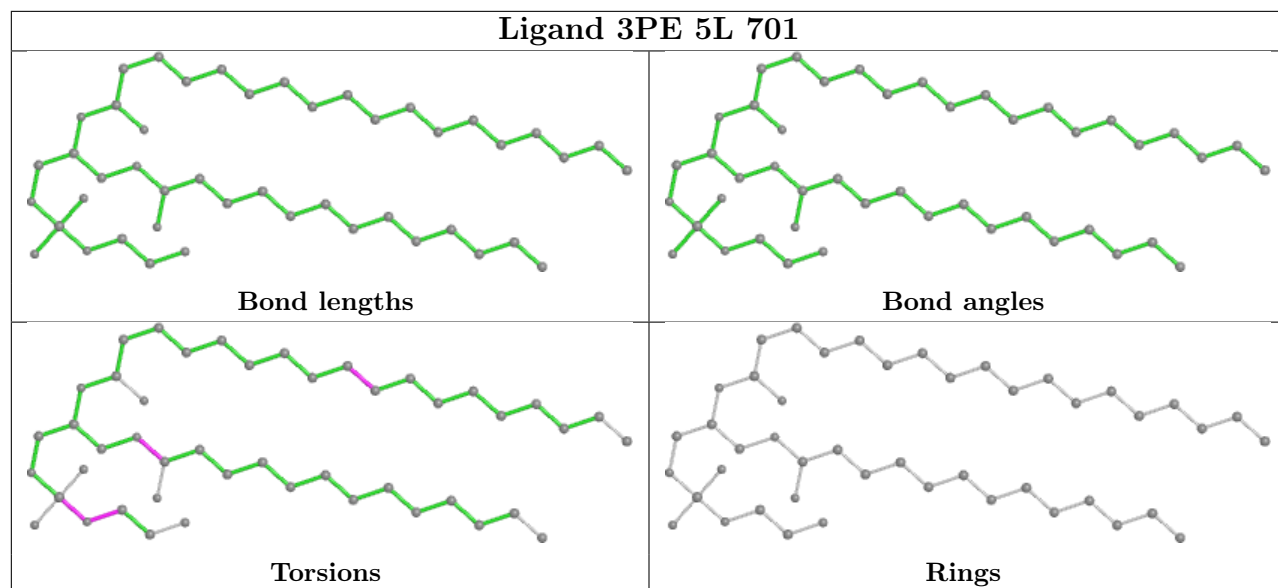


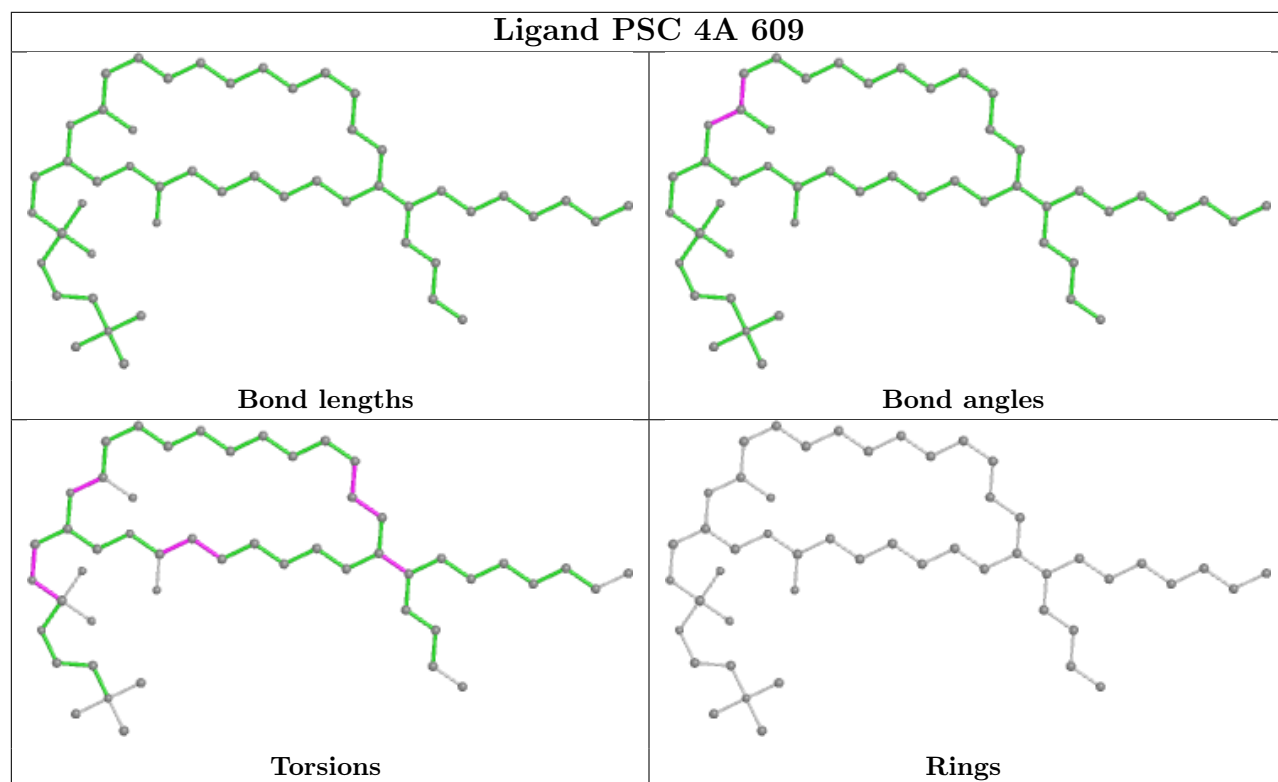
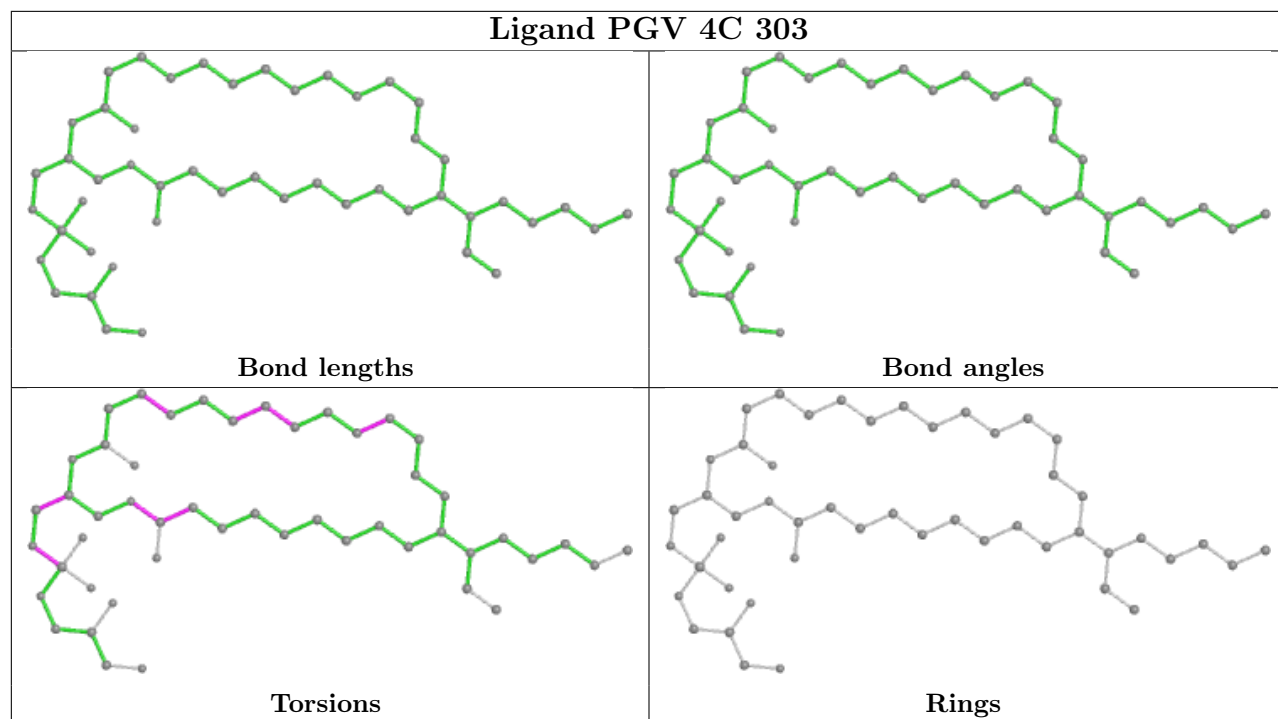


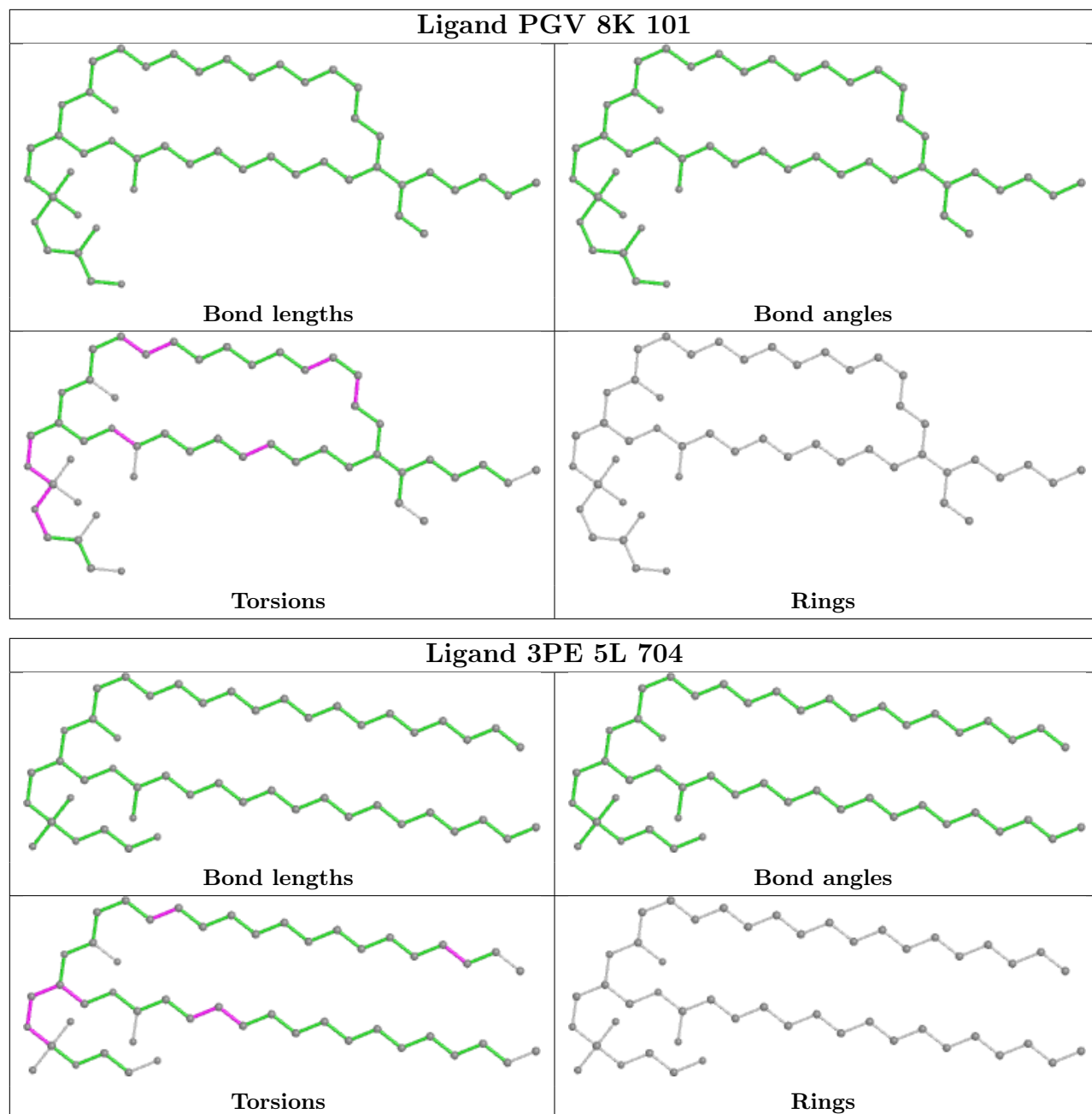


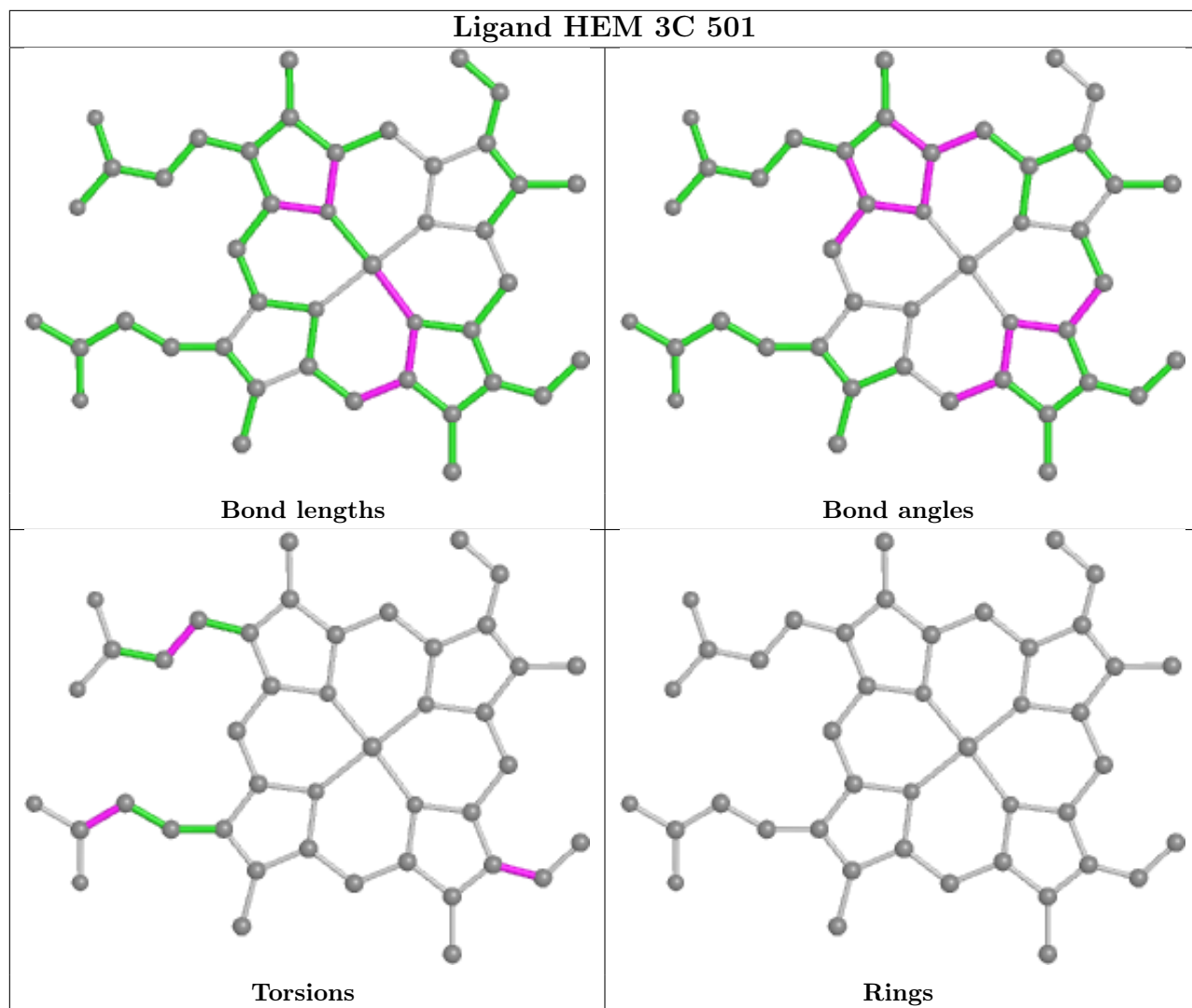




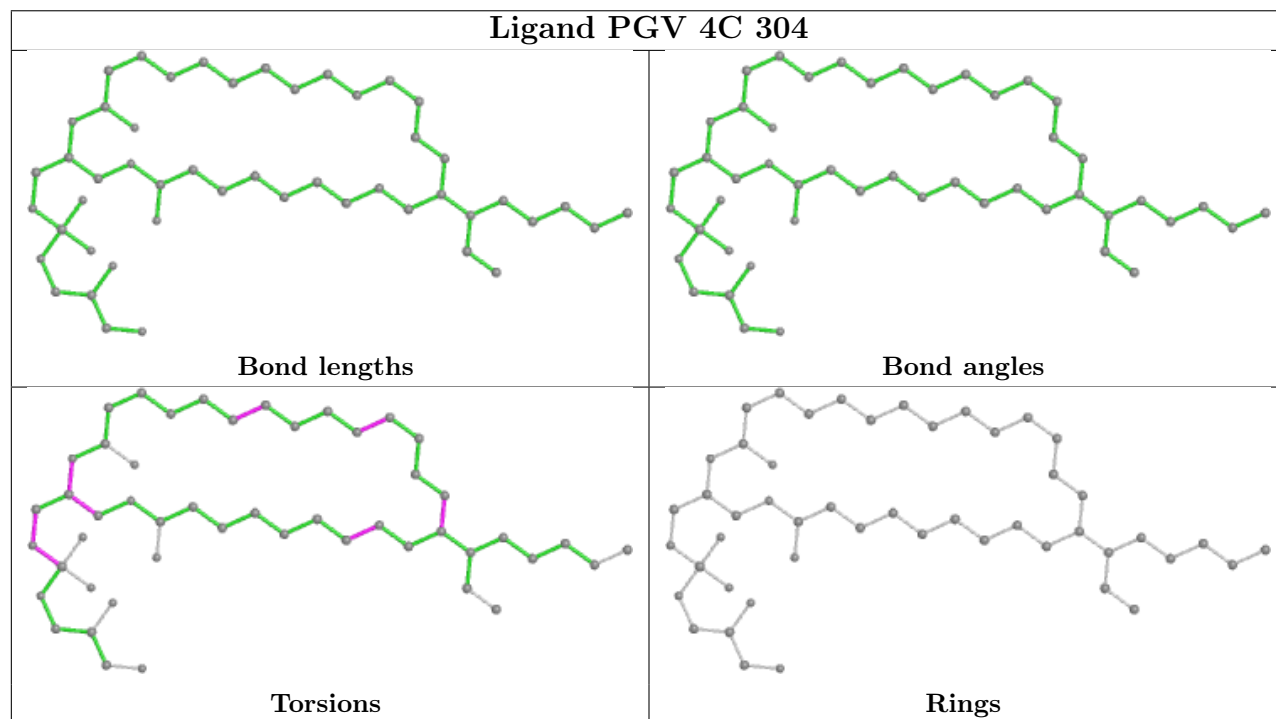
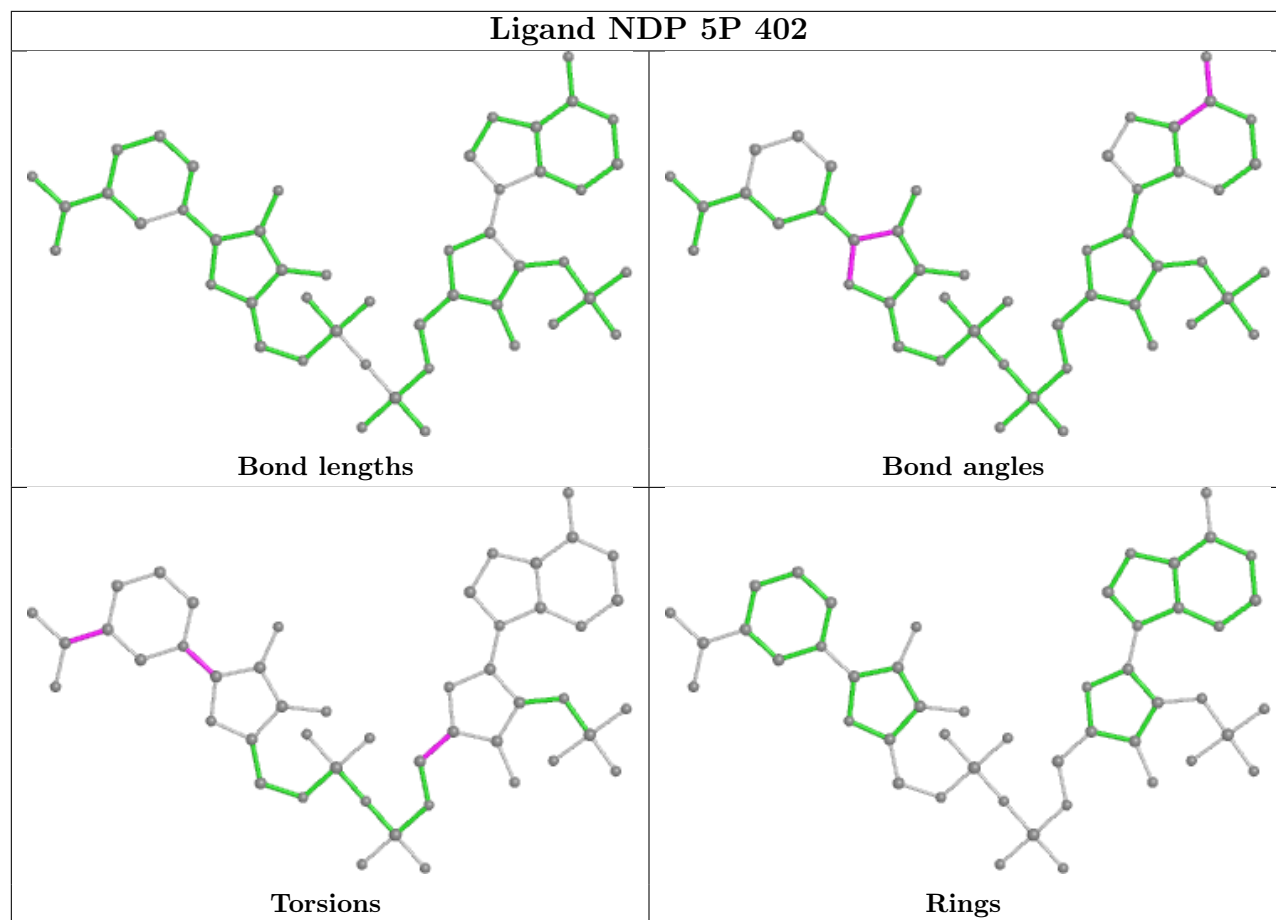


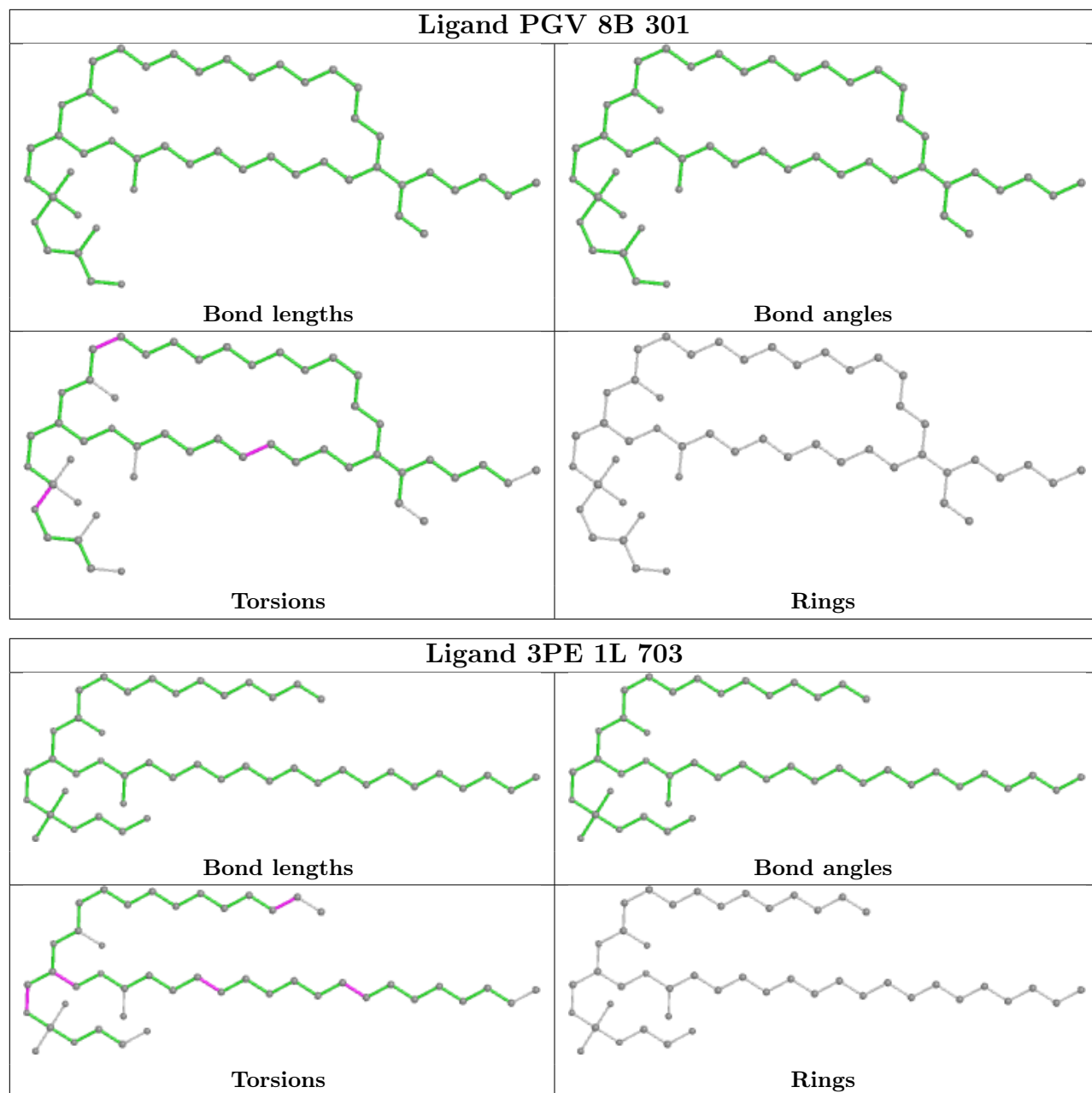


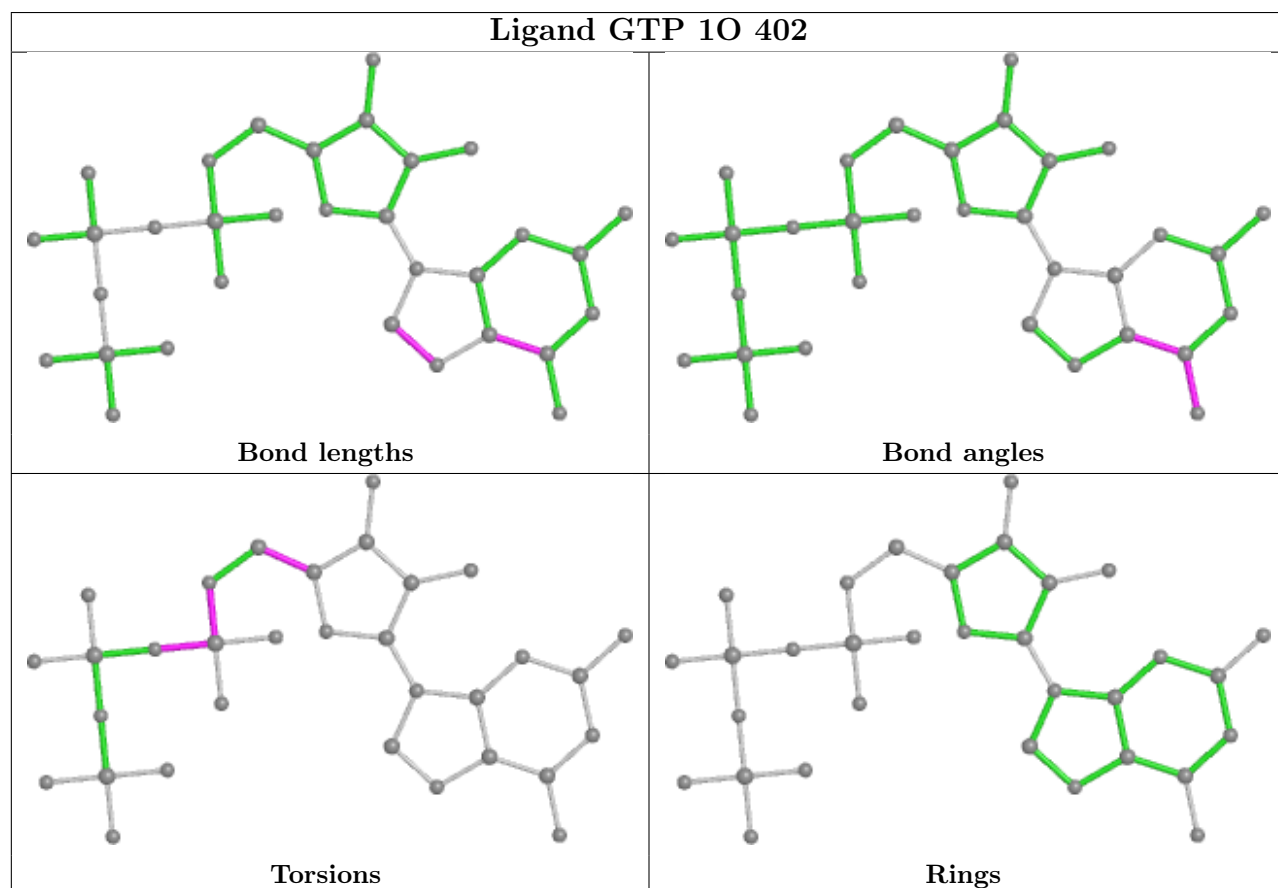
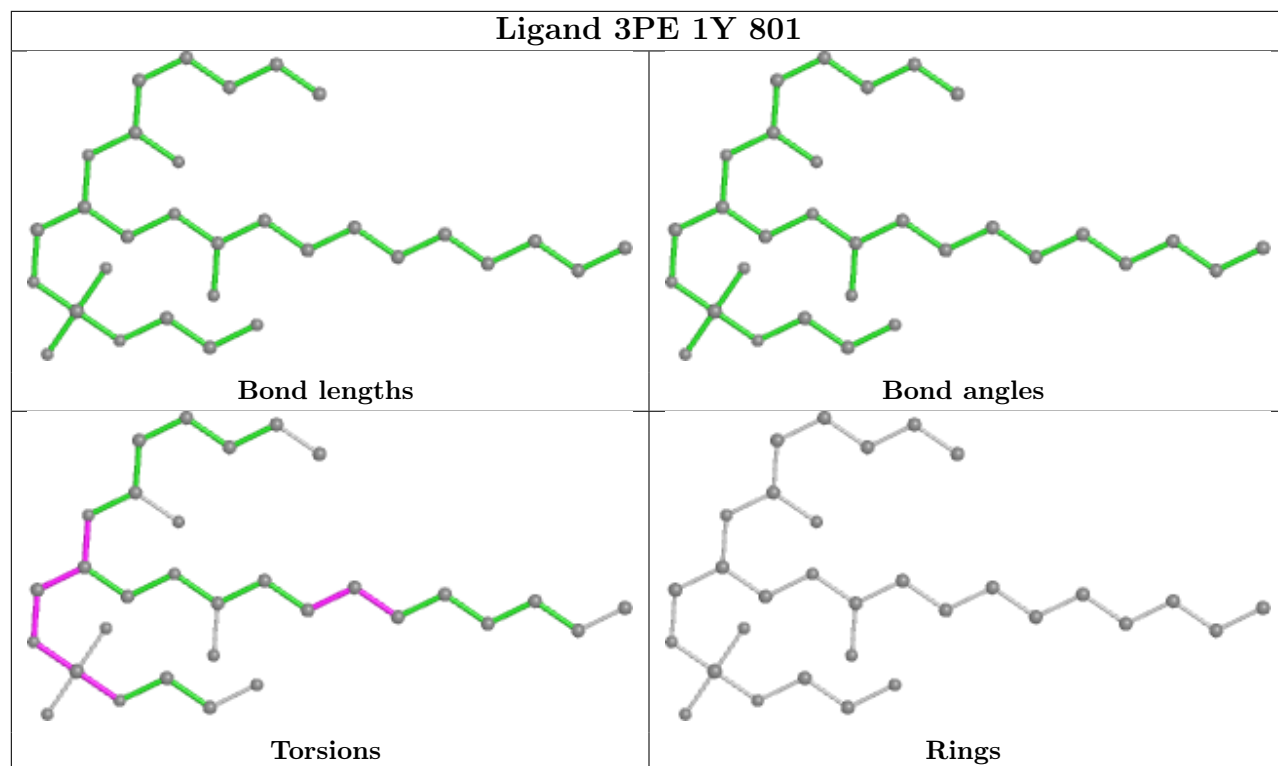


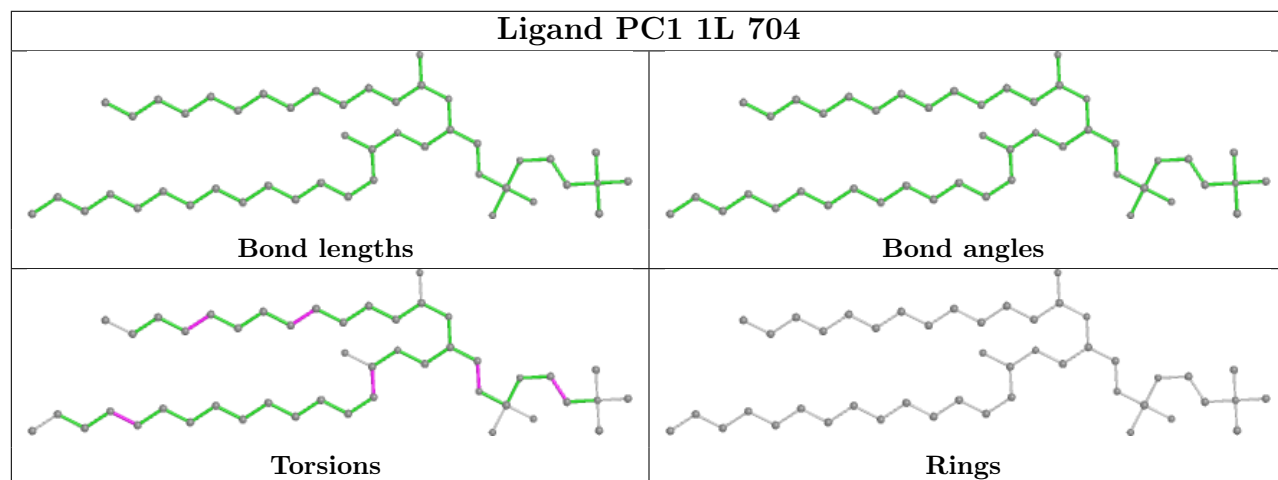
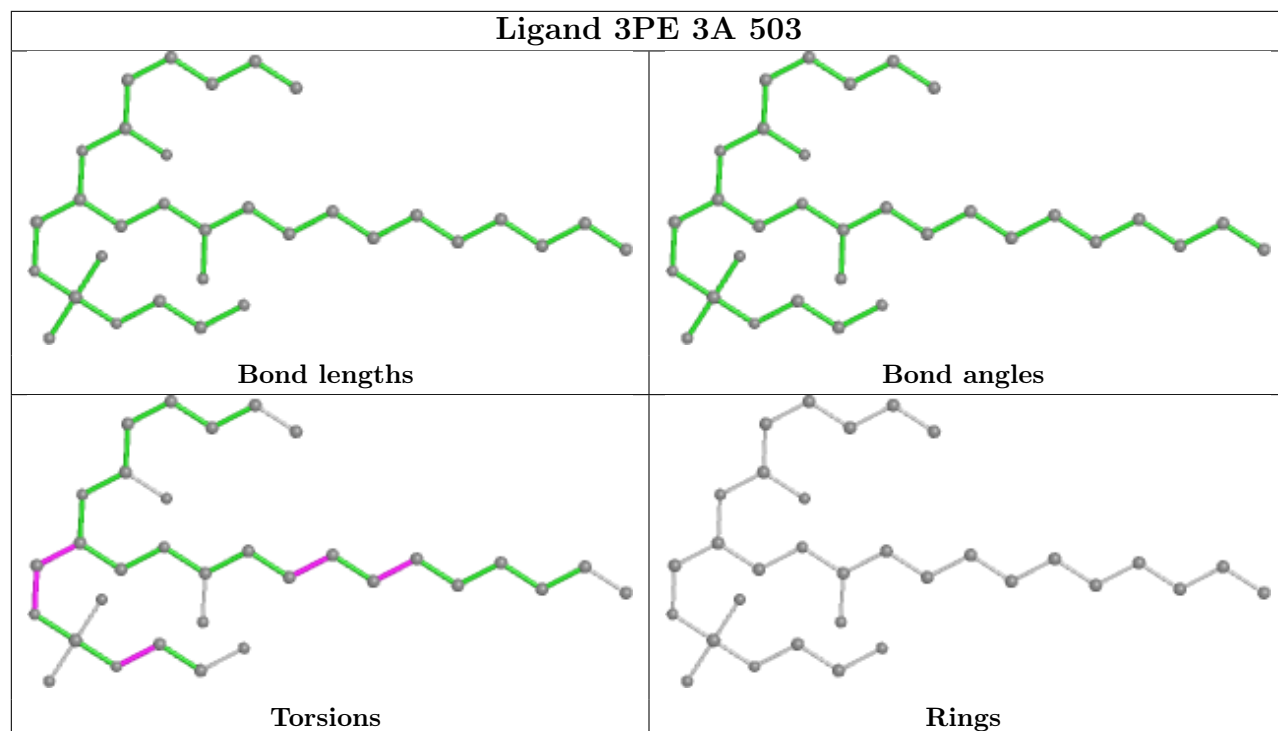


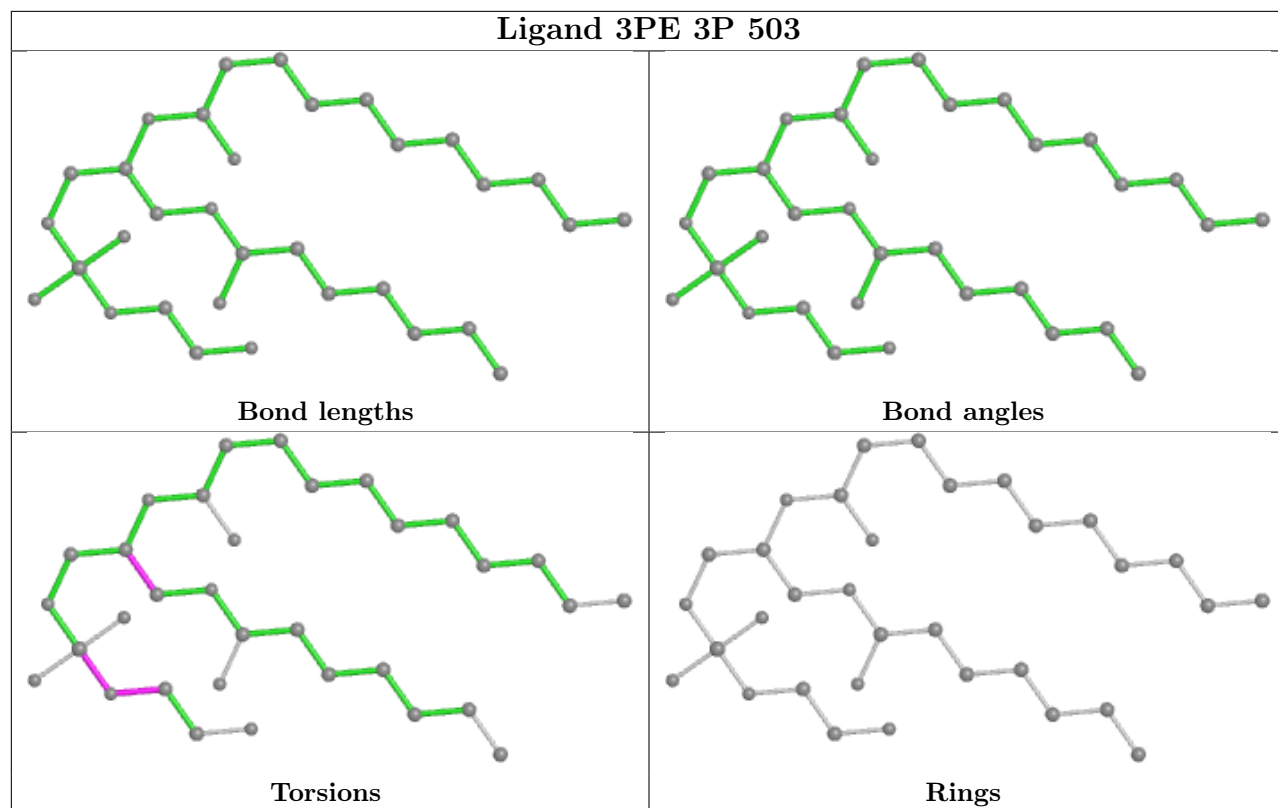


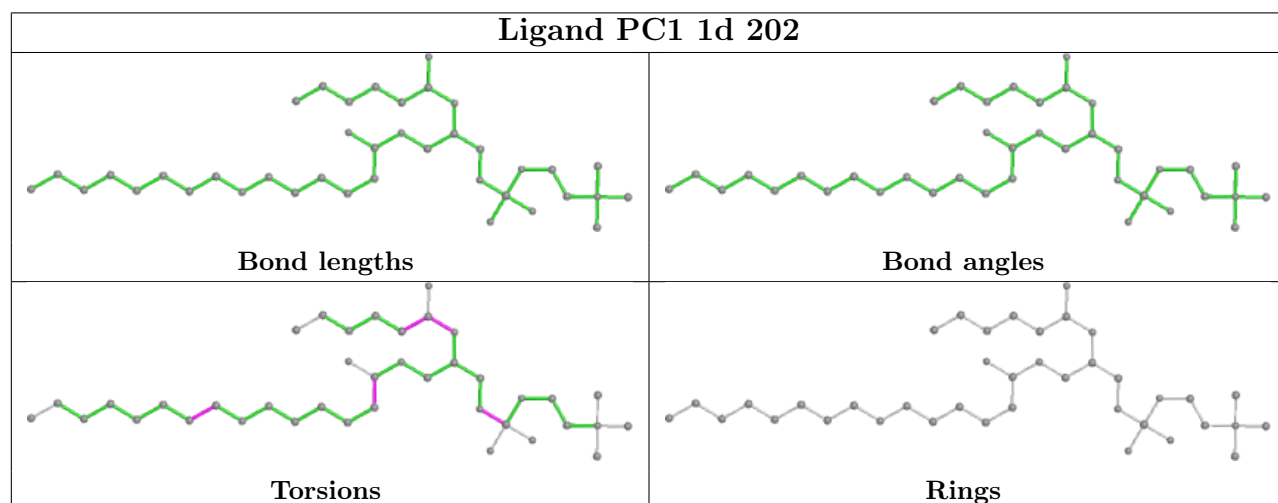
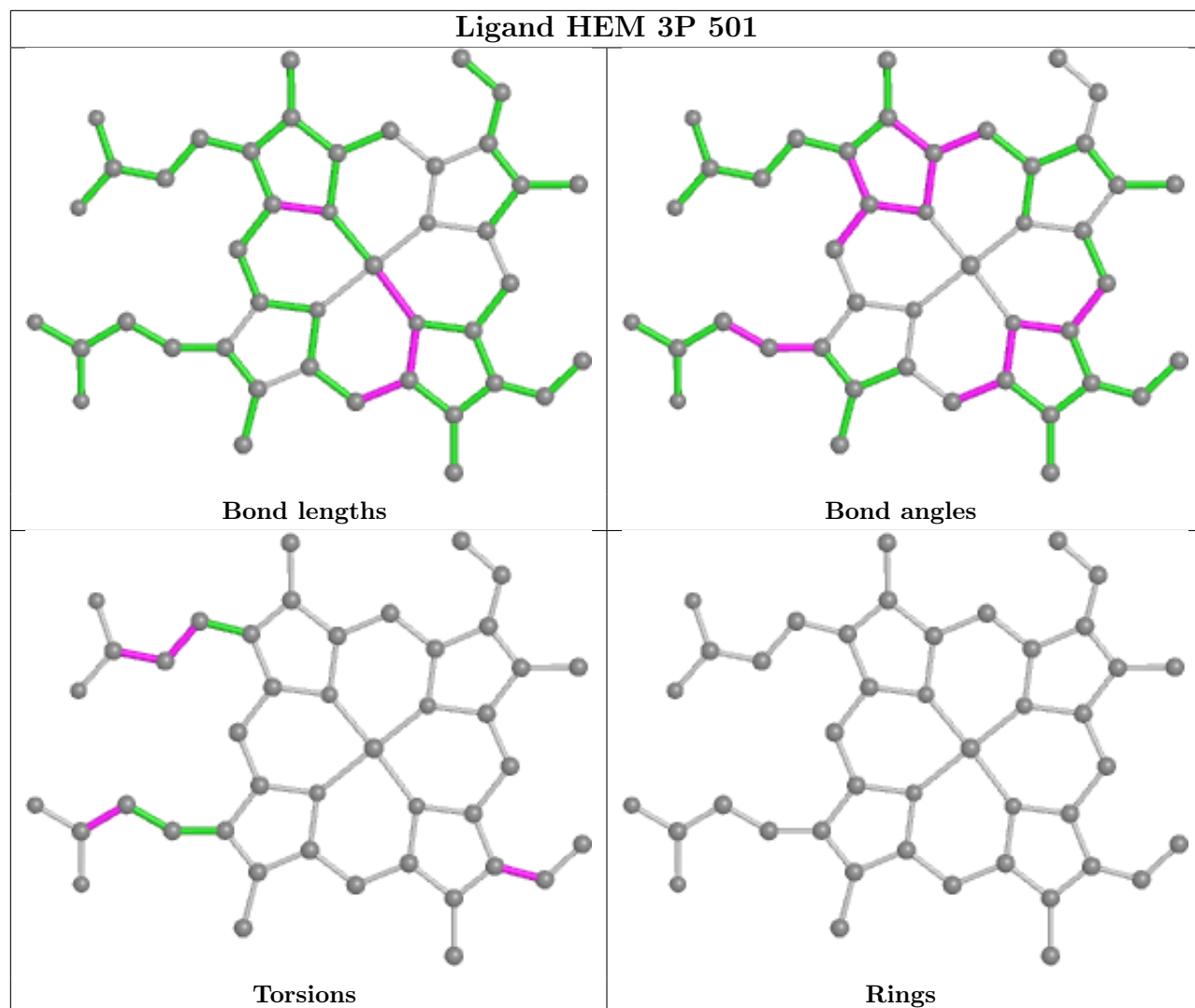


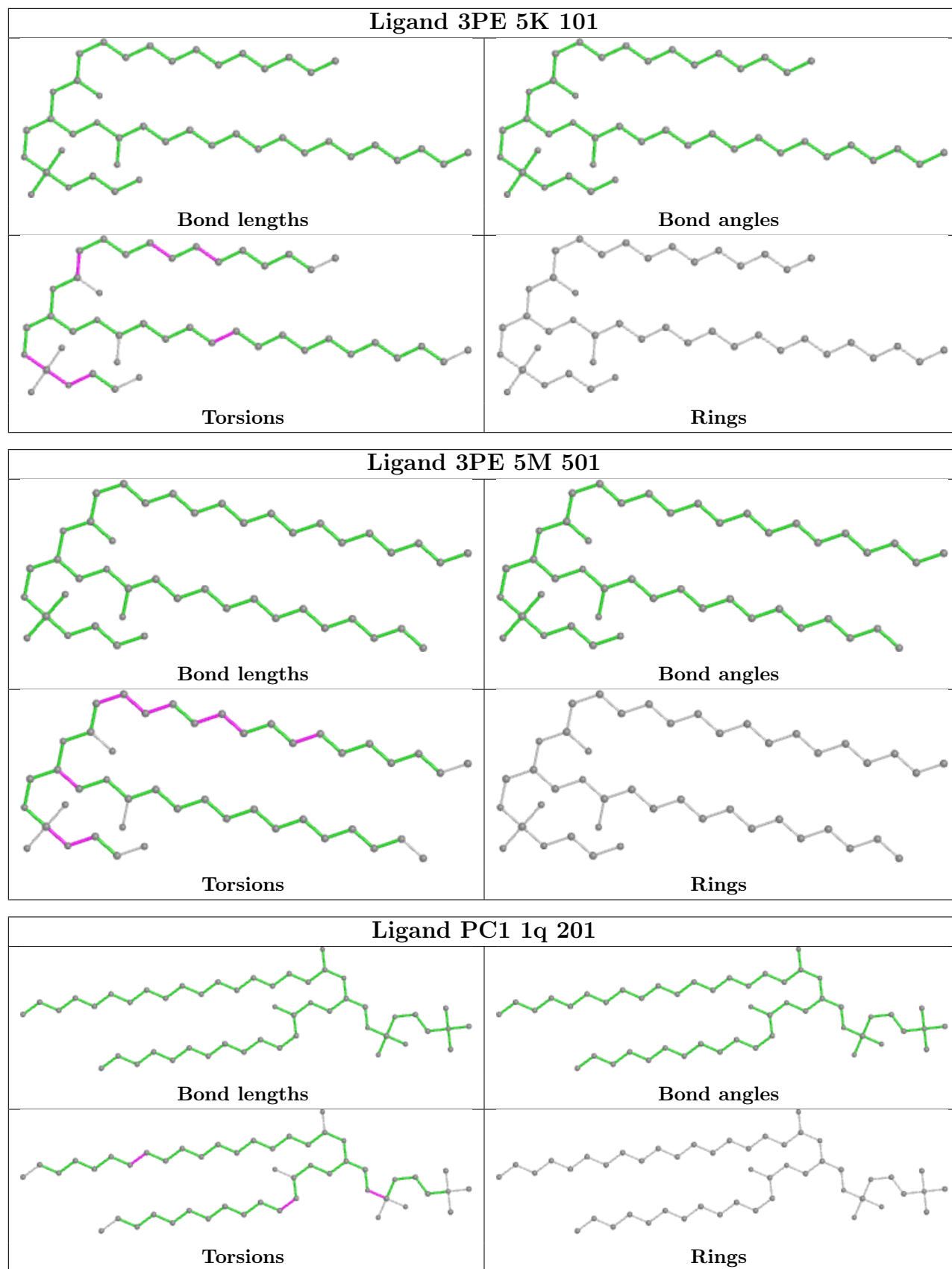


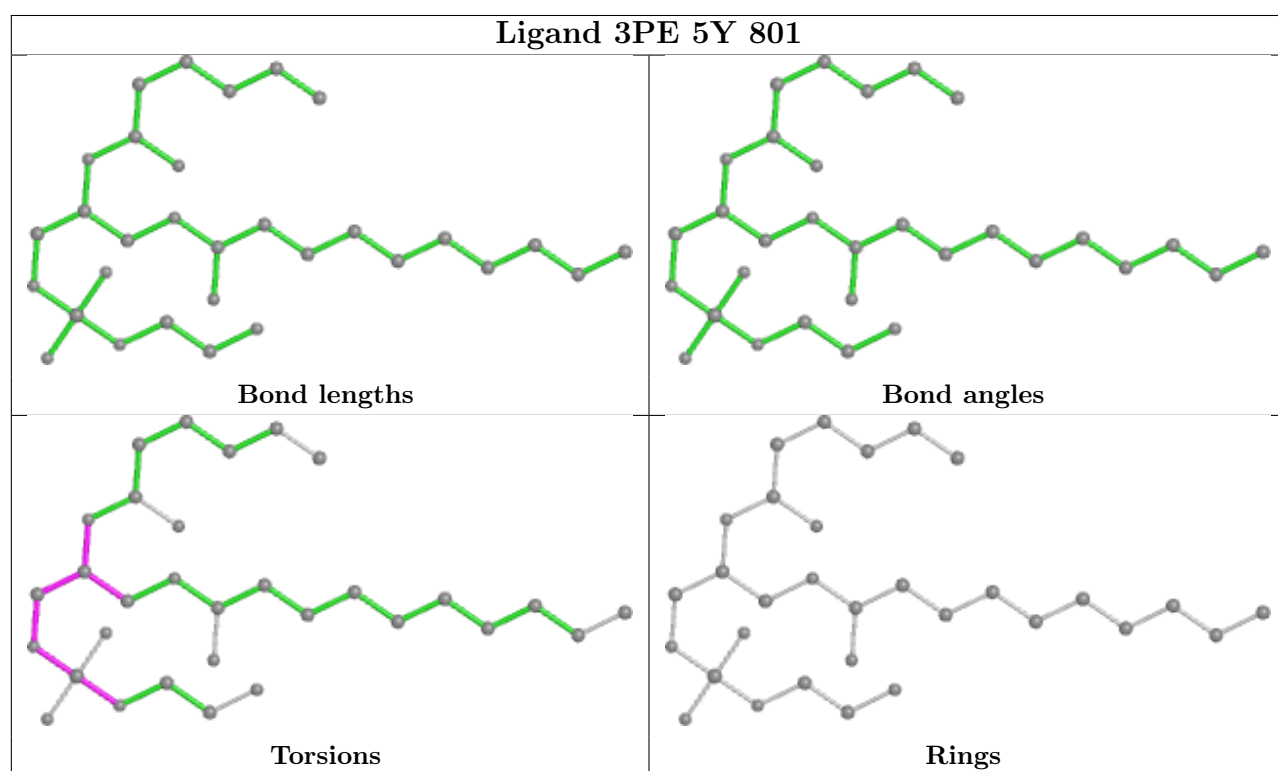
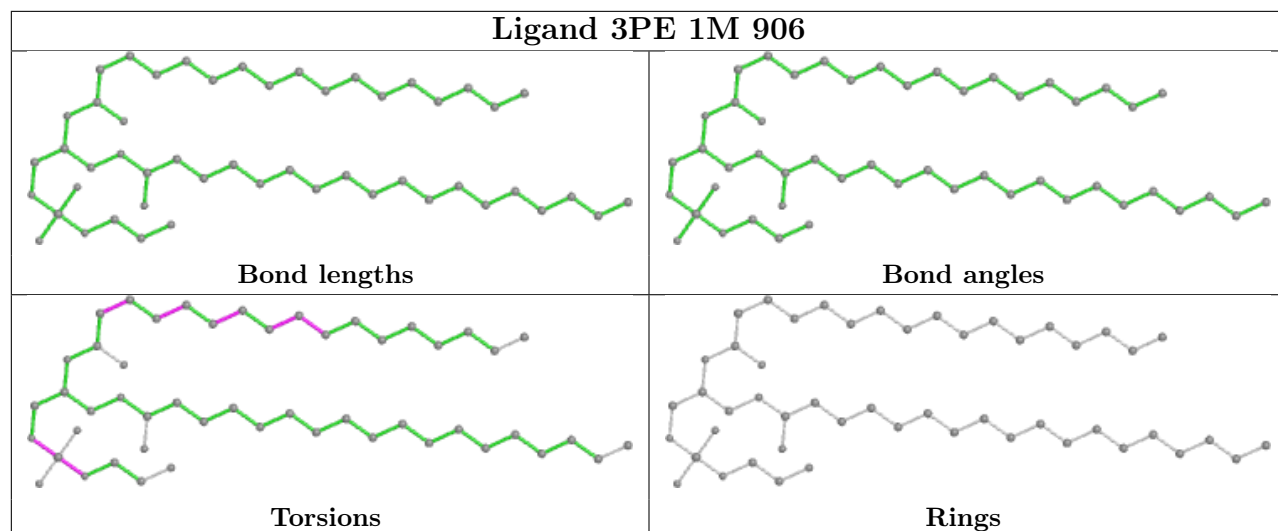




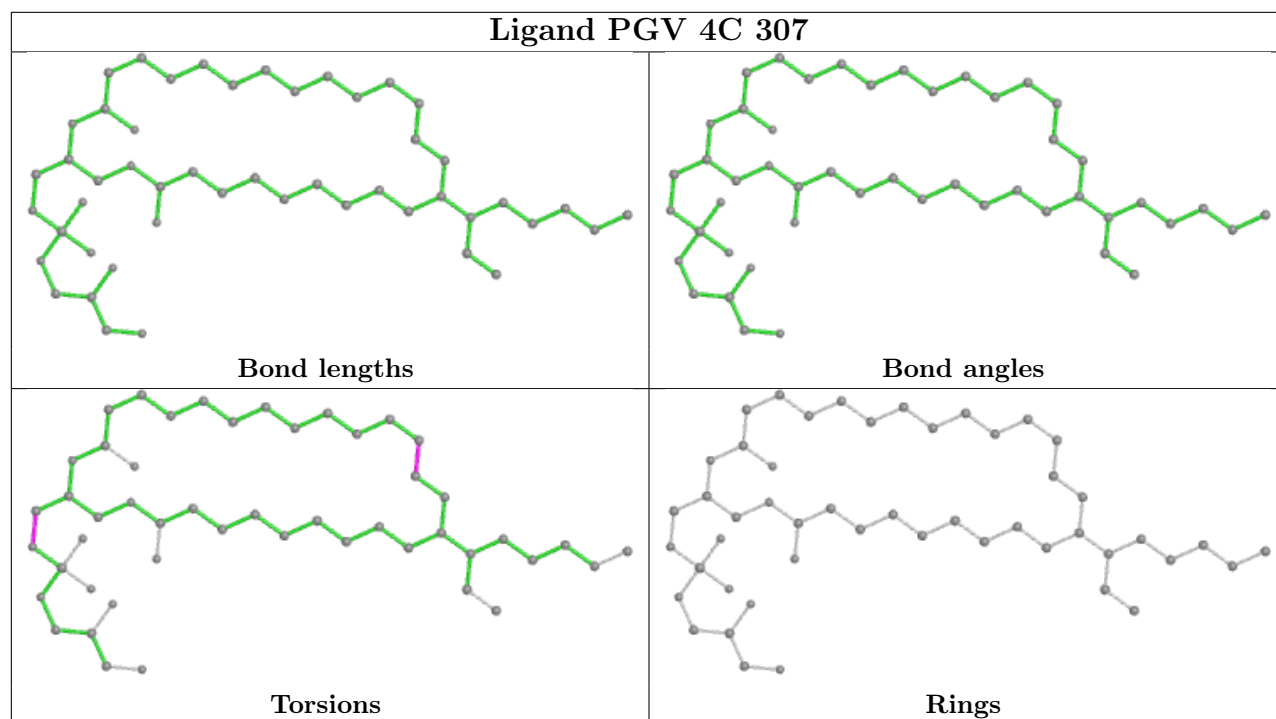
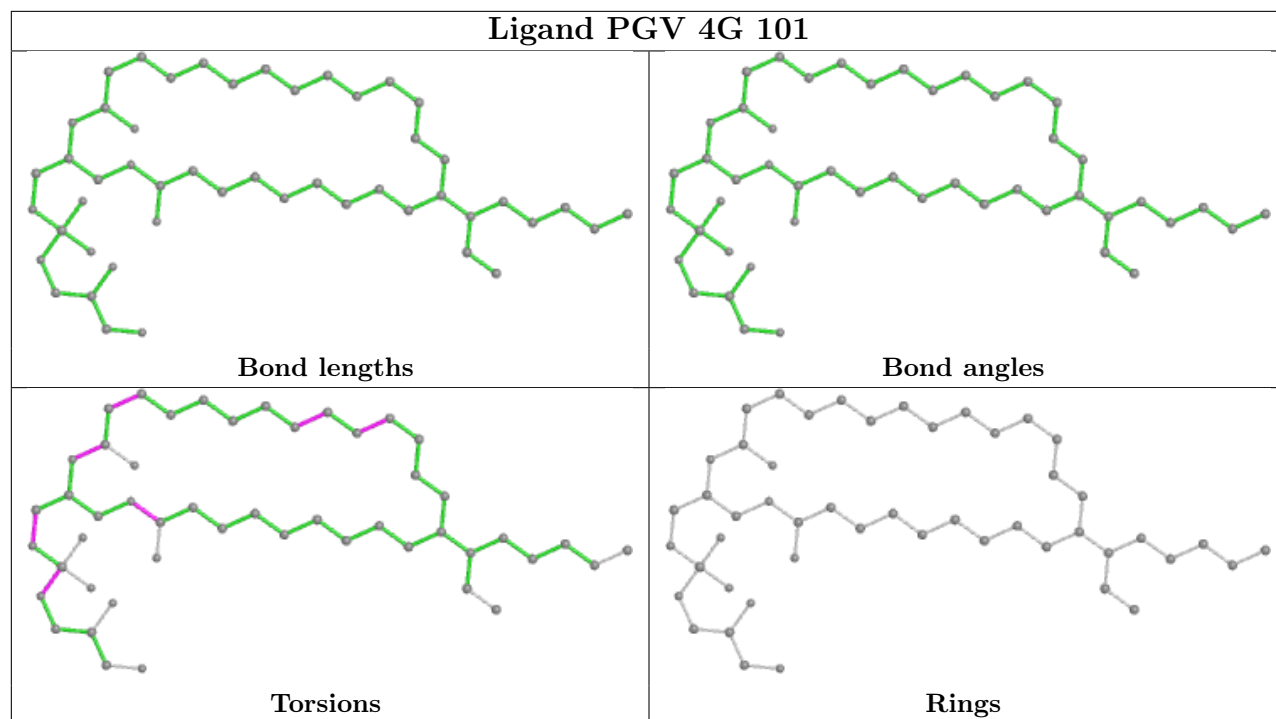


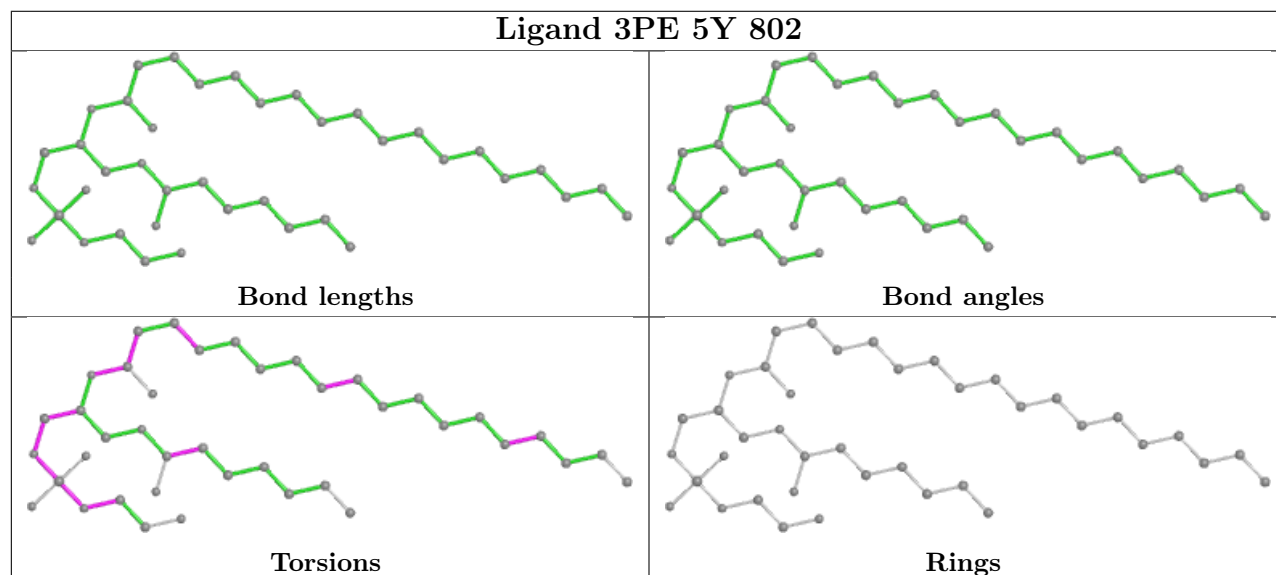
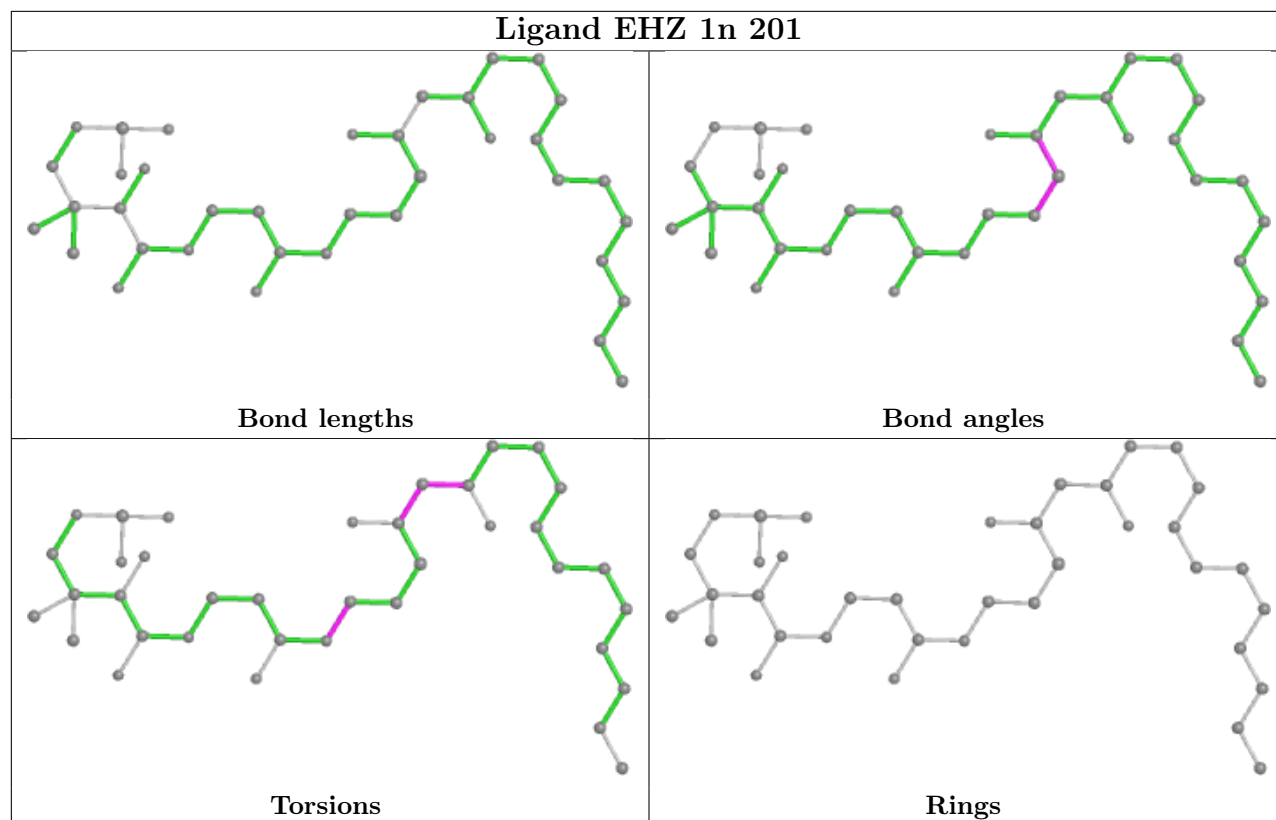


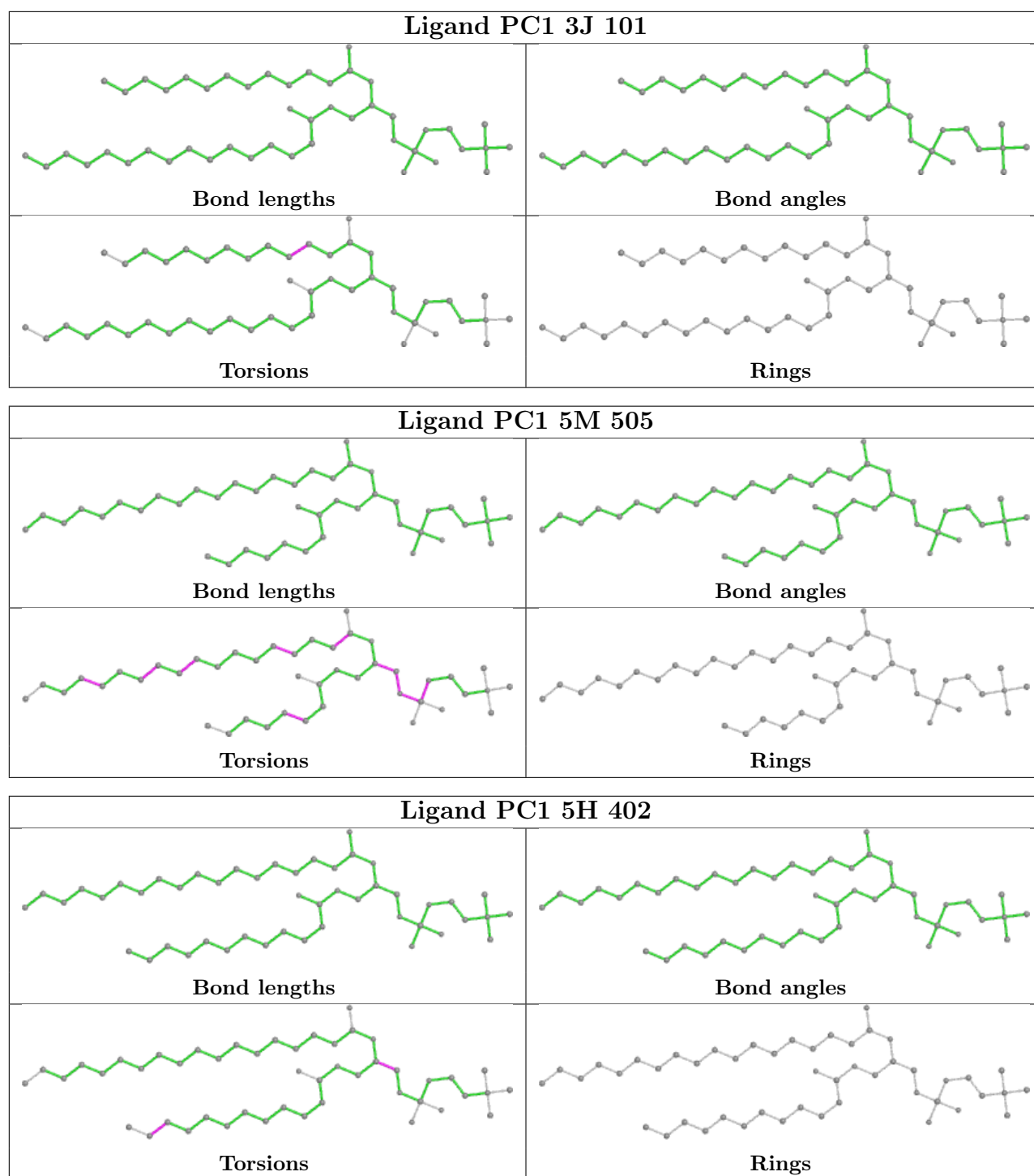


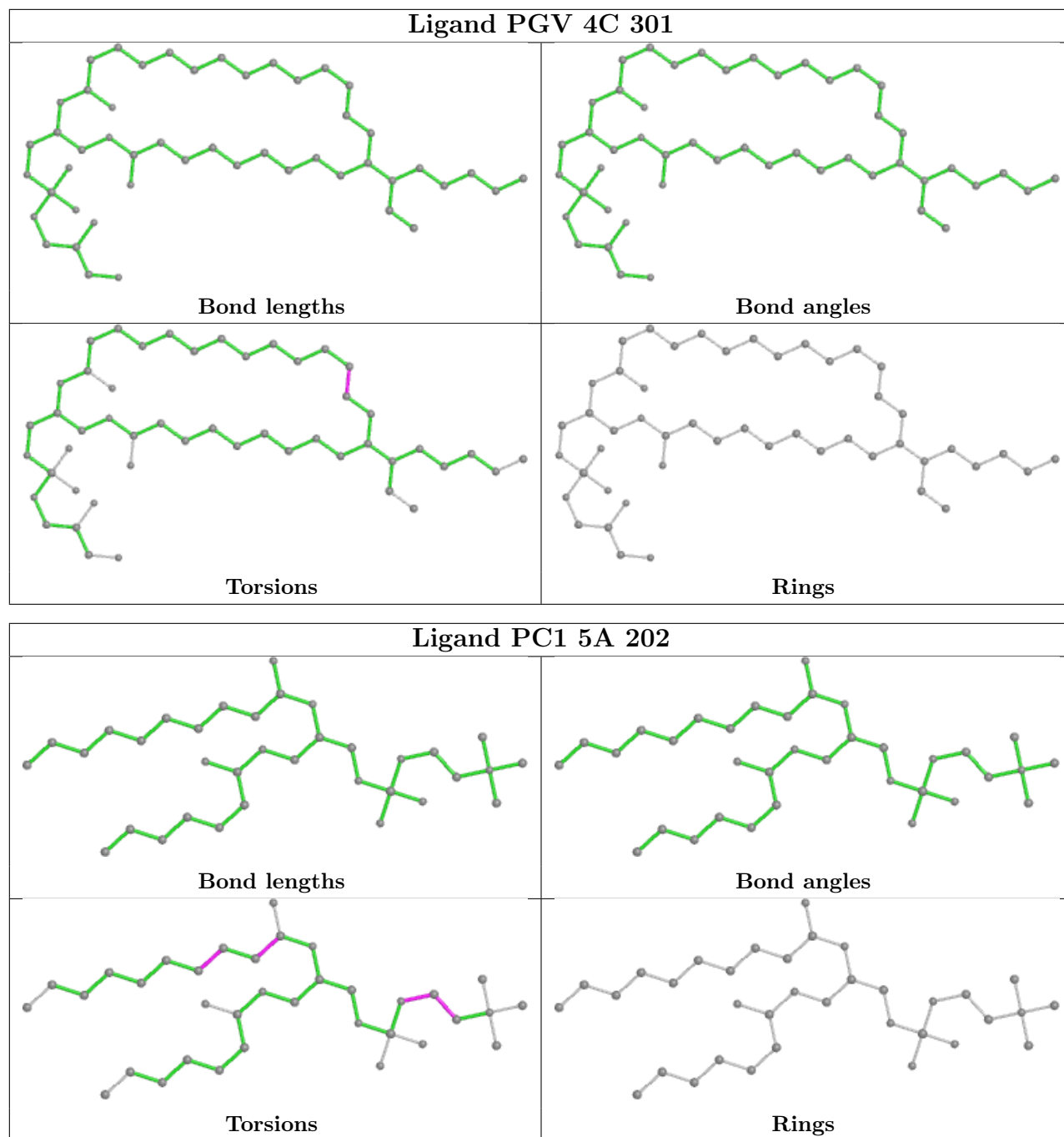


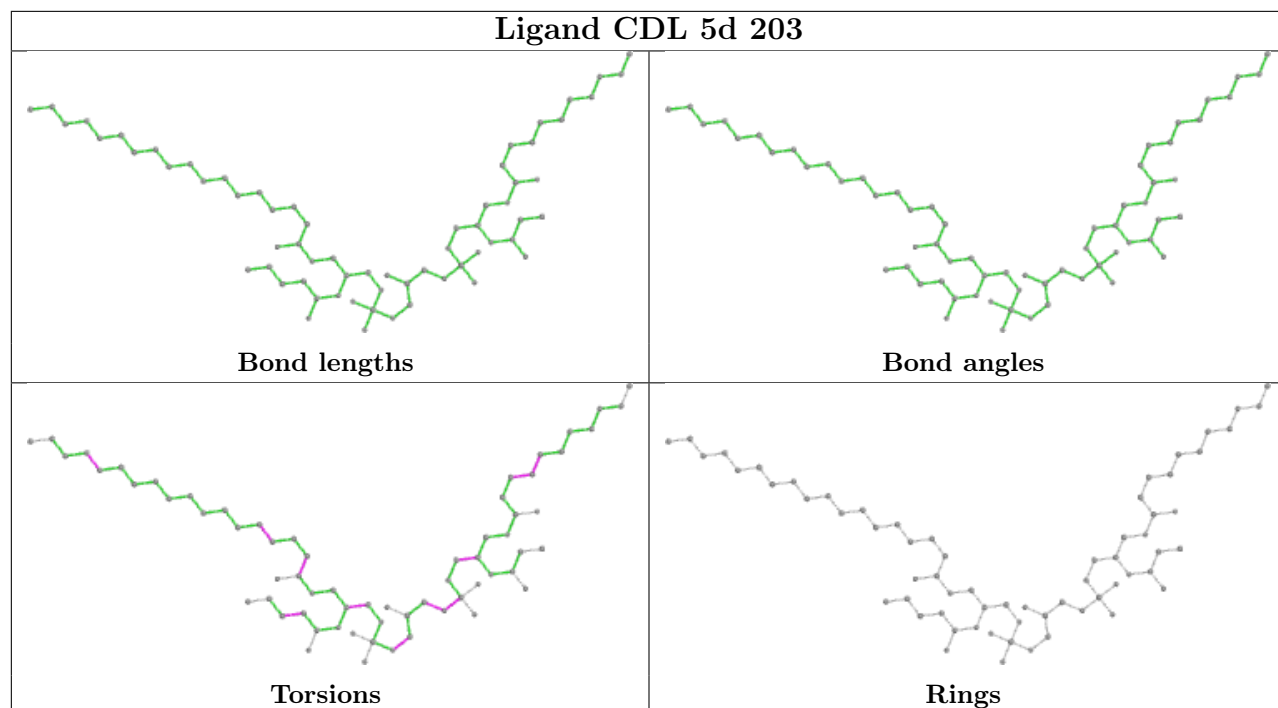


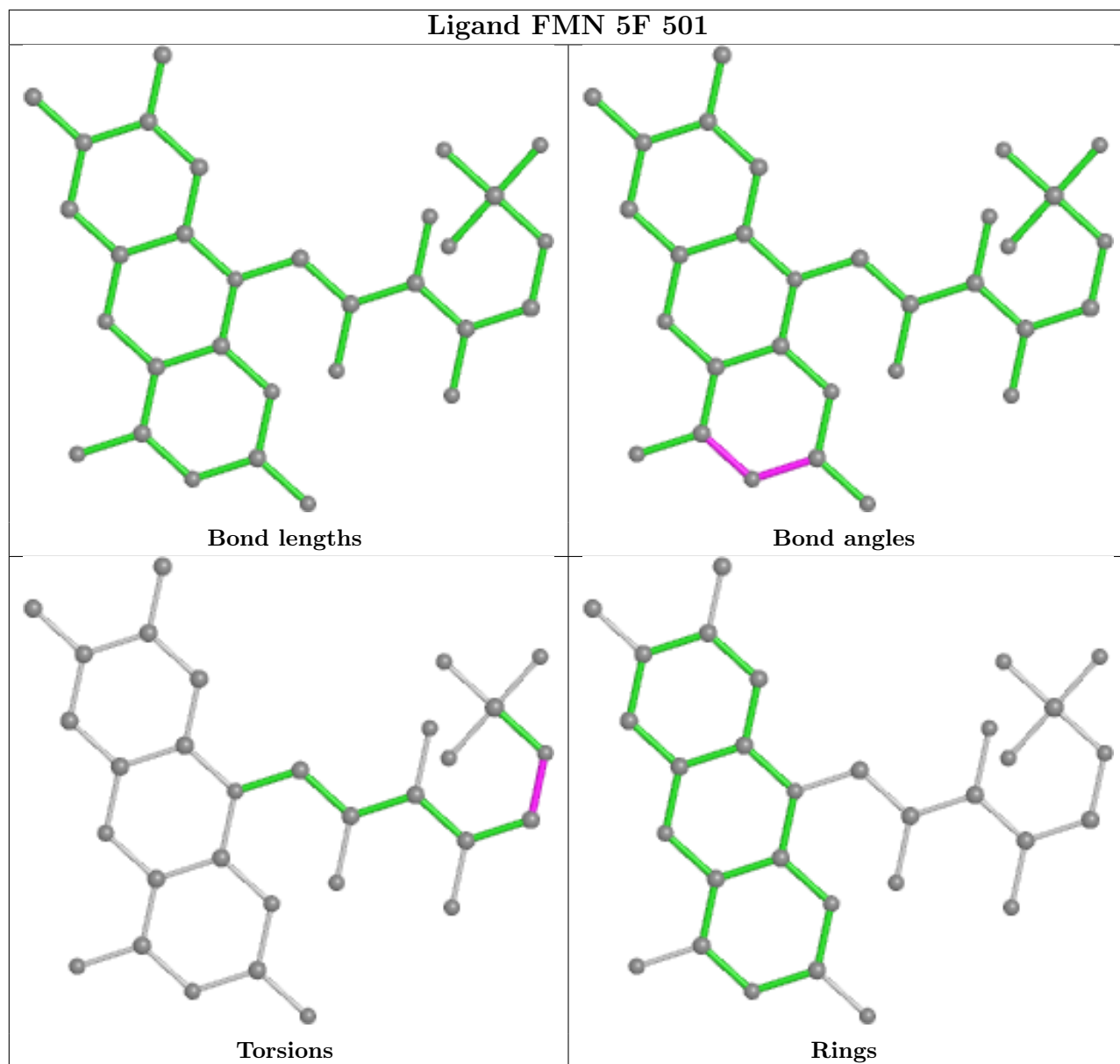


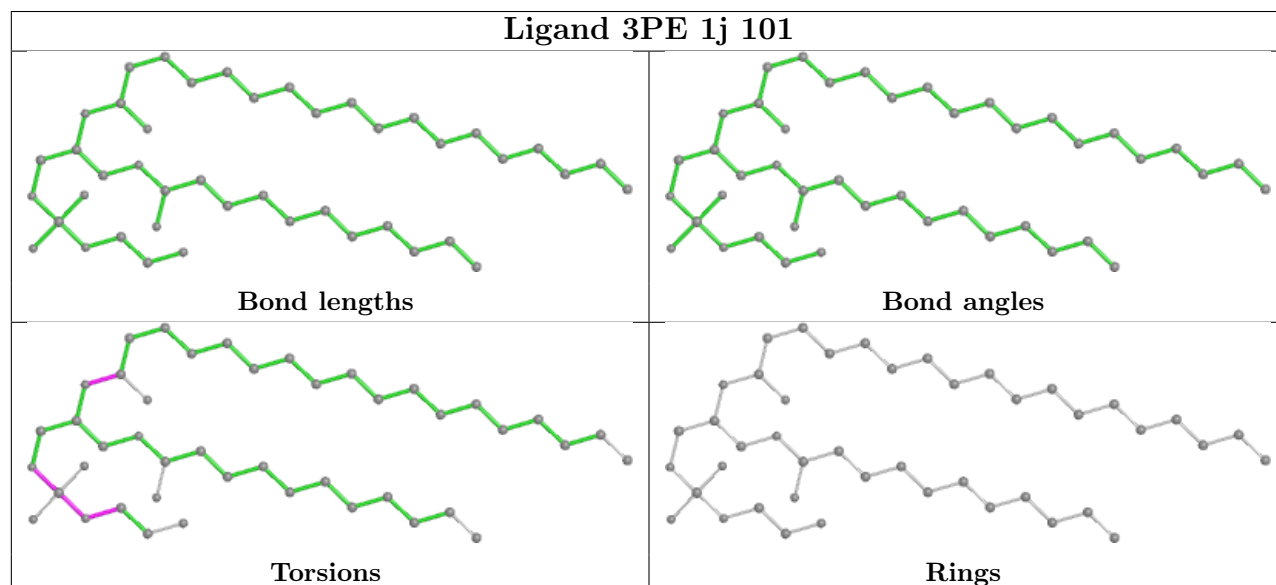
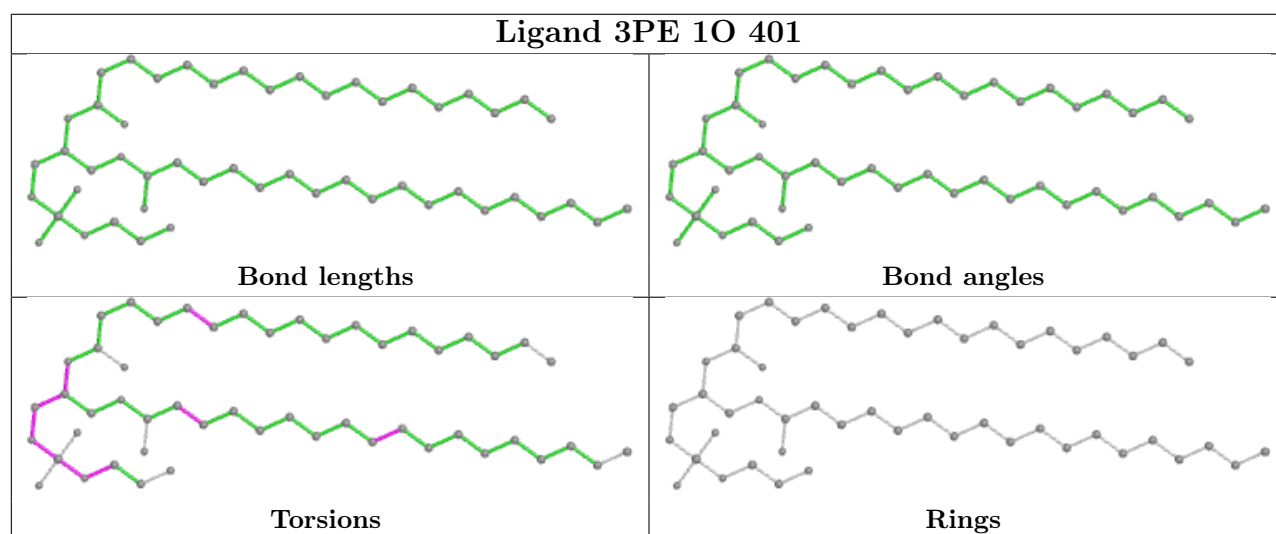
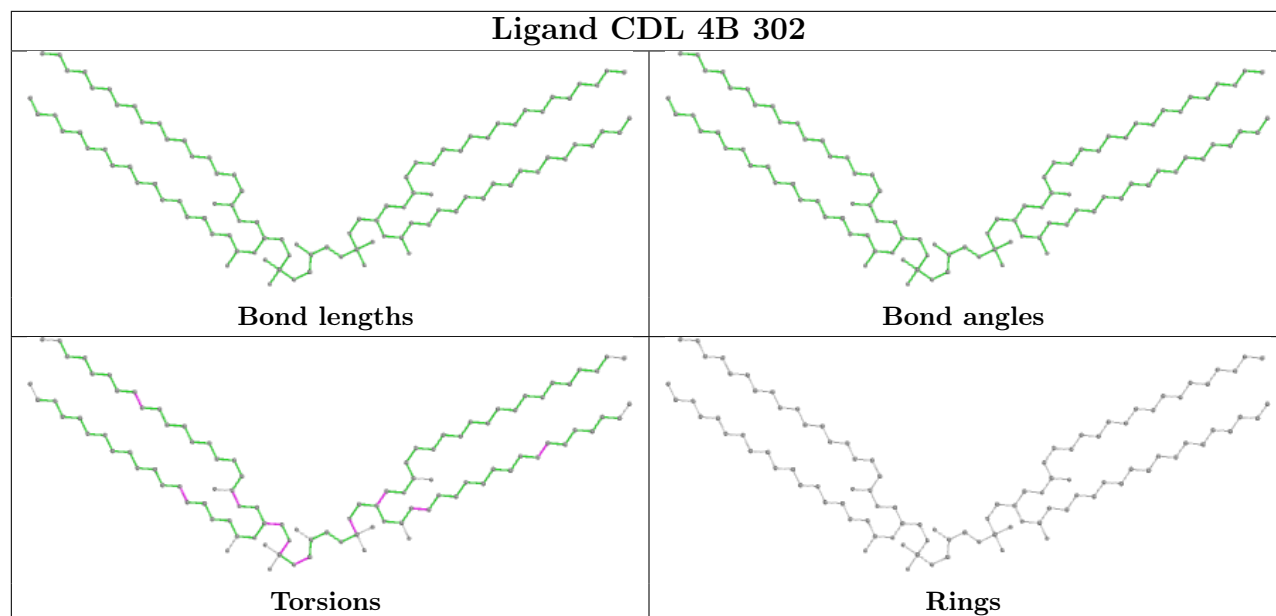


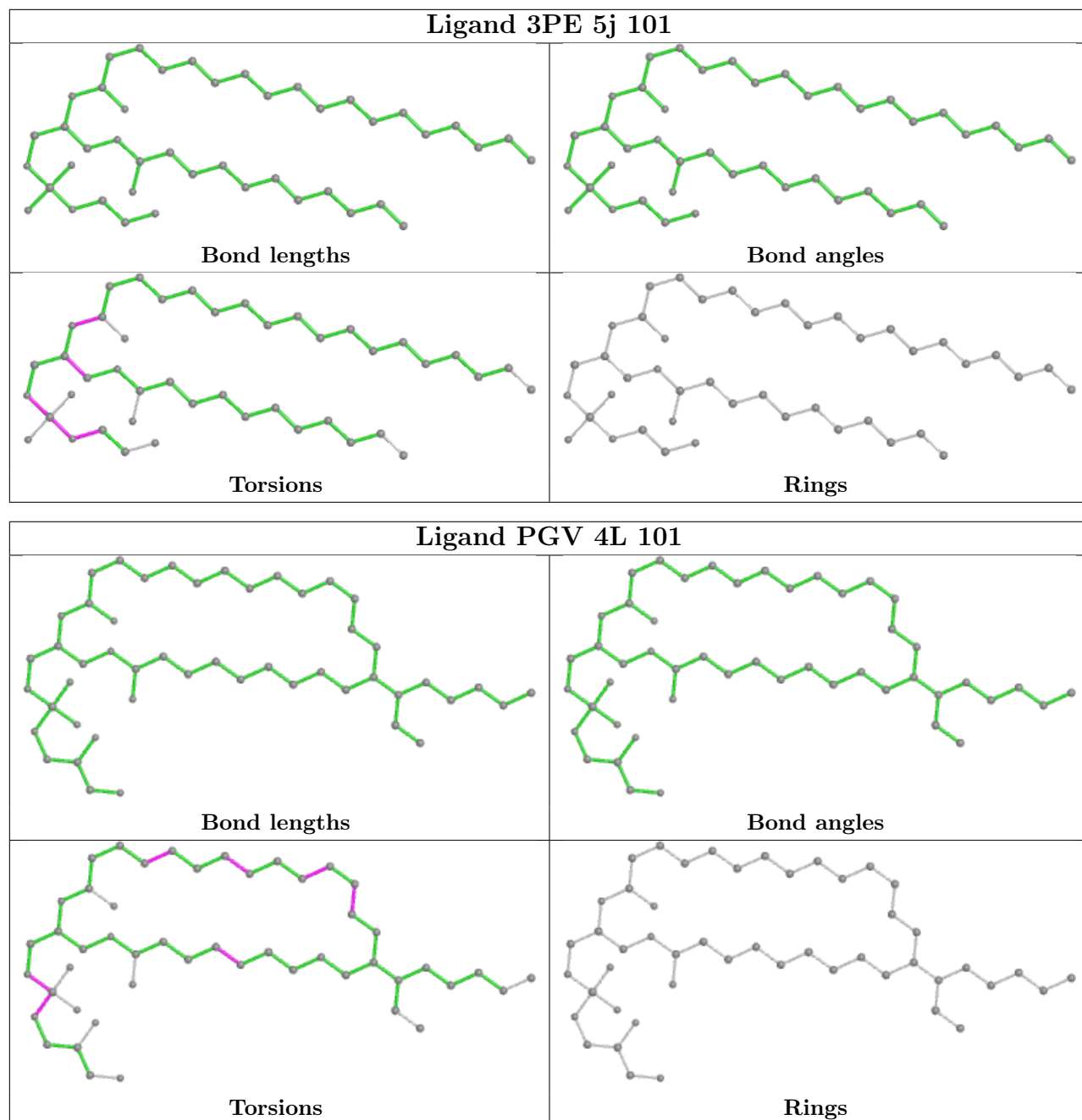




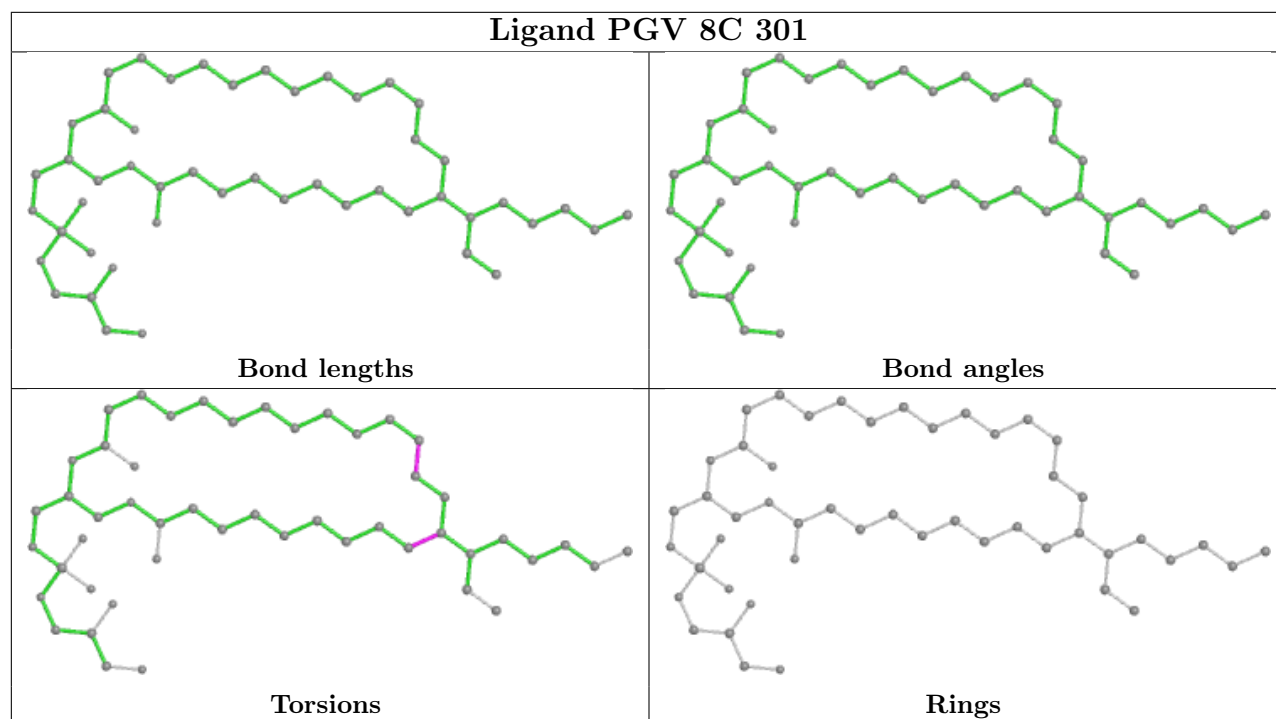
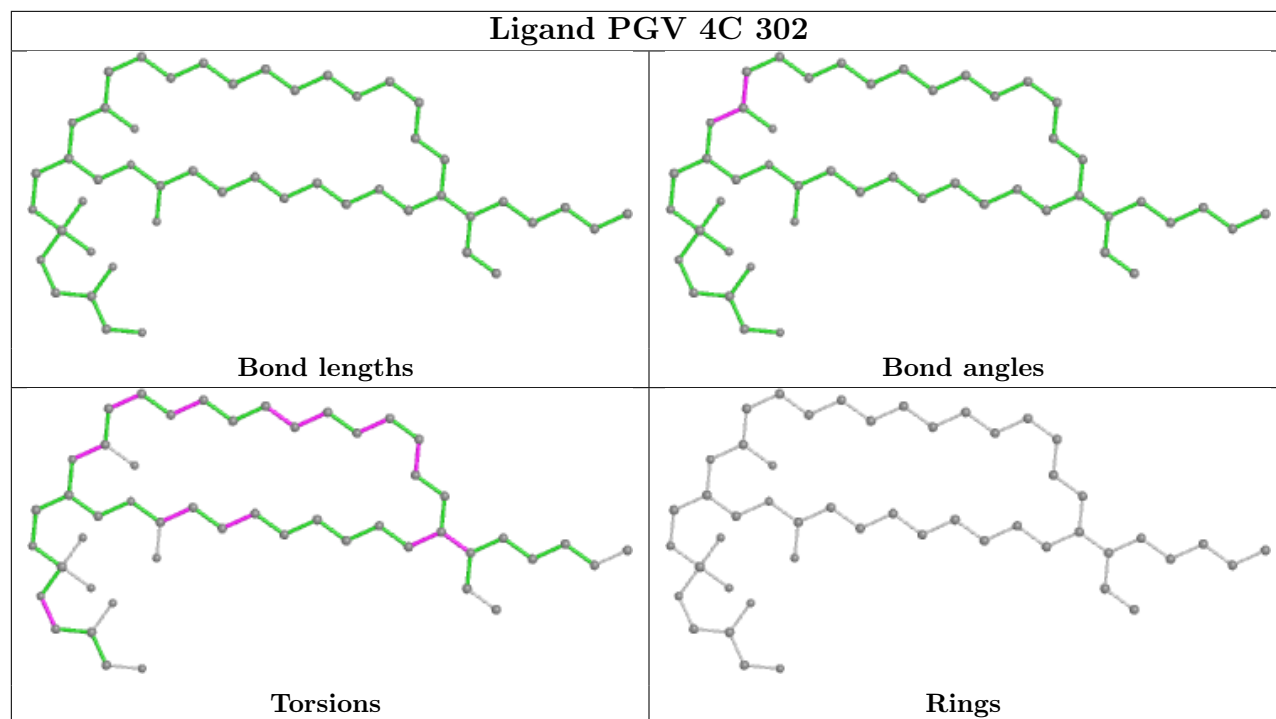


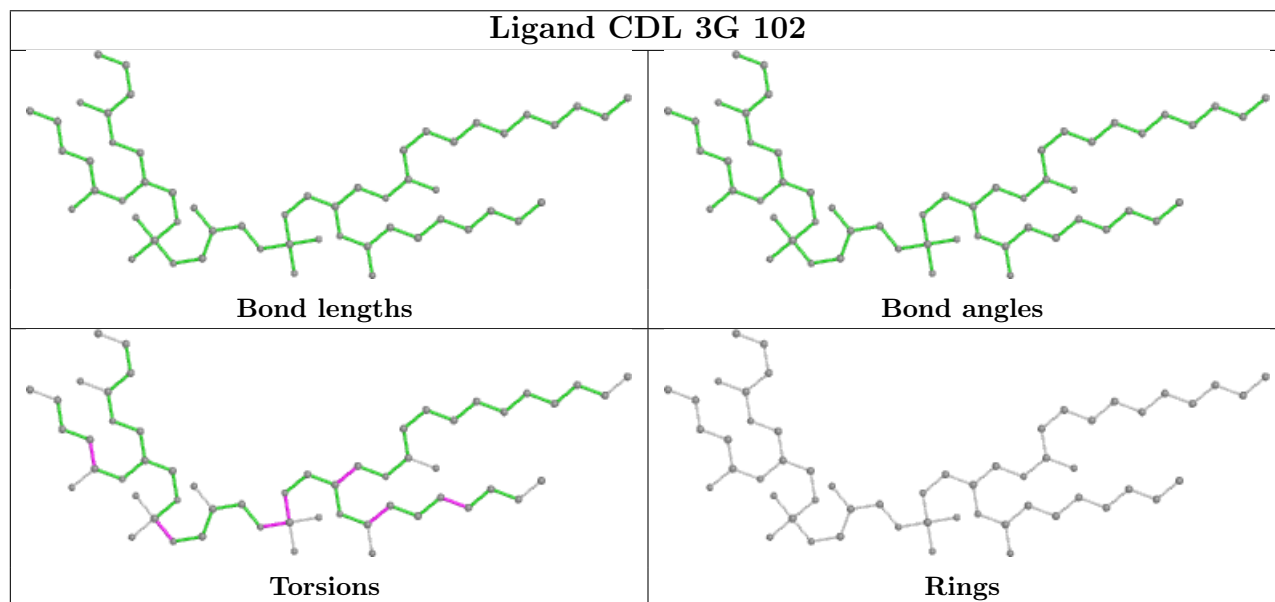
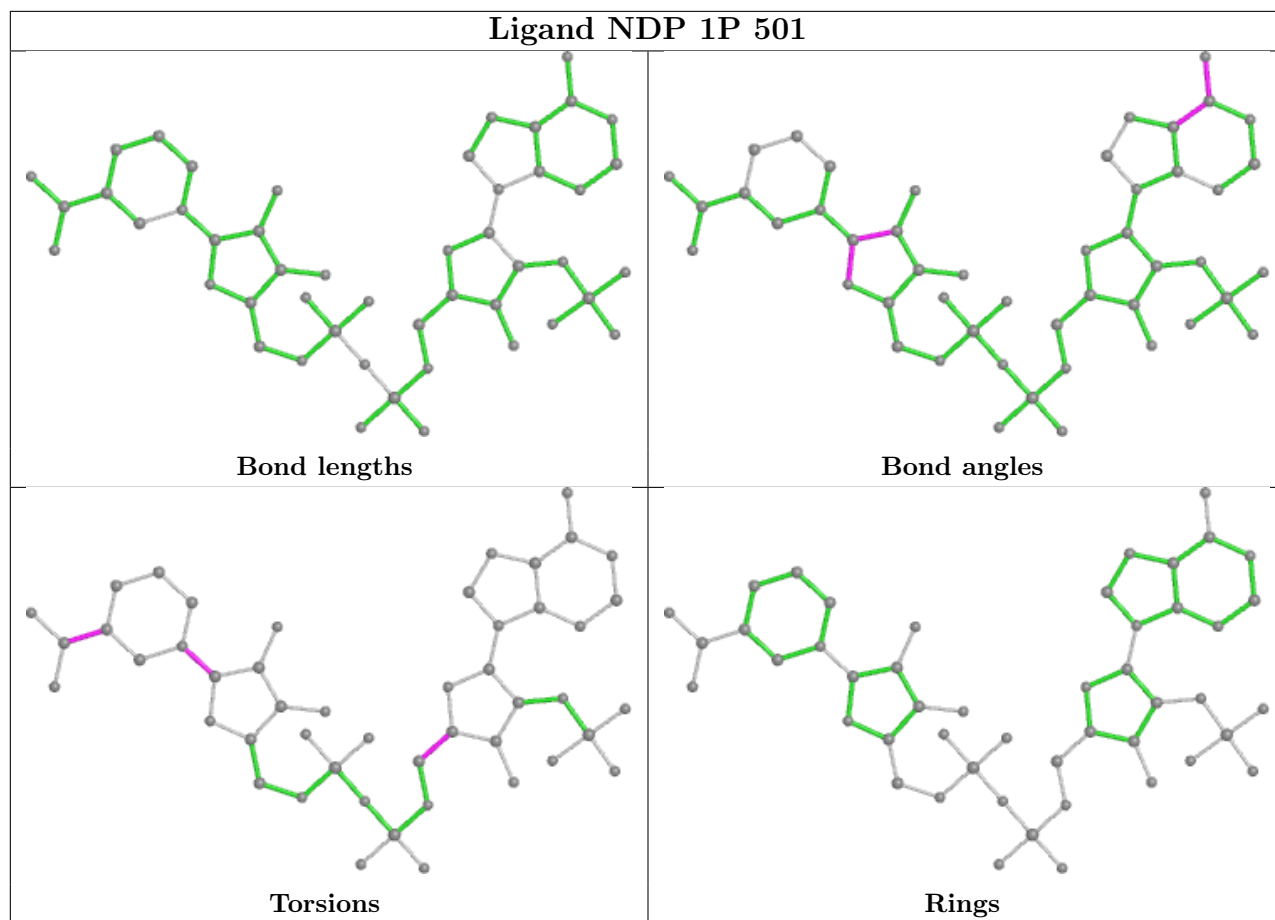


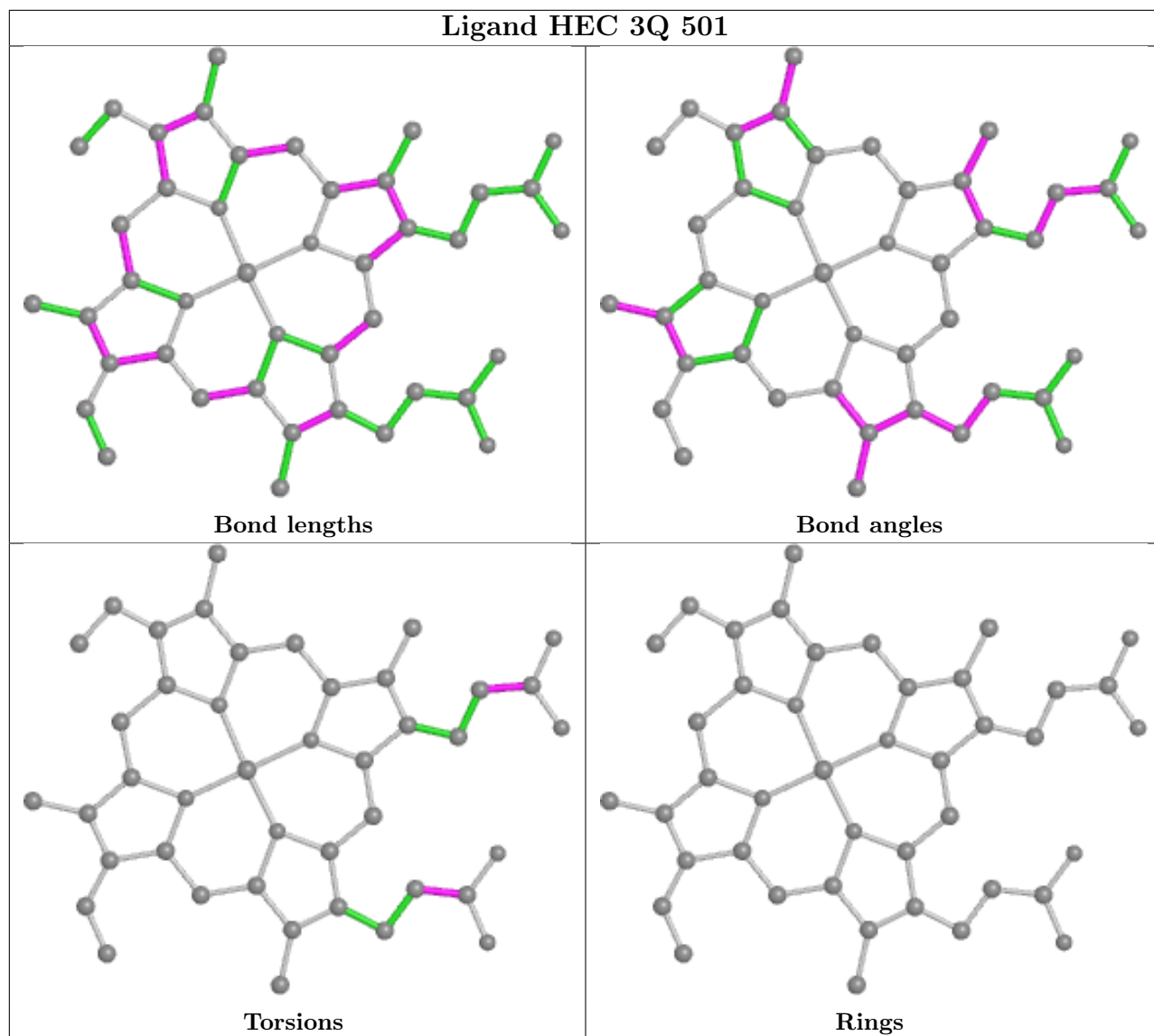


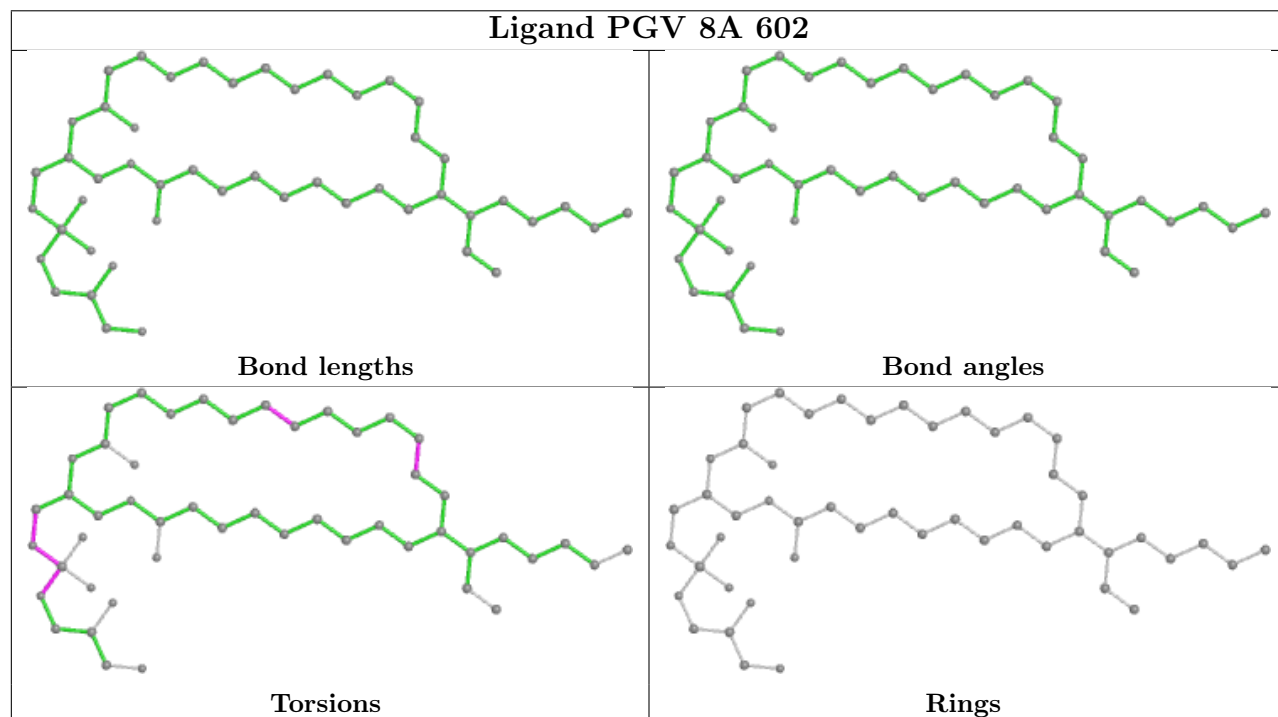
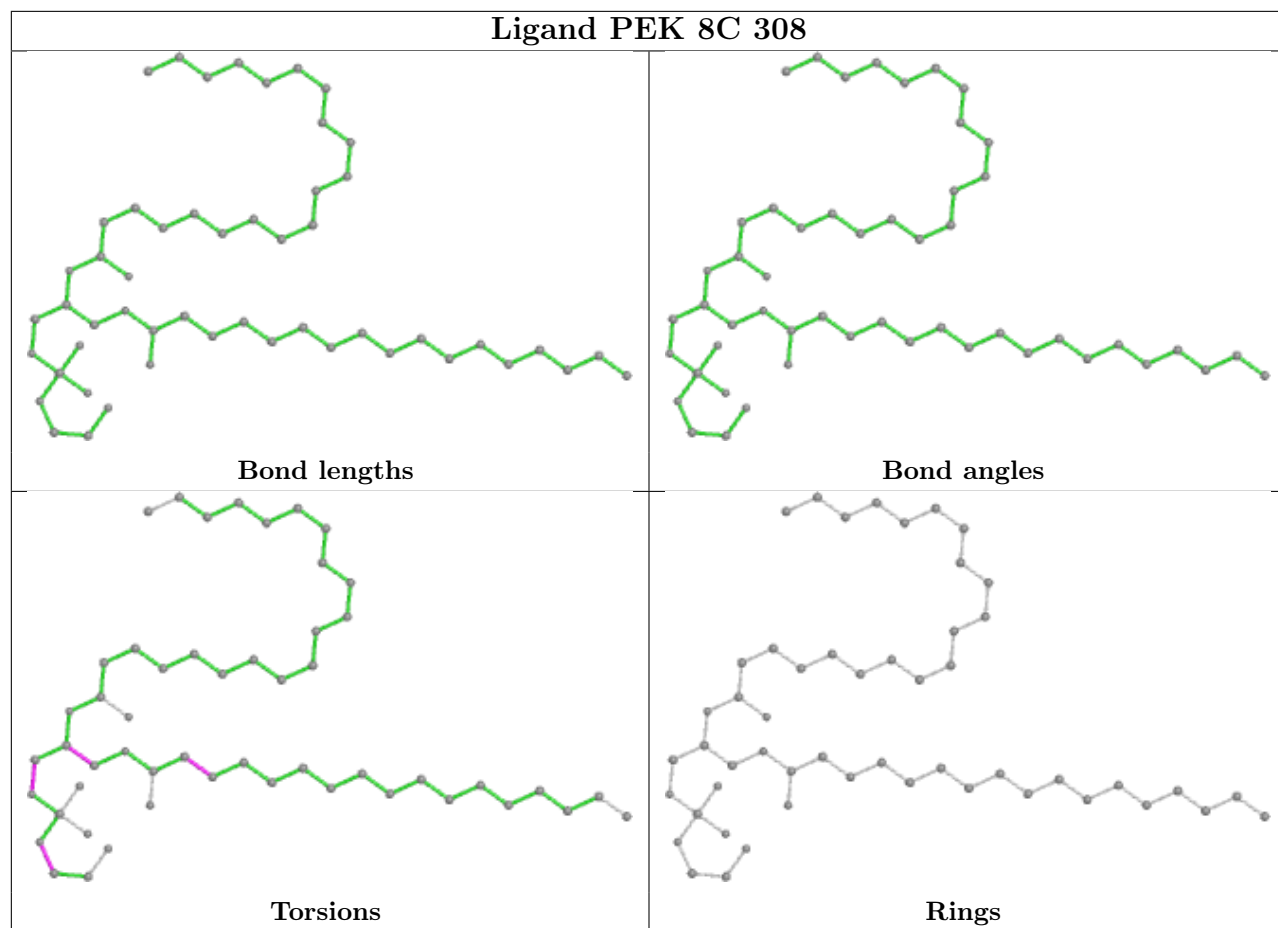


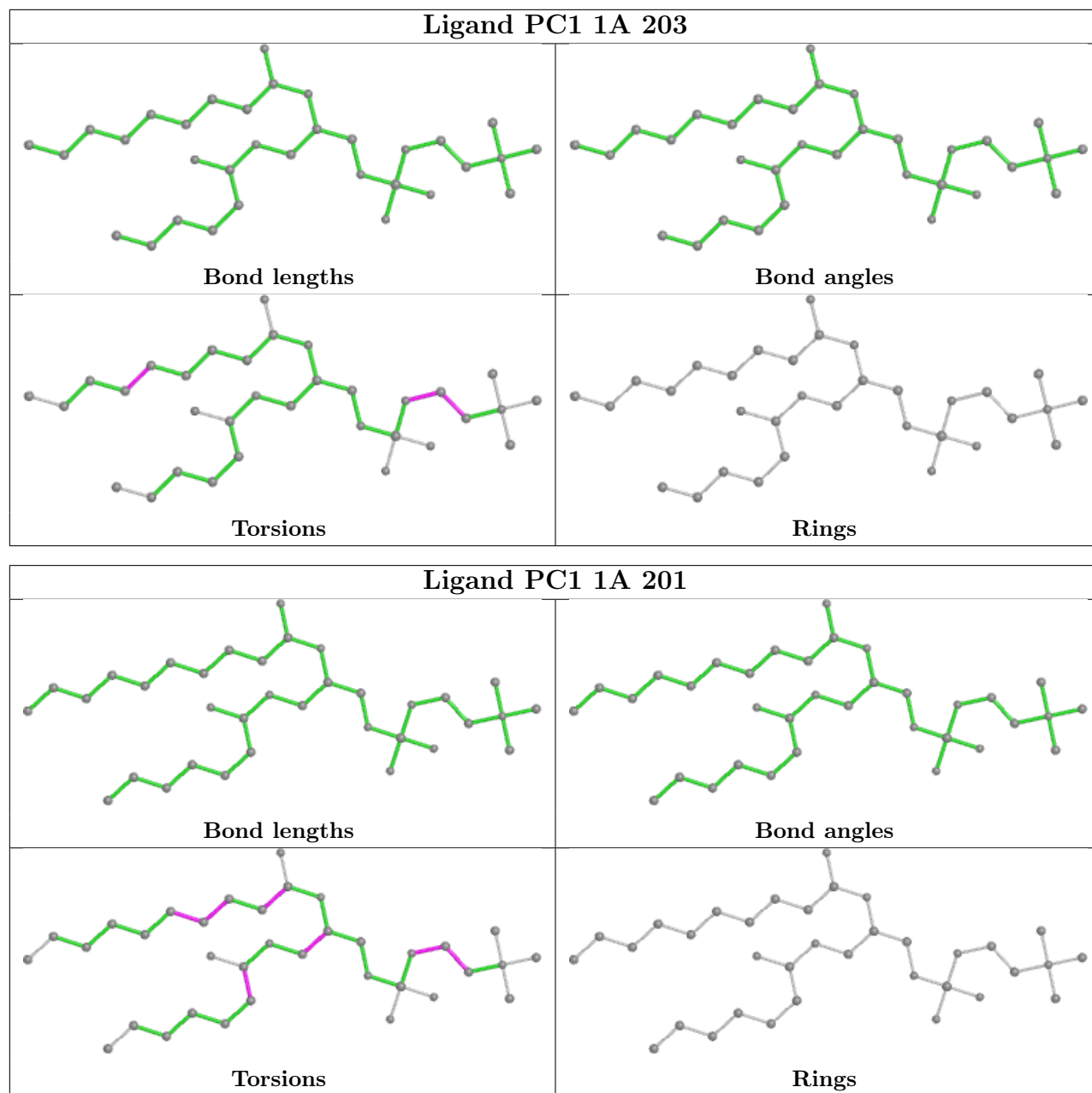


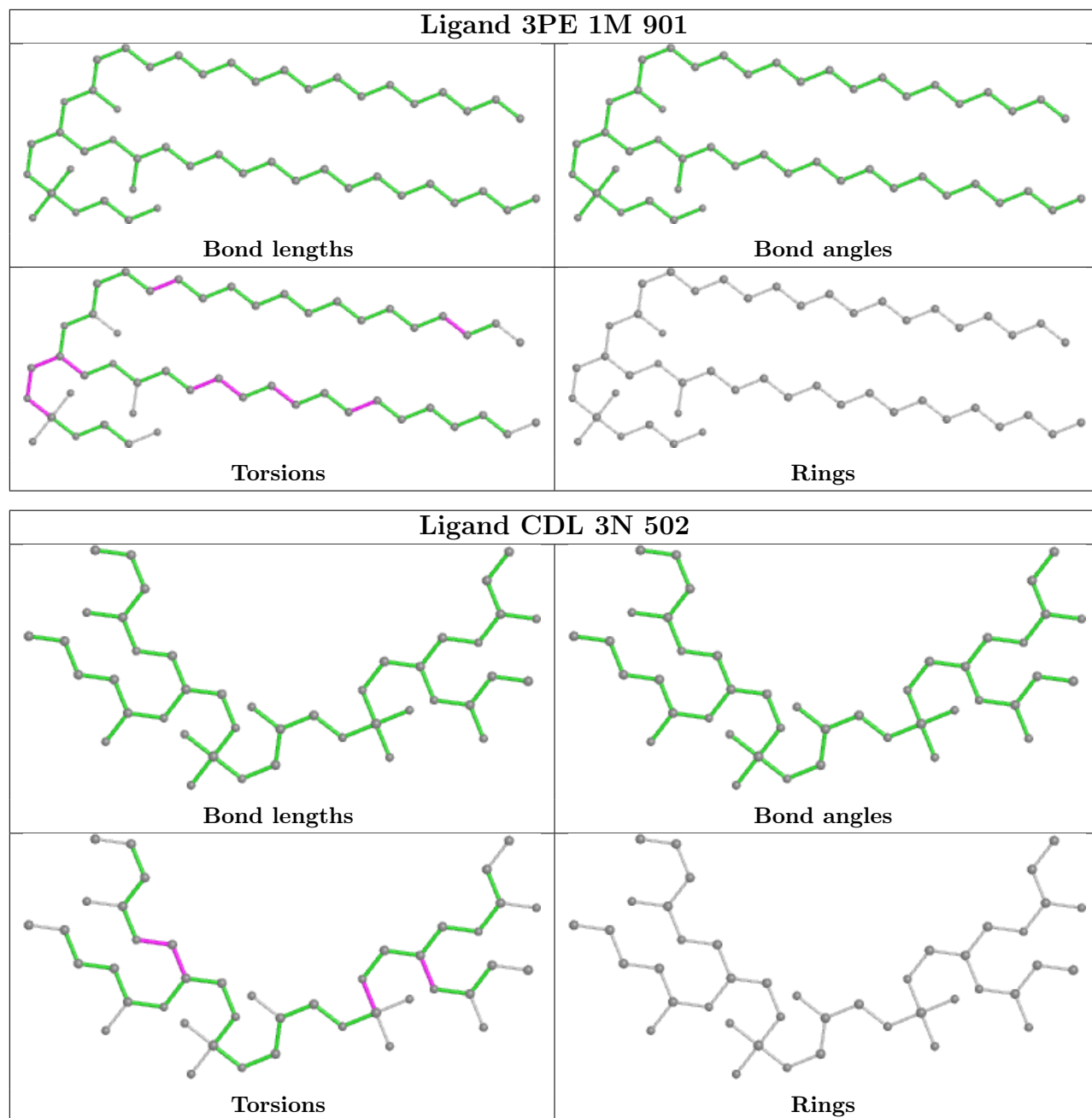


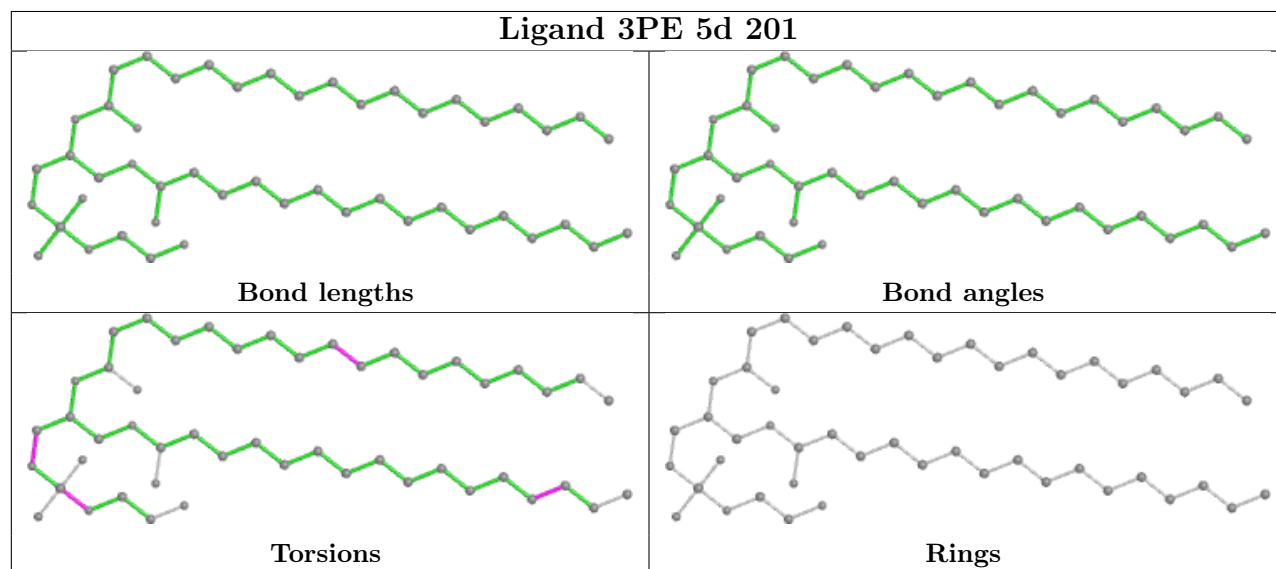
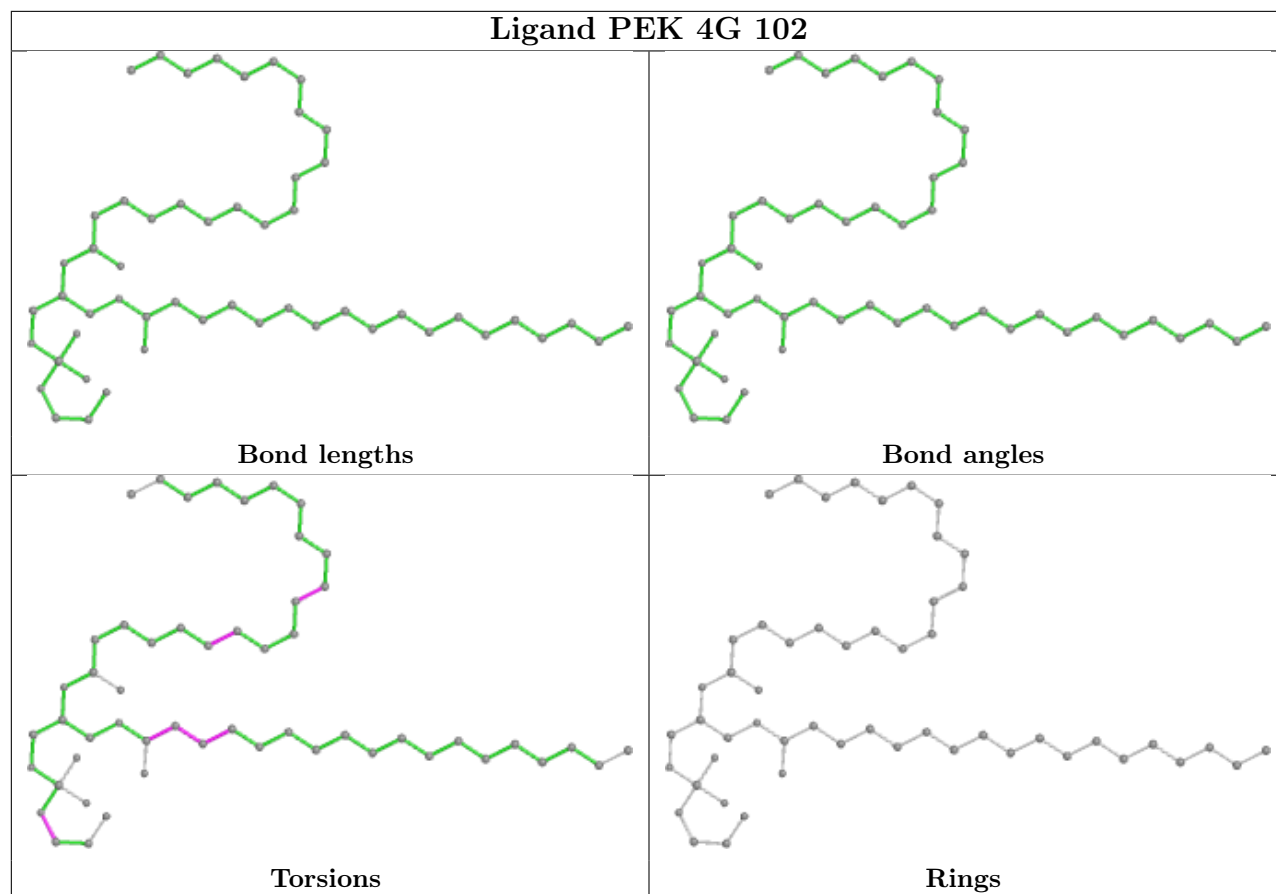


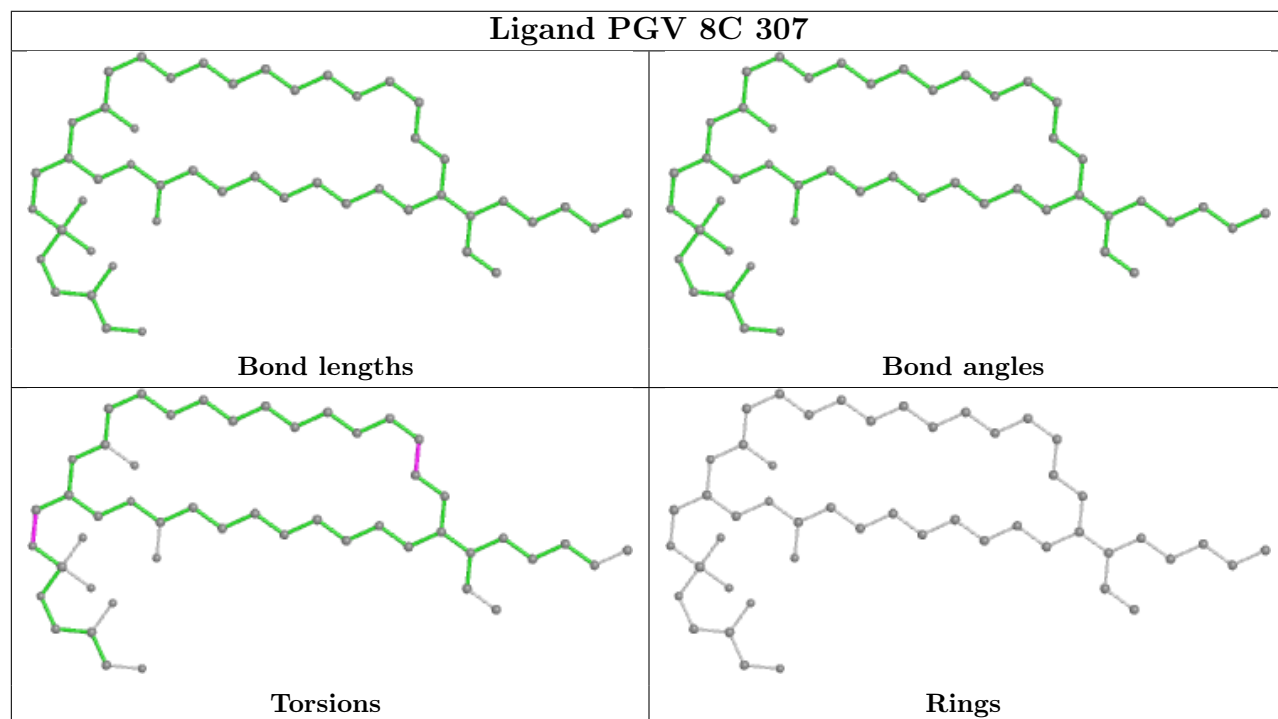
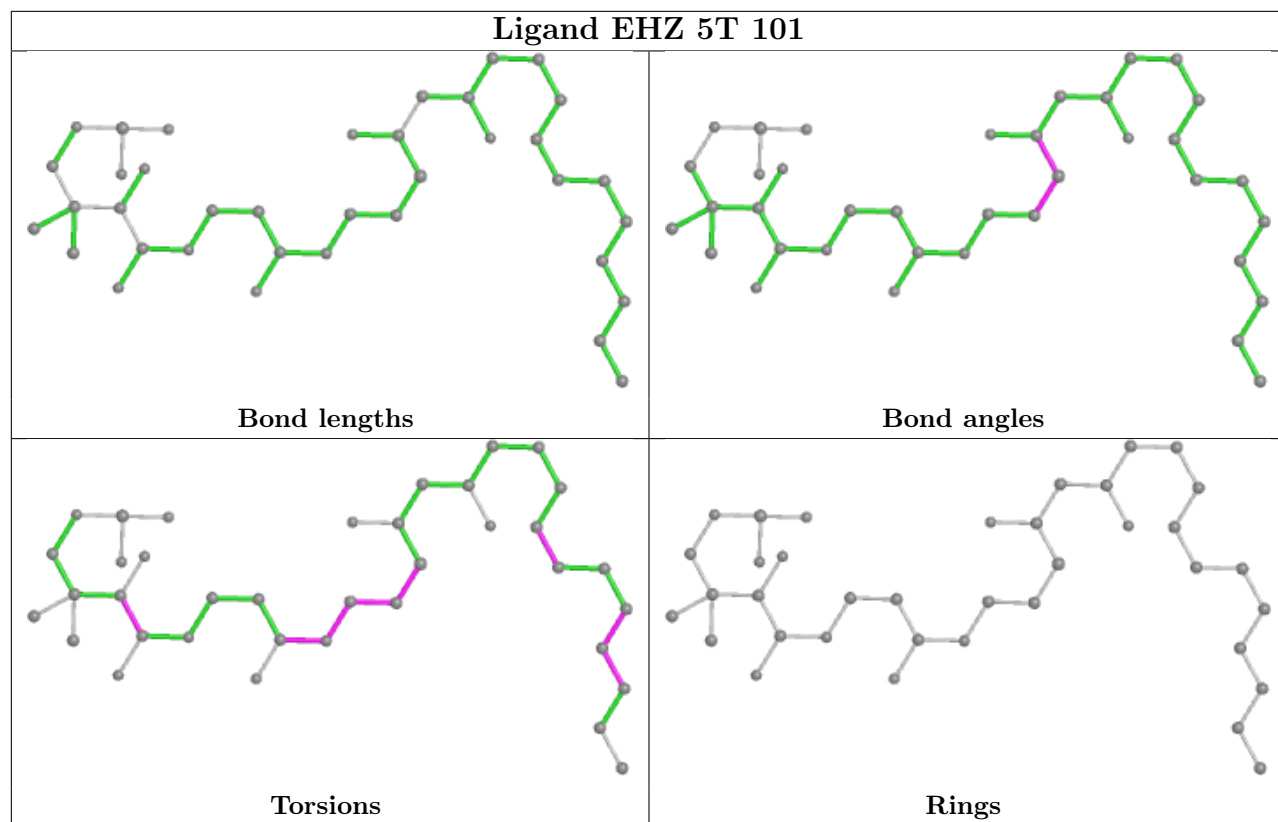




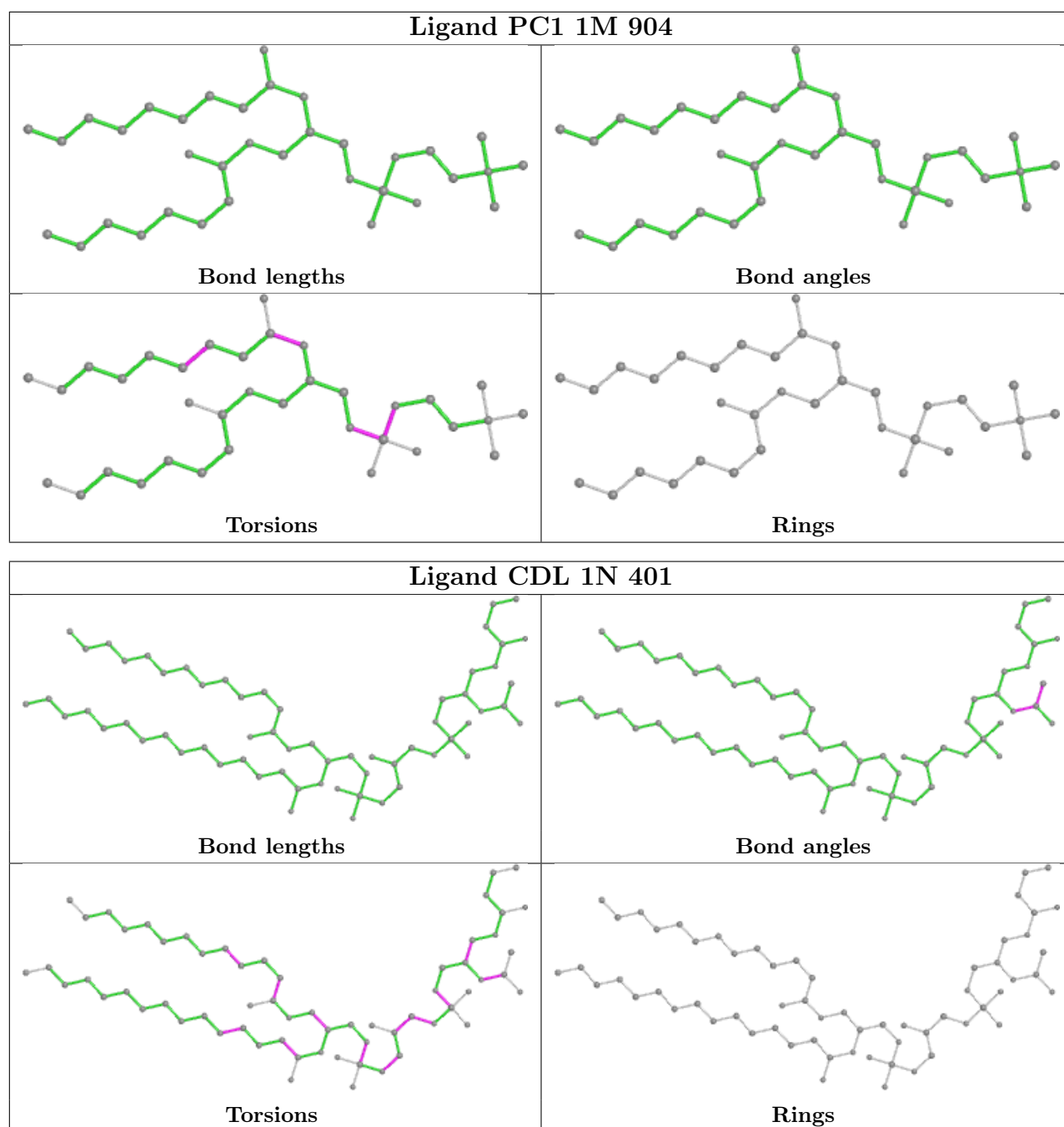


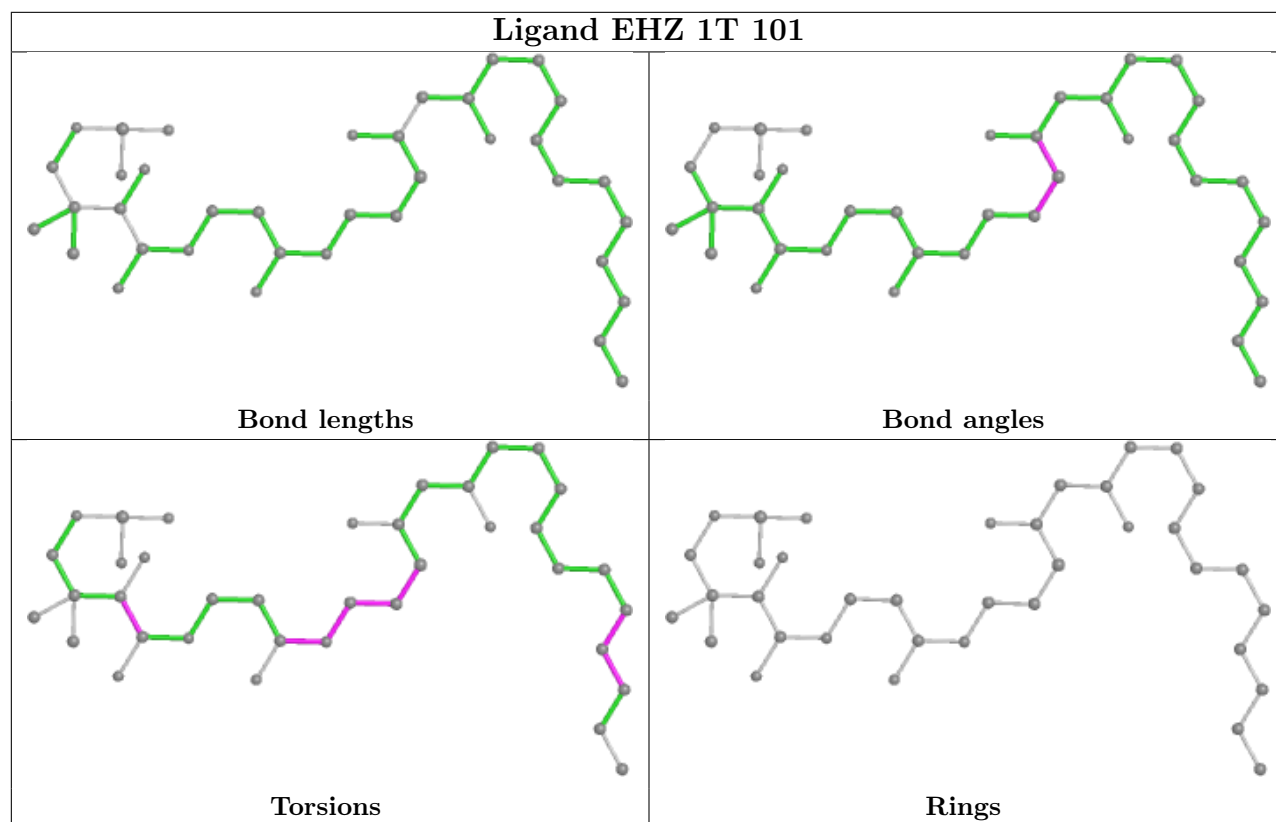
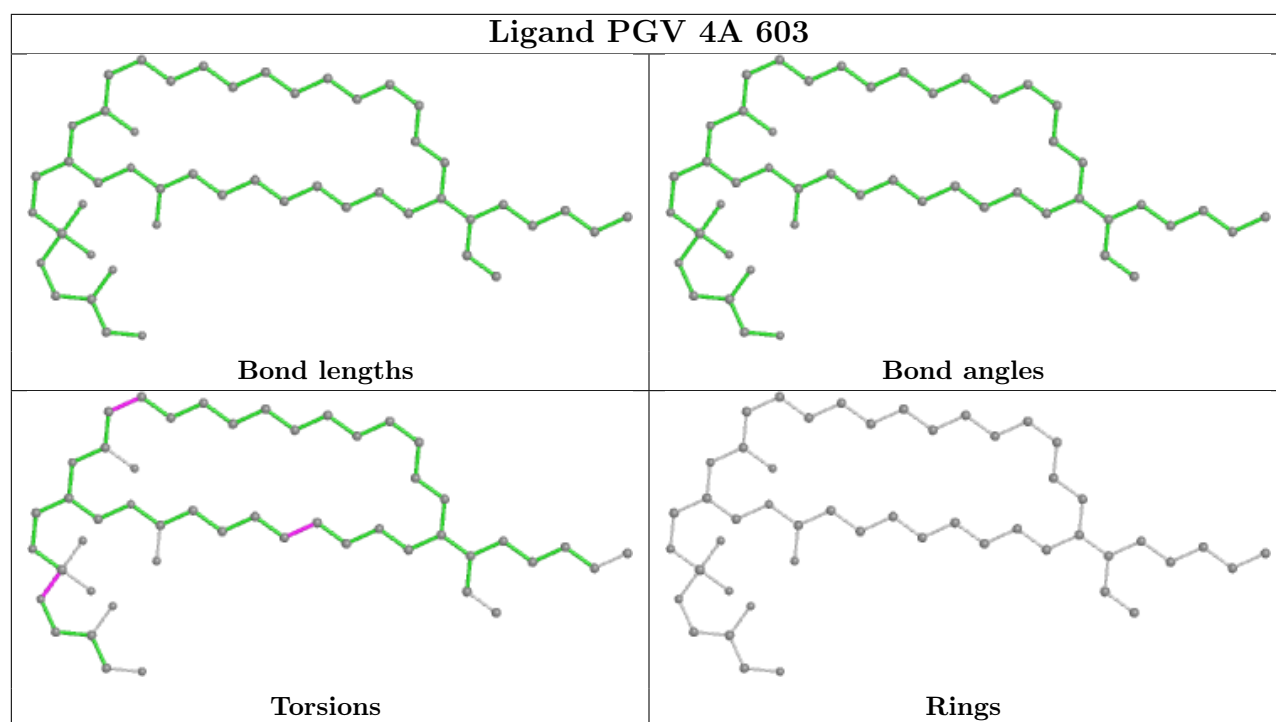


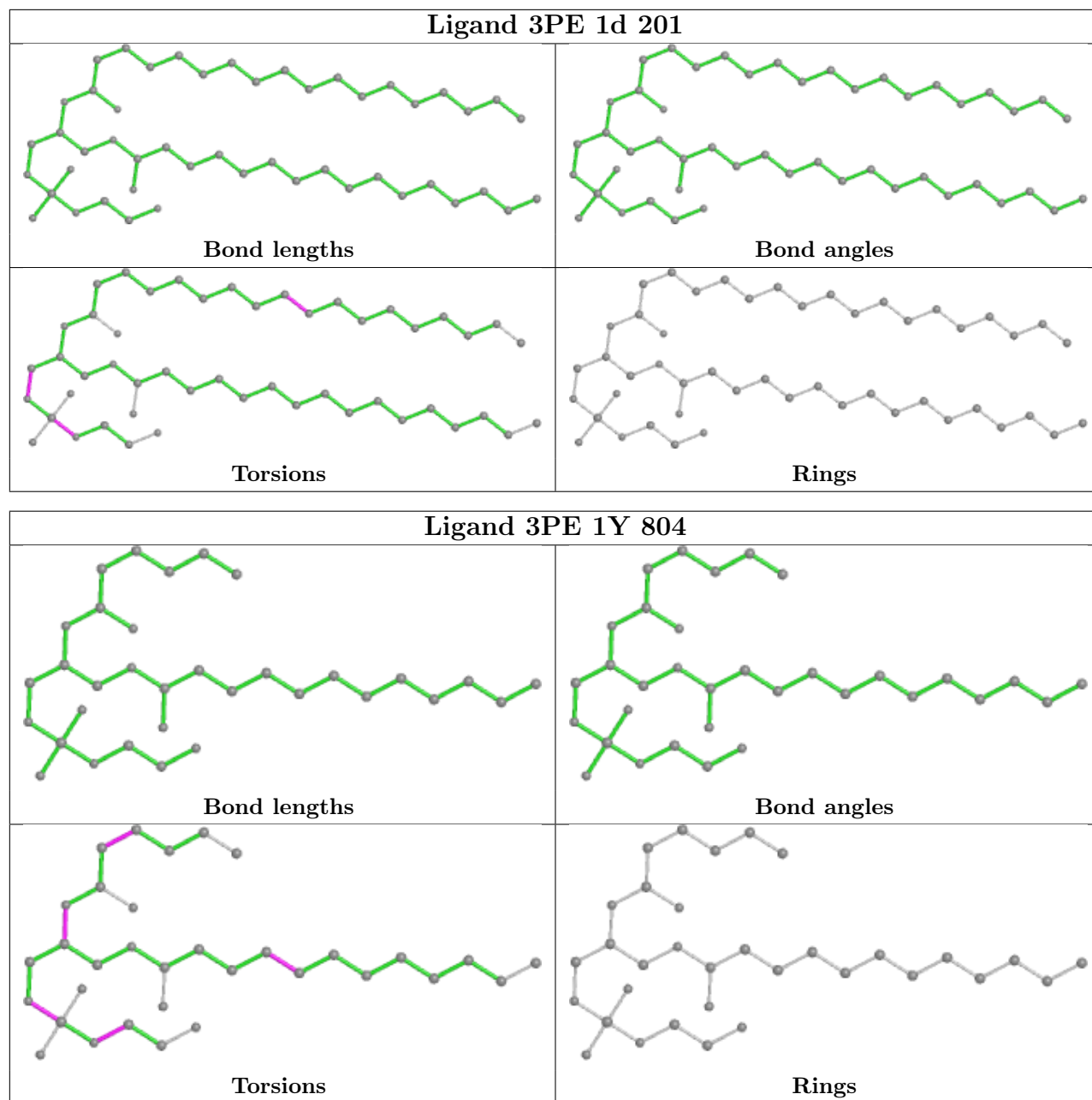


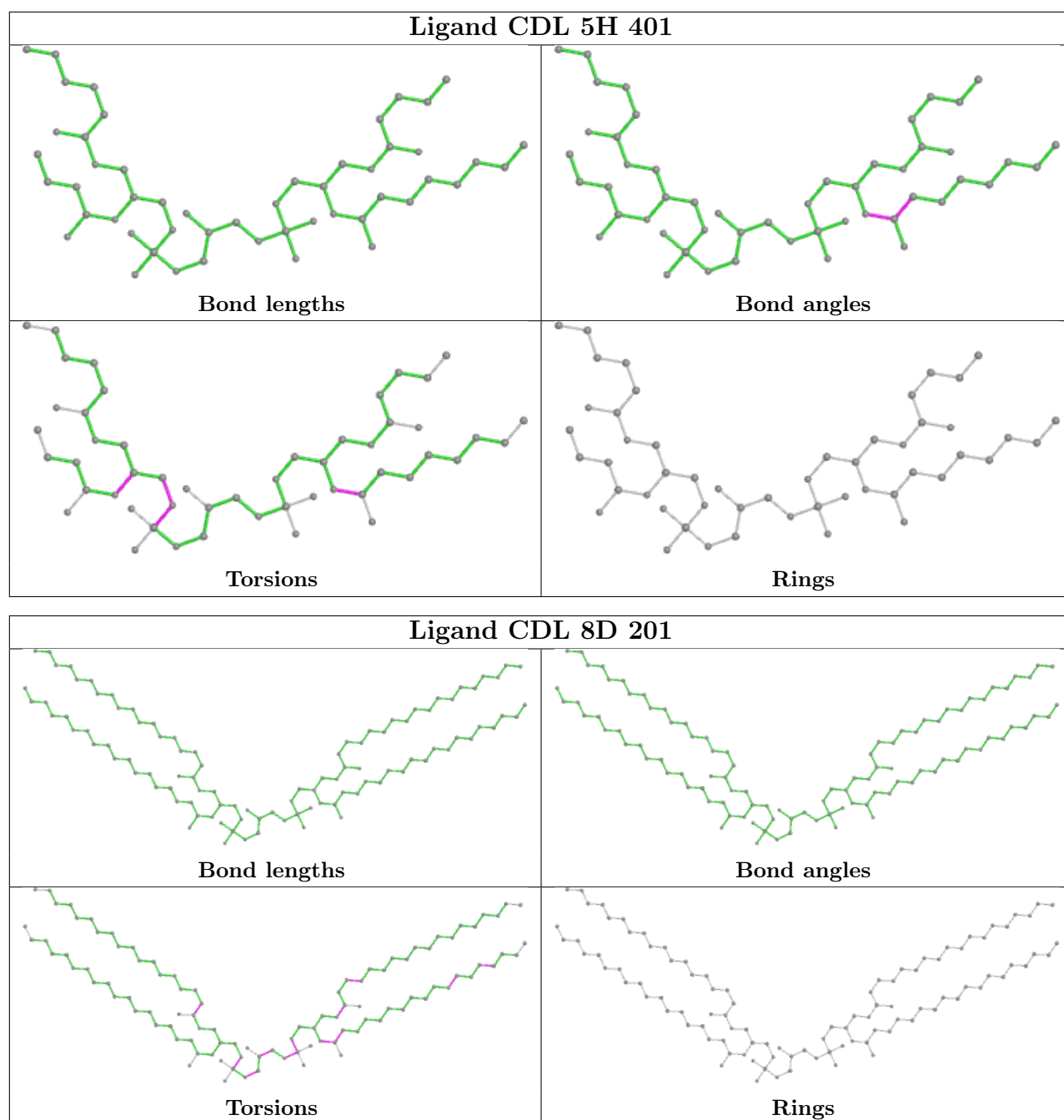












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

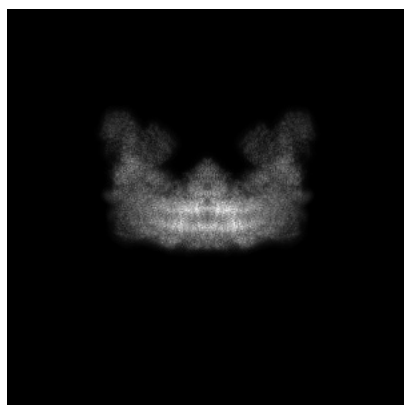
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42230. These allow visual inspection of the internal detail of the map and identification of artifacts.

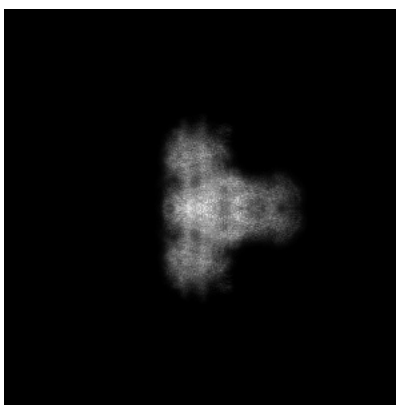
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

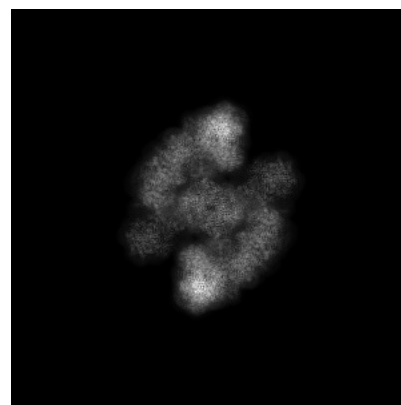
#### 6.1.1 Primary map



X



Y

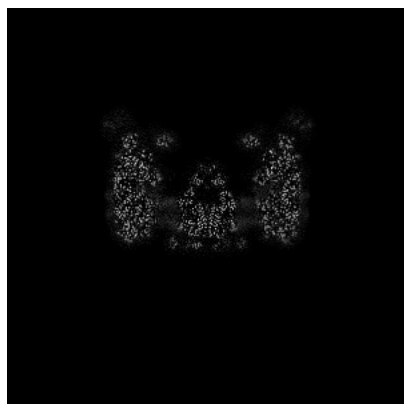


Z

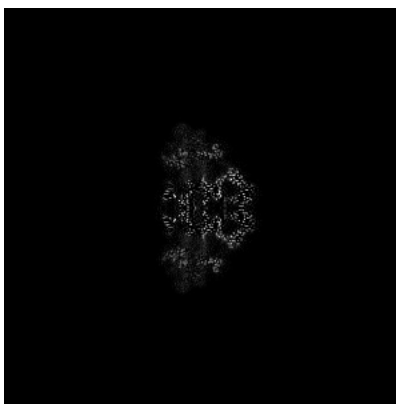
The images above show the map projected in three orthogonal directions.

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

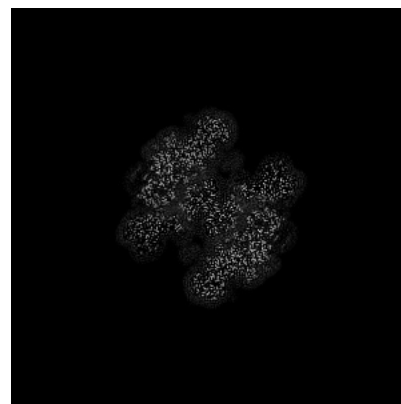
#### 6.2.1 Primary map



X Index: 275



Y Index: 275

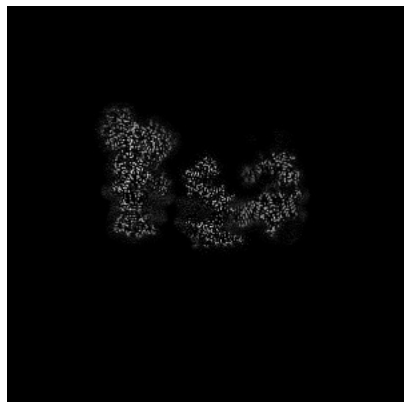


Z Index: 275

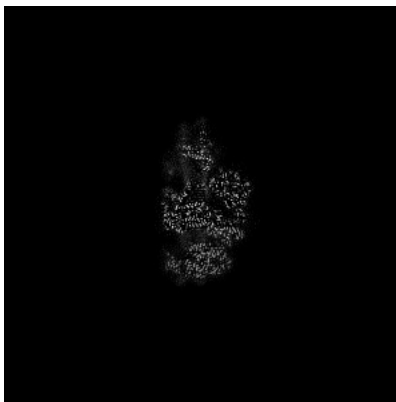
The images above show central slices of the map in three orthogonal directions.

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

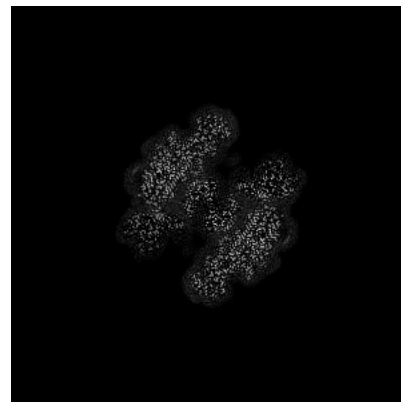
### 6.3.1 Primary map



X Index: 260



Y Index: 288

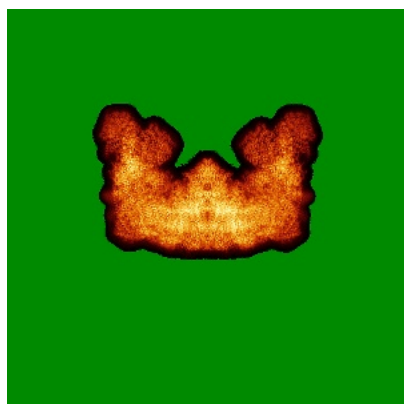


Z Index: 271

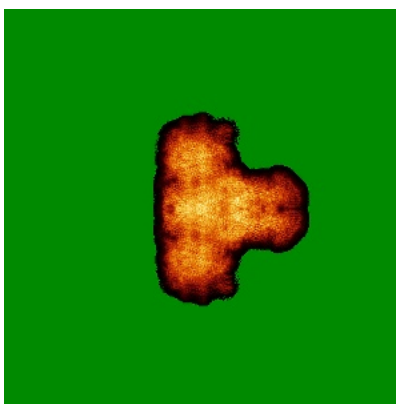
The images above show the largest variance slices of the map in three orthogonal directions.

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

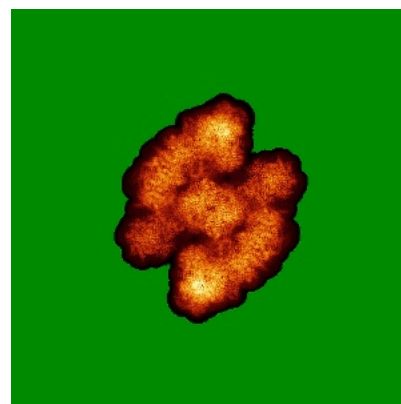
### 6.4.1 Primary map



X



Y

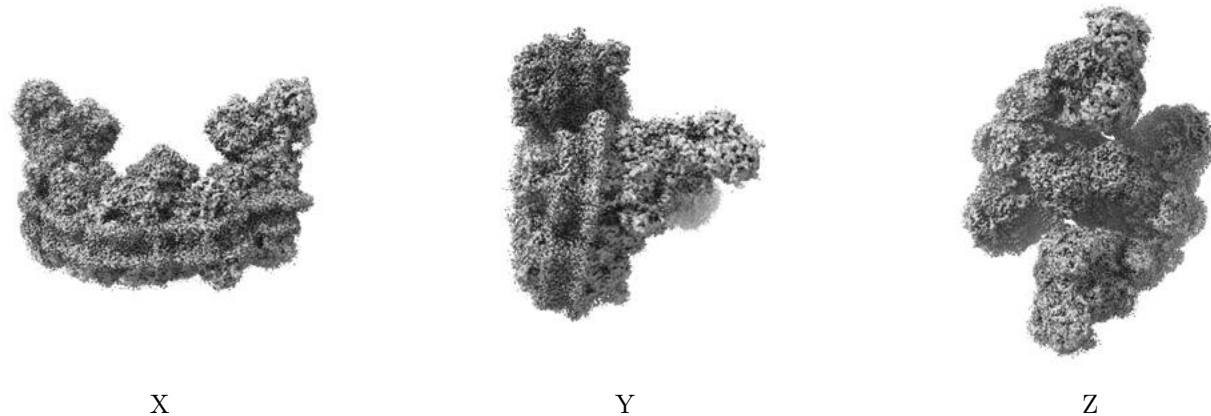


Z

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

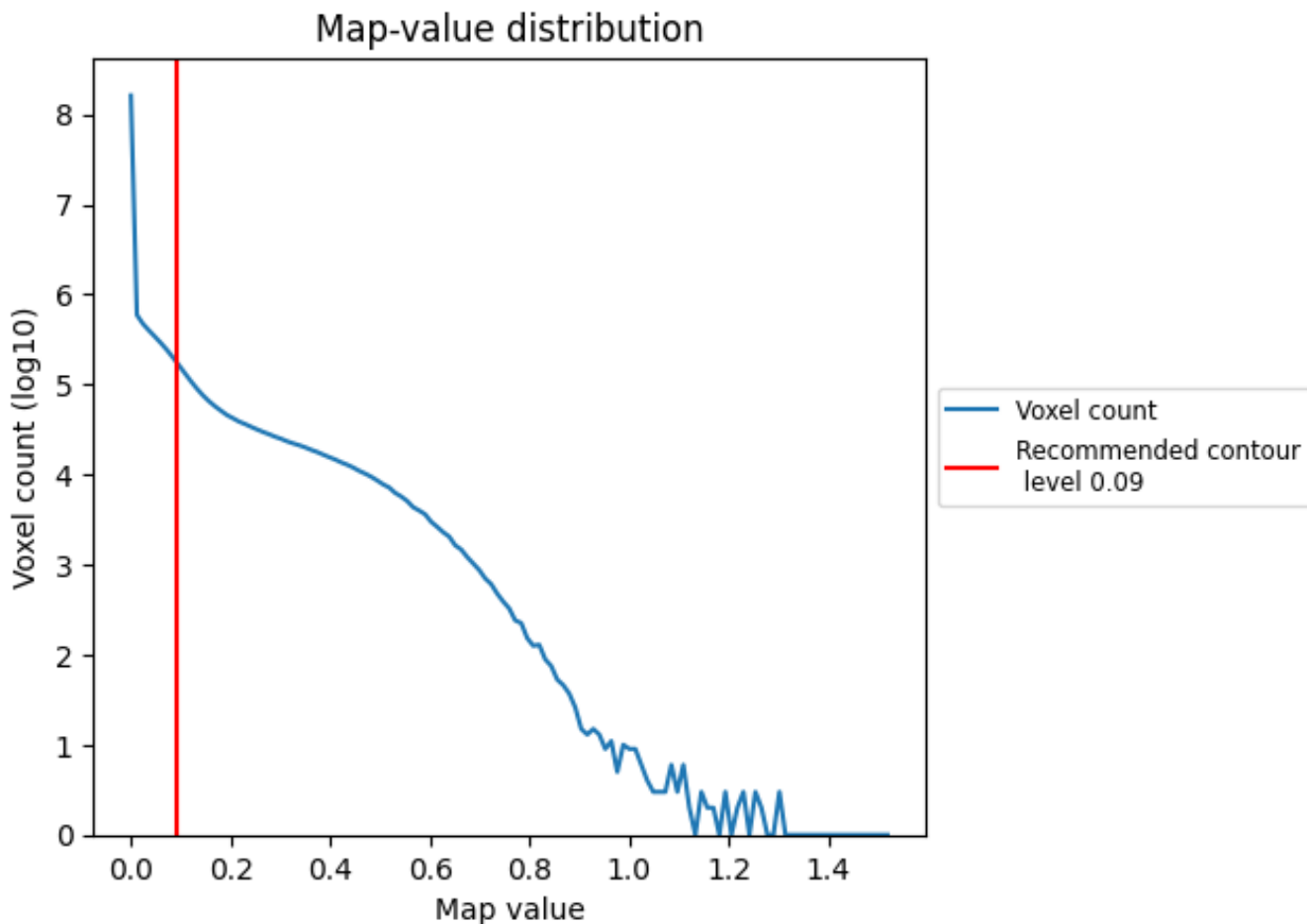
## 6.6 Mask visualisation [i](#)

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.

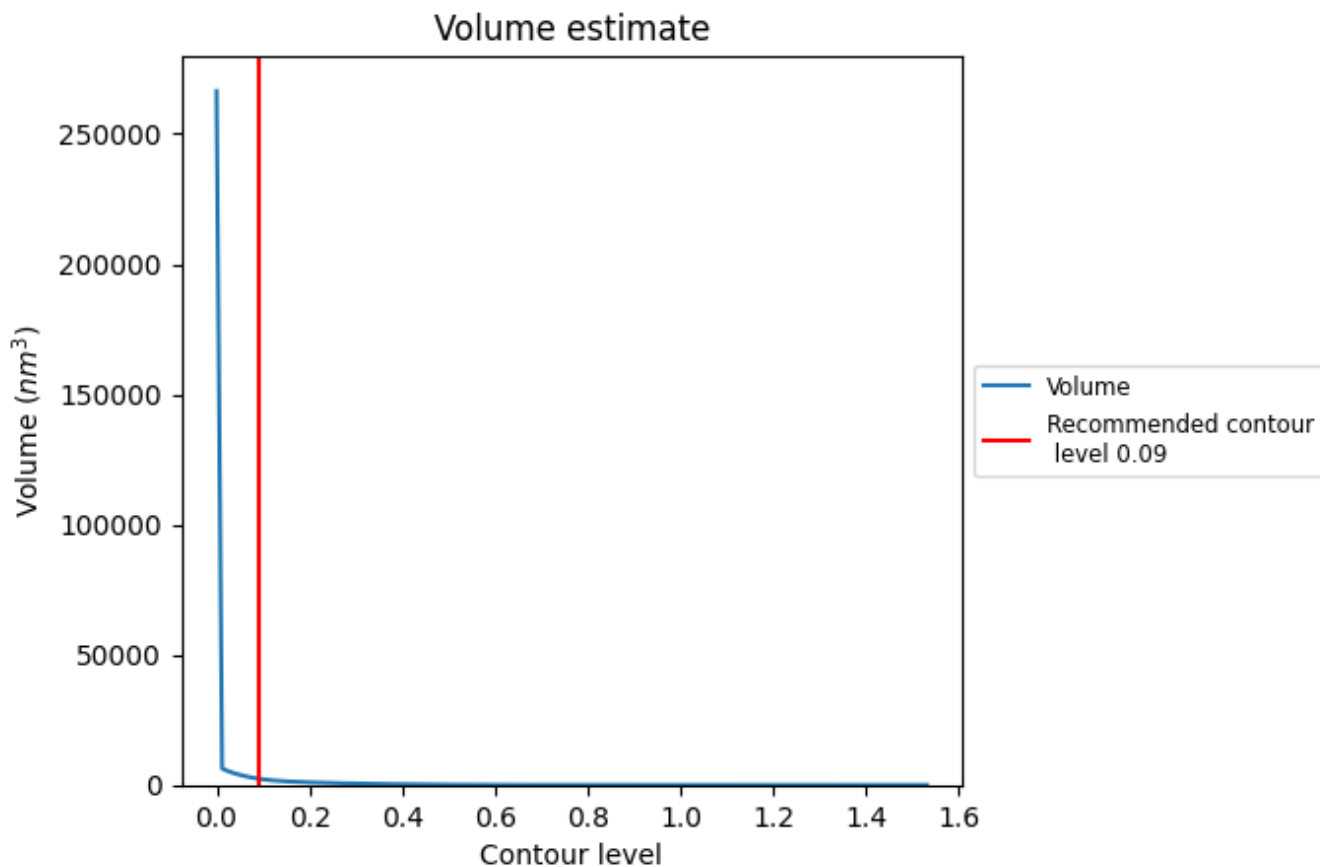
### 7.1 Map-value distribution [i](#)



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.



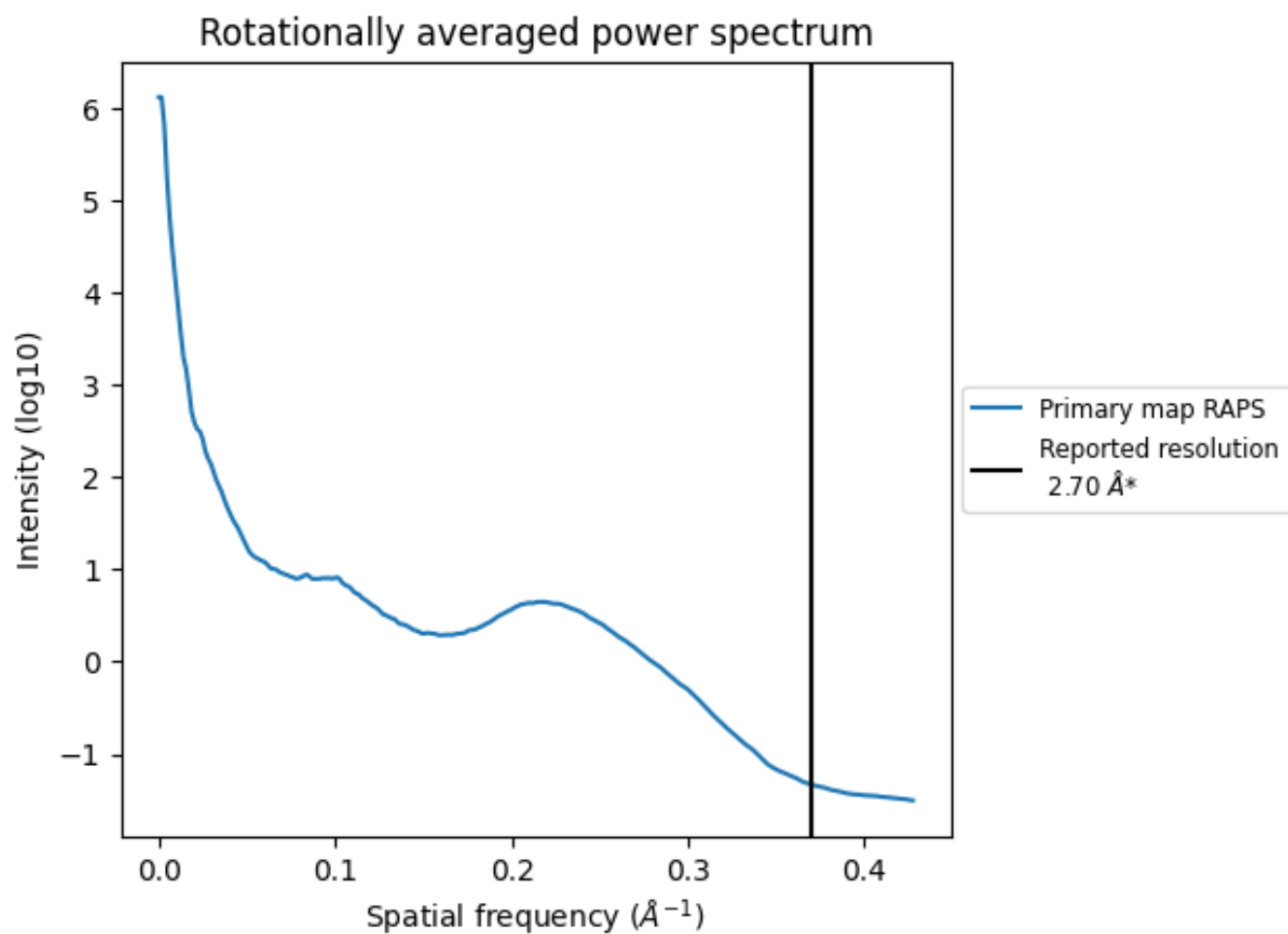
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2412  $\text{nm}^3$ ; this corresponds to an approximate mass of 2179 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 0.370 Å<sup>-1</sup>

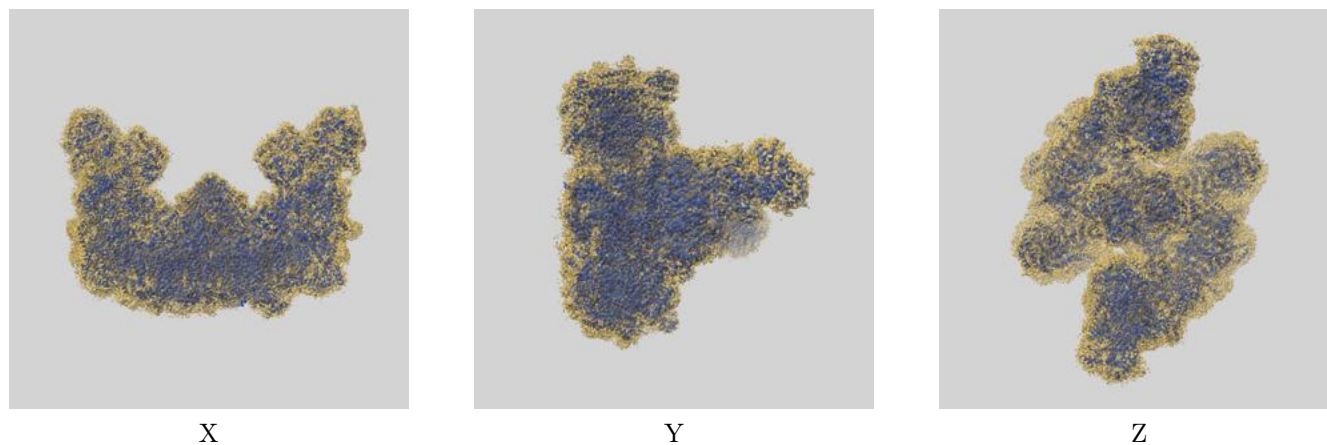
## 8 Fourier-Shell correlation

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

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

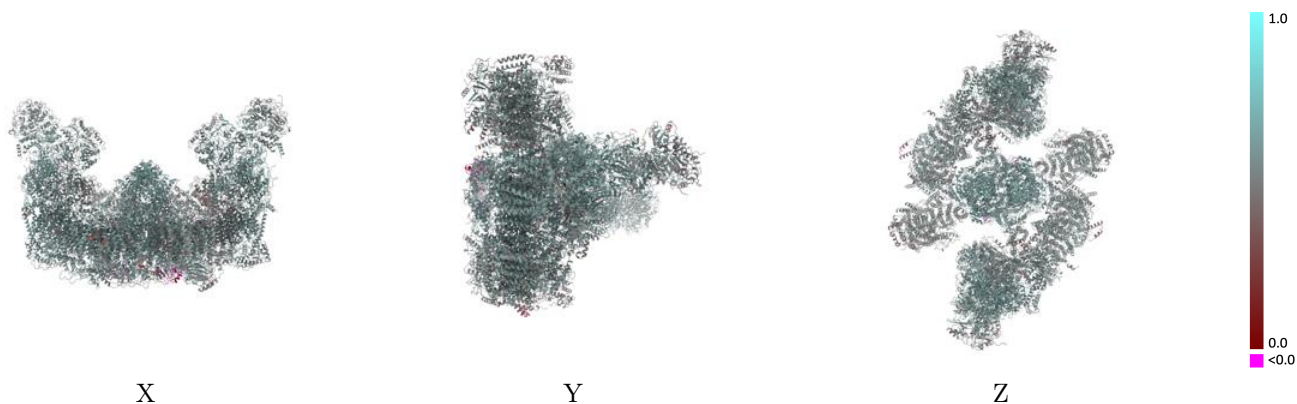
This section contains information regarding the fit between EMDB map EMD-42230 and PDB model 8UGN. Per-residue inclusion information can be found in section [3](#) on page [46](#).

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



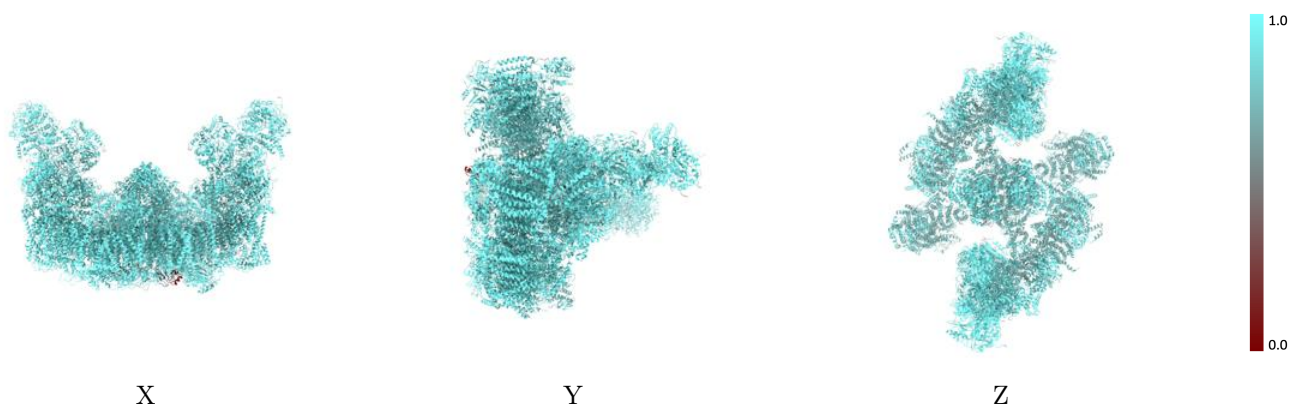
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



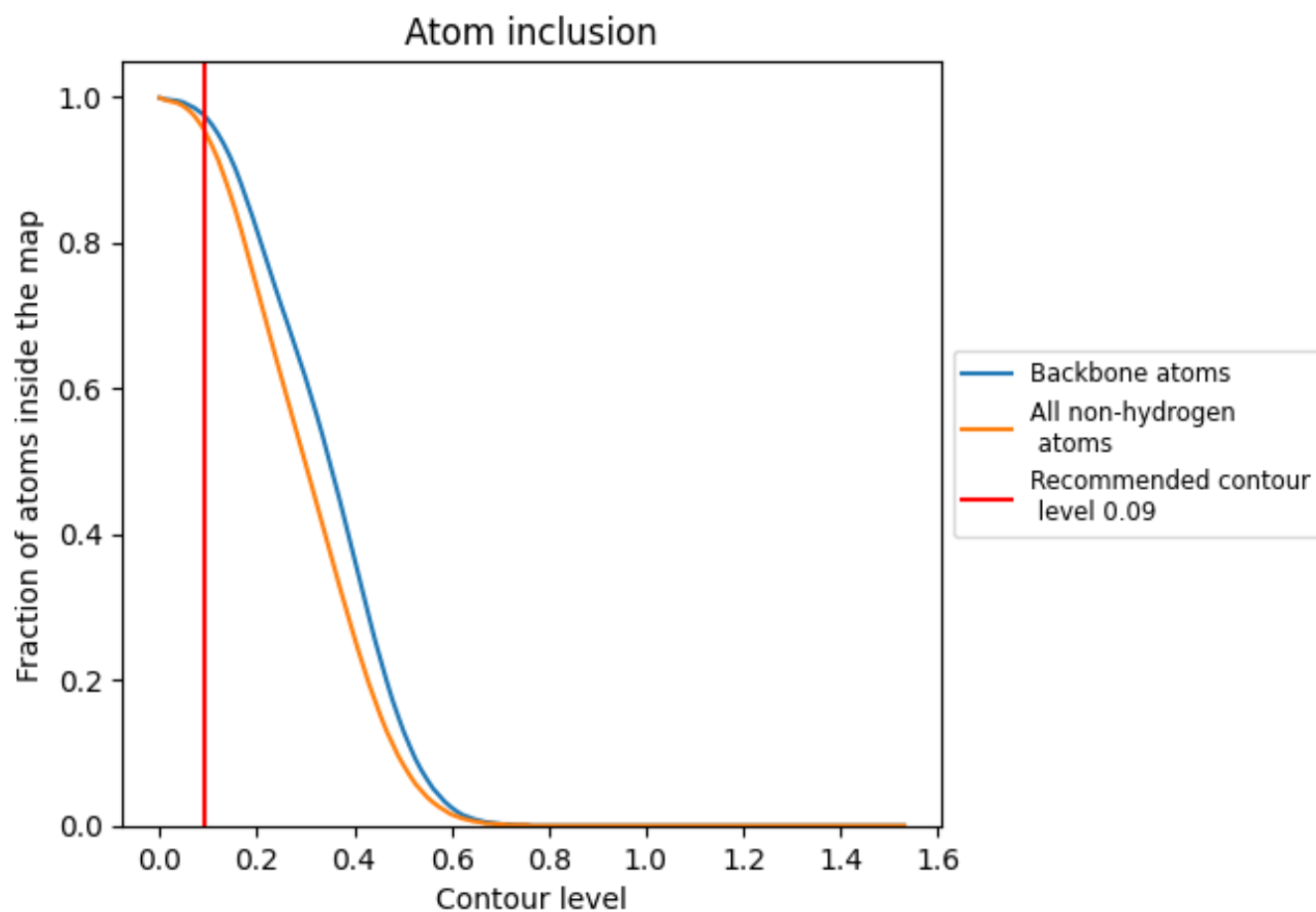
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.5360
1A	 0.8920	 0.4560
1B	 0.9780	 0.5530
1C	 0.9800	 0.5790
1D	 0.9800	 0.5660
1E	 0.9490	 0.5020
1F	 0.9610	 0.5120
1G	 0.9700	 0.5520
1H	 0.9670	 0.5310
1I	 0.9850	 0.5740
1J	 0.9700	 0.4990
1K	 0.9910	 0.5510
1L	 0.9880	 0.5300
1M	 0.9950	 0.5540
1N	 0.9940	 0.5590
1O	 0.9710	 0.5250
1P	 0.9560	 0.5220
1Q	 0.9240	 0.5440
1R	 0.9710	 0.5620
1S	 0.9460	 0.5180
1T	 0.9040	 0.4060
1U	 0.9680	 0.5060
1V	 0.9610	 0.5260
1W	 0.9610	 0.5360
1X	 0.9880	 0.5310
1Y	 0.9790	 0.5110
1Z	 0.9840	 0.5400
1a	 0.9910	 0.5540
1b	 0.9720	 0.5250
1c	 0.9630	 0.5050
1d	 0.9740	 0.5350
1e	 0.9860	 0.5420
1f	 0.9750	 0.5110
1g	 0.9850	 0.5220
1h	 0.9810	 0.5310



*Continued on next page...*





















































































*Continued from previous page...*

Chain	Atom inclusion	Q-score
1i	 0.9200	 0.4570
1j	 0.9440	 0.4770
1k	 0.9420	 0.4800
1l	 0.9800	 0.5360
1m	 0.9790	 0.5360
1n	 0.9870	 0.5360
1o	 0.9740	 0.4870
1p	 0.9770	 0.5160
1q	 0.9760	 0.5580
1r	 0.9860	 0.5610
1s	 0.9570	 0.4960
3A	 0.9750	 0.5960
3B	 0.9760	 0.6000
3C	 0.9890	 0.6140
3D	 0.9900	 0.6130
3E	 0.5600	 0.2830
3F	 0.9840	 0.6070
3G	 0.9800	 0.5740
3H	 0.9690	 0.5670
3I	 0.8390	 0.5010
3J	 0.9880	 0.6000
3N	 0.9830	 0.6030
3O	 0.9790	 0.6080
3P	 0.9870	 0.6170
3Q	 0.9860	 0.6100
3R	 0.5850	 0.3010
3S	 0.9760	 0.6160
3T	 0.9860	 0.5870
3U	 0.9660	 0.5740
3V	 0.9210	 0.5550
3W	 0.9890	 0.6060
3X	 0.9750	 0.5710
3Y	 0.9820	 0.5570
4A	 0.9080	 0.5130
4B	 0.8720	 0.4950
4C	 0.8940	 0.4810
4D	 0.8400	 0.4430
4E	 0.8260	 0.4260
4F	 0.8240	 0.4660
4G	 0.8620	 0.4220
4H	 0.8810	 0.4700
4I	 0.8840	 0.4820

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













































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Chain	Atom inclusion	Q-score
4J	 0.9500	 0.4730
4K	 0.8240	 0.4480
4L	 0.8660	 0.4790
4M	 0.8670	 0.4620
4N	 0.8690	 0.4730
5A	 0.9110	 0.4750
5B	 0.9820	 0.5650
5C	 0.9860	 0.5890
5D	 0.9830	 0.5780
5E	 0.9700	 0.5140
5F	 0.9820	 0.5290
5G	 0.9790	 0.5620
5H	 0.9710	 0.5410
5I	 0.9940	 0.5910
5J	 0.9720	 0.5190
5K	 0.9920	 0.5750
5L	 0.9880	 0.5450
5M	 0.9930	 0.5620
5N	 0.9930	 0.5730
5O	 0.9800	 0.5430
5P	 0.9600	 0.5250
5Q	 0.9330	 0.5480
5R	 0.9780	 0.5720
5S	 0.9570	 0.5110
5T	 0.9110	 0.4100
5U	 0.9750	 0.5210
5V	 0.9740	 0.5510
5W	 0.9580	 0.5460
5X	 0.9890	 0.5430
5Y	 0.9770	 0.5200
5Z	 0.9920	 0.5650
5a	 0.9930	 0.5720
5b	 0.9840	 0.5360
5c	 0.9750	 0.5250
5d	 0.9790	 0.5430
5e	 0.9760	 0.5430
5f	 0.9700	 0.5050
5g	 0.9940	 0.5250
5h	 0.9800	 0.5430
5i	 0.9180	 0.4640
5j	 0.9300	 0.4760
5k	 0.9400	 0.4780

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Chain	Atom inclusion	Q-score
5l	 0.9780	 0.5400
5m	 0.9780	 0.5480
5n	 0.9860	 0.5430
5o	 0.9770	 0.4840
5p	 0.9780	 0.5290
5q	 0.9750	 0.5570
5r	 0.9890	 0.5700
5s	 0.9650	 0.5040
8A	 0.9440	 0.5410
8B	 0.8840	 0.5050
8C	 0.9230	 0.5040
8D	 0.8560	 0.4650
8E	 0.8640	 0.4650
8F	 0.8590	 0.4940
8G	 0.8790	 0.4460
8H	 0.9070	 0.4890
8I	 0.8750	 0.4840
8J	 0.9460	 0.4890
8K	 0.8540	 0.4790
8L	 0.8850	 0.4830
8M	 0.8670	 0.4850
8N	 0.8720	 0.4830