



## wwPDB EM Validation Summary Report ⓘ

Jul 6, 2024 – 06:18 PM EDT

PDB ID : 8UGR  
EMDB ID : EMD-42233  
Title : In-situ structure of typeX supercomplex in respiratory chain (composite)  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-06  
Resolution : 6.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

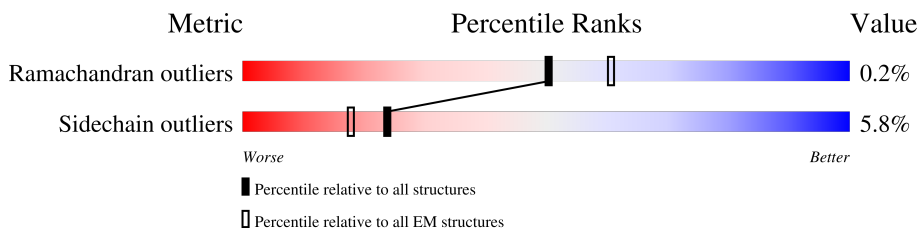
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 6.50 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	7% (red), 91% (green), 9% (yellow)
1	5A	115	17% (red), 87% (green), 12% (yellow), 4% (grey)
2	1B	258	53% (green), 6% (yellow), 40% (grey)
2	5B	258	55% (green), 5% (yellow), 40% (grey)
3	1C	264	76% (green), 21% (grey)
3	5C	264	7% (red), 75% (green), 21% (grey)
4	1D	476	85% (green), 5% (yellow), 10% (grey)
4	5D	476	6% (red), 86% (green), 10% (grey)
5	1E	249	10% (red), 78% (green), 8% (yellow), 14% (grey)

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Mol	Chain	Length	Quality of chain
5	5E	249	10% 80% 6% 14%
6	1F	464	14% 89% 7%
6	5F	464	14% 89% 7%
7	1G	727	11% 90% 6%
7	5G	727	14% 90% 6%
8	1H	318	89% 9%
8	5H	318	92% 6%
9	1I	239	64% 9% 26%
9	5I	239	69% 26%
10	1J	175	91% 8%
10	5J	175	91% 6%
11	1K	98	87% 10%
11	5K	98	90% 10%
12	1L	606	93% 6%
12	5L	606	93% 7%
13	1M	459	96%
13	5M	459	92% 7%
14	1N	347	90% 9%
14	5N	347	90% 9%
15	1O	357	86% 10%
15	5O	357	83% 6% 10%
16	1P	377	87% 9%
16	5P	377	5% 86% 5% 9%
17	1Q	175	11% 69% 26%
17	5Q	175	19% 67% 5% 26%

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Mol	Chain	Length	Quality of chain
18	1R	123	72% 7% 22%
18	5R	123	73% 5% 22%
19	1S	99	9% 80% 8% 12%
19	5S	99	15% 80% 7% 12%
20	1T	156	47% 7% 46%
20	1U	156	6% 52% 45%
20	5T	156	7% 47% 8% 46%
20	5U	156	9% 53% 45%
21	1V	116	9% 96% 3% 2%
21	5V	116	10% 97% 3% 2%
22	1W	128	8% 81% 9% 10%
22	5W	128	8% 79% 10% 10%
23	1X	172	8% 92% 7% 2%
23	5X	172	92% 7% 2%
24	1Y	141	90% 8% 2%
24	5Y	141	89% 5% 6%
25	1Z	144	10% 88% 10% 2%
25	5Z	144	92% 6% 2%
26	1a	70	10% 94% 4% 2%
26	5a	70	90% 10%
27	1b	84	8% 94% 5% 2%
27	5b	84	92% 7% 2%
28	1c	76	57% 7% 36%
28	5c	76	55% 5% 36%
29	1d	122	90% 7% 3%

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Mol	Chain	Length	Quality of chain
29	5d	122	88% 9% ..
30	1e	106	5% 87% 6% • 7%
30	5e	106	84% 8% • 7%
31	1f	135	40% • 58%
31	5f	135	41% • 58%
32	1g	154	62% • 35%
32	5g	154	57% 7% • 35%
33	1h	189	65% 7% • 27%
33	5h	189	68% • 27%
34	1i	128	90% 9% ..
34	5i	128	93% 5% ..
35	1j	105	63% • 32%
35	5j	105	9% 64% • 32%
36	1k	98	7% 82% • 17%
36	5k	98	5% 76% 7% 17%
37	1l	186	78% 5% 16%
37	5l	186	77% 6% • 16%
38	1m	129	97% ..
38	5m	129	94% 5% •
39	1n	179	91% 5% • •
39	5n	179	5% 88% 8% •
40	1o	137	85% • 11%
40	5o	137	84% 5% 11%
41	1p	176	93% 6% •
41	5p	176	93% 5% •





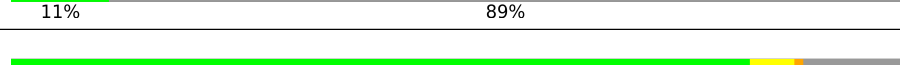
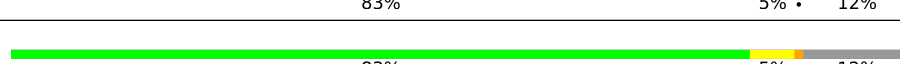
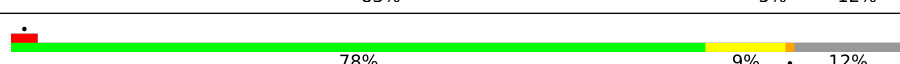
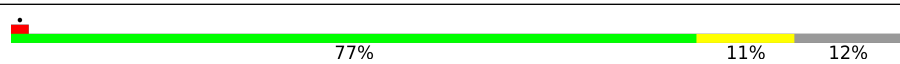

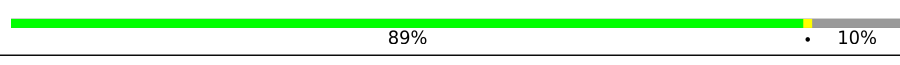
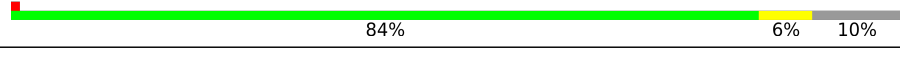
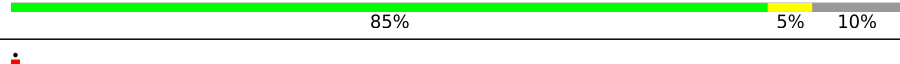

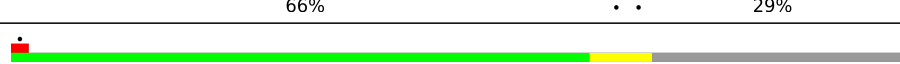
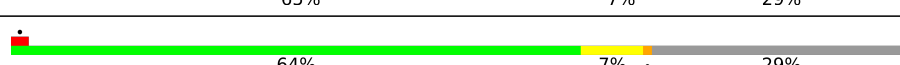




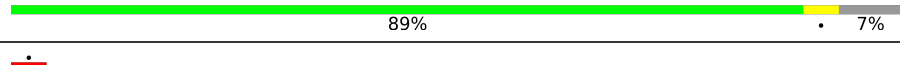





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Mol	Chain	Length	Quality of chain
42	1q	145	92% 8%
42	5q	145	92% 6%
43	1r	113	77% 5% 17%
43	5r	113	74% 9% 17%
44	1s	471	9% 90%
44	5s	471	9% 90%
45	3A	480	10% 88% 8%
45	3N	480	5% 88% 7%
45	6A	480	5% 88% 8%
45	6N	480	87% 5% 7%
46	3B	453	12% 91% 8%
46	3O	453	14% 89% 8%
46	6B	453	6% 88% 8%
46	6O	453	6% 88% 8%
47	3C	379	94% 6%
47	3P	379	98%
47	6C	379	92% 7%
47	6P	379	92% 8%
48	3D	326	70% 27%
48	3Q	326	71% 27%
48	6D	326	68% 27%
48	6Q	326	69% 27%
49	3E	274	68% 28%
49	3I	274	16% 83%
49	3R	274	10% 67% 28%

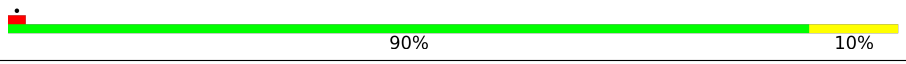
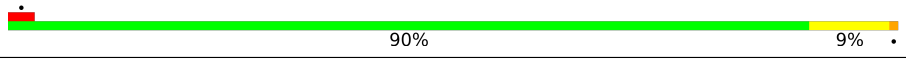
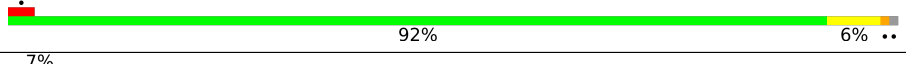
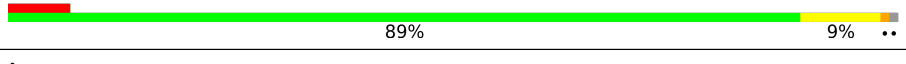
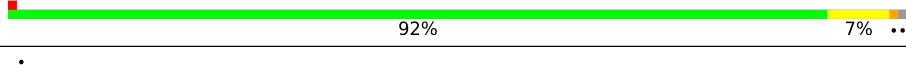
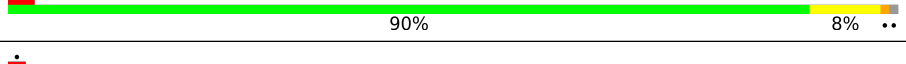


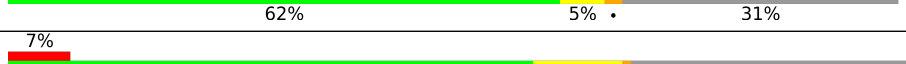
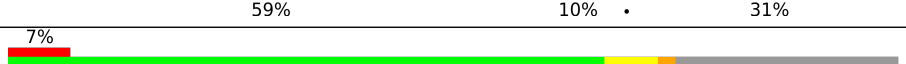
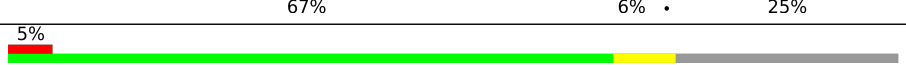
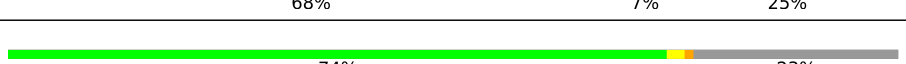
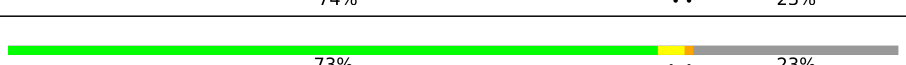
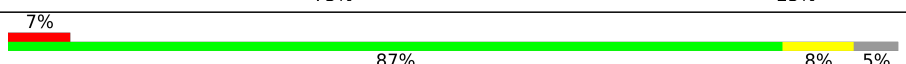
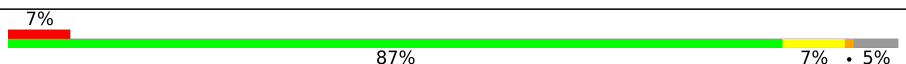
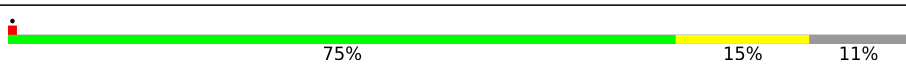
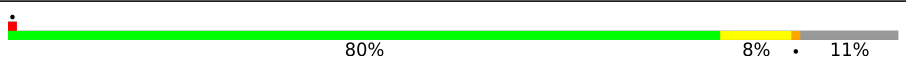


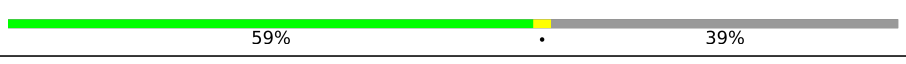

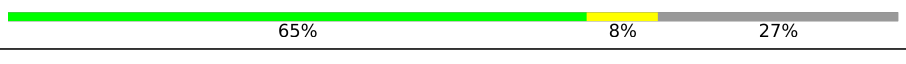



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Mol	Chain	Length	Quality of chain
49	3V	274	 11% 89%
49	6E	274	 8% 67% 5% 20%
49	6I	274	 9% 16% 75% 0%
49	6R	274	 12% 66% 5% 17%
49	6V	274	 11% 89%
50	3F	111	 83% 5% 12%
50	3S	111	 83% 5% 12%
50	6F	111	 78% 9% 13%
50	6S	111	 77% 11% 12%
51	3G	82	 88% 10% 2%
51	3T	82	 89% 10% 1%
51	6G	82	 84% 6% 10%
51	6T	82	 85% 5% 10%
52	3H	91	 63% 8% 29%
52	3U	91	 66% 29% 5%
52	6H	91	 65% 7% 28%
52	6U	91	 64% 7% 29%
53	3J	64	 83% 12% 5%
53	3W	64	 83% 5% 12%
53	6J	64	 77% 9% 14%
53	6W	64	 77% 11% 12%
54	3X	56	 89% 7% 4%
54	3Y	56	 82% 9% 9%
54	6X	56	 84% 9% 7%
54	6Y	56	 82% 9% 9%

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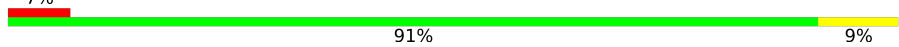
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Mol	Chain	Length	Quality of chain
55	4A	514	 90% 10%
55	8A	514	 90% 9%
56	4B	229	 92% 6%
56	8B	229	 89% 9% 7%
57	4C	261	 92% 7%
57	8C	261	 90% 8%
58	4D	169	 73% 9% 18%
58	8D	169	 72% 9% 18%
59	4E	152	 62% 5% 31%
59	8E	152	 59% 10% 7%
60	4F	129	 67% 6% 7%
60	8F	129	 68% 7% 5%
61	4G	97	 74% 23%
61	8G	97	 73% 23%
62	4H	86	 87% 8% 7%
62	8H	86	 87% 7% 7%
63	4I	75	 75% 15% 11%
63	8I	75	 80% 8% 11%
64	4J	80	 68% 28%
64	8J	80	 62% 6% 28%
65	4K	80	 59% 39%
65	8K	80	 58% 39%
66	4L	63	 65% 8% 27%
66	8L	63	 59% 14% 27%
67	4M	70	 56% 39%

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Mol	Chain	Length	Quality of chain
67	8M	70	 53% 7% 39%
68	4N	82	 5% 84% 16%
68	8N	82	 7% 91% 9%

## 2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 234719 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, mitochond-

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		
45	6A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	6N	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		
46	6B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	6O	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		
47	6C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	6P	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		
48	6D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	6Q	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		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		
49	6E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	6R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6S	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		
51	6G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	6T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace	
53	3J	56	Total	C	N	O		0	0
			454	295	81	78			
53	3W	56	Total	C	N	O		0	0
			454	295	81	78			
53	6J	56	Total	C	N	O		0	0
			454	295	81	78			
53	6W	56	Total	C	N	O		0	0
			454	295	81	78			

There are 16 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

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Chain	Residue	Modelled	Actual	Comment	Reference
3W	59	LYS	TYR	conflict	UNP Q2EN79
6J	60	ASN	LYS	conflict	UNP Q2EN79
6J	61	GLN	HIS	conflict	UNP Q2EN79
6J	62	GLY	LYS	conflict	UNP Q2EN79
6J	63	LYS	TYR	conflict	UNP Q2EN79
6W	56	ASN	LYS	conflict	UNP Q2EN79
6W	57	GLN	HIS	conflict	UNP Q2EN79
6W	58	GLY	LYS	conflict	UNP Q2EN79
6W	59	LYS	TYR	conflict	UNP Q2EN79

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
54	6X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	6Y	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
55	4A	514	Total	C	N	O	S	0	0
			4025	2693	624	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
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
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
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
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
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		

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

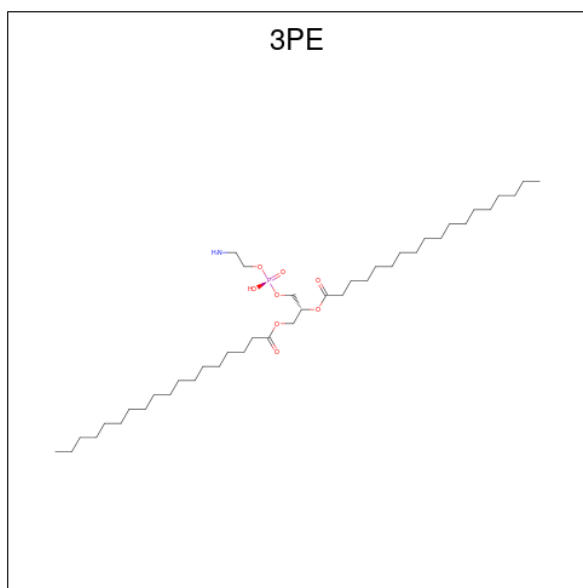
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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

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

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

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1A	1	Total 47	37	1	8	1	0
69	1K	1	Total 44	34	1	8	1	0
69	1L	1	Total 46	36	1	8	1	0
69	1L	1	Total 45	35	1	8	1	0
69	1L	1	Total 49	39	1	8	1	0
69	1L	1	Total 31	21	1	8	1	0
69	1M	1	Total 45	35	1	8	1	0
69	1M	1	Total 51	41	1	8	1	0

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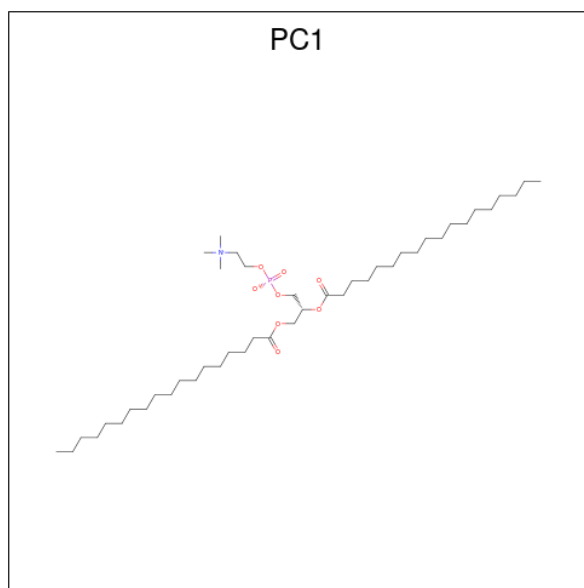
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	1M	1	Total 50	C 40	N 1	O 8	P 1	0
69	1P	1	Total 35	C 25	N 1	O 8	P 1	0
69	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	1d	1	Total 48	C 38	N 1	O 8	P 1	0
69	1d	1	Total 49	C 39	N 1	O 8	P 1	0
69	1j	1	Total 44	C 34	N 1	O 8	P 1	0
69	1m	1	Total 41	C 31	N 1	O 8	P 1	0
69	5A	1	Total 47	C 37	N 1	O 8	P 1	0
69	5K	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	5L	1	Total 45	C 35	N 1	O 8	P 1	0
69	5M	1	Total 49	C 39	N 1	O 8	P 1	0
69	5M	1	Total 45	C 35	N 1	O 8	P 1	0
69	5M	1	Total 48	C 38	N 1	O 8	P 1	0
69	5M	1	Total 51	C 41	N 1	O 8	P 1	0
69	5M	1	Total 50	C 40	N 1	O 8	P 1	0
69	5P	1	Total 35	C 25	N 1	O 8	P 1	0
69	5Y	1	Total 31	C 21	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	5Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	5Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	5Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	5Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	5d	1	Total 49	C 39	N 1	O 8	P 1	0
69	5j	1	Total 44	C 34	N 1	O 8	P 1	0
69	5m	1	Total 41	C 31	N 1	O 8	P 1	0

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
70	1A	1	Total 35	C 25	N 1	O 8	P 1	0
70	1B	1	Total 46	C 36	N 1	O 8	P 1	0
70	1B	1	Total 48	C 38	N 1	O 8	P 1	0
70	1H	1	Total 48	C 38	N 1	O 8	P 1	0

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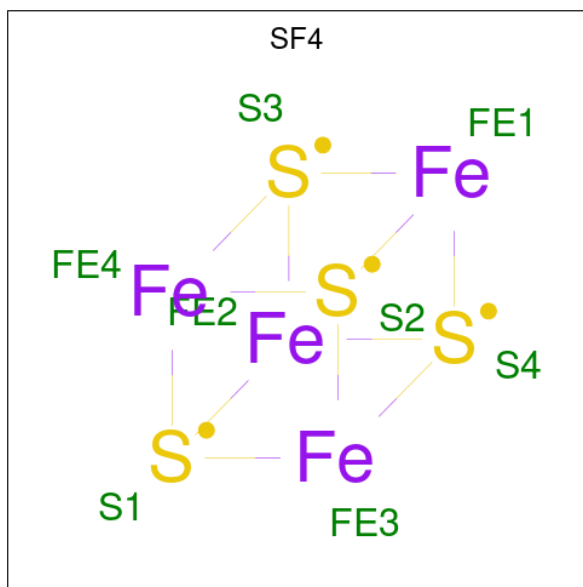
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
70	1I	1	Total 54	C 44	N 1	O 8	P 1	0
70	1I	1	Total 44	C 34	N 1	O 8	P 1	0
70	1J	1	Total 35	C 25	N 1	O 8	P 1	0
70	1L	1	Total 46	C 36	N 1	O 8	P 1	0
70	1M	1	Total 35	C 25	N 1	O 8	P 1	0
70	1M	1	Total 44	C 34	N 1	O 8	P 1	0
70	1P	1	Total 33	C 23	N 1	O 8	P 1	0
70	1d	1	Total 39	C 29	N 1	O 8	P 1	0
70	1h	1	Total 47	C 37	N 1	O 8	P 1	0
70	1q	1	Total 49	C 39	N 1	O 8	P 1	0
70	5A	1	Total 35	C 25	N 1	O 8	P 1	0
70	5A	1	Total 35	C 25	N 1	O 8	P 1	0
70	5B	1	Total 46	C 36	N 1	O 8	P 1	0
70	5B	1	Total 48	C 38	N 1	O 8	P 1	0
70	5H	1	Total 54	C 44	N 1	O 8	P 1	0
70	5H	1	Total 48	C 38	N 1	O 8	P 1	0
70	5I	1	Total 44	C 34	N 1	O 8	P 1	0
70	5M	1	Total 44	C 34	N 1	O 8	P 1	0
70	5P	1	Total 33	C 23	N 1	O 8	P 1	0
70	5Y	1	Total 35	C 25	N 1	O 8	P 1	0
70	5Y	1	Total 46	C 36	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
70	5d	1	Total	C	N	O	P	0
			39	29	1	8	1	
70	5h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	5q	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



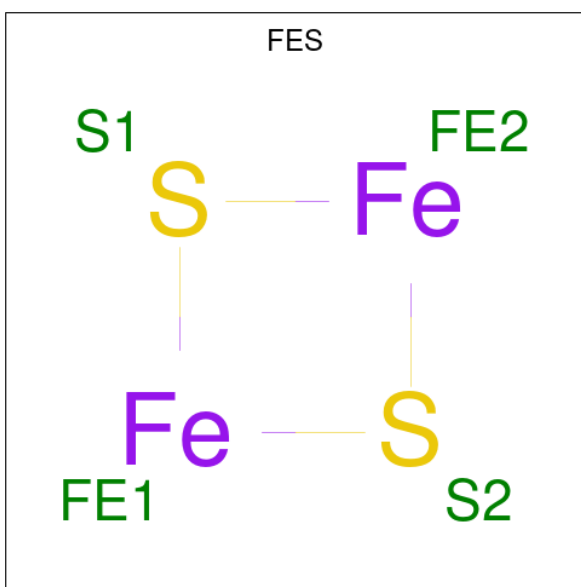
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	5B	1	Total	Fe	S	0
			8	4	4	
71	5F	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
71	5G	1	8	4	4	0
71	5G	1	8	4	4	0
71	5I	1	8	4	4	0
71	5I	1	8	4	4	0

- Molecule 72 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	
72	1E	1	4	2	2	0
72	1G	1	4	2	2	0
72	3E	1	4	2	2	0
72	3R	1	4	2	2	0
72	5E	1	4	2	2	0
72	5G	1	4	2	2	0
72	6E	1	4	2	2	0

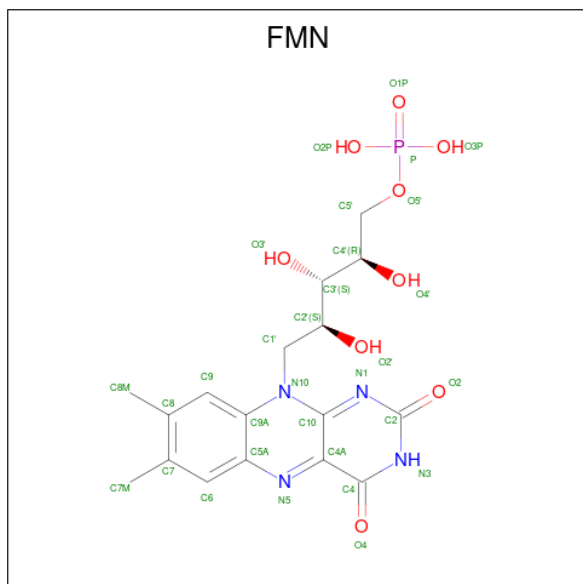
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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
72	6R	1	4	2	2	0

- Molecule 73 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
			Total	C	N	O	P	
73	1F	1	31	17	4	9	1	0
73	5F	1	31	17	4	9	1	0

- Molecule 74 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
74	1G	1	1	1	0
74	5G	1	1	1	0

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



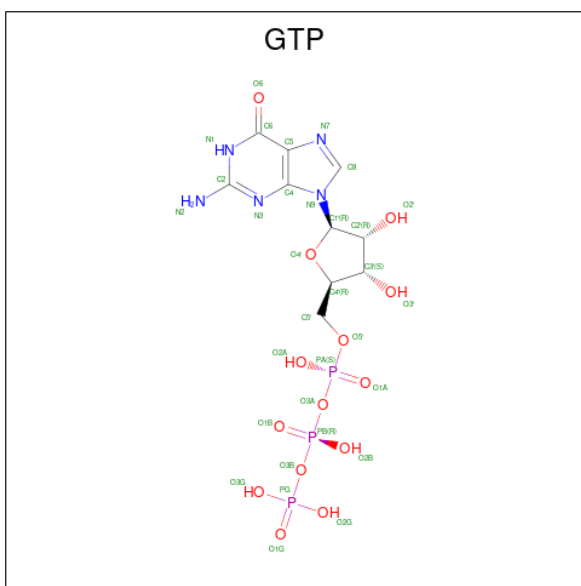
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	1H	1	51	32	17	2	0
75	1L	1	76	57	17	2	0
75	1N	1	62	43	17	2	0
75	1X	1	86	67	17	2	0
75	1a	1	61	42	17	2	0
75	1d	1	65	46	17	2	0
75	1h	1	80	61	17	2	0
75	4B	1	100	81	17	2	0
75	4C	1	100	81	17	2	0
75	4D	1	100	81	17	2	0
75	5H	1	51	32	17	2	0
75	5L	1	76	57	17	2	0
75	5N	1	62	43	17	2	0
75	5a	1	61	42	17	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	5d	1	Total 86	C 67	O 17	P 2	0
75	5d	1	Total 65	C 46	O 17	P 2	0
75	5h	1	Total 80	C 61	O 17	P 2	0
75	8A	1	Total 100	C 81	O 17	P 2	0
75	8C	1	Total 100	C 81	O 17	P 2	0
75	8D	1	Total 100	C 81	O 17	P 2	0

- Molecule 76 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	
76	1O	1	Total 32	C 10	N 5	O 14	P 3	0
76	5O	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 77 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

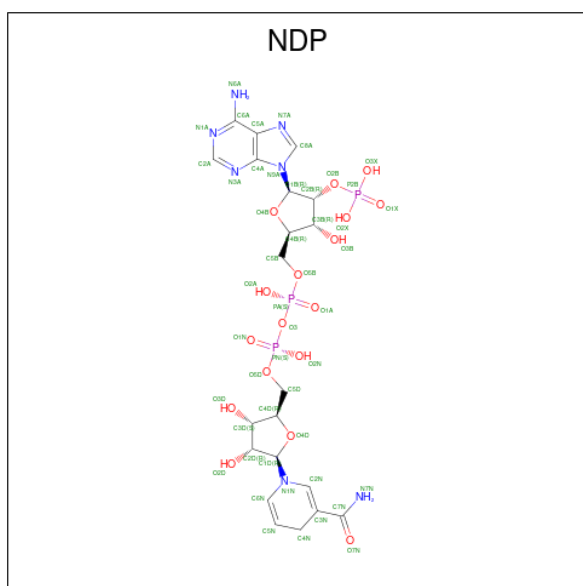
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
77	1O	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
77	4A	1	Total	Mg	0
			1	1	
77	5O	1	Total	Mg	0
			1	1	
77	8A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

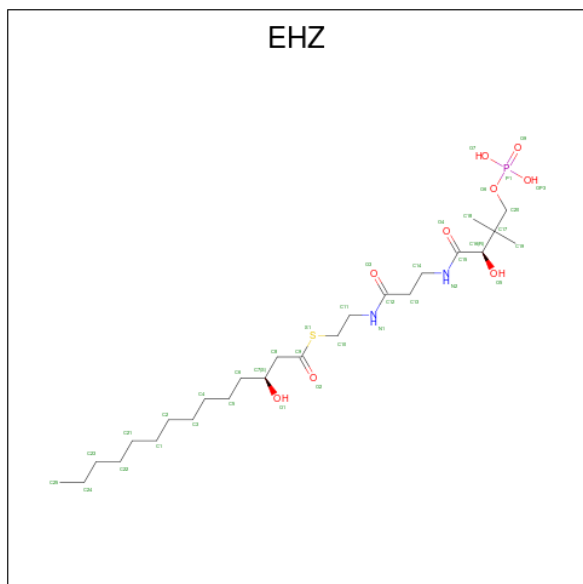


Mol	Chain	Residues	Atoms				AltConf	
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	
78	5P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 79 is ZINC ION (three-letter code: ZN) (formula: Zn).

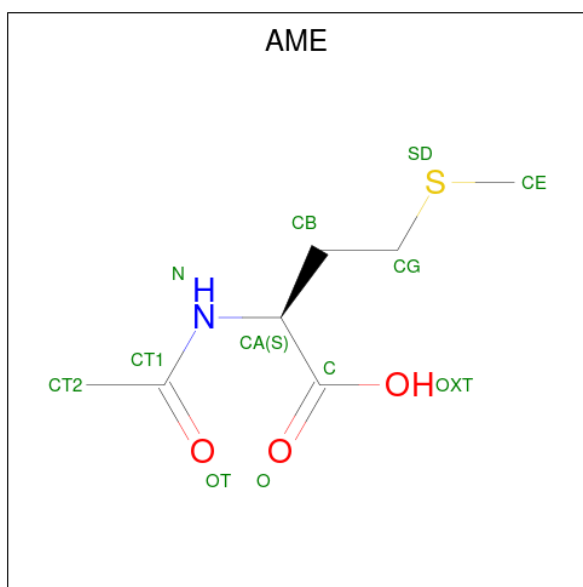
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	
79	5R	1	Total	Zn	0
			1	1	
79	8F	1	Total	Zn	0
			1	1	

- Molecule 80 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<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).



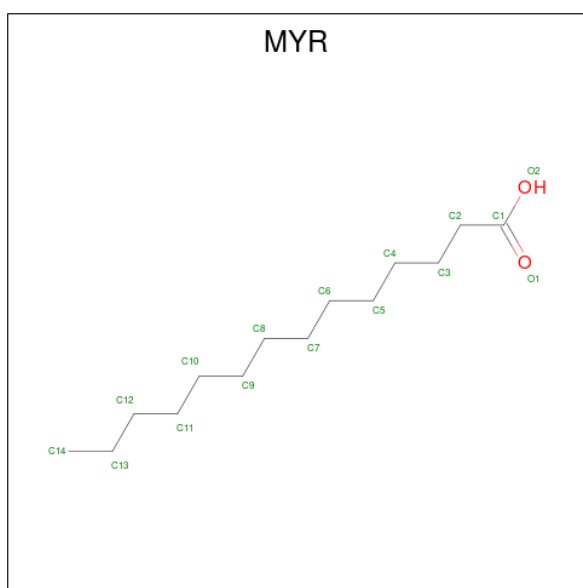
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYL METHIONINE (three-letter code: AME) (formula: C<sub>7</sub>H<sub>13</sub>NO<sub>3</sub>S).



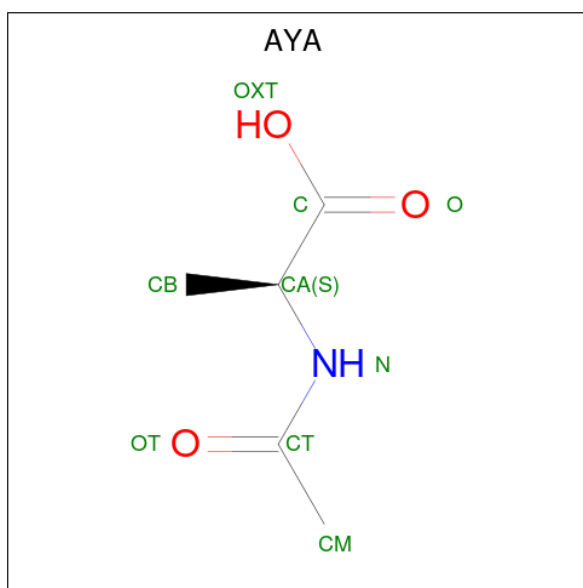
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
81	1h	1	11	7	1	2	1	0
81	5N	1	11	7	1	2	1	0

- Molecule 82 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



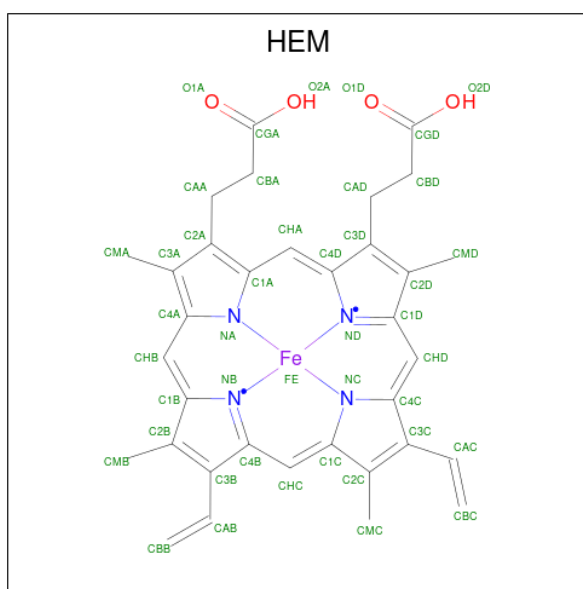
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
82	1l	1	15	14	1	0
82	5l	1	15	14	1	0

- Molecule 83 is N-ACETYLALANINE (three-letter code: AYA) (formula:  $C_5H_9NO_3$ ).



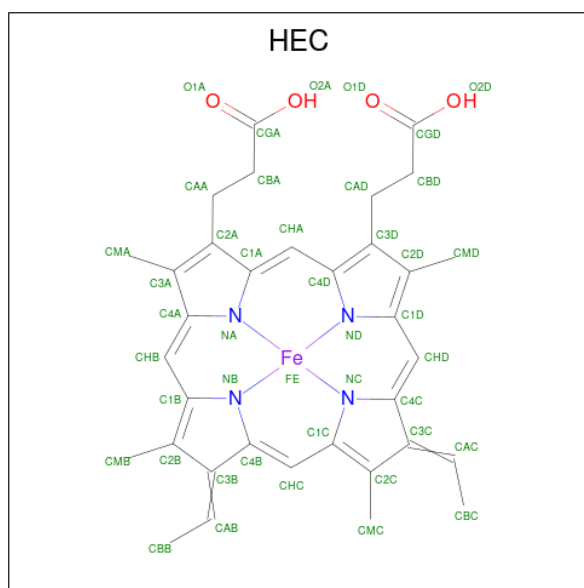
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
83	1q	1	8	5	1	2	0
83	5q	1	8	5	1	2	0

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



Mol	Chain	Residues	Atoms				AltConf	
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	
84	6C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	6C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	6P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	6P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

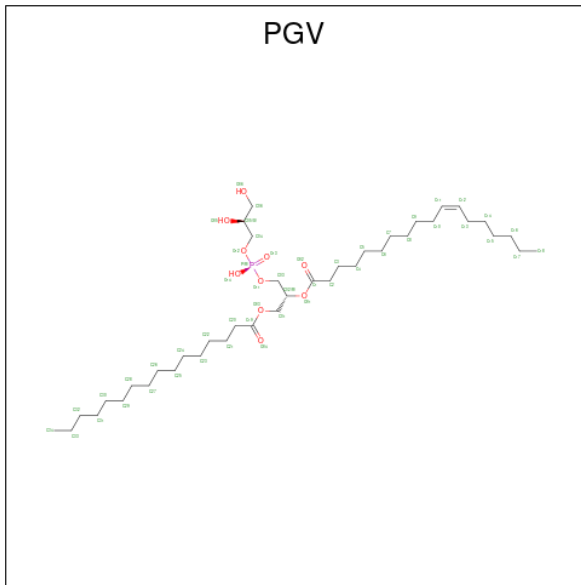
- Molecule 85 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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	
85	6D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
85	6Q	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).



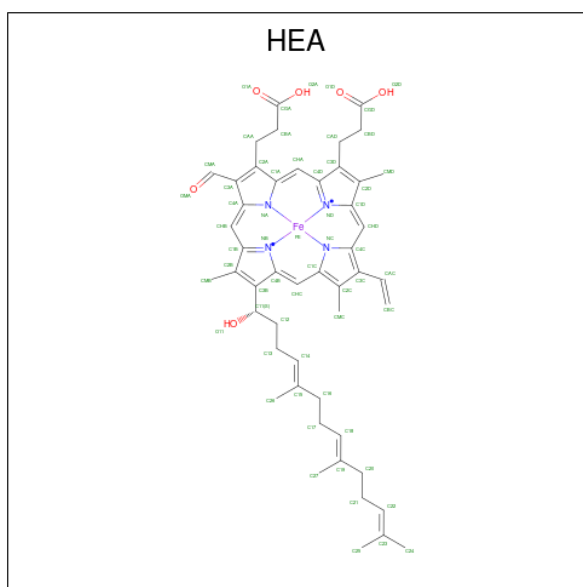
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4B	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
86	4K	1	51	40	10	1	0
86	4L	1	51	40	10	1	0
86	5i	1	51	40	10	1	0
86	8A	1	51	40	10	1	0
86	8A	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	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	8D	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

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
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	

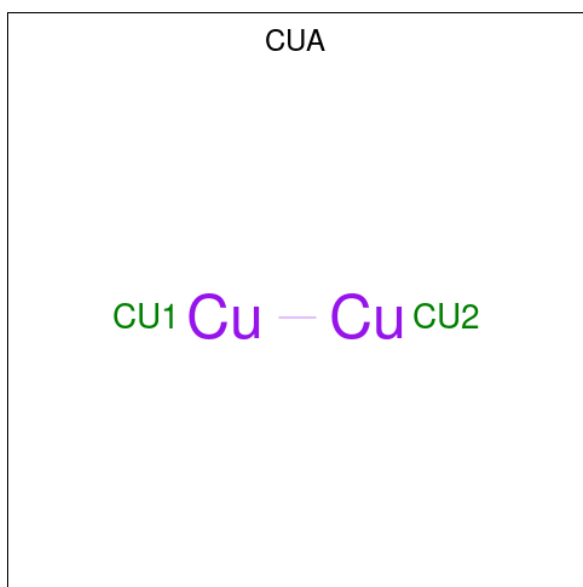
- Molecule 88 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
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).

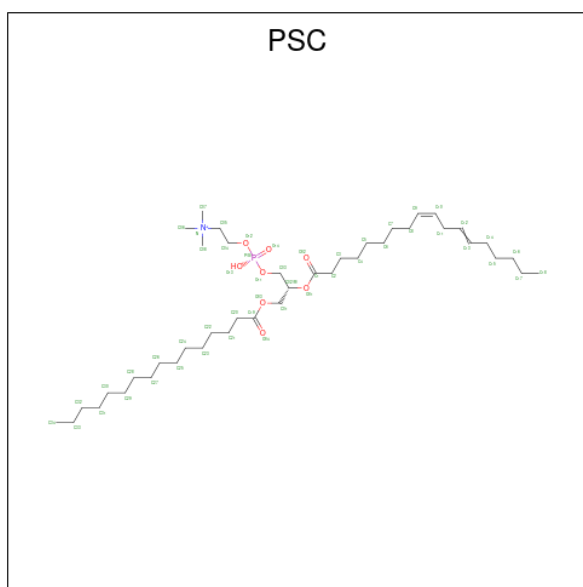
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
89	4A	1	Total	Na	0
			1	1	
89	8A	1	Total	Na	0
			1	1	

- Molecule 90 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	AltConf
90	4B	1	Total Cu 2 2	0
90	8B	1	Total Cu 2 2	0

- Molecule 91 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



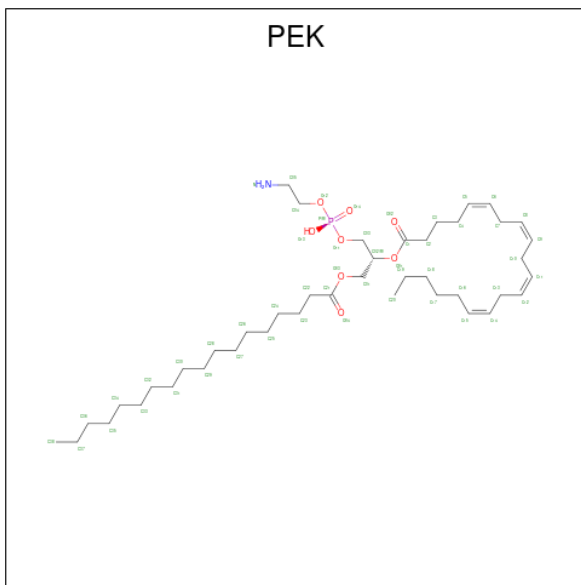
Mol	Chain	Residues	Atoms	AltConf
91	4B	1	Total C N O P 52 42 1 8 1	0

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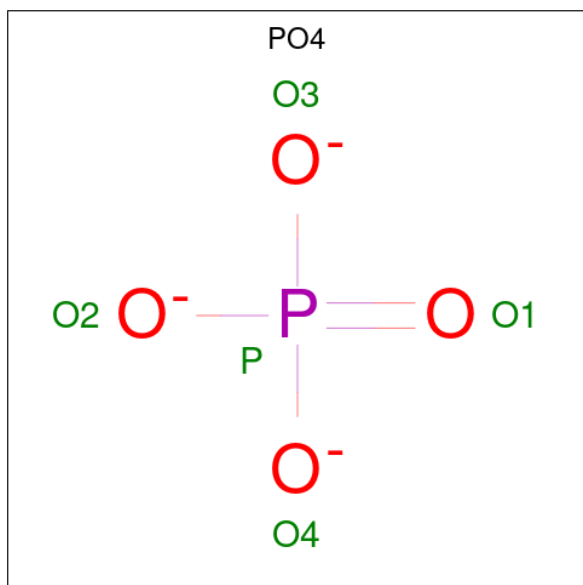
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	8A	1	52	42	1	8	1	0

- Molecule 92 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(STEAROYL)OXY]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
			Total	C	N	O	P	
92	4C	1	53	43	1	8	1	0
92	4C	1	52	42	1	8	1	0
92	8C	1	52	42	1	8	1	0
92	8G	1	53	43	1	8	1	0

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

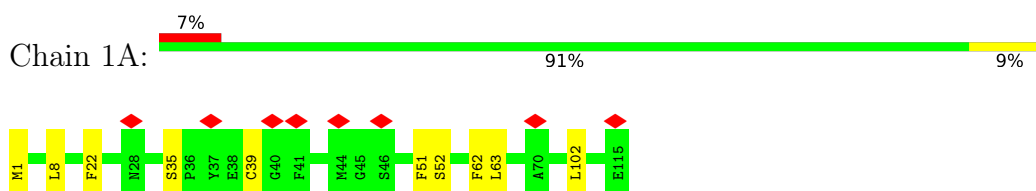


Mol	Chain	Residues	Atoms			AltConf
93	4H	1	Total	O	P	0
			5	4	1	
93	8H	1	Total	O	P	0
			5	4	1	

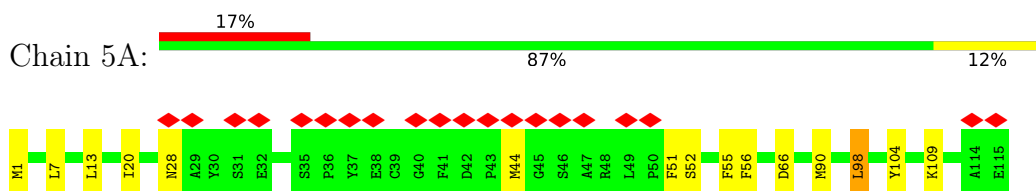
### 3 Residue-property plots [i](#)

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

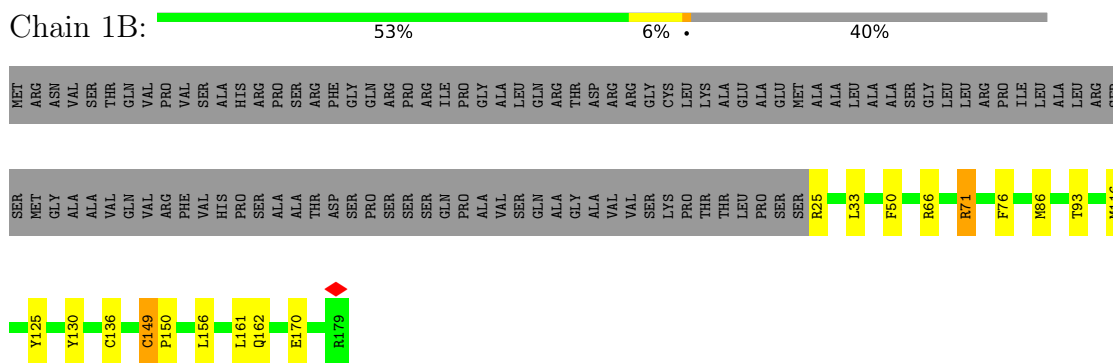
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



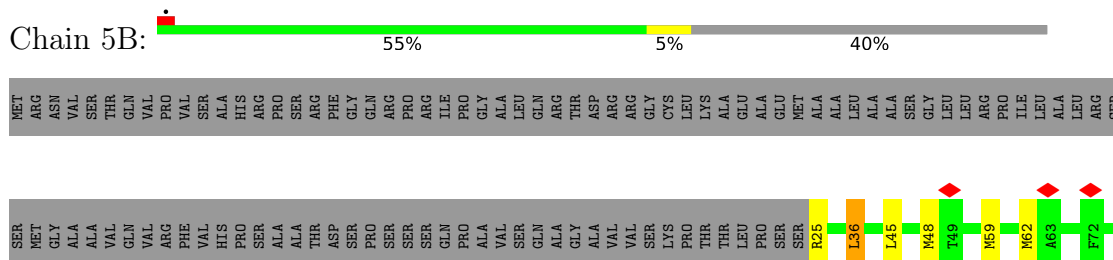
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

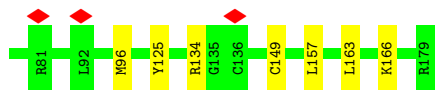


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

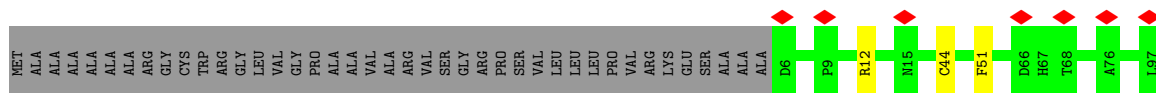
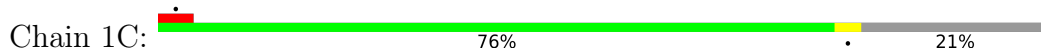


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

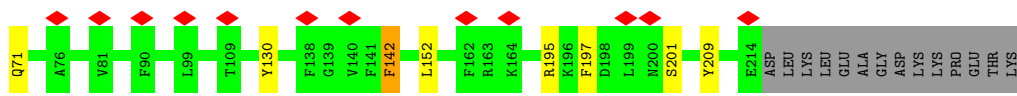
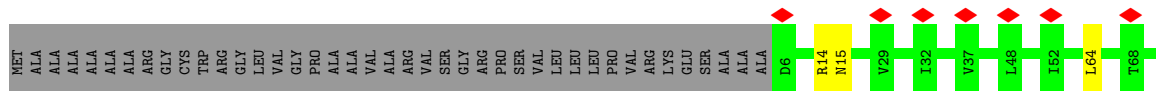
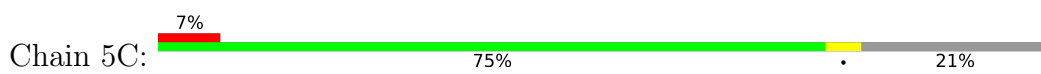




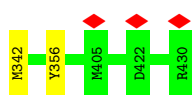
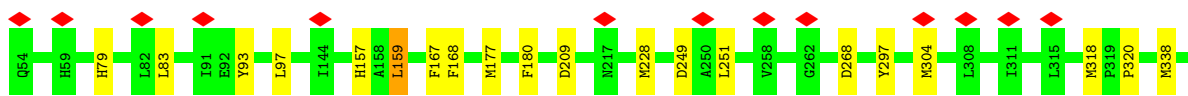
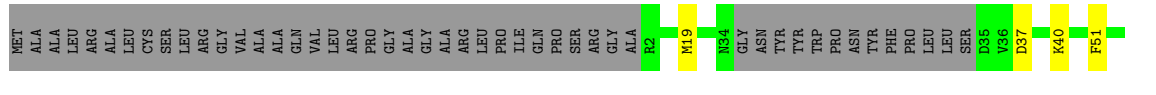
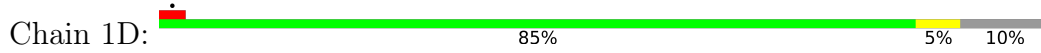
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



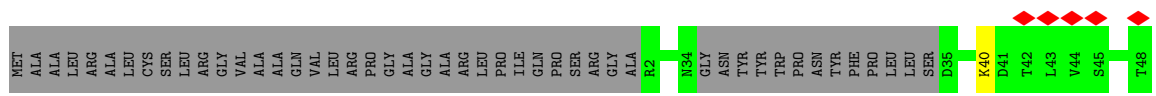
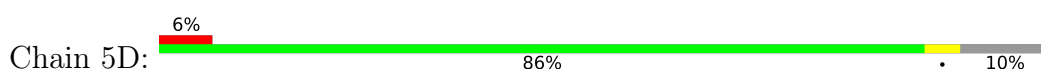
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



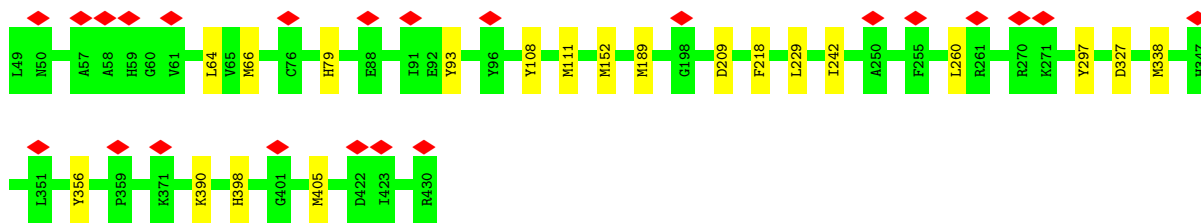
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



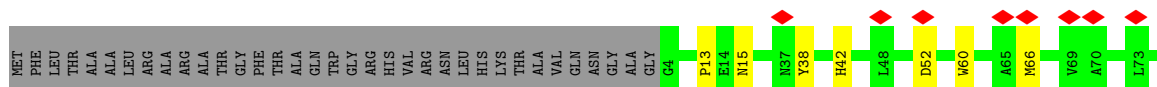
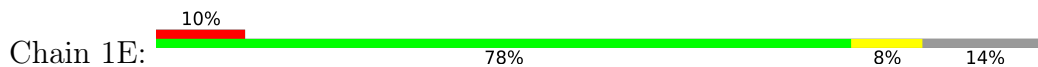
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



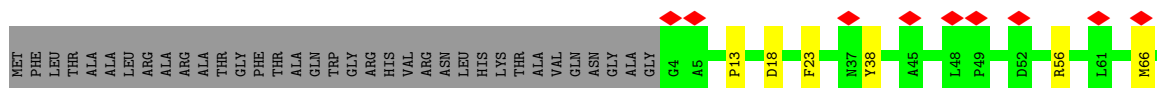
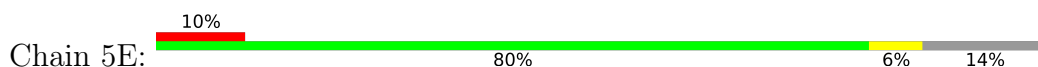




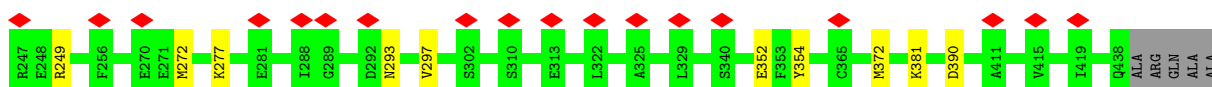
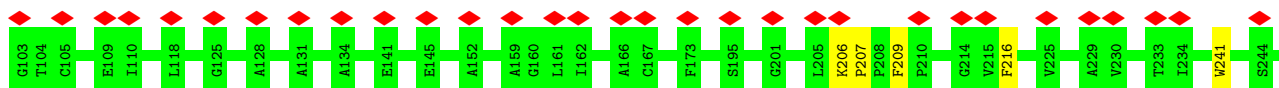
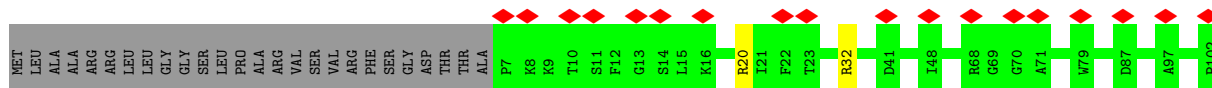
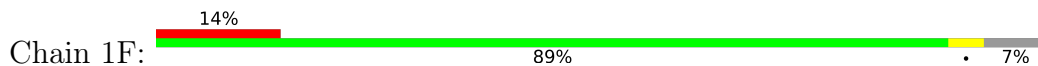
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



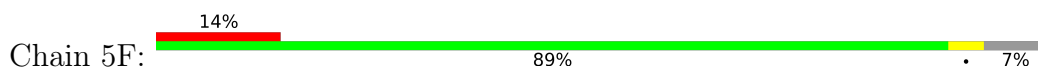
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

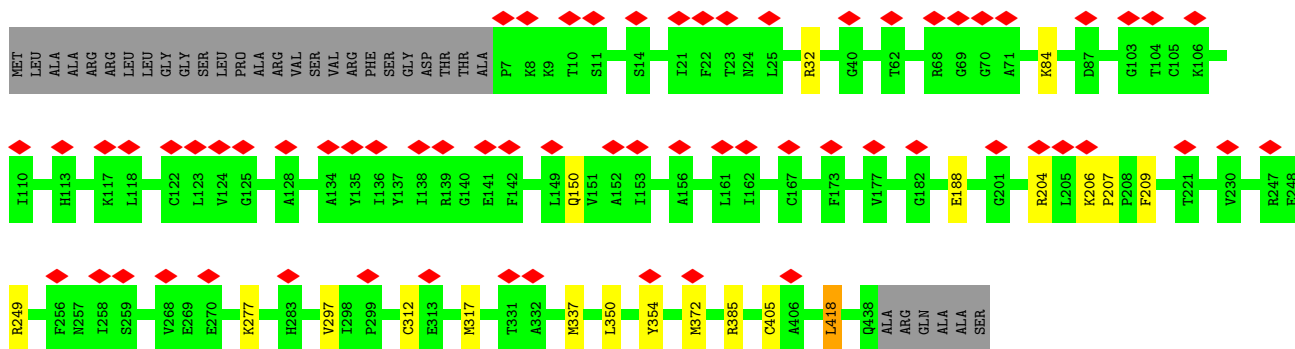


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

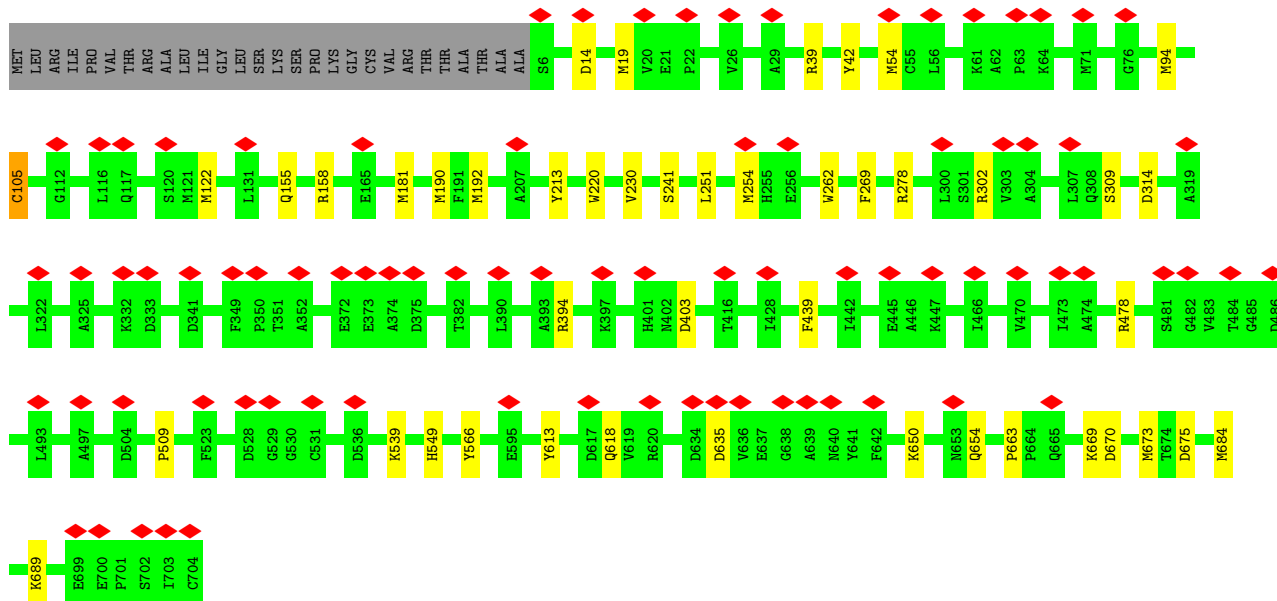
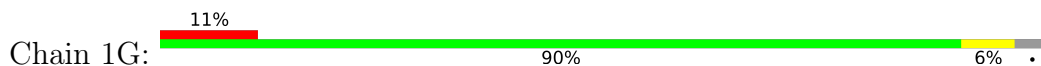


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

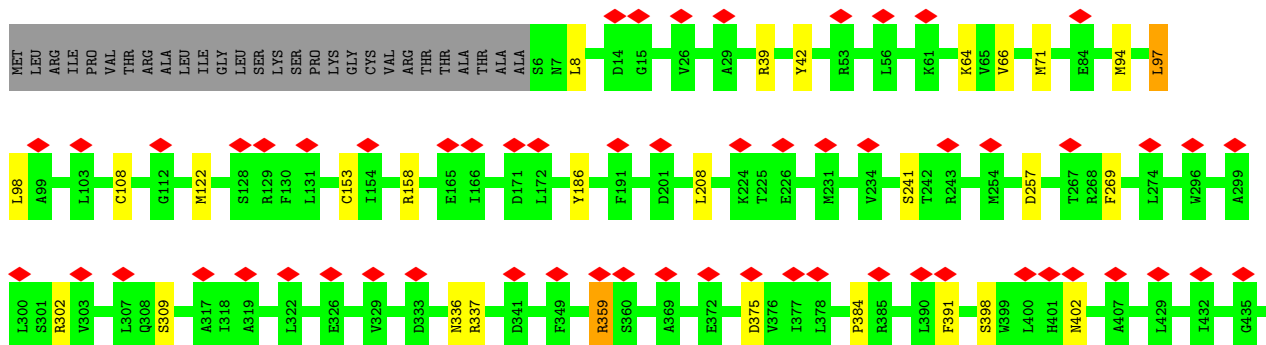
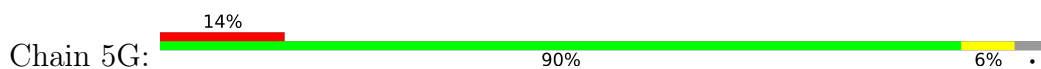


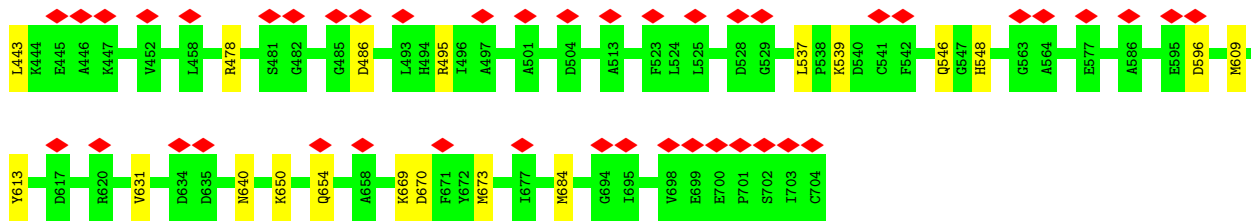


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

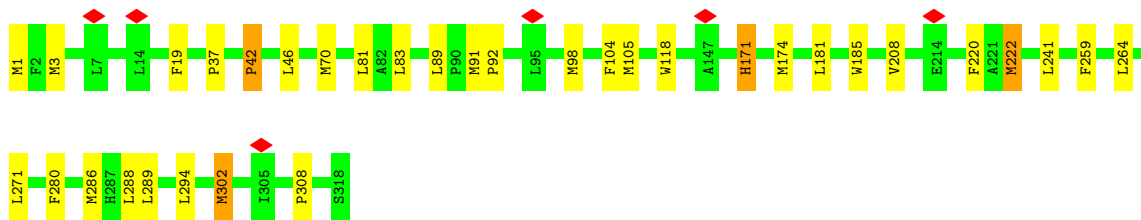
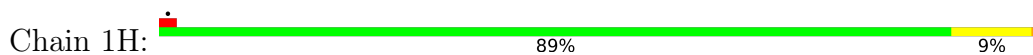


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

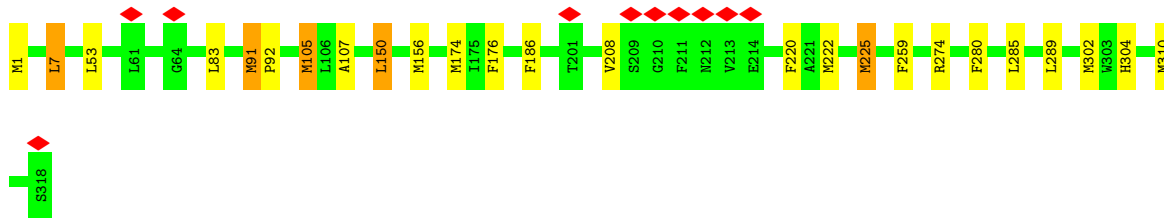




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

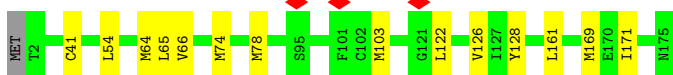


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:  91% 8%




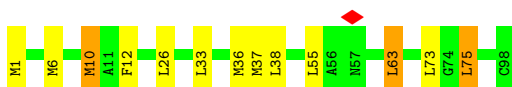
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 5J:  91% 6%




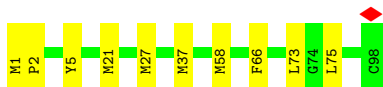
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:  87% 10%



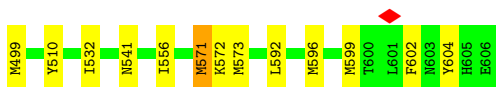
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 5K:  90% 10%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:  93% 6%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

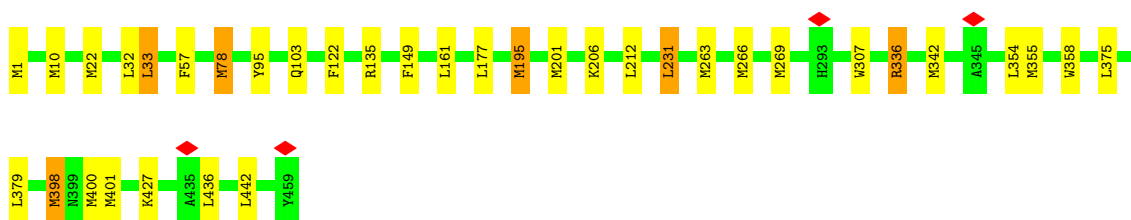
Chain 5L:  93% 7%



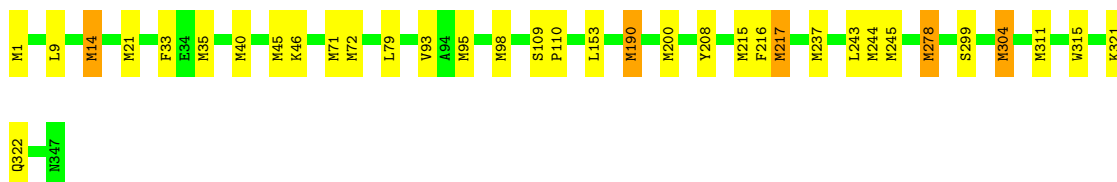
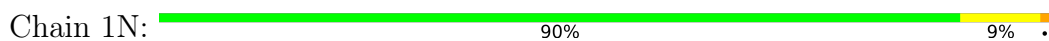
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



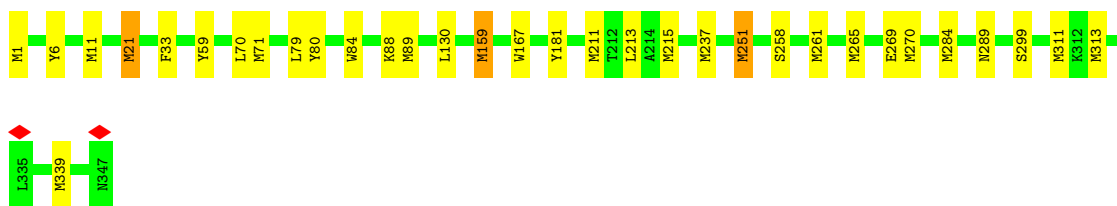
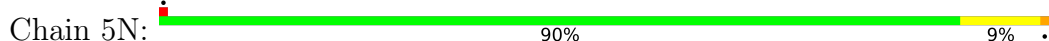
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



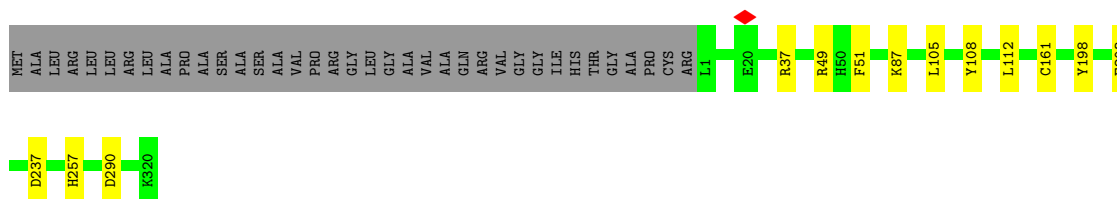
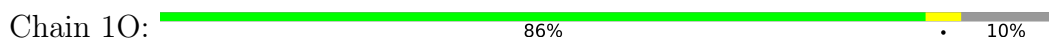
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



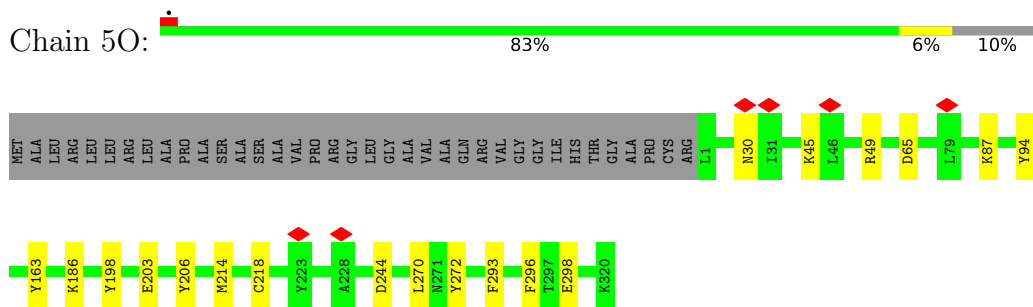
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



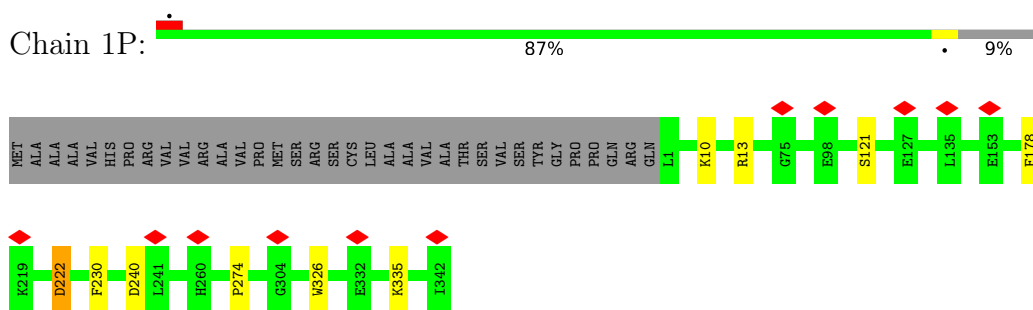
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



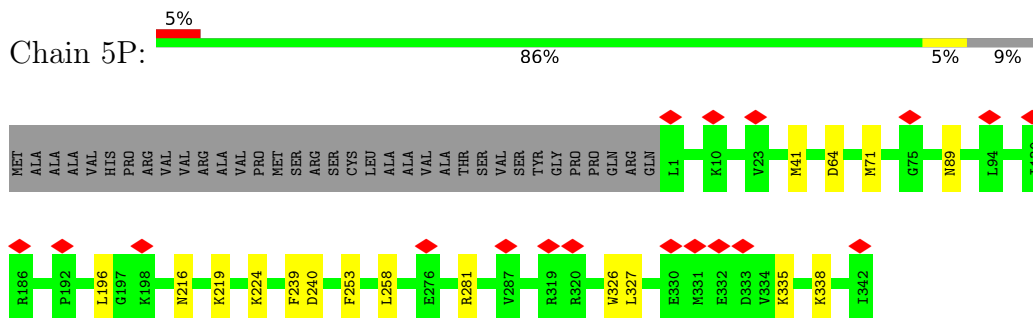
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



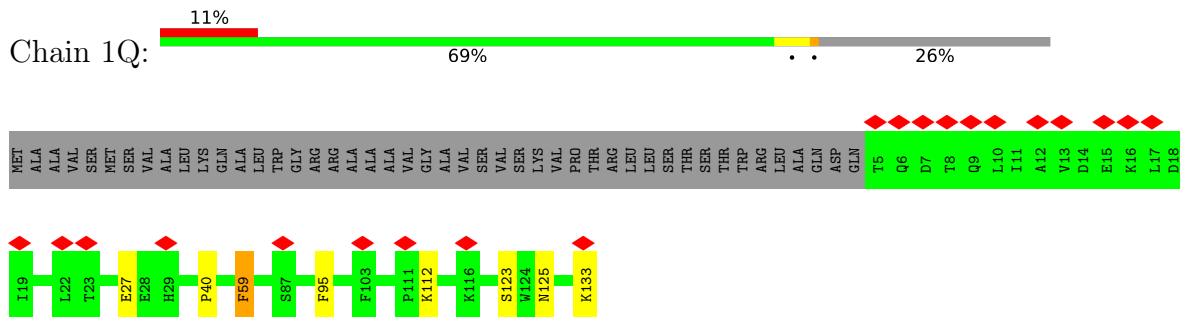
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

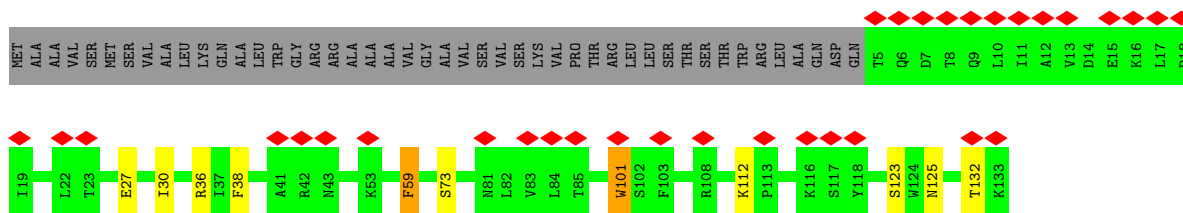


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

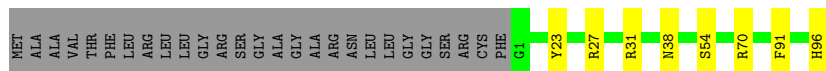


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

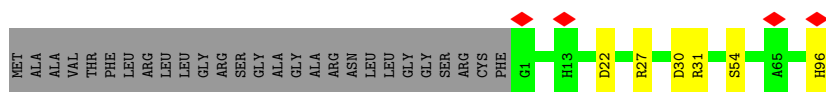




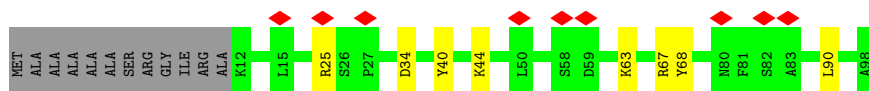
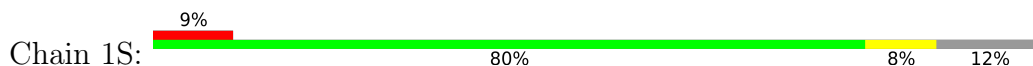
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



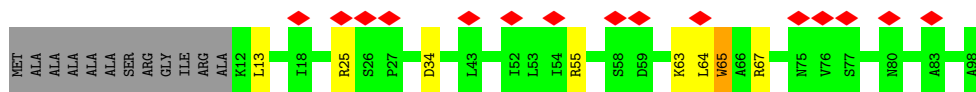
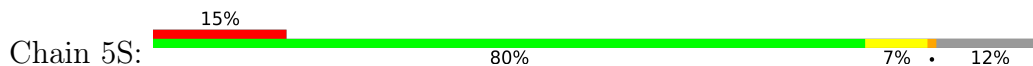
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



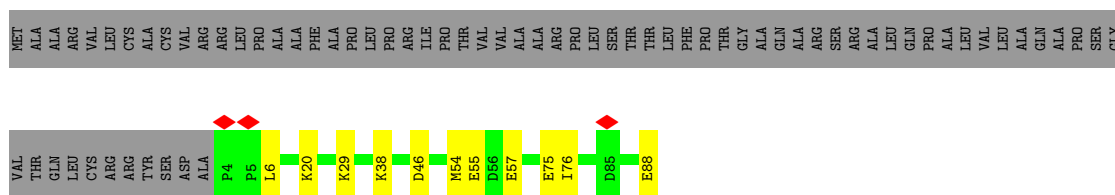
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



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

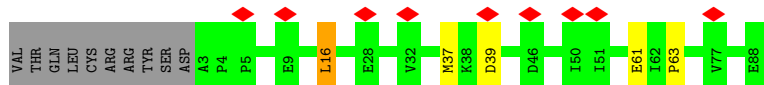
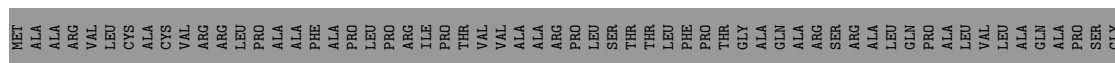


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

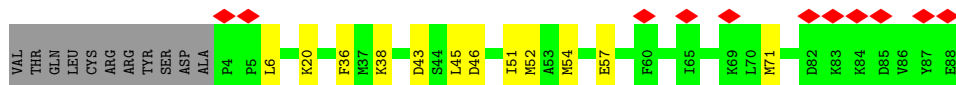
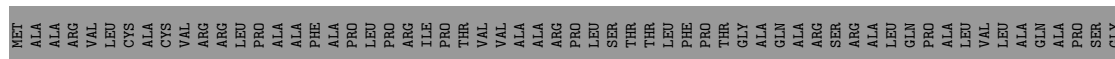


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

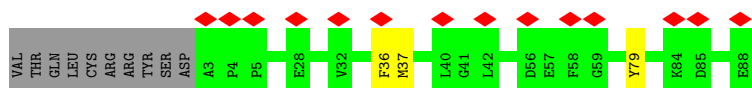




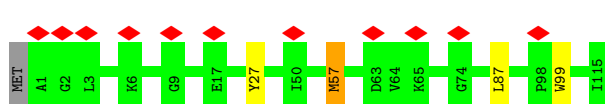
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



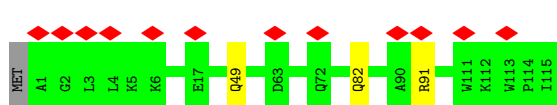
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



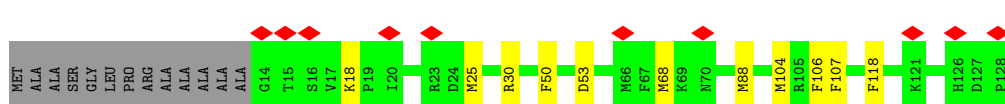
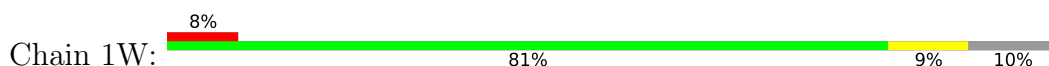
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



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

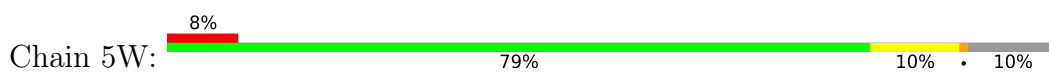


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

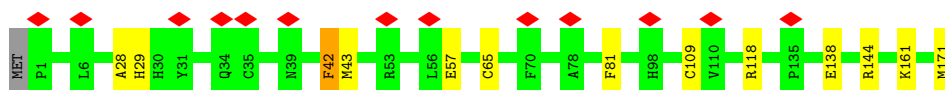
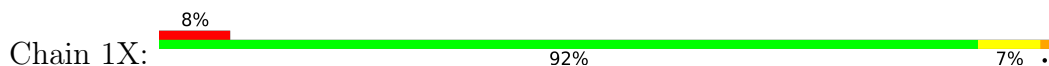


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

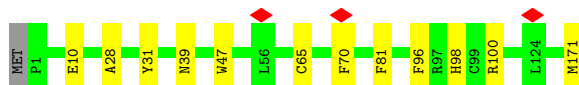




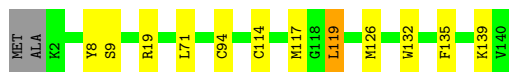
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



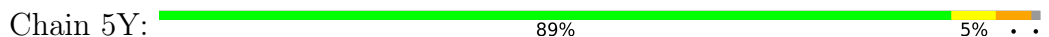
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



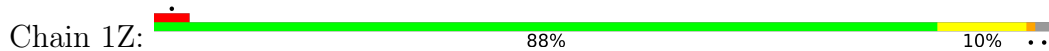
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



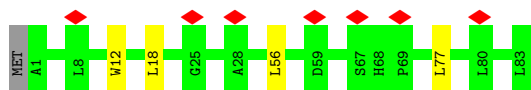
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



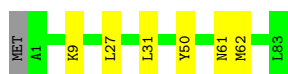
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



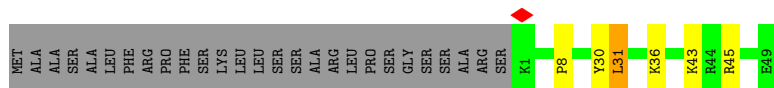
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



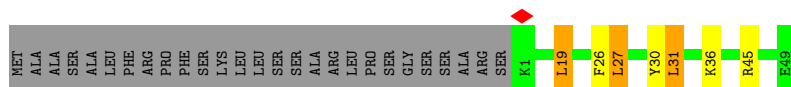
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



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

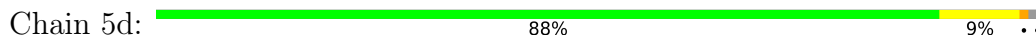


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

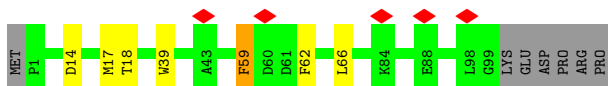
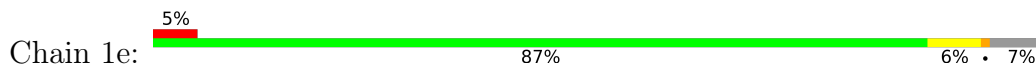




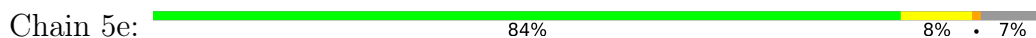
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



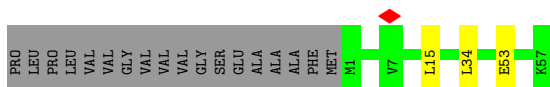
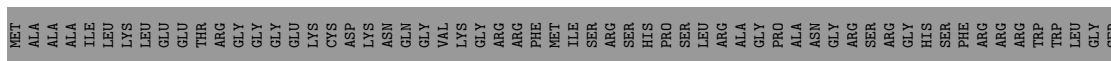
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



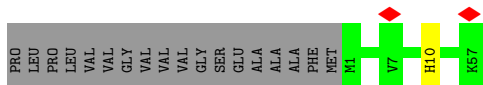
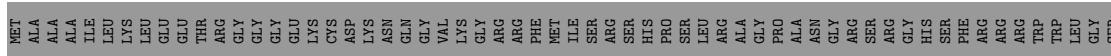
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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

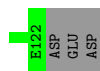
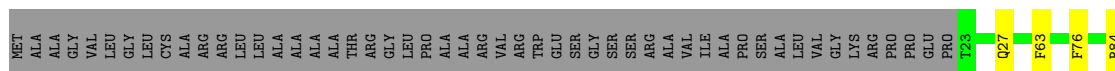


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

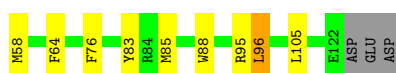
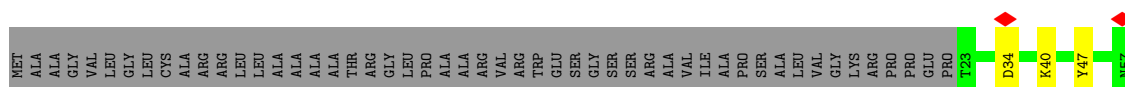


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

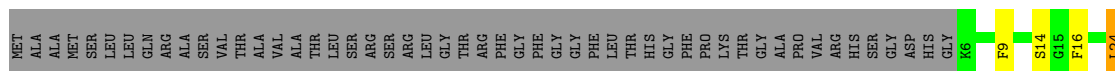




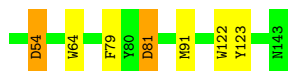
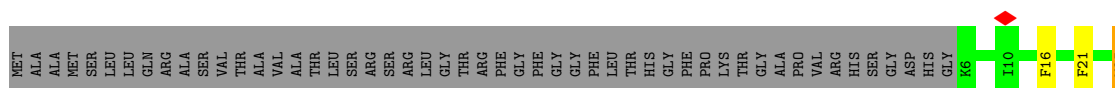
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



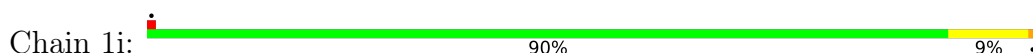
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

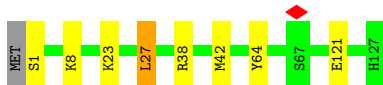


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



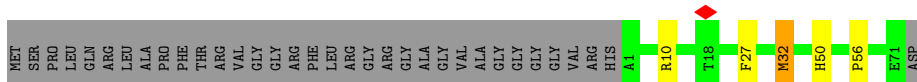
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 5i:  93% 5% ..



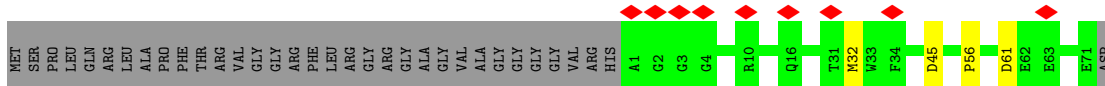
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:  63% .. 32%




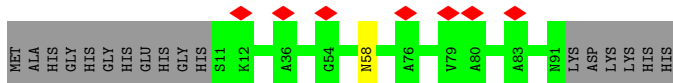
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 5j:  9% 64% . 32%




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

Chain 1k:  7% 82% . 17%




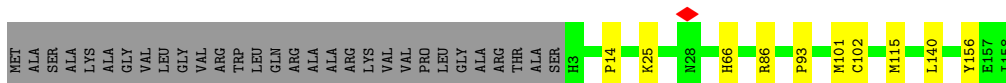
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 5k:  5% 76% 7% 17%




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

Chain 1l:  78% 5% 16%



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

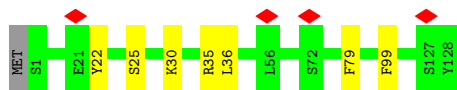
Chain 5l:  77% 6% 16%



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



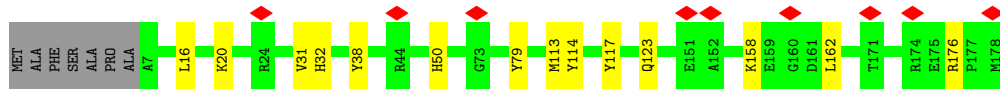
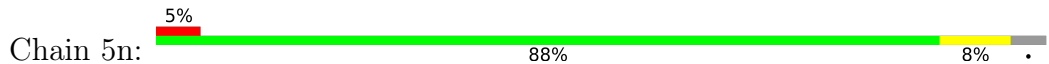
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



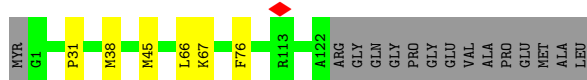
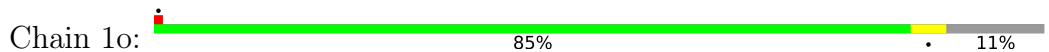
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



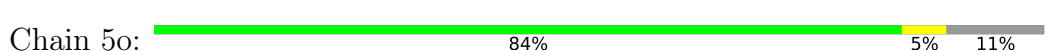
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

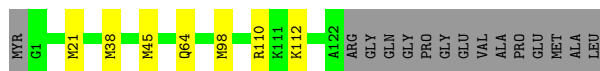


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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





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



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



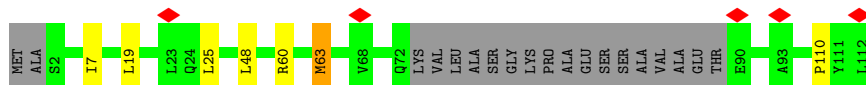
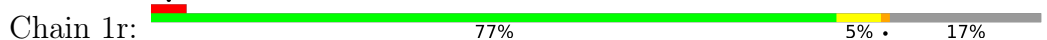
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



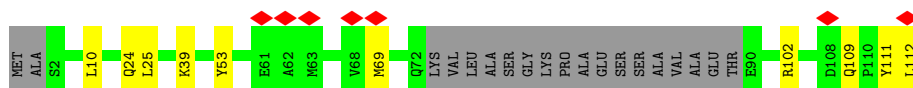
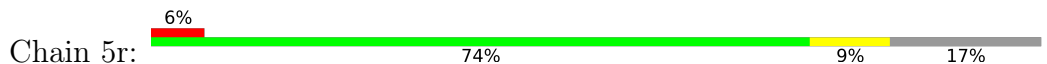
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



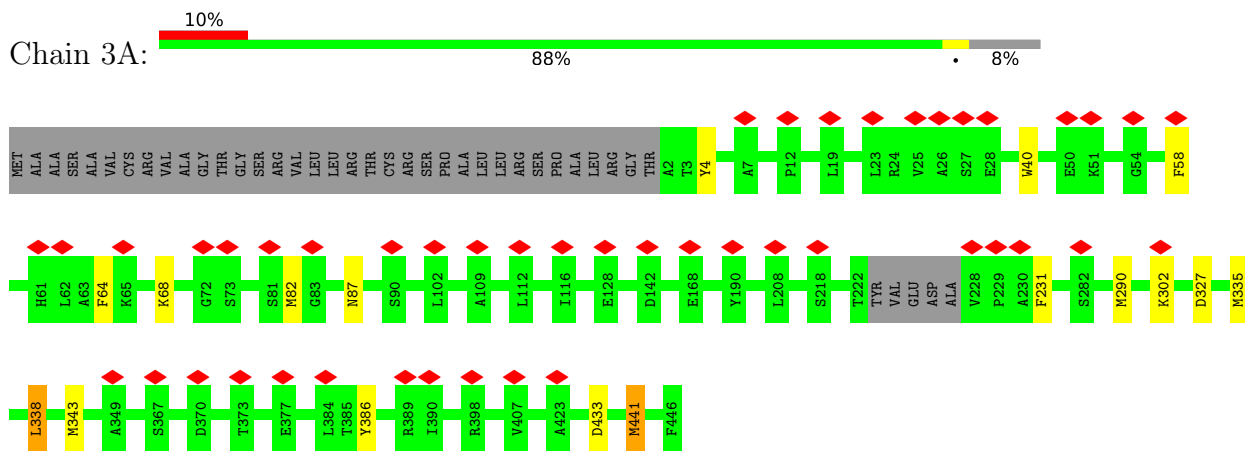
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



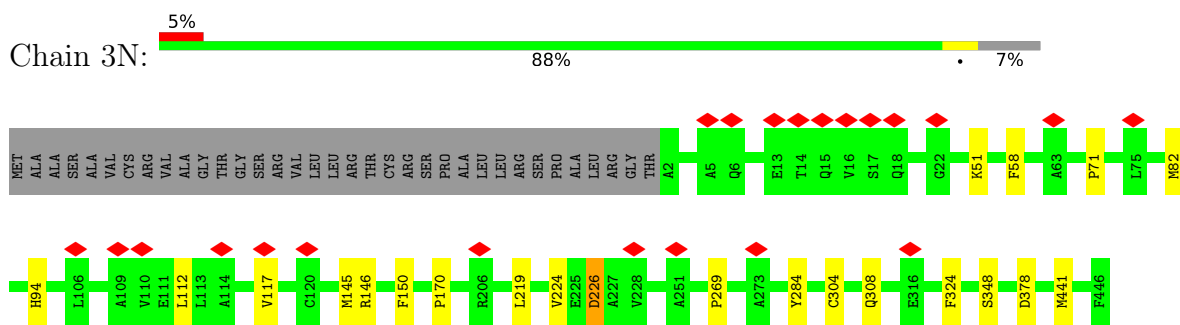
- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



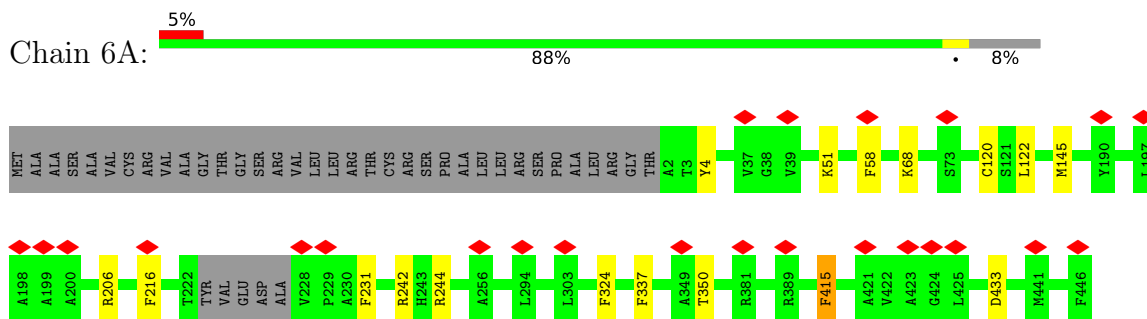




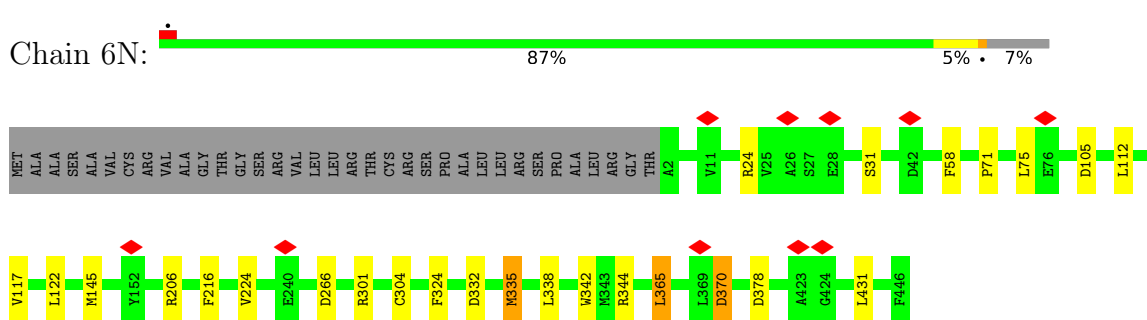
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



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

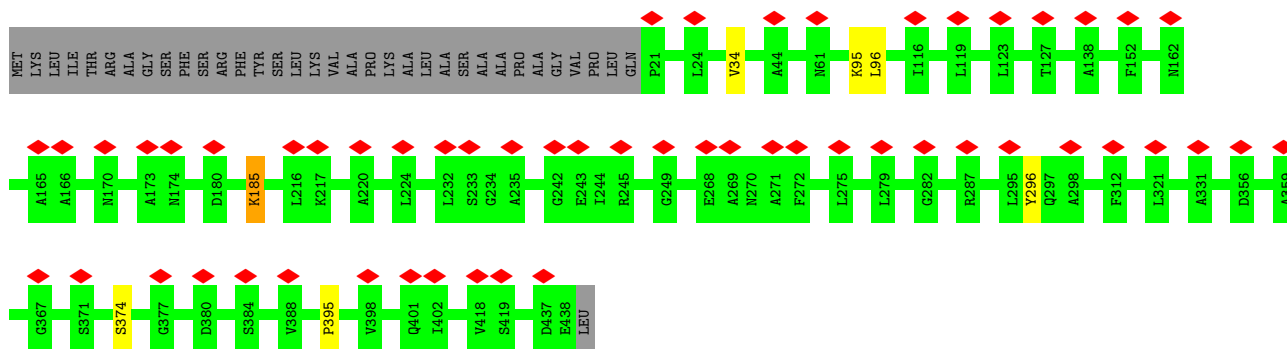


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

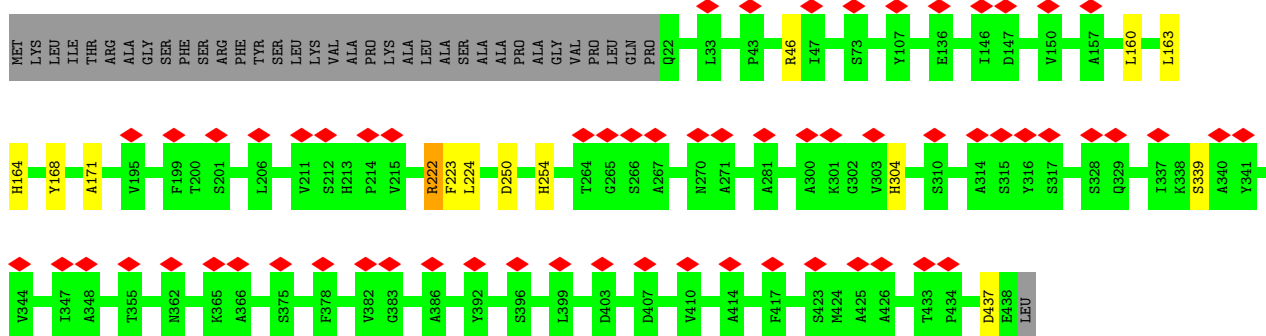
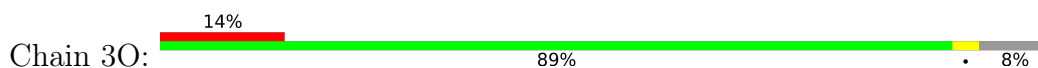


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

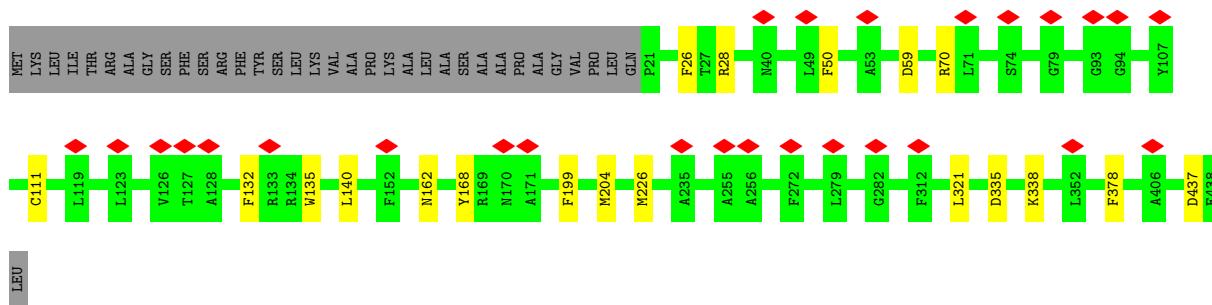
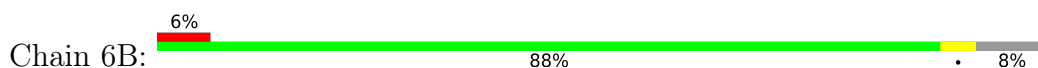




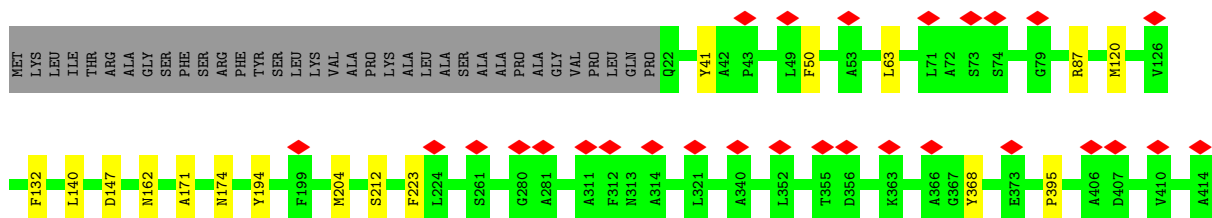
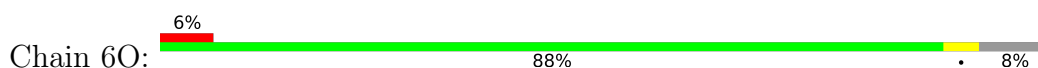
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

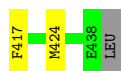


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



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





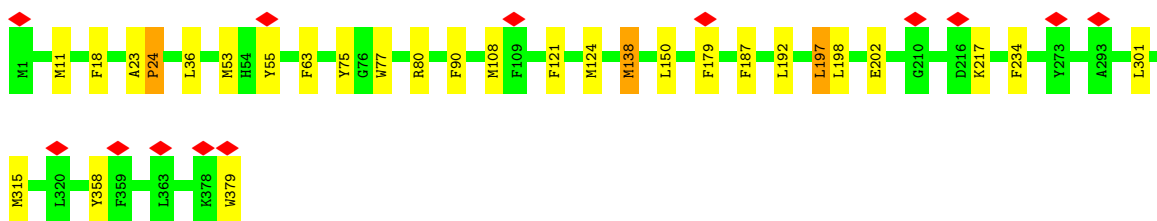
• Molecule 47: Cytochrome b



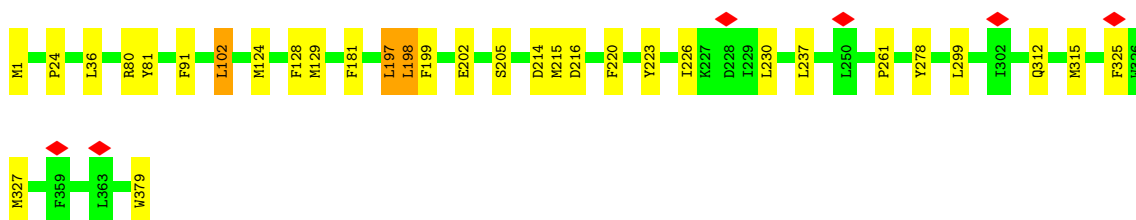
• Molecule 47: Cytochrome b



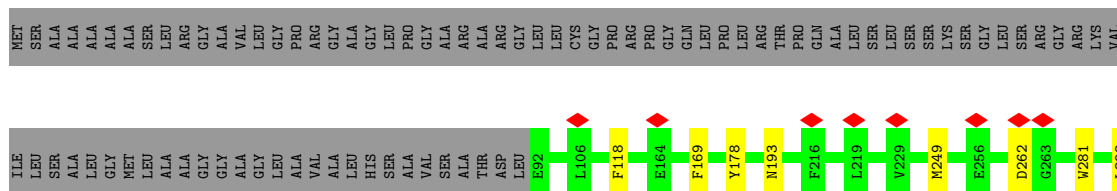
• Molecule 47: Cytochrome b



• Molecule 47: Cytochrome b



• Molecule 48: Cytochrome c1





• Molecule 48: Cytochrome c1



MET	SER	ALA	ALA	ALA	ALA	ALA	ALA	SER	LEU	ARG	GLY	VAL	VAL	LEU	GLY	PRO	ARG	GLY	ALA	ARG	ALA	ARG	ARG	GLY	LEU	LEU	CYS	GLY	PRO	ARG	PRO	GLY	GLN	LEU	PRO	THR	PRO	GLN	ALA	LEU	SER	SER	SER	SER	LYS	GLY	LEU	SER	ARG	GLY	ARG	LYS	VAL
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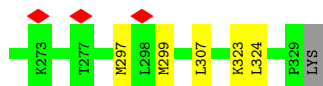
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	------	------	------	------	------	------	------	-----

• Molecule 48: Cytochrome c1



MET	SER	ALA	ALA	ALA	ALA	ALA	SER	LEU	ARG	GLY	VAL	VAL	VAL	ALA	ARG	ALA	THR	ASP	ARG	LEU	LEU	CYS	GLY	PRO	ARG	PRO	GLY	GLN	LEU	PRO	THR	PRO	GLN	ALA	LEU	SER	SER	SER	SER	LYS	SER	GLY	LEU	SER	ARG	GLY	ARG	LYS	VAL
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ILE	LEU	SER	ALA	ALA	LEU	GLY	MET	LEU	ALA	ALA	GLY	VAL	VAL	VAL	LEU	HIS	SER	LEU	ALA	VAL	VAL	THR	E92	M100	K122	M131	L176	F179	M193	R206	G210	Y214	V215	F216	F237	M249	L256	P265	M268	S269
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• Molecule 48: Cytochrome c1



MET	SER	ALA	ALA	ALA	ALA	ALA	SER	LEU	ARG	GLY	VAL	VAL	VAL	ALA	ARG	ALA	THR	ARG	GLY	LEU	LEU	CYS	GLY	PRO	ARG	PRO	GLY	GLN	LEU	PRO	THR	PRO	GLN	ALA	LEU	SER	SER	SER	SER	LYS	SER	GLY	LEU	SER	ARG	GLY	ARG	LYS	VAL
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ILE	LEU	SER	ALA	ALA	LEU	GLY	MET	LEU	ALA	ALA	GLY	VAL	VAL	VAL	LEU	HIS	SER	LEU	ALA	VAL	VAL	THR	D2	L3	E4	S13	L21	P22	H23	F30	L109	Y115	A119	F128	F153	F189	H200	M210	M211	M212	L216	K223
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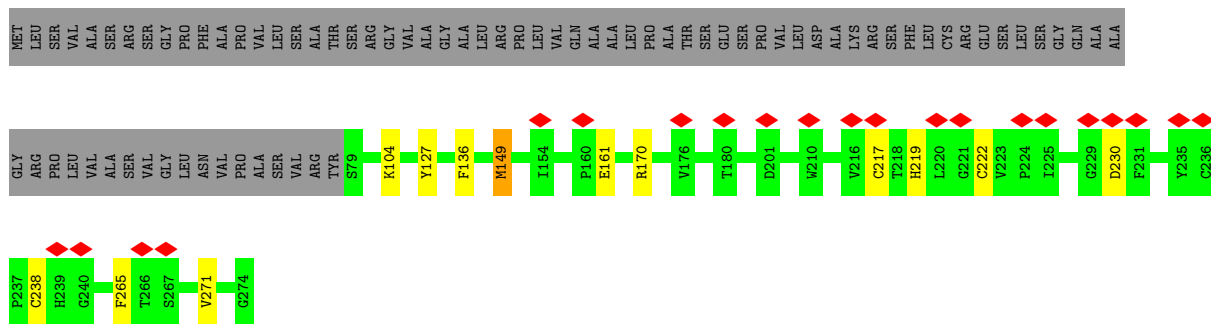
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



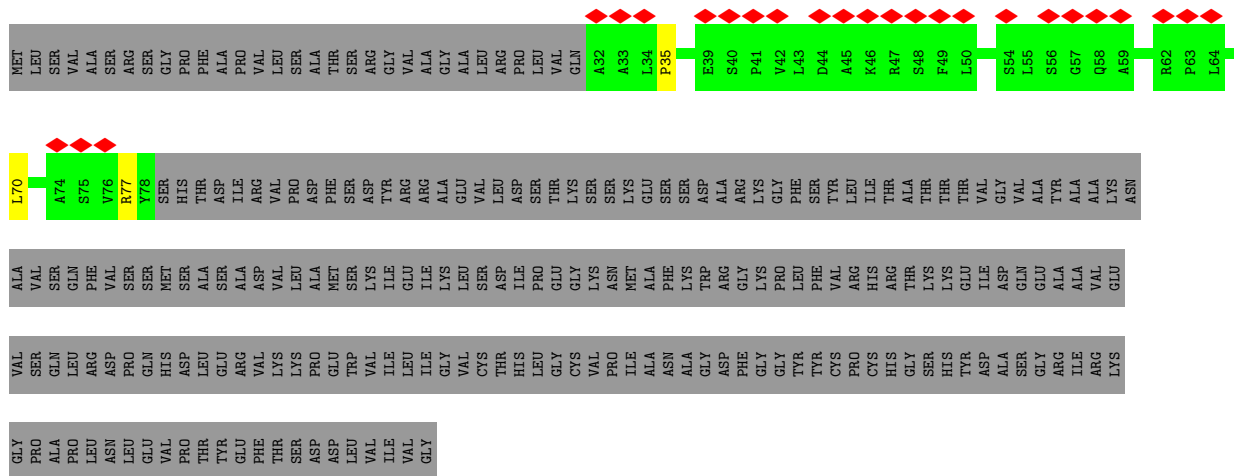
MET	LEU	SER	VAL	VAL	ALA	SER	ARG	SER	VAL	GLY	PRO	PHE	ASN	VAL	PRO	VAL	VAL	LEU	SER	ARG	THR	THR	SER	ARG	ARG	GLY	VAL	VAL	ALA	GLY	ALA	LEU	ARG	PRO	VAL	GLN	VAL	VAL	VAL	GLN	ALA	ALA	PRO	PRO	PRO	ALA	THR	SER	GLU	SER	PRO	VAL	VAL	LEU	ASP	ALA	LYS	ARG	ARG	SER	PHE	LEU	CYS	ARG	GLU	SER	LEU	SER	GLY	GLN	ALA	ALA
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GLY	ARG	PRO	LEU	VAL	VAL	ALA	SER	VAL	VAL	GLY	LEU	ASN	VAL	PRO	VAL	VAL	VAL	LEU	SER	ARG	THR	SER	S79	L116	F136	M149	M165	V176	K181	S193	R196	V216	C217	G229	H242	E264	F265	T266	S267	V271	G274
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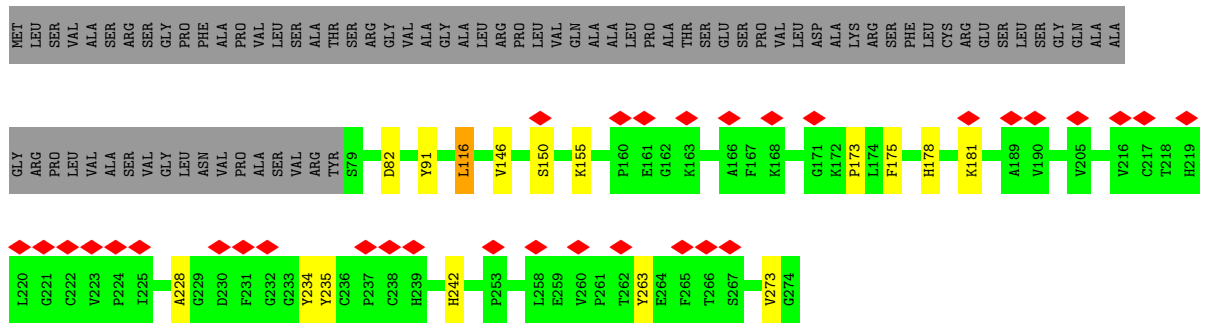




- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

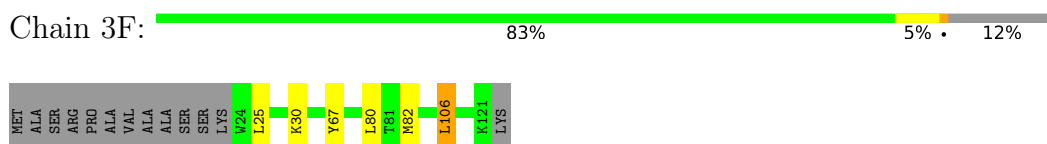


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

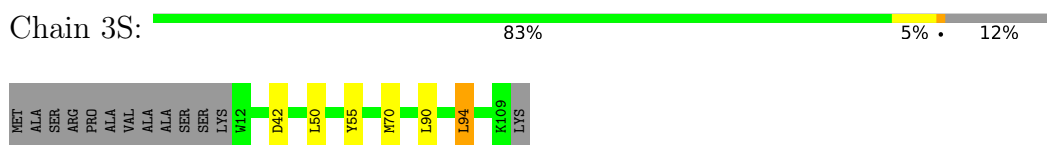




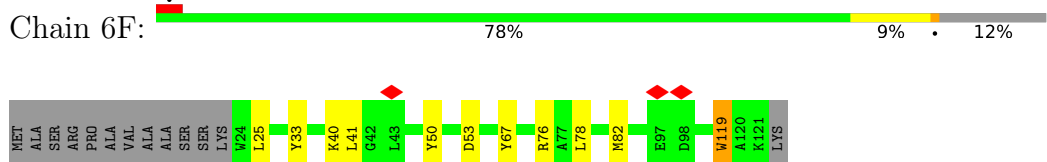
• Molecule 50: Cytochrome b-c1 complex subunit 7



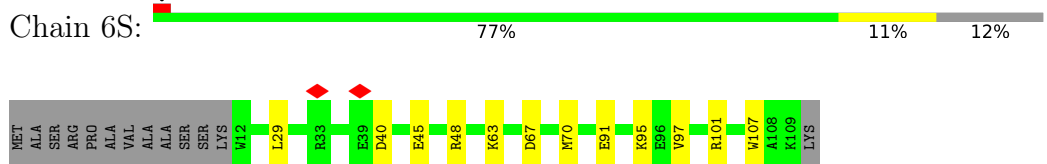
• Molecule 50: Cytochrome b-c1 complex subunit 7



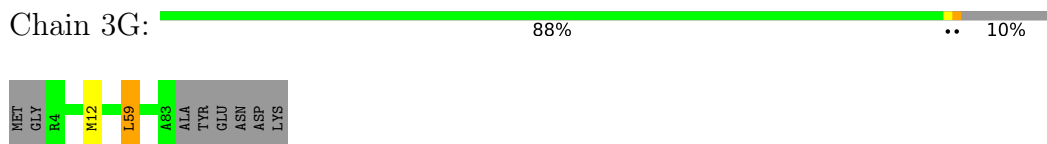
• Molecule 50: Cytochrome b-c1 complex subunit 7



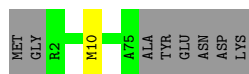
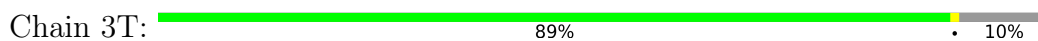
• Molecule 50: Cytochrome b-c1 complex subunit 7



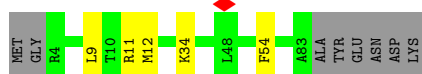
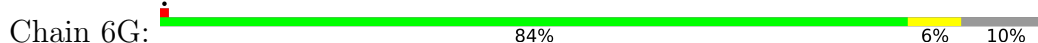
• Molecule 51: Cytochrome b-c1 complex subunit 8



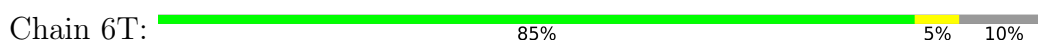
- Molecule 51: Cytochrome b-c1 complex subunit 8



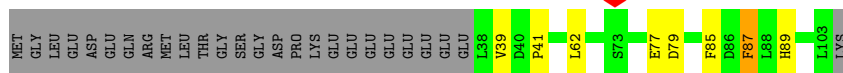
- Molecule 51: Cytochrome b-c1 complex subunit 8



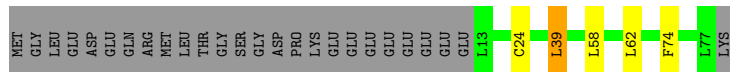
- Molecule 51: Cytochrome b-c1 complex subunit 8



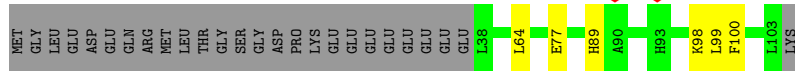
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



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



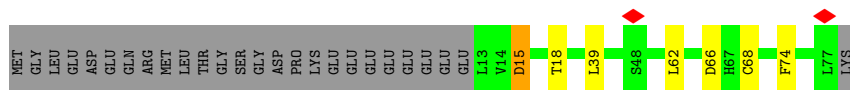
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



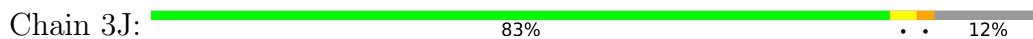
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



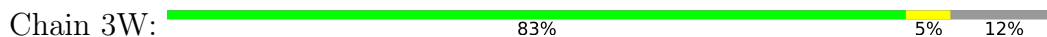




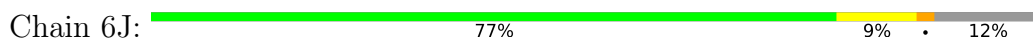
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



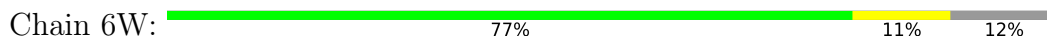
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



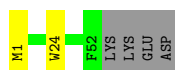
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



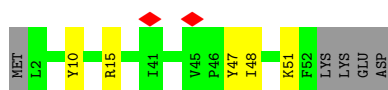
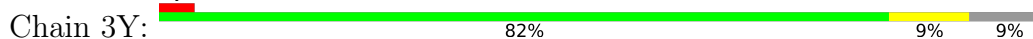
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



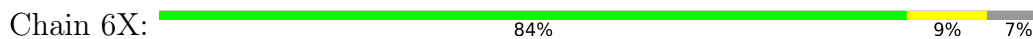
• Molecule 54: Cytochrome b-c1 complex subunit 10



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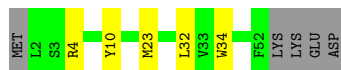
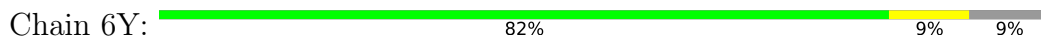


• Molecule 54: Cytochrome b-c1 complex subunit 10

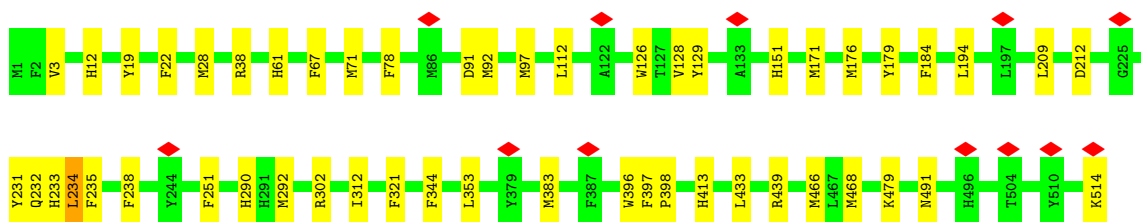




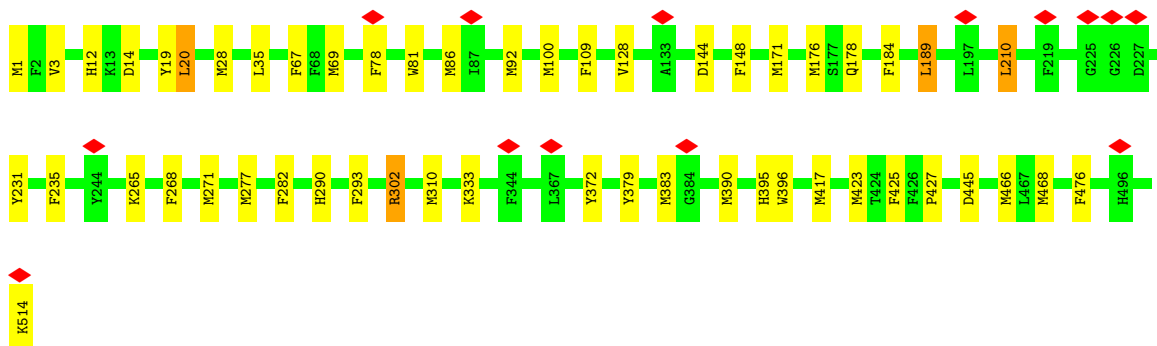
- Molecule 54: Cytochrome b-c1 complex subunit 10



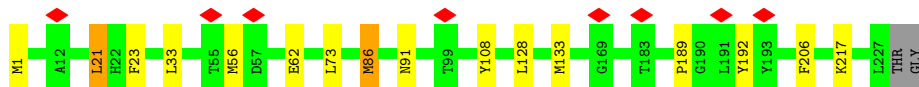
- Molecule 55: Cytochrome c oxidase subunit 1



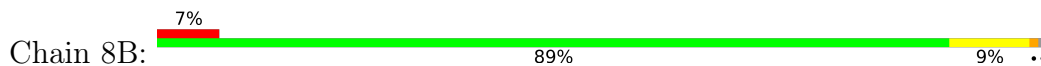
- Molecule 55: Cytochrome c oxidase subunit 1

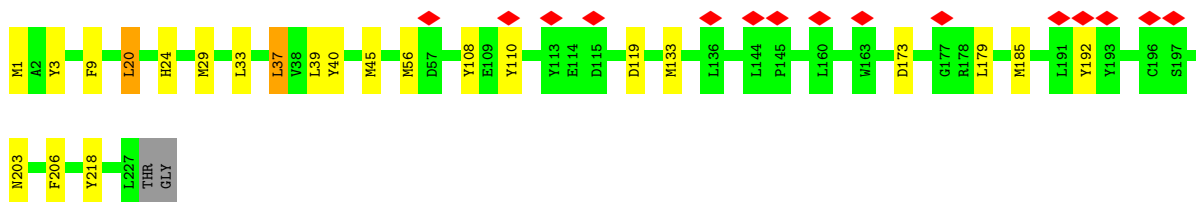


- Molecule 56: Cytochrome c oxidase subunit 2

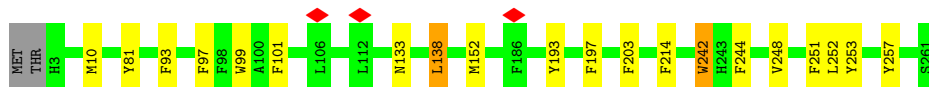


- Molecule 56: Cytochrome c oxidase subunit 2

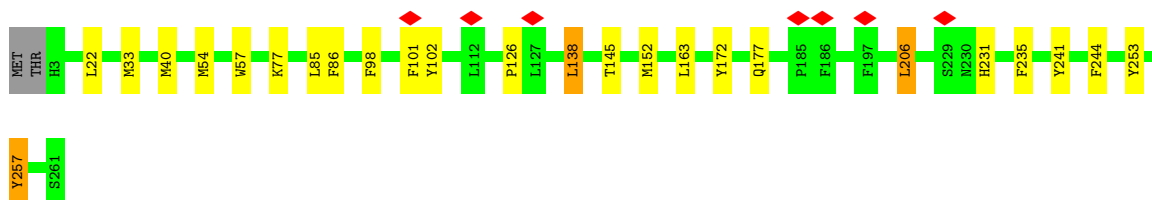
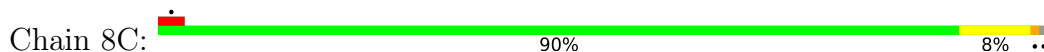




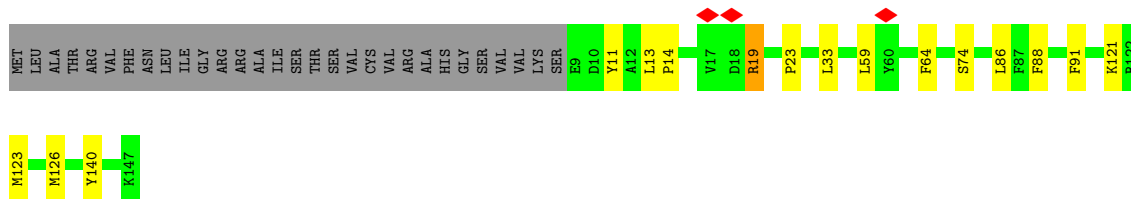
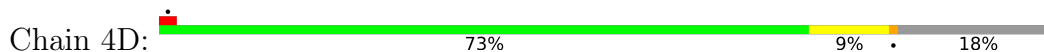
• Molecule 57: Cytochrome c oxidase subunit 3



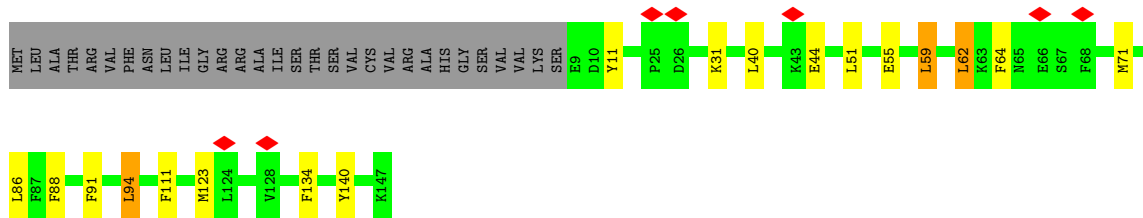
• Molecule 57: Cytochrome c oxidase subunit 3



• Molecule 58: Cytochrome c oxidase subunit 4

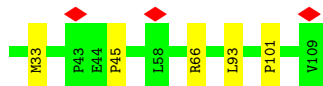
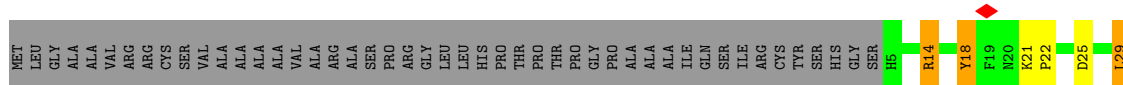


• Molecule 58: Cytochrome c oxidase subunit 4

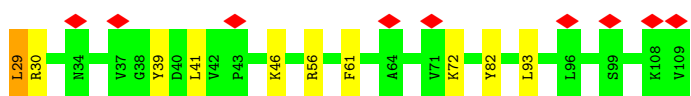
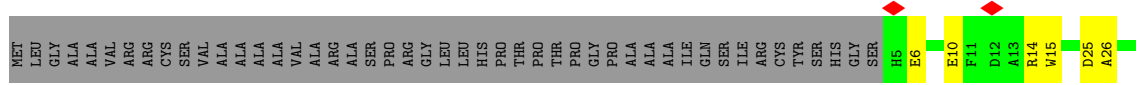


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial





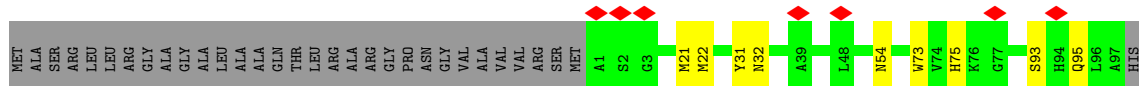
• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



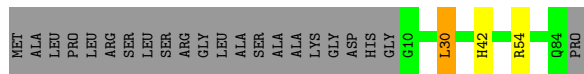
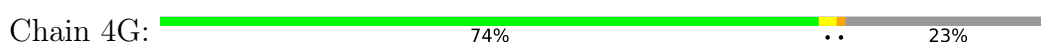
• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



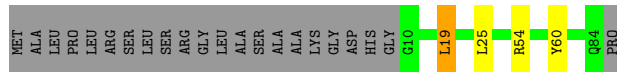
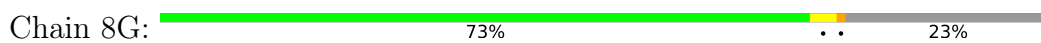
• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



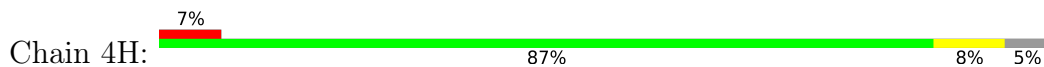
• Molecule 61: Cytochrome c oxidase subunit 6A2



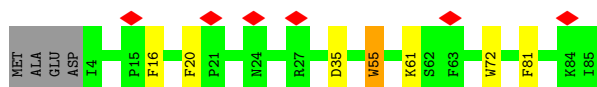
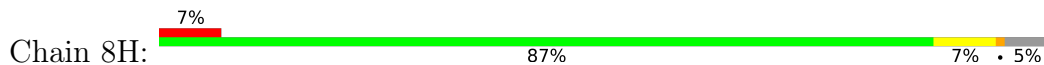
• Molecule 61: Cytochrome c oxidase subunit 6A2



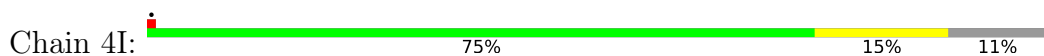
- Molecule 62: Cytochrome c oxidase subunit 6B1



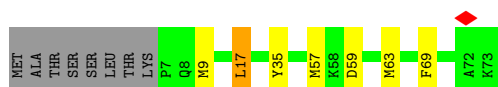
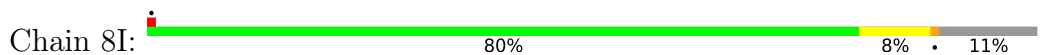
- Molecule 62: Cytochrome c oxidase subunit 6B1



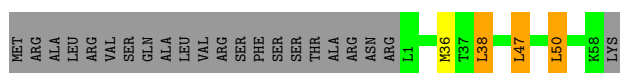
- Molecule 63: Cytochrome c oxidase subunit 6C



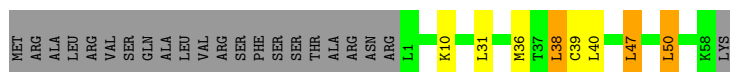
- Molecule 63: Cytochrome c oxidase subunit 6C



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

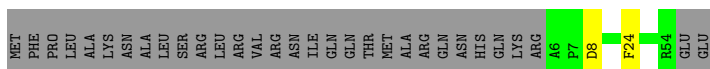


- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

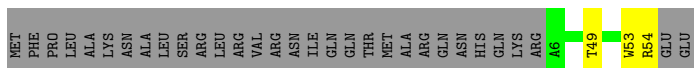


- Molecule 65: Cytochrome c oxidase subunit 7B

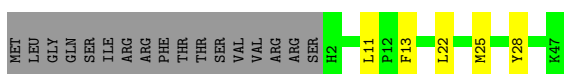




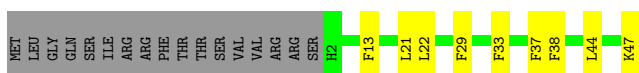
- Molecule 65: Cytochrome c oxidase subunit 7B



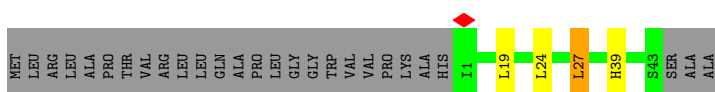
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



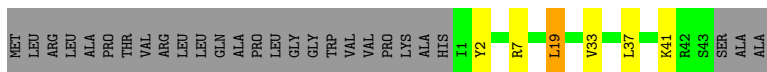
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



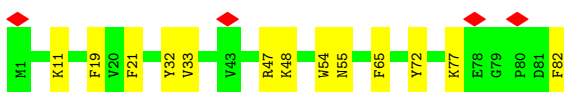
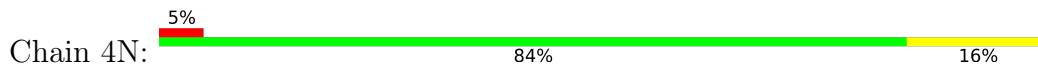
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 67: Cytochrome c oxidase subunit 8

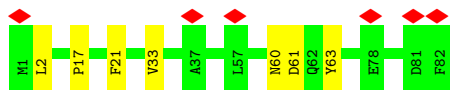


- Molecule 68: Cytochrome c oxidase subunit NDUF4A



- Molecule 68: Cytochrome c oxidase subunit NDUF4A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	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	1.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	798.72, 798.72, 798.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.51	1/930 (0.1%)	0.79	1/1271 (0.1%)
1	5A	0.56	0/930	0.87	5/1271 (0.4%)
2	1B	0.56	2/1273 (0.2%)	0.89	4/1722 (0.2%)
2	5B	0.46	0/1273	0.91	10/1722 (0.6%)
3	1C	0.46	1/1791 (0.1%)	0.69	1/2439 (0.0%)
3	5C	0.61	6/1791 (0.3%)	0.71	3/2439 (0.1%)
4	1D	0.41	1/3545 (0.0%)	0.72	10/4806 (0.2%)
4	5D	0.35	0/3545	0.68	5/4806 (0.1%)
5	1E	0.44	2/1698 (0.1%)	0.67	5/2311 (0.2%)
5	5E	0.49	2/1698 (0.1%)	0.70	4/2311 (0.2%)
6	1F	0.33	0/3401	0.60	1/4595 (0.0%)
6	5F	0.30	0/3401	0.59	4/4595 (0.1%)
7	1G	0.38	2/5451 (0.0%)	0.67	9/7387 (0.1%)
7	5G	0.54	6/5451 (0.1%)	0.83	16/7387 (0.2%)
8	1H	1.08	11/2566 (0.4%)	1.23	28/3509 (0.8%)
8	5H	0.41	0/2566	0.76	11/3509 (0.3%)
9	1I	0.65	4/1443 (0.3%)	0.87	9/1952 (0.5%)
9	5I	0.47	0/1443	0.69	2/1952 (0.1%)
10	1J	0.57	2/1364 (0.1%)	0.84	5/1850 (0.3%)
10	5J	0.43	0/1364	0.72	4/1850 (0.2%)
11	1K	0.68	1/751 (0.1%)	1.34	11/1018 (1.1%)
11	5K	0.39	0/751	0.79	0/1018
12	1L	0.40	1/4939 (0.0%)	0.68	13/6718 (0.2%)
12	5L	0.43	2/4939 (0.0%)	0.80	25/6718 (0.4%)
13	1M	0.34	0/3713	0.68	5/5063 (0.1%)
13	5M	0.39	1/3713 (0.0%)	0.80	13/5063 (0.3%)
14	1N	0.50	2/2765 (0.1%)	0.87	15/3758 (0.4%)
14	5N	0.52	3/2765 (0.1%)	0.88	13/3758 (0.3%)
15	1O	0.31	0/2650	0.57	2/3588 (0.1%)
15	5O	0.42	3/2650 (0.1%)	0.64	2/3588 (0.1%)
16	1P	0.36	1/2828 (0.0%)	0.60	1/3834 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	5P	0.36	1/2828 (0.0%)	0.61	3/3834 (0.1%)
17	1Q	0.62	4/1070 (0.4%)	0.71	1/1446 (0.1%)
17	5Q	0.79	8/1070 (0.7%)	0.77	2/1446 (0.1%)
18	1R	0.31	0/755	0.61	1/1018 (0.1%)
18	5R	0.33	0/755	0.64	1/1018 (0.1%)
19	1S	0.44	0/711	0.81	1/956 (0.1%)
19	5S	0.55	1/711 (0.1%)	0.83	6/956 (0.6%)
20	1T	0.62	2/701 (0.3%)	0.84	4/946 (0.4%)
20	1U	0.46	1/706 (0.1%)	0.80	4/954 (0.4%)
20	5T	0.34	0/701	0.68	1/946 (0.1%)
20	5U	0.62	3/706 (0.4%)	0.71	0/954
21	1V	0.32	0/946	0.65	2/1281 (0.2%)
21	5V	0.29	0/946	0.56	0/1281
22	1W	0.34	0/995	0.75	2/1340 (0.1%)
22	5W	0.49	0/995	0.87	4/1340 (0.3%)
23	1X	0.45	3/1436 (0.2%)	0.59	0/1938
23	5X	0.53	3/1436 (0.2%)	0.61	0/1938
24	1Y	0.33	0/1037	0.74	6/1404 (0.4%)
24	5Y	0.32	0/1037	1.06	8/1404 (0.6%)
25	1Z	0.60	5/1199 (0.4%)	0.78	4/1617 (0.2%)
25	5Z	0.56	1/1199 (0.1%)	0.80	2/1617 (0.1%)
26	1a	0.41	0/577	0.78	2/777 (0.3%)
26	5a	0.37	0/577	0.65	1/777 (0.1%)
27	1b	0.34	0/664	0.62	1/912 (0.1%)
27	5b	0.31	0/664	0.67	2/912 (0.2%)
28	1c	0.68	1/430 (0.2%)	0.86	2/581 (0.3%)
28	5c	0.29	0/430	0.71	3/581 (0.5%)
29	1d	0.45	1/1016 (0.1%)	0.66	0/1374
29	5d	0.55	2/1016 (0.2%)	0.73	3/1374 (0.2%)
30	1e	0.60	2/836 (0.2%)	0.97	6/1118 (0.5%)
30	5e	0.58	3/836 (0.4%)	0.72	1/1118 (0.1%)
31	1f	0.25	0/499	0.65	2/673 (0.3%)
31	5f	0.29	0/499	0.65	0/673
32	1g	0.58	2/858 (0.2%)	0.70	0/1165
32	5g	0.51	1/858 (0.1%)	0.82	2/1165 (0.2%)
33	1h	0.45	1/1184 (0.1%)	0.74	2/1603 (0.1%)
33	5h	0.48	2/1184 (0.2%)	0.73	3/1603 (0.2%)
34	1i	0.49	2/1131 (0.2%)	0.79	4/1541 (0.3%)
34	5i	0.45	1/1131 (0.1%)	0.76	4/1541 (0.3%)
35	1j	0.42	0/627	0.70	2/858 (0.2%)
35	5j	0.33	0/627	0.64	1/858 (0.1%)
36	1k	0.32	0/668	0.54	0/903
36	5k	0.83	3/668 (0.4%)	0.85	3/903 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	1l	0.37	0/1365	0.71	5/1867 (0.3%)
37	5l	0.39	0/1365	0.68	3/1867 (0.2%)
38	1m	0.35	0/1092	0.62	1/1481 (0.1%)
38	5m	0.35	0/1092	0.69	1/1481 (0.1%)
39	1n	0.37	1/1549 (0.1%)	0.67	1/2098 (0.0%)
39	5n	0.61	6/1549 (0.4%)	0.79	4/2098 (0.2%)
40	1o	0.31	0/1069	0.69	2/1430 (0.1%)
40	5o	0.38	0/1069	0.71	1/1430 (0.1%)
41	1p	0.32	0/1481	0.56	0/1997
41	5p	0.38	0/1481	0.68	1/1997 (0.1%)
42	1q	0.55	3/1253 (0.2%)	0.77	3/1704 (0.2%)
42	5q	0.82	9/1253 (0.7%)	0.72	6/1704 (0.4%)
43	1r	0.37	0/777	0.85	5/1051 (0.5%)
43	5r	0.45	0/777	0.75	2/1051 (0.2%)
44	1s	1.04	5/394 (1.3%)	0.82	1/533 (0.2%)
44	5s	0.29	0/394	0.61	0/533
45	3A	0.37	2/3481 (0.1%)	0.62	5/4722 (0.1%)
45	3N	0.57	5/3496 (0.1%)	0.78	8/4723 (0.2%)
45	6A	0.37	0/3481	0.63	2/4722 (0.0%)
45	6N	0.34	0/3496	0.67	7/4723 (0.1%)
46	3B	0.36	2/3190 (0.1%)	0.61	2/4317 (0.0%)
46	3O	0.30	0/3175	0.59	3/4292 (0.1%)
46	6B	0.37	1/3190 (0.0%)	0.62	2/4317 (0.0%)
46	6O	0.33	0/3175	0.62	3/4292 (0.1%)
47	3C	0.41	2/3123 (0.1%)	0.70	9/4269 (0.2%)
47	3P	0.29	0/3122	0.59	4/4269 (0.1%)
47	6C	0.80	6/3123 (0.2%)	0.92	11/4269 (0.3%)
47	6P	0.59	3/3122 (0.1%)	0.92	23/4269 (0.5%)
48	3D	0.38	0/1946	0.69	3/2641 (0.1%)
48	3Q	0.32	0/1962	0.59	2/2663 (0.1%)
48	6D	0.39	0/1946	0.76	7/2641 (0.3%)
48	6Q	0.52	2/1962 (0.1%)	0.86	8/2663 (0.3%)
49	3E	0.31	0/1551	0.61	1/2098 (0.0%)
49	3I	0.64	1/342 (0.3%)	0.78	2/465 (0.4%)
49	3R	0.33	0/1551	0.60	0/2098
49	3V	0.28	0/225	0.62	0/303
49	6E	0.53	3/1551 (0.2%)	0.70	2/2098 (0.1%)
49	6I	0.48	1/342 (0.3%)	0.73	0/465
49	6R	0.60	4/1551 (0.3%)	0.82	4/2098 (0.2%)
49	6V	0.26	0/225	0.68	0/303
50	3F	0.35	0/888	0.71	3/1193 (0.3%)
50	3S	0.28	0/888	0.67	3/1193 (0.3%)
50	6F	0.55	1/888 (0.1%)	0.81	5/1193 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
50	6S	0.50	1/888 (0.1%)	0.87	5/1193 (0.4%)
51	3G	0.37	0/649	0.74	1/878 (0.1%)
51	3T	0.34	0/649	0.61	1/878 (0.1%)
51	6G	0.40	0/649	0.78	1/878 (0.1%)
51	6T	0.40	0/649	0.73	0/878
52	3H	1.11	8/539 (1.5%)	1.23	10/724 (1.4%)
52	3U	0.29	0/539	0.70	3/724 (0.4%)
52	6H	0.34	0/539	0.81	3/724 (0.4%)
52	6U	0.50	0/539	0.85	4/724 (0.6%)
53	3J	0.36	0/464	0.69	2/625 (0.3%)
53	3W	0.53	0/464	0.73	2/625 (0.3%)
53	6J	0.41	0/464	0.82	2/625 (0.3%)
53	6W	0.44	0/464	0.83	4/625 (0.6%)
54	3X	0.27	0/445	0.55	0/608
54	3Y	0.37	0/437	0.71	1/598 (0.2%)
54	6X	0.41	0/445	0.79	3/608 (0.5%)
54	6Y	0.59	1/437 (0.2%)	0.76	2/598 (0.3%)
55	4A	0.51	3/4156 (0.1%)	0.82	13/5679 (0.2%)
55	8A	0.56	6/4156 (0.1%)	0.96	12/5679 (0.2%)
56	4B	0.50	1/1865 (0.1%)	0.79	6/2544 (0.2%)
56	8B	0.43	0/1865	0.83	9/2544 (0.4%)
57	4C	0.55	2/2179 (0.1%)	0.66	3/2981 (0.1%)
57	8C	0.56	2/2179 (0.1%)	0.77	3/2981 (0.1%)
58	4D	0.53	0/1197	0.89	7/1617 (0.4%)
58	8D	0.61	3/1197 (0.3%)	0.86	6/1617 (0.4%)
59	4E	0.63	2/871 (0.2%)	0.97	6/1182 (0.5%)
59	8E	0.56	2/871 (0.2%)	0.93	4/1182 (0.3%)
60	4F	0.65	3/749 (0.4%)	0.76	2/1016 (0.2%)
60	8F	0.31	0/749	0.69	0/1016
61	4G	0.28	0/644	0.60	1/881 (0.1%)
61	8G	0.41	0/644	0.68	2/881 (0.2%)
62	4H	0.83	4/708 (0.6%)	0.86	5/956 (0.5%)
62	8H	0.63	1/708 (0.1%)	0.78	1/956 (0.1%)
63	4I	0.47	0/563	0.98	2/748 (0.3%)
63	8I	0.48	0/563	0.92	3/748 (0.4%)
64	4J	0.31	0/466	0.71	3/631 (0.5%)
64	8J	0.67	1/466 (0.2%)	0.94	5/631 (0.8%)
65	4K	0.29	0/396	0.50	0/543
65	8K	0.31	0/396	0.49	0/543
66	4L	0.49	0/394	0.73	1/528 (0.2%)
66	8L	0.63	0/394	1.07	7/528 (1.3%)
67	4M	0.46	0/349	0.80	3/477 (0.6%)
67	8M	0.45	0/349	0.83	3/477 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
68	4N	0.41	0/680	0.65	0/921
68	8N	0.46	0/680	0.66	1/921 (0.1%)
All	All	0.48	204/232954 (0.1%)	0.75	640/315994 (0.2%)

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
2	1B	0	2
3	1C	0	1
5	1E	0	1
6	1F	0	1
6	5F	0	1
7	5G	0	1
8	1H	0	2
8	5H	0	1
10	1J	0	1
11	5K	0	1
12	1L	0	1
12	5L	0	1
13	5M	0	1
16	1P	0	1
18	5R	0	1
23	5X	0	1
24	1Y	0	1
25	5Z	0	1
26	1a	0	1
33	1h	0	1
38	5m	0	1
39	1n	0	1
43	5r	0	1
45	3N	0	1
45	6A	0	1
45	6N	0	1
47	6C	0	2
48	6D	0	1
49	6E	0	1
52	6H	0	1
59	4E	0	1
59	8E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	4N	0	1
All	All	0	36

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1H	308	PRO	CG-CD	-30.86	0.48	1.50
47	6C	24	PRO	CB-CG	28.68	2.93	1.50
7	5G	384	PRO	CG-CD	-24.08	0.71	1.50
47	6C	24	PRO	CG-CD	-22.70	0.75	1.50
8	1H	42	PRO	CG-CD	-21.25	0.80	1.50

The worst 5 of 640 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	6C	24	PRO	CB-CG-CD	-27.30	0.03	106.50
7	5G	384	PRO	N-CD-CG	-23.64	67.74	103.20
8	1H	42	PRO	CA-CB-CG	-23.19	59.94	104.00
8	1H	308	PRO	N-CD-CG	-21.88	70.38	103.20
55	8A	100	MET	CG-SD-CE	-21.54	65.73	100.20

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	71	ARG	Sidechain
2	1B	93	THR	Peptide
3	1C	106	ARG	Sidechain
5	1E	191	PHE	Sidechain
6	1F	206	LYS	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%)	11 (10%)	2 (2%)	8	40
1	5A	113/115 (98%)	106 (94%)	5 (4%)	2 (2%)	8	40
2	1B	153/258 (59%)	140 (92%)	13 (8%)	0	100	100
2	5B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	187 (90%)	20 (10%)	0	100	100
3	5C	207/264 (78%)	197 (95%)	10 (5%)	0	100	100
4	1D	427/476 (90%)	398 (93%)	29 (7%)	0	100	100
4	5D	427/476 (90%)	400 (94%)	27 (6%)	0	100	100
5	1E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	29	69
5	5E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	29	69
6	1F	430/464 (93%)	401 (93%)	26 (6%)	3 (1%)	22	63
6	5F	430/464 (93%)	404 (94%)	23 (5%)	3 (1%)	22	63
7	1G	697/727 (96%)	657 (94%)	38 (6%)	2 (0%)	41	76
7	5G	697/727 (96%)	661 (95%)	34 (5%)	2 (0%)	41	76
8	1H	316/318 (99%)	289 (92%)	25 (8%)	2 (1%)	25	66
8	5H	316/318 (99%)	290 (92%)	24 (8%)	2 (1%)	25	66
9	1I	174/239 (73%)	163 (94%)	11 (6%)	0	100	100
9	5I	174/239 (73%)	164 (94%)	10 (6%)	0	100	100
10	1J	172/175 (98%)	159 (92%)	12 (7%)	1 (1%)	25	66
10	5J	172/175 (98%)	155 (90%)	16 (9%)	1 (1%)	25	66
11	1K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
11	5K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	545 (90%)	57 (9%)	2 (0%)	41	76
12	5L	604/606 (100%)	559 (92%)	44 (7%)	1 (0%)	47	81
13	1M	457/459 (100%)	441 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5M	457/459 (100%)	436 (95%)	21 (5%)	0	100	100
14	1N	345/347 (99%)	322 (93%)	21 (6%)	2 (1%)	25	66
14	5N	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
15	1O	318/357 (89%)	301 (95%)	17 (5%)	0	100	100
15	5O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	321 (94%)	19 (6%)	0	100	100
16	5P	340/377 (90%)	317 (93%)	22 (6%)	1 (0%)	41	76
17	1Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
17	5Q	127/175 (73%)	116 (91%)	11 (9%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
18	5R	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
19	1S	85/99 (86%)	76 (89%)	9 (11%)	0	100	100
19	5S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	1T	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
20	1U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
20	5T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	5U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
21	5V	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
22	5W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	66
23	5X	169/172 (98%)	160 (95%)	8 (5%)	1 (1%)	25	66
24	1Y	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
24	5Y	137/141 (97%)	130 (95%)	7 (5%)	0	100	100
25	1Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
25	5Z	139/144 (96%)	131 (94%)	8 (6%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
26	5a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	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%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/122 (96%)	111 (95%)	6 (5%)	0	100	100
29	5d	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	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%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	84 (86%)	14 (14%)	0	100	100
32	5g	98/154 (64%)	86 (88%)	12 (12%)	0	100	100
33	1h	136/189 (72%)	127 (93%)	9 (7%)	0	100	100
33	5h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	1i	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	19	60
34	5i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	64 (93%)	5 (7%)	0	100	100
35	5j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	139 (90%)	15 (10%)	0	100	100
37	5l	154/186 (83%)	138 (90%)	16 (10%)	0	100	100
38	1m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
38	5m	126/129 (98%)	116 (92%)	10 (8%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	10 (6%)	0	100	100
39	5n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	25	66
40	1o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
40	5o	120/137 (88%)	110 (92%)	10 (8%)	0	100	100
41	1p	171/176 (97%)	169 (99%)	2 (1%)	0	100	100
41	5p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
42	5q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
43	1r	90/113 (80%)	83 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	5r	90/113 (80%)	84 (93%)	6 (7%)	0	100	100
44	1s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
44	5s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
45	3A	436/480 (91%)	424 (97%)	11 (2%)	1 (0%)	47	81
45	3N	444/480 (92%)	424 (96%)	18 (4%)	2 (0%)	29	69
45	6A	436/480 (91%)	426 (98%)	8 (2%)	2 (0%)	29	69
45	6N	444/480 (92%)	430 (97%)	12 (3%)	2 (0%)	29	69
46	3B	414/453 (91%)	396 (96%)	18 (4%)	0	100	100
46	3O	413/453 (91%)	404 (98%)	8 (2%)	1 (0%)	47	81
46	6B	414/453 (91%)	401 (97%)	13 (3%)	0	100	100
46	6O	413/453 (91%)	403 (98%)	9 (2%)	1 (0%)	47	81
47	3C	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
47	3P	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
47	6C	377/379 (100%)	355 (94%)	22 (6%)	0	100	100
47	6P	377/379 (100%)	364 (97%)	13 (3%)	0	100	100
48	3D	235/326 (72%)	227 (97%)	8 (3%)	0	100	100
48	3Q	237/326 (73%)	230 (97%)	7 (3%)	0	100	100
48	6D	235/326 (72%)	226 (96%)	9 (4%)	0	100	100
48	6Q	237/326 (73%)	225 (95%)	12 (5%)	0	100	100
49	3E	194/274 (71%)	170 (88%)	22 (11%)	2 (1%)	15	54
49	3I	45/274 (16%)	42 (93%)	3 (7%)	0	100	100
49	3R	194/274 (71%)	170 (88%)	20 (10%)	4 (2%)	7	36
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
49	6E	194/274 (71%)	175 (90%)	18 (9%)	1 (0%)	29	69
49	6I	45/274 (16%)	42 (93%)	3 (7%)	0	100	100
49	6R	194/274 (71%)	172 (89%)	18 (9%)	4 (2%)	7	36
49	6V	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
50	6F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	6S	96/111 (86%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	3G	72/82 (88%)	66 (92%)	6 (8%)	0	100	100
51	3T	72/82 (88%)	69 (96%)	3 (4%)	0	100	100
51	6G	72/82 (88%)	68 (94%)	4 (6%)	0	100	100
51	6T	72/82 (88%)	67 (93%)	5 (7%)	0	100	100
52	3H	63/91 (69%)	60 (95%)	3 (5%)	0	100	100
52	3U	63/91 (69%)	63 (100%)	0	0	100	100
52	6H	63/91 (69%)	60 (95%)	3 (5%)	0	100	100
52	6U	63/91 (69%)	61 (97%)	2 (3%)	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	8	38
53	3W	54/64 (84%)	52 (96%)	2 (4%)	0	100	100
53	6J	54/64 (84%)	53 (98%)	0	1 (2%)	8	38
53	6W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
54	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	3Y	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
54	6X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	6Y	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
55	4A	512/514 (100%)	480 (94%)	30 (6%)	2 (0%)	34	72
55	8A	512/514 (100%)	481 (94%)	29 (6%)	2 (0%)	34	72
56	4B	225/229 (98%)	209 (93%)	16 (7%)	0	100	100
56	8B	225/229 (98%)	207 (92%)	18 (8%)	0	100	100
57	4C	257/261 (98%)	241 (94%)	16 (6%)	0	100	100
57	8C	257/261 (98%)	240 (93%)	17 (7%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
58	8D	137/169 (81%)	122 (89%)	15 (11%)	0	100	100
59	4E	103/152 (68%)	100 (97%)	3 (3%)	0	100	100
59	8E	103/152 (68%)	97 (94%)	6 (6%)	0	100	100
60	4F	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14	52
60	8F	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14	52
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	67 (92%)	6 (8%)	0	100	100
62	4H	80/86 (93%)	73 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	8H	80/86 (93%)	71 (89%)	9 (11%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
63	8I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
65	8K	47/80 (59%)	43 (92%)	4 (8%)	0	100	100
66	4L	44/63 (70%)	39 (89%)	5 (11%)	0	100	100
66	8L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
67	4M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
67	8M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
68	4N	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
68	8N	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
All	All	28146/34018 (83%)	26515 (94%)	1569 (6%)	62 (0%)	50	81

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	39	CYS
8	1H	92	PRO
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	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%)	94 (95%)	5 (5%)	24	49
1	5A	99/99 (100%)	91 (92%)	8 (8%)	11	35
2	1B	131/212 (62%)	118 (90%)	13 (10%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5B	131/212 (62%)	123 (94%)	8 (6%)	18	44
3	1C	190/227 (84%)	184 (97%)	6 (3%)	39	61
3	5C	190/227 (84%)	182 (96%)	8 (4%)	30	54
4	1D	371/405 (92%)	354 (95%)	17 (5%)	27	52
4	5D	371/405 (92%)	355 (96%)	16 (4%)	29	53
5	1E	183/207 (88%)	169 (92%)	14 (8%)	13	37
5	5E	183/207 (88%)	172 (94%)	11 (6%)	19	44
6	1F	346/368 (94%)	334 (96%)	12 (4%)	36	59
6	5F	346/368 (94%)	332 (96%)	14 (4%)	31	55
7	1G	588/610 (96%)	553 (94%)	35 (6%)	19	44
7	5G	588/610 (96%)	553 (94%)	35 (6%)	19	44
8	1H	274/274 (100%)	260 (95%)	14 (5%)	24	49
8	5H	274/274 (100%)	259 (94%)	15 (6%)	21	47
9	1I	151/201 (75%)	136 (90%)	15 (10%)	8	26
9	5I	151/201 (75%)	142 (94%)	9 (6%)	19	44
10	1J	140/141 (99%)	133 (95%)	7 (5%)	24	49
10	5J	140/141 (99%)	127 (91%)	13 (9%)	9	29
11	1K	84/84 (100%)	78 (93%)	6 (7%)	14	39
11	5K	84/84 (100%)	76 (90%)	8 (10%)	8	28
12	1L	539/539 (100%)	515 (96%)	24 (4%)	27	52
12	5L	539/539 (100%)	518 (96%)	21 (4%)	32	56
13	1M	408/408 (100%)	395 (97%)	13 (3%)	39	61
13	5M	408/408 (100%)	380 (93%)	28 (7%)	15	40
14	1N	310/310 (100%)	288 (93%)	22 (7%)	14	39
14	5N	310/310 (100%)	288 (93%)	22 (7%)	14	39
15	1O	283/307 (92%)	272 (96%)	11 (4%)	32	56
15	5O	283/307 (92%)	265 (94%)	18 (6%)	17	42
16	1P	296/323 (92%)	285 (96%)	11 (4%)	34	58
16	5P	296/323 (92%)	283 (96%)	13 (4%)	28	53
17	1Q	117/152 (77%)	110 (94%)	7 (6%)	19	44
17	5Q	117/152 (77%)	108 (92%)	9 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1R	79/97 (81%)	72 (91%)	7 (9%)	9	30
18	5R	79/97 (81%)	75 (95%)	4 (5%)	24	49
19	1S	77/82 (94%)	70 (91%)	7 (9%)	9	30
19	5S	77/82 (94%)	73 (95%)	4 (5%)	23	48
20	1T	79/133 (59%)	71 (90%)	8 (10%)	7	25
20	1U	79/133 (59%)	75 (95%)	4 (5%)	24	49
20	5T	79/133 (59%)	68 (86%)	11 (14%)	3	17
20	5U	79/133 (59%)	77 (98%)	2 (2%)	47	68
21	1V	100/101 (99%)	97 (97%)	3 (3%)	41	63
21	5V	100/101 (99%)	97 (97%)	3 (3%)	41	63
22	1W	107/112 (96%)	98 (92%)	9 (8%)	11	34
22	5W	107/112 (96%)	95 (89%)	12 (11%)	6	22
23	1X	153/154 (99%)	141 (92%)	12 (8%)	12	36
23	5X	153/154 (99%)	144 (94%)	9 (6%)	19	45
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	12	36
24	5Y	101/102 (99%)	88 (87%)	13 (13%)	4	18
25	1Z	123/124 (99%)	111 (90%)	12 (10%)	8	27
25	5Z	123/124 (99%)	117 (95%)	6 (5%)	25	50
26	1a	58/58 (100%)	56 (97%)	2 (3%)	37	60
26	5a	58/58 (100%)	52 (90%)	6 (10%)	7	25
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	53
27	5b	69/70 (99%)	65 (94%)	4 (6%)	20	45
28	1c	45/66 (68%)	41 (91%)	4 (9%)	9	30
28	5c	45/66 (68%)	38 (84%)	7 (16%)	2	14
29	1d	106/109 (97%)	98 (92%)	8 (8%)	13	38
29	5d	106/109 (97%)	96 (91%)	10 (9%)	8	28
30	1e	87/94 (93%)	85 (98%)	2 (2%)	50	70
30	5e	87/94 (93%)	78 (90%)	9 (10%)	7	25
31	1f	54/113 (48%)	53 (98%)	1 (2%)	57	75
31	5f	54/113 (48%)	53 (98%)	1 (2%)	57	75
32	1g	92/129 (71%)	89 (97%)	3 (3%)	38	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	5g	92/129 (71%)	82 (89%)	10 (11%)	6	23
33	1h	121/158 (77%)	109 (90%)	12 (10%)	8	26
33	5h	121/158 (77%)	112 (93%)	9 (7%)	13	38
34	1i	119/120 (99%)	112 (94%)	7 (6%)	19	45
34	5i	119/120 (99%)	113 (95%)	6 (5%)	24	49
35	1j	62/84 (74%)	58 (94%)	4 (6%)	17	42
35	5j	62/84 (74%)	59 (95%)	3 (5%)	25	51
36	1k	63/76 (83%)	62 (98%)	1 (2%)	62	79
36	5k	63/76 (83%)	60 (95%)	3 (5%)	25	51
37	1l	141/161 (88%)	136 (96%)	5 (4%)	36	59
37	5l	141/161 (88%)	130 (92%)	11 (8%)	12	36
38	1m	113/114 (99%)	111 (98%)	2 (2%)	59	77
38	5m	113/114 (99%)	108 (96%)	5 (4%)	28	53
39	1n	156/160 (98%)	148 (95%)	8 (5%)	24	49
39	5n	156/160 (98%)	147 (94%)	9 (6%)	20	45
40	1o	110/119 (92%)	106 (96%)	4 (4%)	35	59
40	5o	110/119 (92%)	104 (94%)	6 (6%)	21	47
41	1p	154/156 (99%)	144 (94%)	10 (6%)	17	42
41	5p	154/156 (99%)	146 (95%)	8 (5%)	23	48
42	1q	131/131 (100%)	121 (92%)	10 (8%)	13	37
42	5q	131/131 (100%)	121 (92%)	10 (8%)	13	37
43	1r	85/98 (87%)	81 (95%)	4 (5%)	26	51
43	5r	85/98 (87%)	77 (91%)	8 (9%)	8	28
44	1s	44/351 (12%)	43 (98%)	1 (2%)	50	70
44	5s	44/351 (12%)	42 (96%)	2 (4%)	27	52
45	3A	367/397 (92%)	353 (96%)	14 (4%)	33	57
45	3N	372/397 (94%)	356 (96%)	16 (4%)	29	53
45	6A	367/397 (92%)	354 (96%)	13 (4%)	36	59
45	6N	372/397 (94%)	352 (95%)	20 (5%)	22	47
46	3B	328/355 (92%)	323 (98%)	5 (2%)	65	80
46	3O	327/355 (92%)	316 (97%)	11 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	6B	328/355 (92%)	311 (95%)	17 (5%)	23	48
46	6O	327/355 (92%)	312 (95%)	15 (5%)	27	52
47	3C	332/332 (100%)	316 (95%)	16 (5%)	25	51
47	3P	332/332 (100%)	324 (98%)	8 (2%)	49	69
47	6C	332/332 (100%)	313 (94%)	19 (6%)	20	45
47	6P	332/332 (100%)	313 (94%)	19 (6%)	20	45
48	3D	202/259 (78%)	194 (96%)	8 (4%)	31	55
48	3Q	204/259 (79%)	197 (97%)	7 (3%)	37	60
48	6D	202/259 (78%)	194 (96%)	8 (4%)	31	55
48	6Q	204/259 (79%)	193 (95%)	11 (5%)	22	47
49	3E	166/225 (74%)	160 (96%)	6 (4%)	35	59
49	3I	36/225 (16%)	35 (97%)	1 (3%)	43	65
49	3R	166/225 (74%)	158 (95%)	8 (5%)	25	51
49	3V	24/225 (11%)	23 (96%)	1 (4%)	30	54
49	6E	166/225 (74%)	158 (95%)	8 (5%)	25	51
49	6I	36/225 (16%)	34 (94%)	2 (6%)	21	46
49	6R	166/225 (74%)	157 (95%)	9 (5%)	22	47
49	6V	24/225 (11%)	24 (100%)	0	100	100
50	3F	90/99 (91%)	86 (96%)	4 (4%)	28	53
50	3S	90/99 (91%)	86 (96%)	4 (4%)	28	53
50	6F	90/99 (91%)	83 (92%)	7 (8%)	12	36
50	6S	90/99 (91%)	83 (92%)	7 (8%)	12	36
51	3G	67/73 (92%)	65 (97%)	2 (3%)	41	63
51	3T	67/73 (92%)	67 (100%)	0	100	100
51	6G	67/73 (92%)	63 (94%)	4 (6%)	19	44
51	6T	67/73 (92%)	63 (94%)	4 (6%)	19	44
52	3H	62/85 (73%)	59 (95%)	3 (5%)	25	51
52	3U	62/85 (73%)	59 (95%)	3 (5%)	25	51
52	6H	62/85 (73%)	60 (97%)	2 (3%)	39	61
52	6U	62/85 (73%)	58 (94%)	4 (6%)	17	42
53	3J	45/51 (88%)	44 (98%)	1 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3W	45/51 (88%)	44 (98%)	1 (2%)	52	71
53	6J	45/51 (88%)	40 (89%)	5 (11%)	6	22
53	6W	45/51 (88%)	41 (91%)	4 (9%)	9	30
54	3X	42/46 (91%)	40 (95%)	2 (5%)	25	51
54	3Y	41/46 (89%)	37 (90%)	4 (10%)	8	27
54	6X	42/46 (91%)	40 (95%)	2 (5%)	25	51
54	6Y	41/46 (89%)	39 (95%)	2 (5%)	25	50
55	4A	424/424 (100%)	386 (91%)	38 (9%)	9	30
55	8A	424/424 (100%)	384 (91%)	40 (9%)	8	28
56	4B	210/211 (100%)	200 (95%)	10 (5%)	25	51
56	8B	210/211 (100%)	193 (92%)	17 (8%)	11	35
57	4C	223/225 (99%)	205 (92%)	18 (8%)	11	35
57	8C	223/225 (99%)	200 (90%)	23 (10%)	7	25
58	4D	124/149 (83%)	113 (91%)	11 (9%)	9	30
58	8D	124/149 (83%)	110 (89%)	14 (11%)	6	21
59	4E	92/124 (74%)	86 (94%)	6 (6%)	17	42
59	8E	92/124 (74%)	82 (89%)	10 (11%)	6	23
60	4F	80/101 (79%)	72 (90%)	8 (10%)	7	26
60	8F	80/101 (79%)	72 (90%)	8 (10%)	7	26
61	4G	65/80 (81%)	62 (95%)	3 (5%)	27	52
61	8G	65/80 (81%)	62 (95%)	3 (5%)	27	52
62	4H	73/76 (96%)	69 (94%)	4 (6%)	21	47
62	8H	73/76 (96%)	67 (92%)	6 (8%)	11	34
63	4I	54/61 (88%)	45 (83%)	9 (17%)	2	12
63	8I	54/61 (88%)	49 (91%)	5 (9%)	9	29
64	4J	49/68 (72%)	45 (92%)	4 (8%)	11	34
64	8J	49/68 (72%)	43 (88%)	6 (12%)	5	20
65	4K	38/66 (58%)	36 (95%)	2 (5%)	22	47
65	8K	38/66 (58%)	35 (92%)	3 (8%)	12	36
66	4L	39/55 (71%)	35 (90%)	4 (10%)	7	25
66	8L	39/55 (71%)	33 (85%)	6 (15%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	4M	37/57 (65%)	35 (95%)	2 (5%)	22	47
67	8M	37/57 (65%)	33 (89%)	4 (11%)	6	23
68	4N	70/70 (100%)	59 (84%)	11 (16%)	2	14
68	8N	70/70 (100%)	65 (93%)	5 (7%)	14	39
All	All	24526/28666 (86%)	23099 (94%)	1427 (6%)	24	45

5 of 1427 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	5V	82	GLN
48	6D	179	PHE
24	5Y	33	LEU
21	5V	49	GLN
37	5l	62	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

Mol	Chain	Res	Type
10	5J	86	ASN
39	5n	13	GLN
12	5L	135	ASN
16	5P	180	ASN
43	5r	46	HIS

### 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
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
1	FME	1A	1	1	8,9,10	0.52	0	7,9,11	1.09	1 (14%)
13	FME	5M	1	13	8,9,10	0.52	0	7,9,11	1.04	1 (14%)
34	SAC	5i	1	34	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	1.21	1 (14%)
12	FME	5L	1	12	8,9,10	0.51	0	7,9,11	0.95	1 (14%)
14	FME	5N	1	14	8,9,10	0.52	0	7,9,11	0.99	1 (14%)
34	SAC	1i	1	34	7,8,9	0.54	0	8,9,11	0.89	1 (12%)
8	FME	5H	1	8	8,9,10	0.52	0	7,9,11	1.08	1 (14%)
1	FME	5A	1	1	8,9,10	0.53	0	7,9,11	2.61	3 (42%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	0.88	1 (14%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
11	FME	5K	1	11	8,9,10	0.47	0	7,9,11	1.25	1 (14%)
56	FME	8B	1	56	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
55	FME	8A	1	55	8,9,10	0.52	0	7,9,11	1.38	2 (28%)
56	FME	4B	1	56	8,9,10	0.53	0	7,9,11	0.84	1 (14%)
55	FME	4A	1	55	6,7,10	0.55	0	5,5,11	0.64	0
14	FME	1N	1	14	8,9,10	0.51	0	7,9,11	1.05	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
13	FME	1M	1	13	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
13	FME	5M	1	13	-	0/7/9/11	-
34	SAC	5i	1	34	-	0/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
14	FME	5N	1	14	-	2/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
8	FME	5H	1	8	-	1/7/9/11	-
1	FME	5A	1	1	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
11	FME	5K	1	11	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	8B	1	56	-	1/7/9/11	-
55	FME	8A	1	55	-	3/7/9/11	-
56	FME	4B	1	56	-	1/7/9/11	-
55	FME	4A	1	55	-	2/3/4/11	-
14	FME	1N	1	14	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5A	1	FME	CA-N-CN	4.68	130.02	122.82
1	5A	1	FME	O-C-CA	-3.64	115.24	124.78
1	5A	1	FME	C-CA-N	3.37	115.81	109.73
11	5K	1	FME	O-C-CA	-3.17	116.47	124.78
11	1K	1	FME	O-C-CA	-2.74	117.59	124.78

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	CB-CA-N-CN
8	1H	1	FME	O1-CN-N-CA
11	1K	1	FME	CB-CA-N-CN
13	1M	1	FME	O-C-CA-CB
14	1N	1	FME	O1-CN-N-CA

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 [i](#)

Of 190 ligands modelled in this entry, 14 are monoatomic - leaving 176 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
75	CDL	1a	201	-	60,60,99	0.34	0	66,72,111	0.43	0
86	PGV	4A	602	-	50,50,50	0.33	0	53,56,56	1.00	2 (3%)
70	PC1	5q	201	-	48,48,53	0.27	0	54,56,61	0.33	0
75	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.43	1 (0%)
75	CDL	8A	605	-	99,99,99	0.26	0	105,111,111	0.30	0
69	3PE	1d	202	-	48,48,50	0.26	0	51,53,55	0.35	0
75	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.38	0
82	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.39	0
86	PGV	4C	303	-	50,50,50	0.28	0	53,56,56	0.31	0
69	3PE	1A	201	-	46,46,50	0.27	0	49,51,55	0.35	0
75	CDL	1N	401	-	61,61,99	0.31	0	67,73,111	0.65	1 (1%)
75	CDL	5d	201	-	85,85,99	0.31	0	91,97,111	0.54	1 (1%)
69	3PE	5M	906	-	49,49,50	0.26	0	52,54,55	0.31	0
69	3PE	5Y	203	-	39,39,50	0.31	0	42,44,55	0.49	0
75	CDL	5N	401	-	61,61,99	0.31	0	67,73,111	0.61	1 (1%)
80	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.08	1 (2%)
84	HEM	3P	502	47	41,50,50	1.35	6 (14%)	45,82,82	1.74	7 (15%)
92	PEK	8G	102	-	52,52,52	0.27	0	55,57,57	0.41	0
70	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.34	0
69	3PE	1j	101	-	43,43,50	0.28	0	46,48,55	0.42	0
69	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.33	0
69	3PE	5M	903	-	47,47,50	0.27	0	50,52,55	0.35	0
72	FES	6E	301	49	0,4,4	-	-	-	-	-
70	PC1	5M	905	-	43,43,53	0.30	0	49,51,61	0.37	0
70	PC1	5H	403	-	47,47,53	0.29	0	53,55,61	0.37	0
72	FES	3R	301	49	0,4,4	-	-	-	-	-
86	PGV	5i	201	34	50,50,50	0.28	0	53,56,56	0.36	0
69	3PE	5P	403	-	34,34,50	0.32	0	37,39,55	0.43	0
70	PC1	5H	402	-	53,53,53	0.26	0	59,61,61	0.35	0
70	PC1	5B	203	-	47,47,53	0.28	0	53,55,61	0.41	0
70	PC1	5h	202	-	46,46,53	0.28	0	52,54,61	0.30	0
73	FMN	5F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
72	FES	1G	803	7	0,4,4	-	-	-	-	-
72	FES	1E	301	5	0,4,4	-	-	-	-	-
84	HEM	6C	502	-	41,50,50	1.34	7 (17%)	45,82,82	1.72	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
72	FES	5E	301	5	0,4,4	-	-	-		
84	HEM	6C	501	47	41,50,50	1.34	6 (14%)	45,82,82	1.87	8 (17%)
71	SF4	5B	201	2	0,12,12	-	-	-		
70	PC1	5B	202	-	45,45,53	0.28	0	51,53,61	0.37	0
75	CDL	4D	201	-	99,99,99	0.26	0	105,111,111	0.41	0
70	PC1	1M	504	-	43,43,53	0.36	0	49,51,61	0.42	0
70	PC1	1B	203	-	47,47,53	0.28	0	53,55,61	0.39	0
86	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.74	1 (1%)
75	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.46	0
71	SF4	1I	203	9	0,12,12	-	-	-		
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.31	0
69	3PE	1Y	203	-	32,32,50	0.32	0	35,37,55	0.50	0
75	CDL	5a	201	-	60,60,99	0.33	0	66,72,111	0.42	0
75	CDL	5d	204	-	64,64,99	0.32	0	70,76,111	0.47	0
69	3PE	1Y	204	-	26,26,50	0.35	0	29,31,55	0.54	0
92	PEK	4C	308	-	52,52,52	0.26	0	55,57,57	0.38	0
76	GTP	5O	401	77	26,34,34	0.95	2 (7%)	32,54,54	0.82	1 (3%)
86	PGV	8A	604	-	50,50,50	0.28	0	53,56,56	0.41	0
69	3PE	1d	201	-	47,47,50	0.27	0	50,52,55	0.33	0
86	PGV	4C	305	-	50,50,50	0.29	0	53,56,56	0.47	1 (1%)
69	3PE	5Y	204	-	29,29,50	0.34	0	32,34,55	0.75	1 (3%)
86	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
73	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.70	1 (2%)
70	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.38	0
85	HEC	3D	501	48	31,49,50	2.45	12 (38%)	22,80,82	2.24	4 (18%)
87	HEA	8A	606	55	57,67,67	2.23	20 (35%)	61,103,103	2.35	26 (42%)
69	3PE	5d	202	-	48,48,50	0.26	0	51,53,55	0.35	0
86	PGV	8C	306	-	50,50,50	0.29	0	53,56,56	0.35	0
71	SF4	1I	202	9	0,12,12	-	-	-		
71	SF4	5I	202	9	0,12,12	-	-	-		
69	3PE	1K	101	-	43,43,50	0.28	0	46,48,55	0.33	0
69	3PE	5M	904	-	50,50,50	0.27	0	53,55,55	0.48	0
71	SF4	1G	802	7	0,12,12	-	-	-		
86	PGV	8B	301	56	50,50,50	0.27	0	53,56,56	0.41	0
86	PGV	8D	202	-	50,50,50	0.30	0	53,56,56	0.40	0
69	3PE	1m	201	-	40,40,50	0.28	0	43,45,55	0.38	0
93	PO4	8H	101	-	4,4,4	0.92	0	6,6,6	0.43	0
75	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.58	0
86	PGV	8C	302	-	50,50,50	0.28	0	53,56,56	0.30	0
90	CUA	4B	303	56	0,1,1	-	-	-		
86	PGV	8A	601	-	50,50,50	0.28	0	53,56,56	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.34	0
86	PGV	8C	301	-	50,50,50	0.29	0	53,56,56	0.65	1 (1%)
69	3PE	5L	701	-	45,45,50	0.28	0	48,50,55	0.32	0
87	HEA	8A	607	55	57,67,67	2.02	16 (28%)	61,103,103	2.55	26 (42%)
78	NDP	5P	402	-	45,52,52	0.61	0	53,80,80	0.76	2 (3%)
75	CDL	5L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
70	PC1	5Y	201	-	34,34,53	0.32	0	40,42,61	0.54	1 (2%)
70	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.41	0
84	HEM	6P	502	47	41,50,50	1.35	7 (17%)	45,82,82	1.76	7 (15%)
69	3PE	1M	505	-	49,49,50	0.27	0	52,54,55	0.32	0
85	HEC	3Q	501	-	32,50,50	2.44	12 (37%)	24,82,82	2.27	4 (16%)
69	3PE	1M	501	-	44,44,50	0.28	0	47,49,55	0.37	0
70	PC1	1d	203	-	38,38,53	0.30	0	44,46,61	0.46	0
71	SF4	5F	502	6	0,12,12	-	-	-	-	-
84	HEM	6P	501	47	41,50,50	1.36	6 (14%)	45,82,82	1.83	8 (17%)
69	3PE	1M	503	-	50,50,50	0.28	0	53,55,55	0.43	0
75	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.39	0
69	3PE	1P	403	-	34,34,50	0.32	0	37,39,55	0.43	0
70	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.36	0
86	PGV	4G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
86	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.33	0
91	PSC	4B	304	-	51,51,51	0.29	0	57,59,59	0.45	1 (1%)
71	SF4	1G	801	7	0,12,12	-	-	-	-	-
69	3PE	1L	704	-	48,48,50	0.27	0	51,53,55	0.37	0
69	3PE	5L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
70	PC1	5d	203	-	38,38,53	0.30	0	44,46,61	0.46	0
69	3PE	1Y	202	-	29,29,50	0.34	0	32,34,55	0.82	1 (3%)
71	SF4	5G	801	7	0,12,12	-	-	-	-	-
71	SF4	5I	201	9	0,12,12	-	-	-	-	-
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
80	EHZ	1T	101	20	29,36,37	0.17	0	35,44,47	1.04	1 (2%)
91	PSC	8A	611	-	51,51,51	0.31	0	57,59,59	0.54	1 (1%)
90	CUA	8B	302	56	0,1,1	-	-	-	-	-
86	PGV	4L	101	-	50,50,50	0.28	0	53,56,56	0.42	0
69	3PE	5m	201	-	40,40,50	0.28	0	43,45,55	0.38	0
84	HEM	3C	502	-	41,50,50	1.35	6 (14%)	45,82,82	1.77	8 (17%)
80	EHZ	5n	201	-	29,36,37	0.14	0	35,44,47	1.02	1 (2%)
81	AME	5N	402	-	9,10,11	0.49	0	9,11,13	1.01	1 (11%)
69	3PE	5A	201	-	46,46,50	0.27	0	49,51,55	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
80	EHZ	5T	101	20	29,36,37	0.17	0	35,44,47	1.24	1 (2%)
81	AME	1h	201	-	9,10,11	0.49	0	9,11,13	0.95	1 (11%)
69	3PE	1Y	201	-	39,39,50	0.31	0	42,44,55	0.49	0
83	AYA	5q	202	-	6,7,8	0.65	0	5,8,10	0.40	0
70	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.45	0
70	PC1	1q	201	-	48,48,53	0.27	0	54,56,61	0.39	0
70	PC1	1M	502	-	34,34,53	0.33	0	40,42,61	0.63	1 (2%)
75	CDL	5h	201	-	79,79,99	0.30	0	85,91,111	0.40	0
70	PC1	1I	201	-	53,53,53	0.32	0	59,61,61	0.81	3 (5%)
82	MYR	5l	201	-	14,14,15	0.34	0	13,13,15	0.38	0
86	PGV	8J	101	-	50,50,50	0.27	0	53,56,56	0.41	0
69	3PE	5Y	205	-	32,32,50	0.33	0	35,37,55	0.56	0
69	3PE	5j	101	-	43,43,50	0.29	0	46,48,55	0.49	1 (2%)
75	CDL	8C	305	-	99,99,99	0.39	1 (1%)	105,111,111	0.56	0
86	PGV	8G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
69	3PE	5K	101	-	43,43,50	0.29	0	46,48,55	0.35	0
71	SF4	1B	201	2	0,12,12	-	-	-	-	-
84	HEM	3C	501	47	41,50,50	1.33	7 (17%)	45,82,82	1.83	9 (20%)
75	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.30	0
69	3PE	1L	705	-	30,30,50	0.33	0	33,35,55	0.55	0
86	PGV	4A	601	-	50,50,50	0.29	0	53,56,56	0.42	0
78	NDP	1P	402	-	45,52,52	0.60	0	53,80,80	0.79	2 (3%)
86	PGV	4C	301	-	50,50,50	0.29	0	53,56,56	0.32	0
76	GTP	1O	401	77	26,34,34	0.95	2 (7%)	32,54,54	0.80	0
75	CDL	1d	204	-	64,64,99	0.31	0	70,76,111	0.43	0
86	PGV	8L	101	-	50,50,50	0.28	0	53,56,56	0.37	0
85	HEC	6Q	501	48	32,50,50	2.50	12 (37%)	24,82,82	2.29	4 (16%)
84	HEM	3P	501	47	41,50,50	1.34	5 (12%)	45,82,82	1.91	11 (24%)
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
71	SF4	5G	802	7	0,12,12	-	-	-	-	-
69	3PE	5Y	206	-	26,26,50	0.34	0	29,31,55	0.53	0
69	3PE	5Y	202	-	30,30,50	0.33	0	33,35,55	0.50	0
70	PC1	1L	706	-	45,45,53	0.29	0	51,53,61	0.31	0
70	PC1	5I	203	-	43,43,53	0.29	0	49,51,61	0.32	0
72	FES	6R	301	49	0,4,4	-	-	-	-	-
87	HEA	4A	604	55	57,67,67	2.24	21 (36%)	61,103,103	2.38	24 (39%)
92	PEK	8C	307	-	51,51,52	0.29	0	54,56,57	0.68	2 (3%)
92	PEK	4C	309	-	51,51,52	0.27	0	54,56,57	0.43	0
70	PC1	1H	402	-	47,47,53	0.42	0	53,55,61	1.17	5 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	PC1	5A	203	-	34,34,53	0.32	0	40,42,61	0.38	0
86	PGV	4C	304	-	50,50,50	0.29	0	53,56,56	0.52	0
86	PGV	8C	304	-	50,50,50	0.30	0	53,56,56	0.45	0
72	FES	3E	301	49	0,4,4	-	-	-	-	-
72	FES	5G	803	7	0,4,4	-	-	-	-	-
86	PGV	8A	603	-	50,50,50	0.28	0	53,56,56	0.35	0
69	3PE	5M	901	-	48,48,50	0.27	0	51,53,55	0.38	0
86	PGV	4C	307	-	50,50,50	0.28	0	53,56,56	0.35	0
87	HEA	4A	605	55	57,67,67	2.06	18 (31%)	61,103,103	2.50	26 (42%)
70	PC1	5Y	207	-	45,45,53	0.28	0	51,53,61	0.31	0
70	PC1	1B	202	-	45,45,53	0.27	0	51,53,61	0.36	0
86	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.43	0
83	AYA	1q	202	-	6,7,8	0.64	0	5,8,10	0.41	0
86	PGV	4A	603	-	50,50,50	0.29	0	53,56,56	0.37	0
86	PGV	4B	301	56	50,50,50	0.29	0	53,56,56	0.44	1 (1%)
86	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.40	0
75	CDL	5H	401	-	50,50,99	0.36	0	56,62,111	0.58	0
69	3PE	5M	902	-	44,44,50	0.29	0	47,49,55	0.37	0
93	PO4	4H	101	-	4,4,4	0.93	0	6,6,6	0.42	0
70	PC1	1P	401	-	32,32,53	0.34	0	38,40,61	0.37	0
71	SF4	1F	502	6	0,12,12	-	-	-	-	-
85	HEC	6D	501	48	31,49,50	2.49	12 (38%)	22,80,82	2.34	5 (22%)

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
75	CDL	1a	201	-	-	10/71/71/110	-
86	PGV	4A	602	-	-	9/55/55/55	-
71	SF4	1F	502	6	-	-	0/6/5/5
70	PC1	5q	201	-	-	4/52/52/57	-
75	CDL	4C	306	-	-	25/110/110/110	-
75	CDL	8A	605	-	-	15/110/110/110	-
69	3PE	1d	202	-	-	11/52/52/54	-
75	CDL	1X	201	-	-	20/96/96/110	-
82	MYR	1l	201	-	-	1/11/12/13	-
86	PGV	4C	303	-	-	10/55/55/55	-
69	3PE	1A	201	-	-	8/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	1N	401	-	-	17/71/71/110	-
75	CDL	5d	201	-	-	22/96/96/110	-
69	3PE	5M	906	-	-	7/53/53/54	-
69	3PE	5Y	203	-	-	12/43/43/54	-
75	CDL	5N	401	-	-	18/71/71/110	-
80	EHZ	1n	201	-	-	5/42/44/45	-
84	HEM	3P	502	47	-	6/12/54/54	-
92	PEK	8G	102	-	-	5/56/56/56	-
70	PC1	1I	204	-	-	5/47/47/57	-
69	3PE	1j	101	-	-	5/47/47/54	-
69	3PE	1L	701	-	-	5/49/49/54	-
69	3PE	5M	903	-	-	18/51/51/54	-
72	FES	6E	301	49	-	-	0/1/1/1
70	PC1	5M	905	-	-	13/47/47/57	-
70	PC1	5H	403	-	-	8/51/51/57	-
86	PGV	5i	201	34	-	4/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
69	3PE	5P	403	-	-	8/38/38/54	-
70	PC1	5H	402	-	-	9/57/57/57	-
70	PC1	5B	203	-	-	11/51/51/57	-
70	PC1	5h	202	-	-	14/50/50/57	-
73	FMN	5F	501	-	-	7/18/18/18	0/3/3/3
72	FES	1G	803	7	-	-	0/1/1/1
72	FES	1E	301	5	-	-	0/1/1/1
84	HEM	6C	502	-	-	4/12/54/54	-
84	HEM	6C	501	47	-	5/12/54/54	-
72	FES	5E	301	5	-	-	0/1/1/1
71	SF4	5B	201	2	-	-	0/6/5/5
70	PC1	5B	202	-	-	4/49/49/57	-
75	CDL	4D	201	-	-	24/110/110/110	-
70	PC1	1M	504	-	-	17/47/47/57	-
70	PC1	1B	203	-	-	10/51/51/57	-
86	PGV	4C	302	-	-	13/55/55/55	-
75	CDL	1h	202	-	-	23/90/90/110	-
71	SF4	1I	203	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1h	203	-	-	13/50/50/57	-
69	3PE	1Y	203	-	-	6/36/36/54	-
75	CDL	5a	201	-	-	9/71/71/110	-
75	CDL	5d	204	-	-	21/75/75/110	-
69	3PE	1Y	204	-	-	7/30/30/54	-
92	PEK	4C	308	-	-	8/56/56/56	-
76	GTP	5O	401	77	-	4/18/38/38	0/3/3/3
86	PGV	8A	604	-	-	3/55/55/55	-
69	3PE	1d	201	-	-	16/51/51/54	-
86	PGV	4C	305	-	-	7/55/55/55	-
69	3PE	5Y	204	-	-	12/33/33/54	-
86	PGV	8K	101	-	-	13/55/55/55	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
70	PC1	5P	401	-	-	4/36/36/57	-
85	HEC	3D	501	48	-	3/8/53/54	-
87	HEA	8A	606	55	-	12/32/76/76	-
69	3PE	5d	202	-	-	8/52/52/54	-
86	PGV	8C	306	-	-	3/55/55/55	-
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	1K	101	-	-	11/47/47/54	-
71	SF4	5I	202	9	-	-	0/6/5/5
69	3PE	5M	904	-	-	12/54/54/54	-
86	PGV	8B	301	56	-	6/55/55/55	-
71	SF4	1G	802	7	-	-	0/6/5/5
86	PGV	8D	202	-	-	15/55/55/55	-
69	3PE	1m	201	-	-	12/44/44/54	-
75	CDL	1H	401	-	-	10/61/61/110	-
86	PGV	8C	302	-	-	10/55/55/55	-
86	PGV	8A	601	-	-	18/55/55/55	-
86	PGV	8A	602	-	-	6/55/55/55	-
86	PGV	8C	301	-	-	12/55/55/55	-
69	3PE	5L	701	-	-	7/49/49/54	-
87	HEA	8A	607	55	-	4/32/76/76	-
78	NDP	5P	402	-	-	5/30/77/77	0/5/5/5
75	CDL	5L	702	-	-	19/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	5Y	201	-	-	10/38/38/57	-
70	PC1	1A	202	-	-	5/38/38/57	-
84	HEM	6P	502	47	-	6/12/54/54	-
69	3PE	1M	505	-	-	9/53/53/54	-
85	HEC	3Q	501	-	-	2/10/54/54	-
69	3PE	1M	501	-	-	9/48/48/54	-
70	PC1	1d	203	-	-	10/42/42/57	-
71	SF4	5F	502	6	-	-	0/6/5/5
84	HEM	6P	501	47	-	6/12/54/54	-
69	3PE	1M	503	-	-	10/54/54/54	-
75	CDL	8D	201	-	-	21/110/110/110	-
69	3PE	1P	403	-	-	7/38/38/54	-
70	PC1	1J	201	-	-	4/38/38/57	-
86	PGV	4G	101	-	-	10/55/55/55	-
86	PGV	4K	101	-	-	11/55/55/55	-
91	PSC	4B	304	-	-	18/55/55/55	-
71	SF4	1G	801	7	-	-	0/6/5/5
69	3PE	1L	704	-	-	12/52/52/54	-
69	3PE	5L	703	-	-	6/48/48/54	-
70	PC1	5d	203	-	-	8/42/42/57	-
69	3PE	1Y	202	-	-	13/33/33/54	-
71	SF4	5G	801	7	-	-	0/6/5/5
75	CDL	1L	702	-	-	24/86/86/110	-
80	EHZ	1T	101	20	-	10/42/44/45	-
91	PSC	8A	611	-	-	23/55/55/55	-
71	SF4	5I	201	9	-	-	0/6/5/5
86	PGV	4L	101	-	-	14/55/55/55	-
69	3PE	5m	201	-	-	14/44/44/54	-
84	HEM	3C	502	-	-	4/12/54/54	-
80	EHZ	5n	201	-	-	4/42/44/45	-
81	AME	5N	402	-	-	0/9/10/12	-
69	3PE	5A	201	-	-	8/50/50/54	-
80	EHZ	5T	101	20	-	9/42/44/45	-
81	AME	1h	201	-	-	1/9/10/12	-
69	3PE	1Y	201	-	-	12/43/43/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	AYA	5q	202	-	-	0/4/6/8	-
70	PC1	5A	202	-	-	12/38/38/57	-
70	PC1	1q	201	-	-	4/52/52/57	-
70	PC1	1M	502	-	-	10/38/38/57	-
75	CDL	5h	201	-	-	22/90/90/110	-
70	PC1	1I	201	-	-	9/57/57/57	-
82	MYR	5l	201	-	-	0/11/12/13	-
86	PGV	8J	101	-	-	7/55/55/55	-
69	3PE	5Y	205	-	-	5/36/36/54	-
69	3PE	5j	101	-	-	8/47/47/54	-
75	CDL	8C	305	-	-	23/110/110/110	-
86	PGV	8G	101	-	-	9/55/55/55	-
69	3PE	5K	101	-	-	10/47/47/54	-
84	HEM	3C	501	47	-	5/12/54/54	-
71	SF4	1B	201	2	-	-	0/6/5/5
75	CDL	4B	302	-	-	20/110/110/110	-
69	3PE	1L	705	-	-	10/34/34/54	-
86	PGV	4A	601	-	-	17/55/55/55	-
78	NDP	1P	402	-	-	6/30/77/77	0/5/5/5
86	PGV	4C	301	-	-	6/55/55/55	-
76	GTP	1O	401	77	-	5/18/38/38	0/3/3/3
75	CDL	1d	204	-	-	16/75/75/110	-
86	PGV	8L	101	-	-	7/55/55/55	-
85	HEC	6Q	501	48	-	2/10/54/54	-
84	HEM	3P	501	47	-	7/12/54/54	-
69	3PE	1L	703	-	-	8/48/48/54	-
69	3PE	5Y	206	-	-	7/30/30/54	-
69	3PE	5Y	202	-	-	12/34/34/54	-
70	PC1	1L	706	-	-	9/49/49/57	-
70	PC1	5I	203	-	-	6/47/47/57	-
71	SF4	5G	802	7	-	-	0/6/5/5
72	FES	6R	301	49	-	-	0/1/1/1
87	HEA	4A	604	55	-	10/32/76/76	-
92	PEK	8C	307	-	-	5/55/55/56	-
92	PEK	4C	309	-	-	3/55/55/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1H	402	-	-	6/51/51/57	-
70	PC1	5A	203	-	-	4/38/38/57	-
86	PGV	8C	304	-	-	6/55/55/55	-
72	FES	3E	301	49	-	-	0/1/1/1
72	FES	5G	803	7	-	-	0/1/1/1
86	PGV	8A	603	-	-	8/55/55/55	-
69	3PE	5M	901	-	-	13/52/52/54	-
86	PGV	4C	307	-	-	7/55/55/55	-
87	HEA	4A	605	55	-	5/32/76/76	-
70	PC1	5Y	207	-	-	8/49/49/57	-
70	PC1	1B	202	-	-	3/49/49/57	-
86	PGV	8C	303	-	-	10/55/55/55	-
83	AYA	1q	202	-	-	0/4/6/8	-
86	PGV	4A	603	-	-	8/55/55/55	-
86	PGV	4B	301	56	-	7/55/55/55	-
86	PGV	4J	101	-	-	9/55/55/55	-
75	CDL	5H	401	-	-	8/61/61/110	-
69	3PE	5M	902	-	-	11/48/48/54	-
70	PC1	1P	401	-	-	3/36/36/57	-
86	PGV	4C	304	-	-	14/55/55/55	-
85	HEC	6D	501	48	-	4/8/53/54	-

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	6Q	501	HEC	C2B-C3B	7.45	1.48	1.40
85	6Q	501	HEC	C3C-C2C	7.23	1.48	1.40
85	3Q	501	HEC	C2B-C3B	7.12	1.48	1.40
85	6D	501	HEC	C2B-C3B	7.08	1.48	1.40
85	3Q	501	HEC	C3C-C2C	7.03	1.48	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	607	HEA	C3D-C4D-ND	6.91	117.05	110.36
87	4A	604	HEA	C4D-CHA-C1A	-6.65	113.78	122.56
80	5T	101	EHZ	C10-S1-C9	6.61	122.46	101.87
86	4A	602	PGV	O01-C1-C2	6.33	125.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	6D	501	HEC	CMC-C2C-C3C	6.24	133.16	125.82

There are no chirality outliers.

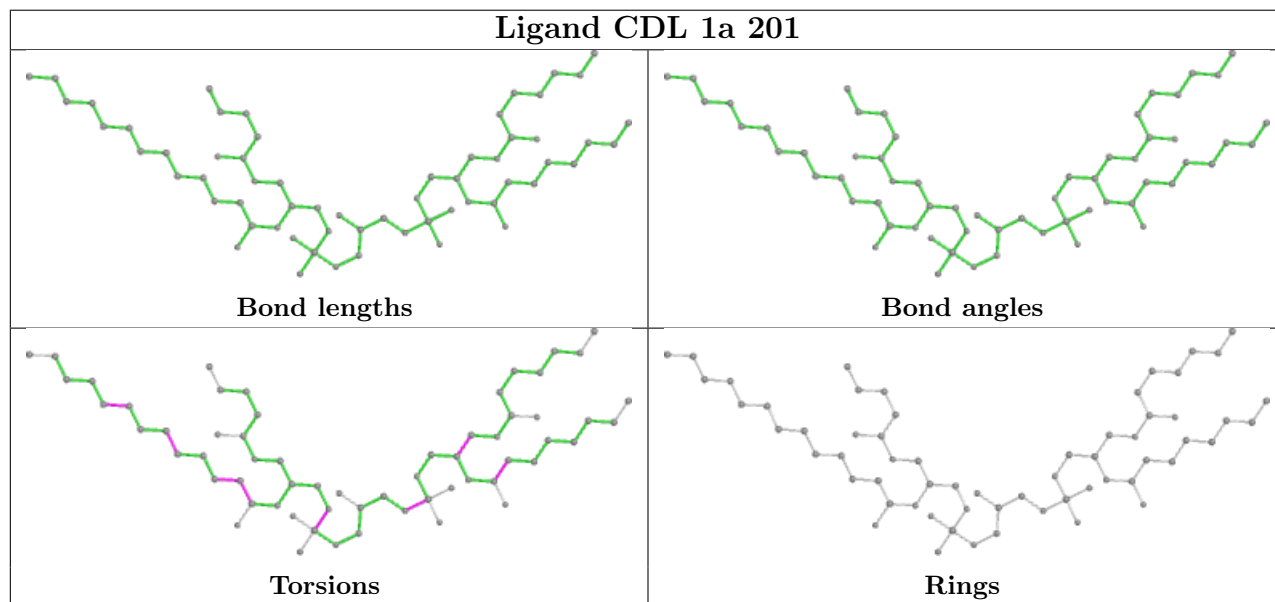
5 of 1424 torsion outliers are listed below:

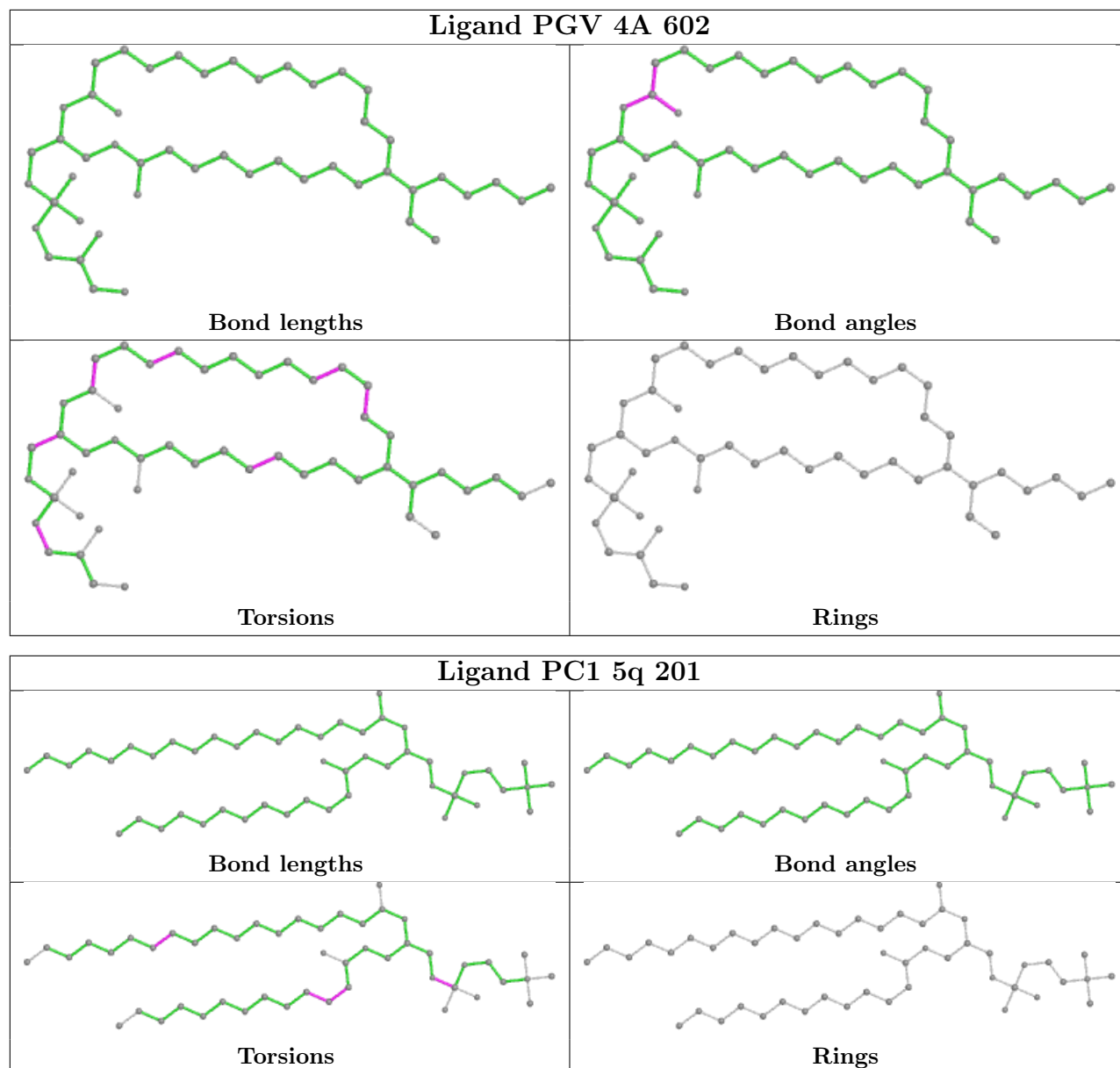
Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O12
69	1K	101	3PE	C1-O11-P-O14
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3
69	1L	704	3PE	C1-O11-P-O12

There are no ring outliers.

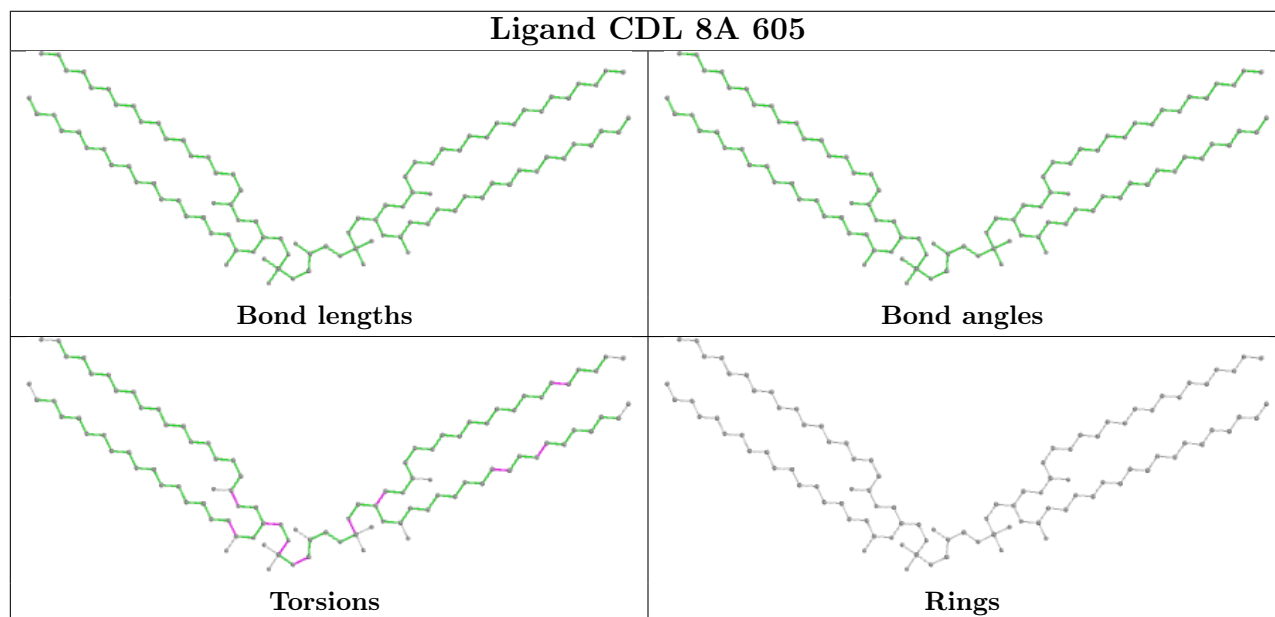
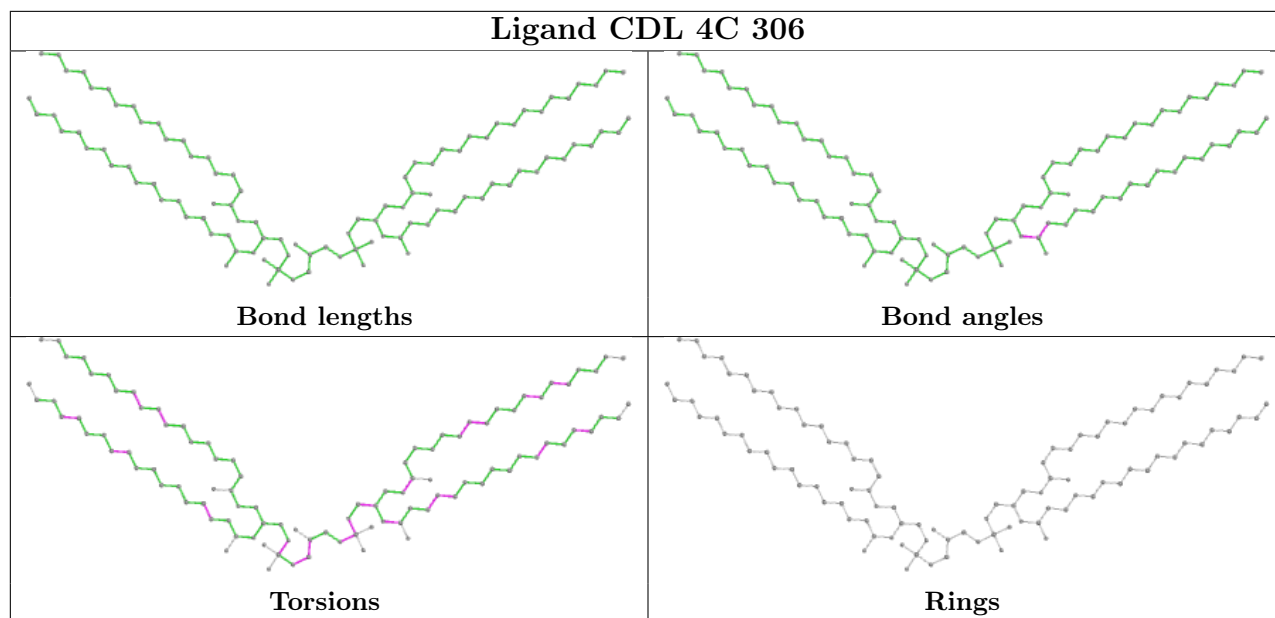
No monomer is involved in short contacts.

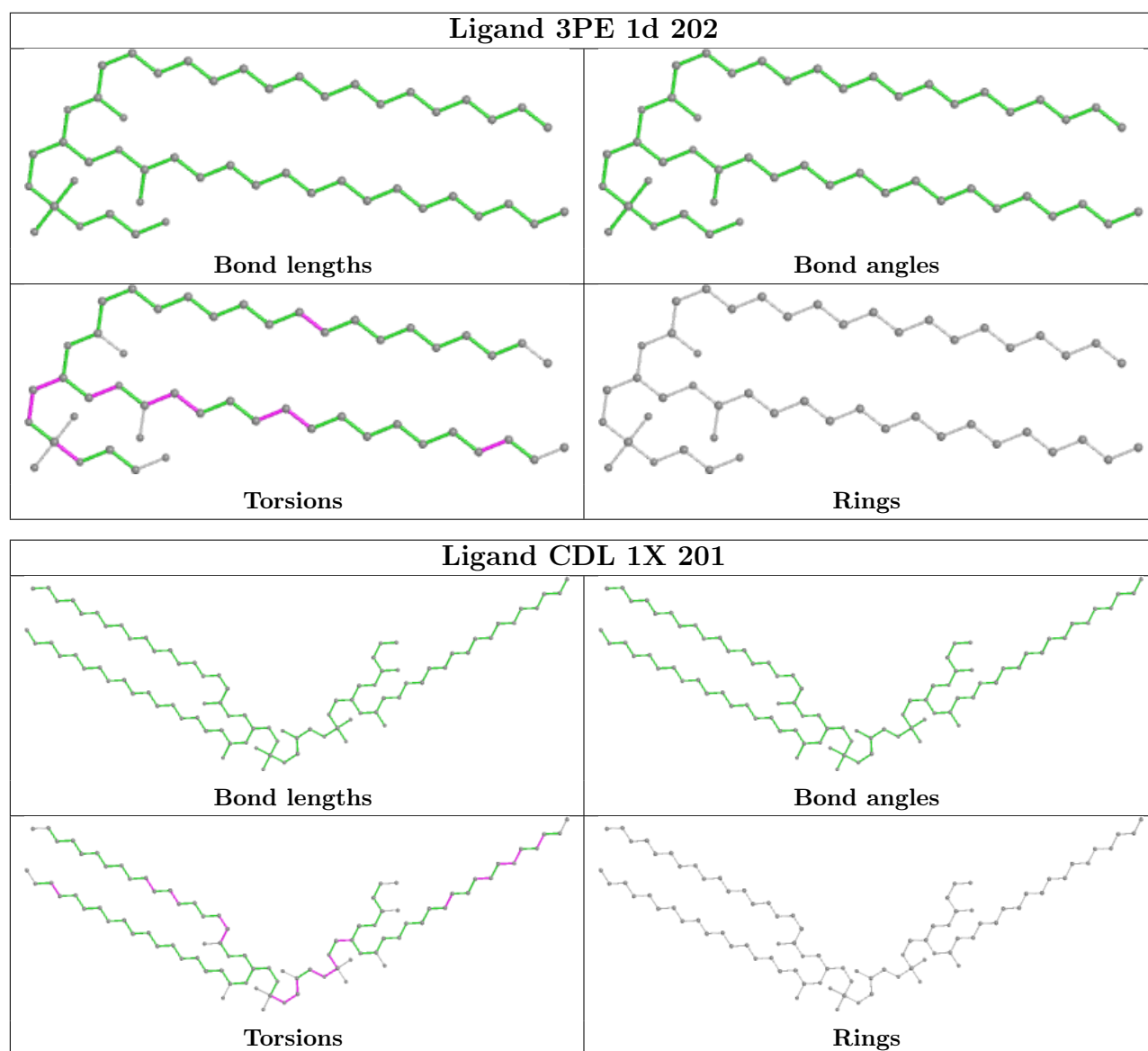
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

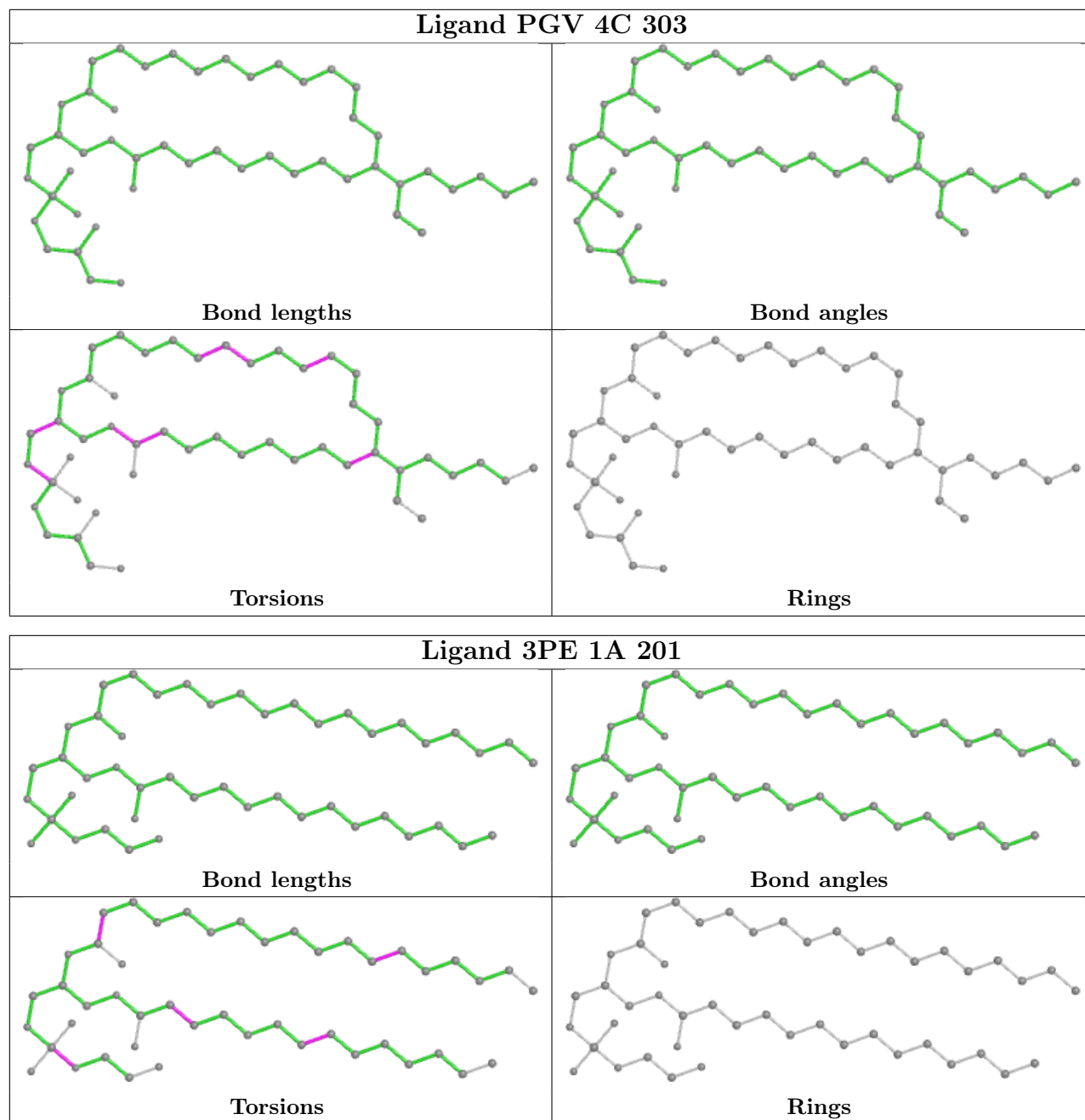


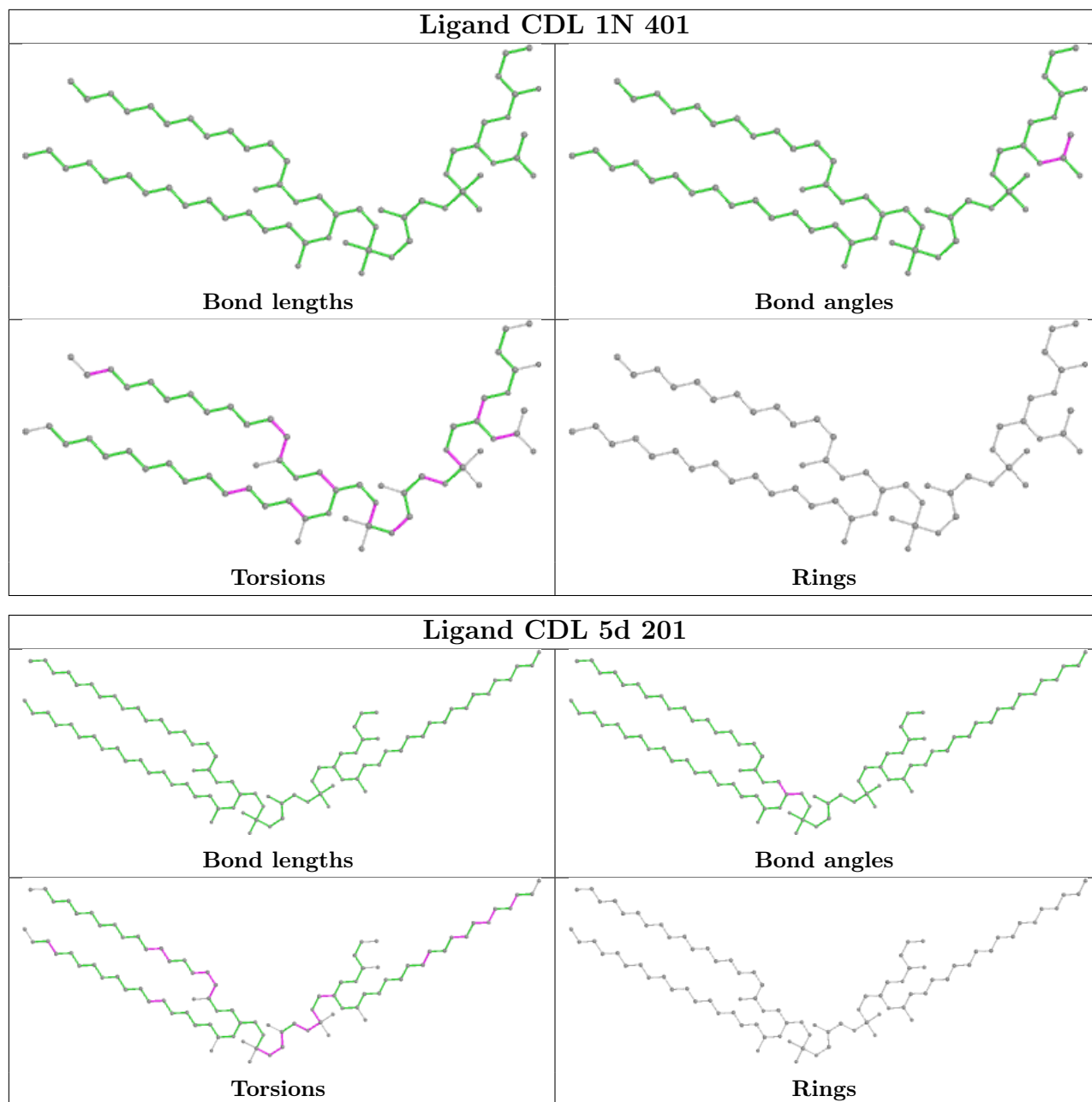


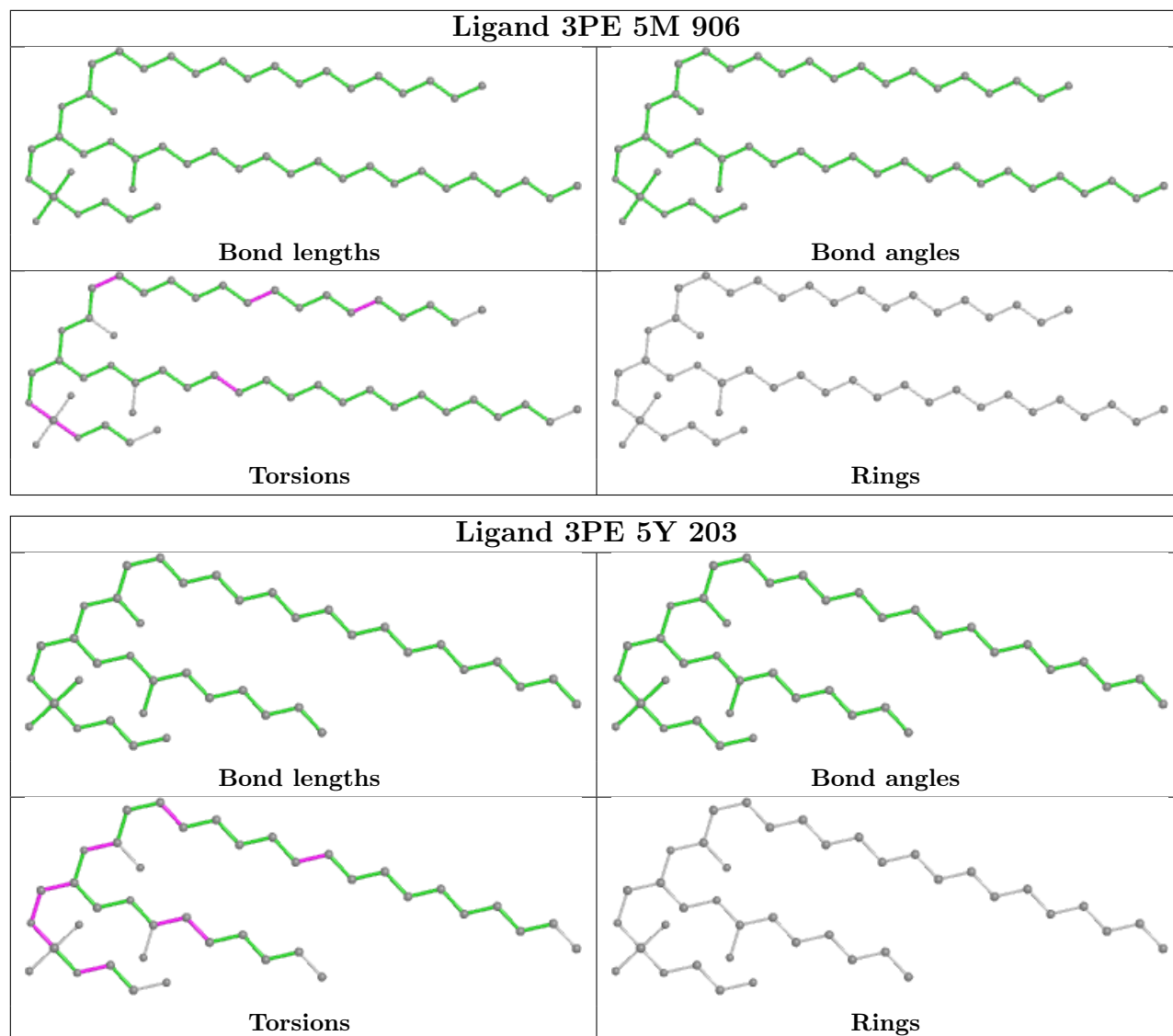


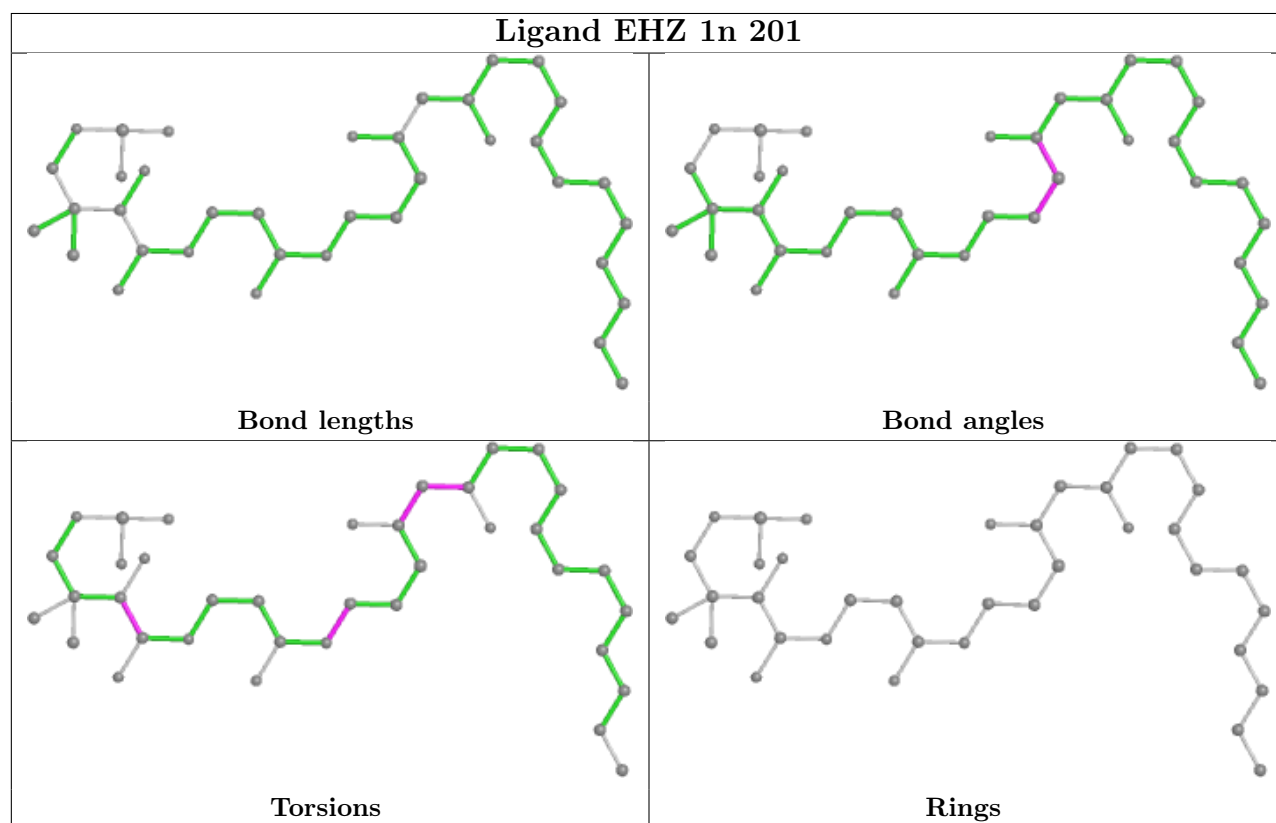
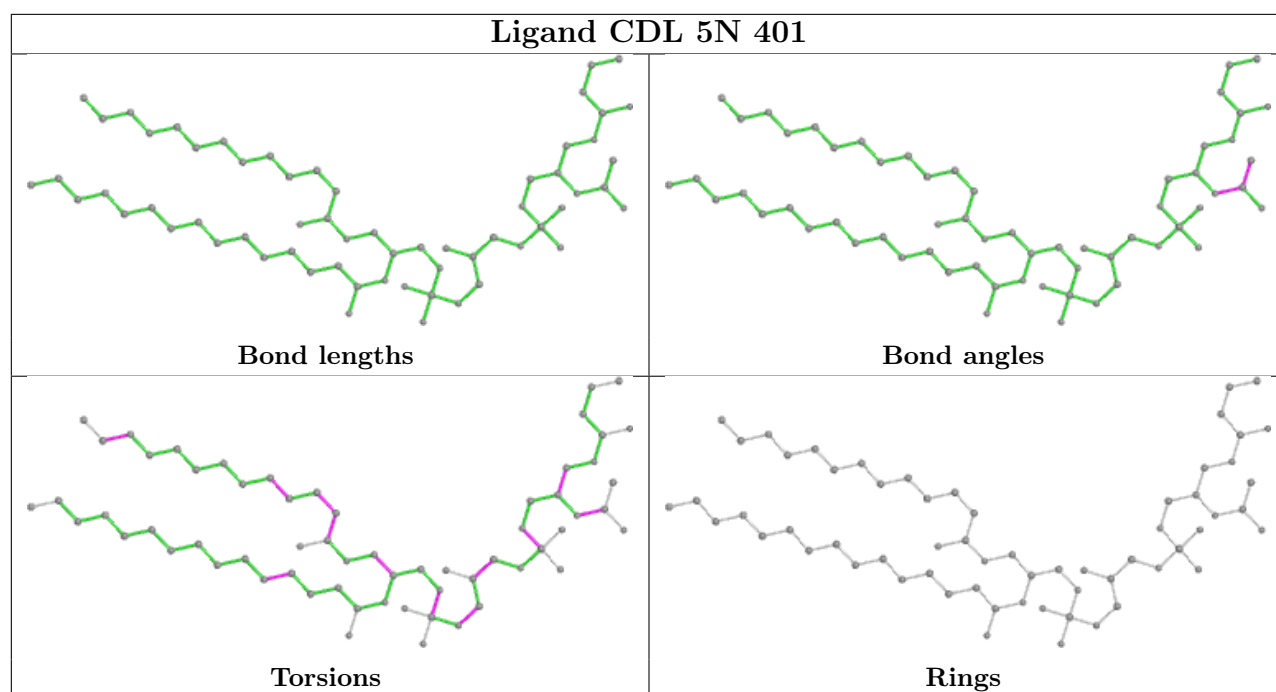


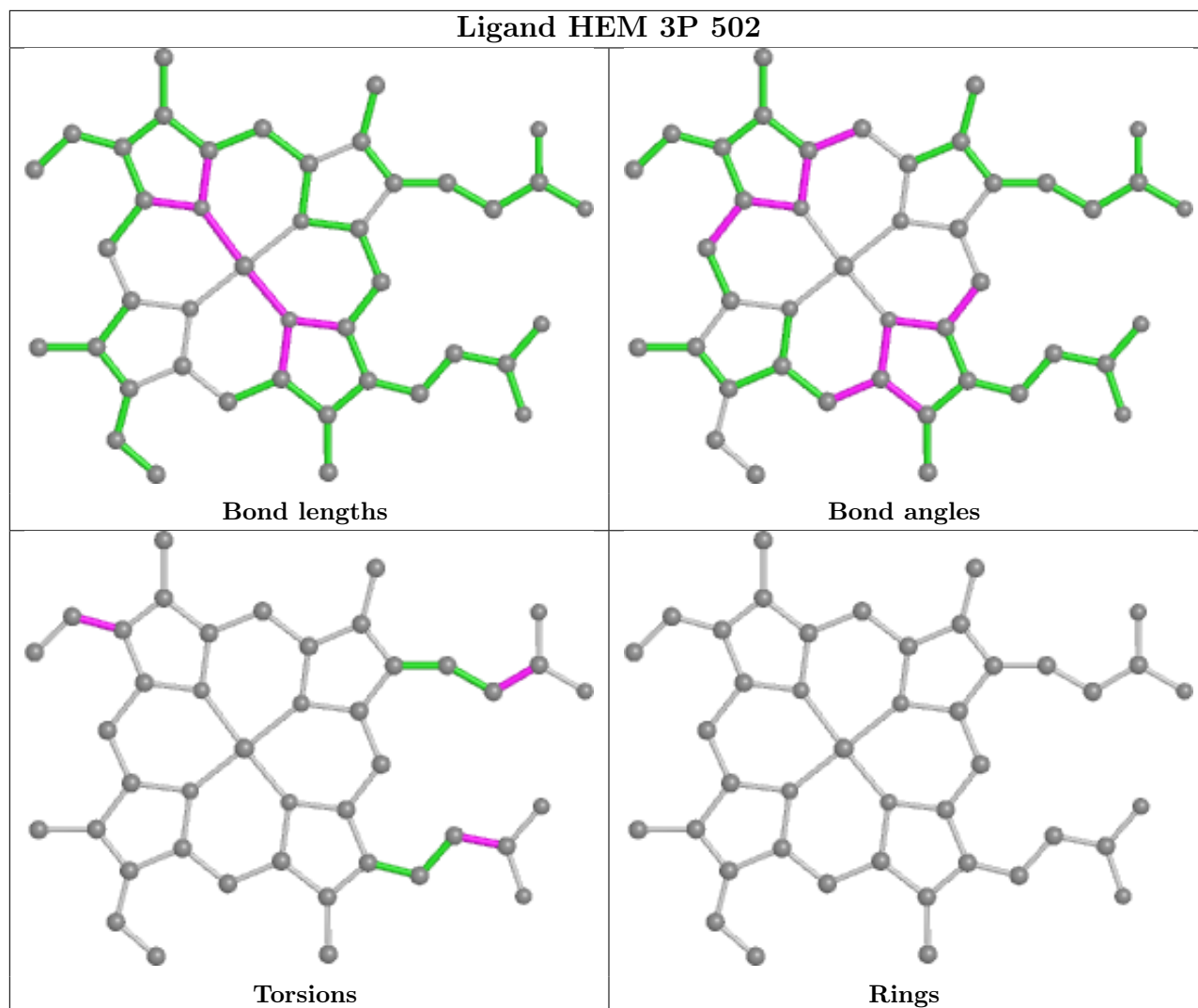


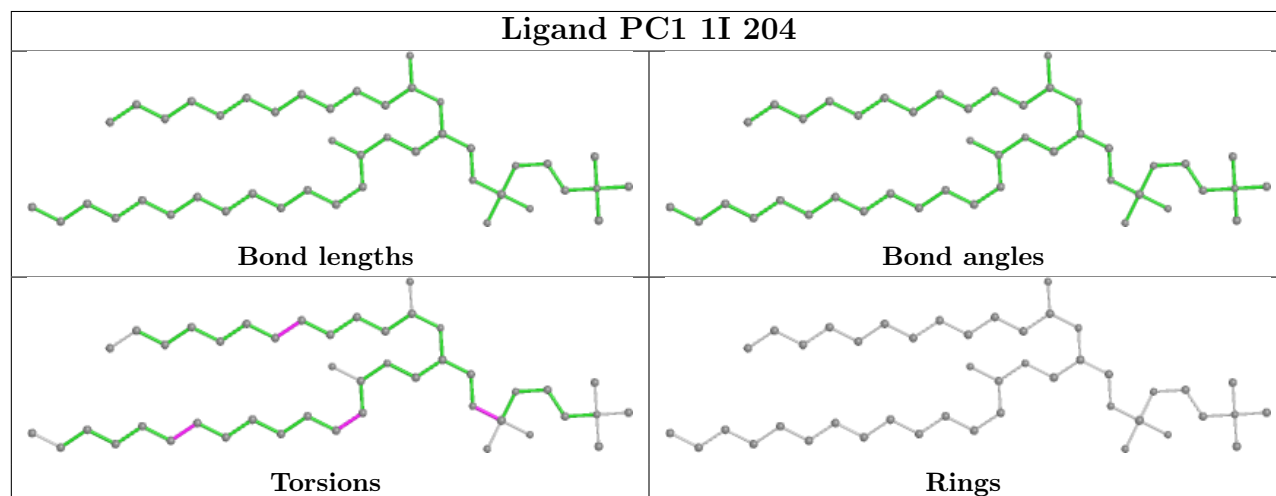
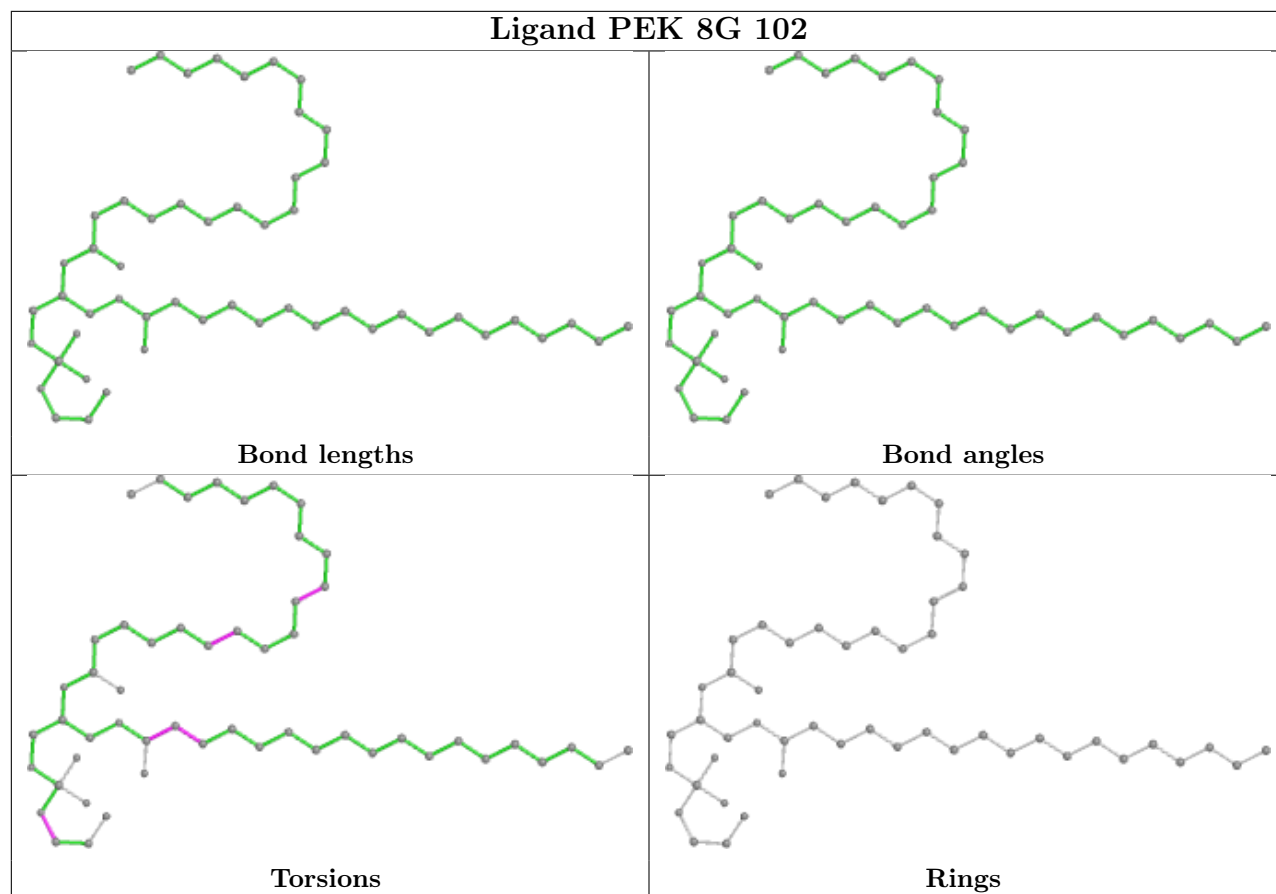




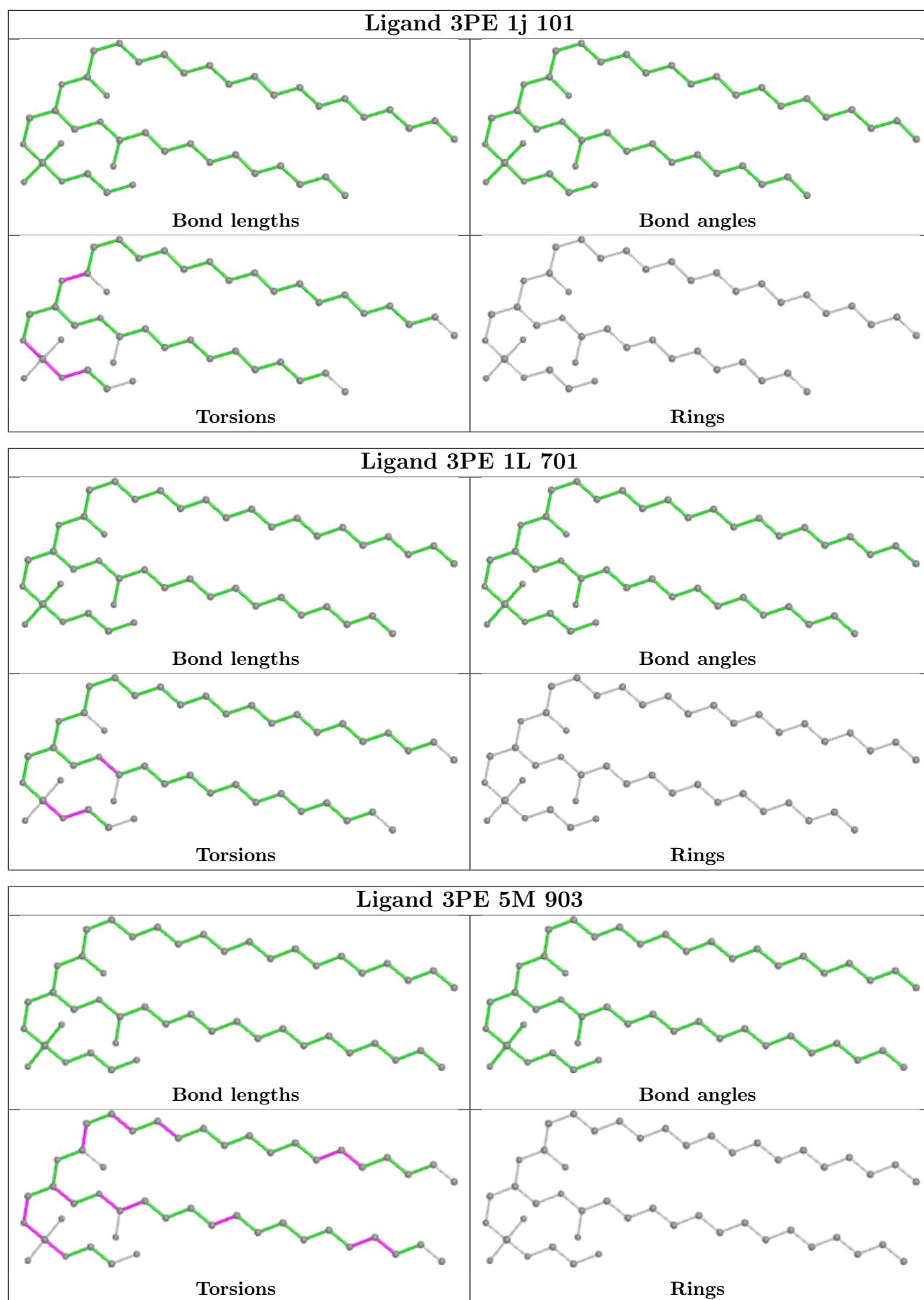


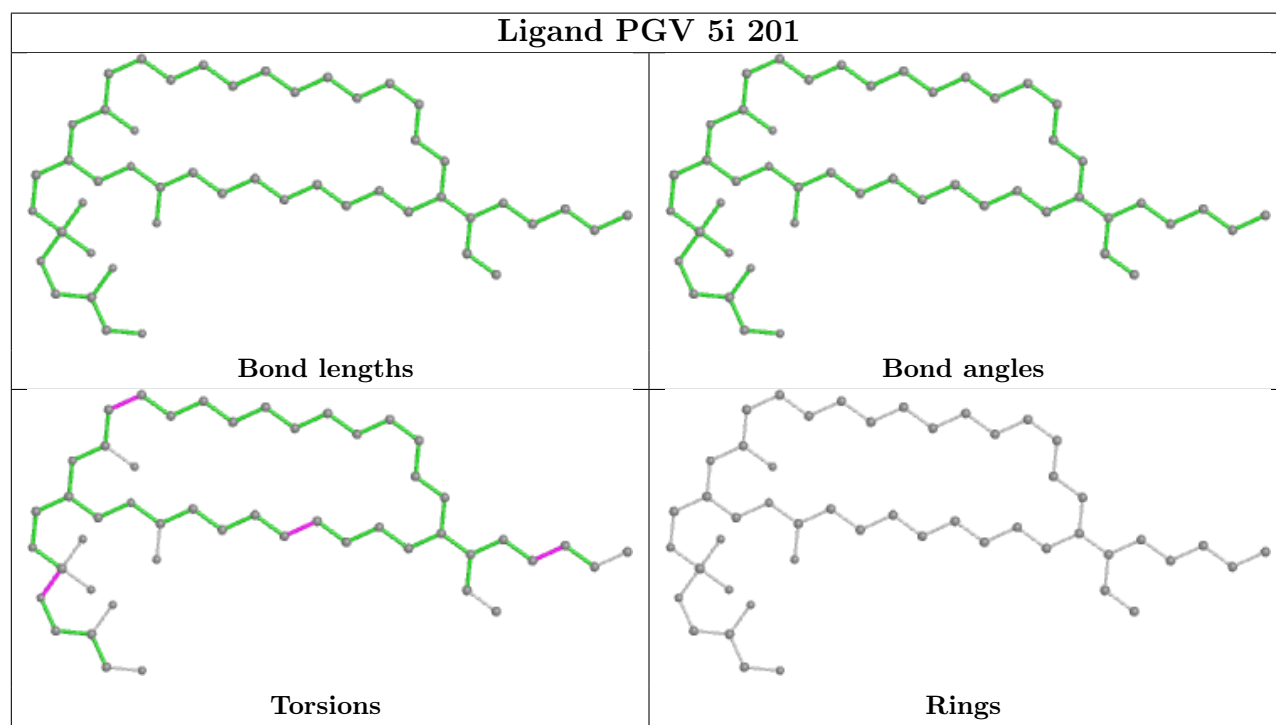
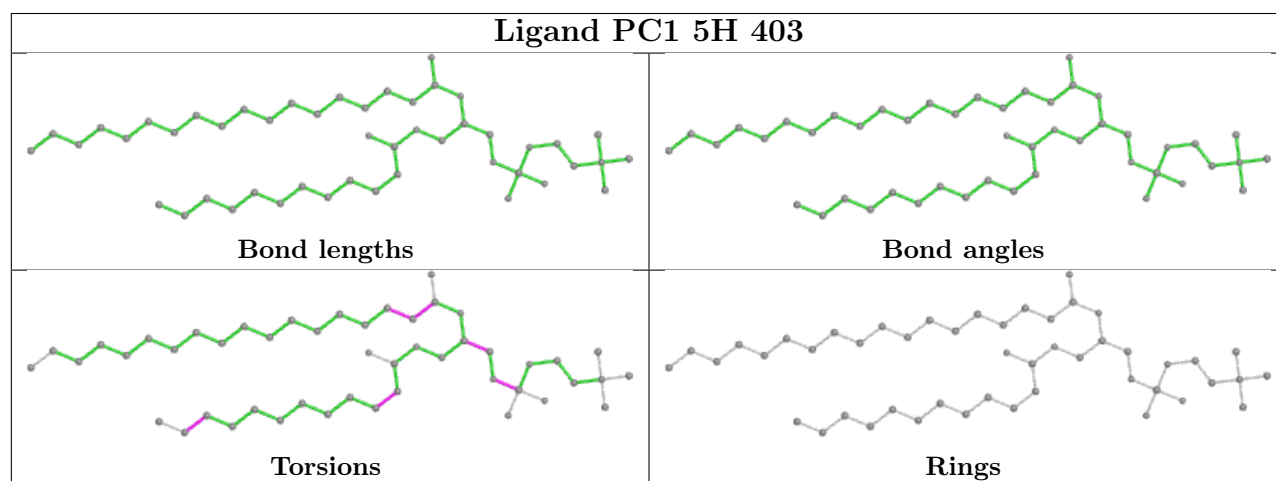
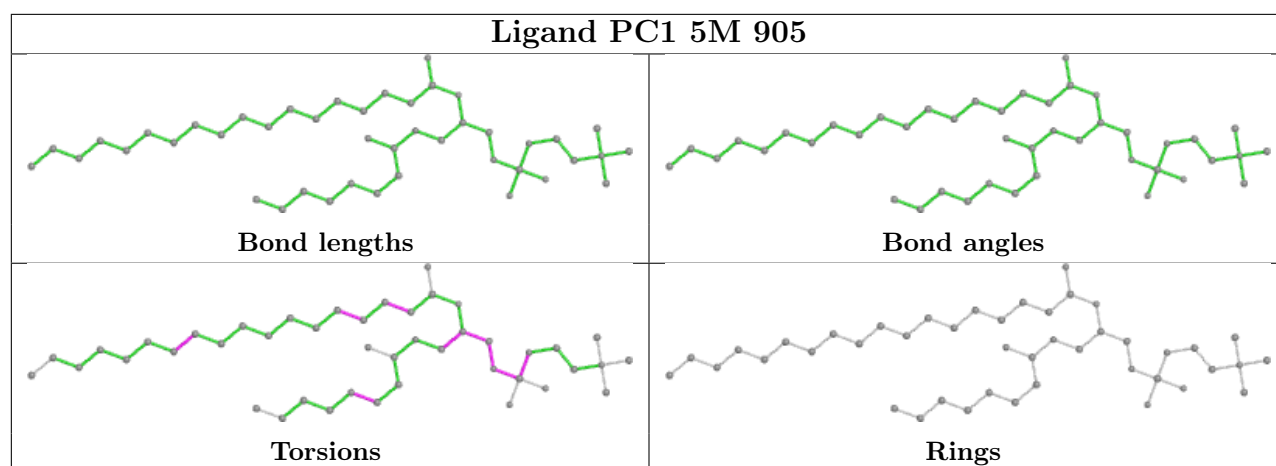


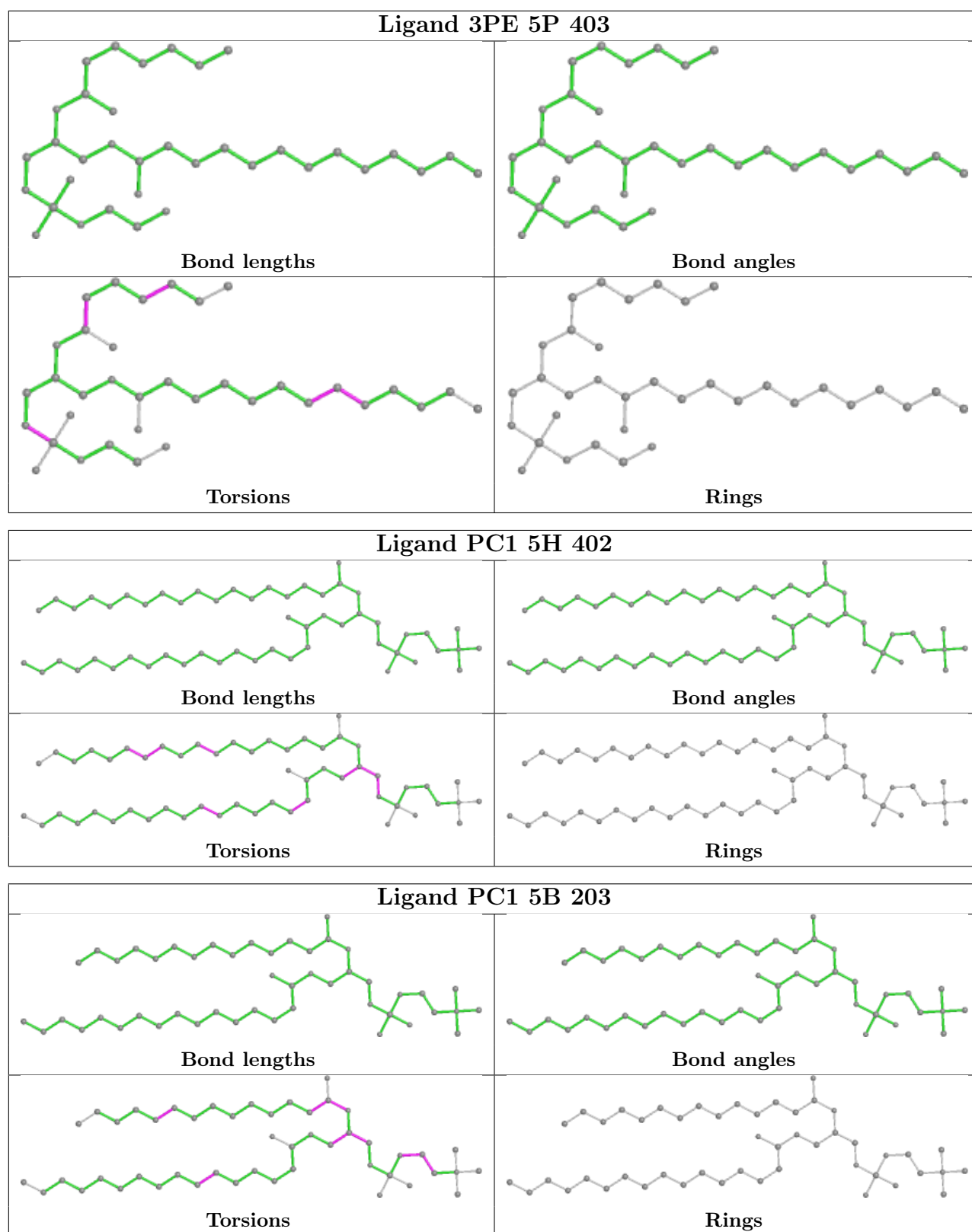


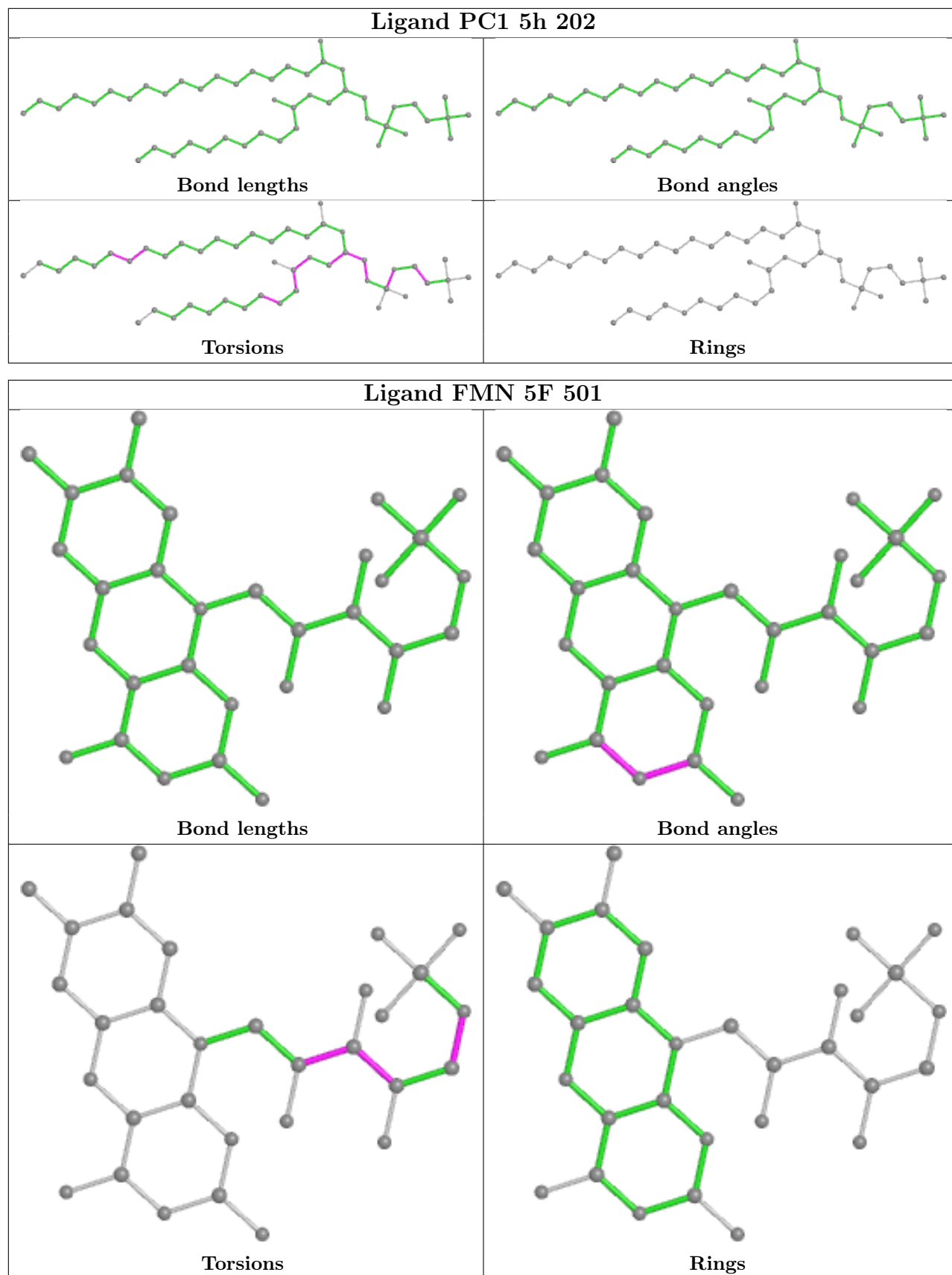


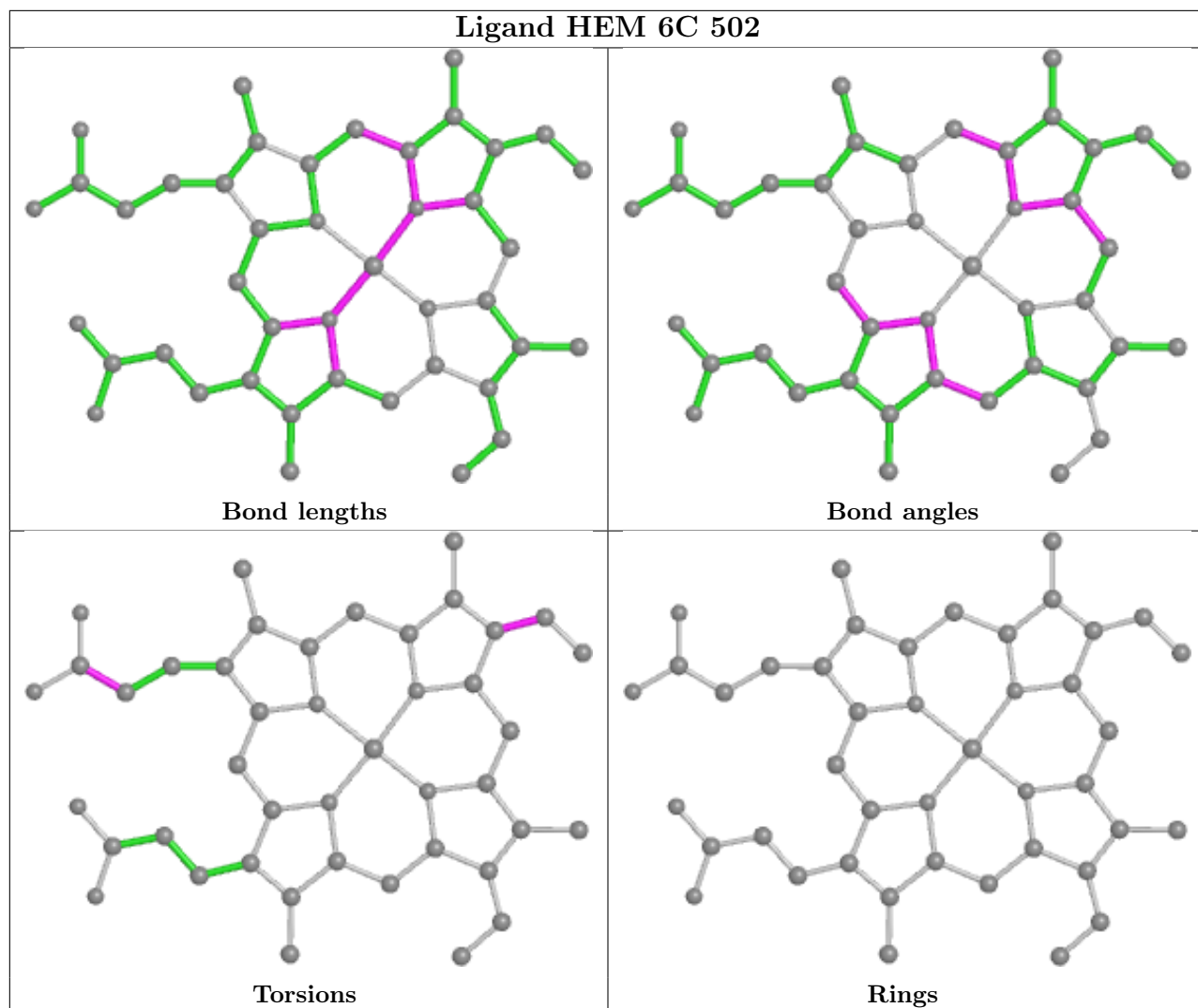


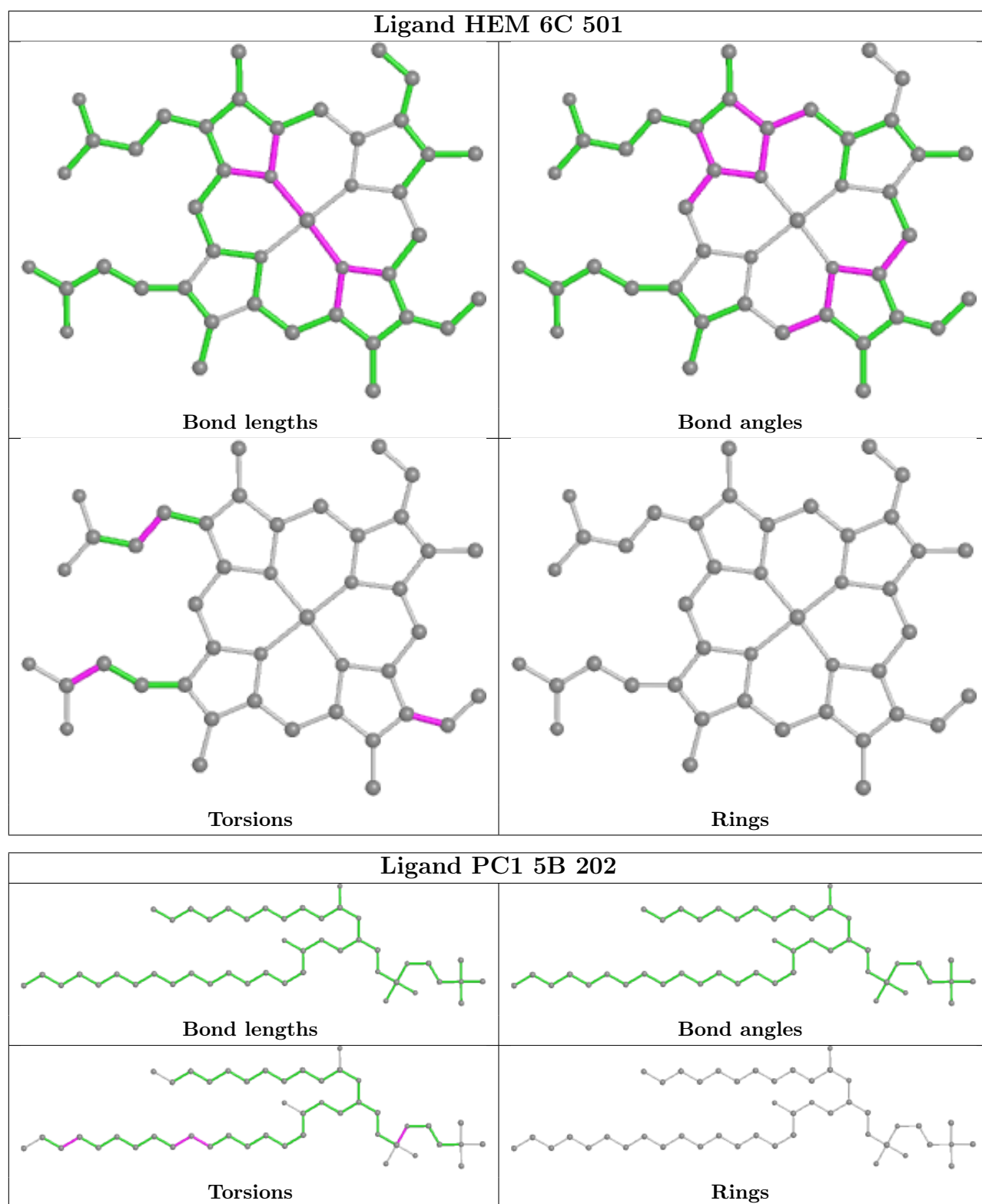


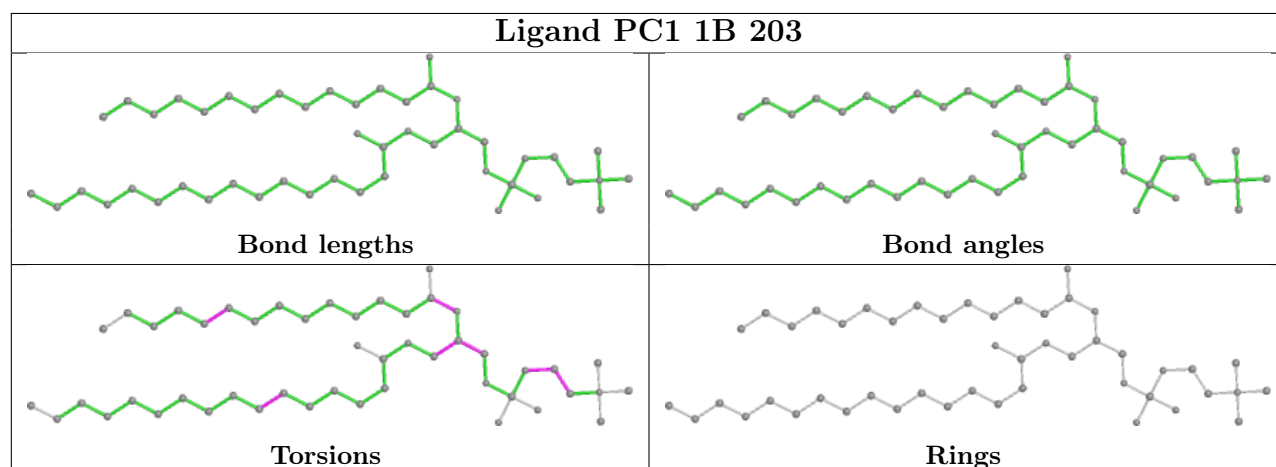
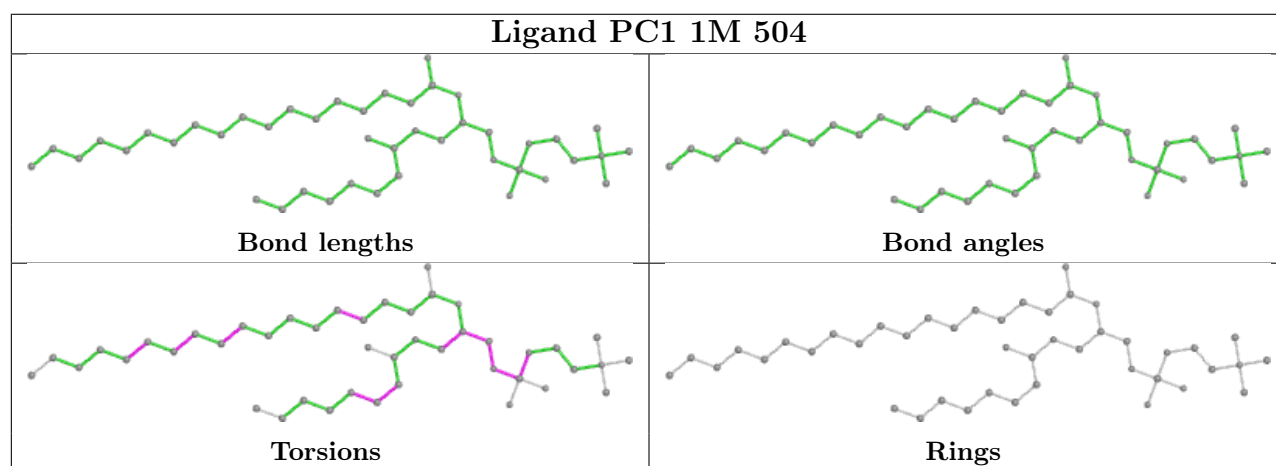
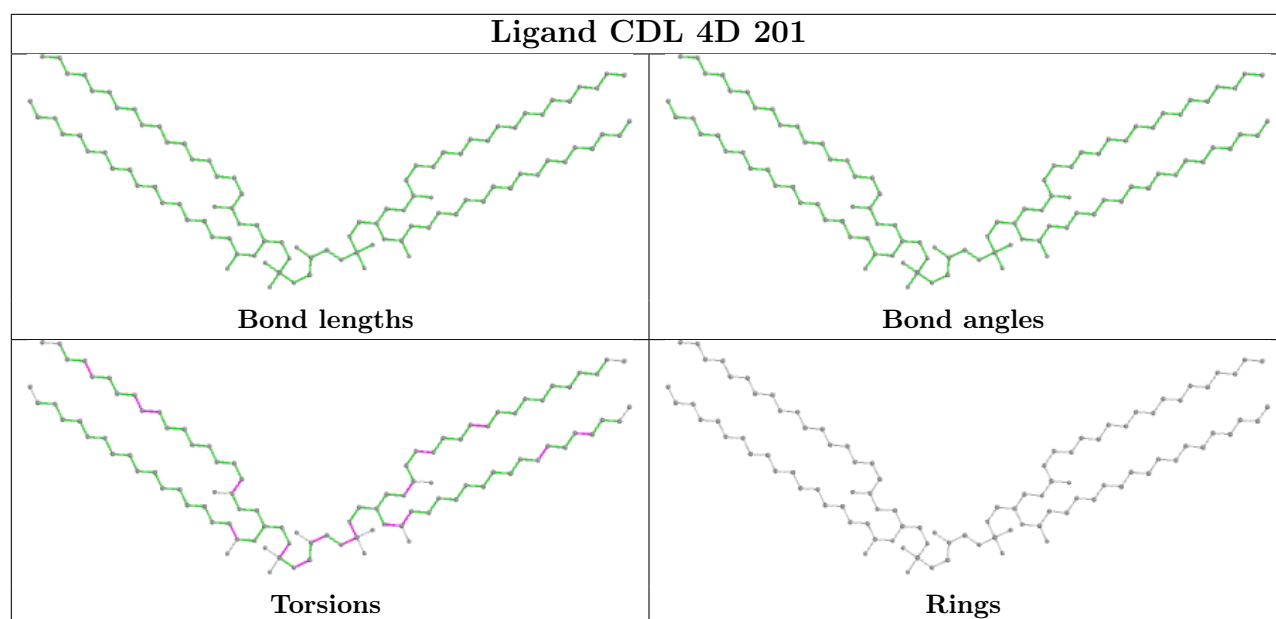


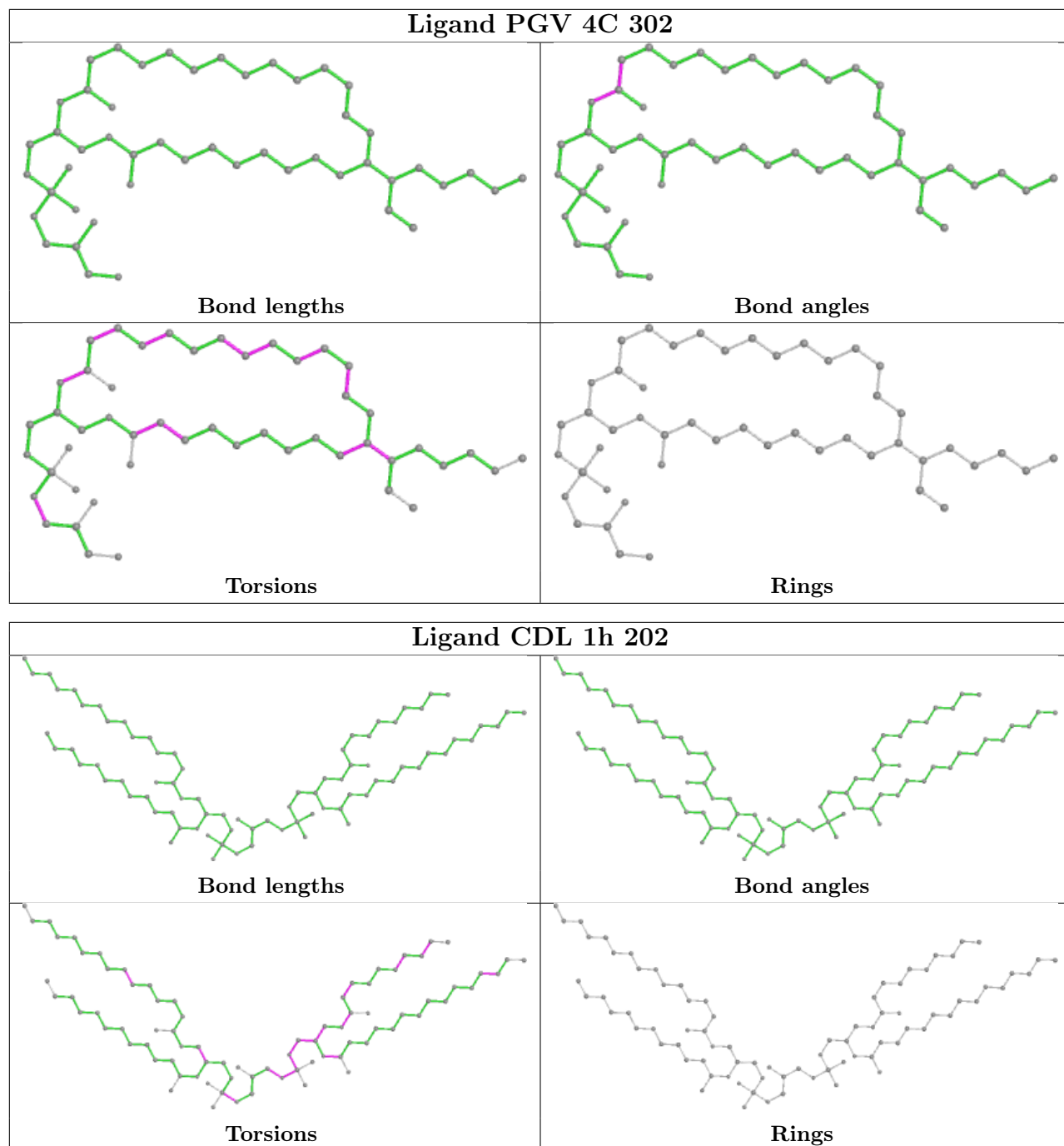




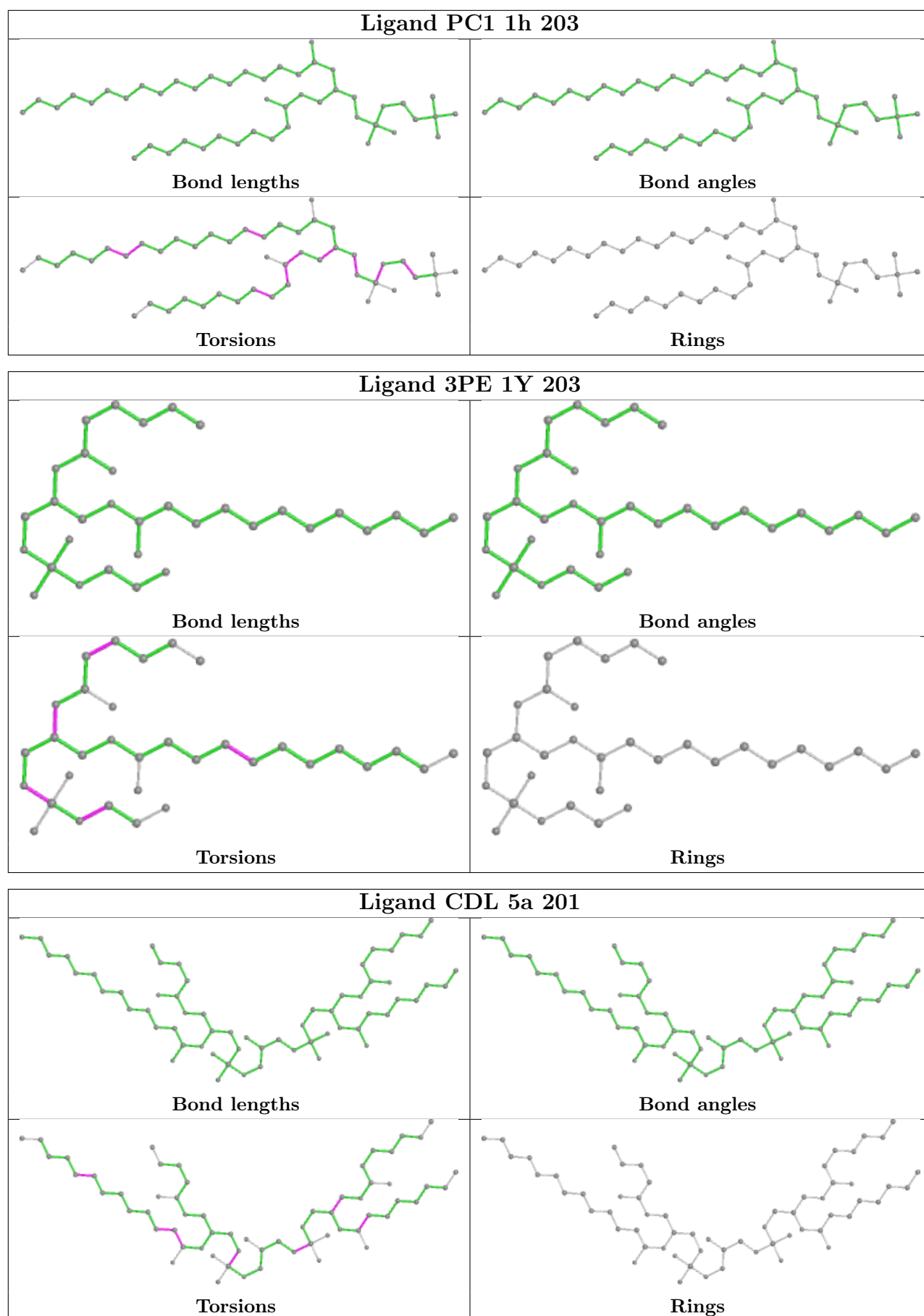


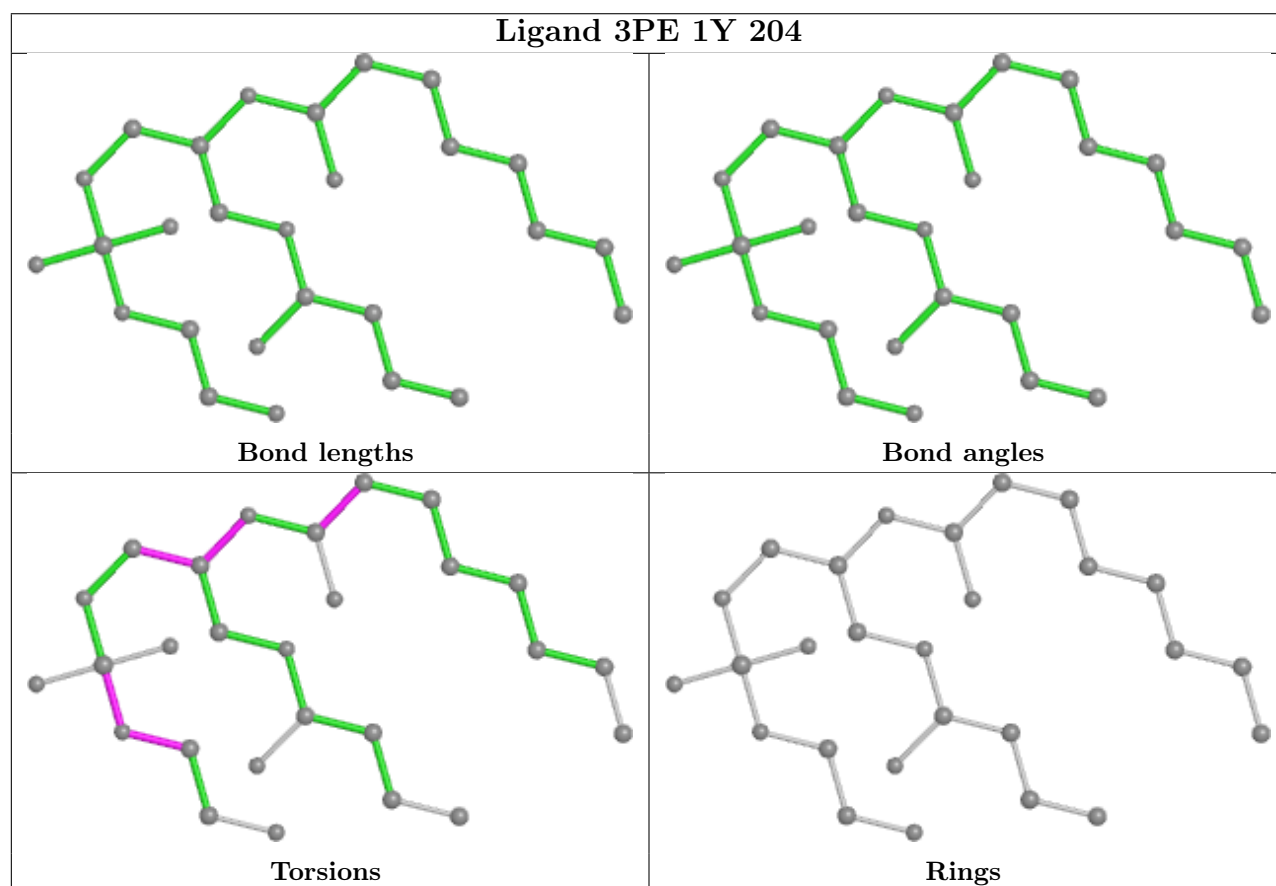
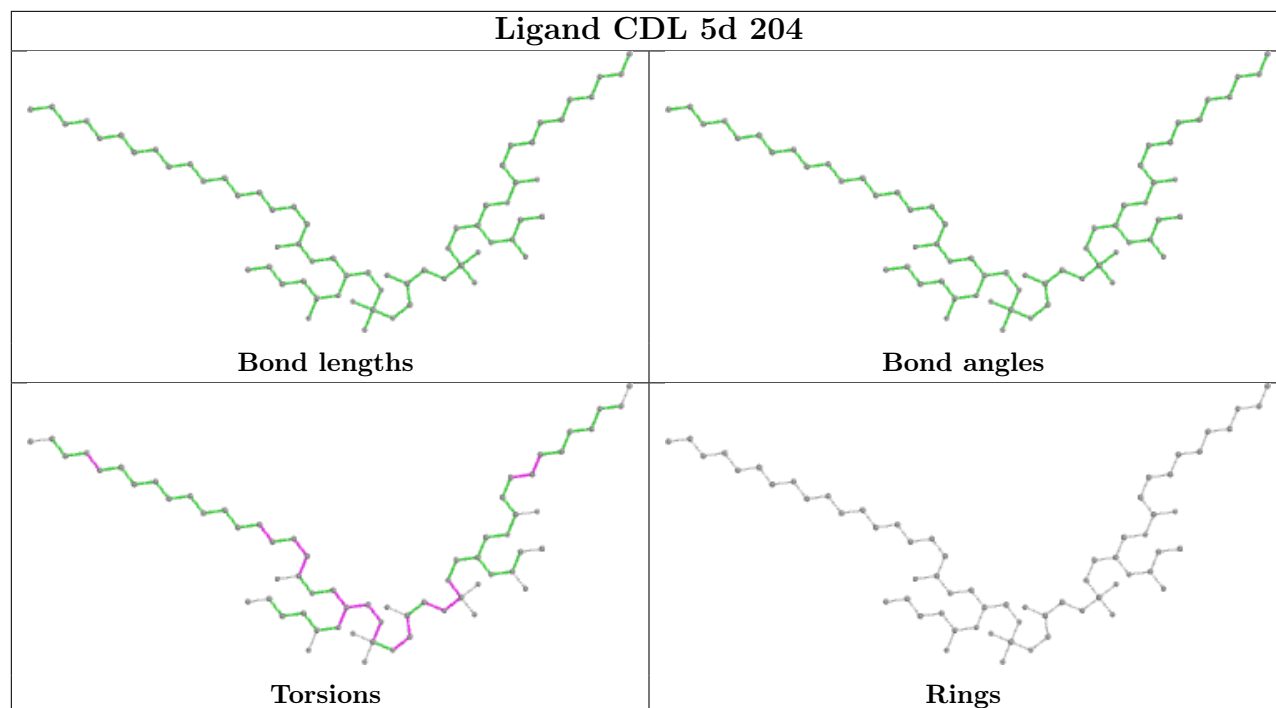


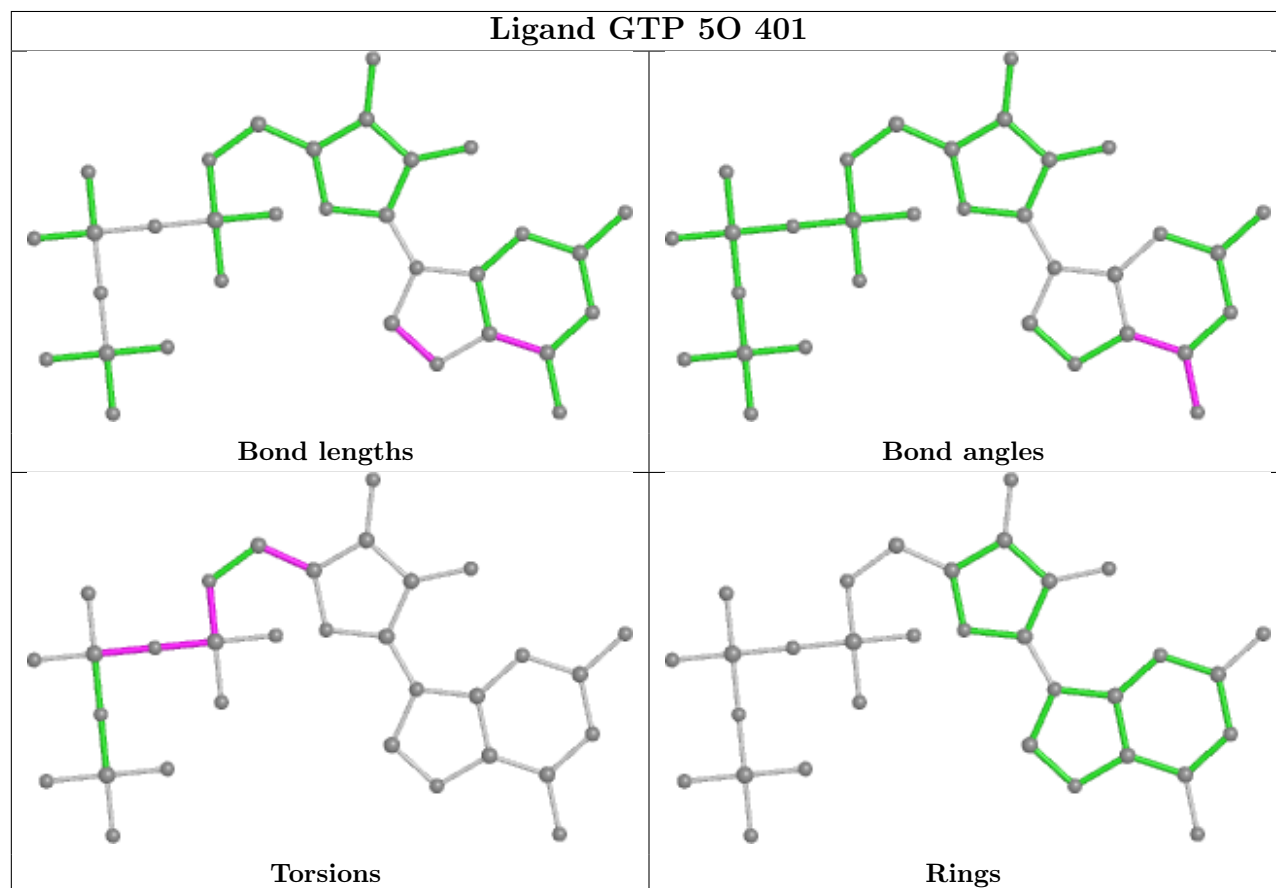
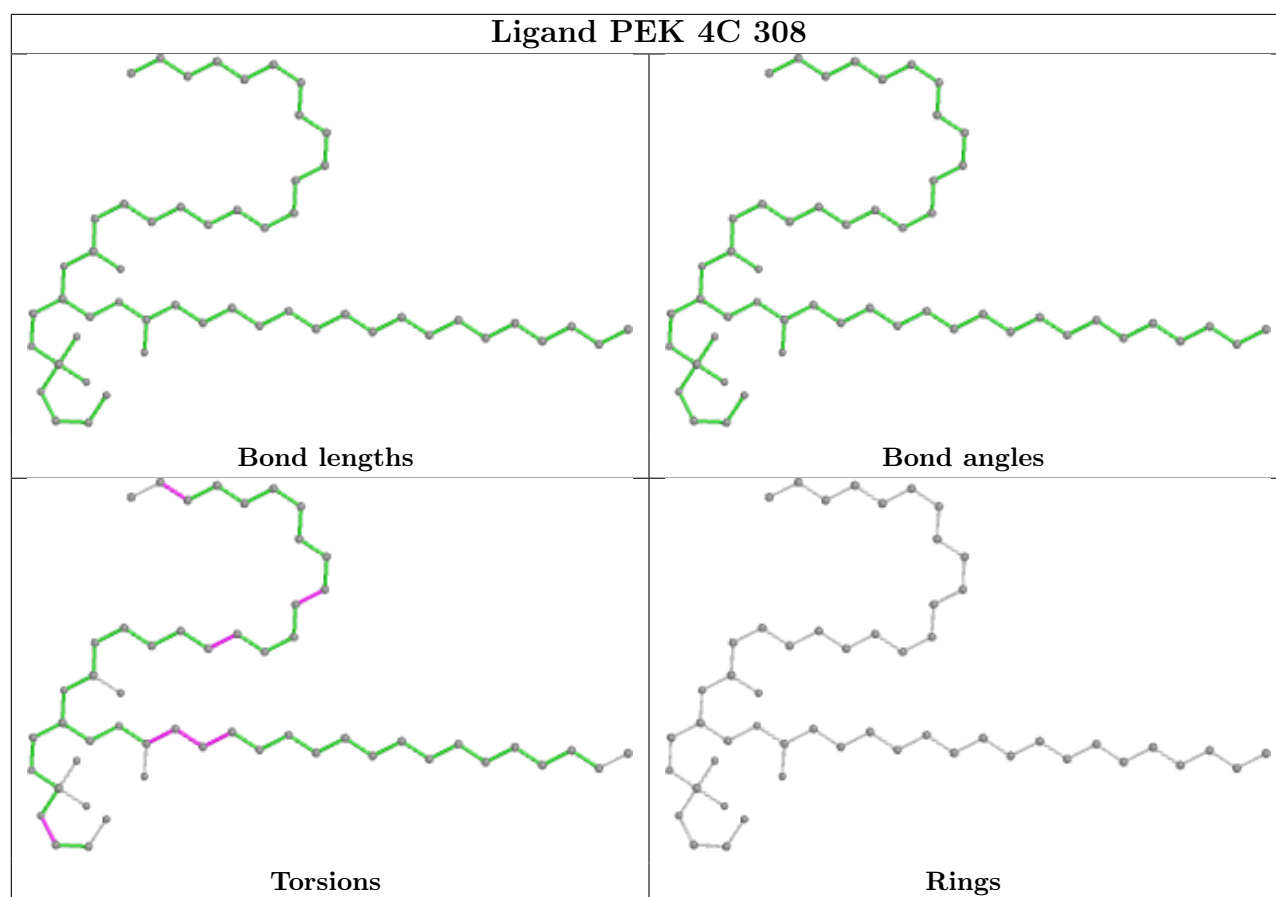


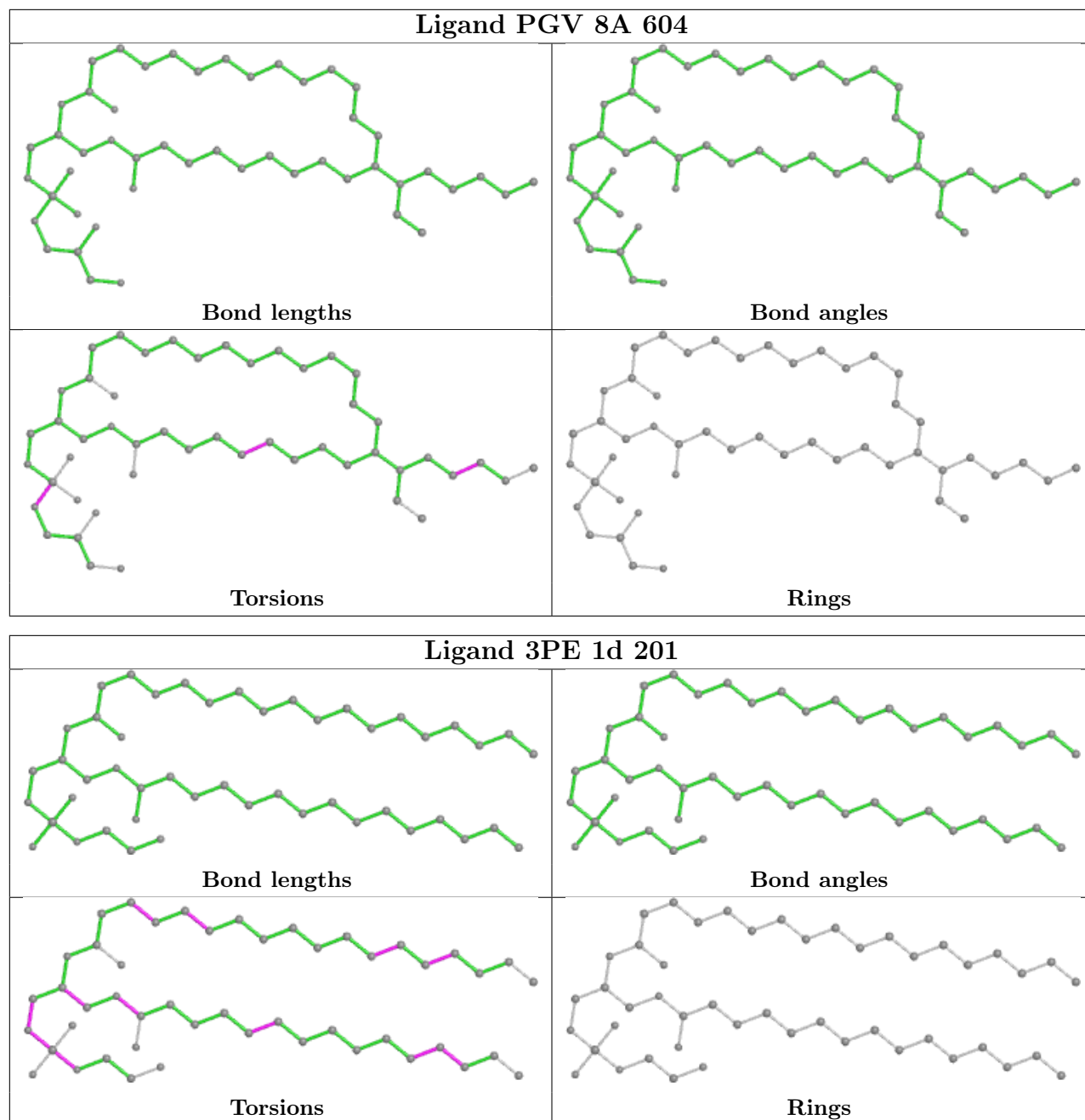


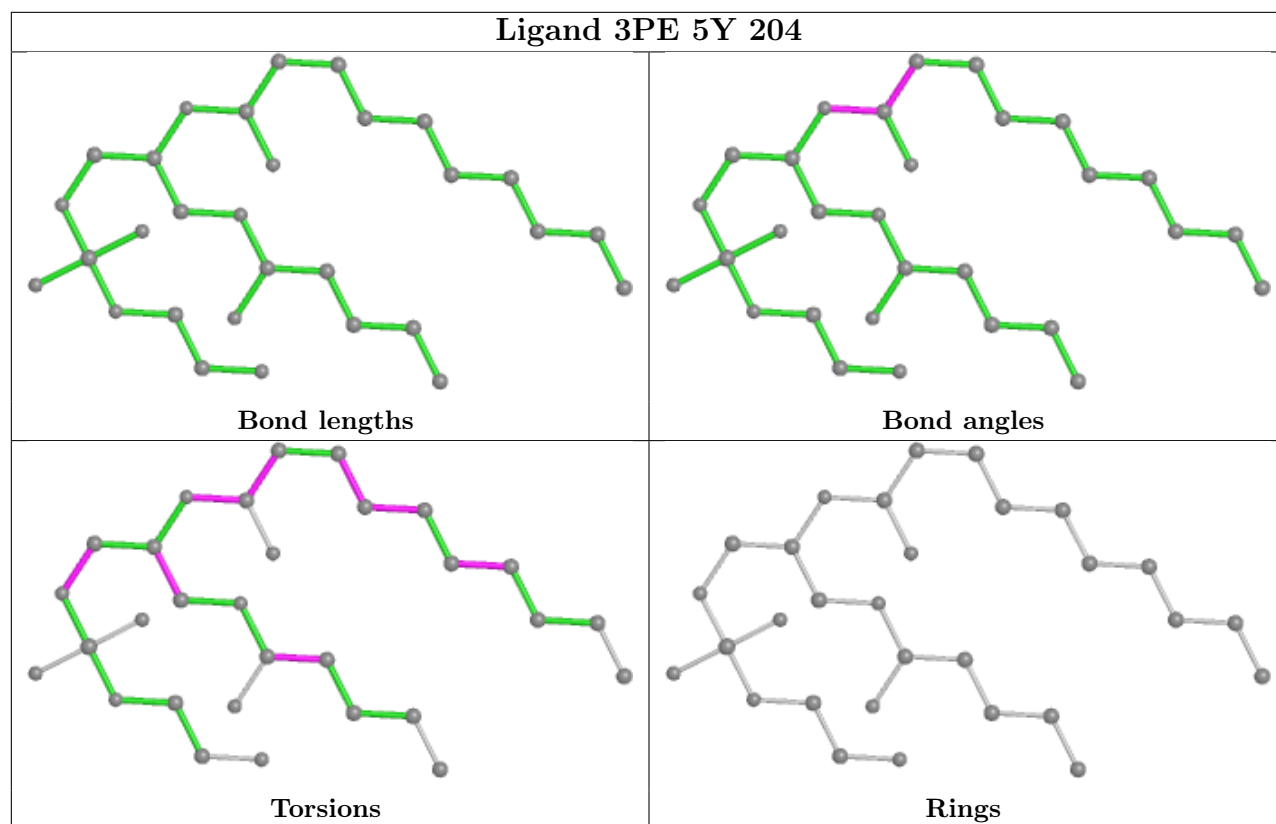
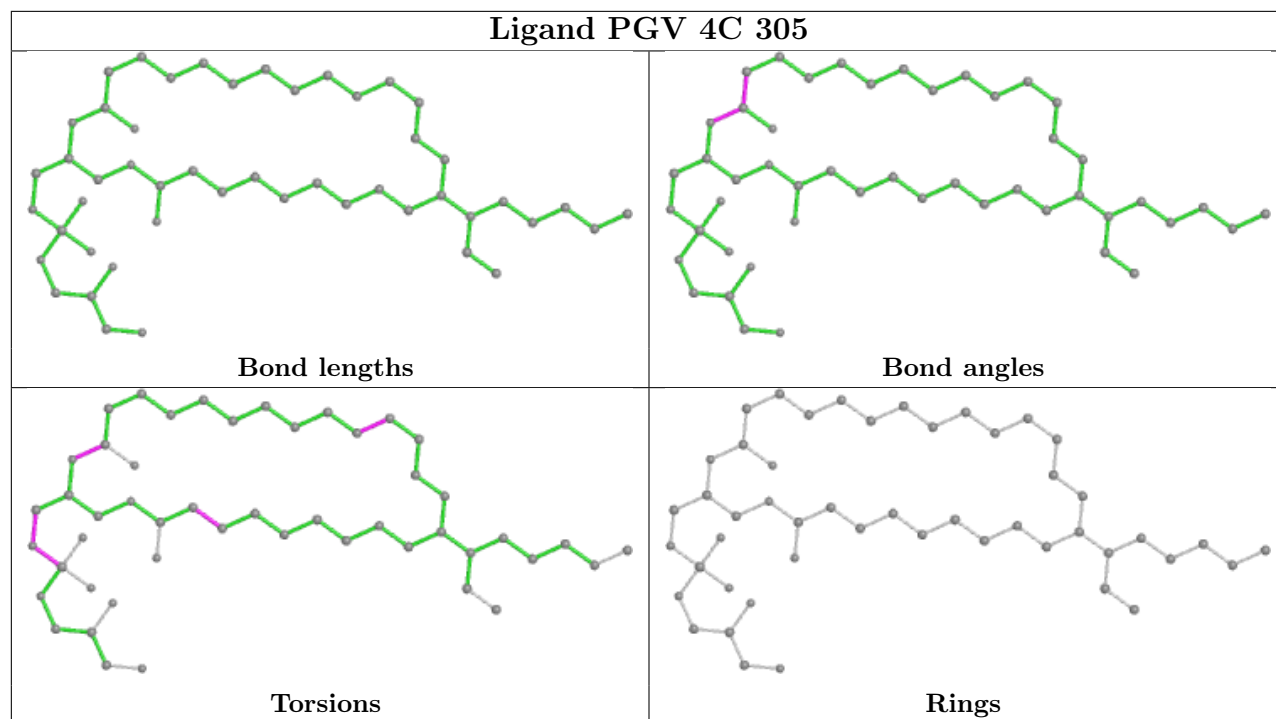


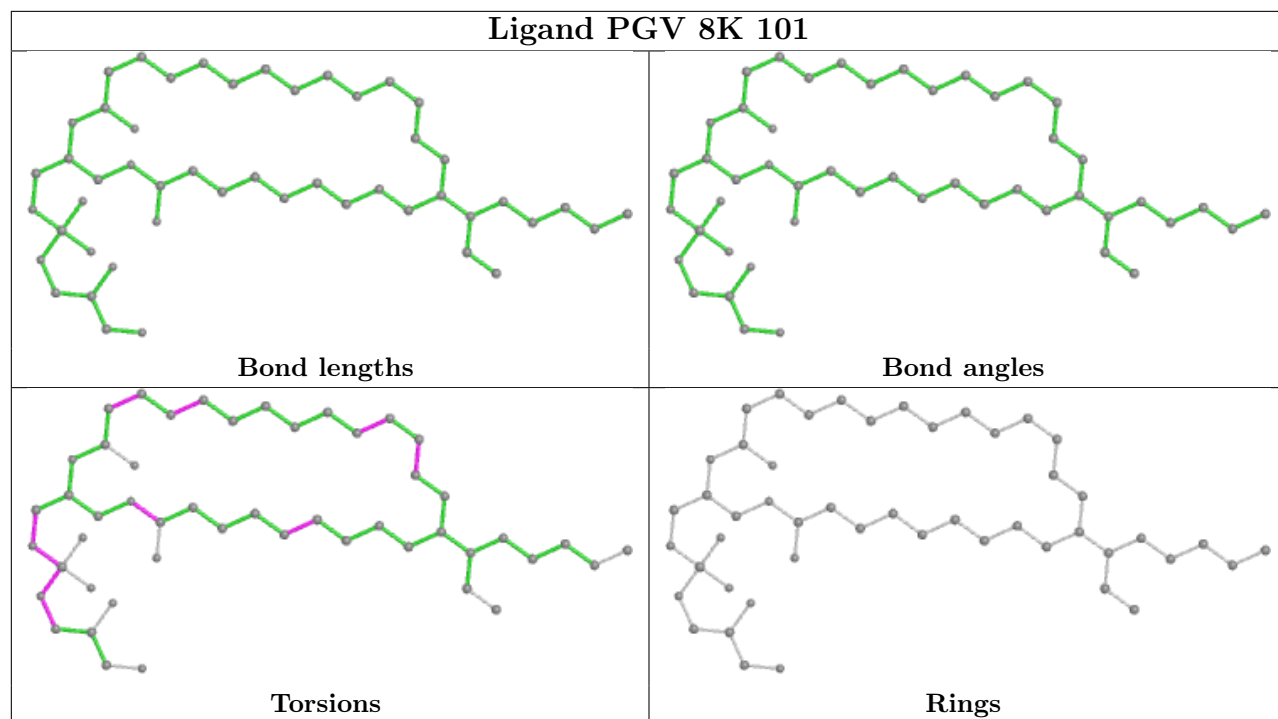


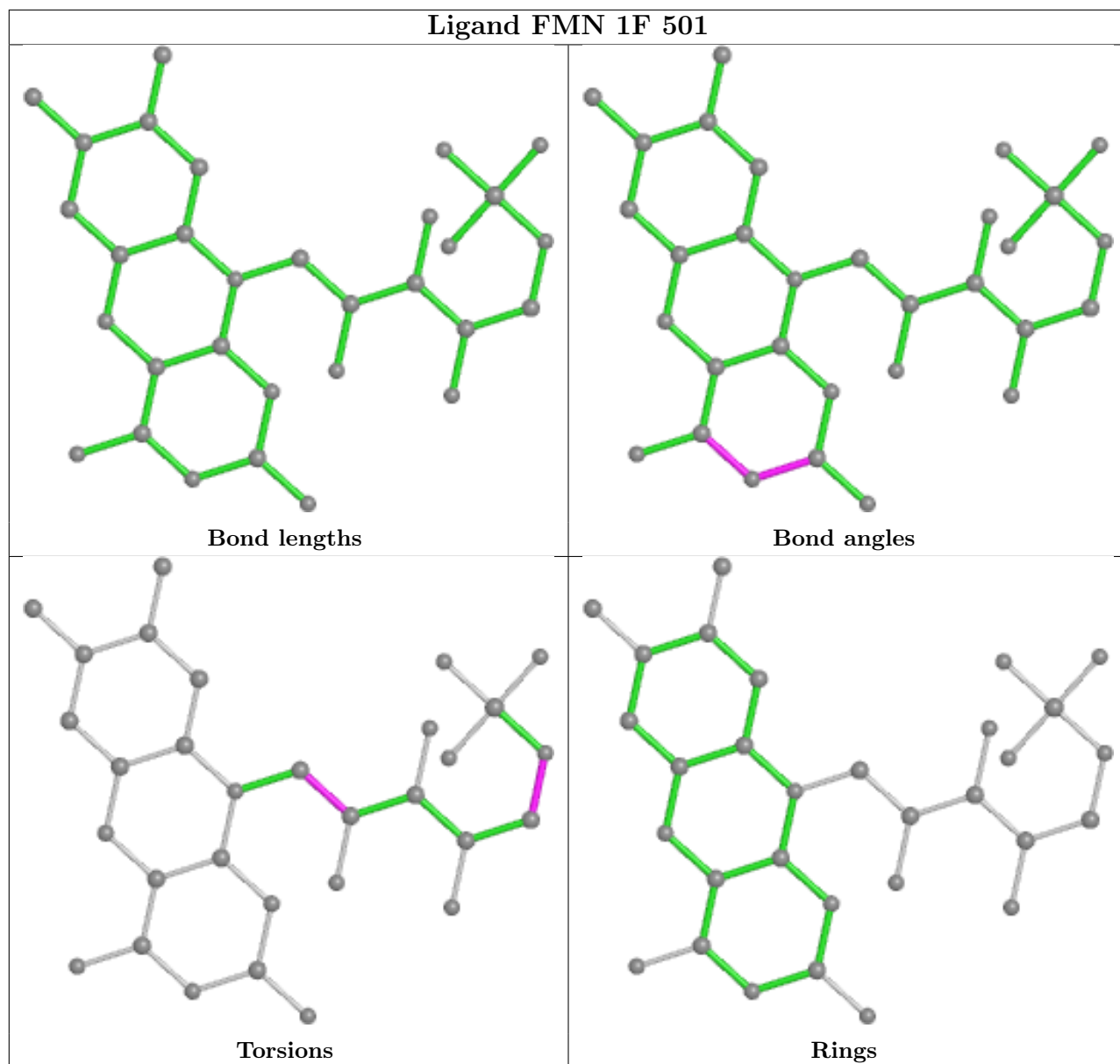


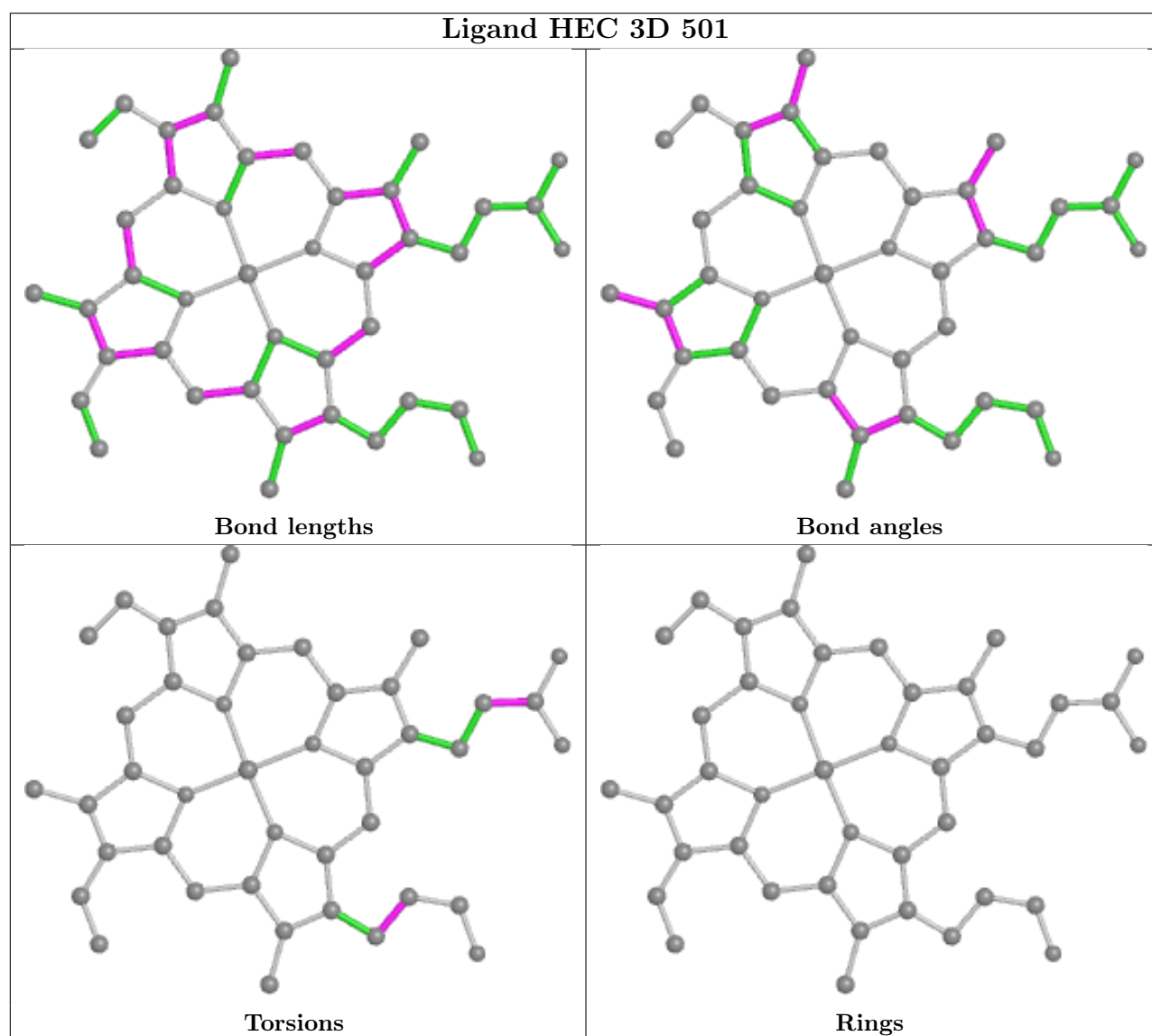
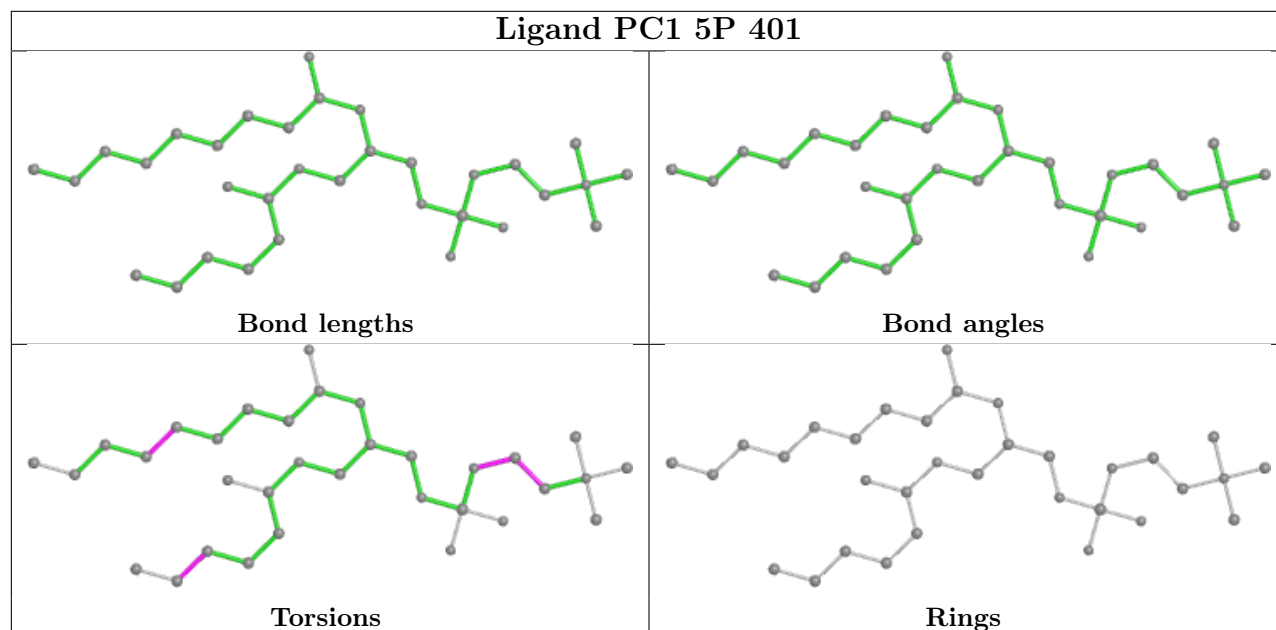




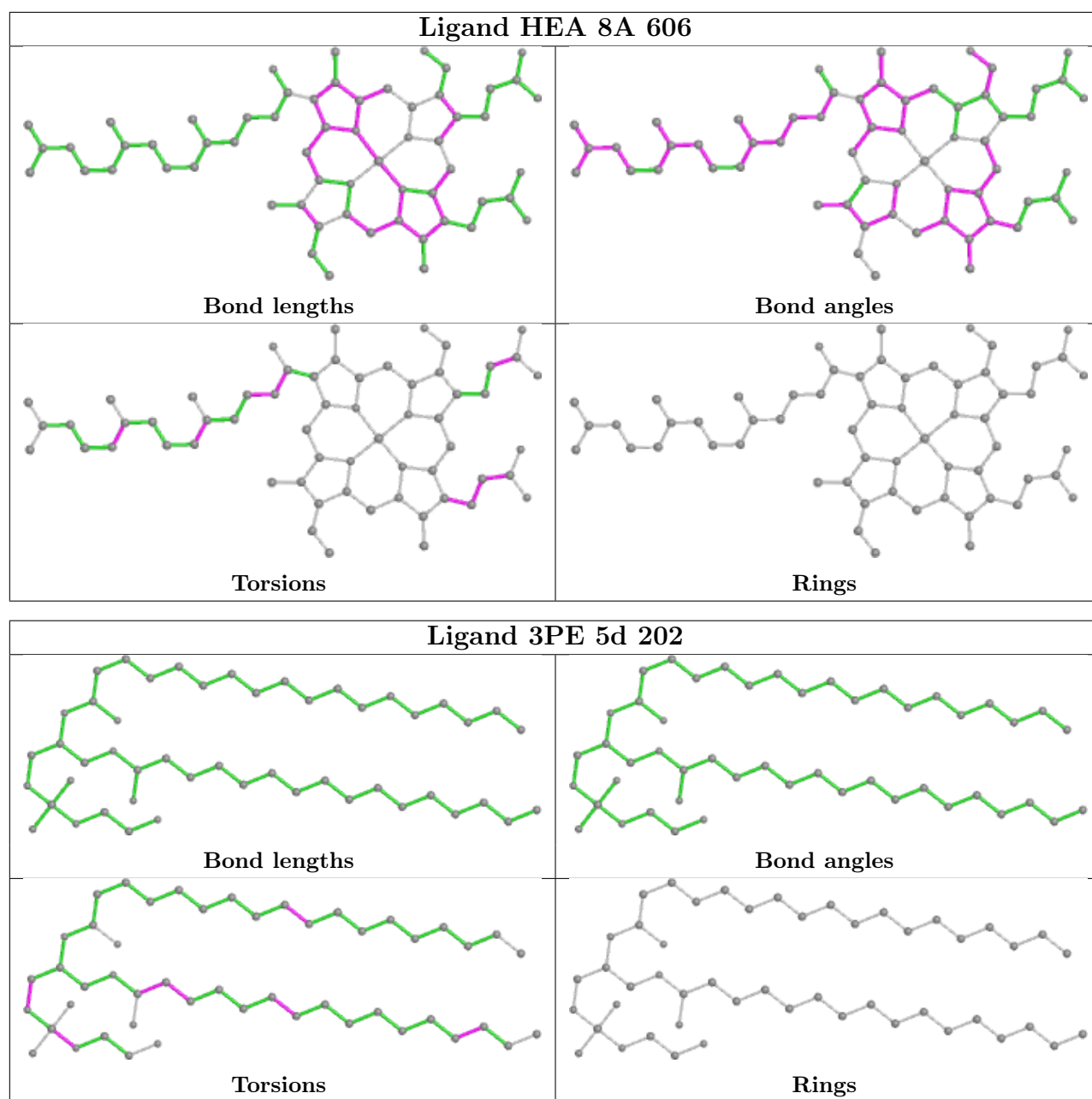


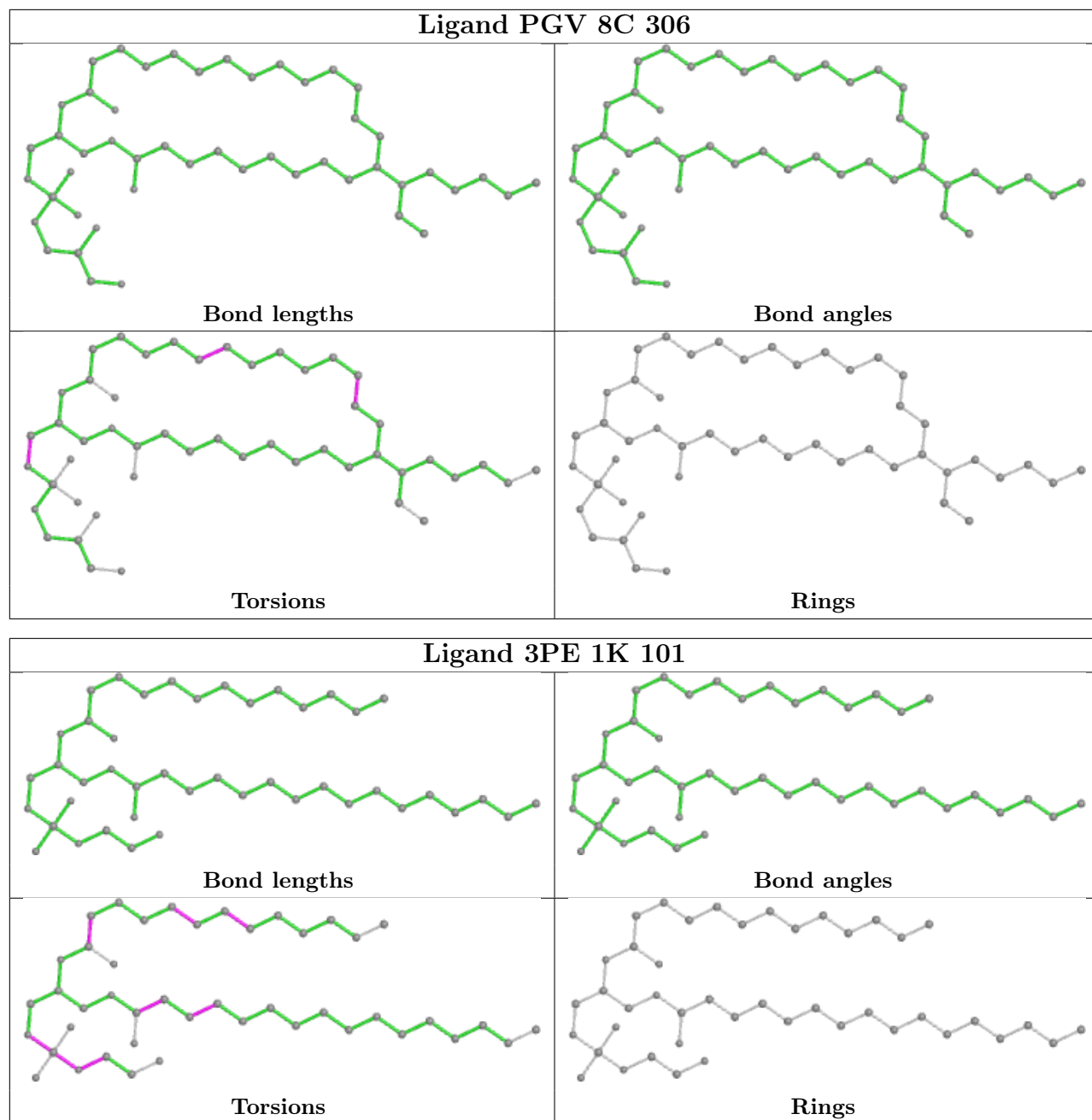


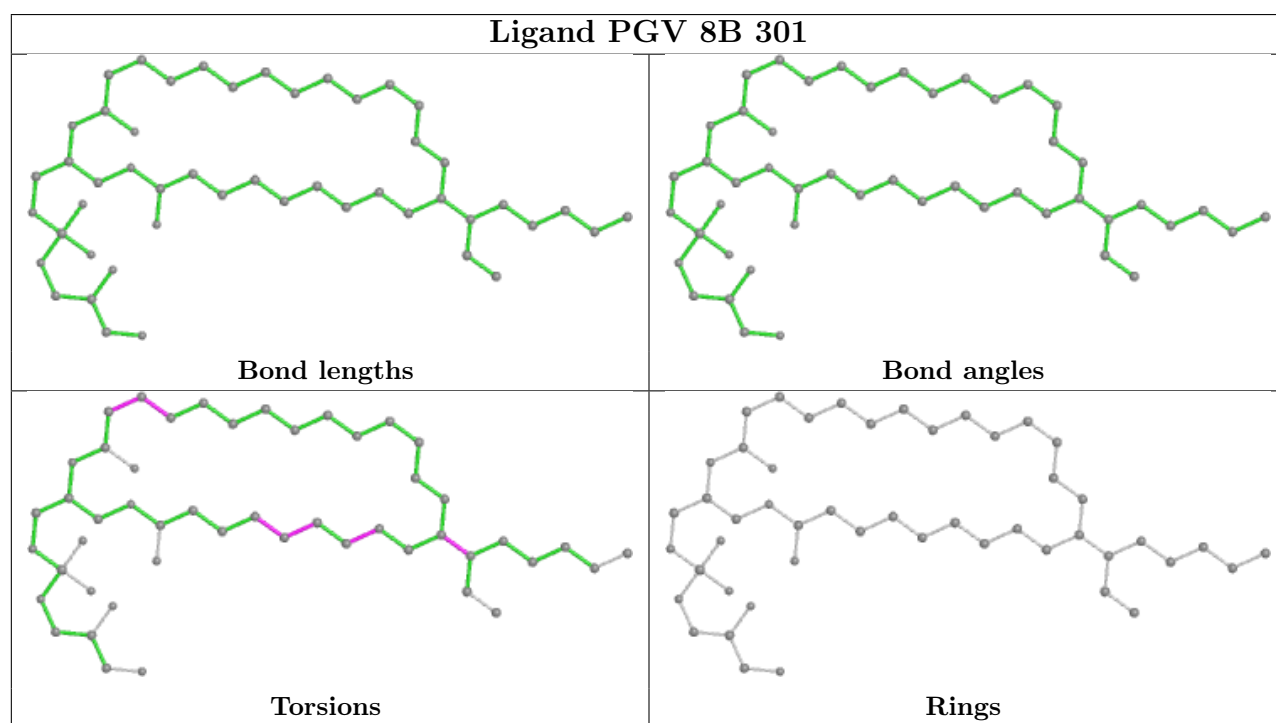
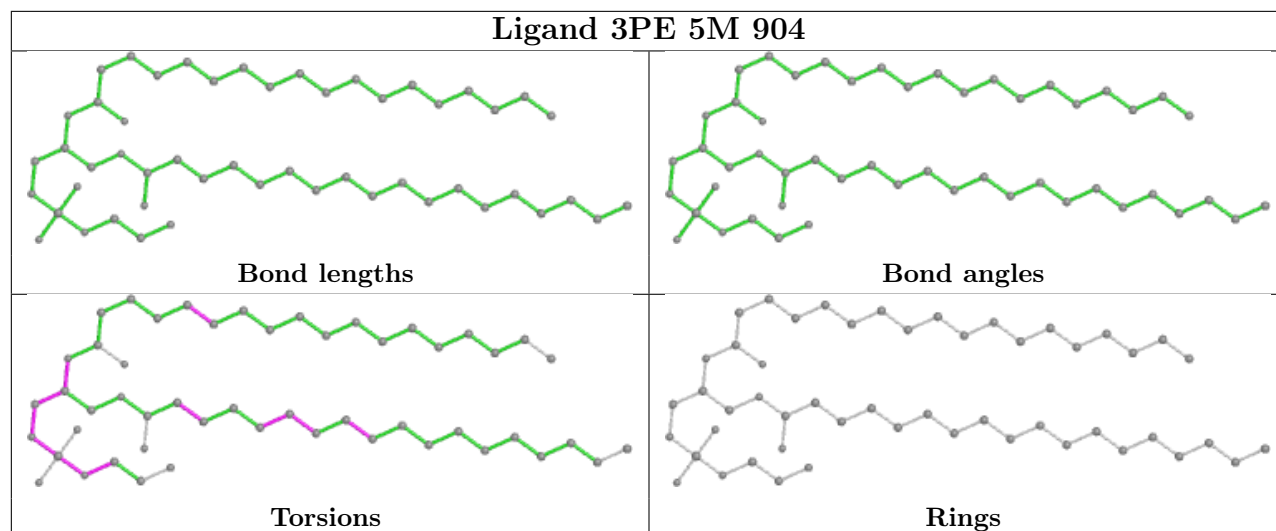


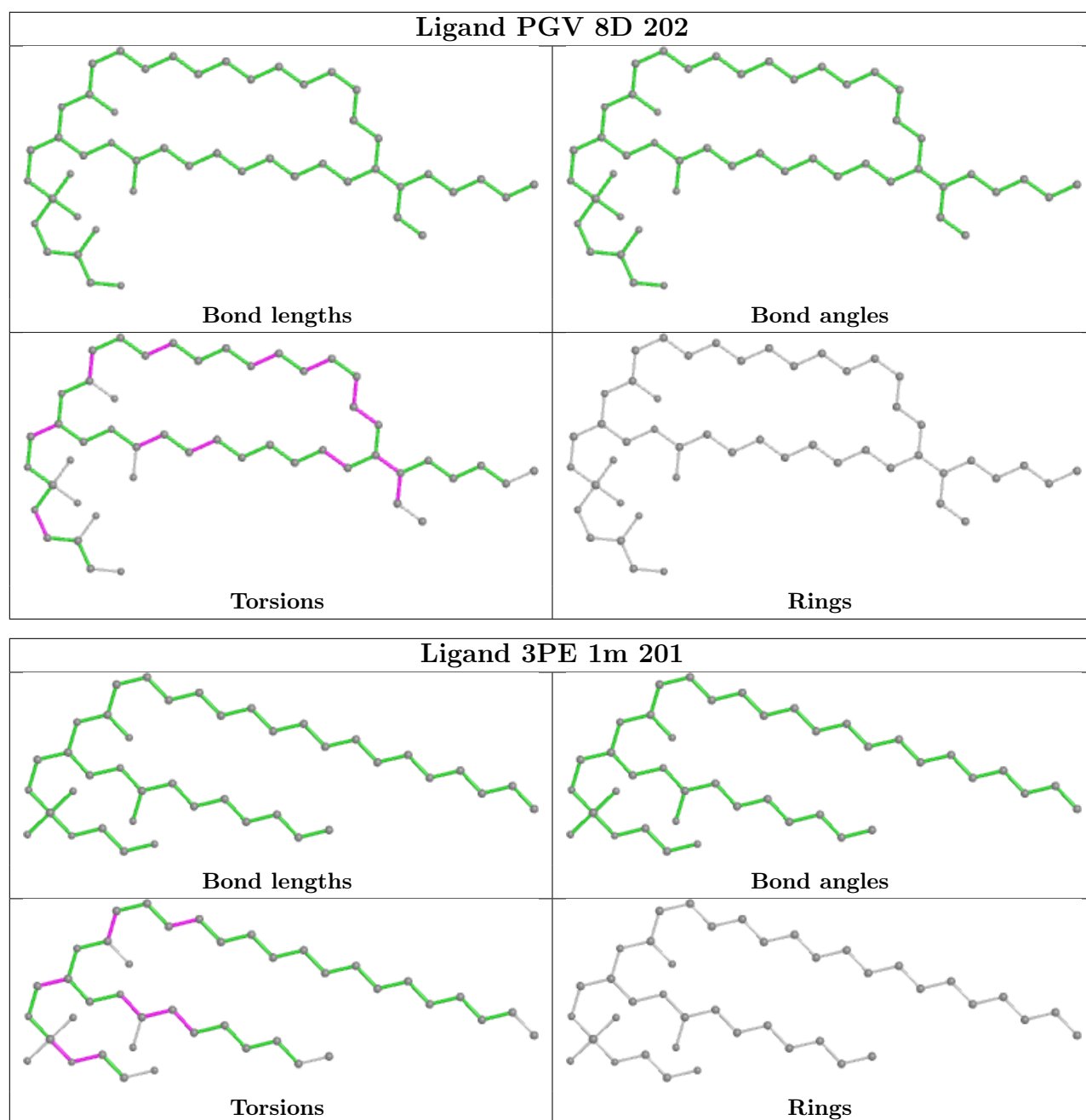


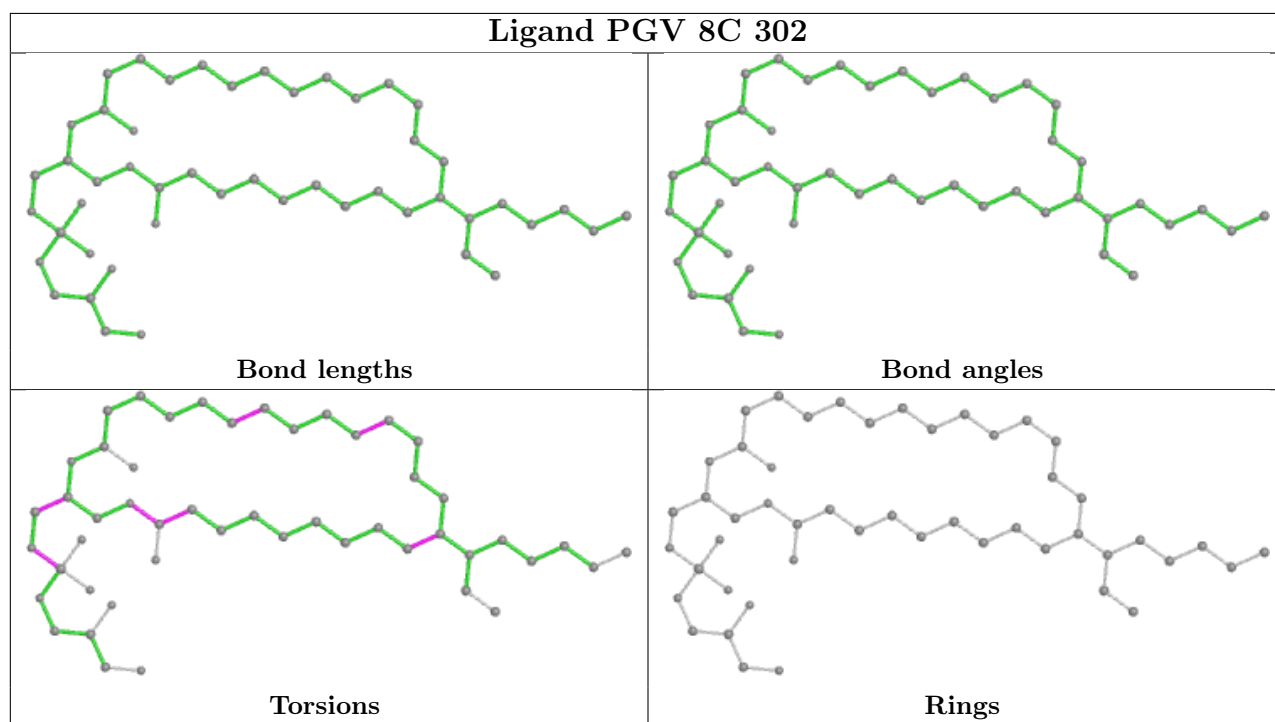
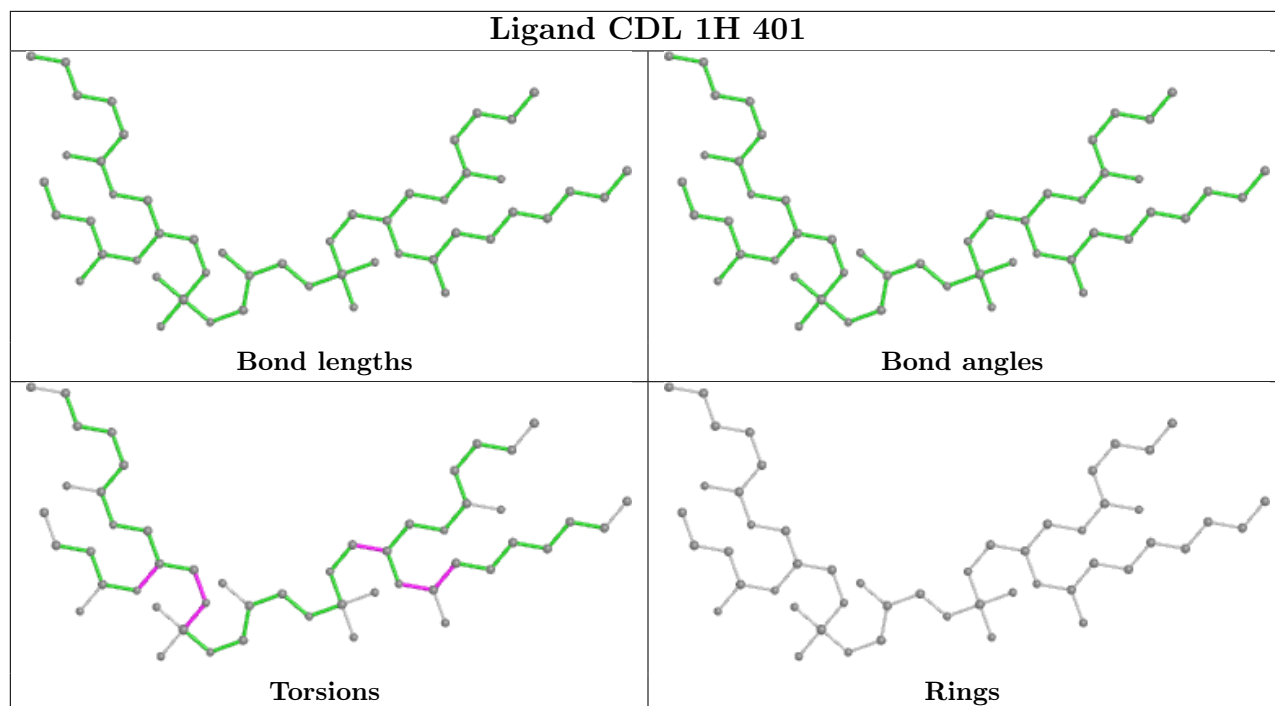


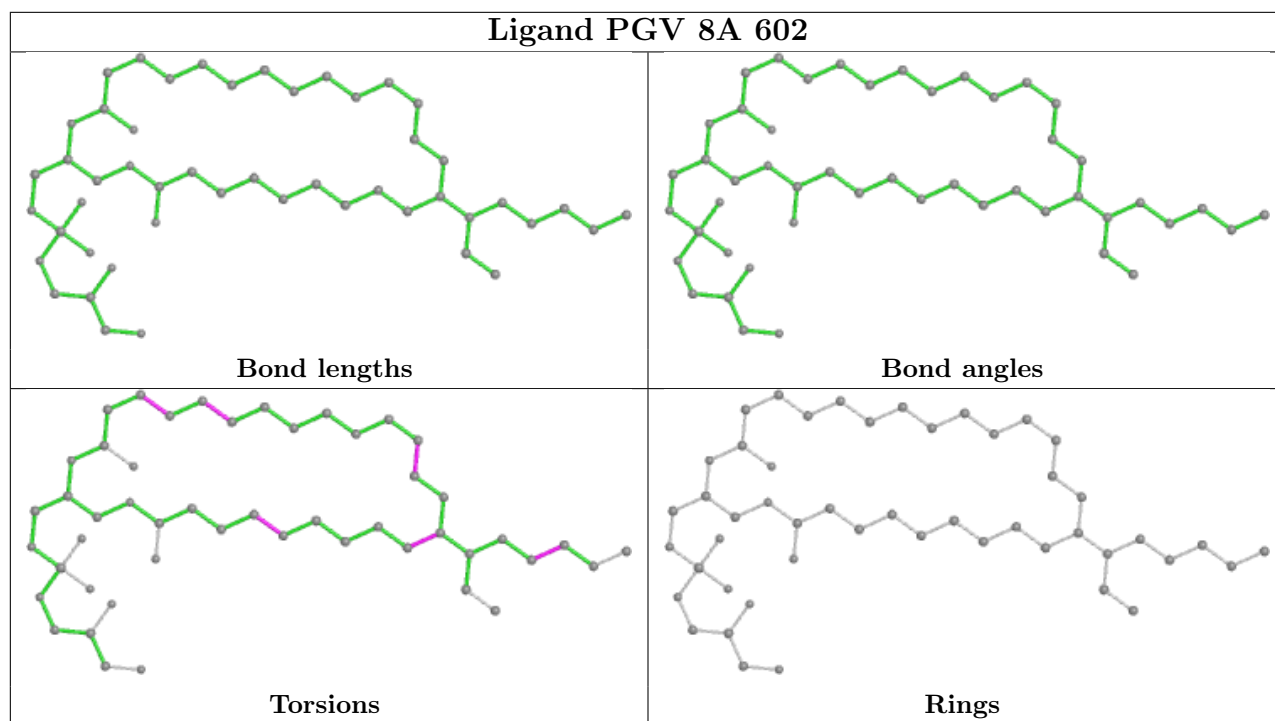
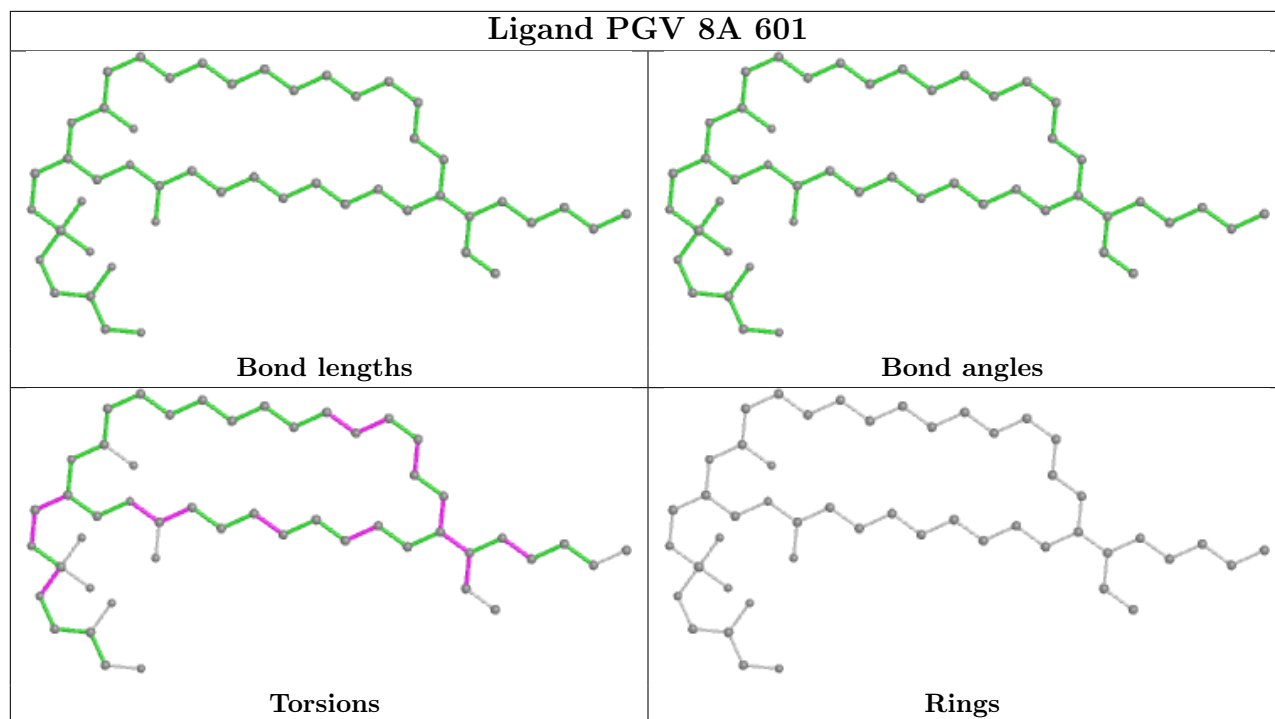


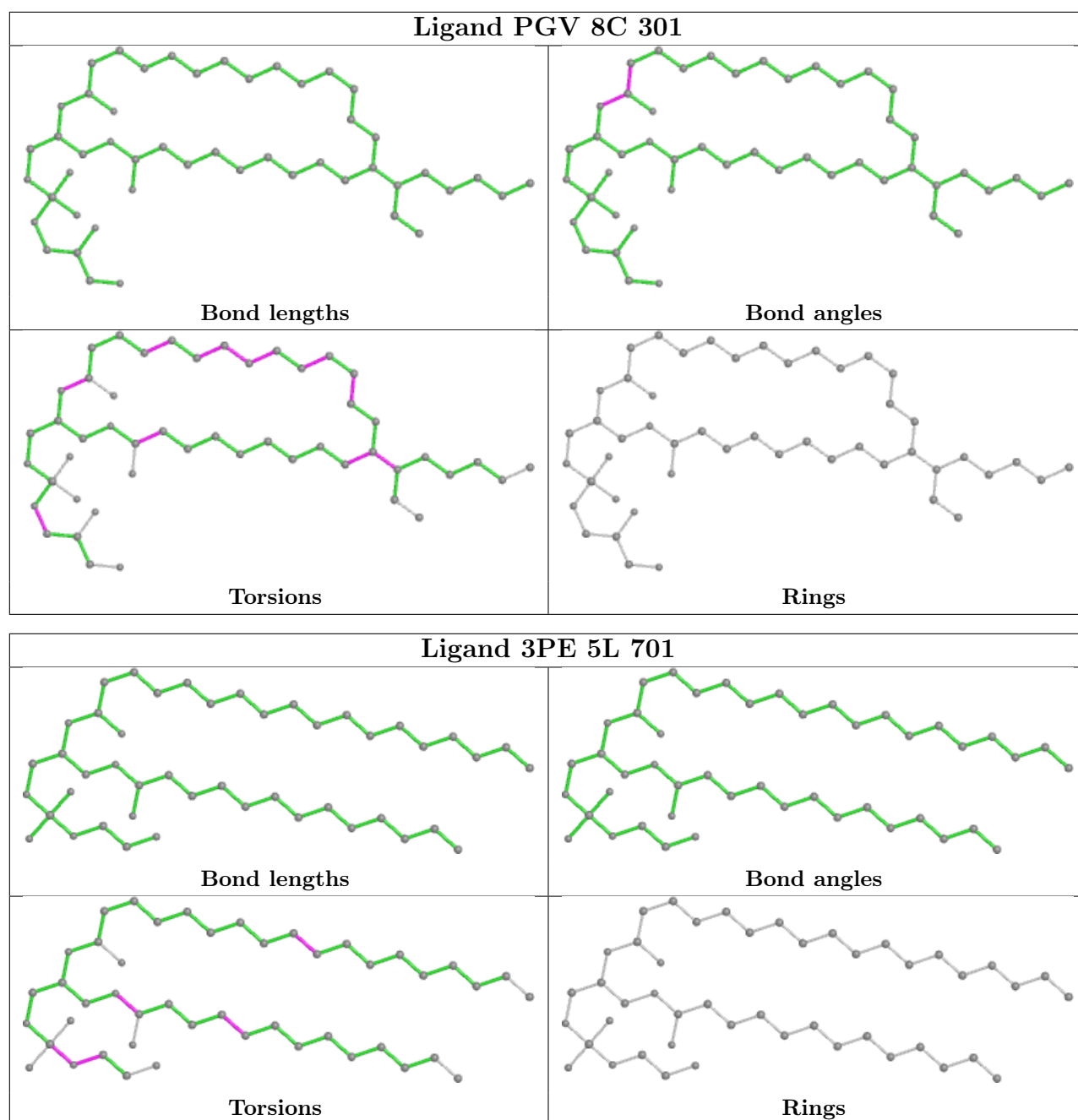


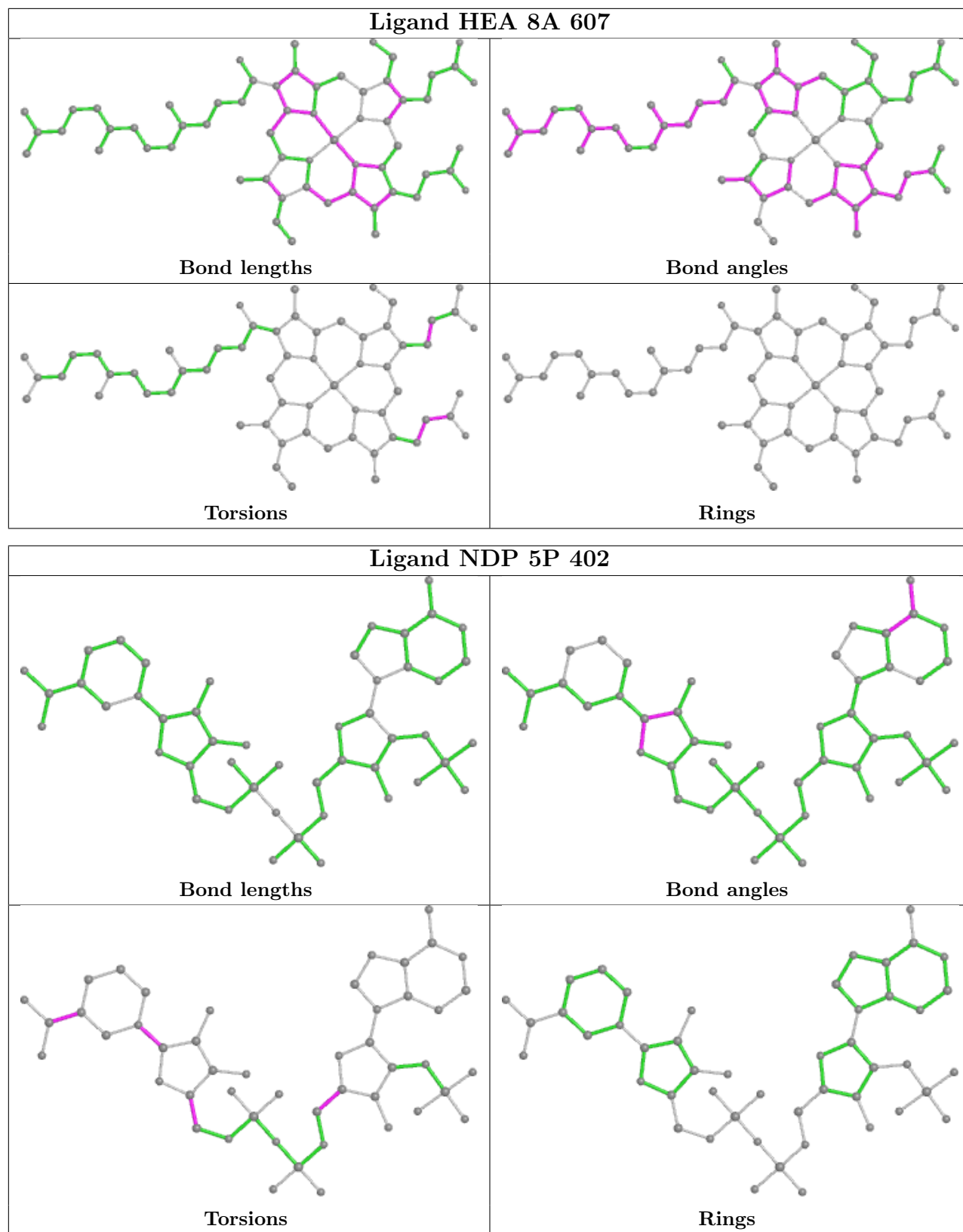




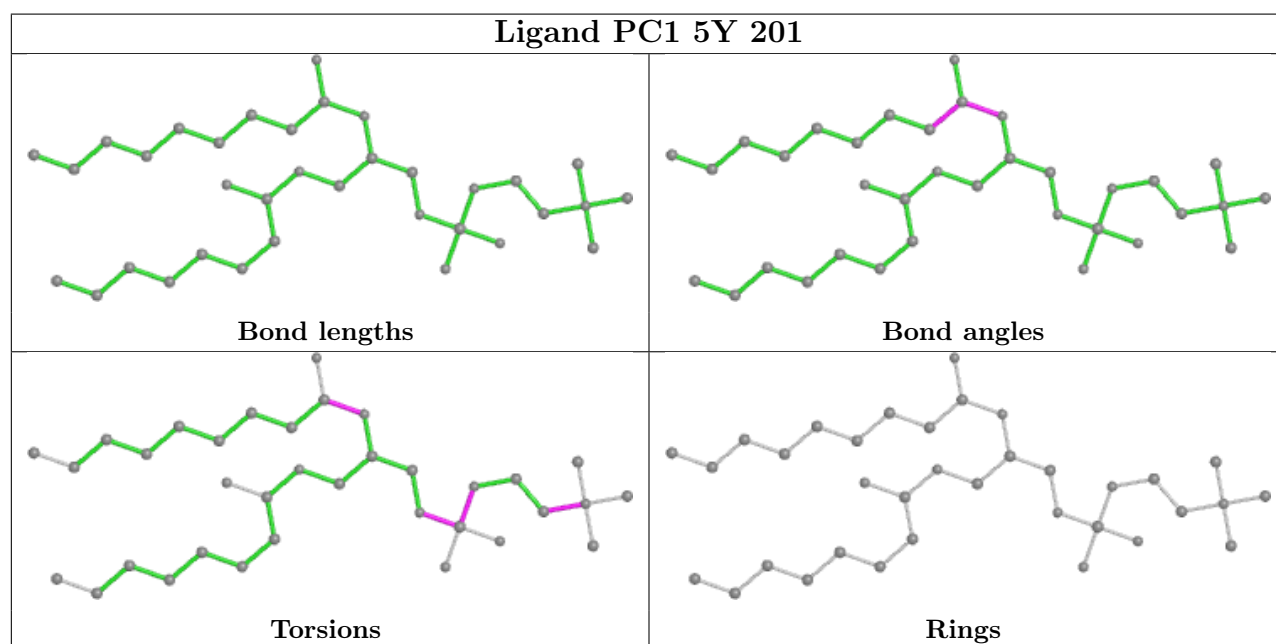
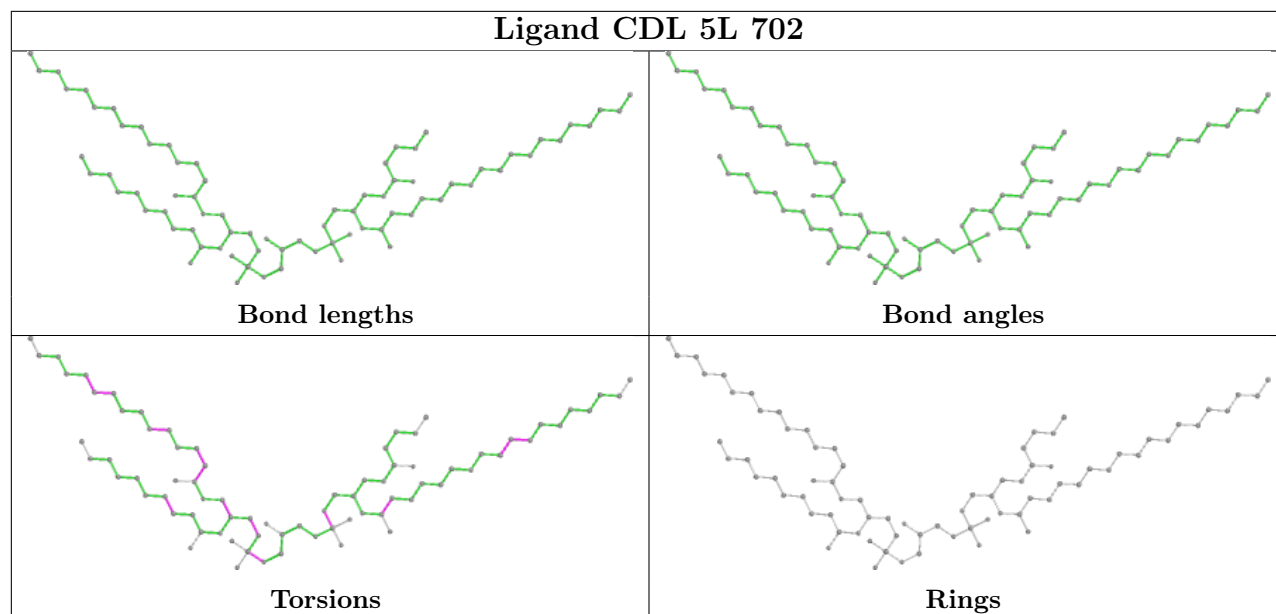


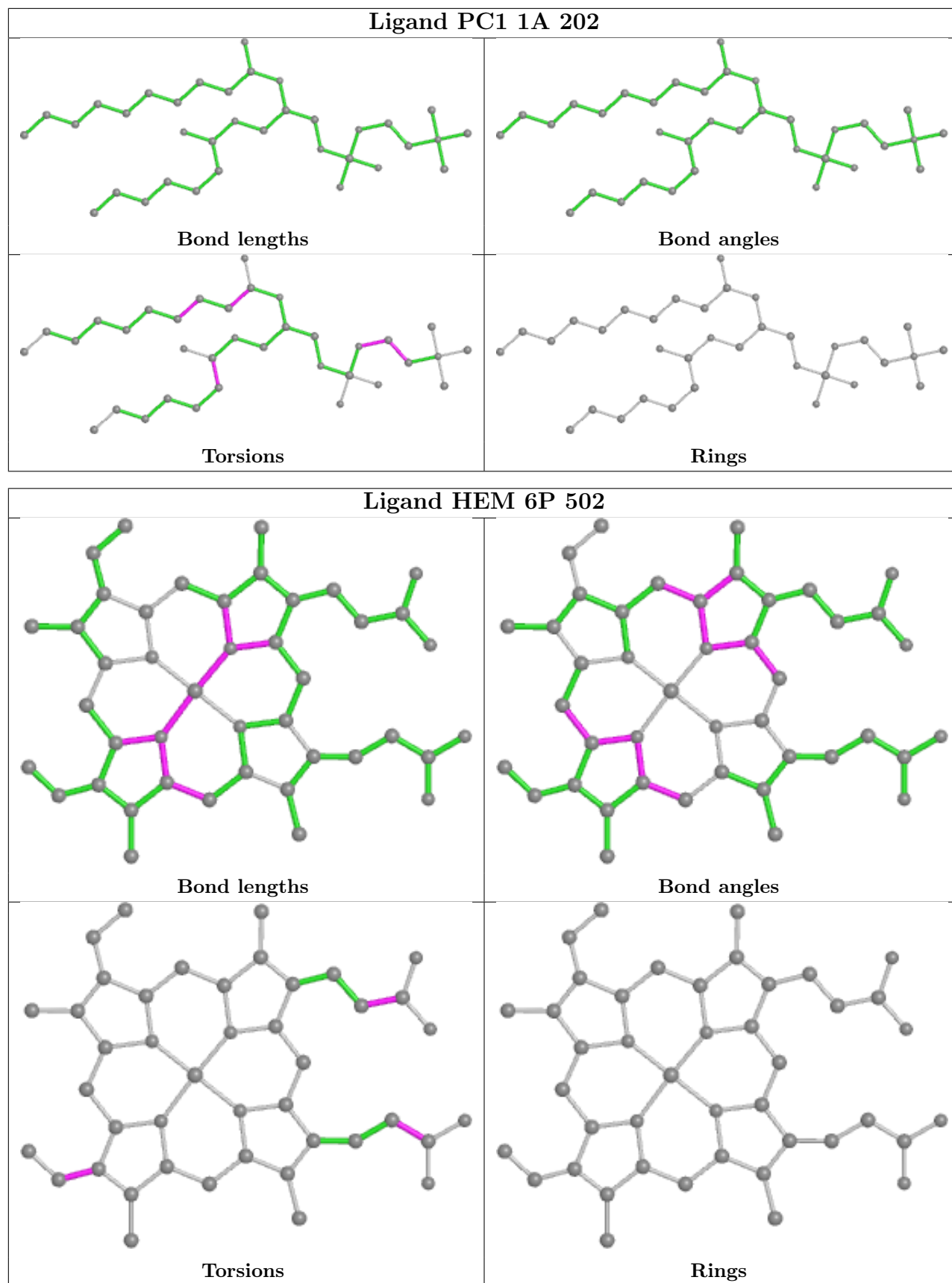


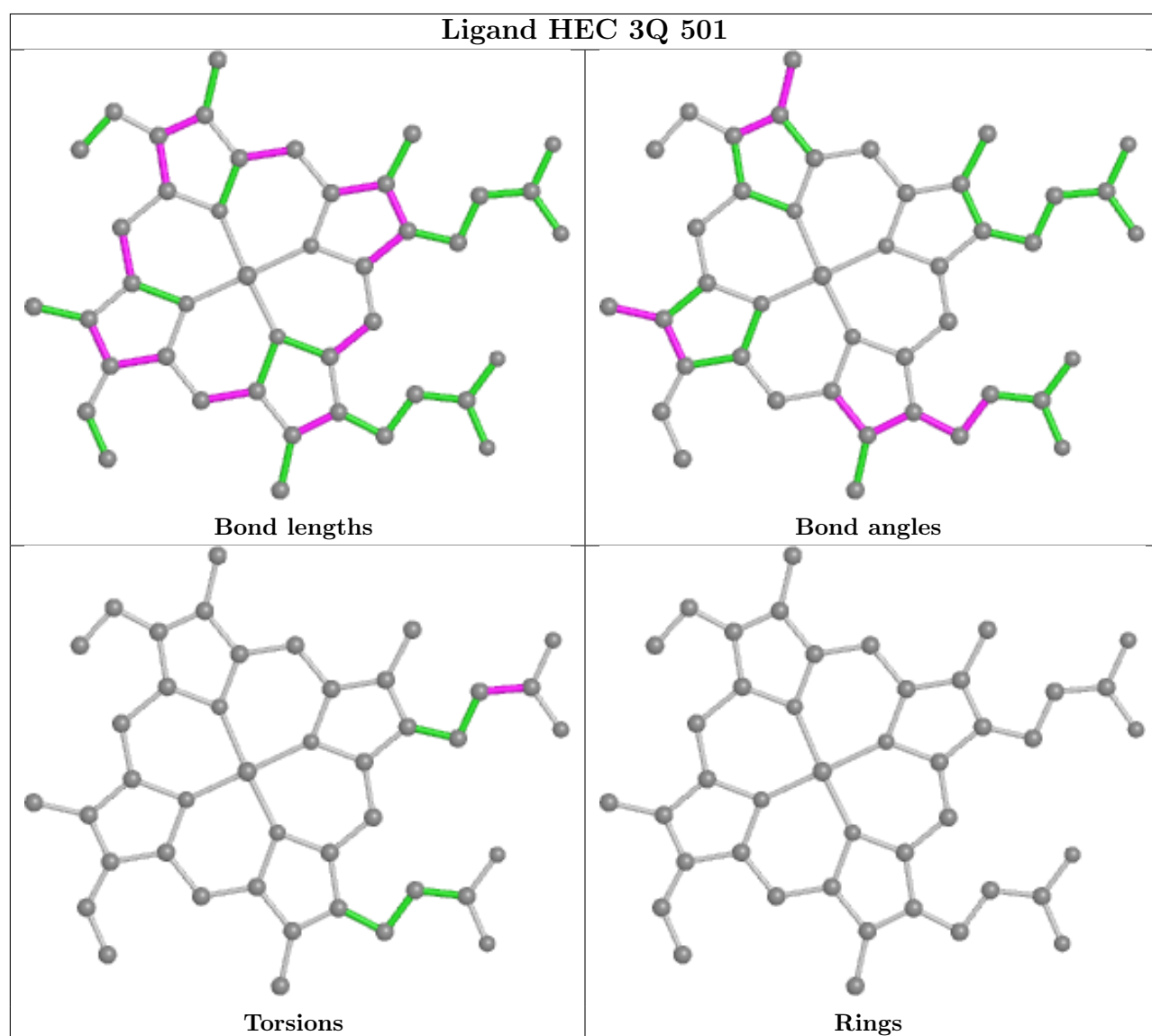
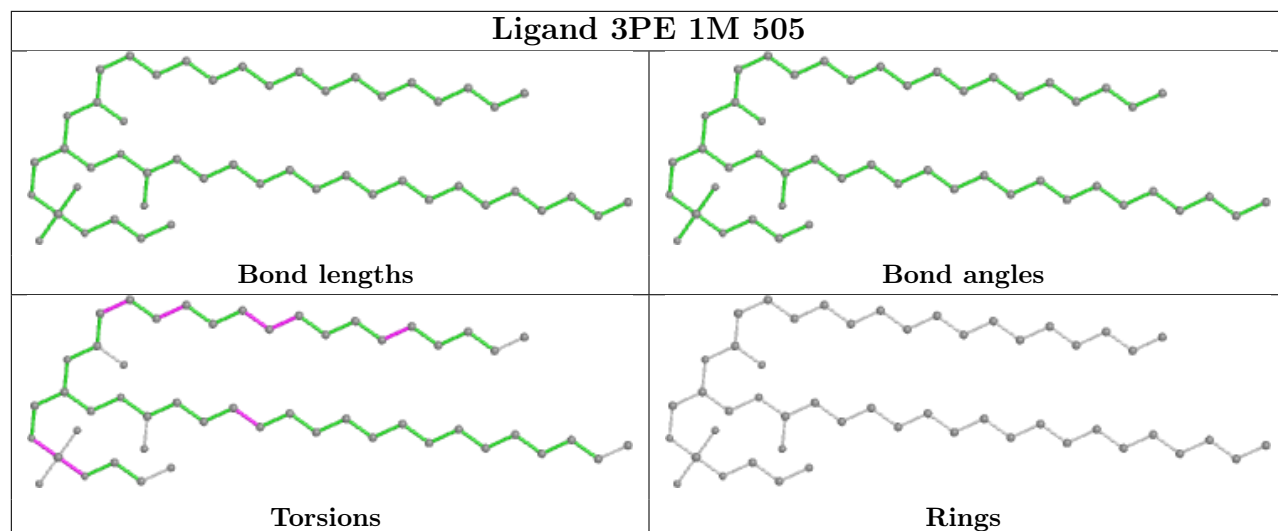


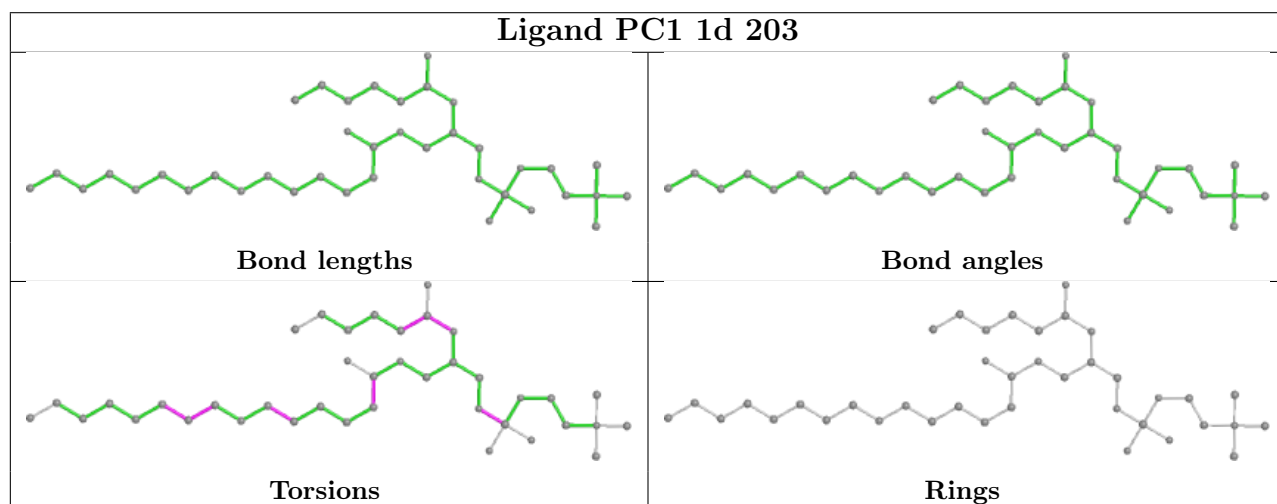
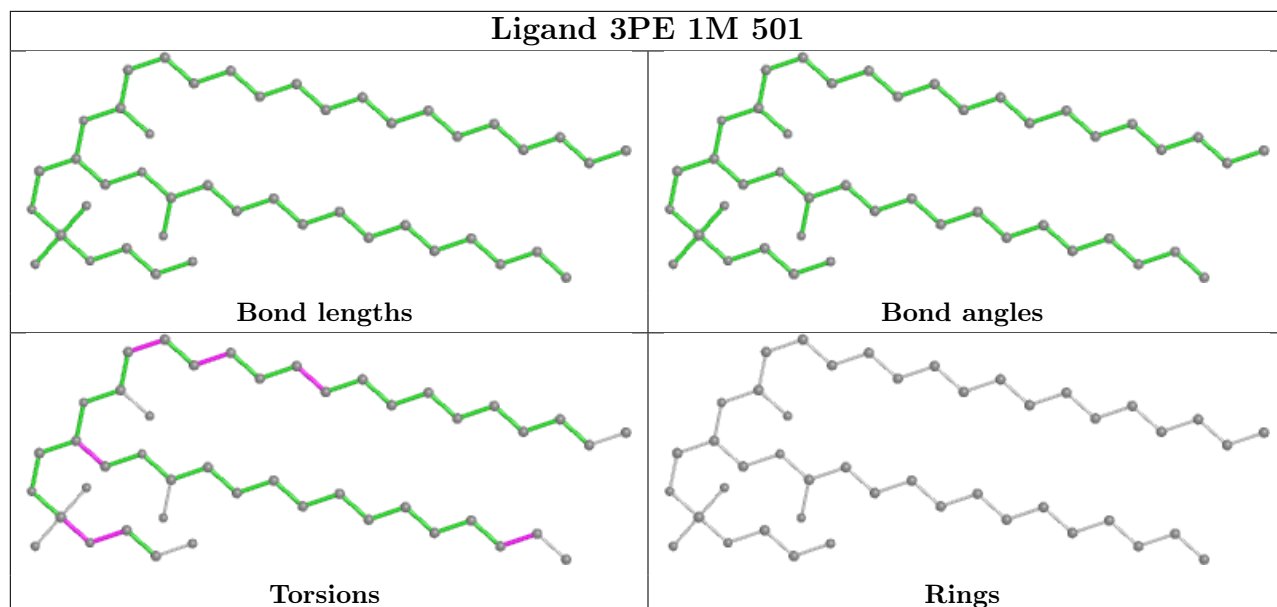


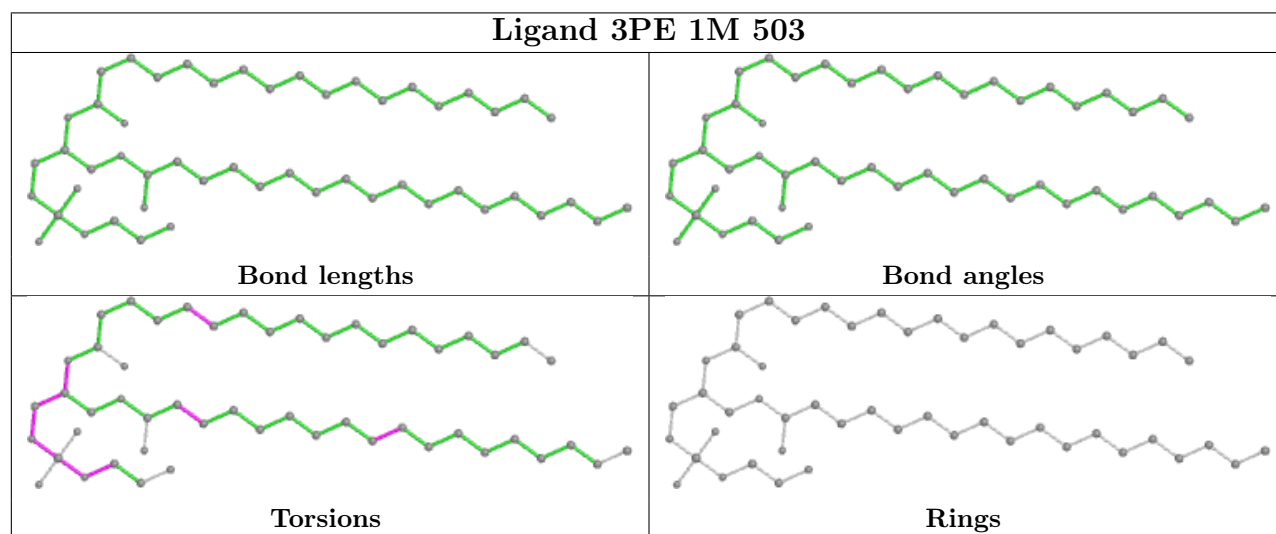
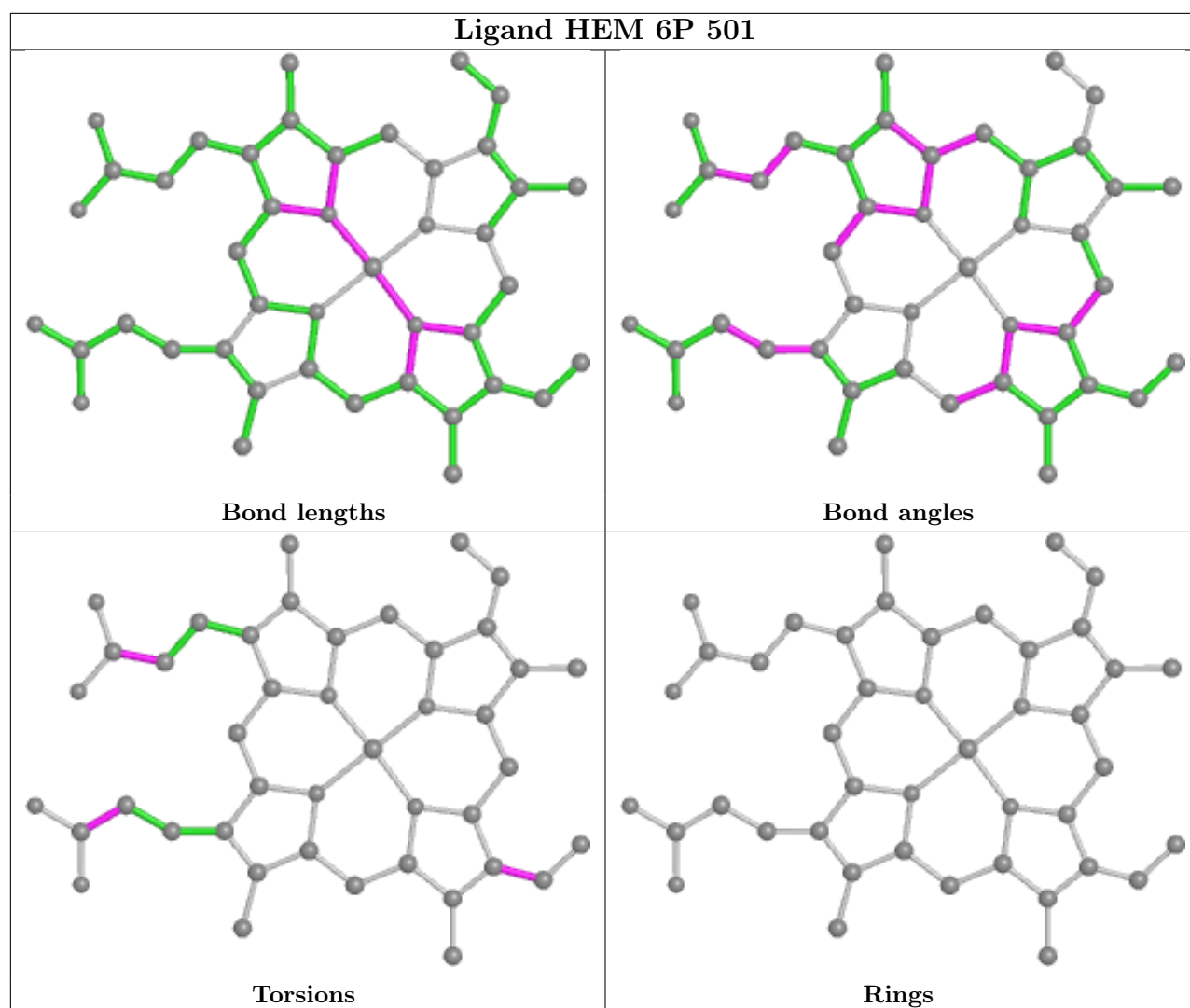


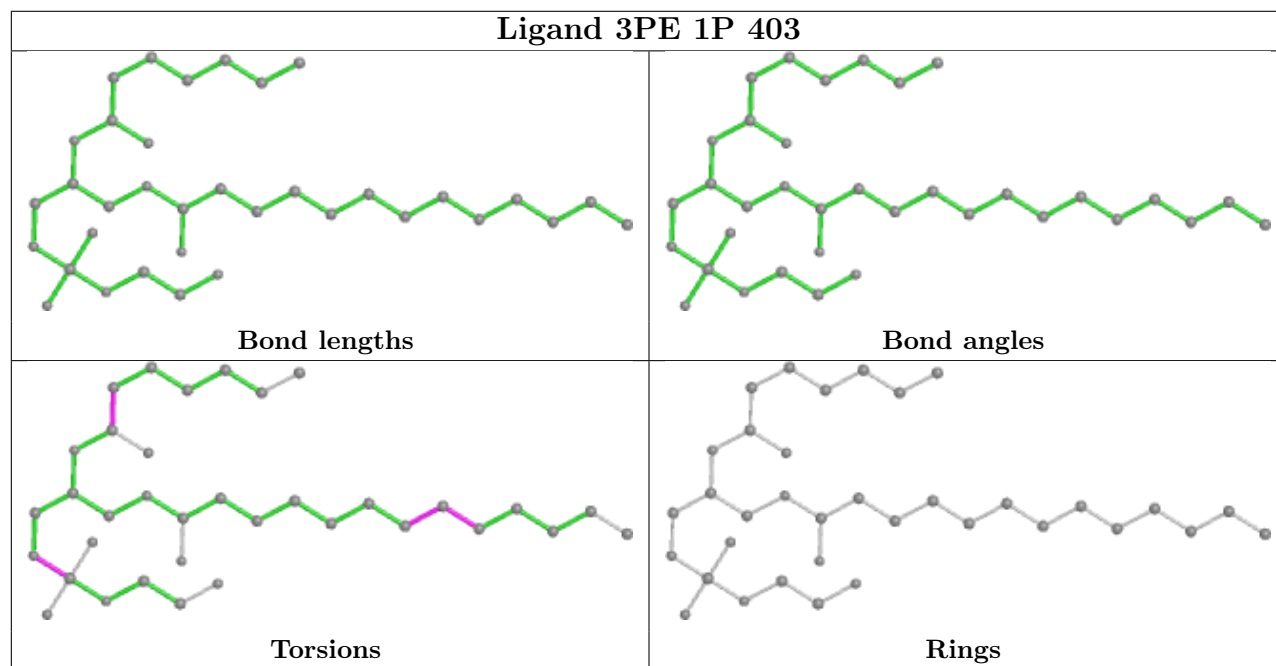
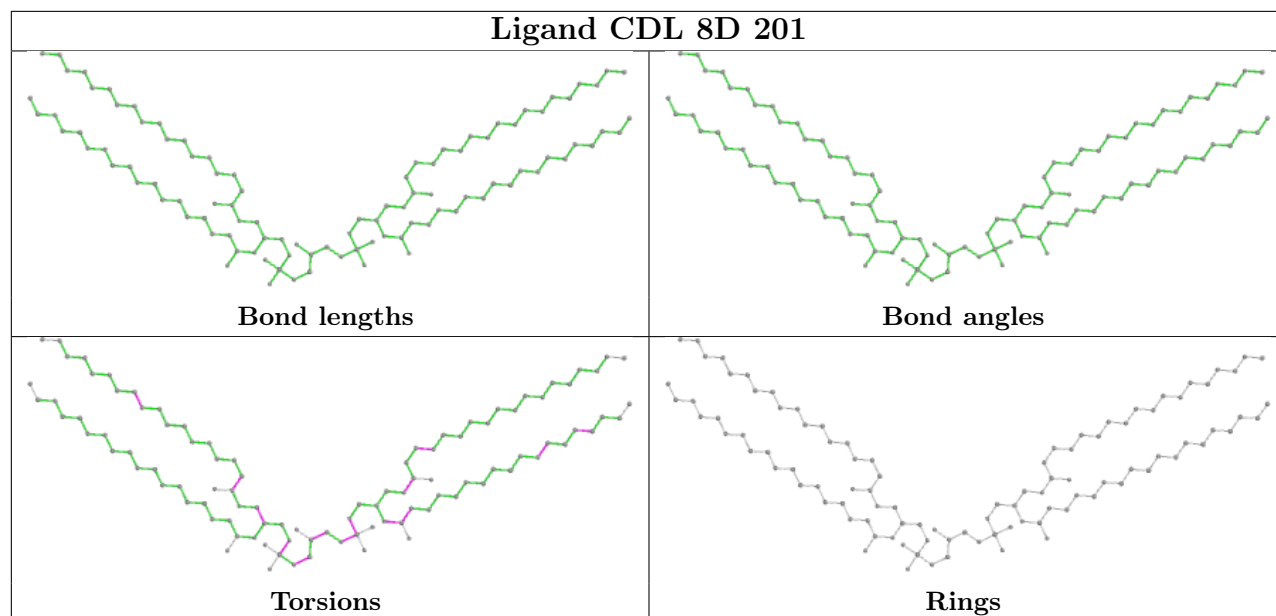


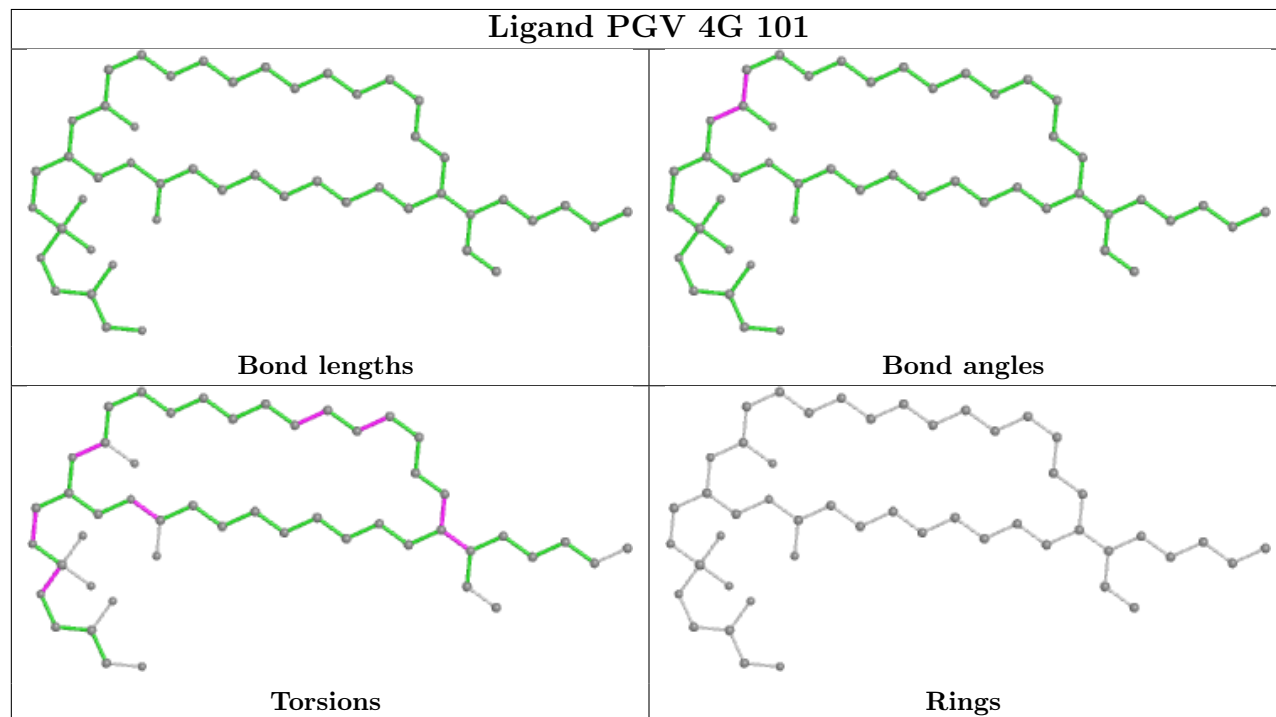
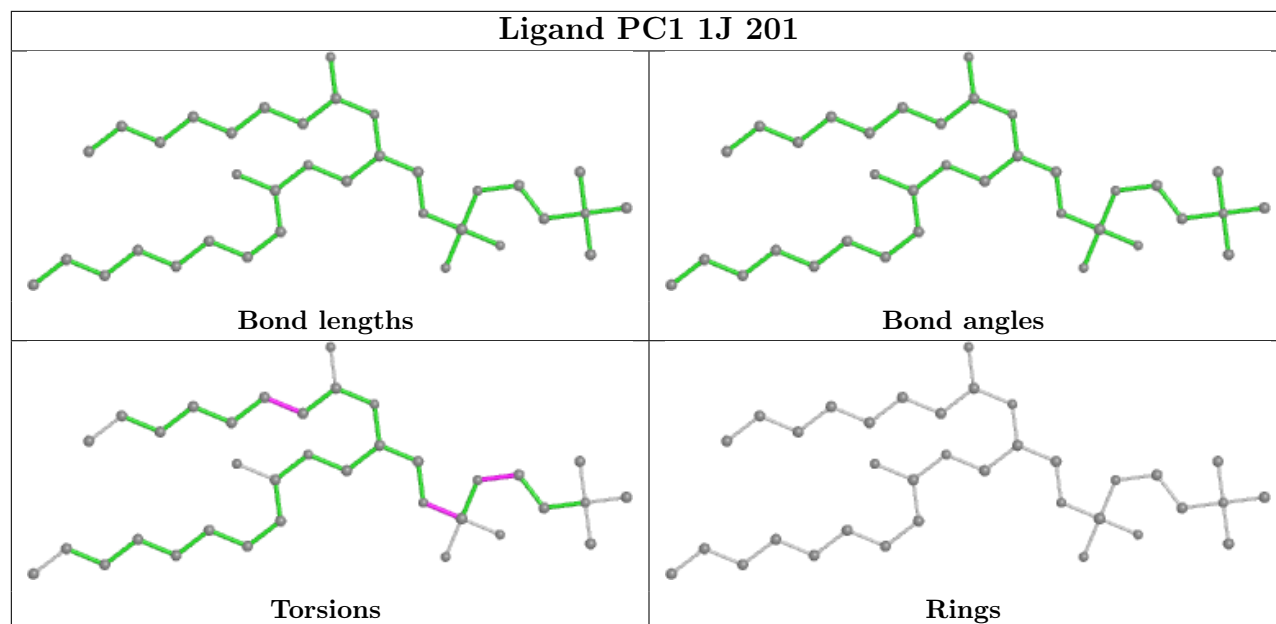


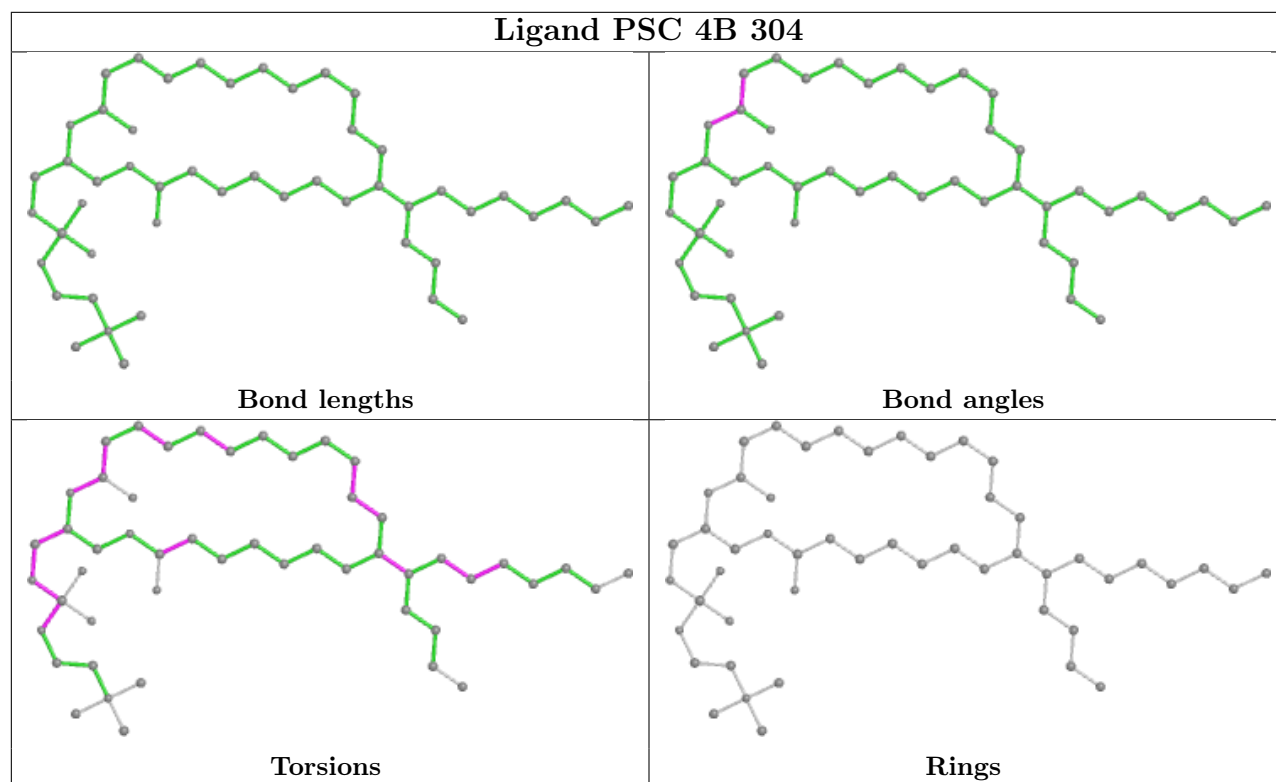
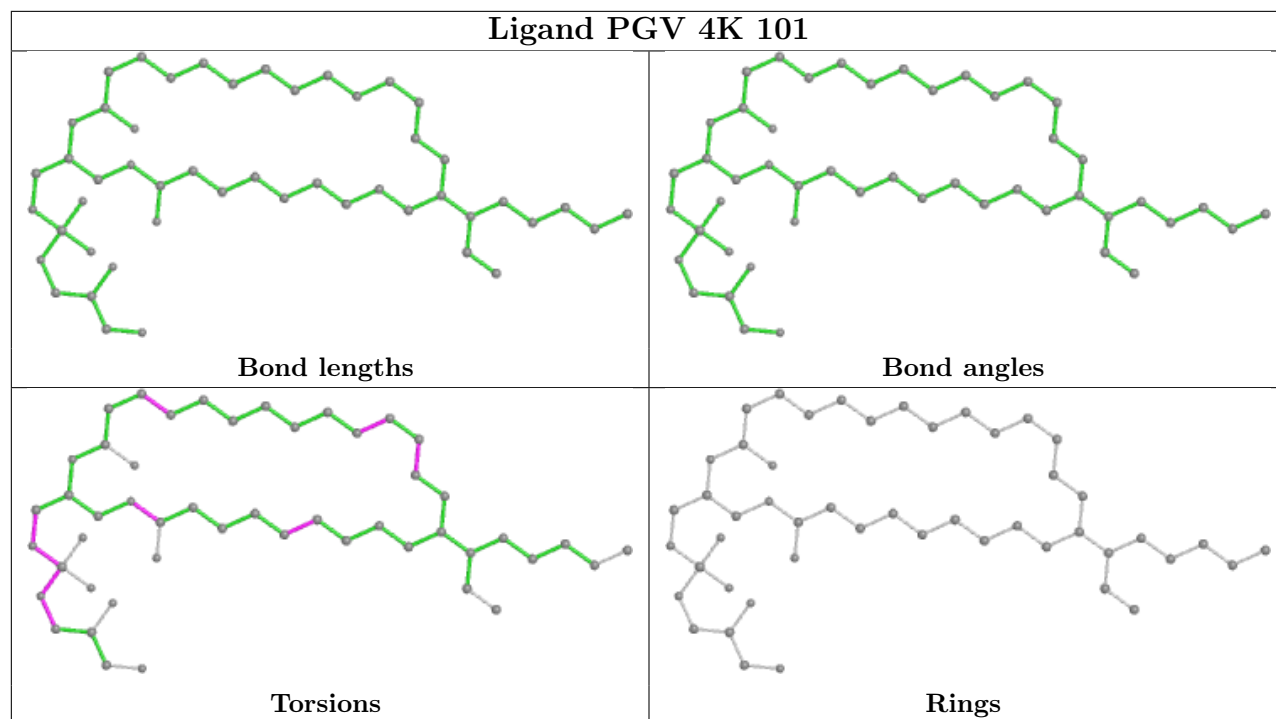




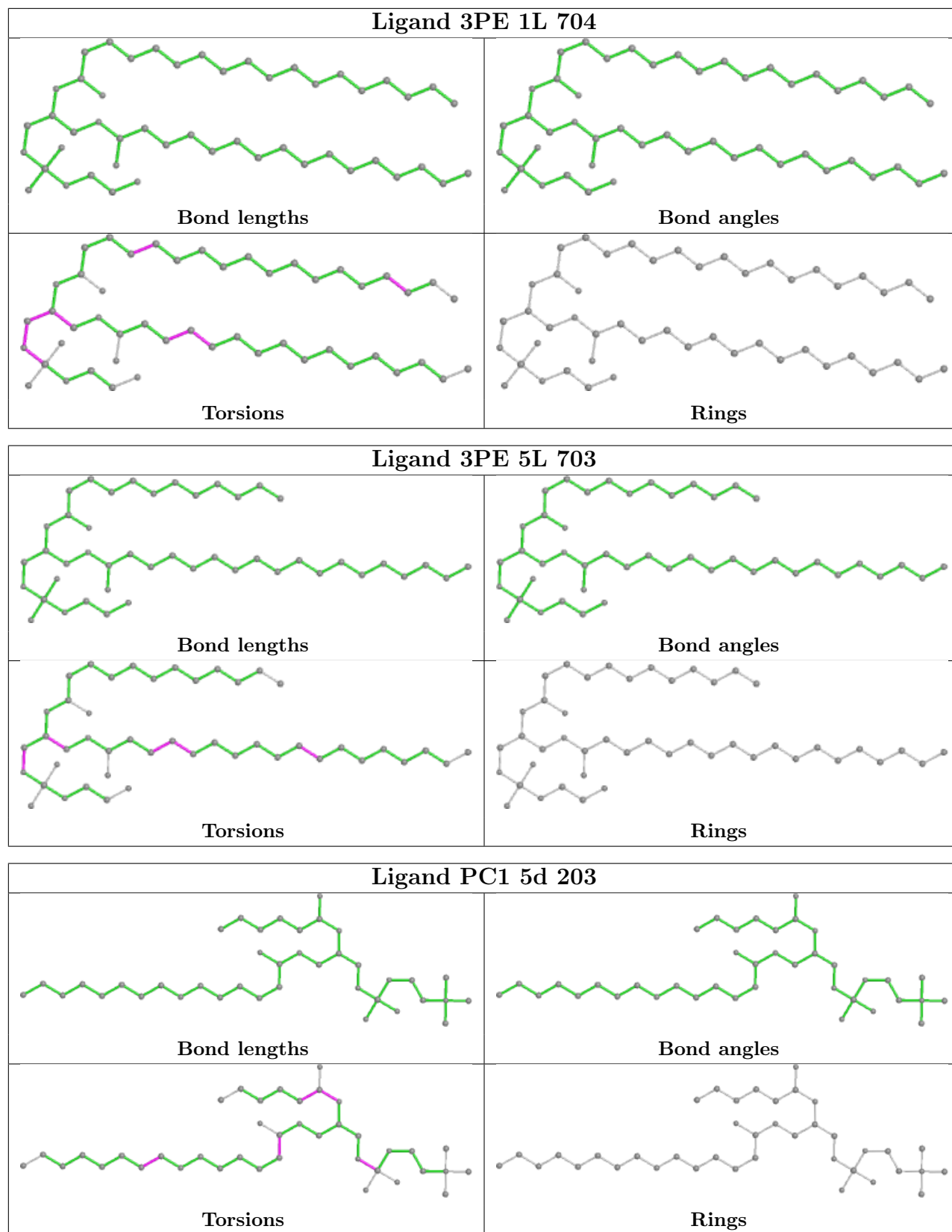


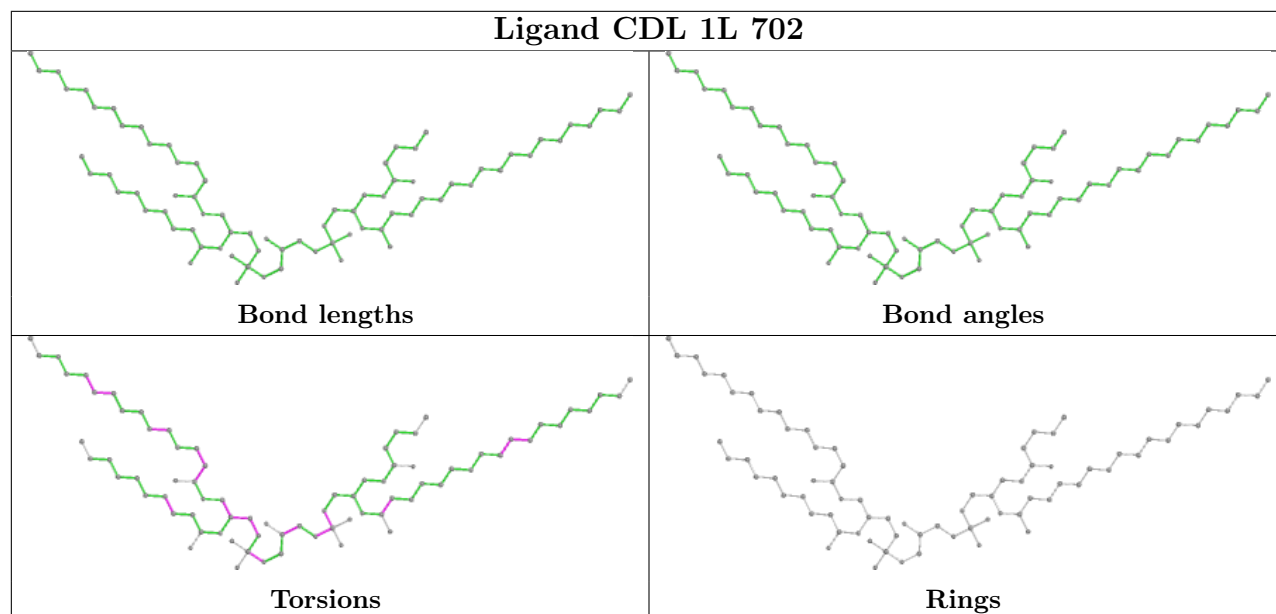
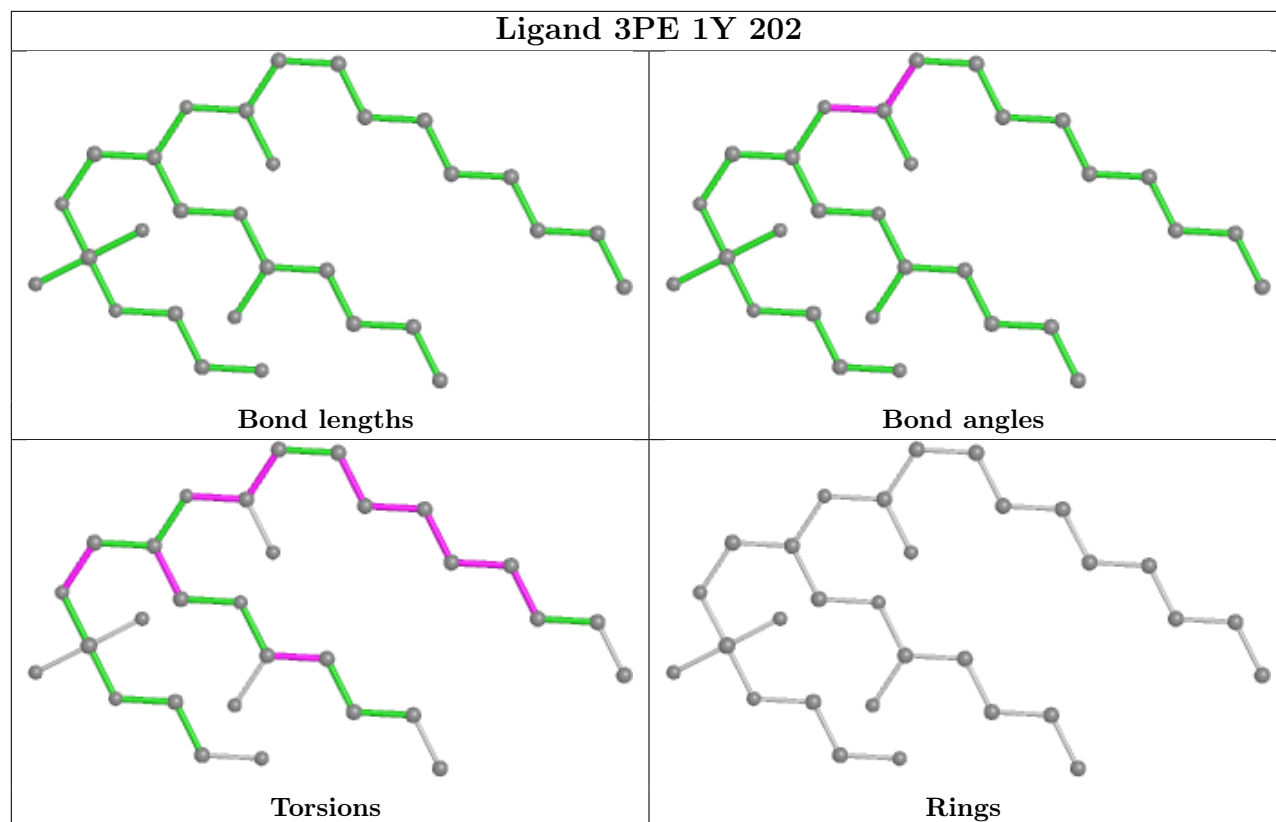


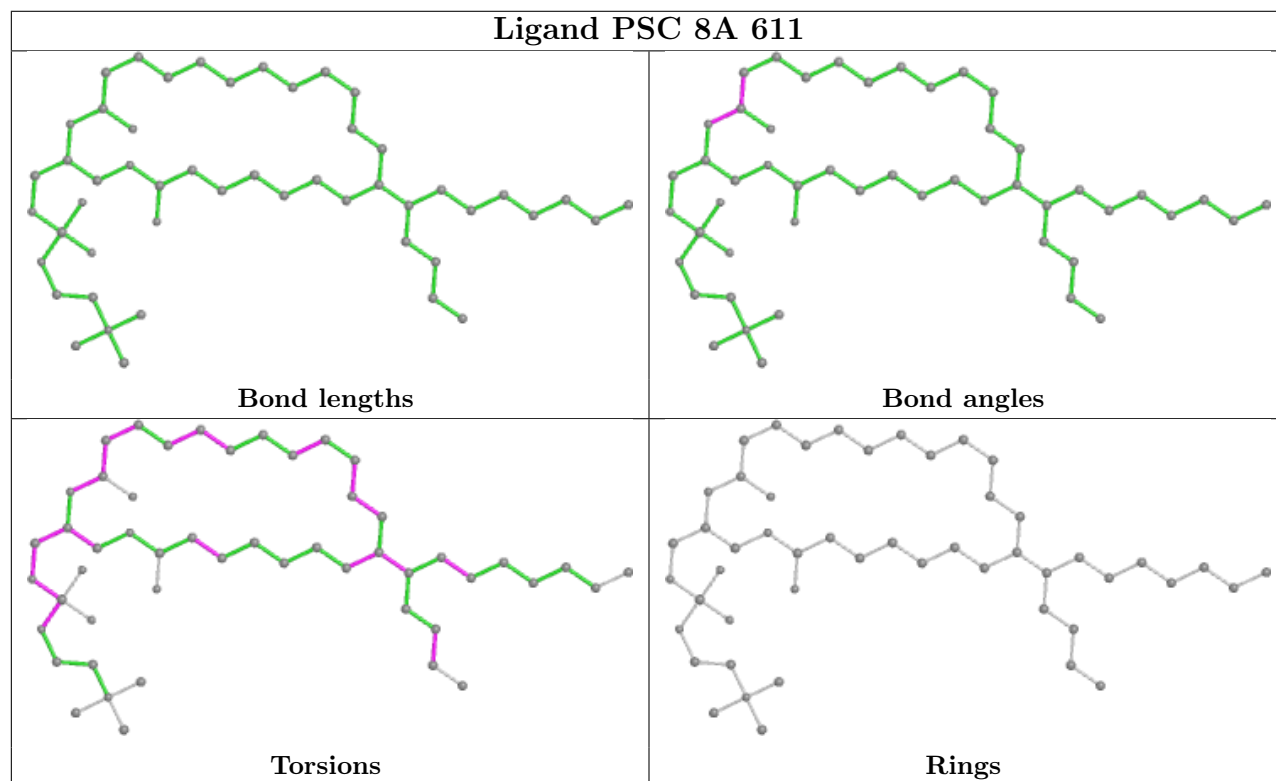
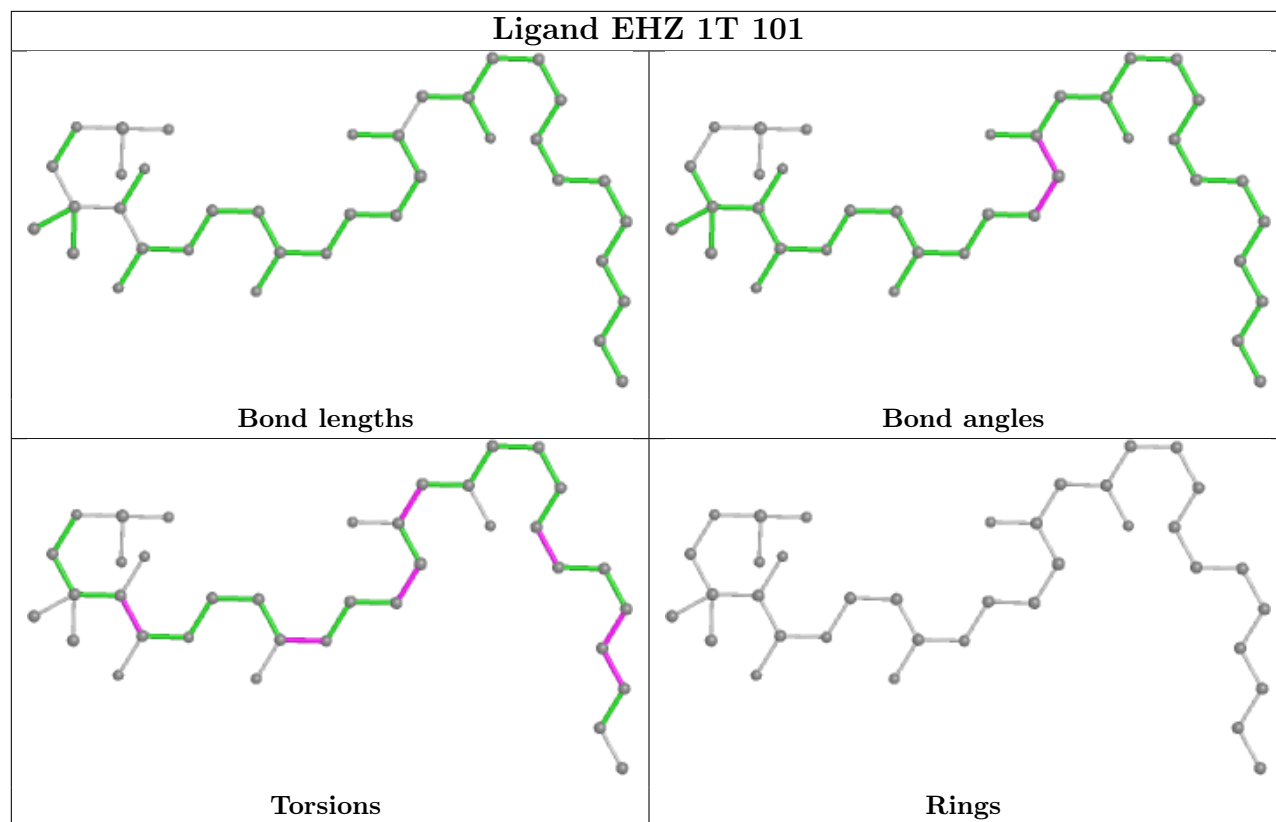


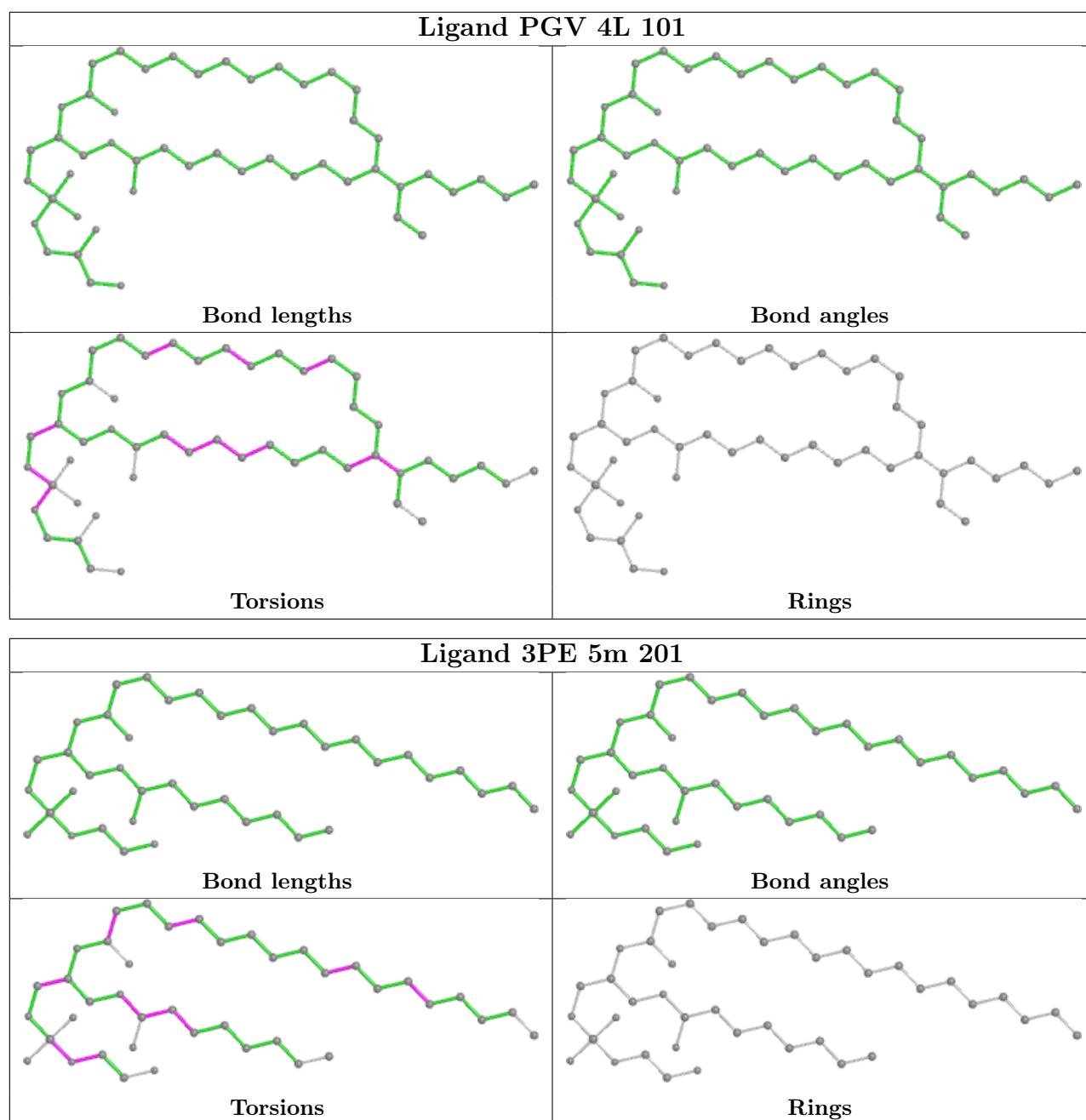


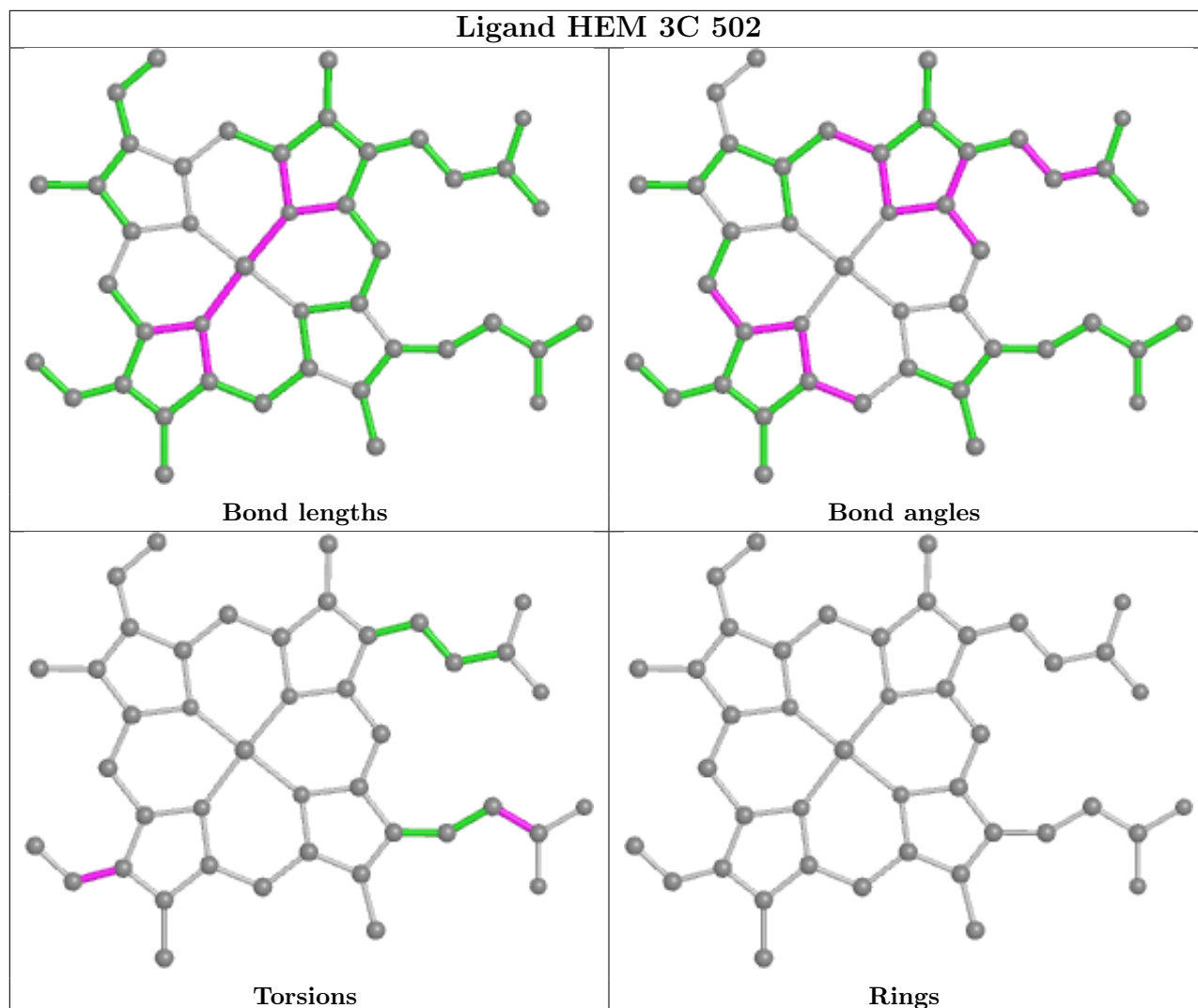


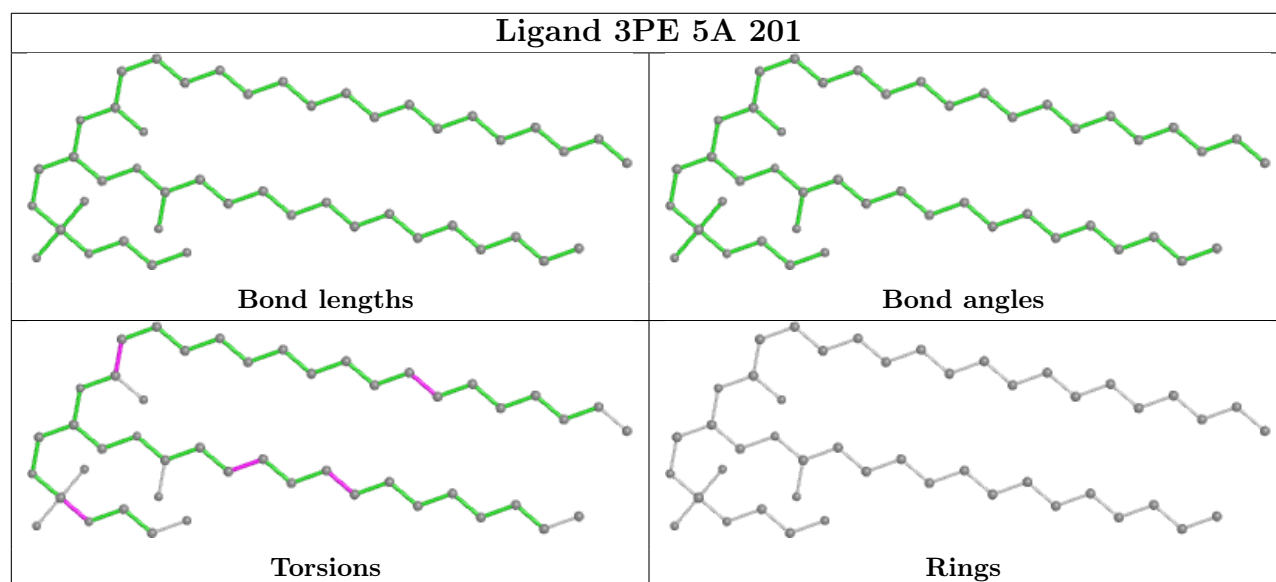
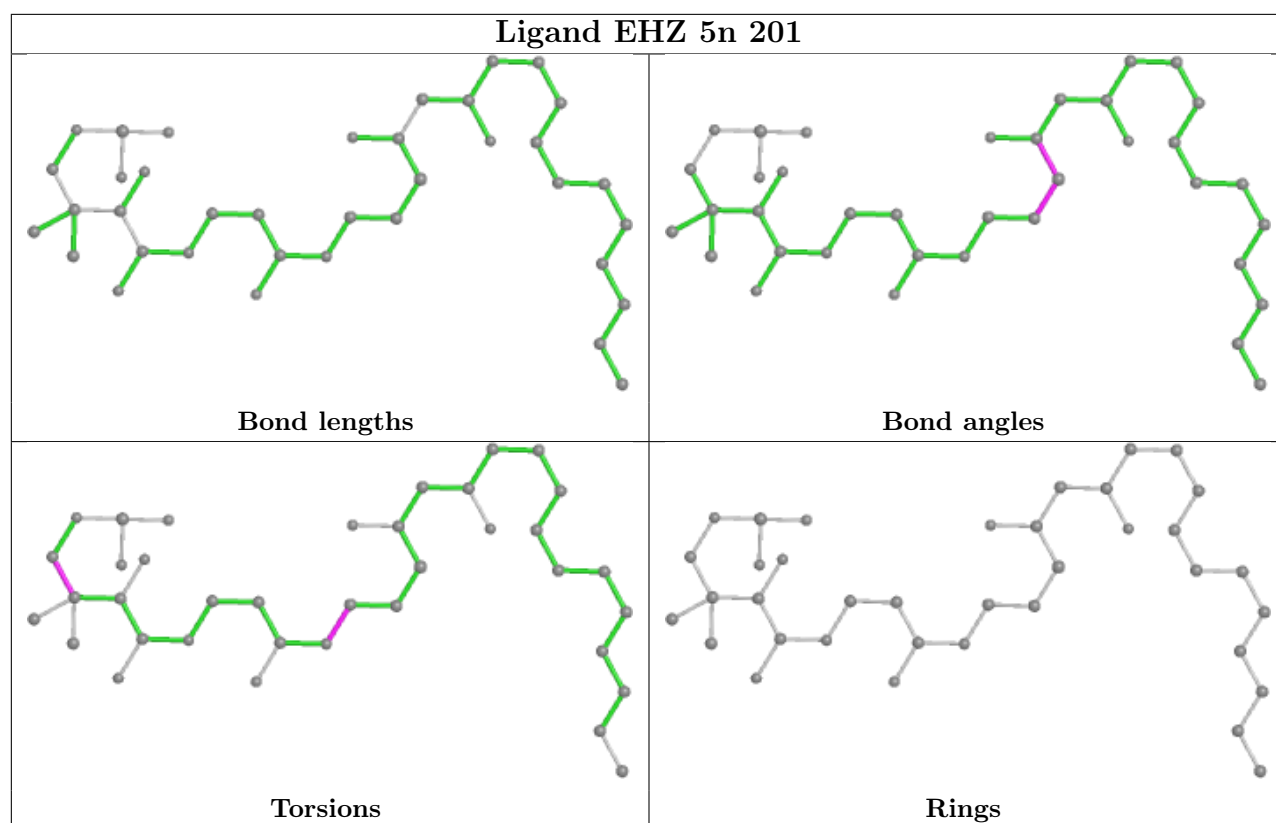


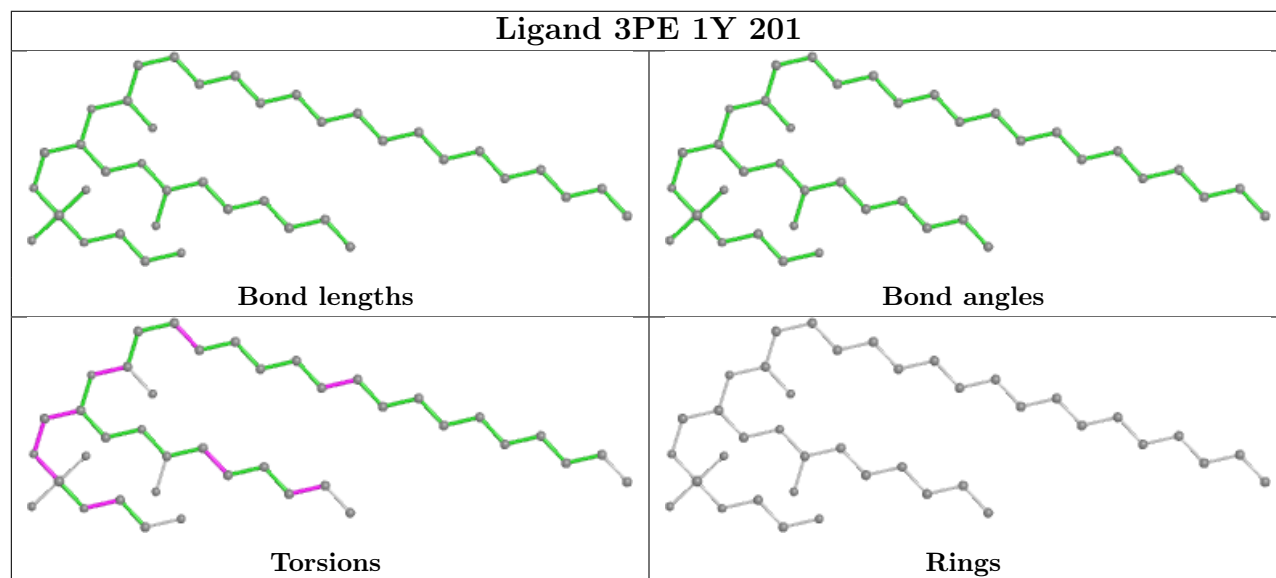
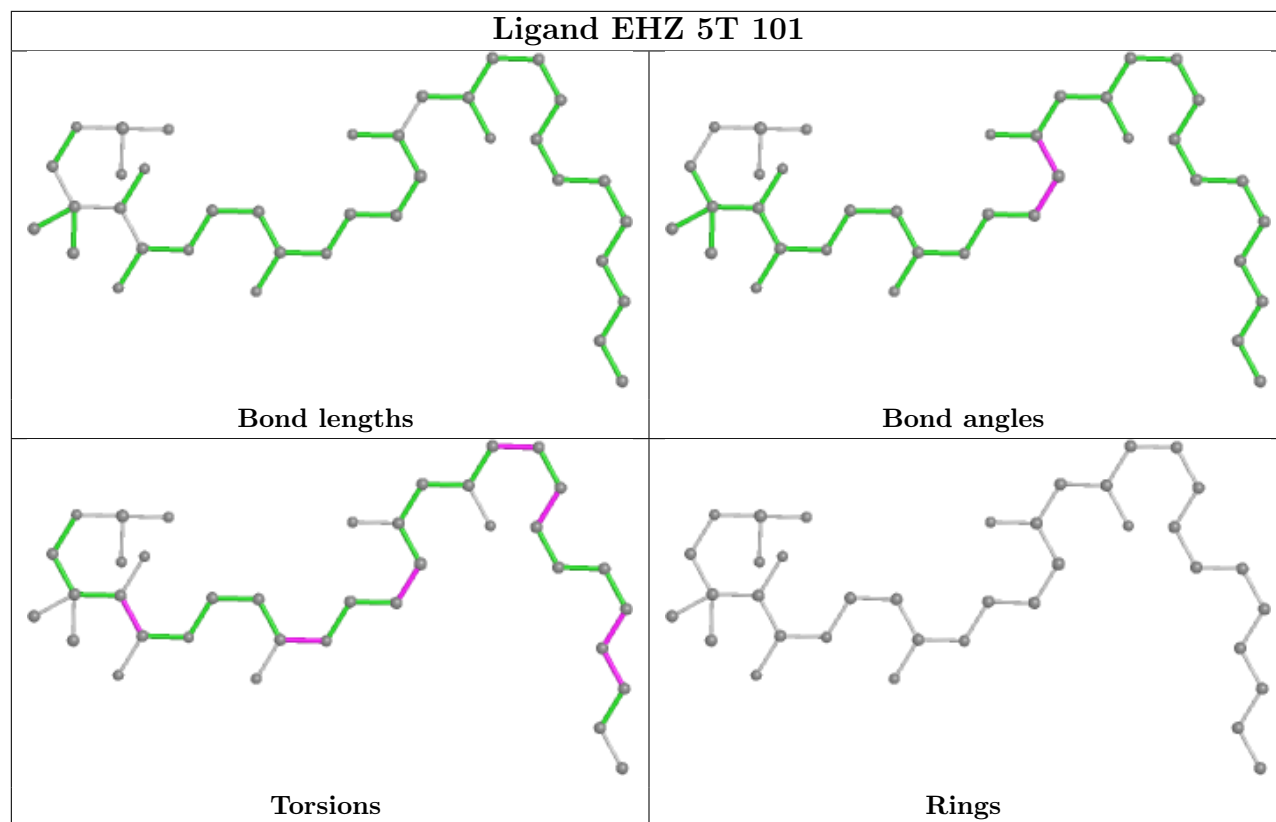


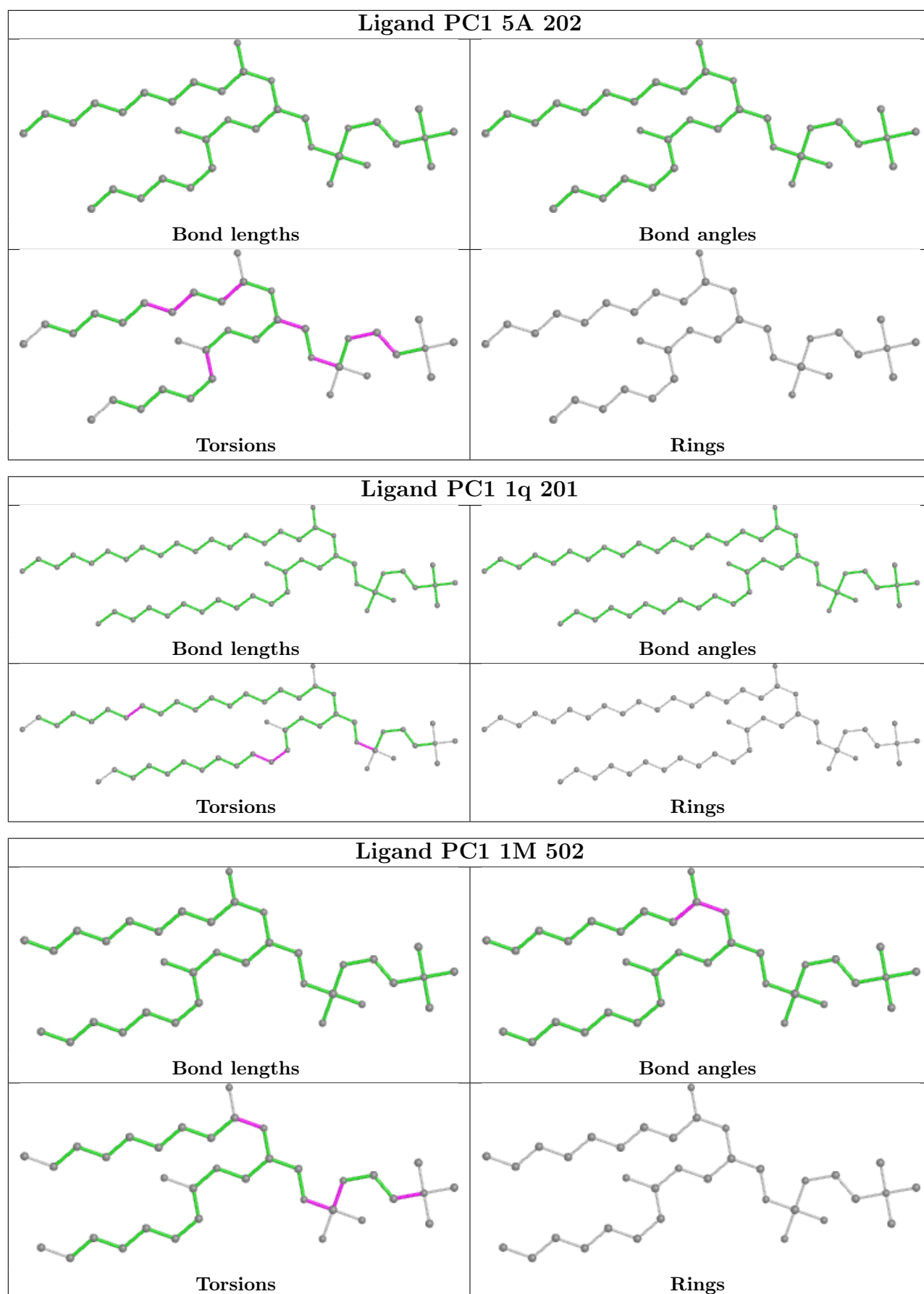




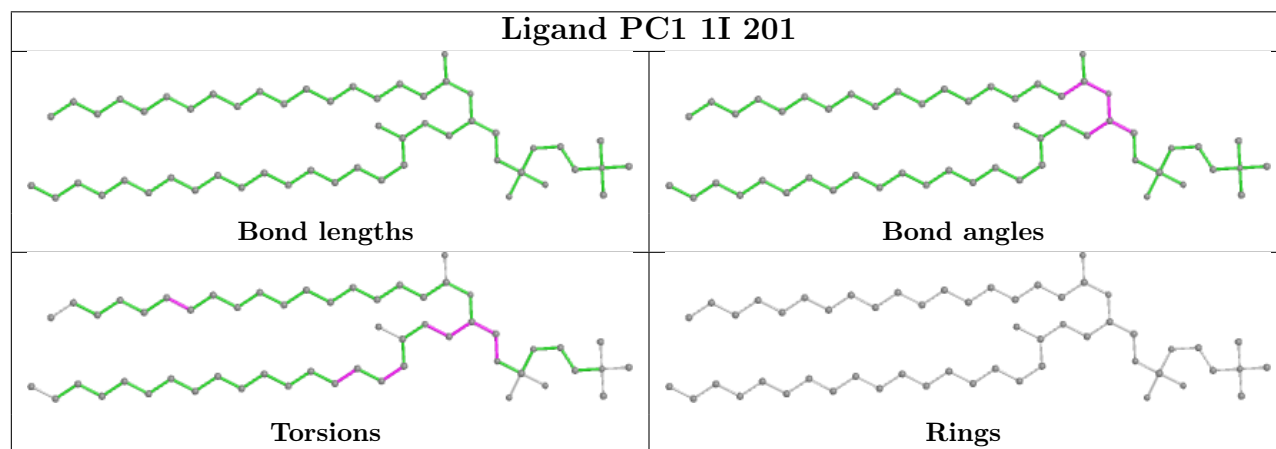
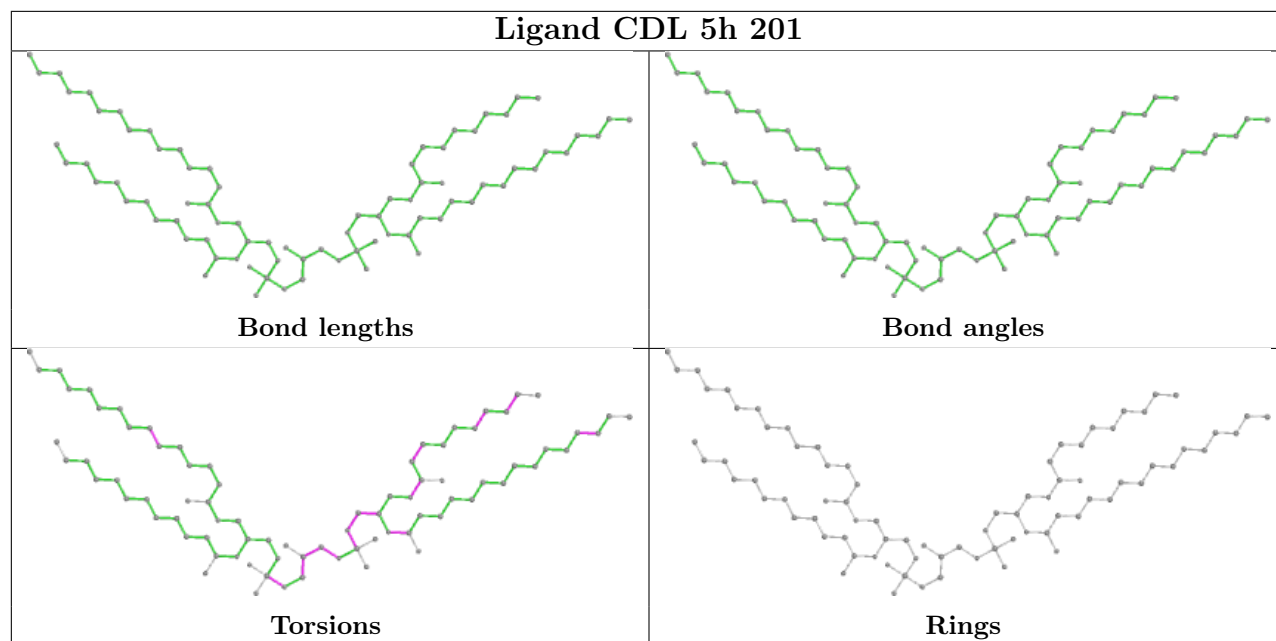


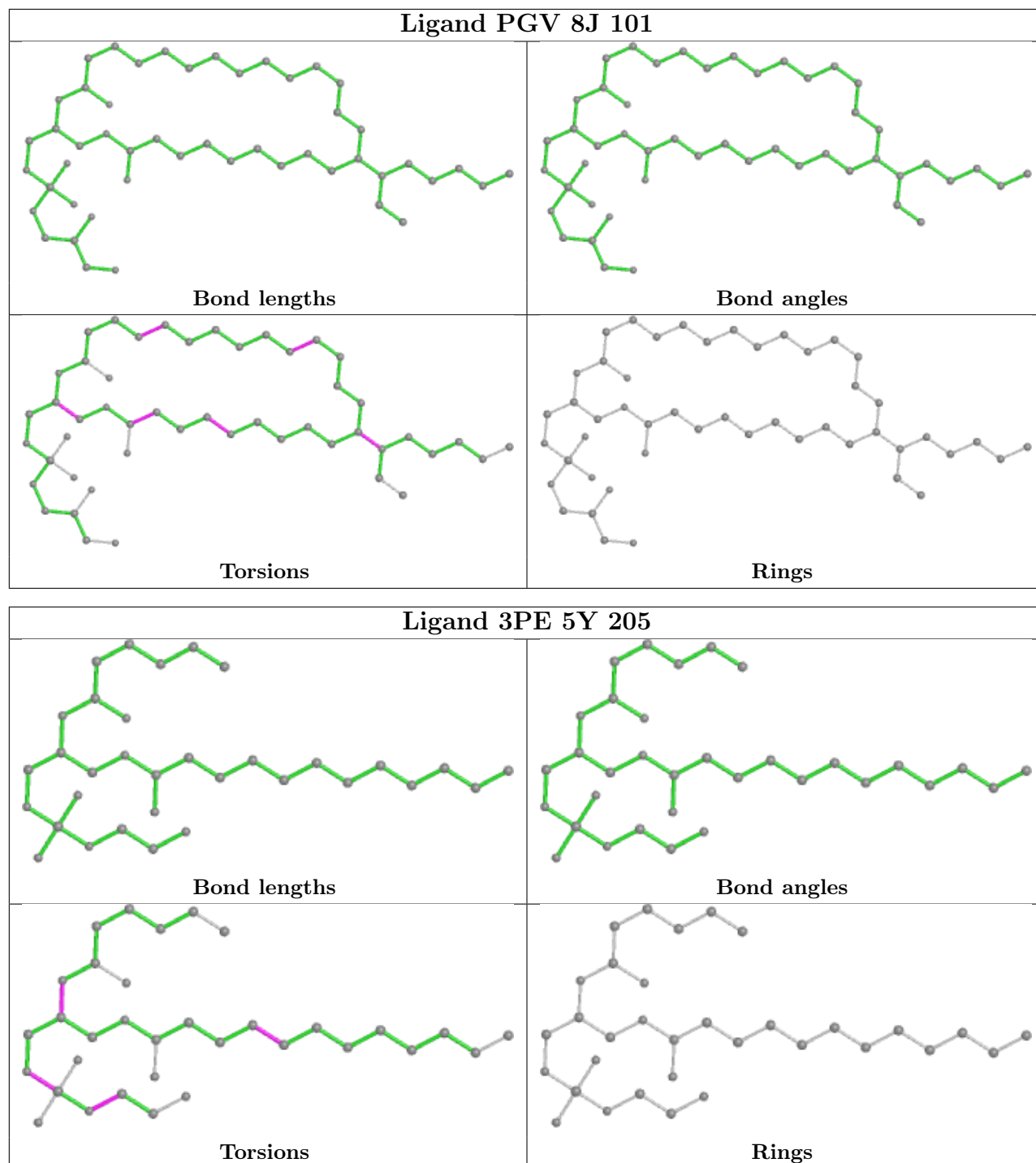


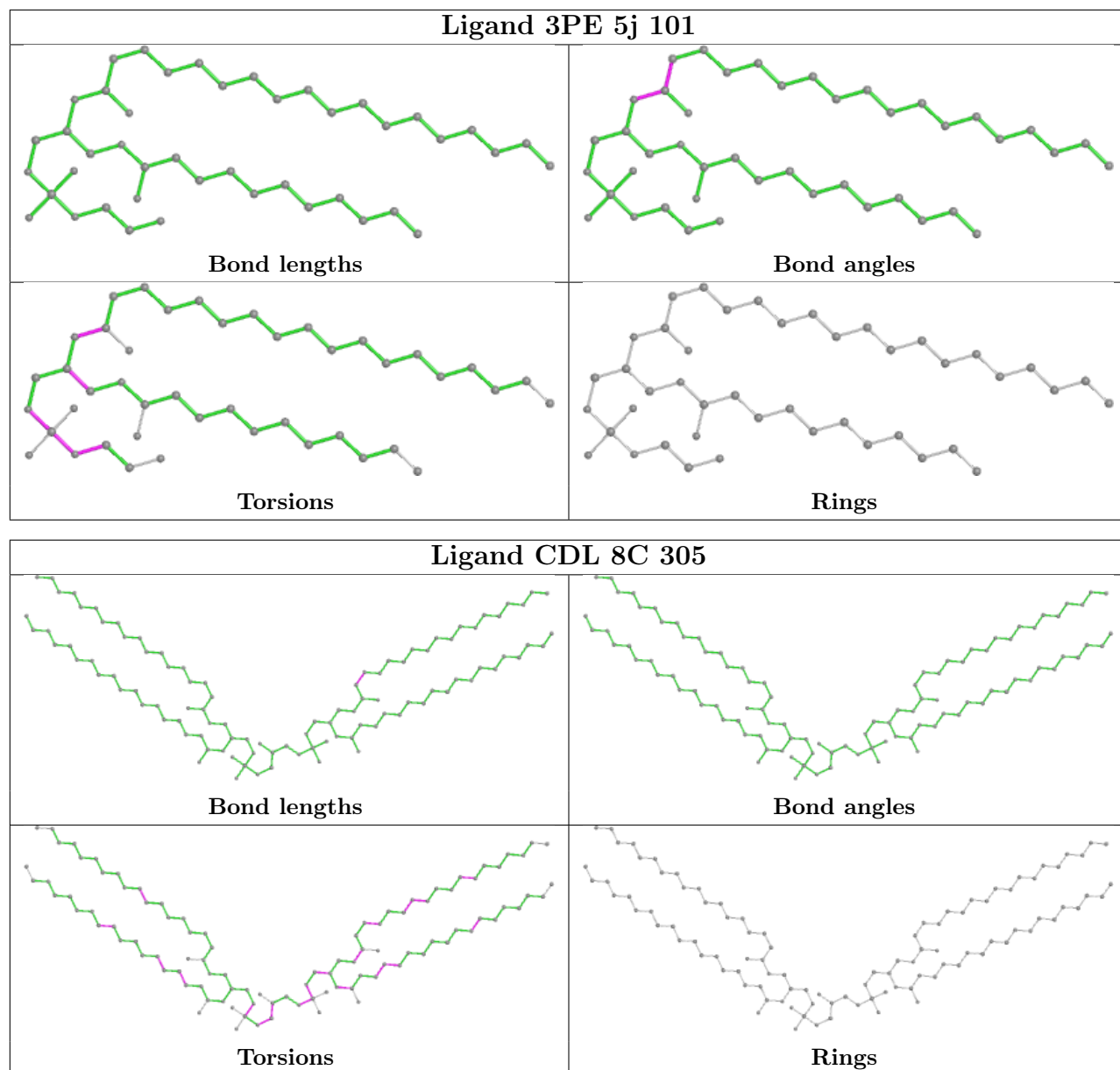


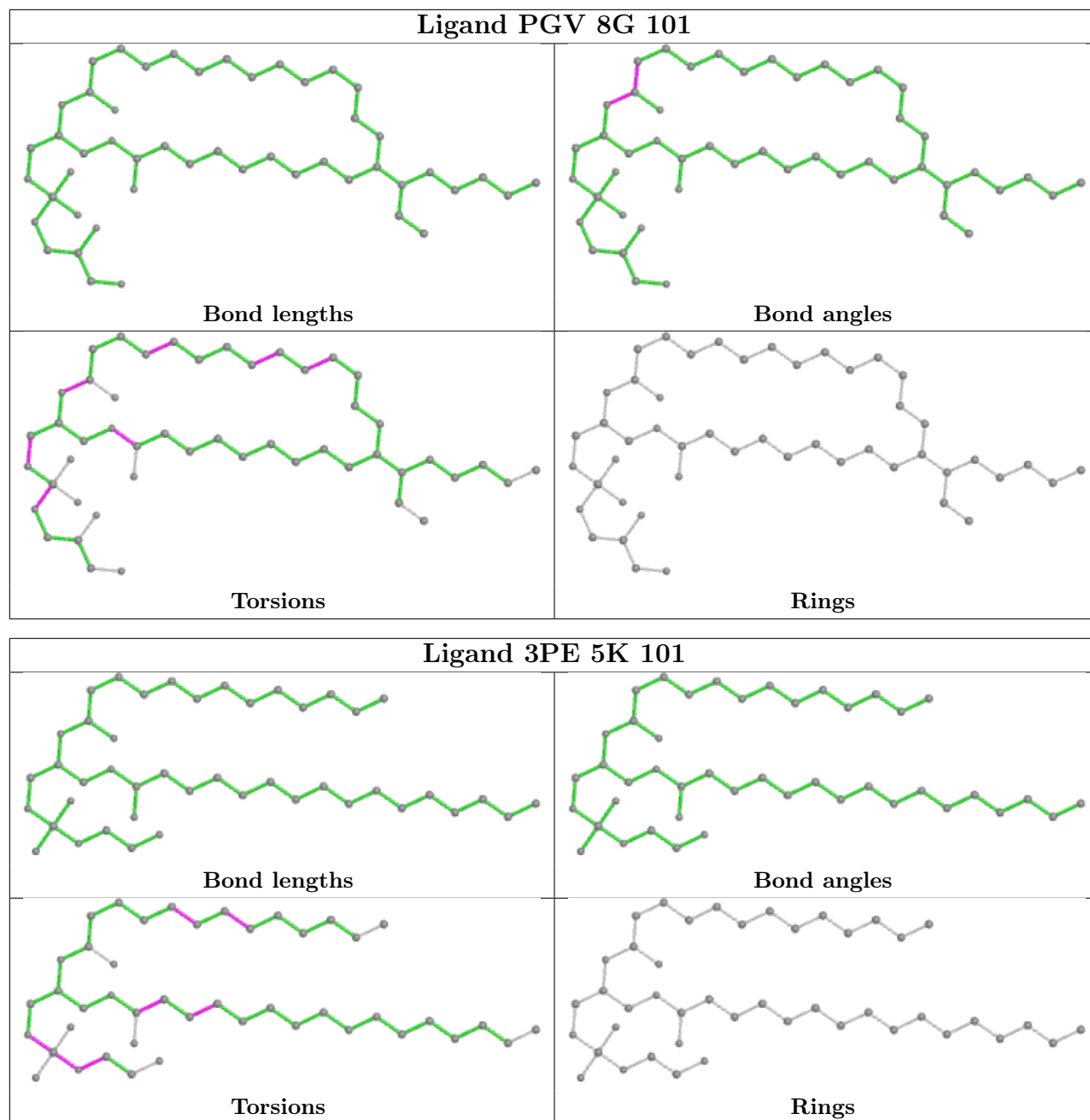


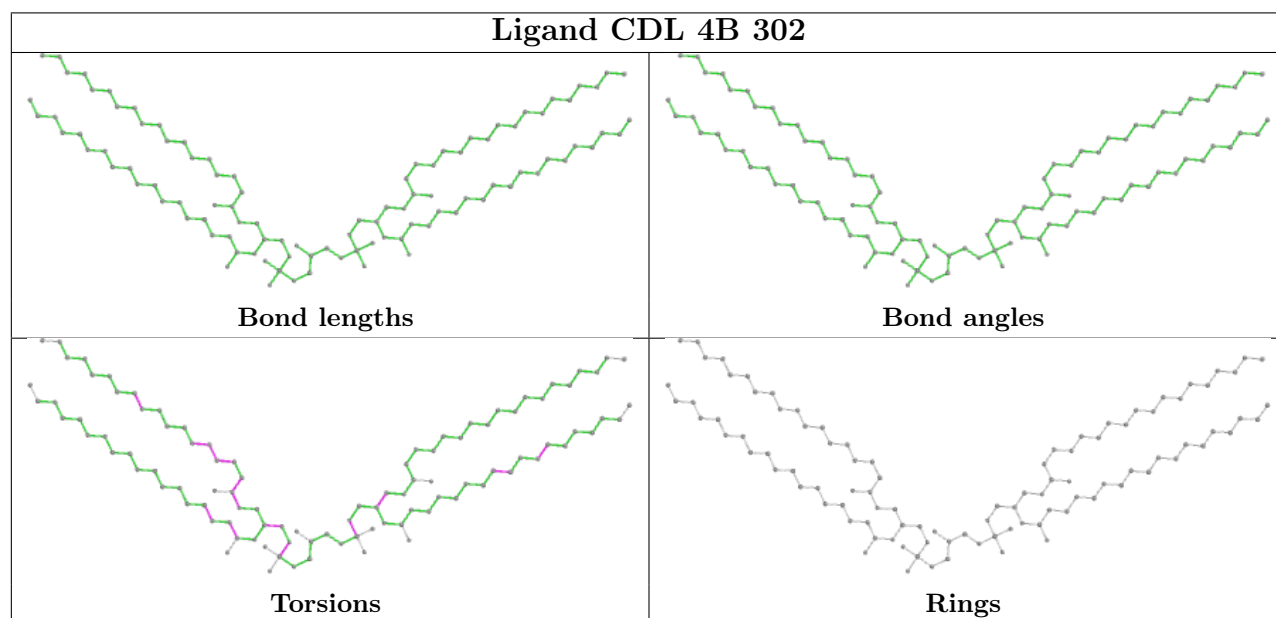
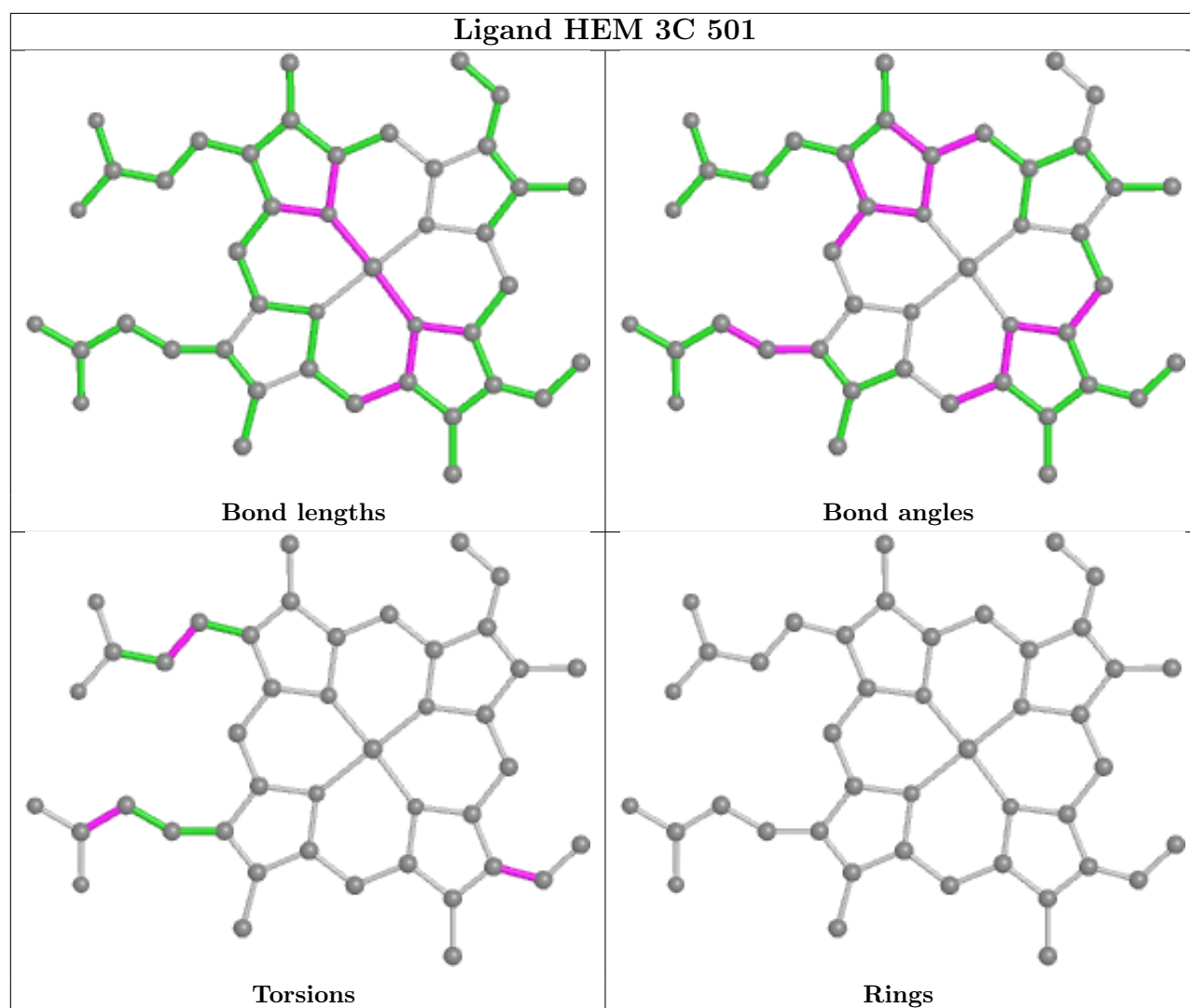


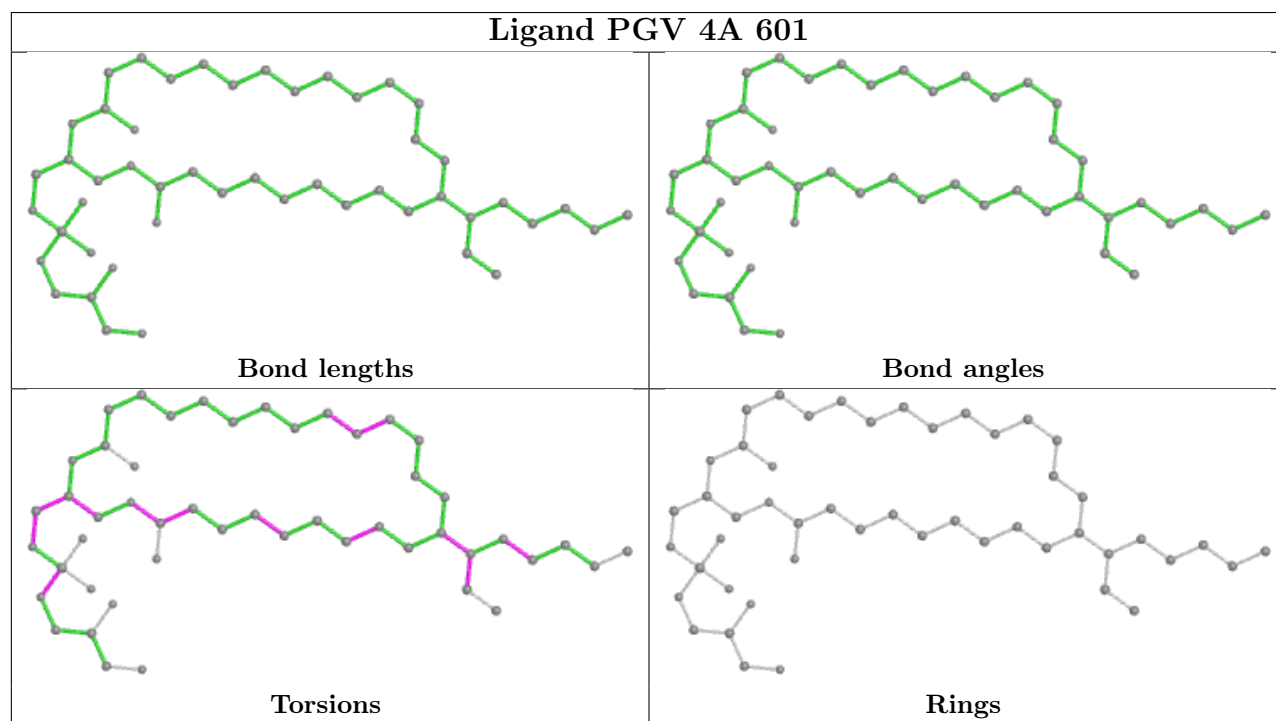
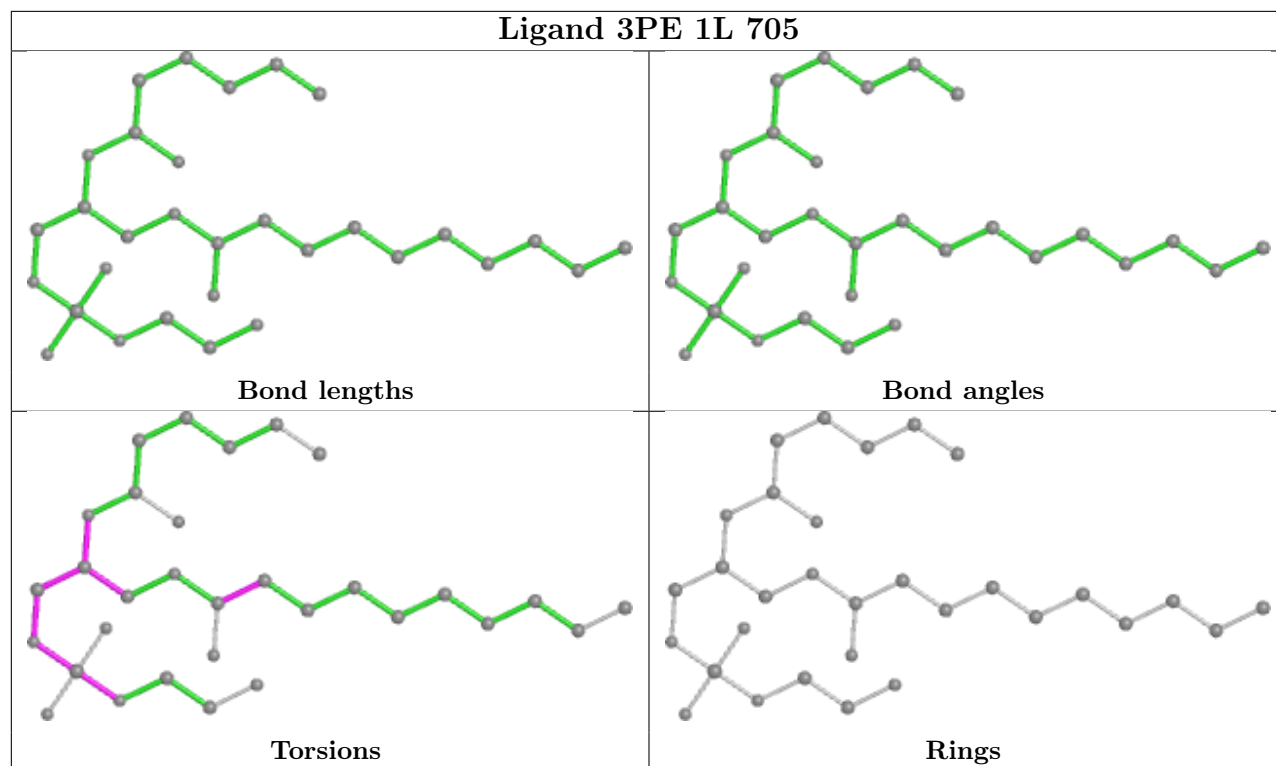


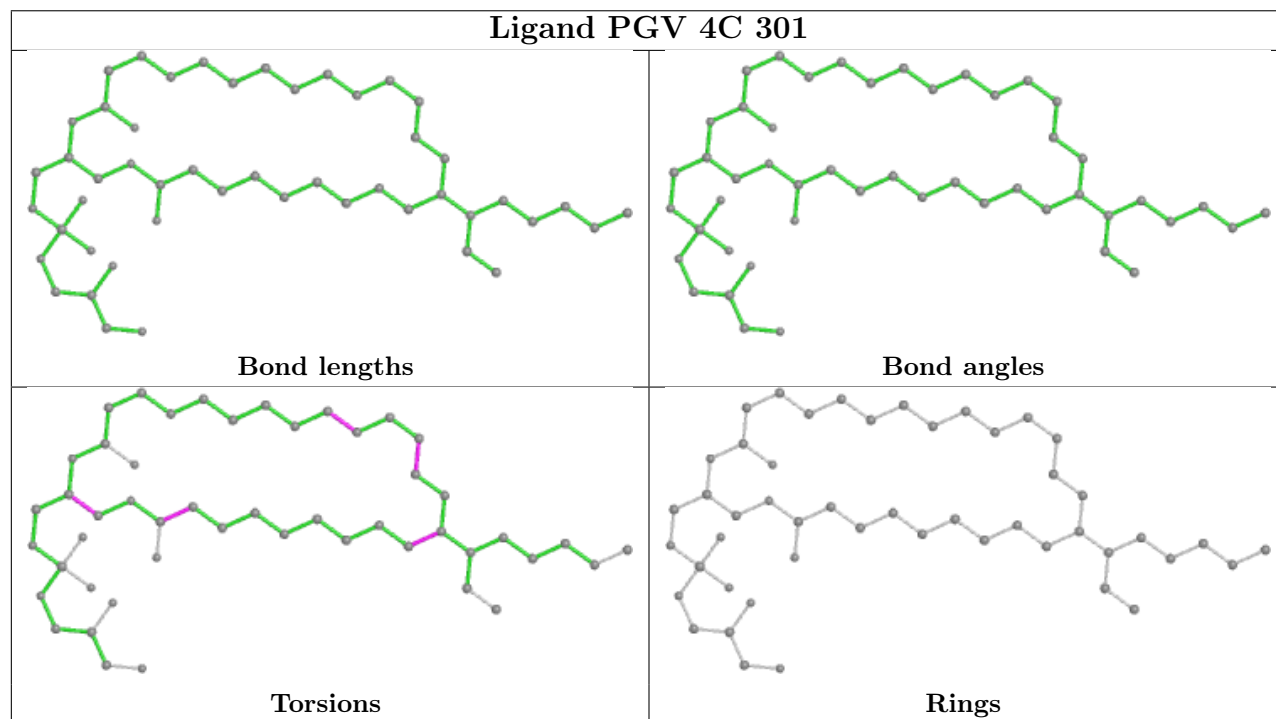
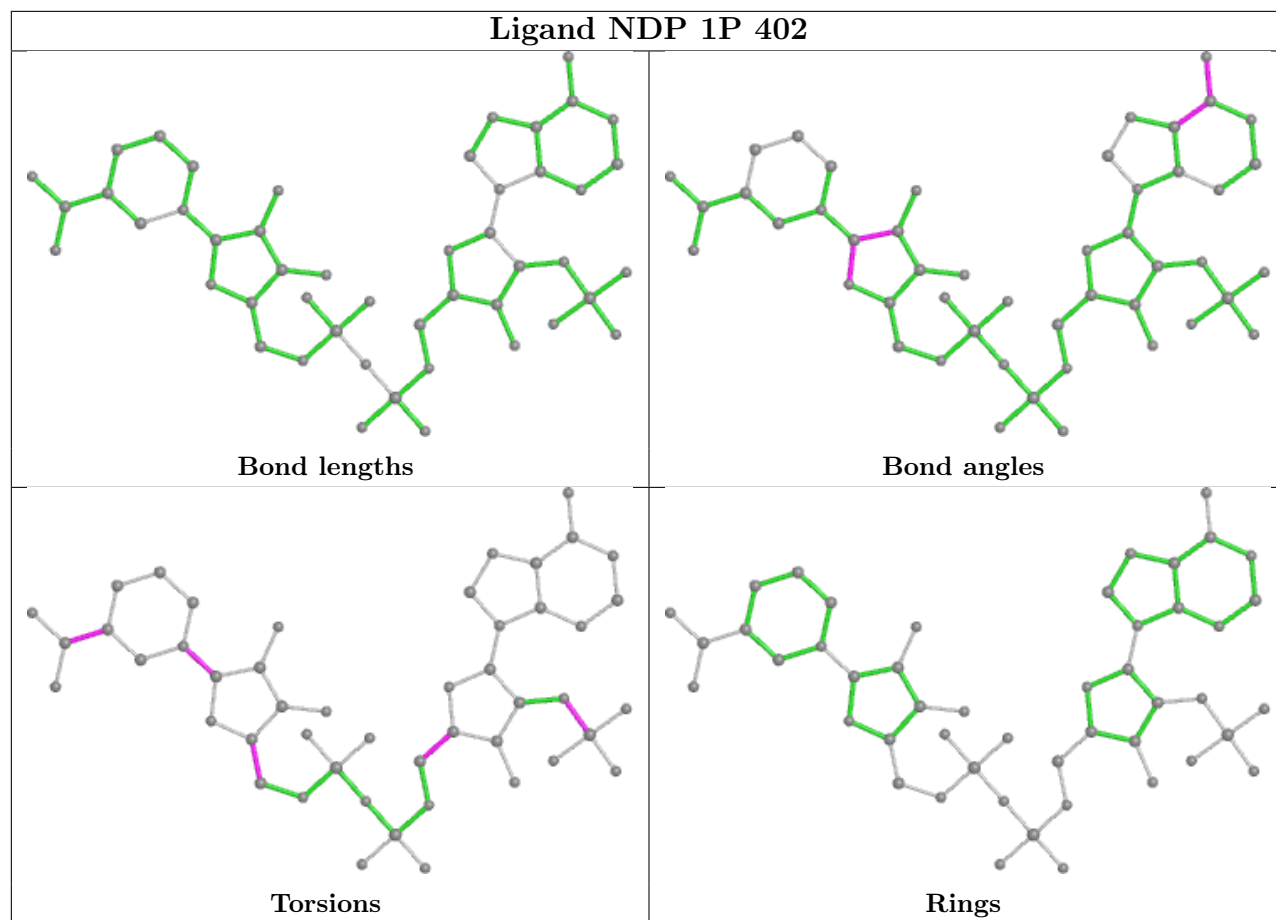


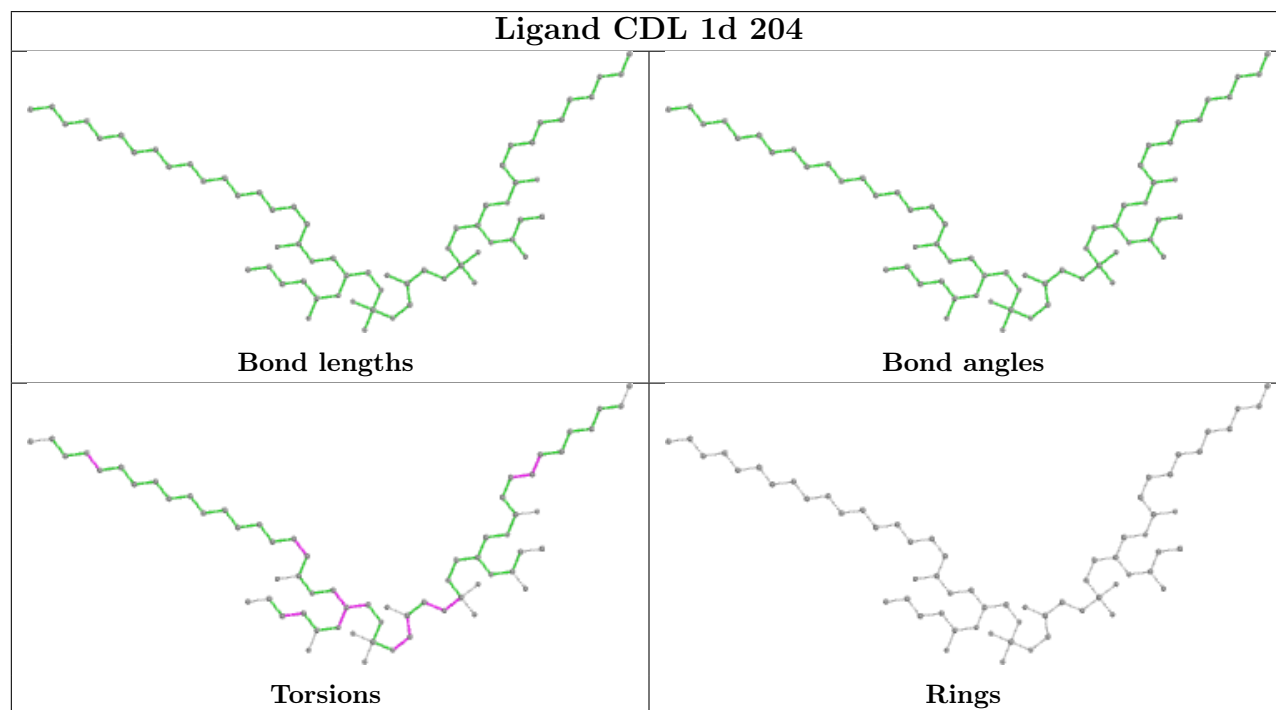
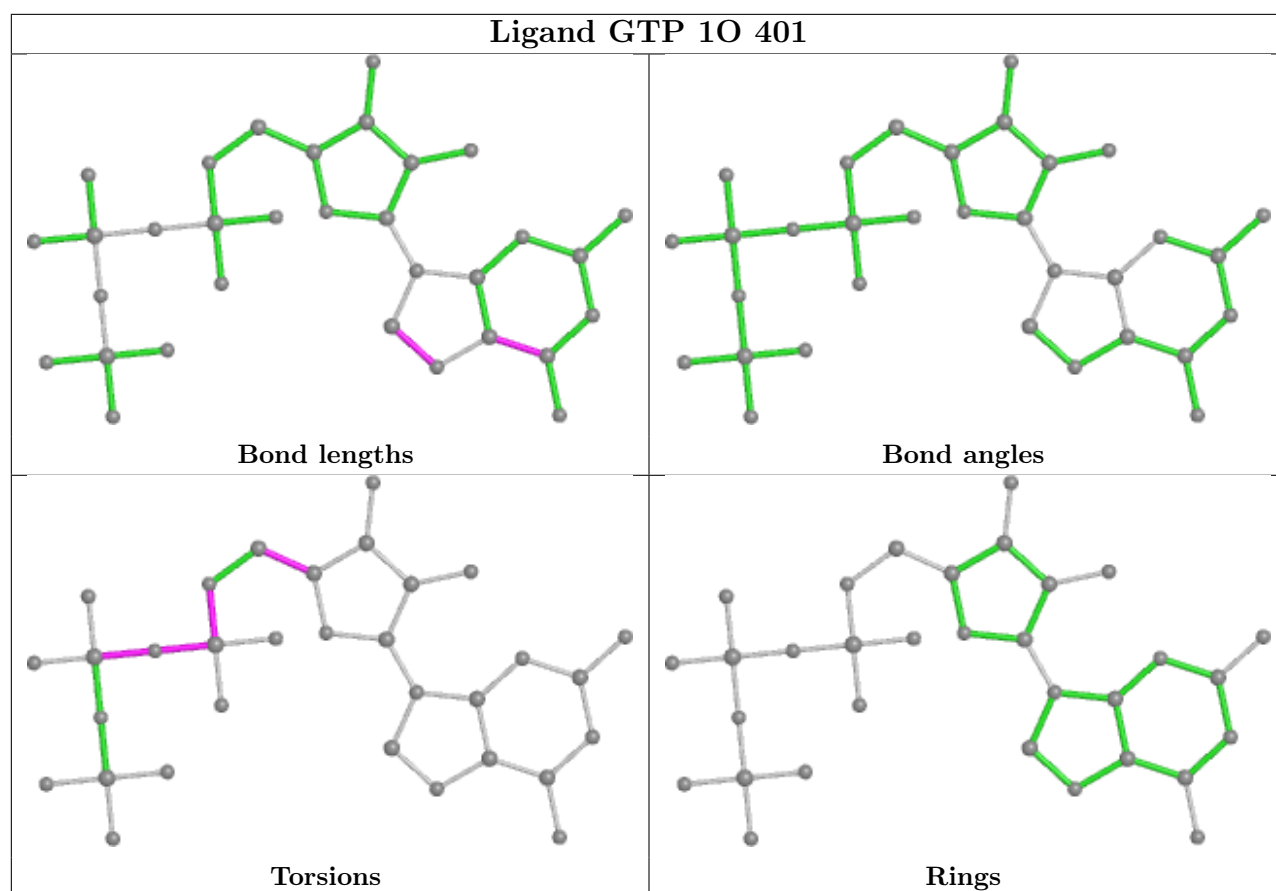




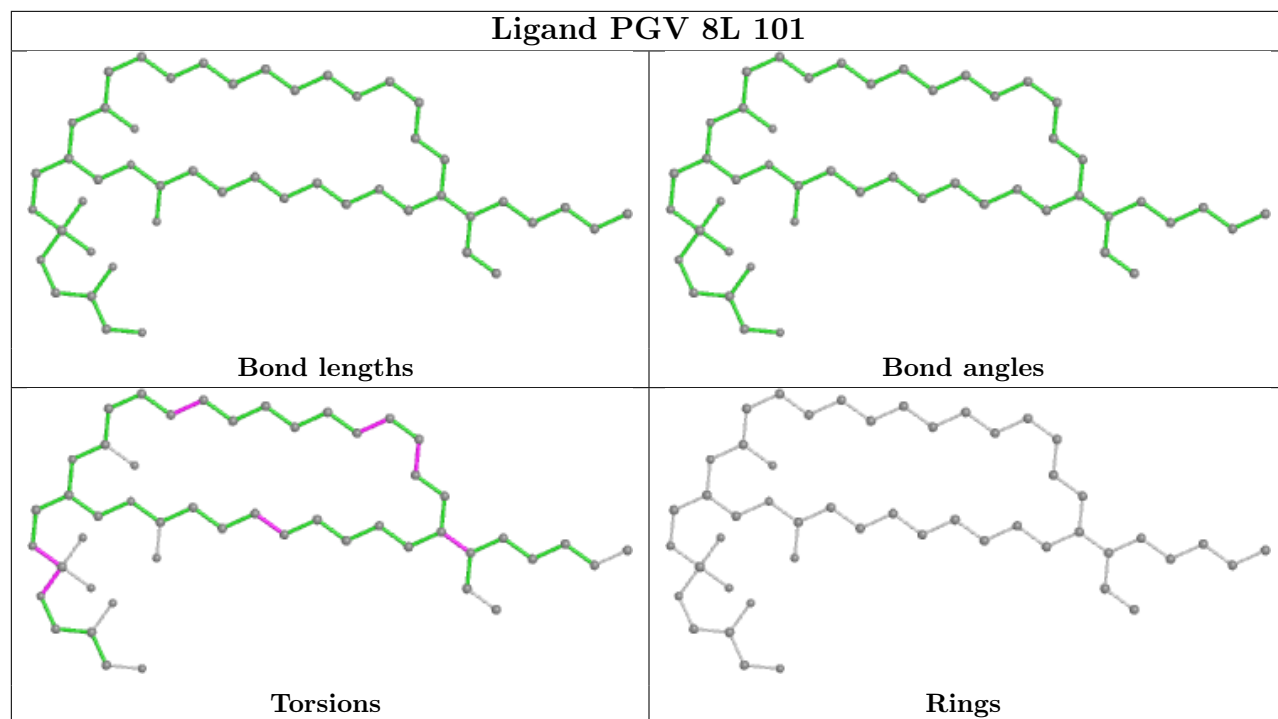


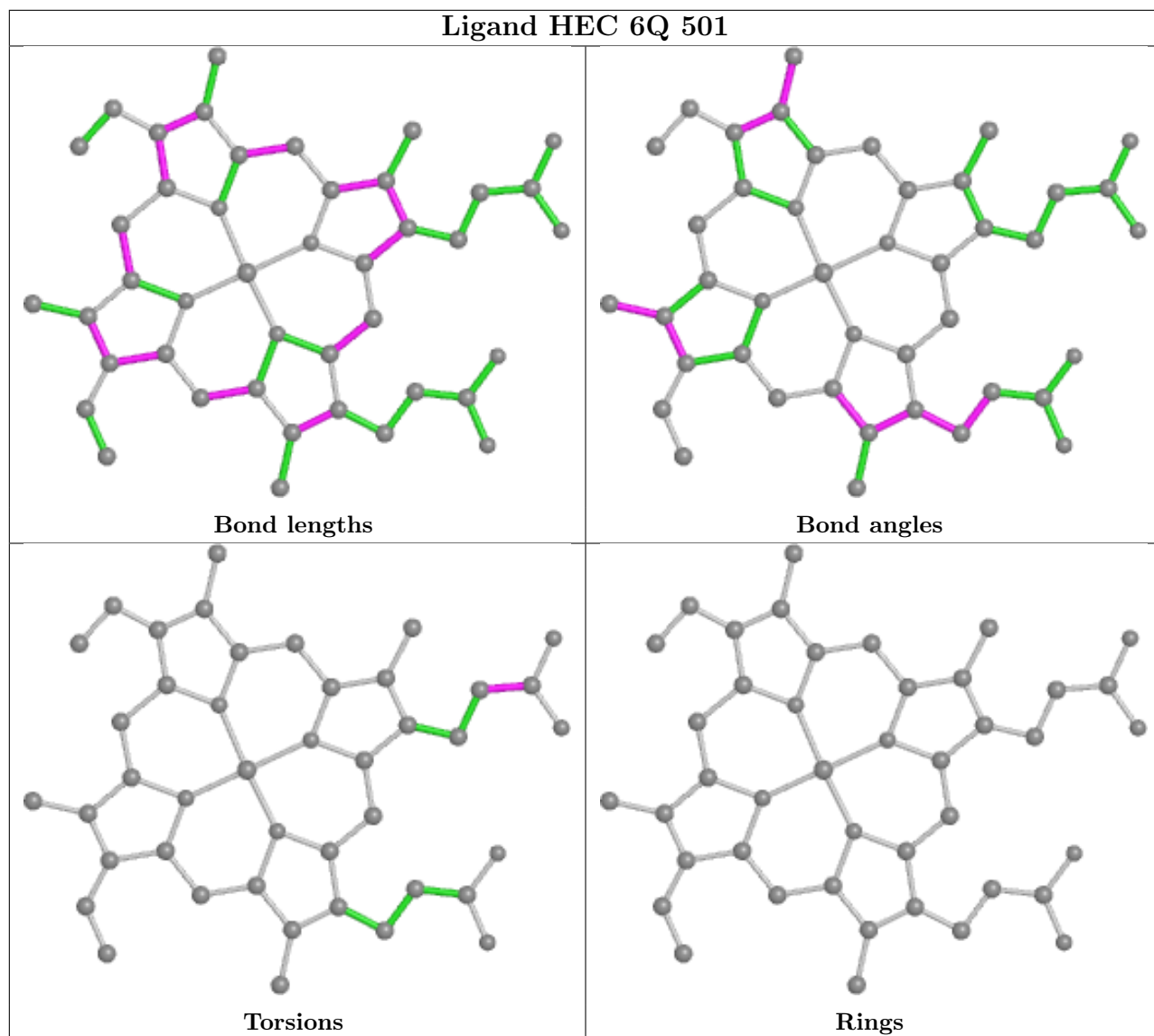


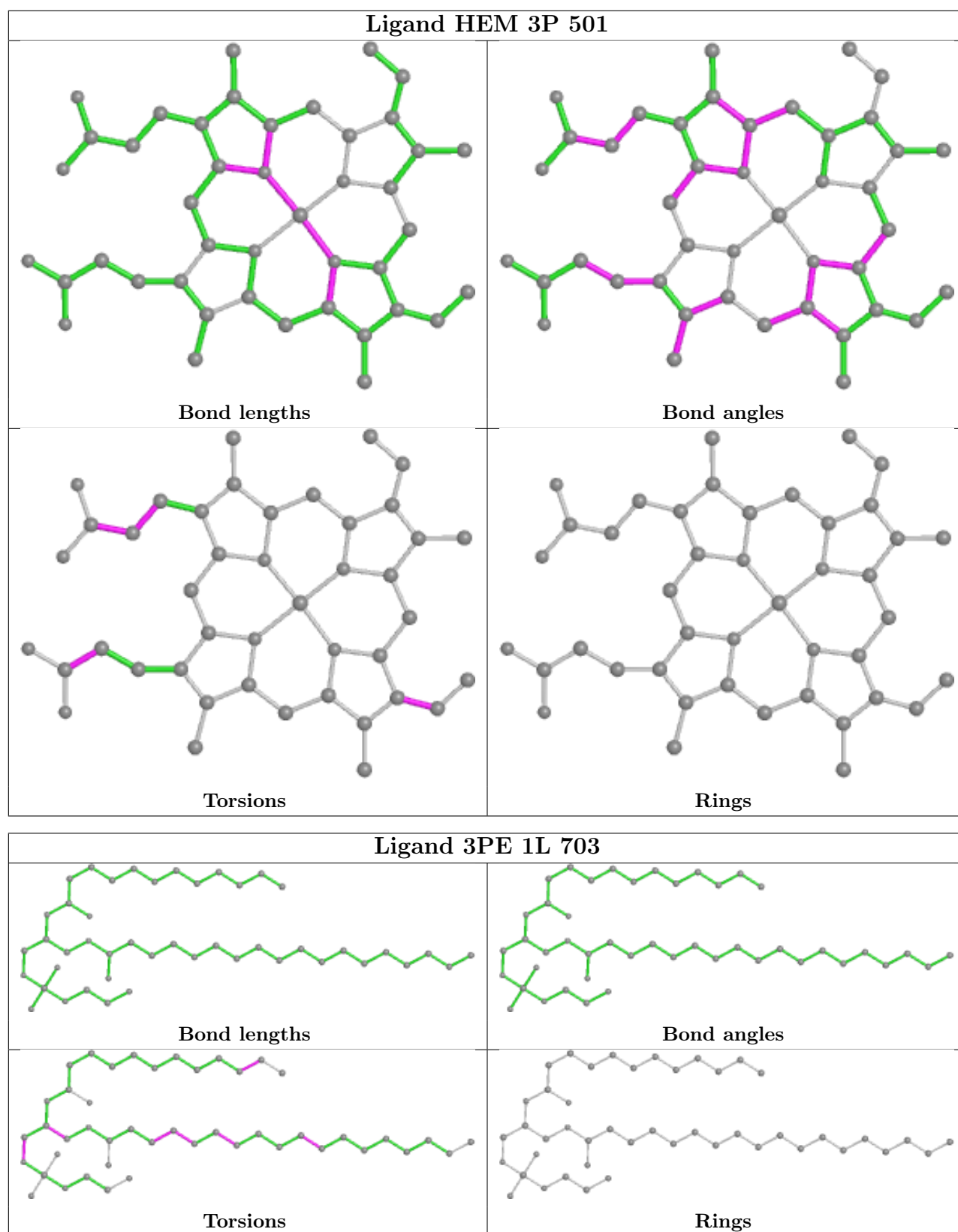


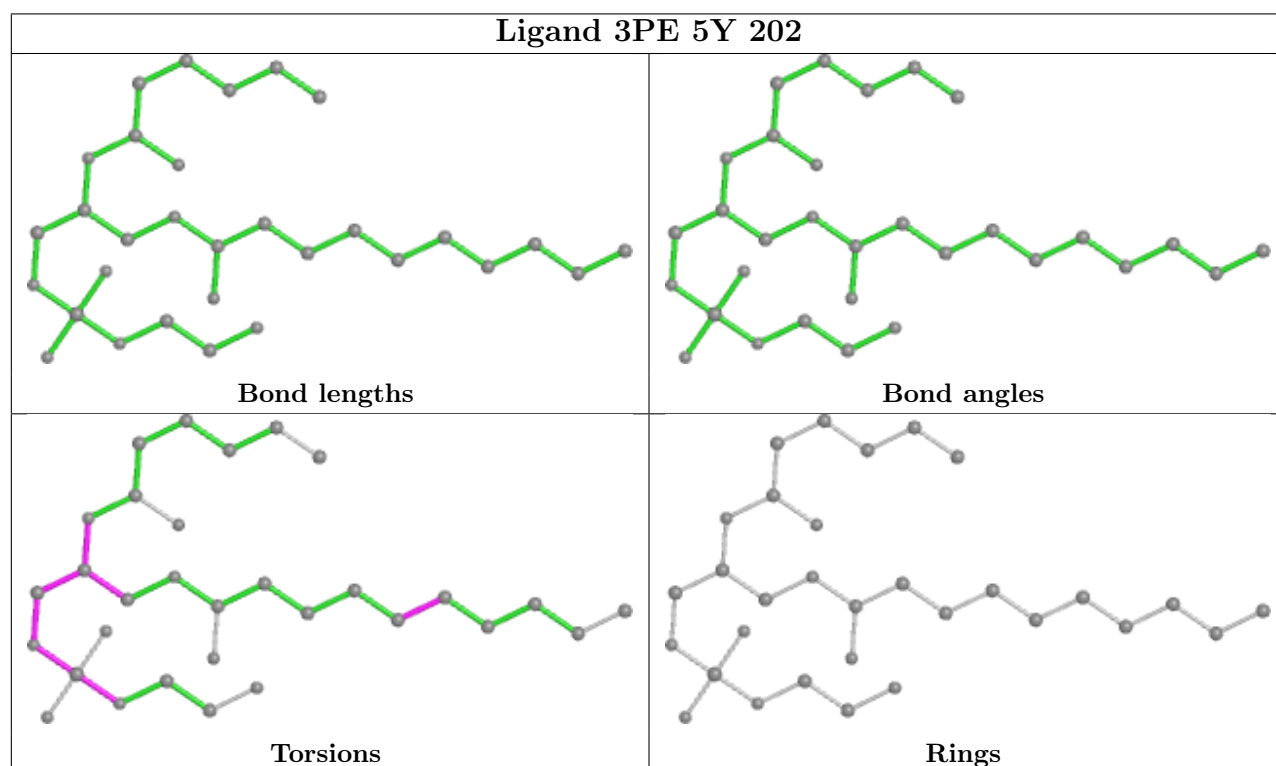
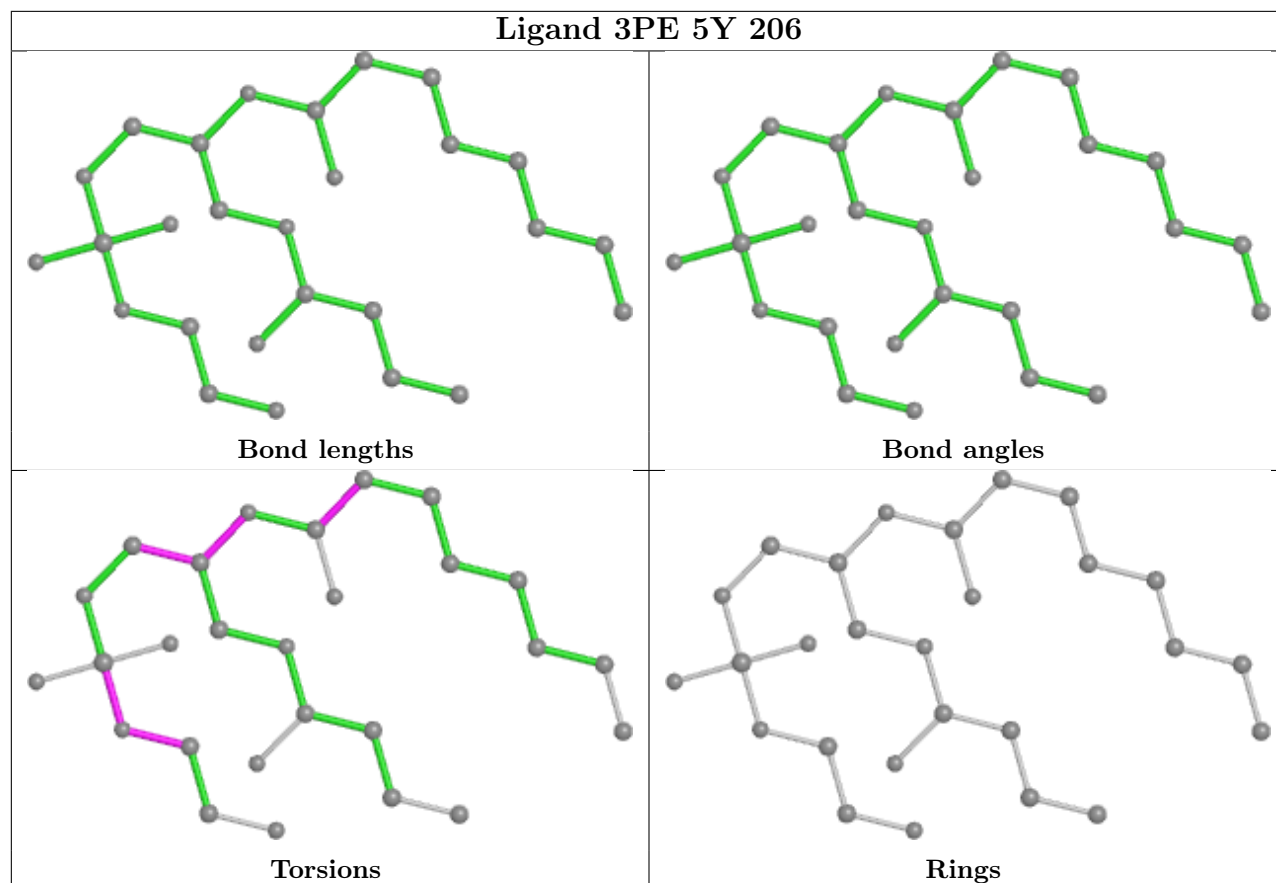


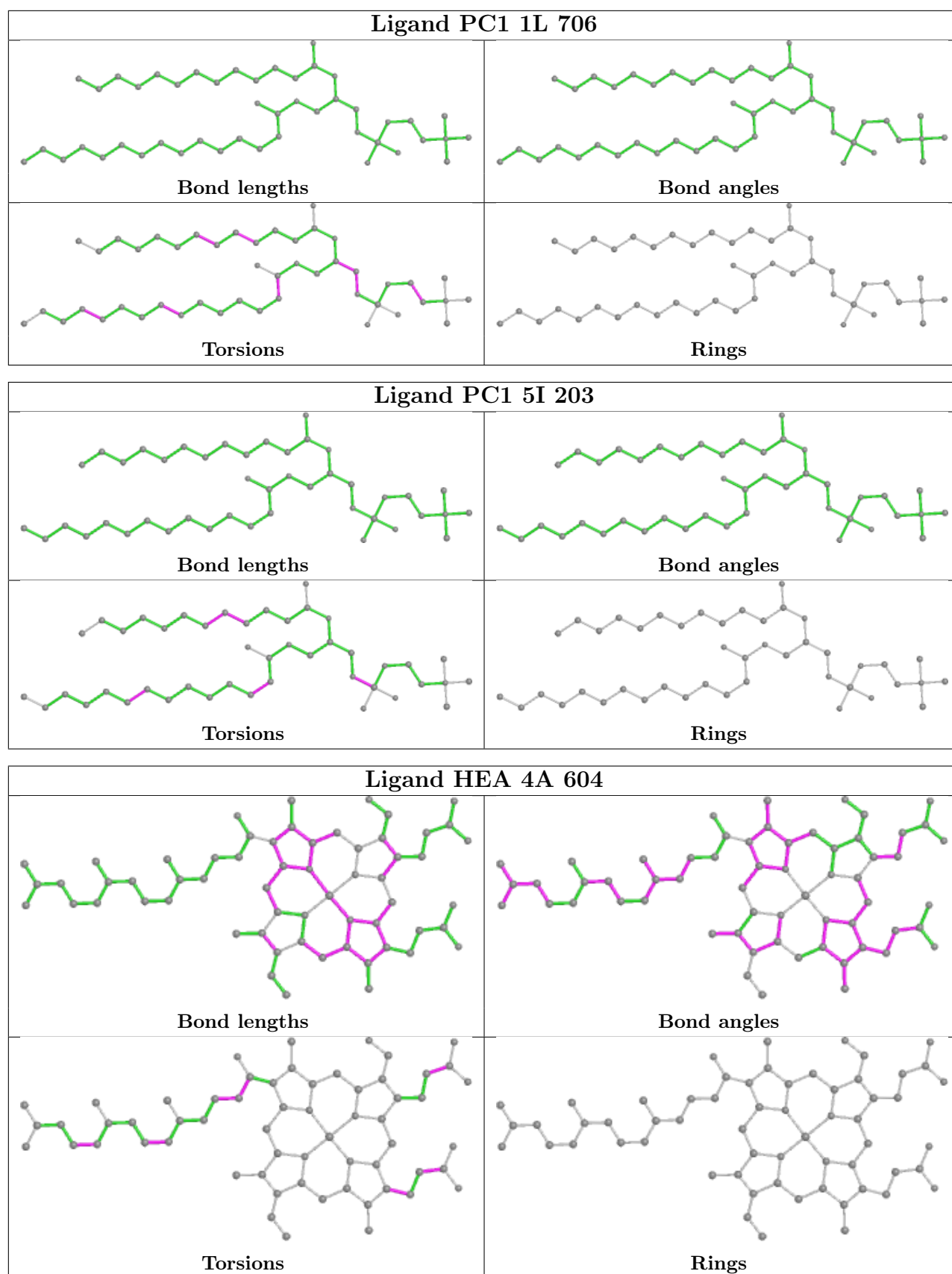


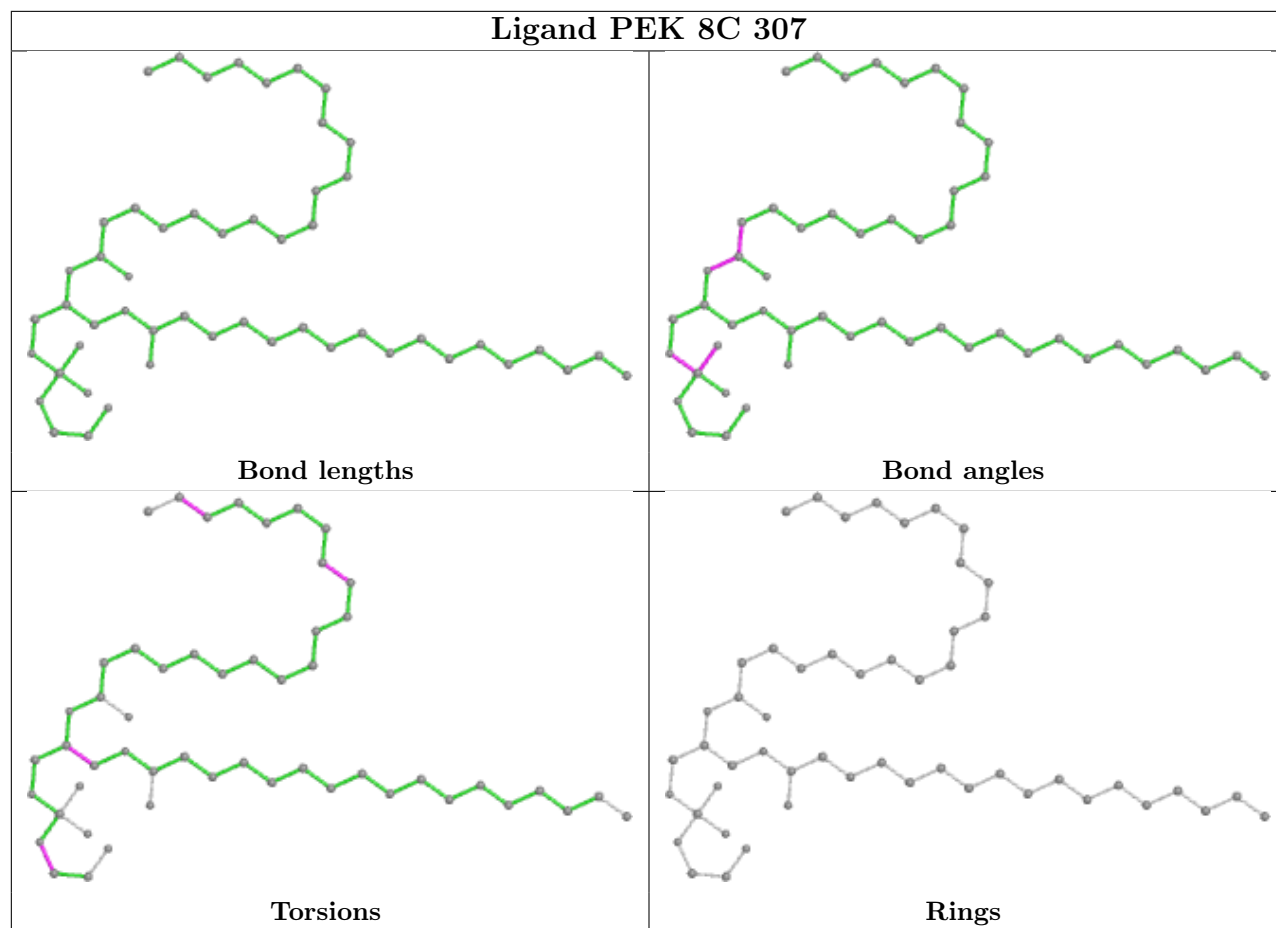


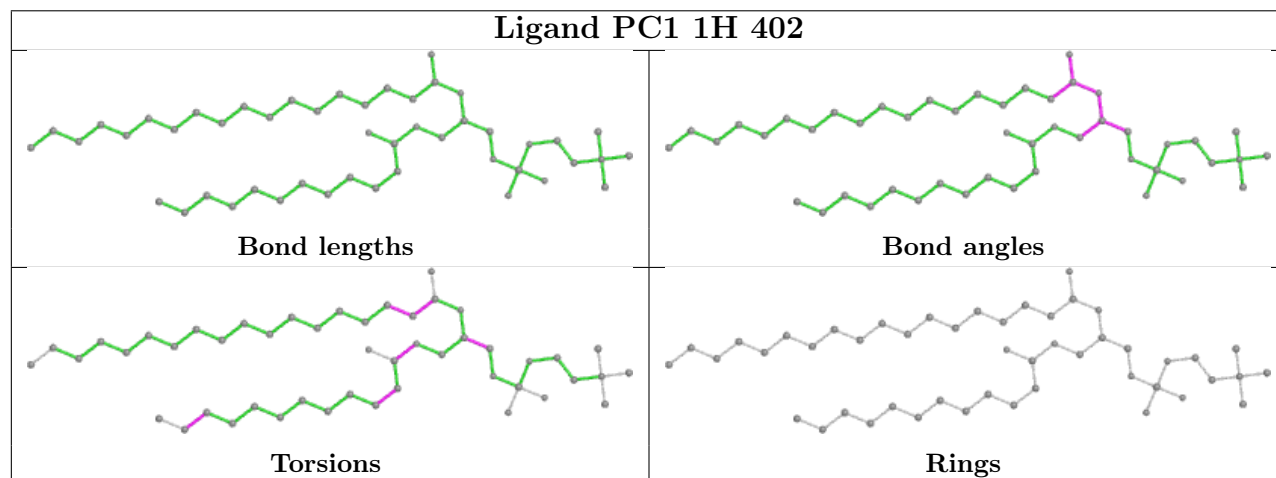
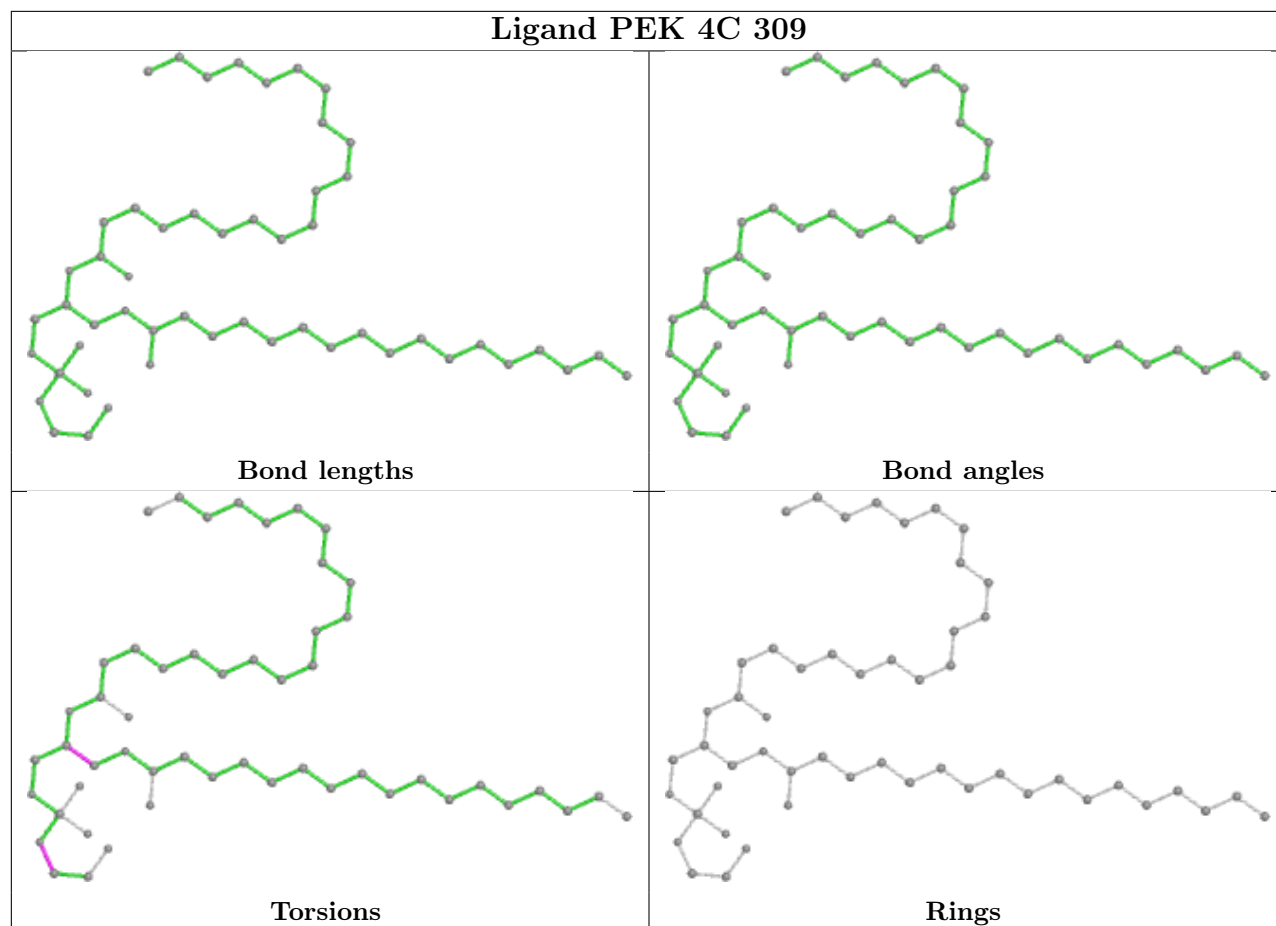


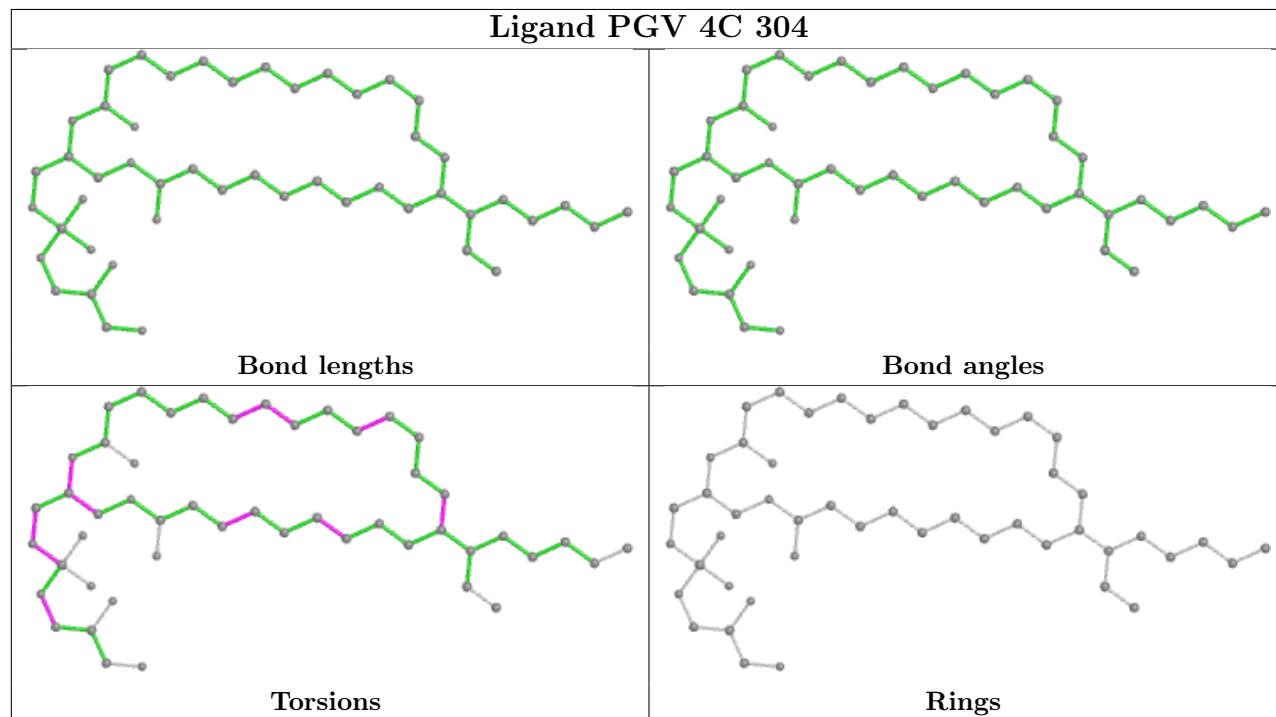
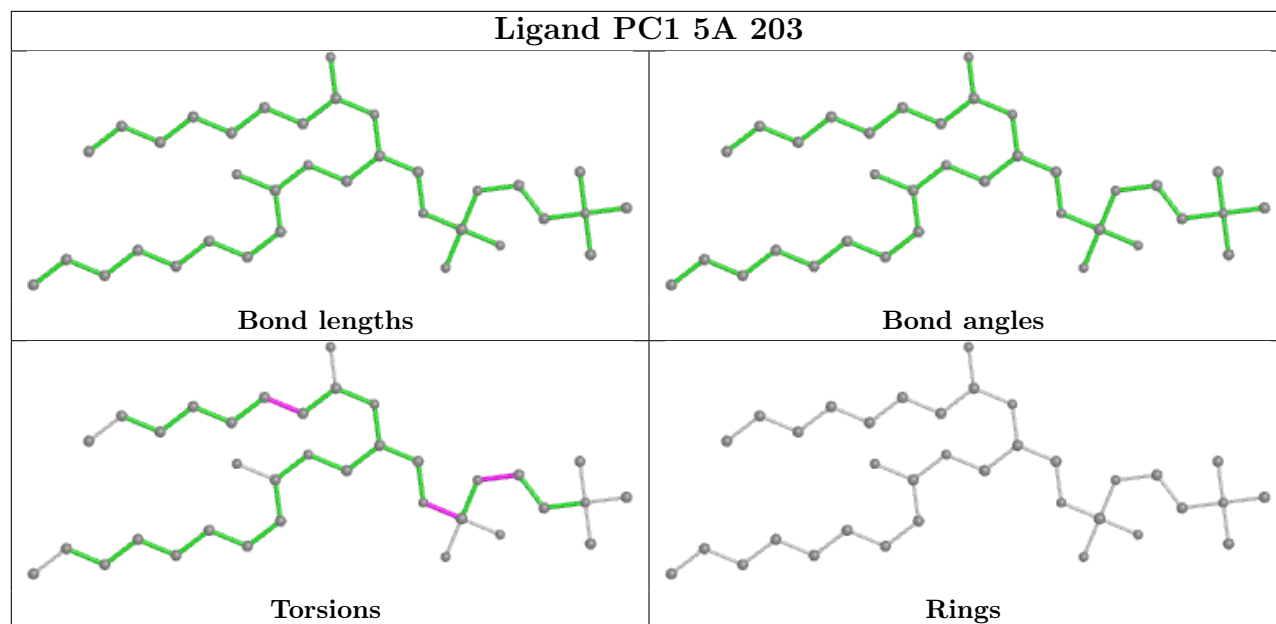




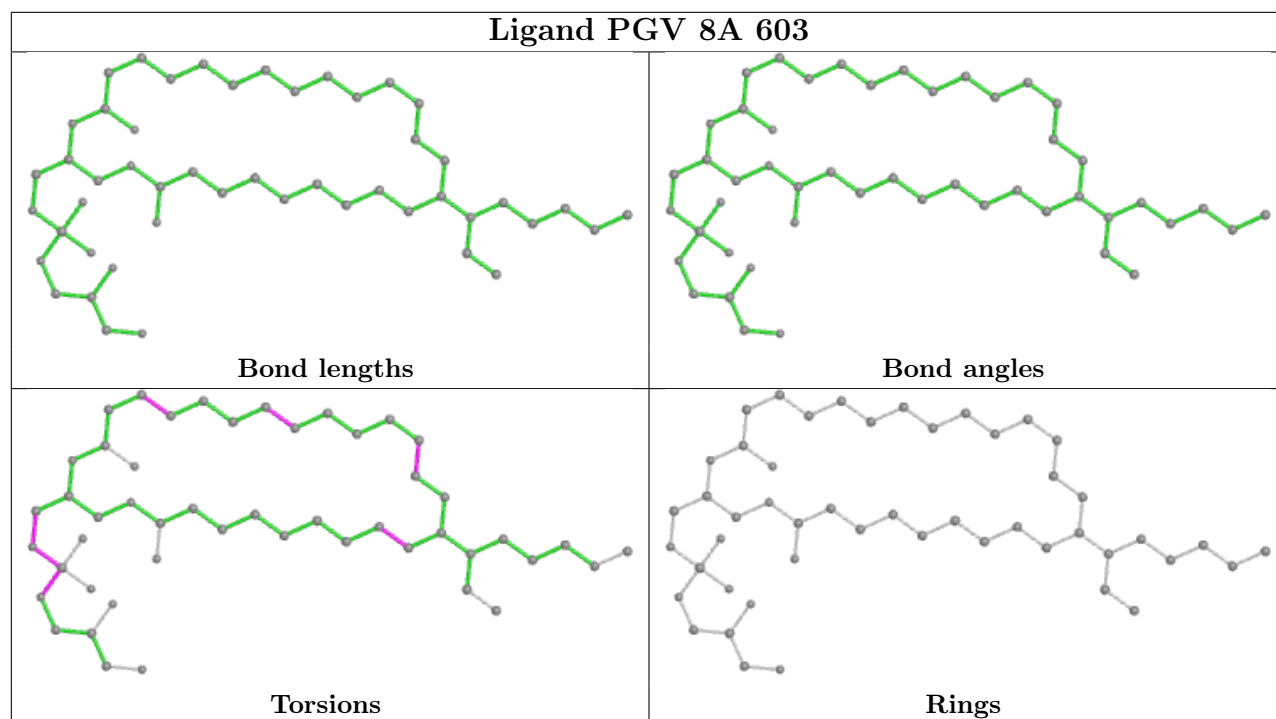
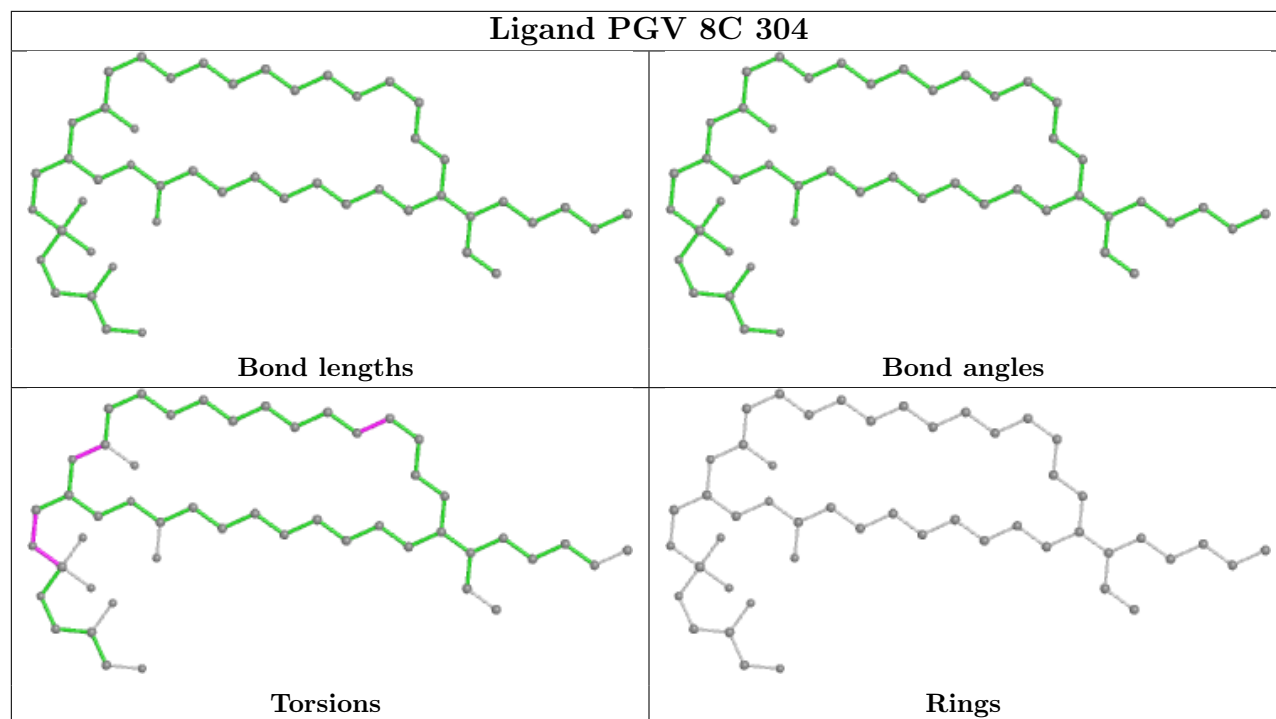


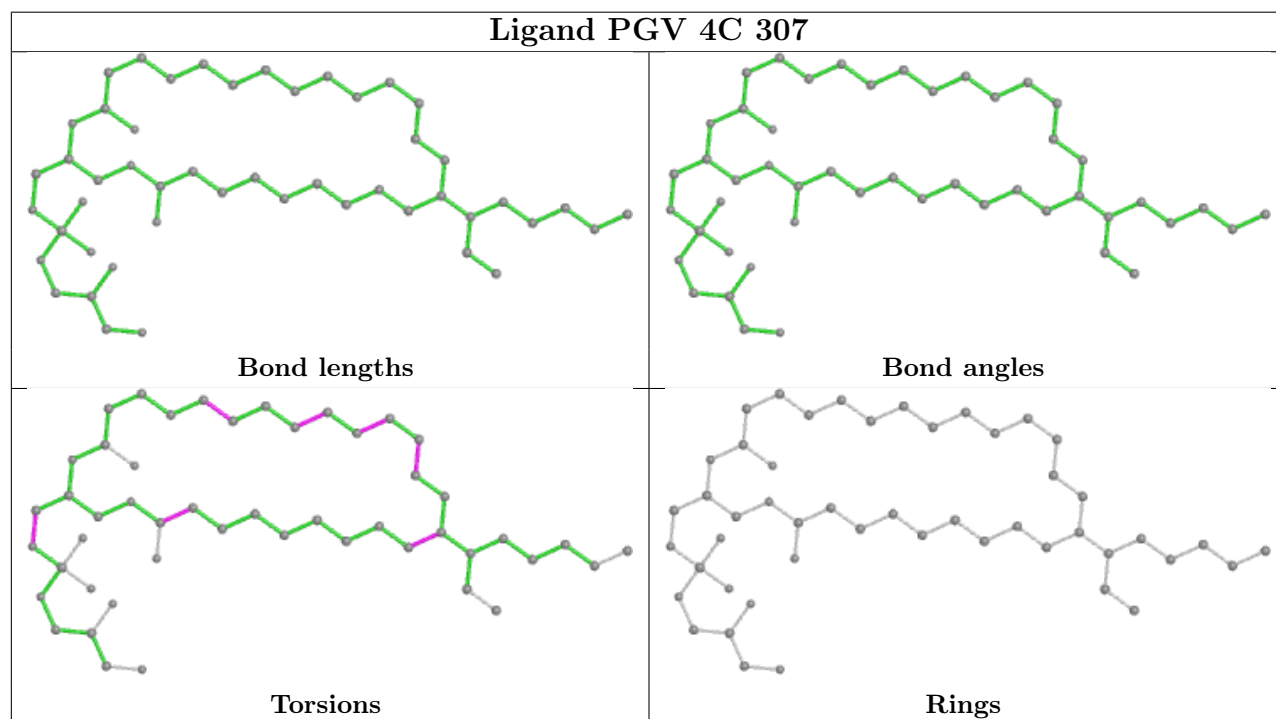
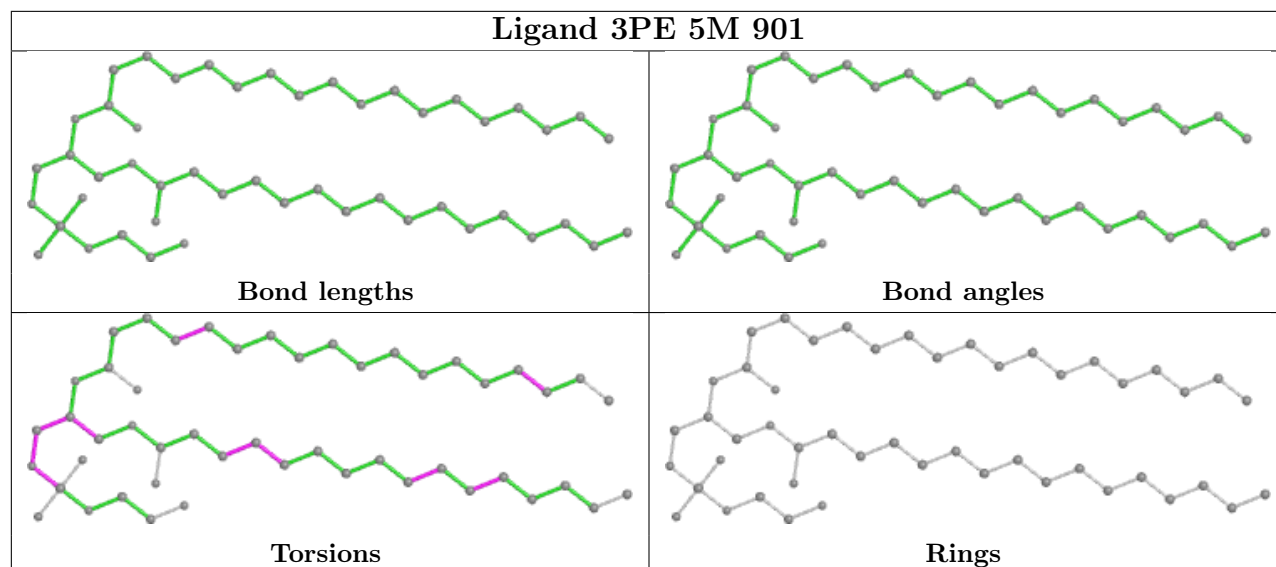


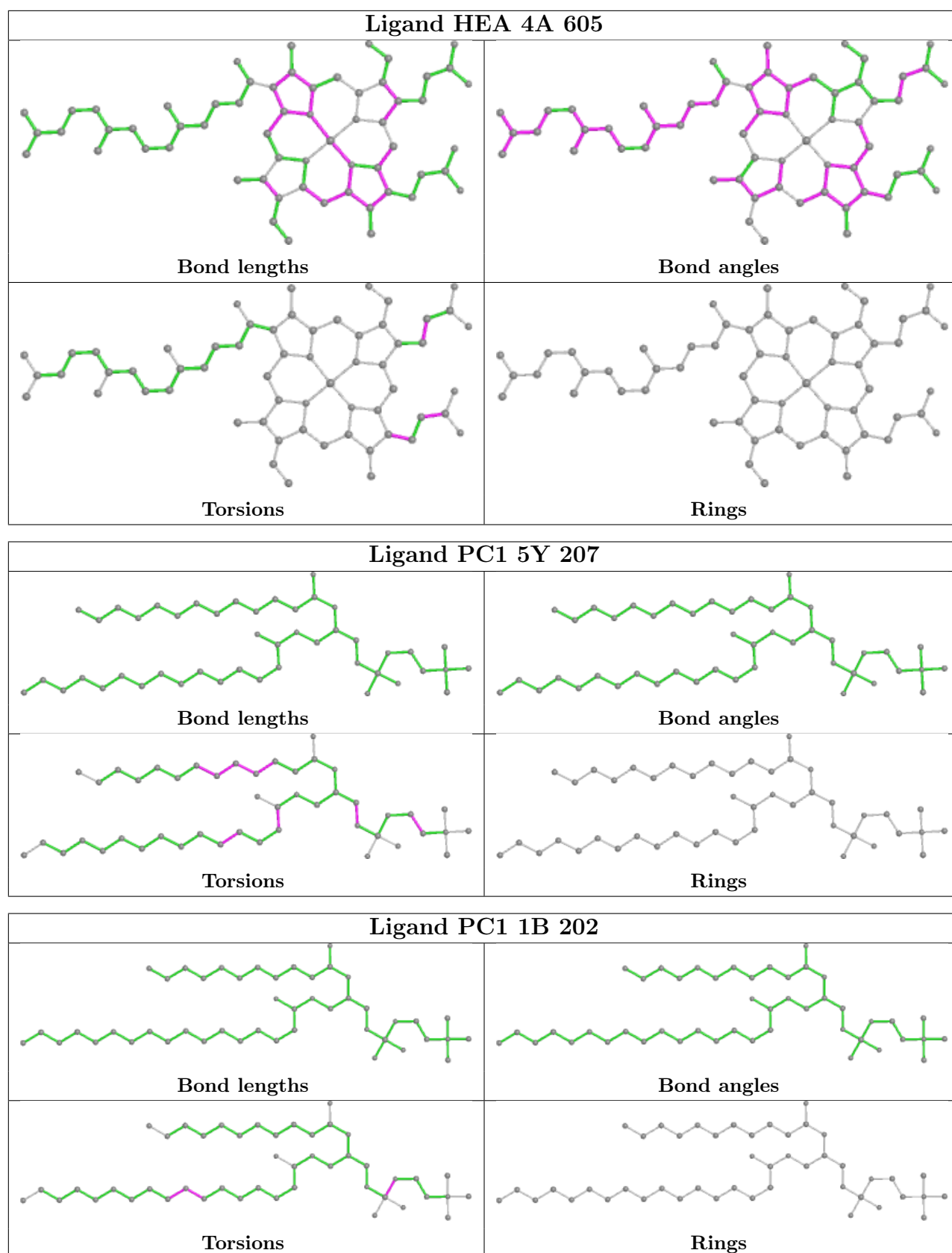


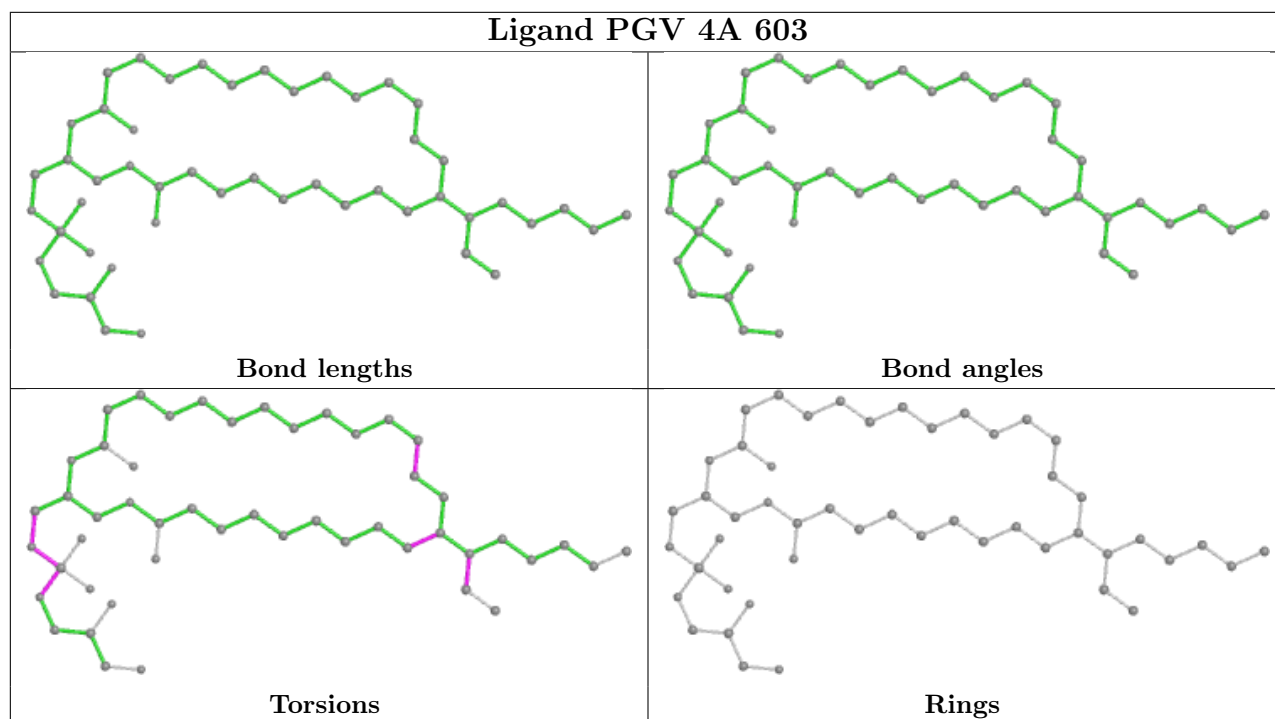
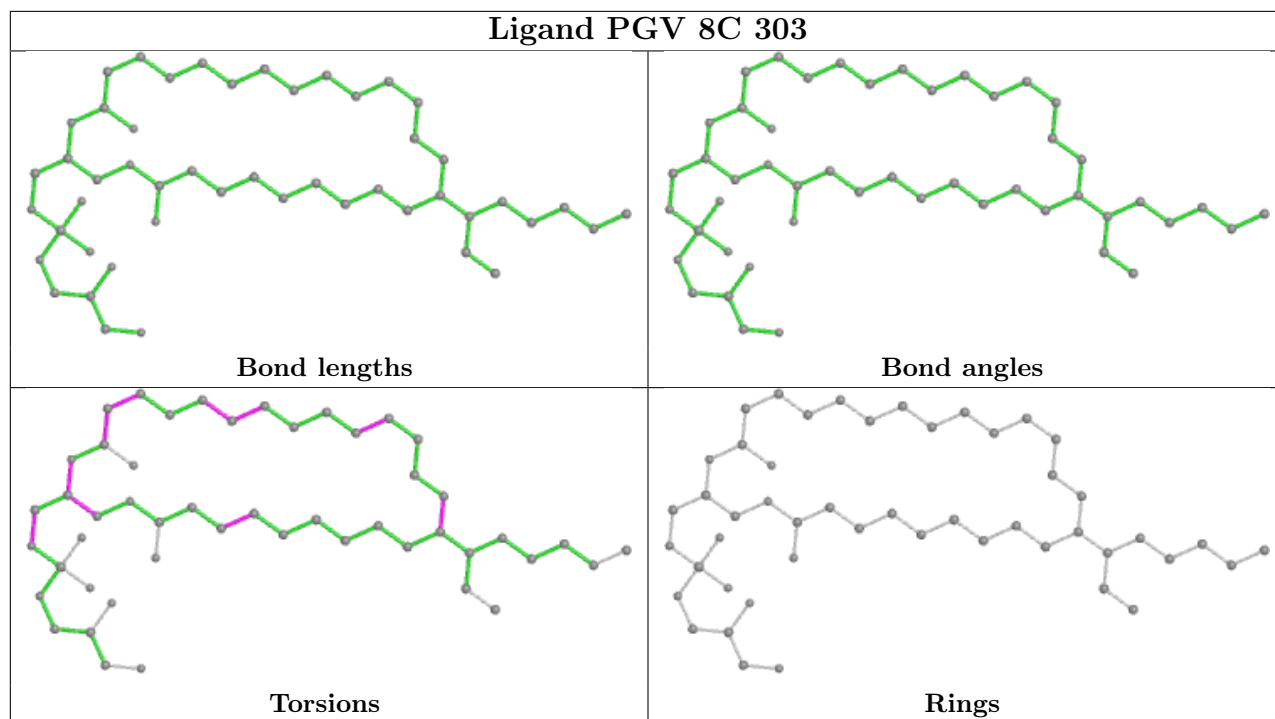


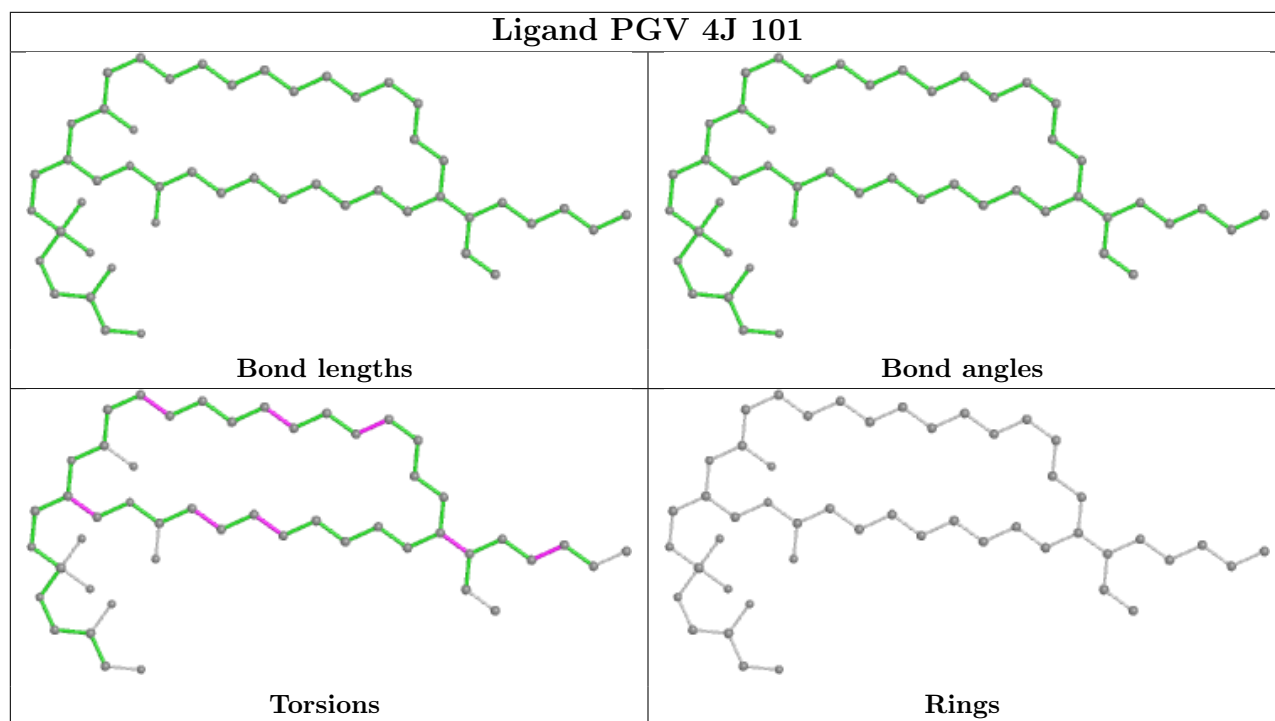
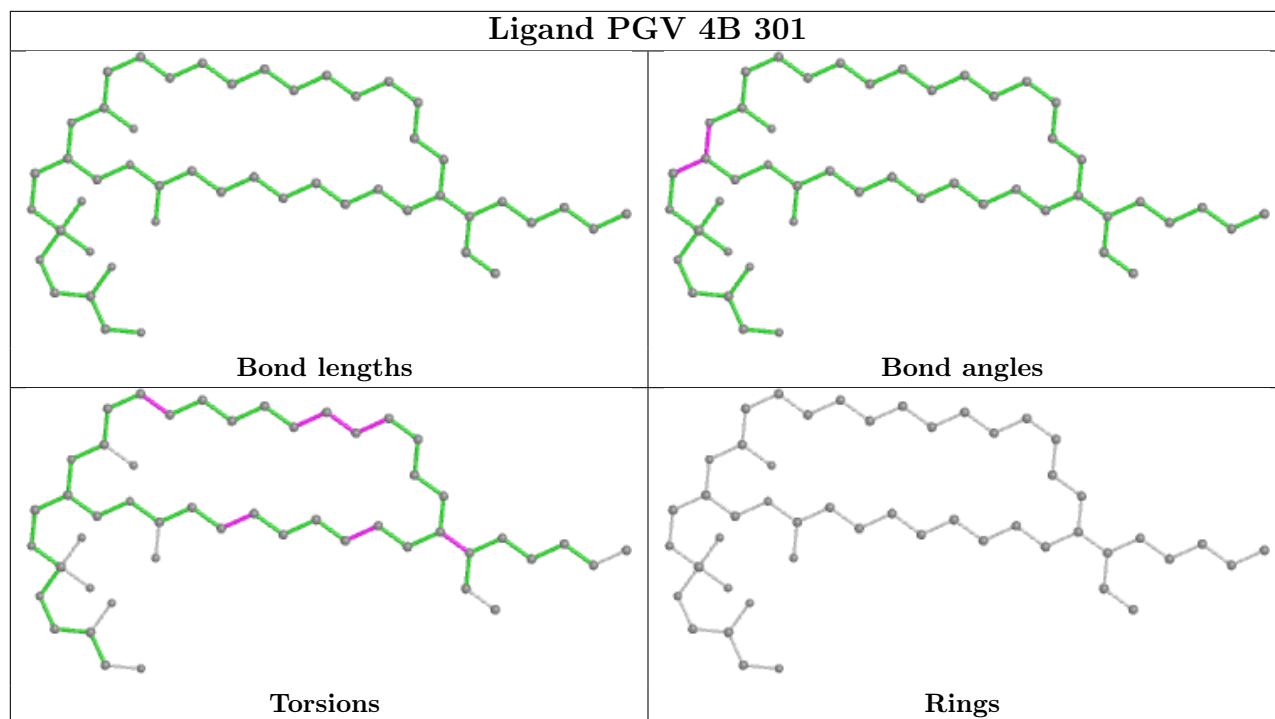


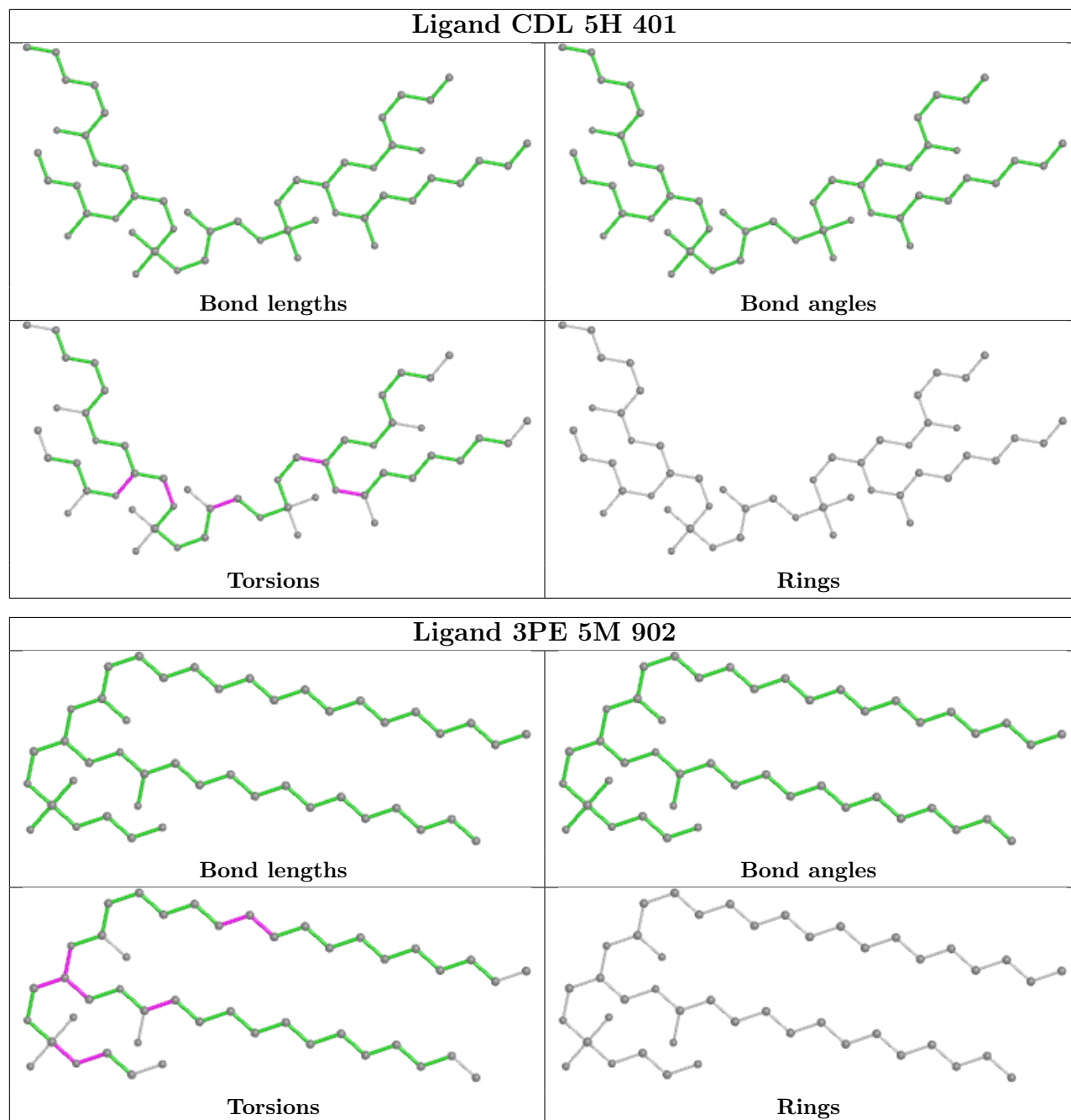


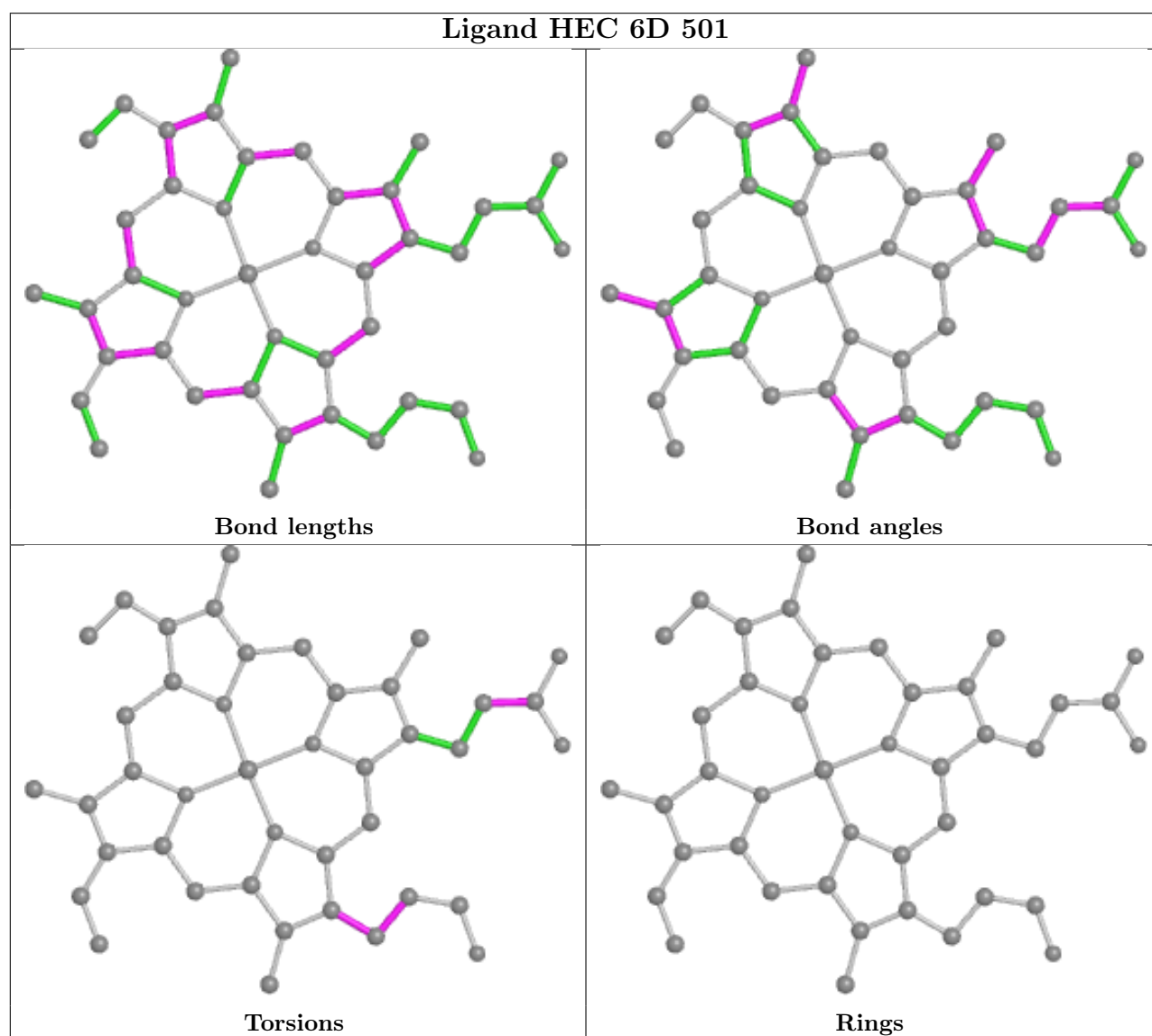
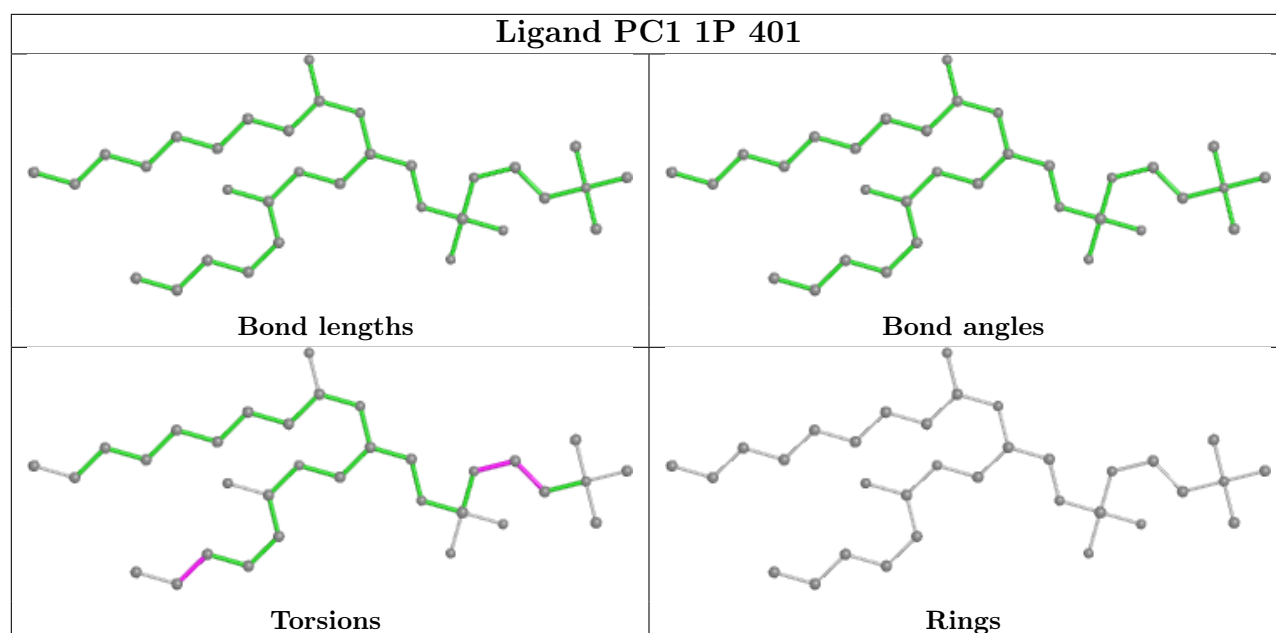












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	1h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1h	124:GLN	C	125:TYR	N	1.12



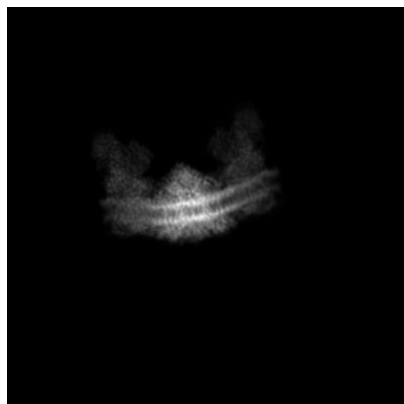
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42233. These allow visual inspection of the internal detail of the map and identification of artifacts.

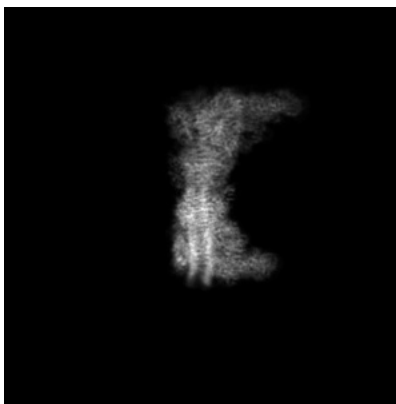
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

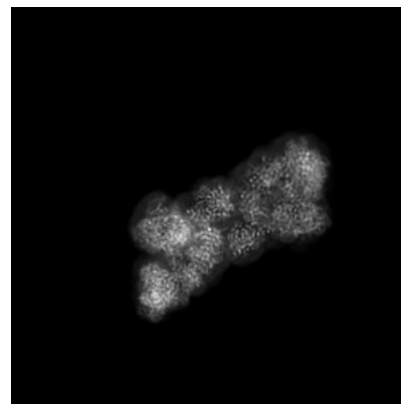
#### 6.1.1 Primary map



X

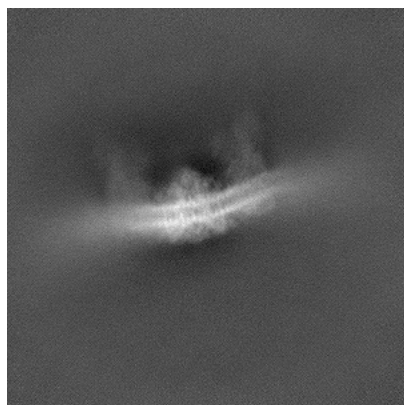


Y

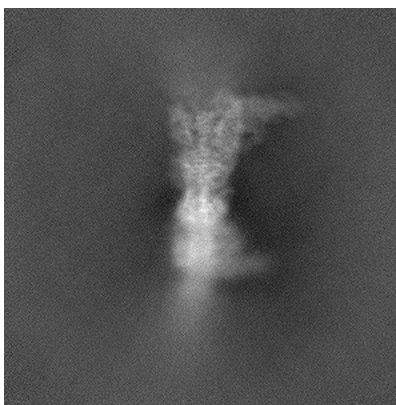


Z

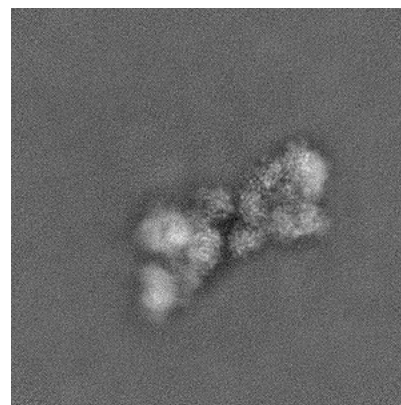
#### 6.1.2 Raw map



X



Y

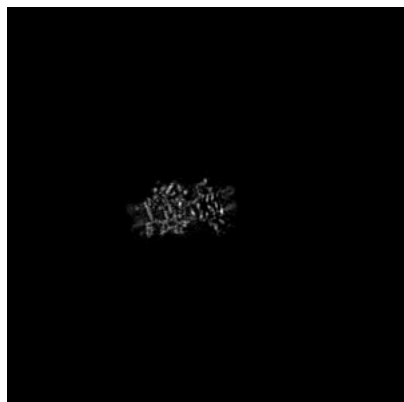


Z

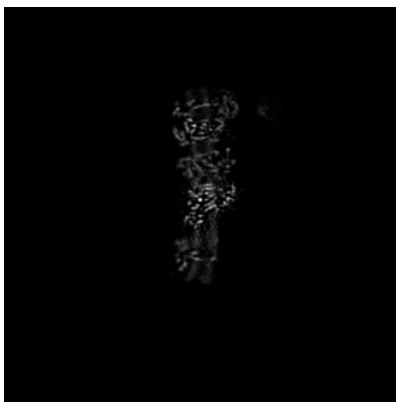
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

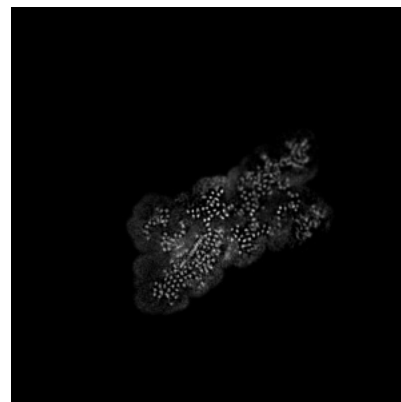
### 6.2.1 Primary map



X Index: 256

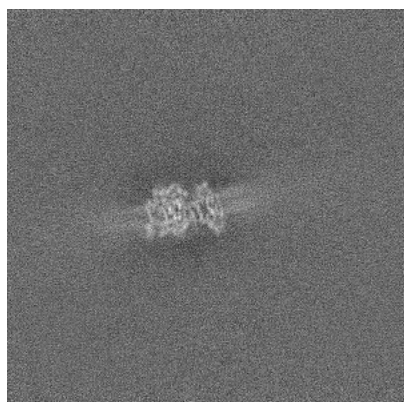


Y Index: 256



Z Index: 256

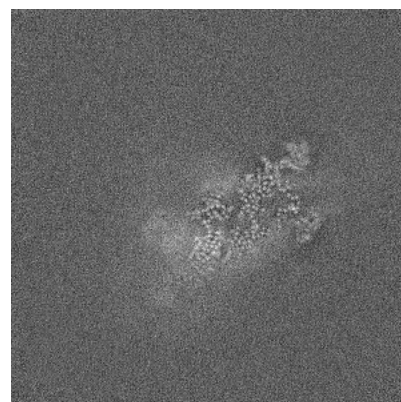
### 6.2.2 Raw map



X Index: 256



Y Index: 256

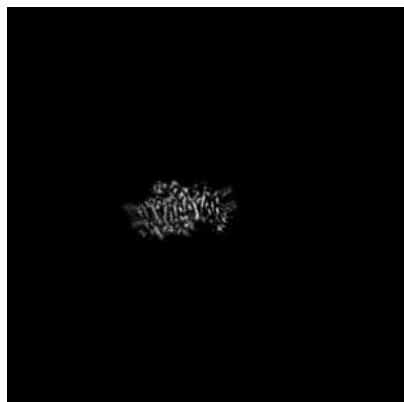


Z Index: 256

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

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

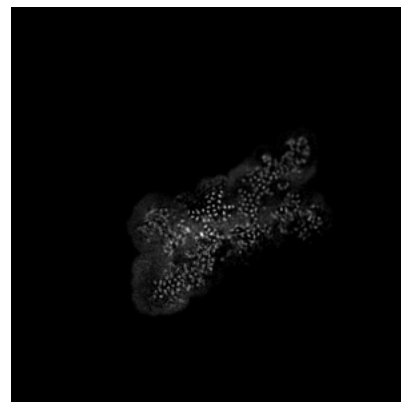
### 6.3.1 Primary map



X Index: 252

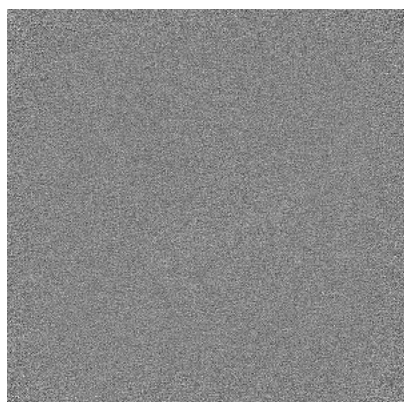


Y Index: 222

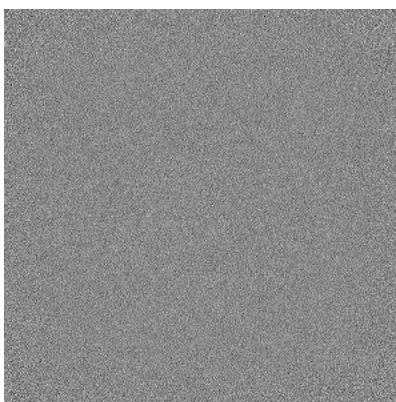


Z Index: 260

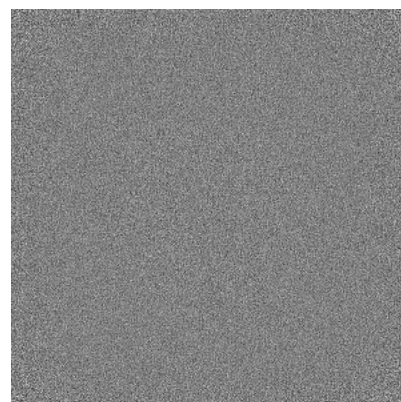
### 6.3.2 Raw map



X Index: 0



Y Index: 0

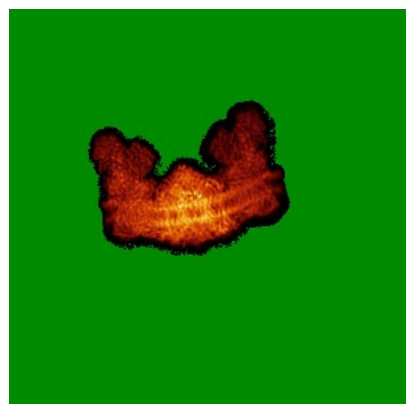


Z Index: 0

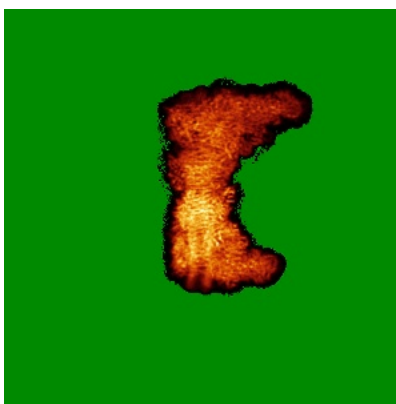
The images above show the largest variance slices of the map in three orthogonal directions.

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

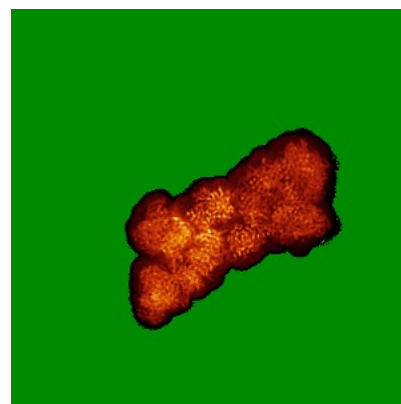
### 6.4.1 Primary map



X

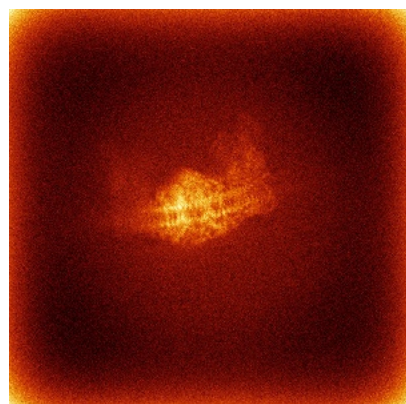


Y

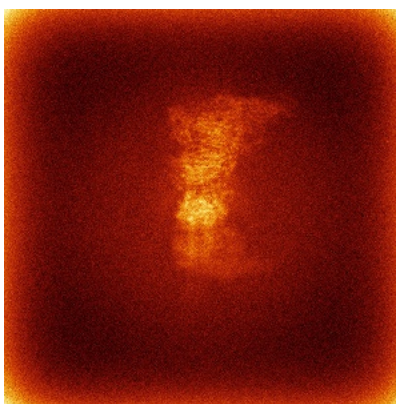


Z

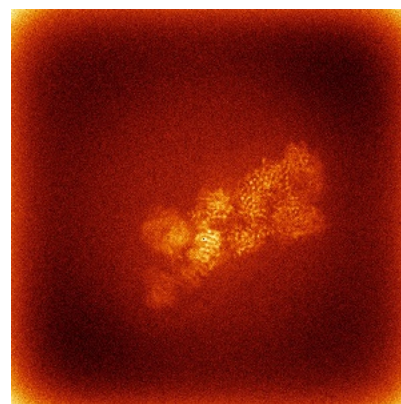
### 6.4.2 Raw map



X



Y

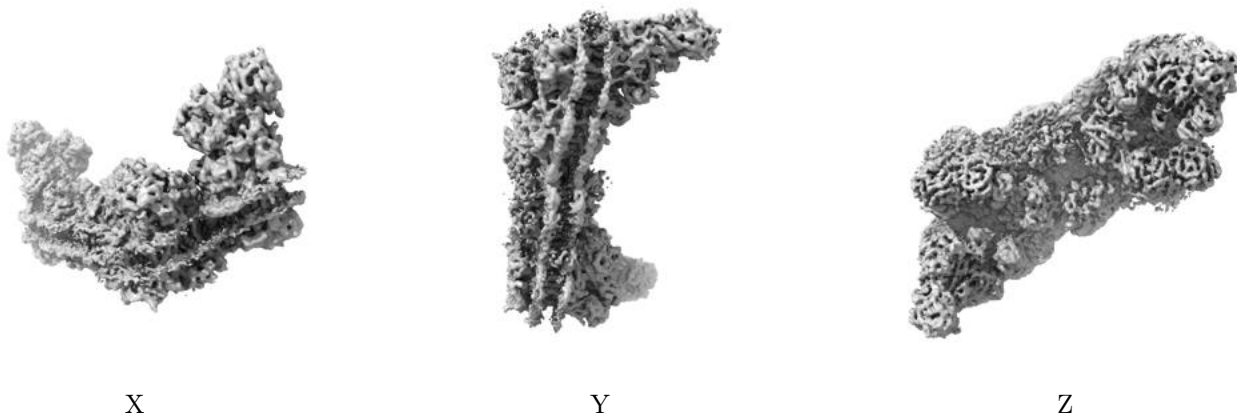


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

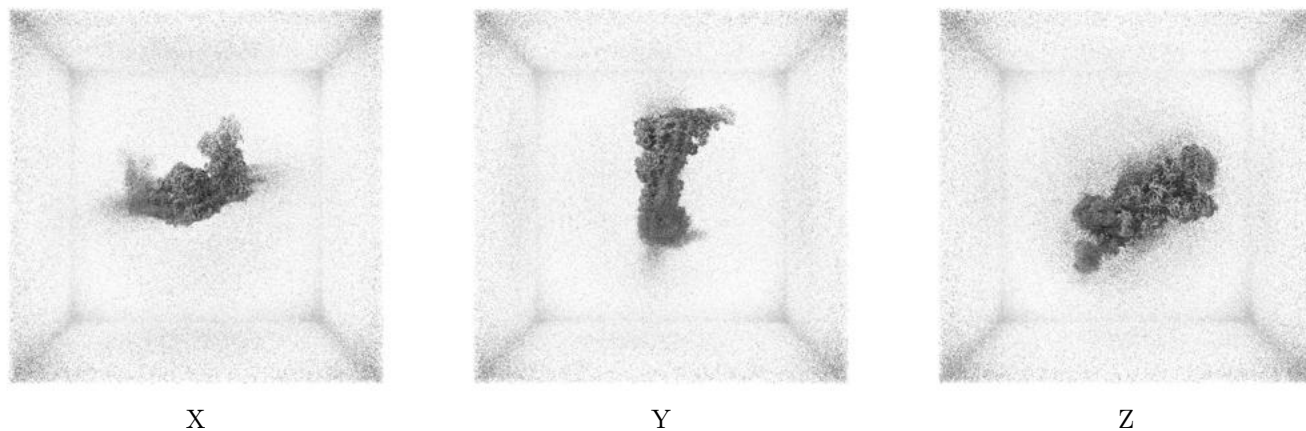
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

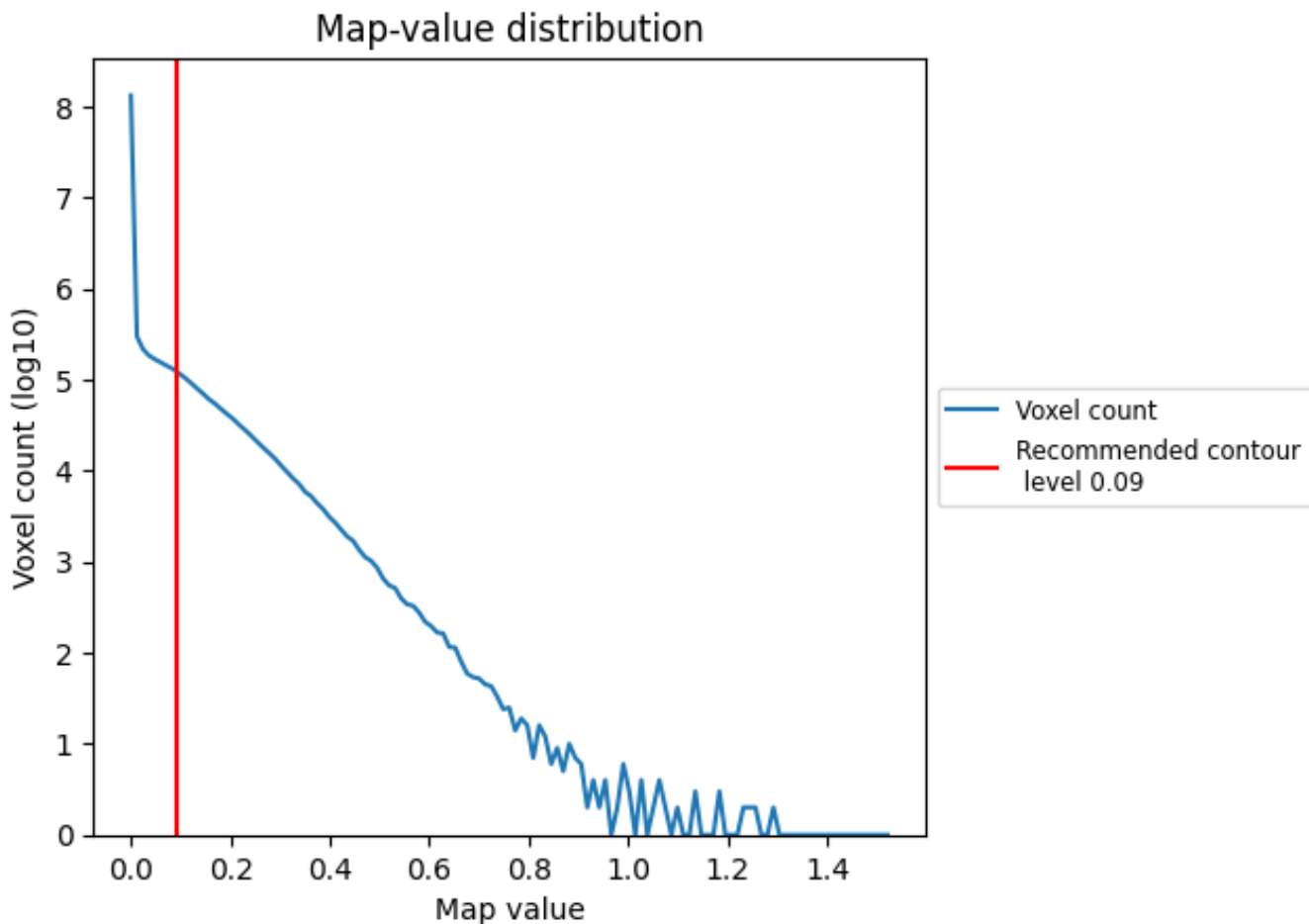
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

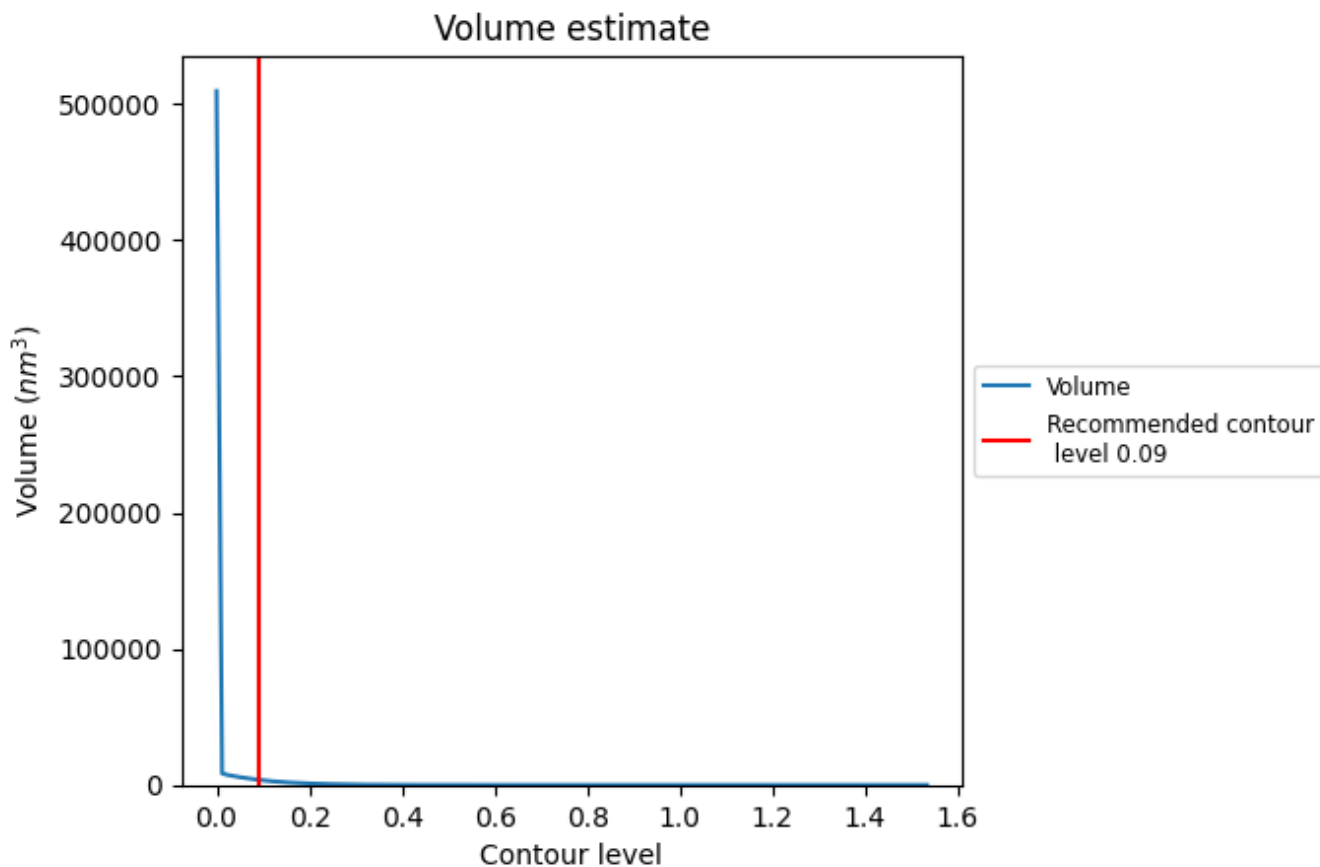
This section contains the results of statistical analysis of the map.

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



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

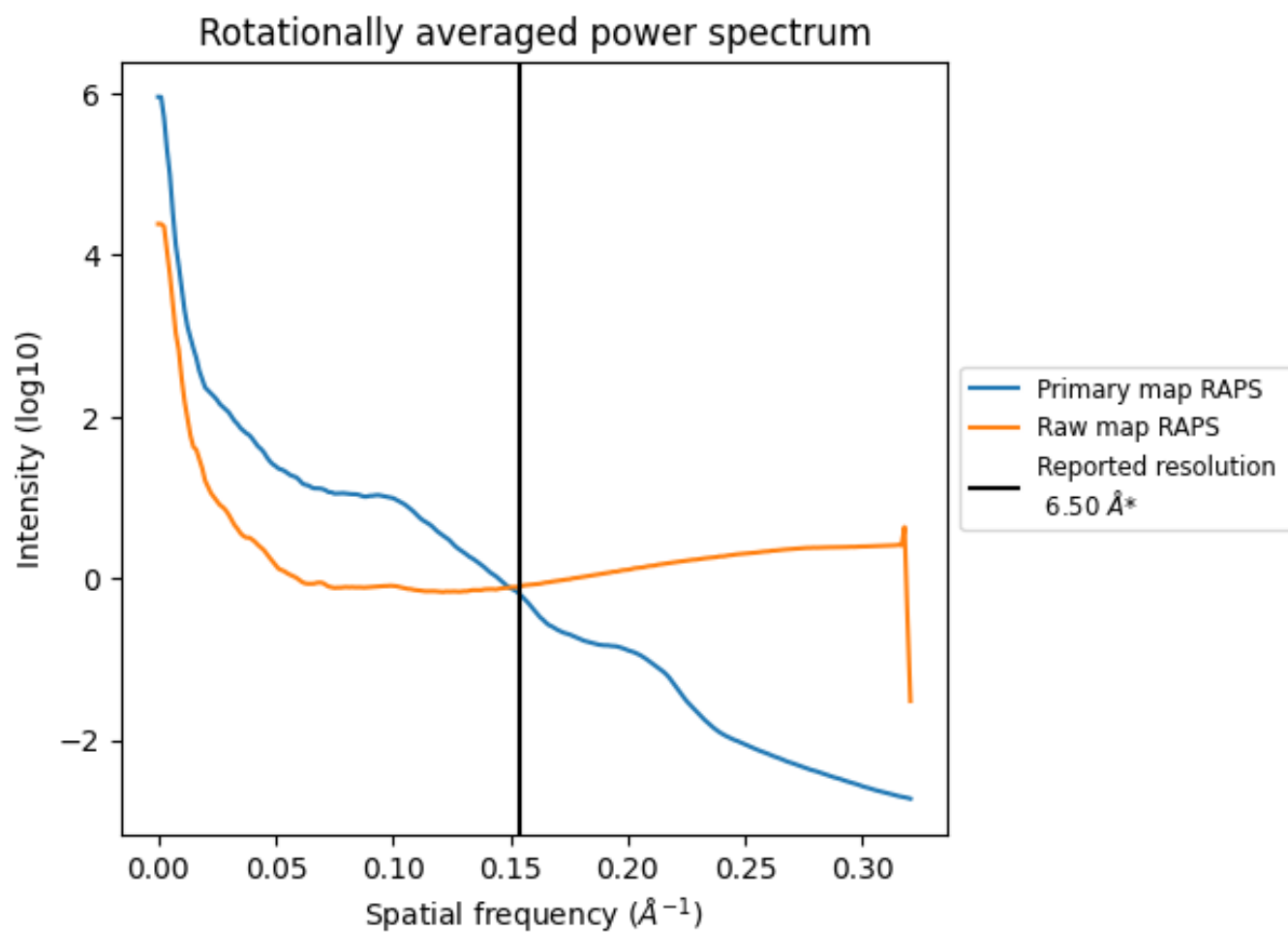
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3822  $\text{nm}^3$ ; this corresponds to an approximate mass of 3453 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



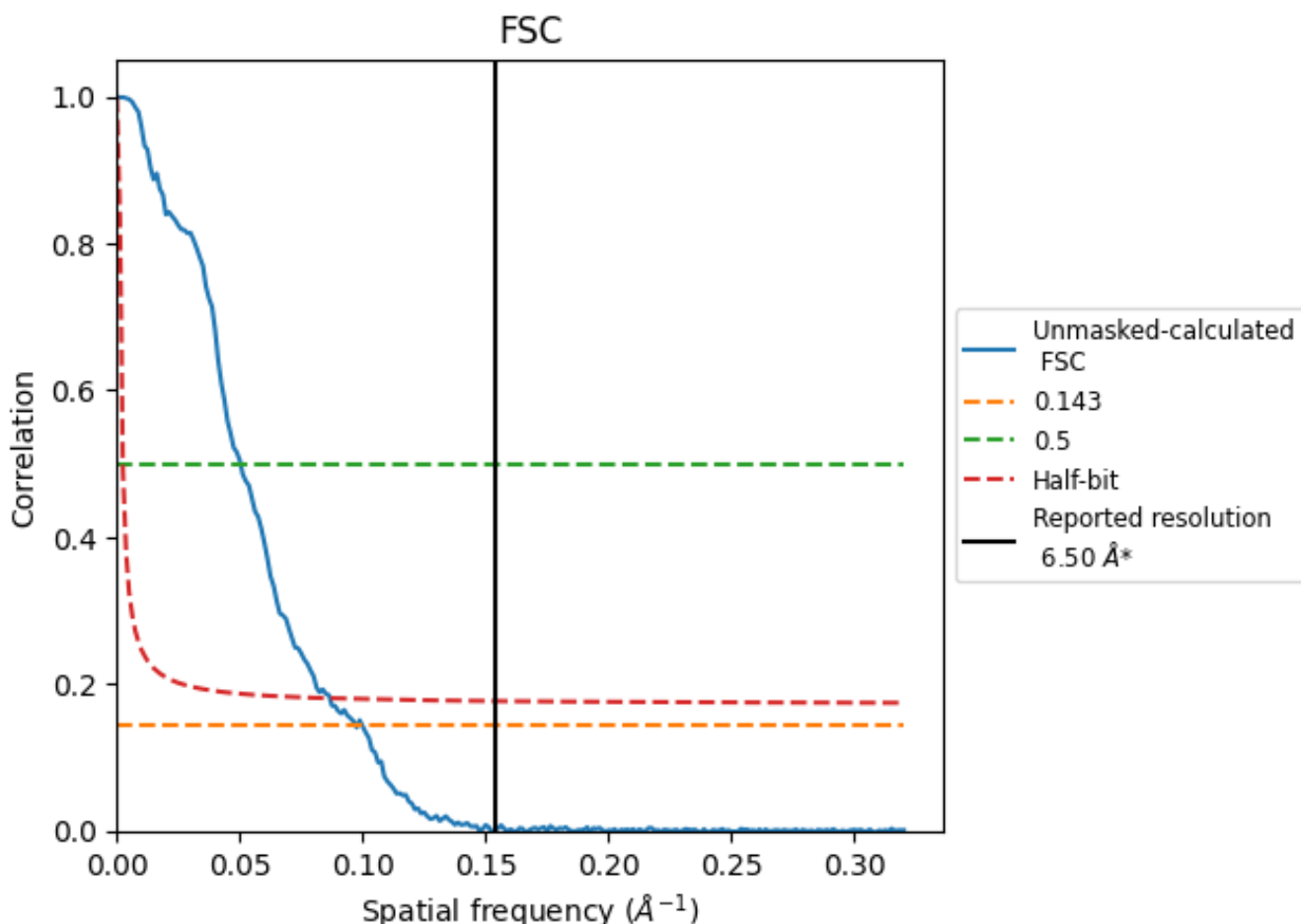
\*Reported resolution corresponds to spatial frequency of  $0.154 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.154 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

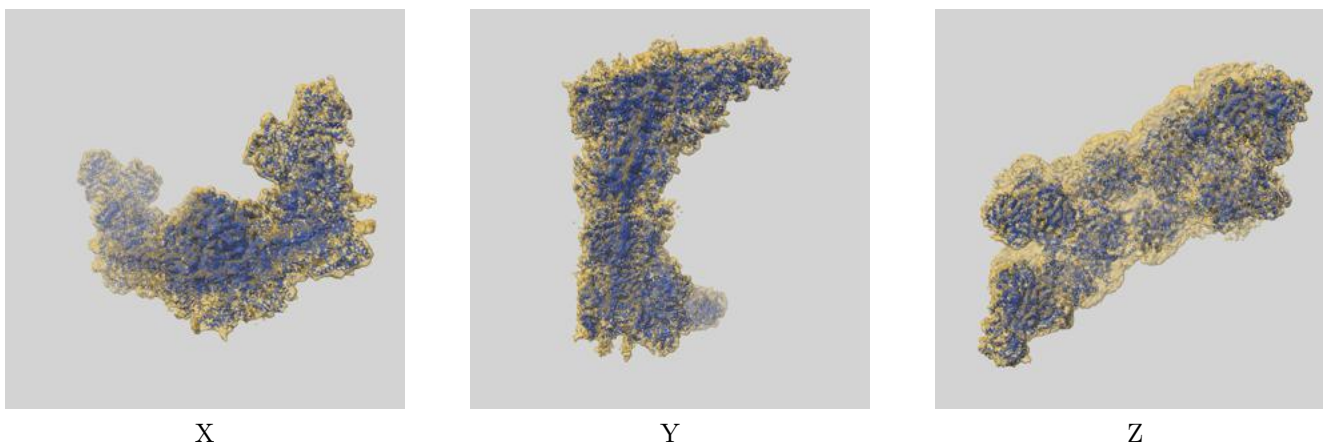
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	19.84	11.52

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.28 differs from the reported value 6.5 by more than 10 %

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

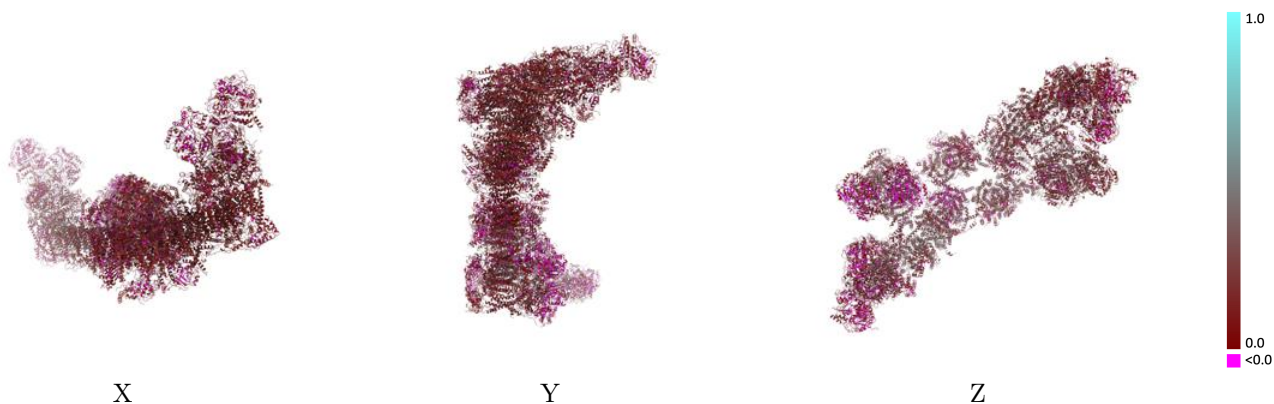
This section contains information regarding the fit between EMDB map EMD-42233 and PDB model 8UGR. Per-residue inclusion information can be found in section [3](#) on page [47](#).

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



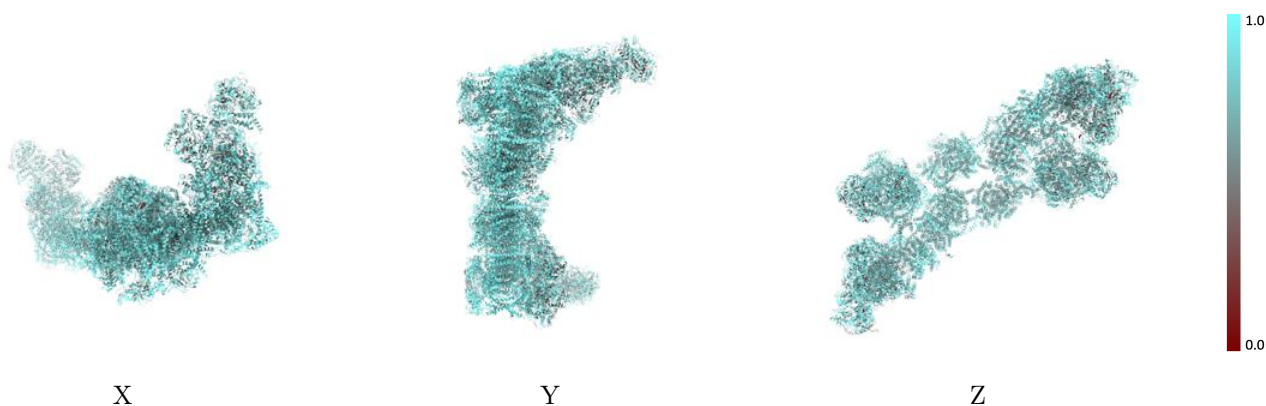
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



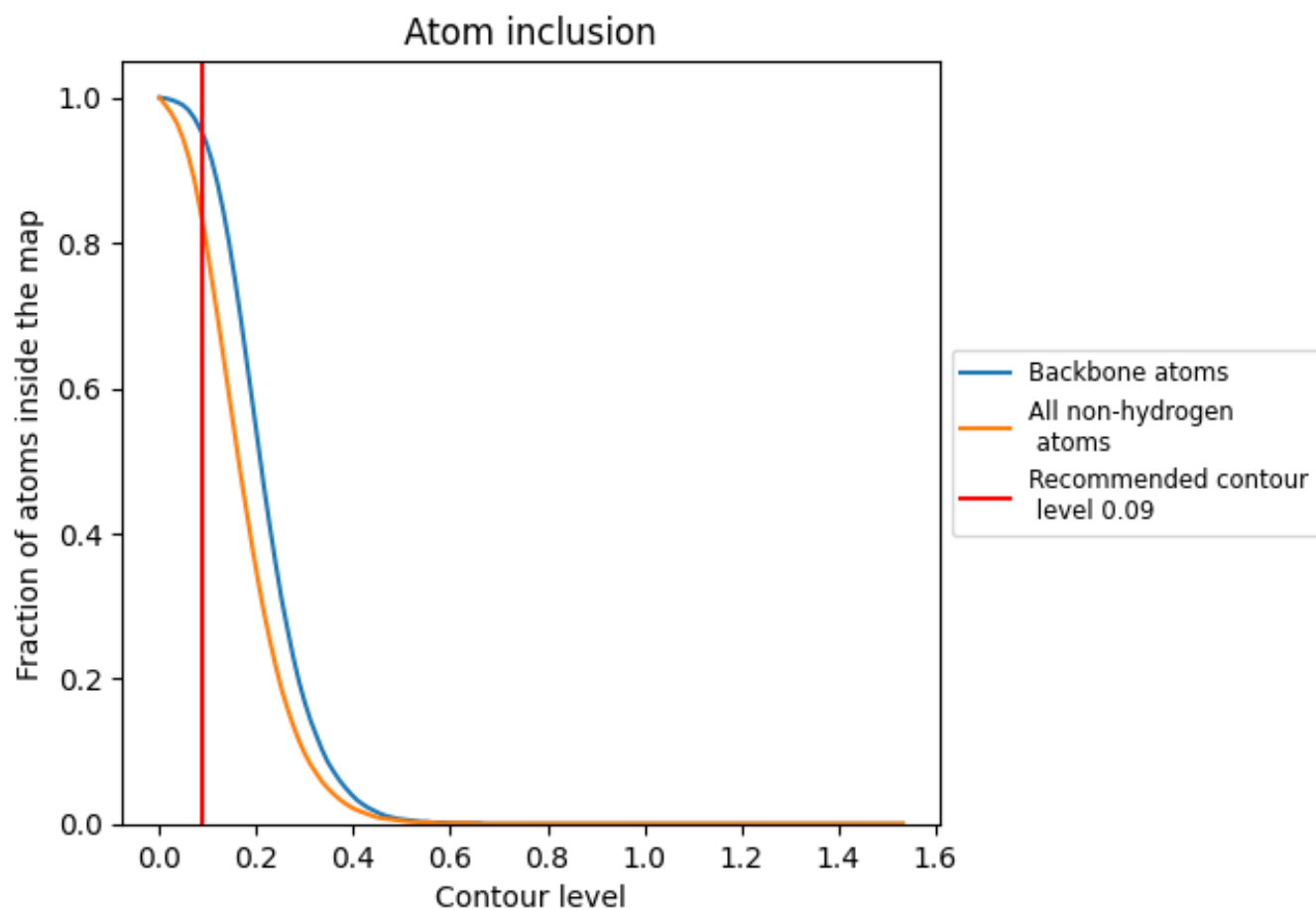
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 82% 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	0.8250	0.1640
1A	0.7810	0.1770
1B	0.8050	0.2190
1C	0.8000	0.1750
1D	0.8160	0.1950
1E	0.7730	0.1490
1F	0.7460	0.0960
1G	0.7630	0.1300
1H	0.8300	0.1690
1I	0.8500	0.2150
1J	0.8640	0.1710
1K	0.8430	0.1960
1L	0.8990	0.1430
1M	0.9080	0.2170
1N	0.8990	0.2450
1O	0.9130	0.1940
1P	0.8220	0.1840
1Q	0.7280	0.1670
1R	0.9180	0.2740
1S	0.7860	0.1280
1T	0.8500	0.1710
1U	0.8110	0.0840
1V	0.7570	0.1290
1W	0.7880	0.2200
1X	0.8550	0.1170
1Y	0.9300	0.1460
1Z	0.8650	0.1450
1a	0.8490	0.1500
1b	0.8790	0.1350
1c	0.9410	0.1880
1d	0.8990	0.2020
1e	0.8730	0.1950
1f	0.9600	0.2150
1g	0.9420	0.2150
1h	0.9000	0.2050























































































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Chain	Atom inclusion	Q-score
1i	 0.9340	 0.1700
1j	 0.9080	 0.1040
1k	 0.8890	 0.1040
1l	 0.9310	 0.1500
1m	 0.9690	 0.1570
1n	 0.9040	 0.1210
1o	 0.9550	 0.0990
1p	 0.9640	 0.2230
1q	 0.8860	 0.2210
1r	 0.8340	 0.1970
1s	 0.8190	 0.1440
3A	 0.7990	 0.1440
3B	 0.7850	 0.1130
3C	 0.8970	 0.2060
3D	 0.8690	 0.1830
3E	 0.8660	 0.1660
3F	 0.9090	 0.1920
3G	 0.9320	 0.2200
3H	 0.8890	 0.1880
3I	 0.5060	 0.1000
3J	 0.9340	 0.1950
3N	 0.9090	 0.0730
3O	 0.7770	 0.0680
3P	 0.9560	 0.2070
3Q	 0.9400	 0.1550
3R	 0.8070	 0.0940
3S	 0.9690	 0.1920
3T	 0.9980	 0.2110
3U	 0.9790	 0.1550
3V	 0.7260	 0.0540
3W	 0.9640	 0.0990
3X	 0.9900	 0.1100
3Y	 0.9160	 0.1960
4A	 0.8040	 0.1340
4B	 0.7970	 0.1320
4C	 0.8150	 0.1280
4D	 0.8760	 0.1460
4E	 0.8650	 0.1650
4F	 0.8550	 0.1950
4G	 0.9620	 0.1570
4H	 0.8330	 0.1530
4I	 0.9030	 0.1600

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






















































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Chain	Atom inclusion	Q-score
4J	 0.9360	 0.1790
4K	 0.9690	 0.1790
4L	 0.8780	 0.1360
4M	 0.9270	 0.1730
4N	 0.8490	 0.1880
5A	 0.6690	 0.1480
5B	 0.7630	 0.1710
5C	 0.7090	 0.1680
5D	 0.7110	 0.1670
5E	 0.7260	 0.1680
5F	 0.7090	 0.1420
5G	 0.7110	 0.1380
5H	 0.7540	 0.1630
5I	 0.8000	 0.1580
5J	 0.8290	 0.1710
5K	 0.8010	 0.1620
5L	 0.8130	 0.1490
5M	 0.7790	 0.1580
5N	 0.8230	 0.1820
5O	 0.8270	 0.1800
5P	 0.7980	 0.1540
5Q	 0.6260	 0.1510
5R	 0.8460	 0.1950
5S	 0.7230	 0.1580
5T	 0.6920	 0.1580
5U	 0.6990	 0.1460
5V	 0.7170	 0.1800
5W	 0.7340	 0.1850
5X	 0.9300	 0.1860
5Y	 0.8280	 0.1740
5Z	 0.8680	 0.1990
5a	 0.8660	 0.1750
5b	 0.8980	 0.1810
5c	 0.8990	 0.1810
5d	 0.8240	 0.1740
5e	 0.9400	 0.2020
5f	 0.8860	 0.1940
5g	 0.8590	 0.1980
5h	 0.8410	 0.1670
5i	 0.8680	 0.1670
5j	 0.8350	 0.1640
5k	 0.8690	 0.1640

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Chain	Atom inclusion	Q-score
5l	 0.8910	 0.1890
5m	 0.8490	 0.1700
5n	 0.8120	 0.1630
5o	 0.9260	 0.1740
5p	 0.9190	 0.1880
5q	 0.8750	 0.2050
5r	 0.7860	 0.2200
5s	 0.8280	 0.1690
6A	 0.7840	 0.1820
6B	 0.7560	 0.2090
6C	 0.7690	 0.1910
6D	 0.8500	 0.1770
6E	 0.7830	 0.1330
6F	 0.7520	 0.2040
6G	 0.8310	 0.1980
6H	 0.8390	 0.1970
6I	 0.4390	 0.1080
6J	 0.8890	 0.1770
6N	 0.8100	 0.1730
6O	 0.7600	 0.2010
6P	 0.8020	 0.1850
6Q	 0.8520	 0.1810
6R	 0.7420	 0.1360
6S	 0.8250	 0.1910
6T	 0.9190	 0.1890
6U	 0.9100	 0.1870
6V	 0.5950	 0.1620
6W	 0.8850	 0.1770
6X	 0.9420	 0.2070
6Y	 0.8860	 0.2100
8A	 0.7410	 0.1270
8B	 0.7730	 0.1400
8C	 0.7210	 0.1170
8D	 0.8260	 0.1590
8E	 0.7620	 0.1590
8F	 0.7720	 0.1790
8G	 0.8490	 0.1450
8H	 0.8370	 0.1620
8I	 0.8800	 0.1760
8J	 0.9120	 0.1780
8K	 0.9360	 0.1510
8L	 0.8280	 0.1400

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Chain	Atom inclusion	Q-score
8M	 0.9370	 0.1760
8N	 0.8230	 0.1840