



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 06:01 AM EDT

PDB ID : 8UGN / pdb_00008ugn
EMDB ID : EMD-42230
Title : In-situ structure of typeO supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

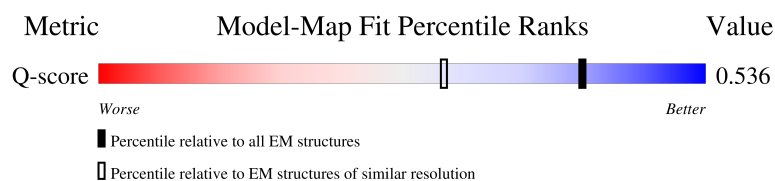
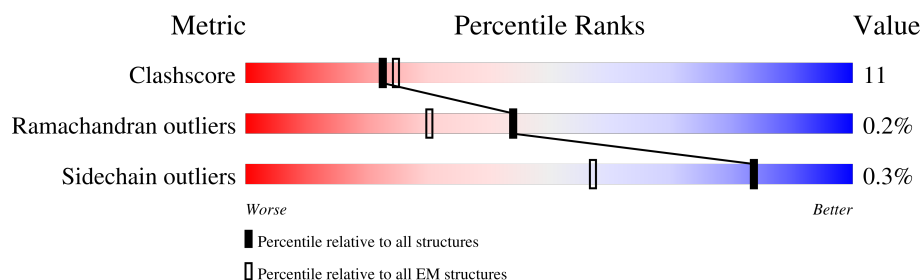
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	1A	115	 63% 37%
1	5A	115	 57% 43%
2	1B	258	 43% 17% 40%
2	5B	258	 40% 20% 40%

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Mol	Chain	Length	Quality of chain
3	1C	264	
3	5C	264	
4	1D	476	
4	5D	476	
5	1E	249	
5	5E	249	
6	1F	464	
6	5F	464	
7	1G	727	
7	5G	727	
8	1H	318	
8	5H	318	
9	1I	239	
9	5I	239	
10	1J	175	
10	5J	175	
11	1K	98	
11	5K	98	
12	1L	606	
12	5L	606	
13	1M	459	
13	5M	459	
14	1N	347	
14	5N	347	
15	1O	357	

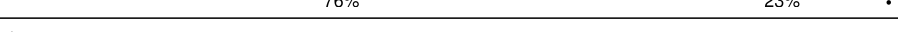
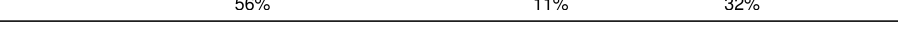
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Mol	Chain	Length	Quality of chain
15	5O	357	
16	1P	377	
16	5P	377	
17	1Q	175	
17	5Q	175	
18	1R	123	
18	5R	123	
19	1S	99	
19	5S	99	
20	1T	156	
20	1U	156	
20	5T	156	
20	5U	156	
21	1V	116	
21	5V	116	
22	1W	128	
22	5W	128	
23	1X	172	
23	5X	172	
24	1Y	141	
24	5Y	141	
25	1Z	144	
25	5Z	144	
26	1a	70	
26	5a	70	

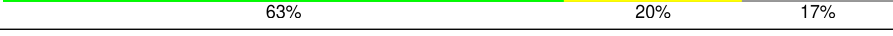
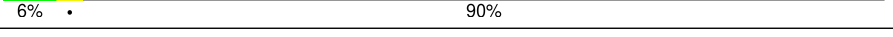
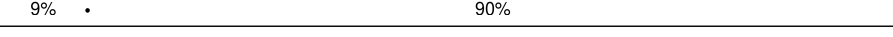
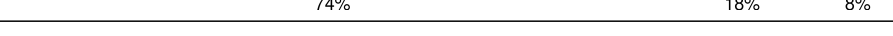
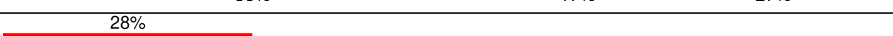
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Mol	Chain	Length	Quality of chain
27	1b	84	
27	5b	84	
28	1c	76	
28	5c	76	
29	1d	122	
29	5d	122	
30	1e	106	
30	5e	106	
31	1f	135	
31	5f	135	
32	1g	154	
32	5g	154	
33	1h	189	
33	5h	189	
34	1i	128	
34	5i	128	
35	1j	105	
35	5j	105	
36	1k	98	
36	5k	98	
37	1l	186	
37	5l	186	
38	1m	129	
38	5m	129	
39	1n	179	

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Mol	Chain	Length	Quality of chain
39	5n	179	
40	1o	137	
40	5o	137	
41	1p	176	
41	5p	176	
42	1q	145	
42	5q	145	
43	1r	113	
43	5r	113	
44	1s	471	
44	5s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	

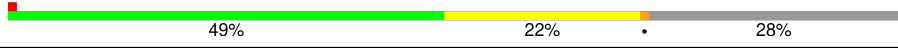
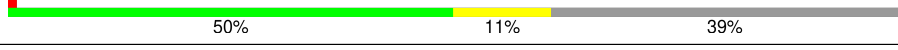
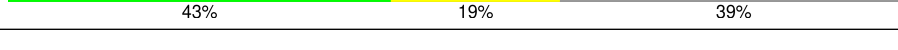
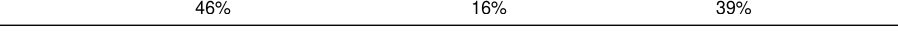
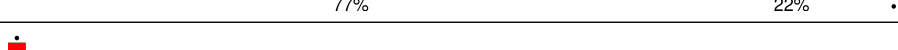
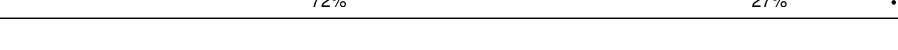
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Mol	Chain	Length	Quality of chain
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	128	
60	8F	128	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	

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Mol	Chain	Length	Quality of chain
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
71	FES	1G	803	-	-	X	-
71	FES	5G	803	-	-	X	-
85	HEC	3D	501	X	-	-	-
85	HEC	3Q	501	X	-	-	-
91	CUA	4B	303	-	-	X	-

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 202910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		
1	5A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		
2	5B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		
3	5C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		

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
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		
4	5D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

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
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		
5	5E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		
6	5F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		
7	5G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	5H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		
9	5I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		
10	5J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		
11	5K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		
12	5L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	5M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		
14	5N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		
15	5O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		
16	5P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		
17	5Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- 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
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
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
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
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
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
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		
32	5g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		
33	5h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		
34	5i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	5j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		
36	5k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		
37	5l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1m	128	Total	C	N	O		0	0
			1062	691	182	189			
38	5m	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		
39	5n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1
5o	0	MYR	-	insertion	UNP F1SCH1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		
41	5p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Cytochrome b.

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

- Molecule 48 is a protein called Cytochrome c1.

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	3I	47	Total	C	N	O	S	0	0
			340	211	65	63	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			224	136	48	39	1		

There are 16 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		
55	8A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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		
62	8H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		
63	8I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		
64	8J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		
65	8K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

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

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

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

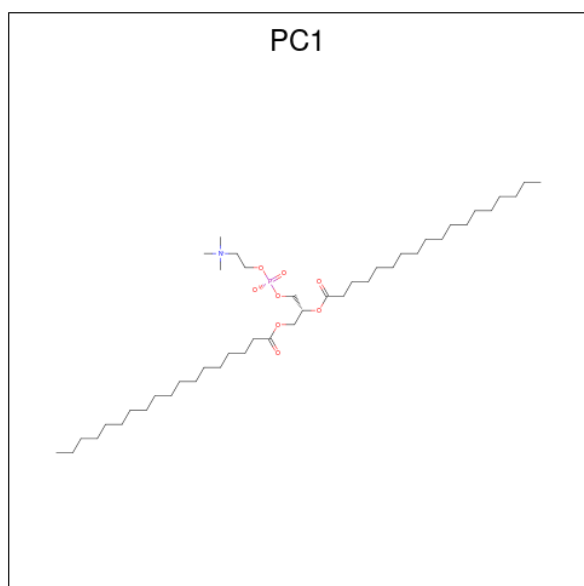
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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 NDUF44.

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

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	

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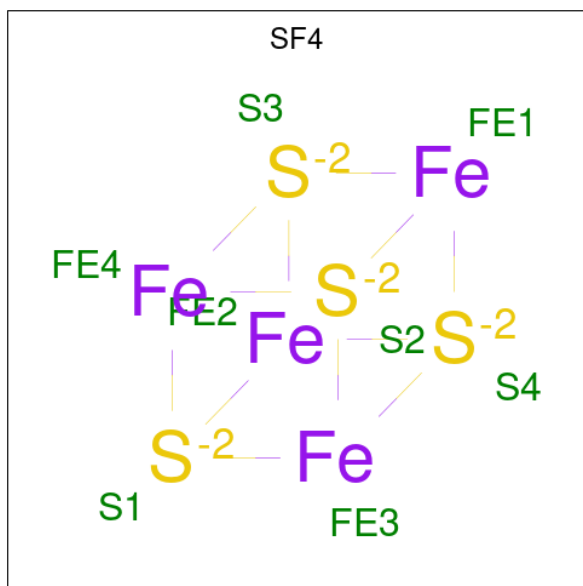
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	1A	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
69	1I	1	Total	C	N	O	P	0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

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

- Molecule 70 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



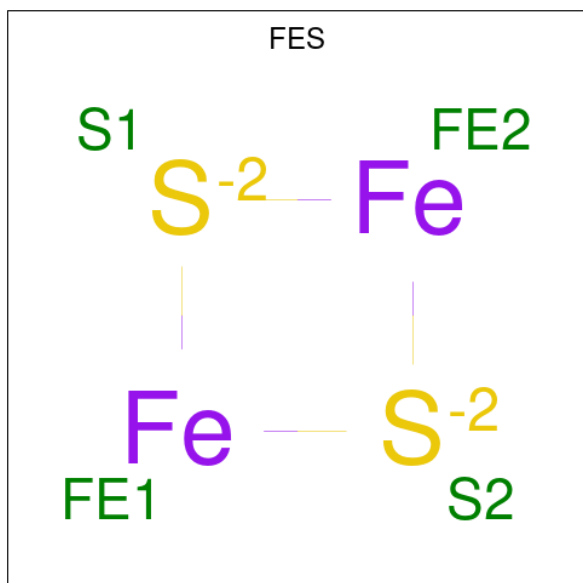
Mol	Chain	Residues	Atoms			AltConf
70	1B	1	Total	Fe	S	0
			8	4	4	
70	1F	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



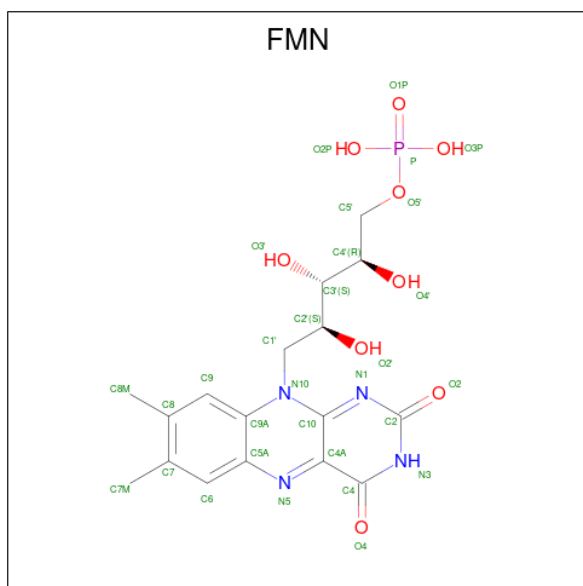
Mol	Chain	Residues	Atoms			AltConf
71	1E	1	Total	Fe	S	0
			4	2	2	

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

- Molecule 72 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

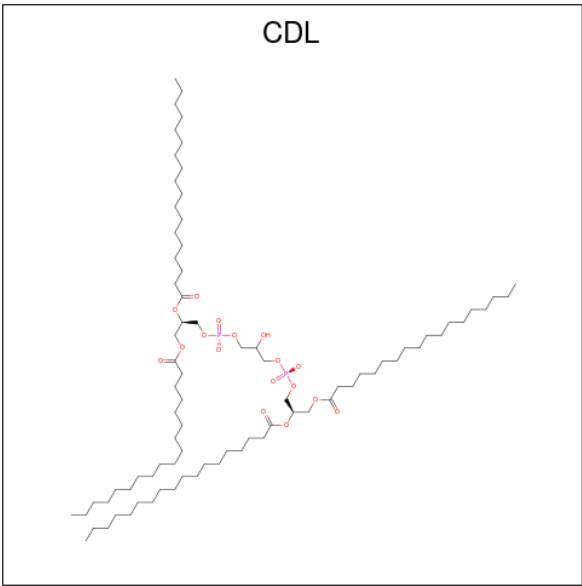


Mol	Chain	Residues	Atoms					AltConf
72	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	
72	5F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 73 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 74 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



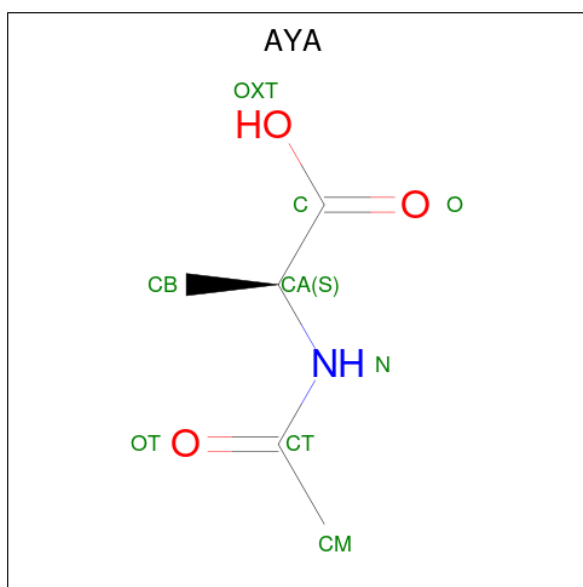
Mol	Chain	Residues	Atoms				AltConf
74	1H	1	Total	C	O	P	0
			51	32	17	2	
74	1L	1	Total	C	O	P	0
			76	57	17	2	
74	1N	1	Total	C	O	P	0
			62	43	17	2	
74	1X	1	Total	C	O	P	0
			86	67	17	2	
74	1d	1	Total	C	O	P	0
			65	46	17	2	
74	1h	1	Total	C	O	P	0
			80	61	17	2	
74	1q	1	Total	C	O	P	0
			61	42	17	2	
74	3A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

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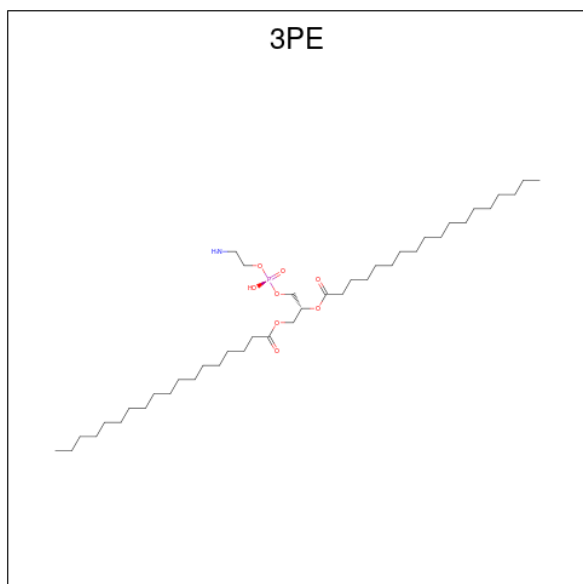
Mol	Chain	Residues	Atoms				AltConf
74	4B	1	Total 100	C 81	O 17	P 2	0
74	4C	1	Total 100	C 81	O 17	P 2	0
74	4D	1	Total 100	C 81	O 17	P 2	0
74	5H	1	Total 51	C 32	O 17	P 2	0
74	5L	1	Total 76	C 57	O 17	P 2	0
74	5N	1	Total 62	C 43	O 17	P 2	0
74	5X	1	Total 86	C 67	O 17	P 2	0
74	5d	1	Total 65	C 46	O 17	P 2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

- Molecule 75 is N-ACETYLALANINE (CCD ID: AYA) (formula: C₅H₉NO₃).



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

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



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

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

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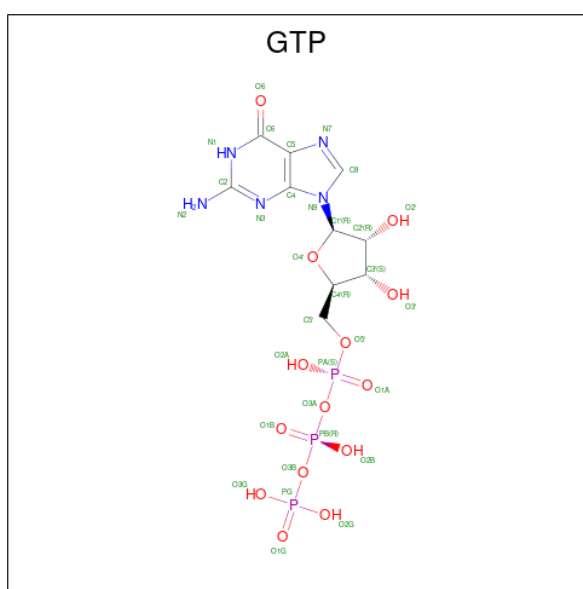
Mol	Chain	Residues	Atoms					AltConf
76	3D	1	Total 33	C 23	N 1	O 8	P 1	0
76	3G	1	Total 29	C 19	N 1	O 8	P 1	0
76	3N	1	Total 33	C 23	N 1	O 8	P 1	0
76	3N	1	Total 25	C 15	N 1	O 8	P 1	0
76	3P	1	Total 33	C 23	N 1	O 8	P 1	0
76	3Q	1	Total 47	C 37	N 1	O 8	P 1	0
76	3Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	5A	1	Total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

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

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



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

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

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

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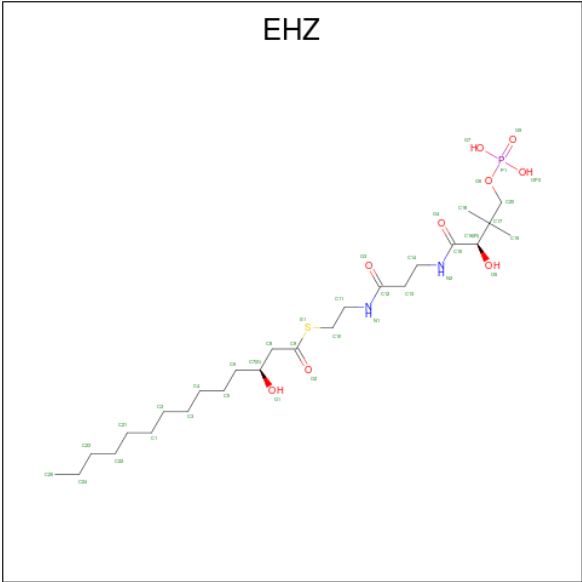
Mol	Chain	Residues	Atoms	AltConf
78	8A	1	Total Mg 1 1	0

- # NDP

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

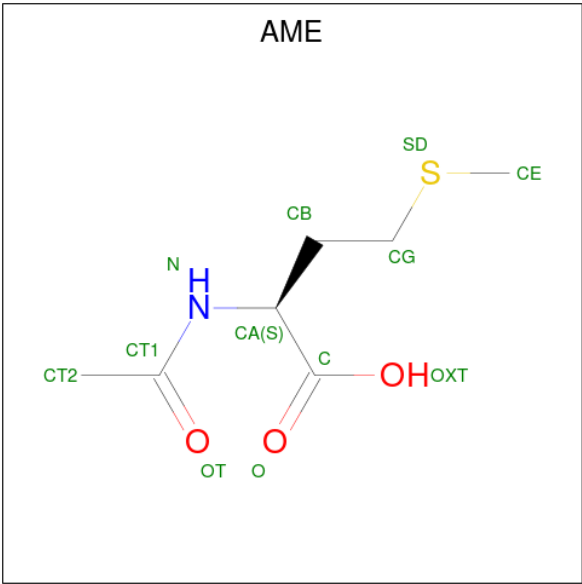
- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 80 | 1R | 1 | Total Zn
1 1 | 0 |
| 80 | 4F | 1 | Total Zn
1 1 | 0 |
| 80 | 5R | 1 | Total Zn
1 1 | 0 |
| 80 | 8F | 1 | Total Zn
1 1 | 0 |

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



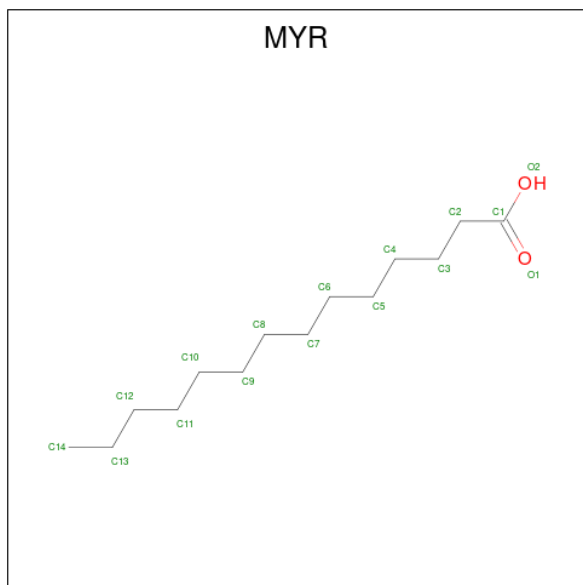
Mol	Chain	Residues	Atoms						AltConf
81	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 82 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



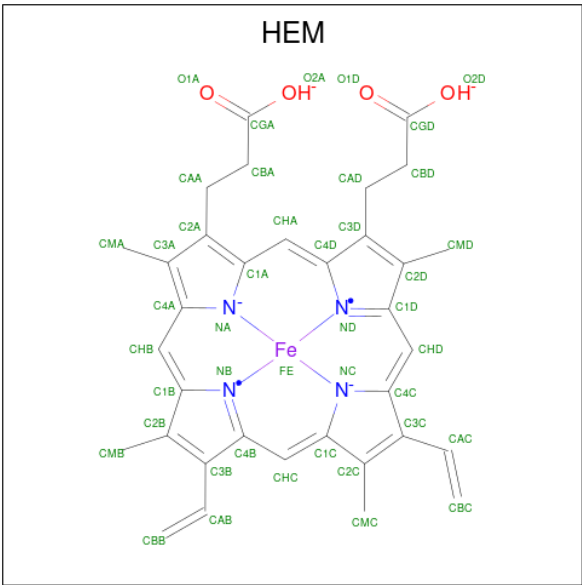
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
82	5h	1	Total	C	N	O	S	0
			11	7	1	2	1	

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



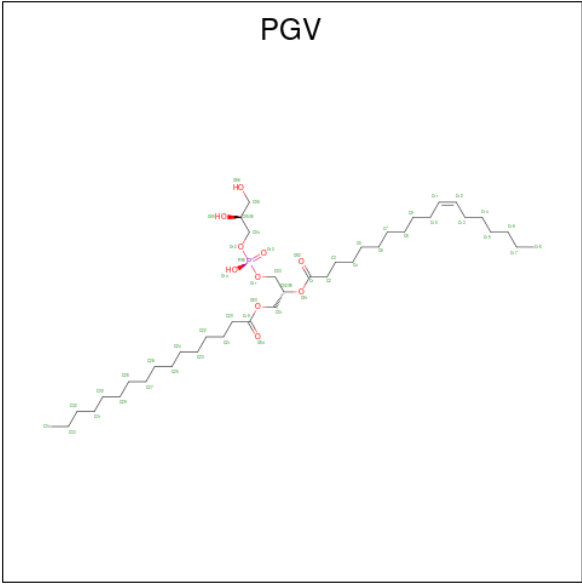
Mol	Chain	Residues	Atoms			AltConf
83	1o	1	Total	C	O	0
			15	14	1	
83	5o	1	Total	C	O	0
			15	14	1	

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



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

- Molecule 86 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



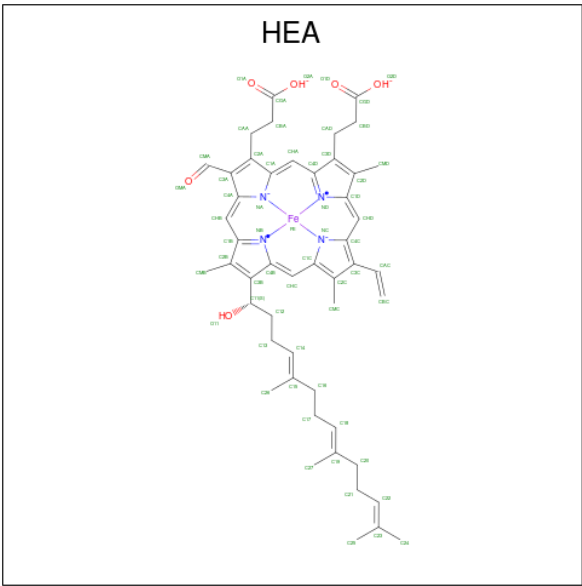
Mol	Chain	Residues	Atoms				AltConf
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4B	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C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

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

- Molecule 87 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 88 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

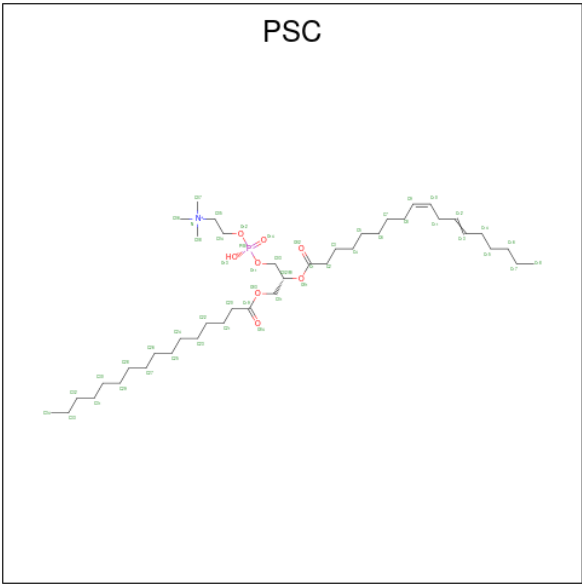
Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Cu	0
			1	1	
88	8A	1	Total	Cu	0
			1	1	

- Molecule 89 is SODIUM ION (CCD ID: NA) (formula: Na).

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

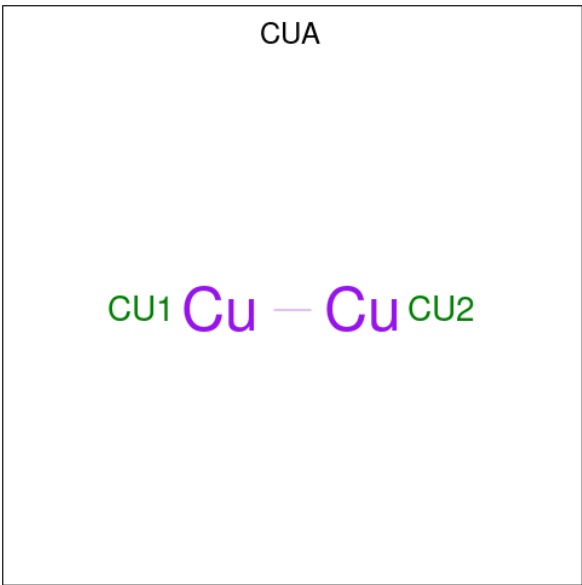
- Molecule 90 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO

YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM
4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



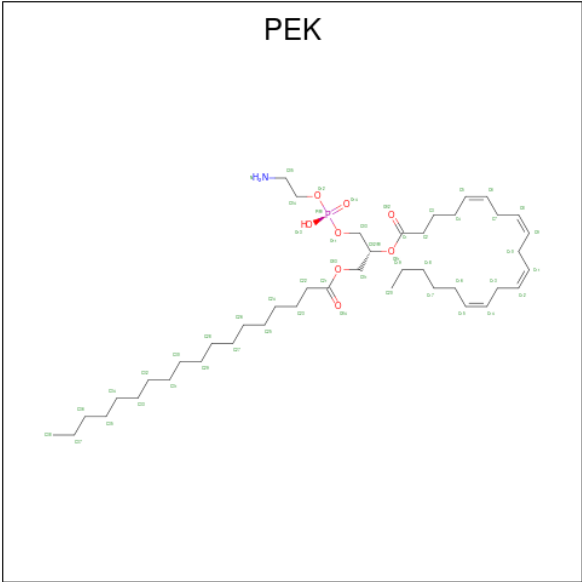
Mol	Chain	Residues	Atoms					AltConf
90	4A	1	Total	C	N	O	P	0
			52	42	1	8	1	
90	8I	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 91 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



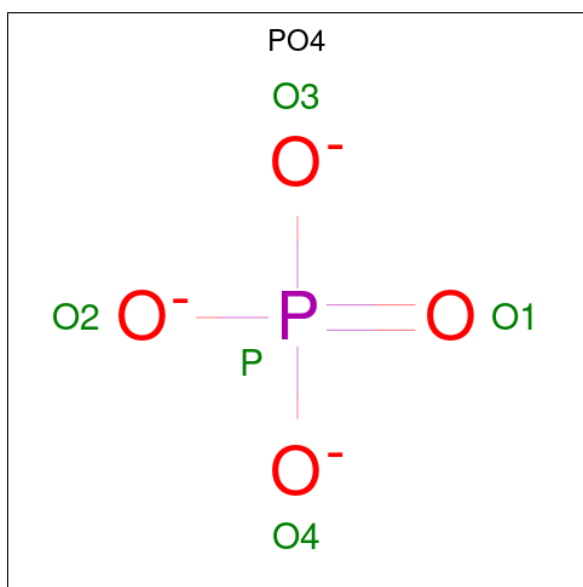
Mol	Chain	Residues	Atoms		AltConf
91	4B	1	Total	Cu	0
			2	2	
91	8B	1	Total	Cu	0
			2	2	

- 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 (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).

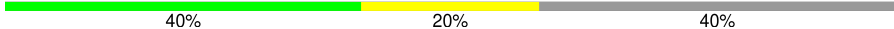


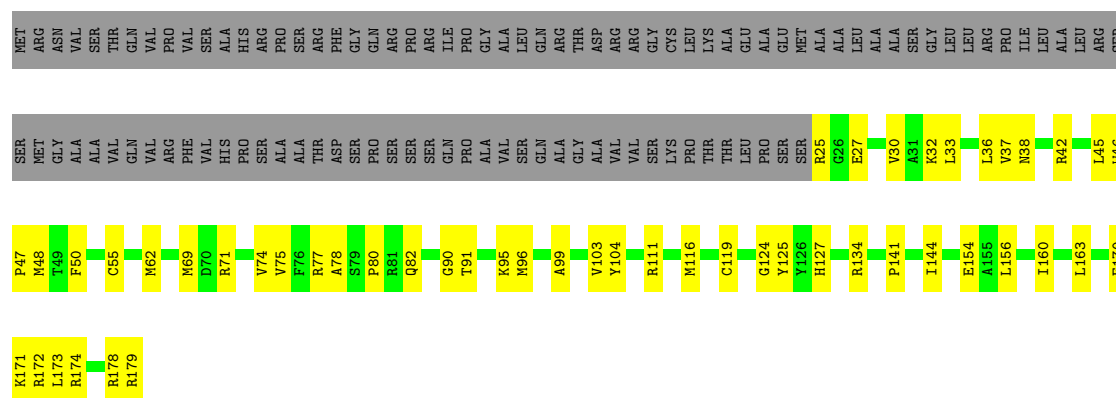
Mol	Chain	Residues	Atoms					AltConf
92	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
92	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	8G	1	Total	C	N	O	P	0
			53	43	1	8	1	

- Molecule 93 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



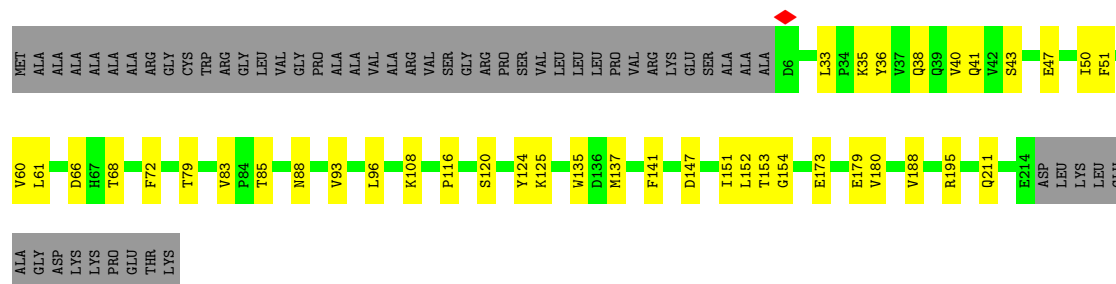
Mol	Chain	Residues	Atoms			AltConf
93	4H	1	Total	O	P	0
			5	4	1	
93	8H	1	Total	O	P	0
			5	4	1	

Chain 5B: 



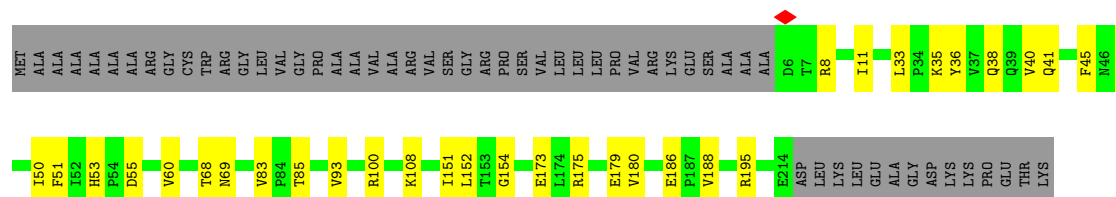
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 1C: 



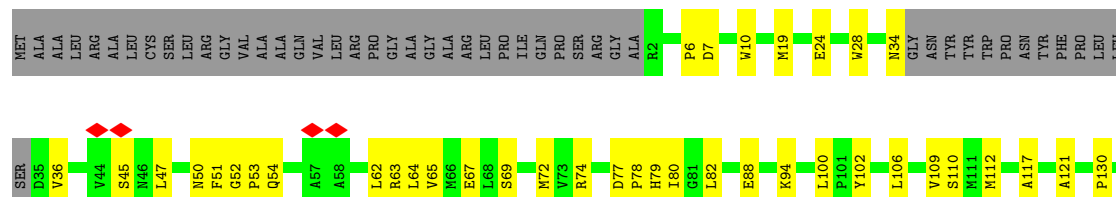
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

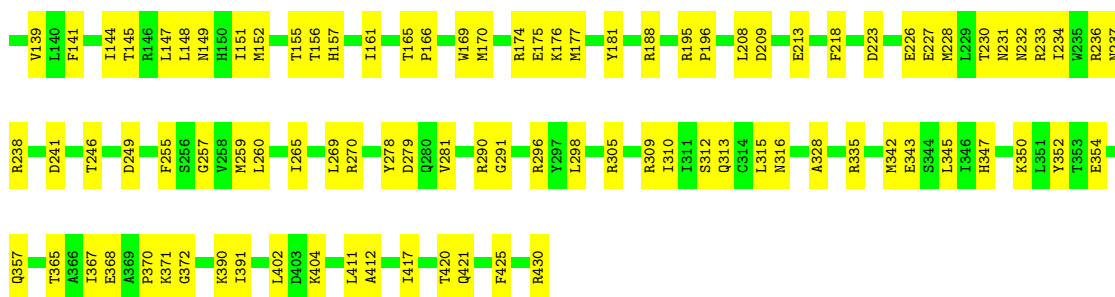
Chain 5C: 



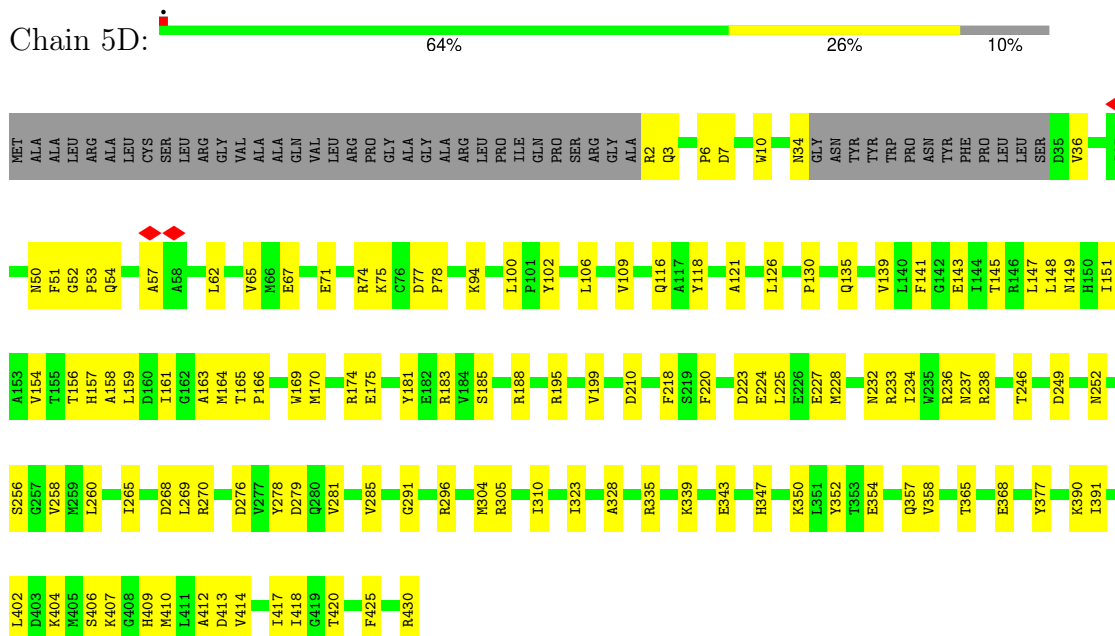
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D: 

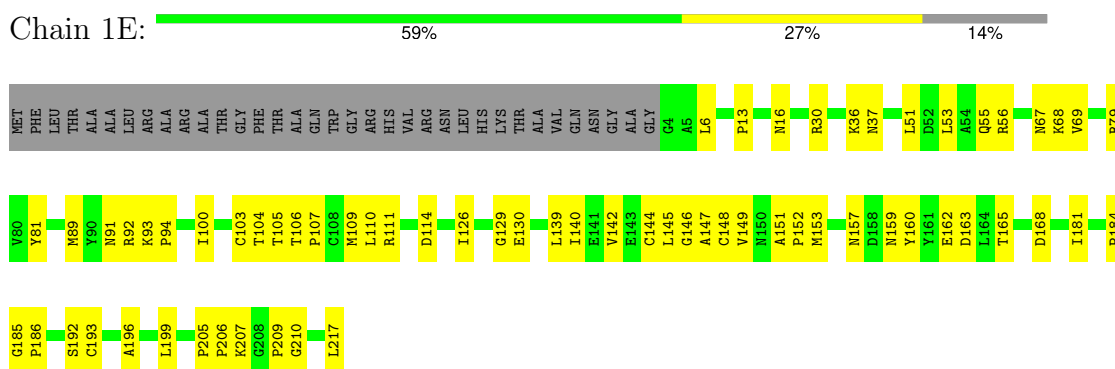




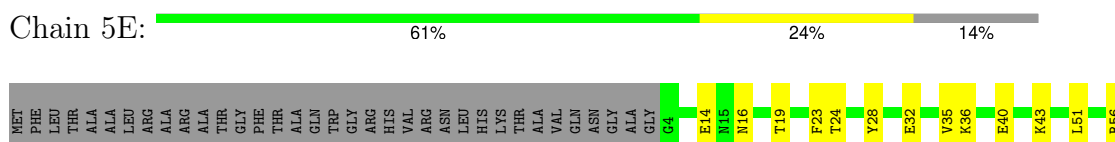
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

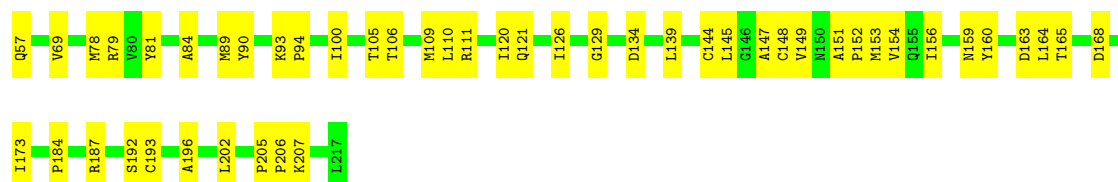


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



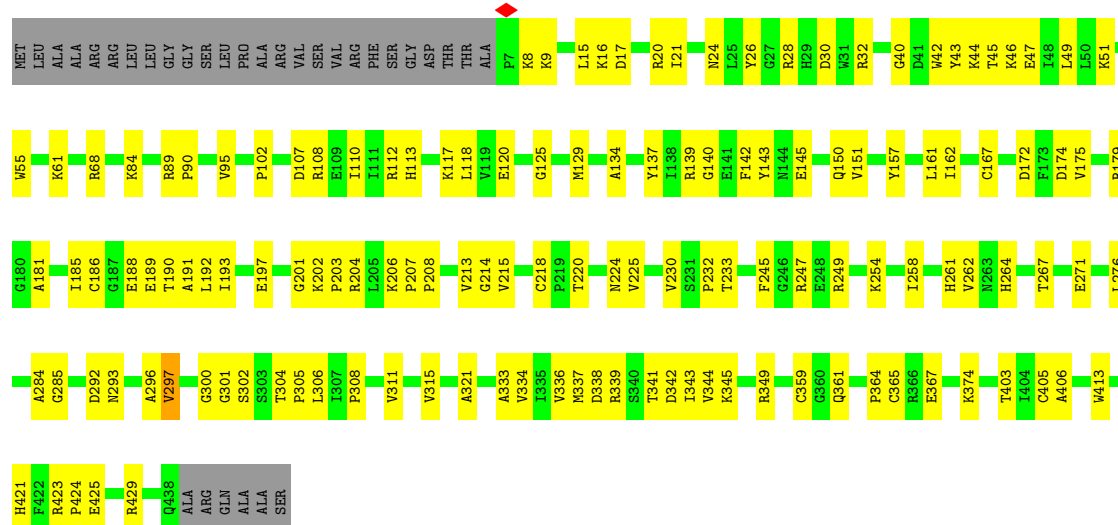
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





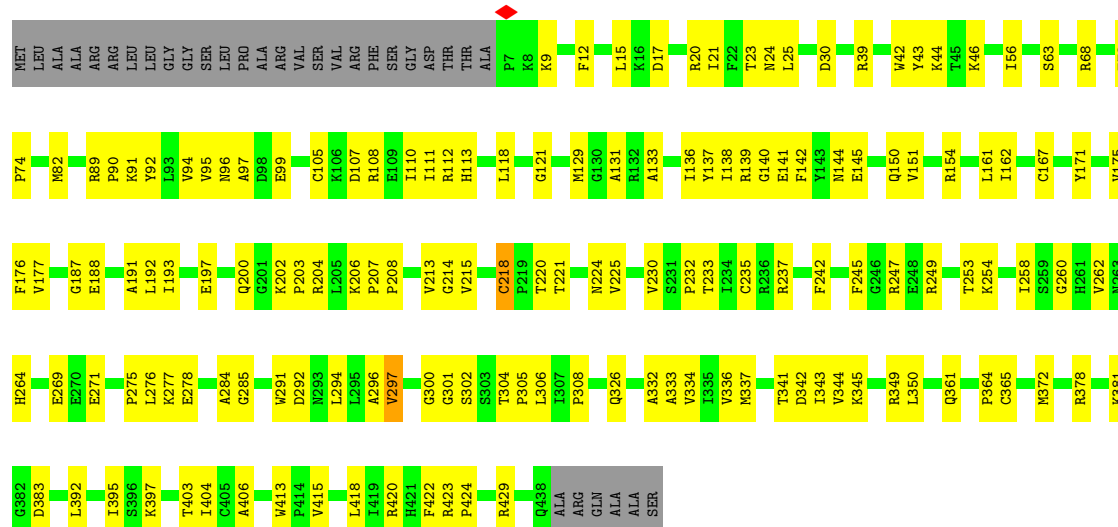
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F: 64% 29% 7%



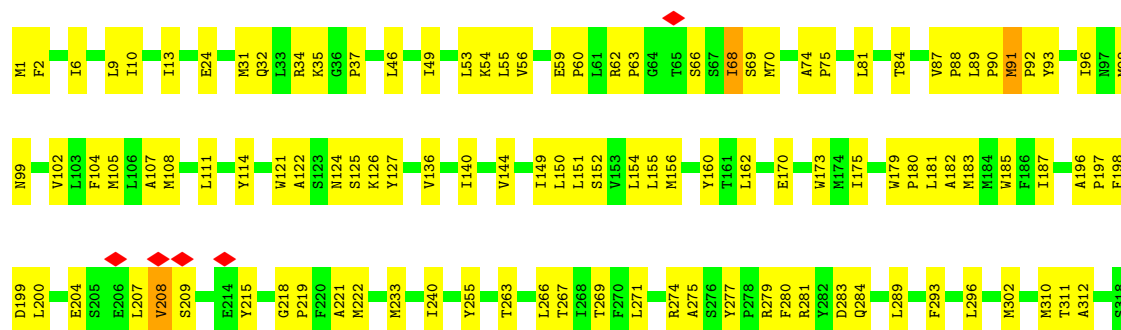
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 5F: 61% 32% 7%



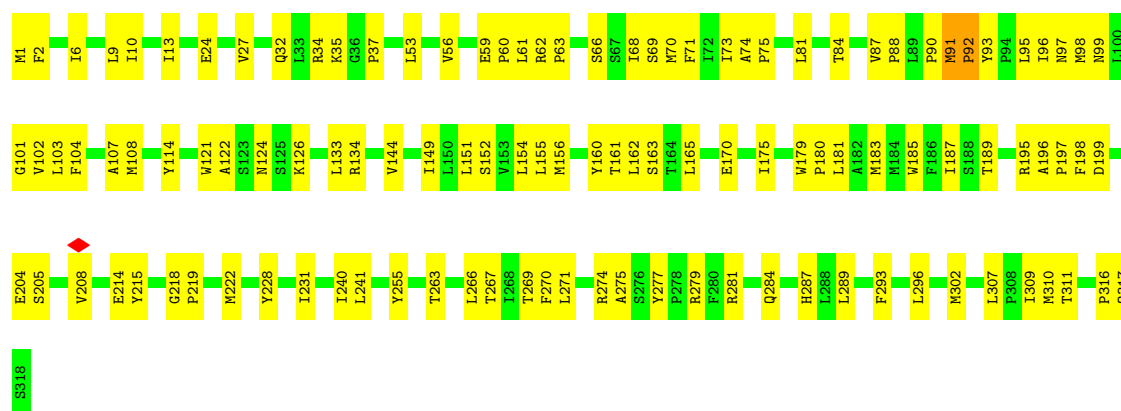
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G: 68% 28% 4%



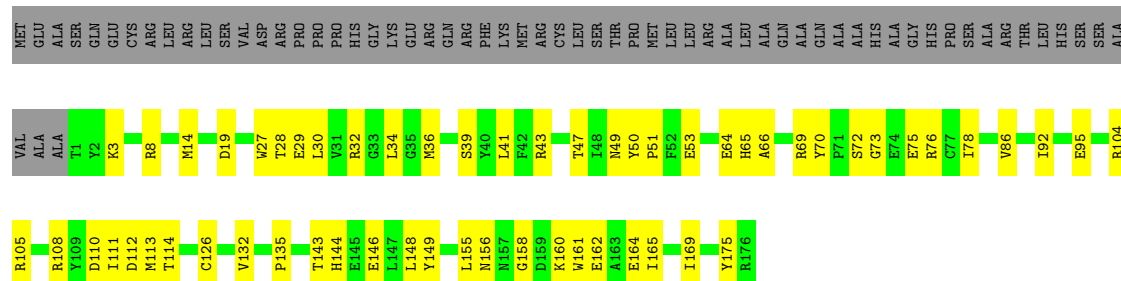
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 5H: 64% 36%



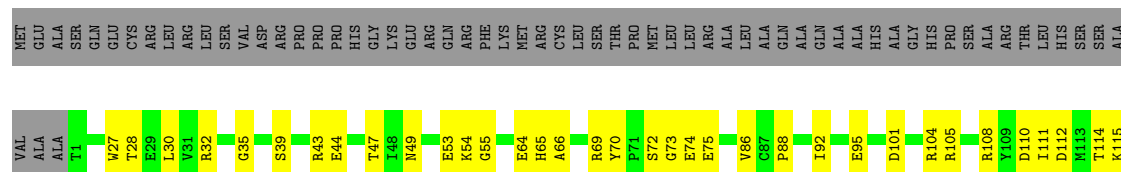
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 49% 24% 26%



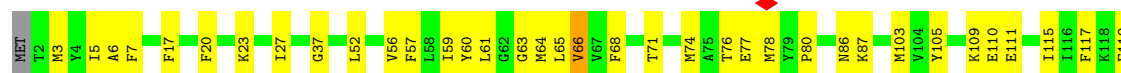
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 5I: 49% 25% 26%

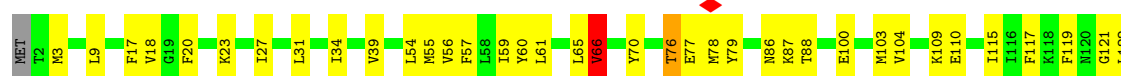




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

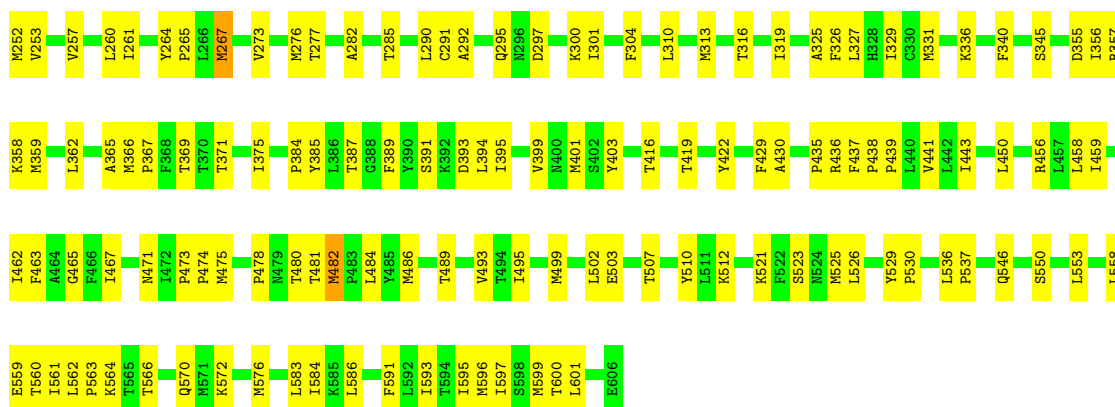


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



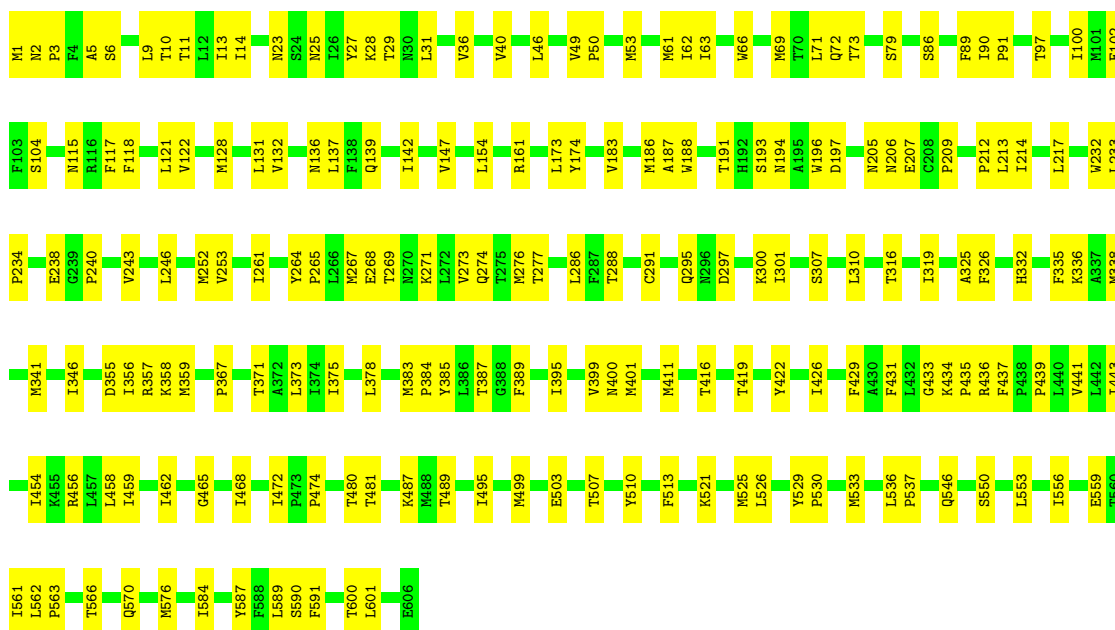
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5





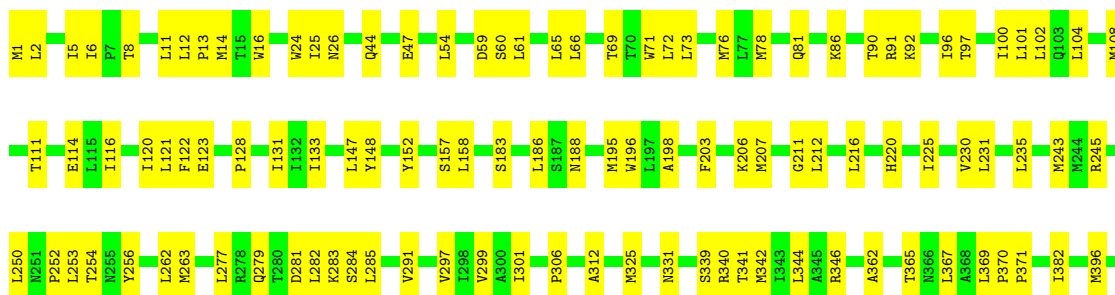
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 5L: 68% 32%



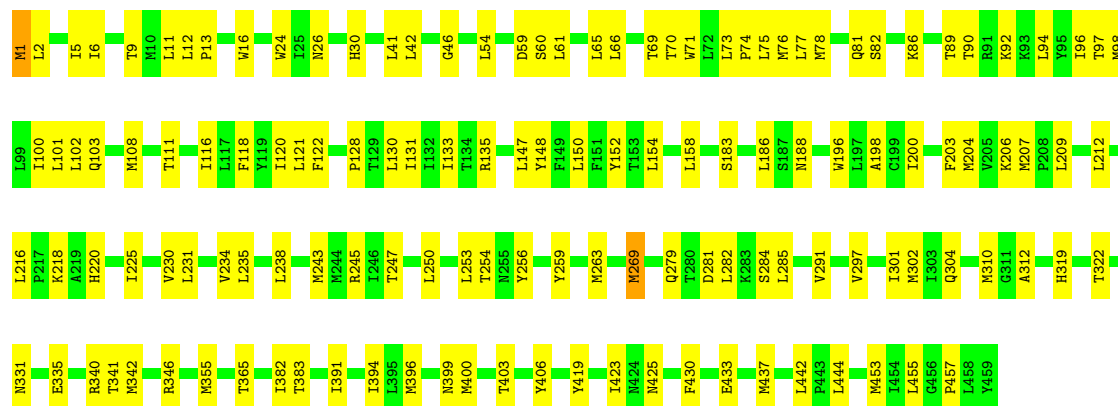
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M: 72% 28%





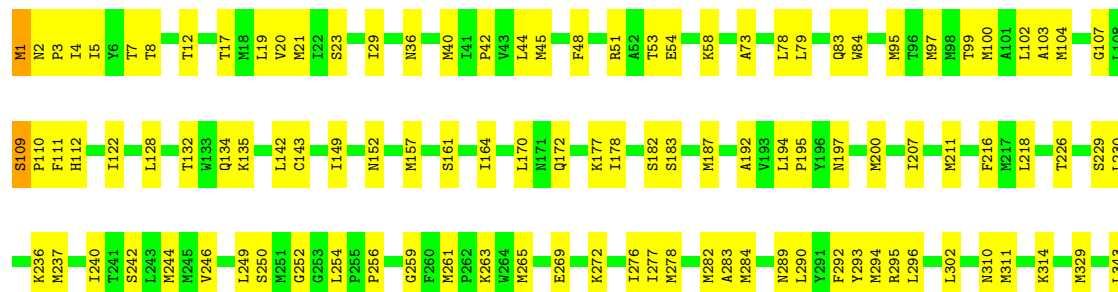
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

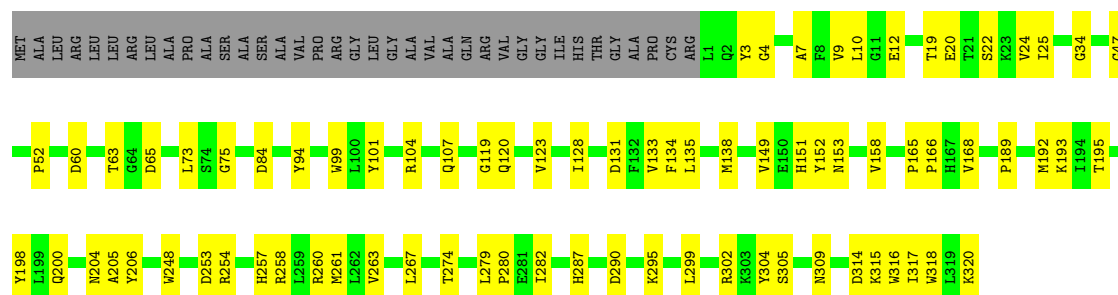


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

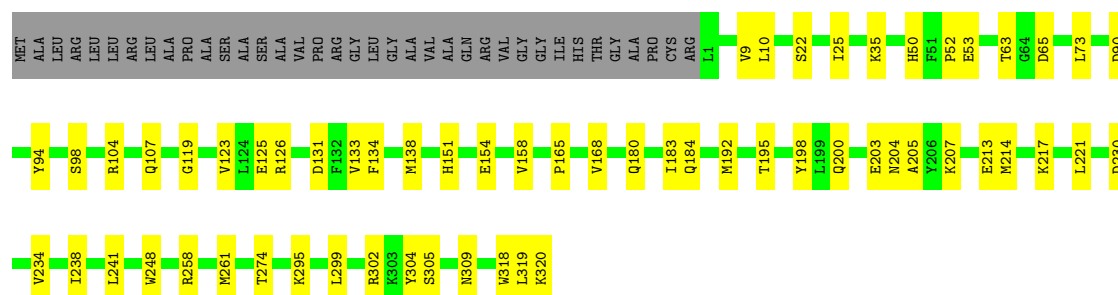


R347

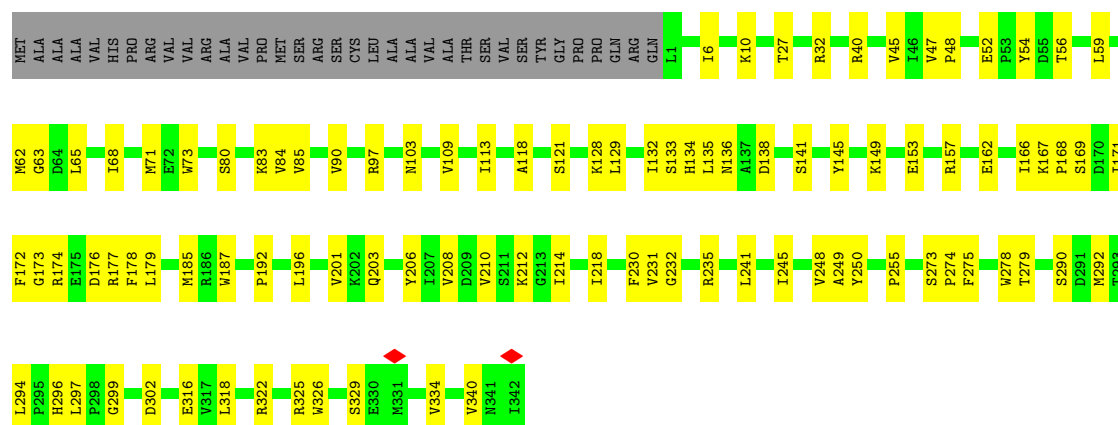
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 10:  68% 22% 10%

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

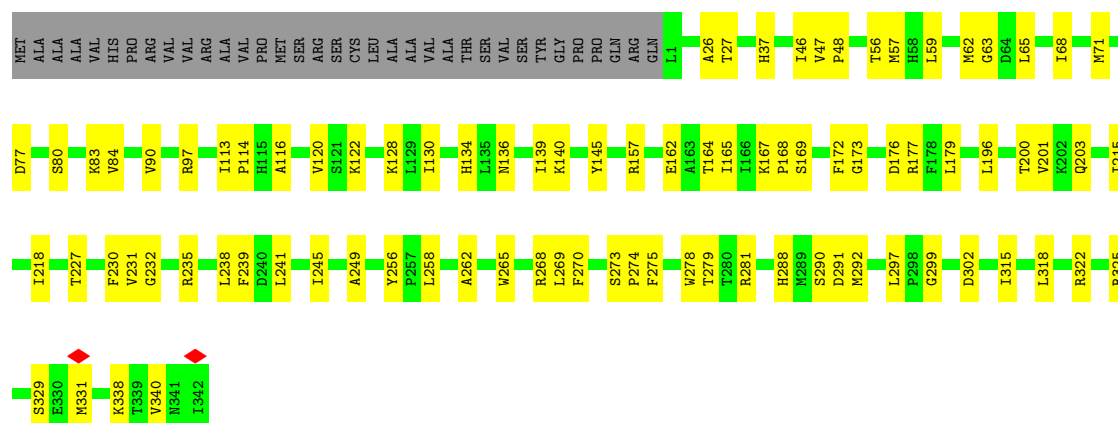
Chain 50:  73% 17% 10%

- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  65% 26% 9%

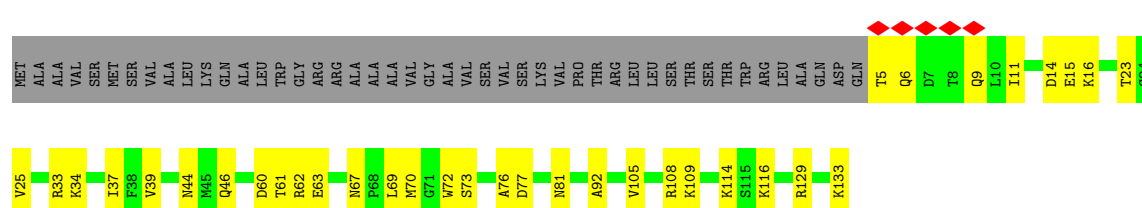
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P: 



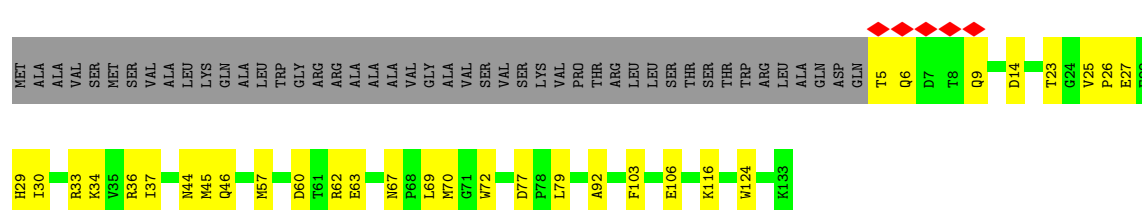
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q: 



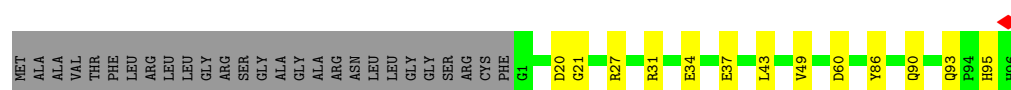
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 5Q: 



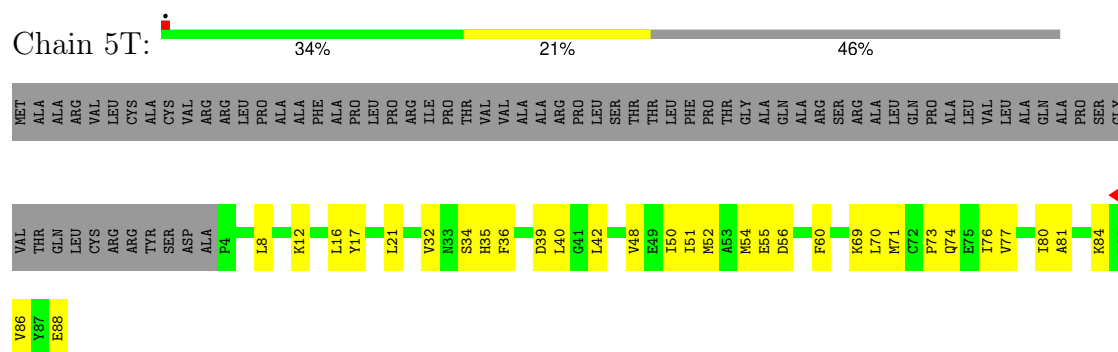
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R: 

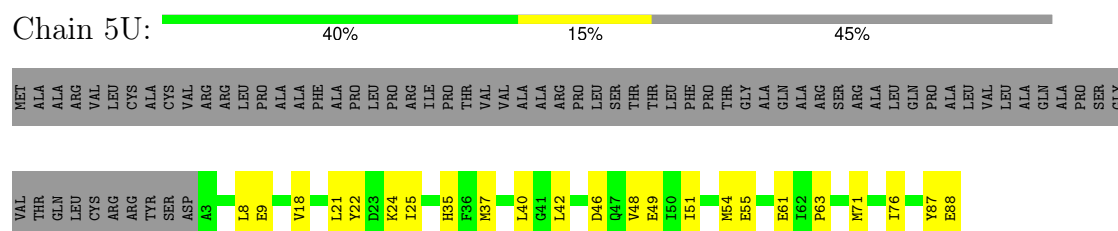


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

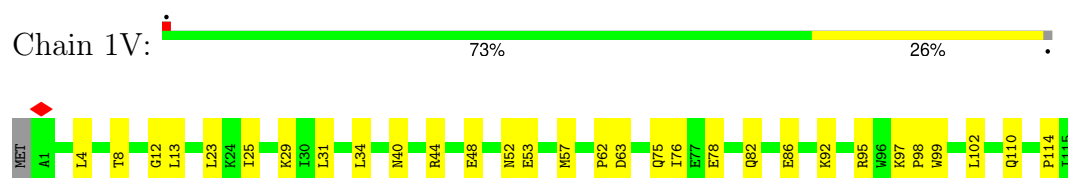
Chain 5R: 



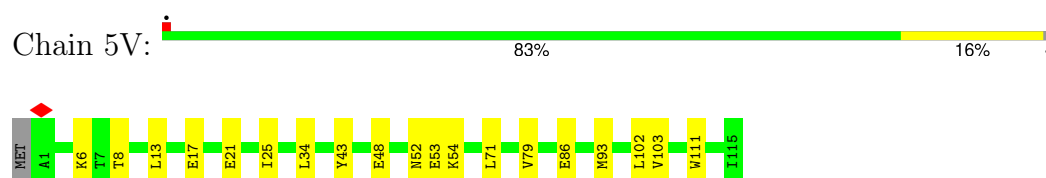
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



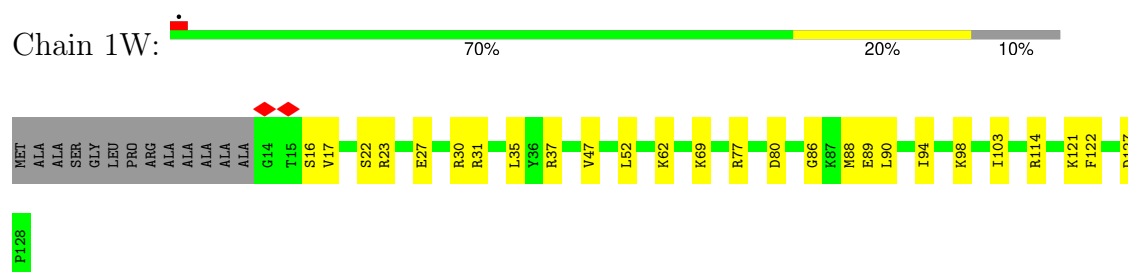
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



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

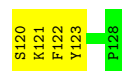


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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





- Chain 1X: 77% 23%



- Chain 5X: 77% 22% .

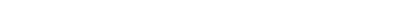


- Chain 1Y: 75% 23%



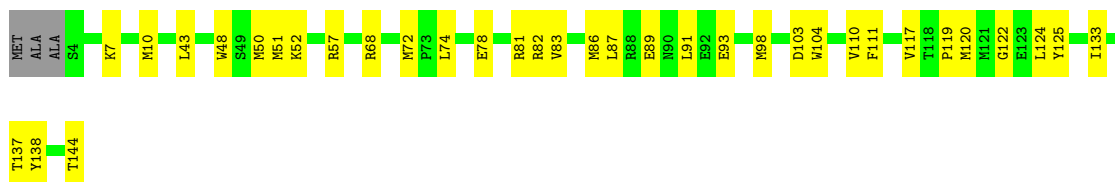
- Chain 5Y:  79% 19%



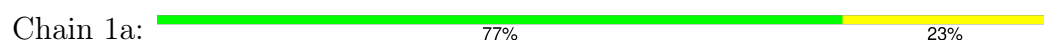
- Chain 1Z:  77% 20% ..



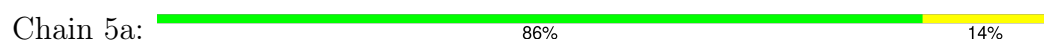
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



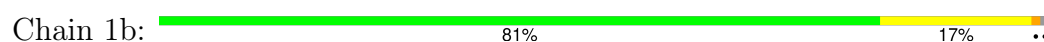
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



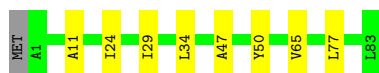
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



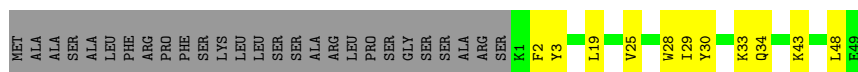
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

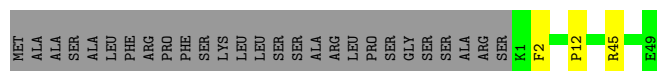


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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

Chain 5c:  61% 36%



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

Chain 1d:  80% 16%



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

Chain 5d:  79% 19%



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

Chain 1e:  67% 26% 7%



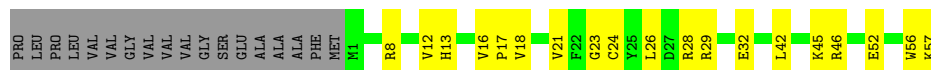
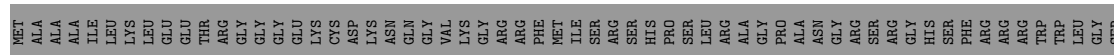
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 5e:  72% 22% 7%



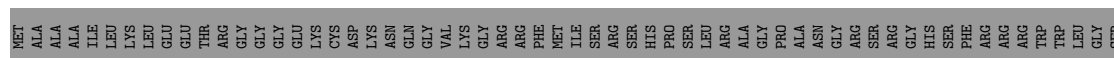
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f:  28% 14% 58%



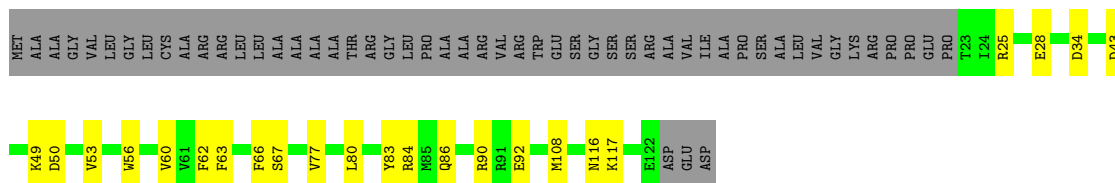
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 5f:  32% 10% 58%

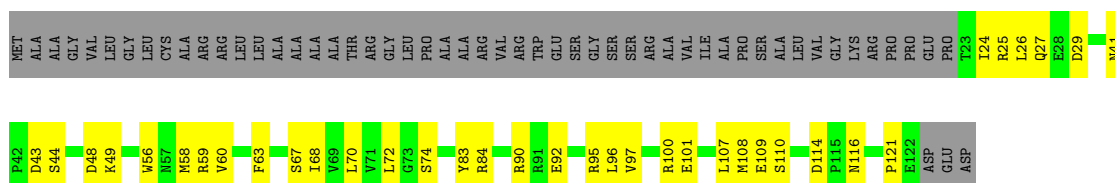




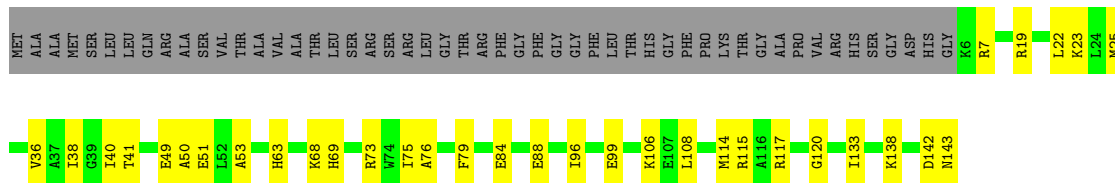
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



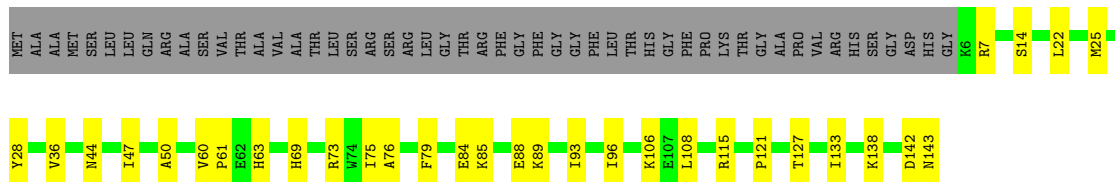
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

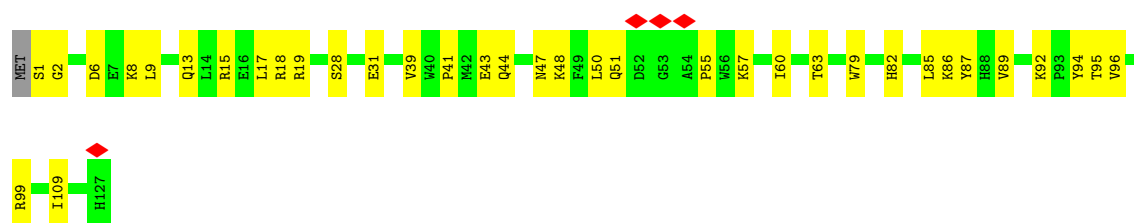


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

Chain 1i: 



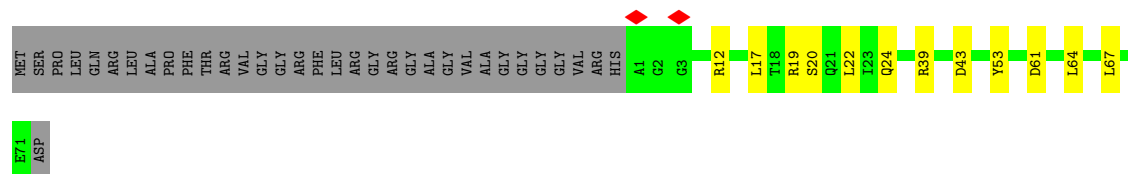
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 5i: 

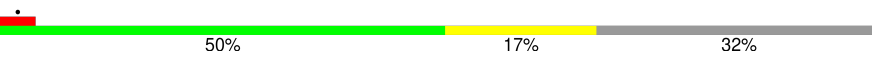


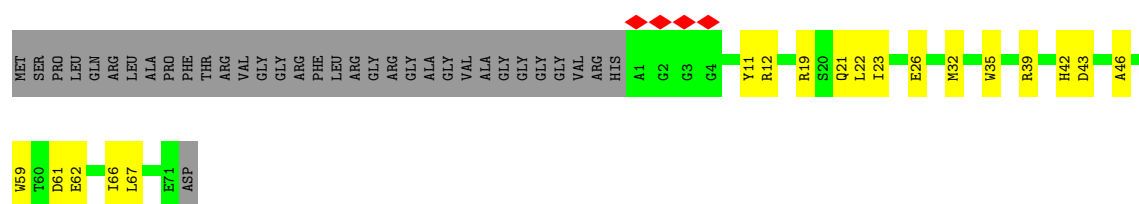
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j: 



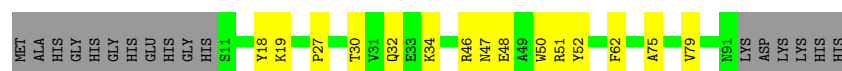
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 5j: 



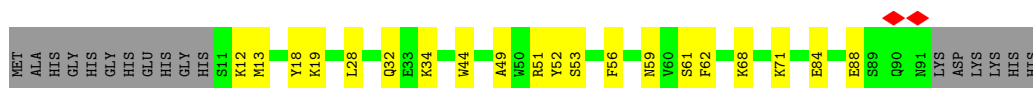
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k: 



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

Chain 5k: 



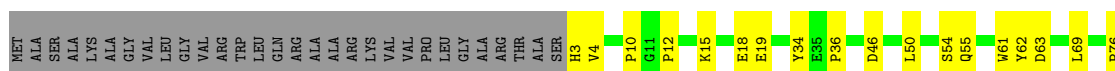
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 11l: 65% 19% 16%



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

Chain 5l: 67% 17% 16%



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

Chain 1m: 78% 22%



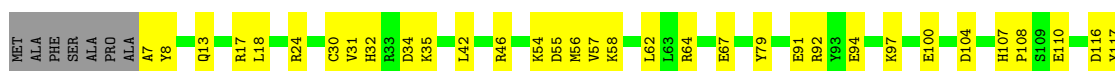
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 5m: 75% 24%

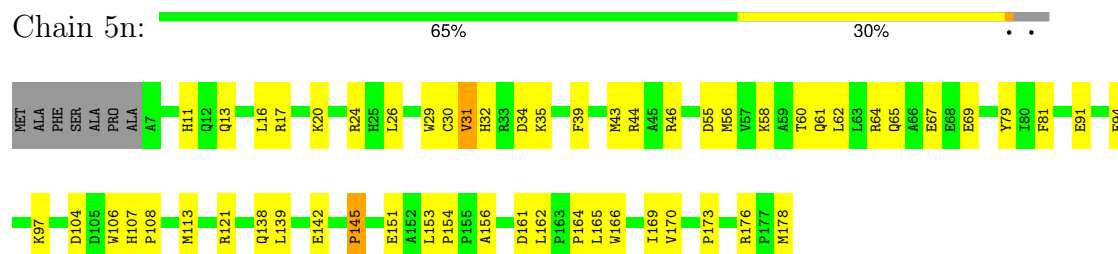


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

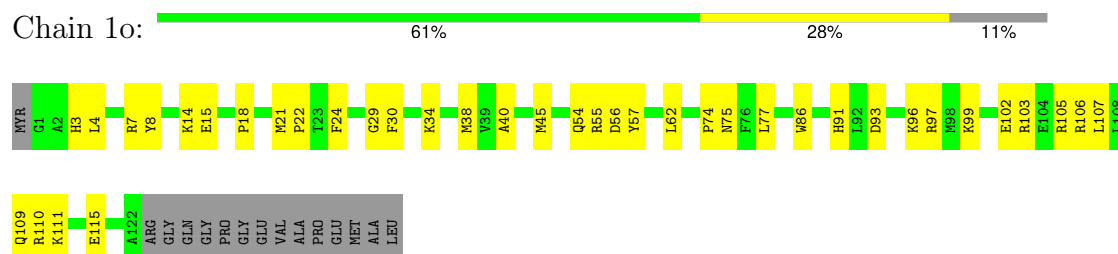
Chain 1n: 68% 28%



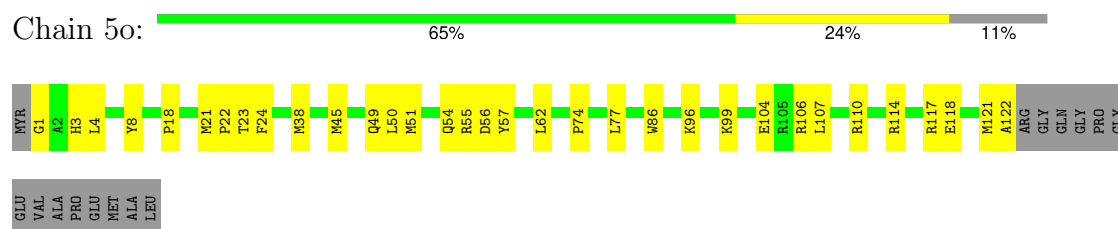
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



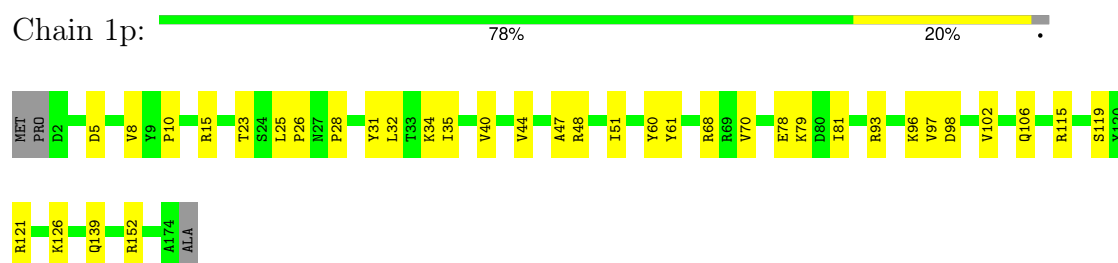
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



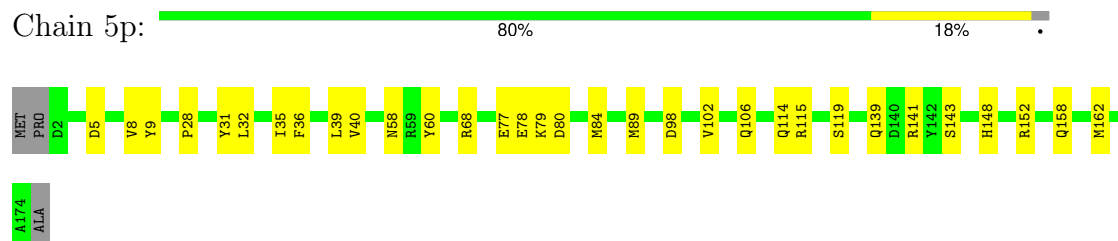
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

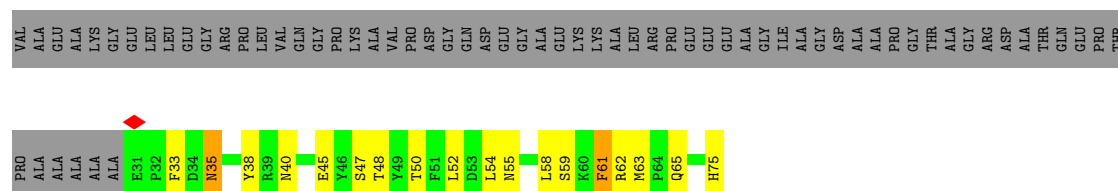


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



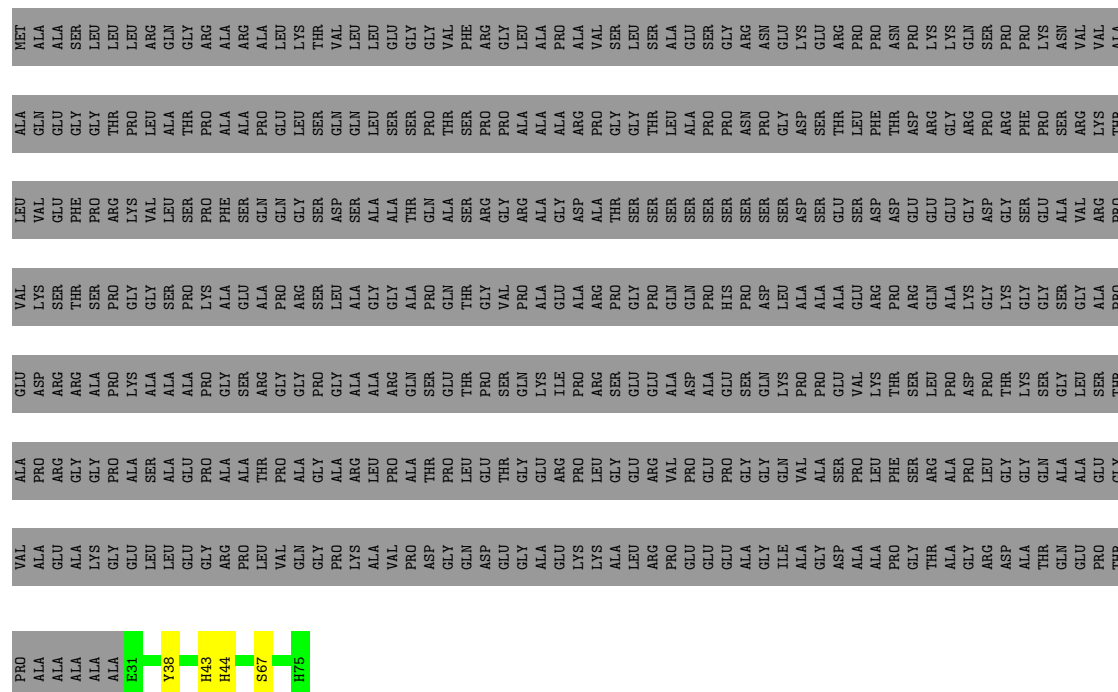
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10





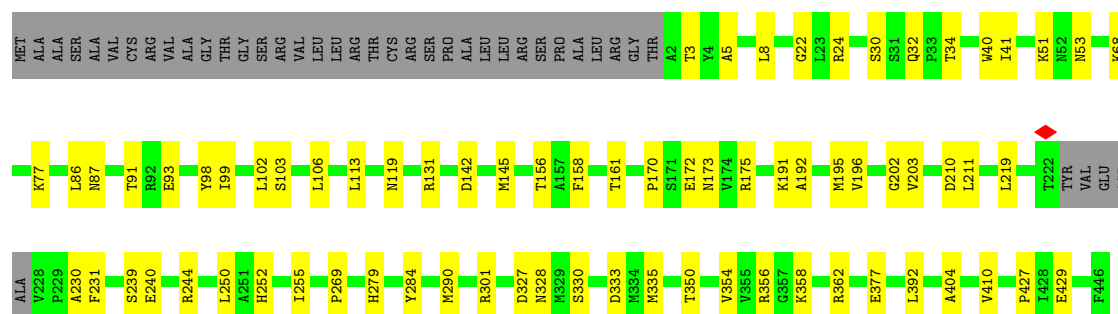
- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain 5s: 9% 90%



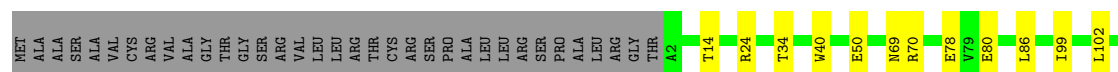
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

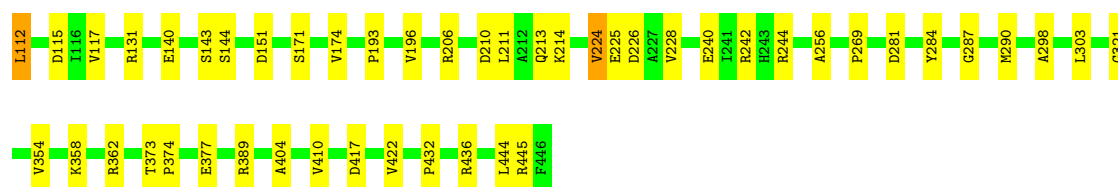
Chain 3A: 76% 15% 8%



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

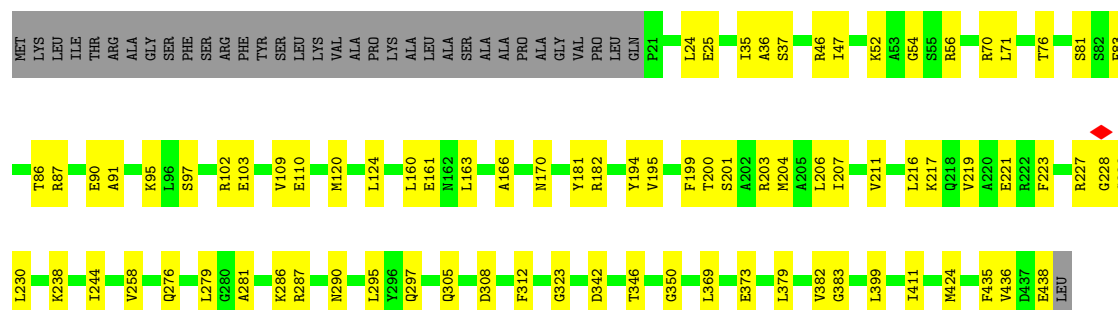
Chain 3N: 80% 12% 7%





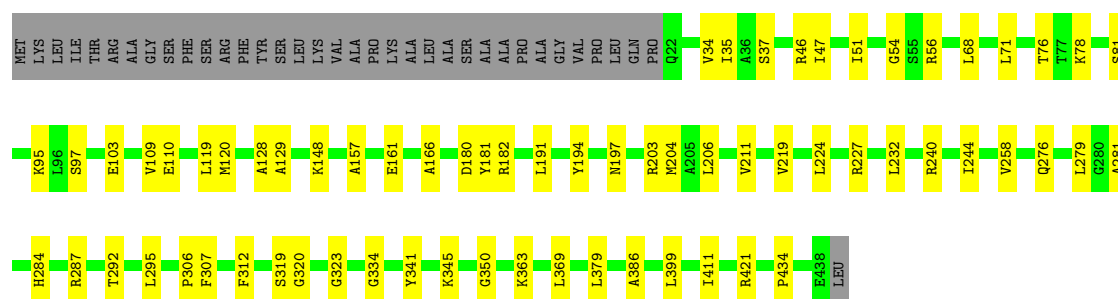
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 74% 18% 8%



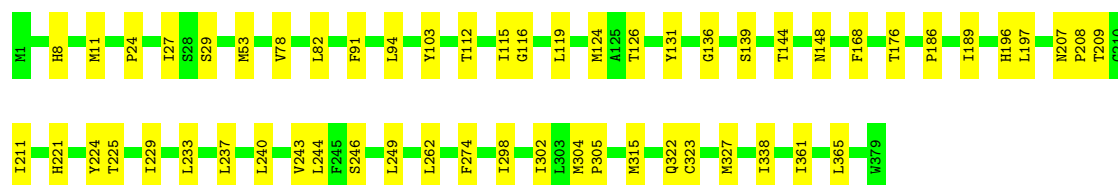
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 77% 15% 8%



- Molecule 47: Cytochrome b

Chain 3C: 85% 15%



- Molecule 47: Cytochrome b

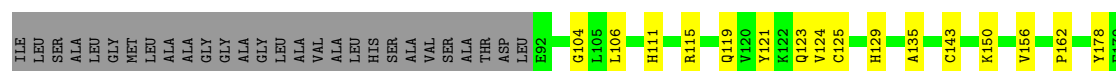
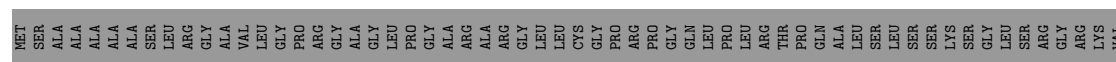
Chain 3P: 84% 16%





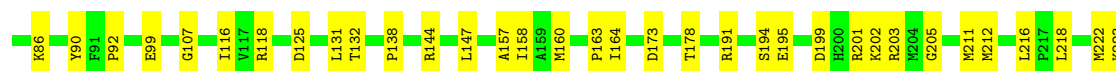
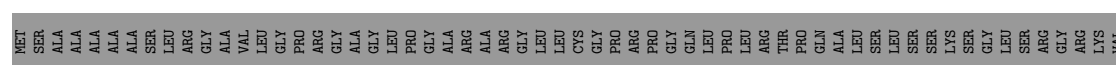
• Molecule 48: Cytochrome c1

Chain 3D: 59% 14% 27%



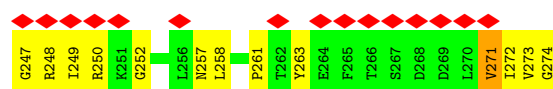
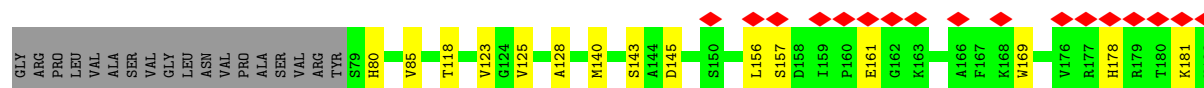
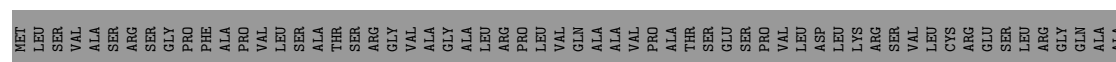
• Molecule 48: Cytochrome c1

Chain 3Q: 56% 17% 27%

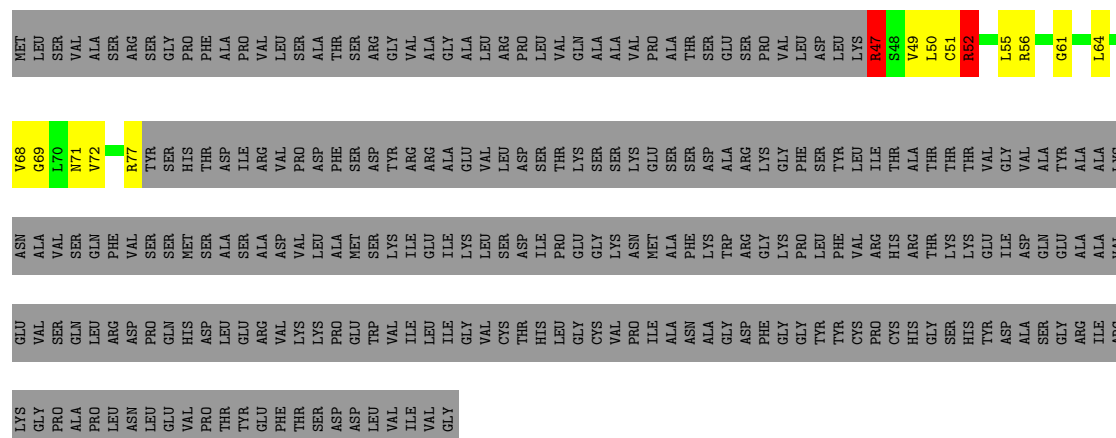


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3E: 28% 54% 18% 28%



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



- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F: 



- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S: 



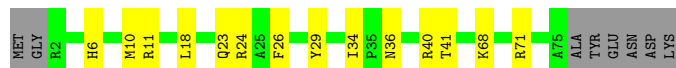
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G: 



- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T: 



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

Chain 3H: 



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

Chain 3U: 



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

Chain 3J: 



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

Chain 3W:  66% 19% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X:  82% 11% 7%



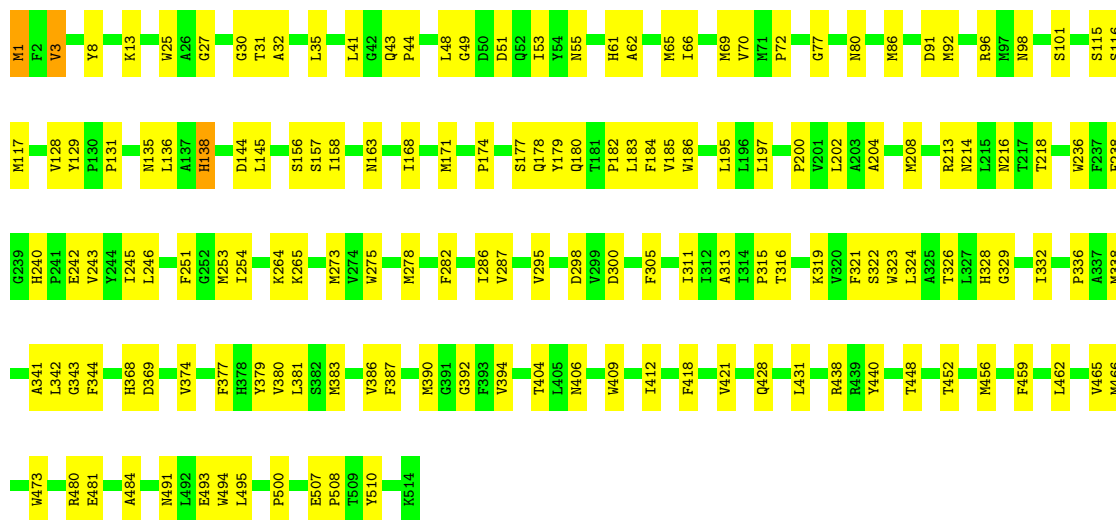
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y:  75% 16% 9%



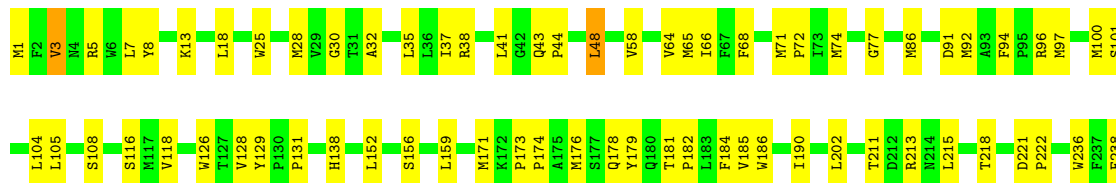
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A:  70% 29% 1%



- Molecule 55: Cytochrome c oxidase subunit 1

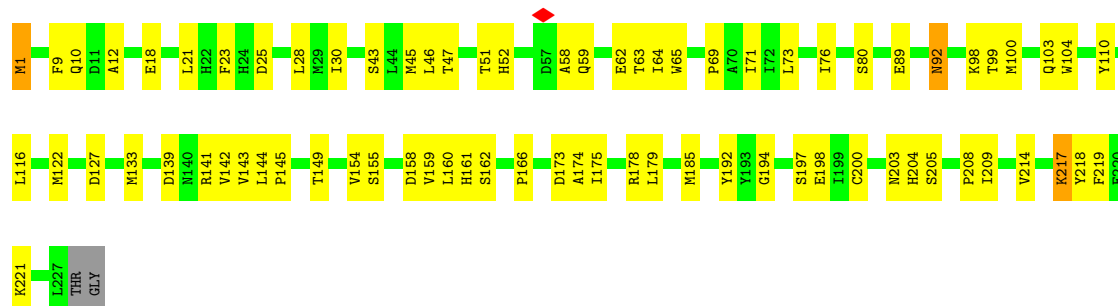
Chain 8A:  69% 30%





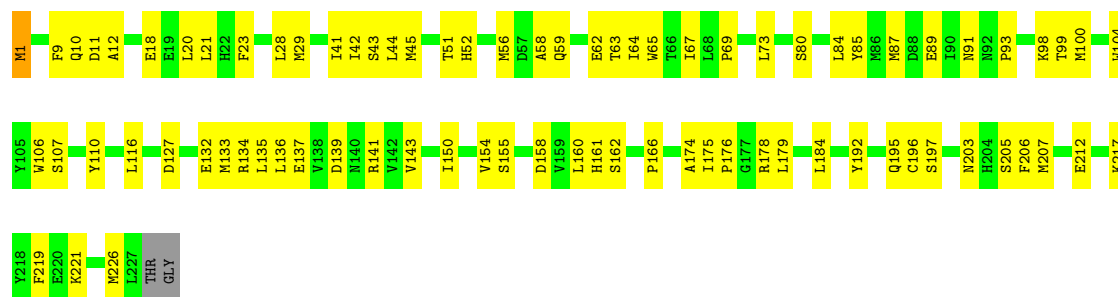
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 66% 31%



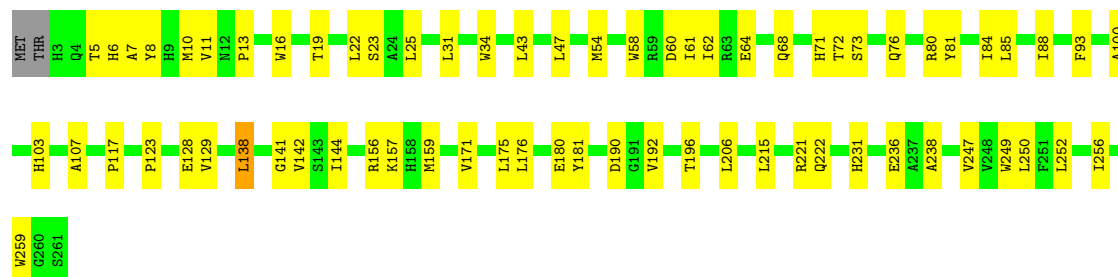
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 8B: 64% 34%



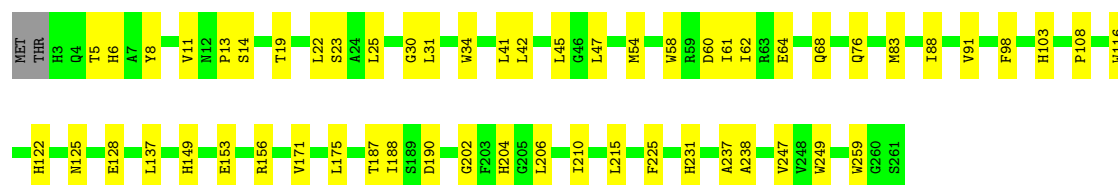
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C: 73% 26%



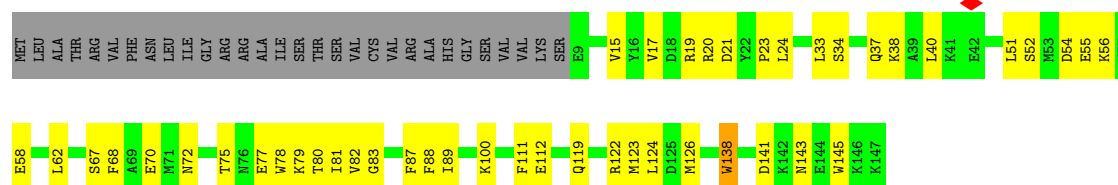
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 8C:  78% 21%



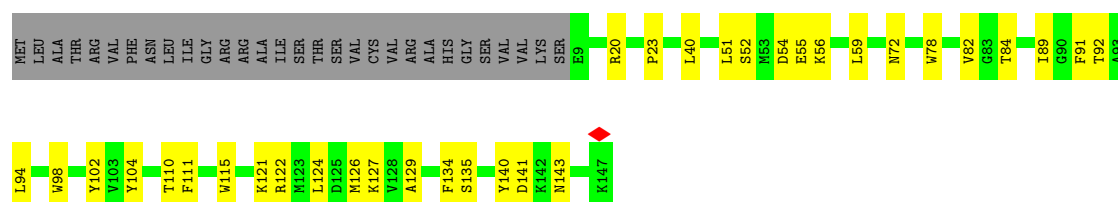
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 4D:  55% 27% 18%



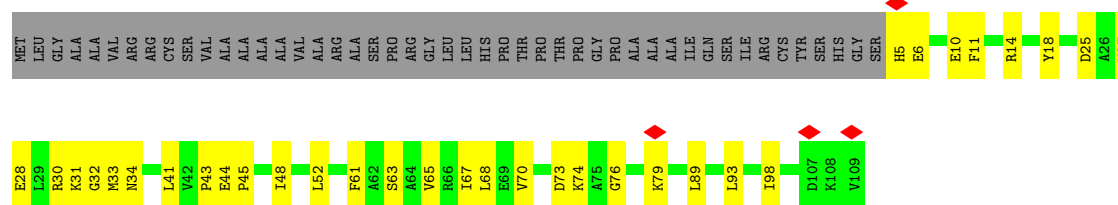
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 8D:  62% 20% 18%



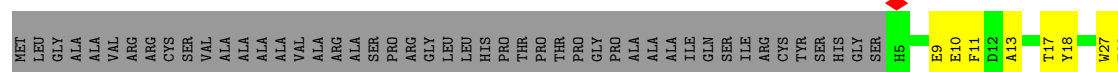
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

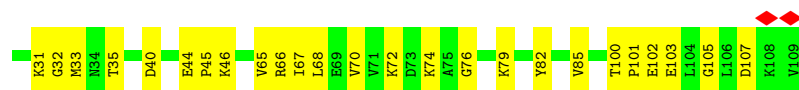
Chain 4E:  47% 22% 31%



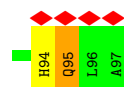
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 8E:  47% 22% 31%





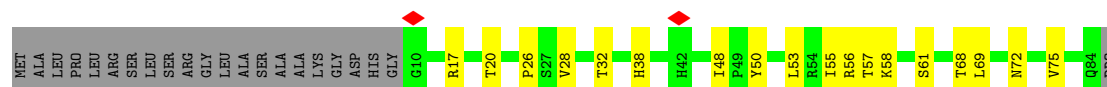
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



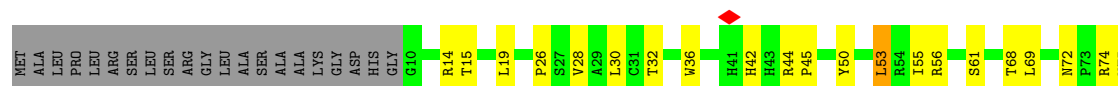
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



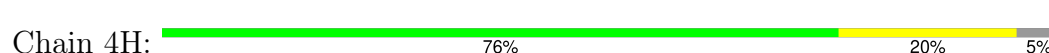
- Molecule 61: Cytochrome c oxidase subunit 6A2



- Molecule 61: Cytochrome c oxidase subunit 6A2



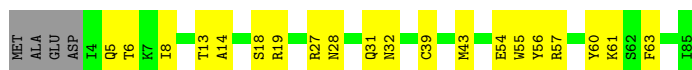
- Molecule 62: Cytochrome c oxidase subunit 6B1





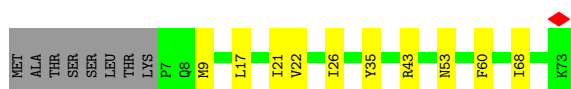
- Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 8H: 72% 23% 5%



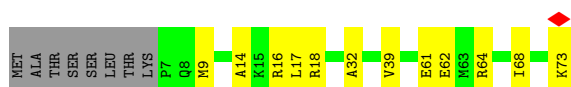
- Molecule 63: Cytochrome c oxidase subunit 6C

Chain 4I: 76% 13% 11%



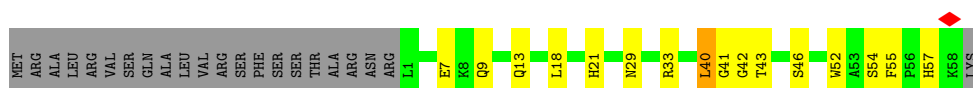
- Molecule 63: Cytochrome c oxidase subunit 6C

Chain 8I: 73% 16% 11%



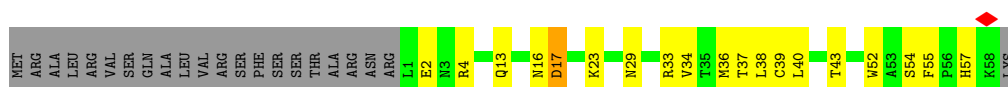
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 4J: 52% 19% 28%



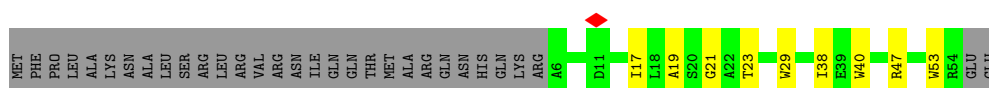
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 8J: 49% 22% 28%

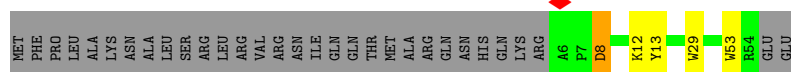


- Molecule 65: Cytochrome c oxidase subunit 7B

Chain 4K: 50% 11% 39%



- Molecule 65: Cytochrome c oxidase subunit 7B



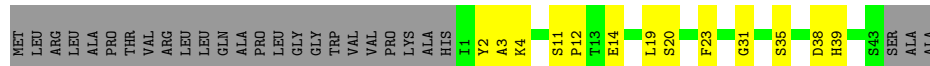
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



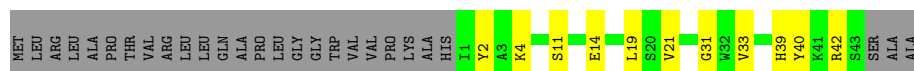
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



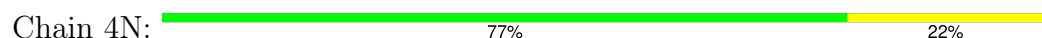
- Molecule 67: Cytochrome c oxidase subunit 8



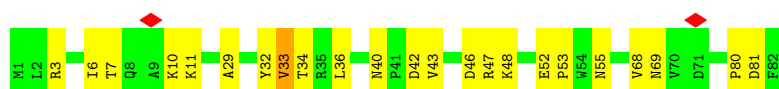
- Molecule 67: Cytochrome c oxidase subunit 8



- 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	80000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.531	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	643.50006, 643.50006, 643.50006	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1700001, 1.1700001, 1.1700001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEK, NA, FMN, GTP, HEC, CU, ZN, HEA, CUA, FES, SF4, AYA, FME, PC1, MYR, AME, PSC, MG, 3PE, CDL, K, PGV, SAC, HEM, NDP, PO4, EH2

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	0.14	0/930	0.34	0/1271
1	5A	0.17	0/930	0.40	0/1271
2	1B	0.17	0/1273	0.40	0/1722
2	5B	0.15	0/1273	0.34	0/1722
3	1C	0.13	0/1791	0.29	0/2439
3	5C	0.13	0/1791	0.27	0/2439
4	1D	0.13	0/3545	0.28	0/4806
4	5D	0.14	0/3545	0.29	0/4806
5	1E	0.12	0/1698	0.30	0/2311
5	5E	0.13	0/1698	0.30	0/2311
6	1F	0.11	0/3401	0.28	0/4595
6	5F	0.15	0/3401	0.33	1/4595 (0.0%)
7	1G	0.13	0/5451	0.31	0/7387
7	5G	0.13	0/5451	0.31	1/7387 (0.0%)
8	1H	0.14	0/2566	0.36	0/3509
8	5H	0.14	0/2566	0.35	0/3509
9	1I	0.13	0/1443	0.28	0/1952
9	5I	0.14	0/1443	0.27	0/1952
10	1J	0.13	0/1364	0.39	0/1850
10	5J	0.14	0/1364	0.39	0/1850
11	1K	0.14	0/751	0.31	0/1018
11	5K	0.14	0/751	0.32	0/1018
12	1L	0.13	0/4939	0.31	0/6718
12	5L	0.13	0/4939	0.32	0/6718
13	1M	0.13	0/3713	0.28	0/5063
13	5M	0.13	0/3713	0.28	0/5063
14	1N	0.13	0/2765	0.30	0/3758
14	5N	0.14	0/2765	0.30	0/3758
15	1O	0.11	0/2650	0.26	0/3588
15	5O	0.11	0/2650	0.25	0/3588
16	1P	0.12	0/2828	0.28	0/3834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	5P	0.12	0/2828	0.28	0/3834
17	1Q	0.15	0/1070	0.32	0/1446
17	5Q	0.15	0/1070	0.34	0/1446
18	1R	0.14	0/755	0.30	0/1018
18	5R	0.14	0/755	0.29	0/1018
19	1S	0.14	0/711	0.37	0/956
19	5S	0.13	0/711	0.35	0/956
20	1T	0.15	0/701	0.44	0/946
20	1U	0.20	0/706	0.47	1/954 (0.1%)
20	5T	0.16	0/701	0.37	0/946
20	5U	0.16	0/706	0.39	0/954
21	1V	0.12	0/946	0.29	0/1281
21	5V	0.11	0/946	0.25	0/1281
22	1W	0.13	0/995	0.30	0/1340
22	5W	0.17	0/995	0.45	1/1340 (0.1%)
23	1X	0.10	0/1436	0.26	0/1938
23	5X	0.11	0/1436	0.28	0/1938
24	1Y	0.14	0/1037	0.32	0/1404
24	5Y	0.13	0/1037	0.28	0/1404
25	1Z	0.16	0/1199	0.40	1/1617 (0.1%)
25	5Z	0.13	0/1199	0.27	0/1617
26	1a	0.13	0/577	0.26	0/777
26	5a	0.11	0/577	0.24	0/777
27	1b	0.13	0/664	0.36	0/912
27	5b	0.13	0/664	0.34	0/912
28	1c	0.14	0/430	0.36	0/581
28	5c	0.13	0/430	0.31	0/581
29	1d	0.12	0/1016	0.26	0/1374
29	5d	0.12	0/1016	0.27	0/1374
30	1e	0.12	0/836	0.31	0/1118
30	5e	0.12	0/836	0.28	0/1118
31	1f	0.11	0/499	0.31	0/673
31	5f	0.12	0/499	0.30	0/673
32	1g	0.14	0/858	0.38	0/1165
32	5g	0.13	0/858	0.35	0/1165
33	1h	0.11	0/1184	0.28	0/1603
33	5h	0.12	0/1184	0.28	0/1603
34	1i	0.17	0/1131	0.42	1/1541 (0.1%)
34	5i	0.12	0/1131	0.32	0/1541
35	1j	0.11	0/627	0.31	0/858
35	5j	0.14	0/627	0.38	0/858
36	1k	0.14	0/668	0.35	0/903
36	5k	0.13	0/668	0.34	0/903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	1l	0.13	0/1365	0.34	0/1867
37	5l	0.13	0/1365	0.32	0/1867
38	1m	0.12	0/1092	0.35	0/1481
38	5m	0.14	0/1092	0.32	0/1481
39	1n	0.12	0/1549	0.31	0/2098
39	5n	0.21	1/1549 (0.1%)	0.45	3/2098 (0.1%)
40	1o	0.13	0/1069	0.32	0/1430
40	5o	0.12	0/1069	0.34	0/1430
41	1p	0.10	0/1481	0.29	0/1997
41	5p	0.11	0/1481	0.31	0/1997
42	1q	0.11	0/1253	0.29	1/1704 (0.1%)
42	5q	0.13	0/1253	0.30	1/1704 (0.1%)
43	1r	0.11	0/777	0.27	0/1051
43	5r	0.13	0/777	0.32	0/1051
44	1s	0.14	0/394	0.38	0/533
44	5s	0.15	0/394	0.37	0/533
45	3A	0.12	0/3481	0.27	0/4722
45	3N	0.13	0/3496	0.29	0/4723
46	3B	0.12	0/3190	0.26	0/4317
46	3O	0.18	0/3175	0.31	0/4292
47	3C	0.13	0/3123	0.29	0/4269
47	3P	0.13	0/3122	0.29	0/4269
48	3D	0.13	0/1946	0.28	0/2641
48	3Q	0.13	0/1962	0.27	0/2663
49	3E	0.15	0/1551	0.37	0/2098
49	3I	0.14	0/344	0.41	0/468
49	3R	0.18	0/1551	0.44	1/2098 (0.0%)
49	3V	0.63	0/225	0.83	0/303
50	3F	0.11	0/888	0.21	0/1193
50	3S	0.11	0/888	0.21	0/1193
51	3G	0.13	0/649	0.28	0/878
51	3T	0.13	0/649	0.28	0/878
52	3H	0.13	0/539	0.62	2/724 (0.3%)
52	3U	0.12	0/539	0.31	0/724
53	3J	0.11	0/464	0.30	0/625
53	3W	0.31	0/464	0.48	0/625
54	3X	0.10	0/445	0.23	0/608
54	3Y	0.15	0/437	0.37	0/598
55	4A	0.14	0/4156	0.31	0/5679
55	8A	0.14	0/4156	0.29	0/5679
56	4B	0.14	0/1865	0.35	0/2544
56	8B	0.14	0/1865	0.31	0/2544
57	4C	0.12	0/2179	0.27	0/2981

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
57	8C	0.13	0/2179	0.29	2/2981 (0.1%)
58	4D	0.11	0/1197	0.28	0/1617
58	8D	0.12	0/1197	0.33	0/1617
59	4E	0.14	0/871	0.37	0/1182
59	8E	0.15	0/871	0.37	0/1182
60	4F	0.13	0/749	0.32	0/1016
60	8F	0.14	0/749	0.35	0/1016
61	4G	0.11	0/644	0.28	0/881
61	8G	0.13	0/644	0.29	0/881
62	4H	0.13	0/708	0.31	0/956
62	8H	0.12	0/708	0.30	0/956
63	4I	0.10	0/563	0.24	0/748
63	8I	0.10	0/563	0.23	0/748
64	4J	0.13	0/466	0.35	0/631
64	8J	0.13	0/466	0.34	0/631
65	4K	0.17	0/396	0.32	0/543
65	8K	0.13	0/396	0.33	0/543
66	4L	0.12	0/394	0.28	0/528
66	8L	0.11	0/394	0.24	0/528
67	4M	0.13	0/349	0.31	0/477
67	8M	0.09	0/349	0.26	0/477
68	4N	0.13	0/680	0.33	0/921
68	8N	0.16	0/680	0.41	0/921
All	All	0.14	1/199830 (0.0%)	0.31	16/271091 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5n	145	PRO	CG-CD	-5.54	1.31	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5W	115	PRO	CA-N-CD	-10.69	97.04	112.00
25	1Z	18	PRO	CA-N-CD	-10.18	97.75	112.00
52	3H	77	GLU	CA-C-N	10.17	140.01	121.70
52	3H	77	GLU	C-N-CA	10.17	140.01	121.70
39	5n	145	PRO	N-CD-CG	-9.20	89.40	103.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	47	0
1	5A	916	0	950	48	0
2	1B	1242	0	1249	48	0
2	5B	1242	0	1249	42	0
3	1C	1740	0	1691	33	0
3	5C	1740	0	1691	28	0
4	1D	3452	0	3389	104	0
4	5D	3452	0	3389	87	0
5	1E	1658	0	1662	48	0
5	5E	1658	0	1662	47	0
6	1F	3325	0	3288	100	0
6	5F	3325	0	3288	105	0
7	1G	5362	0	5388	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5G	5362	0	5388	131	0
8	1H	2504	0	2602	97	0
8	5H	2504	0	2602	95	0
9	1I	1412	0	1366	53	0
9	5I	1412	0	1366	57	0
10	1J	1329	0	1326	63	0
10	5J	1329	0	1326	56	0
11	1K	750	0	798	34	0
11	5K	750	0	798	30	0
12	1L	4818	0	4956	152	0
12	5L	4818	0	4956	150	0
13	1M	3632	0	3836	99	0
13	5M	3632	0	3836	104	0
14	1N	2712	0	2873	94	0
14	5N	2712	0	2873	88	0
15	1O	2590	0	2556	56	0
15	5O	2590	0	2555	47	0
16	1P	2751	0	2776	72	0
16	5P	2751	0	2776	60	0
17	1Q	1047	0	1042	36	0
17	5Q	1047	0	1042	32	0
18	1R	741	0	704	11	0
18	5R	741	0	704	10	0
19	1S	700	0	719	22	0
19	5S	700	0	719	22	0
20	1T	689	0	687	35	0
20	1U	694	0	691	26	0
20	5T	689	0	687	22	0
20	5U	694	0	691	22	0
21	1V	927	0	972	23	0
21	5V	927	0	972	16	0
22	1W	971	0	975	23	0
22	5W	971	0	975	24	0
23	1X	1398	0	1378	34	0
23	5X	1398	0	1378	32	0
24	1Y	1016	0	1020	27	0
24	5Y	1016	0	1020	24	0
25	1Z	1168	0	1161	30	0
25	5Z	1168	0	1161	36	0
26	1a	562	0	557	13	0
26	5a	562	0	557	9	0
27	1b	643	0	645	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	5b	643	0	645	7	0
28	1c	417	0	425	11	0
28	5c	417	0	425	3	0
29	1d	985	0	978	22	0
29	5d	985	0	978	24	0
30	1e	816	0	823	24	0
30	5e	816	0	823	22	0
31	1f	487	0	498	15	0
31	5f	487	0	498	15	0
32	1g	835	0	795	24	0
32	5g	835	0	795	28	0
33	1h	1151	0	1164	34	0
33	5h	1151	0	1164	31	0
34	1i	1100	0	1107	35	0
34	5i	1100	0	1107	27	0
35	1j	601	0	546	11	0
35	5j	601	0	546	17	0
36	1k	649	0	626	15	0
36	5k	649	0	626	23	0
37	1l	1310	0	1204	30	0
37	5l	1310	0	1204	25	0
38	1m	1062	0	1075	22	0
38	5m	1062	0	1075	29	0
39	1n	1495	0	1434	42	0
39	5n	1495	0	1434	48	0
40	1o	1045	0	1016	39	0
40	5o	1045	0	1016	26	0
41	1p	1449	0	1416	34	0
41	5p	1449	0	1416	29	0
42	1q	1212	0	1174	14	0
42	5q	1212	0	1174	30	0
43	1r	759	0	783	15	0
43	5r	759	0	783	21	0
44	1s	382	0	351	21	0
44	5s	382	0	351	4	0
45	3A	3411	0	3308	46	0
45	3N	3424	0	3350	40	0
46	3B	3138	0	3116	51	0
46	3O	3124	0	3108	45	0
47	3C	3025	0	3090	46	0
47	3P	3024	0	3090	40	0
48	3D	1888	0	1834	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	3Q	1904	0	1849	46	0
49	3E	1518	0	1498	43	0
49	3I	340	0	359	13	0
49	3R	1518	0	1498	74	0
49	3V	224	0	241	11	0
50	3F	868	0	857	6	0
50	3S	868	0	857	8	0
51	3G	628	0	634	7	0
51	3T	628	0	634	12	0
52	3H	533	0	513	9	0
52	3U	533	0	513	9	0
53	3J	454	0	455	4	0
53	3W	454	0	455	10	0
54	3X	429	0	430	5	0
54	3Y	421	0	418	6	0
55	4A	4026	0	4005	127	0
55	8A	4026	0	4005	135	0
56	4B	1828	0	1835	63	0
56	8B	1828	0	1835	62	0
57	4C	2096	0	2027	57	0
57	8C	2096	0	2027	50	0
58	4D	1163	0	1143	40	0
58	8D	1163	0	1143	33	0
59	4E	852	0	845	26	0
59	8E	852	0	845	27	0
60	4F	734	0	718	15	0
60	8F	734	0	718	20	0
61	4G	617	0	585	14	0
61	8G	617	0	585	17	0
62	4H	687	0	645	12	0
62	8H	687	0	645	15	0
63	4I	550	0	560	11	0
63	8I	550	0	560	12	0
64	4J	456	0	459	16	0
64	8J	456	0	459	18	0
65	4K	383	0	366	8	0
65	8K	383	0	366	5	0
66	4L	381	0	380	9	0
66	8L	381	0	380	12	0
67	4M	338	0	345	12	0
67	8M	338	0	345	10	0
68	4N	660	0	664	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	8N	660	0	664	19	0
69	1A	103	0	128	6	0
69	1B	94	0	136	12	0
69	1H	48	0	73	2	0
69	1I	98	0	150	8	0
69	1L	46	0	66	3	0
69	1M	79	0	109	8	0
69	1d	39	0	52	6	0
69	1h	47	0	71	3	0
69	1q	49	0	75	3	0
69	3J	47	0	68	4	0
69	3R	45	0	64	6	0
69	3X	29	0	32	2	0
69	5A	70	0	88	4	0
69	5B	94	0	136	12	0
69	5H	48	0	73	2	0
69	5I	98	0	150	9	0
69	5L	46	0	66	3	0
69	5M	79	0	109	10	0
69	5P	33	0	40	0	0
69	5d	39	0	52	8	0
69	5h	47	0	71	3	0
69	5q	49	0	75	4	0
70	1B	8	0	0	1	0
70	1F	8	0	0	1	0
70	1G	16	0	0	1	0
70	1I	16	0	0	0	0
70	5B	8	0	0	1	0
70	5F	8	0	0	1	0
70	5G	16	0	0	1	0
70	5I	16	0	0	0	0
71	1E	4	0	0	0	0
71	1G	4	0	0	3	0
71	3E	4	0	0	0	0
71	3R	4	0	0	1	0
71	5E	4	0	0	0	0
71	5G	4	0	0	3	0
72	1F	31	0	19	3	0
72	5F	31	0	19	3	0
73	1G	1	0	0	0	0
73	5G	1	0	0	0	0
74	1H	51	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	1L	76	0	99	8	0
74	1N	62	0	68	3	0
74	1X	86	0	125	10	0
74	1d	65	0	77	9	0
74	1h	80	0	104	11	0
74	1q	61	0	66	1	0
74	3A	58	0	60	5	0
74	3C	52	0	48	3	0
74	3G	56	0	56	5	0
74	3N	43	0	30	1	0
74	3P	56	0	56	9	0
74	3T	57	0	58	11	0
74	4B	100	0	156	7	0
74	4C	100	0	156	15	0
74	4D	100	0	156	18	0
74	5H	51	0	46	2	0
74	5L	76	0	99	6	0
74	5N	62	0	68	3	0
74	5X	86	0	125	6	0
74	5d	65	0	77	3	0
74	5h	80	0	104	10	0
74	5q	61	0	66	2	0
74	8B	100	0	156	9	0
74	8C	100	0	156	14	0
74	8D	100	0	156	18	0
75	1I	8	0	8	1	0
75	5q	8	0	8	3	0
76	1K	44	0	62	2	0
76	1L	91	0	136	8	0
76	1M	192	0	289	22	0
76	1O	51	0	82	10	0
76	1P	35	0	44	3	0
76	1Y	202	0	254	16	0
76	1b	47	0	71	1	0
76	1d	49	0	75	4	0
76	1j	44	0	65	2	0
76	3A	59	0	66	5	0
76	3C	69	0	86	6	0
76	3D	33	0	40	2	0
76	3G	29	0	32	0	0
76	3N	58	0	62	5	0
76	3P	33	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	3Q	47	0	71	3	0
76	3Y	30	0	34	2	0
76	5A	47	0	71	3	0
76	5K	44	0	62	3	0
76	5L	140	0	211	8	0
76	5M	194	0	296	22	0
76	5P	35	0	44	1	0
76	5Y	202	0	254	18	0
76	5d	49	0	75	7	0
76	5j	44	0	65	5	0
77	1O	32	0	12	2	0
77	5O	32	0	12	1	0
78	1O	1	0	0	0	0
78	4A	1	0	0	0	0
78	5O	1	0	0	0	0
78	8A	1	0	0	0	0
79	1P	48	0	26	3	0
79	5P	48	0	26	5	0
80	1R	1	0	0	0	0
80	4F	1	0	0	0	0
80	5R	1	0	0	0	0
80	8F	1	0	0	0	0
81	1T	37	0	0	0	0
81	1n	37	0	0	2	0
81	5T	37	0	0	1	0
81	5n	37	0	0	1	0
82	1h	11	0	12	1	0
82	5h	11	0	12	1	0
83	1o	15	0	27	0	0
83	5o	15	0	27	1	0
84	3C	86	0	60	4	0
84	3P	86	0	60	3	0
85	3D	42	0	32	3	0
85	3Q	43	0	32	2	0
86	4A	153	0	228	21	0
86	4B	51	0	75	4	0
86	4C	306	0	456	27	0
86	4G	51	0	76	6	0
86	4J	51	0	76	3	0
86	4K	51	0	76	1	0
86	4L	51	0	76	3	0
86	4M	51	0	76	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	8A	102	0	152	10	0
86	8B	102	0	151	14	0
86	8C	306	0	456	22	0
86	8G	51	0	76	6	0
86	8J	51	0	76	3	0
86	8K	51	0	76	1	0
86	8L	51	0	76	3	0
86	8M	51	0	76	3	0
87	4A	120	0	108	9	0
87	8A	120	0	108	10	0
88	4A	1	0	0	0	0
88	8A	1	0	0	0	0
89	4A	1	0	0	0	0
89	8A	1	0	0	0	0
90	4A	52	0	80	7	0
90	8I	52	0	80	5	0
91	4B	2	0	0	3	0
91	8B	2	0	0	1	0
92	4C	52	0	72	4	0
92	4G	53	0	77	4	0
92	8C	52	0	72	6	0
92	8G	53	0	77	4	0
93	4H	5	0	0	0	0
93	8H	5	0	0	0	0
All	All	202910	0	204833	4594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 4594 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:77:ARG:HD2	2:1B:78:ALA:H	1.28	0.97
56:4B:200:CYS:HG	91:4B:303:CUA:CU2	0.67	0.97
2:1B:77:ARG:HD2	2:1B:78:ALA:N	1.88	0.89
45:3N:444:LEU:HB2	74:3N:502:CDL:HB31	1.59	0.85
12:5L:600:THR:HG22	12:5L:601:LEU:H	1.41	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	100 (88%)	12 (11%)	1 (1%)	14	35
1	5A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6	18
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
2	5B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
3	5C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
4	1D	427/476 (90%)	411 (96%)	16 (4%)	0	100	100
4	5D	427/476 (90%)	408 (96%)	19 (4%)	0	100	100
5	1E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	24	48
5	5E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
6	1F	430/464 (93%)	409 (95%)	18 (4%)	3 (1%)	18	41
6	5F	430/464 (93%)	403 (94%)	24 (6%)	3 (1%)	18	41
7	1G	697/727 (96%)	666 (96%)	29 (4%)	2 (0%)	36	60
7	5G	697/727 (96%)	669 (96%)	25 (4%)	3 (0%)	30	54
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	36	60
8	5H	316/318 (99%)	300 (95%)	14 (4%)	2 (1%)	21	44
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
9	5I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	44
10	5J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	44
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
11	5K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	32
12	1L	604/606 (100%)	562 (93%)	42 (7%)	0	100	100
12	5L	604/606 (100%)	562 (93%)	41 (7%)	1 (0%)	43	68
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	5M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	1N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	36	60
14	5N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	36	60
15	1O	318/357 (89%)	307 (96%)	11 (4%)	0	100	100
15	5O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
16	5P	340/377 (90%)	330 (97%)	10 (3%)	0	100	100
17	1Q	127/175 (73%)	116 (91%)	11 (9%)	0	100	100
17	5Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
18	5R	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
19	1S	85/99 (86%)	78 (92%)	7 (8%)	0	100	100
19	5S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	80 (95%)	4 (5%)	0	100	100
20	5T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	5U	84/156 (54%)	82 (98%)	2 (2%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
21	5V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
22	5W	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	44
23	5X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	44
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
24	5Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
25	1Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
25	5Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
26	5a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
27	5b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
28	5c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
29	5d	117/122 (96%)	115 (98%)	2 (2%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/135 (41%)	52 (94%)	3 (6%)	0	100	100
32	1g	98/154 (64%)	89 (91%)	9 (9%)	0	100	100
32	5g	98/154 (64%)	91 (93%)	7 (7%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
33	5h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	1i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
34	5i	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
35	5j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100
37	5l	154/186 (83%)	144 (94%)	10 (6%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
38	5m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
39	5n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	21	44
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
40	5o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
41	5p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
42	5q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	5r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
44	5s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
45	3A	436/480 (91%)	429 (98%)	5 (1%)	2 (0%)	24	48
45	3N	444/480 (92%)	425 (96%)	18 (4%)	1 (0%)	43	68
46	3B	414/453 (91%)	405 (98%)	9 (2%)	0	100	100
46	3O	413/453 (91%)	406 (98%)	7 (2%)	0	100	100
47	3C	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
47	3P	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	230 (97%)	7 (3%)	0	100	100
49	3E	194/274 (71%)	176 (91%)	17 (9%)	1 (0%)	24	48
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	175 (90%)	16 (8%)	3 (2%)	8	22
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	96 (100%)	0	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	63/91 (69%)	61 (97%)	2 (3%)	0	100	100
52	3U	63/91 (69%)	63 (100%)	0	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	6	17
53	3W	54/64 (84%)	54 (100%)	0	0	100	100
54	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
55	4A	512/514 (100%)	492 (96%)	18 (4%)	2 (0%)	30	54
55	8A	512/514 (100%)	489 (96%)	21 (4%)	2 (0%)	30	54
56	4B	225/229 (98%)	219 (97%)	6 (3%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	4D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
58	8D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	100 (97%)	3 (3%)	0	100	100
60	4F	95/128 (74%)	91 (96%)	3 (3%)	1 (1%)	11	29
60	8F	95/128 (74%)	89 (94%)	5 (5%)	1 (1%)	11	29
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	71 (97%)	2 (3%)	0	100	100
62	4H	80/86 (93%)	76 (95%)	4 (5%)	0	100	100
62	8H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
63	4I	65/75 (87%)	65 (100%)	0	0	100	100
63	8I	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
64	4J	56/80 (70%)	52 (93%)	4 (7%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	47 (100%)	0	0	100	100
65	8K	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
66	8L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	25
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	25
All	All	24082/28836 (84%)	23087 (96%)	952 (4%)	43 (0%)	44	68

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	208	VAL
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	98 (99%)	1 (1%)	68	86
1	5A	99/99 (100%)	99 (100%)	0	100	100
2	1B	131/212 (62%)	131 (100%)	0	100	100
2	5B	131/212 (62%)	131 (100%)	0	100	100
3	1C	190/227 (84%)	190 (100%)	0	100	100
3	5C	190/227 (84%)	190 (100%)	0	100	100
4	1D	371/405 (92%)	371 (100%)	0	100	100
4	5D	371/405 (92%)	370 (100%)	1 (0%)	86	94
5	1E	183/207 (88%)	183 (100%)	0	100	100
5	5E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	346 (100%)	0	100	100
6	5F	346/368 (94%)	345 (100%)	1 (0%)	86	94
7	1G	588/610 (96%)	587 (100%)	1 (0%)	87	95
7	5G	588/610 (96%)	587 (100%)	1 (0%)	87	95
8	1H	274/274 (100%)	272 (99%)	2 (1%)	76	90
8	5H	274/274 (100%)	273 (100%)	1 (0%)	84	93
9	1I	151/201 (75%)	151 (100%)	0	100	100
9	5I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/141 (99%)	140 (100%)	0	100	100
10	5J	140/141 (99%)	138 (99%)	2 (1%)	59	82
11	1K	84/84 (100%)	84 (100%)	0	100	100
11	5K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	537 (100%)	2 (0%)	84	93
12	5L	539/539 (100%)	539 (100%)	0	100	100
13	1M	408/408 (100%)	407 (100%)	1 (0%)	87	95
13	5M	408/408 (100%)	406 (100%)	2 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1N	310/310 (100%)	309 (100%)	1 (0%)	86	94
14	5N	310/310 (100%)	309 (100%)	1 (0%)	86	94
15	1O	283/307 (92%)	283 (100%)	0	100	100
15	5O	283/307 (92%)	282 (100%)	1 (0%)	84	93
16	1P	296/323 (92%)	296 (100%)	0	100	100
16	5P	296/323 (92%)	295 (100%)	1 (0%)	86	94
17	1Q	117/152 (77%)	117 (100%)	0	100	100
17	5Q	117/152 (77%)	116 (99%)	1 (1%)	70	87
18	1R	79/97 (81%)	79 (100%)	0	100	100
18	5R	79/97 (81%)	79 (100%)	0	100	100
19	1S	77/82 (94%)	77 (100%)	0	100	100
19	5S	77/82 (94%)	76 (99%)	1 (1%)	61	83
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	77 (98%)	2 (2%)	42	71
20	5T	79/133 (59%)	79 (100%)	0	100	100
20	5U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	86
21	5V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	107 (100%)	0	100	100
22	5W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	152 (99%)	1 (1%)	76	90
23	5X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	100 (99%)	1 (1%)	68	86
24	5Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	122 (99%)	1 (1%)	73	88
25	5Z	123/124 (99%)	123 (100%)	0	100	100
26	1a	58/58 (100%)	58 (100%)	0	100	100
26	5a	58/58 (100%)	57 (98%)	1 (2%)	53	79
27	1b	69/70 (99%)	66 (96%)	3 (4%)	26	54
27	5b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	5c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	105 (99%)	1 (1%)	70	87
29	5d	106/109 (97%)	106 (100%)	0	100	100
30	1e	87/94 (93%)	87 (100%)	0	100	100
30	5e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
31	5f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	92 (100%)	0	100	100
32	5g	92/129 (71%)	92 (100%)	0	100	100
33	1h	121/158 (77%)	121 (100%)	0	100	100
33	5h	121/158 (77%)	121 (100%)	0	100	100
34	1i	119/120 (99%)	119 (100%)	0	100	100
34	5i	119/120 (99%)	119 (100%)	0	100	100
35	1j	62/84 (74%)	62 (100%)	0	100	100
35	5j	62/84 (74%)	61 (98%)	1 (2%)	55	80
36	1k	63/76 (83%)	63 (100%)	0	100	100
36	5k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
37	5l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	113 (100%)	0	100	100
38	5m	113/114 (99%)	113 (100%)	0	100	100
39	1n	156/160 (98%)	156 (100%)	0	100	100
39	5n	156/160 (98%)	155 (99%)	1 (1%)	78	91
40	1o	110/119 (92%)	110 (100%)	0	100	100
40	5o	110/119 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	154 (100%)	0	100	100
41	5p	154/156 (99%)	154 (100%)	0	100	100
42	1q	131/131 (100%)	131 (100%)	0	100	100
42	5q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100
43	5r	85/98 (87%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1s	44/351 (12%)	42 (96%)	2 (4%)	24	52
44	5s	44/351 (12%)	44 (100%)	0	100	100
45	3A	367/397 (92%)	367 (100%)	0	100	100
45	3N	372/397 (94%)	370 (100%)	2 (0%)	81	92
46	3B	328/355 (92%)	328 (100%)	0	100	100
46	3O	327/355 (92%)	327 (100%)	0	100	100
47	3C	332/332 (100%)	332 (100%)	0	100	100
47	3P	332/332 (100%)	332 (100%)	0	100	100
48	3D	202/259 (78%)	201 (100%)	1 (0%)	81	92
48	3Q	204/259 (79%)	203 (100%)	1 (0%)	81	92
49	3E	166/226 (74%)	166 (100%)	0	100	100
49	3I	37/226 (16%)	37 (100%)	0	100	100
49	3R	166/226 (74%)	165 (99%)	1 (1%)	78	91
49	3V	24/226 (11%)	18 (75%)	6 (25%)	0	2
50	3F	90/99 (91%)	90 (100%)	0	100	100
50	3S	90/99 (91%)	90 (100%)	0	100	100
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	66 (98%)	1 (2%)	57	81
52	3H	62/85 (73%)	62 (100%)	0	100	100
52	3U	62/85 (73%)	61 (98%)	1 (2%)	55	80
53	3J	45/51 (88%)	45 (100%)	0	100	100
53	3W	45/51 (88%)	41 (91%)	4 (9%)	9	23
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	41 (100%)	0	100	100
55	4A	424/424 (100%)	420 (99%)	4 (1%)	70	87
55	8A	424/424 (100%)	423 (100%)	1 (0%)	87	95
56	4B	210/211 (100%)	208 (99%)	2 (1%)	68	86
56	8B	210/211 (100%)	209 (100%)	1 (0%)	81	92
57	4C	223/225 (99%)	222 (100%)	1 (0%)	84	93
57	8C	223/225 (99%)	223 (100%)	0	100	100
58	4D	124/149 (83%)	123 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	8D	124/149 (83%)	124 (100%)	0	100	100
59	4E	92/124 (74%)	92 (100%)	0	100	100
59	8E	92/124 (74%)	92 (100%)	0	100	100
60	4F	80/100 (80%)	80 (100%)	0	100	100
60	8F	80/100 (80%)	79 (99%)	1 (1%)	61	83
61	4G	65/80 (81%)	65 (100%)	0	100	100
61	8G	65/80 (81%)	64 (98%)	1 (2%)	57	81
62	4H	73/76 (96%)	73 (100%)	0	100	100
62	8H	73/76 (96%)	72 (99%)	1 (1%)	59	82
63	4I	54/61 (88%)	54 (100%)	0	100	100
63	8I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	48 (98%)	1 (2%)	48	76
64	8J	49/68 (72%)	48 (98%)	1 (2%)	48	76
65	4K	38/66 (58%)	38 (100%)	0	100	100
65	8K	38/66 (58%)	37 (97%)	1 (3%)	40	70
66	4L	39/55 (71%)	39 (100%)	0	100	100
66	8L	39/55 (71%)	39 (100%)	0	100	100
67	4M	37/57 (65%)	37 (100%)	0	100	100
67	8M	37/57 (65%)	37 (100%)	0	100	100
68	4N	70/70 (100%)	70 (100%)	0	100	100
68	8N	70/70 (100%)	70 (100%)	0	100	100
All	All	21060/24374 (86%)	20991 (100%)	69 (0%)	84	94

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	5Q	44	ASN
26	5a	1	MET
61	8G	53	LEU
49	3R	222	CYS
48	3Q	43	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 215 such sidechains are listed below:

Mol	Chain	Res	Type
56	4B	24	HIS
12	5L	400	ASN
55	8A	291	HIS
58	4D	29	HIS
5	5E	57	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
11	FME	5K	1	11	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
1	FME	1A	1	1	8,9,10	0.53	0	8,9,11	1.07	1 (12%)
12	FME	5L	1	12	8,9,10	0.55	0	8,9,11	0.88	1 (12%)
34	SAC	5i	1	34	7,8,9	0.57	0	7,9,11	0.91	1 (14%)
55	FME	8A	1	55	8,9,10	0.55	0	8,9,11	0.99	1 (12%)
14	FME	5N	1	14	8,9,10	0.56	0	8,9,11	1.00	1 (12%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.98	1 (12%)
56	FME	4B	1	56	8,9,10	0.57	0	8,9,11	0.96	1 (12%)
34	SAC	1i	1	34	7,8,9	0.58	0	7,9,11	0.93	1 (14%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
55	FME	4A	1	55	8,9,10	0.56	0	8,9,11	0.96	1 (12%)
13	FME	5M	1	13	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.04	1 (12%)
8	FME	5H	1	8	8,9,10	0.55	0	8,9,11	1.05	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	0.86	1 (12%)
1	FME	5A	1	1	8,9,10	0.53	0	8,9,11	1.06	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	FME	8B	1	56	8,9,10	0.56	0	8,9,11	1.04	1 (12%)
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	0.99	1 (12%)

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

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

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5H	1	FME	O-C-CA	-2.69	117.86	124.77
8	1H	1	FME	O-C-CA	-2.67	117.90	124.77
11	1K	1	FME	O-C-CA	-2.67	117.92	124.77
1	1A	1	FME	O-C-CA	-2.62	118.02	124.77
11	5K	1	FME	O-C-CA	-2.61	118.05	124.77

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	5K	1	FME	2	0
1	1A	1	FME	1	0
14	5N	1	FME	1	0
14	1N	1	FME	1	0
56	4B	1	FME	2	0
11	1K	1	FME	2	0
55	4A	1	FME	2	0
13	5M	1	FME	1	0
1	5A	1	FME	2	0
56	8B	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 14 are monoatomic - leaving 188 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
71	FES	5E	301	5	0,4,4	-	-	-		
83	MYR	5o	201	-	13,14,15	0.32	0	12,13,15	0.29	0
86	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.37	0
86	PGV	4A	602	-	50,50,50	0.29	0	53,56,56	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
91	CUA	4B	303	56	0,1,1	-	-	-		
69	PC1	1A	203	-	32,32,53	0.34	0	38,40,61	0.35	0
76	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.31	0
76	3PE	1M	901	-	48,48,50	0.28	0	51,53,55	0.35	0
76	3PE	1M	906	-	49,49,50	0.28	0	52,54,55	0.33	0
71	FES	5G	803	7	0,4,4	-	-	-		
74	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.41	1 (0%)
76	3PE	5Y	804	-	32,32,50	0.33	0	35,37,55	0.49	0
77	GTP	1O	402	78	33,34,34	0.57	0	50,54,54	0.60	0
74	CDL	5H	401	-	50,50,99	0.36	0	56,62,111	0.61	1 (1%)
69	PC1	5I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
74	CDL	5N	401	-	61,61,99	0.31	0	67,73,111	0.62	1 (1%)
92	PEK	4G	102	-	52,52,52	0.27	0	55,57,57	0.41	0
76	3PE	1Y	801	-	30,30,50	0.33	0	33,35,55	0.51	0
76	3PE	5M	504	-	50,50,50	0.29	0	53,55,55	0.46	0
76	3PE	3Q	502	-	46,46,50	0.28	0	49,51,55	0.38	0
70	SF4	5G	802	7	0,12,12	-	-	-		
87	HEA	4A	605	55	67,67,67	2.44	24 (35%)	81,103,103	2.51	35 (43%)
76	3PE	1O	401	-	50,50,50	0.28	0	53,55,55	0.46	0
76	3PE	3A	503	45	31,31,50	0.34	0	34,36,55	0.38	0
86	PGV	8C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
91	CUA	8B	304	56	0,1,1	-	-	-		
76	3PE	1b	201	-	46,46,50	0.28	0	49,51,55	0.36	0
71	FES	1G	803	7	0,4,4	-	-	-		
76	3PE	5L	701	-	45,45,50	0.29	0	48,50,55	0.32	0
76	3PE	3C	505	-	33,33,50	0.34	0	36,38,55	0.40	0
69	PC1	5H	402	-	47,47,53	0.28	0	53,55,61	0.34	0
82	AME	5h	201	-	9,10,11	0.52	0	9,11,13	1.01	1 (11%)
74	CDL	3P	504	-	55,55,99	0.36	0	61,67,111	0.52	0
76	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
76	3PE	5M	502	-	47,47,50	0.28	0	50,52,55	0.34	0
69	PC1	3J	101	-	46,46,53	0.29	0	52,54,61	0.33	0
69	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.44	0
69	PC1	5B	203	-	47,47,53	0.30	0	53,55,61	0.44	0
92	PEK	4C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
71	FES	3E	301	49	0,4,4	-	-	-		
85	HEC	3Q	501	48	50,50,50	2.87	26 (52%)	68,82,82	2.50	27 (39%)
70	SF4	5I	203	9	0,12,12	-	-	-		
69	PC1	3R	302	-	44,44,53	0.29	0	50,52,61	0.36	0
70	SF4	1G	802	7	0,12,12	-	-	-		
76	3PE	3P	503	-	32,32,50	0.34	0	35,37,55	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.70	1 (1%)
69	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
81	EHZ	1T	101	20	31,36,37	0.19	0	36,44,47	1.07	1 (2%)
86	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.32	0
76	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.50	0
74	CDL	1d	203	-	64,64,99	0.32	0	70,76,111	0.42	0
76	3PE	1Y	804	-	32,32,50	0.33	0	35,37,55	0.49	0
74	CDL	8B	303	-	99,99,99	0.26	0	105,111,111	0.31	0
74	CDL	5h	202	-	79,79,99	0.31	0	85,91,111	0.41	0
69	PC1	5A	203	-	34,34,53	0.33	0	40,42,61	0.39	0
76	3PE	5M	501	-	44,44,50	0.30	0	47,49,55	0.36	0
76	3PE	5Y	806	-	40,40,50	0.29	0	43,45,55	0.40	0
76	3PE	5A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
86	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.42	0
74	CDL	5X	201	-	85,85,99	0.29	0	91,97,111	0.38	0
86	PGV	8C	304	-	50,50,50	0.27	0	53,56,56	0.38	0
90	PSC	8I	101	-	51,51,51	0.30	0	57,59,59	0.48	1 (1%)
76	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.46	0
70	SF4	5I	202	9	0,12,12	-	-	-		
86	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
76	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.62	0
81	EHZ	5T	101	20	31,36,37	0.20	0	36,44,47	1.06	1 (2%)
86	PGV	8A	602	-	50,50,50	0.29	0	53,56,56	0.36	0
76	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.41	0
76	3PE	5L	703	-	44,44,50	0.29	0	47,49,55	0.33	0
70	SF4	1I	203	9	0,12,12	-	-	-		
74	CDL	5L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
76	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.45	0
72	FMN	1F	501	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
81	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.05	1 (2%)
86	PGV	8G	101	-	50,50,50	0.28	0	53,56,56	0.47	1 (1%)
93	PO4	4H	101	-	4,4,4	0.96	0	6,6,6	0.47	0
79	NDP	5P	402	-	51,52,52	0.52	0	71,80,80	0.78	2 (2%)
74	CDL	3T	101	-	56,56,99	0.34	0	62,68,111	0.44	0
70	SF4	1G	801	7	0,12,12	-	-	-		
76	3PE	1K	101	-	43,43,50	0.30	0	46,48,55	0.35	0
84	HEM	3C	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.63	11 (16%)
69	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.33	0
86	PGV	4B	301	56	50,50,50	0.28	0	53,56,56	0.33	0
75	AYA	1I	205	-	6,7,8	0.65	0	6,8,10	0.94	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PGV	8M	101	-	50,50,50	0.29	0	53,56,56	0.30	0
86	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
87	HEA	4A	604	55	67,67,67	2.44	25 (37%)	81,103,103	2.57	36 (44%)
86	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.40	0
74	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
74	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.43	0
83	MYR	1o	201	-	13,14,15	0.32	0	12,13,15	0.30	0
76	3PE	1M	902	-	44,44,50	0.30	0	47,49,55	0.35	0
86	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
69	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.37	0
69	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.51	0
76	3PE	5Y	802	-	39,39,50	0.31	0	42,44,55	0.46	0
86	PGV	8B	302	56	50,50,50	0.28	0	53,56,56	0.36	0
86	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.33	0
71	FES	1E	301	5	0,4,4	-	-	-	-	-
76	3PE	5L	704	-	48,48,50	0.28	0	51,53,55	0.36	0
76	3PE	1P	502	-	34,34,50	0.32	0	37,39,55	0.37	0
75	AYA	5q	202	-	6,7,8	0.65	0	6,8,10	0.93	1 (16%)
92	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
84	HEM	3C	502	-	50,50,50	1.57	8 (16%)	67,82,82	1.57	11 (16%)
69	PC1	1A	201	-	34,34,53	0.32	0	40,42,61	0.39	0
70	SF4	5G	801	7	0,12,12	-	-	-	-	-
69	PC1	5L	705	-	45,45,53	0.30	0	51,53,61	0.37	0
86	PGV	8L	101	-	50,50,50	0.29	0	53,56,56	0.37	0
74	CDL	3G	102	-	55,55,99	0.34	0	61,67,111	0.48	0
69	PC1	1d	202	-	38,38,53	0.30	0	44,46,61	0.48	0
74	CDL	3N	502	-	42,42,99	0.38	0	48,54,111	0.52	0
86	PGV	4L	101	-	50,50,50	0.29	0	53,56,56	0.38	0
74	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.41	0
69	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
69	PC1	5I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
86	PGV	8C	307	-	50,50,50	0.28	0	53,56,56	0.38	0
76	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.33	0
69	PC1	5M	505	-	43,43,53	0.30	0	49,51,61	0.38	0
69	PC1	1H	402	-	47,47,53	0.29	0	53,55,61	0.34	0
76	3PE	1Y	806	-	40,40,50	0.29	0	43,45,55	0.41	0
69	PC1	5B	202	-	45,45,53	0.29	0	51,53,61	0.36	0
69	PC1	1M	905	-	43,43,53	0.30	0	49,51,61	0.37	0
76	3PE	1M	903	-	47,47,50	0.28	0	50,52,55	0.35	0
76	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.66	1 (3%)
74	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.42	0
86	PGV	8A	601	-	50,50,50	0.28	0	53,56,56	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	FES	3R	301	49	0,4,4	-	-	-		
74	CDL	1h	202	-	79,79,99	0.31	0	85,91,111	0.40	0
69	PC1	5h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
70	SF4	5F	502	6	0,12,12	-	-	-		
76	3PE	5Y	803	-	29,29,50	0.34	0	32,34,55	0.77	1 (3%)
87	HEA	8A	603	55	67,67,67	2.42	24 (35%)	81,103,103	2.58	37 (45%)
86	PGV	4A	603	-	50,50,50	0.27	0	53,56,56	0.32	0
76	3PE	5j	101	-	43,43,50	0.29	0	46,48,55	0.46	0
69	PC1	5M	503	-	34,34,53	0.32	0	40,42,61	0.47	0
74	CDL	5d	203	-	64,64,99	0.32	0	70,76,111	0.42	0
74	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.40	0
76	3PE	5K	101	-	43,43,50	0.30	0	46,48,55	0.35	0
69	PC1	5q	201	-	48,48,53	0.28	0	54,56,61	0.34	0
69	PC1	5d	202	-	38,38,53	0.30	0	44,46,61	0.49	1 (2%)
86	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.31	0
74	CDL	1L	702	-	75,75,99	0.30	0	81,87,111	0.38	0
82	AME	1h	201	-	9,10,11	0.51	0	9,11,13	1.00	1 (11%)
70	SF4	1F	502	6	0,12,12	-	-	-		
69	PC1	1L	704	-	45,45,53	0.30	0	51,53,61	0.37	0
74	CDL	3C	503	-	51,51,99	0.35	0	57,63,111	0.54	1 (1%)
86	PGV	4C	304	-	50,50,50	0.28	0	53,56,56	0.39	0
92	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
70	SF4	5B	201	2	0,12,12	-	-	-		
76	3PE	1Y	805	-	26,26,50	0.34	0	29,31,55	0.55	0
86	PGV	8B	301	-	50,50,50	0.27	0	53,56,56	0.33	0
86	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.31	0
76	3PE	5M	506	-	49,49,50	0.27	0	52,54,55	0.33	0
72	FMN	5F	501	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
74	CDL	5q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
76	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.38	0
84	HEM	3P	502	47	50,50,50	1.57	9 (18%)	67,82,82	1.59	12 (17%)
79	NDP	1P	501	-	51,52,52	0.52	0	71,80,80	0.80	2 (2%)
69	PC1	1M	904	-	34,34,53	0.33	0	40,42,61	0.47	0
74	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.30	0
86	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.69	1 (1%)
69	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
70	SF4	1I	202	9	0,12,12	-	-	-		
87	HEA	8A	604	55	67,67,67	2.43	25 (37%)	81,103,103	2.54	34 (41%)
76	3PE	1Y	803	-	29,29,50	0.34	0	32,34,55	0.80	1 (3%)
69	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	3PE	1Y	802	-	39,39,50	0.32	0	42,44,55	0.44	0
69	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.37	0
74	CDL	1N	401	-	61,61,99	0.31	0	67,73,111	0.63	1 (1%)
86	PGV	4J	101	-	50,50,50	0.28	0	53,56,56	0.39	0
74	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.61	1 (1%)
86	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.43	0
76	3PE	5Y	805	-	26,26,50	0.34	0	29,31,55	0.55	0
77	GTP	5O	401	78	33,34,34	0.56	0	50,54,54	0.58	0
76	3PE	5d	201	-	48,48,50	0.27	0	51,53,55	0.33	0
74	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.42	0
76	3PE	5P	403	-	34,34,50	0.32	0	37,39,55	0.38	0
70	SF4	1B	201	2	0,12,12	-	-	-	-	-
86	PGV	4C	305	-	50,50,50	0.29	0	53,56,56	0.49	1 (1%)
85	HEC	3D	501	48	48,49,50	2.91	25 (52%)	66,80,82	2.57	28 (42%)
84	HEM	3P	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.63	11 (16%)
69	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.41	0
76	3PE	5Y	801	-	30,30,50	0.33	0	33,35,55	0.50	0
93	PO4	8H	101	-	4,4,4	0.96	0	6,6,6	0.48	0
76	3PE	3C	504	-	34,34,50	0.33	0	37,39,55	0.47	0
90	PSC	4A	609	-	51,51,51	0.29	0	57,59,59	0.46	1 (1%)
81	EHZ	5n	201	-	31,36,37	0.18	0	36,44,47	1.09	1 (2%)

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
71	FES	5E	301	5	-	-	0/1/1/1
83	MYR	5o	201	-	-	2/12/12/13	-
86	PGV	4C	307	-	-	3/55/55/55	-
86	PGV	4A	602	-	-	4/55/55/55	-
69	PC1	1A	203	-	-	3/36/36/57	-
76	3PE	1L	701	-	-	5/49/49/54	-
76	3PE	1M	901	-	-	14/52/52/54	-
76	3PE	1M	906	-	-	7/53/53/54	-
71	FES	5G	803	7	-	-	0/1/1/1
74	CDL	4C	306	-	-	19/110/110/110	-
76	3PE	5Y	804	-	-	5/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	GTP	1O	402	78	-	3/22/38/38	0/3/3/3
74	CDL	5H	401	-	-	5/61/61/110	-
69	PC1	5I	204	-	-	5/47/47/57	-
74	CDL	5N	401	-	-	14/71/71/110	-
92	PEK	4G	102	-	-	7/56/56/56	-
76	3PE	1Y	801	-	-	7/34/34/54	-
76	3PE	5M	504	-	-	9/54/54/54	-
76	3PE	3Q	502	-	-	4/50/50/54	-
87	HEA	4A	605	55	-	6/36/76/76	-
70	SF4	5G	802	7	-	-	0/6/5/5
76	3PE	1O	401	-	-	8/54/54/54	-
76	3PE	3A	503	45	-	5/35/35/54	-
86	PGV	8C	301	-	-	2/55/55/55	-
76	3PE	1b	201	-	-	8/50/50/54	-
71	FES	1G	803	7	-	-	0/1/1/1
76	3PE	5L	701	-	-	4/49/49/54	-
76	3PE	3C	505	-	-	5/37/37/54	-
69	PC1	5H	402	-	-	2/51/51/57	-
82	AME	5h	201	-	-	2/9/10/12	-
74	CDL	3P	504	-	-	13/66/66/110	-
76	3PE	1L	703	-	-	6/48/48/54	-
76	3PE	5M	502	-	-	16/51/51/54	-
69	PC1	3J	101	-	-	1/50/50/57	-
69	PC1	1B	203	-	-	11/51/51/57	-
69	PC1	5B	203	-	-	10/51/51/57	-
92	PEK	4C	308	-	-	4/55/55/56	-
71	FES	3E	301	49	-	-	0/1/1/1
85	HEC	3Q	501	48	1/1/3/7	6/14/54/54	-
70	SF4	5I	203	9	-	-	0/6/5/5
69	PC1	3R	302	-	-	3/48/48/57	-
70	SF4	1G	802	7	-	-	0/6/5/5
76	3PE	3P	503	-	-	6/36/36/54	-
86	PGV	8C	302	-	-	10/55/55/55	-
69	PC1	1I	201	-	-	6/57/57/57	-
81	EHZ	1T	101	20	-	7/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PGV	8C	303	-	-	12/55/55/55	-
76	3PE	3D	502	-	-	2/36/36/54	-
74	CDL	1d	203	-	-	13/75/75/110	-
76	3PE	1Y	804	-	-	5/36/36/54	-
74	CDL	8B	303	-	-	13/110/110/110	-
74	CDL	5h	202	-	-	16/90/90/110	-
69	PC1	5A	203	-	-	2/38/38/57	-
76	3PE	5M	501	-	-	9/48/48/54	-
76	3PE	5Y	806	-	-	9/44/44/54	-
76	3PE	5A	201	-	-	6/50/50/54	-
86	PGV	4A	601	-	-	13/55/55/55	-
74	CDL	5X	201	-	-	17/96/96/110	-
86	PGV	8C	304	-	-	9/55/55/55	-
90	PSC	8I	101	-	-	12/55/55/55	-
76	3PE	3N	501	-	-	9/35/35/54	-
86	PGV	8C	305	-	-	6/55/55/55	-
70	SF4	5I	202	9	-	-	0/6/5/5
76	3PE	3N	503	-	-	6/28/28/54	-
81	EHZ	5T	101	20	-	8/42/44/45	-
86	PGV	8A	602	-	-	3/55/55/55	-
76	3PE	3Y	101	-	-	5/33/33/54	-
76	3PE	5L	703	-	-	6/48/48/54	-
70	SF4	1I	203	9	-	-	0/6/5/5
74	CDL	5L	702	-	-	14/86/86/110	-
76	3PE	1j	101	-	-	5/47/47/54	-
72	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
81	EHZ	1n	201	-	-	4/42/44/45	-
86	PGV	8G	101	-	-	9/55/55/55	-
79	NDP	5P	402	-	-	2/34/77/77	0/5/5/5
74	CDL	3T	101	-	-	7/67/67/110	-
84	HEM	3C	501	47	-	7/14/54/54	-
76	3PE	1K	101	-	-	8/47/47/54	-
70	SF4	1G	801	7	-	-	0/6/5/5
69	PC1	1I	204	-	-	3/47/47/57	-
86	PGV	4B	301	56	-	5/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	AYA	1I	205	-	-	0/5/6/8	-
86	PGV	8M	101	-	-	6/55/55/55	-
86	PGV	8K	101	-	-	12/55/55/55	-
87	HEA	4A	604	55	-	8/36/76/76	-
86	PGV	8J	101	-	-	6/55/55/55	-
74	CDL	8C	306	-	-	20/110/110/110	-
74	CDL	1q	202	-	-	5/71/71/110	-
83	MYR	1o	201	-	-	1/12/12/13	-
76	3PE	1M	902	-	-	9/48/48/54	-
86	PGV	4K	101	-	-	10/55/55/55	-
69	PC1	5P	401	-	-	3/36/36/57	-
69	PC1	3X	101	-	-	2/32/32/57	-
76	3PE	5Y	802	-	-	13/43/43/54	-
86	PGV	8B	302	56	-	5/55/55/55	-
86	PGV	4M	101	-	-	4/55/55/55	-
71	FES	1E	301	5	-	-	0/1/1/1
76	3PE	5L	704	-	-	12/52/52/54	-
76	3PE	1P	502	-	-	1/38/38/54	-
75	AYA	5q	202	-	-	0/5/6/8	-
92	PEK	8C	308	-	-	4/55/55/56	-
84	HEM	3C	502	-	-	6/14/54/54	-
69	PC1	1A	201	-	-	6/38/38/57	-
70	SF4	5G	801	7	-	-	0/6/5/5
69	PC1	5L	705	-	-	6/49/49/57	-
86	PGV	8L	101	-	-	5/55/55/55	-
74	CDL	3G	102	-	-	7/66/66/110	-
69	PC1	1d	202	-	-	6/42/42/57	-
74	CDL	3N	502	-	-	5/53/53/110	-
86	PGV	4L	101	-	-	5/55/55/55	-
74	CDL	8D	201	-	-	14/110/110/110	-
69	PC1	1A	202	-	-	2/38/38/57	-
69	PC1	5I	201	-	-	7/57/57/57	-
86	PGV	8C	307	-	-	2/55/55/55	-
76	3PE	1d	201	-	-	2/52/52/54	-
69	PC1	5M	505	-	-	9/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	PC1	1H	402	-	-	3/51/51/57	-
76	3PE	1Y	806	-	-	10/44/44/54	-
69	PC1	5B	202	-	-	3/49/49/57	-
69	PC1	1M	905	-	-	14/47/47/57	-
76	3PE	1M	903	-	-	16/51/51/54	-
76	3PE	3A	502	-	-	7/30/30/54	-
74	CDL	3A	501	-	-	2/68/68/110	-
86	PGV	8A	601	-	-	14/55/55/55	-
71	FES	3R	301	49	-	-	0/1/1/1
74	CDL	1h	202	-	-	18/90/90/110	-
69	PC1	5h	203	-	-	10/50/50/57	-
76	3PE	5Y	803	-	-	9/33/33/54	-
87	HEA	8A	603	55	-	12/36/76/76	-
70	SF4	5F	502	6	-	-	0/6/5/5
86	PGV	4A	603	-	-	2/55/55/55	-
76	3PE	5j	101	-	-	6/47/47/54	-
69	PC1	5M	503	-	-	5/38/38/57	-
74	CDL	5d	203	-	-	13/75/75/110	-
74	CDL	1X	201	-	-	15/96/96/110	-
76	3PE	5K	101	-	-	9/47/47/54	-
69	PC1	5q	201	-	-	2/52/52/57	-
69	PC1	5d	202	-	-	6/42/42/57	-
86	PGV	4C	301	-	-	2/55/55/55	-
74	CDL	1L	702	-	-	15/86/86/110	-
82	AME	1h	201	-	-	2/9/10/12	-
70	SF4	1F	502	6	-	-	0/6/5/5
69	PC1	1L	704	-	-	6/49/49/57	-
74	CDL	3C	503	-	-	9/62/62/110	-
86	PGV	4C	304	-	-	10/55/55/55	-
92	PEK	8G	102	-	-	7/56/56/56	-
70	SF4	5B	201	2	-	-	0/6/5/5
76	3PE	1Y	805	-	-	7/30/30/54	-
86	PGV	8B	301	-	-	3/55/55/55	-
86	PGV	4C	303	-	-	8/55/55/55	-
76	3PE	5M	506	-	-	6/53/53/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	FMN	5F	501	-	-	1/18/18/18	0/3/3/3
74	CDL	5q	203	-	-	6/71/71/110	-
76	3PE	3G	101	-	-	4/32/32/54	-
84	HEM	3P	502	47	-	8/14/54/54	-
79	NDP	1P	501	-	-	2/34/77/77	0/5/5/5
69	PC1	1M	904	-	-	5/38/38/57	-
74	CDL	4B	302	-	-	13/110/110/110	-
86	PGV	4C	302	-	-	12/55/55/55	-
69	PC1	1h	203	-	-	11/50/50/57	-
70	SF4	1I	202	9	-	-	0/6/5/5
87	HEA	8A	604	55	-	6/36/76/76	-
76	3PE	1Y	803	-	-	8/33/33/54	-
69	PC1	1q	201	-	-	2/52/52/57	-
76	3PE	1Y	802	-	-	15/43/43/54	-
69	PC1	1B	202	-	-	4/49/49/57	-
74	CDL	1N	401	-	-	16/71/71/110	-
86	PGV	4J	101	-	-	5/55/55/55	-
74	CDL	1H	401	-	-	4/61/61/110	-
86	PGV	4G	101	-	-	9/55/55/55	-
76	3PE	5Y	805	-	-	5/30/30/54	-
77	GTP	5O	401	78	-	1/22/38/38	0/3/3/3
76	3PE	5d	201	-	-	3/52/52/54	-
74	CDL	4D	201	-	-	15/110/110/110	-
76	3PE	5P	403	-	-	2/38/38/54	-
86	PGV	4C	305	-	-	5/55/55/55	-
70	SF4	1B	201	2	-	-	0/6/5/5
85	HEC	3D	501	48	1/1/2/7	7/13/53/54	-
84	HEM	3P	501	47	-	9/14/54/54	-
69	PC1	5A	202	-	-	2/38/38/57	-
76	3PE	5Y	801	-	-	9/34/34/54	-
76	3PE	3C	504	-	-	11/38/38/54	-
90	PSC	4A	609	-	-	10/55/55/55	-
81	EHZ	5n	201	-	-	3/42/44/45	-

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4A	604	HEA	FE-ND	5.64	2.12	1.94
87	4A	604	HEA	FE-NB	5.62	2.12	1.94
87	8A	603	HEA	FE-NB	5.61	2.12	1.94
87	8A	603	HEA	FE-ND	5.58	2.12	1.94
87	4A	605	HEA	FE-ND	5.55	2.12	1.94

The worst 5 of 273 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	604	HEA	C3D-C4D-ND	6.64	116.77	110.35
87	8A	603	HEA	C3D-C4D-ND	6.61	116.74	110.35
87	4A	605	HEA	C3D-C4D-ND	6.50	116.63	110.35
87	4A	604	HEA	C3D-C4D-ND	6.45	116.59	110.35
85	3Q	501	HEC	C1B-C2B-C3B	-6.00	100.67	106.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	3D	501	HEC	NA
85	3Q	501	HEC	NA

5 of 1171 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1B	203	PC1	O22-C21-O21-C2
69	1B	203	PC1	C22-C21-O21-C2
69	1I	204	PC1	C1-O11-P-O14
69	1M	904	PC1	O22-C21-O21-C2
69	1M	904	PC1	C22-C21-O21-C2

There are no ring outliers.

171 monomers are involved in 656 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	5o	201	MYR	1	0
86	4C	307	PGV	7	0
86	4A	602	PGV	6	0
91	4B	303	CUA	3	0
69	1A	203	PC1	1	0
76	1L	701	3PE	3	0
76	1M	901	3PE	4	0
76	1M	906	3PE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	5G	803	FES	3	0
74	4C	306	CDL	15	0
76	5Y	804	3PE	2	0
77	1O	402	GTP	2	0
74	5H	401	CDL	2	0
69	5I	204	PC1	4	0
74	5N	401	CDL	3	0
92	4G	102	PEK	4	0
76	1Y	801	3PE	4	0
76	5M	504	3PE	7	0
76	3Q	502	3PE	3	0
87	4A	605	HEA	2	0
76	1O	401	3PE	10	0
76	3A	503	3PE	4	0
86	8C	301	PGV	2	0
91	8B	304	CUA	1	0
76	1b	201	3PE	1	0
71	1G	803	FES	3	0
76	5L	701	3PE	2	0
76	3C	505	3PE	3	0
69	5H	402	PC1	2	0
82	5h	201	AME	1	0
74	3P	504	CDL	9	0
76	1L	703	3PE	5	0
76	5M	502	3PE	11	0
69	3J	101	PC1	4	0
69	1B	203	PC1	7	0
69	5B	203	PC1	7	0
92	4C	308	PEK	4	0
85	3Q	501	HEC	2	0
69	3R	302	PC1	6	0
86	8C	302	PGV	2	0
69	1I	201	PC1	5	0
86	8C	303	PGV	4	0
76	3D	502	3PE	2	0
74	1d	203	CDL	9	0
76	1Y	804	3PE	2	0
74	8B	303	CDL	9	0
74	5h	202	CDL	10	0
69	5A	203	PC1	1	0
76	5M	501	3PE	4	0
76	5Y	806	3PE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	5A	201	3PE	3	0
86	4A	601	PGV	7	0
74	5X	201	CDL	6	0
86	8C	304	PGV	6	0
90	8I	101	PSC	5	0
76	3N	501	3PE	2	0
86	8C	305	PGV	2	0
76	3N	503	3PE	3	0
81	5T	101	EHZ	1	0
86	8A	602	PGV	5	0
76	3Y	101	3PE	2	0
76	5L	703	3PE	3	0
74	5L	702	CDL	6	0
76	1j	101	3PE	2	0
72	1F	501	FMN	3	0
81	1n	201	EHZ	2	0
86	8G	101	PGV	6	0
79	5P	402	NDP	5	0
74	3T	101	CDL	11	0
70	1G	801	SF4	1	0
76	1K	101	3PE	2	0
69	1I	204	PC1	3	0
86	4B	301	PGV	4	0
75	1I	205	AYA	1	0
86	8M	101	PGV	3	0
86	8K	101	PGV	1	0
87	4A	604	HEA	7	0
86	8J	101	PGV	3	0
74	8C	306	CDL	14	0
74	1q	202	CDL	1	0
76	1M	902	3PE	5	0
86	4K	101	PGV	1	0
69	3X	101	PC1	2	0
76	5Y	802	3PE	3	0
86	8B	302	PGV	5	0
86	4M	101	PGV	9	0
76	5L	704	3PE	3	0
76	1P	502	3PE	3	0
75	5q	202	AYA	3	0
92	8C	308	PEK	6	0
84	3C	502	HEM	4	0
69	1A	201	PC1	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	5G	801	SF4	1	0
69	5L	705	PC1	3	0
86	8L	101	PGV	3	0
74	3G	102	CDL	5	0
69	1d	202	PC1	6	0
74	3N	502	CDL	1	0
86	4L	101	PGV	3	0
74	8D	201	CDL	18	0
69	1A	202	PC1	1	0
69	5I	201	PC1	5	0
86	8C	307	PGV	7	0
76	1d	201	3PE	4	0
69	5M	505	PC1	6	0
69	1H	402	PC1	2	0
76	1Y	806	3PE	1	0
69	5B	202	PC1	6	0
69	1M	905	PC1	6	0
76	1M	903	3PE	11	0
76	3A	502	3PE	1	0
74	3A	501	CDL	5	0
86	8A	601	PGV	5	0
71	3R	301	FES	1	0
74	1h	202	CDL	11	0
69	5h	203	PC1	3	0
70	5F	502	SF4	1	0
76	5Y	803	3PE	3	0
87	8A	603	HEA	6	0
86	4A	603	PGV	8	0
76	5j	101	3PE	5	0
69	5M	503	PC1	4	0
74	5d	203	CDL	3	0
74	1X	201	CDL	10	0
76	5K	101	3PE	3	0
69	5q	201	PC1	4	0
69	5d	202	PC1	8	0
86	4C	301	PGV	6	0
74	1L	702	CDL	8	0
82	1h	201	AME	1	0
70	1F	502	SF4	1	0
69	1L	704	PC1	3	0
74	3C	503	CDL	3	0
86	4C	304	PGV	6	0

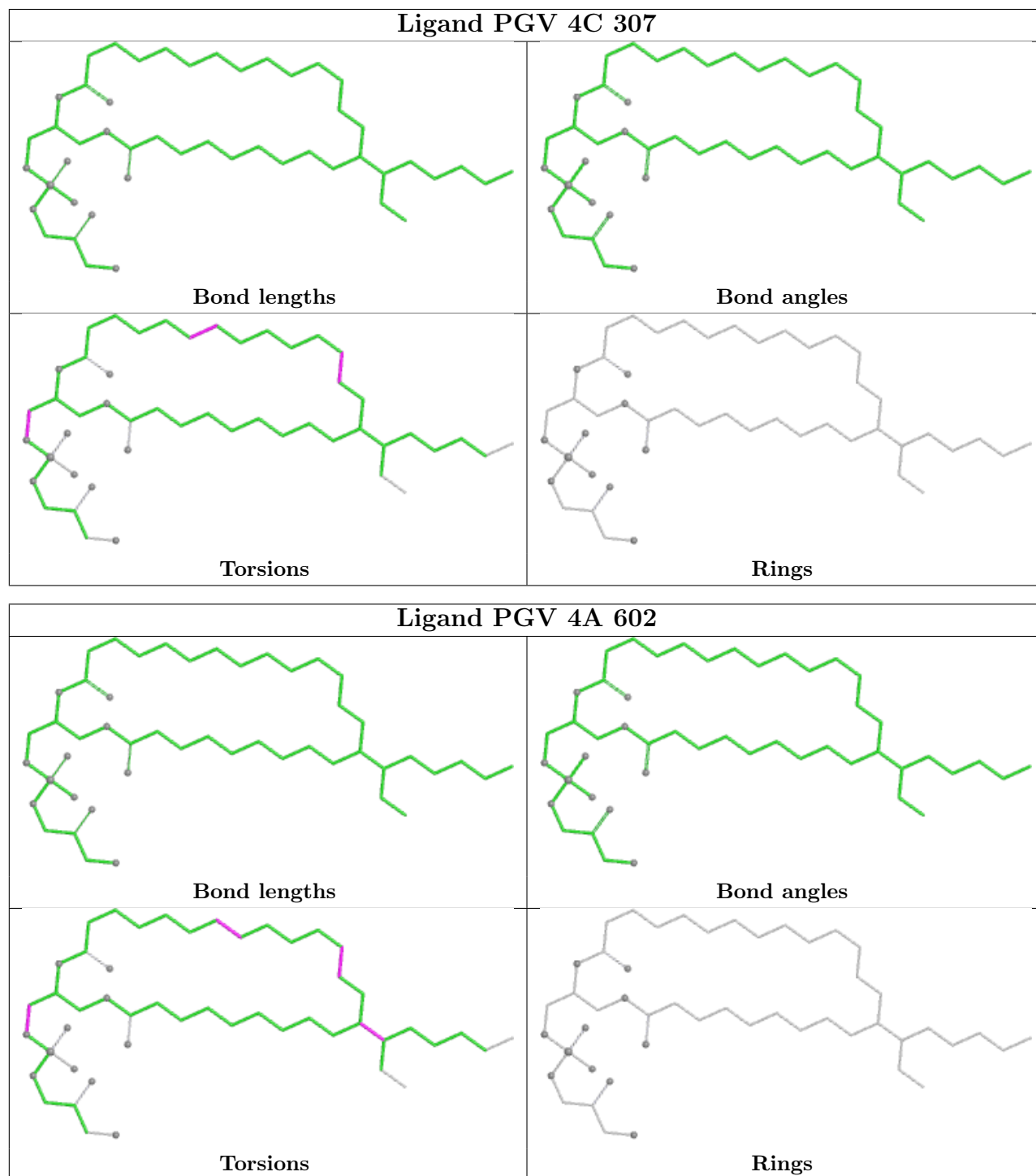
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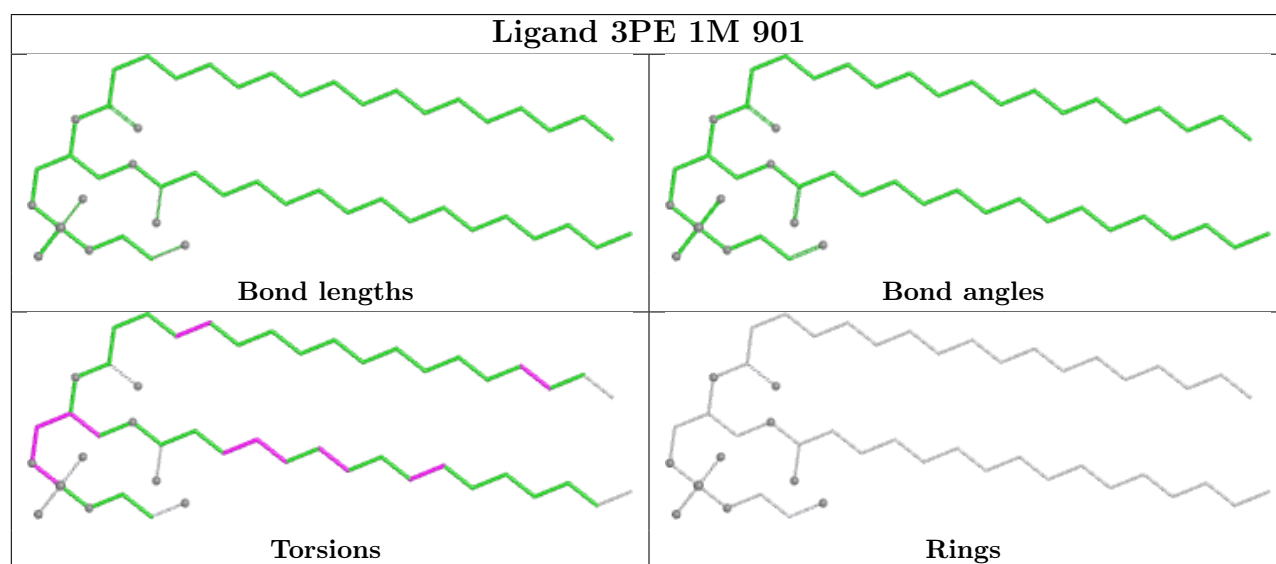
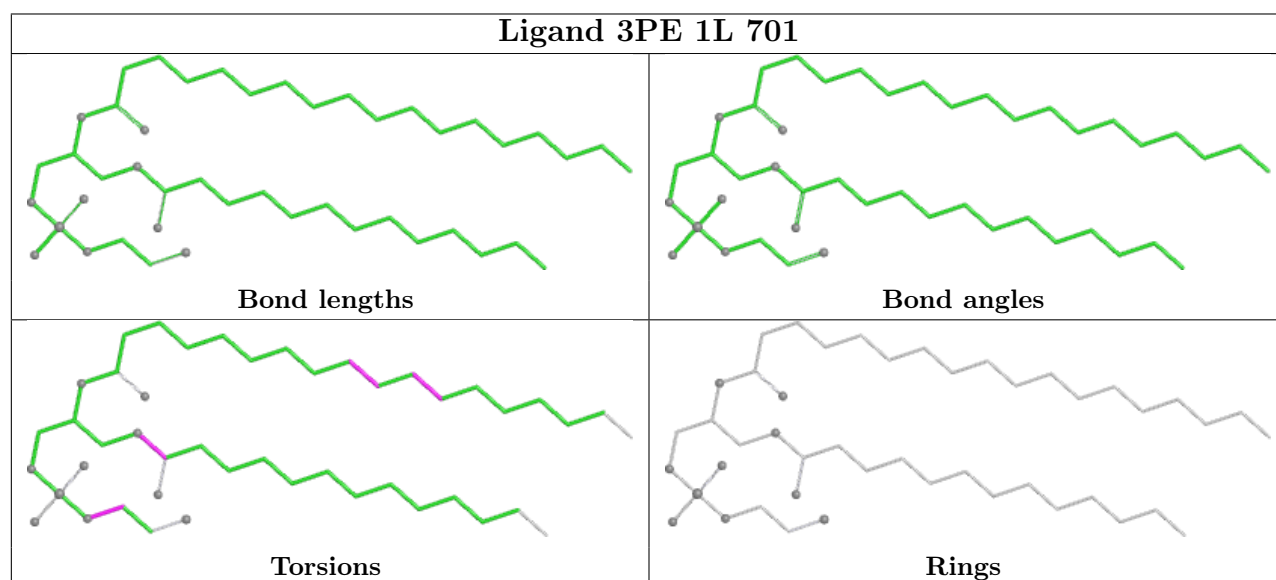
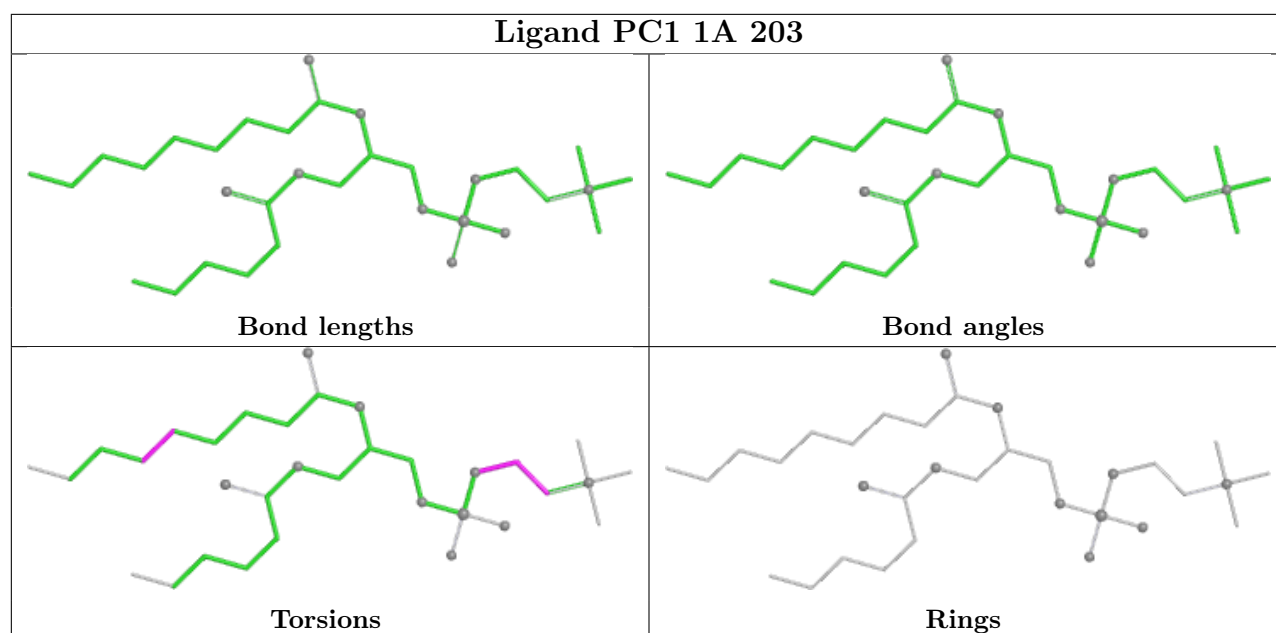
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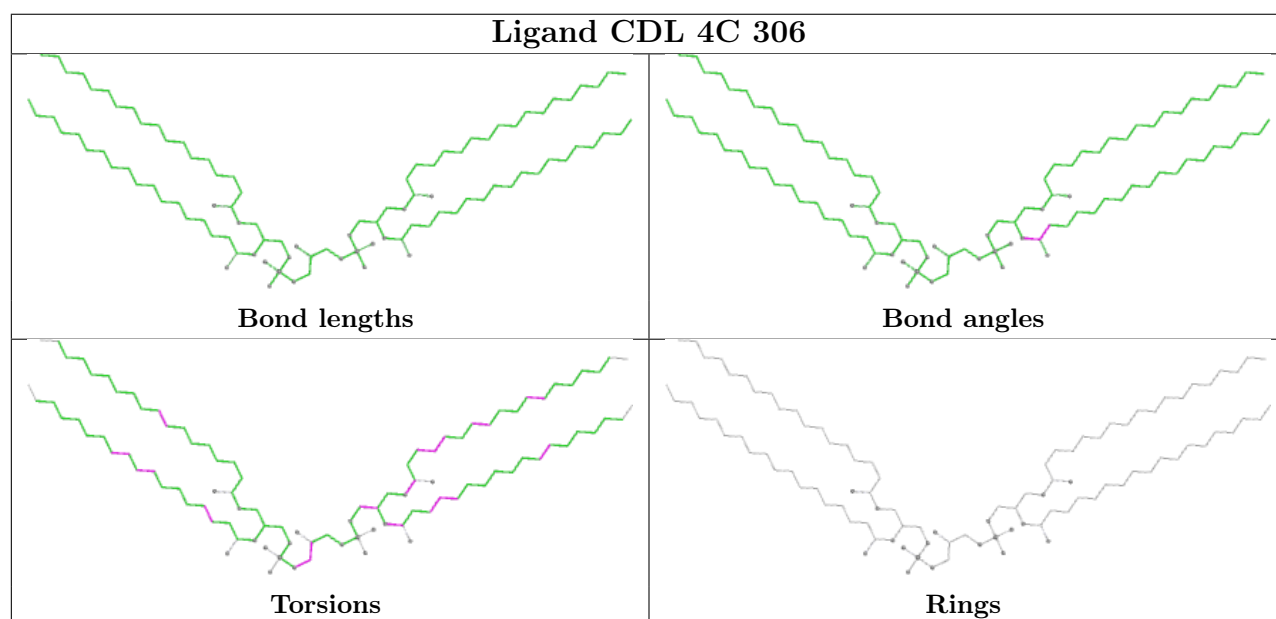
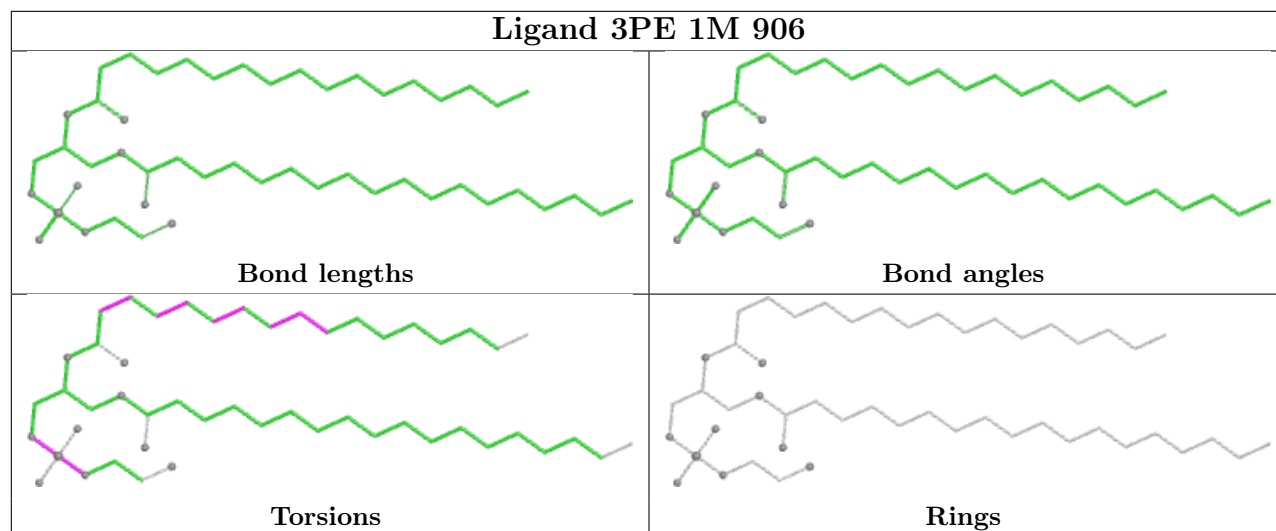
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	8G	102	PEK	4	0
70	5B	201	SF4	1	0
76	1Y	805	3PE	2	0
86	8B	301	PGV	9	0
86	4C	303	PGV	5	0
76	5M	506	3PE	2	0
72	5F	501	FMN	3	0
74	5q	203	CDL	2	0
84	3P	502	HEM	2	0
79	1P	501	NDP	3	0
69	1M	904	PC1	2	0
74	4B	302	CDL	7	0
86	4C	302	PGV	3	0
69	1h	203	PC1	3	0
87	8A	604	HEA	4	0
76	1Y	803	3PE	3	0
69	1q	201	PC1	3	0
76	1Y	802	3PE	4	0
69	1B	202	PC1	5	0
74	1N	401	CDL	3	0
86	4J	101	PGV	3	0
74	1H	401	CDL	3	0
86	4G	101	PGV	6	0
76	5Y	805	3PE	1	0
77	5O	401	GTP	1	0
76	5d	201	3PE	7	0
74	4D	201	CDL	18	0
76	5P	403	3PE	1	0
70	1B	201	SF4	1	0
86	4C	305	PGV	1	0
85	3D	501	HEC	3	0
84	3P	501	HEM	1	0
69	5A	202	PC1	3	0
76	5Y	801	3PE	6	0
76	3C	504	3PE	3	0
90	4A	609	PSC	7	0
81	5n	201	EHZ	1	0

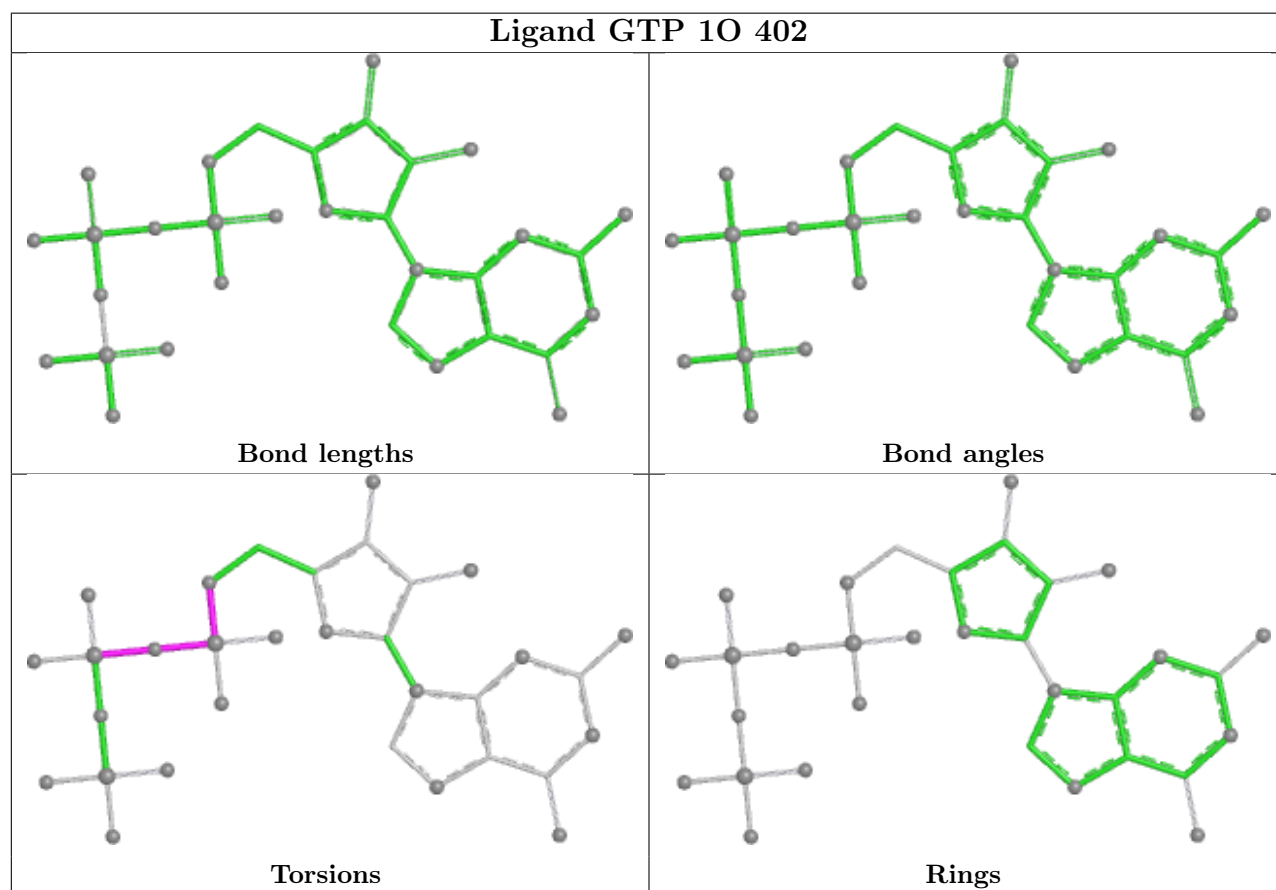
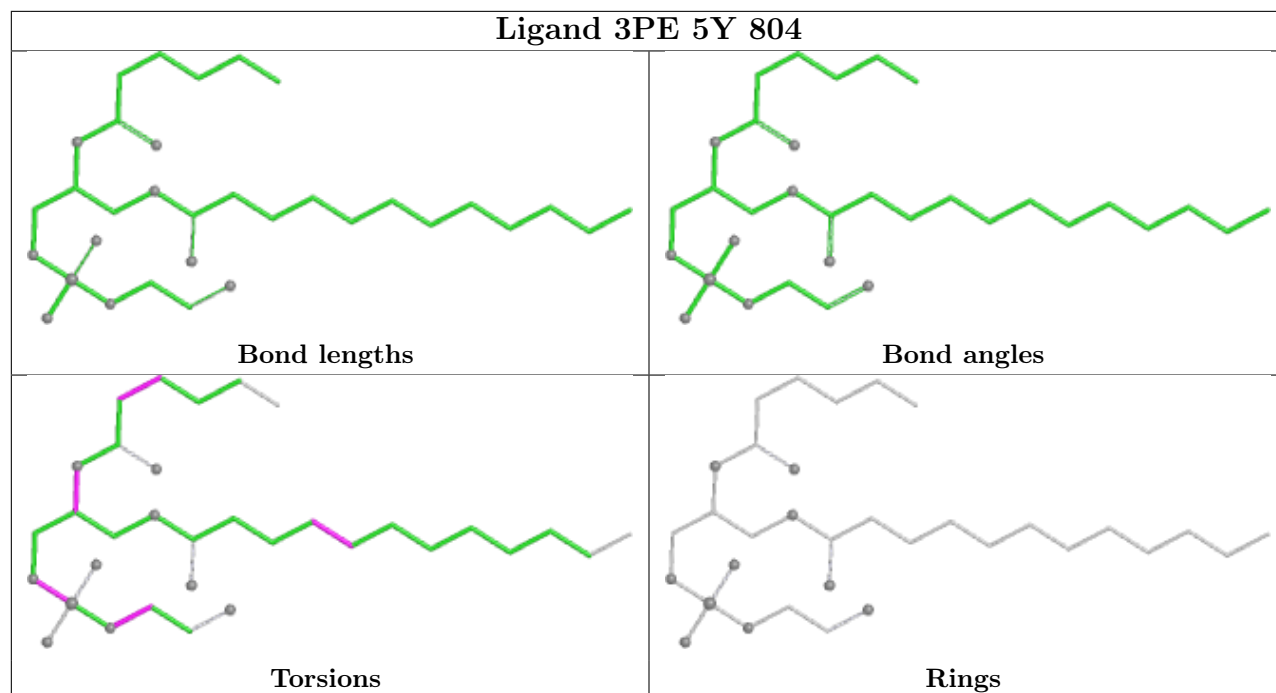
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

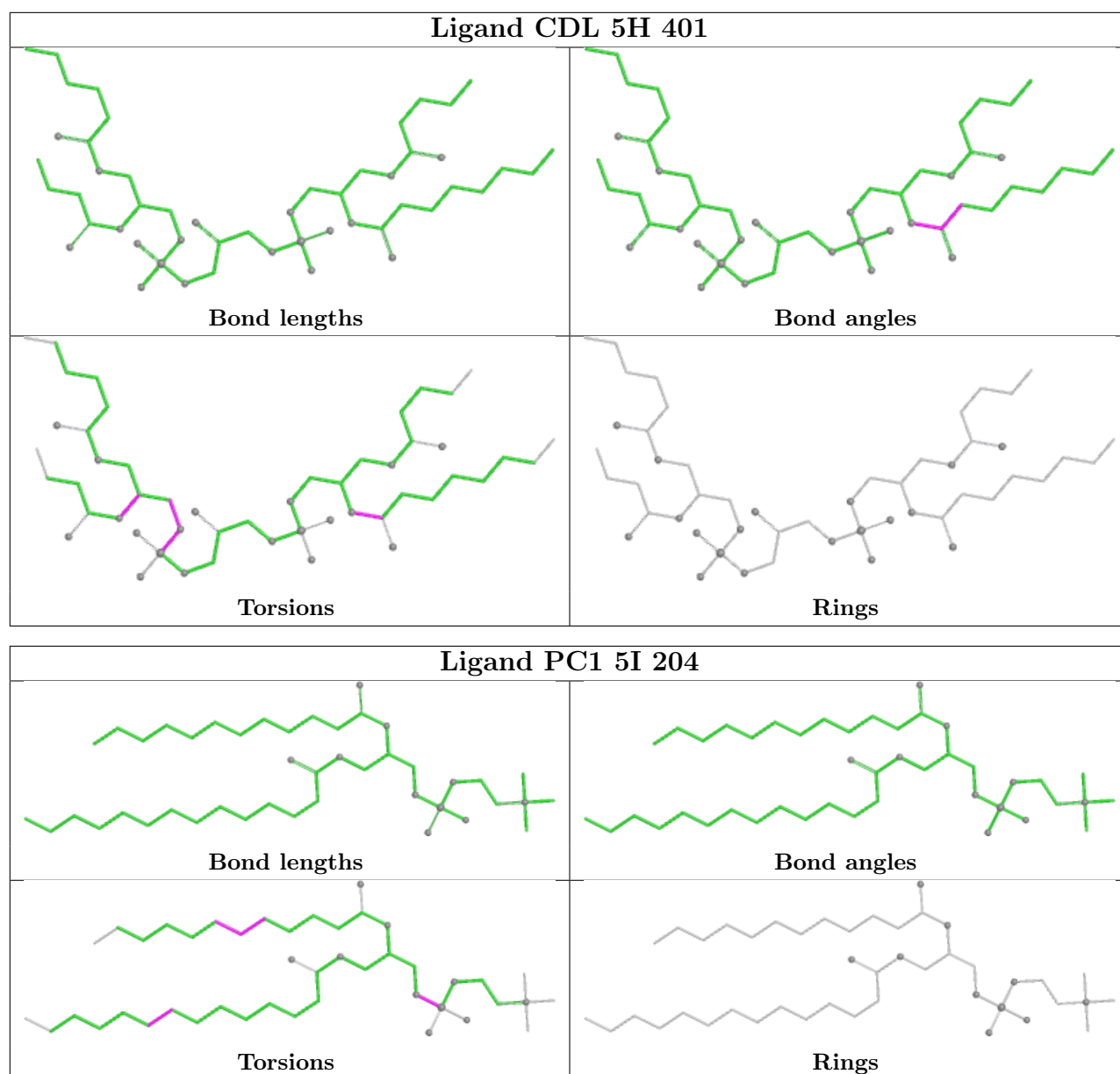
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

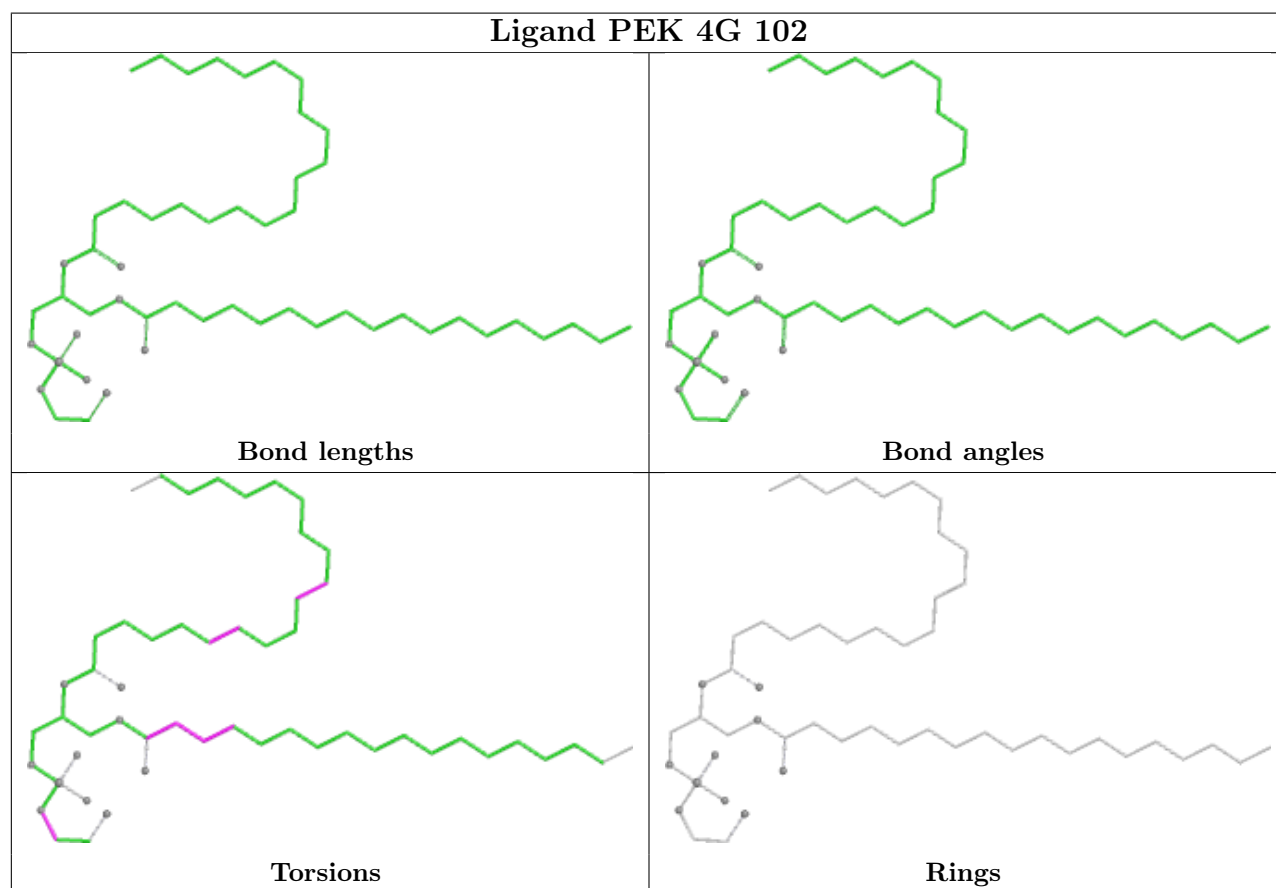
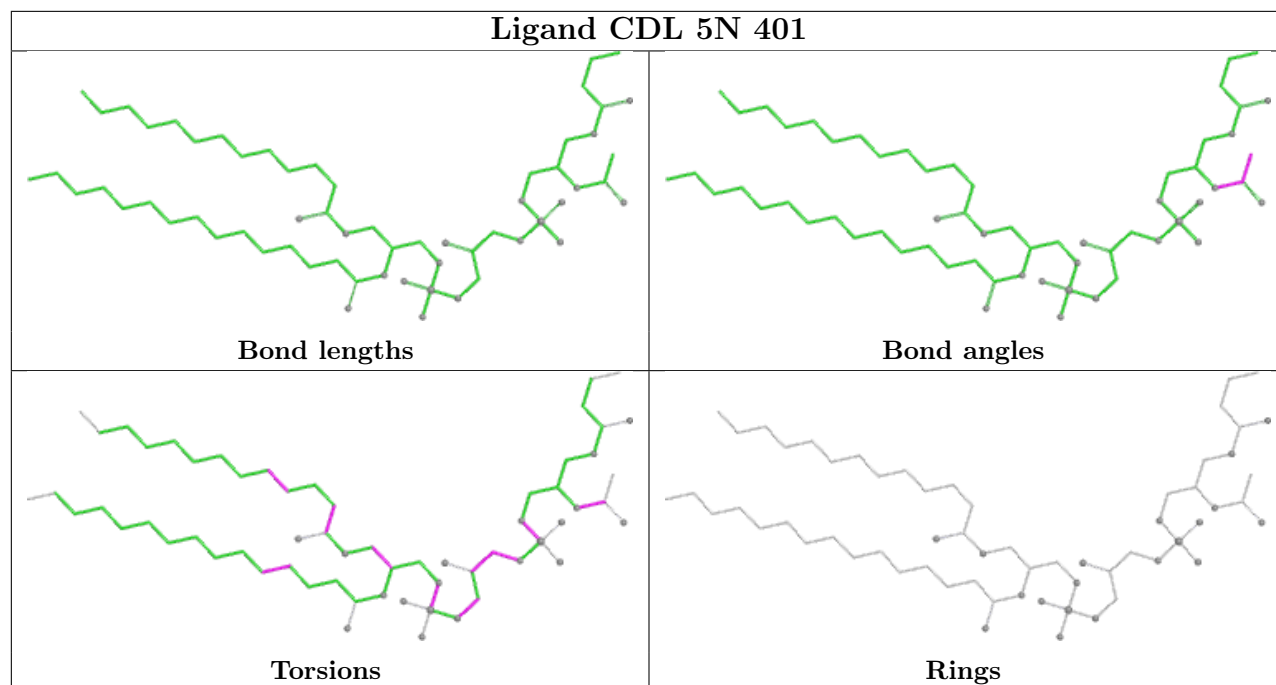


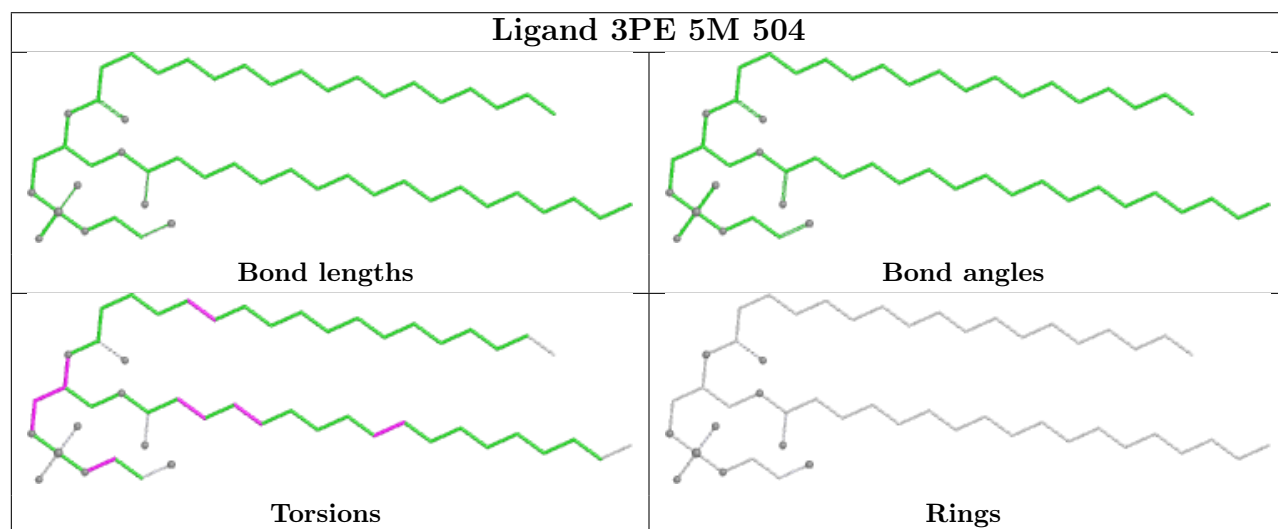
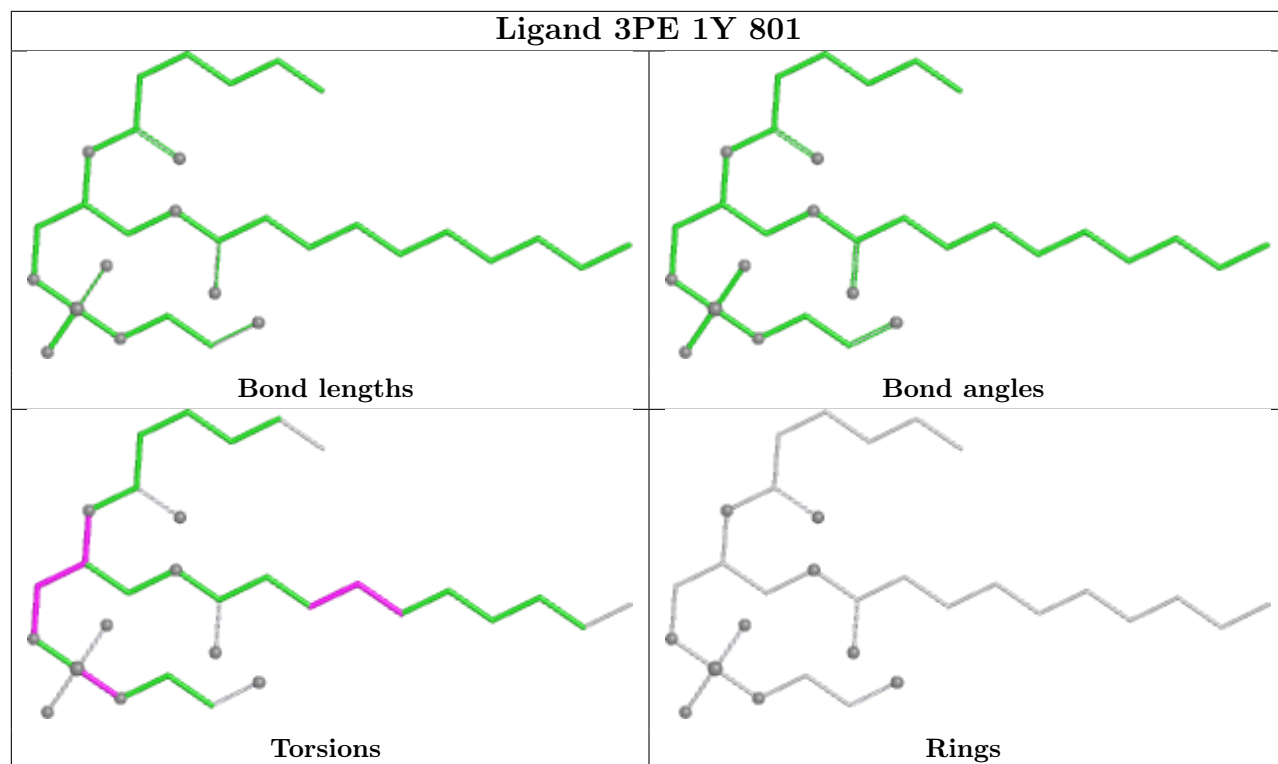


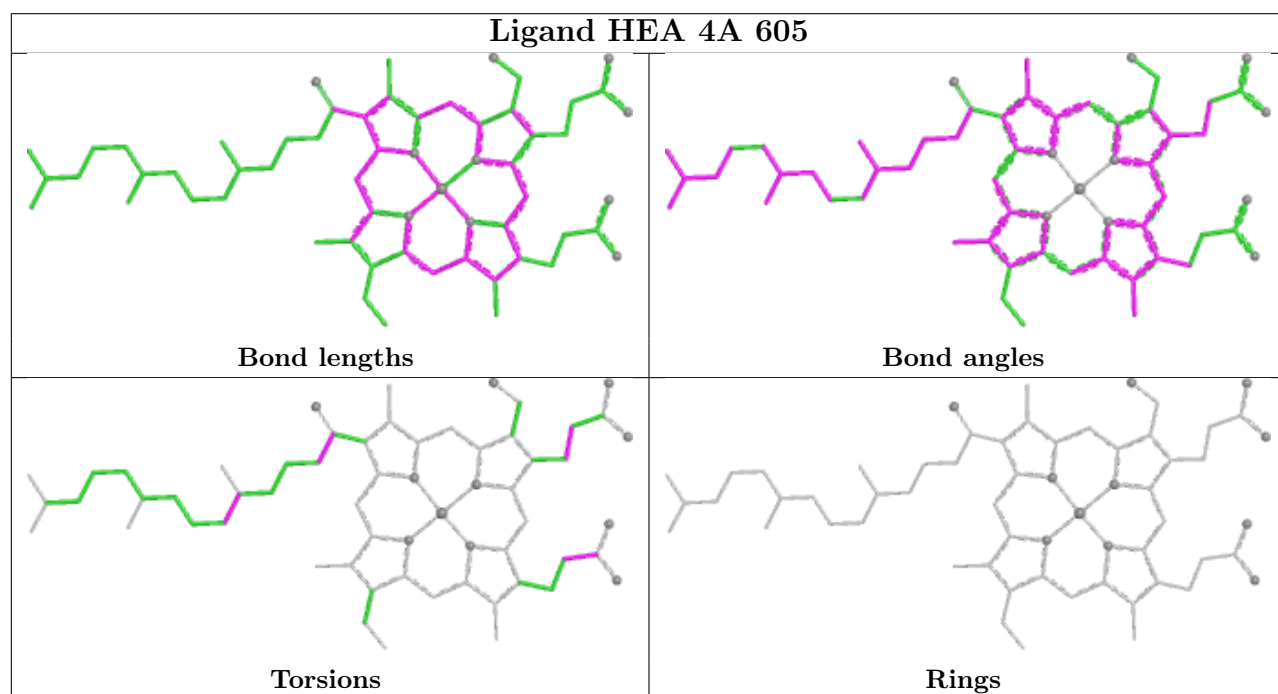
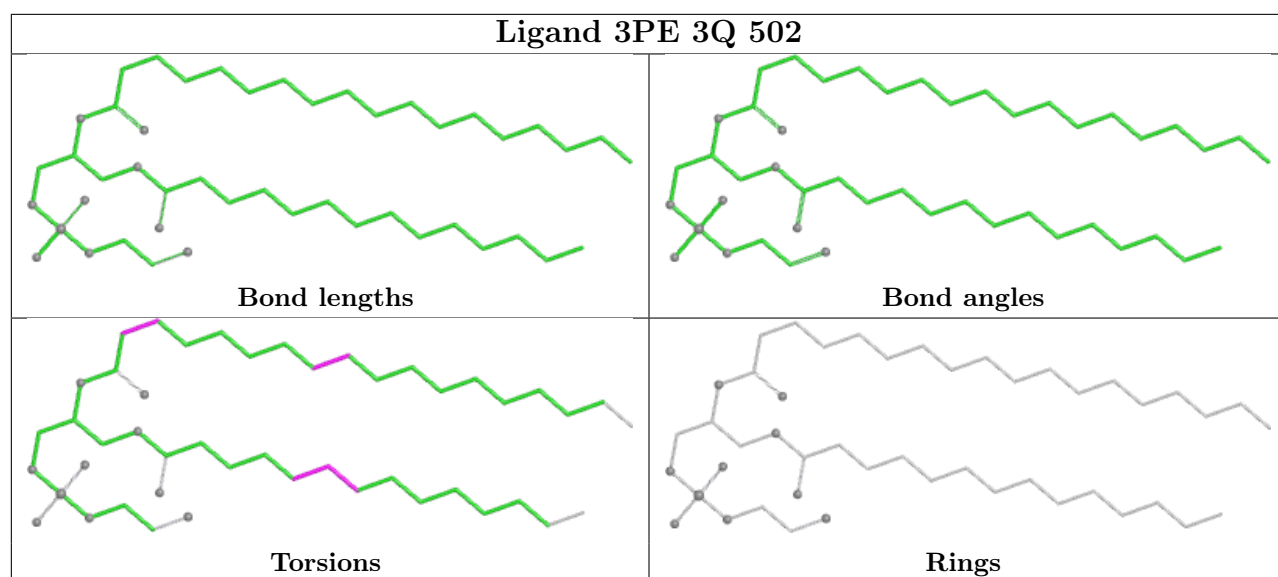


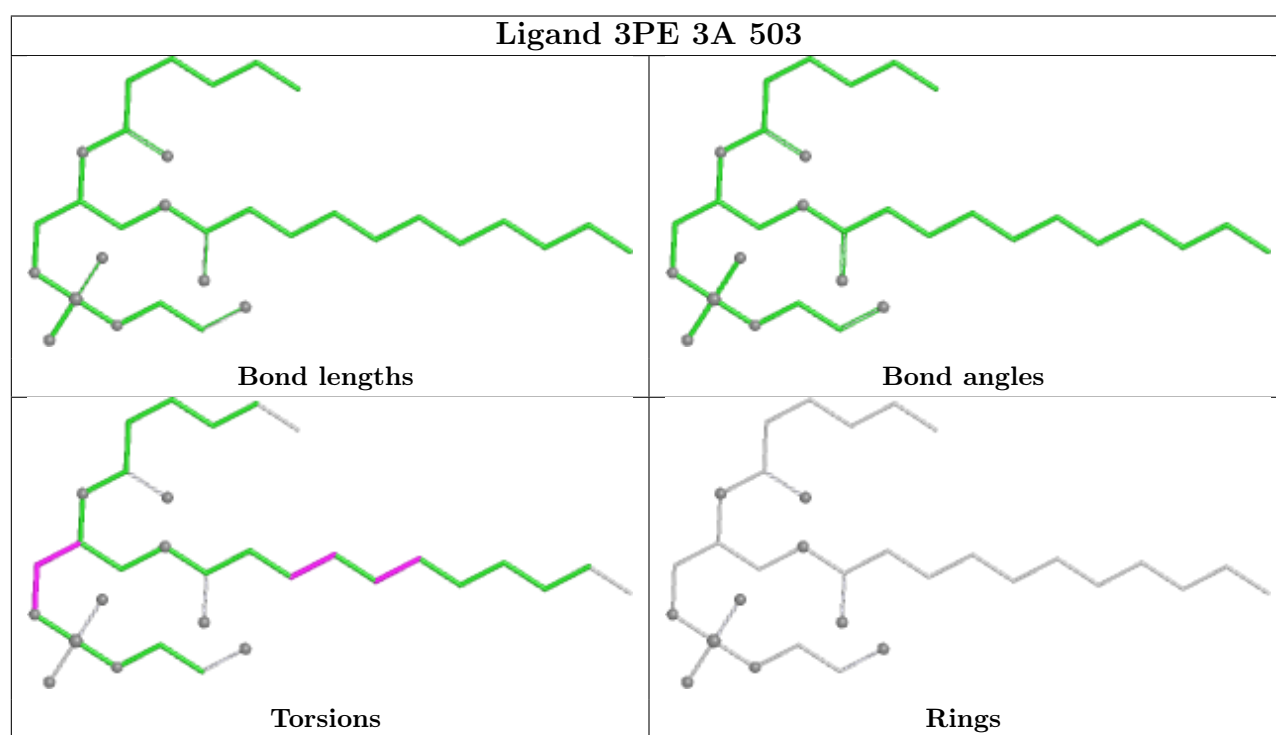
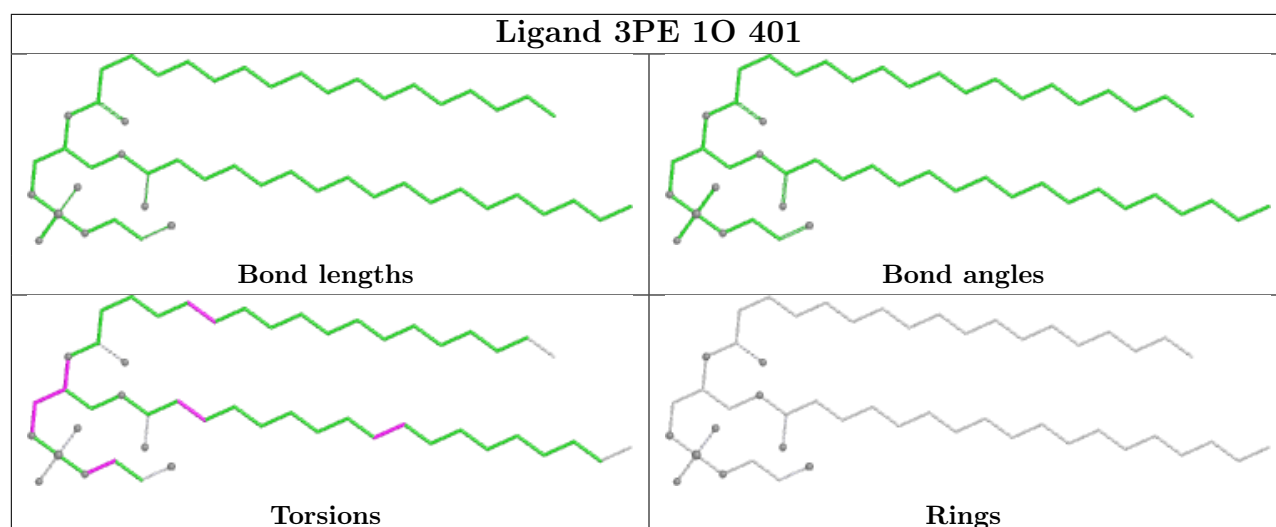


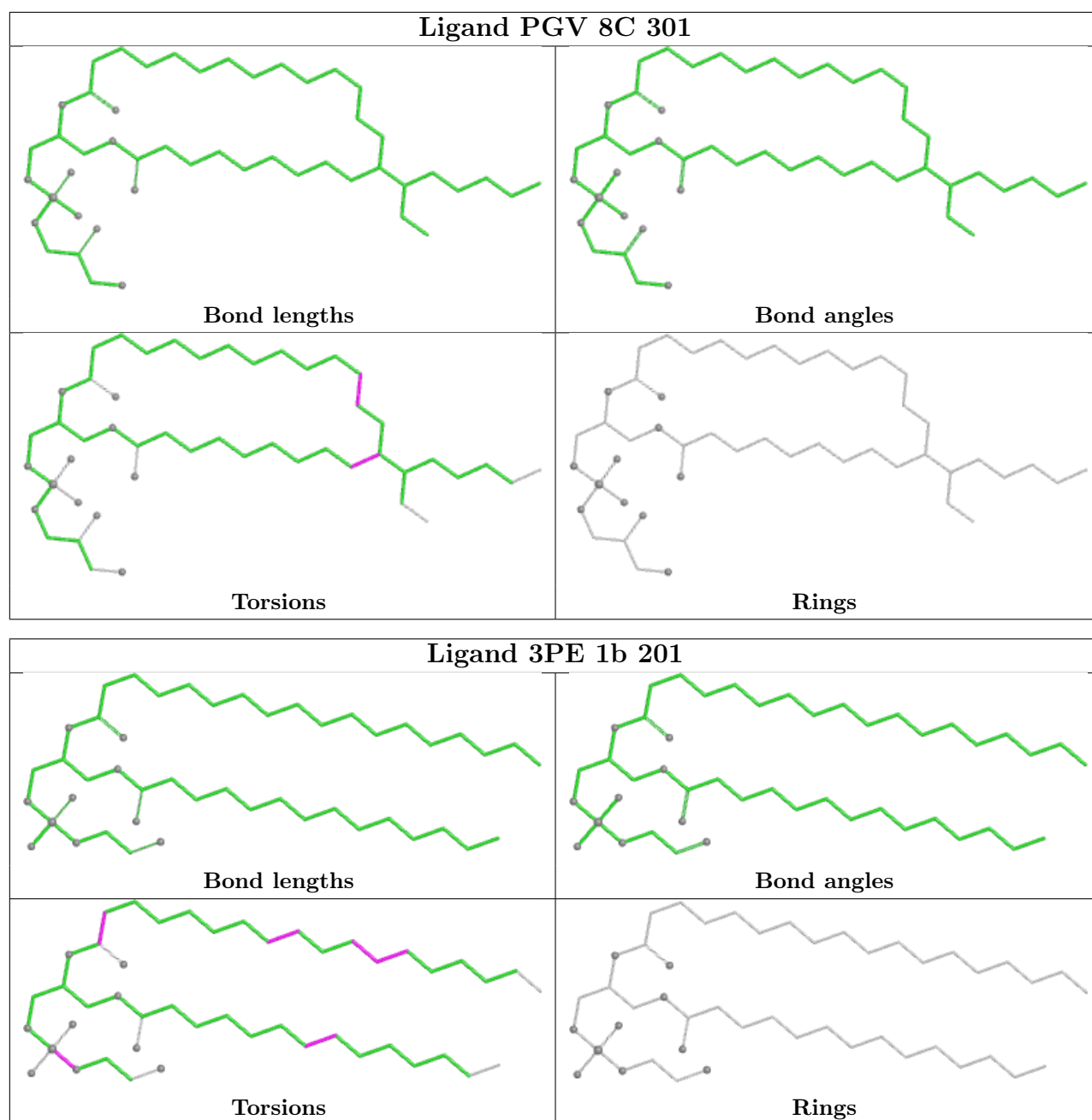


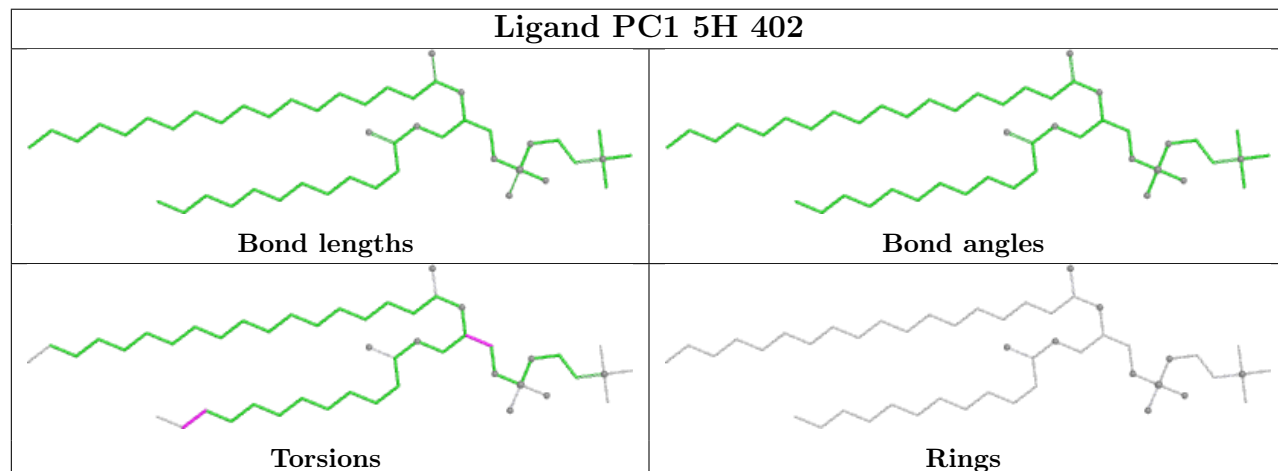
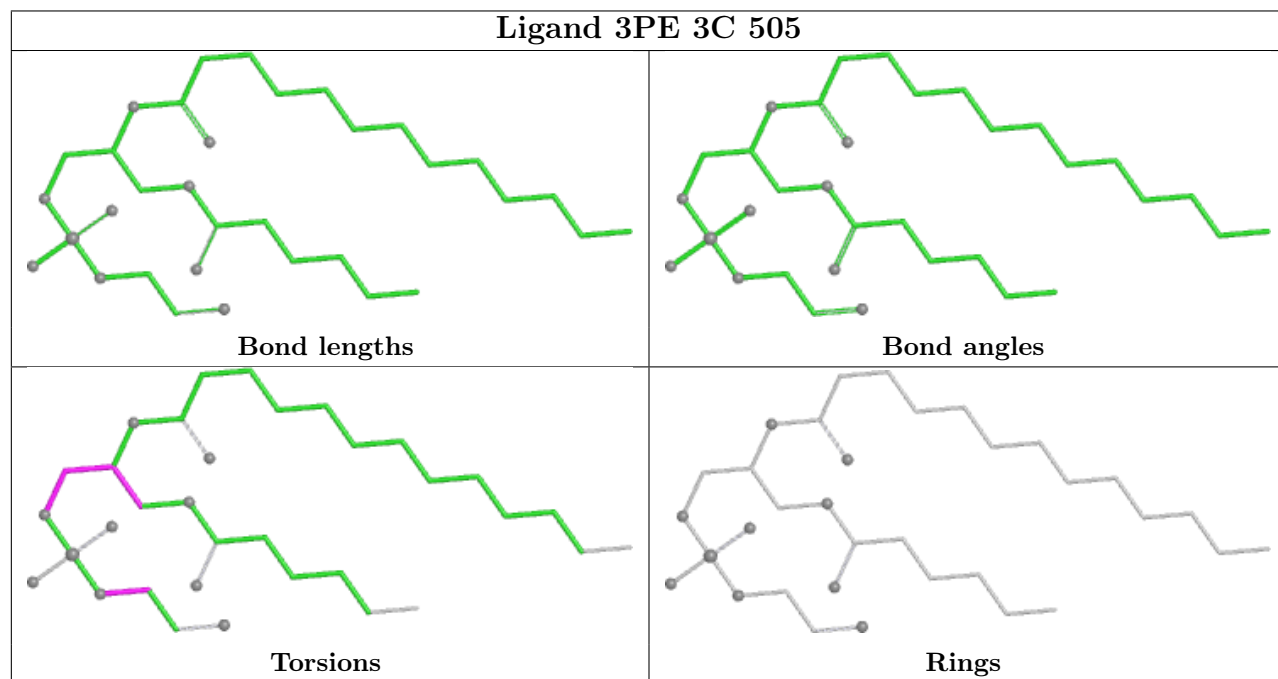
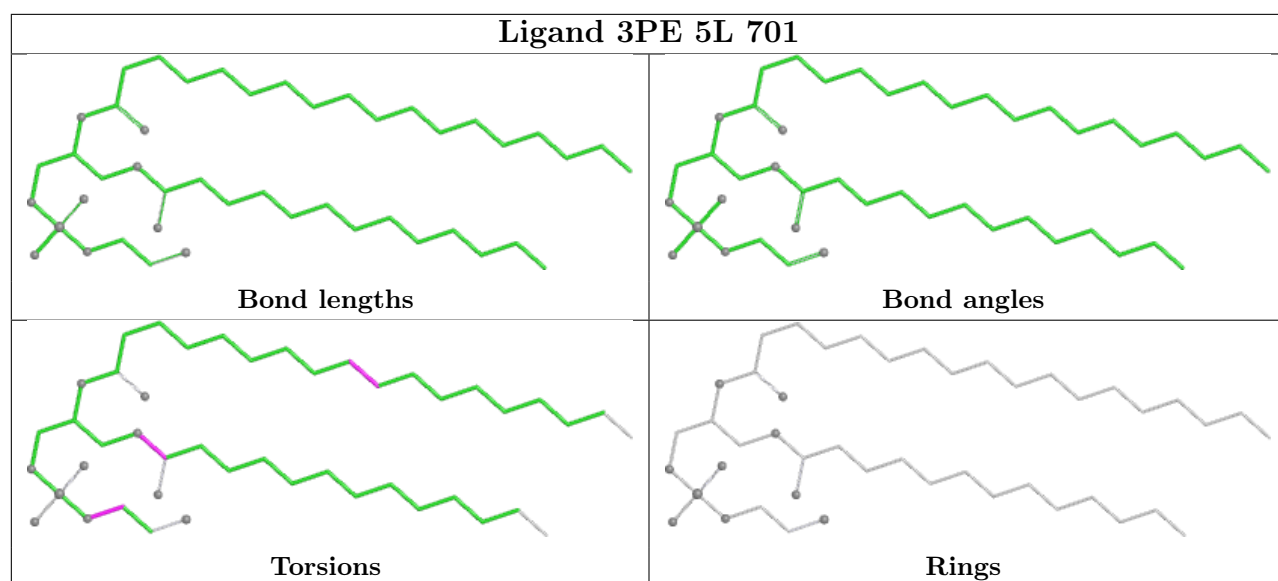


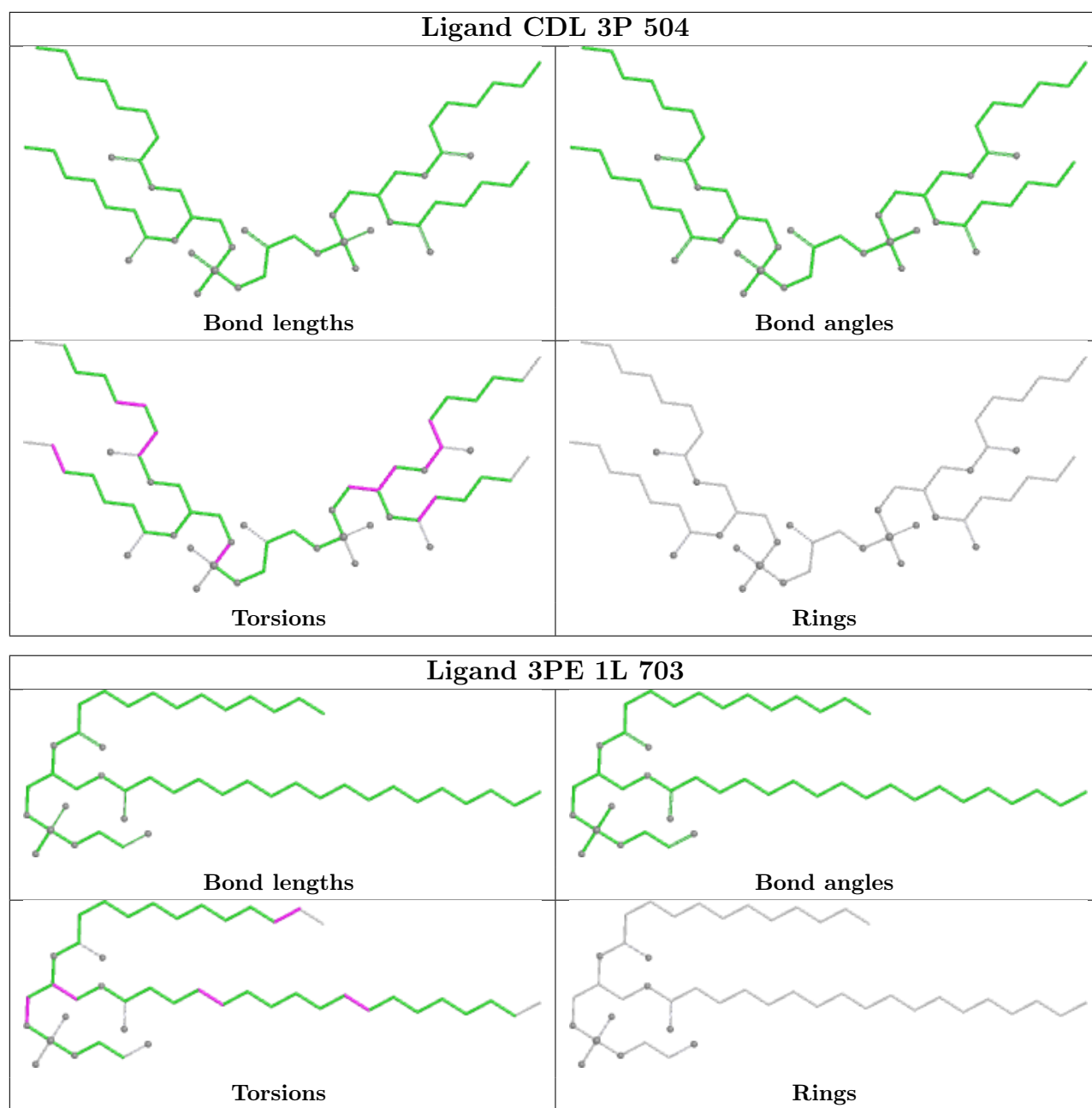


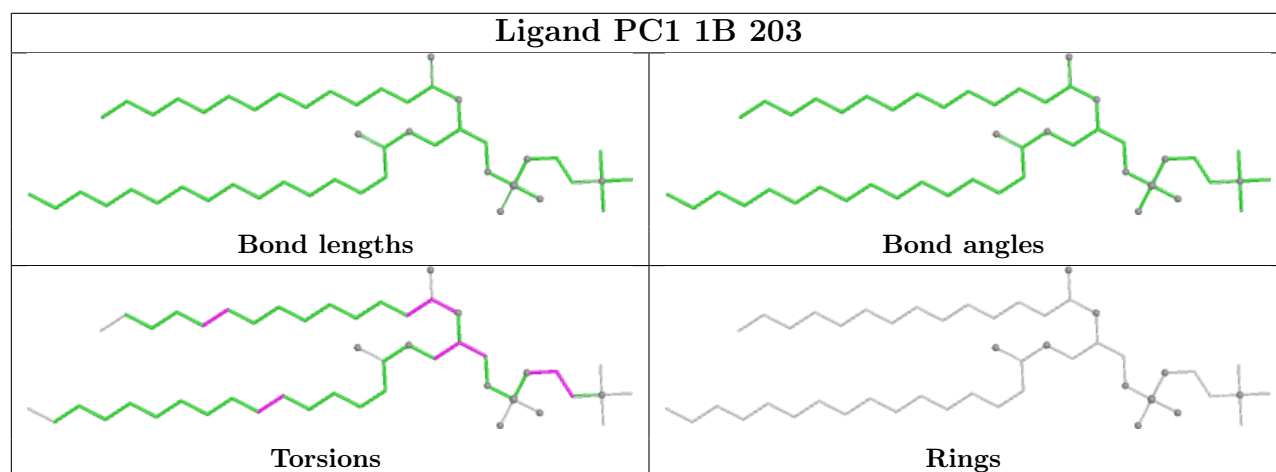
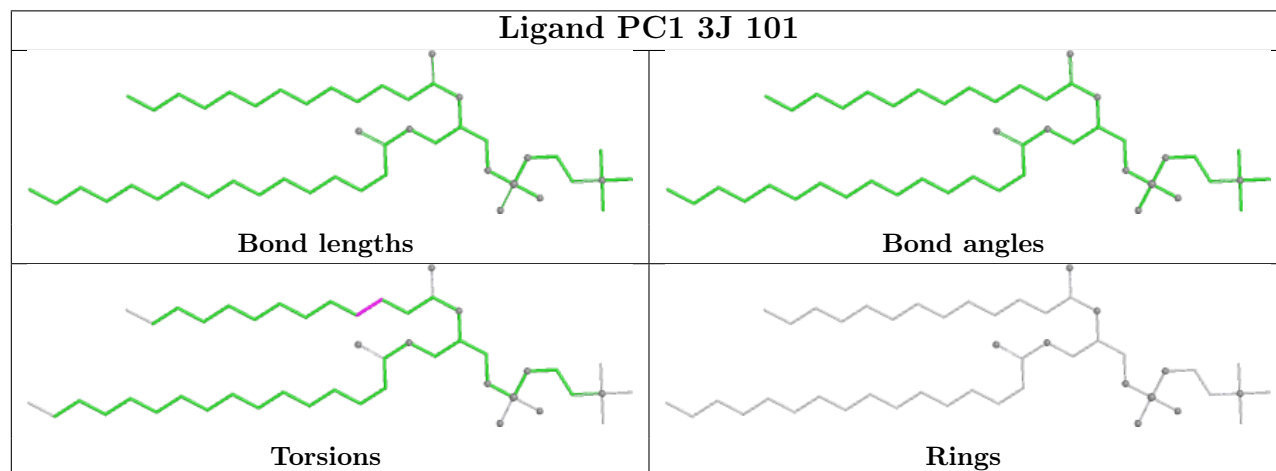
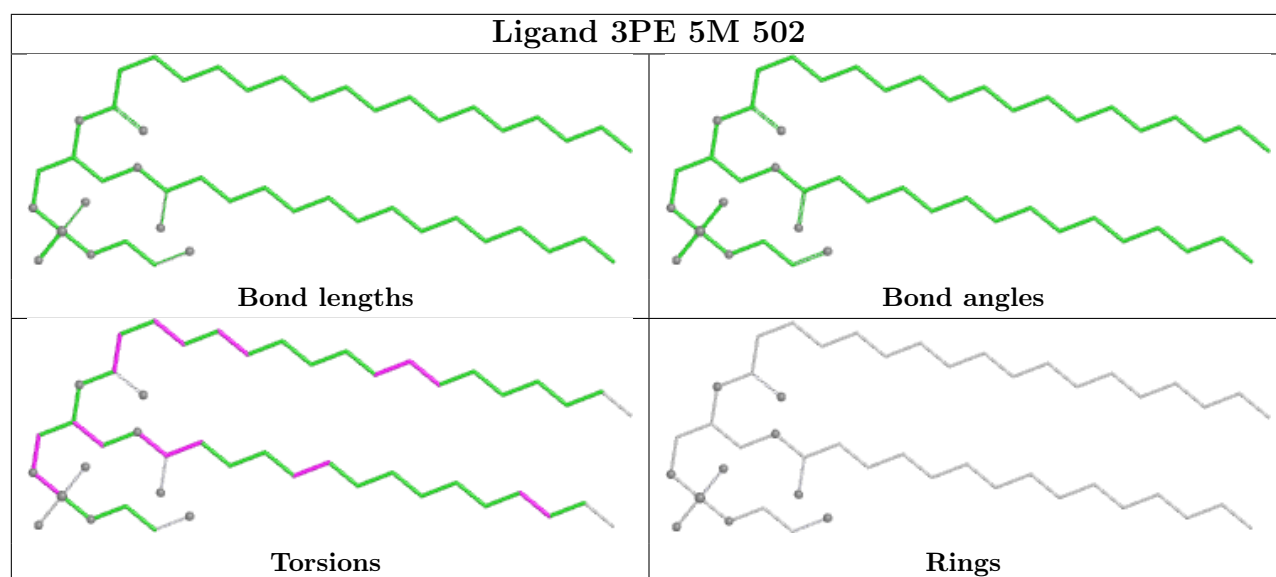


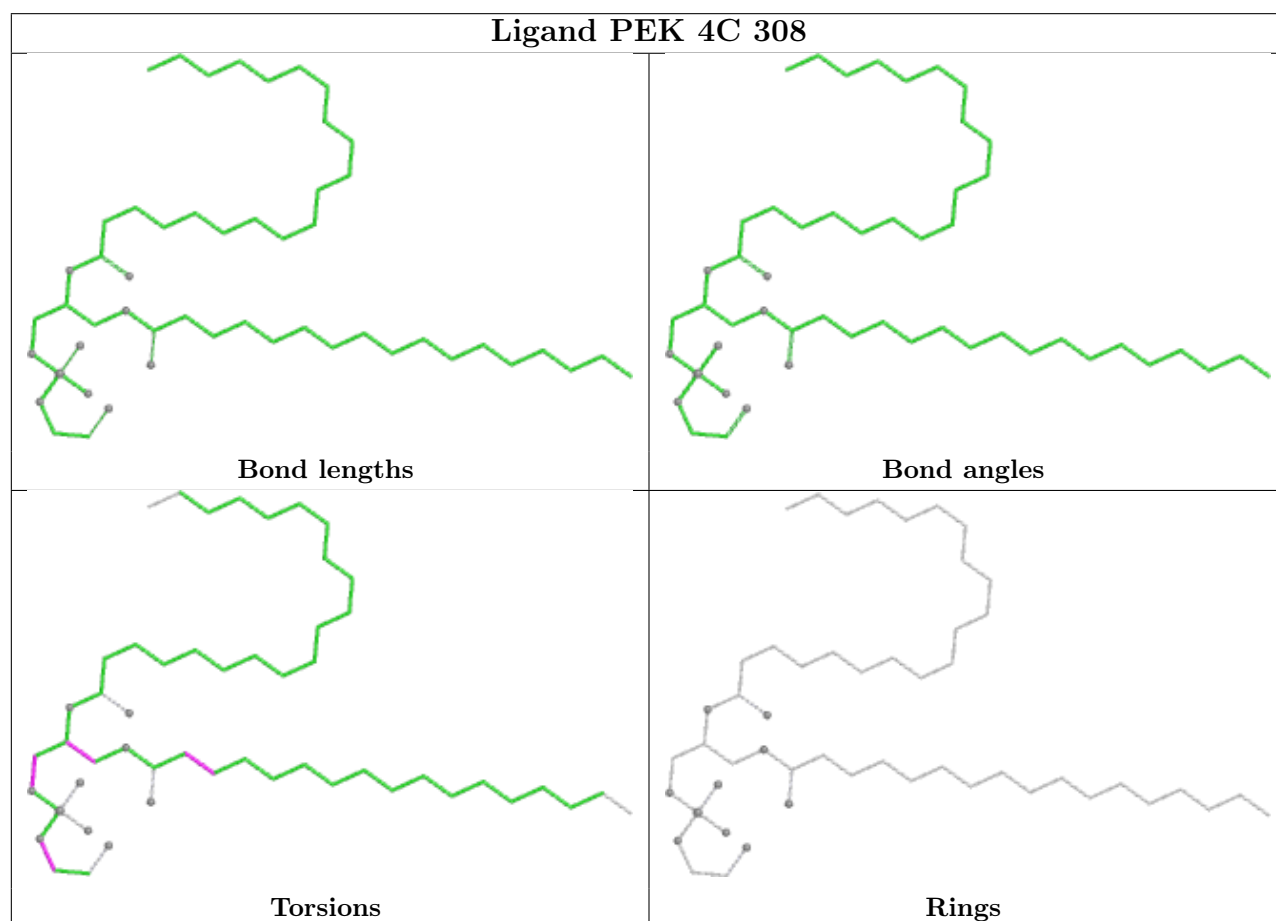
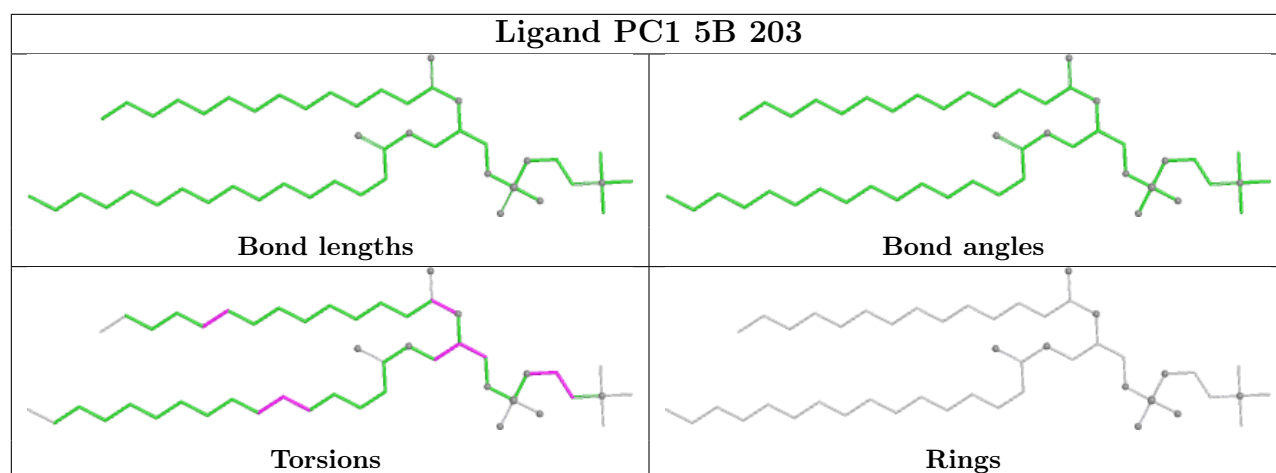




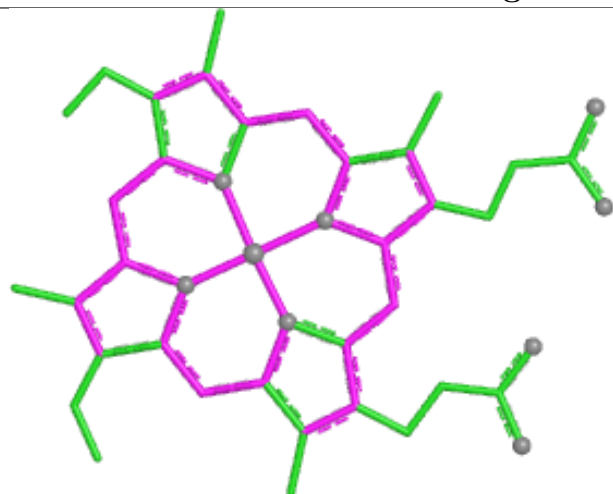




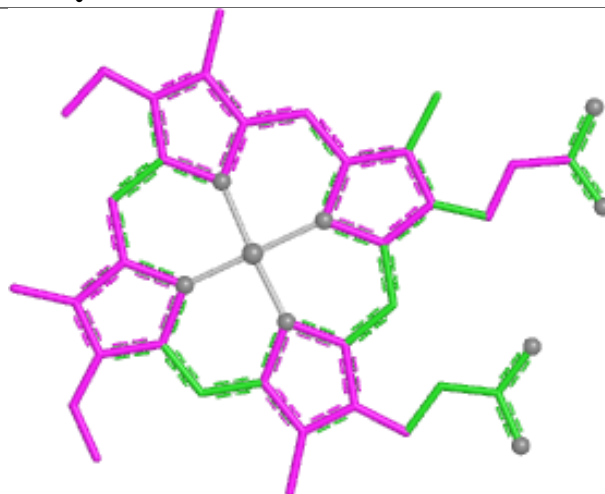




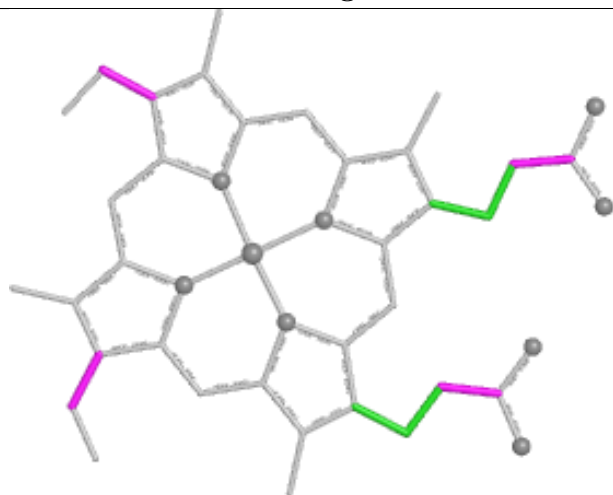
Ligand HEC 3Q 501



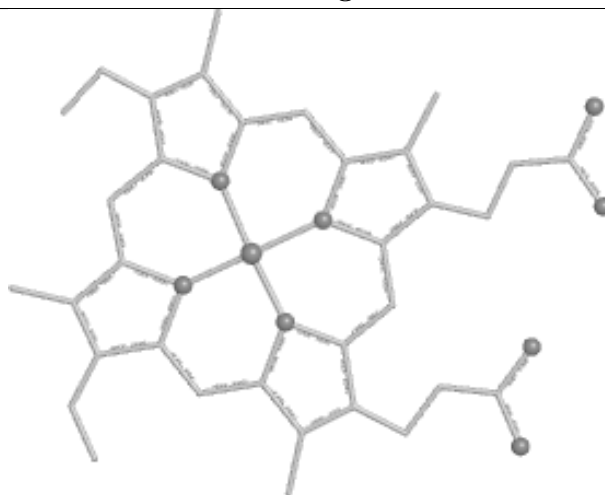
Bond lengths



Bond angles

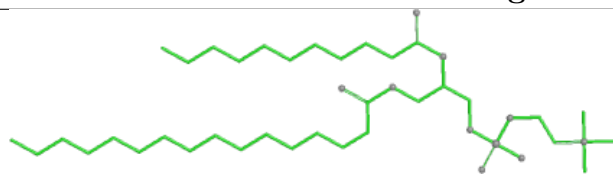


Torsions

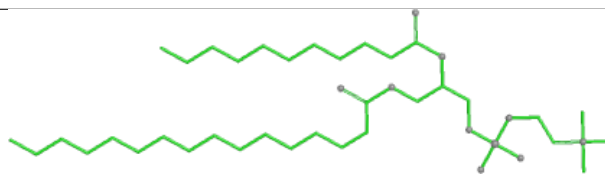


Rings

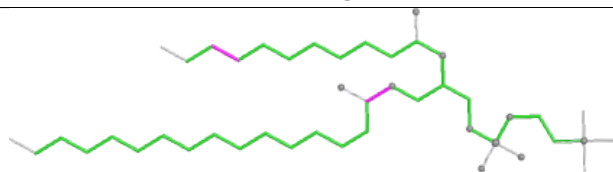
Ligand PC1 3R 302



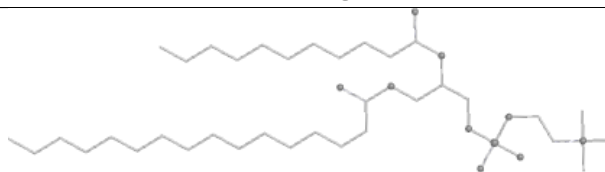
Bond lengths



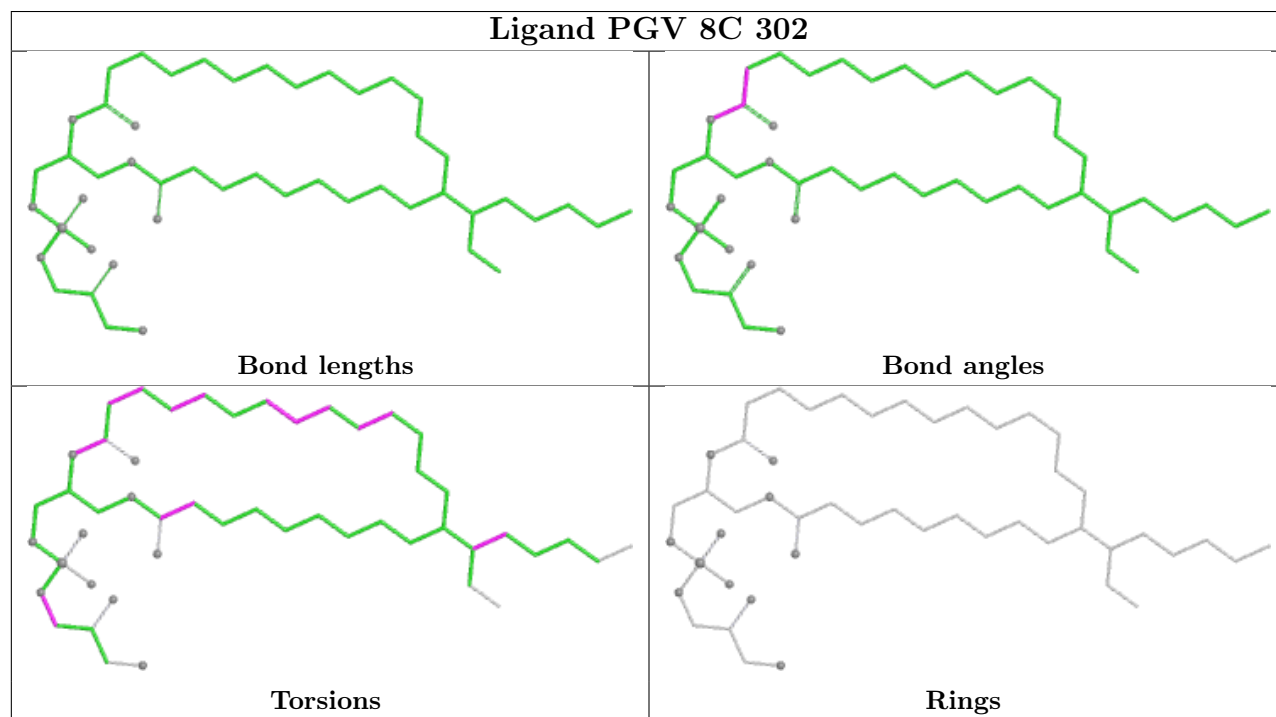
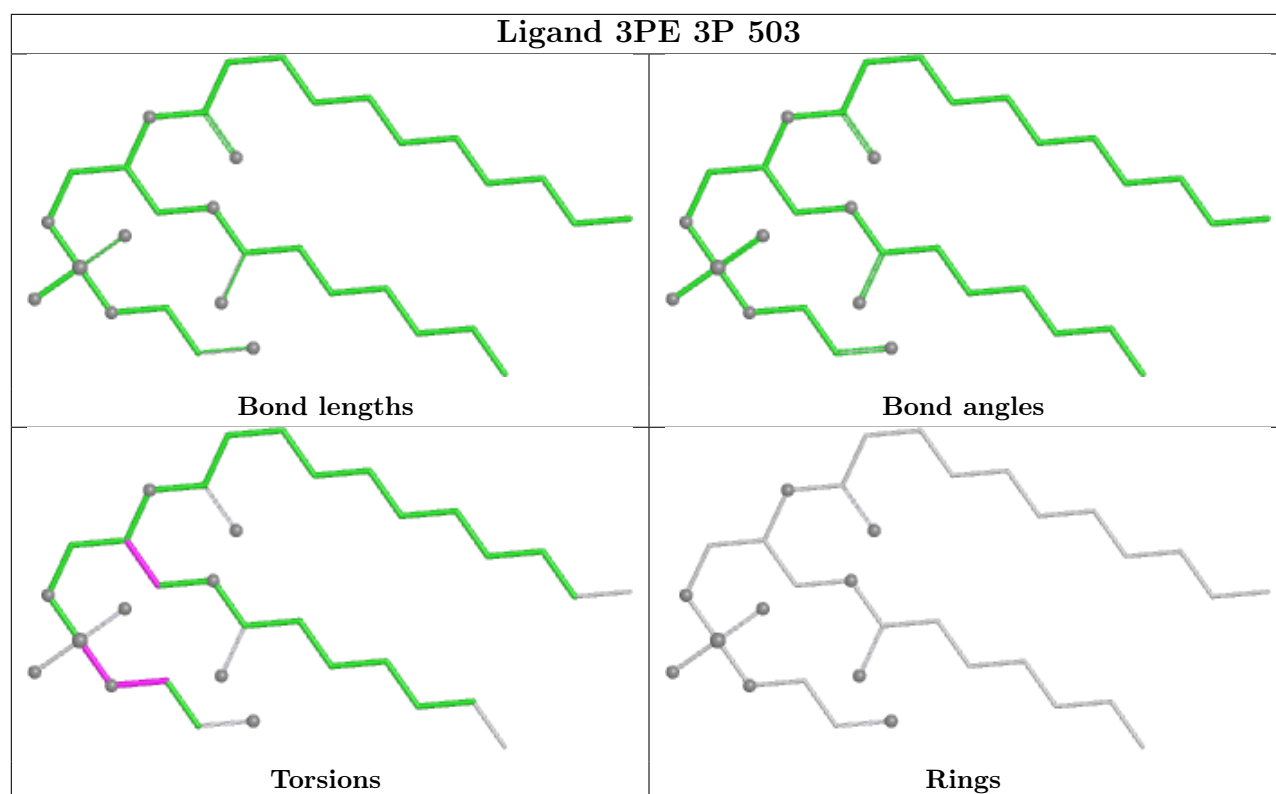
Bond angles

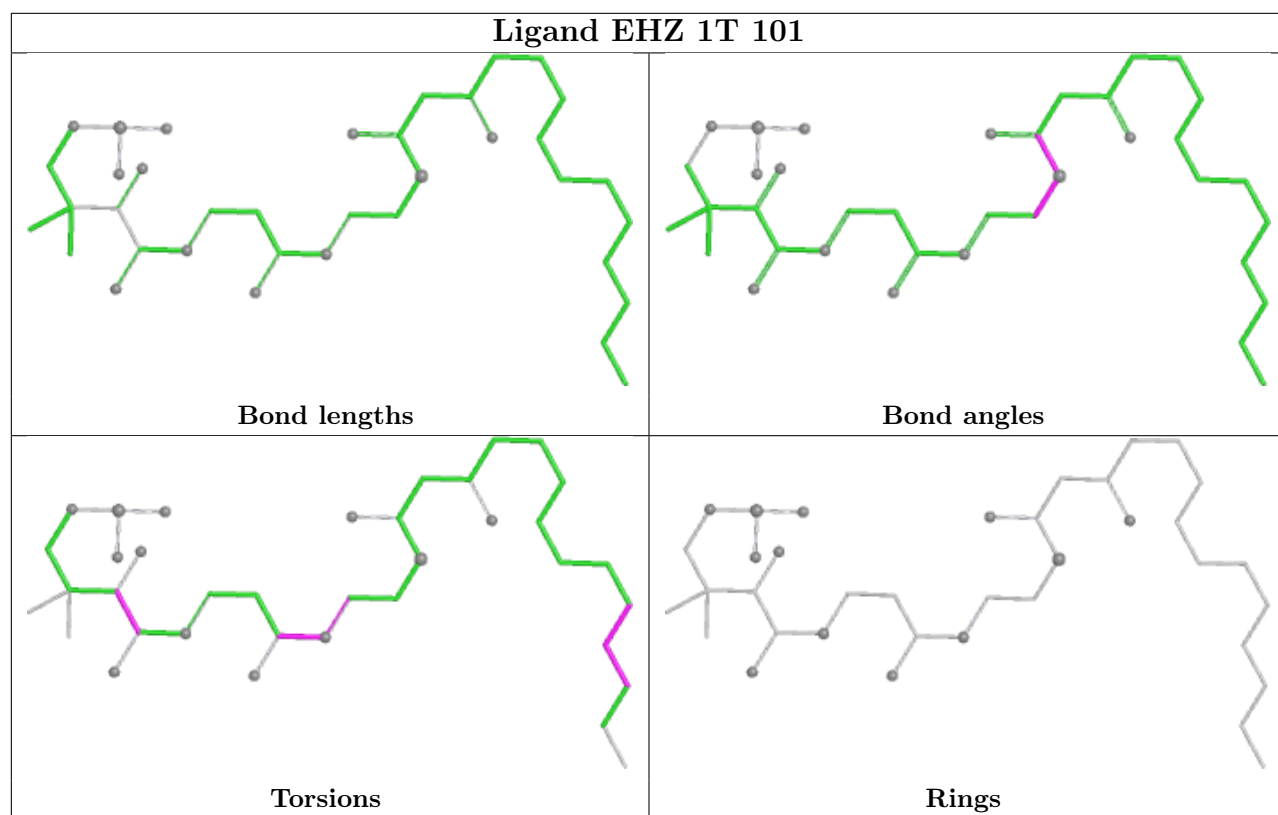
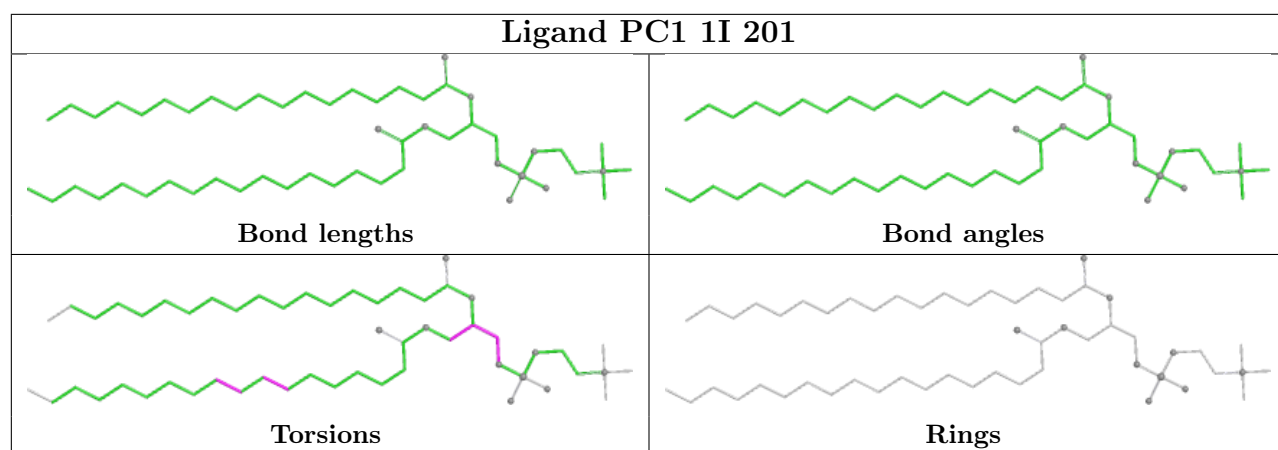


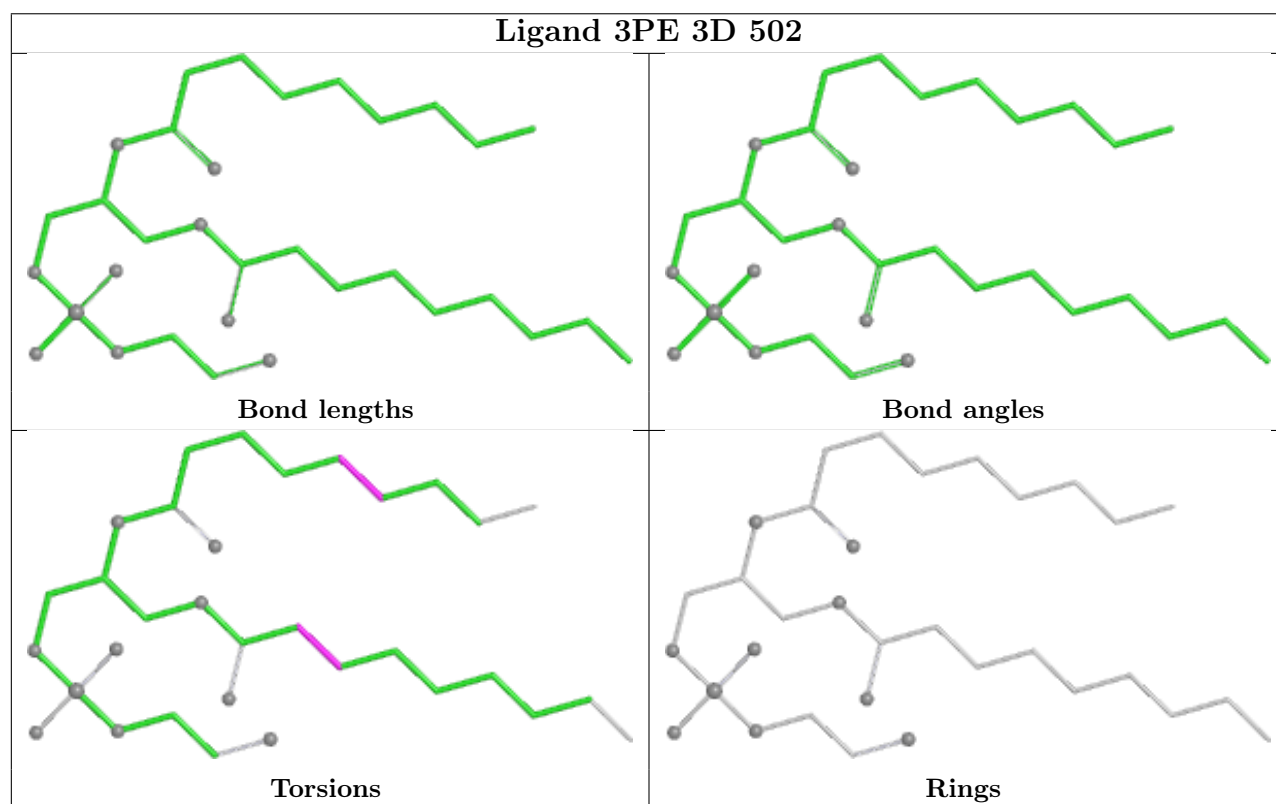
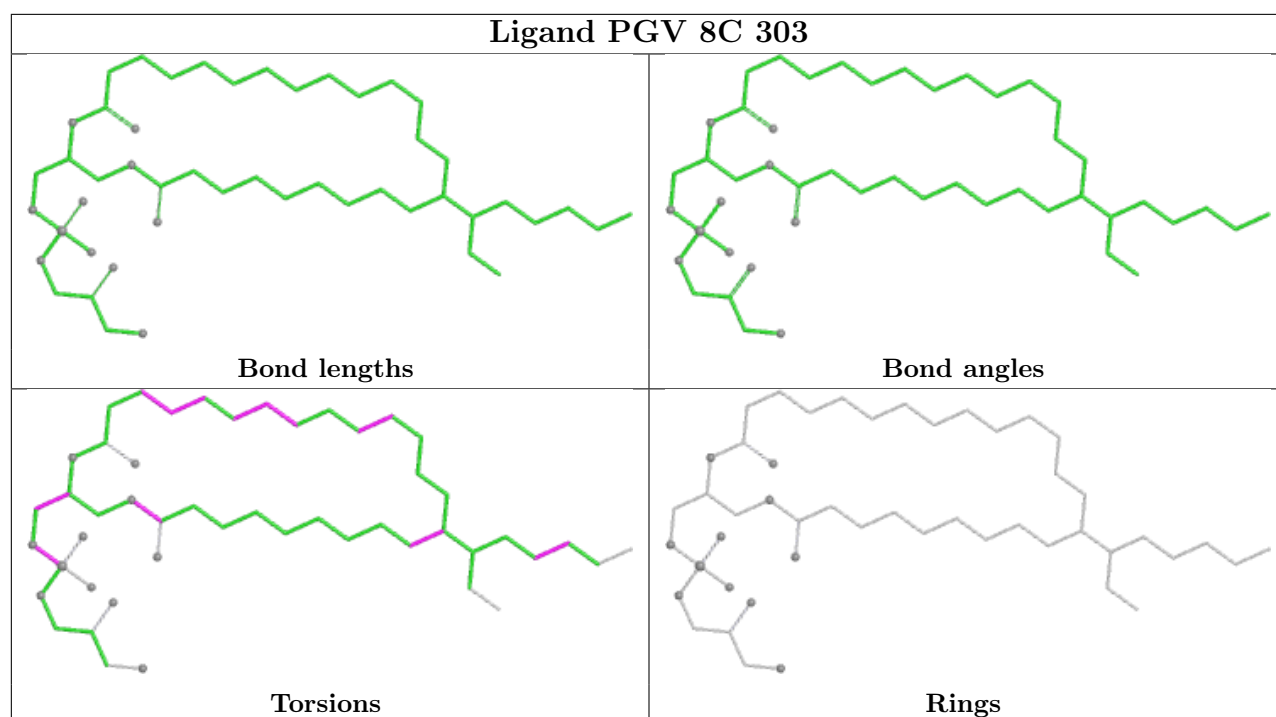
Torsions

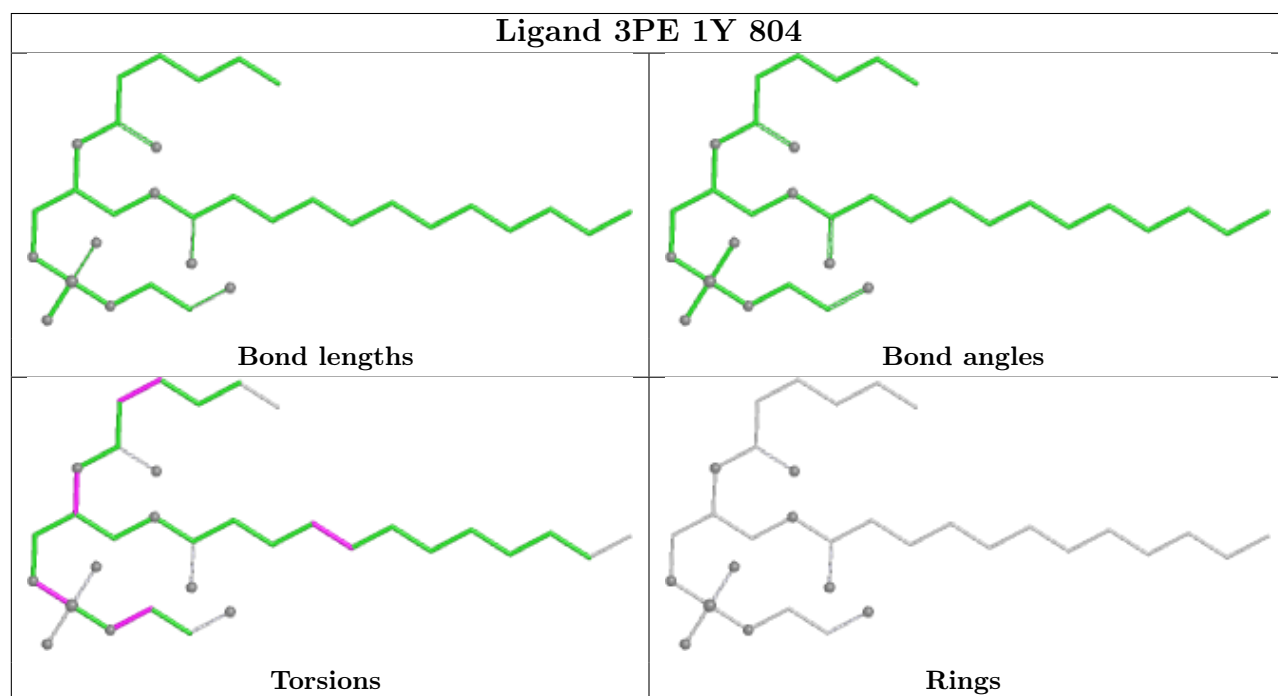
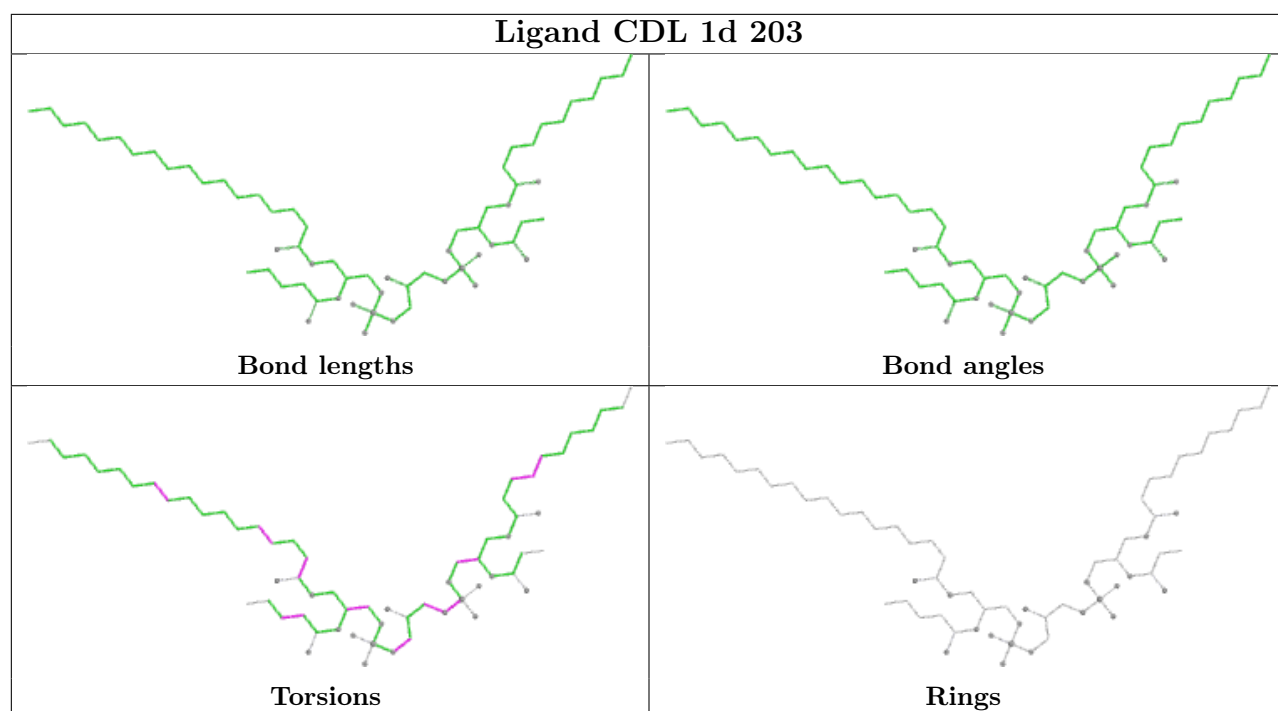


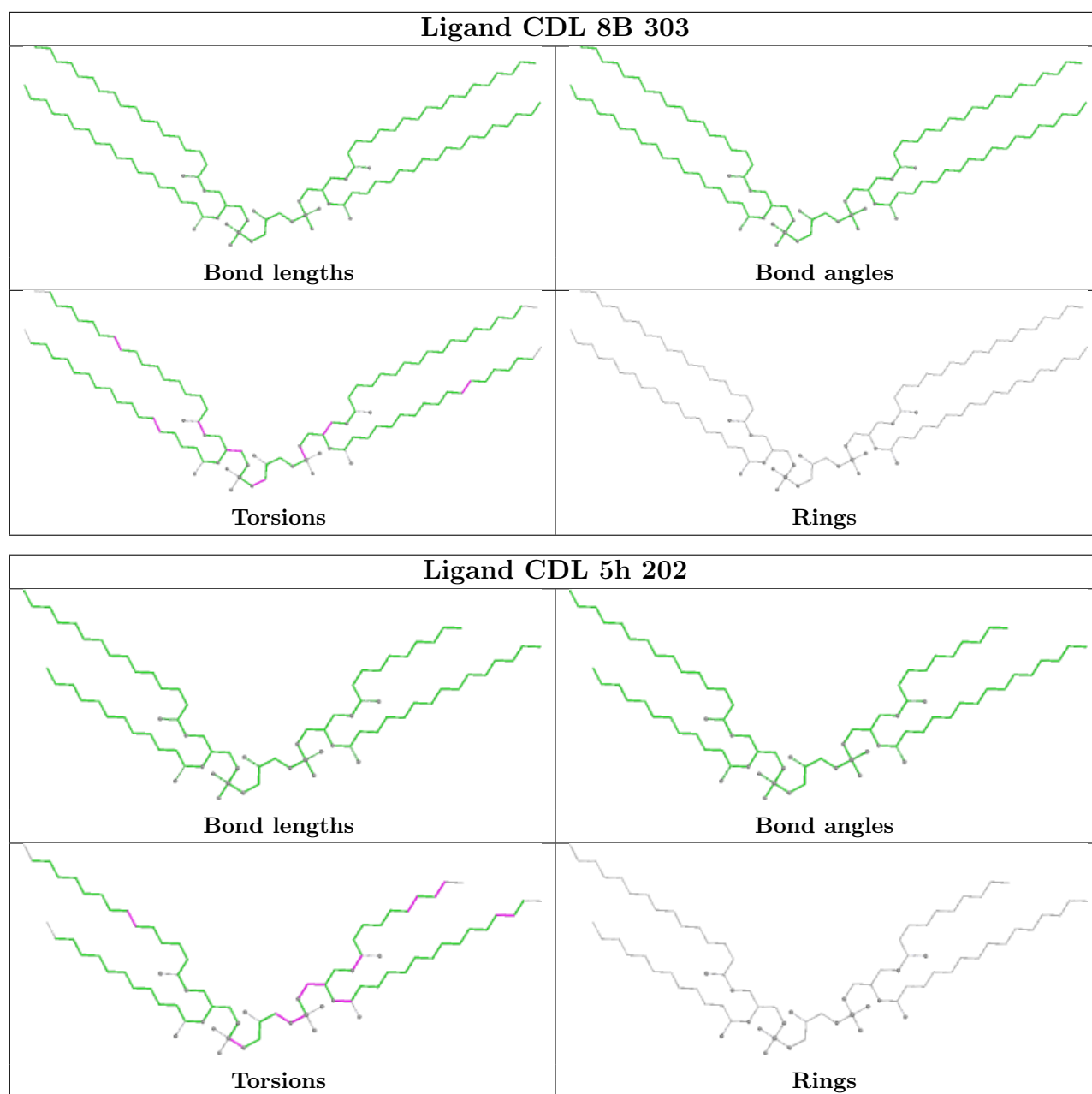
Rings

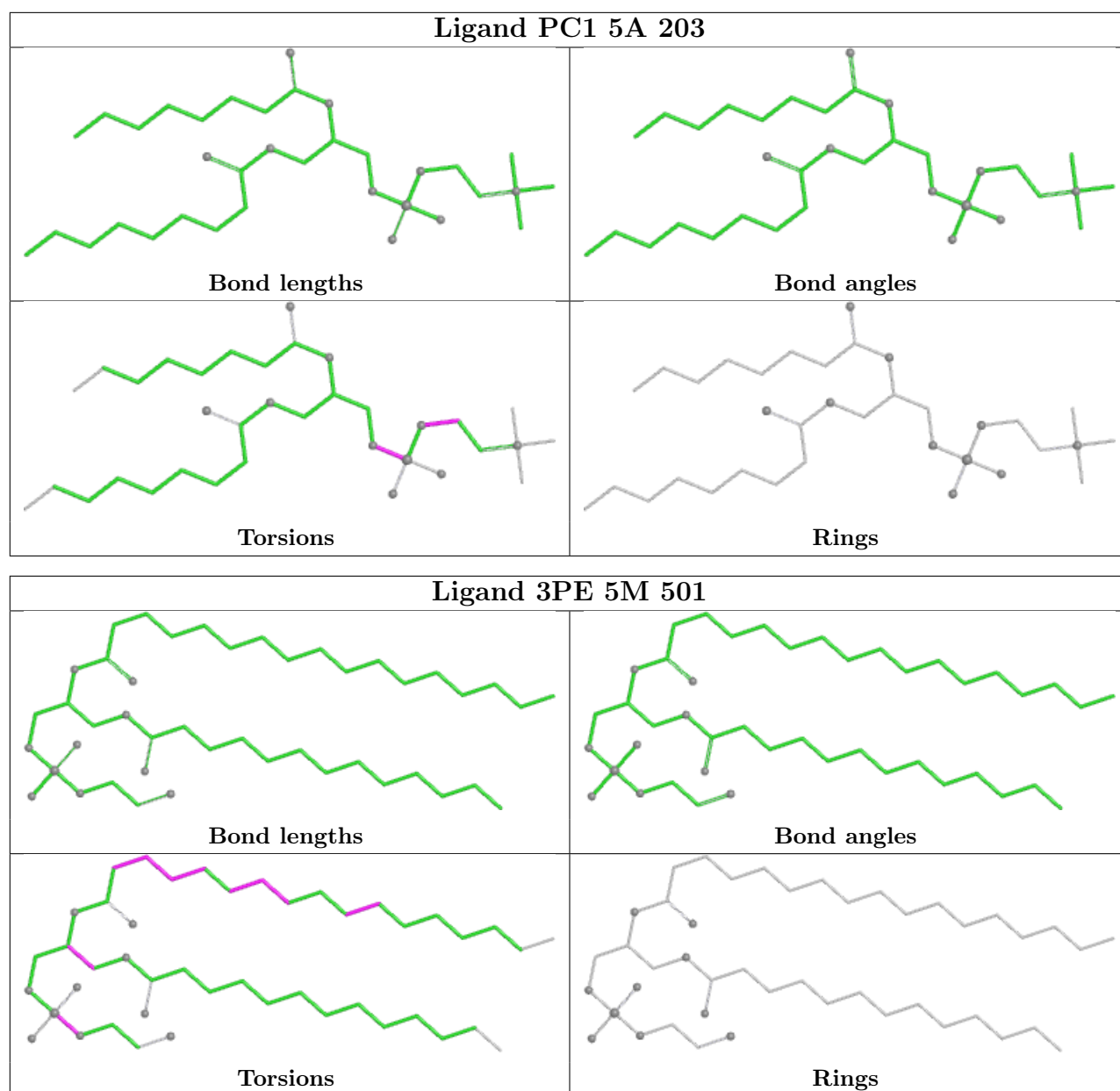


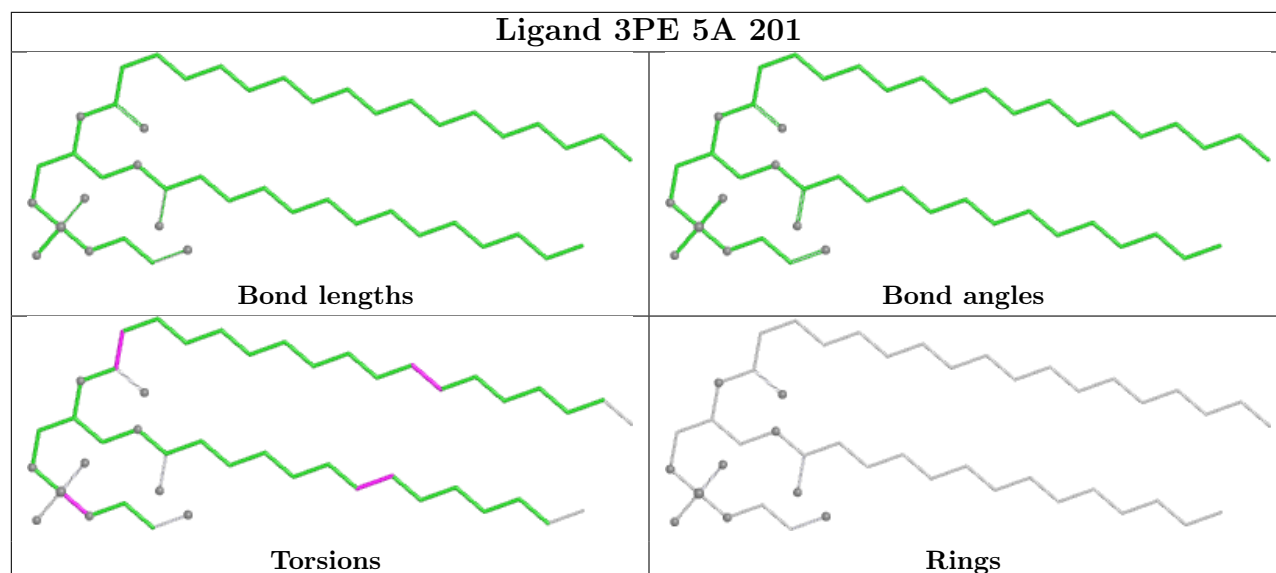
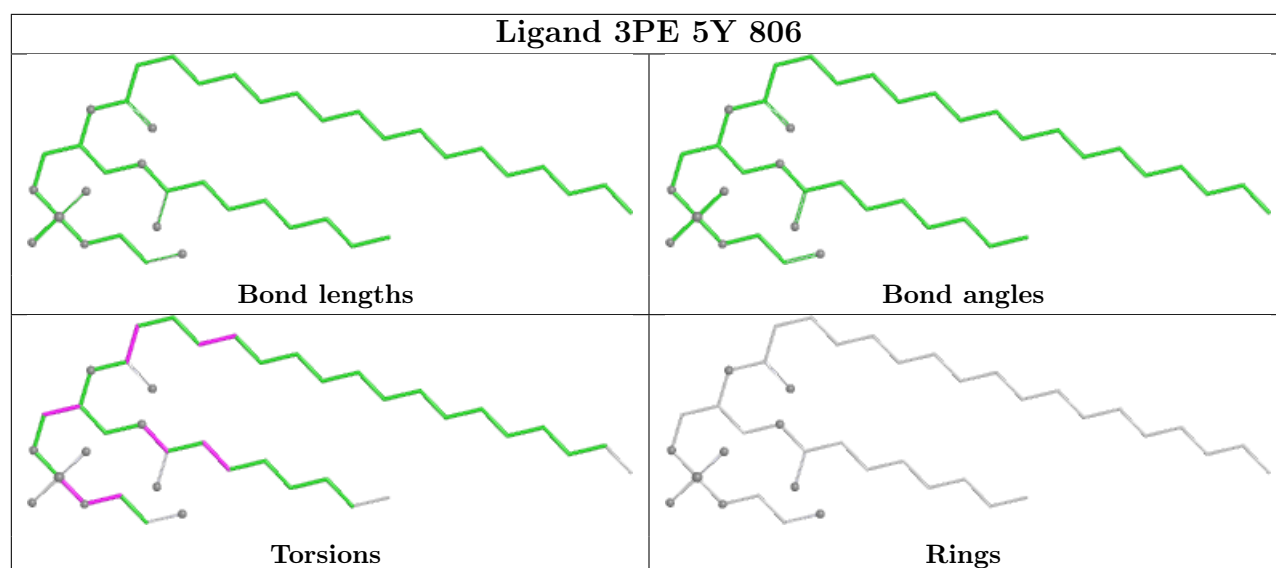


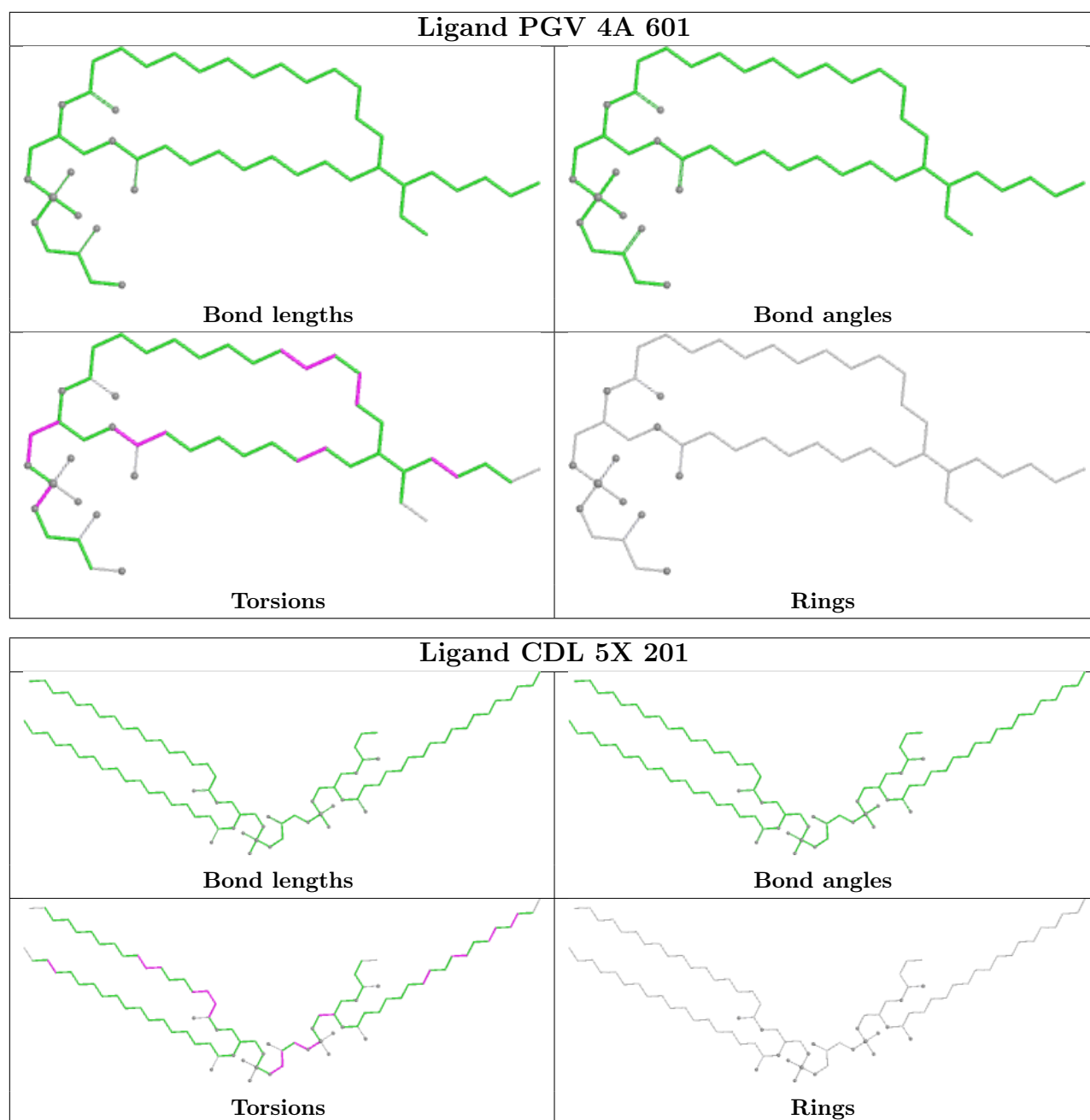


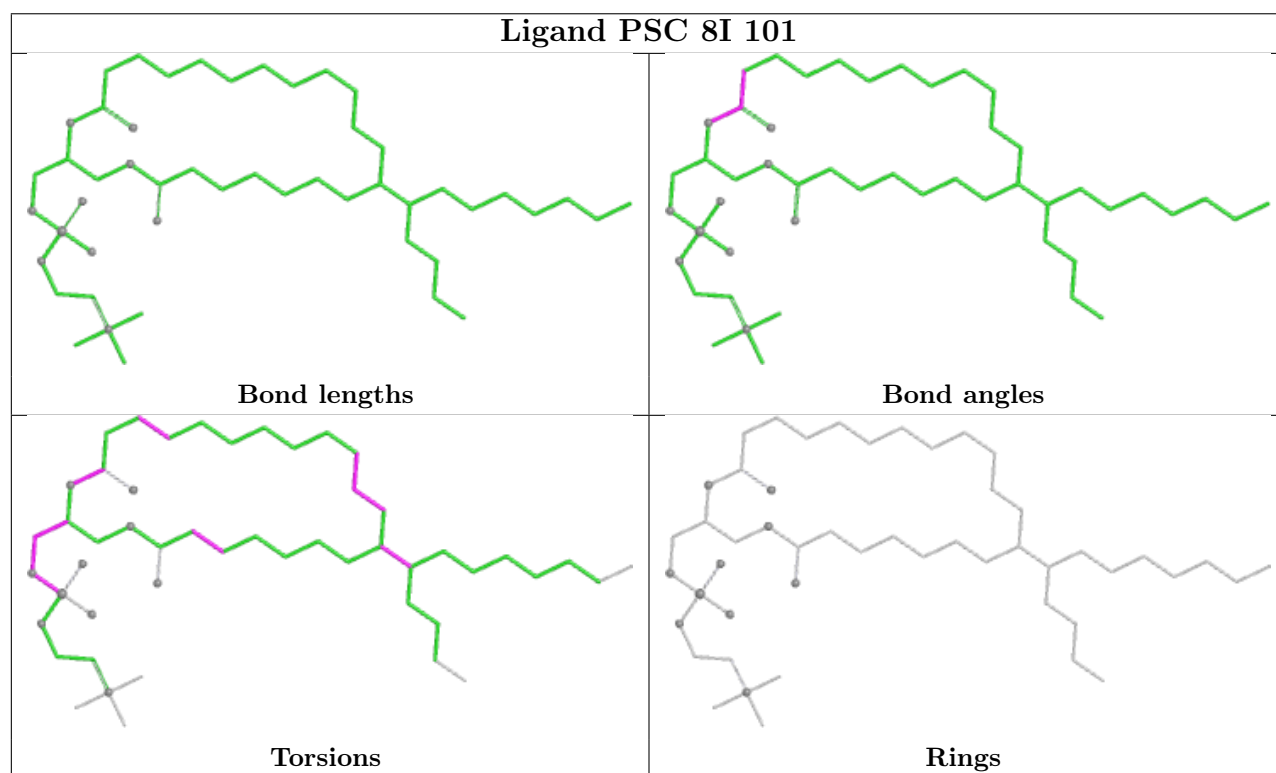
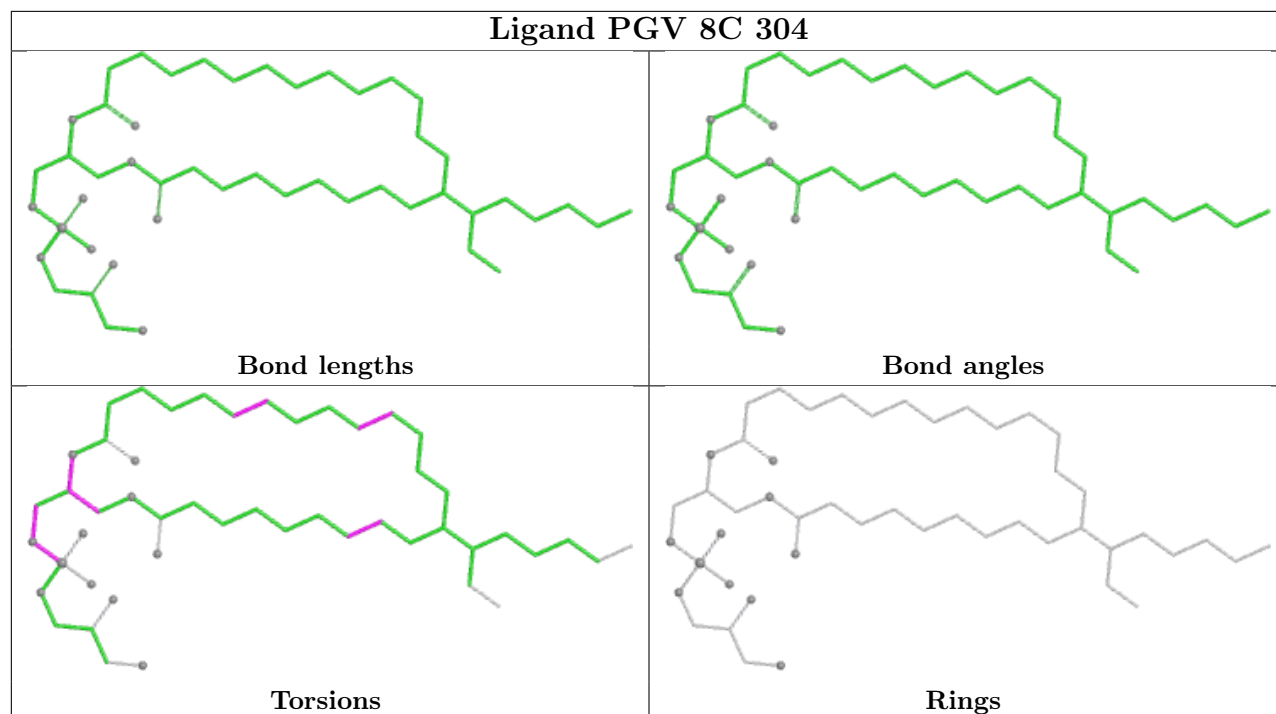


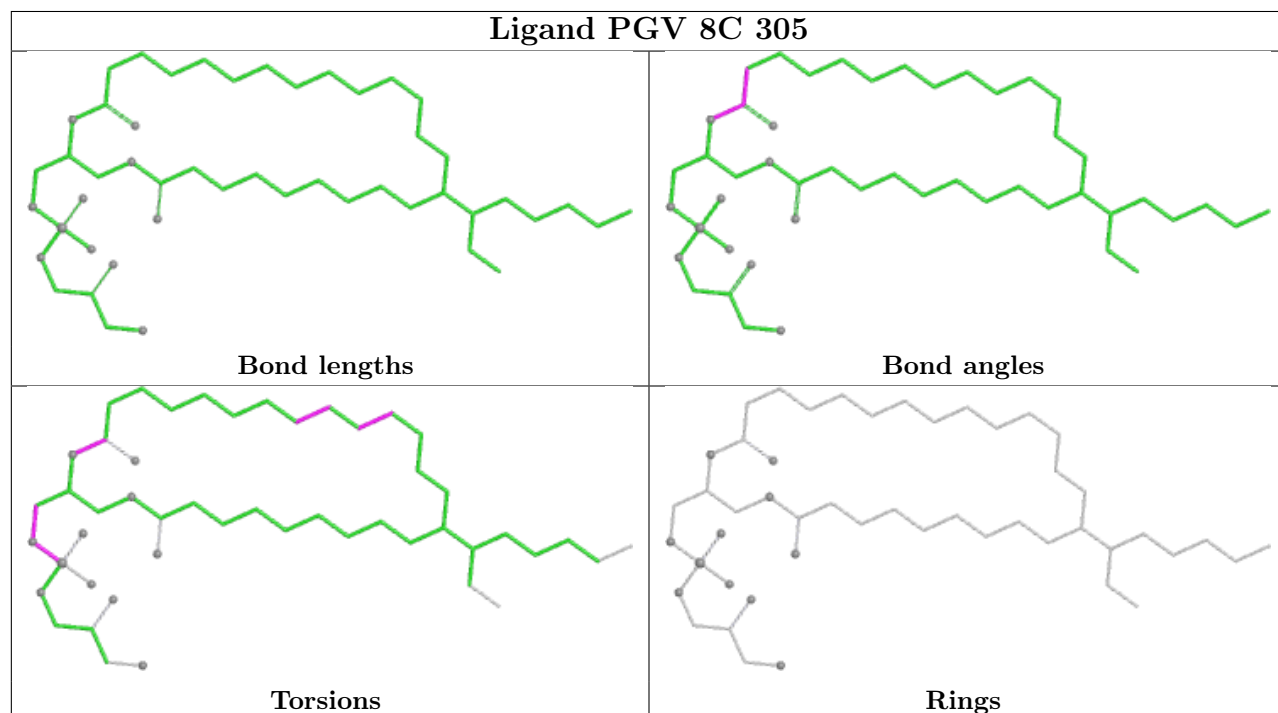
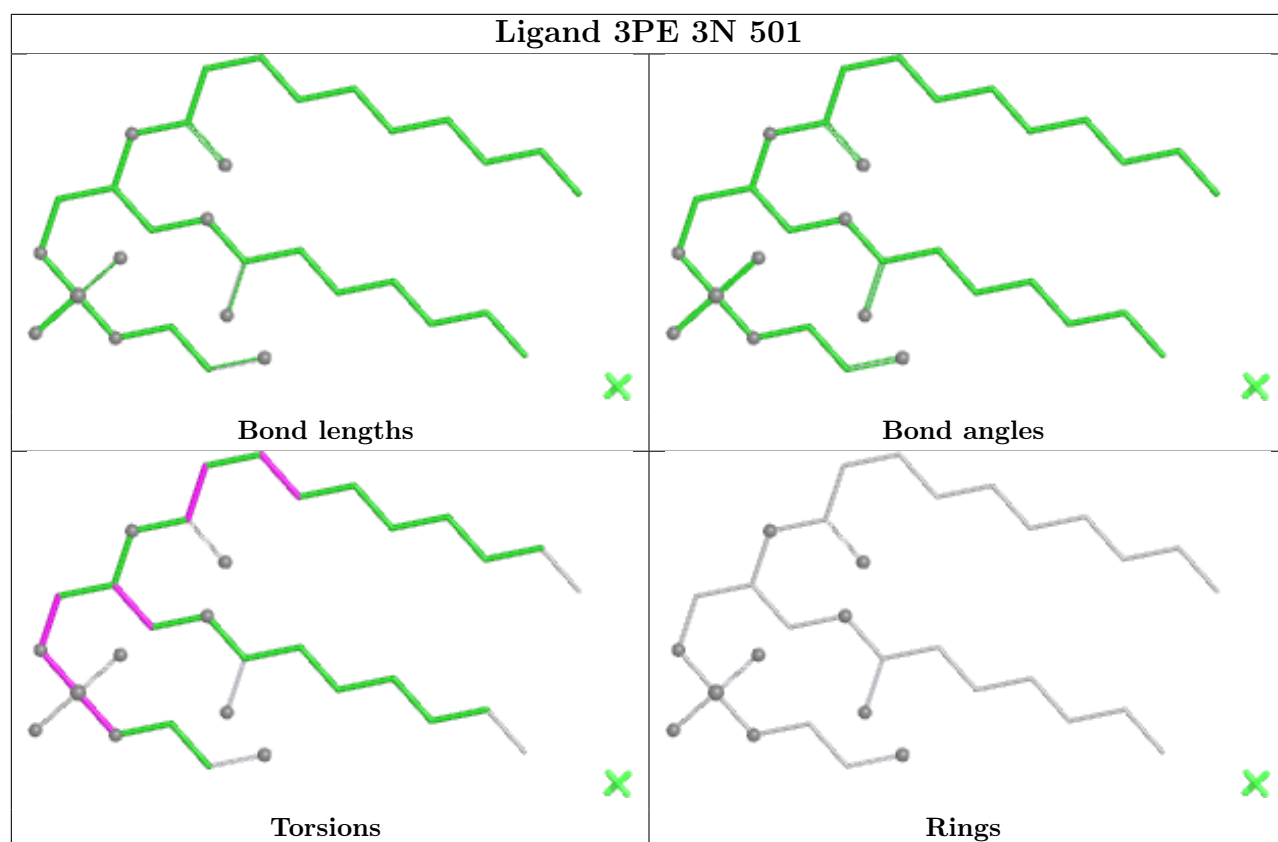


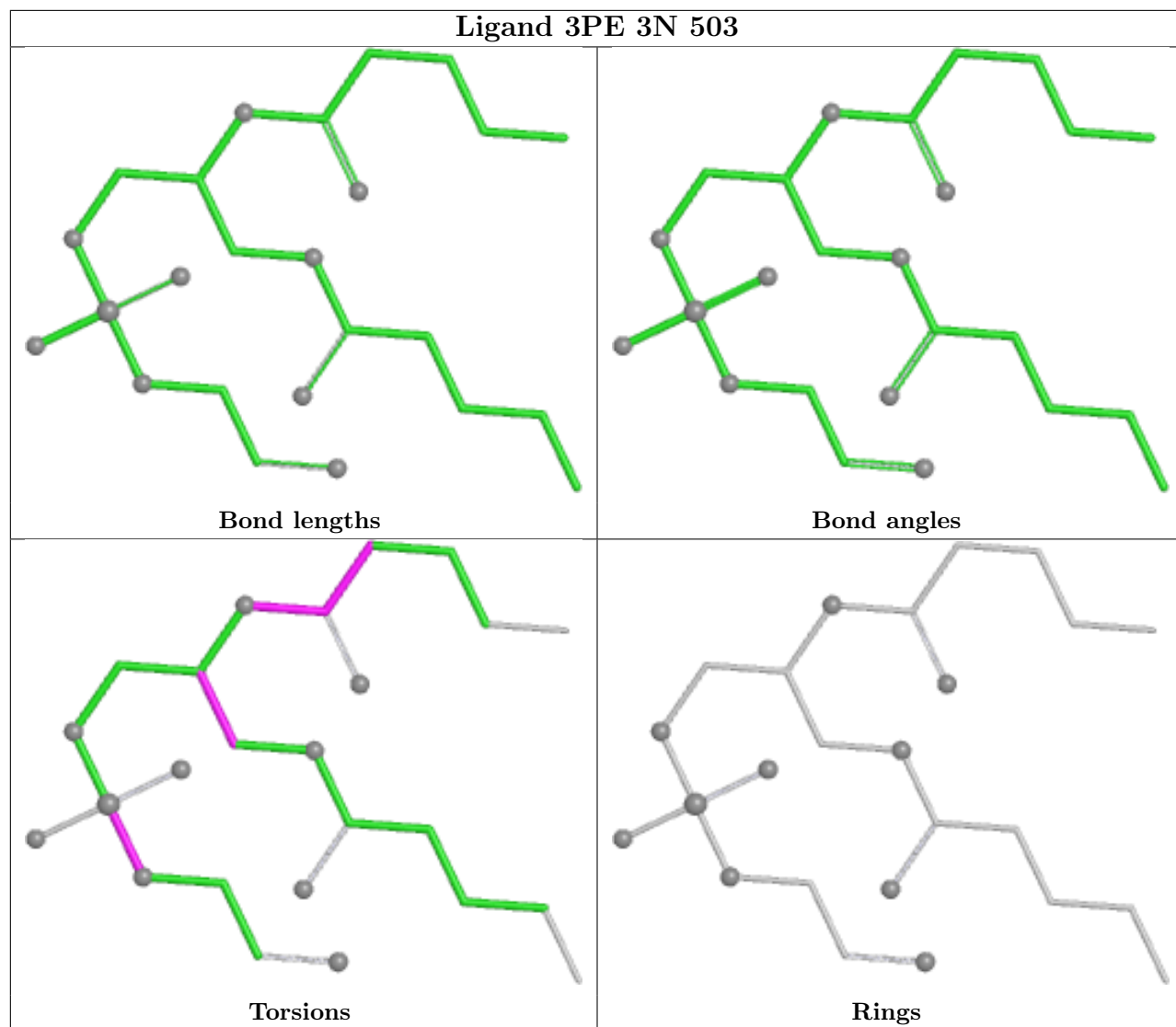


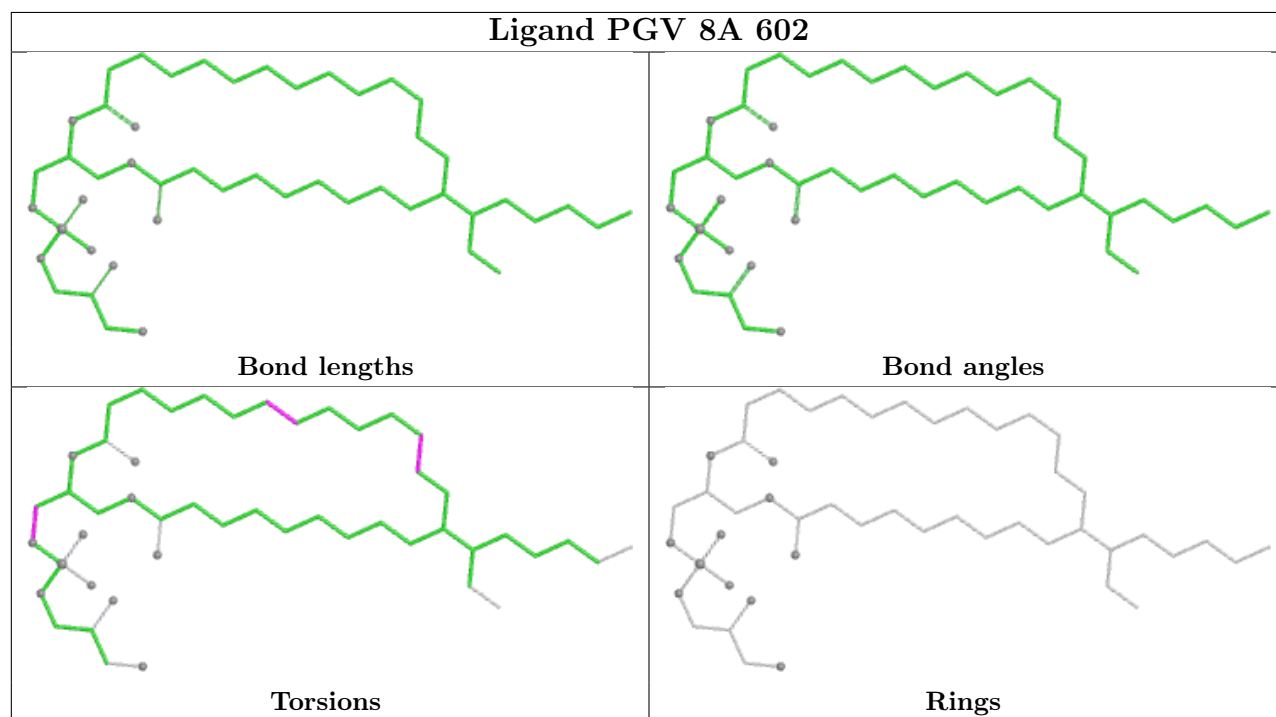
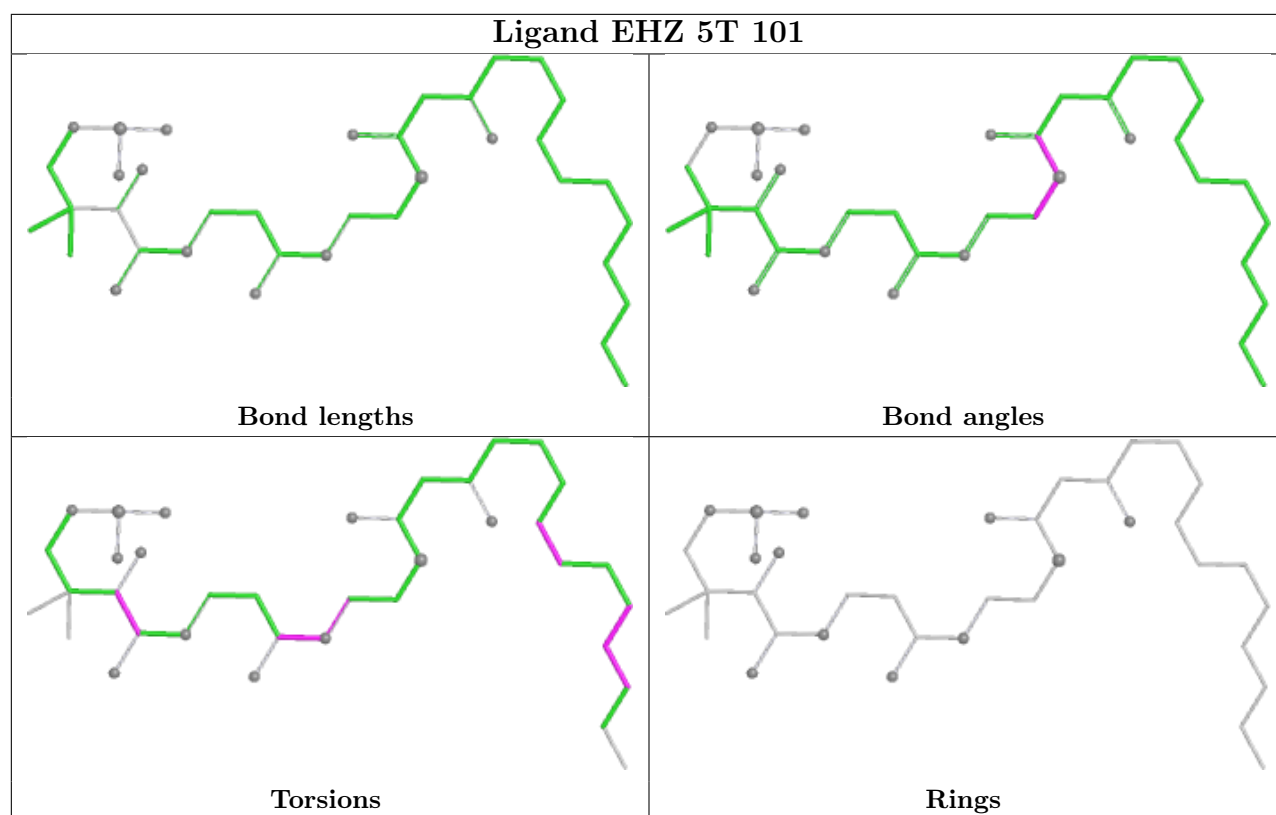


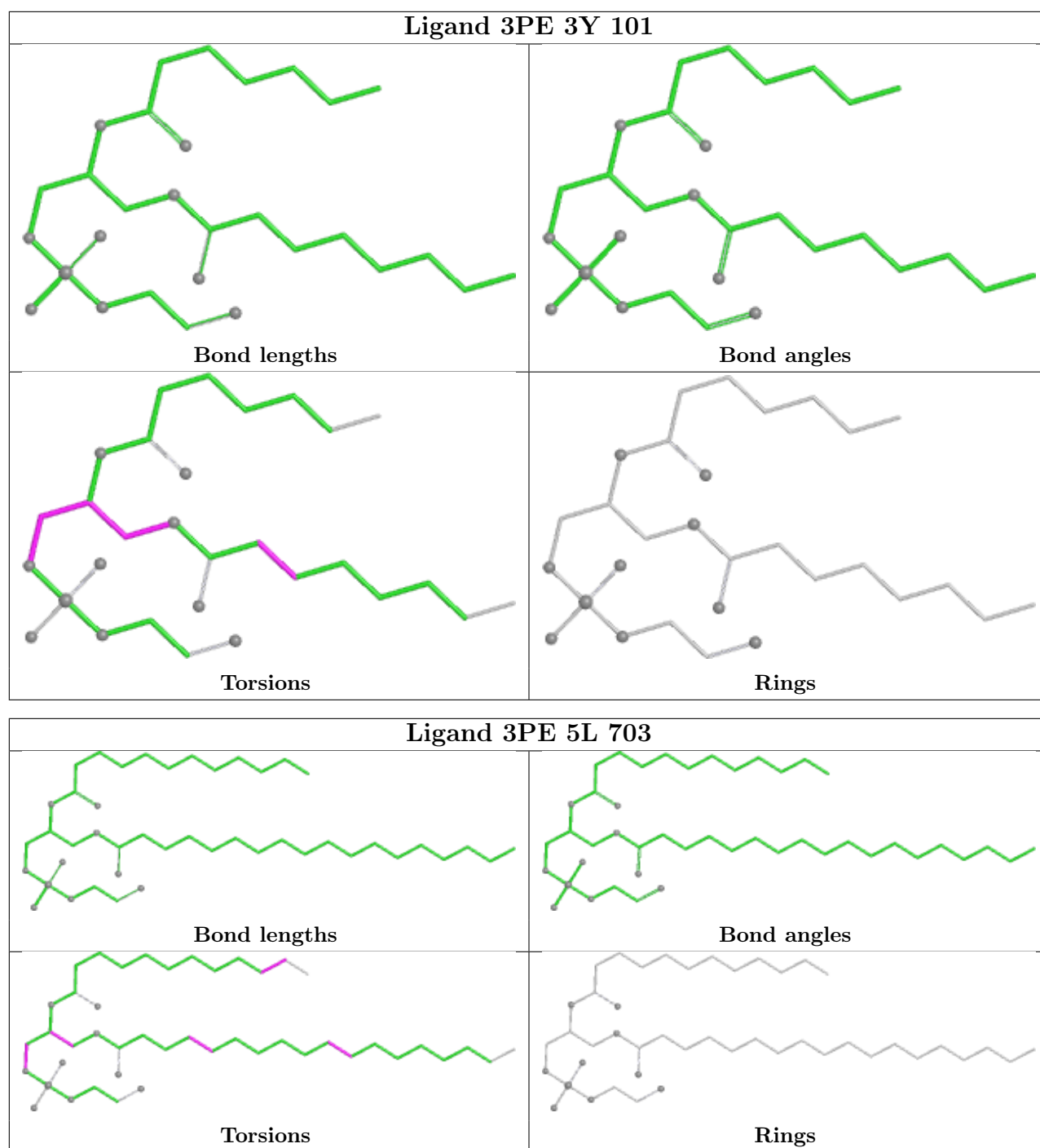


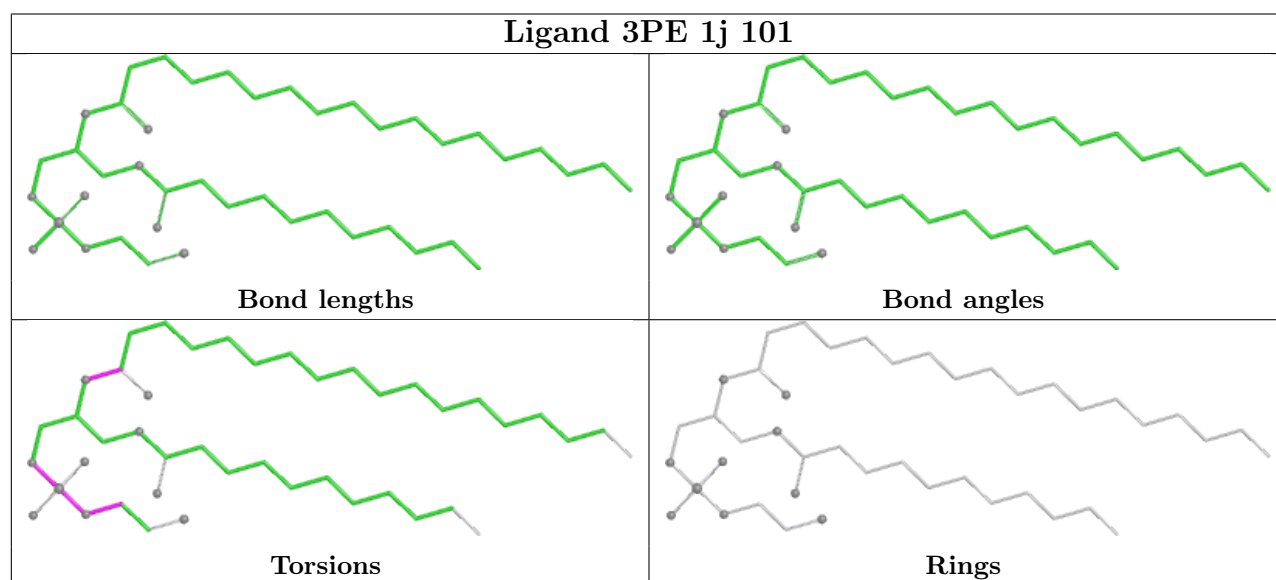
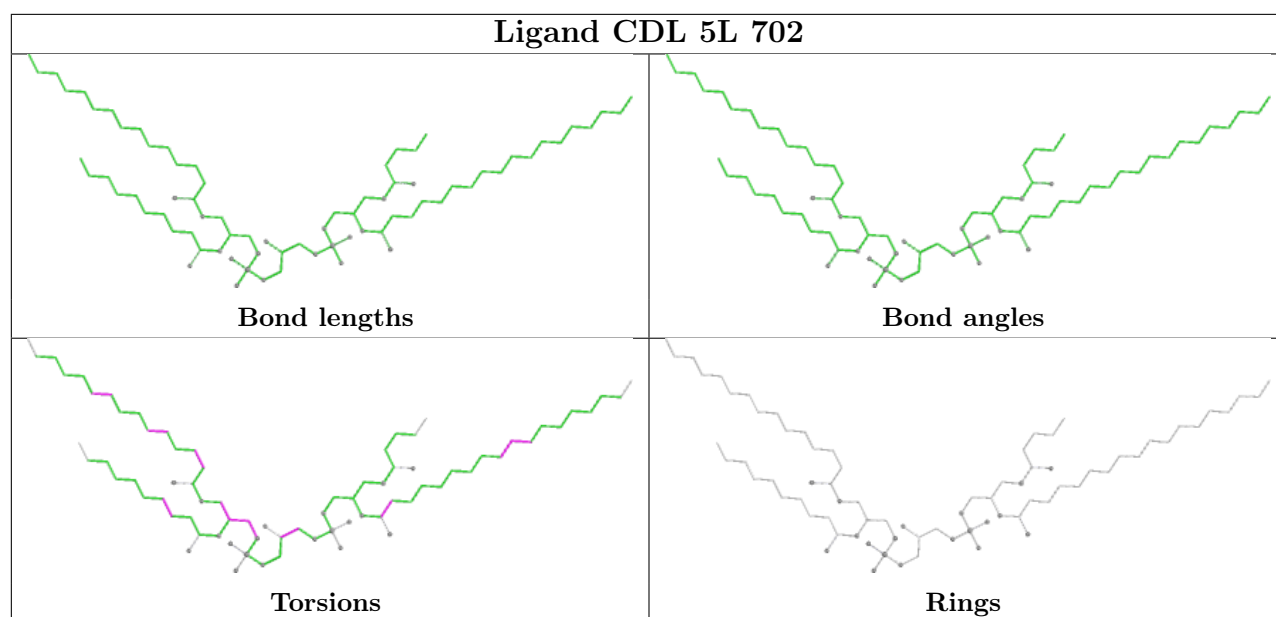




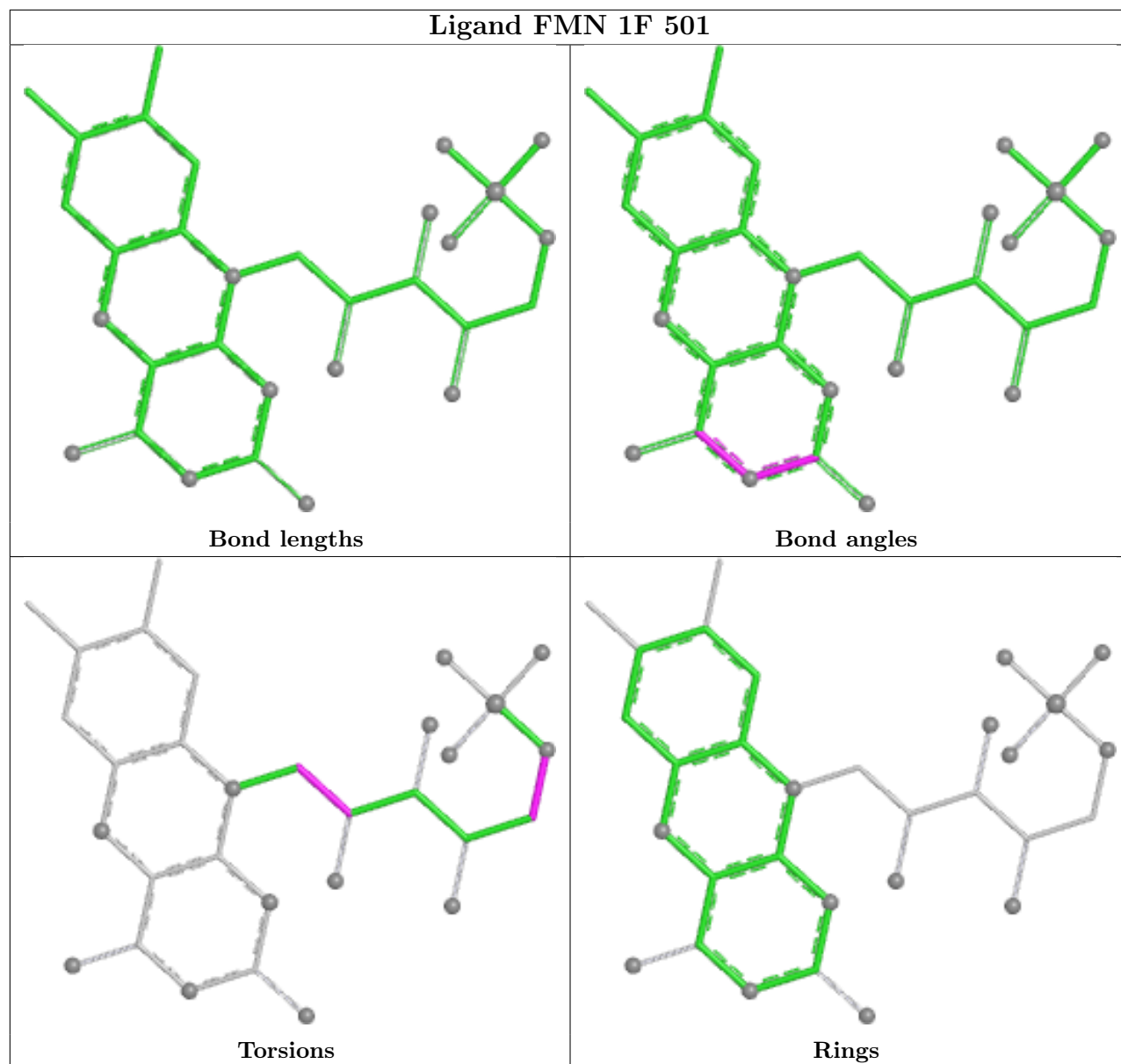


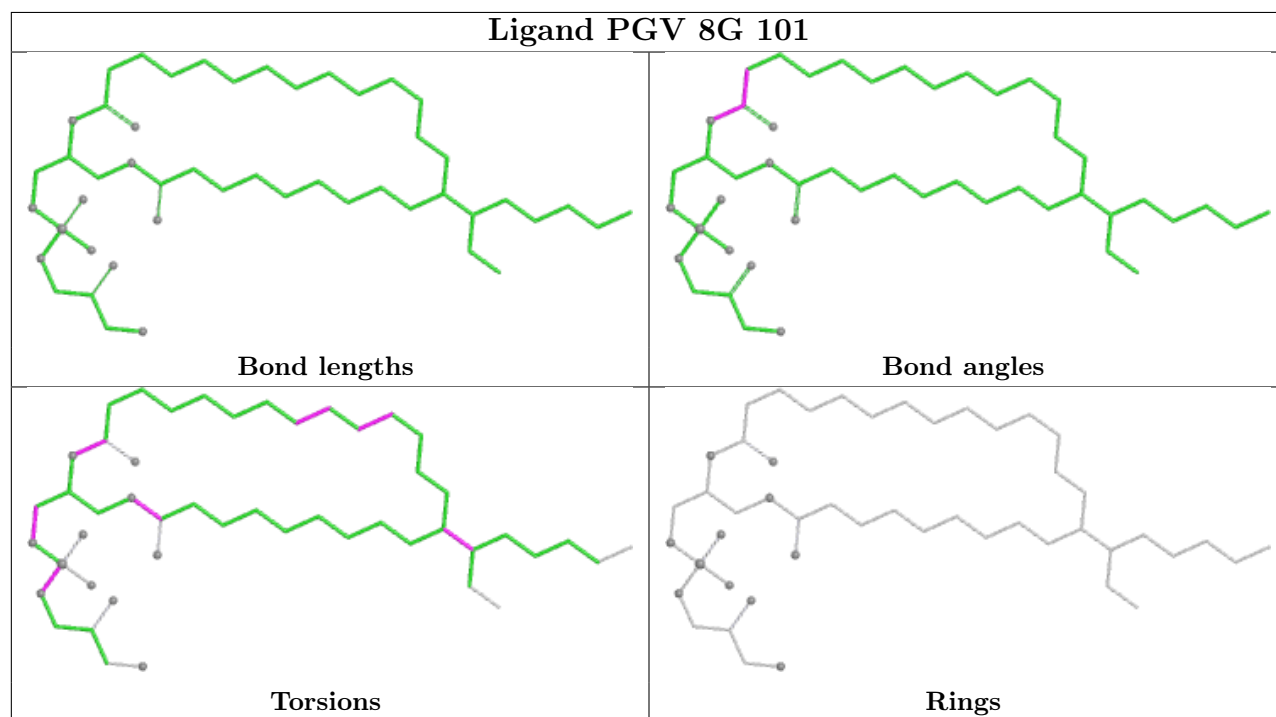
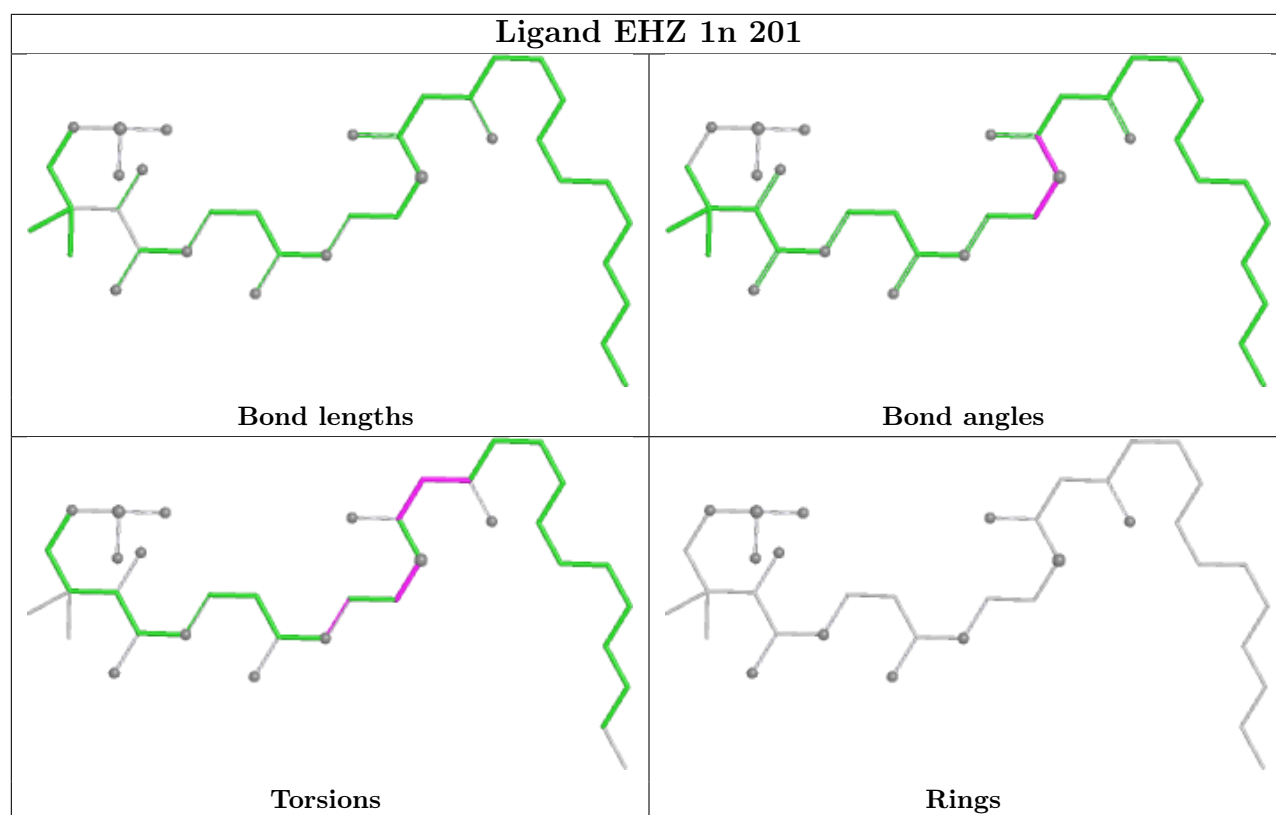


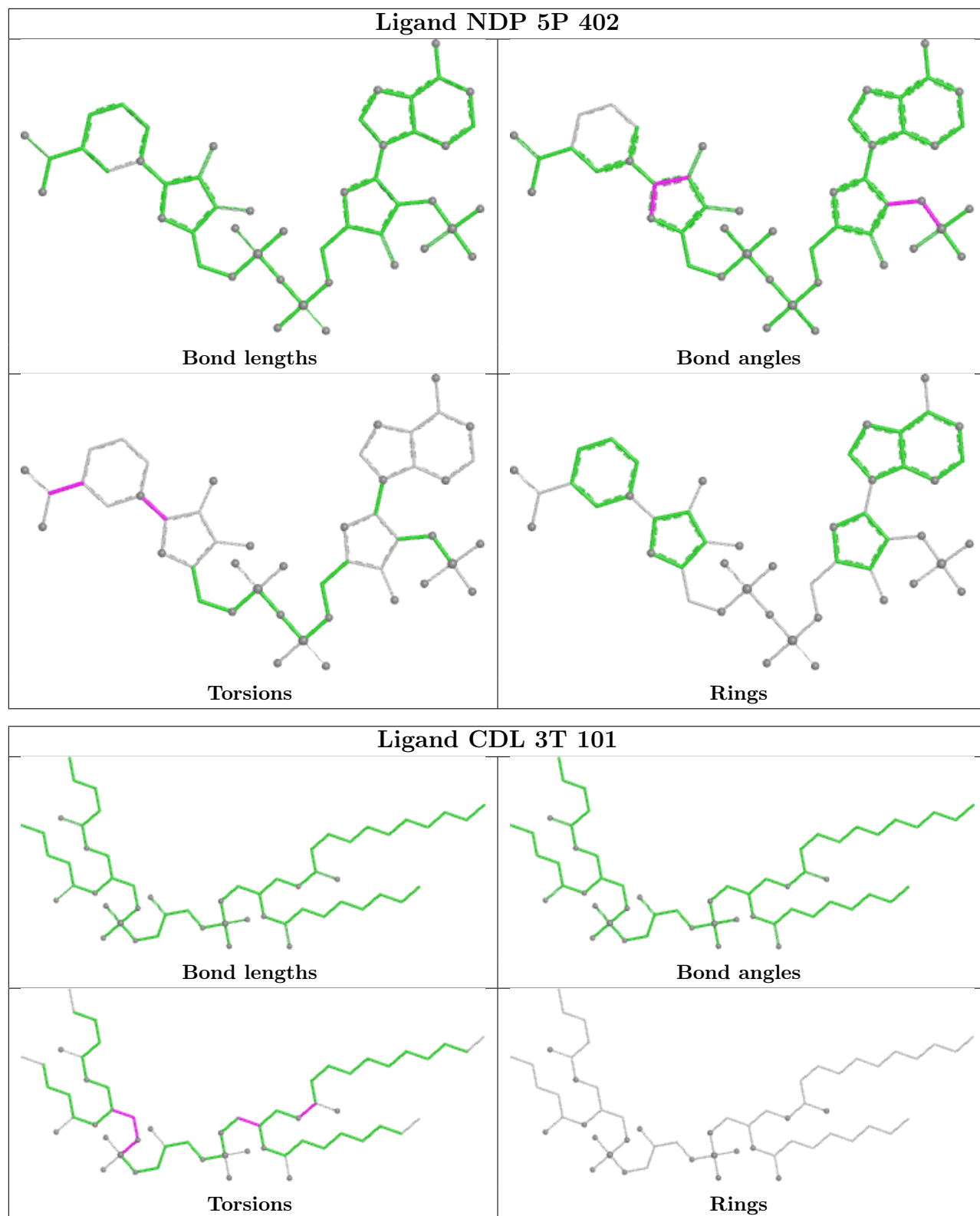


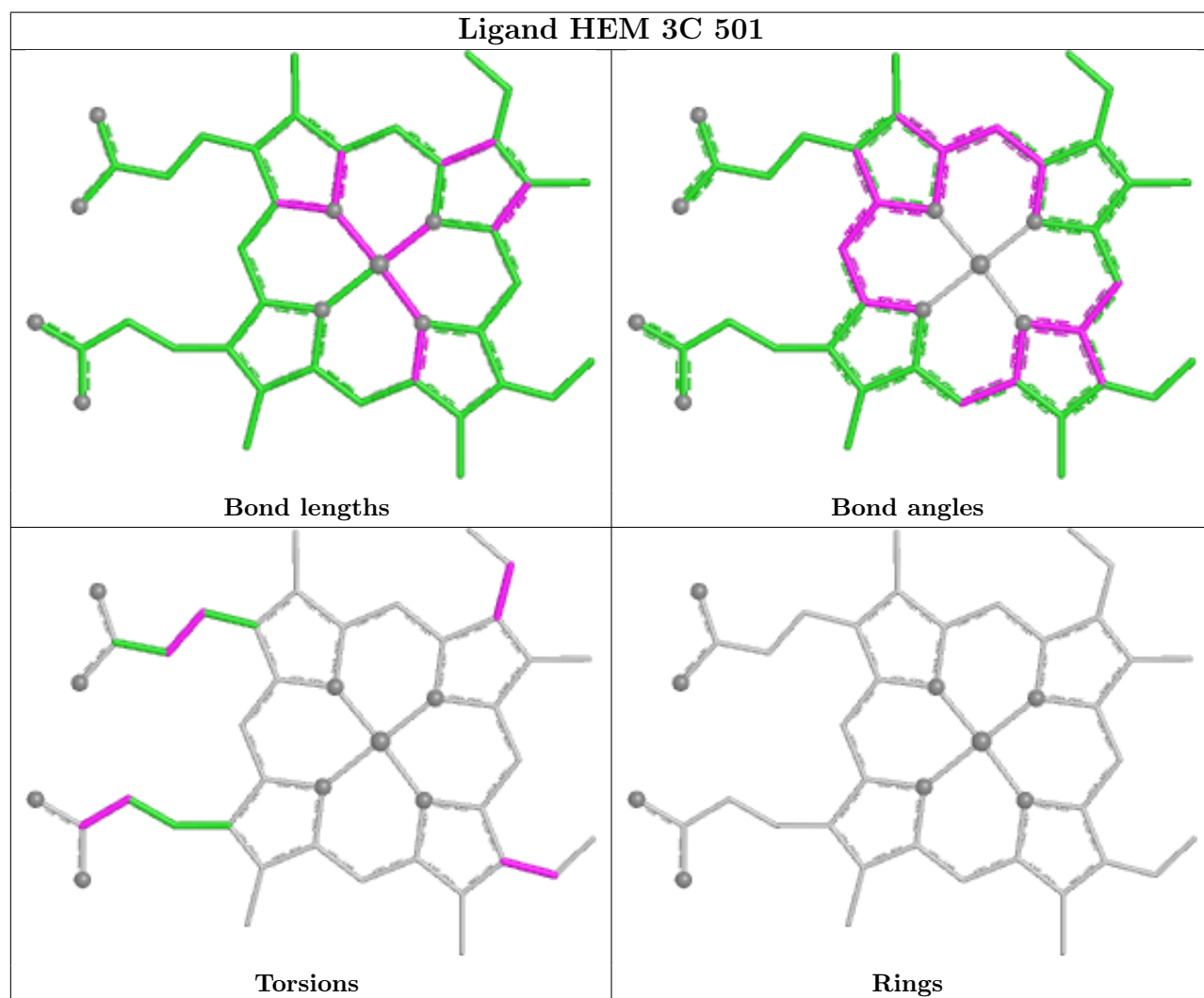
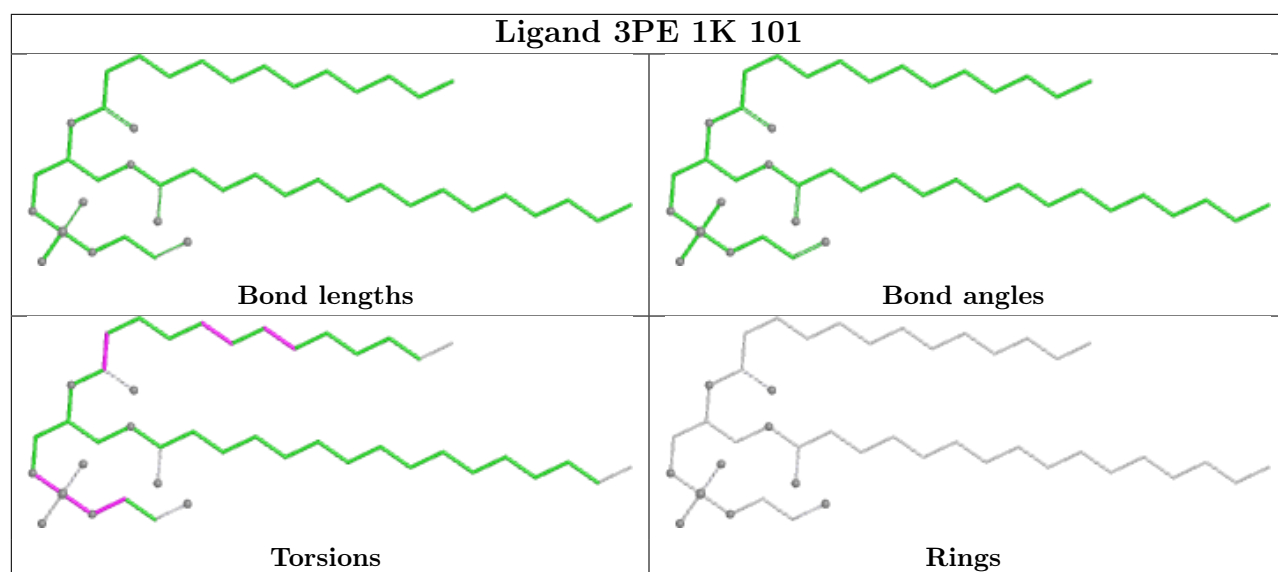


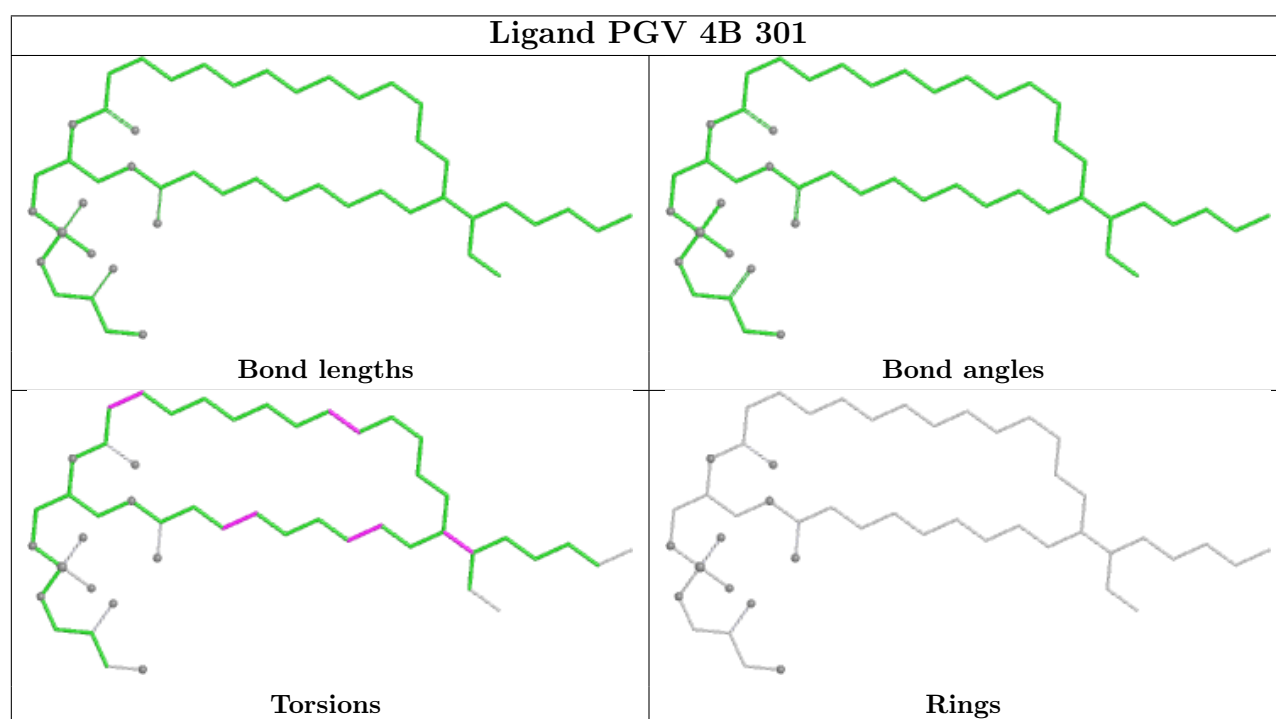
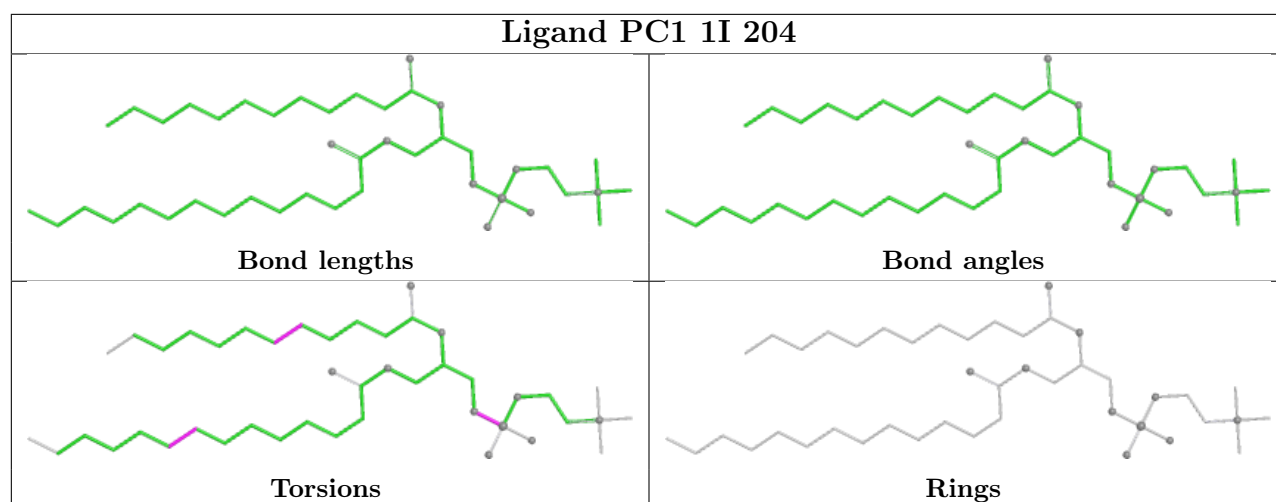
Ligand FMN 1F 501

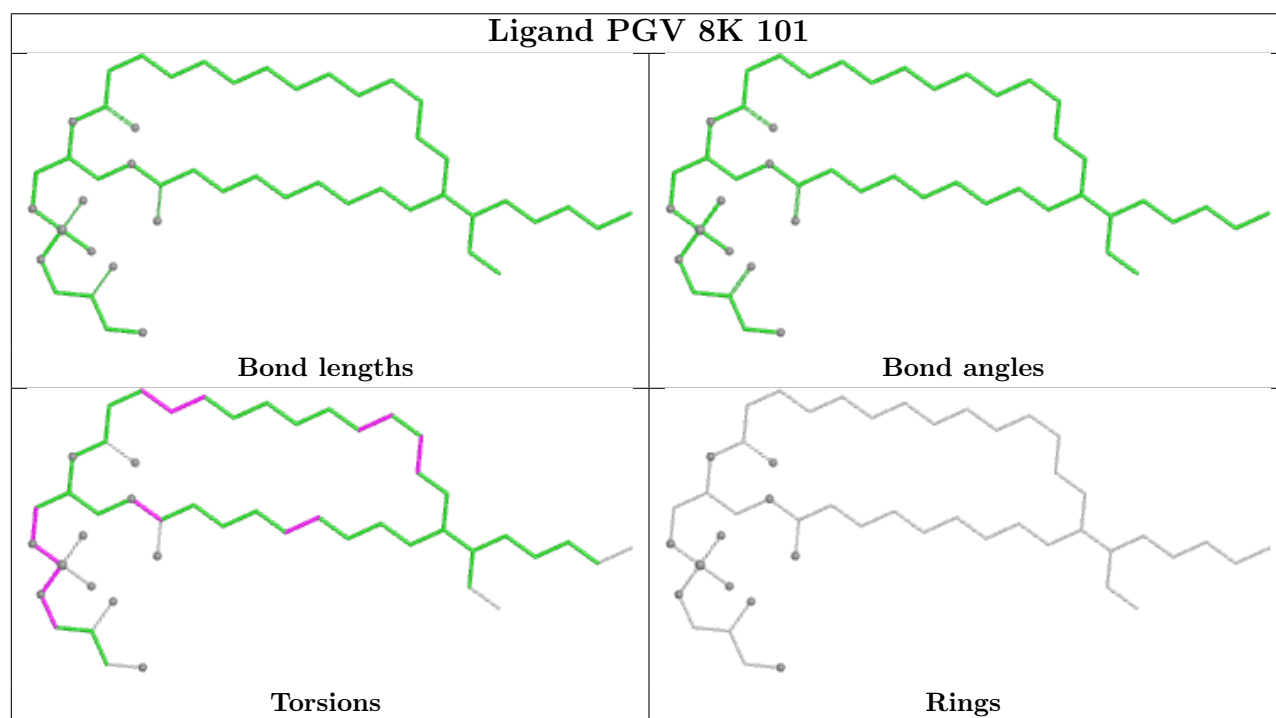
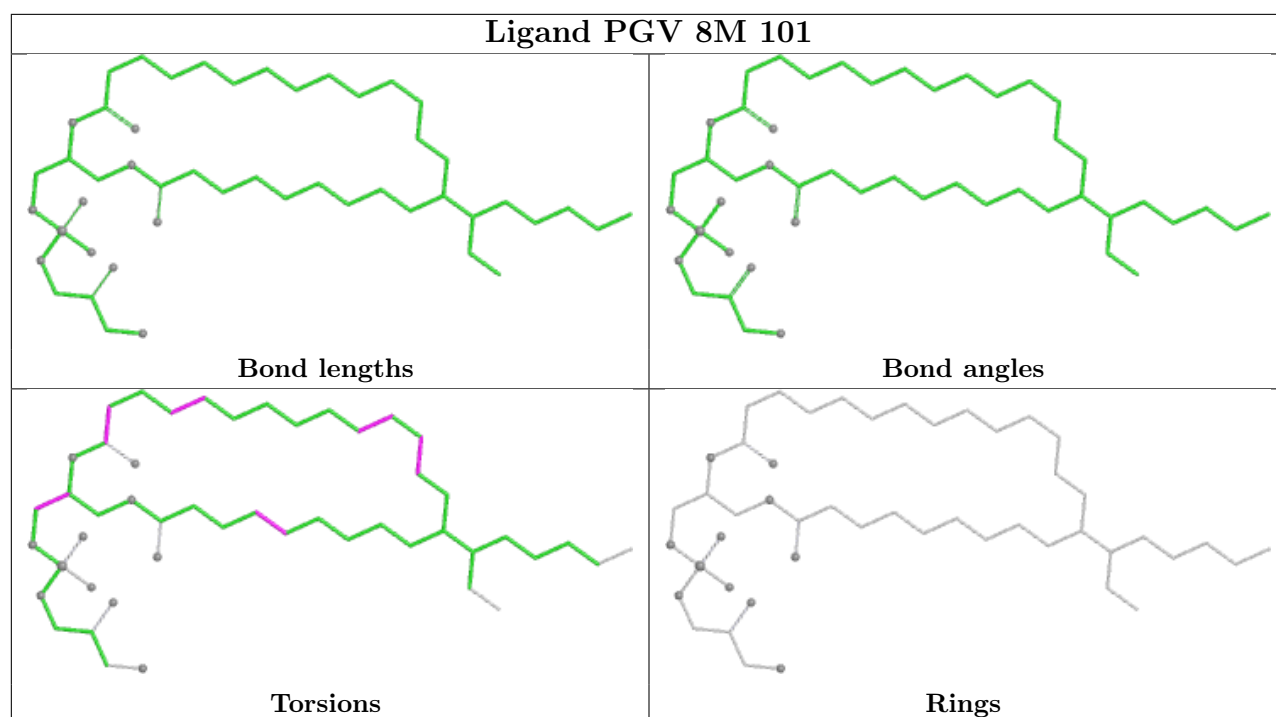


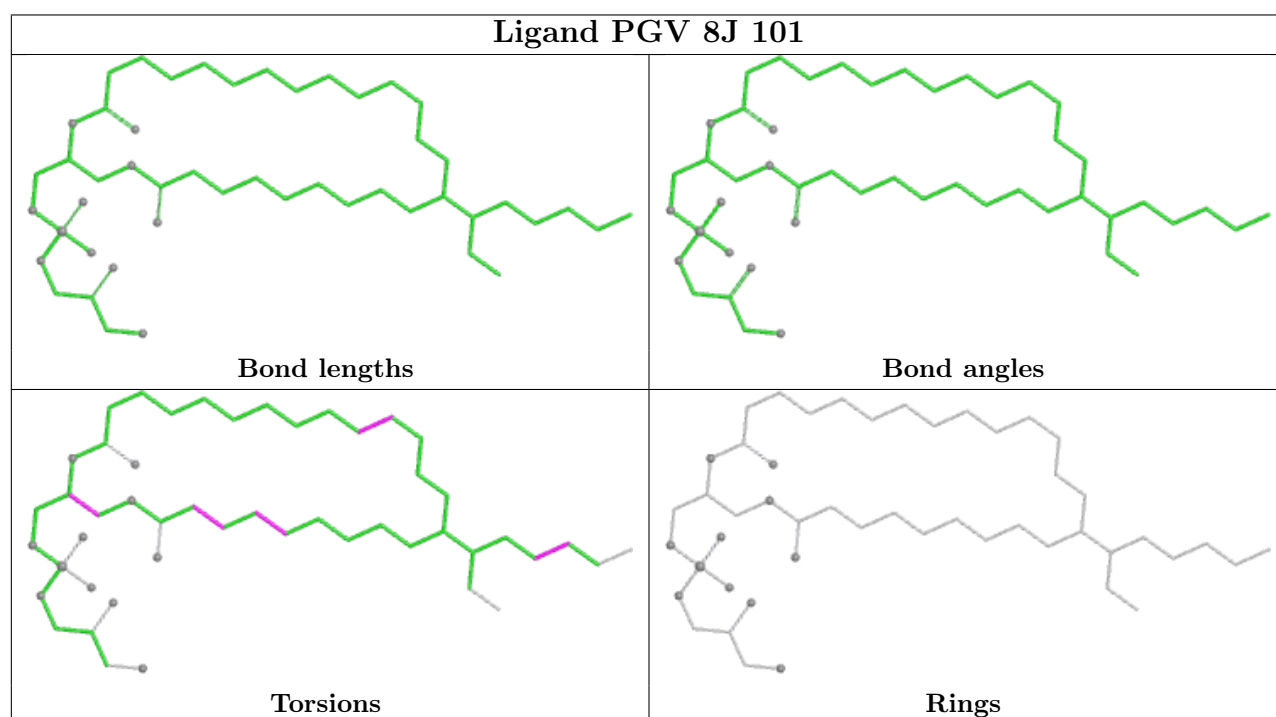
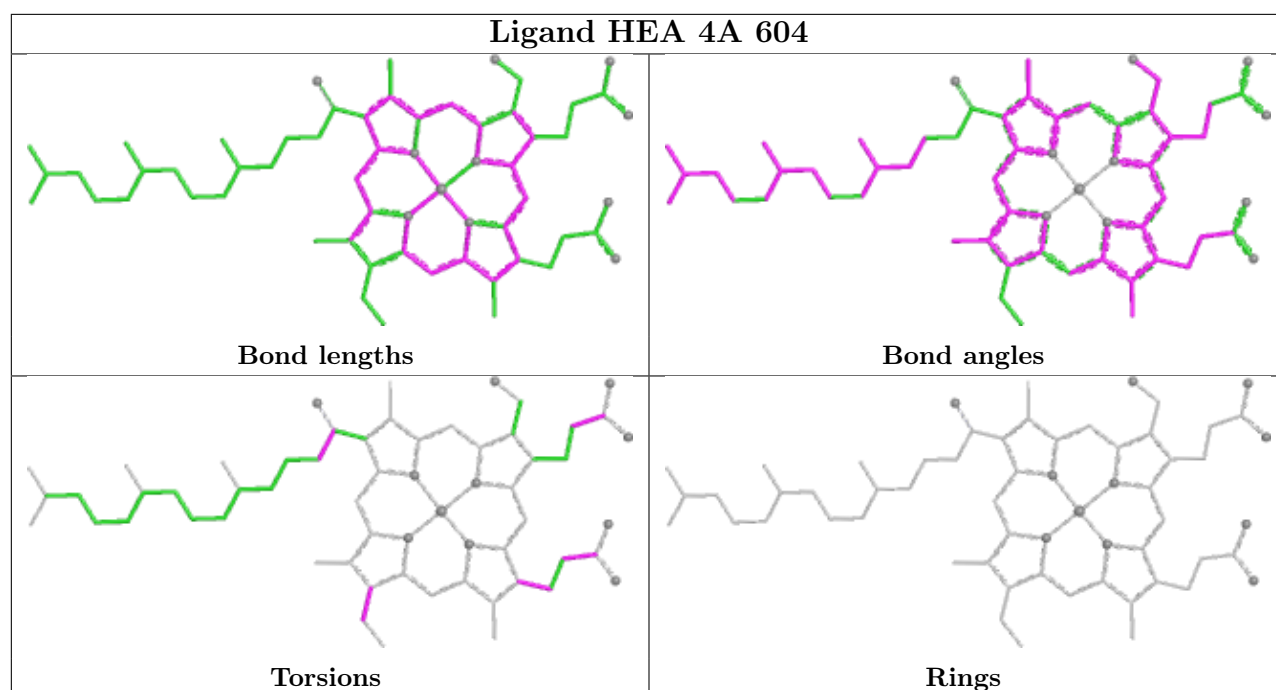


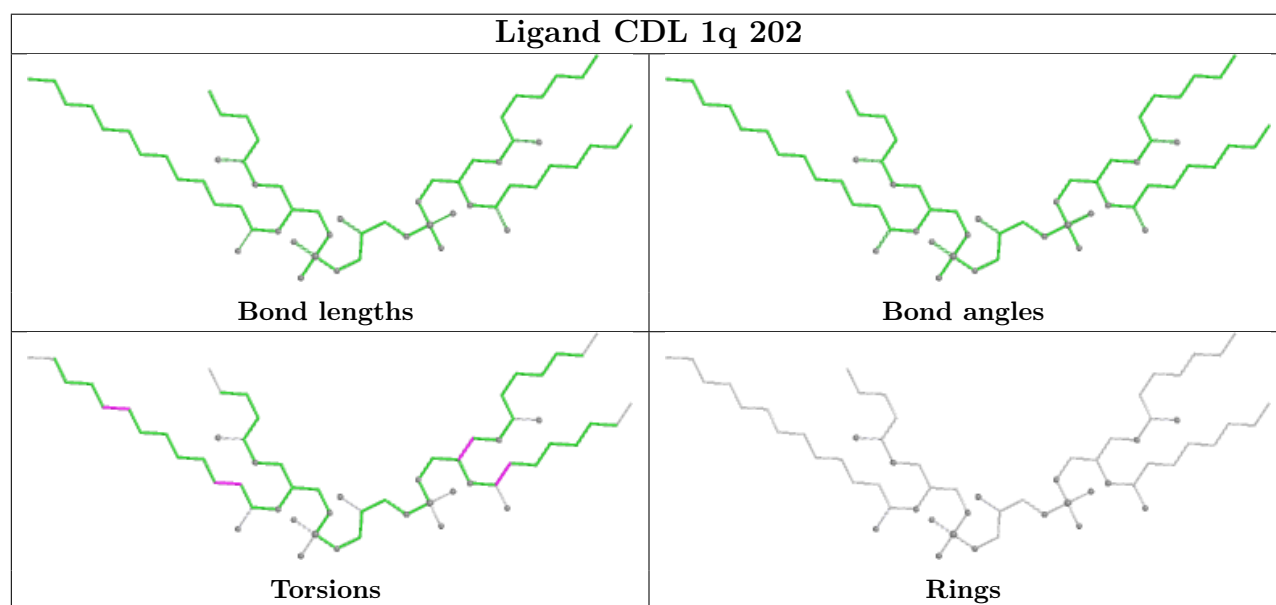
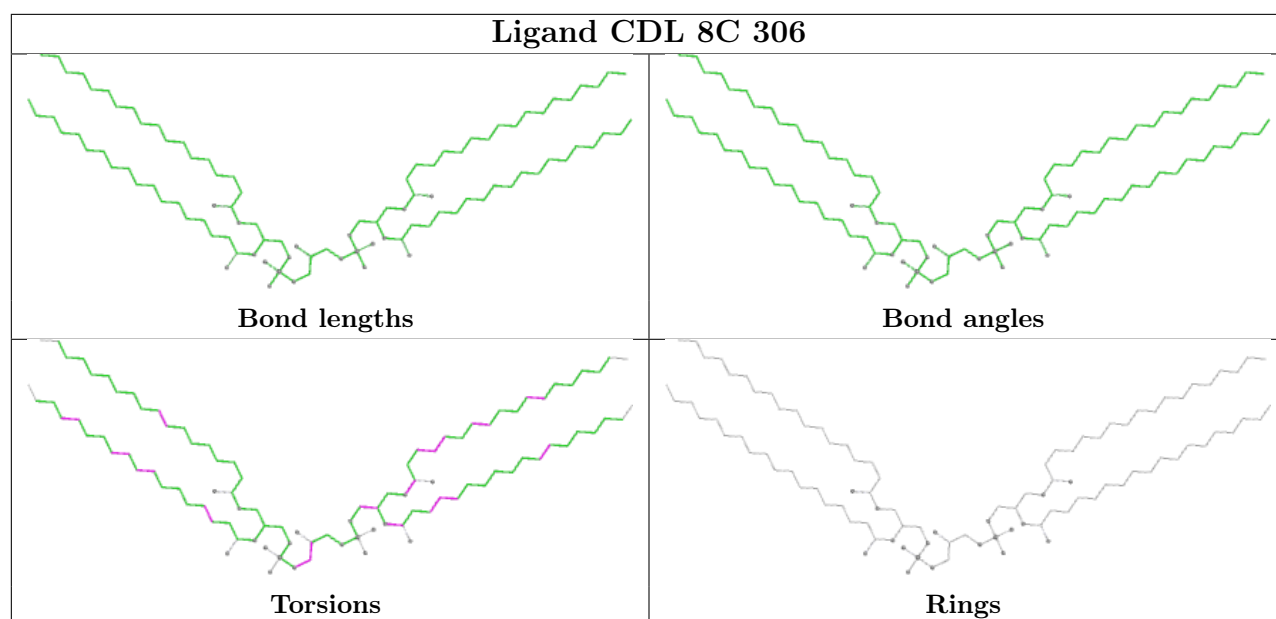


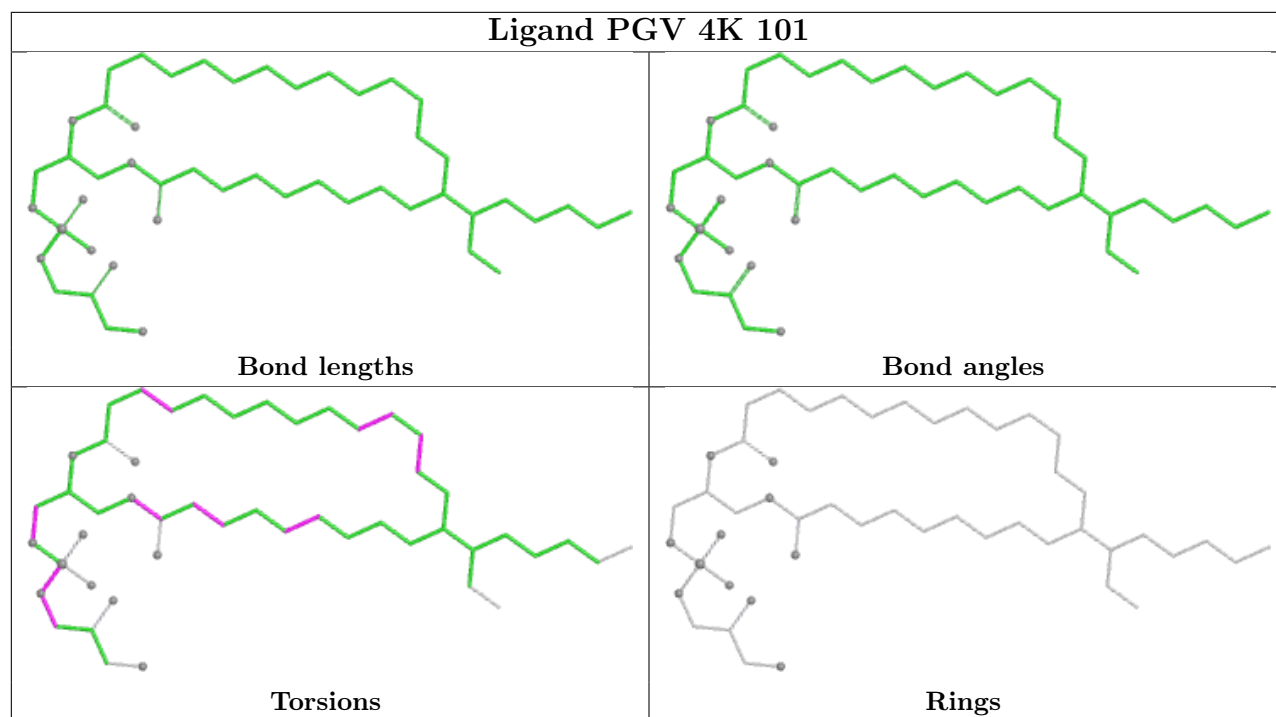
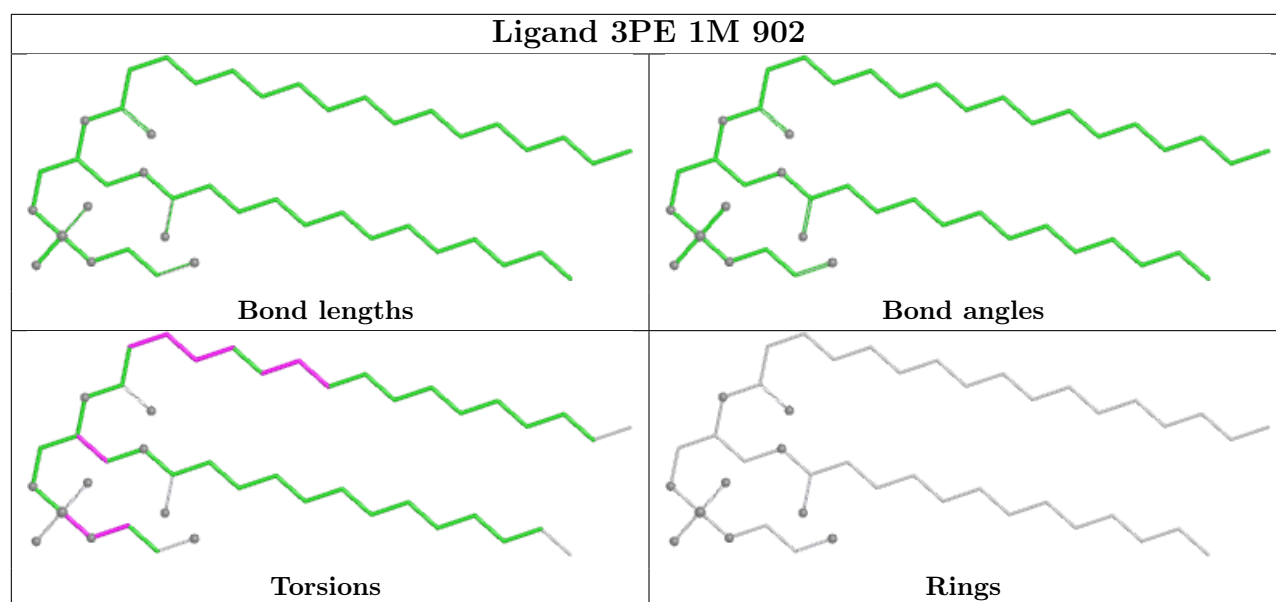


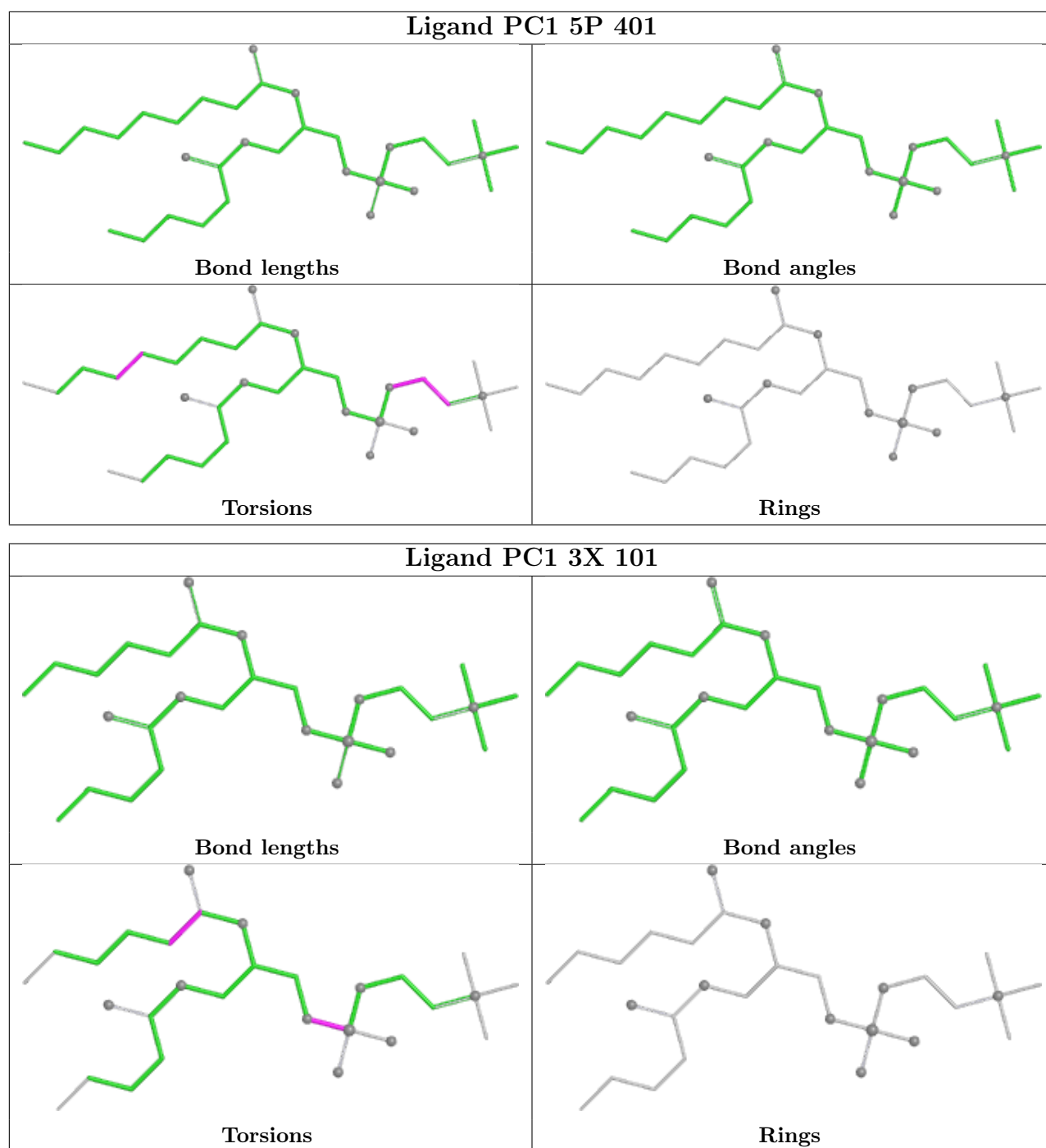


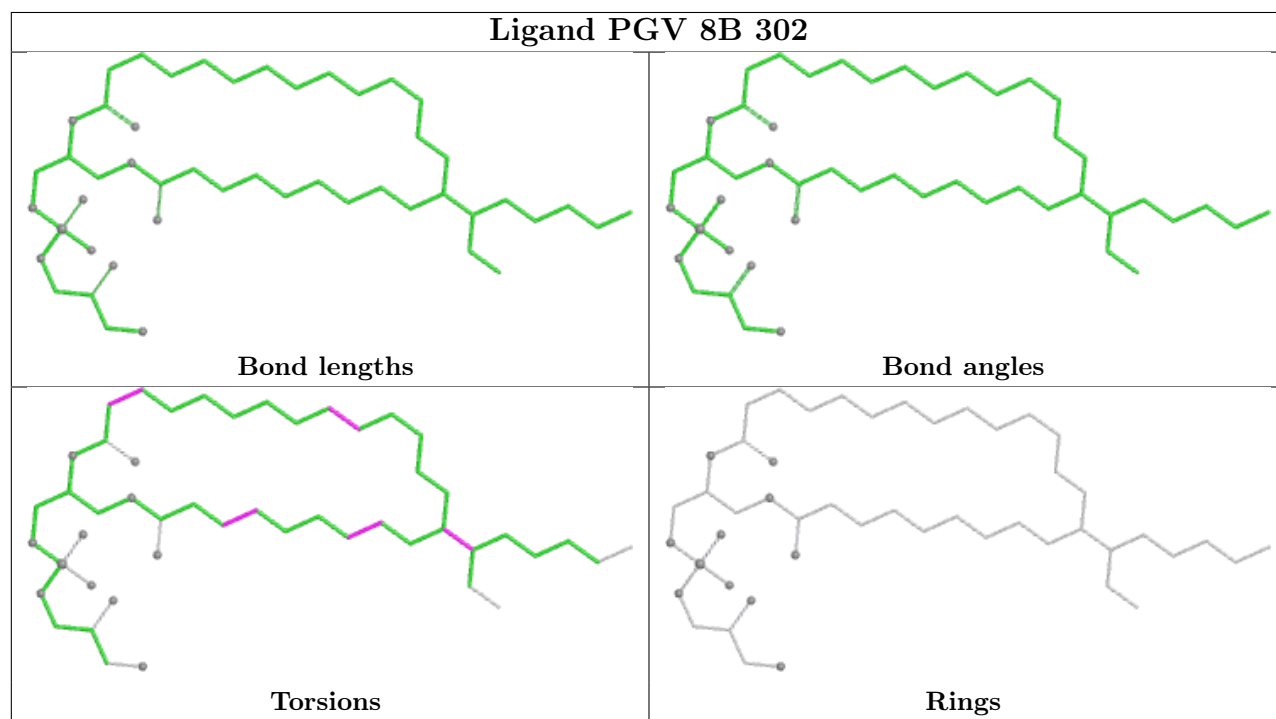
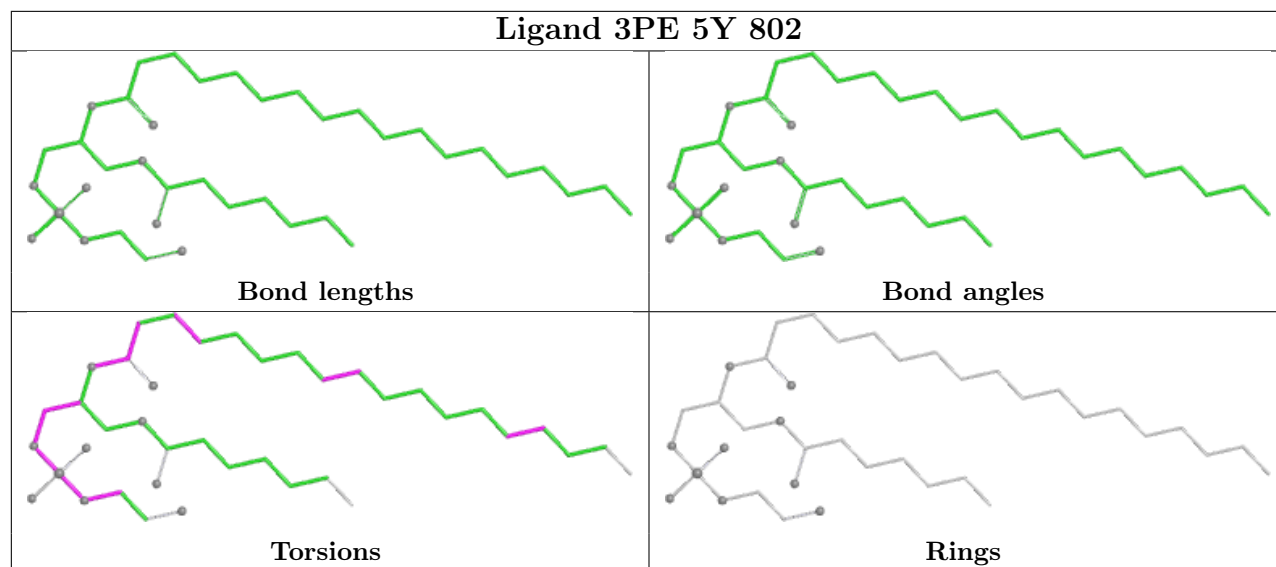


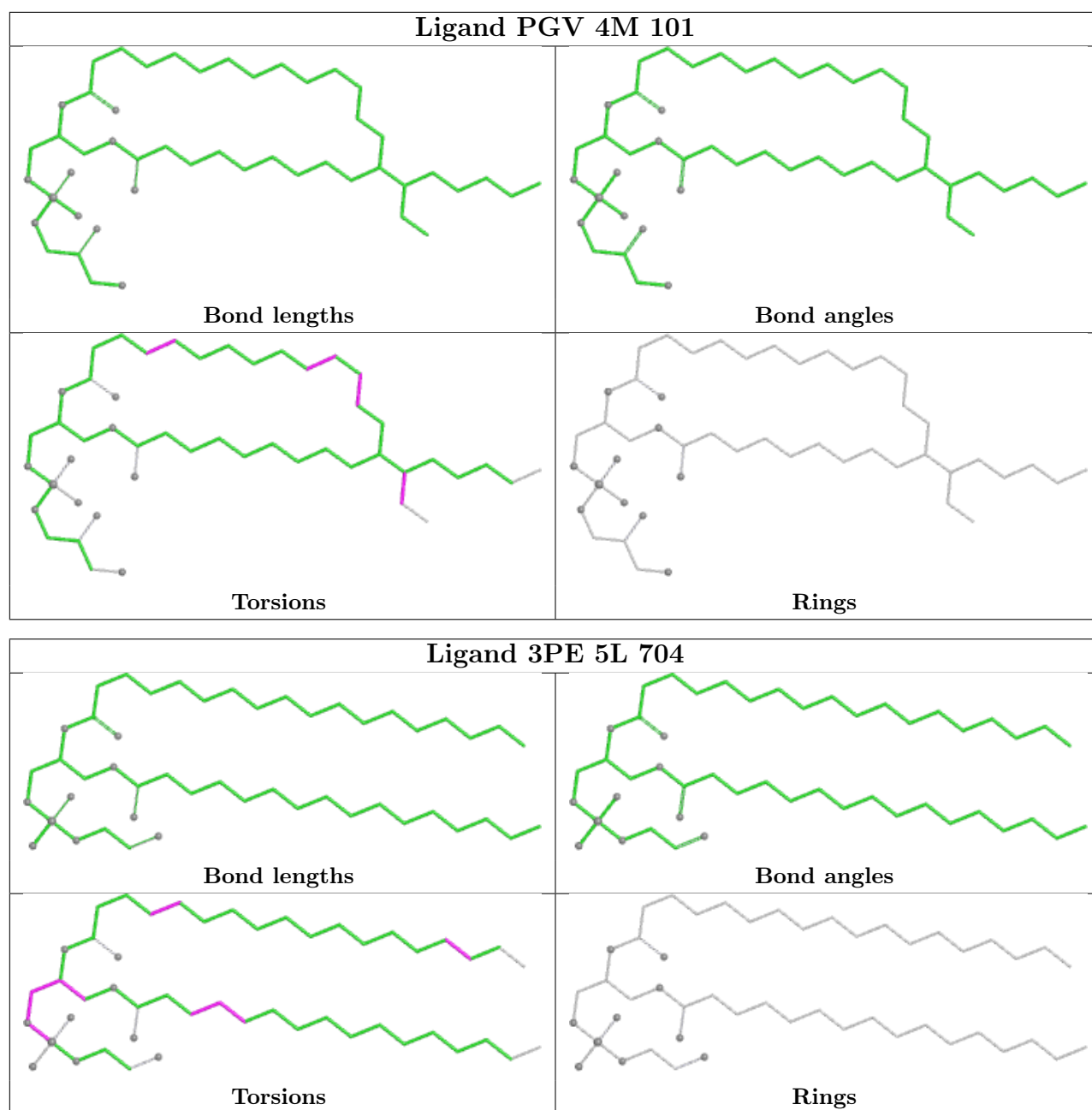


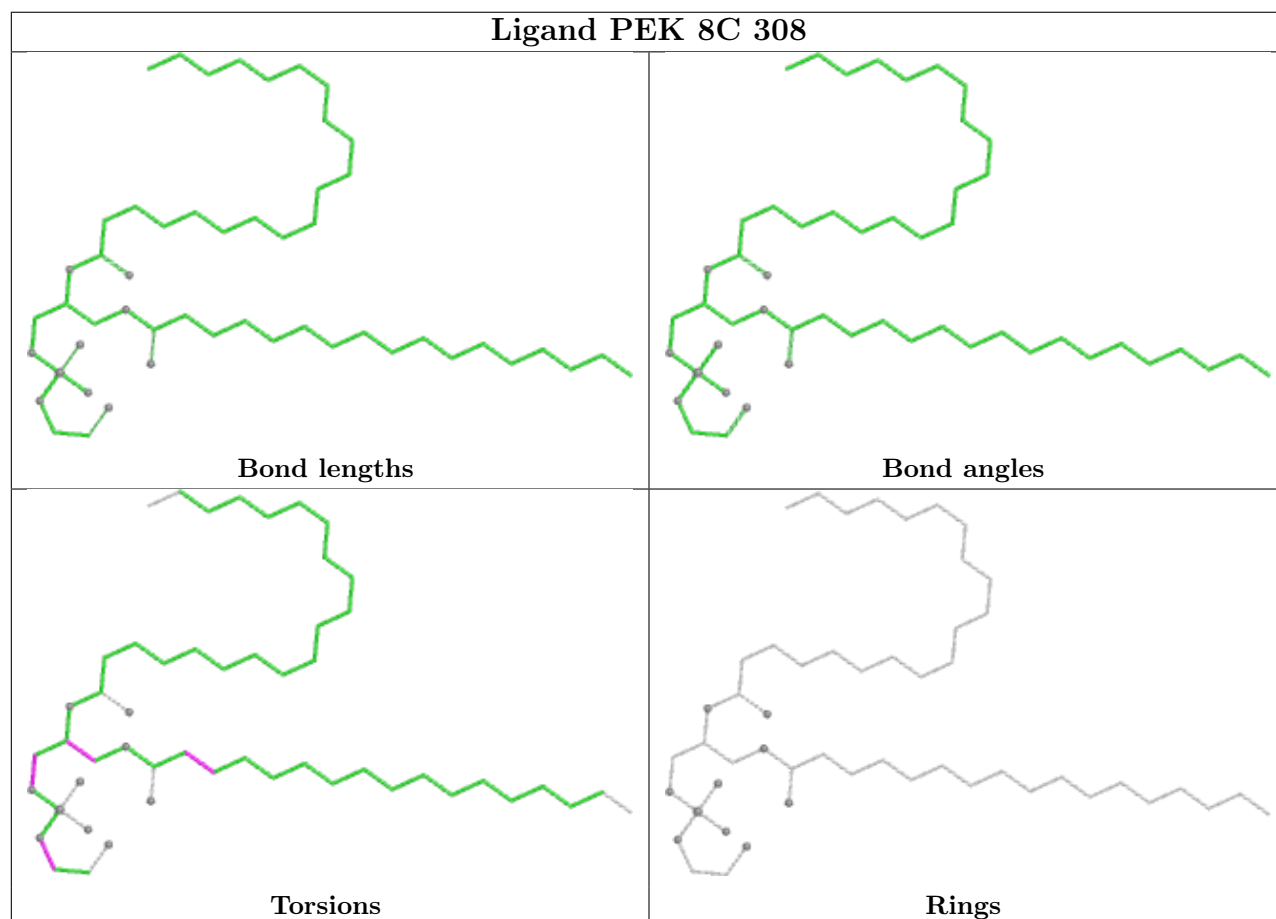
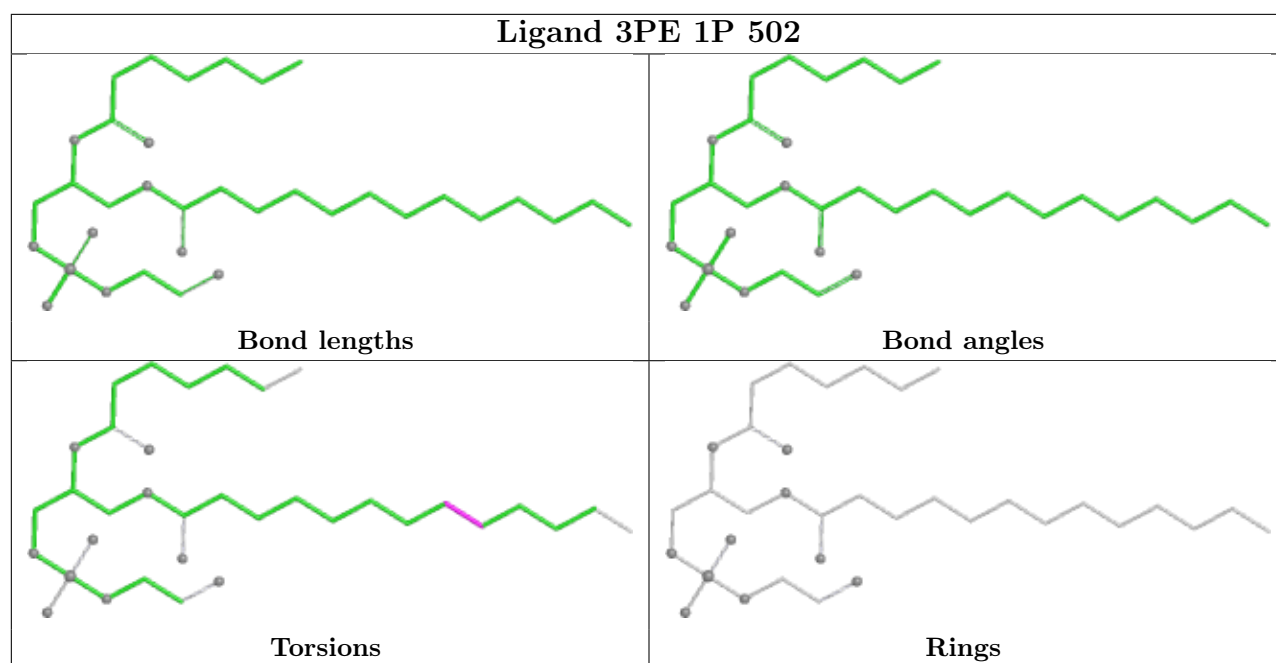




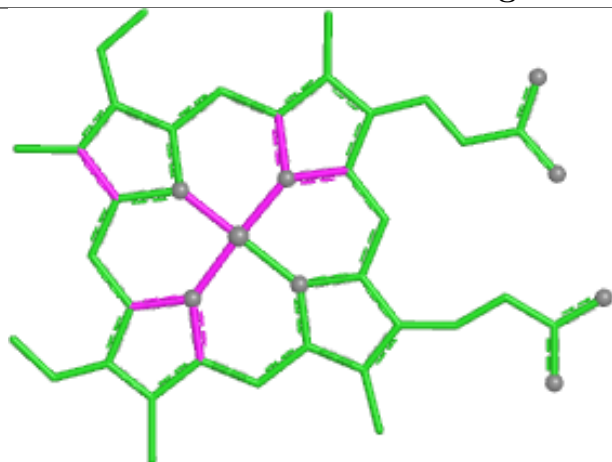




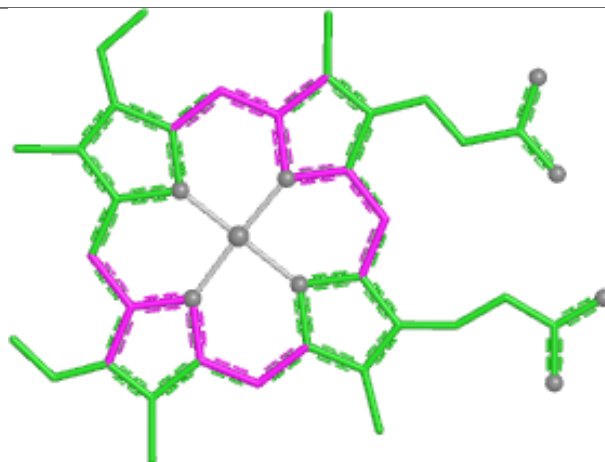




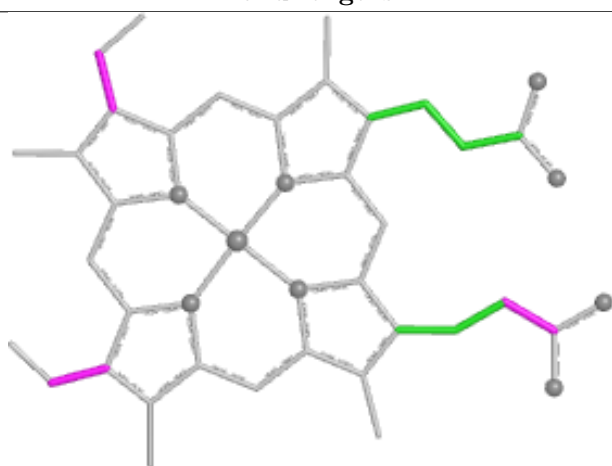
Ligand HEM 3C 502



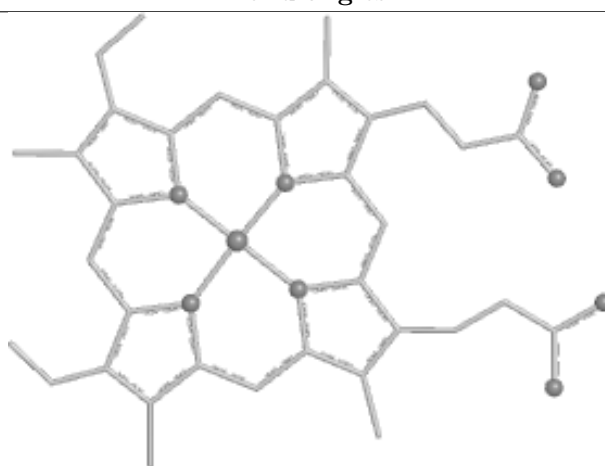
Bond lengths



Bond angles

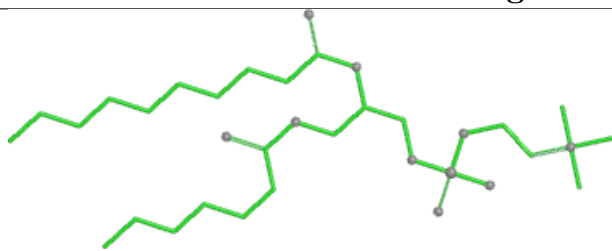


Torsions

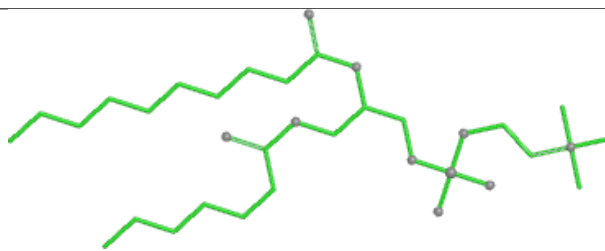


Rings

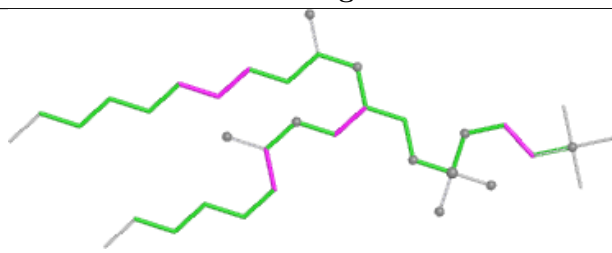
Ligand PC1 1A 201



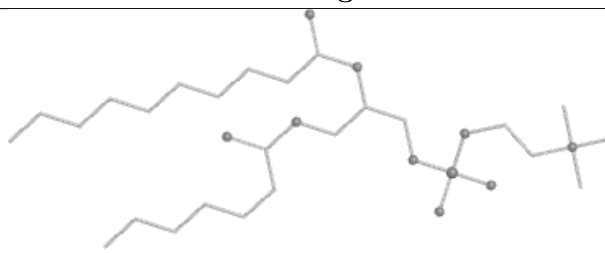
Bond lengths



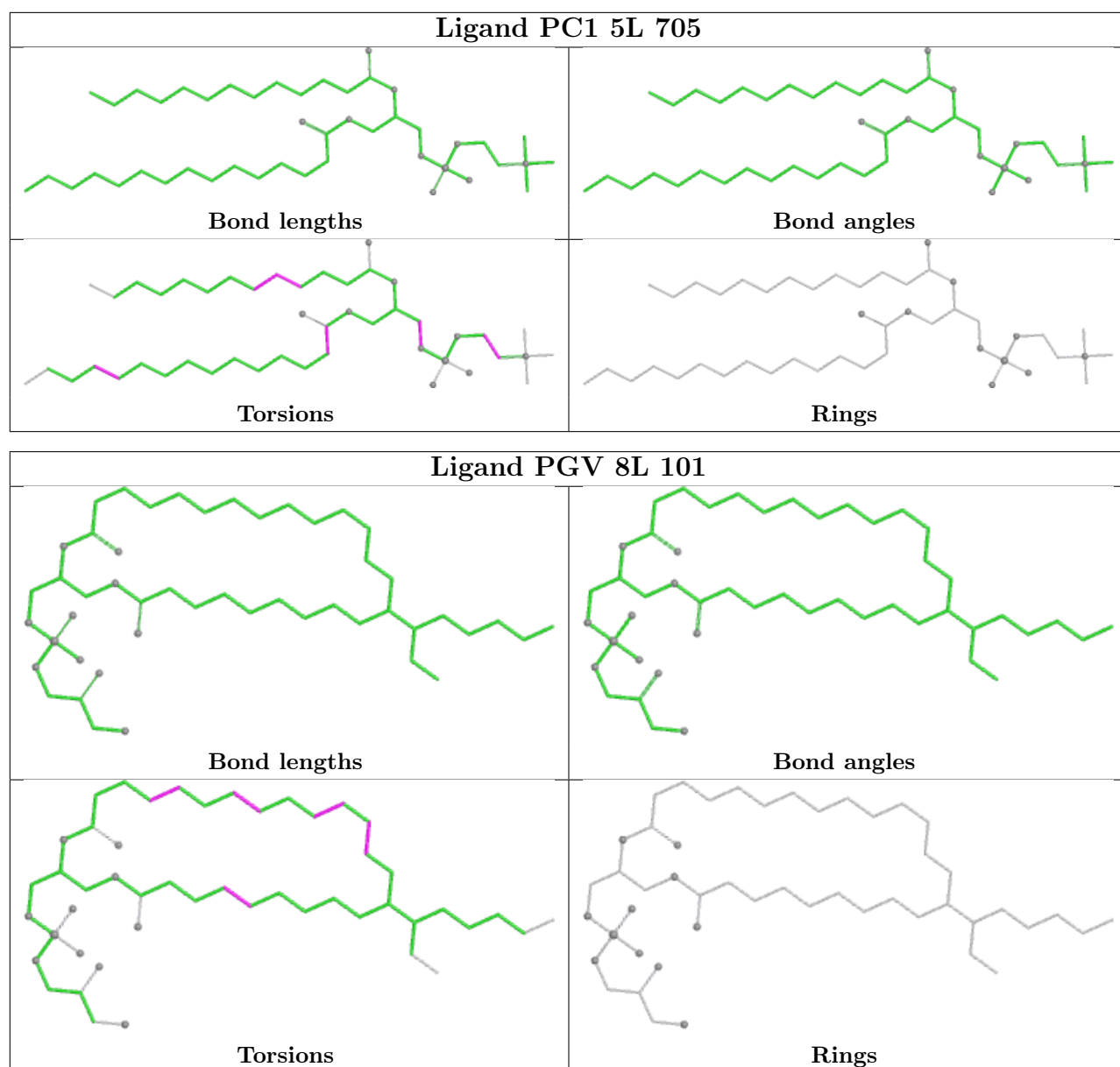
Bond angles

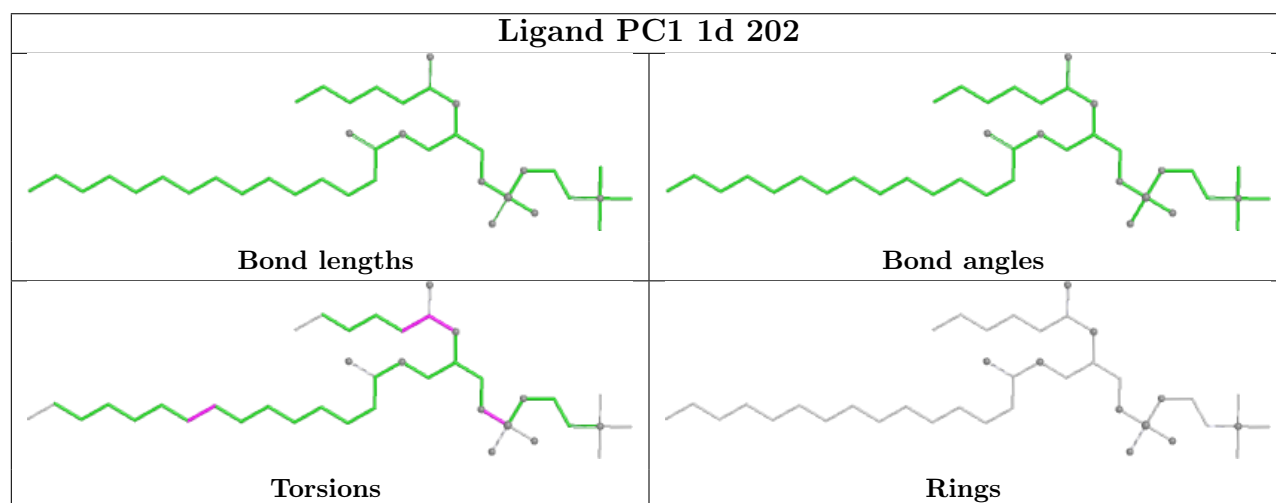
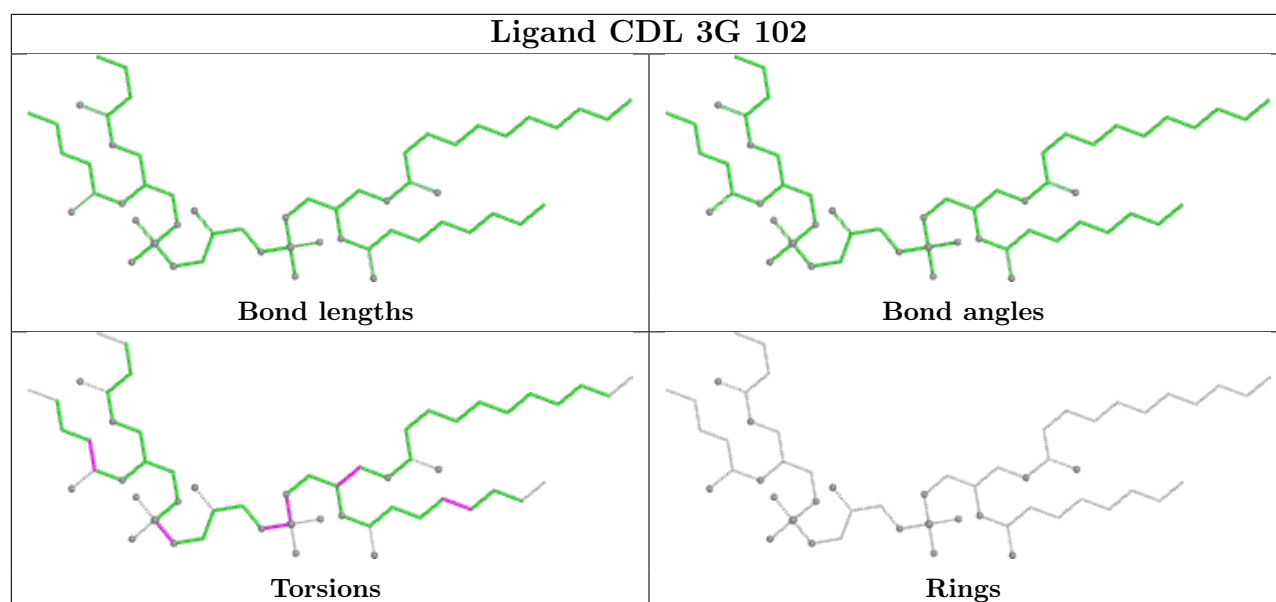


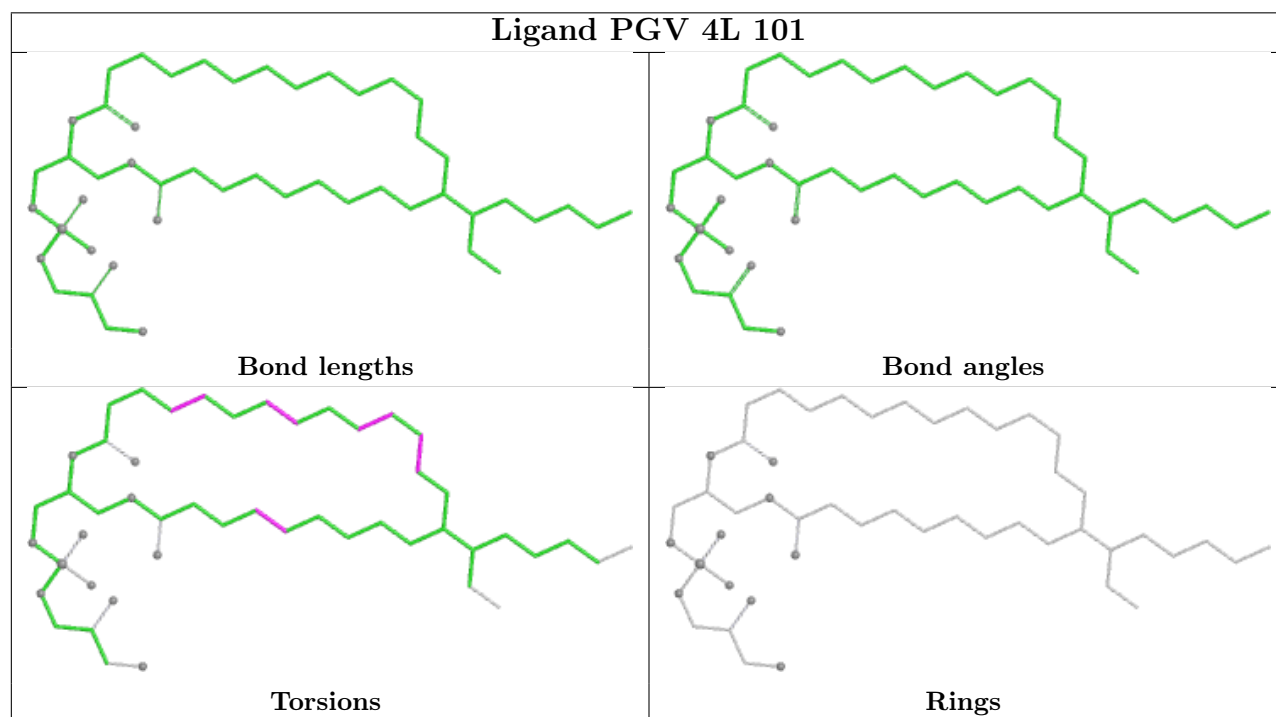
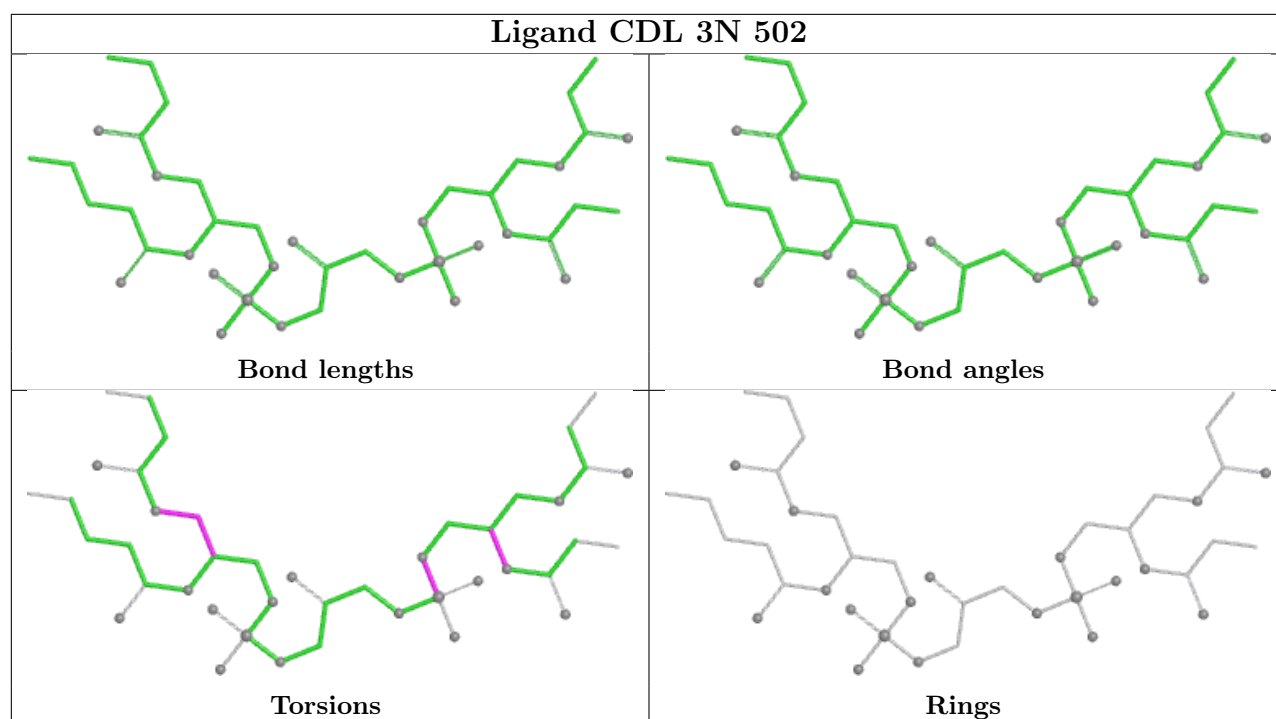
Torsions

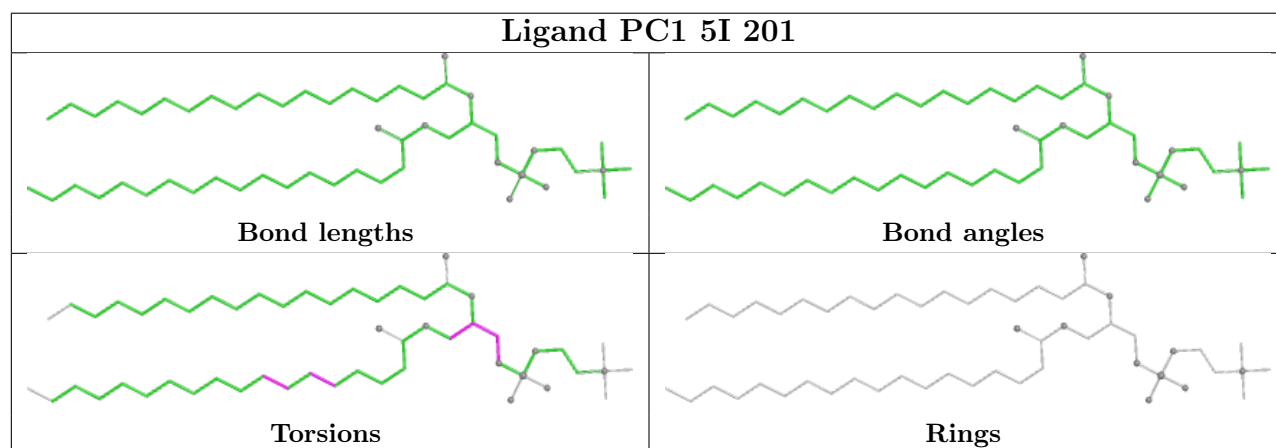
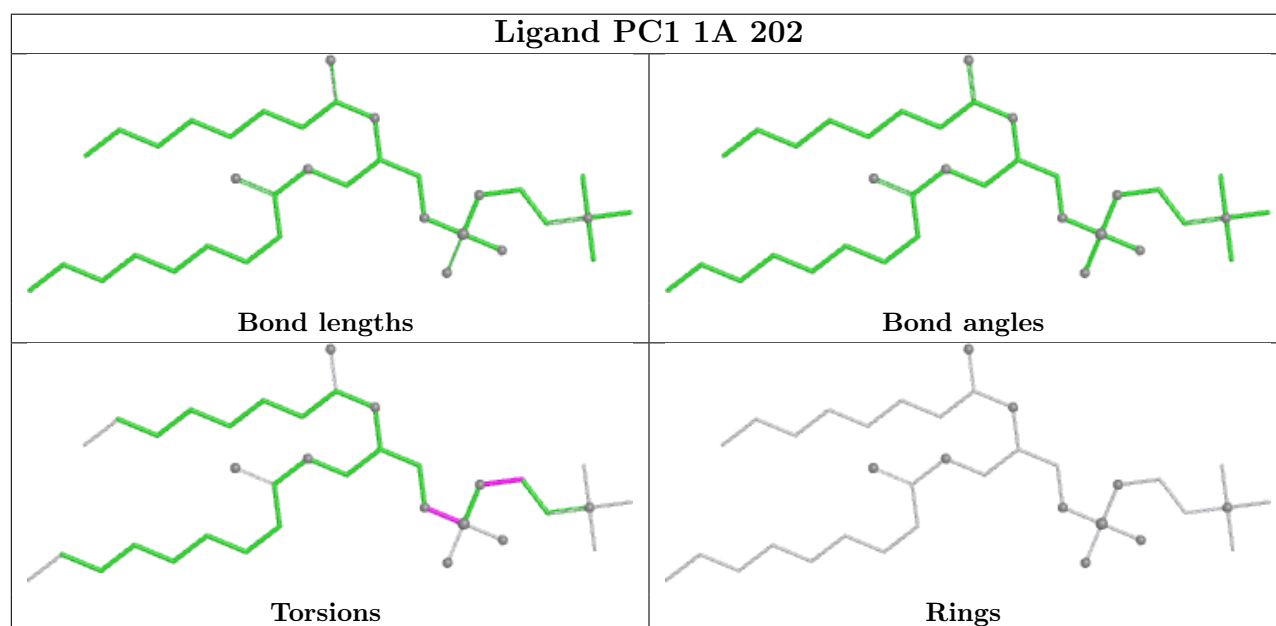
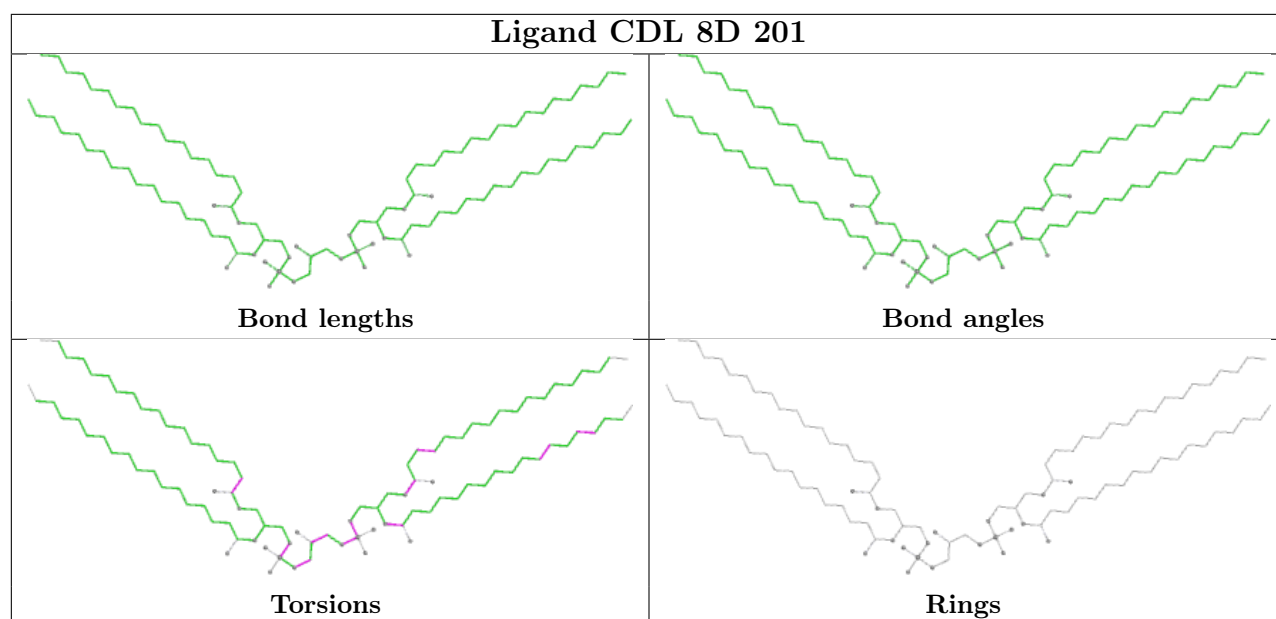


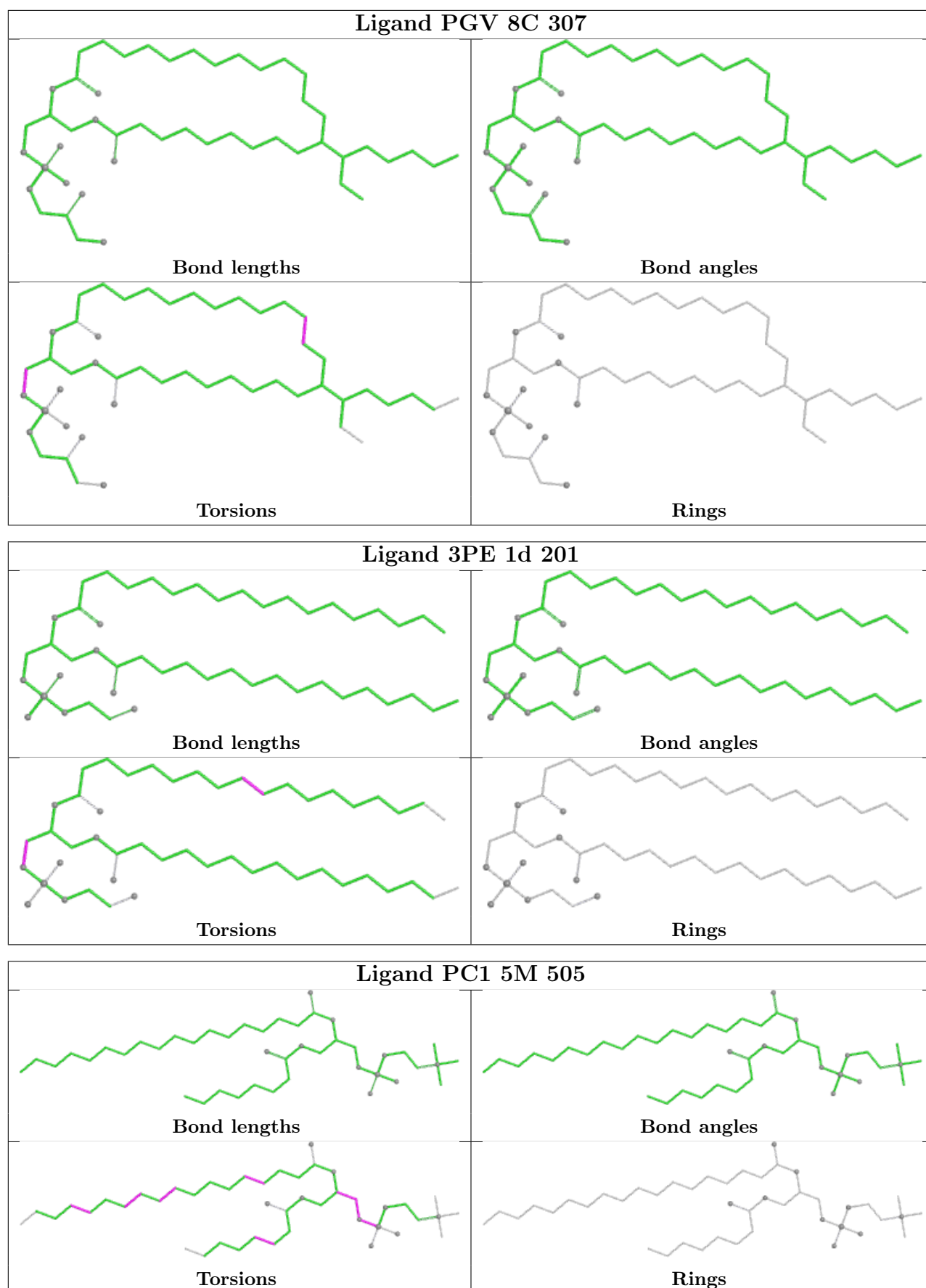
Rings

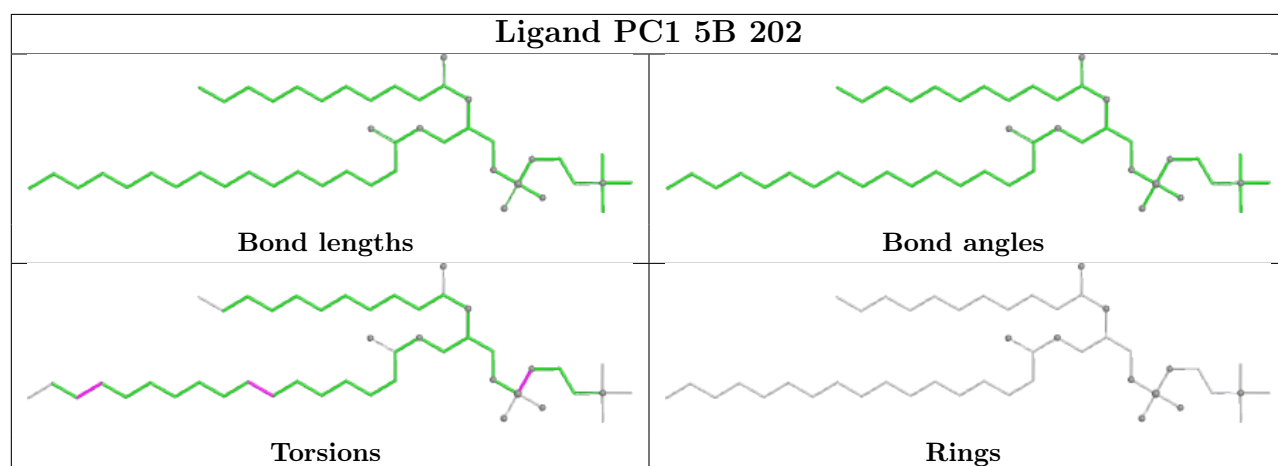
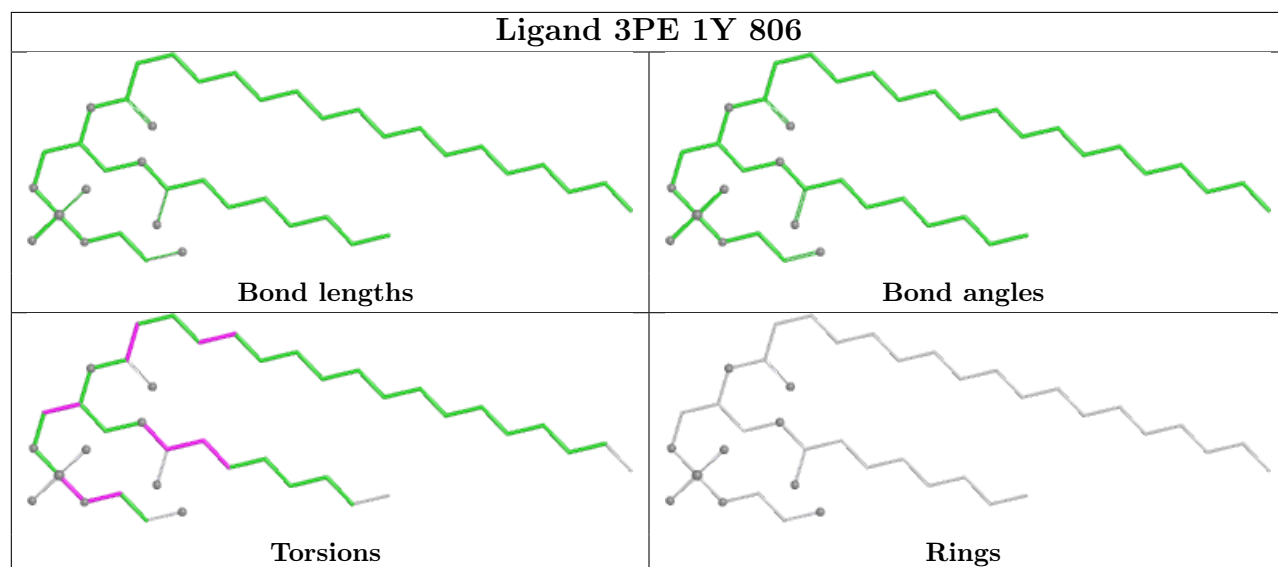
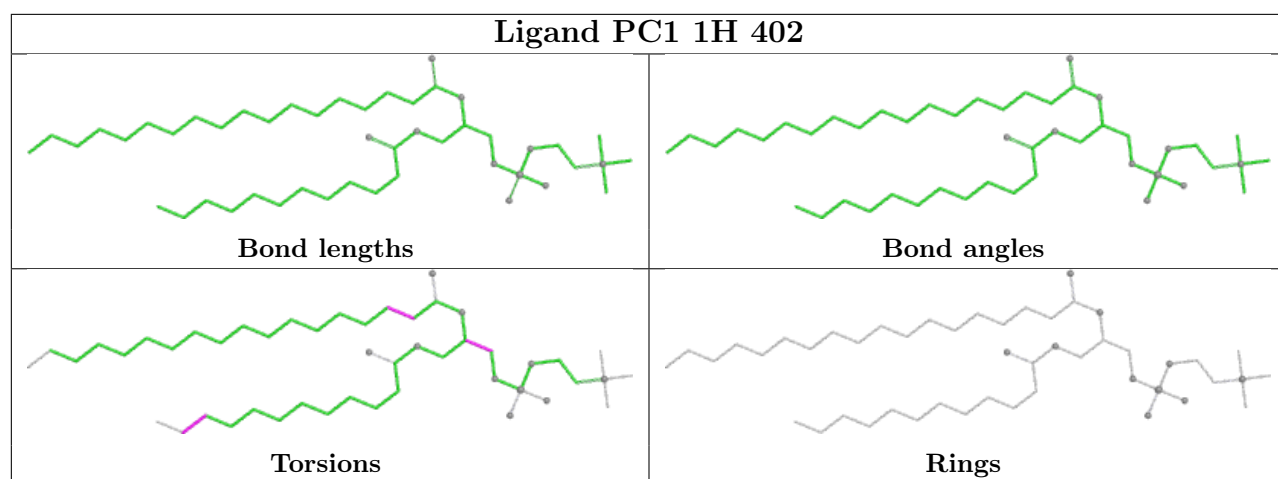


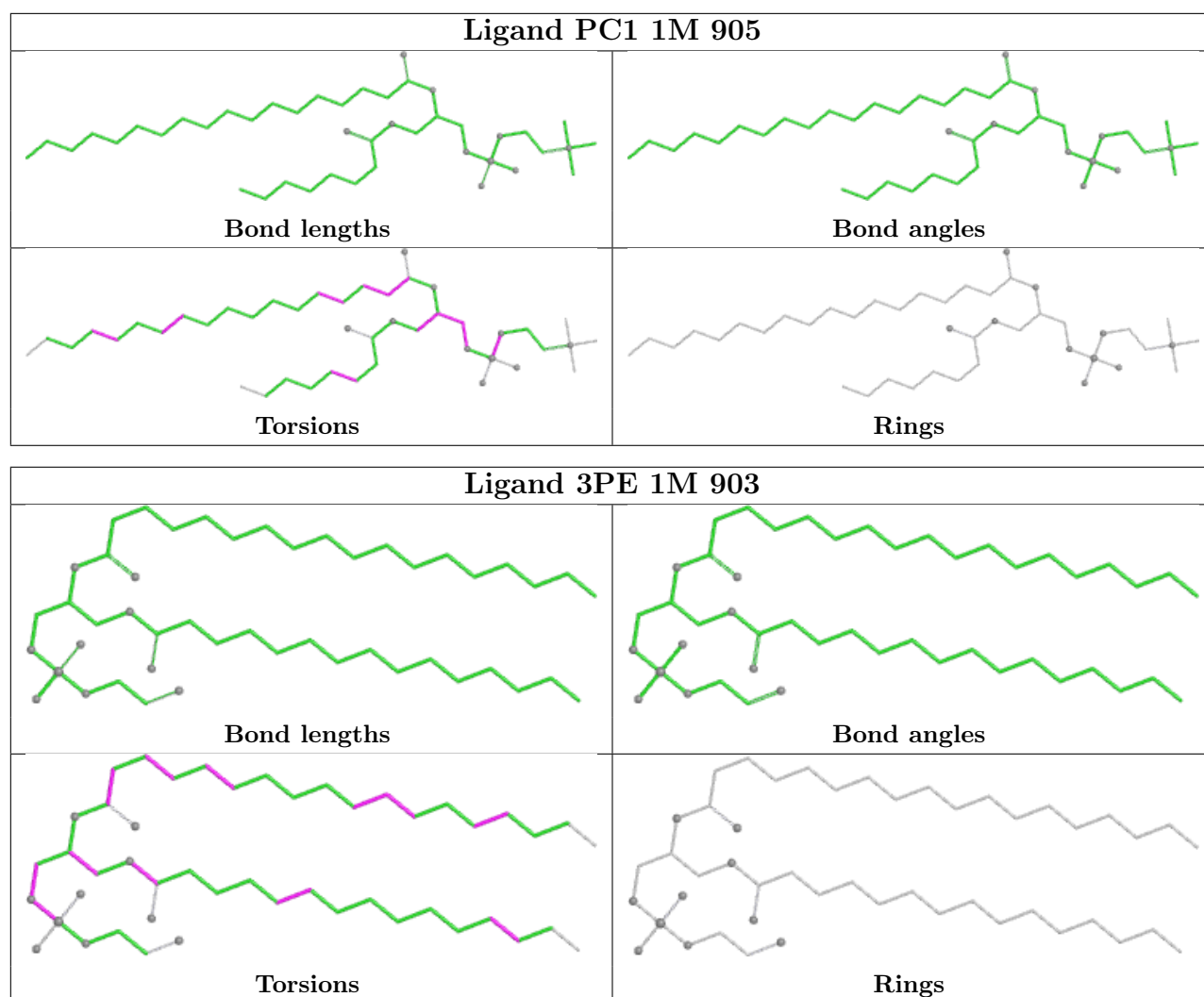


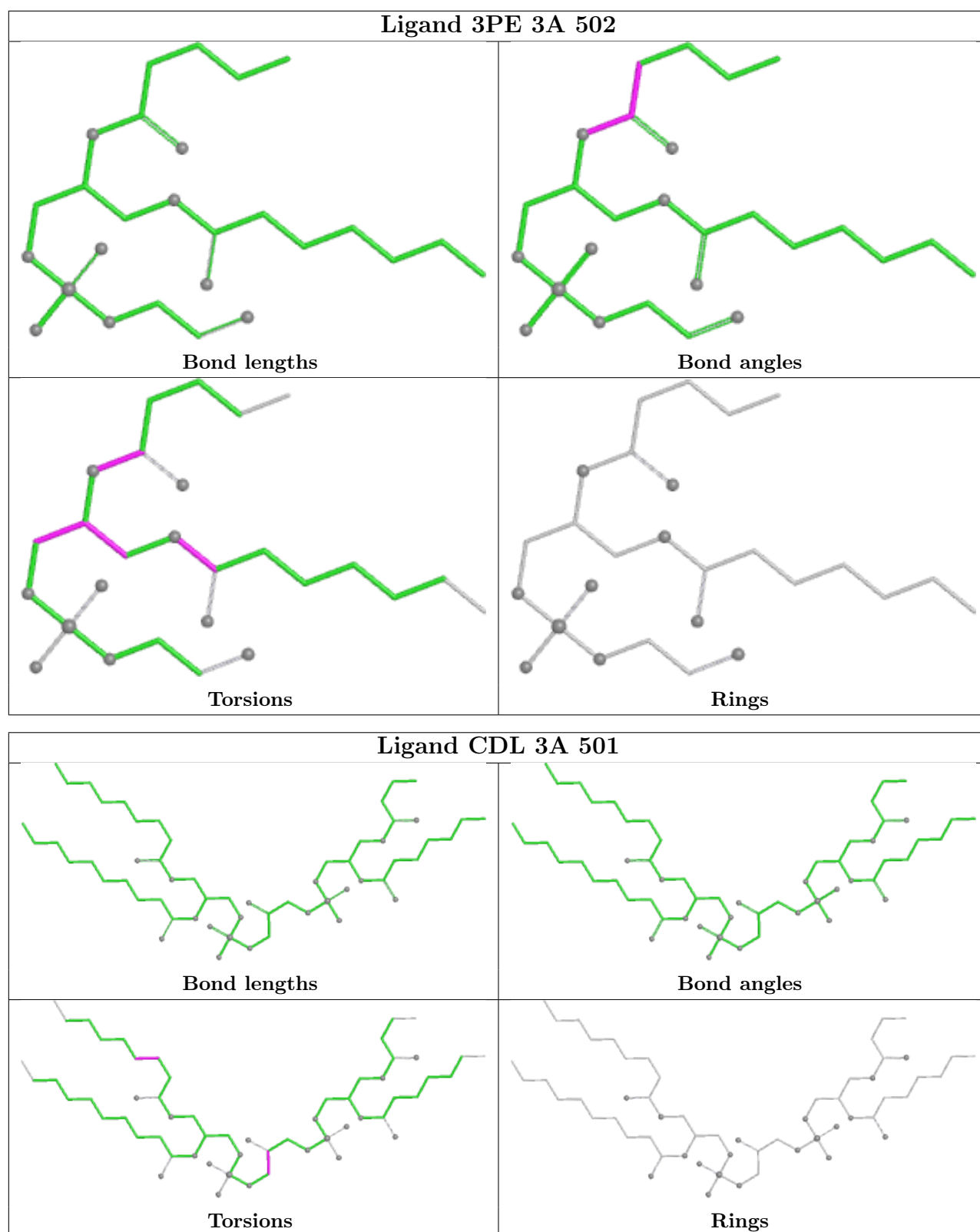


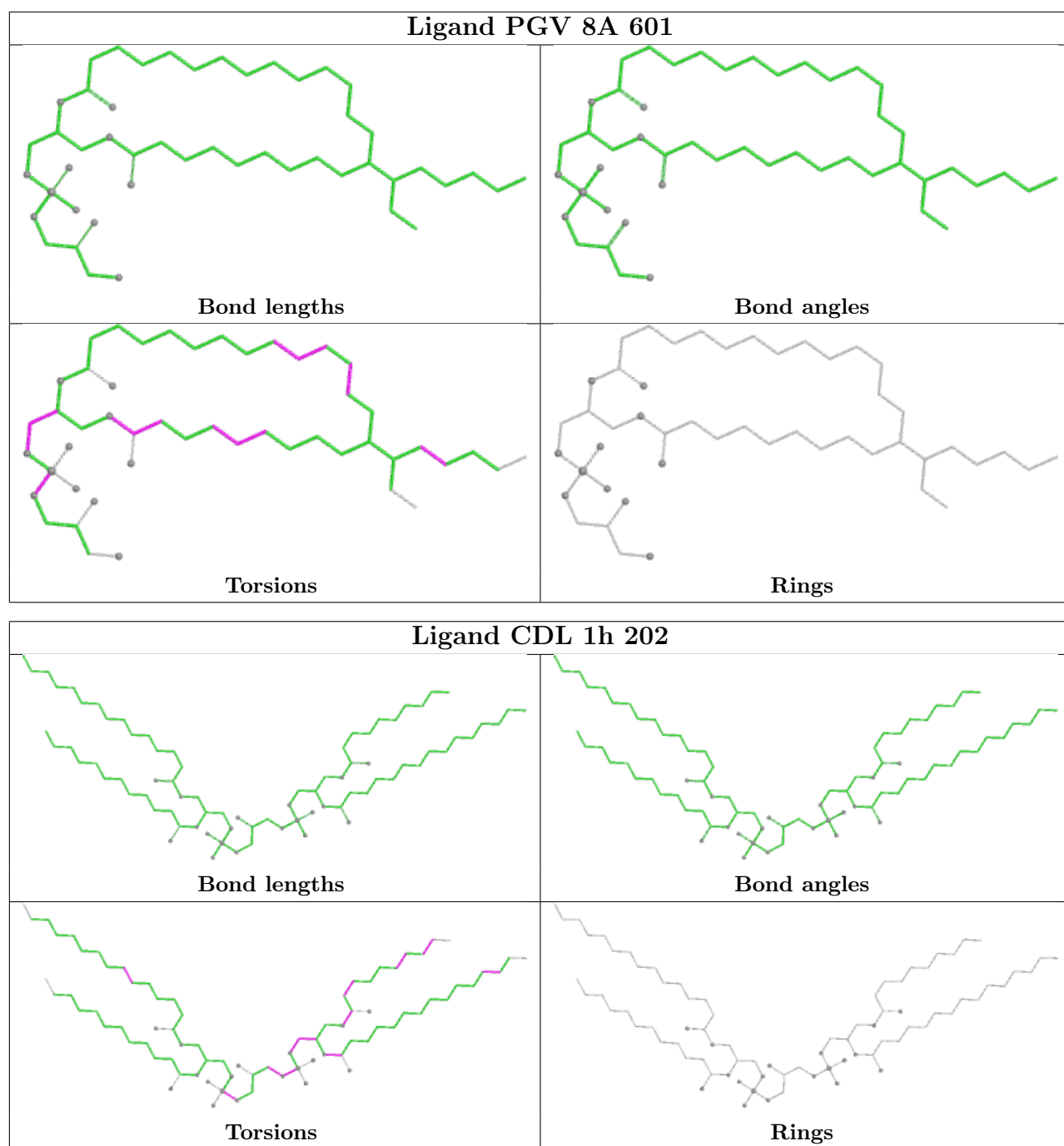


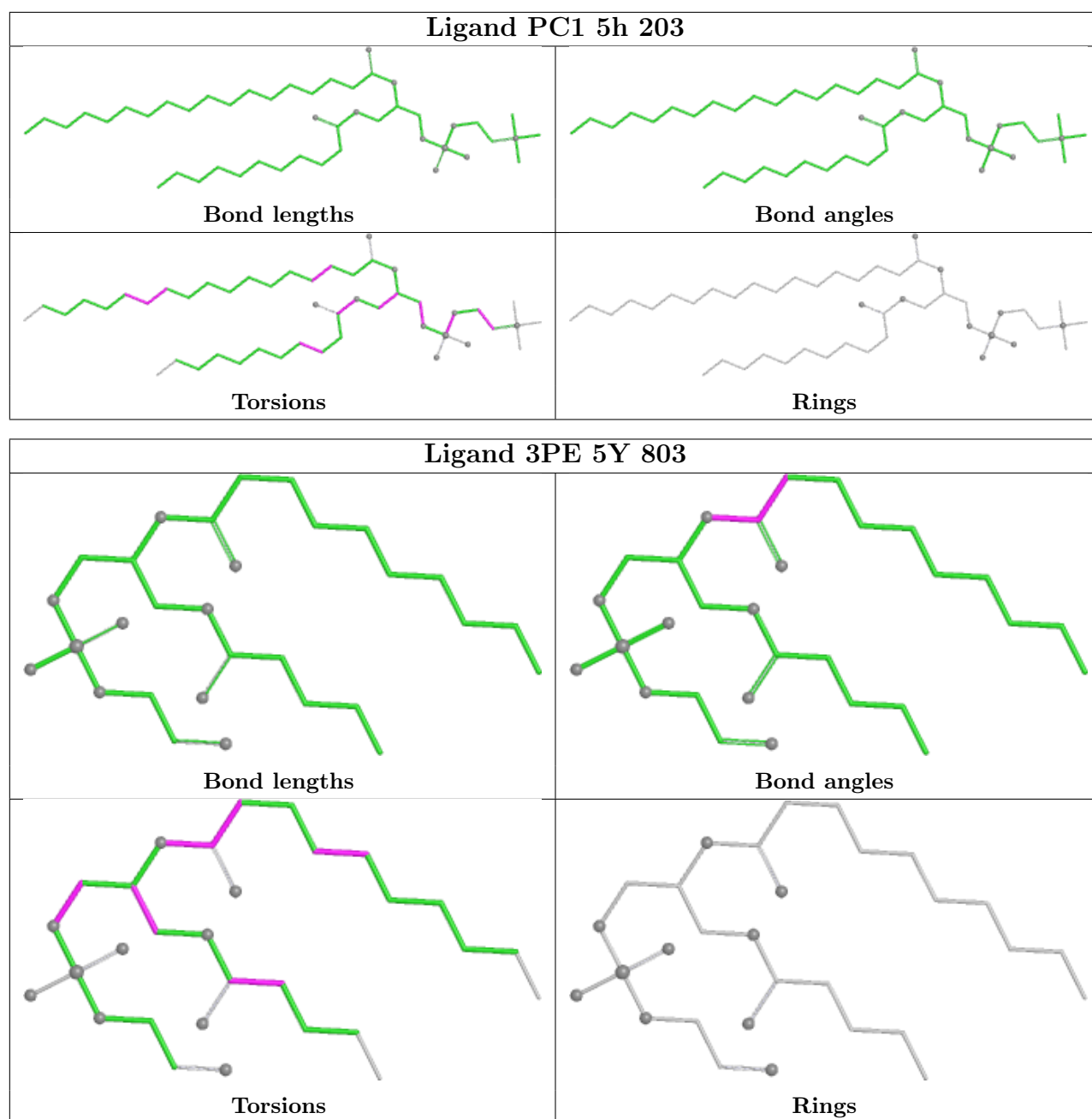


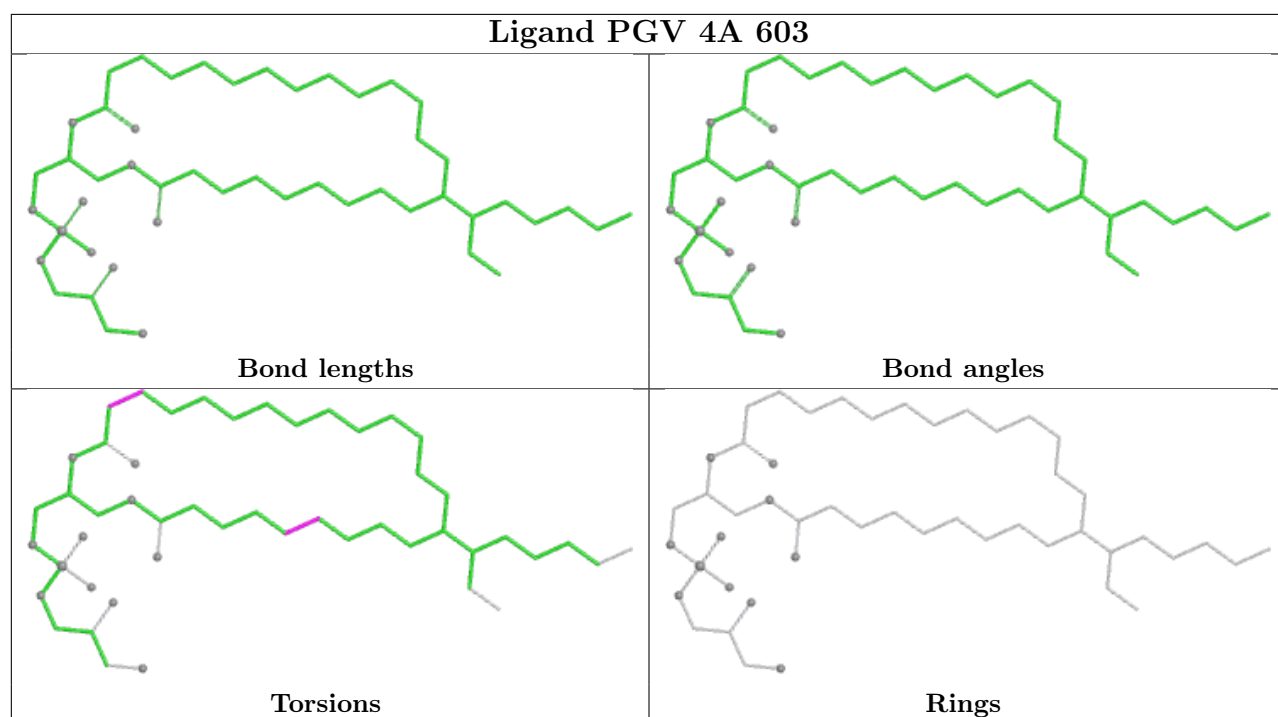
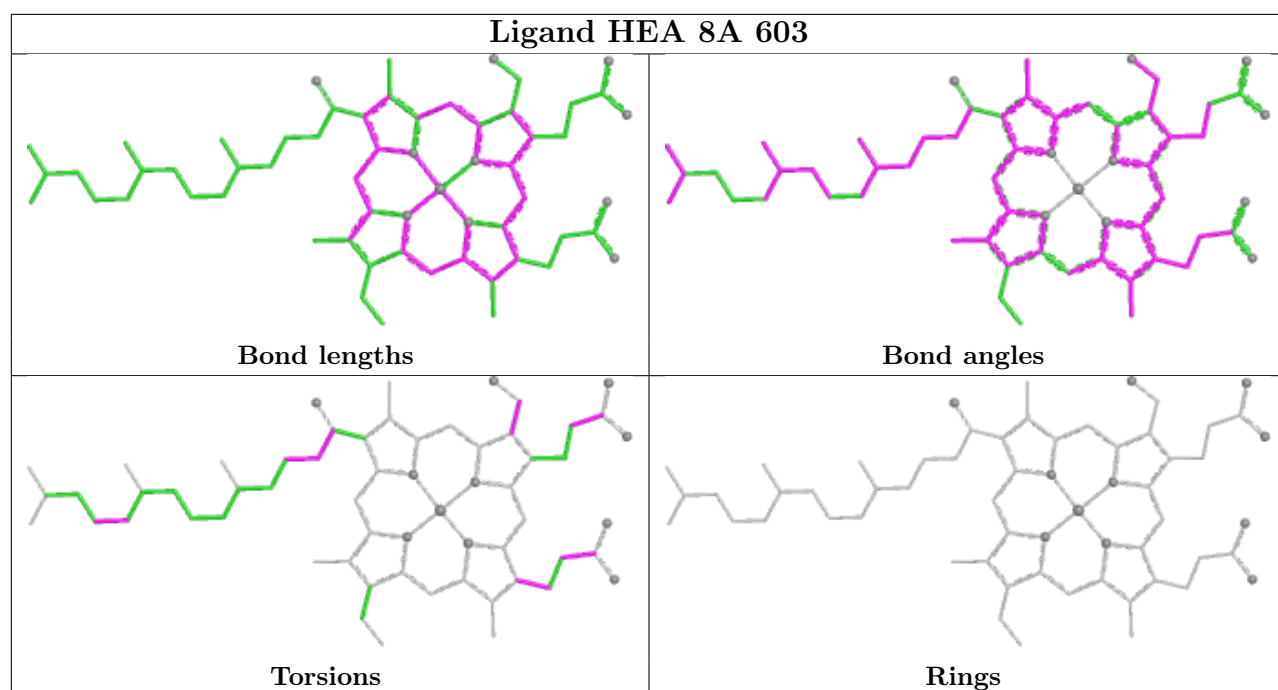


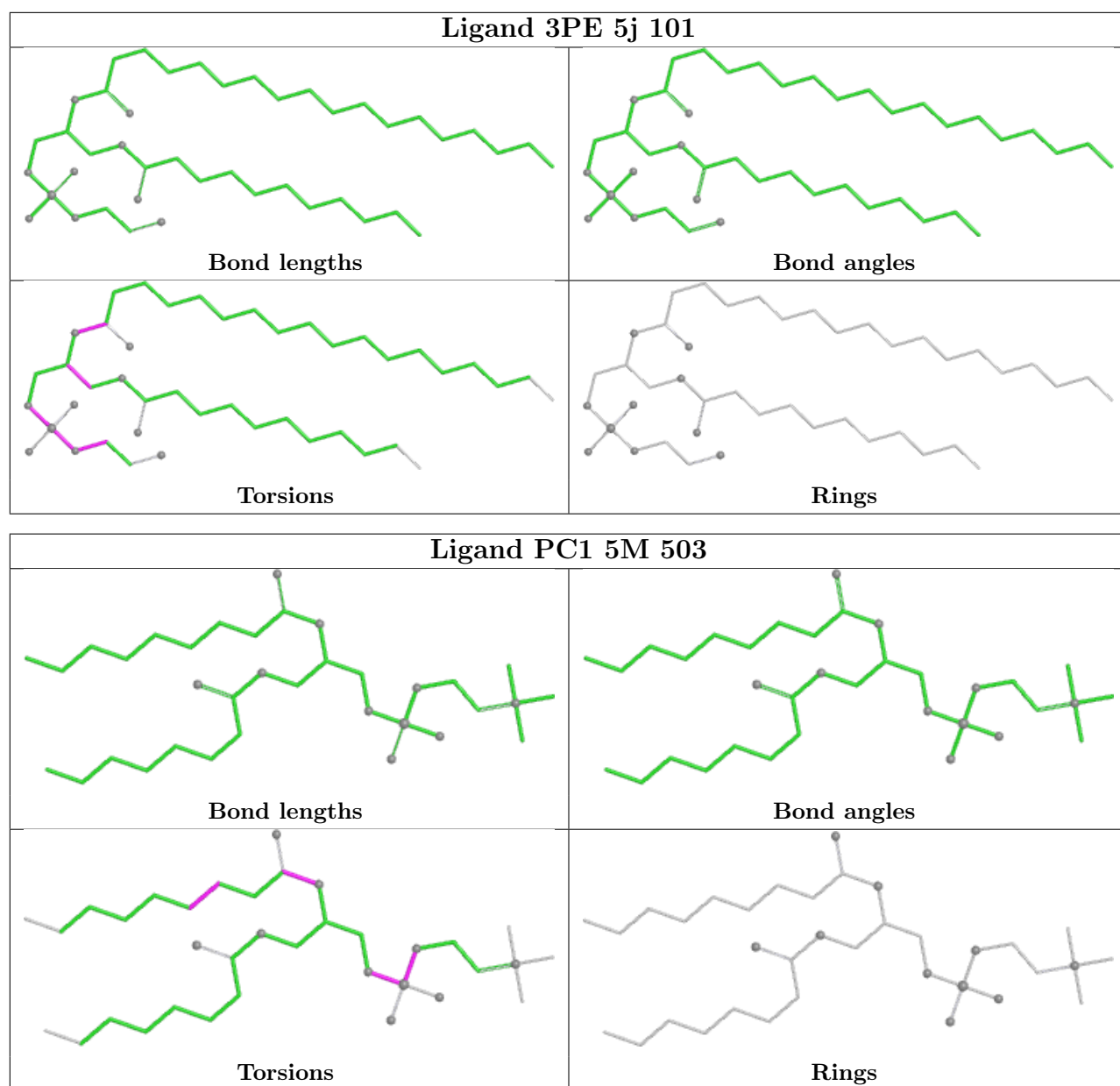


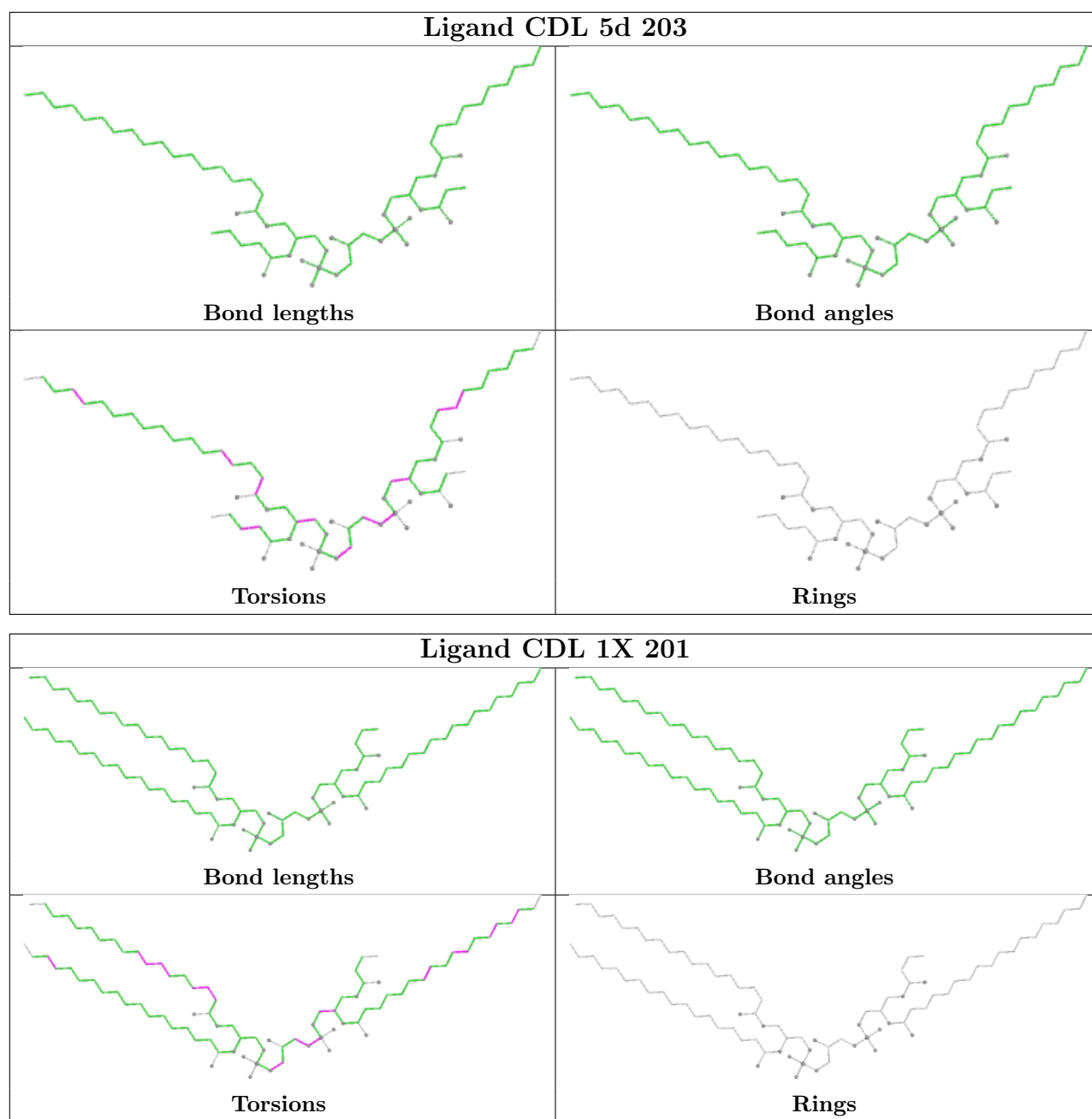


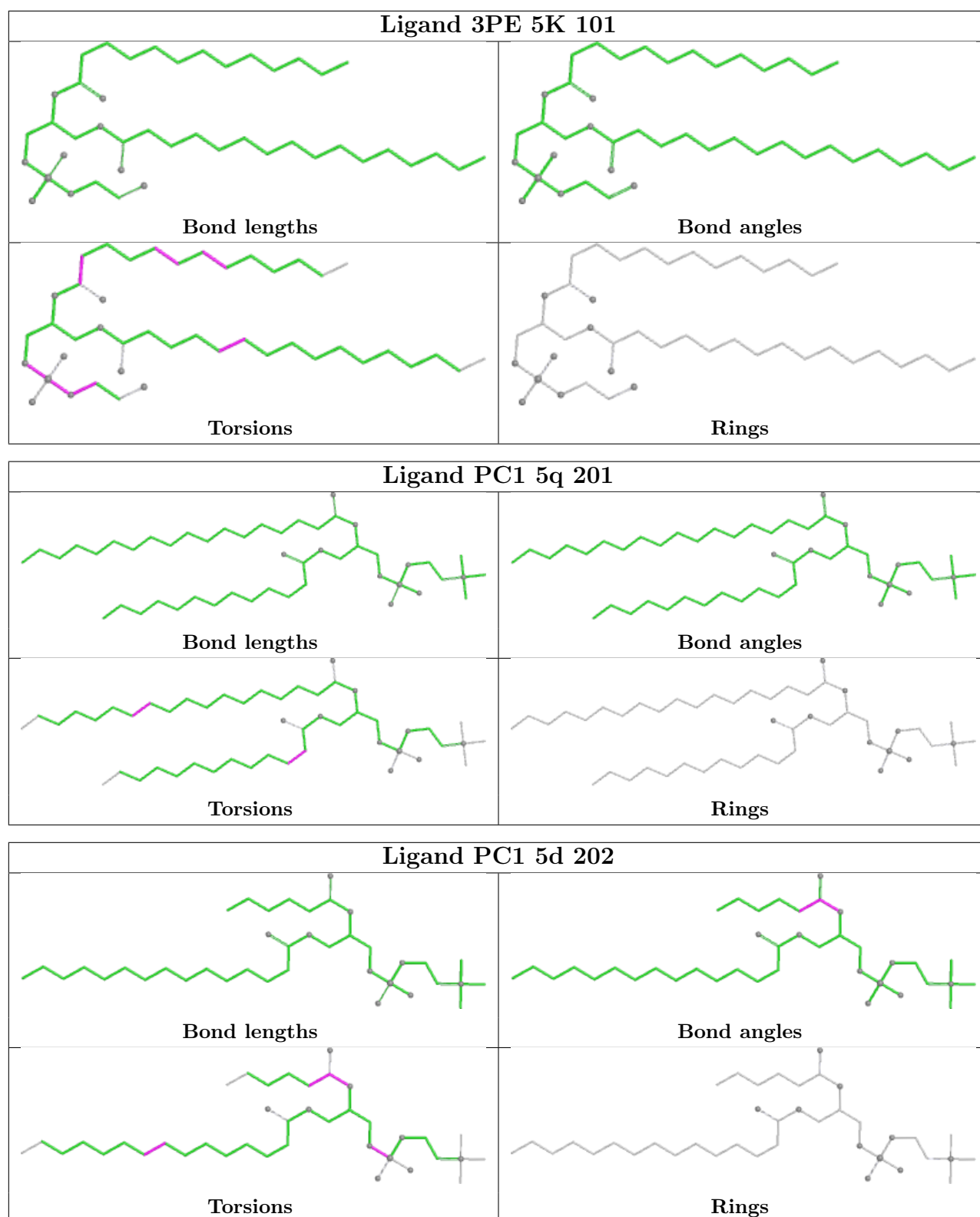


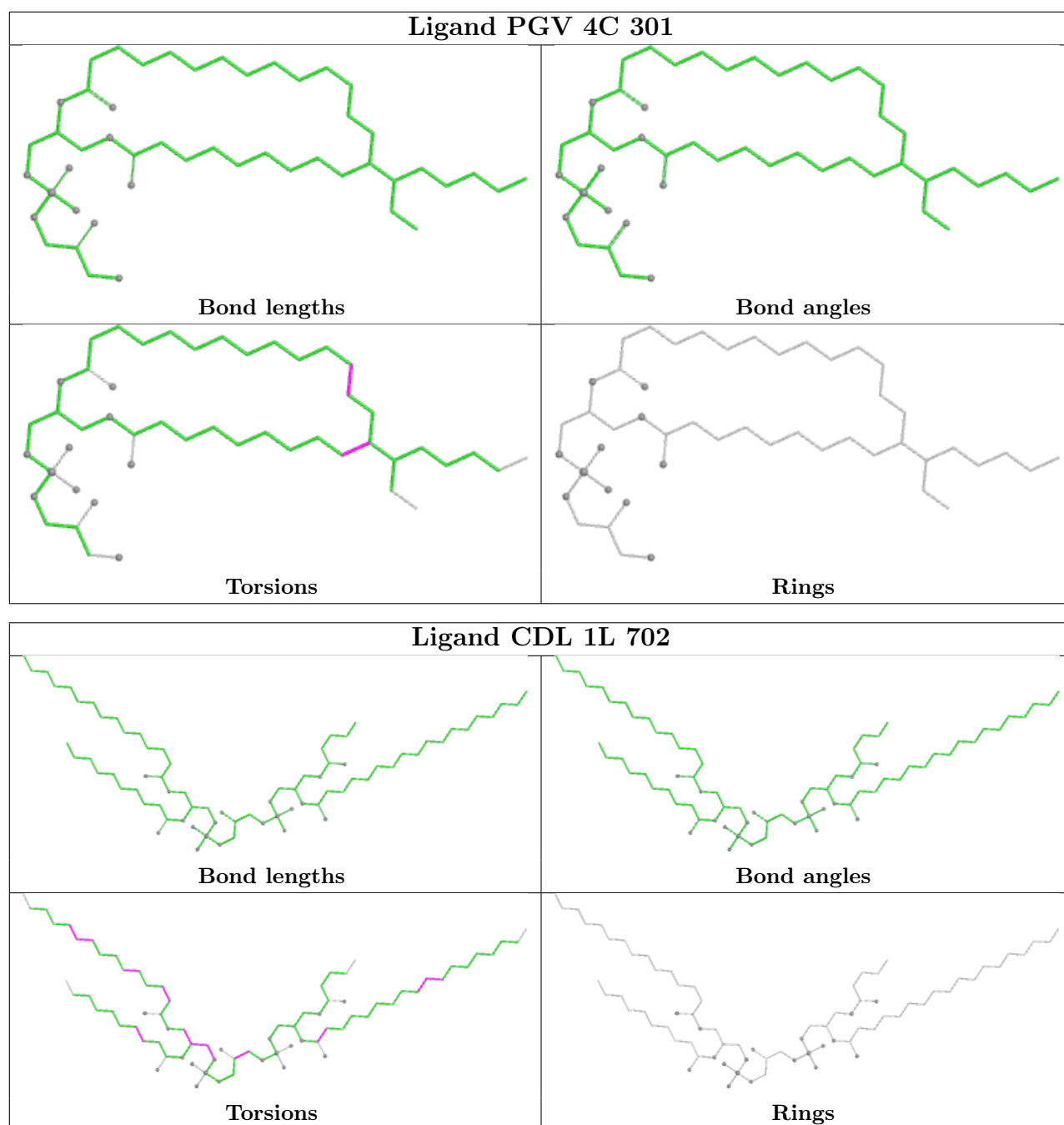


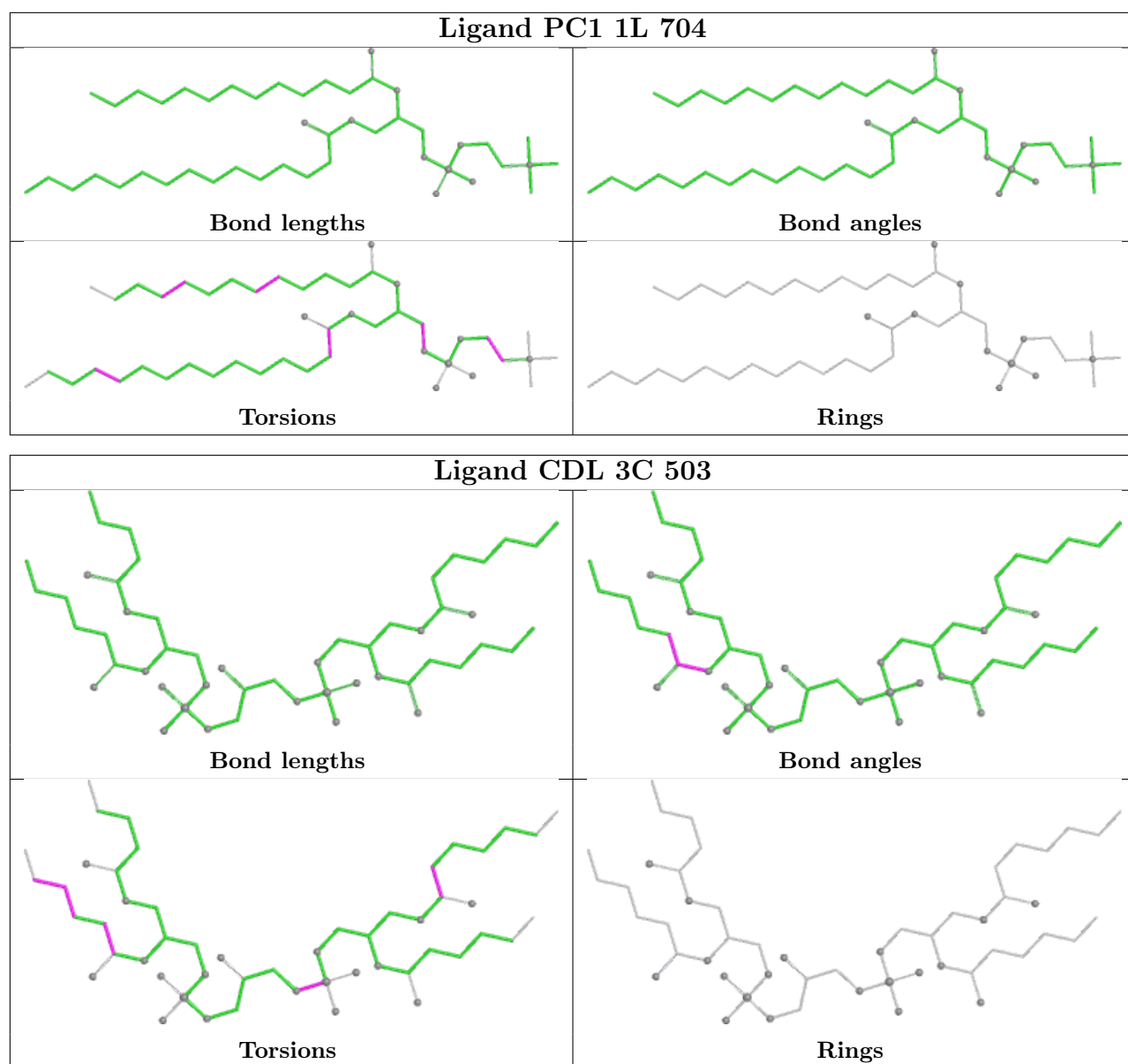


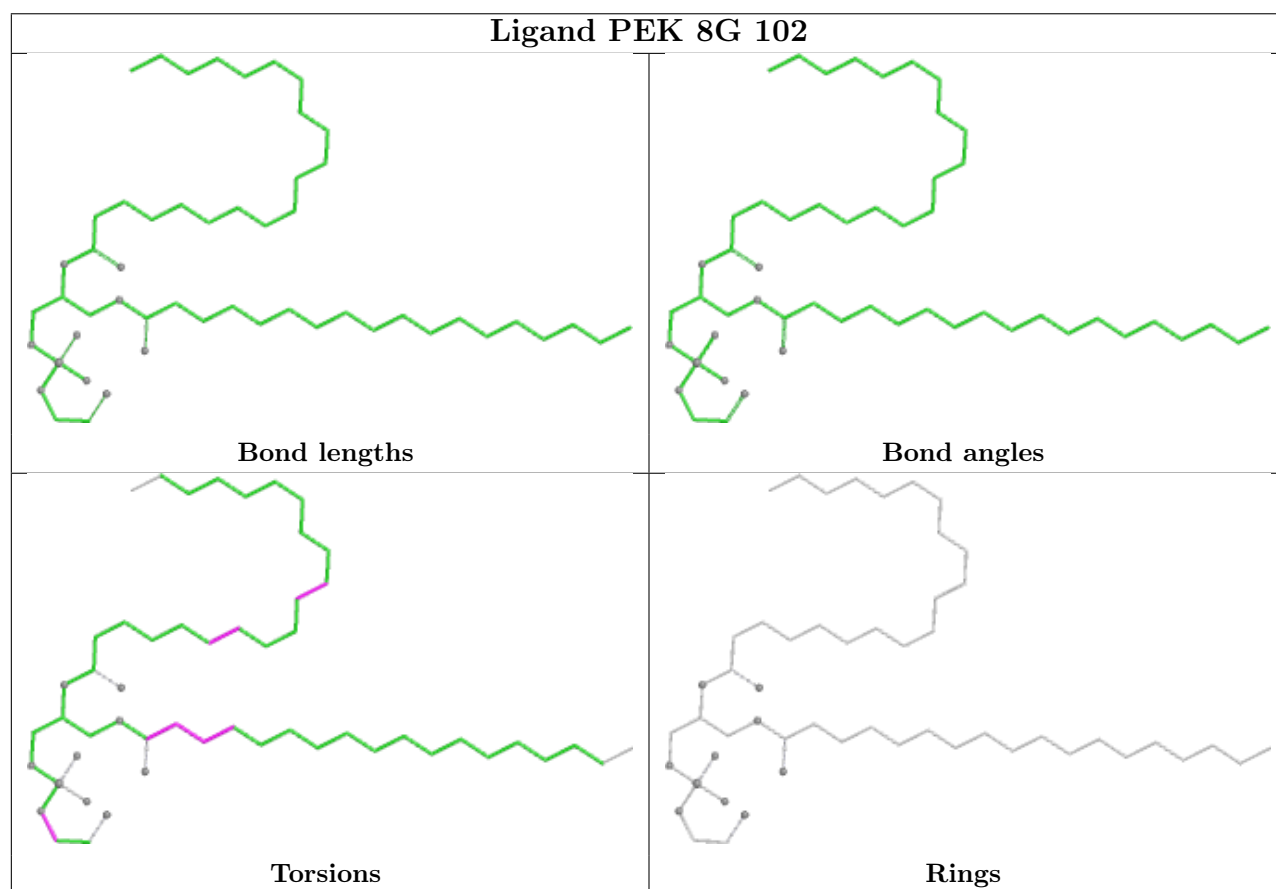
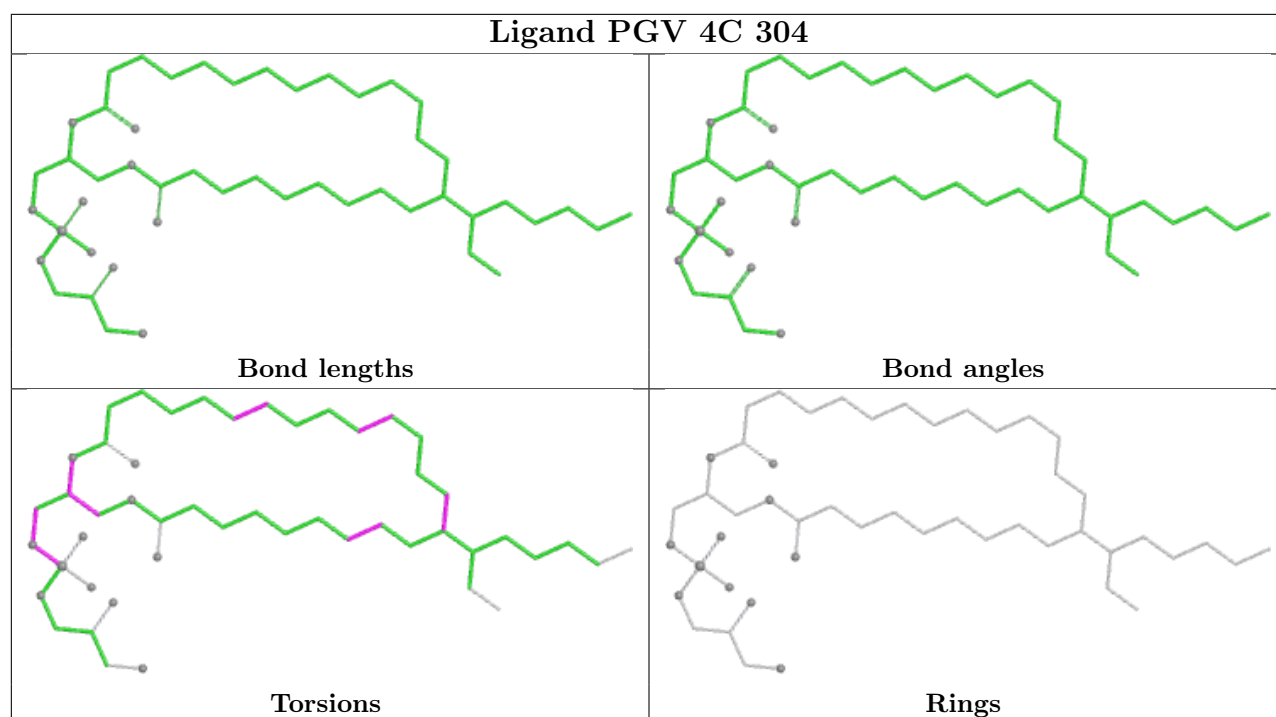


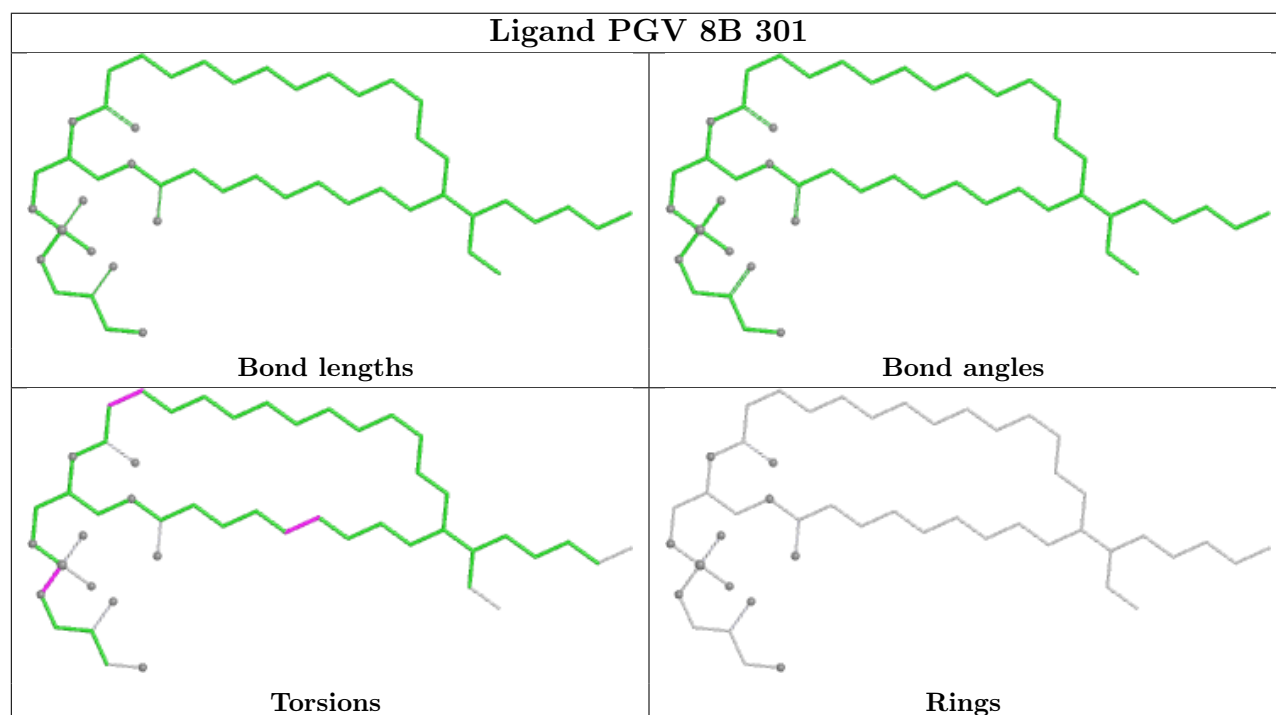
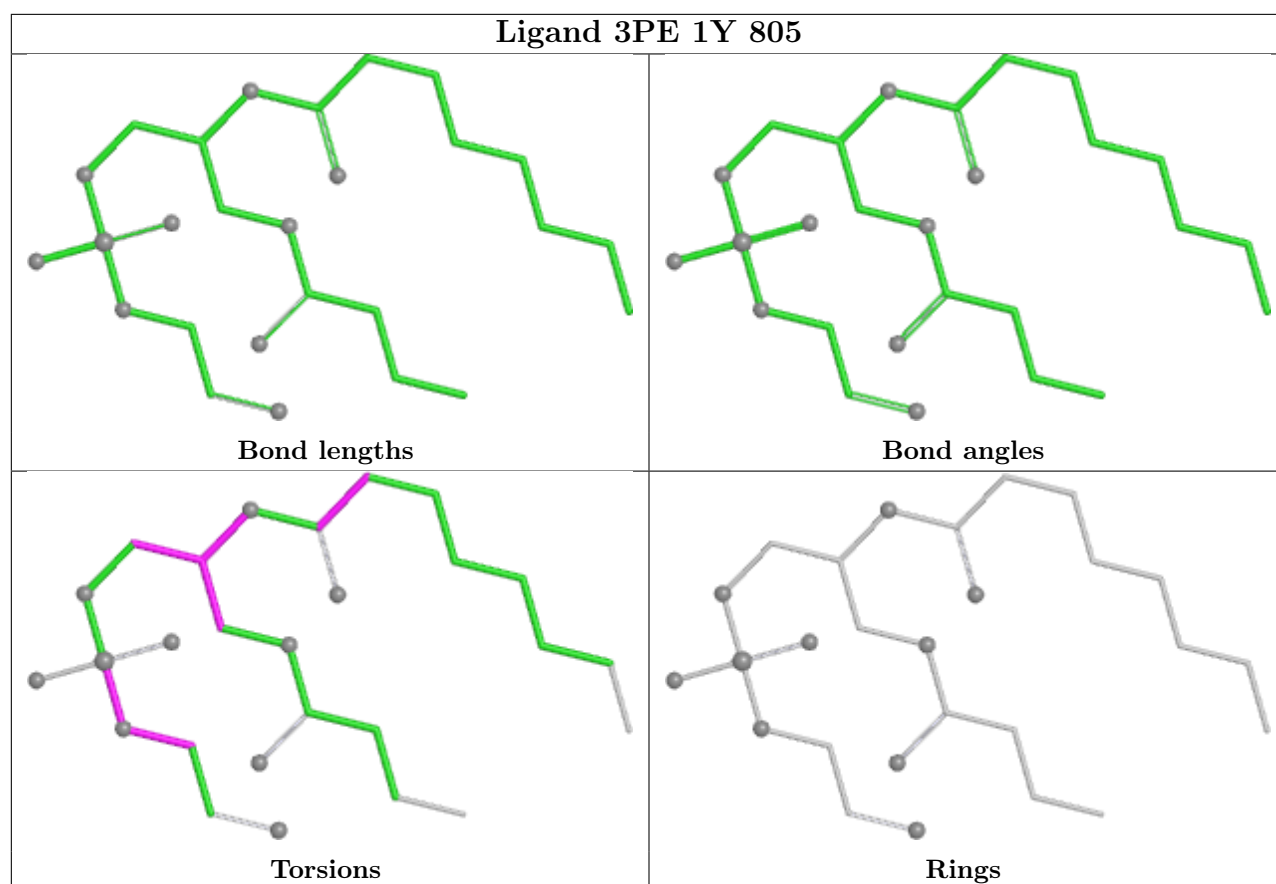


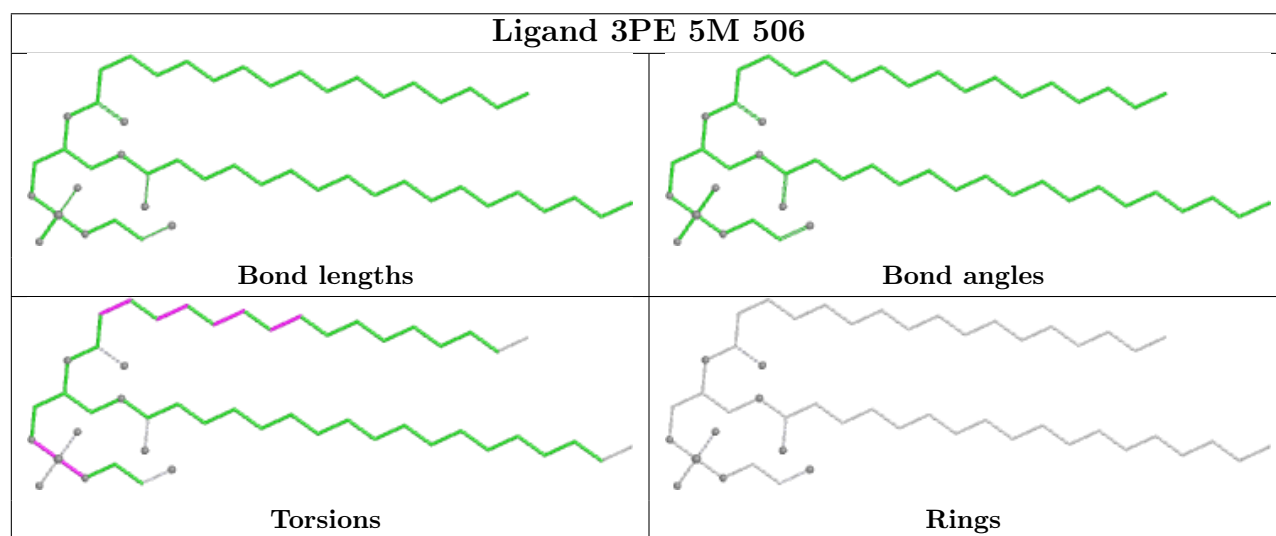
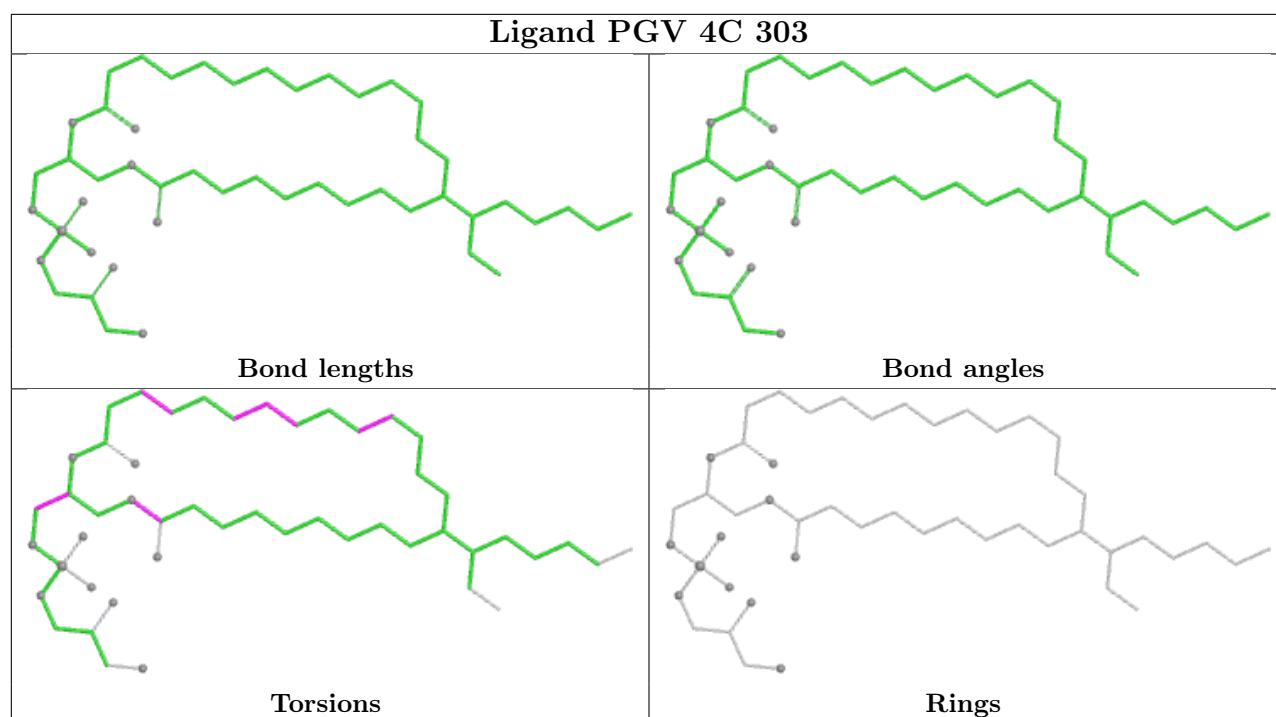




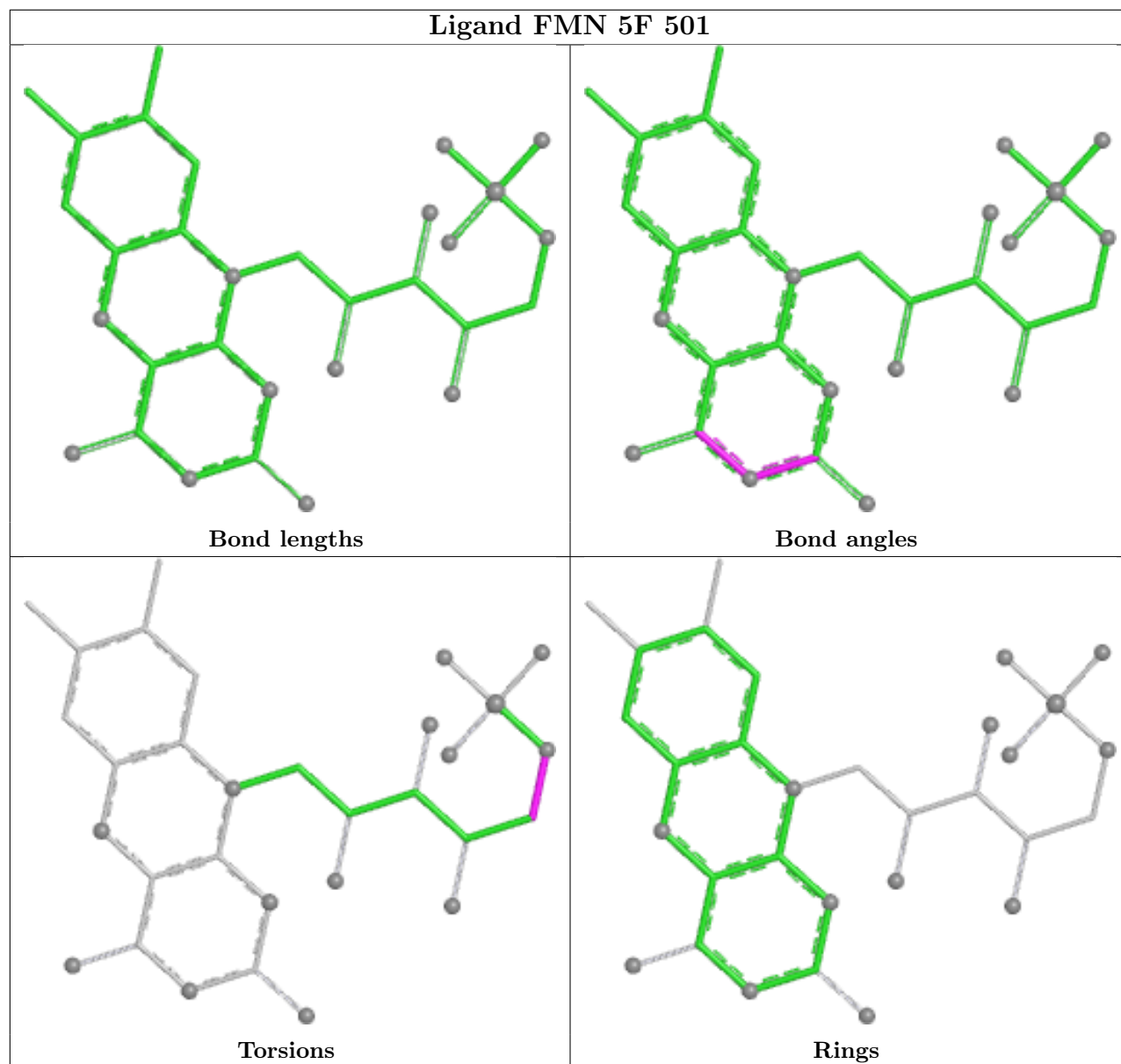


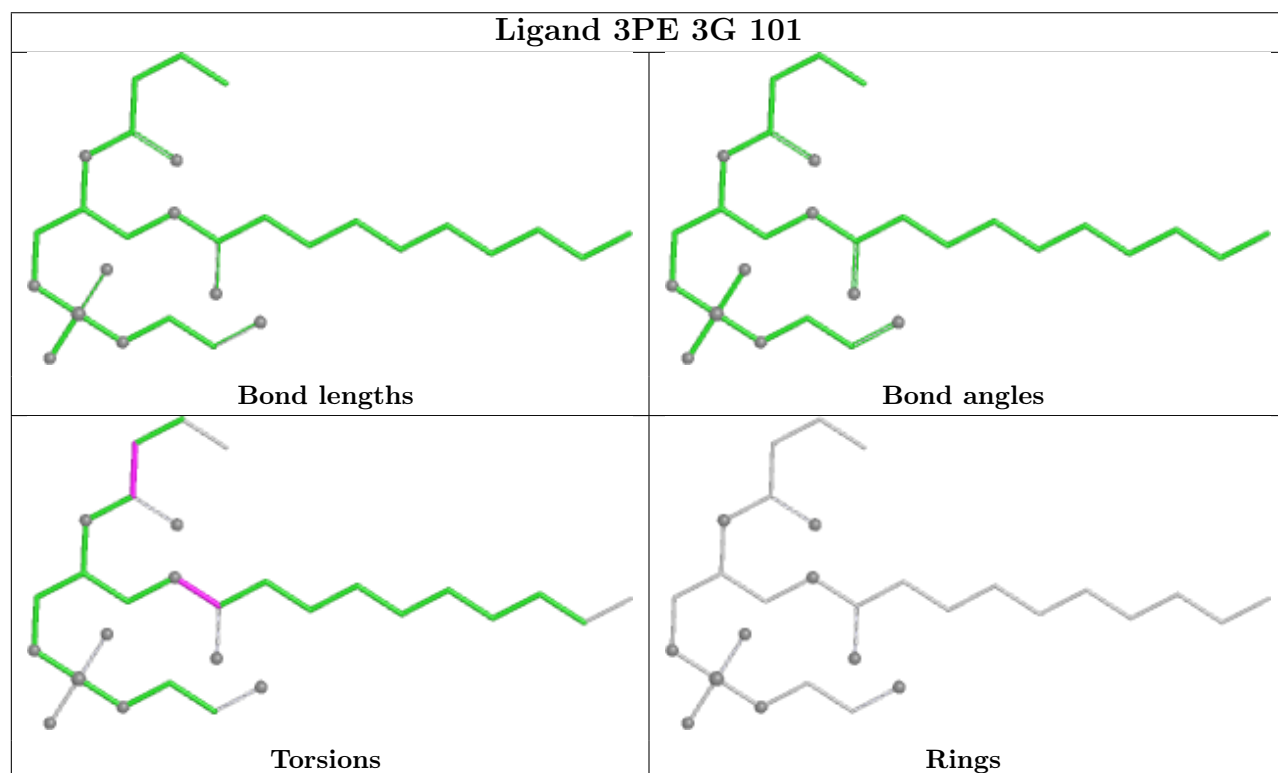
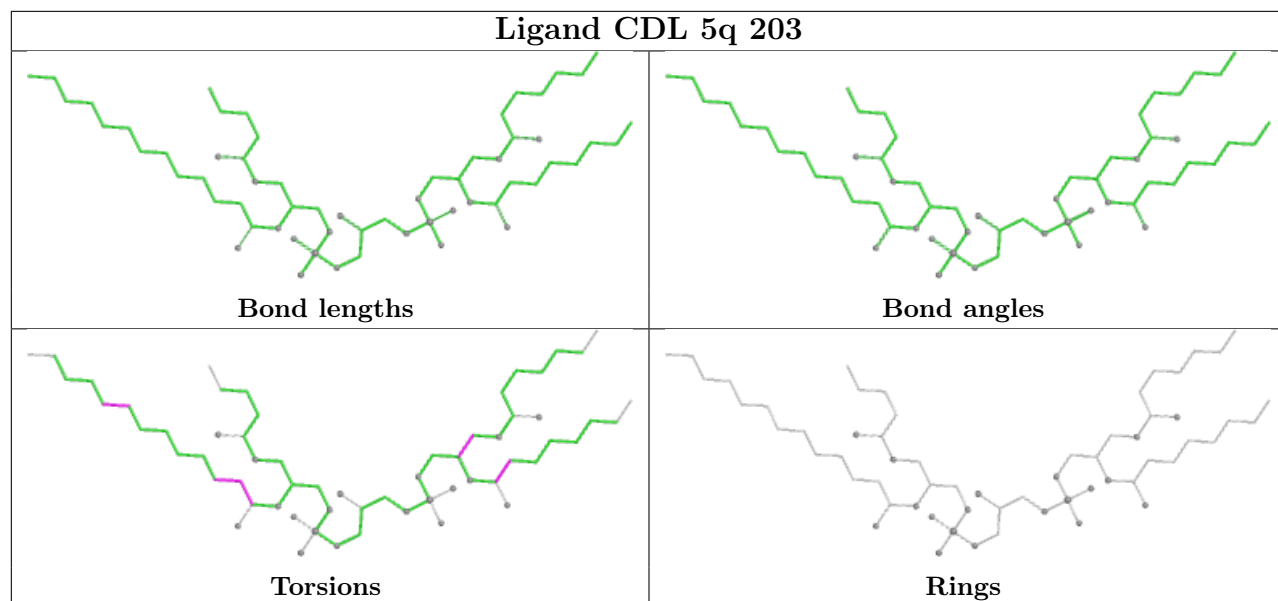




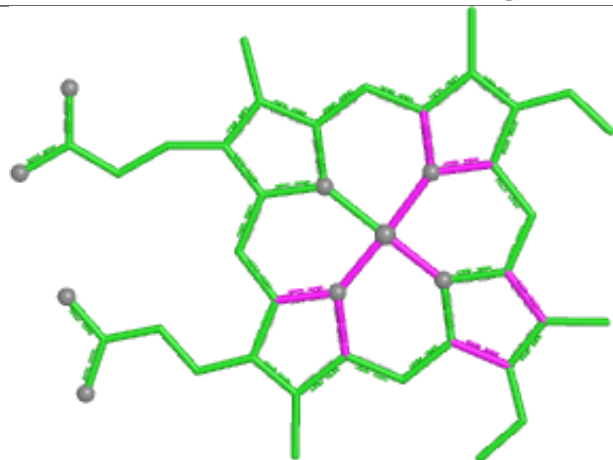


Ligand FMN 5F 501

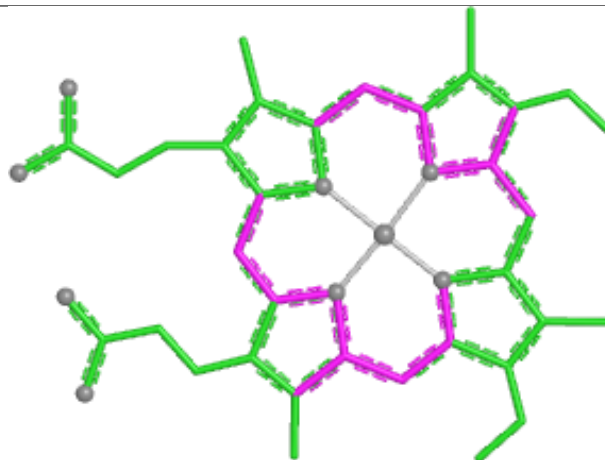




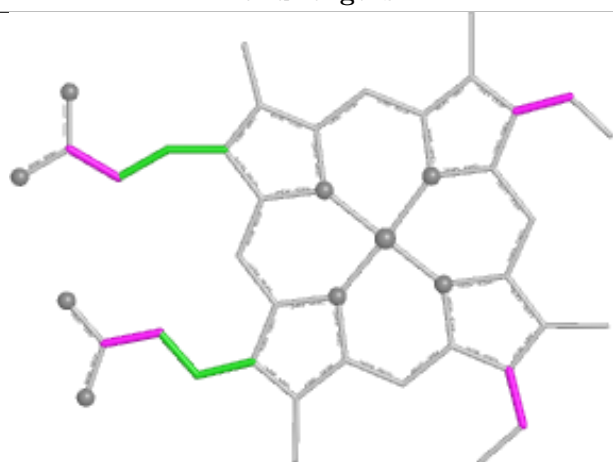
Ligand HEM 3P 502



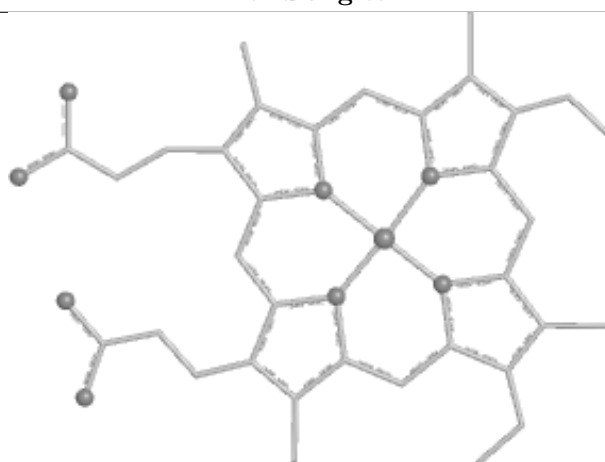
Bond lengths



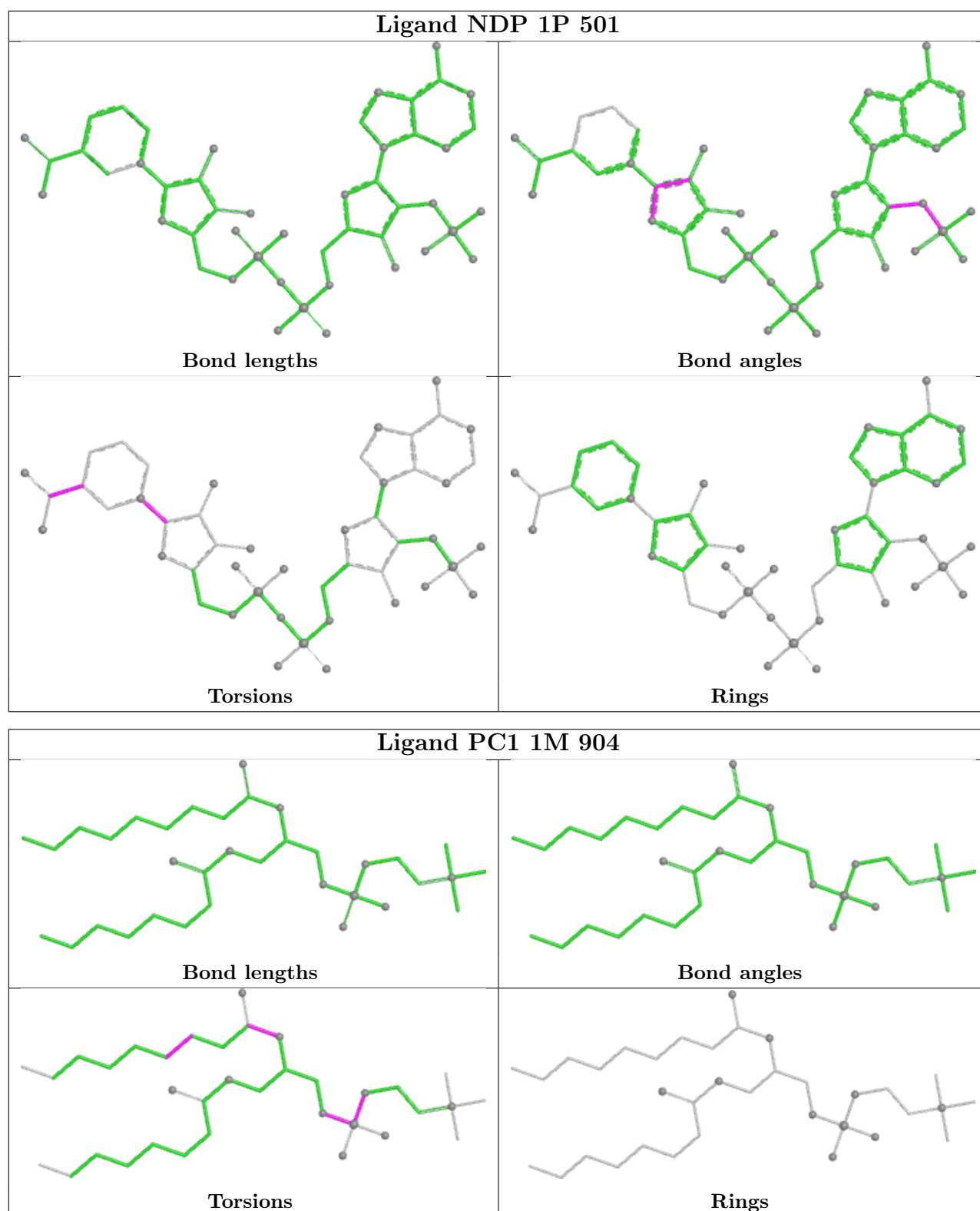
Bond angles

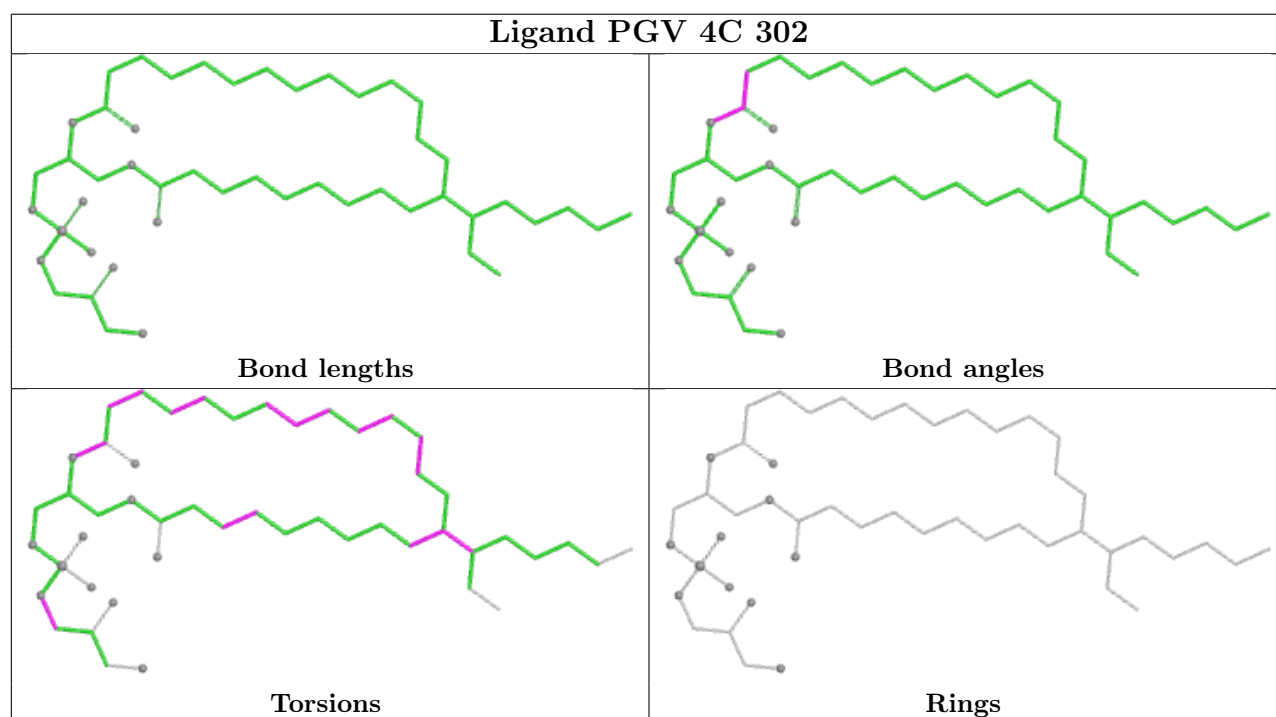
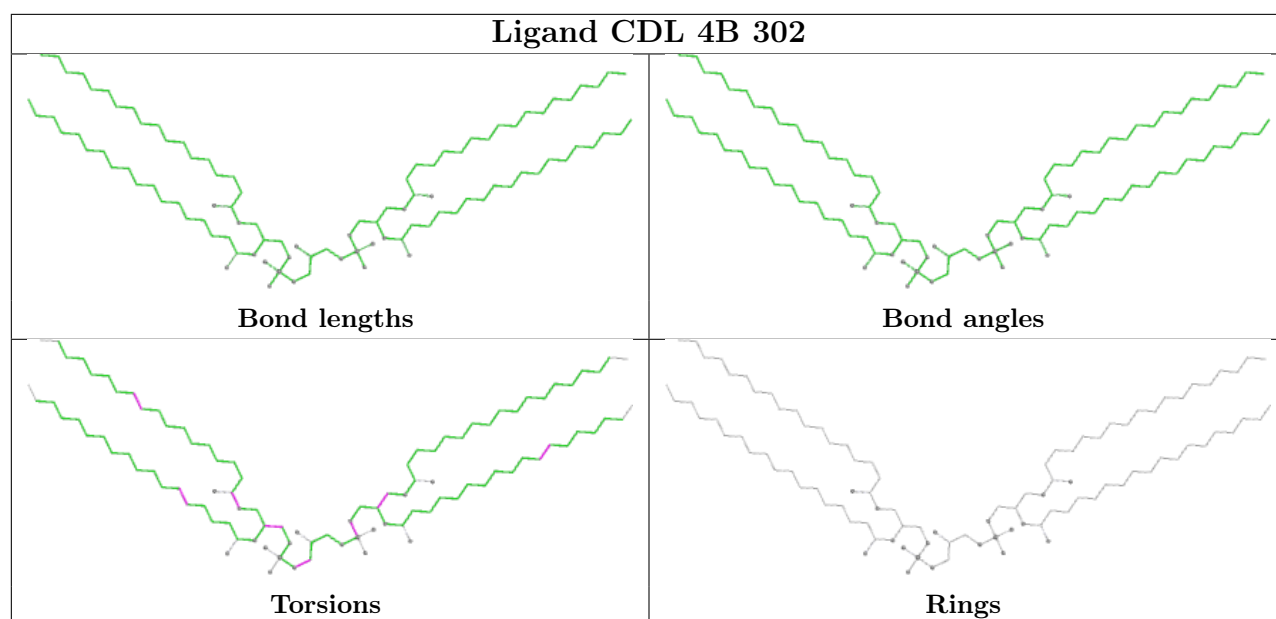


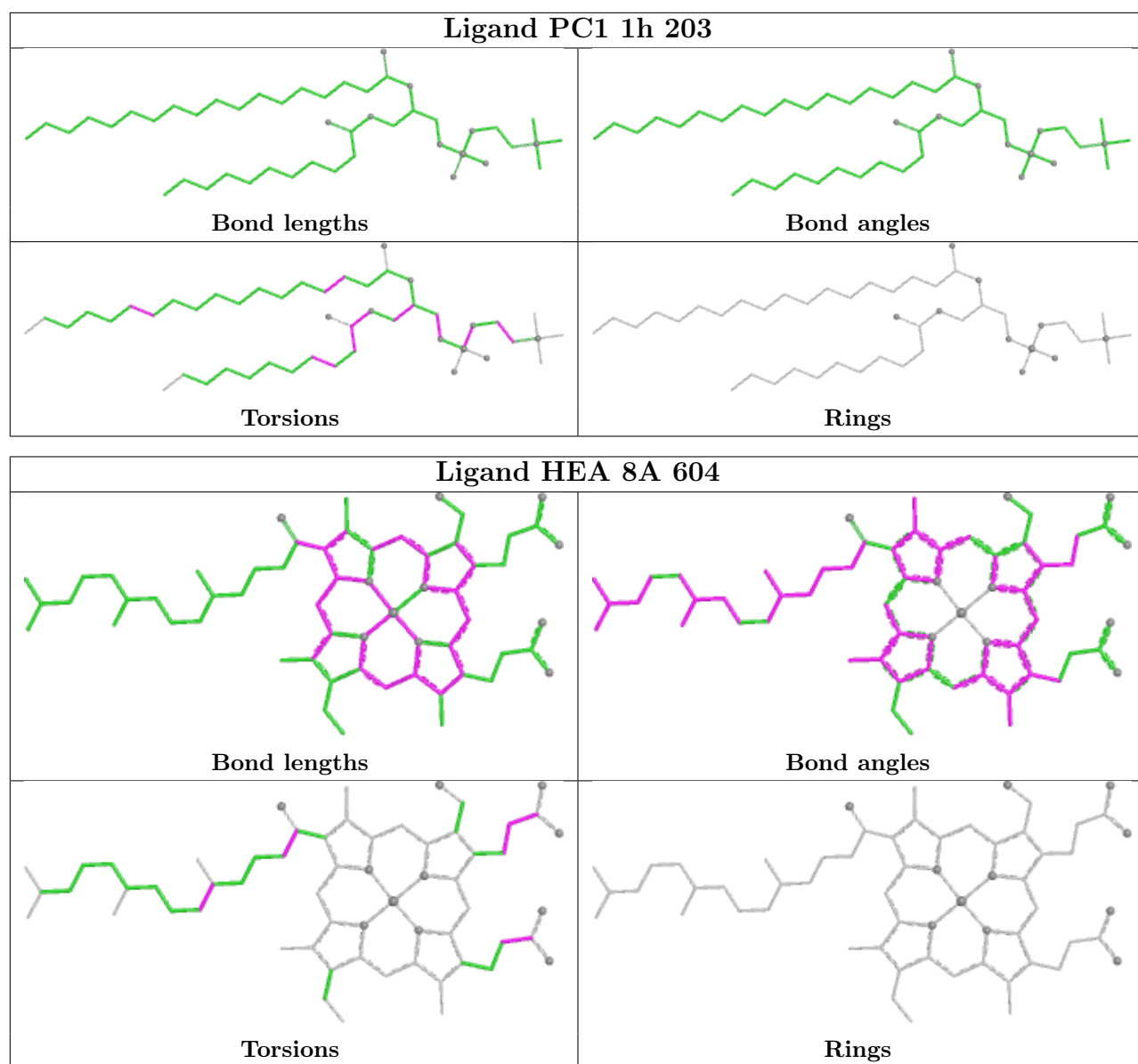
Torsions

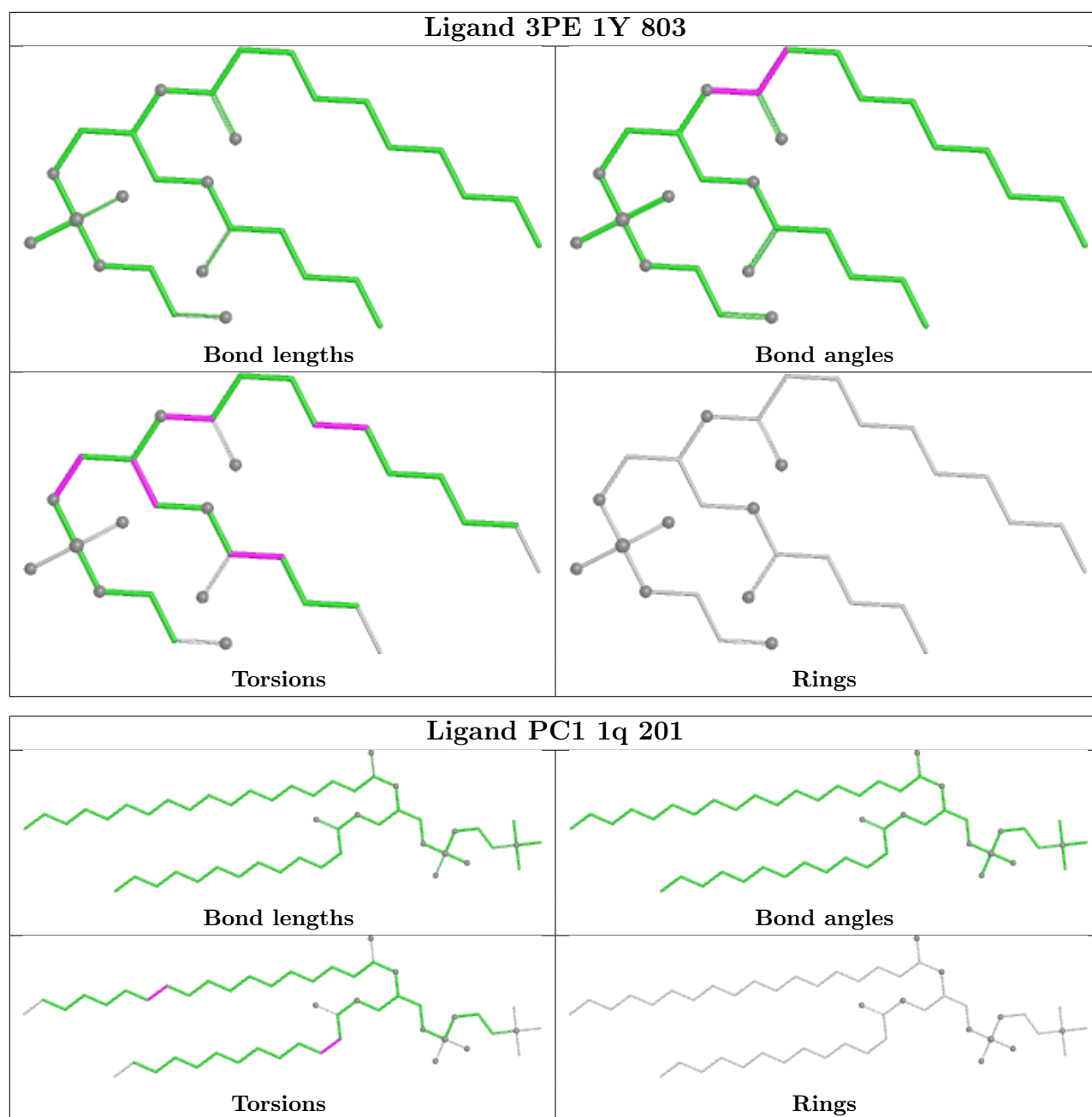


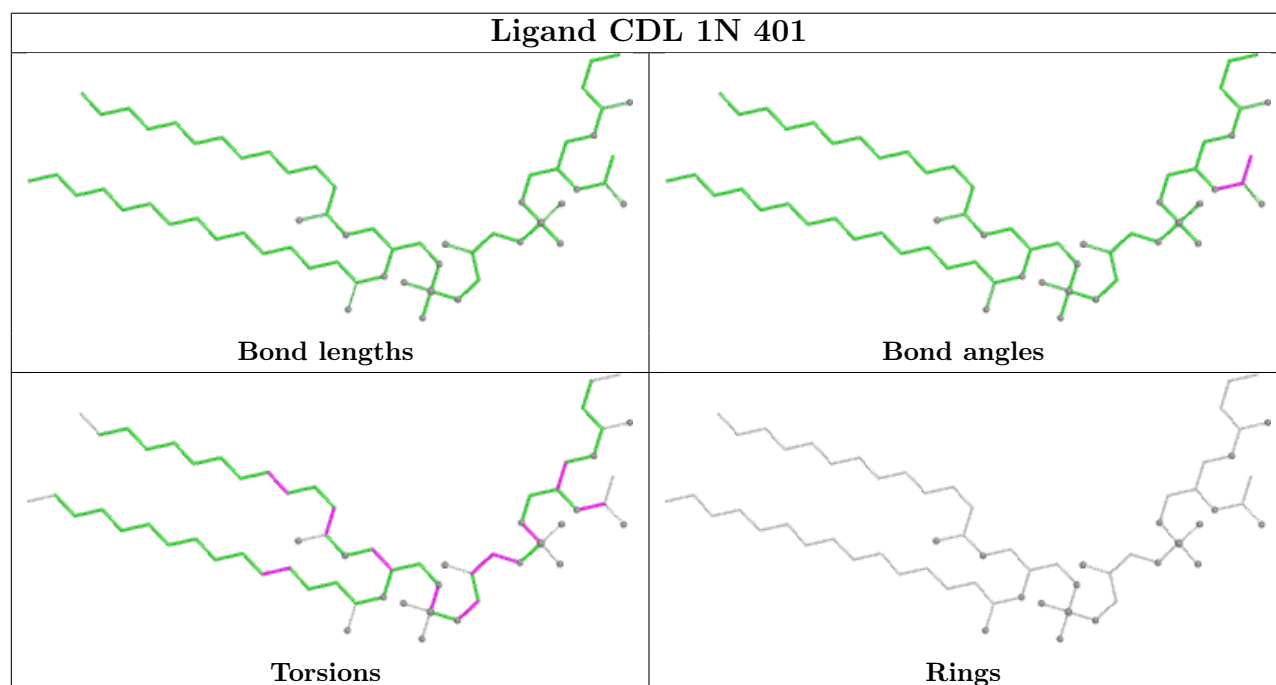
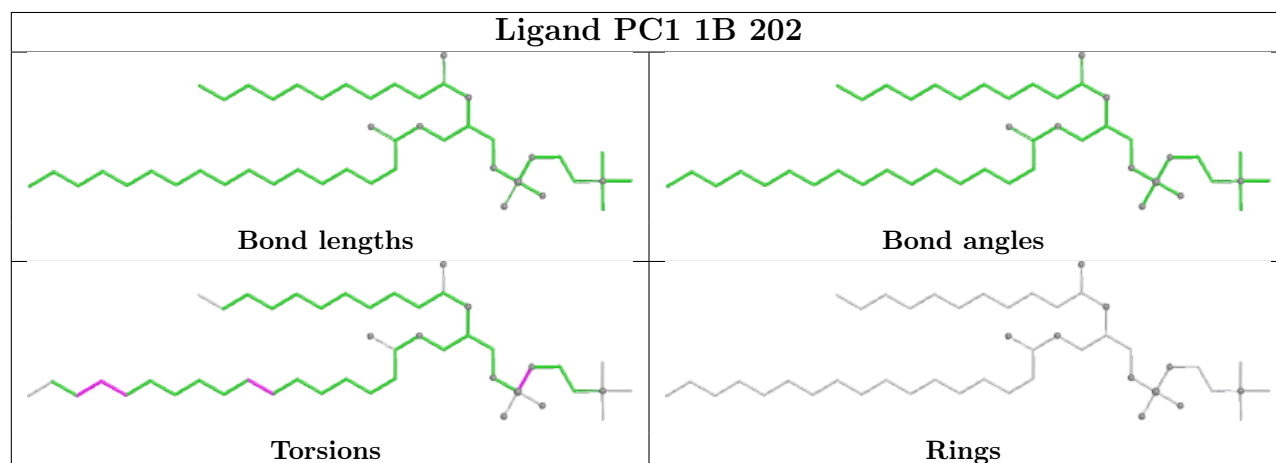
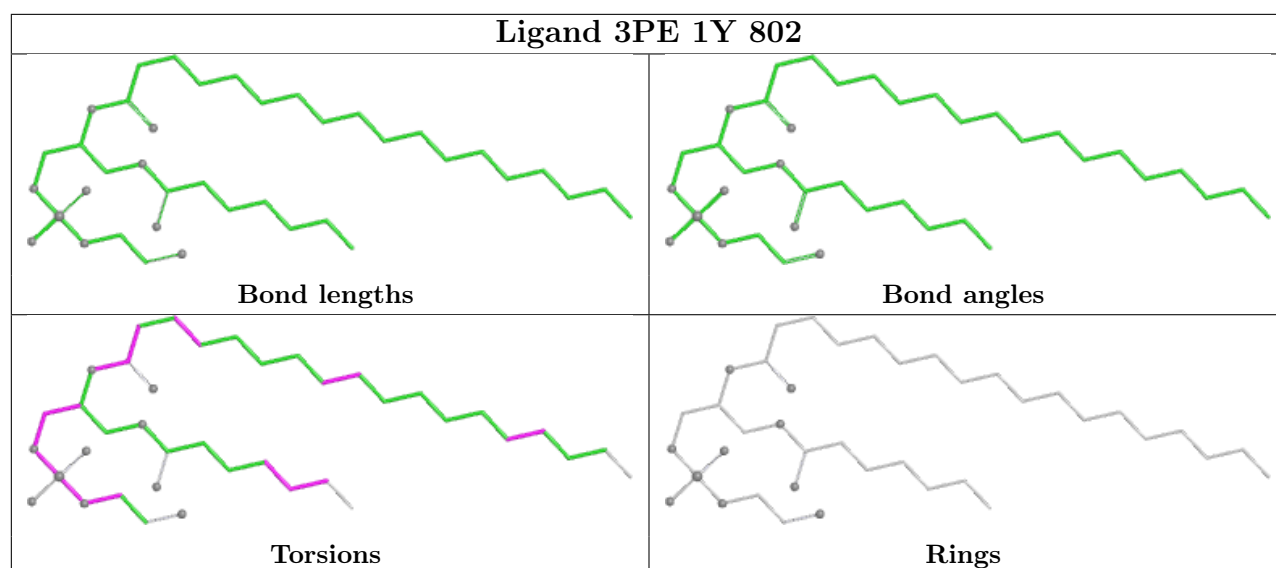
Rings

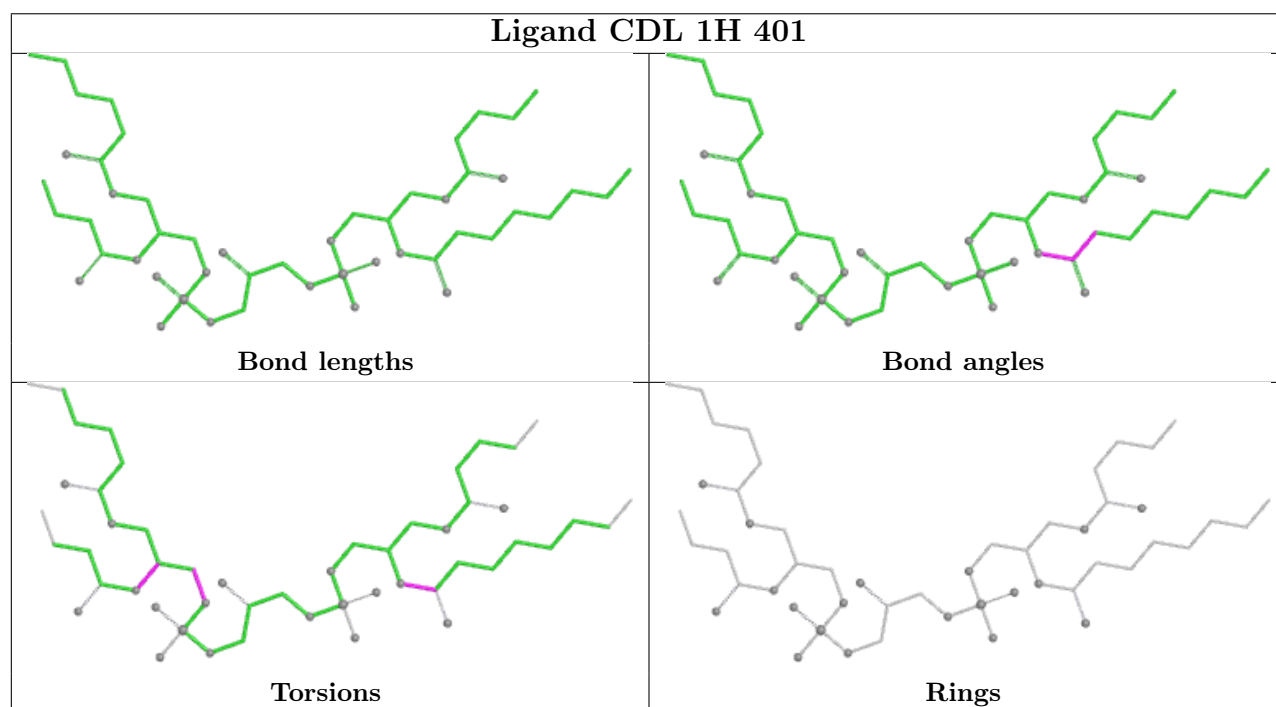
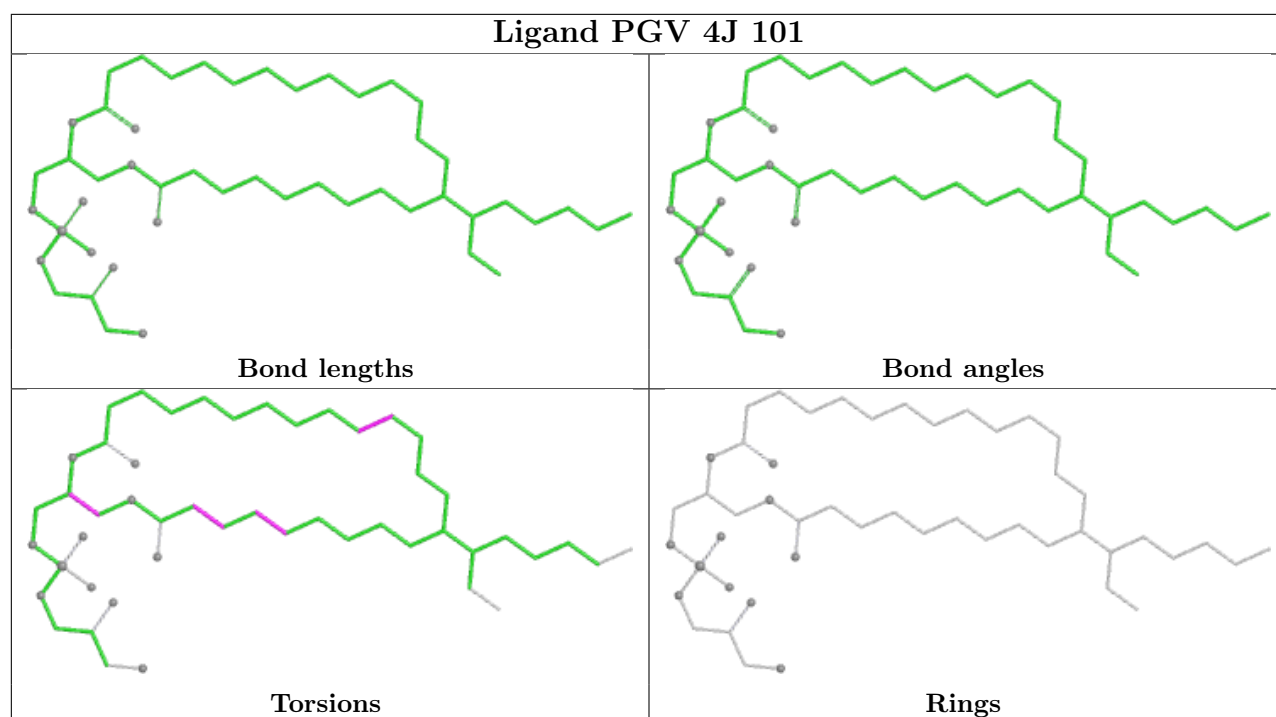


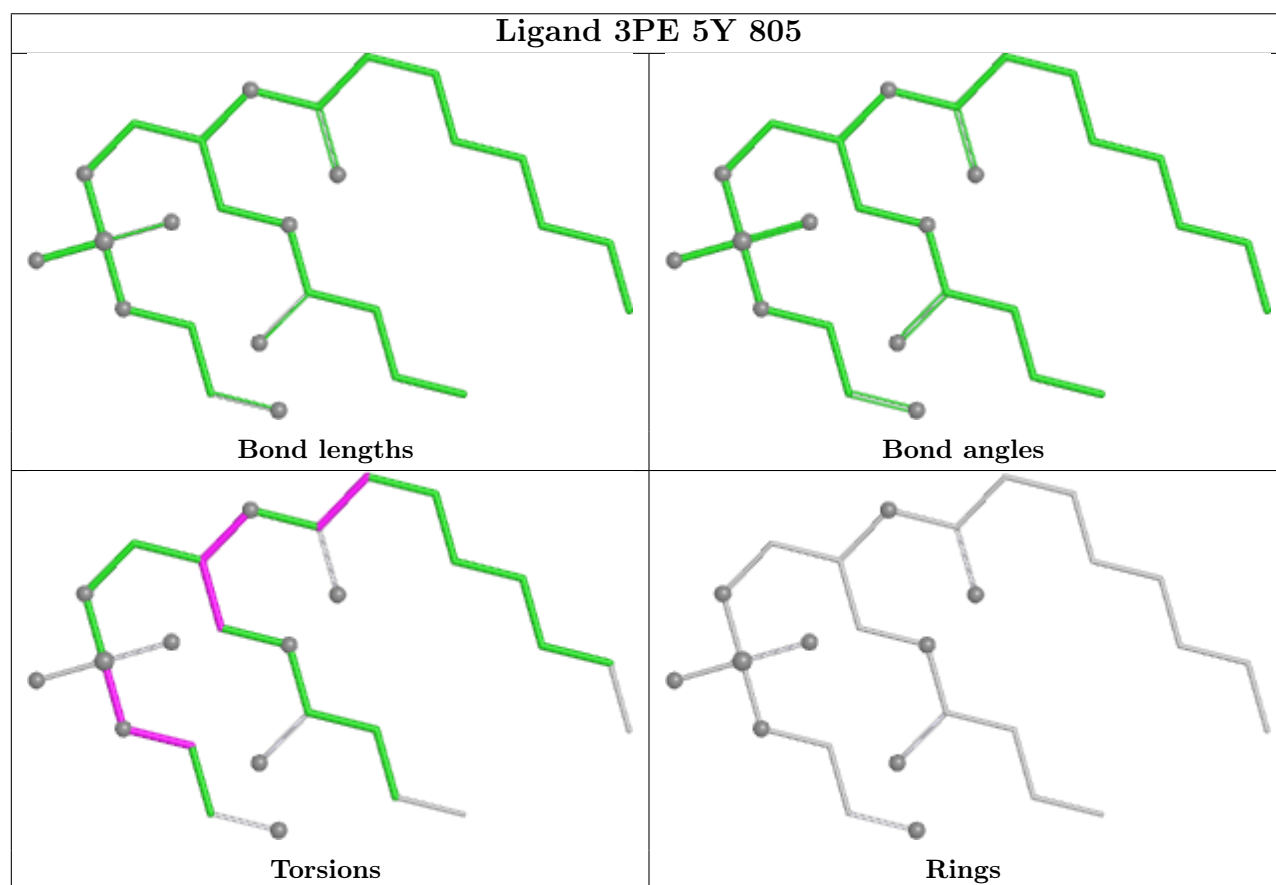
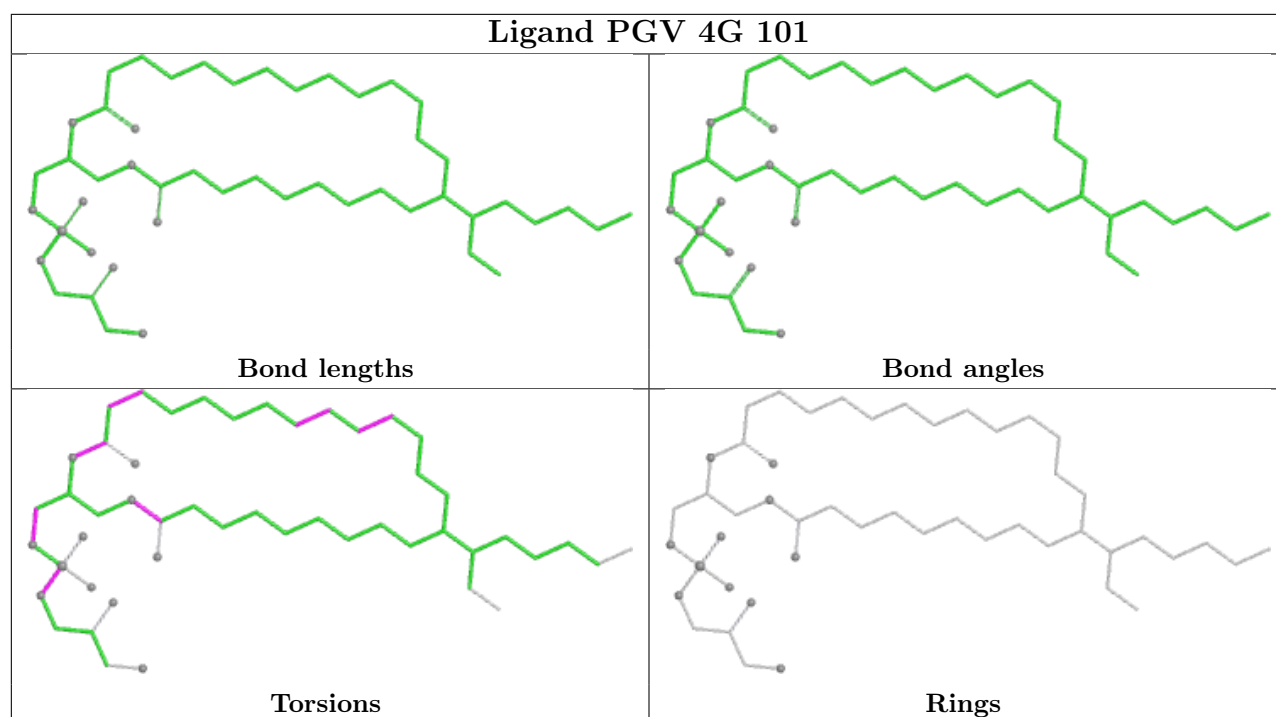


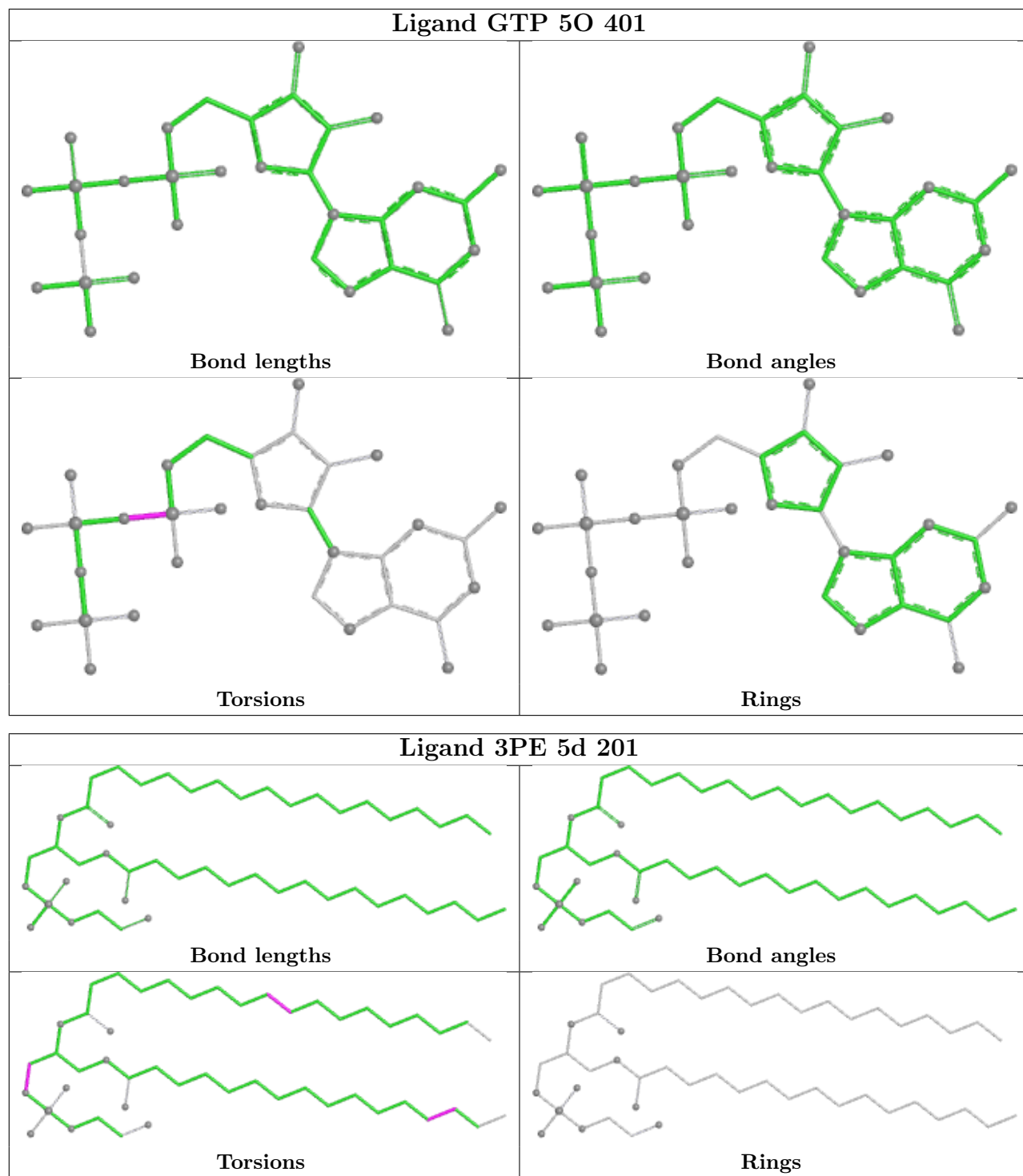


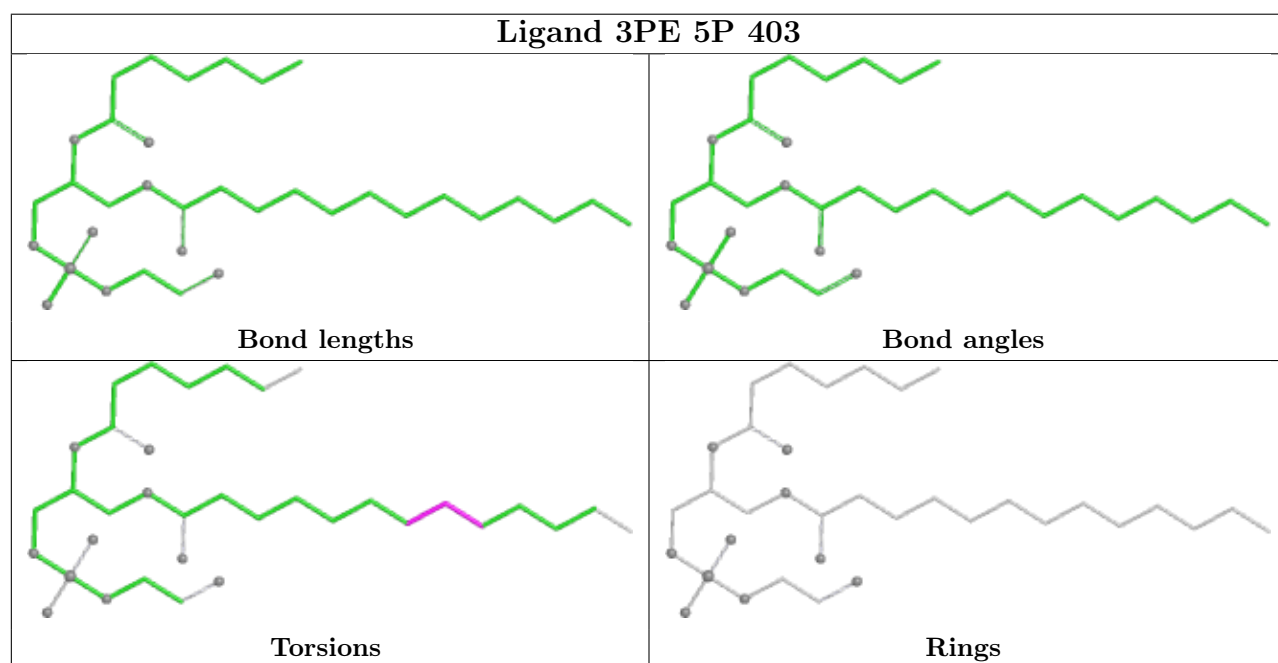
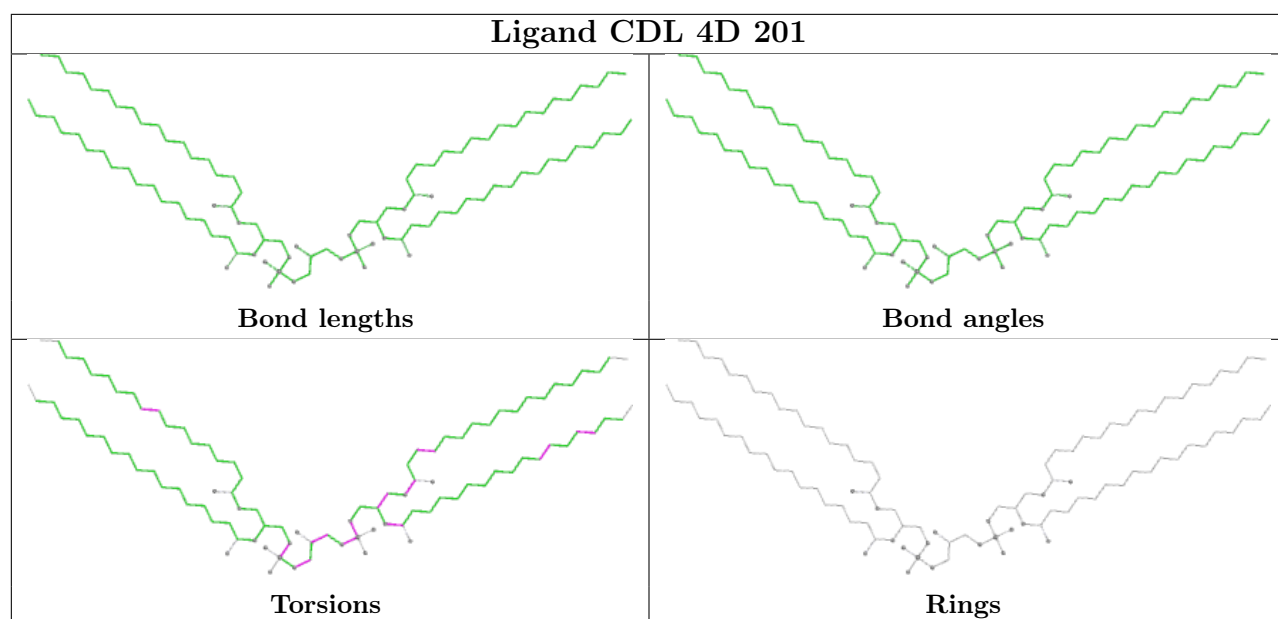


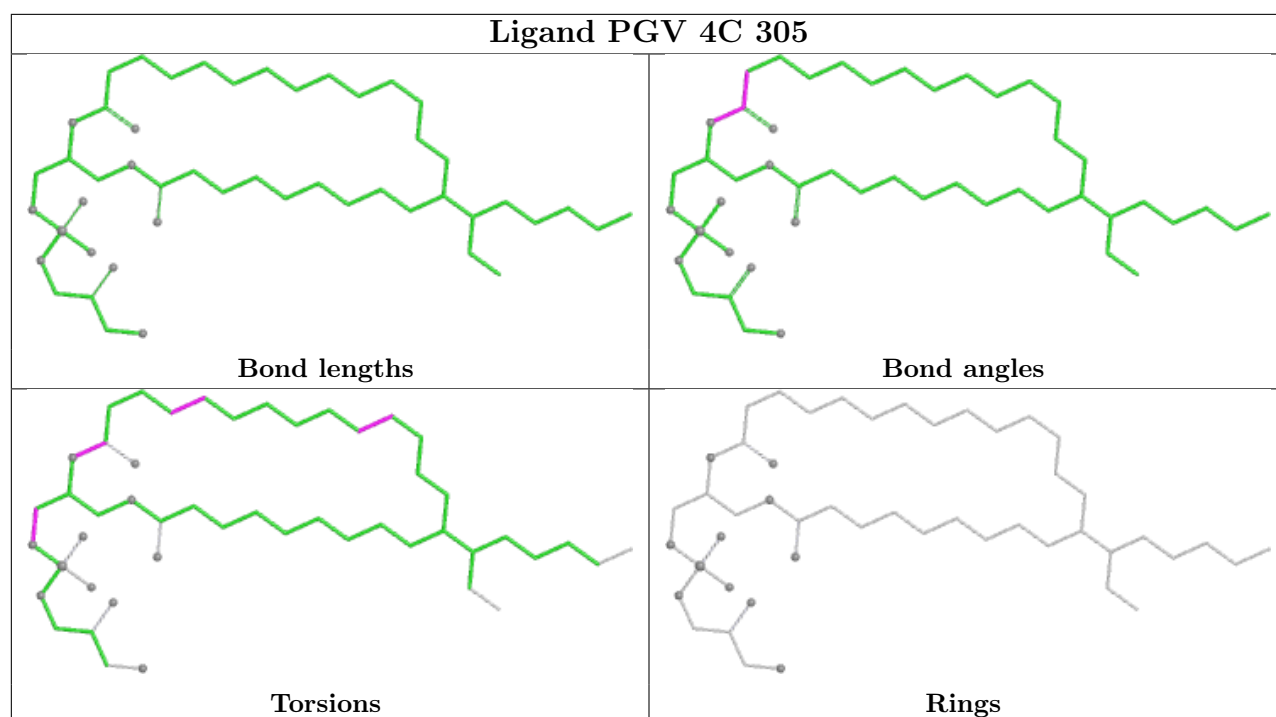


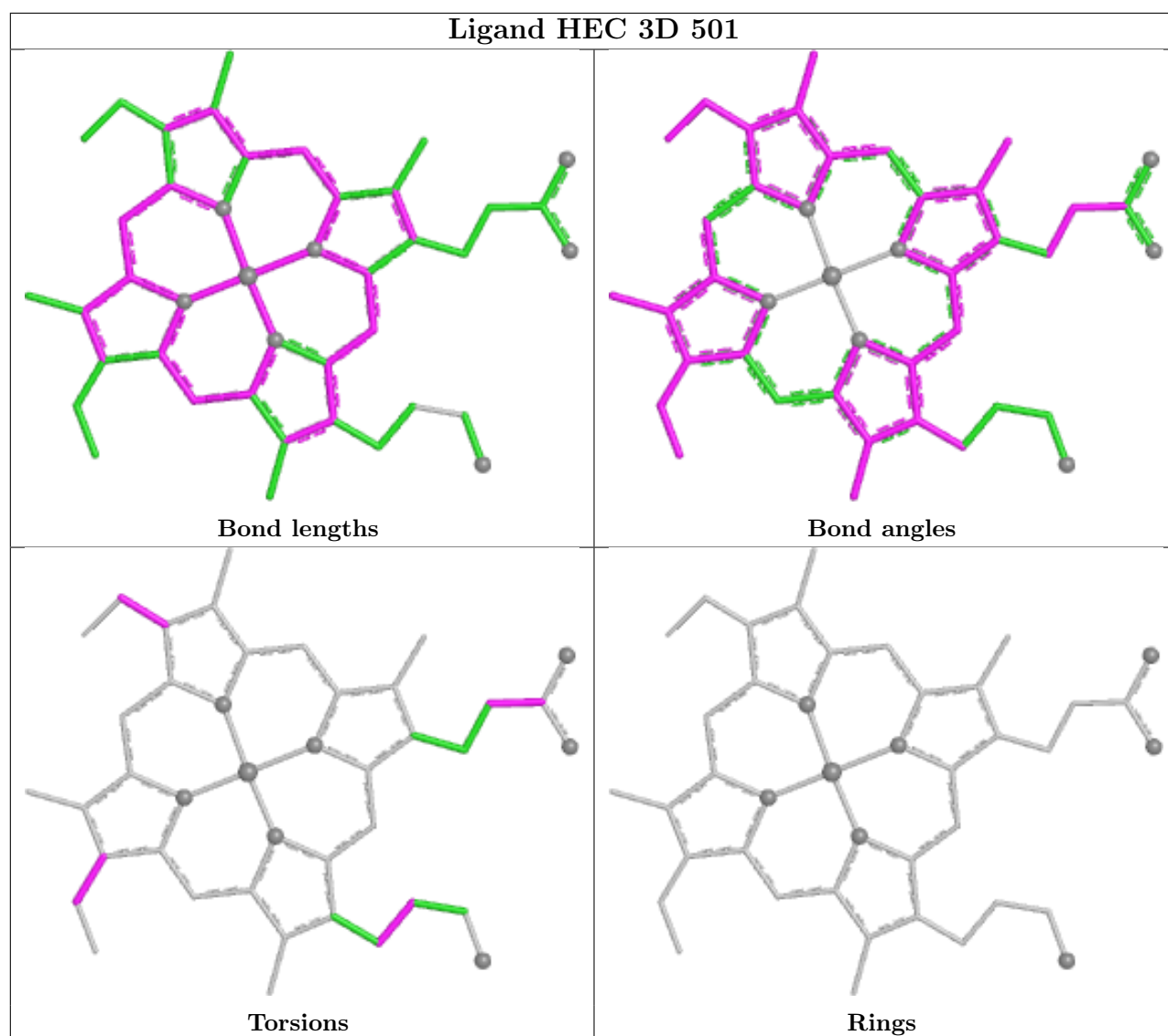




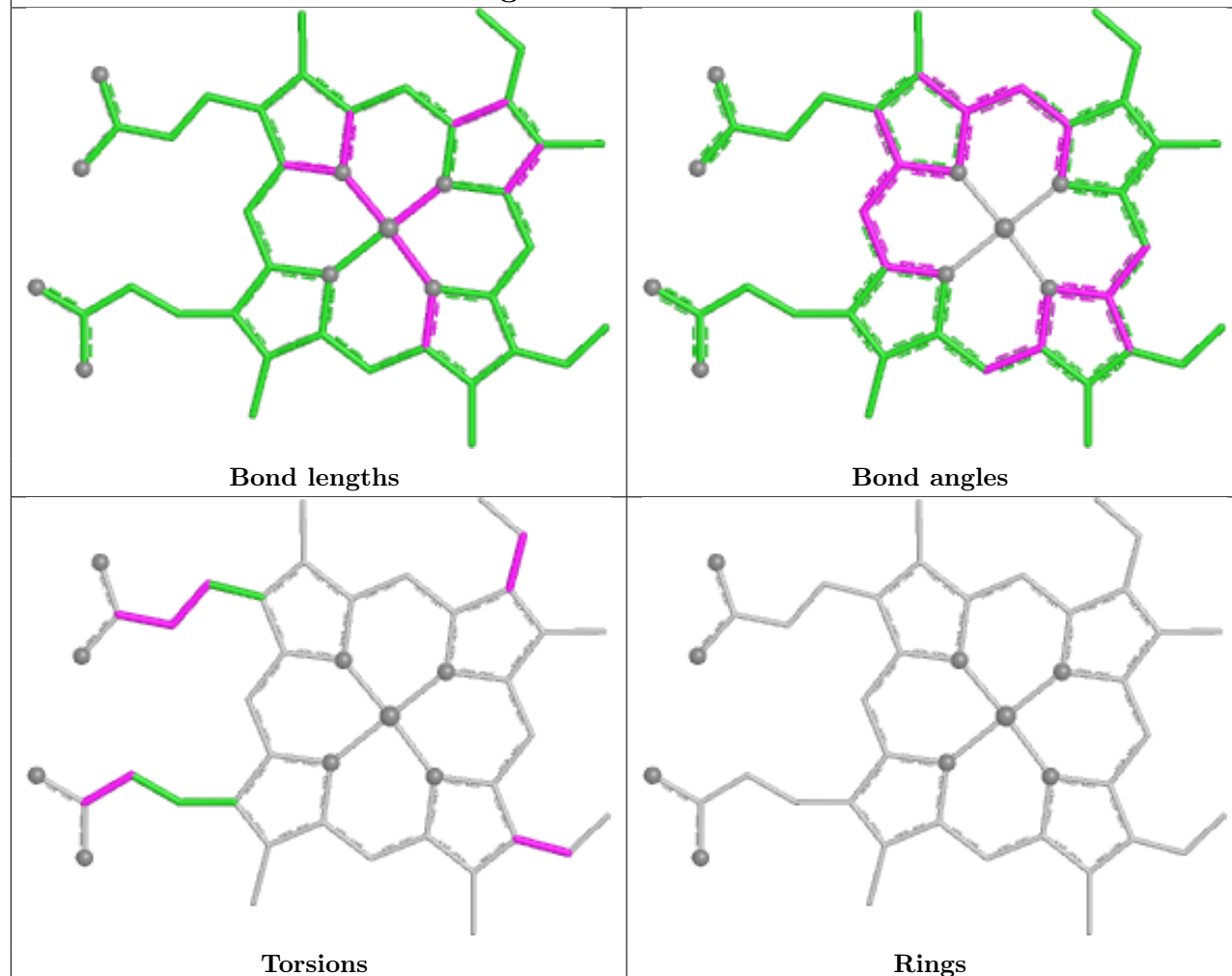




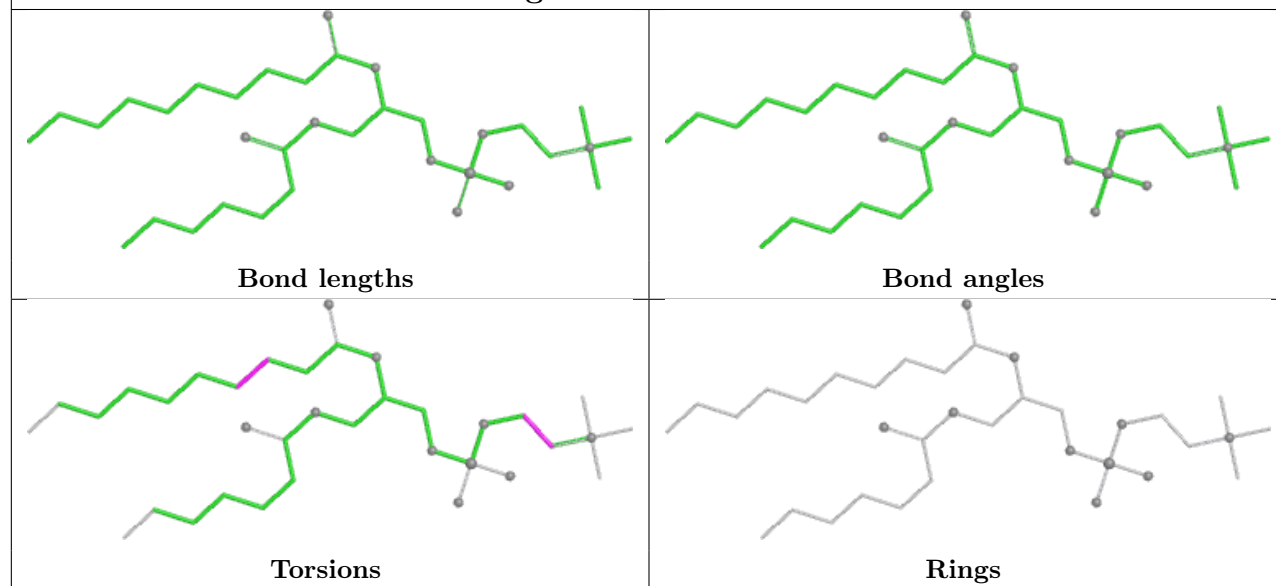


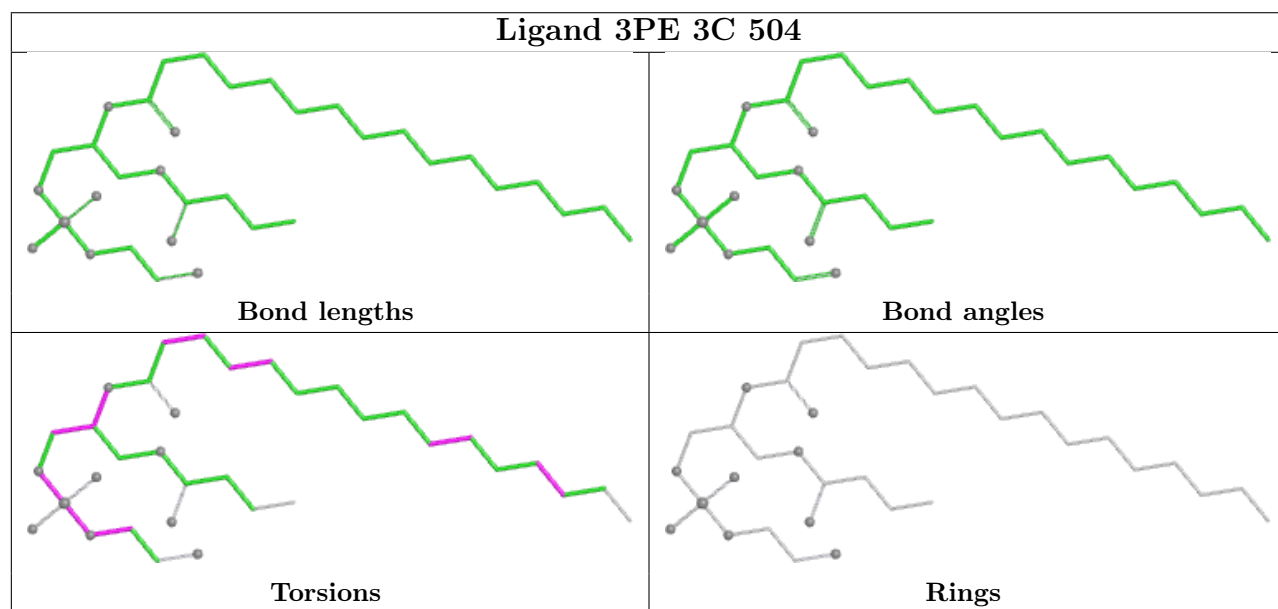
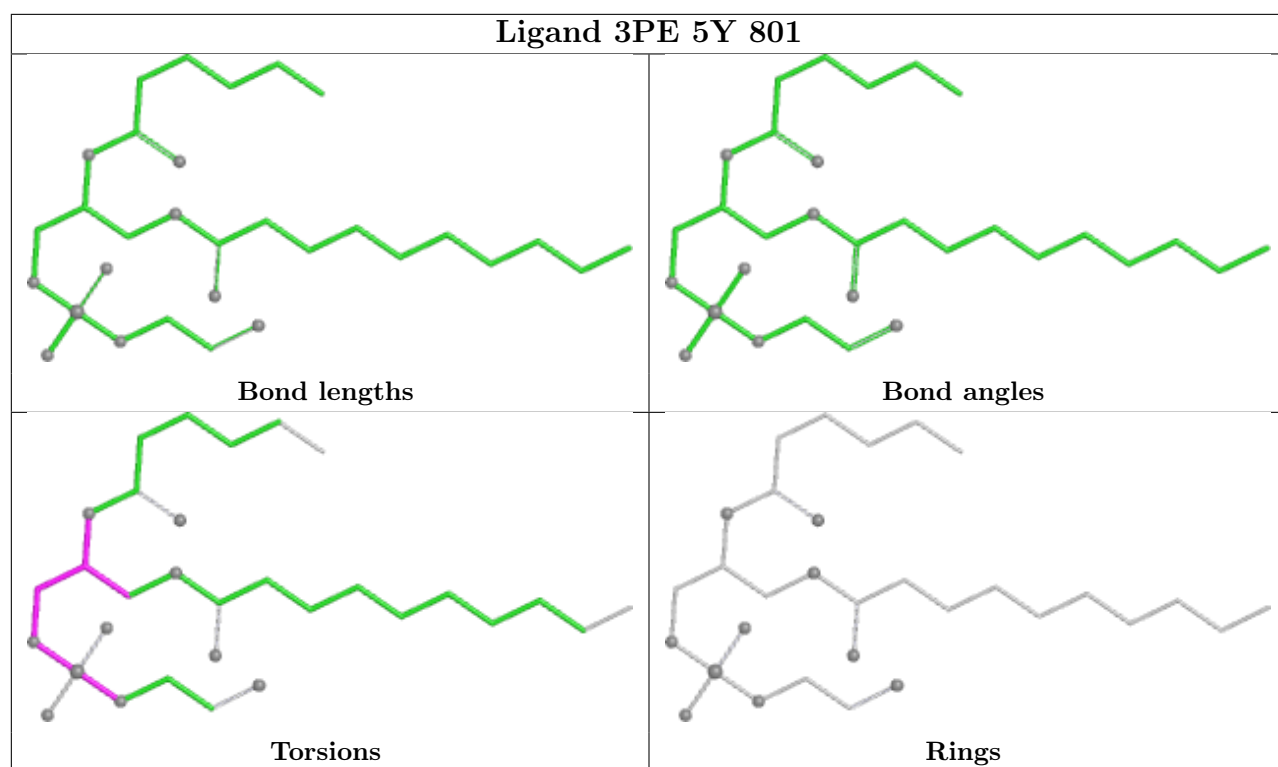


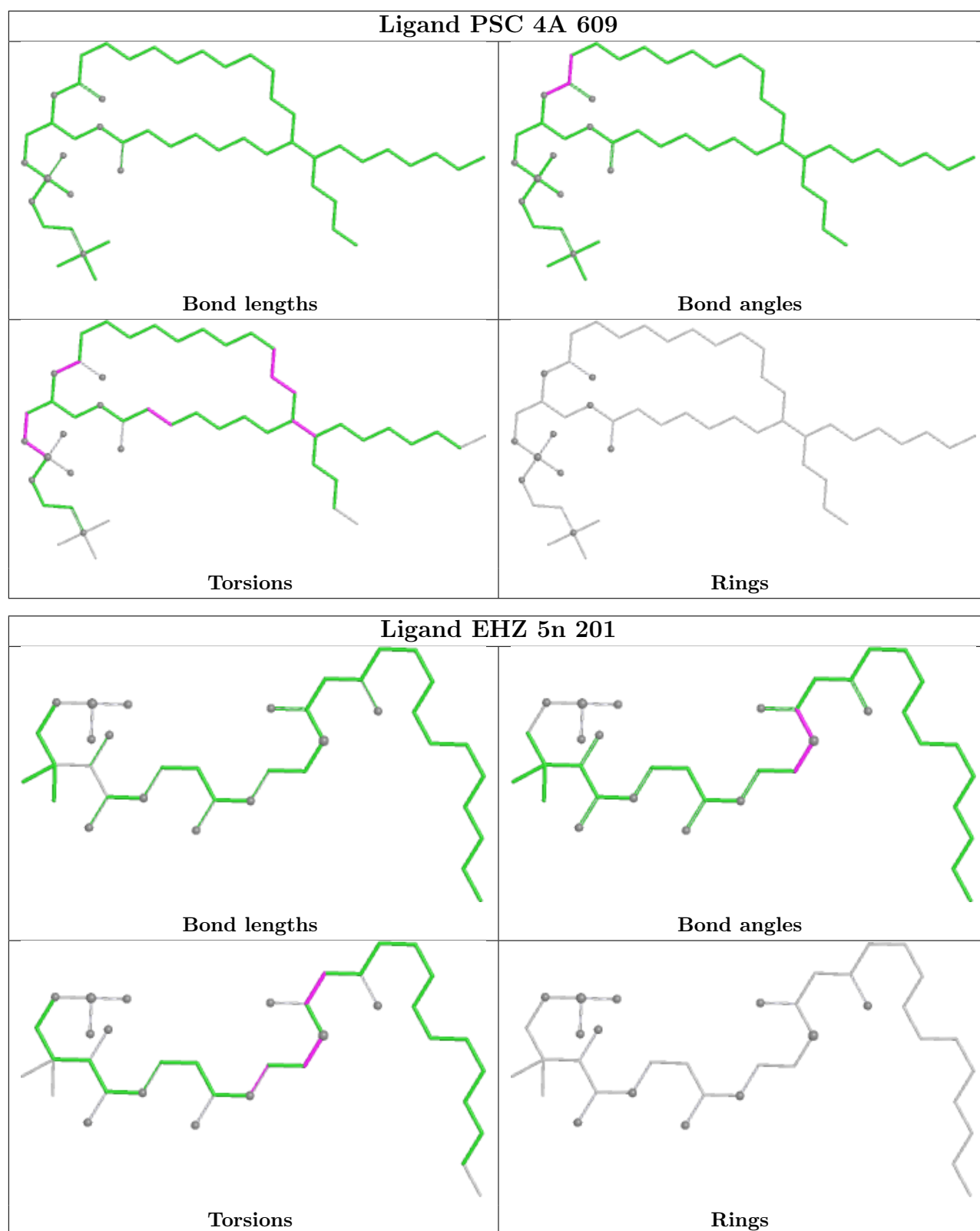
Ligand HEM 3P 501



Ligand PC1 5A 202







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

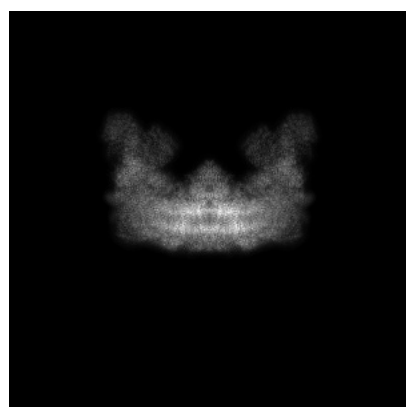
6 Map visualisation [i](#)

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

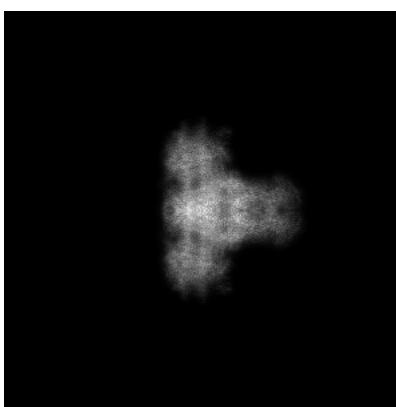
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

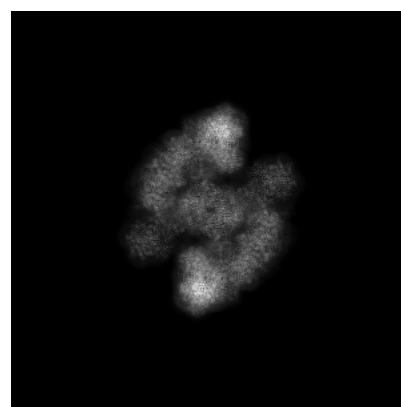
6.1.1 Primary map



X



Y

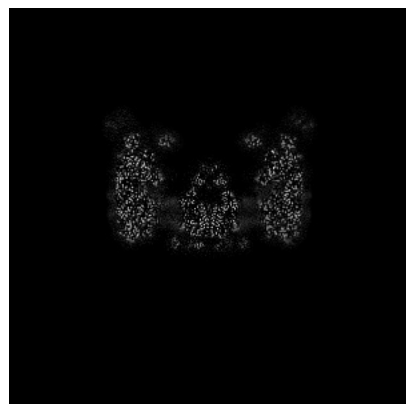


Z

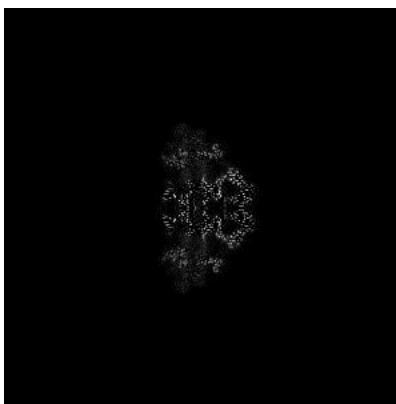
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

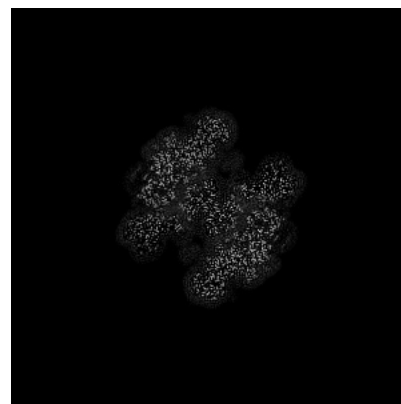
6.2.1 Primary map



X Index: 275



Y Index: 275

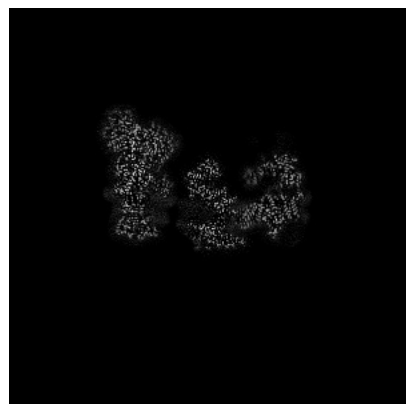


Z Index: 275

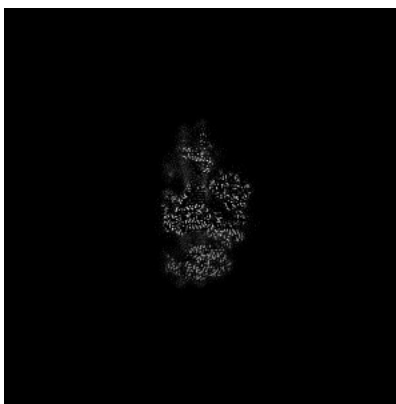
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

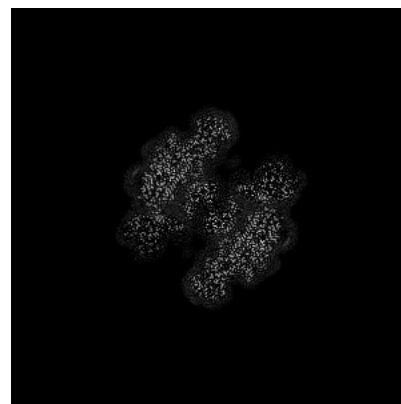
6.3.1 Primary map



X Index: 260



Y Index: 288

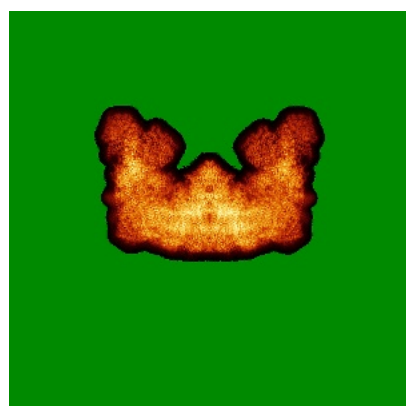


Z Index: 271

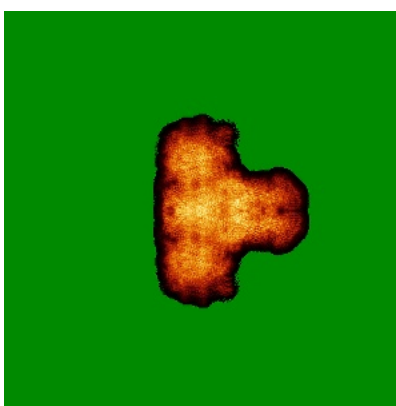
The images above show the largest variance slices of the map in three orthogonal directions.

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

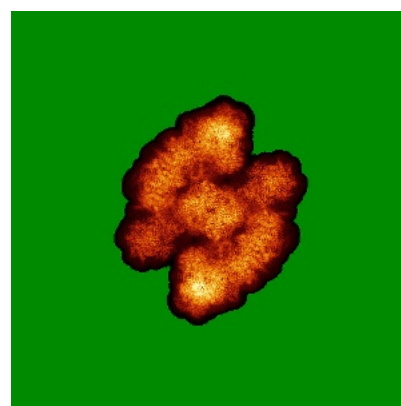
6.4.1 Primary map



X



Y

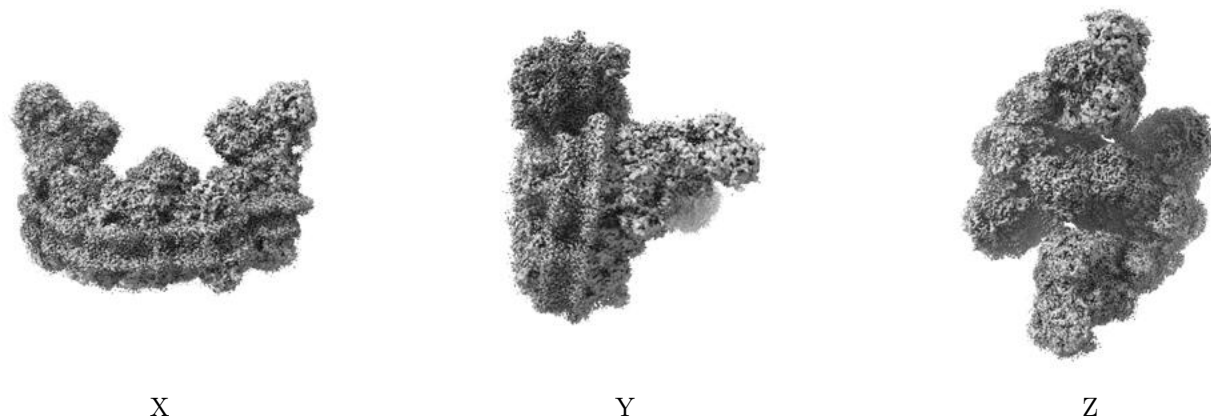


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

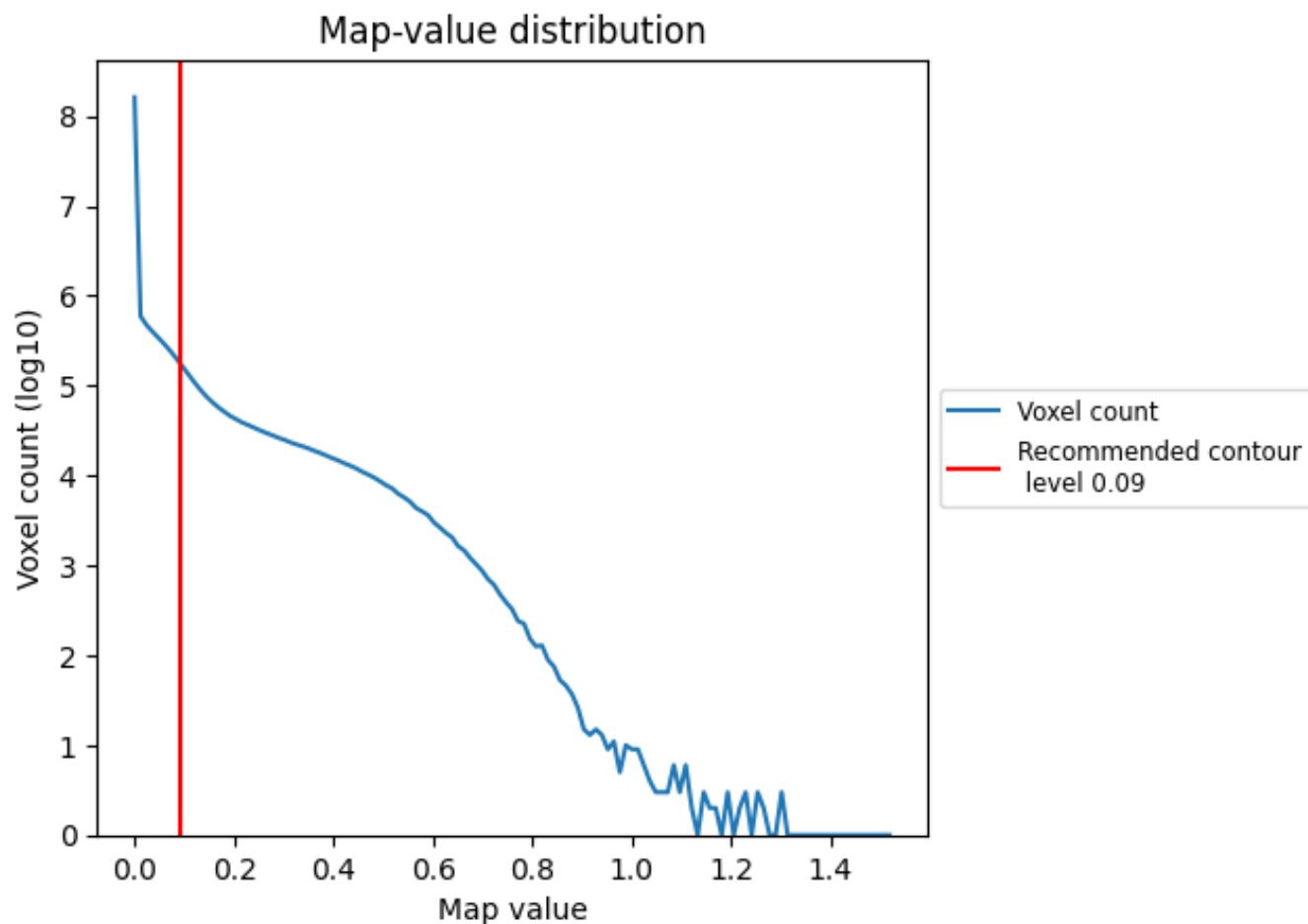
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

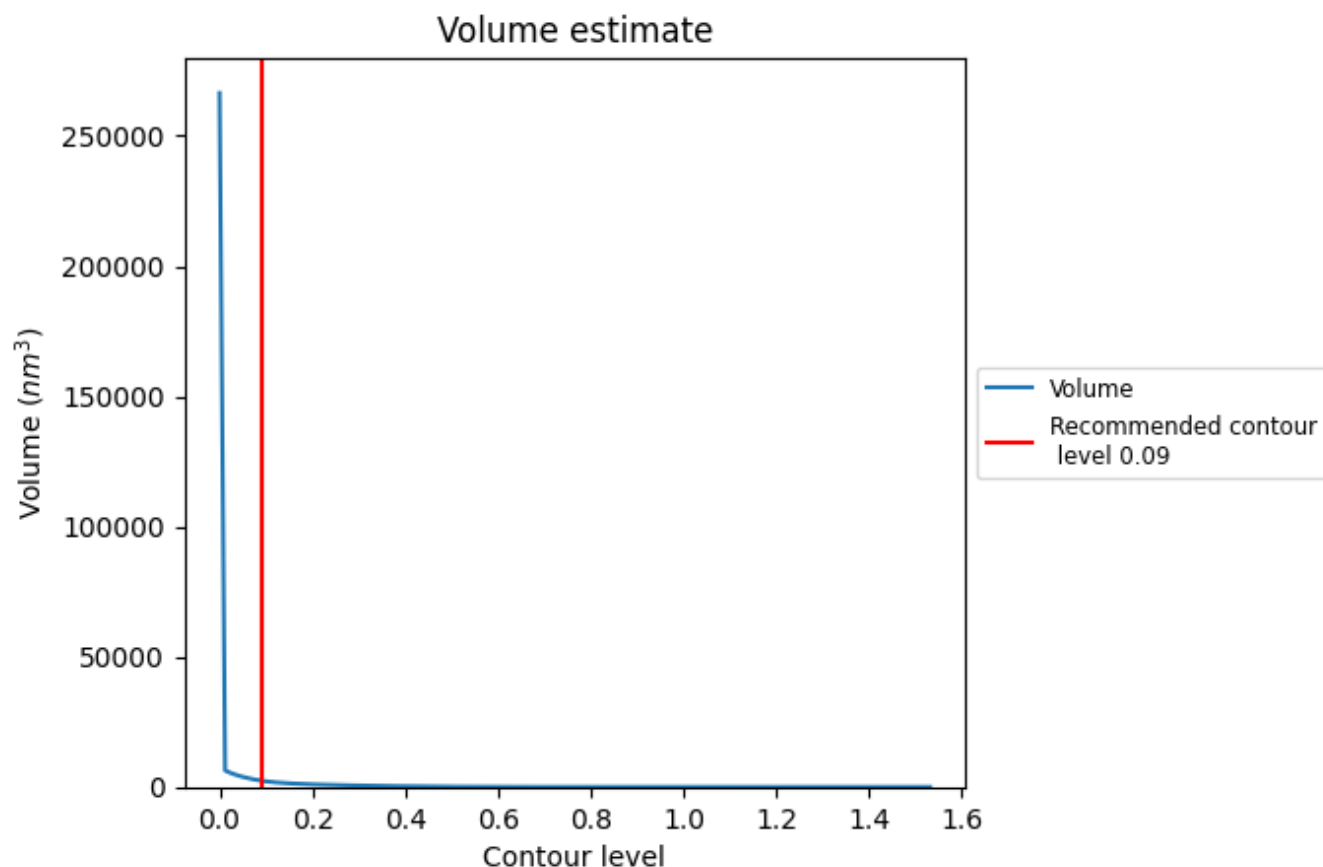
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

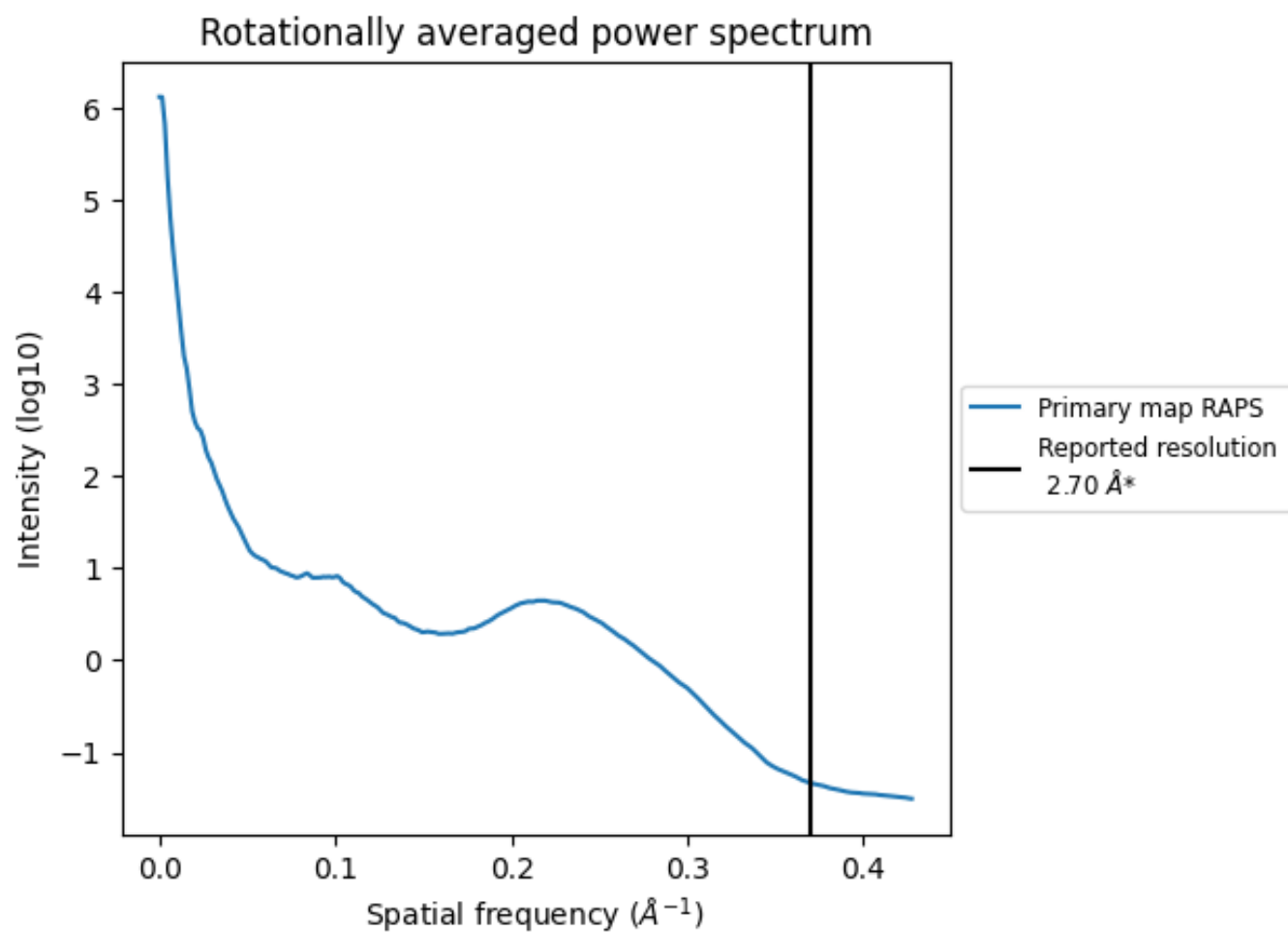
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2412 nm^3 ; this corresponds to an approximate mass of 2179 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

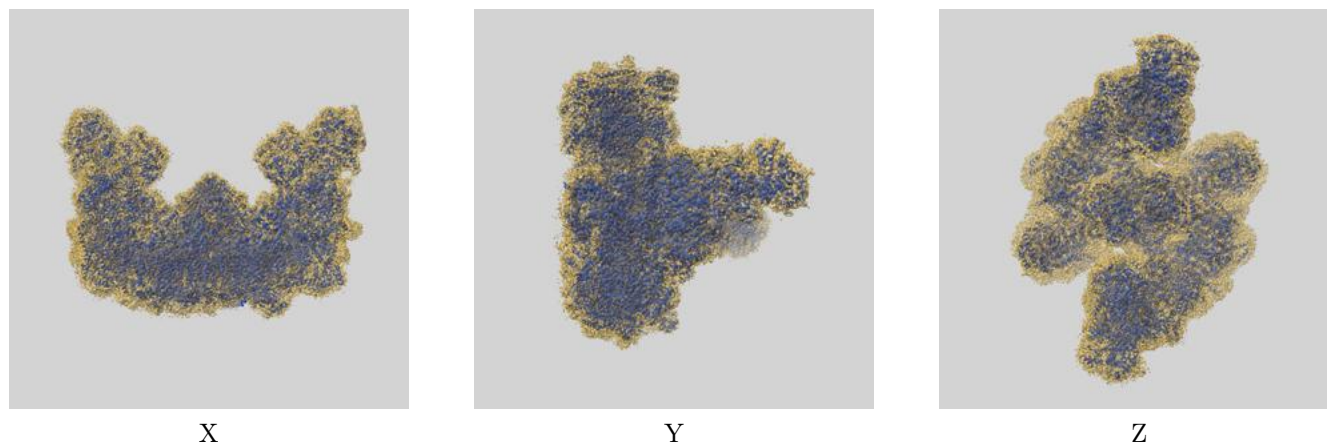
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

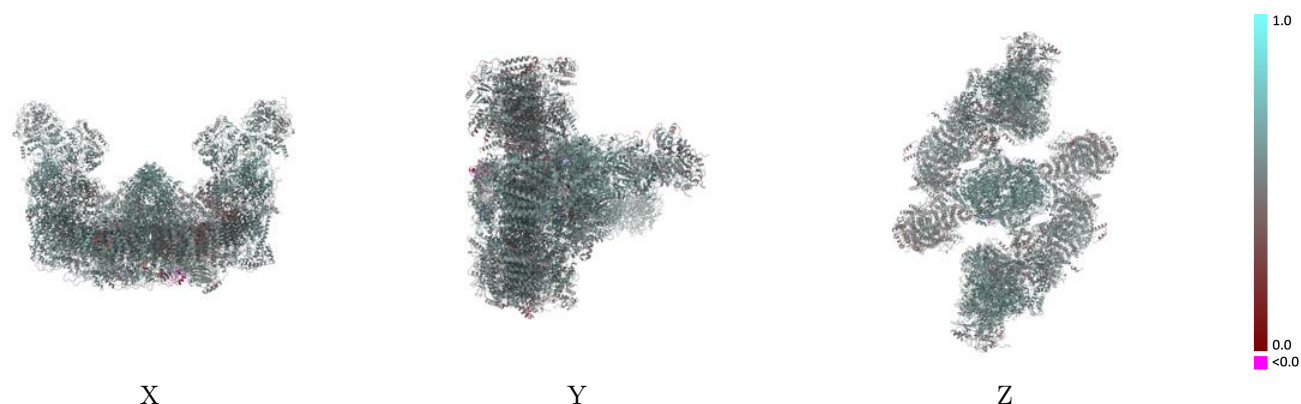
This section contains information regarding the fit between EMDB map EMD-42230 and PDB model 8UGN. Per-residue inclusion information can be found in [section 3](#) on [page 46](#).

9.1 Map-model overlay [i](#)



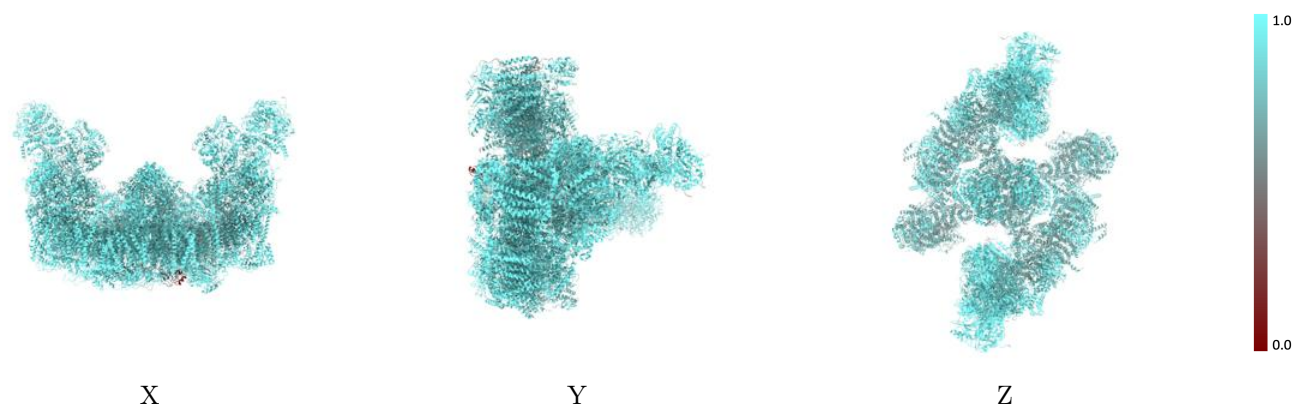
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



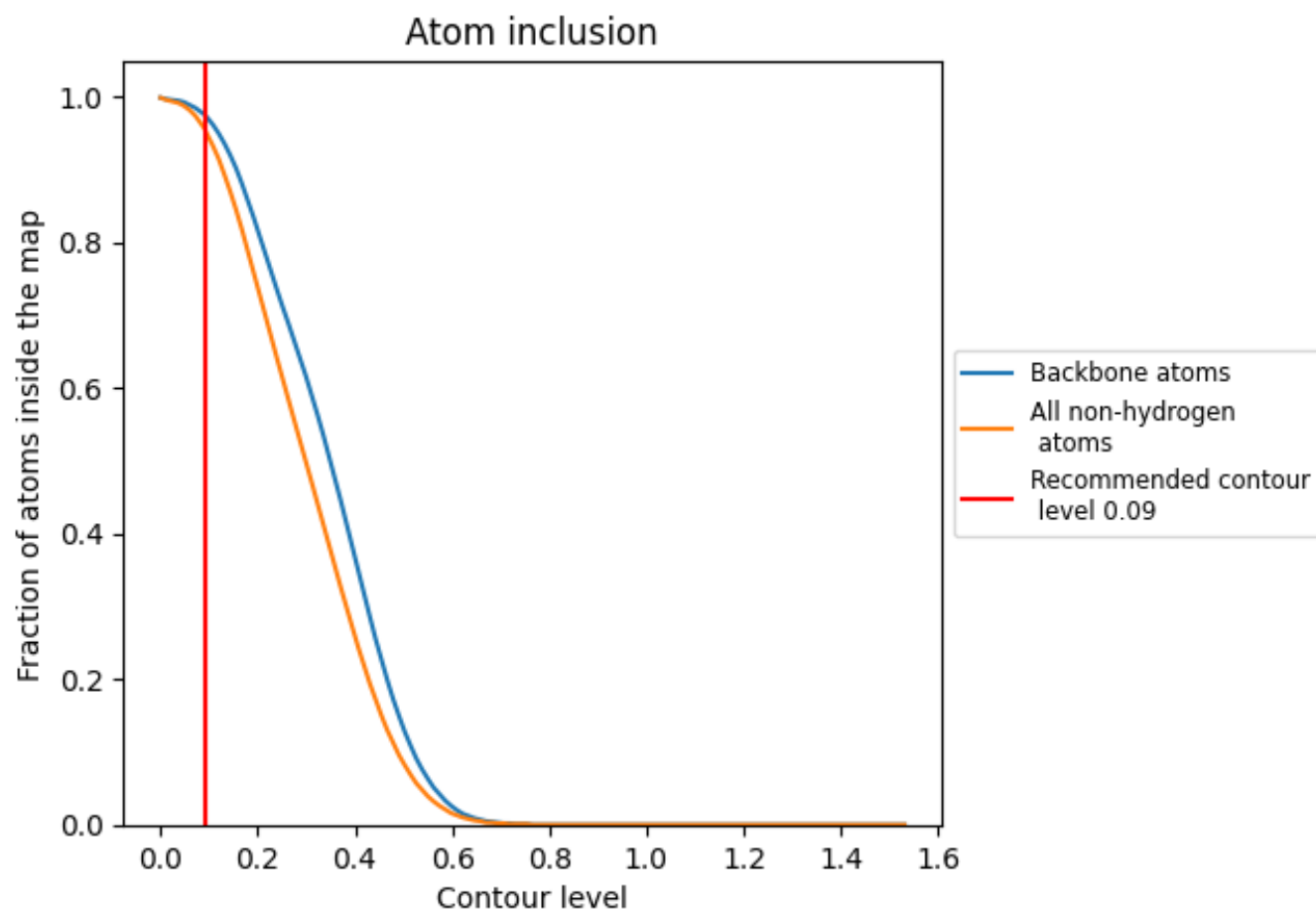
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

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



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Chain	Atom inclusion	Q-score
1i	 0.9200	 0.4570
1j	 0.9440	 0.4770
1k	 0.9420	 0.4800
1l	 0.9800	 0.5360
1m	 0.9790	 0.5360
1n	 0.9870	 0.5360
1o	 0.9740	 0.4870
1p	 0.9770	 0.5160
1q	 0.9760	 0.5580
1r	 0.9860	 0.5610
1s	 0.9570	 0.4960
3A	 0.9750	 0.5960
3B	 0.9760	 0.6000
3C	 0.9890	 0.6140
3D	 0.9900	 0.6130
3E	 0.5600	 0.2830
3F	 0.9840	 0.6070
3G	 0.9800	 0.5740
3H	 0.9690	 0.5670
3I	 0.8390	 0.5010
3J	 0.9880	 0.6000
3N	 0.9830	 0.6030
3O	 0.9790	 0.6080
3P	 0.9870	 0.6170
3Q	 0.9860	 0.6100
3R	 0.5850	 0.3000
3S	 0.9760	 0.6160
3T	 0.9860	 0.5870
3U	 0.9660	 0.5740
3V	 0.9210	 0.5550
3W	 0.9890	 0.6060
3X	 0.9750	 0.5710
3Y	 0.9820	 0.5570
4A	 0.9080	 0.5130
4B	 0.8720	 0.4950
4C	 0.8940	 0.4810
4D	 0.8400	 0.4430
4E	 0.8260	 0.4260
4F	 0.8240	 0.4660
4G	 0.8620	 0.4220
4H	 0.8810	 0.4700
4I	 0.8840	 0.4820

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

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