



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2023 – 01:29 PM JST

PDB ID : 7YMM
EMDB ID : EMD-33933
Title : PSII-Pcb Tetramer of Acaryochloris Marina
Authors : Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on : 2022-07-28
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

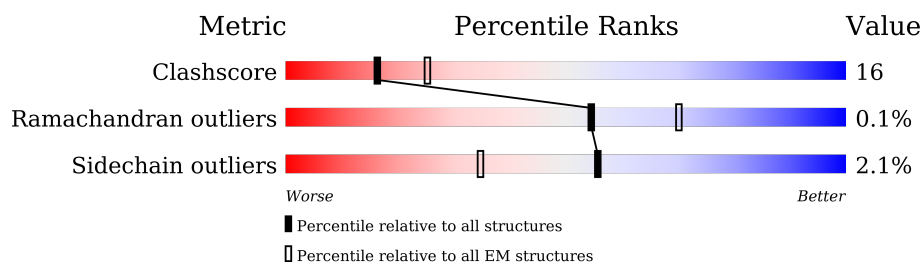
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	360	
1	2A	360	
1	3A	360	
1	4A	360	
2	1B	506	
2	2B	506	
2	3B	506	
2	4B	506	

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Mol	Chain	Length	Quality of chain
3	1C	490	
3	2C	490	
3	3C	490	
3	4C	490	
4	1D	351	
4	2D	351	
4	3D	351	
4	4D	351	
5	1E	83	
5	2E	83	
5	3E	83	
5	4E	83	
6	1F	99	
6	2F	99	
6	3F	99	
6	4F	99	
7	1H	71	
7	2H	71	
7	3H	71	
7	4H	71	
8	1I	34	
8	2I	34	
8	3I	34	
8	4I	34	
9	1K	45	

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Mol	Chain	Length	Quality of chain
9	2K	45	
9	3K	45	
9	4K	45	
10	1L	38	
10	2L	38	
10	3L	38	
10	4L	38	
11	1M	34	
11	2M	34	
11	3M	34	
11	4M	34	
12	1T	46	
12	2T	46	
12	3T	46	
12	4T	46	
13	1X	40	
13	2X	40	
13	3X	40	
13	4X	40	
14	1Y	39	
14	2Y	39	
14	3Y	39	
14	4Y	39	
15	1Z	62	
15	2Z	62	

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Mol	Chain	Length	Quality of chain
15	3Z	62	<div>85%</div> <div>82% 13% 5%</div>
15	4Z	62	<div>95%</div> <div>84% 11% 5%</div>
16	12	352	<div>57%</div> <div>70% 29%</div>
16	22	352	<div>33%</div> <div>70% 29%</div>
16	32	352	<div>32%</div> <div>69% 30%</div>
16	42	352	<div>58%</div> <div>70% 29%</div>
17	1G	41	<div>61%</div> <div>93% 7%</div>
17	2G	41	<div>51%</div> <div>93% 7%</div>
17	3G	41	<div>51%</div> <div>93% 7%</div>
17	4G	41	<div>63%</div> <div>93% 7%</div>
18	11	356	<div>83%</div> <div>63% 30% 8%</div>
18	21	356	<div>43%</div> <div>62% 30% 8%</div>
18	31	356	<div>43%</div> <div>62% 30% 8%</div>
18	41	356	<div>83%</div> <div>61% 31% 8%</div>
19	13	349	<div>42%</div> <div>75% 23% ..</div>
19	23	349	<div>38%</div> <div>75% 23% ..</div>
19	33	349	<div>38%</div> <div>75% 23% ..</div>
19	43	349	<div>42%</div> <div>75% 23% ..</div>
20	14	353	<div>71%</div> <div>69% 25% 6%</div>
20	24	353	<div>36%</div> <div>69% 25% 6%</div>
20	34	353	<div>37%</div> <div>69% 25% 6%</div>
20	44	353	<div>71%</div> <div>69% 24% 6%</div>

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
21	CL7	11	402	X	-	-	-
21	CL7	11	403	X	-	-	-
21	CL7	11	404	X	-	-	-
21	CL7	11	405	X	-	-	-
21	CL7	11	406	X	-	-	-
21	CL7	11	407	X	-	-	-
21	CL7	11	408	X	-	-	-
21	CL7	11	409	X	-	-	-
21	CL7	11	410	X	-	-	-
21	CL7	11	411	X	-	-	-
21	CL7	11	412	X	-	-	-
21	CL7	11	413	X	-	-	-
21	CL7	11	414	X	-	-	-
21	CL7	11	415	X	-	-	-
21	CL7	11	416	X	-	-	-
21	CL7	11	417	X	-	-	-
21	CL7	11	418	X	-	-	-
21	CL7	11	419	X	-	-	-
21	CL7	11	420	X	-	-	-
21	CL7	12	501	X	-	-	-
21	CL7	12	502	X	-	-	-
21	CL7	12	503	X	-	-	-
21	CL7	12	504	X	-	-	-
21	CL7	12	505	X	-	-	-
21	CL7	12	506	X	-	-	-
21	CL7	12	507	X	-	-	-
21	CL7	12	508	X	-	-	-
21	CL7	12	509	X	-	-	-
21	CL7	12	510	X	-	-	-
21	CL7	12	511	X	-	-	-
21	CL7	12	512	X	-	-	-
21	CL7	12	513	X	-	-	-
21	CL7	12	514	X	-	-	-
21	CL7	12	515	X	-	-	-
21	CL7	12	516	X	-	-	-
21	CL7	12	517	X	-	-	-
21	CL7	12	518	X	-	-	-
21	CL7	13	501	X	-	-	-
21	CL7	13	502	X	-	-	-
21	CL7	13	503	X	-	-	-
21	CL7	13	504	X	-	-	-
21	CL7	13	505	X	-	-	-
21	CL7	13	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	13	507	X	-	-	-
21	CL7	13	508	X	-	-	-
21	CL7	13	509	X	-	-	-
21	CL7	13	510	X	-	-	-
21	CL7	13	511	X	-	-	-
21	CL7	13	512	X	-	-	-
21	CL7	13	513	X	-	-	-
21	CL7	13	514	X	-	-	-
21	CL7	13	515	X	-	-	-
21	CL7	13	516	X	-	-	-
21	CL7	13	517	X	-	-	-
21	CL7	13	518	X	-	-	-
21	CL7	14	404	X	-	-	-
21	CL7	14	405	X	-	-	-
21	CL7	14	406	X	-	-	-
21	CL7	14	407	X	-	-	-
21	CL7	14	408	X	-	-	-
21	CL7	14	409	X	-	-	-
21	CL7	14	410	X	-	-	-
21	CL7	14	411	X	-	-	-
21	CL7	14	412	X	-	-	-
21	CL7	14	413	X	-	-	-
21	CL7	14	414	X	-	-	-
21	CL7	14	415	X	-	-	-
21	CL7	14	416	X	-	-	-
21	CL7	14	417	X	-	-	-
21	CL7	1A	401	X	-	-	-
21	CL7	1A	403	X	-	-	-
21	CL7	1A	407	X	-	-	-
21	CL7	1B	601	X	-	-	-
21	CL7	1B	602	X	-	-	-
21	CL7	1B	603	X	-	-	-
21	CL7	1B	604	X	-	-	-
21	CL7	1B	605	X	-	-	-
21	CL7	1B	606	X	-	-	-
21	CL7	1B	607	X	-	-	-
21	CL7	1B	608	X	-	-	-
21	CL7	1B	609	X	-	-	-
21	CL7	1B	610	X	-	-	-
21	CL7	1B	611	X	-	-	-
21	CL7	1B	612	X	-	-	-
21	CL7	1B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	1B	614	X	-	-	-
21	CL7	1B	615	X	-	-	-
21	CL7	1B	616	X	-	-	-
21	CL7	1B	622	X	-	-	-
21	CL7	1C	501	X	-	-	-
21	CL7	1C	502	X	-	-	-
21	CL7	1C	503	X	-	-	-
21	CL7	1C	504	X	-	-	-
21	CL7	1C	505	X	-	-	-
21	CL7	1C	506	X	-	-	-
21	CL7	1C	507	X	-	-	-
21	CL7	1C	508	X	-	-	-
21	CL7	1C	509	X	-	-	-
21	CL7	1C	510	X	-	-	-
21	CL7	1C	511	X	-	-	-
21	CL7	1C	512	X	-	-	-
21	CL7	1C	513	X	-	-	-
21	CL7	1C	517	X	-	-	-
21	CL7	1D	402	X	-	-	-
21	CL7	1D	404	X	-	-	-
21	CL7	1D	405	X	-	-	-
21	CL7	21	402	X	-	-	-
21	CL7	21	403	X	-	-	-
21	CL7	21	404	X	-	-	-
21	CL7	21	405	X	-	-	-
21	CL7	21	406	X	-	-	-
21	CL7	21	407	X	-	-	-
21	CL7	21	408	X	-	-	-
21	CL7	21	409	X	-	-	-
21	CL7	21	410	X	-	-	-
21	CL7	21	411	X	-	-	-
21	CL7	21	412	X	-	-	-
21	CL7	21	413	X	-	-	-
21	CL7	21	414	X	-	-	-
21	CL7	21	415	X	-	-	-
21	CL7	21	416	X	-	-	-
21	CL7	21	417	X	-	-	-
21	CL7	21	418	X	-	-	-
21	CL7	21	419	X	-	-	-
21	CL7	21	420	X	-	-	-
21	CL7	22	501	X	-	-	-
21	CL7	22	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	22	503	X	-	-	-
21	CL7	22	504	X	-	-	-
21	CL7	22	505	X	-	-	-
21	CL7	22	506	X	-	-	-
21	CL7	22	507	X	-	-	-
21	CL7	22	508	X	-	-	-
21	CL7	22	509	X	-	-	-
21	CL7	22	510	X	-	-	-
21	CL7	22	511	X	-	-	-
21	CL7	22	512	X	-	-	-
21	CL7	22	513	X	-	-	-
21	CL7	22	514	X	-	-	-
21	CL7	22	515	X	-	-	-
21	CL7	22	516	X	-	-	-
21	CL7	22	517	X	-	-	-
21	CL7	22	518	X	-	-	-
21	CL7	23	402	X	-	-	-
21	CL7	23	403	X	-	-	-
21	CL7	23	404	X	-	-	-
21	CL7	23	405	X	-	-	-
21	CL7	23	406	X	-	-	-
21	CL7	23	407	X	-	-	-
21	CL7	23	408	X	-	-	-
21	CL7	23	409	X	-	-	-
21	CL7	23	410	X	-	-	-
21	CL7	23	411	X	-	-	-
21	CL7	23	412	X	-	-	-
21	CL7	23	413	X	-	-	-
21	CL7	23	414	X	-	-	-
21	CL7	23	415	X	-	-	-
21	CL7	23	416	X	-	-	-
21	CL7	23	417	X	-	-	-
21	CL7	23	418	X	-	-	-
21	CL7	23	419	X	-	-	-
21	CL7	24	404	X	-	-	-
21	CL7	24	405	X	-	-	-
21	CL7	24	406	X	-	-	-
21	CL7	24	407	X	-	-	-
21	CL7	24	408	X	-	-	-
21	CL7	24	409	X	-	-	-
21	CL7	24	410	X	-	-	-
21	CL7	24	411	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	24	412	X	-	-	-
21	CL7	24	413	X	-	-	-
21	CL7	24	414	X	-	-	-
21	CL7	24	415	X	-	-	-
21	CL7	24	416	X	-	-	-
21	CL7	24	417	X	-	-	-
21	CL7	2A	401	X	-	-	-
21	CL7	2A	403	X	-	-	-
21	CL7	2A	407	X	-	-	-
21	CL7	2B	602	X	-	-	-
21	CL7	2B	603	X	-	-	-
21	CL7	2B	604	X	-	-	-
21	CL7	2B	605	X	-	-	-
21	CL7	2B	606	X	-	-	-
21	CL7	2B	607	X	-	-	-
21	CL7	2B	608	X	-	-	-
21	CL7	2B	609	X	-	-	-
21	CL7	2B	610	X	-	-	-
21	CL7	2B	611	X	-	-	-
21	CL7	2B	612	X	-	-	-
21	CL7	2B	613	X	-	-	-
21	CL7	2B	614	X	-	-	-
21	CL7	2B	615	X	-	-	-
21	CL7	2B	616	X	-	-	-
21	CL7	2B	617	X	-	-	-
21	CL7	2B	623	X	-	-	-
21	CL7	2C	501	X	-	-	-
21	CL7	2C	502	X	-	-	-
21	CL7	2C	503	X	-	-	-
21	CL7	2C	504	X	-	-	-
21	CL7	2C	505	X	-	-	-
21	CL7	2C	506	X	-	-	-
21	CL7	2C	507	X	-	-	-
21	CL7	2C	508	X	-	-	-
21	CL7	2C	509	X	-	-	-
21	CL7	2C	510	X	-	-	-
21	CL7	2C	511	X	-	-	-
21	CL7	2C	512	X	-	-	-
21	CL7	2C	513	X	-	-	-
21	CL7	2C	517	X	-	-	-
21	CL7	2D	402	X	-	-	-
21	CL7	2D	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	2D	405	X	-	-	-
21	CL7	31	402	X	-	-	-
21	CL7	31	403	X	-	-	-
21	CL7	31	404	X	-	-	-
21	CL7	31	405	X	-	-	-
21	CL7	31	406	X	-	-	-
21	CL7	31	407	X	-	-	-
21	CL7	31	408	X	-	-	-
21	CL7	31	409	X	-	-	-
21	CL7	31	410	X	-	-	-
21	CL7	31	411	X	-	-	-
21	CL7	31	412	X	-	-	-
21	CL7	31	413	X	-	-	-
21	CL7	31	414	X	-	-	-
21	CL7	31	415	X	-	-	-
21	CL7	31	416	X	-	-	-
21	CL7	31	417	X	-	-	-
21	CL7	31	418	X	-	-	-
21	CL7	31	419	X	-	-	-
21	CL7	31	420	X	-	-	-
21	CL7	32	501	X	-	-	-
21	CL7	32	502	X	-	-	-
21	CL7	32	503	X	-	-	-
21	CL7	32	504	X	-	-	-
21	CL7	32	505	X	-	-	-
21	CL7	32	506	X	-	-	-
21	CL7	32	507	X	-	-	-
21	CL7	32	508	X	-	-	-
21	CL7	32	509	X	-	-	-
21	CL7	32	510	X	-	-	-
21	CL7	32	511	X	-	-	-
21	CL7	32	512	X	-	-	-
21	CL7	32	513	X	-	-	-
21	CL7	32	514	X	-	-	-
21	CL7	32	515	X	-	-	-
21	CL7	32	516	X	-	-	-
21	CL7	32	517	X	-	-	-
21	CL7	32	518	X	-	-	-
21	CL7	33	501	X	-	-	-
21	CL7	33	502	X	-	-	-
21	CL7	33	503	X	-	-	-
21	CL7	33	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	33	505	X	-	-	-
21	CL7	33	506	X	-	-	-
21	CL7	33	507	X	-	-	-
21	CL7	33	508	X	-	-	-
21	CL7	33	509	X	-	-	-
21	CL7	33	510	X	-	-	-
21	CL7	33	511	X	-	-	-
21	CL7	33	512	X	-	-	-
21	CL7	33	513	X	-	-	-
21	CL7	33	514	X	-	-	-
21	CL7	33	515	X	-	-	-
21	CL7	33	516	X	-	-	-
21	CL7	33	517	X	-	-	-
21	CL7	33	518	X	-	-	-
21	CL7	34	404	X	-	-	-
21	CL7	34	405	X	-	-	-
21	CL7	34	406	X	-	-	-
21	CL7	34	407	X	-	-	-
21	CL7	34	408	X	-	-	-
21	CL7	34	409	X	-	-	-
21	CL7	34	410	X	-	-	-
21	CL7	34	411	X	-	-	-
21	CL7	34	412	X	-	-	-
21	CL7	34	413	X	-	-	-
21	CL7	34	414	X	-	-	-
21	CL7	34	415	X	-	-	-
21	CL7	34	416	X	-	-	-
21	CL7	34	417	X	-	-	-
21	CL7	3A	401	X	-	X	-
21	CL7	3A	403	X	-	-	-
21	CL7	3A	407	X	-	-	-
21	CL7	3B	601	X	-	-	-
21	CL7	3B	602	X	-	-	-
21	CL7	3B	603	X	-	-	-
21	CL7	3B	604	X	-	-	-
21	CL7	3B	605	X	-	-	-
21	CL7	3B	606	X	-	-	-
21	CL7	3B	607	X	-	-	-
21	CL7	3B	608	X	-	-	-
21	CL7	3B	609	X	-	-	-
21	CL7	3B	610	X	-	-	-
21	CL7	3B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	3B	612	X	-	-	-
21	CL7	3B	613	X	-	-	-
21	CL7	3B	614	X	-	-	-
21	CL7	3B	615	X	-	-	-
21	CL7	3B	616	X	-	-	-
21	CL7	3B	622	X	-	-	-
21	CL7	3C	501	X	-	-	-
21	CL7	3C	502	X	-	-	-
21	CL7	3C	503	X	-	-	-
21	CL7	3C	504	X	-	-	-
21	CL7	3C	505	X	-	-	-
21	CL7	3C	506	X	-	-	-
21	CL7	3C	507	X	-	-	-
21	CL7	3C	508	X	-	-	-
21	CL7	3C	509	X	-	-	-
21	CL7	3C	510	X	-	-	-
21	CL7	3C	511	X	-	-	-
21	CL7	3C	512	X	-	-	-
21	CL7	3C	513	X	-	-	-
21	CL7	3C	517	X	-	-	-
21	CL7	3D	402	X	-	-	-
21	CL7	3D	404	X	-	-	-
21	CL7	3D	405	X	-	-	-
21	CL7	41	402	X	-	-	-
21	CL7	41	403	X	-	-	-
21	CL7	41	404	X	-	-	-
21	CL7	41	405	X	-	-	-
21	CL7	41	406	X	-	-	-
21	CL7	41	407	X	-	-	-
21	CL7	41	408	X	-	-	-
21	CL7	41	409	X	-	-	-
21	CL7	41	410	X	-	-	-
21	CL7	41	411	X	-	-	-
21	CL7	41	412	X	-	-	-
21	CL7	41	413	X	-	-	-
21	CL7	41	414	X	-	-	-
21	CL7	41	415	X	-	-	-
21	CL7	41	416	X	-	-	-
21	CL7	41	417	X	-	-	-
21	CL7	41	418	X	-	-	-
21	CL7	41	419	X	-	-	-
21	CL7	41	420	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	42	501	X	-	-	-
21	CL7	42	502	X	-	-	-
21	CL7	42	503	X	-	-	-
21	CL7	42	504	X	-	-	-
21	CL7	42	505	X	-	-	-
21	CL7	42	506	X	-	-	-
21	CL7	42	507	X	-	-	-
21	CL7	42	508	X	-	-	-
21	CL7	42	509	X	-	-	-
21	CL7	42	510	X	-	-	-
21	CL7	42	511	X	-	-	-
21	CL7	42	512	X	-	-	-
21	CL7	42	513	X	-	-	-
21	CL7	42	514	X	-	-	-
21	CL7	42	515	X	-	-	-
21	CL7	42	516	X	-	-	-
21	CL7	42	517	X	-	-	-
21	CL7	42	518	X	-	-	-
21	CL7	43	402	X	-	-	-
21	CL7	43	403	X	-	-	-
21	CL7	43	404	X	-	-	-
21	CL7	43	405	X	-	-	-
21	CL7	43	406	X	-	-	-
21	CL7	43	407	X	-	-	-
21	CL7	43	408	X	-	-	-
21	CL7	43	409	X	-	-	-
21	CL7	43	410	X	-	-	-
21	CL7	43	411	X	-	-	-
21	CL7	43	412	X	-	-	-
21	CL7	43	413	X	-	-	-
21	CL7	43	414	X	-	-	-
21	CL7	43	415	X	-	-	-
21	CL7	43	416	X	-	-	-
21	CL7	43	417	X	-	-	-
21	CL7	43	418	X	-	-	-
21	CL7	43	419	X	-	-	-
21	CL7	44	404	X	-	-	-
21	CL7	44	405	X	-	-	-
21	CL7	44	406	X	-	-	-
21	CL7	44	407	X	-	-	-
21	CL7	44	408	X	-	-	-
21	CL7	44	409	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	44	410	X	-	-	-
21	CL7	44	411	X	-	-	-
21	CL7	44	412	X	-	-	-
21	CL7	44	413	X	-	-	-
21	CL7	44	414	X	-	-	-
21	CL7	44	415	X	-	-	-
21	CL7	44	416	X	-	-	-
21	CL7	44	417	X	-	-	-
21	CL7	4A	401	X	-	-	-
21	CL7	4A	403	X	-	-	-
21	CL7	4A	407	X	-	-	-
21	CL7	4B	602	X	-	-	-
21	CL7	4B	603	X	-	-	-
21	CL7	4B	604	X	-	-	-
21	CL7	4B	605	X	-	-	-
21	CL7	4B	606	X	-	-	-
21	CL7	4B	607	X	-	-	-
21	CL7	4B	608	X	-	-	-
21	CL7	4B	609	X	-	-	-
21	CL7	4B	610	X	-	-	-
21	CL7	4B	611	X	-	-	-
21	CL7	4B	612	X	-	-	-
21	CL7	4B	613	X	-	-	-
21	CL7	4B	614	X	-	-	-
21	CL7	4B	615	X	-	-	-
21	CL7	4B	616	X	-	-	-
21	CL7	4B	617	X	-	-	-
21	CL7	4B	623	X	-	-	-
21	CL7	4C	501	X	-	-	-
21	CL7	4C	502	X	-	-	-
21	CL7	4C	503	X	-	-	-
21	CL7	4C	504	X	-	-	-
21	CL7	4C	505	X	-	-	-
21	CL7	4C	506	X	-	-	-
21	CL7	4C	507	X	-	-	-
21	CL7	4C	508	X	-	-	-
21	CL7	4C	509	X	-	-	-
21	CL7	4C	510	X	-	-	-
21	CL7	4C	511	X	-	-	-
21	CL7	4C	512	X	-	-	-
21	CL7	4C	513	X	-	-	-
21	CL7	4C	517	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	4D	402	X	-	-	-
21	CL7	4D	404	X	-	-	-
21	CL7	4D	405	X	-	-	-
22	PHO	1D	408	X	-	-	-
22	PHO	2D	408	X	-	-	-
22	PHO	3D	408	X	-	-	-
22	PHO	4D	408	X	-	-	-
24	LMG	1A	405	X	-	-	-
24	LMG	2A	405	X	-	-	-
24	LMG	3A	405	X	-	-	-
24	LMG	4A	405	X	-	-	-
32	ZEX	12	520	-	-	X	-
32	ZEX	13	522	-	-	X	-
32	ZEX	13	525	-	-	X	-
32	ZEX	14	403	-	-	X	-
32	ZEX	22	520	-	-	X	-
32	ZEX	23	401	-	-	X	-
32	ZEX	23	423	-	-	X	-
32	ZEX	24	403	-	-	X	-
32	ZEX	31	422	-	-	X	-
32	ZEX	32	520	-	-	X	-
32	ZEX	33	522	-	-	X	-
32	ZEX	33	525	-	-	X	-
32	ZEX	34	403	-	-	X	-
32	ZEX	41	422	-	-	X	-
32	ZEX	42	520	-	-	X	-
32	ZEX	43	401	-	-	X	-
32	ZEX	43	423	-	-	X	-
32	ZEX	44	403	-	-	X	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 136856 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 Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	2A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	3A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	4A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	2B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	3B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	4B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	2C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	3C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	4C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	2D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	3D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	4D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	2E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	3E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	4E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	2F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	3F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	4F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	2H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	3H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	4H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

- Molecule 8 is a protein called Photosystem II protein PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	2I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	3I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	4I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	2K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	3K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	4K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1L	36	Total	C	N	O	0	0
			288	194	45	49		
10	2L	36	Total	C	N	O	0	0
			288	194	45	49		
10	3L	36	Total	C	N	O	0	0
			288	194	45	49		
10	4L	36	Total	C	N	O	0	0
			288	194	45	49		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	2M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	3M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	4M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	2T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	3T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	4T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		

- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	1X	35	Total	C	N	O	0	0
			269	185	39	45		
13	2X	35	Total	C	N	O	0	0
			269	185	39	45		
13	3X	35	Total	C	N	O	0	0
			269	185	39	45		
13	4X	35	Total	C	N	O	0	0
			269	185	39	45		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	2Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	3Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	4Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	2Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	3Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	4Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	12	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	22	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	32	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	42	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1G	41	Total	C	N	O	0	0
			205	123	41	41		
17	2G	41	Total	C	N	O	0	0
			205	123	41	41		
17	3G	41	Total	C	N	O	0	0
			205	123	41	41		
17	4G	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	11	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	21	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	31	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	41	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

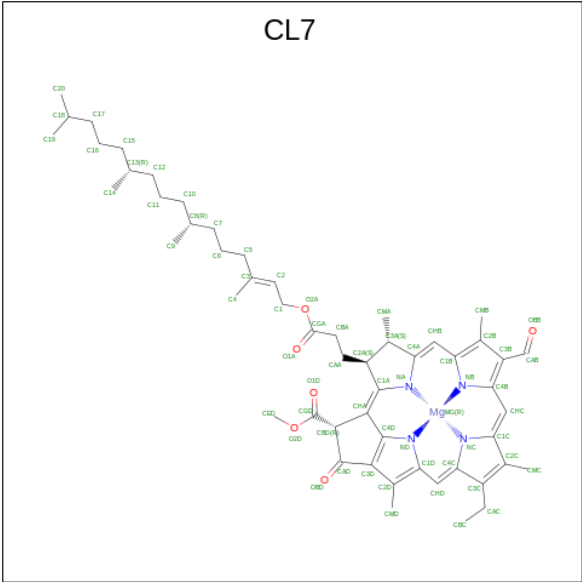
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	13	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	23	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	33	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	43	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	14	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	24	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	34	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	44	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (three-letter code: CL7) (formula: C₅₄H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1A	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	1A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	1B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1B	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	1D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	1D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	11	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	11	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	11	1	Total 62	C 51	Mg 1	N 4	O 6	0
21	11	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	11	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	11	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	11	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	11	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	11	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	11	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	11	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	11	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	11	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	13	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	13	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	13	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	13	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	13	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	13	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	13	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	14	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	14	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	14	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	14	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	14	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	14	1	Total 60	C 49	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	14	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	14	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	14	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	14	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	14	1	Total 53	C 42	Mg 1	N 4	O 6	0
21	14	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	14	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	14	1	Total 42	C 33	Mg 1	N 4	O 4	0
21	2A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2A	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	2A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2B	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	2B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	2B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2B	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	2B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	2B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	2B	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	2D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	21	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	21	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	21	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	21	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	21	1	Total 62	C 51	Mg 1	N 4	O 6	0
21	21	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	21	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	21	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	21	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	21	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	21	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	21	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	21	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	21	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	21	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	21	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	21	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	21	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 58	C 47	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	23	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	23	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	23	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	23	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	23	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	23	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	23	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	24	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	24	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	24	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	24	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	24	1	Total 45	C 34	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	24	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	24	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	24	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	24	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	24	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	24	1	Total 53	C 42	Mg 1	N 4	O 6	0
21	24	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	24	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	24	1	Total 42	C 33	Mg 1	N 4	O 4	0
21	3A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3A	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	3A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3B	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	3B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	3B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3B	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	3B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	3B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3B	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	3C	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	3D	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	3D	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	3D	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	32	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	31	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	31	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	31	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	31	1	Total 62	C 51	Mg 1	N 4	O 6	0
21	31	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	31	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	31	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	31	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	31	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	31	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	31	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	31	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	31	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	33	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	33	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	34	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	34	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	34	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	34	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	34	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	34	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	34	1	Total 53	C 42	Mg 1	N 4	O 6	0
21	34	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	34	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	34	1	Total 42	C 33	Mg 1	N 4	O 4	0
21	4A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4A	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	4A	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4B	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	4B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	4B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4B	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4B	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	4B	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	4B	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	4C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	4C	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	4C	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	4D	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	4D	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	4D	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	42	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	41	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	41	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	41	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	41	1	Total 62	C 51	Mg 1	N 4	O 6	0
21	41	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	41	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	41	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	41	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	41	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	41	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	41	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	41	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	41	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	41	1	Total 45	C 34	Mg 1	N 4	O 6	0

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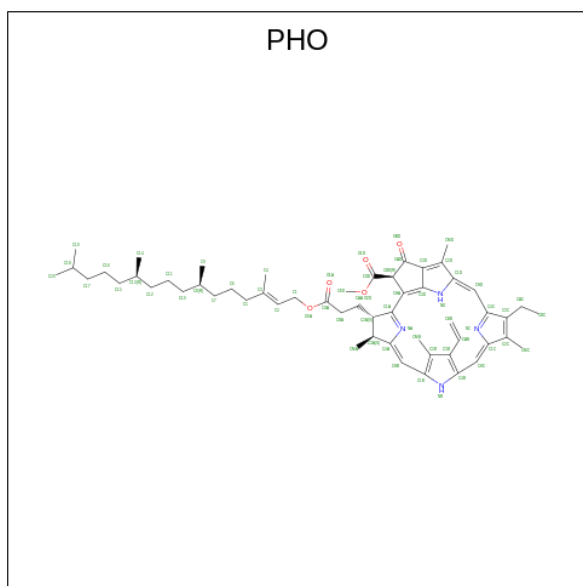
Mol	Chain	Residues	Atoms					AltConf
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	43	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	43	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	43	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	43	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	43	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	43	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	43	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	44	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	44	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	44	1	Total 65	C 54	Mg 1	N 4	O 6	0

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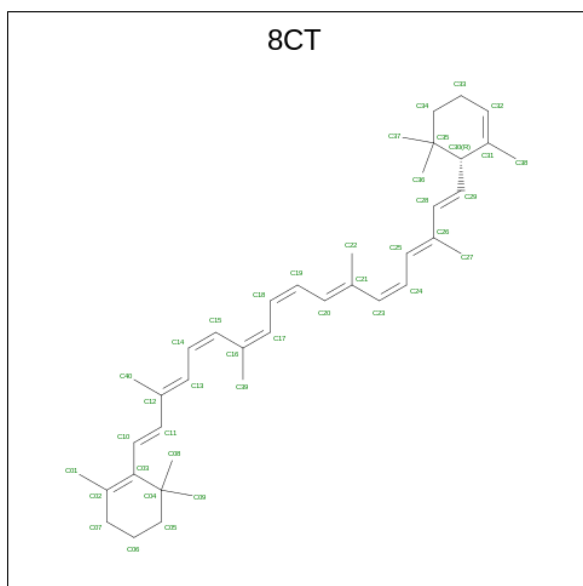
Mol	Chain	Residues	Atoms					AltConf
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	1A	1	Total	C	N	O	0
			64	55	4	5	
22	1D	1	Total	C	N	O	0
			64	55	4	5	
22	2A	1	Total	C	N	O	0
			64	55	4	5	
22	2D	1	Total	C	N	O	0
			64	55	4	5	
22	3A	1	Total	C	N	O	0
			64	55	4	5	
22	3D	1	Total	C	N	O	0
			64	55	4	5	
22	4A	1	Total	C	N	O	0
			64	55	4	5	
22	4D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	1A	1	Total	C	0
			40	40	
23	1B	1	Total	C	0
			40	40	
23	1B	1	Total	C	0
			40	40	

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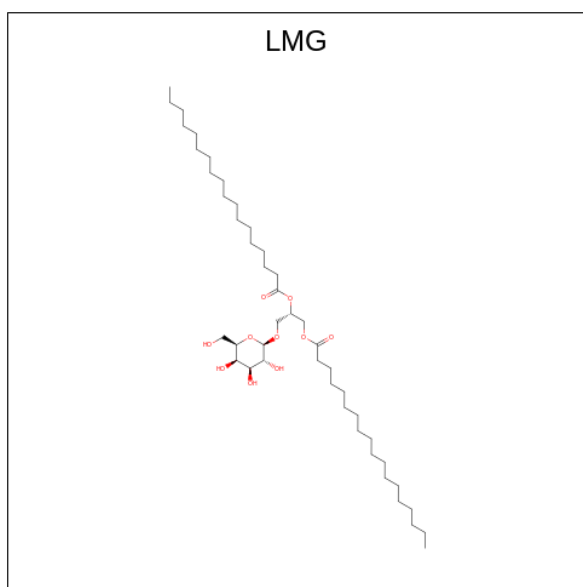
Mol	Chain	Residues	Atoms	AltConf
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1D	1	Total C 40 40	0
23	1K	1	Total C 40 40	0
23	14	1	Total C 40 40	0
23	2A	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2D	1	Total C 40 40	0
23	2K	1	Total C 40 40	0
23	24	1	Total C 40 40	0
23	3A	1	Total C 40 40	0
23	3B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3D	1	Total C 40 40	0
23	3K	1	Total C 40 40	0
23	34	1	Total C 40 40	0
23	4A	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4D	1	Total C 40 40	0
23	4K	1	Total C 40 40	0
23	44	1	Total C 40 40	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



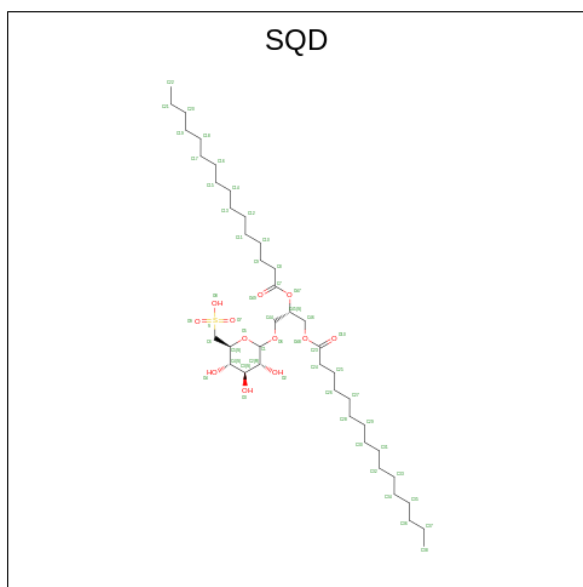
Mol	Chain	Residues	Atoms			AltConf
24	1A	1	Total	C	O	0
			50	40	10	
24	1B	1	Total	C	O	0
			51	41	10	
24	1D	1	Total	C	O	0
			33	23	10	
24	1I	1	Total	C	O	0
			51	41	10	
24	2A	1	Total	C	O	0
			50	40	10	
24	2B	1	Total	C	O	0
			51	41	10	
24	2D	1	Total	C	O	0
			33	23	10	
24	2I	1	Total	C	O	0
			51	41	10	
24	3A	1	Total	C	O	0
			50	40	10	
24	3B	1	Total	C	O	0
			51	41	10	
24	3D	1	Total	C	O	0
			33	23	10	
24	3I	1	Total	C	O	0
			51	41	10	
24	4A	1	Total	C	O	0
			50	40	10	
24	4B	1	Total	C	O	0
			51	41	10	

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Mol	Chain	Residues	Atoms			AltConf
24	4D	1	Total	C	O	0
			33	23	10	
24	41	1	Total	C	O	0
			51	41	10	

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
25	1A	1	Total	C	O	S	0
			34	21	12	1	
25	1B	1	Total	C	O	S	0
			54	41	12	1	
25	12	1	Total	C	O	S	0
			50	37	12	1	
25	12	1	Total	C	O	S	0
			41	28	12	1	
25	11	1	Total	C	O	S	0
			32	19	12	1	
25	13	1	Total	C	O	S	0
			46	33	12	1	
25	13	1	Total	C	O	S	0
			50	37	12	1	
25	2A	1	Total	C	O	S	0
			34	21	12	1	

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Mol	Chain	Residues	Atoms				AltConf
25	2B	1	Total	C	O	S	0
			54	41	12	1	
25	22	1	Total	C	O	S	0
			50	37	12	1	
25	22	1	Total	C	O	S	0
			41	28	12	1	
25	21	1	Total	C	O	S	0
			32	19	12	1	
25	23	1	Total	C	O	S	0
			46	33	12	1	
25	23	1	Total	C	O	S	0
			50	37	12	1	
25	3A	1	Total	C	O	S	0
			34	21	12	1	
25	3B	1	Total	C	O	S	0
			54	41	12	1	
25	32	1	Total	C	O	S	0
			50	37	12	1	
25	32	1	Total	C	O	S	0
			41	28	12	1	
25	31	1	Total	C	O	S	0
			32	19	12	1	
25	33	1	Total	C	O	S	0
			46	33	12	1	
25	33	1	Total	C	O	S	0
			50	37	12	1	
25	4A	1	Total	C	O	S	0
			34	21	12	1	
25	4B	1	Total	C	O	S	0
			54	41	12	1	
25	42	1	Total	C	O	S	0
			50	37	12	1	
25	42	1	Total	C	O	S	0
			41	28	12	1	
25	41	1	Total	C	O	S	0
			32	19	12	1	
25	43	1	Total	C	O	S	0
			46	33	12	1	
25	43	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

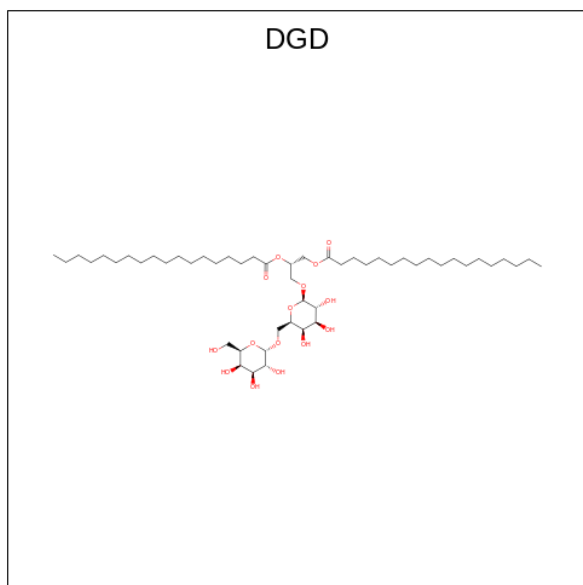


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Mol	Chain	Residues	Atoms				AltConf
26	3B	1	Total	C	O	P	0
			49	38	10	1	
26	3D	1	Total	C	O	P	0
			49	38	10	1	
26	33	1	Total	C	O	P	0
			36	25	10	1	
26	34	1	Total	C	O	P	0
			49	38	10	1	
26	4A	1	Total	C	O	P	0
			46	35	10	1	
26	4B	1	Total	C	O	P	0
			45	34	10	1	
26	4B	1	Total	C	O	P	0
			49	38	10	1	
26	4D	1	Total	C	O	P	0
			49	38	10	1	
26	43	1	Total	C	O	P	0
			36	25	10	1	
26	44	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	1B	1	Total	C	O	0
			62	47	15	

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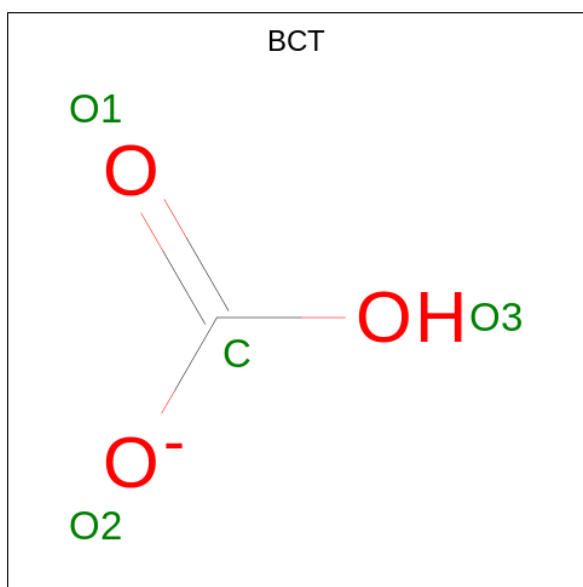
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Mol	Chain	Residues	Atoms			AltConf
27	1C	1	Total 62	C 47	O 15	0
27	2B	1	Total 62	C 47	O 15	0
27	2C	1	Total 62	C 47	O 15	0
27	3B	1	Total 62	C 47	O 15	0
27	3C	1	Total 62	C 47	O 15	0
27	4B	1	Total 62	C 47	O 15	0
27	4C	1	Total 62	C 47	O 15	0

- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

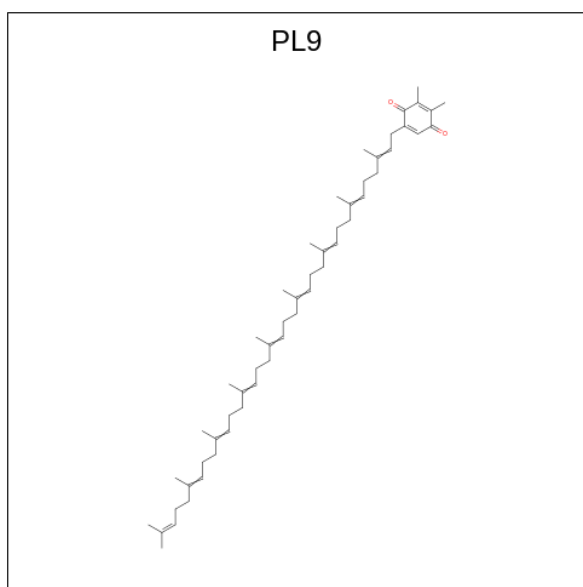
Mol	Chain	Residues	Atoms		AltConf
28	1D	1	Total 1	Fe 1	0
28	2D	1	Total 1	Fe 1	0
28	3D	1	Total 1	Fe 1	0
28	4D	1	Total 1	Fe 1	0

- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



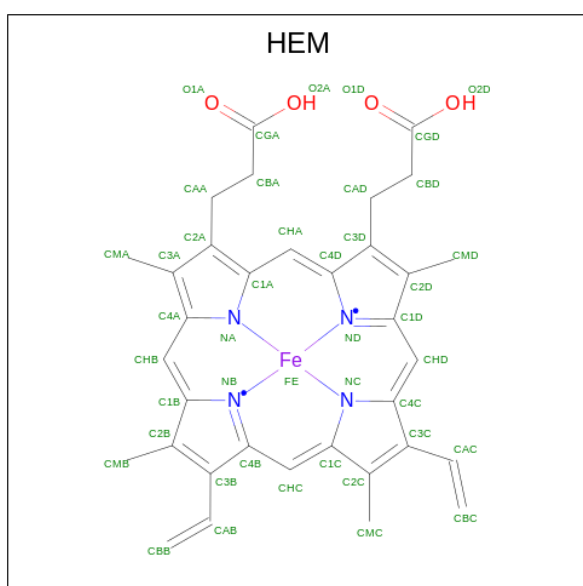
Mol	Chain	Residues	Atoms			AltConf
29	1D	1	Total	C	O	0
			4	1	3	
29	2D	1	Total	C	O	0
			4	1	3	
29	3D	1	Total	C	O	0
			4	1	3	
29	4D	1	Total	C	O	0
			4	1	3	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



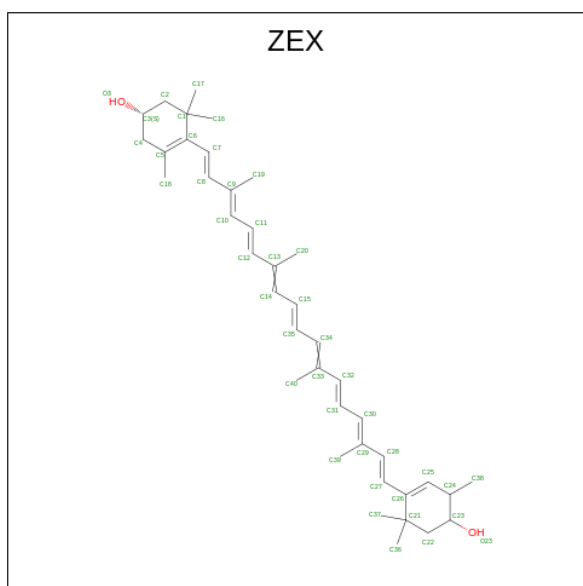
Mol	Chain	Residues	Atoms			AltConf
30	1D	1	Total	C	O	0
			55	53	2	
30	2D	1	Total	C	O	0
			55	53	2	
30	3D	1	Total	C	O	0
			55	53	2	
30	4D	1	Total	C	O	0
			55	53	2	

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	2F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	3F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	4F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	

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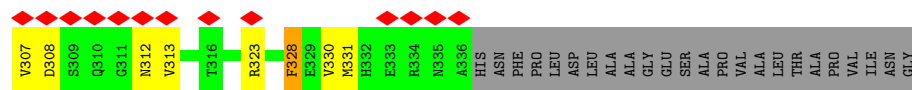
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Mol	Chain	Residues	Atoms			AltConf
32	24	1	Total 42	C 40	O 2	0
32	32	1	Total 42	C 40	O 2	0
32	32	1	Total 42	C 40	O 2	0
32	32	1	Total 42	C 40	O 2	0
32	32	1	Total 42	C 40	O 2	0
32	31	1	Total 42	C 40	O 2	0
32	31	1	Total 42	C 40	O 2	0
32	33	1	Total 42	C 40	O 2	0
32	33	1	Total 42	C 40	O 2	0
32	33	1	Total 42	C 40	O 2	0
32	33	1	Total 42	C 40	O 2	0
32	34	1	Total 42	C 40	O 2	0
32	34	1	Total 42	C 40	O 2	0
32	34	1	Total 42	C 40	O 2	0
32	34	1	Total 42	C 40	O 2	0
32	42	1	Total 42	C 40	O 2	0
32	42	1	Total 42	C 40	O 2	0
32	42	1	Total 42	C 40	O 2	0
32	42	1	Total 42	C 40	O 2	0
32	41	1	Total 42	C 40	O 2	0
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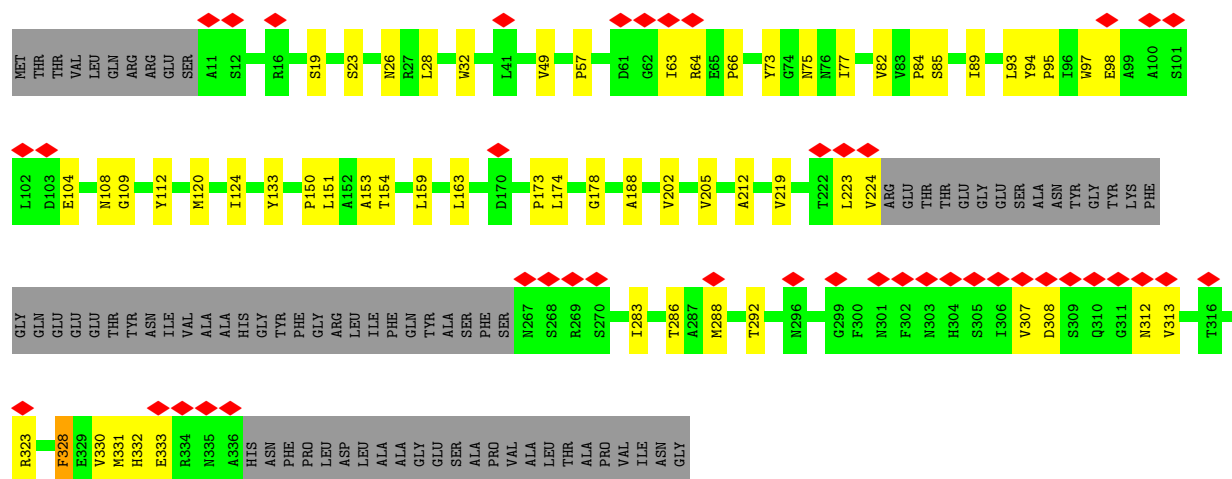
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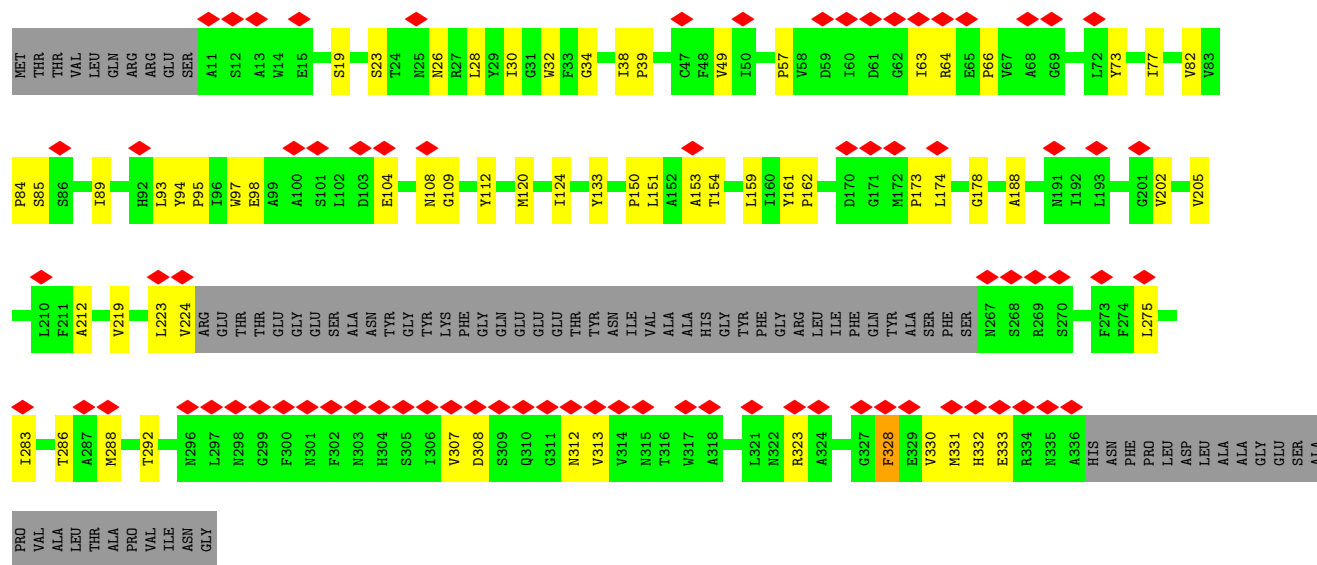
Mol	Chain	Residues	Atoms			AltConf
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			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	



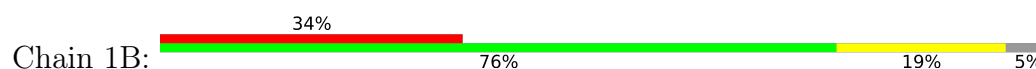
• Molecule 1: Photosystem II protein D1 2

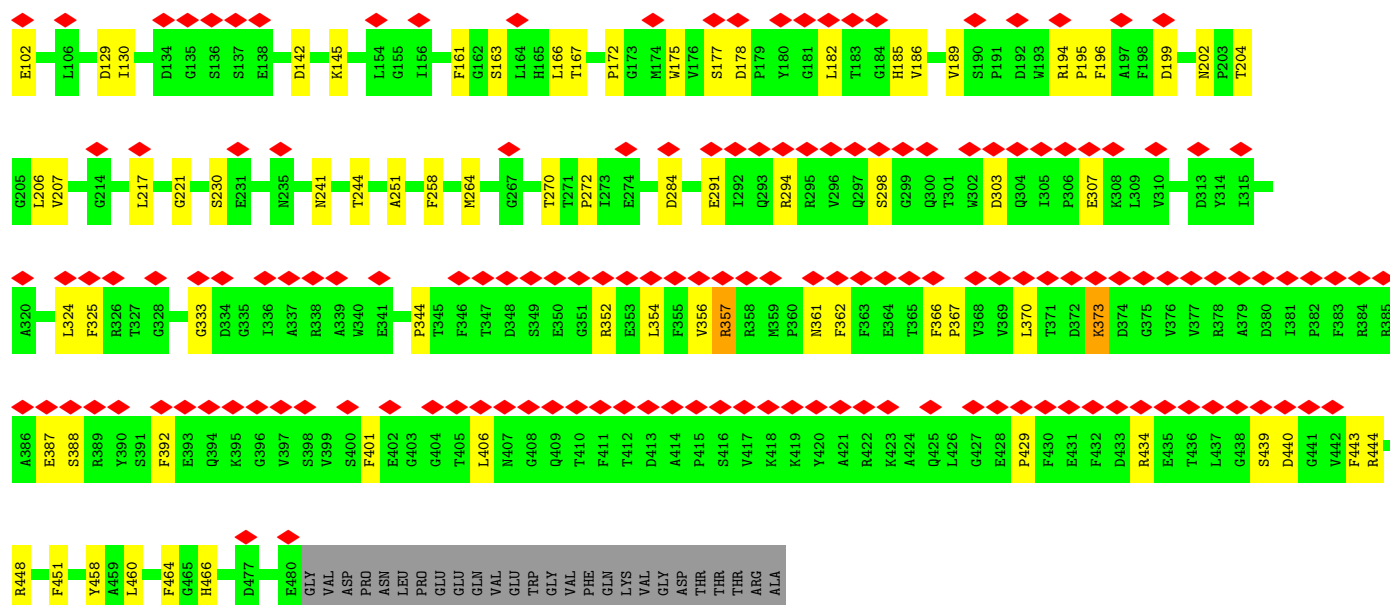


• Molecule 1: Photosystem II protein D1 2



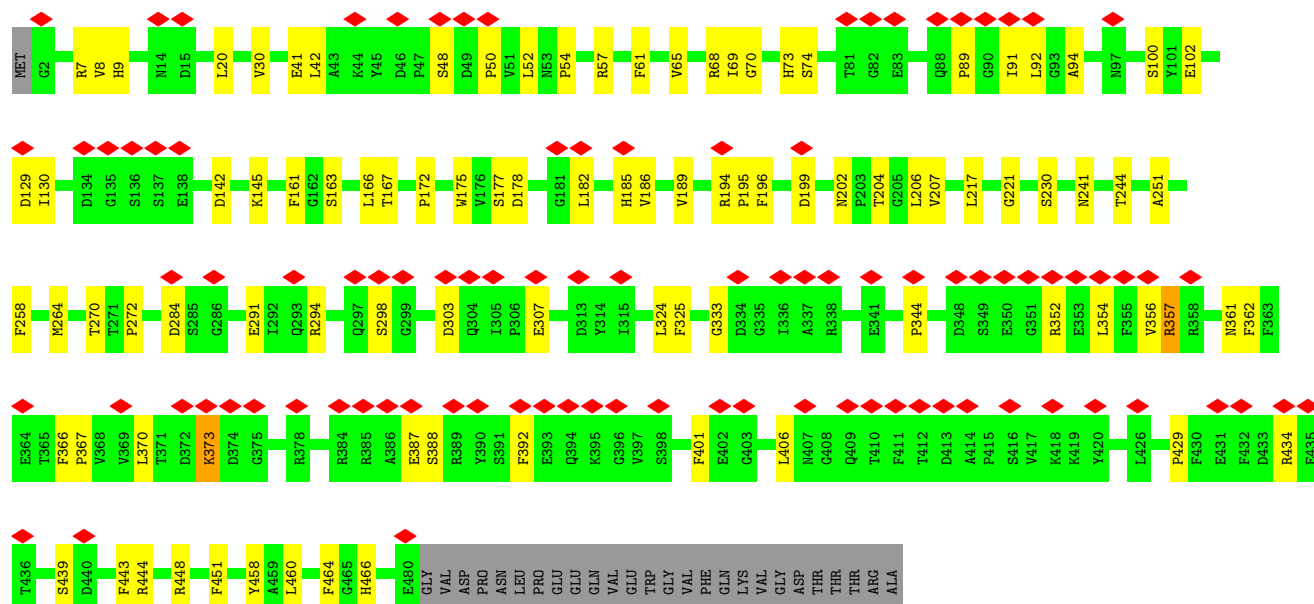
• Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 2: Photosystem II CP47 reaction center protein

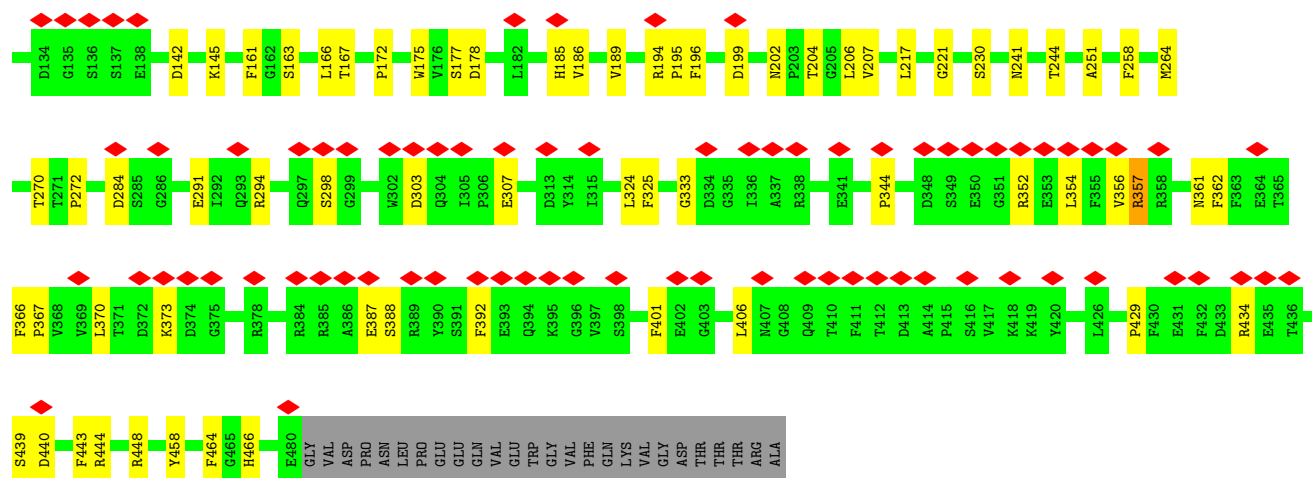
Chain 2B: 19% 76% 18% 5%



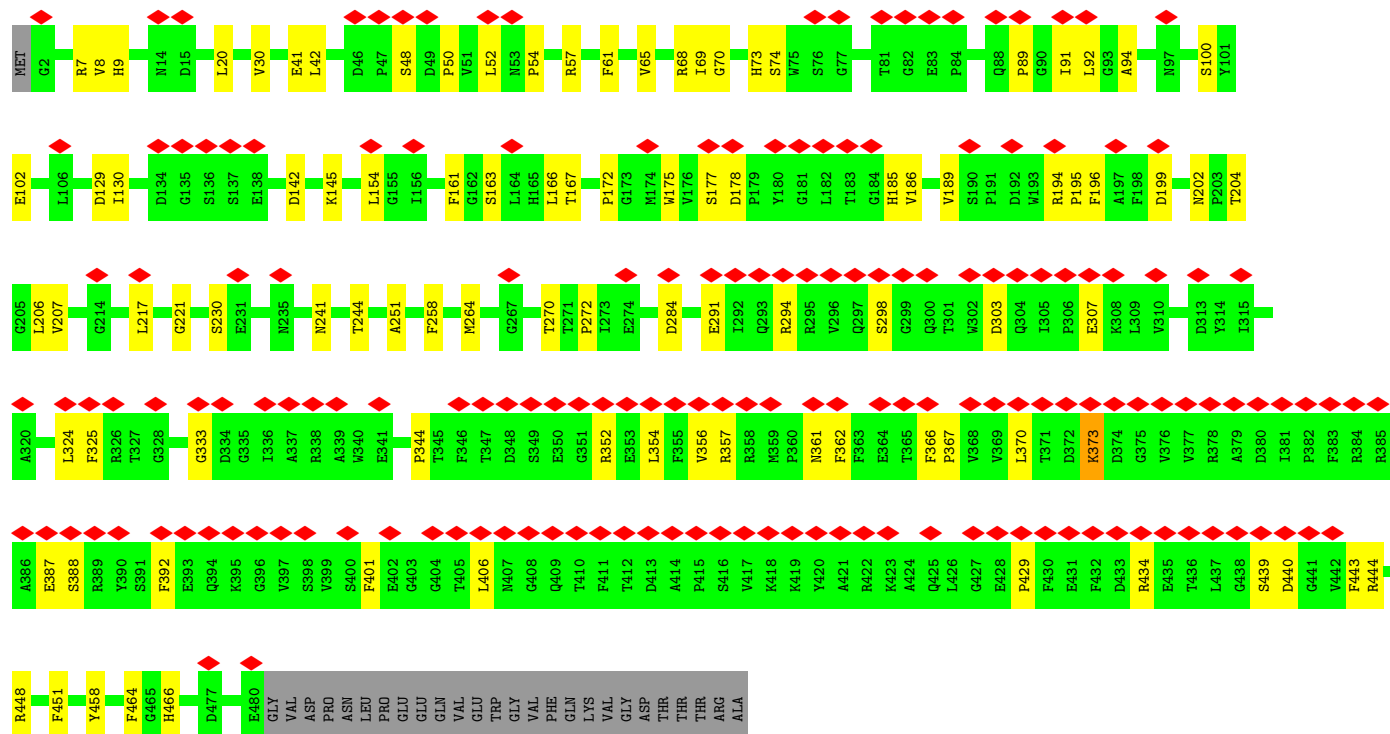
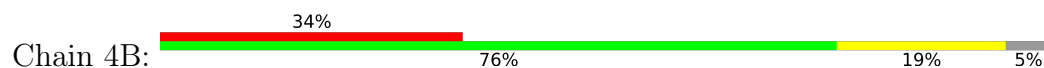
• Molecule 2: Photosystem II CP47 reaction center protein

Chain 3B: 19% 76% 18% 5%

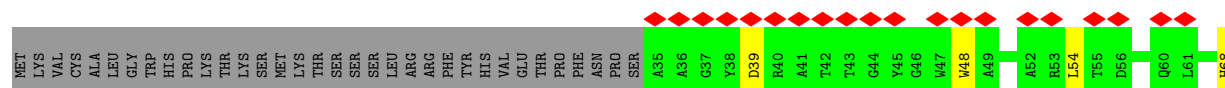


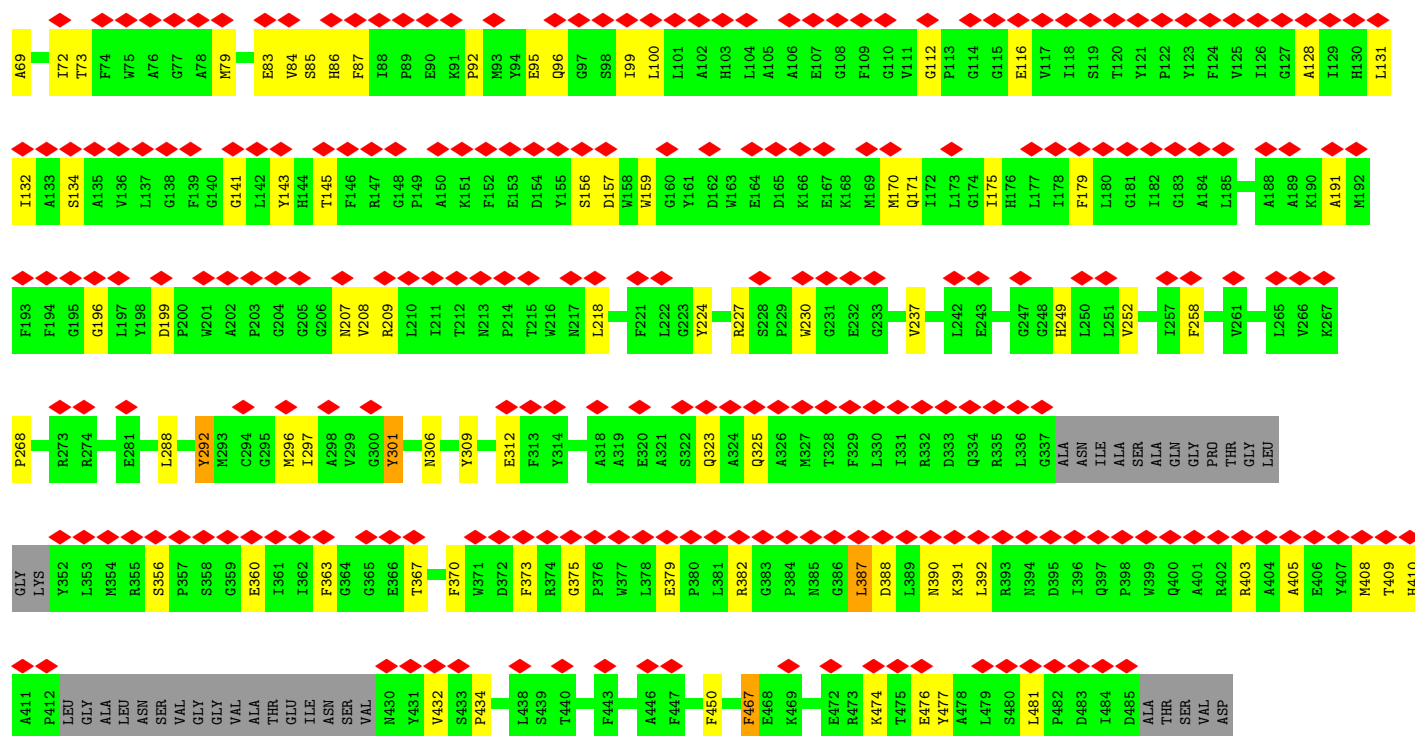


• Molecule 2: Photosystem II CP47 reaction center protein

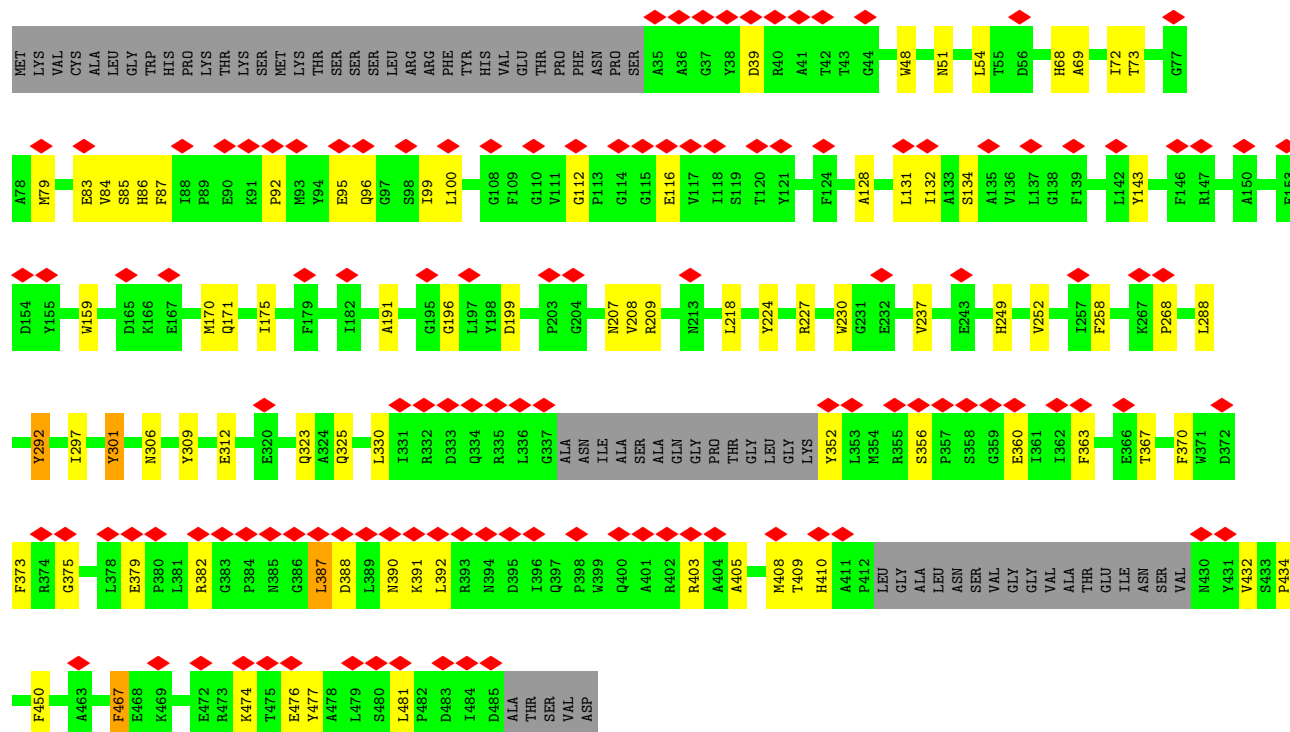


• Molecule 3: Photosystem II CP43 reaction center protein



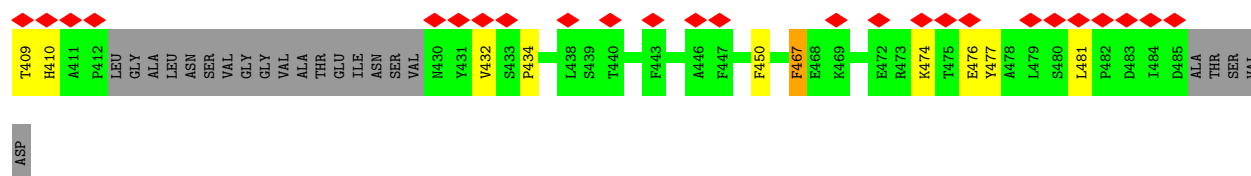


• Molecule 3: Photosystem II CP43 reaction center protein

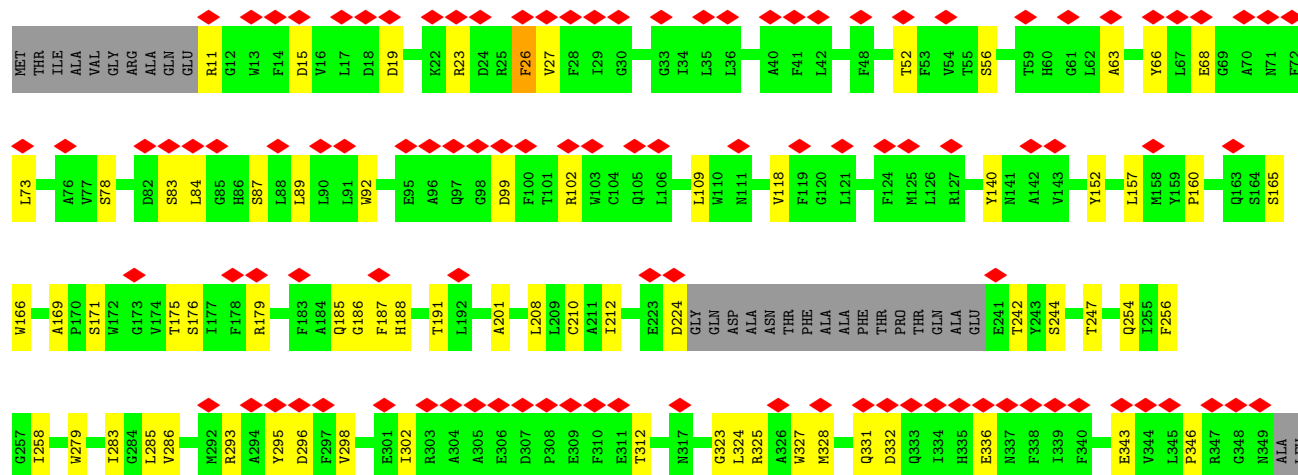
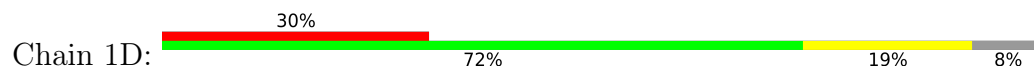


• Molecule 3: Photosystem II CP43 reaction center protein

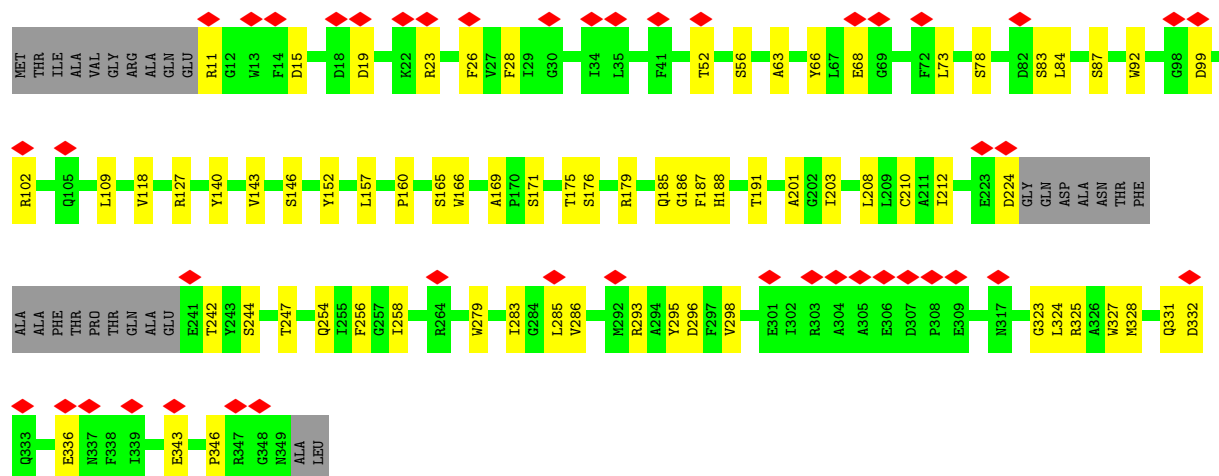
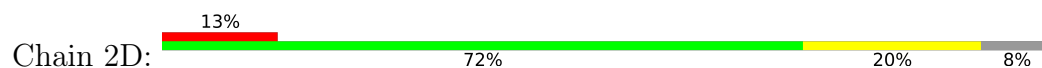




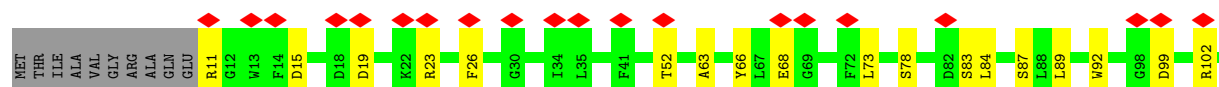
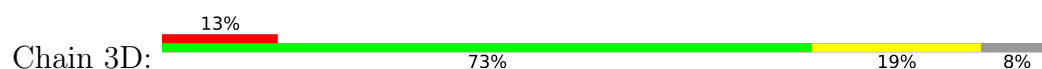
• Molecule 4: Photosystem II D2 protein 1

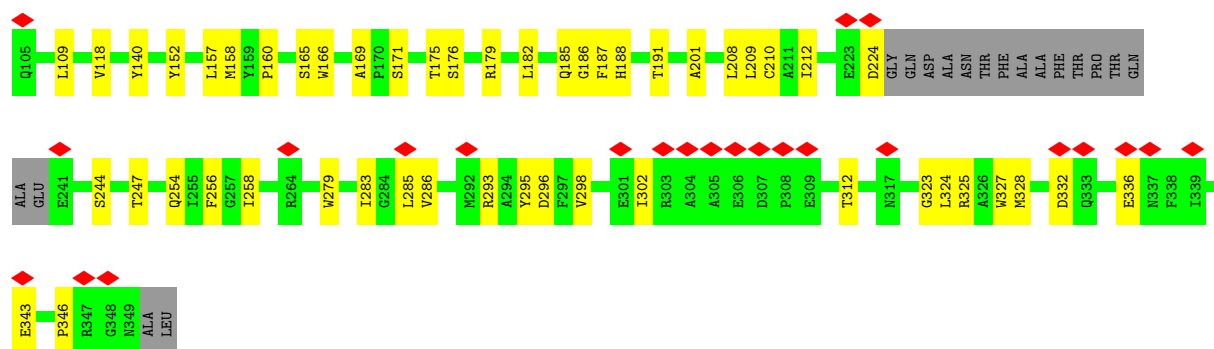


• Molecule 4: Photosystem II D2 protein 1

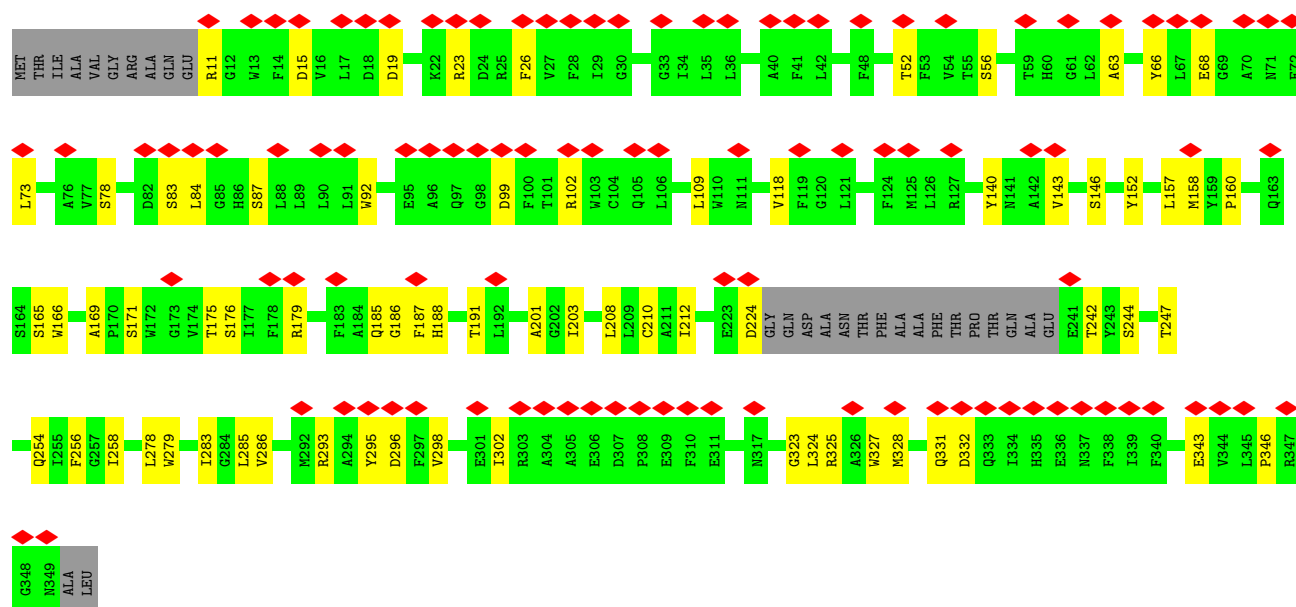


• Molecule 4: Photosystem II D2 protein 1

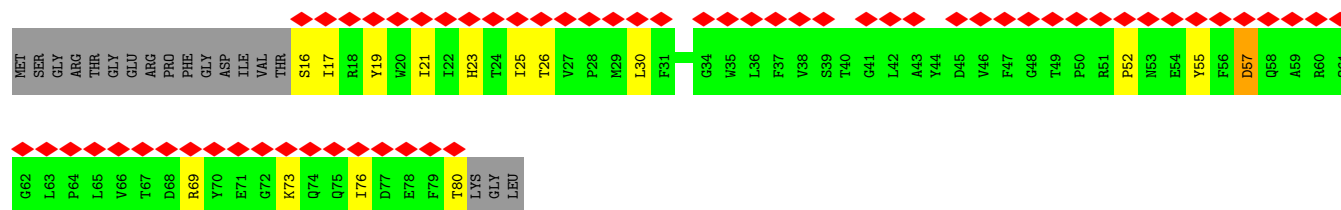
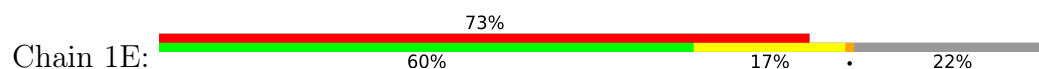




• Molecule 4: Photosystem II D2 protein 1

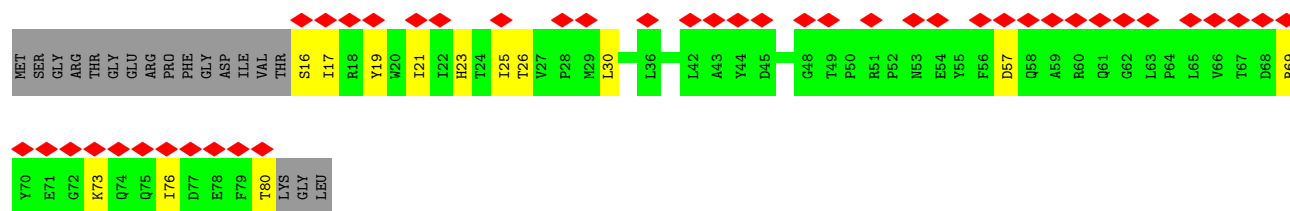


• Molecule 5: Cytochrome b559 subunit alpha

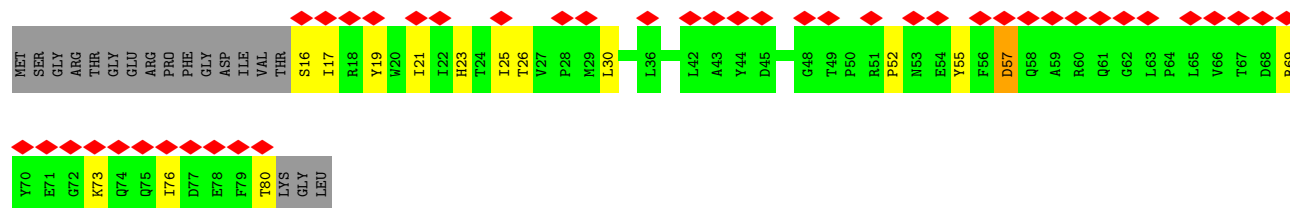


• Molecule 5: Cytochrome b559 subunit alpha

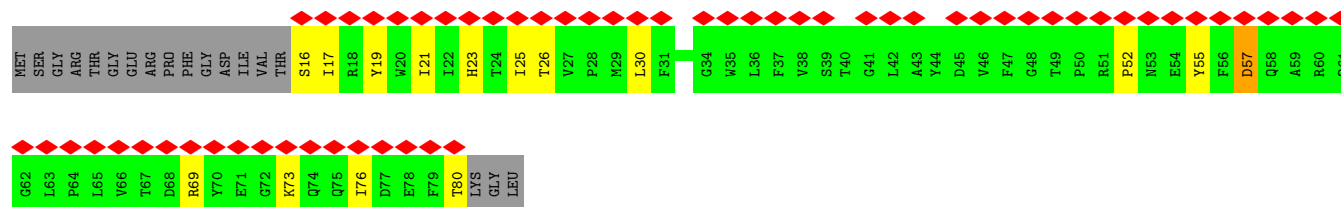
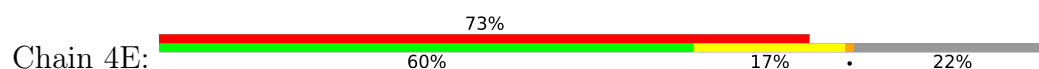




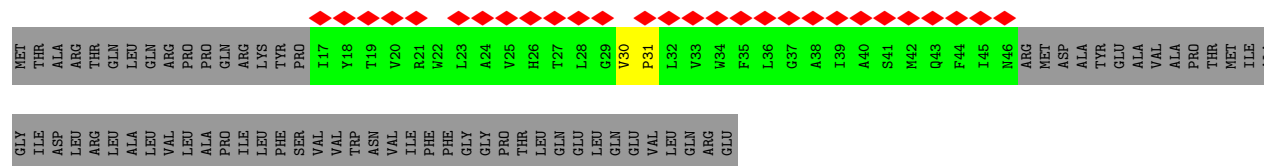
• Molecule 5: Cytochrome b559 subunit alpha



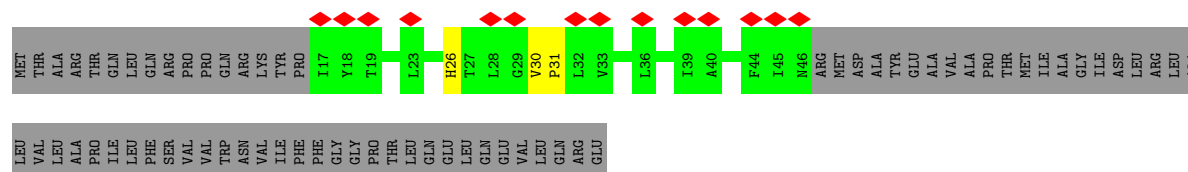
• Molecule 5: Cytochrome b559 subunit alpha



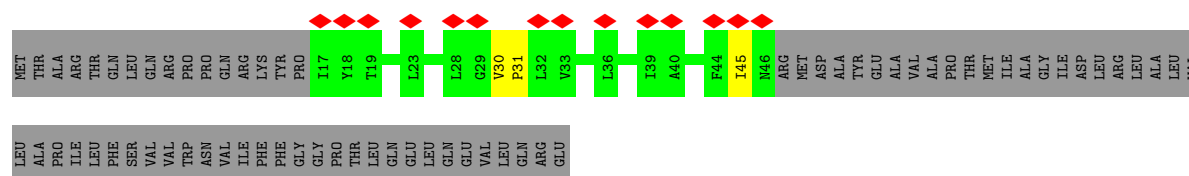
• Molecule 6: Photosystem II protein Y



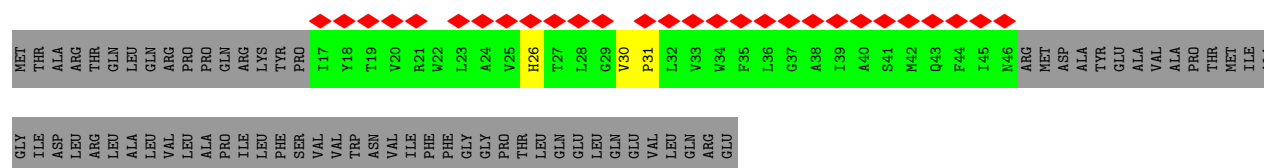
• Molecule 6: Photosystem II protein Y



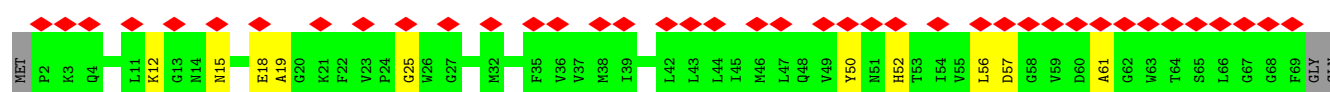
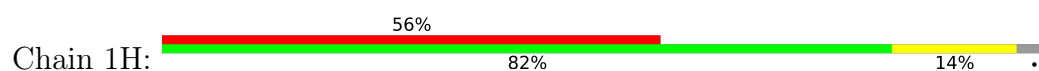
• Molecule 6: Photosystem II protein Y



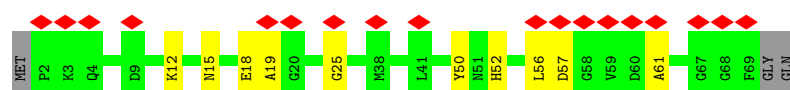
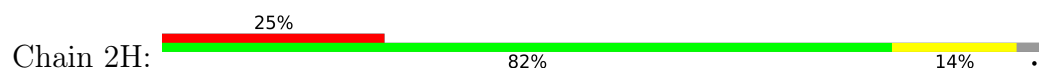
- Molecule 6: Photosystem II protein Y



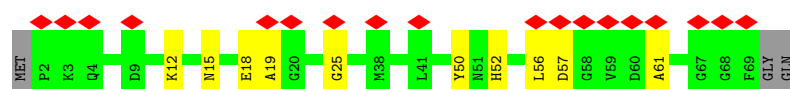
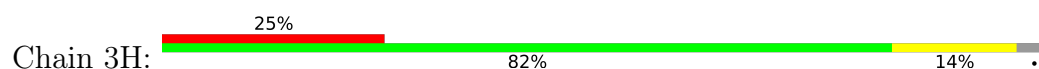
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



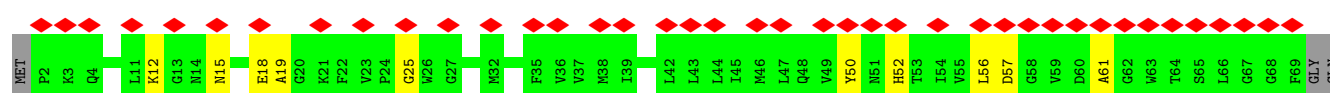
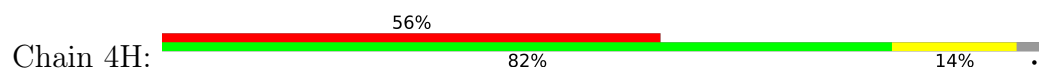
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



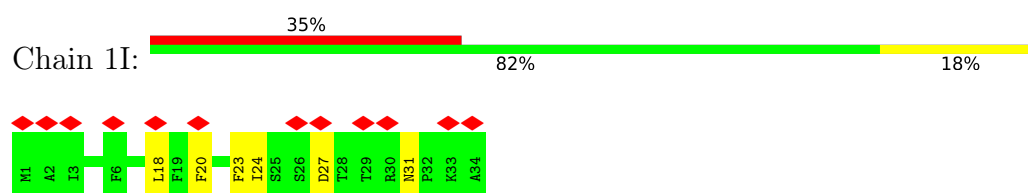
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



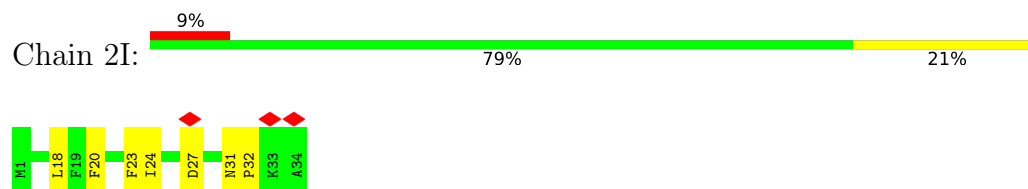
- Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



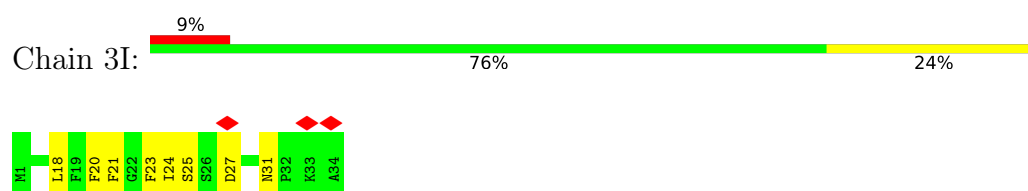
- Molecule 8: Photosystem II protein PsbI



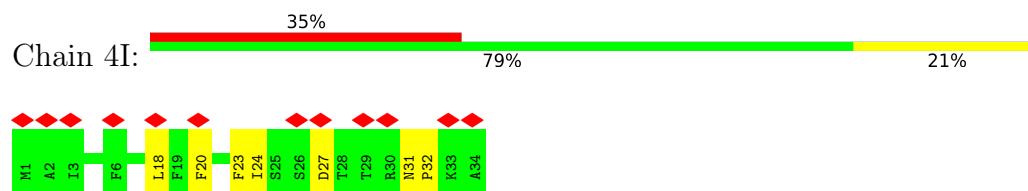
- Molecule 8: Photosystem II protein PsbI



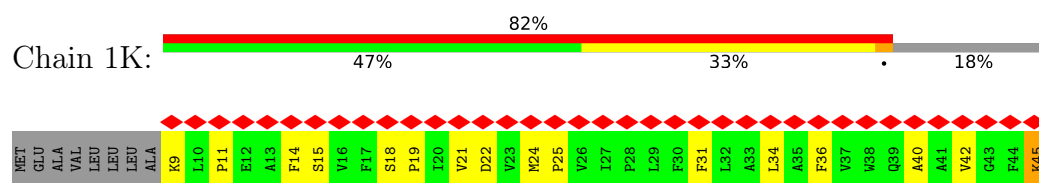
- Molecule 8: Photosystem II protein PsbI



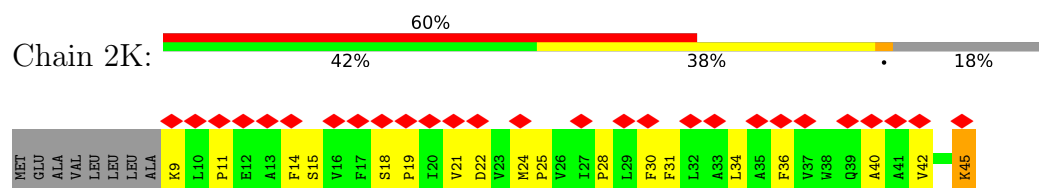
- Molecule 8: Photosystem II protein PsbI



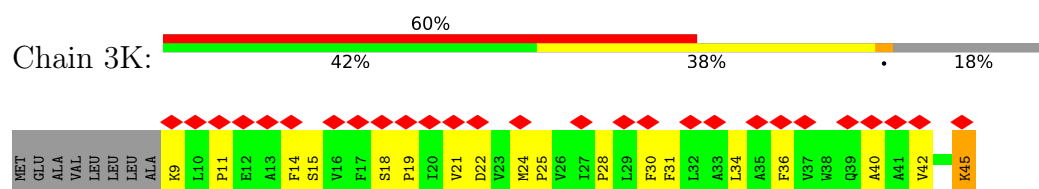
- Molecule 9: Photosystem II reaction center protein K



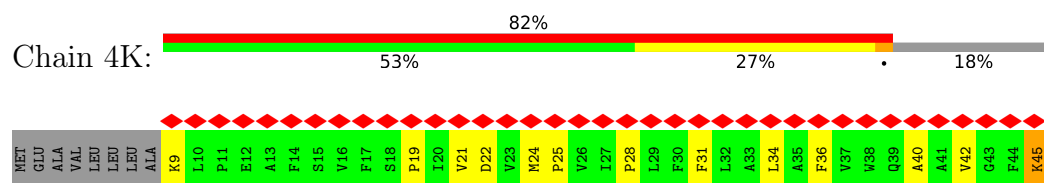
- Molecule 9: Photosystem II reaction center protein K



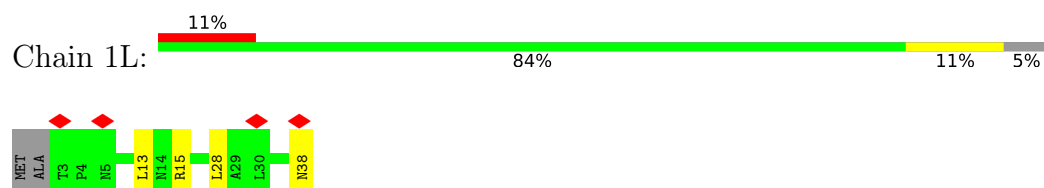
- Molecule 9: Photosystem II reaction center protein K



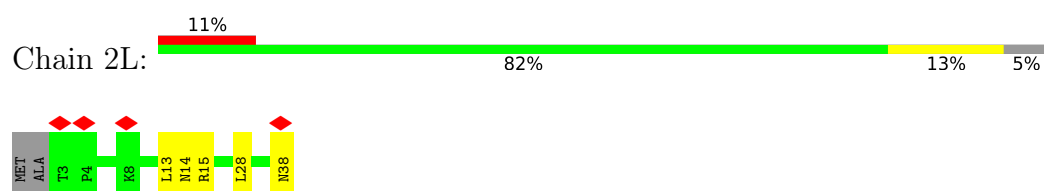
- Molecule 9: Photosystem II reaction center protein K



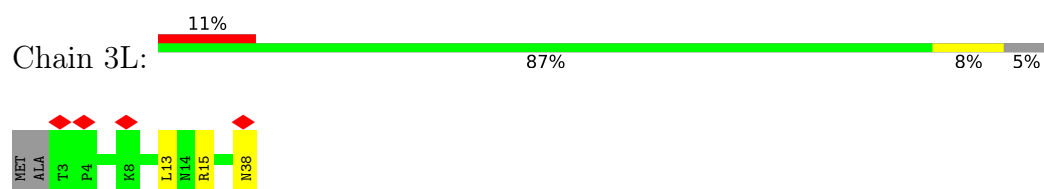
- Molecule 10: Photosystem II reaction center protein L



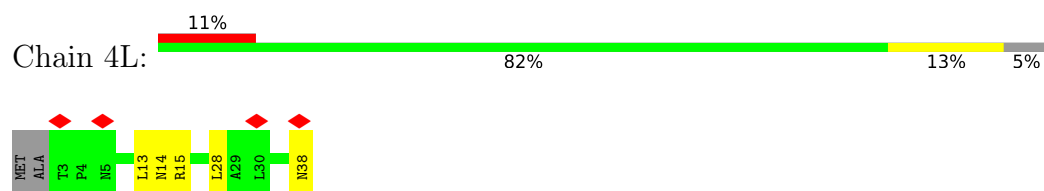
- Molecule 10: Photosystem II reaction center protein L



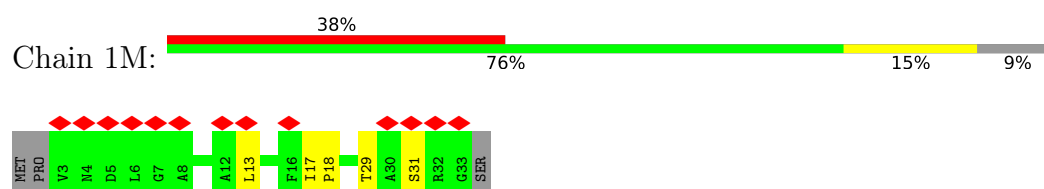
- Molecule 10: Photosystem II reaction center protein L



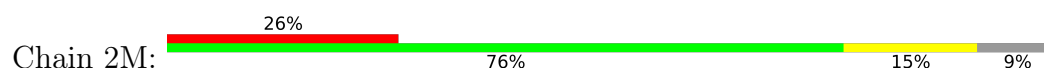
- Molecule 10: Photosystem II reaction center protein L

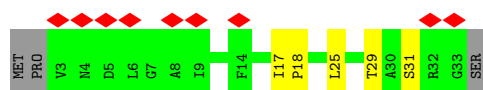


- Molecule 11: Photosystem II reaction center protein M

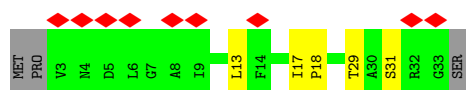
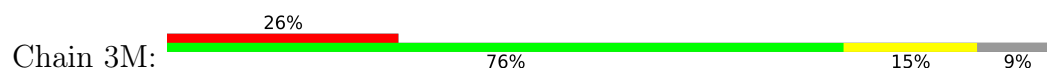


- Molecule 11: Photosystem II reaction center protein M

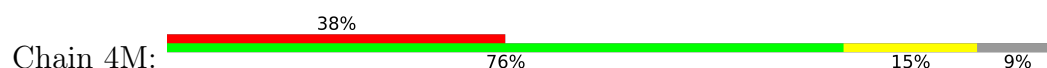




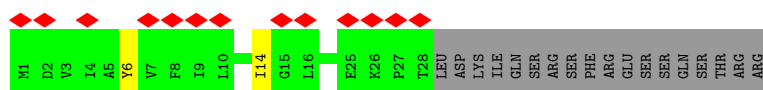
- Molecule 11: Photosystem II reaction center protein M



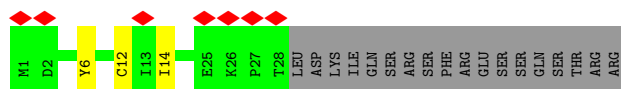
- Molecule 11: Photosystem II reaction center protein M



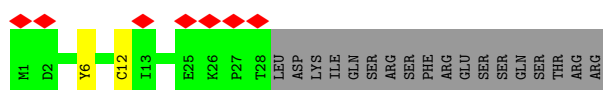
- Molecule 12: Photosystem II reaction center protein T



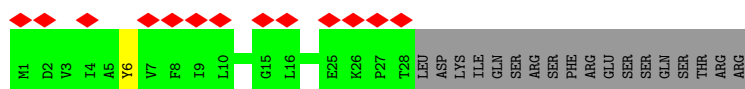
- Molecule 12: Photosystem II reaction center protein T



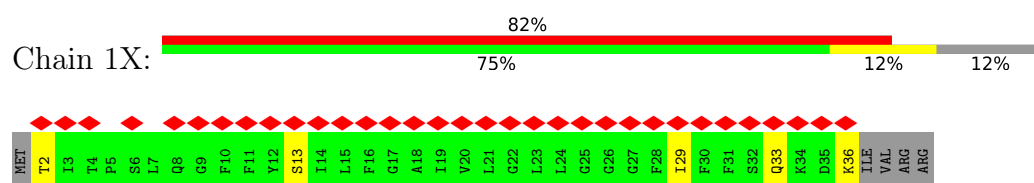
- Molecule 12: Photosystem II reaction center protein T



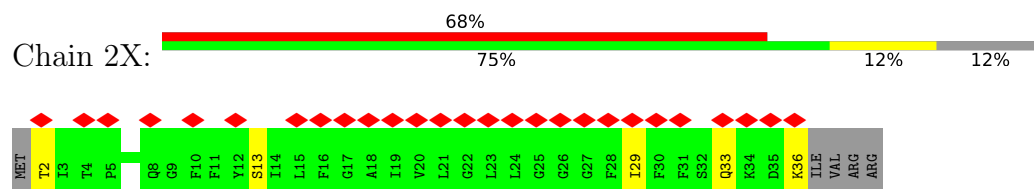
- Molecule 12: Photosystem II reaction center protein T



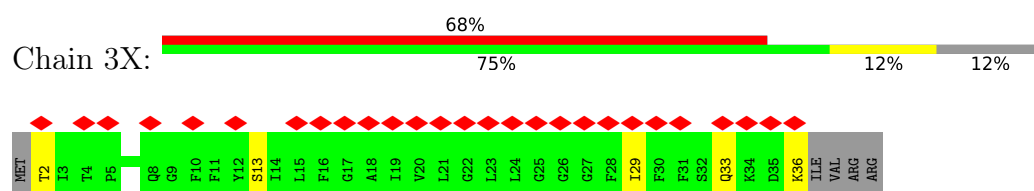
- Molecule 13: Photosystem II reaction center X protein



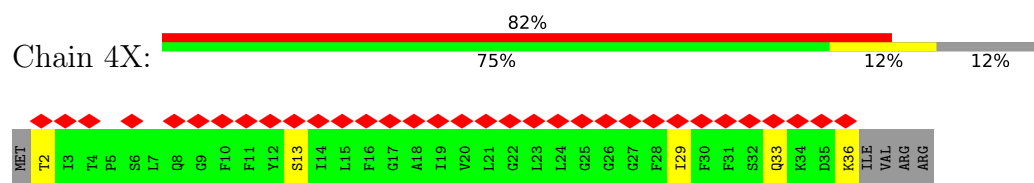
- Molecule 13: Photosystem II reaction center X protein



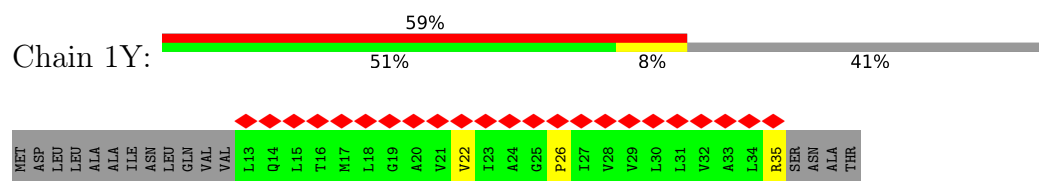
- Molecule 13: Photosystem II reaction center X protein



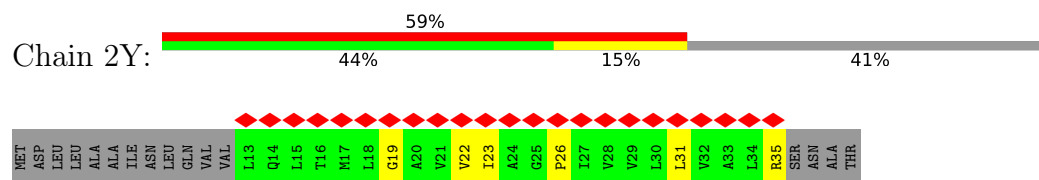
- Molecule 13: Photosystem II reaction center X protein



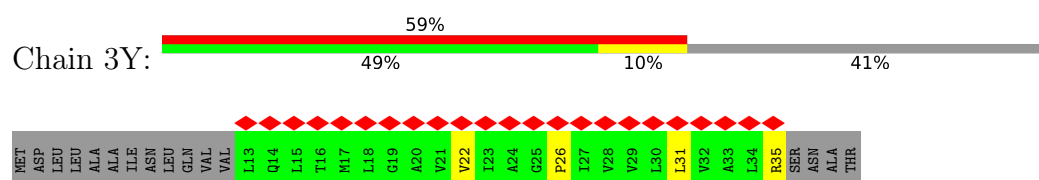
- Molecule 14: Photosystem II reaction center protein Ycf12



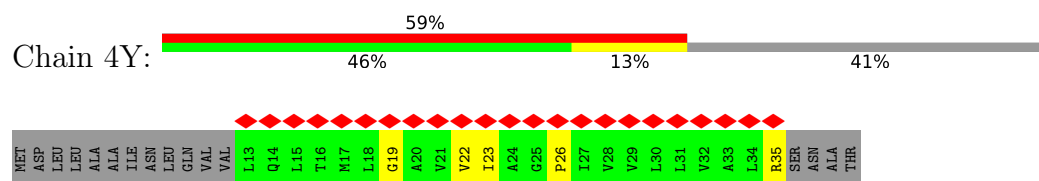
- Molecule 14: Photosystem II reaction center protein Ycf12



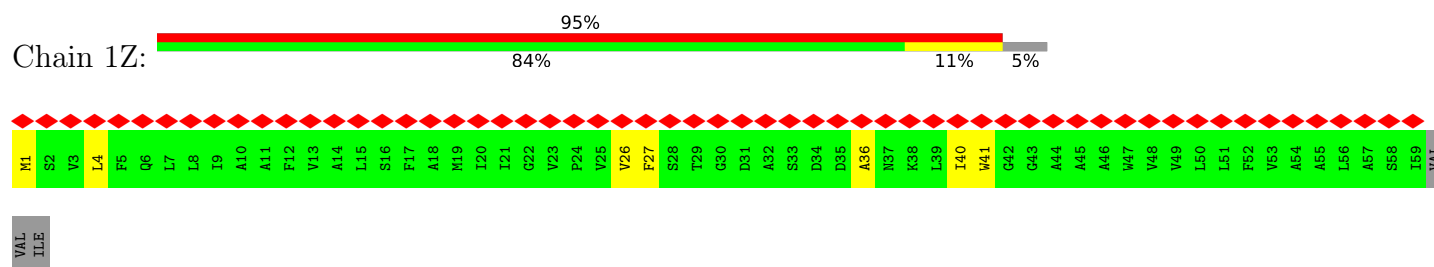
- Molecule 14: Photosystem II reaction center protein Ycf12



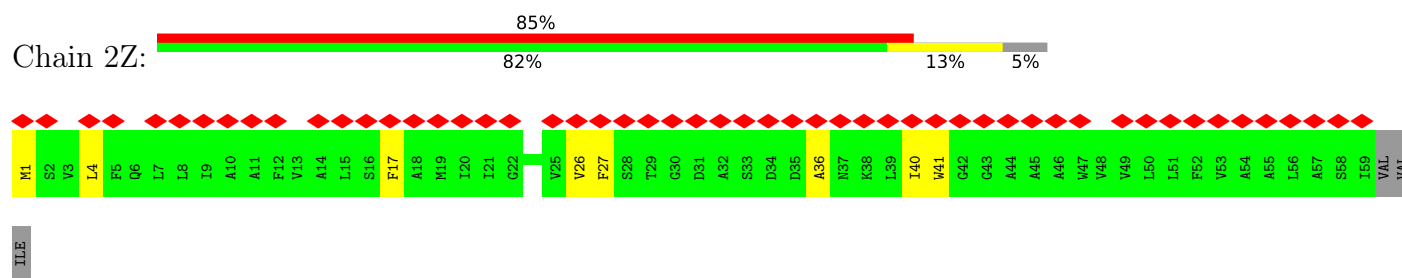
- Molecule 14: Photosystem II reaction center protein Ycf12



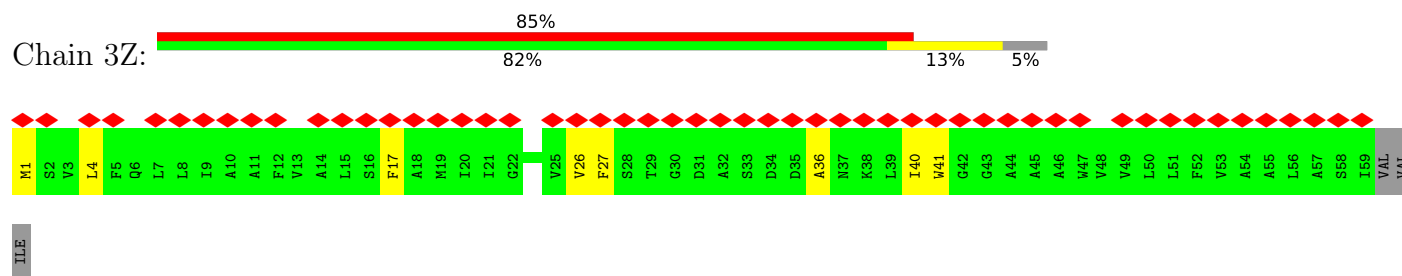
- Molecule 15: Photosystem II reaction center protein Z



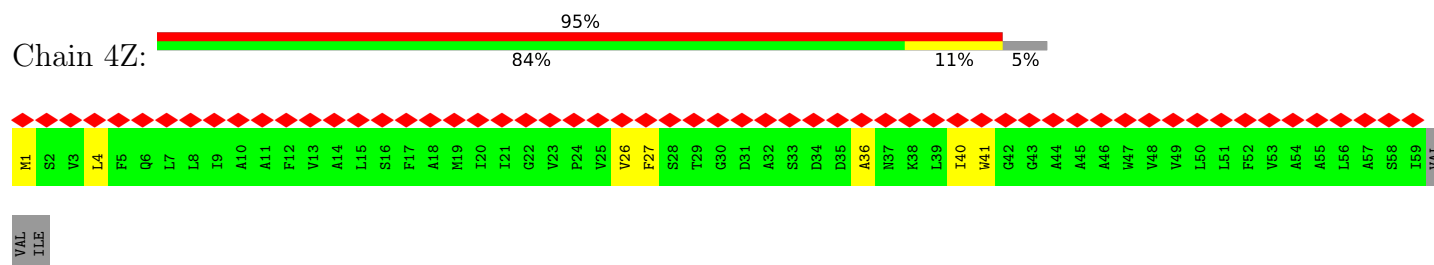
- Molecule 15: Photosystem II reaction center protein Z



- Molecule 15: Photosystem II reaction center protein Z

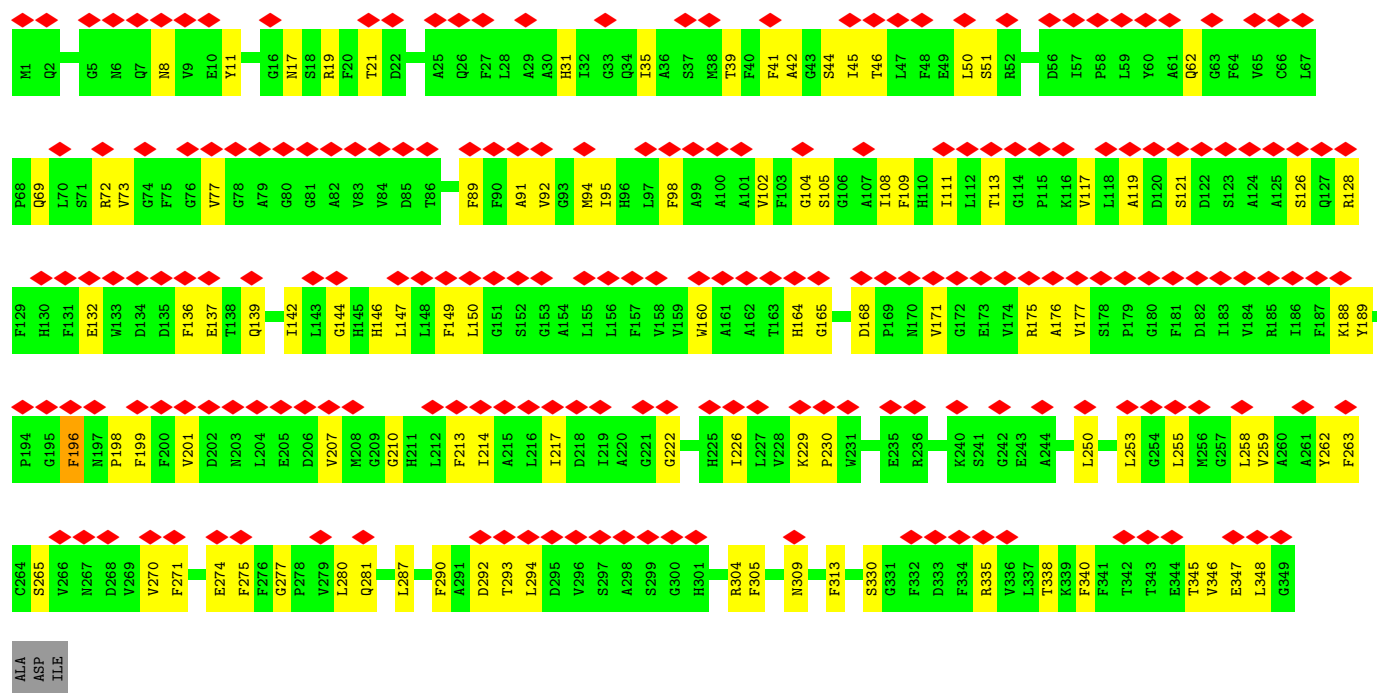


- Molecule 15: Photosystem II reaction center protein Z



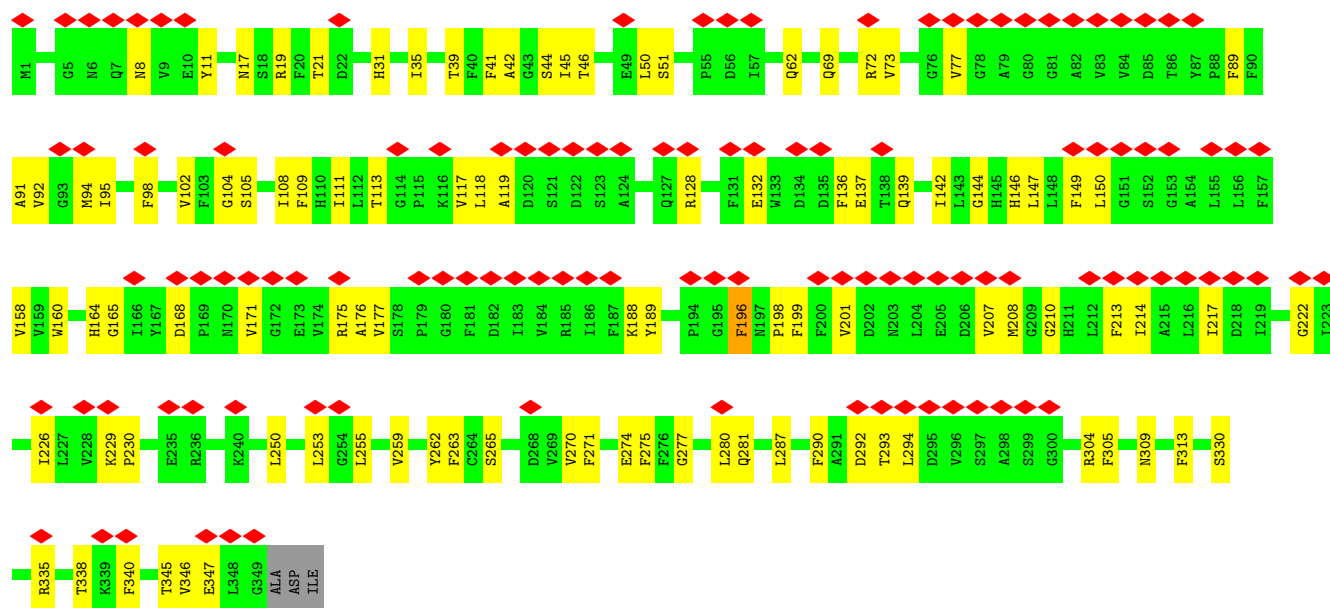
- Molecule 16: High light inducible protein





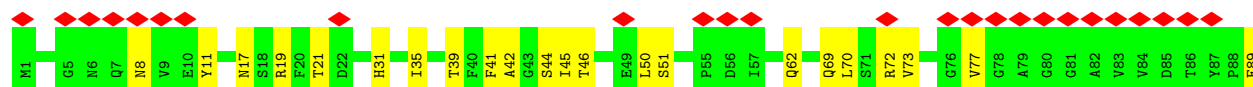
• Molecule 16: High light inducible protein

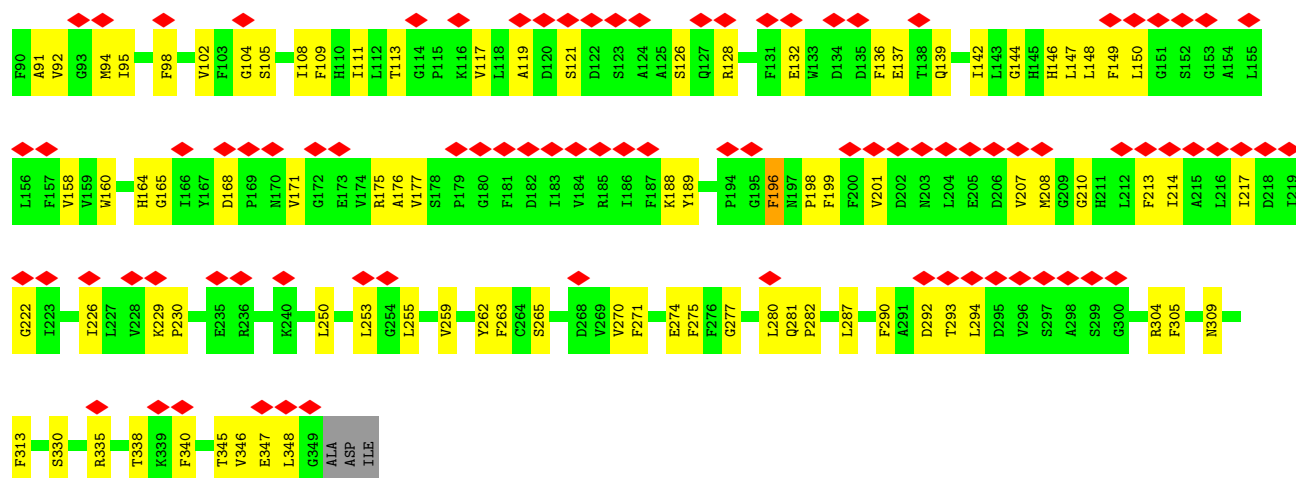
Chain 22: 33% 70% 29%



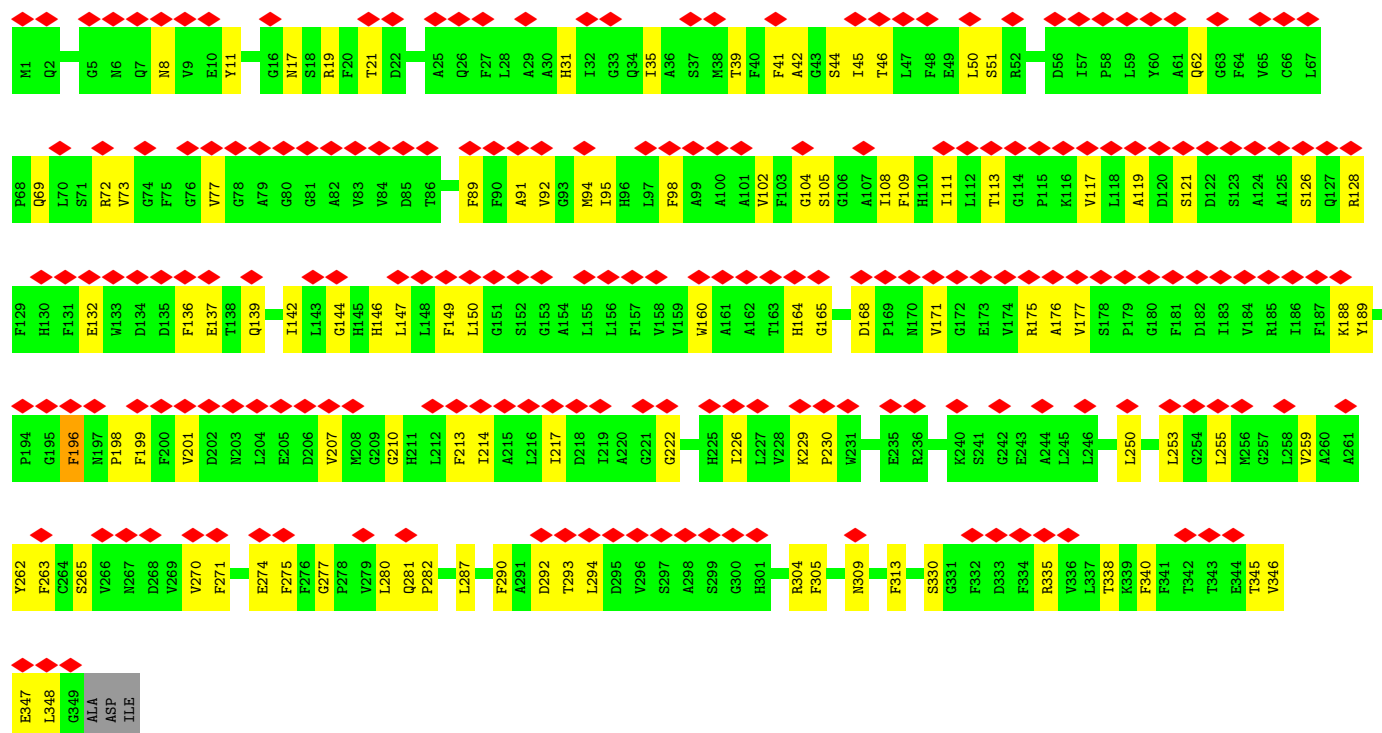
• Molecule 16: High light inducible protein

Chain 32: 32% 69% 30%

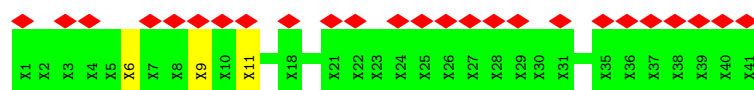




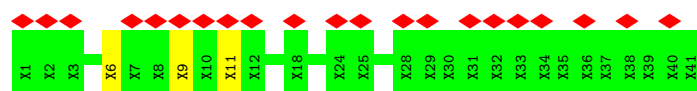
• Molecule 16: High light inducible protein



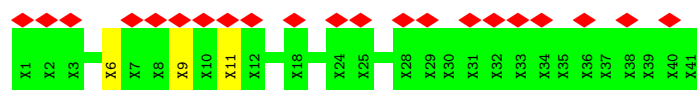
• Molecule 17: Unknown protein



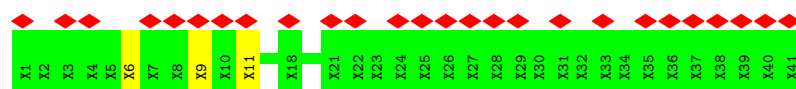
• Molecule 17: Unknown protein



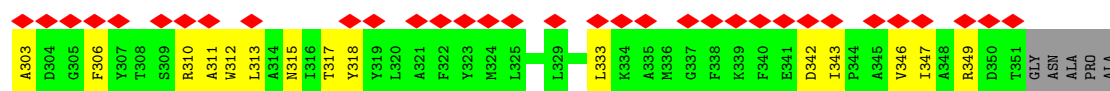
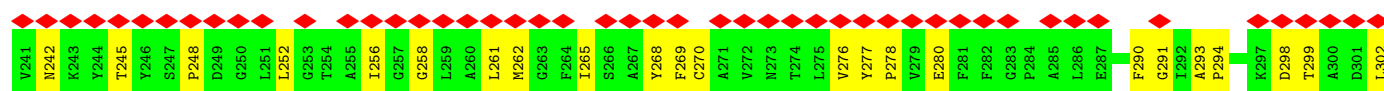
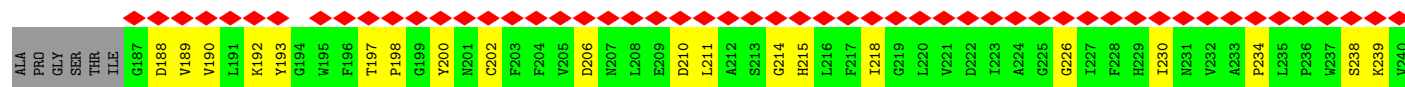
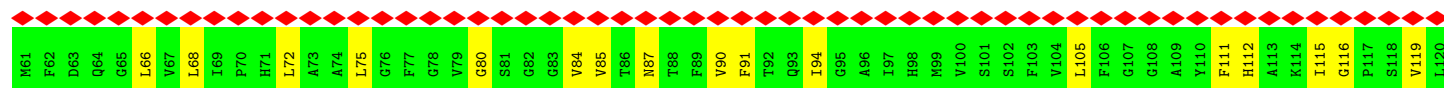
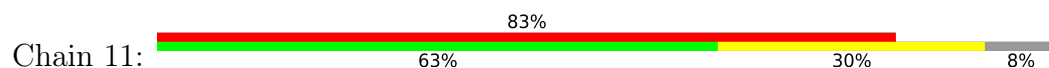
- Molecule 17: Unknown protein



- Molecule 17: Unknown protein

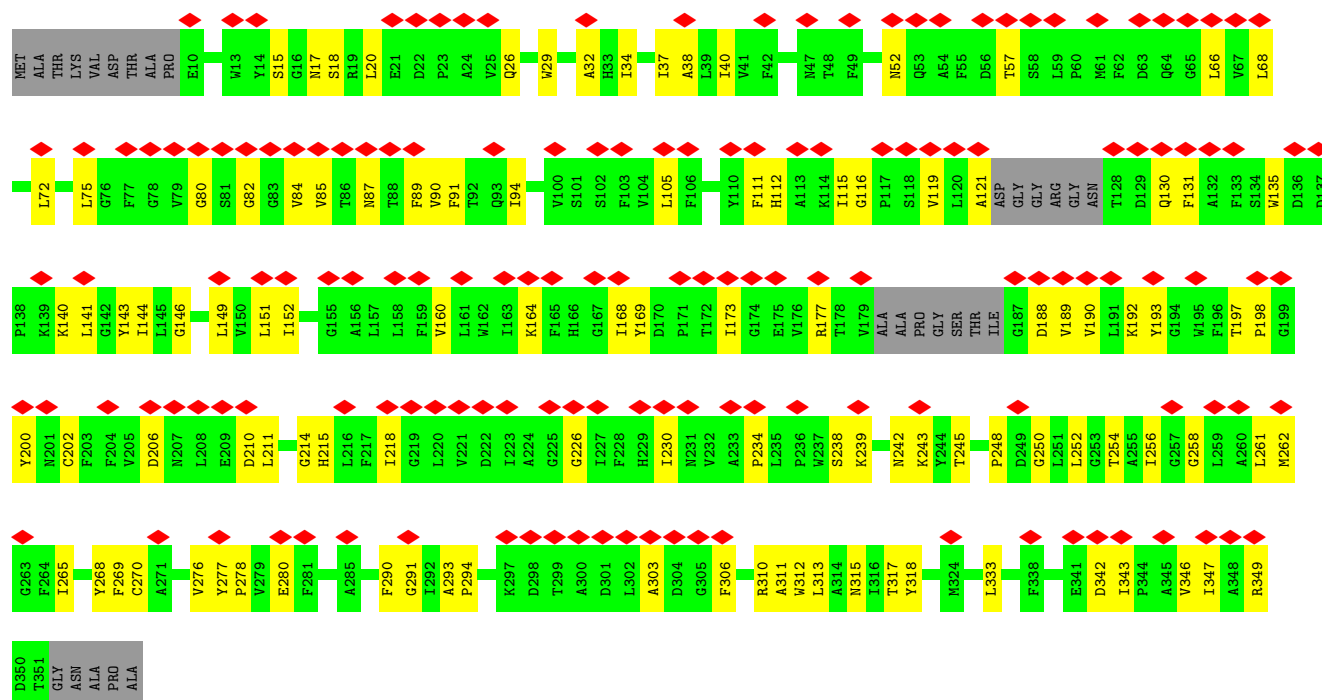


- Molecule 18: High light inducible protein

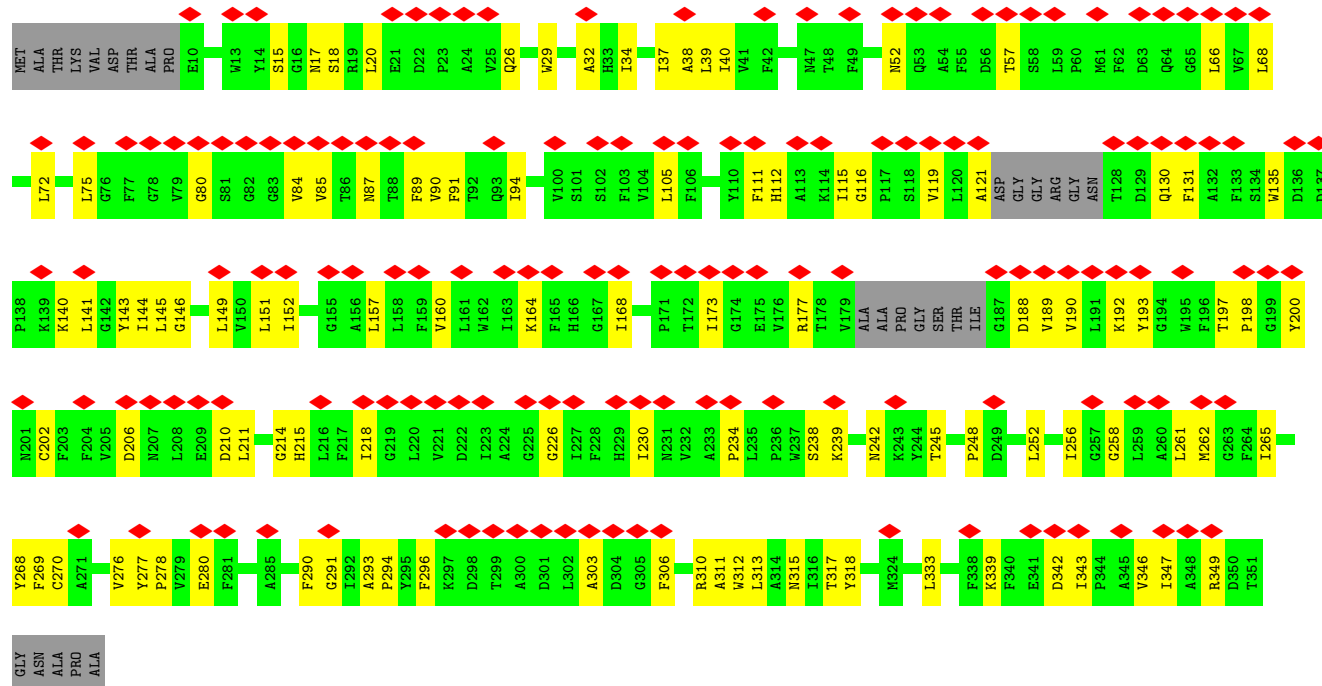
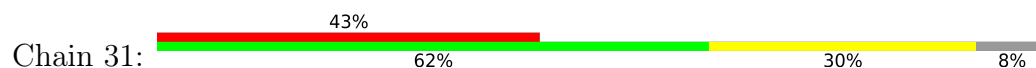


- Molecule 18: High light inducible protein

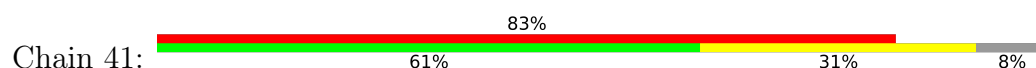


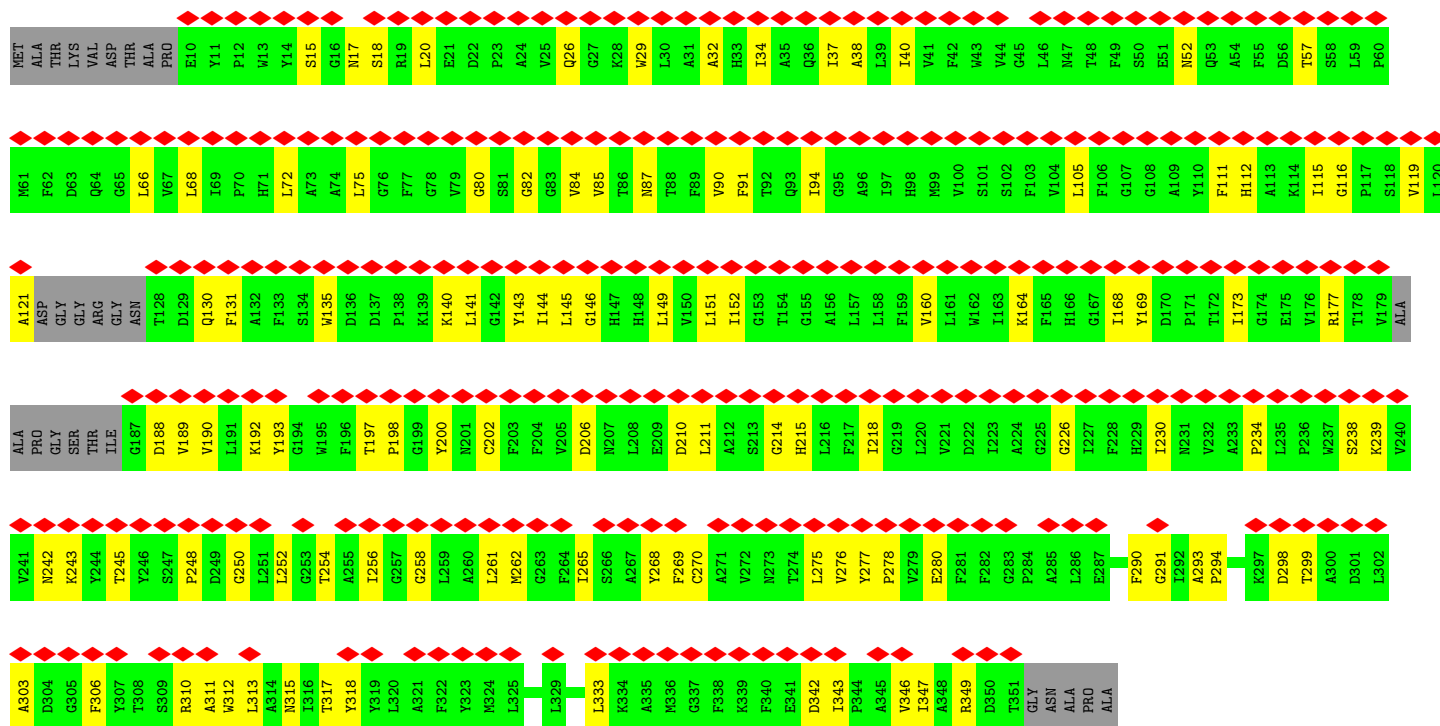


- Molecule 18: High light inducible protein

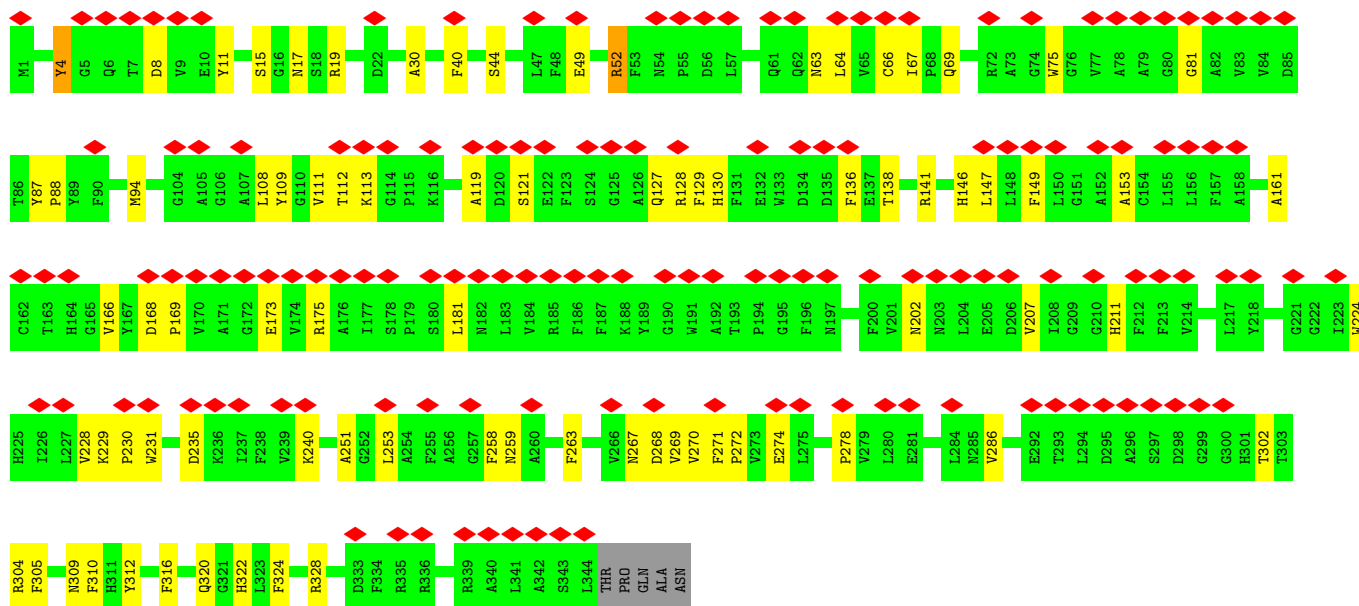
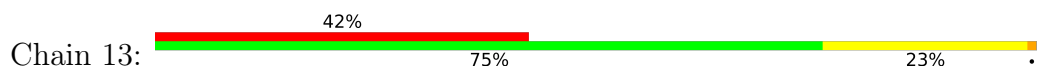


- Molecule 18: High light inducible protein

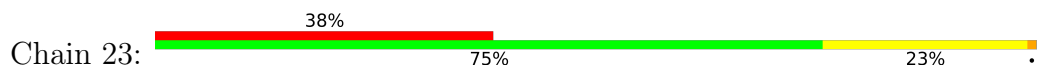


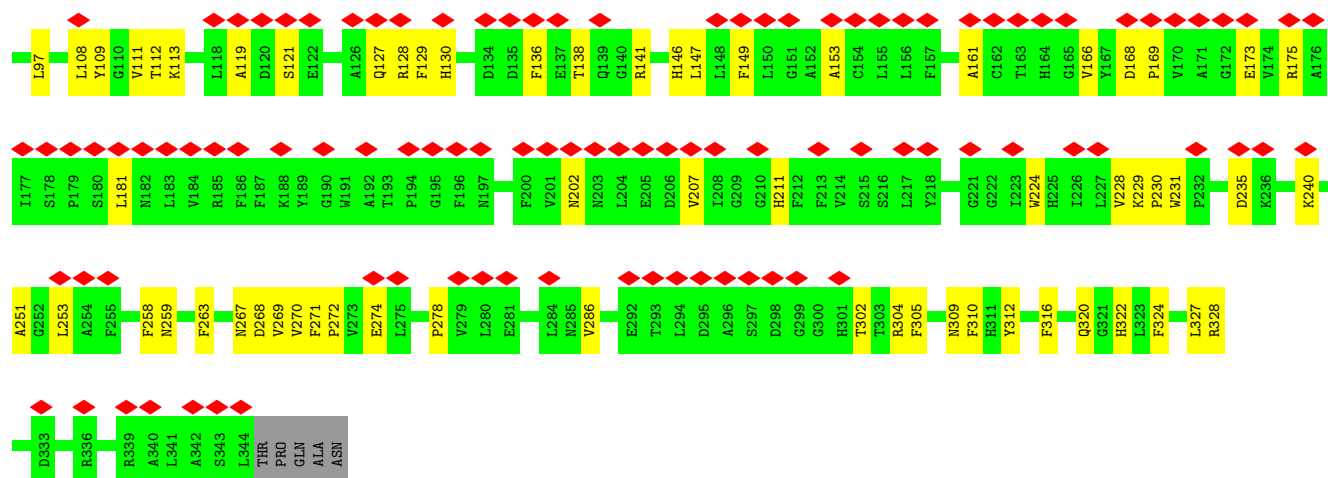


• Molecule 19: High light inducible protein



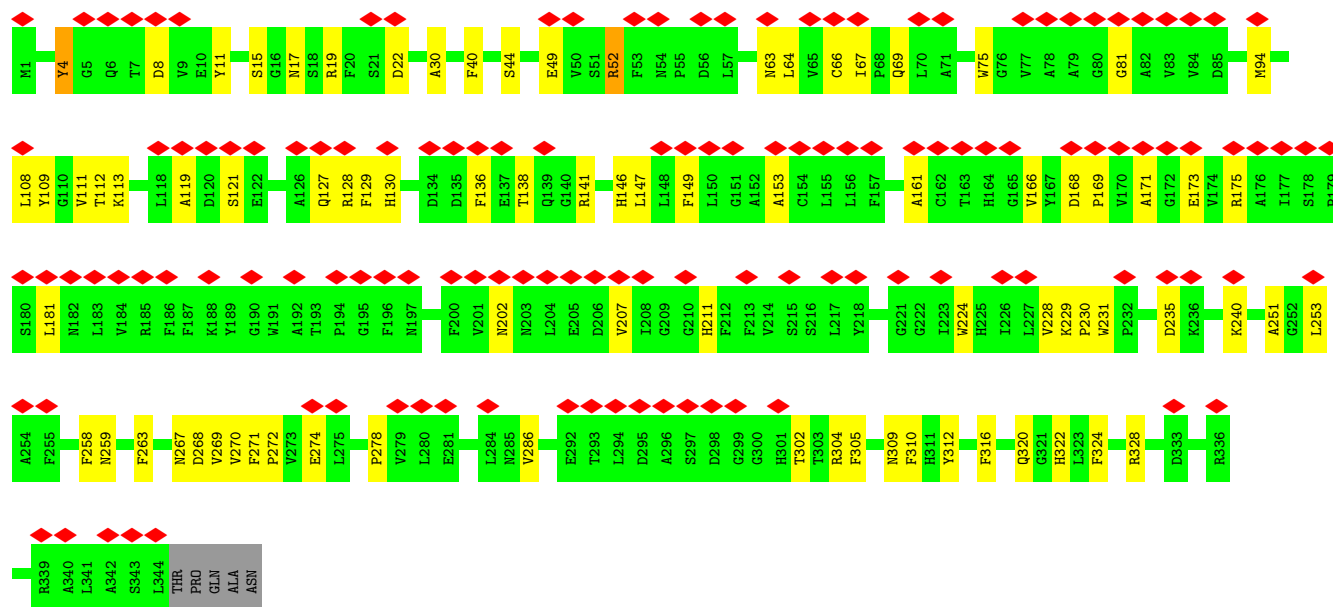
• Molecule 19: High light inducible protein





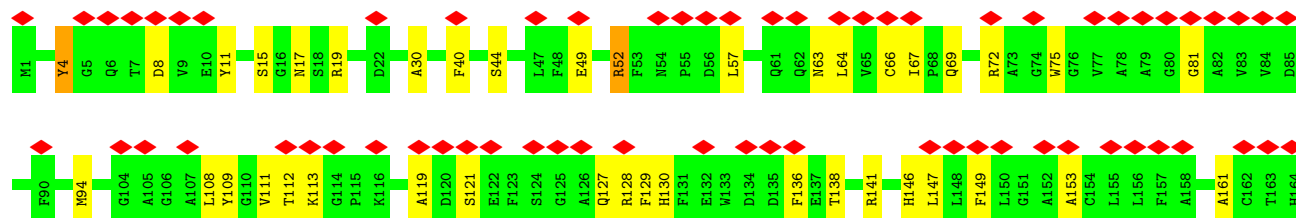
- Molecule 19: High light inducible protein

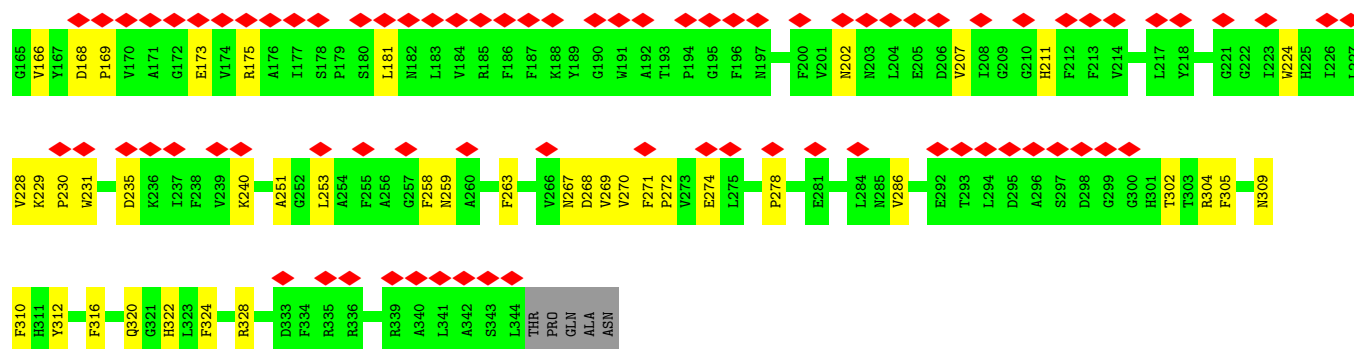
Chain 33: 38% 75% 23% ..



- Molecule 19: High light inducible protein

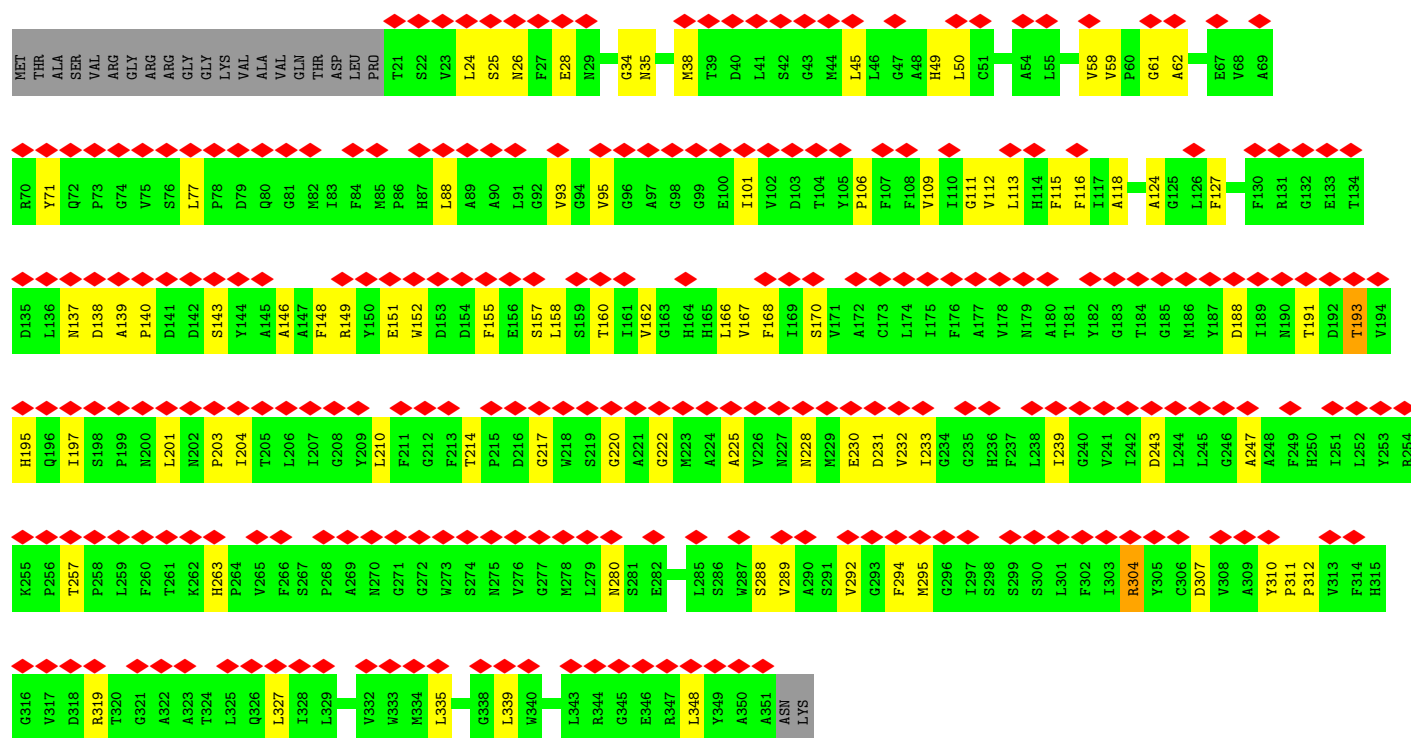
Chain 43: 42% 75% 23% ..





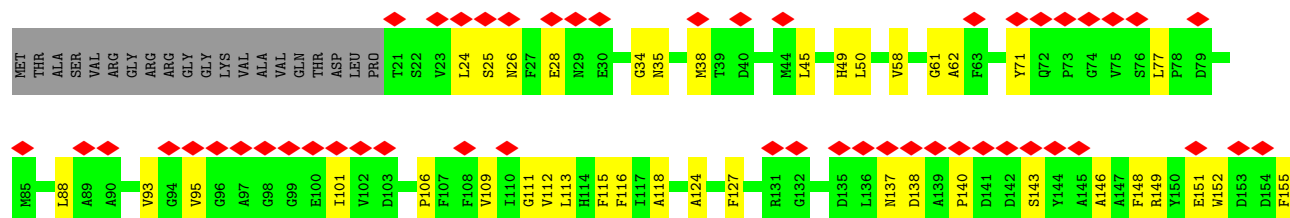
• Molecule 20: High light inducible protein

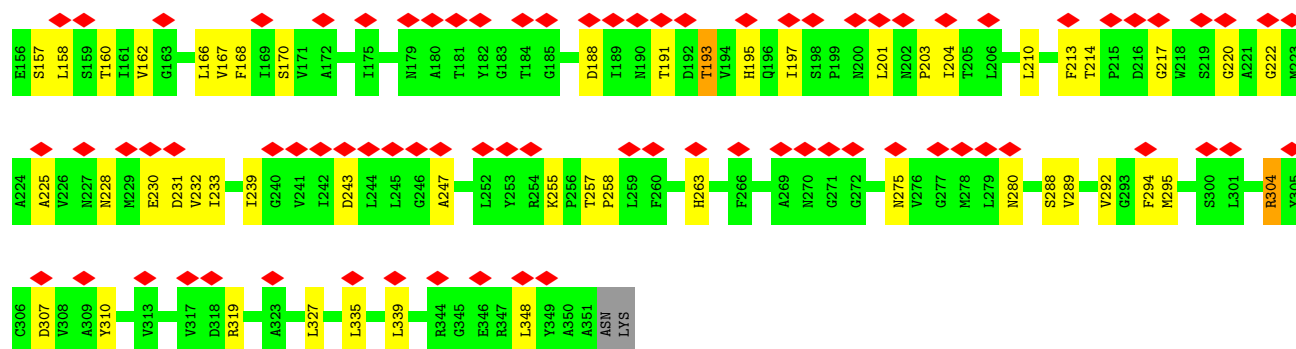
Chain 14: 71%
69% 25% 6%



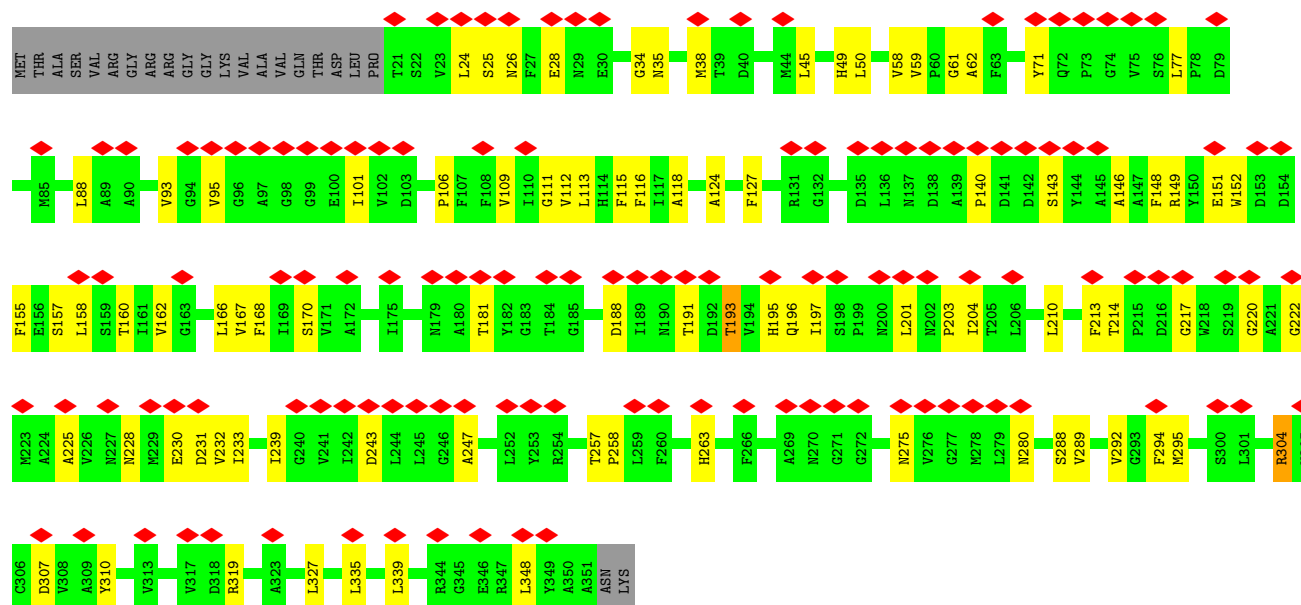
• Molecule 20: High light inducible protein

Chain 24: 36%
69% 25% 6%



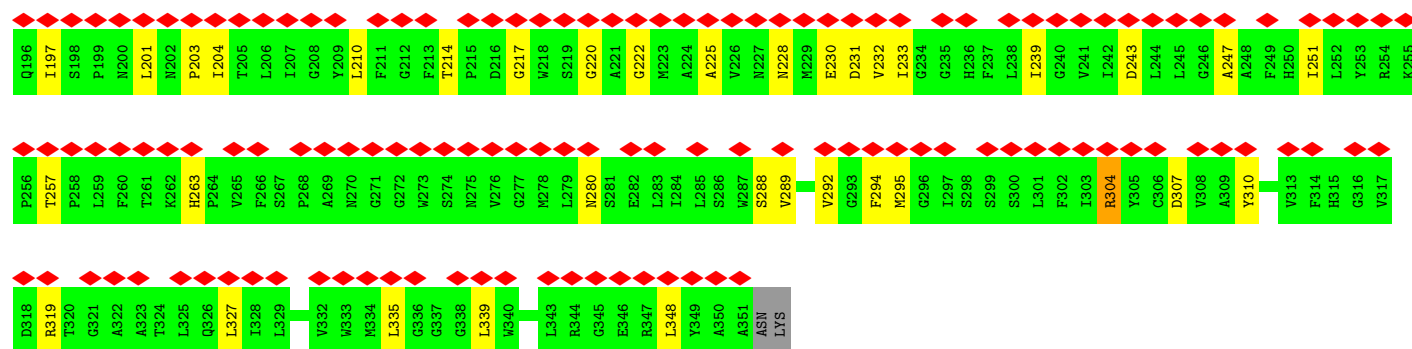


- Molecule 20: High light inducible protein



- Molecule 20: High light inducible protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LMG, HEM, SQD, CL7, LHG, FE2, PHO, BCT, PL9, 8CT, ZEX

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	0.47	0/2280	0.48	0/3112
1	2A	0.47	0/2280	0.48	0/3112
1	3A	0.47	0/2280	0.48	0/3112
1	4A	0.47	0/2280	0.48	0/3112
2	1B	0.46	0/3929	0.47	0/5360
2	2B	0.46	0/3929	0.47	0/5360
2	3B	0.46	0/3929	0.47	0/5360
2	4B	0.46	0/3929	0.47	0/5360
3	1C	0.43	0/3431	0.48	1/4669 (0.0%)
3	2C	0.43	0/3431	0.48	1/4669 (0.0%)
3	3C	0.43	0/3431	0.48	1/4669 (0.0%)
3	4C	0.43	0/3431	0.48	1/4669 (0.0%)
4	1D	0.45	0/2672	0.47	0/3641
4	2D	0.45	0/2672	0.47	0/3641
4	3D	0.45	0/2672	0.47	0/3641
4	4D	0.45	0/2672	0.47	0/3641
5	1E	0.34	0/555	0.44	0/757
5	2E	0.35	0/555	0.44	0/757
5	3E	0.35	0/555	0.44	0/757
5	4E	0.35	0/555	0.44	0/757
6	1F	0.37	0/250	0.42	0/343
6	2F	0.38	0/250	0.42	0/343
6	3F	0.37	0/250	0.42	0/343
6	4F	0.38	0/250	0.42	0/343
7	1H	0.37	0/534	0.49	0/729
7	2H	0.37	0/534	0.49	0/729
7	3H	0.38	0/534	0.49	0/729
7	4H	0.37	0/534	0.49	0/729
8	1I	0.49	0/290	0.43	0/391
8	2I	0.49	0/290	0.43	0/391
8	3I	0.49	0/290	0.43	0/391
8	4I	0.49	0/290	0.43	0/391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	1K	0.35	0/303	0.43	0/413
9	2K	0.35	0/303	0.43	0/413
9	3K	0.35	0/303	0.43	0/413
9	4K	0.35	0/303	0.43	0/413
10	1L	0.44	0/295	0.45	0/401
10	2L	0.44	0/295	0.45	0/401
10	3L	0.44	0/295	0.45	0/401
10	4L	0.44	0/295	0.45	0/401
11	1M	0.40	0/236	0.48	0/322
11	2M	0.40	0/236	0.48	0/322
11	3M	0.40	0/236	0.48	0/322
11	4M	0.41	0/236	0.48	0/322
12	1T	0.43	0/238	0.44	0/321
12	2T	0.42	0/238	0.44	0/321
12	3T	0.42	0/238	0.43	0/321
12	4T	0.43	0/238	0.43	0/321
13	1X	0.34	0/276	0.40	0/370
13	2X	0.34	0/276	0.40	0/370
13	3X	0.34	0/276	0.40	0/370
13	4X	0.34	0/276	0.40	0/370
14	1Y	0.26	0/164	0.42	0/224
14	2Y	0.26	0/164	0.42	0/224
14	3Y	0.26	0/164	0.42	0/224
14	4Y	0.26	0/164	0.42	0/224
15	1Z	0.29	0/438	0.38	0/599
15	2Z	0.29	0/438	0.38	0/599
15	3Z	0.29	0/438	0.38	0/599
15	4Z	0.29	0/438	0.38	0/599
16	12	0.44	0/2830	0.47	0/3855
16	22	0.44	0/2830	0.47	0/3855
16	32	0.44	0/2830	0.47	0/3855
16	42	0.44	0/2830	0.47	0/3855
18	11	0.37	0/2652	0.45	0/3618
18	21	0.37	0/2652	0.45	0/3618
18	31	0.37	0/2652	0.45	0/3618
18	41	0.37	0/2652	0.45	0/3618
19	13	0.46	0/2814	0.48	0/3841
19	23	0.46	0/2814	0.48	0/3841
19	33	0.46	0/2814	0.48	0/3841
19	43	0.46	0/2814	0.48	0/3841
20	14	0.39	0/2590	0.47	0/3537
20	24	0.38	0/2590	0.47	0/3537
20	34	0.39	0/2590	0.47	0/3537

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	44	0.39	0/2590	0.47	0/3537
All	All	0.43	0/107108	0.47	4/146012 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3C	387	LEU	CA-CB-CG	5.61	128.21	115.30
3	1C	387	LEU	CA-CB-CG	5.61	128.20	115.30
3	4C	387	LEU	CA-CB-CG	5.60	128.18	115.30
3	2C	387	LEU	CA-CB-CG	5.60	128.17	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2209	0	2142	54	0
1	2A	2209	0	2142	55	0
1	3A	2209	0	2142	52	0
1	4A	2209	0	2142	56	0
2	1B	3794	0	3626	67	0
2	2B	3794	0	3626	68	0
2	3B	3794	0	3626	64	0
2	4B	3794	0	3626	66	0
3	1C	3313	0	3162	58	0
3	2C	3313	0	3162	56	0
3	3C	3313	0	3162	57	0
3	4C	3313	0	3162	56	0
4	1D	2583	0	2493	58	0
4	2D	2583	0	2493	57	0
4	3D	2583	0	2493	58	0
4	4D	2583	0	2493	58	0
5	1E	538	0	520	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2E	538	0	520	18	0
5	3E	538	0	520	20	0
5	4E	538	0	520	14	0
6	1F	242	0	249	1	0
6	2F	242	0	249	2	0
6	3F	242	0	249	2	0
6	4F	242	0	249	2	0
7	1H	519	0	518	9	0
7	2H	519	0	518	9	0
7	3H	519	0	518	9	0
7	4H	519	0	518	9	0
8	1I	281	0	289	6	0
8	2I	281	0	289	7	0
8	3I	281	0	289	7	0
8	4I	281	0	289	7	0
9	1K	292	0	302	9	0
9	2K	292	0	302	11	0
9	3K	292	0	302	11	0
9	4K	292	0	302	8	0
10	1L	288	0	301	7	0
10	2L	288	0	301	8	0
10	3L	288	0	301	6	0
10	4L	288	0	301	8	0
11	1M	232	0	243	4	0
11	2M	232	0	243	4	0
11	3M	232	0	243	4	0
11	4M	232	0	243	4	0
12	1T	231	0	240	2	0
12	2T	231	0	240	3	0
12	3T	231	0	240	2	0
12	4T	231	0	240	1	0
13	1X	269	0	275	4	0
13	2X	269	0	275	4	0
13	3X	269	0	275	4	0
13	4X	269	0	275	5	0
14	1Y	164	0	197	1	0
14	2Y	164	0	197	4	0
14	3Y	164	0	197	3	0
14	4Y	164	0	197	2	0
15	1Z	429	0	450	3	0
15	2Z	429	0	450	7	0
15	3Z	429	0	450	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	4Z	429	0	450	3	0
16	12	2734	0	2611	106	0
16	22	2734	0	2611	103	0
16	32	2734	0	2611	108	0
16	42	2734	0	2611	106	0
17	1G	205	0	46	2	0
17	2G	205	0	46	2	0
17	3G	205	0	46	2	0
17	4G	205	0	46	2	0
18	11	2567	0	2508	100	0
18	21	2567	0	2508	108	0
18	31	2567	0	2508	110	0
18	41	2567	0	2508	104	0
19	13	2715	0	2580	77	0
19	23	2715	0	2580	79	0
19	33	2715	0	2580	80	0
19	43	2715	0	2580	77	0
20	14	2514	0	2436	79	0
20	24	2514	0	2436	91	0
20	34	2514	0	2436	89	0
20	44	2514	0	2436	78	0
21	11	972	0	822	84	0
21	12	1065	0	1050	110	0
21	13	1024	0	962	125	0
21	14	757	0	681	64	0
21	1A	185	0	187	32	0
21	1B	991	0	947	63	0
21	1C	799	0	763	46	0
21	1D	153	0	121	11	0
21	21	972	0	822	93	0
21	22	1065	0	1050	112	0
21	23	1024	0	962	126	0
21	24	757	0	681	62	0
21	2A	185	0	187	30	0
21	2B	991	0	947	64	0
21	2C	799	0	763	44	0
21	2D	153	0	121	12	0
21	31	972	0	821	92	0
21	32	1065	0	1050	111	0
21	33	1024	0	962	125	0
21	34	757	0	681	64	0
21	3A	185	0	187	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3B	991	0	946	57	0
21	3C	799	0	763	44	0
21	3D	153	0	121	11	0
21	41	972	0	822	90	0
21	42	1065	0	1050	109	0
21	43	1024	0	962	132	0
21	44	757	0	681	63	0
21	4A	185	0	187	30	0
21	4B	991	0	947	60	0
21	4C	799	0	763	43	0
21	4D	153	0	121	12	0
22	1A	64	0	74	5	0
22	1D	64	0	74	5	0
22	2A	64	0	74	5	0
22	2D	64	0	74	4	0
22	3A	64	0	74	5	0
22	3D	64	0	74	5	0
22	4A	64	0	74	5	0
22	4D	64	0	74	4	0
23	14	40	0	0	0	0
23	1A	40	0	0	0	0
23	1B	160	0	0	0	0
23	1C	120	0	0	1	0
23	1D	40	0	0	0	0
23	1K	40	0	0	0	0
23	24	40	0	0	0	0
23	2A	40	0	0	0	0
23	2B	160	0	0	0	0
23	2C	120	0	0	1	0
23	2D	40	0	0	0	0
23	2K	40	0	0	0	0
23	34	40	0	0	0	0
23	3A	40	0	0	0	0
23	3B	160	0	0	0	0
23	3C	120	0	0	1	0
23	3D	40	0	0	0	0
23	3K	40	0	0	0	0
23	44	40	0	0	0	0
23	4A	40	0	0	0	0
23	4B	160	0	0	0	0
23	4C	120	0	0	1	0
23	4D	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	4K	40	0	0	0	0
24	11	51	0	72	2	0
24	1A	50	0	70	2	0
24	1B	51	0	72	5	0
24	1D	33	0	36	1	0
24	21	51	0	72	2	0
24	2A	50	0	70	2	0
24	2B	51	0	72	5	0
24	2D	33	0	36	1	0
24	31	51	0	72	3	0
24	3A	50	0	70	2	0
24	3B	51	0	72	6	0
24	3D	33	0	36	1	0
24	41	51	0	72	2	0
24	4A	50	0	70	2	0
24	4B	51	0	72	6	0
24	4D	33	0	36	1	0
25	11	32	0	28	0	0
25	12	91	0	113	2	0
25	13	96	0	123	6	0
25	1A	34	0	32	3	0
25	1B	54	0	78	3	0
25	21	32	0	28	0	0
25	22	91	0	113	2	0
25	23	96	0	123	6	0
25	2A	34	0	32	3	0
25	2B	54	0	78	2	0
25	31	32	0	28	0	0
25	32	91	0	113	1	0
25	33	96	0	123	5	0
25	3A	34	0	32	1	0
25	3B	54	0	78	2	0
25	41	32	0	28	0	0
25	42	91	0	113	2	0
25	43	96	0	123	5	0
25	4A	34	0	32	2	0
25	4B	54	0	78	3	0
26	13	36	0	42	1	0
26	14	49	0	74	1	0
26	1A	46	0	65	1	0
26	1B	94	0	137	7	0
26	1D	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	23	36	0	42	1	0
26	24	49	0	74	1	0
26	2A	46	0	65	1	0
26	2B	94	0	137	8	0
26	2D	49	0	74	4	0
26	33	36	0	42	1	0
26	34	49	0	74	1	0
26	3A	46	0	65	1	0
26	3B	94	0	137	7	0
26	3D	49	0	74	3	0
26	43	36	0	42	1	0
26	44	49	0	74	1	0
26	4A	46	0	65	1	0
26	4B	94	0	137	8	0
26	4D	49	0	74	3	0
27	1B	62	0	82	2	0
27	1C	62	0	82	5	0
27	2B	62	0	82	2	0
27	2C	62	0	82	3	0
27	3B	62	0	82	2	0
27	3C	62	0	82	4	0
27	4B	62	0	82	2	0
27	4C	62	0	82	3	0
28	1D	1	0	0	0	0
28	2D	1	0	0	0	0
28	3D	1	0	0	0	0
28	4D	1	0	0	0	0
29	1D	4	0	0	0	0
29	2D	4	0	0	0	0
29	3D	4	0	0	0	0
29	4D	4	0	0	0	0
30	1D	55	0	80	7	0
30	2D	55	0	80	7	0
30	3D	55	0	80	7	0
30	4D	55	0	80	7	0
31	1F	43	0	30	3	0
31	2F	43	0	30	4	0
31	3F	43	0	30	3	0
31	4F	43	0	30	4	0
32	11	84	0	112	34	0
32	12	168	0	224	69	0
32	13	168	0	224	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	14	168	0	224	51	0
32	21	84	0	112	36	0
32	22	168	0	224	65	0
32	23	168	0	224	80	0
32	24	168	0	224	53	0
32	31	84	0	112	36	0
32	32	168	0	224	68	0
32	33	168	0	224	80	0
32	34	168	0	224	50	0
32	41	84	0	112	37	0
32	42	168	0	224	69	0
32	43	168	0	224	82	0
32	44	168	0	224	53	0
All	All	136856	0	131770	4245	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 16.

The worst 5 of 4245 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)
18:41:315:ASN:HB3	32:41:421:ZEX:C36	1.32	1.58
18:11:315:ASN:CB	32:11:421:ZEX:C36	1.81	1.58
18:41:315:ASN:CB	32:41:421:ZEX:C36	1.81	1.57
18:21:315:ASN:CB	32:21:421:ZEX:C36	1.81	1.57
18:31:315:ASN:CB	32:31:421:ZEX:C36	1.81	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	2A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	3A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	4A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
2	1B	477/506 (94%)	451 (94%)	26 (6%)	0	100	100
2	2B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	3B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	4B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
3	1C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	2C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	3C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	4C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	1D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	2D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
4	3D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	4D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	1E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	2E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	3E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	4E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	1F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	2F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	3F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	4F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	1H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	2H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	3H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	4H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	1I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	2I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	3I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	4I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1K	35/45 (78%)	35 (100%)	0	0	100	100
9	2K	35/45 (78%)	35 (100%)	0	0	100	100
9	3K	35/45 (78%)	35 (100%)	0	0	100	100
9	4K	35/45 (78%)	35 (100%)	0	0	100	100
10	1L	34/38 (90%)	34 (100%)	0	0	100	100
10	2L	34/38 (90%)	34 (100%)	0	0	100	100
10	3L	34/38 (90%)	34 (100%)	0	0	100	100
10	4L	34/38 (90%)	34 (100%)	0	0	100	100
11	1M	29/34 (85%)	29 (100%)	0	0	100	100
11	2M	29/34 (85%)	29 (100%)	0	0	100	100
11	3M	29/34 (85%)	29 (100%)	0	0	100	100
11	4M	29/34 (85%)	29 (100%)	0	0	100	100
12	1T	26/46 (56%)	26 (100%)	0	0	100	100
12	2T	26/46 (56%)	26 (100%)	0	0	100	100
12	3T	26/46 (56%)	26 (100%)	0	0	100	100
12	4T	26/46 (56%)	26 (100%)	0	0	100	100
13	1X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	2X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	3X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	4X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	1Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	2Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	3Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	4Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	1Z	57/62 (92%)	57 (100%)	0	0	100	100
15	2Z	57/62 (92%)	57 (100%)	0	0	100	100
15	3Z	57/62 (92%)	57 (100%)	0	0	100	100
15	4Z	57/62 (92%)	57 (100%)	0	0	100	100
16	12	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	22	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	32	347/352 (99%)	325 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	42	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	11	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	75
18	21	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	75
18	31	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	75
18	41	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	75
19	13	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	75
19	23	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	75
19	33	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	75
19	43	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	75
20	14	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	24	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	34	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	44	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
All	All	13020/14832 (88%)	12413 (95%)	599 (5%)	8 (0%)	54	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	13	4	TYR
19	23	4	TYR
19	33	4	TYR
19	43	4	TYR
18	11	202	CYS

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	232/292 (80%)	229 (99%)	3 (1%)	69	86
1	2A	232/292 (80%)	229 (99%)	3 (1%)	69	86
1	3A	232/292 (80%)	229 (99%)	3 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4A	232/292 (80%)	229 (99%)	3 (1%)	69	86
2	1B	395/418 (94%)	385 (98%)	10 (2%)	47	75
2	2B	395/418 (94%)	385 (98%)	10 (2%)	47	75
2	3B	395/418 (94%)	385 (98%)	10 (2%)	47	75
2	4B	395/418 (94%)	385 (98%)	10 (2%)	47	75
3	1C	322/378 (85%)	313 (97%)	9 (3%)	43	72
3	2C	322/378 (85%)	313 (97%)	9 (3%)	43	72
3	3C	322/378 (85%)	313 (97%)	9 (3%)	43	72
3	4C	322/378 (85%)	313 (97%)	9 (3%)	43	72
4	1D	265/284 (93%)	261 (98%)	4 (2%)	65	84
4	2D	265/284 (93%)	261 (98%)	4 (2%)	65	84
4	3D	265/284 (93%)	261 (98%)	4 (2%)	65	84
4	4D	265/284 (93%)	261 (98%)	4 (2%)	65	84
5	1E	57/71 (80%)	56 (98%)	1 (2%)	59	81
5	2E	57/71 (80%)	56 (98%)	1 (2%)	59	81
5	3E	57/71 (80%)	56 (98%)	1 (2%)	59	81
5	4E	57/71 (80%)	56 (98%)	1 (2%)	59	81
6	1F	25/84 (30%)	25 (100%)	0	100	100
6	2F	25/84 (30%)	25 (100%)	0	100	100
6	3F	25/84 (30%)	25 (100%)	0	100	100
6	4F	25/84 (30%)	25 (100%)	0	100	100
7	1H	55/57 (96%)	54 (98%)	1 (2%)	59	81
7	2H	55/57 (96%)	54 (98%)	1 (2%)	59	81
7	3H	55/57 (96%)	54 (98%)	1 (2%)	59	81
7	4H	55/57 (96%)	54 (98%)	1 (2%)	59	81
8	1I	30/30 (100%)	29 (97%)	1 (3%)	38	69
8	2I	30/30 (100%)	29 (97%)	1 (3%)	38	69
8	3I	30/30 (100%)	29 (97%)	1 (3%)	38	69
8	4I	30/30 (100%)	29 (97%)	1 (3%)	38	69
9	1K	31/37 (84%)	30 (97%)	1 (3%)	39	70
9	2K	31/37 (84%)	30 (97%)	1 (3%)	39	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	3K	31/37 (84%)	30 (97%)	1 (3%)	39	70
9	4K	31/37 (84%)	30 (97%)	1 (3%)	39	70
10	1L	33/34 (97%)	33 (100%)	0	100	100
10	2L	33/34 (97%)	33 (100%)	0	100	100
10	3L	33/34 (97%)	33 (100%)	0	100	100
10	4L	33/34 (97%)	33 (100%)	0	100	100
11	1M	24/27 (89%)	24 (100%)	0	100	100
11	2M	24/27 (89%)	24 (100%)	0	100	100
11	3M	24/27 (89%)	24 (100%)	0	100	100
11	4M	24/27 (89%)	24 (100%)	0	100	100
12	1T	24/42 (57%)	24 (100%)	0	100	100
12	2T	24/42 (57%)	24 (100%)	0	100	100
12	3T	24/42 (57%)	24 (100%)	0	100	100
12	4T	24/42 (57%)	24 (100%)	0	100	100
13	1X	28/33 (85%)	28 (100%)	0	100	100
13	2X	28/33 (85%)	28 (100%)	0	100	100
13	3X	28/33 (85%)	28 (100%)	0	100	100
13	4X	28/33 (85%)	28 (100%)	0	100	100
14	1Y	18/31 (58%)	17 (94%)	1 (6%)	21	56
14	2Y	18/31 (58%)	17 (94%)	1 (6%)	21	56
14	3Y	18/31 (58%)	17 (94%)	1 (6%)	21	56
14	4Y	18/31 (58%)	17 (94%)	1 (6%)	21	56
15	1Z	43/46 (94%)	42 (98%)	1 (2%)	50	76
15	2Z	43/46 (94%)	42 (98%)	1 (2%)	50	76
15	3Z	43/46 (94%)	42 (98%)	1 (2%)	50	76
15	4Z	43/46 (94%)	42 (98%)	1 (2%)	50	76
16	12	276/278 (99%)	270 (98%)	6 (2%)	52	77
16	22	276/278 (99%)	270 (98%)	6 (2%)	52	77
16	32	276/278 (99%)	270 (98%)	6 (2%)	52	77
16	42	276/278 (99%)	270 (98%)	6 (2%)	52	77
18	11	262/278 (94%)	258 (98%)	4 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	21	262/278 (94%)	258 (98%)	4 (2%)	65	84
18	31	262/278 (94%)	258 (98%)	4 (2%)	65	84
18	41	262/278 (94%)	258 (98%)	4 (2%)	65	84
19	13	269/273 (98%)	261 (97%)	8 (3%)	41	71
19	23	269/273 (98%)	261 (97%)	8 (3%)	41	71
19	33	269/273 (98%)	261 (97%)	8 (3%)	41	71
19	43	269/273 (98%)	261 (97%)	8 (3%)	41	71
20	14	260/277 (94%)	254 (98%)	6 (2%)	50	76
20	24	260/277 (94%)	254 (98%)	6 (2%)	50	76
20	34	260/277 (94%)	254 (98%)	6 (2%)	50	76
20	44	260/277 (94%)	254 (98%)	6 (2%)	50	76
All	All	10596/11880 (89%)	10372 (98%)	224 (2%)	56	78

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3B	129	ASP
20	44	204	ILE
15	3Z	27	PHE
20	44	28	GLU
15	4Z	27	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
16	32	62	GLN
20	34	195	HIS
20	44	195	HIS
19	33	34	GLN
20	34	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 624 ligands modelled in this entry, 4 are monoatomic - leaving 620 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	$\# Z > 2$
21	CL7	34	417	20	43,50,73	2.67	11 (25%)	36,85,113	2.89	13 (36%)
21	CL7	4B	614	-	56,63,73	2.38	14 (25%)	53,101,113	2.41	17 (32%)
21	CL7	12	515	-	46,53,73	2.63	12 (26%)	41,89,113	2.66	15 (36%)
25	SQD	1A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
27	DGD	1C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
23	8CT	3C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	24	414	-	54,61,73	2.40	13 (24%)	50,98,113	2.53	16 (32%)
23	8CT	1D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	22	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	23	409	-	66,73,73	2.20	14 (21%)	65,113,113	2.24	18 (27%)
21	CL7	23	416	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
21	CL7	1C	517	-	42,49,73	2.62	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	2C	504	-	56,63,73	2.42	12 (21%)	53,101,113	2.37	14 (26%)
21	CL7	33	516	19	56,63,73	2.41	13 (23%)	53,101,113	2.42	19 (35%)
23	8CT	3C	515	-	40,41,41	4.64	20 (50%)	50,56,56	3.06	22 (44%)
32	ZEX	21	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	42	518	16	66,73,73	2.22	12 (18%)	65,113,113	2.16	17 (26%)
21	CL7	1B	607	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	24	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	21	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.60	13 (31%)
21	CL7	43	411	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	24	412	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	18 (27%)
21	CL7	4B	613	-	66,73,73	2.16	13 (19%)	65,113,113	2.28	18 (27%)
22	PHO	4A	402	-	51,69,69	0.73	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	2B	604	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	2B	606	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
29	BCT	1D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	3D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	43	407	-	46,53,73	2.59	14 (30%)	41,89,113	2.73	14 (34%)
24	LMG	4B	622	-	51,51,55	0.24	0	59,59,63	0.33	0
26	LHG	14	401	-	48,48,48	0.29	0	51,54,54	0.34	0
21	CL7	3B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	42	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
23	8CT	3A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
26	LHG	4A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	43	414	-	46,53,73	2.66	15 (32%)	41,89,113	2.68	13 (31%)
31	HEM	1F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	32	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.67	15 (36%)
21	CL7	31	420	18	46,53,73	2.62	12 (26%)	41,89,113	2.75	14 (34%)
23	8CT	1C	518	-	40,41,41	4.65	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	3D	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.73	16 (39%)
21	CL7	31	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	24	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	20 (33%)
21	CL7	4B	616	-	51,58,73	2.45	14 (27%)	47,95,113	2.64	16 (34%)
21	CL7	12	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.64	14 (34%)
21	CL7	14	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.20	16 (24%)
25	SQD	43	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
23	8CT	1C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	2D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.37	17 (30%)
21	CL7	11	403	-	61,68,73	2.29	12 (19%)	59,107,113	2.38	15 (25%)
21	CL7	1B	602	-	61,68,73	2.31	12 (19%)	59,107,113	2.39	17 (28%)
21	CL7	12	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.25	17 (26%)
21	CL7	2C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	2B	613	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	2B	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	15 (23%)
21	CL7	42	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.19	17 (26%)
31	HEM	2F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
23	8CT	2B	619	-	40,41,41	4.70	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	3A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	4B	607	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	18 (33%)
21	CL7	3C	507	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	17 (26%)
21	CL7	12	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	17 (26%)
21	CL7	4C	502	-	61,68,73	2.29	14 (22%)	59,107,113	2.30	15 (25%)
27	DGD	3C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	23	411	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	3C	510	-	66,73,73	2.24	11 (16%)	65,113,113	2.20	18 (27%)
21	CL7	44	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	19 (32%)
24	LMG	3D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	3B	610	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
21	CL7	14	406	-	66,73,73	2.22	12 (18%)	65,113,113	2.22	17 (26%)
32	ZEX	24	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	21	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.75	14 (34%)
25	SQD	33	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	23	408	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	32	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	17 (26%)
21	CL7	21	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
32	ZEX	33	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	11	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.77	14 (38%)
21	CL7	2C	508	-	66,73,73	2.21	13 (19%)	65,113,113	2.29	21 (32%)
21	CL7	23	403	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
21	CL7	21	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	4C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.90	14 (38%)
21	CL7	31	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.92	14 (38%)
21	CL7	32	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.18	16 (24%)
21	CL7	31	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.38	15 (25%)
21	CL7	31	405	-	46,53,73	2.62	13 (28%)	41,89,113	2.58	12 (29%)
21	CL7	1A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	19 (35%)
21	CL7	1C	513	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	14	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	20 (33%)
21	CL7	43	410	-	66,73,73	2.21	11 (16%)	65,113,113	2.20	16 (24%)
23	8CT	3B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
32	ZEX	13	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	3C	513	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)
21	CL7	43	416	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
21	CL7	11	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
21	CL7	1B	603	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)
23	8CT	2D	406	-	40,41,41	4.63	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	41	405	-	46,53,73	2.63	13 (28%)	41,89,113	2.61	12 (29%)
21	CL7	14	413	20	61,68,73	2.28	14 (22%)	59,107,113	2.33	16 (27%)
21	CL7	41	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
32	ZEX	13	525	-	42,43,43	1.18	5 (11%)	55,60,60	2.44	18 (32%)
21	CL7	22	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	16 (39%)
23	8CT	2C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
32	ZEX	11	421	-	42,43,43	0.93	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	13	506	-	46,53,73	2.59	15 (32%)	41,89,113	2.72	14 (34%)
21	CL7	24	408	-	46,53,73	2.66	14 (30%)	41,89,113	2.66	13 (31%)
21	CL7	1A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	44	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
23	8CT	2C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	3B	602	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	12	505	-	66,73,73	2.23	13 (19%)	65,113,113	2.41	19 (29%)
21	CL7	3C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.40	18 (30%)
21	CL7	1A	401	-	66,73,73	2.28	14 (21%)	65,113,113	2.33	19 (29%)
21	CL7	42	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	24	407	-	42,49,73	2.65	10 (23%)	36,84,113	2.84	14 (38%)
23	8CT	1B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	21	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.30	19 (29%)
21	CL7	33	502	-	59,66,73	2.35	13 (22%)	56,104,113	2.25	17 (30%)
21	CL7	23	417	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
32	ZEX	12	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	24	405	-	66,73,73	2.21	13 (19%)	65,113,113	2.31	20 (30%)
23	8CT	4B	619	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
21	CL7	2C	513	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	3D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	12	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.65	13 (31%)
21	CL7	14	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
32	ZEX	31	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.22	20 (36%)
25	SQD	33	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	4B	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	17 (28%)
21	CL7	41	408	-	66,73,73	2.18	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	41	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
21	CL7	2A	403	-	56,63,73	2.41	14 (25%)	53,101,113	2.58	18 (33%)
21	CL7	12	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
31	HEM	3F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	13	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	3C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.89	14 (38%)
25	SQD	23	422	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
26	LHG	3B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	3C	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.19	15 (23%)
21	CL7	2B	610	-	66,73,73	2.24	14 (21%)	65,113,113	2.16	15 (23%)
29	BCT	3D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	1B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.36	19 (32%)
21	CL7	4C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	17 (26%)
21	CL7	24	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	43	419	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
23	8CT	14	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.77	21 (42%)
26	LHG	3B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	24	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.87	14 (34%)
21	CL7	1C	503	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	17 (26%)
26	LHG	3A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
26	LHG	33	524	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	11	405	-	46,53,73	2.64	13 (28%)	41,89,113	2.60	12 (29%)
26	LHG	3D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	3C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
21	CL7	3B	605	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	2C	507	-	66,73,73	2.17	14 (21%)	65,113,113	2.25	18 (27%)
24	LMG	2B	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	13	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	1C	501	-	66,73,73	2.18	13 (19%)	65,113,113	2.18	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	4I	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
21	CL7	1B	609	-	66,73,73	2.24	15 (22%)	65,113,113	2.16	15 (23%)
23	8CT	2B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
23	8CT	3B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.24	21 (42%)
21	CL7	4C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
26	LHG	4D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	4C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.24	16 (24%)
25	SQD	2B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
21	CL7	2C	506	-	61,68,73	2.31	13 (21%)	59,107,113	2.38	18 (30%)
32	ZEX	43	423	-	42,43,43	1.01	4 (9%)	55,60,60	2.39	17 (30%)
21	CL7	43	417	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
24	LMG	11	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
23	8CT	3K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
23	8CT	2C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
26	LHG	2D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	4B	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	2A	401	-	66,73,73	2.27	14 (21%)	65,113,113	2.34	19 (29%)
25	SQD	3B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
32	ZEX	22	522	-	42,43,43	1.04	3 (7%)	55,60,60	2.47	17 (30%)
21	CL7	23	419	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
21	CL7	1B	616	-	46,53,73	2.61	14 (30%)	41,89,113	2.59	16 (39%)
21	CL7	33	511	19	66,73,73	2.19	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	44	407	-	42,49,73	2.65	10 (23%)	36,84,113	2.85	14 (38%)
21	CL7	3B	607	-	61,68,73	2.29	13 (21%)	59,107,113	2.26	17 (28%)
21	CL7	32	511	16	61,68,73	2.33	13 (21%)	59,107,113	2.22	15 (25%)
21	CL7	42	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.67	15 (36%)
32	ZEX	41	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	2C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.88	14 (38%)
21	CL7	33	517	19	51,58,73	2.48	13 (25%)	47,95,113	2.54	14 (29%)
32	ZEX	44	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
26	LHG	4B	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	3A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	19 (35%)
21	CL7	41	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.24	16 (24%)
24	LMG	31	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
23	8CT	4C	514	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	34	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
32	ZEX	43	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
32	ZEX	33	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
23	8CT	4C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
23	8CT	3C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	4C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
21	CL7	4C	513	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)
25	SQD	42	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
24	LMG	41	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
29	BCT	2D	403	28	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
26	LHG	24	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	22	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
21	CL7	12	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.66	15 (36%)
21	CL7	4B	604	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
27	DGD	2B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
27	DGD	4C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	22	505	-	66,73,73	2.23	13 (19%)	65,113,113	2.41	19 (29%)
21	CL7	33	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.66	14 (34%)
21	CL7	3C	504	-	56,63,73	2.42	13 (23%)	53,101,113	2.38	14 (26%)
21	CL7	24	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.20	16 (24%)
21	CL7	14	411	-	66,73,73	2.23	12 (18%)	65,113,113	2.21	17 (26%)
21	CL7	3A	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
23	8CT	1B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	34	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
32	ZEX	43	401	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	23	420	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
25	SQD	3A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	22	513	-	46,53,73	2.66	13 (28%)	41,89,113	2.67	15 (36%)
21	CL7	2C	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.19	15 (23%)
21	CL7	3B	603	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	1B	605	-	66,73,73	2.23	14 (21%)	65,113,113	2.22	15 (23%)
23	8CT	1C	514	-	40,41,41	4.63	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	22	501	-	66,73,73	2.17	13 (19%)	65,113,113	2.24	15 (23%)
21	CL7	32	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
25	SQD	2A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	SQD	13	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
30	PL9	1D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	31	403	-	61,68,73	2.30	12 (19%)	59,107,113	2.38	15 (25%)
26	LHG	1D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	44	408	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
21	CL7	13	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
23	8CT	1B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	41	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.29	14 (22%)
21	CL7	44	404	-	66,73,73	2.23	14 (21%)	65,113,113	2.20	16 (24%)
21	CL7	11	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
24	LMG	1A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	13	515	-	42,49,73	2.65	10 (23%)	36,84,113	2.85	15 (41%)
21	CL7	42	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.20	16 (24%)
26	LHG	23	425	-	35,35,48	0.35	0	38,41,54	0.47	0
21	CL7	2C	502	-	61,68,73	2.29	14 (22%)	59,107,113	2.30	15 (25%)
21	CL7	22	508	-	46,53,73	2.60	13 (28%)	41,89,113	2.65	14 (34%)
21	CL7	13	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	4C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.39	18 (30%)
21	CL7	4C	507	-	66,73,73	2.18	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	42	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	43	415	-	46,53,73	2.63	14 (30%)	41,89,113	2.81	14 (34%)
32	ZEX	21	421	-	42,43,43	0.92	2 (4%)	55,60,60	2.23	20 (36%)
21	CL7	12	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	44	405	-	66,73,73	2.20	14 (21%)	65,113,113	2.30	21 (32%)
32	ZEX	22	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	11	411	-	46,53,73	2.65	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	34	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
32	ZEX	24	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	1B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	1B	606	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
23	8CT	3D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	31	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
32	ZEX	22	524	-	42,43,43	1.03	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	42	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.25	18 (27%)
24	LMG	2A	405	-	50,50,55	0.24	0	58,58,63	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	13	516	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
21	CL7	41	412	-	46,53,73	2.60	12 (26%)	41,89,113	2.71	15 (36%)
24	LMG	4A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
27	DGD	4B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	33	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
26	LHG	2A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	22	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.25	18 (27%)
32	ZEX	33	520	-	42,43,43	0.92	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	41	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.76	14 (34%)
21	CL7	43	412	19	66,73,73	2.18	15 (22%)	65,113,113	2.42	19 (29%)
21	CL7	42	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.38	19 (29%)
26	LHG	2B	624	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	1C	507	-	66,73,73	2.18	14 (21%)	65,113,113	2.27	18 (27%)
21	CL7	23	415	-	46,53,73	2.64	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	22	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.68	12 (29%)
21	CL7	4C	501	-	66,73,73	2.19	13 (19%)	65,113,113	2.20	15 (23%)
26	LHG	13	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	13	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	23	402	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
23	8CT	24	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
22	PHO	2D	408	-	51,69,69	0.60	2 (3%)	47,99,99	0.88	1 (2%)
21	CL7	3B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
32	ZEX	12	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	4C	504	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
21	CL7	13	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	3C	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.22	16 (24%)
32	ZEX	32	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	41	403	-	61,68,73	2.29	12 (19%)	59,107,113	2.38	15 (25%)
21	CL7	4D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.73	16 (39%)
21	CL7	3C	502	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
21	CL7	32	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.69	12 (29%)
21	CL7	42	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
32	ZEX	42	522	-	42,43,43	1.04	5 (11%)	55,60,60	2.47	15 (27%)
21	CL7	1B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.18	15 (23%)
21	CL7	33	515	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	15 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PHO	1A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	32	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
32	ZEX	32	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	17 (30%)
32	ZEX	43	420	-	42,43,43	1.01	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	3B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	3B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	18 (27%)
25	SQD	4A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	33	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	11	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
21	CL7	13	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
26	LHG	34	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	13	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.67	14 (34%)
21	CL7	31	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	11	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
21	CL7	3C	503	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
21	CL7	4B	615	-	61,68,73	2.30	15 (24%)	59,107,113	2.36	19 (32%)
32	ZEX	14	403	-	42,43,43	1.02	4 (9%)	55,60,60	2.56	19 (34%)
32	ZEX	12	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	21	405	-	46,53,73	2.63	14 (30%)	41,89,113	2.60	12 (29%)
21	CL7	12	517	16	66,73,73	2.17	11 (16%)	65,113,113	2.20	17 (26%)
23	8CT	1K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
25	SQD	32	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	24	410	-	46,53,73	2.62	12 (26%)	41,89,113	2.65	14 (34%)
24	LMG	4D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	3B	616	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)
21	CL7	1D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	4B	610	-	66,73,73	2.24	13 (19%)	65,113,113	2.15	15 (23%)
23	8CT	34	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	41	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	23	413	-	56,63,73	2.38	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	11	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	12	514	-	46,53,73	2.62	13 (28%)	41,89,113	2.69	12 (29%)
21	CL7	2B	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.59	16 (39%)
21	CL7	22	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
21	CL7	1C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.20	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMG	1B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
22	PHO	4D	408	-	51,69,69	0.59	1 (1%)	47,99,99	0.88	2 (4%)
21	CL7	43	405	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)
21	CL7	21	402	-	61,68,73	2.32	14 (22%)	59,107,113	2.37	15 (25%)
25	SQD	22	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
32	ZEX	23	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	11	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.95	15 (41%)
21	CL7	1B	610	-	66,73,73	2.15	13 (19%)	65,113,113	2.32	15 (23%)
21	CL7	2B	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.26	16 (27%)
32	ZEX	14	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	31	418	18	66,73,73	2.17	13 (19%)	65,113,113	2.31	21 (32%)
22	PHO	1D	408	-	51,69,69	0.59	2 (3%)	47,99,99	0.88	1 (2%)
21	CL7	11	418	18	66,73,73	2.18	12 (18%)	65,113,113	2.32	19 (29%)
21	CL7	21	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	19 (29%)
21	CL7	1B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.27	18 (27%)
21	CL7	21	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.70	15 (36%)
21	CL7	11	420	18	46,53,73	2.62	12 (26%)	41,89,113	2.75	14 (34%)
21	CL7	1C	502	-	61,68,73	2.30	14 (22%)	59,107,113	2.31	15 (25%)
21	CL7	24	413	20	61,68,73	2.28	13 (21%)	59,107,113	2.32	16 (27%)
21	CL7	21	417	18	56,63,73	2.43	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	1C	504	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
21	CL7	3C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.26	17 (26%)
21	CL7	44	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	2D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.74	16 (39%)
21	CL7	41	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	20 (30%)
25	SQD	1B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
25	SQD	4B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
25	SQD	31	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
25	SQD	13	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	33	506	-	46,53,73	2.58	13 (28%)	41,89,113	2.73	14 (34%)
21	CL7	34	412	-	66,73,73	2.21	12 (18%)	65,113,113	2.19	18 (27%)
21	CL7	14	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	41	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
25	SQD	11	423	-	31,32,54	0.49	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	1B	611	-	66,73,73	2.18	14 (21%)	65,113,113	2.25	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PHO	2A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	3B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.29	18 (27%)
21	CL7	33	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	33	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	2B	615	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	19 (32%)
21	CL7	22	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.22	15 (25%)
21	CL7	23	414	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
21	CL7	41	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	23	406	-	66,73,73	2.16	13 (19%)	65,113,113	2.33	15 (23%)
21	CL7	33	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.23	18 (27%)
26	LHG	4B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	21	414	-	42,49,73	2.73	10 (23%)	36,84,113	2.93	14 (38%)
32	ZEX	11	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.23	18 (32%)
25	SQD	42	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	32	508	-	46,53,73	2.60	13 (28%)	41,89,113	2.65	14 (34%)
21	CL7	23	404	-	66,73,73	2.20	14 (21%)	65,113,113	2.29	18 (27%)
21	CL7	2C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	18 (27%)
25	SQD	12	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
32	ZEX	13	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	31	406	-	63,70,73	2.27	12 (19%)	61,109,113	2.30	14 (22%)
32	ZEX	24	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	42	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	43	402	-	66,73,73	2.21	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	23	412	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	41	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.93	14 (38%)
21	CL7	1B	601	-	42,49,73	2.68	11 (26%)	36,84,113	2.82	12 (33%)
24	LMG	3B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	31	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	2B	623	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	34	411	-	66,73,73	2.23	14 (21%)	65,113,113	2.21	17 (26%)
23	8CT	4A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
32	ZEX	14	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	21	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.90	14 (38%)
21	CL7	31	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
25	SQD	21	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	4B	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.59	16 (39%)
21	CL7	3C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
32	ZEX	32	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
32	ZEX	23	423	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	18 (32%)
26	LHG	1A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
23	8CT	1B	618	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	21	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
30	PL9	4D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	42	514	-	46,53,73	2.64	13 (28%)	41,89,113	2.69	12 (29%)
23	8CT	1A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	34	407	-	42,49,73	2.64	10 (23%)	36,84,113	2.85	14 (38%)
21	CL7	1B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	1B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	18 (27%)
25	SQD	41	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	2B	611	-	66,73,73	2.15	12 (18%)	65,113,113	2.31	15 (23%)
23	8CT	2B	620	-	40,41,41	4.58	21 (52%)	50,56,56	2.91	18 (36%)
21	CL7	2C	503	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
21	CL7	3B	609	-	66,73,73	2.25	14 (21%)	65,113,113	2.16	15 (23%)
21	CL7	11	417	18	56,63,73	2.41	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	32	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.39	19 (29%)
21	CL7	32	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	4D	402	-	51,58,73	2.54	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	4B	623	-	46,53,73	2.68	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	4A	407	-	66,73,73	2.23	13 (19%)	65,113,113	2.29	16 (24%)
21	CL7	33	513	-	46,53,73	2.66	14 (30%)	41,89,113	2.67	13 (31%)
26	LHG	44	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	1D	405	-	46,53,73	2.58	13 (28%)	41,89,113	2.74	16 (39%)
21	CL7	4B	605	-	66,73,73	2.15	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	2B	607	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	17 (32%)
21	CL7	14	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	15 (30%)
21	CL7	4A	401	-	66,73,73	2.27	14 (21%)	65,113,113	2.34	19 (29%)
21	CL7	22	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.18	15 (23%)
21	CL7	1C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.25	17 (26%)
23	8CT	2B	601	-	40,41,41	4.71	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	1C	508	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	21	410	-	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	43	408	-	66,73,73	2.15	13 (19%)	65,113,113	2.30	17 (26%)
21	CL7	11	414	-	42,49,73	2.74	11 (26%)	36,84,113	2.93	15 (41%)
29	BCT	4D	403	28	2,3,3	0.99	0	2,3,3	1.66	1 (50%)
21	CL7	21	416	-	42,49,73	2.72	10 (23%)	36,84,113	2.75	14 (38%)
21	CL7	21	404	-	66,73,73	2.28	12 (18%)	65,113,113	2.25	16 (24%)
21	CL7	33	504	-	66,73,73	2.20	13 (19%)	65,113,113	2.25	17 (26%)
21	CL7	43	404	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	43	403	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
21	CL7	22	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	32	504	-	46,53,73	2.63	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	12	503	-	66,73,73	2.19	15 (22%)	65,113,113	2.39	19 (29%)
21	CL7	31	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	12	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.21	15 (25%)
21	CL7	14	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.89	15 (36%)
21	CL7	4B	602	-	42,49,73	2.67	11 (26%)	36,84,113	2.82	12 (33%)
21	CL7	44	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
32	ZEX	22	520	-	42,43,43	0.99	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	32	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	11	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	34	404	-	66,73,73	2.23	13 (19%)	65,113,113	2.21	16 (24%)
21	CL7	2B	602	-	42,49,73	2.66	10 (23%)	36,84,113	2.81	12 (33%)
21	CL7	43	409	-	66,73,73	2.19	14 (21%)	65,113,113	2.23	18 (27%)
21	CL7	24	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
26	LHG	1B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	12	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	13	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
23	8CT	4K	101	-	40,41,41	4.76	25 (62%)	50,56,56	2.66	16 (32%)
21	CL7	3C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.83	14 (38%)
21	CL7	21	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	2A	407	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	22	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	3B	611	-	66,73,73	2.19	14 (21%)	65,113,113	2.25	15 (23%)
21	CL7	32	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	4C	510	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	34	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.51	19 (32%)
21	CL7	2B	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	42	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.29	17 (26%)
32	ZEX	34	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	42	511	16	61,68,73	2.33	13 (21%)	59,107,113	2.22	15 (25%)
21	CL7	3B	606	-	56,63,73	2.42	14 (25%)	53,101,113	2.48	16 (30%)
21	CL7	4D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	44	412	-	66,73,73	2.22	12 (18%)	65,113,113	2.21	18 (27%)
23	8CT	2A	404	-	40,41,41	4.63	20 (50%)	50,56,56	2.97	20 (40%)
21	CL7	33	512	-	56,63,73	2.38	14 (25%)	53,101,113	2.44	18 (33%)
21	CL7	14	412	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	18 (27%)
21	CL7	11	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
32	ZEX	33	519	-	42,43,43	1.01	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	34	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
23	8CT	4B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	43	406	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
21	CL7	44	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.88	13 (36%)
24	LMG	3A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	33	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	24	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.21	17 (26%)
21	CL7	4C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	44	406	-	66,73,73	2.20	11 (16%)	65,113,113	2.22	17 (26%)
23	8CT	4C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
32	ZEX	42	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.18	17 (30%)
21	CL7	13	508	-	66,73,73	2.21	14 (21%)	65,113,113	2.24	18 (27%)
21	CL7	13	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
25	SQD	22	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	33	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	43	413	-	56,63,73	2.39	14 (25%)	53,101,113	2.45	18 (33%)
21	CL7	4C	503	-	66,73,73	2.19	13 (19%)	65,113,113	2.22	17 (26%)
32	ZEX	34	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	13	513	-	46,53,73	2.66	14 (30%)	41,89,113	2.66	13 (31%)
21	CL7	32	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.41	19 (29%)
21	CL7	23	405	-	66,73,73	2.20	13 (19%)	65,113,113	2.25	17 (26%)
23	8CT	2K	101	-	40,41,41	4.75	25 (62%)	50,56,56	2.65	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	12	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
23	8CT	3B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.66	20 (40%)
21	CL7	1D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	41	409	-	46,53,73	2.62	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	4B	606	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
32	ZEX	34	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
22	PHO	3A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
26	LHG	2B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	42	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.62	14 (34%)
21	CL7	2C	511	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	12 (33%)
32	ZEX	23	401	-	42,43,43	1.18	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	13	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
23	8CT	44	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	44	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	4B	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.27	15 (23%)
32	ZEX	44	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
25	SQD	23	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	32	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	16 (24%)
21	CL7	31	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
32	ZEX	14	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	19 (34%)
25	SQD	12	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	11	410	-	66,73,73	2.23	13 (19%)	65,113,113	2.17	16 (24%)
24	LMG	21	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	3B	601	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	12 (33%)
21	CL7	43	418	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	32	509	-	66,73,73	2.20	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	44	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	2B	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.26	16 (24%)
21	CL7	42	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
23	8CT	4D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.98	19 (38%)
21	CL7	32	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	17 (26%)
21	CL7	42	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.40	19 (29%)
26	LHG	1B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	42	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.66	14 (34%)
21	CL7	23	407	-	46,53,73	2.58	14 (30%)	41,89,113	2.72	14 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	32	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.24	19 (29%)
21	CL7	2B	614	-	56,63,73	2.39	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	31	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	22	510	16	66,73,73	2.19	14 (21%)	65,113,113	2.23	18 (27%)
21	CL7	13	512	-	56,63,73	2.39	14 (25%)	53,101,113	2.44	18 (33%)
32	ZEX	44	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	34	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.66	13 (31%)
21	CL7	21	411	-	46,53,73	2.65	12 (26%)	41,89,113	2.62	14 (34%)
32	ZEX	42	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	1C	506	-	61,68,73	2.32	13 (21%)	59,107,113	2.39	18 (30%)
21	CL7	3B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.64	17 (36%)
21	CL7	12	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	14	407	-	42,49,73	2.64	9 (21%)	36,84,113	2.84	14 (38%)
21	CL7	2B	616	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	17 (36%)
21	CL7	41	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	16 (44%)
24	LMG	2D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	34	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	31	410	-	66,73,73	2.25	13 (19%)	65,113,113	2.18	16 (24%)
21	CL7	13	504	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)
21	CL7	14	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.65	13 (31%)
27	DGD	1B	624	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
21	CL7	12	510	16	66,73,73	2.19	13 (19%)	65,113,113	2.24	18 (27%)
21	CL7	14	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.30	19 (29%)
21	CL7	44	410	-	46,53,73	2.62	13 (28%)	41,89,113	2.66	13 (31%)
21	CL7	41	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
23	8CT	4B	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	24	417	20	43,50,73	2.68	11 (25%)	36,85,113	2.89	13 (36%)
24	LMG	1D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
32	ZEX	42	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
30	PL9	3D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	22	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	17 (26%)
21	CL7	23	418	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
32	ZEX	31	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	1C	512	-	42,49,73	2.56	9 (21%)	36,84,113	2.91	14 (38%)
21	CL7	14	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.89	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	11	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	1C	511	3	43,50,73	2.70	11 (25%)	36,85,113	2.78	13 (36%)
21	CL7	13	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
27	DGD	2C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
27	DGD	3B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	12	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
21	CL7	22	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.39	19 (29%)
21	CL7	4B	611	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
23	8CT	4B	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	32	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
32	ZEX	12	522	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	17 (30%)
21	CL7	4A	403	-	56,63,73	2.41	14 (25%)	53,101,113	2.58	18 (33%)
21	CL7	33	507	-	66,73,73	2.15	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	21	403	-	61,68,73	2.28	13 (21%)	59,107,113	2.38	15 (25%)
21	CL7	31	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	15 (41%)
26	LHG	43	425	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	34	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	15 (30%)
21	CL7	1C	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)
30	PL9	2D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
32	ZEX	34	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	22	518	16	66,73,73	2.23	13 (19%)	65,113,113	2.17	17 (26%)
21	CL7	31	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
22	PHO	3D	408	-	51,69,69	0.59	2 (3%)	47,99,99	0.87	2 (4%)
21	CL7	31	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
21	CL7	34	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.66	13 (31%)
25	SQD	43	422	-	45,46,54	0.42	0	54,57,65	0.48	0
21	CL7	2C	505	-	66,73,73	2.22	14 (21%)	65,113,113	2.26	17 (26%)
21	CL7	1B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.62	17 (36%)
23	8CT	3B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.76	19 (38%)
21	CL7	11	402	-	61,68,73	2.32	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	2B	605	-	66,73,73	2.16	13 (19%)	65,113,113	2.23	17 (26%)
25	SQD	32	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	44	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	16 (32%)
21	CL7	3B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	15 (23%)
21	CL7	41	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	4I	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.57	13 (31%)
31	HEM	4F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	23	410	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	2C	517	-	42,49,73	2.63	10 (23%)	36,84,113	2.84	14 (38%)
21	CL7	4B	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
21	CL7	2D	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.47	15 (31%)

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
21	CL7	34	417	20	2/2/10/20	4/10/88/115	-
21	CL7	4B	614	-	2/2/13/20	4/25/103/115	-
21	CL7	12	515	-	2/2/11/20	6/13/91/115	-
25	SQD	1A	406	-	-	3/29/49/69	0/1/1/1
27	DGD	1C	516	-	-	9/51/91/95	0/2/2/2
23	8CT	3C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	24	414	-	2/2/12/20	6/23/101/115	-
23	8CT	1D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	22	506	-	2/2/15/20	12/37/115/115	-
21	CL7	23	409	-	2/2/15/20	14/37/115/115	-
21	CL7	23	416	-	2/2/10/20	0/8/86/115	-
21	CL7	1C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	2C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	33	516	19	2/2/13/20	14/25/103/115	-
23	8CT	3C	515	-	-	10/29/63/63	0/2/2/2
32	ZEX	21	422	-	-	6/29/67/67	0/2/2/2
21	CL7	42	518	16	2/2/15/20	10/37/115/115	-
21	CL7	1B	607	-	2/2/14/20	9/31/109/115	-
32	ZEX	24	419	-	-	9/29/67/67	0/2/2/2
21	CL7	21	419	-	2/2/11/20	7/13/91/115	-
21	CL7	43	411	-	2/2/15/20	14/37/115/115	-
21	CL7	24	412	-	2/2/15/20	17/37/115/115	-
21	CL7	4B	613	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHO	4A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	2B	604	-	2/2/15/20	12/37/115/115	-
21	CL7	2B	606	-	2/2/15/20	16/37/115/115	-
21	CL7	3D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	43	407	-	2/2/11/20	11/13/91/115	-
24	LMG	4B	622	-	-	7/46/66/70	0/1/1/1
26	LHG	14	401	-	-	8/53/53/53	-
21	CL7	3B	613	-	2/2/13/20	4/25/103/115	-
21	CL7	42	507	-	2/2/15/20	18/37/115/115	-
23	8CT	3A	404	-	-	5/29/63/63	0/2/2/2
26	LHG	4A	408	-	-	5/50/50/53	-
21	CL7	43	414	-	2/2/11/20	7/13/91/115	-
31	HEM	1F	101	-	-	6/12/54/54	-
21	CL7	32	513	-	2/2/11/20	6/13/91/115	-
21	CL7	31	420	18	2/2/11/20	4/13/91/115	-
23	8CT	1C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	3D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	31	408	-	2/2/15/20	14/37/115/115	-
21	CL7	24	409	-	2/2/14/20	15/31/109/115	-
21	CL7	4B	616	-	2/2/12/20	8/19/97/115	-
21	CL7	12	504	-	2/2/11/20	4/13/91/115	-
21	CL7	14	404	-	2/2/15/20	15/37/115/115	-
25	SQD	43	424	-	-	7/45/65/69	0/1/1/1
23	8CT	1C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	2D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	11	403	-	2/2/14/20	9/31/109/115	-
21	CL7	1B	602	-	2/2/14/20	7/31/109/115	-
21	CL7	12	502	-	2/2/15/20	15/37/115/115	-
21	CL7	2C	509	-	2/2/15/20	18/37/115/115	-
21	CL7	2B	613	-	2/2/15/20	15/37/115/115	-
21	CL7	2B	609	-	2/2/15/20	15/37/115/115	-
21	CL7	42	517	16	2/2/15/20	19/37/115/115	-
31	HEM	2F	101	-	-	6/12/54/54	-
23	8CT	2B	619	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	3A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	4B	607	-	2/2/13/20	4/25/103/115	-
21	CL7	3C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	12	518	16	2/2/15/20	10/37/115/115	-
21	CL7	4C	502	-	2/2/14/20	10/31/109/115	-
27	DGD	3C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	23	411	-	2/2/15/20	13/37/115/115	-
21	CL7	3C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	44	409	-	2/2/14/20	15/31/109/115	-
24	LMG	3D	410	-	-	5/28/48/70	0/1/1/1
21	CL7	3B	610	-	2/2/15/20	11/37/115/115	-
21	CL7	14	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	24	403	-	-	10/29/67/67	0/2/2/2
21	CL7	21	420	18	2/2/11/20	4/13/91/115	-
25	SQD	33	521	-	-	3/41/61/69	0/1/1/1
21	CL7	23	408	-	2/2/15/20	13/37/115/115	-
21	CL7	32	507	-	2/2/15/20	18/37/115/115	-
21	CL7	21	406	-	2/2/14/20	11/34/112/115	-
32	ZEX	33	522	-	-	5/29/67/67	0/2/2/2
21	CL7	11	416	-	2/2/10/20	2/8/86/115	-
21	CL7	2C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	23	403	-	2/2/13/20	10/29/107/115	-
21	CL7	21	409	-	2/2/11/20	4/13/91/115	-
21	CL7	4C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	31	415	-	2/2/10/20	5/8/86/115	-
21	CL7	32	506	-	2/2/15/20	12/37/115/115	-
21	CL7	31	402	-	2/2/14/20	14/31/109/115	-
21	CL7	31	405	-	2/2/11/20	9/13/91/115	-
21	CL7	1A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	1C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	14	409	-	2/2/14/20	15/31/109/115	-
21	CL7	43	410	-	2/2/15/20	15/37/115/115	-
23	8CT	3B	619	-	-	4/29/63/63	0/2/2/2
32	ZEX	13	522	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	3C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	43	416	-	2/2/10/20	0/8/86/115	-
21	CL7	11	415	-	2/2/10/20	5/8/86/115	-
21	CL7	1B	603	-	2/2/15/20	12/37/115/115	-
23	8CT	2D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	41	405	-	2/2/11/20	9/13/91/115	-
21	CL7	14	413	20	2/2/14/20	7/31/109/115	-
21	CL7	41	402	-	2/2/14/20	14/31/109/115	-
32	ZEX	13	525	-	-	7/29/67/67	0/2/2/2
21	CL7	22	515	-	2/2/11/20	6/13/91/115	-
23	8CT	2C	514	-	-	14/29/63/63	0/2/2/2
32	ZEX	11	421	-	-	14/29/67/67	0/2/2/2
21	CL7	13	506	-	2/2/11/20	11/13/91/115	-
21	CL7	24	408	-	2/2/11/20	2/13/91/115	-
21	CL7	1A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	44	413	20	2/2/14/20	7/31/109/115	-
23	8CT	2C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	3B	602	-	2/2/14/20	7/31/109/115	-
21	CL7	12	505	-	2/2/15/20	16/37/115/115	-
21	CL7	3C	506	-	2/2/14/20	13/31/109/115	-
21	CL7	1A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	42	509	-	2/2/15/20	14/37/115/115	-
21	CL7	24	407	-	2/2/10/20	1/8/86/115	-
23	8CT	1B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	21	408	-	2/2/15/20	14/37/115/115	-
21	CL7	33	502	-	2/2/13/20	10/29/107/115	-
21	CL7	23	417	19	2/2/13/20	14/25/103/115	-
32	ZEX	12	519	-	-	11/29/67/67	0/2/2/2
21	CL7	24	405	-	2/2/15/20	16/37/115/115	-
23	8CT	4B	619	-	-	10/29/63/63	0/2/2/2
21	CL7	2C	513	-	2/2/11/20	6/13/91/115	-
21	CL7	3D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	12	508	-	2/2/11/20	3/13/91/115	-
21	CL7	14	408	-	2/2/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	31	421	-	-	14/29/67/67	0/2/2/2
25	SQD	33	523	-	-	7/45/65/69	0/1/1/1
21	CL7	4B	608	-	2/2/14/20	9/31/109/115	-
21	CL7	41	408	-	2/2/15/20	14/37/115/115	-
21	CL7	41	415	-	2/2/10/20	5/8/86/115	-
21	CL7	2A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	12	512	-	2/2/15/20	16/37/115/115	-
31	HEM	3F	101	-	-	6/12/54/54	-
21	CL7	13	501	-	2/2/15/20	19/37/115/115	-
21	CL7	3C	512	-	2/2/10/20	2/8/86/115	-
25	SQD	23	422	-	-	3/41/61/69	0/1/1/1
26	LHG	3B	625	-	-	6/53/53/53	-
21	CL7	3C	501	-	2/2/15/20	18/37/115/115	-
21	CL7	2B	610	-	2/2/15/20	12/37/115/115	-
21	CL7	1B	614	-	2/2/14/20	12/31/109/115	-
21	CL7	4C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	24	416	-	2/2/10/20	5/8/86/115	-
21	CL7	43	419	19	2/2/11/20	5/13/91/115	-
23	8CT	14	402	-	-	4/29/63/63	0/2/2/2
26	LHG	3B	623	-	-	3/49/49/53	-
21	CL7	24	415	-	2/2/11/20	10/13/91/115	-
21	CL7	1C	503	-	2/2/15/20	17/37/115/115	-
26	LHG	3A	408	-	-	5/50/50/53	-
26	LHG	33	524	-	-	3/40/40/53	-
21	CL7	11	405	-	2/2/11/20	9/13/91/115	-
26	LHG	3D	409	-	-	7/53/53/53	-
21	CL7	3C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	3B	605	-	2/2/15/20	16/37/115/115	-
21	CL7	2C	507	-	2/2/15/20	15/37/115/115	-
24	LMG	2B	622	-	-	7/46/66/70	0/1/1/1
21	CL7	13	503	-	2/2/15/20	18/37/115/115	-
21	CL7	1C	501	-	2/2/15/20	18/37/115/115	-
21	CL7	41	416	-	2/2/10/20	2/8/86/115	-
21	CL7	1B	609	-	2/2/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	2B	618	-	-	7/29/63/63	0/2/2/2
23	8CT	3B	626	-	-	10/29/63/63	0/2/2/2
21	CL7	4C	508	-	2/2/15/20	15/37/115/115	-
26	LHG	4D	409	-	-	7/53/53/53	-
21	CL7	4C	509	-	2/2/15/20	18/37/115/115	-
25	SQD	2B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	2C	506	-	2/2/14/20	13/31/109/115	-
32	ZEX	43	423	-	-	5/29/67/67	0/2/2/2
21	CL7	43	417	19	2/2/13/20	14/25/103/115	-
24	LMG	11	401	-	-	5/46/66/70	0/1/1/1
23	8CT	3K	101	-	-	10/29/63/63	0/2/2/2
23	8CT	2C	518	-	-	8/29/63/63	0/2/2/2
26	LHG	2D	409	-	-	7/53/53/53	-
21	CL7	4B	603	-	2/2/14/20	7/31/109/115	-
21	CL7	2A	401	-	2/2/15/20	16/37/115/115	-
25	SQD	3B	620	-	-	5/49/69/69	0/1/1/1
32	ZEX	22	522	-	-	6/29/67/67	0/2/2/2
21	CL7	23	419	19	2/2/11/20	5/13/91/115	-
21	CL7	1B	616	-	2/2/11/20	4/13/91/115	-
21	CL7	33	511	19	2/2/15/20	17/37/115/115	-
21	CL7	44	407	-	2/2/10/20	1/8/86/115	-
21	CL7	3B	607	-	2/2/14/20	9/31/109/115	-
21	CL7	32	511	16	2/2/14/20	14/31/109/115	-
21	CL7	42	513	-	2/2/11/20	6/13/91/115	-
32	ZEX	41	421	-	-	14/29/67/67	0/2/2/2
21	CL7	2C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	33	517	19	2/2/12/20	7/19/97/115	-
32	ZEX	44	418	-	-	9/29/67/67	0/2/2/2
26	LHG	4B	624	-	-	3/49/49/53	-
21	CL7	3A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	41	404	-	2/2/15/20	13/37/115/115	-
24	LMG	31	401	-	-	5/46/66/70	0/1/1/1
23	8CT	4C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	34	405	-	2/2/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	43	421	-	-	10/29/67/67	0/2/2/2
32	ZEX	33	525	-	-	7/29/67/67	0/2/2/2
23	8CT	4C	515	-	-	10/29/63/63	0/2/2/2
23	8CT	3C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	4C	511	3	2/2/10/20	3/10/88/115	-
21	CL7	4C	513	-	2/2/11/20	6/13/91/115	-
25	SQD	42	523	-	-	0/36/56/69	0/1/1/1
24	LMG	41	401	-	-	5/46/66/70	0/1/1/1
26	LHG	24	401	-	-	8/53/53/53	-
21	CL7	22	516	-	2/2/15/20	14/37/115/115	-
21	CL7	12	513	-	2/2/11/20	6/13/91/115	-
21	CL7	4B	604	-	2/2/15/20	12/37/115/115	-
27	DGD	2B	625	-	-	7/51/91/95	0/2/2/2
27	DGD	4C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	22	505	-	2/2/15/20	16/37/115/115	-
21	CL7	33	518	19	2/2/11/20	5/13/91/115	-
21	CL7	3C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	24	404	-	2/2/15/20	15/37/115/115	-
21	CL7	14	411	-	2/2/15/20	12/37/115/115	-
21	CL7	3A	401	-	2/2/15/20	16/37/115/115	-
23	8CT	1B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	34	415	-	2/2/11/20	10/13/91/115	-
32	ZEX	43	401	-	-	7/29/67/67	0/2/2/2
32	ZEX	23	420	-	-	10/29/67/67	0/2/2/2
25	SQD	3A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	22	513	-	2/2/11/20	6/13/91/115	-
21	CL7	2C	501	-	2/2/15/20	18/37/115/115	-
21	CL7	3B	603	-	2/2/15/20	12/37/115/115	-
21	CL7	1B	605	-	2/2/15/20	16/37/115/115	-
23	8CT	1C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	22	501	-	2/2/15/20	15/37/115/115	-
21	CL7	32	501	-	2/2/15/20	15/37/115/115	-
25	SQD	2A	406	-	-	3/29/49/69	0/1/1/1
25	SQD	13	523	-	-	7/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PL9	1D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	31	403	-	2/2/14/20	9/31/109/115	-
26	LHG	1D	409	-	-	7/53/53/53	-
21	CL7	44	408	-	2/2/11/20	2/13/91/115	-
21	CL7	13	514	-	2/2/11/20	5/13/91/115	-
23	8CT	1B	626	-	-	10/29/63/63	0/2/2/2
21	CL7	41	406	-	2/2/14/20	11/34/112/115	-
21	CL7	44	404	-	2/2/15/20	14/37/115/115	-
21	CL7	11	412	-	2/2/11/20	8/13/91/115	-
24	LMG	1A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	13	515	-	2/2/10/20	0/8/86/115	-
21	CL7	42	506	-	2/2/15/20	12/37/115/115	-
26	LHG	23	425	-	-	3/40/40/53	-
21	CL7	2C	502	-	2/2/14/20	10/31/109/115	-
21	CL7	22	508	-	2/2/11/20	3/13/91/115	-
21	CL7	13	511	19	2/2/15/20	17/37/115/115	-
21	CL7	4C	506	-	2/2/14/20	13/31/109/115	-
21	CL7	4C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	42	510	16	2/2/15/20	20/37/115/115	-
21	CL7	43	415	-	2/2/11/20	5/13/91/115	-
32	ZEX	21	421	-	-	14/29/67/67	0/2/2/2
21	CL7	12	501	-	2/2/15/20	15/37/115/115	-
21	CL7	44	405	-	2/2/15/20	16/37/115/115	-
32	ZEX	22	519	-	-	11/29/67/67	0/2/2/2
21	CL7	11	411	-	2/2/11/20	5/13/91/115	-
21	CL7	34	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	24	420	-	-	12/29/67/67	0/2/2/2
21	CL7	1B	613	-	2/2/13/20	4/25/103/115	-
21	CL7	1B	606	-	2/2/13/20	4/25/103/115	-
23	8CT	3D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	31	404	-	2/2/15/20	13/37/115/115	-
32	ZEX	22	524	-	-	11/29/67/67	0/2/2/2
21	CL7	42	502	-	2/2/15/20	15/37/115/115	-
24	LMG	2A	405	-	2/2/8/8	8/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	13	516	19	2/2/13/20	14/25/103/115	-
21	CL7	41	412	-	2/2/11/20	8/13/91/115	-
24	LMG	4A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
27	DGD	4B	625	-	-	7/51/91/95	0/2/2/2
21	CL7	33	505	-	2/2/15/20	14/37/115/115	-
26	LHG	2A	408	-	-	5/50/50/53	-
21	CL7	22	502	-	2/2/15/20	15/37/115/115	-
32	ZEX	33	520	-	-	10/29/67/67	0/2/2/2
21	CL7	41	420	18	2/2/11/20	4/13/91/115	-
21	CL7	43	412	19	2/2/15/20	17/37/115/115	-
21	CL7	42	503	-	2/2/15/20	17/37/115/115	-
26	LHG	2B	624	-	-	3/49/49/53	-
21	CL7	1C	507	-	2/2/15/20	15/37/115/115	-
21	CL7	23	415	-	2/2/11/20	5/13/91/115	-
21	CL7	22	514	-	2/2/11/20	7/13/91/115	-
21	CL7	4C	501	-	2/2/15/20	18/37/115/115	-
26	LHG	13	524	-	-	3/40/40/53	-
32	ZEX	13	519	-	-	10/29/67/67	0/2/2/2
21	CL7	23	402	-	2/2/15/20	19/37/115/115	-
23	8CT	24	402	-	-	4/29/63/63	0/2/2/2
22	PHO	2D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	3B	614	-	2/2/14/20	12/31/109/115	-
32	ZEX	12	524	-	-	11/29/67/67	0/2/2/2
21	CL7	4C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	13	517	19	2/2/12/20	7/19/97/115	-
21	CL7	3C	509	-	2/2/15/20	18/37/115/115	-
32	ZEX	32	519	-	-	11/29/67/67	0/2/2/2
21	CL7	41	403	-	2/2/14/20	9/31/109/115	-
21	CL7	4D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	3C	502	-	2/2/14/20	10/31/109/115	-
21	CL7	32	514	-	2/2/11/20	7/13/91/115	-
21	CL7	42	501	-	2/2/15/20	15/37/115/115	-
32	ZEX	42	522	-	-	6/29/67/67	0/2/2/2
21	CL7	1B	608	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	515	-	2/2/10/20	0/8/86/115	-
22	PHO	1A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	32	515	-	2/2/11/20	6/13/91/115	-
32	ZEX	32	522	-	-	6/29/67/67	0/2/2/2
32	ZEX	43	420	-	-	10/29/67/67	0/2/2/2
21	CL7	3B	622	-	2/2/11/20	6/13/91/115	-
21	CL7	3B	604	-	2/2/15/20	15/37/115/115	-
25	SQD	4A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	33	501	-	2/2/15/20	19/37/115/115	-
21	CL7	11	406	-	2/2/14/20	11/34/112/115	-
21	CL7	13	510	-	2/2/15/20	13/37/115/115	-
26	LHG	34	401	-	-	8/53/53/53	-
21	CL7	13	518	19	2/2/11/20	5/13/91/115	-
21	CL7	31	413	-	2/2/10/20	2/8/86/115	-
21	CL7	11	404	-	2/2/15/20	13/37/115/115	-
21	CL7	3C	503	-	2/2/15/20	17/37/115/115	-
21	CL7	4B	615	-	2/2/14/20	12/31/109/115	-
32	ZEX	14	403	-	-	10/29/67/67	0/2/2/2
32	ZEX	12	520	-	-	6/29/67/67	0/2/2/2
21	CL7	21	405	-	2/2/11/20	9/13/91/115	-
21	CL7	12	517	16	2/2/15/20	19/37/115/115	-
23	8CT	1K	101	-	-	10/29/63/63	0/2/2/2
25	SQD	32	523	-	-	0/36/56/69	0/1/1/1
21	CL7	24	410	-	2/2/11/20	7/13/91/115	-
24	LMG	4D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	3B	616	-	2/2/11/20	4/13/91/115	-
21	CL7	1D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	4B	610	-	2/2/15/20	12/37/115/115	-
23	8CT	34	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	41	422	-	-	6/29/67/67	0/2/2/2
21	CL7	23	413	-	2/2/13/20	12/25/103/115	-
21	CL7	11	409	-	2/2/11/20	4/13/91/115	-
21	CL7	12	514	-	2/2/11/20	7/13/91/115	-
21	CL7	2B	617	-	2/2/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	512	-	2/2/15/20	16/37/115/115	-
21	CL7	1C	510	-	2/2/15/20	20/37/115/115	-
24	LMG	1B	621	-	-	7/46/66/70	0/1/1/1
22	PHO	4D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	43	405	-	2/2/15/20	14/37/115/115	-
21	CL7	21	402	-	2/2/14/20	14/31/109/115	-
25	SQD	22	521	-	-	7/45/65/69	0/1/1/1
32	ZEX	23	421	-	-	10/29/67/67	0/2/2/2
21	CL7	11	413	-	2/2/10/20	2/8/86/115	-
21	CL7	1B	610	-	2/2/15/20	11/37/115/115	-
21	CL7	2B	608	-	2/2/14/20	9/31/109/115	-
32	ZEX	14	419	-	-	9/29/67/67	0/2/2/2
21	CL7	31	418	18	2/2/15/20	20/37/115/115	-
22	PHO	1D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	11	418	18	2/2/15/20	20/37/115/115	-
21	CL7	21	418	18	2/2/15/20	20/37/115/115	-
21	CL7	1B	612	-	2/2/15/20	15/37/115/115	-
21	CL7	21	412	-	2/2/11/20	8/13/91/115	-
21	CL7	11	420	18	2/2/11/20	4/13/91/115	-
21	CL7	1C	502	-	2/2/14/20	10/31/109/115	-
21	CL7	24	413	20	2/2/14/20	7/31/109/115	-
21	CL7	21	417	18	2/2/13/20	7/25/103/115	-
21	CL7	1C	504	-	2/2/13/20	11/25/103/115	-
21	CL7	3C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	44	416	-	2/2/10/20	5/8/86/115	-
21	CL7	2D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	41	418	18	2/2/15/20	20/37/115/115	-
25	SQD	1B	620	-	-	5/49/69/69	0/1/1/1
25	SQD	4B	621	-	-	5/49/69/69	0/1/1/1
25	SQD	31	423	-	-	3/27/47/69	0/1/1/1
25	SQD	13	521	-	-	3/41/61/69	0/1/1/1
21	CL7	33	506	-	2/2/11/20	11/13/91/115	-
21	CL7	34	412	-	2/2/15/20	17/37/115/115	-
21	CL7	14	416	-	2/2/10/20	5/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	41	417	18	2/2/13/20	7/25/103/115	-
25	SQD	11	423	-	-	3/27/47/69	0/1/1/1
21	CL7	1B	611	-	2/2/15/20	15/37/115/115	-
22	PHO	2A	402	-	-	3/37/103/103	0/5/6/6
21	CL7	3B	612	-	2/2/15/20	15/37/115/115	-
21	CL7	33	503	-	2/2/15/20	18/37/115/115	-
21	CL7	33	510	-	2/2/15/20	13/37/115/115	-
21	CL7	2B	615	-	2/2/14/20	12/31/109/115	-
21	CL7	22	511	16	2/2/14/20	14/31/109/115	-
21	CL7	23	414	-	2/2/11/20	7/13/91/115	-
21	CL7	41	413	-	2/2/10/20	2/8/86/115	-
21	CL7	23	406	-	2/2/15/20	14/37/115/115	-
21	CL7	33	508	-	2/2/15/20	14/37/115/115	-
26	LHG	4B	626	-	-	6/53/53/53	-
21	CL7	21	414	-	2/2/10/20	1/8/86/115	-
32	ZEX	11	422	-	-	6/29/67/67	0/2/2/2
25	SQD	42	521	-	-	7/45/65/69	0/1/1/1
21	CL7	32	508	-	2/2/11/20	3/13/91/115	-
21	CL7	23	404	-	2/2/15/20	18/37/115/115	-
21	CL7	2C	510	-	2/2/15/20	20/37/115/115	-
25	SQD	12	523	-	-	0/36/56/69	0/1/1/1
32	ZEX	13	520	-	-	10/29/67/67	0/2/2/2
21	CL7	31	406	-	2/2/14/20	11/34/112/115	-
32	ZEX	24	418	-	-	9/29/67/67	0/2/2/2
21	CL7	42	515	-	2/2/11/20	6/13/91/115	-
21	CL7	43	402	-	2/2/15/20	19/37/115/115	-
21	CL7	23	412	19	2/2/15/20	17/37/115/115	-
21	CL7	41	414	-	2/2/10/20	1/8/86/115	-
21	CL7	1B	601	-	2/2/10/20	4/8/86/115	-
24	LMG	3B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	31	409	-	2/2/11/20	4/13/91/115	-
21	CL7	2B	623	-	2/2/11/20	6/13/91/115	-
21	CL7	34	411	-	2/2/15/20	12/37/115/115	-
23	8CT	4A	404	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	14	418	-	-	9/29/67/67	0/2/2/2
21	CL7	21	415	-	2/2/10/20	5/8/86/115	-
21	CL7	31	416	-	2/2/10/20	2/8/86/115	-
25	SQD	21	423	-	-	3/27/47/69	0/1/1/1
21	CL7	4B	617	-	2/2/11/20	4/13/91/115	-
21	CL7	3C	511	3	2/2/10/20	3/10/88/115	-
32	ZEX	32	524	-	-	11/29/67/67	0/2/2/2
32	ZEX	23	423	-	-	5/29/67/67	0/2/2/2
26	LHG	1A	408	-	-	5/50/50/53	-
23	8CT	1B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	21	407	-	2/2/10/20	2/8/86/115	-
30	PL9	4D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	42	514	-	2/2/11/20	7/13/91/115	-
23	8CT	1A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	34	407	-	2/2/10/20	1/8/86/115	-
21	CL7	1B	622	-	2/2/11/20	6/13/91/115	-
21	CL7	1B	604	-	2/2/15/20	15/37/115/115	-
25	SQD	41	423	-	-	3/27/47/69	0/1/1/1
21	CL7	2B	611	-	2/2/15/20	11/37/115/115	-
23	8CT	2B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	2C	503	-	2/2/15/20	17/37/115/115	-
21	CL7	3B	609	-	2/2/15/20	12/37/115/115	-
21	CL7	11	417	18	2/2/13/20	7/25/103/115	-
21	CL7	32	503	-	2/2/15/20	17/37/115/115	-
21	CL7	32	518	16	2/2/15/20	10/37/115/115	-
21	CL7	4D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	4B	623	-	2/2/11/20	6/13/91/115	-
21	CL7	4A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	33	513	-	2/2/11/20	7/13/91/115	-
26	LHG	44	401	-	-	8/53/53/53	-
21	CL7	1D	405	-	2/2/11/20	6/13/91/115	-
21	CL7	4B	605	-	2/2/15/20	15/37/115/115	-
21	CL7	2B	607	-	2/2/13/20	4/25/103/115	-
21	CL7	14	414	-	2/2/12/20	6/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	22	509	-	2/2/15/20	14/37/115/115	-
21	CL7	1C	505	-	2/2/15/20	14/37/115/115	-
23	8CT	2B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	1C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	21	410	-	2/2/15/20	15/37/115/115	-
21	CL7	43	408	-	2/2/15/20	13/37/115/115	-
21	CL7	11	414	-	2/2/10/20	1/8/86/115	-
21	CL7	21	416	-	2/2/10/20	2/8/86/115	-
21	CL7	21	404	-	2/2/15/20	13/37/115/115	-
21	CL7	33	504	-	2/2/15/20	14/37/115/115	-
21	CL7	43	404	-	2/2/15/20	18/37/115/115	-
21	CL7	43	403	-	2/2/13/20	10/29/107/115	-
21	CL7	22	504	-	2/2/11/20	4/13/91/115	-
21	CL7	32	504	-	2/2/11/20	4/13/91/115	-
21	CL7	12	503	-	2/2/15/20	17/37/115/115	-
21	CL7	31	411	-	2/2/11/20	5/13/91/115	-
21	CL7	12	511	16	2/2/14/20	14/31/109/115	-
21	CL7	14	415	-	2/2/11/20	10/13/91/115	-
21	CL7	4B	602	-	2/2/10/20	4/8/86/115	-
21	CL7	44	415	-	2/2/11/20	10/13/91/115	-
32	ZEX	22	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	32	520	-	-	6/29/67/67	0/2/2/2
21	CL7	11	408	-	2/2/15/20	14/37/115/115	-
21	CL7	34	404	-	2/2/15/20	14/37/115/115	-
21	CL7	2B	602	-	2/2/10/20	4/8/86/115	-
21	CL7	43	409	-	2/2/15/20	14/37/115/115	-
21	CL7	24	406	-	2/2/15/20	22/37/115/115	-
26	LHG	1B	623	-	-	3/49/49/53	-
21	CL7	12	509	-	2/2/15/20	14/37/115/115	-
21	CL7	13	509	-	2/2/15/20	15/37/115/115	-
23	8CT	4K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	3C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	21	413	-	2/2/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2A	407	-	2/2/15/20	14/37/115/115	-
21	CL7	22	517	16	2/2/15/20	19/37/115/115	-
21	CL7	3B	611	-	2/2/15/20	15/37/115/115	-
21	CL7	32	517	16	2/2/15/20	19/37/115/115	-
21	CL7	4C	510	-	2/2/15/20	20/37/115/115	-
21	CL7	34	409	-	2/2/14/20	15/31/109/115	-
21	CL7	2B	603	-	2/2/14/20	7/31/109/115	-
21	CL7	42	512	-	2/2/15/20	16/37/115/115	-
32	ZEX	34	403	-	-	10/29/67/67	0/2/2/2
21	CL7	42	511	16	2/2/14/20	14/31/109/115	-
21	CL7	3B	606	-	2/2/13/20	4/25/103/115	-
21	CL7	4D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	44	412	-	2/2/15/20	17/37/115/115	-
23	8CT	2A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	33	512	-	2/2/13/20	12/25/103/115	-
21	CL7	14	412	-	2/2/15/20	17/37/115/115	-
21	CL7	11	407	-	2/2/10/20	2/8/86/115	-
32	ZEX	33	519	-	-	10/29/67/67	0/2/2/2
21	CL7	34	413	20	2/2/14/20	7/31/109/115	-
23	8CT	4B	618	-	-	7/29/63/63	0/2/2/2
21	CL7	43	406	-	2/2/15/20	14/37/115/115	-
21	CL7	44	417	20	2/2/10/20	4/10/88/115	-
24	LMG	3A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	33	509	-	2/2/15/20	15/37/115/115	-
21	CL7	24	411	-	2/2/15/20	12/37/115/115	-
21	CL7	4C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	44	406	-	2/2/15/20	22/37/115/115	-
23	8CT	4C	518	-	-	8/29/63/63	0/2/2/2
32	ZEX	42	520	-	-	6/29/67/67	0/2/2/2
21	CL7	13	508	-	2/2/15/20	14/37/115/115	-
21	CL7	13	505	-	2/2/15/20	14/37/115/115	-
25	SQD	22	523	-	-	0/36/56/69	0/1/1/1
21	CL7	33	514	-	2/2/11/20	5/13/91/115	-
21	CL7	43	413	-	2/2/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	4C	503	-	2/2/15/20	17/37/115/115	-
32	ZEX	34	419	-	-	9/29/67/67	0/2/2/2
21	CL7	13	513	-	2/2/11/20	7/13/91/115	-
21	CL7	32	505	-	2/2/15/20	16/37/115/115	-
21	CL7	23	405	-	2/2/15/20	14/37/115/115	-
23	8CT	2K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	12	516	-	2/2/15/20	14/37/115/115	-
23	8CT	3B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	1D	404	-	2/2/13/20	11/29/107/115	-
21	CL7	41	409	-	2/2/11/20	4/13/91/115	-
21	CL7	4B	606	-	2/2/15/20	16/37/115/115	-
32	ZEX	34	418	-	-	9/29/67/67	0/2/2/2
22	PHO	3A	402	-	-	3/37/103/103	0/5/6/6
26	LHG	2B	626	-	-	6/53/53/53	-
21	CL7	42	504	-	2/2/11/20	4/13/91/115	-
21	CL7	2C	511	3	2/2/10/20	3/10/88/115	-
32	ZEX	23	401	-	-	7/29/67/67	0/2/2/2
21	CL7	13	507	-	2/2/15/20	13/37/115/115	-
23	8CT	44	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	44	420	-	-	12/29/67/67	0/2/2/2
21	CL7	4B	612	-	2/2/15/20	15/37/115/115	-
32	ZEX	44	419	-	-	9/29/67/67	0/2/2/2
25	SQD	23	424	-	-	7/45/65/69	0/1/1/1
21	CL7	32	512	-	2/2/15/20	16/37/115/115	-
21	CL7	31	417	18	2/2/13/20	7/25/103/115	-
32	ZEX	14	420	-	-	12/29/67/67	0/2/2/2
25	SQD	12	521	-	-	7/45/65/69	0/1/1/1
21	CL7	11	410	-	2/2/15/20	15/37/115/115	-
24	LMG	21	401	-	-	5/46/66/70	0/1/1/1
21	CL7	3B	601	-	2/2/10/20	4/8/86/115	-
21	CL7	43	418	19	2/2/12/20	7/19/97/115	-
21	CL7	32	509	-	2/2/15/20	14/37/115/115	-
21	CL7	44	411	-	2/2/15/20	12/37/115/115	-
21	CL7	2B	612	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	42	516	-	2/2/15/20	14/37/115/115	-
23	8CT	4D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	32	502	-	2/2/15/20	15/37/115/115	-
21	CL7	42	505	-	2/2/15/20	16/37/115/115	-
26	LHG	1B	625	-	-	6/53/53/53	-
21	CL7	42	508	-	2/2/11/20	3/13/91/115	-
21	CL7	23	407	-	2/2/11/20	11/13/91/115	-
21	CL7	32	516	-	2/2/15/20	14/37/115/115	-
21	CL7	2B	614	-	2/2/13/20	4/25/103/115	-
21	CL7	31	414	-	2/2/10/20	1/8/86/115	-
21	CL7	22	510	16	2/2/15/20	20/37/115/115	-
21	CL7	13	512	-	2/2/13/20	12/25/103/115	-
32	ZEX	44	403	-	-	10/29/67/67	0/2/2/2
21	CL7	34	410	-	2/2/11/20	7/13/91/115	-
21	CL7	21	411	-	2/2/11/20	5/13/91/115	-
32	ZEX	42	519	-	-	11/29/67/67	0/2/2/2
21	CL7	1C	506	-	2/2/14/20	13/31/109/115	-
21	CL7	3B	615	-	2/2/12/20	8/19/97/115	-
21	CL7	12	506	-	2/2/15/20	12/37/115/115	-
21	CL7	14	407	-	2/2/10/20	1/8/86/115	-
21	CL7	2B	616	-	2/2/12/20	8/19/97/115	-
21	CL7	41	407	-	2/2/10/20	2/8/86/115	-
24	LMG	2D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	34	416	-	2/2/10/20	5/8/86/115	-
21	CL7	31	410	-	2/2/15/20	15/37/115/115	-
21	CL7	13	504	-	2/2/15/20	14/37/115/115	-
21	CL7	14	410	-	2/2/11/20	7/13/91/115	-
27	DGD	1B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	12	510	16	2/2/15/20	20/37/115/115	-
21	CL7	14	405	-	2/2/15/20	16/37/115/115	-
21	CL7	44	410	-	2/2/11/20	7/13/91/115	-
21	CL7	41	411	-	2/2/11/20	5/13/91/115	-
23	8CT	4B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	24	417	20	2/2/10/20	4/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	1D	410	-	-	6/28/48/70	0/1/1/1
32	ZEX	42	524	-	-	11/29/67/67	0/2/2/2
30	PL9	3D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	22	507	-	2/2/15/20	18/37/115/115	-
21	CL7	23	418	19	2/2/12/20	7/19/97/115	-
32	ZEX	31	422	-	-	6/29/67/67	0/2/2/2
21	CL7	1C	512	-	2/2/10/20	2/8/86/115	-
21	CL7	14	417	20	2/2/10/20	4/10/88/115	-
21	CL7	11	419	-	2/2/11/20	7/13/91/115	-
21	CL7	1C	511	3	2/2/10/20	3/10/88/115	-
21	CL7	13	502	-	2/2/13/20	10/29/107/115	-
27	DGD	2C	516	-	-	9/51/91/95	0/2/2/2
27	DGD	3B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	12	507	-	2/2/15/20	18/37/115/115	-
21	CL7	22	503	-	2/2/15/20	17/37/115/115	-
21	CL7	4B	611	-	2/2/15/20	11/37/115/115	-
23	8CT	4B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	32	510	16	2/2/15/20	20/37/115/115	-
32	ZEX	12	522	-	-	6/29/67/67	0/2/2/2
21	CL7	4A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	33	507	-	2/2/15/20	13/37/115/115	-
21	CL7	21	403	-	2/2/14/20	9/31/109/115	-
21	CL7	31	407	-	2/2/10/20	2/8/86/115	-
26	LHG	43	425	-	-	3/40/40/53	-
21	CL7	34	414	-	2/2/12/20	6/23/101/115	-
21	CL7	1C	509	-	2/2/15/20	18/37/115/115	-
30	PL9	2D	407	-	-	9/53/73/73	0/1/1/1
32	ZEX	34	420	-	-	12/29/67/67	0/2/2/2
21	CL7	22	518	16	2/2/15/20	10/37/115/115	-
21	CL7	31	419	-	2/2/11/20	7/13/91/115	-
22	PHO	3D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	31	412	-	2/2/11/20	8/13/91/115	-
21	CL7	34	408	-	2/2/11/20	2/13/91/115	-
25	SQD	43	422	-	-	3/41/61/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2C	505	-	2/2/15/20	14/37/115/115	-
21	CL7	1B	615	-	2/2/12/20	8/19/97/115	-
23	8CT	3B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	11	402	-	2/2/14/20	14/31/109/115	-
21	CL7	2B	605	-	2/2/15/20	15/37/115/115	-
25	SQD	32	521	-	-	7/45/65/69	0/1/1/1
21	CL7	44	414	-	2/2/12/20	6/23/101/115	-
21	CL7	3B	608	-	2/2/15/20	15/37/115/115	-
21	CL7	41	410	-	2/2/15/20	15/37/115/115	-
21	CL7	41	419	-	2/2/11/20	7/13/91/115	-
31	HEM	4F	101	-	-	6/12/54/54	-
21	CL7	23	410	-	2/2/15/20	15/37/115/115	-
21	CL7	2C	517	-	2/2/10/20	3/8/86/115	-
21	CL7	4B	609	-	2/2/15/20	15/37/115/115	-
21	CL7	2D	402	-	2/2/12/20	7/19/97/115	-

The worst 5 of 6635 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2B	601	8CT	C02-C03	14.85	1.60	1.34
23	1B	626	8CT	C02-C03	14.83	1.60	1.34
23	4B	619	8CT	C02-C03	14.82	1.60	1.34
23	4B	601	8CT	C02-C03	14.80	1.60	1.34
23	3B	626	8CT	C02-C03	14.80	1.60	1.34

The worst 5 of 8780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1A	403	CL7	C3C-C4C-NC	10.55	117.82	110.18
21	2A	403	CL7	C3C-C4C-NC	10.52	117.81	110.18
21	3A	403	CL7	C3C-C4C-NC	10.51	117.80	110.18
21	4A	403	CL7	C3C-C4C-NC	10.50	117.78	110.18
21	33	505	CL7	C3C-C4C-NC	10.30	117.64	110.18

5 of 860 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1A	401	CL7	NA

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Mol	Chain	Res	Type	Atom
21	1A	401	CL7	NC
21	1A	403	CL7	NA
21	1A	403	CL7	NC
21	1A	407	CL7	NA

5 of 5870 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1A	403	CL7	O1A-CGA-O2A-C1
21	1A	403	CL7	CBA-CGA-O2A-C1
21	1A	403	CL7	C1A-C2A-CAA-CBA
21	1A	403	CL7	C3A-C2A-CAA-CBA
21	1A	407	CL7	C1A-C2A-CAA-CBA

There are no ring outliers.

552 monomers are involved in 2778 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	34	417	CL7	5	0
21	4B	614	CL7	2	0
21	12	515	CL7	2	0
25	1A	406	SQD	3	0
27	1C	516	DGD	5	0
21	24	414	CL7	4	0
21	22	506	CL7	4	0
21	23	409	CL7	14	0
21	23	416	CL7	3	0
21	1C	517	CL7	1	0
21	2C	504	CL7	4	0
21	33	516	CL7	6	0
23	3C	515	8CT	1	0
32	21	422	ZEX	20	0
21	42	518	CL7	11	0
21	1B	607	CL7	8	0
32	24	419	ZEX	7	0
21	43	411	CL7	8	0
21	24	412	CL7	4	0
21	4B	613	CL7	6	0
22	4A	402	PHO	5	0
21	2B	604	CL7	9	0
21	2B	606	CL7	7	0
21	3D	404	CL7	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	43	407	CL7	5	0
24	4B	622	LMG	6	0
26	14	401	LHG	1	0
21	3B	613	CL7	2	0
21	42	507	CL7	6	0
26	4A	408	LHG	1	0
21	43	414	CL7	13	0
31	1F	101	HEM	3	0
21	32	513	CL7	6	0
21	31	420	CL7	6	0
21	3D	405	CL7	2	0
21	31	408	CL7	7	0
21	24	409	CL7	3	0
21	4B	616	CL7	4	0
21	12	504	CL7	2	0
21	14	404	CL7	6	0
25	43	424	SQD	2	0
23	1C	515	8CT	1	0
21	2D	404	CL7	8	0
21	11	403	CL7	5	0
21	1B	602	CL7	5	0
21	12	502	CL7	8	0
21	2C	509	CL7	3	0
21	2B	613	CL7	5	0
21	2B	609	CL7	4	0
21	42	517	CL7	11	0
31	2F	101	HEM	4	0
21	3A	407	CL7	15	0
21	4B	607	CL7	4	0
21	3C	507	CL7	4	0
21	12	518	CL7	12	0
21	4C	502	CL7	3	0
27	3C	516	DGD	4	0
21	23	411	CL7	6	0
21	3C	510	CL7	5	0
21	44	409	CL7	3	0
24	3D	410	LMG	1	0
21	3B	610	CL7	1	0
21	14	406	CL7	13	0
32	24	403	ZEX	22	0
21	21	420	CL7	5	0
25	33	521	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	23	408	CL7	9	0
21	32	507	CL7	6	0
21	21	406	CL7	14	0
32	33	522	ZEX	26	0
21	11	416	CL7	2	0
21	2C	508	CL7	5	0
21	23	403	CL7	7	0
21	21	409	CL7	4	0
21	4C	512	CL7	1	0
21	32	506	CL7	3	0
21	31	402	CL7	9	0
21	31	405	CL7	5	0
21	1A	403	CL7	2	0
21	1C	513	CL7	3	0
21	14	409	CL7	3	0
21	43	410	CL7	8	0
32	13	522	ZEX	27	0
21	3C	513	CL7	3	0
21	43	416	CL7	3	0
21	1B	603	CL7	7	0
21	41	405	CL7	4	0
21	14	413	CL7	6	0
21	41	402	CL7	9	0
32	13	525	ZEX	24	0
21	22	515	CL7	2	0
32	11	421	ZEX	14	0
21	13	506	CL7	5	0
21	24	408	CL7	4	0
21	1A	407	CL7	16	0
21	44	413	CL7	5	0
23	2C	515	8CT	1	0
21	3B	602	CL7	4	0
21	12	505	CL7	15	0
21	3C	506	CL7	5	0
21	1A	401	CL7	20	0
21	42	509	CL7	9	0
21	24	407	CL7	10	0
21	21	408	CL7	7	0
21	33	502	CL7	7	0
21	23	417	CL7	6	0
32	12	519	ZEX	4	0
21	24	405	CL7	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2C	513	CL7	3	0
21	3D	402	CL7	3	0
21	12	508	CL7	4	0
21	14	408	CL7	4	0
32	31	421	ZEX	15	0
25	33	523	SQD	1	0
21	4B	608	CL7	8	0
21	41	408	CL7	8	0
21	2A	403	CL7	2	0
21	12	512	CL7	9	0
31	3F	101	HEM	3	0
21	13	501	CL7	8	0
21	3C	512	CL7	2	0
25	23	422	SQD	4	0
26	3B	625	LHG	1	0
21	3C	501	CL7	3	0
21	2B	610	CL7	5	0
21	1B	614	CL7	2	0
21	4C	505	CL7	6	0
21	43	419	CL7	4	0
26	3B	623	LHG	6	0
21	24	415	CL7	4	0
21	1C	503	CL7	6	0
26	3A	408	LHG	1	0
26	33	524	LHG	1	0
21	11	405	CL7	4	0
26	3D	409	LHG	3	0
21	3C	508	CL7	4	0
21	3B	605	CL7	6	0
21	2C	507	CL7	5	0
24	2B	622	LMG	5	0
21	13	503	CL7	10	0
21	1C	501	CL7	3	0
21	41	416	CL7	2	0
21	1B	609	CL7	5	0
21	4C	508	CL7	6	0
26	4D	409	LHG	3	0
21	4C	509	CL7	4	0
25	2B	621	SQD	2	0
21	2C	506	CL7	4	0
32	43	423	ZEX	28	0
21	43	417	CL7	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	11	401	LMG	2	0
26	2D	409	LHG	4	0
21	4B	603	CL7	3	0
21	2A	401	CL7	20	0
25	3B	620	SQD	2	0
32	22	522	ZEX	17	0
21	23	419	CL7	4	0
21	1B	616	CL7	1	0
21	33	511	CL7	7	0
21	44	407	CL7	10	0
21	3B	607	CL7	8	0
21	32	511	CL7	9	0
21	42	513	CL7	6	0
32	41	421	ZEX	15	0
21	2C	512	CL7	1	0
21	33	517	CL7	3	0
32	44	418	ZEX	11	0
26	4B	624	LHG	6	0
21	3A	403	CL7	2	0
21	41	404	CL7	9	0
24	31	401	LMG	3	0
21	34	405	CL7	6	0
32	43	421	ZEX	13	0
32	33	525	ZEX	24	0
23	4C	515	8CT	1	0
21	4C	511	CL7	2	0
21	4C	513	CL7	3	0
24	41	401	LMG	2	0
26	24	401	LHG	1	0
21	22	516	CL7	7	0
21	12	513	CL7	6	0
21	4B	604	CL7	8	0
27	2B	625	DGD	2	0
27	4C	516	DGD	3	0
21	22	505	CL7	17	0
21	33	518	CL7	4	0
21	3C	504	CL7	4	0
21	24	404	CL7	6	0
21	14	411	CL7	6	0
21	3A	401	CL7	21	0
21	34	415	CL7	4	0
32	43	401	ZEX	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	23	420	ZEX	17	0
25	3A	406	SQD	1	0
21	22	513	CL7	6	0
21	2C	501	CL7	4	0
21	3B	603	CL7	6	0
21	1B	605	CL7	7	0
21	22	501	CL7	8	0
21	32	501	CL7	7	0
25	2A	406	SQD	3	0
25	13	523	SQD	2	0
30	1D	407	PL9	7	0
21	31	403	CL7	6	0
26	1D	409	LHG	3	0
21	44	408	CL7	4	0
21	13	514	CL7	2	0
21	41	406	CL7	15	0
21	44	404	CL7	6	0
21	11	412	CL7	3	0
24	1A	405	LMG	2	0
21	13	515	CL7	3	0
21	42	506	CL7	3	0
26	23	425	LHG	1	0
21	2C	502	CL7	4	0
21	22	508	CL7	4	0
21	13	511	CL7	6	0
21	4C	506	CL7	5	0
21	4C	507	CL7	3	0
21	42	510	CL7	7	0
21	43	415	CL7	2	0
32	21	421	ZEX	16	0
21	12	501	CL7	6	0
21	44	405	CL7	7	0
32	22	519	ZEX	4	0
21	11	411	CL7	3	0
21	34	406	CL7	13	0
32	24	420	ZEX	12	0
21	1B	613	CL7	2	0
21	1B	606	CL7	5	0
21	31	404	CL7	9	0
32	22	524	ZEX	16	0
21	42	502	CL7	8	0
24	2A	405	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	13	516	CL7	6	0
21	41	412	CL7	3	0
24	4A	405	LMG	2	0
27	4B	625	DGD	2	0
21	33	505	CL7	19	0
26	2A	408	LHG	1	0
21	22	502	CL7	8	0
32	33	520	ZEX	13	0
21	41	420	CL7	5	0
21	43	412	CL7	6	0
21	42	503	CL7	7	0
26	2B	624	LHG	6	0
21	1C	507	CL7	5	0
21	23	415	CL7	2	0
21	22	514	CL7	2	0
21	4C	501	CL7	3	0
26	13	524	LHG	1	0
32	13	519	ZEX	16	0
21	23	402	CL7	10	0
22	2D	408	PHO	4	0
21	3B	614	CL7	2	0
32	12	524	ZEX	16	0
21	4C	504	CL7	4	0
21	13	517	CL7	3	0
21	3C	509	CL7	5	0
32	32	519	ZEX	5	0
21	41	403	CL7	6	0
21	4D	405	CL7	2	0
21	3C	502	CL7	3	0
21	32	514	CL7	2	0
21	42	501	CL7	7	0
32	42	522	ZEX	18	0
21	1B	608	CL7	4	0
21	33	515	CL7	3	0
22	1A	402	PHO	5	0
21	32	515	CL7	1	0
32	32	522	ZEX	17	0
32	43	420	ZEX	17	0
21	3B	604	CL7	10	0
25	4A	406	SQD	2	0
21	33	501	CL7	8	0
21	11	406	CL7	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	13	510	CL7	8	0
26	34	401	LHG	1	0
21	13	518	CL7	4	0
21	31	413	CL7	5	0
21	11	404	CL7	8	0
21	3C	503	CL7	7	0
21	4B	615	CL7	2	0
32	14	403	ZEX	22	0
32	12	520	ZEX	31	0
21	21	405	CL7	4	0
21	12	517	CL7	9	0
21	24	410	CL7	2	0
24	4D	410	LMG	1	0
21	3B	616	CL7	1	0
21	1D	402	CL7	3	0
21	4B	610	CL7	5	0
32	41	422	ZEX	22	0
21	23	413	CL7	7	0
21	11	409	CL7	3	0
21	12	514	CL7	2	0
21	2B	617	CL7	1	0
21	22	512	CL7	10	0
21	1C	510	CL7	5	0
24	1B	621	LMG	5	0
22	4D	408	PHO	4	0
21	43	405	CL7	10	0
21	21	402	CL7	9	0
25	22	521	SQD	2	0
32	23	421	ZEX	12	0
21	11	413	CL7	5	0
21	1B	610	CL7	4	0
21	2B	608	CL7	7	0
32	14	419	ZEX	8	0
21	31	418	CL7	8	0
22	1D	408	PHO	5	0
21	11	418	CL7	7	0
21	21	418	CL7	8	0
21	1B	612	CL7	3	0
21	21	412	CL7	3	0
21	11	420	CL7	6	0
21	1C	502	CL7	4	0
21	24	413	CL7	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	21	417	CL7	6	0
21	1C	504	CL7	4	0
21	3C	505	CL7	5	0
21	2D	405	CL7	2	0
21	41	418	CL7	7	0
25	1B	620	SQD	3	0
25	4B	621	SQD	3	0
25	13	521	SQD	4	0
21	33	506	CL7	5	0
21	34	412	CL7	5	0
21	41	417	CL7	7	0
21	1B	611	CL7	4	0
22	2A	402	PHO	5	0
21	3B	612	CL7	3	0
21	33	503	CL7	10	0
21	33	510	CL7	7	0
21	2B	615	CL7	2	0
21	22	511	CL7	8	0
21	23	414	CL7	12	0
21	41	413	CL7	5	0
21	23	406	CL7	18	0
21	33	508	CL7	14	0
26	4B	626	LHG	2	0
21	21	414	CL7	7	0
32	11	422	ZEX	20	0
25	42	521	SQD	2	0
21	32	508	CL7	4	0
21	23	404	CL7	11	0
21	2C	510	CL7	5	0
32	13	520	ZEX	13	0
21	31	406	CL7	13	0
32	24	418	ZEX	12	0
21	42	515	CL7	1	0
21	43	402	CL7	9	0
21	23	412	CL7	6	0
21	41	414	CL7	2	0
21	1B	601	CL7	1	0
24	3B	621	LMG	6	0
21	31	409	CL7	3	0
21	34	411	CL7	7	0
32	14	418	ZEX	11	0
21	31	416	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4B	617	CL7	1	0
21	3C	511	CL7	2	0
32	32	524	ZEX	17	0
32	23	423	ZEX	27	0
26	1A	408	LHG	1	0
21	21	407	CL7	2	0
30	4D	407	PL9	7	0
21	42	514	CL7	2	0
21	34	407	CL7	10	0
21	1B	604	CL7	10	0
21	2B	611	CL7	4	0
21	2C	503	CL7	6	0
21	3B	609	CL7	4	0
21	11	417	CL7	4	0
21	32	503	CL7	9	0
21	32	518	CL7	11	0
21	4D	402	CL7	3	0
21	4A	407	CL7	14	0
21	33	513	CL7	12	0
26	44	401	LHG	1	0
21	1D	405	CL7	2	0
21	4B	605	CL7	9	0
21	2B	607	CL7	6	0
21	14	414	CL7	5	0
21	4A	401	CL7	20	0
21	22	509	CL7	6	0
21	1C	505	CL7	6	0
21	1C	508	CL7	4	0
21	21	410	CL7	6	0
21	43	408	CL7	10	0
21	11	414	CL7	2	0
21	21	416	CL7	2	0
21	21	404	CL7	9	0
21	33	504	CL7	10	0
21	43	404	CL7	11	0
21	43	403	CL7	8	0
21	22	504	CL7	2	0
21	32	504	CL7	2	0
21	12	503	CL7	8	0
21	31	411	CL7	3	0
21	12	511	CL7	8	0
21	14	415	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4B	602	CL7	1	0
21	44	415	CL7	4	0
32	22	520	ZEX	28	0
32	32	520	ZEX	29	0
21	11	408	CL7	7	0
21	34	404	CL7	5	0
21	2B	602	CL7	1	0
21	43	409	CL7	14	0
21	24	406	CL7	13	0
26	1B	623	LHG	6	0
21	12	509	CL7	7	0
21	13	509	CL7	9	0
21	3C	517	CL7	1	0
21	21	413	CL7	5	0
21	2A	407	CL7	14	0
21	22	517	CL7	10	0
21	3B	611	CL7	5	0
21	32	517	CL7	11	0
21	4C	510	CL7	4	0
21	34	409	CL7	3	0
21	2B	603	CL7	4	0
21	42	512	CL7	9	0
32	34	403	ZEX	21	0
21	42	511	CL7	7	0
21	3B	606	CL7	5	0
21	4D	404	CL7	8	0
21	44	412	CL7	3	0
21	33	512	CL7	7	0
21	14	412	CL7	4	0
21	11	407	CL7	3	0
32	33	519	ZEX	17	0
21	34	413	CL7	5	0
21	43	406	CL7	19	0
21	44	417	CL7	5	0
24	3A	405	LMG	2	0
21	33	509	CL7	8	0
21	24	411	CL7	6	0
21	4C	517	CL7	1	0
21	44	406	CL7	12	0
32	42	520	ZEX	30	0
21	13	508	CL7	15	0
21	13	505	CL7	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	33	514	CL7	2	0
21	43	413	CL7	8	0
21	4C	503	CL7	7	0
32	34	419	ZEX	8	0
21	13	513	CL7	12	0
21	32	505	CL7	15	0
21	23	405	CL7	9	0
21	12	516	CL7	6	0
21	1D	404	CL7	7	0
21	41	409	CL7	4	0
21	4B	606	CL7	6	0
32	34	418	ZEX	11	0
22	3A	402	PHO	5	0
26	2B	626	LHG	2	0
21	42	504	CL7	2	0
21	2C	511	CL7	2	0
32	23	401	ZEX	24	0
21	13	507	CL7	10	0
32	44	420	ZEX	12	0
21	4B	612	CL7	4	0
32	44	419	ZEX	9	0
25	23	424	SQD	2	0
21	32	512	CL7	9	0
21	31	417	CL7	4	0
32	14	420	ZEX	10	0
25	12	521	SQD	2	0
21	11	410	CL7	7	0
24	21	401	LMG	2	0
21	3B	601	CL7	1	0
21	43	418	CL7	3	0
21	32	509	CL7	7	0
21	44	411	CL7	7	0
21	2B	612	CL7	4	0
21	42	516	CL7	7	0
21	32	502	CL7	9	0
21	42	505	CL7	14	0
26	1B	625	LHG	1	0
21	42	508	CL7	4	0
21	23	407	CL7	5	0
21	32	516	CL7	6	0
21	2B	614	CL7	2	0
21	31	414	CL7	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	22	510	CL7	6	0
21	13	512	CL7	6	0
32	44	403	ZEX	21	0
21	34	410	CL7	2	0
21	21	411	CL7	3	0
32	42	519	ZEX	4	0
21	1C	506	CL7	6	0
21	3B	615	CL7	4	0
21	12	506	CL7	3	0
21	14	407	CL7	10	0
21	2B	616	CL7	4	0
21	41	407	CL7	3	0
24	2D	410	LMG	1	0
21	31	410	CL7	6	0
21	13	504	CL7	9	0
21	14	410	CL7	2	0
27	1B	624	DGD	2	0
21	12	510	CL7	6	0
21	14	405	CL7	6	0
21	44	410	CL7	2	0
21	41	411	CL7	3	0
21	24	417	CL7	5	0
24	1D	410	LMG	1	0
32	42	524	ZEX	17	0
30	3D	407	PL9	7	0
21	22	507	CL7	6	0
21	23	418	CL7	3	0
32	31	422	ZEX	21	0
21	1C	512	CL7	2	0
21	14	417	CL7	5	0
21	1C	511	CL7	2	0
21	13	502	CL7	7	0
27	2C	516	DGD	3	0
27	3B	624	DGD	2	0
21	12	507	CL7	7	0
21	22	503	CL7	5	0
21	4B	611	CL7	2	0
21	32	510	CL7	6	0
32	12	522	ZEX	18	0
21	4A	403	CL7	2	0
21	33	507	CL7	10	0
21	21	403	CL7	6	0

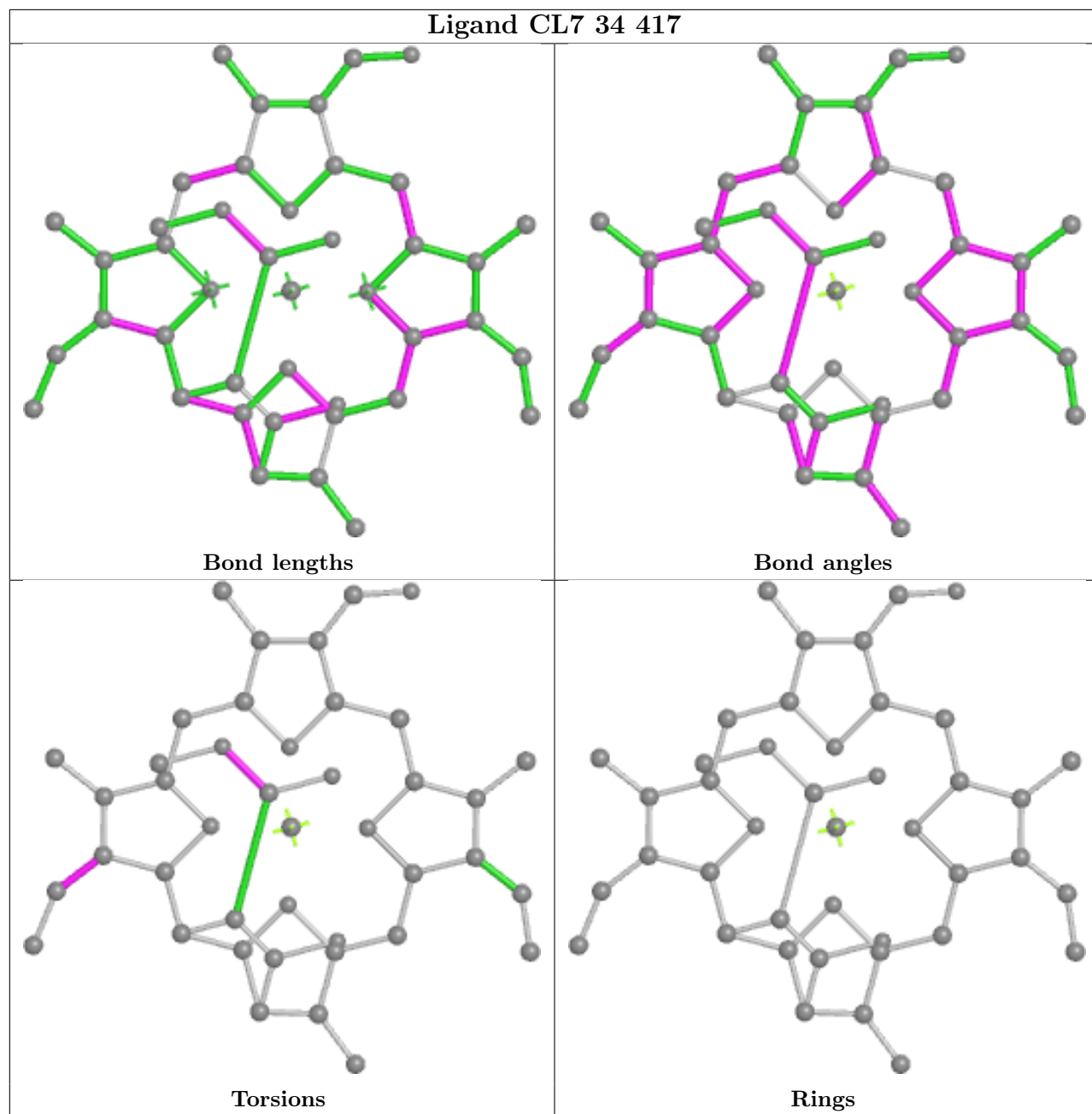
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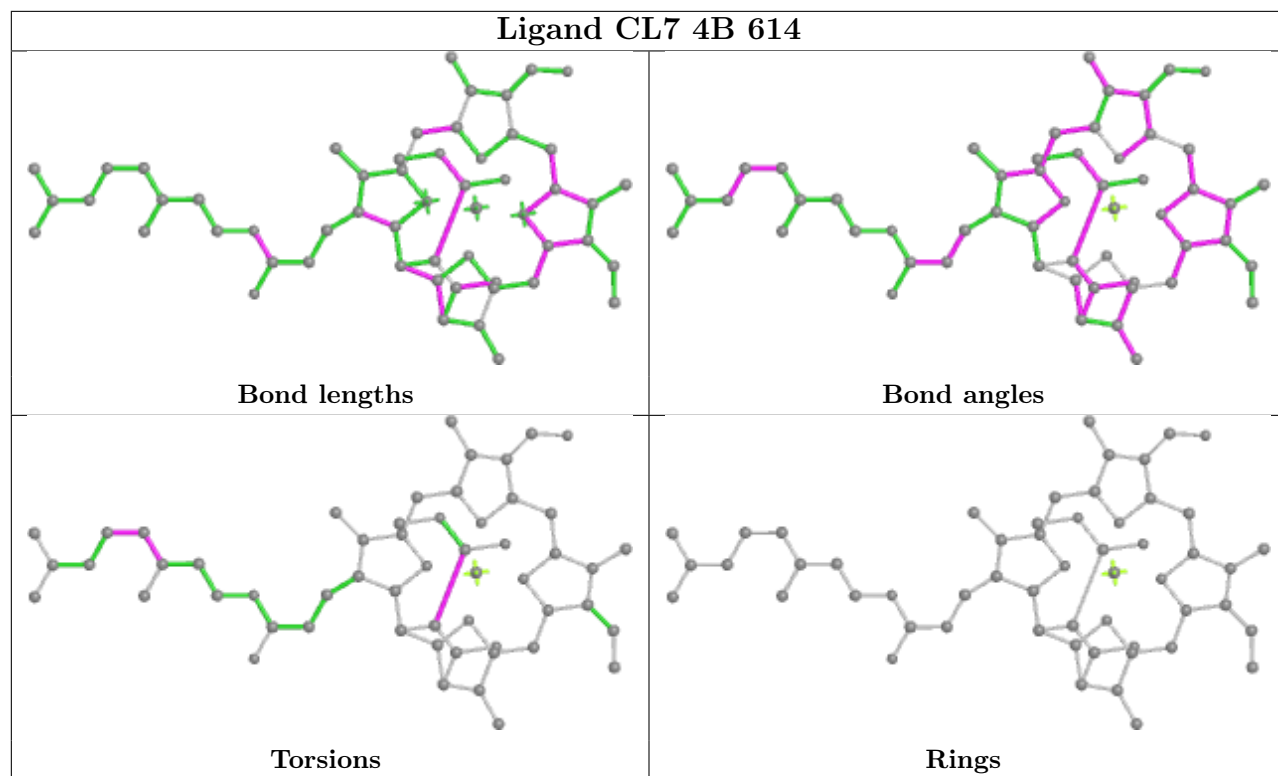
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	407	CL7	3	0
26	43	425	LHG	1	0
21	34	414	CL7	5	0
21	1C	509	CL7	4	0
30	2D	407	PL9	7	0
32	34	420	ZEX	10	0
21	22	518	CL7	12	0
22	3D	408	PHO	5	0
21	31	412	CL7	3	0
21	34	408	CL7	4	0
25	43	422	SQD	3	0
21	2C	505	CL7	6	0
21	1B	615	CL7	4	0
21	11	402	CL7	9	0
21	2B	605	CL7	8	0
25	32	521	SQD	1	0
21	44	414	CL7	5	0
21	3B	608	CL7	4	0
21	41	410	CL7	5	0
31	4F	101	HEM	4	0
21	23	410	CL7	10	0
21	2C	517	CL7	1	0
21	4B	609	CL7	4	0
21	2D	402	CL7	3	0

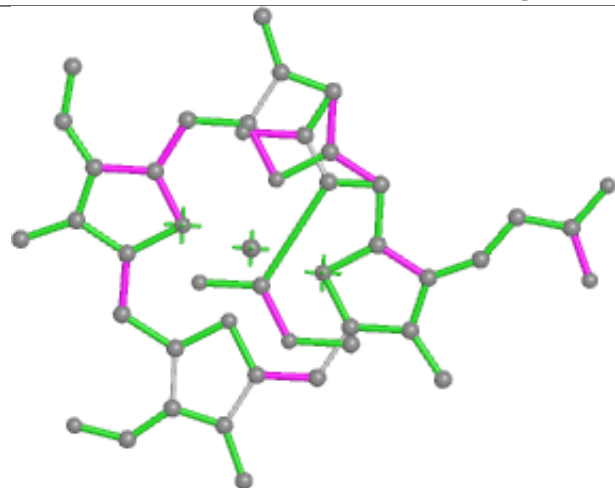
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CL7 34 417

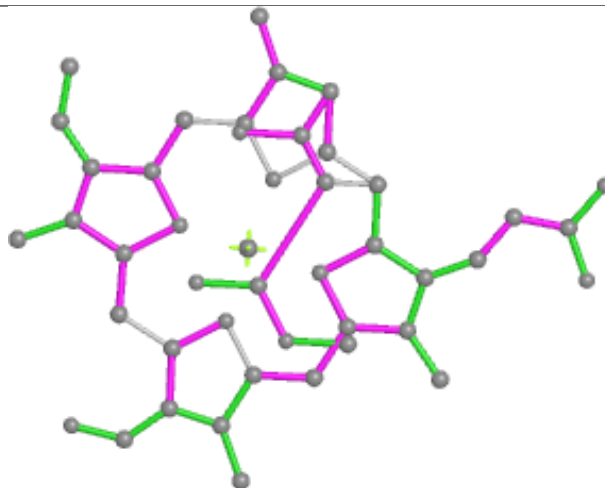




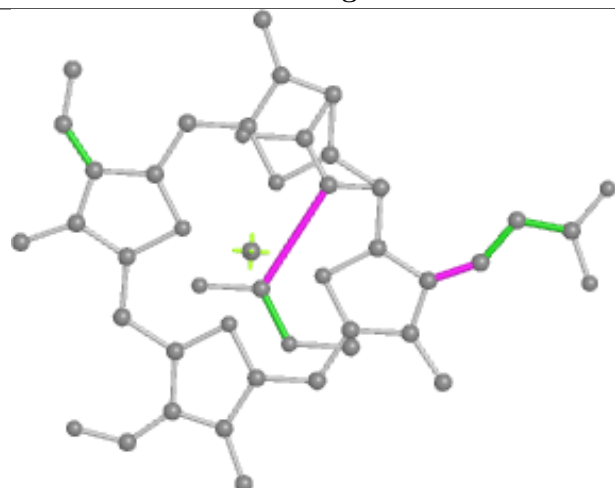
Ligand CL7 12 515



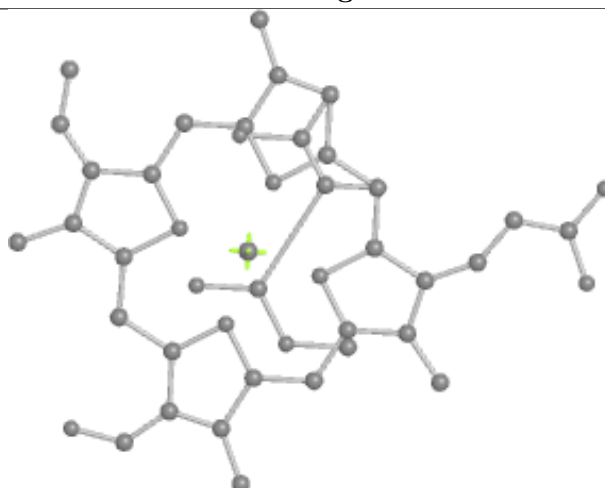
Bond lengths



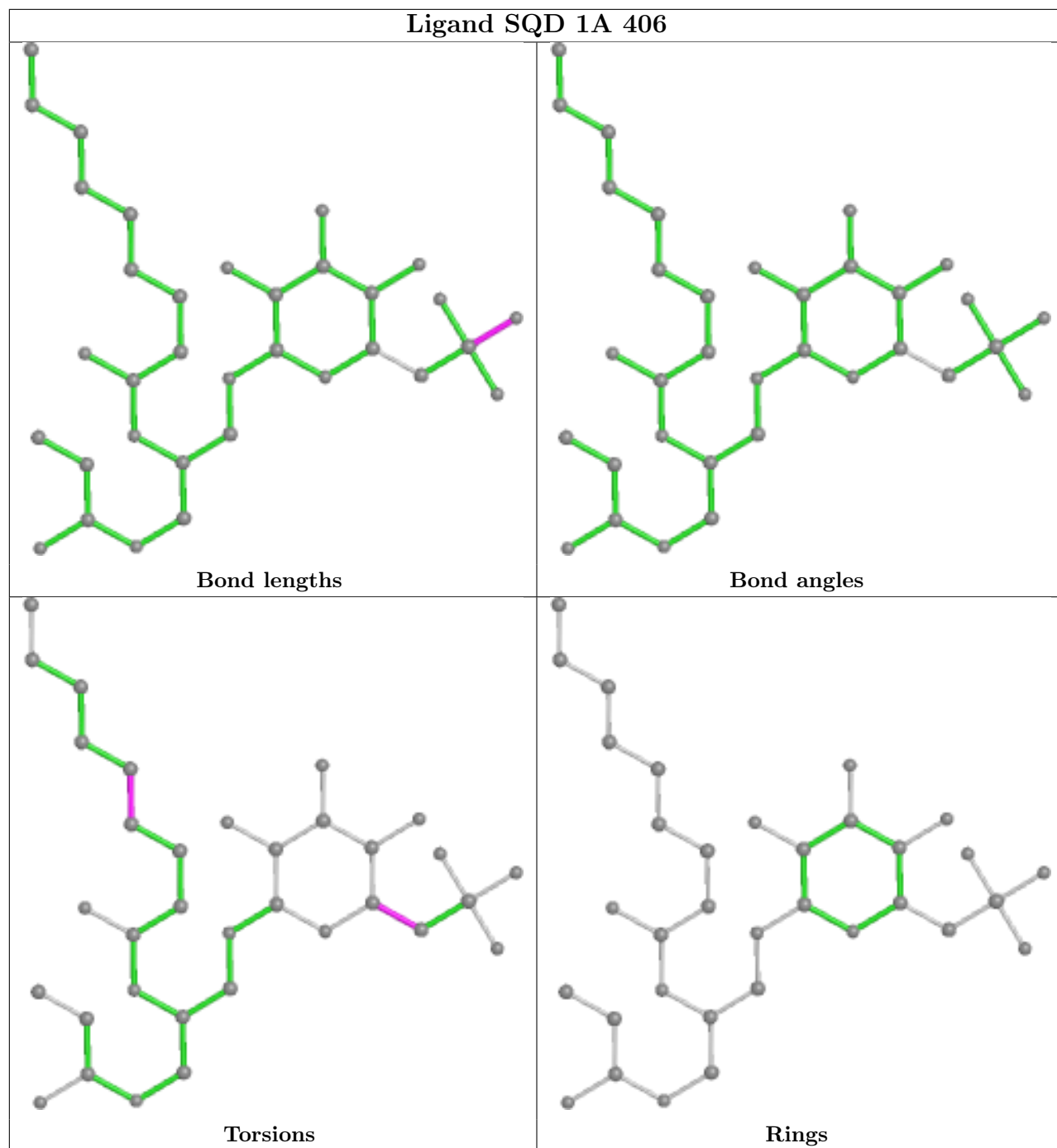
Bond angles

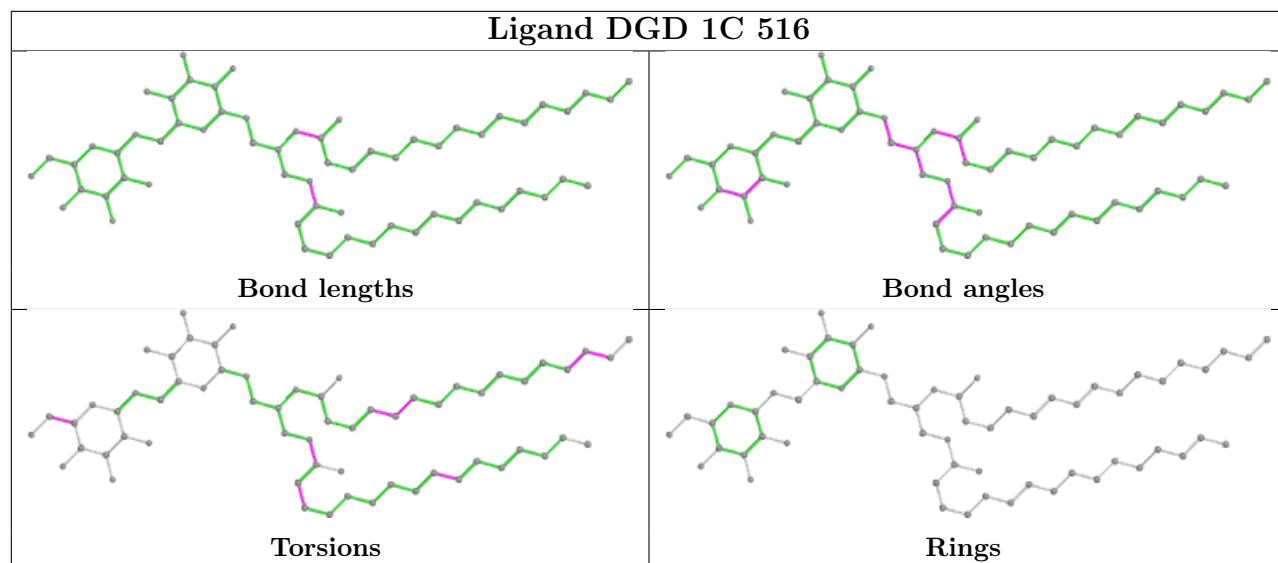
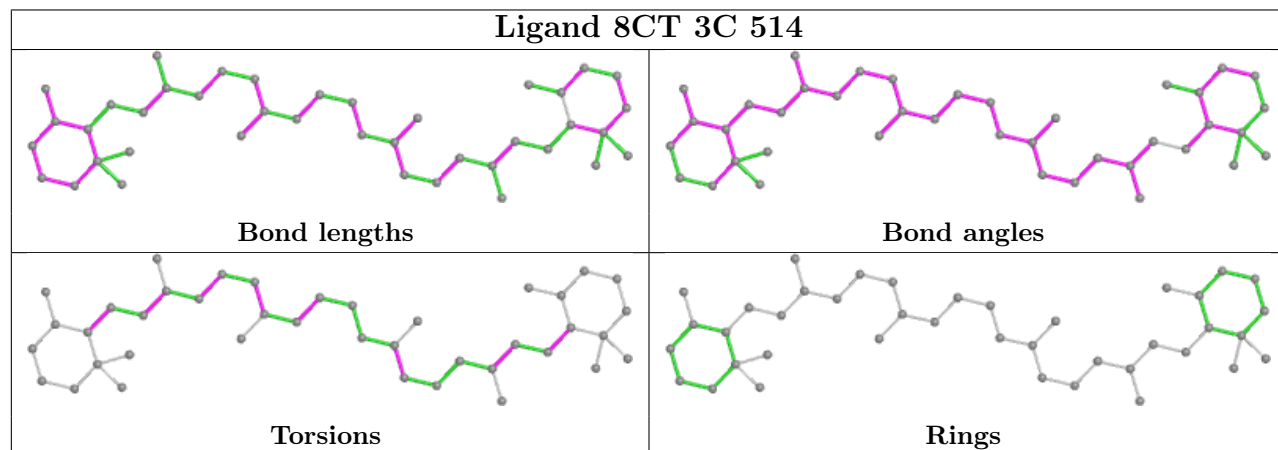


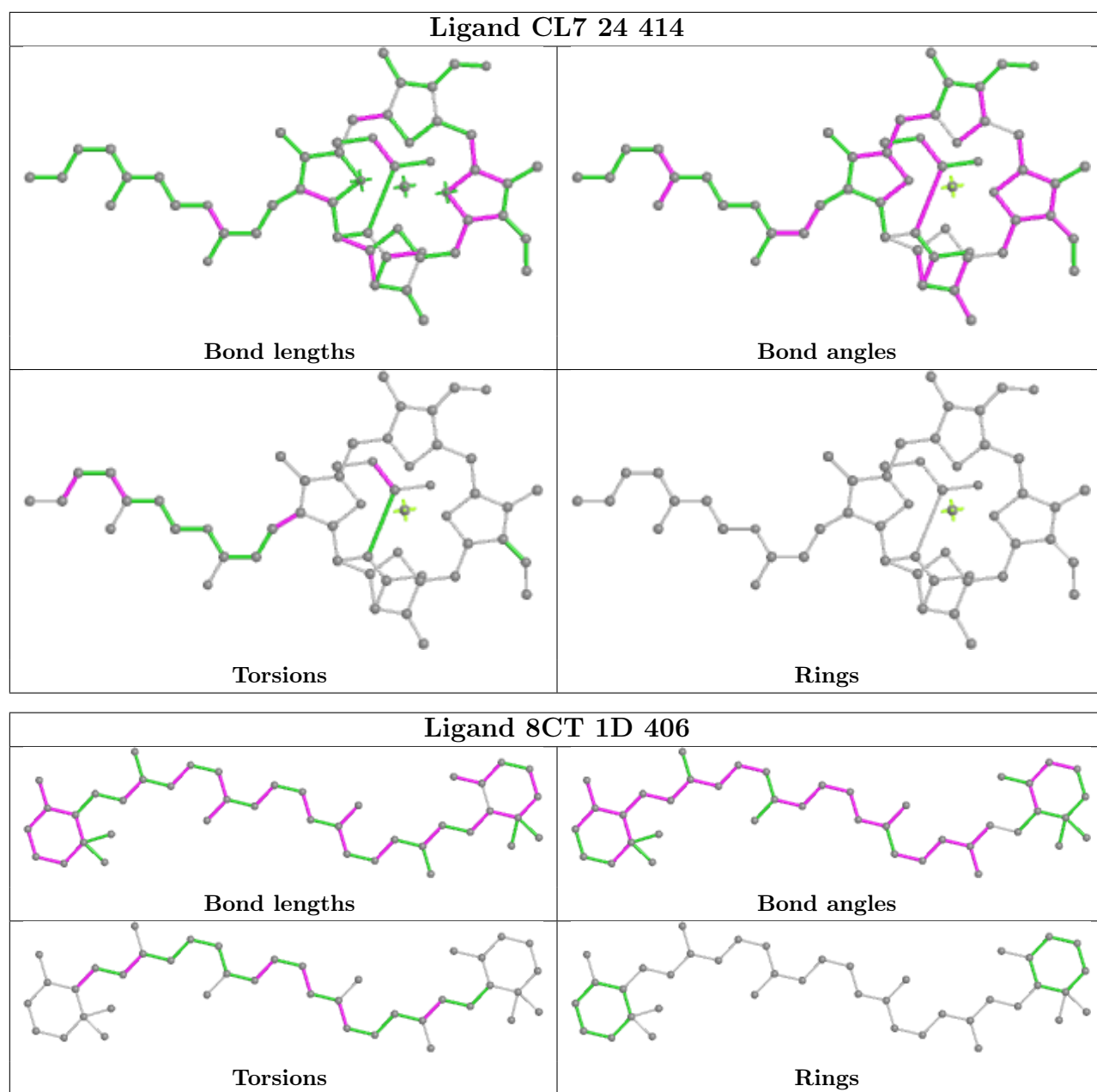
Torsions

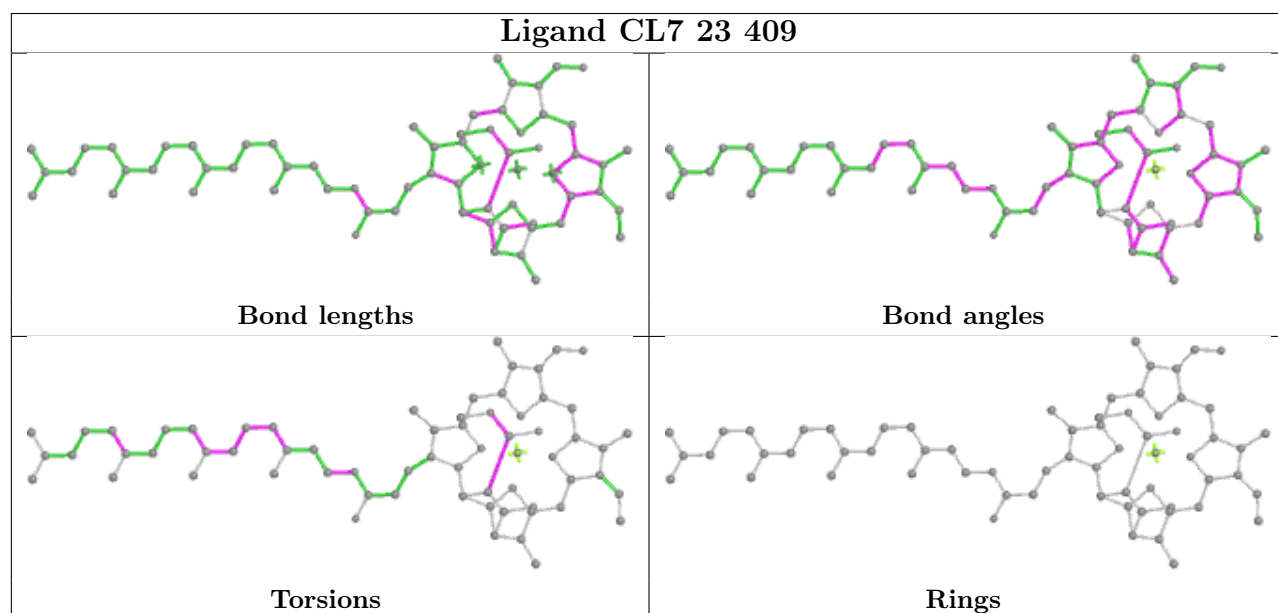
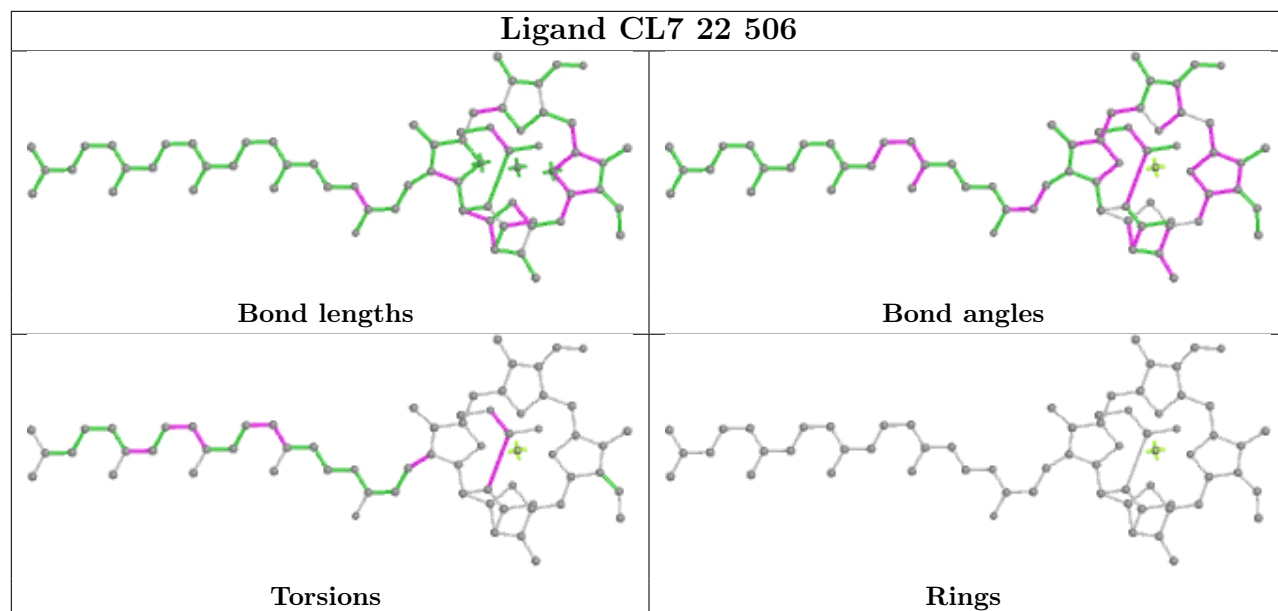


Rings

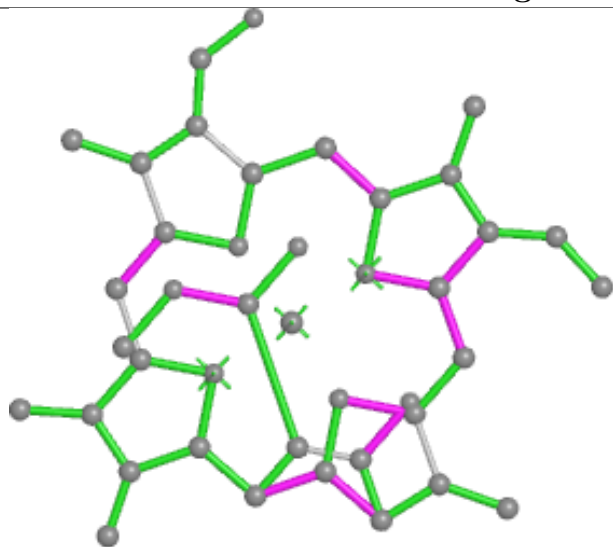


Ligand DGD 1C 516**Ligand 8CT 3C 514**

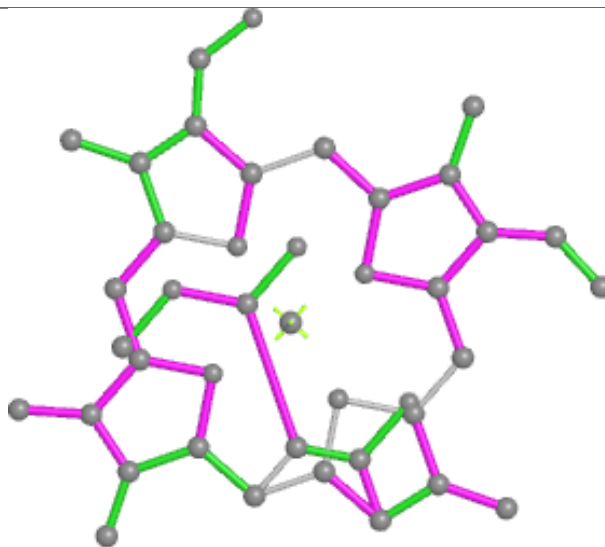




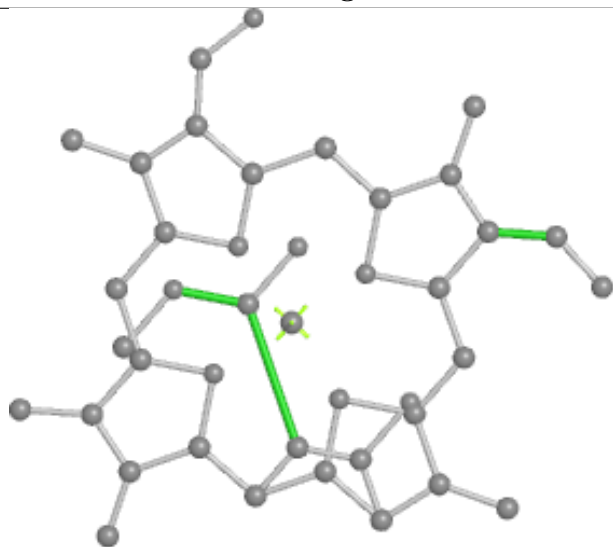
Ligand CL7 23 416



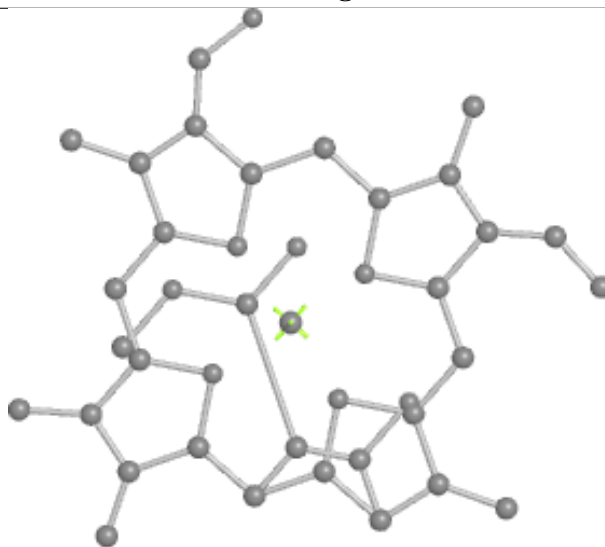
Bond lengths



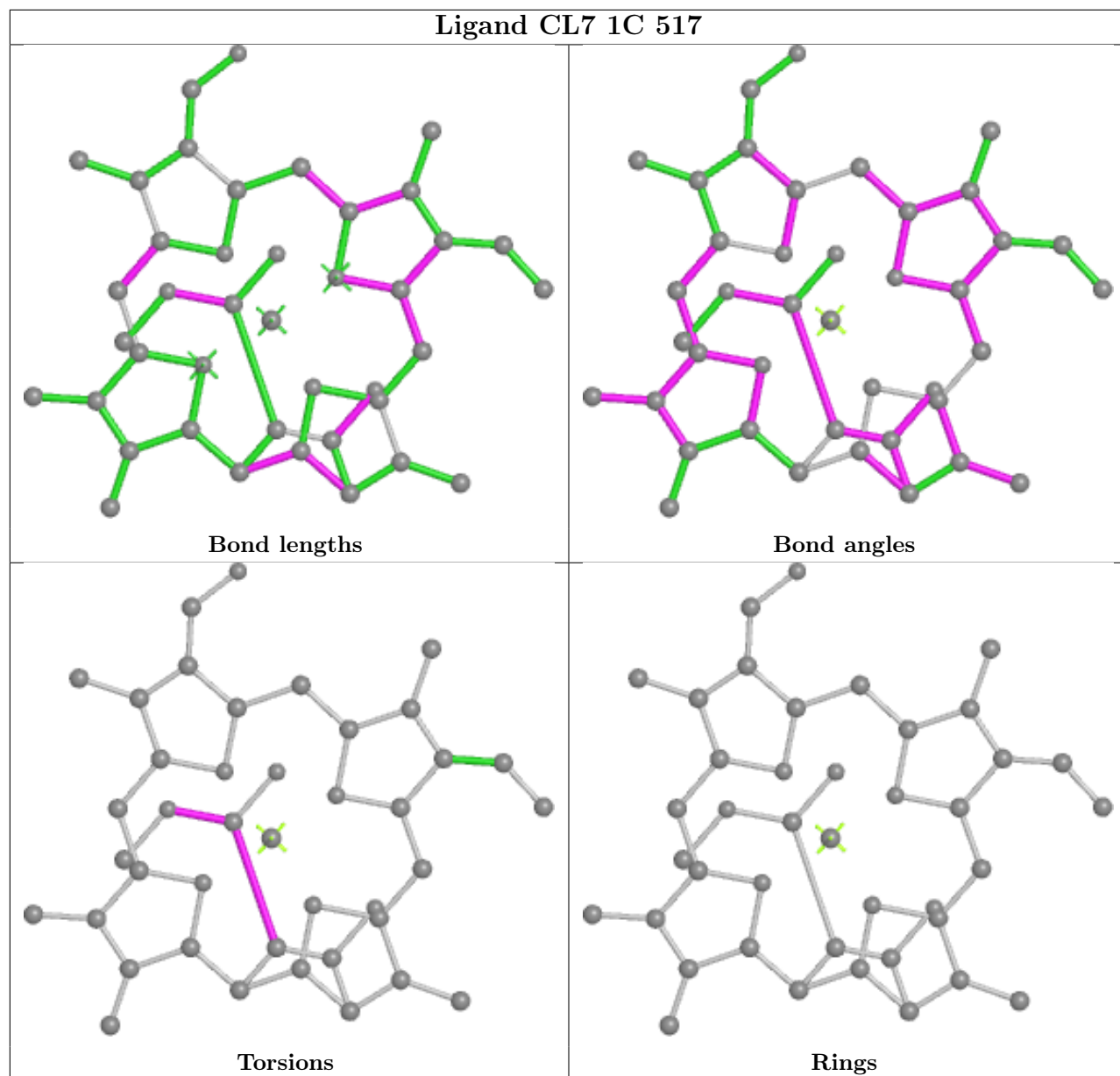
Bond angles

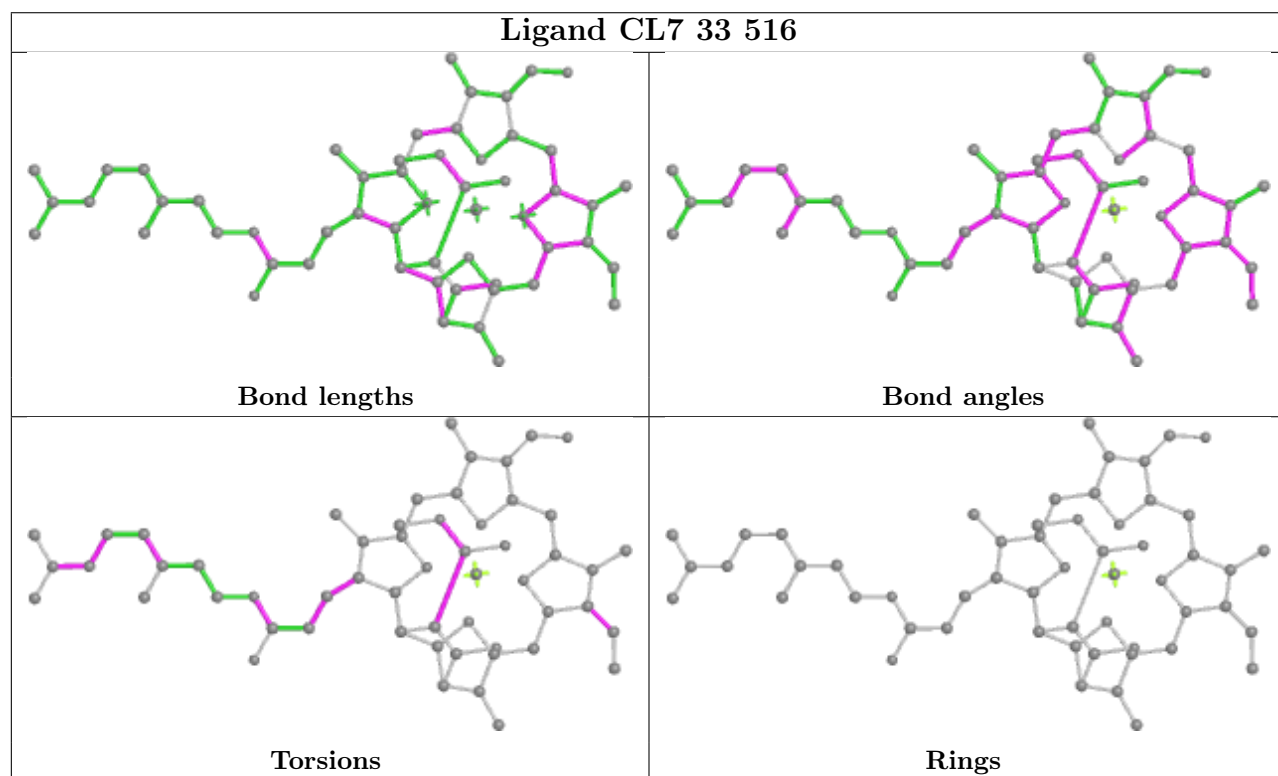
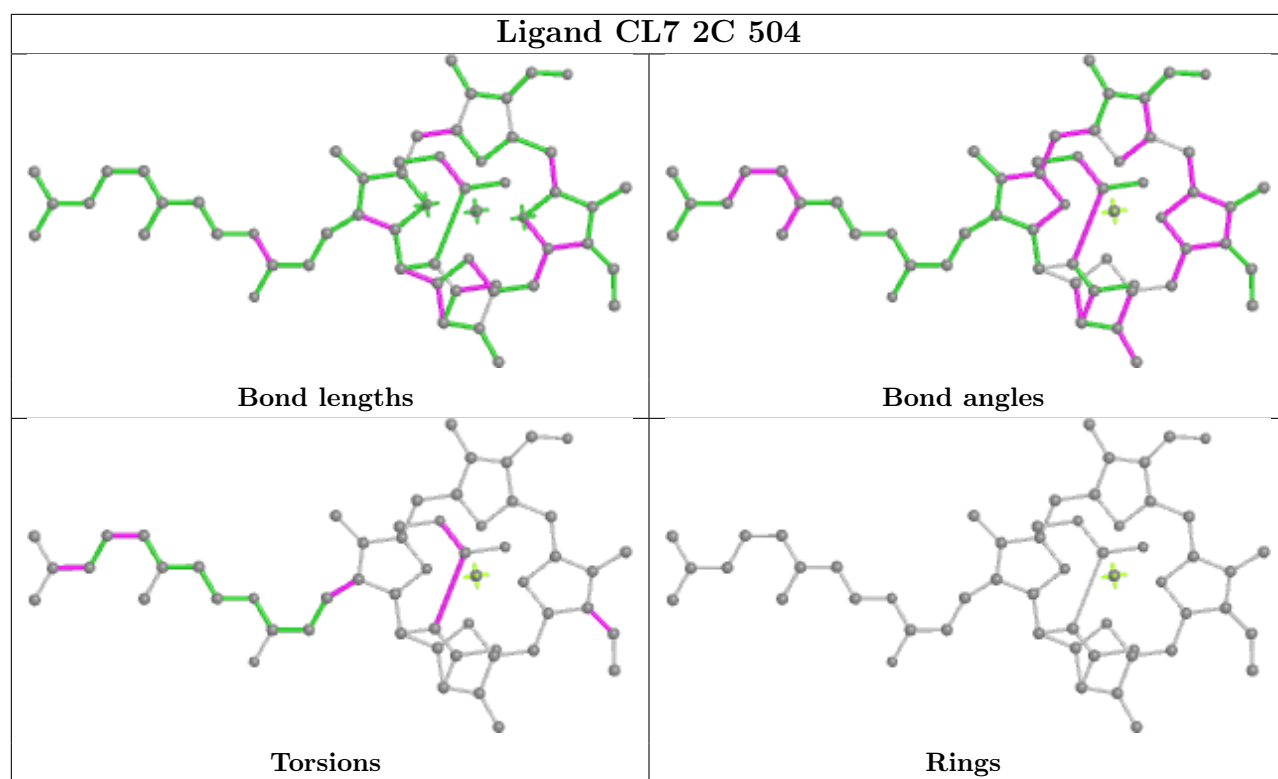


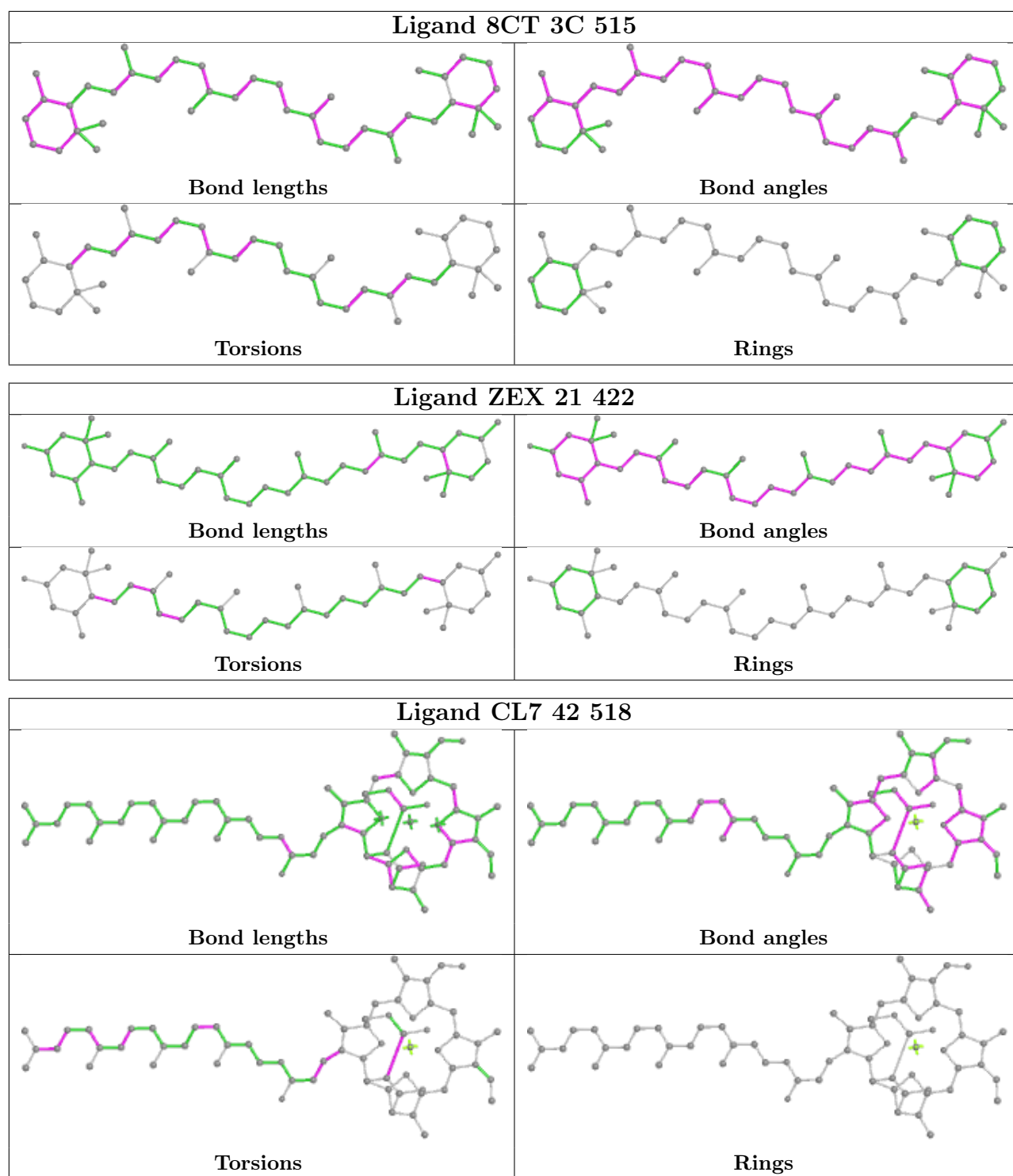
Torsions

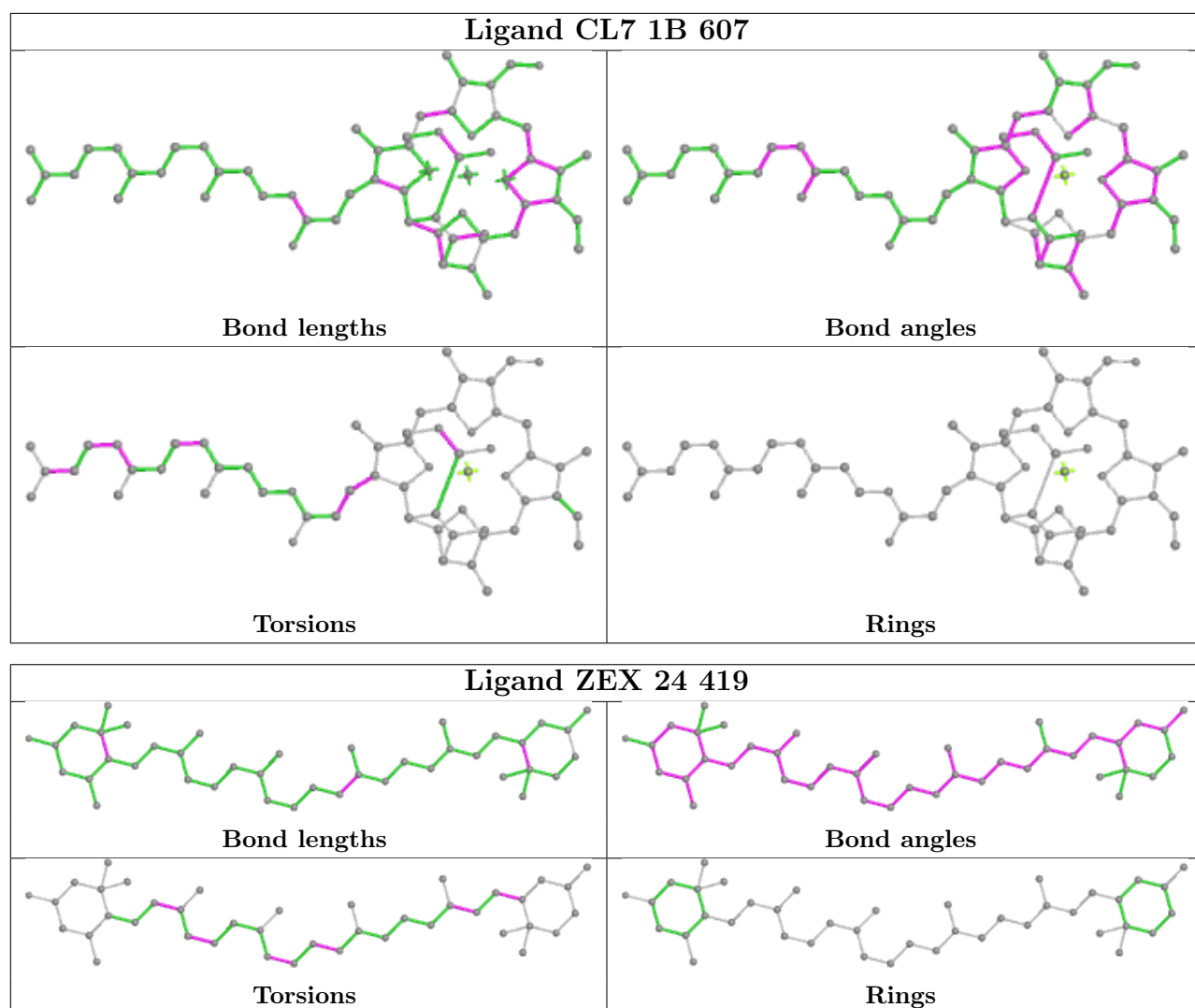


Rings

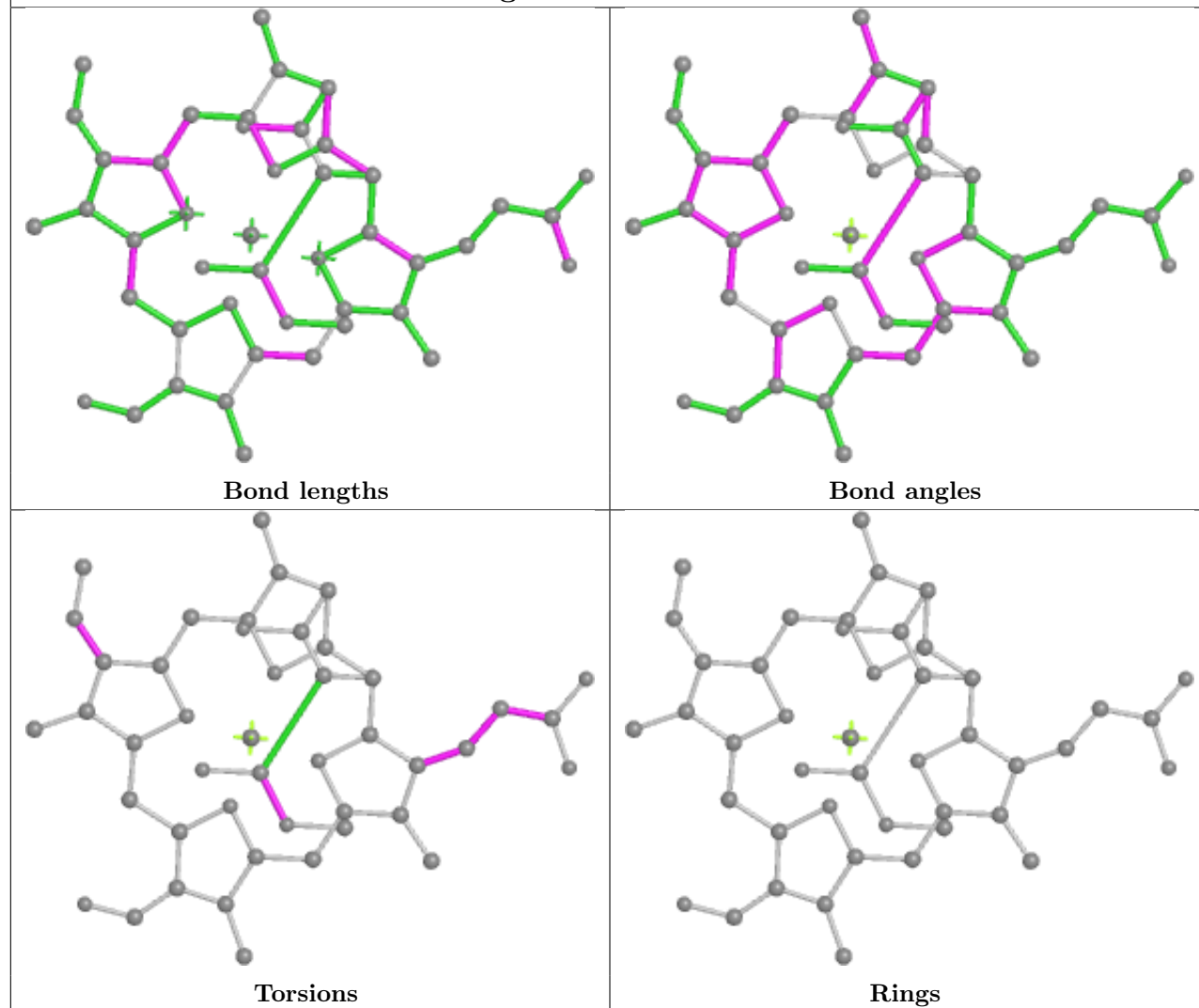




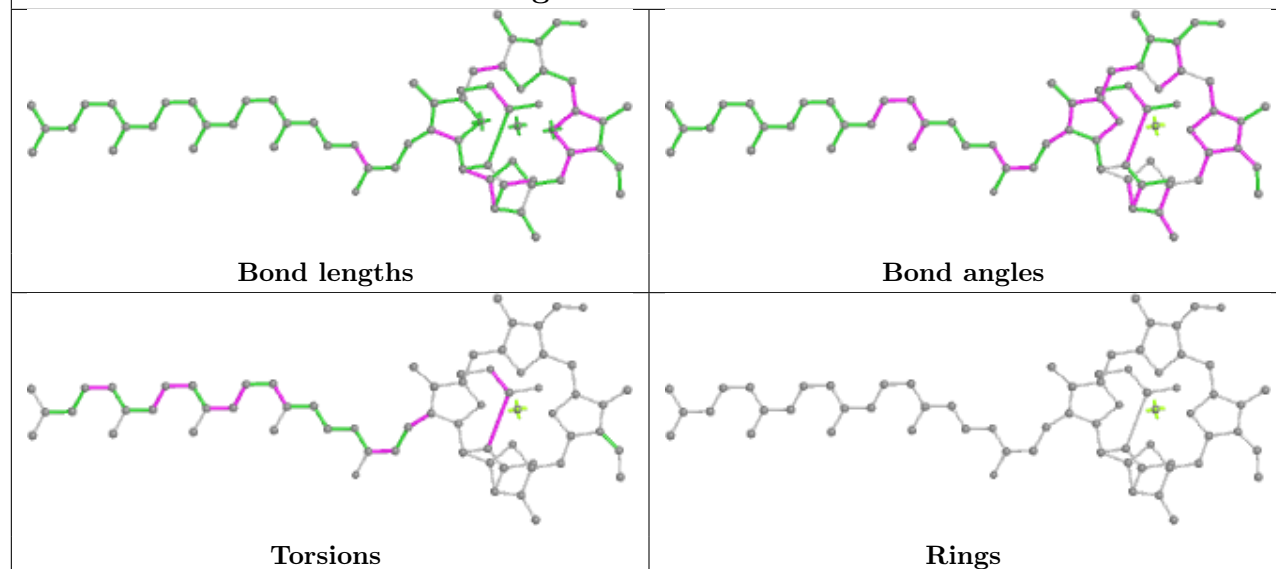


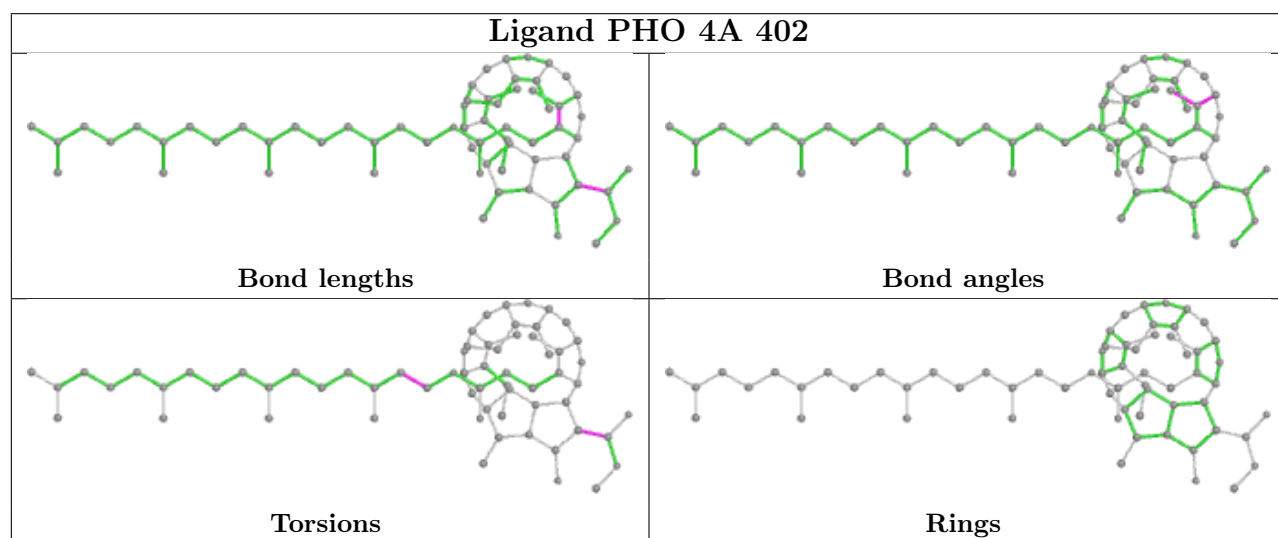
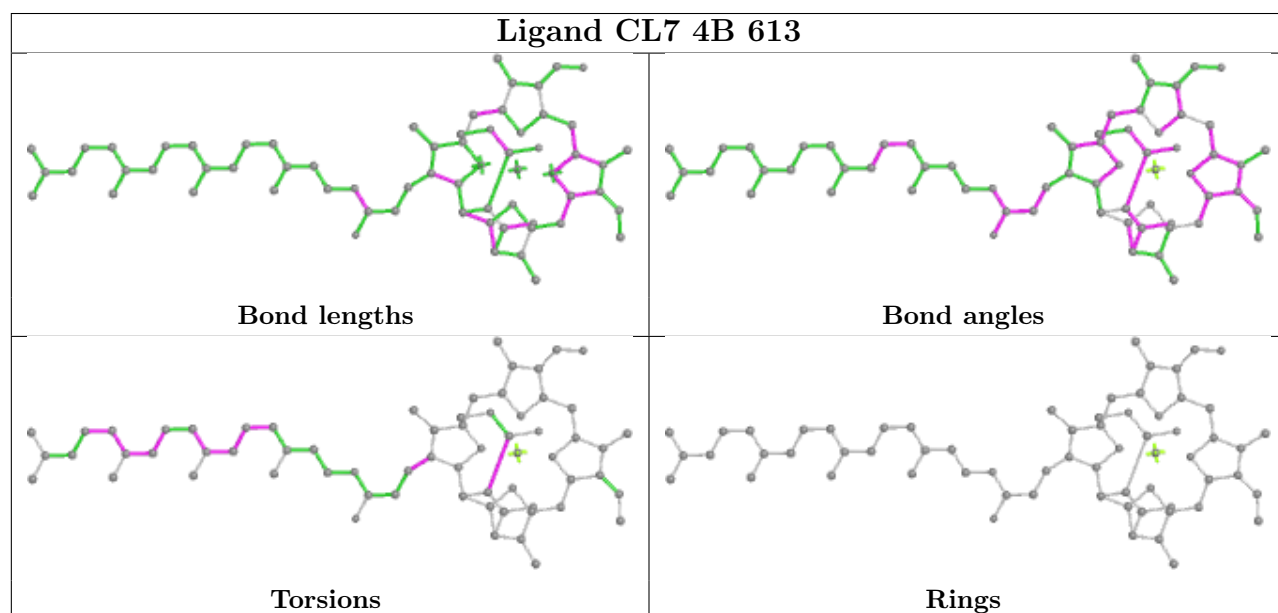
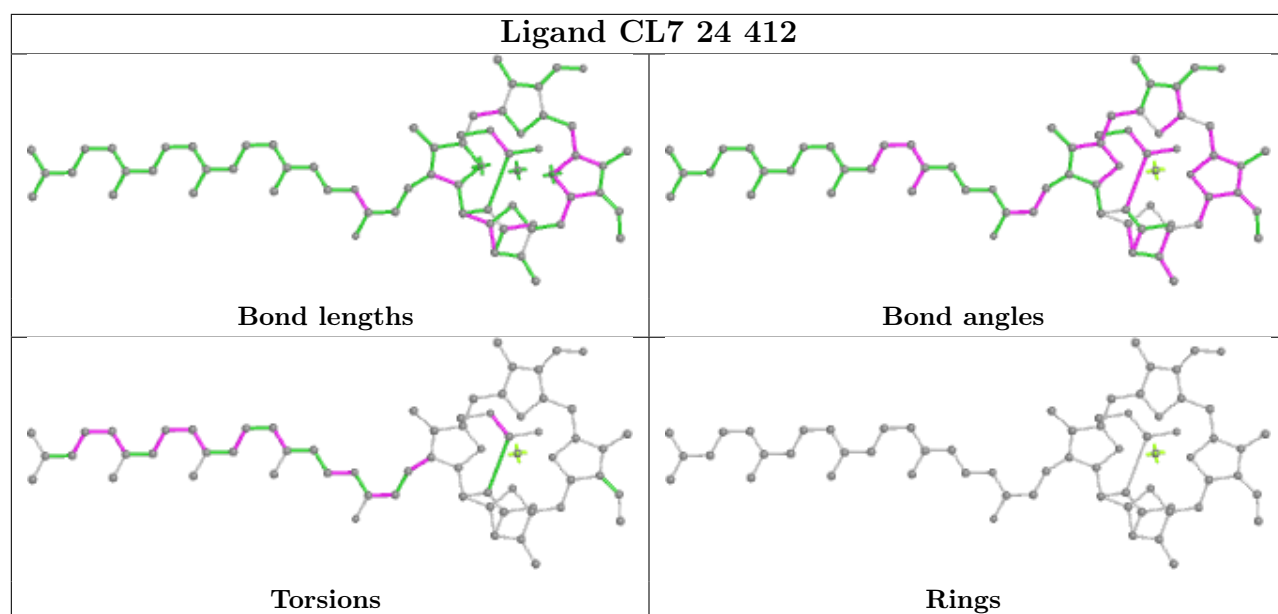


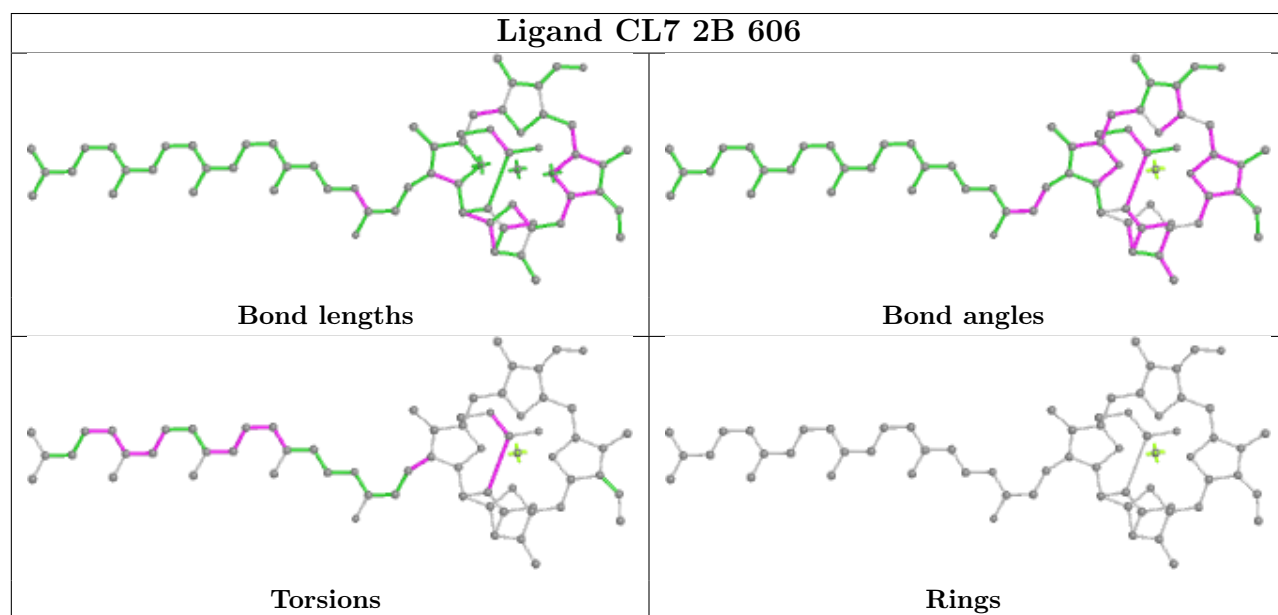
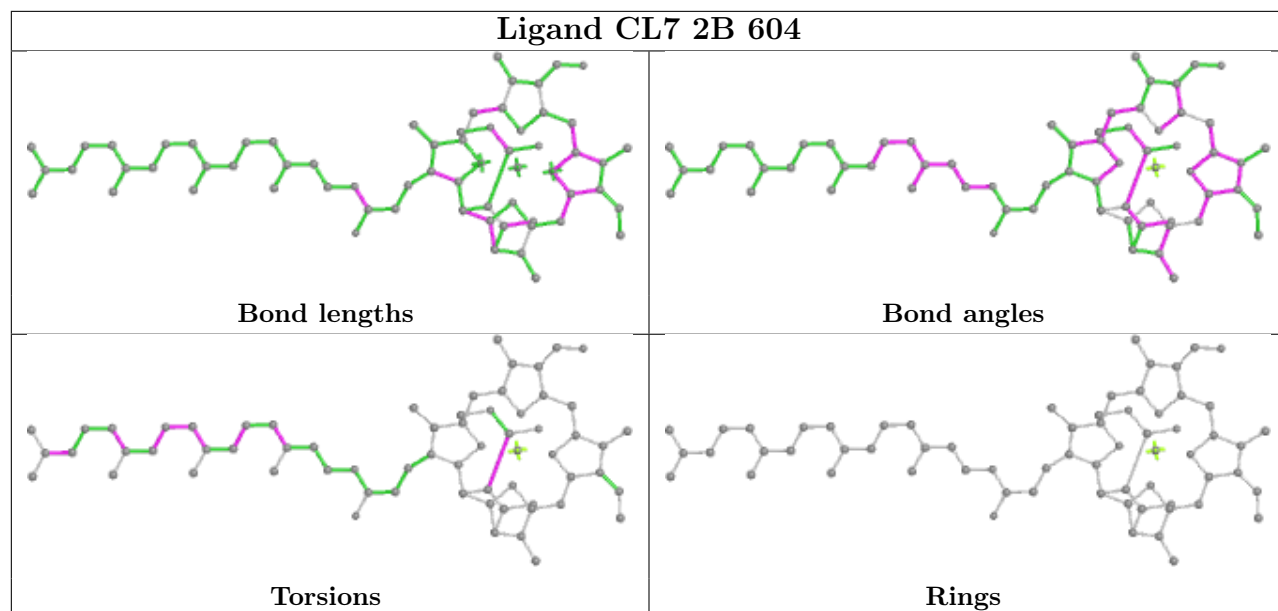
Ligand CL7 21 419

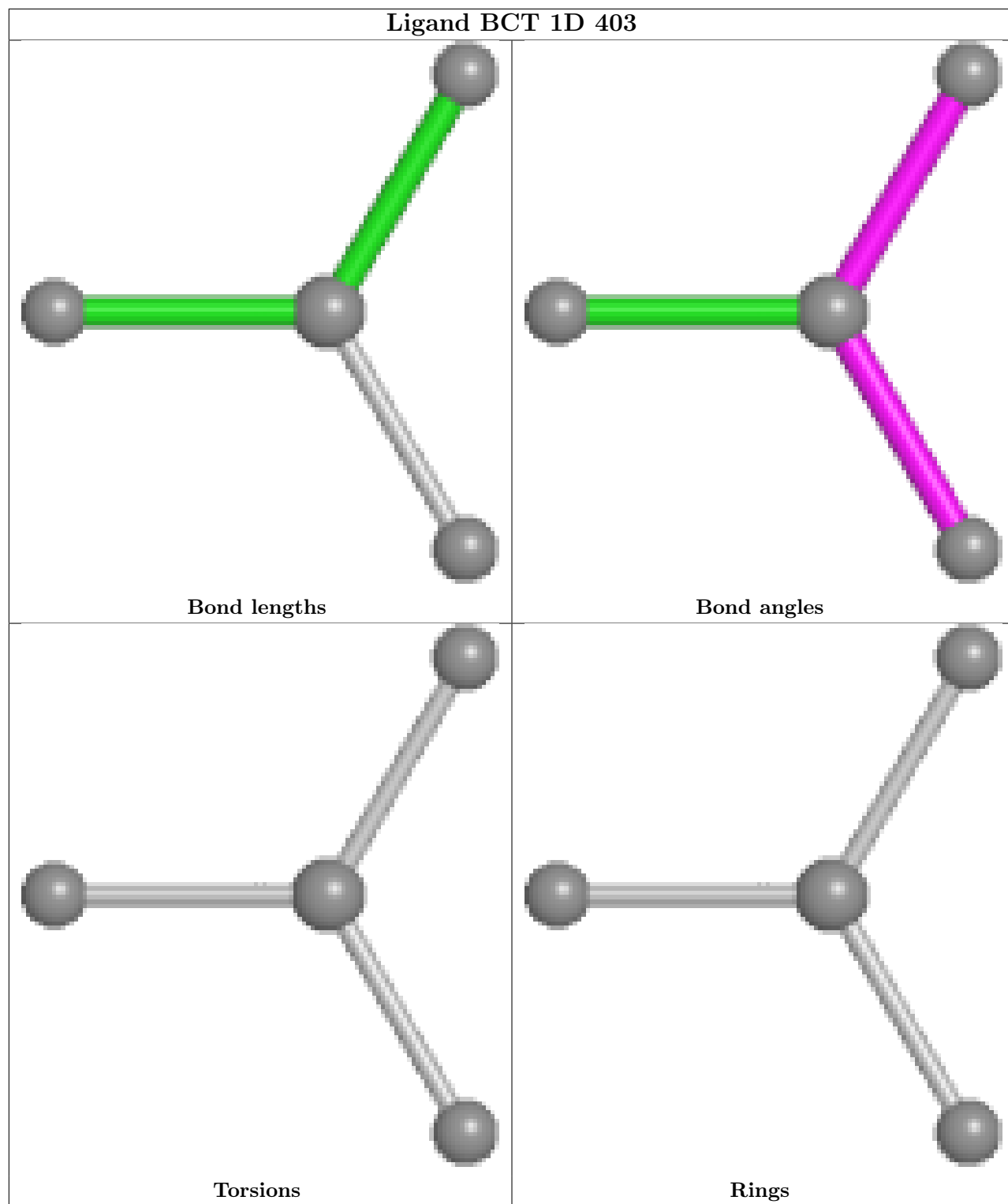


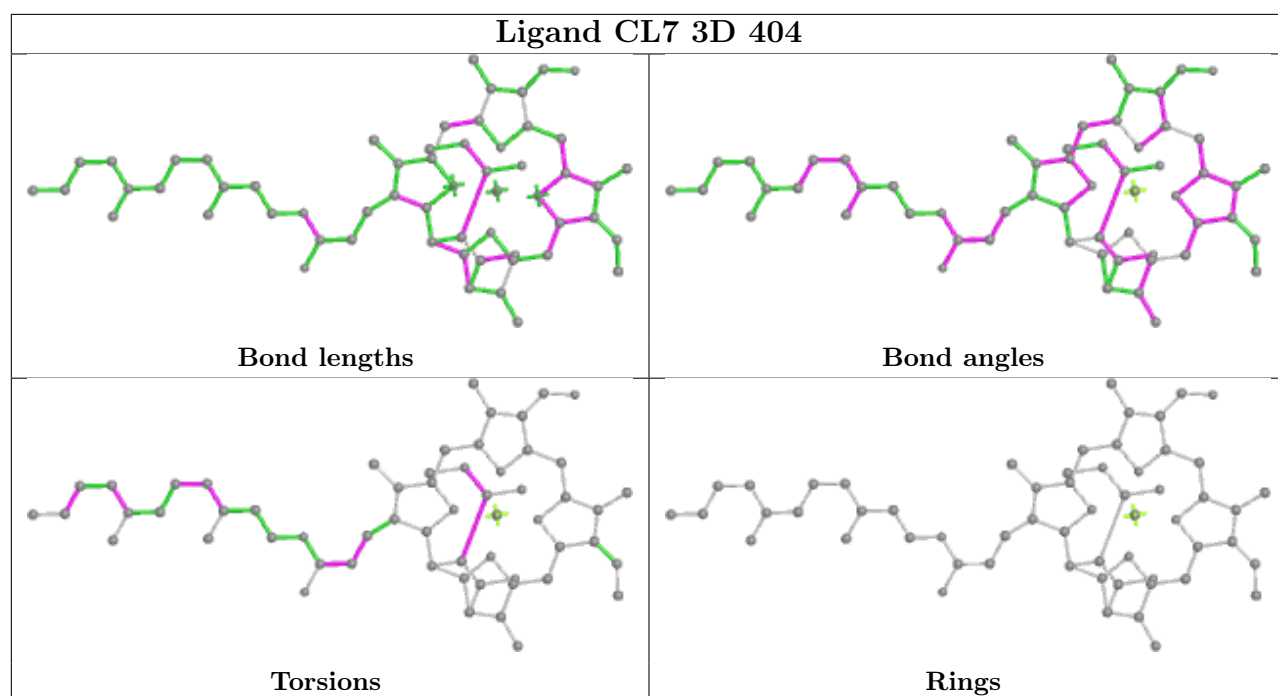
Ligand CL7 43 411



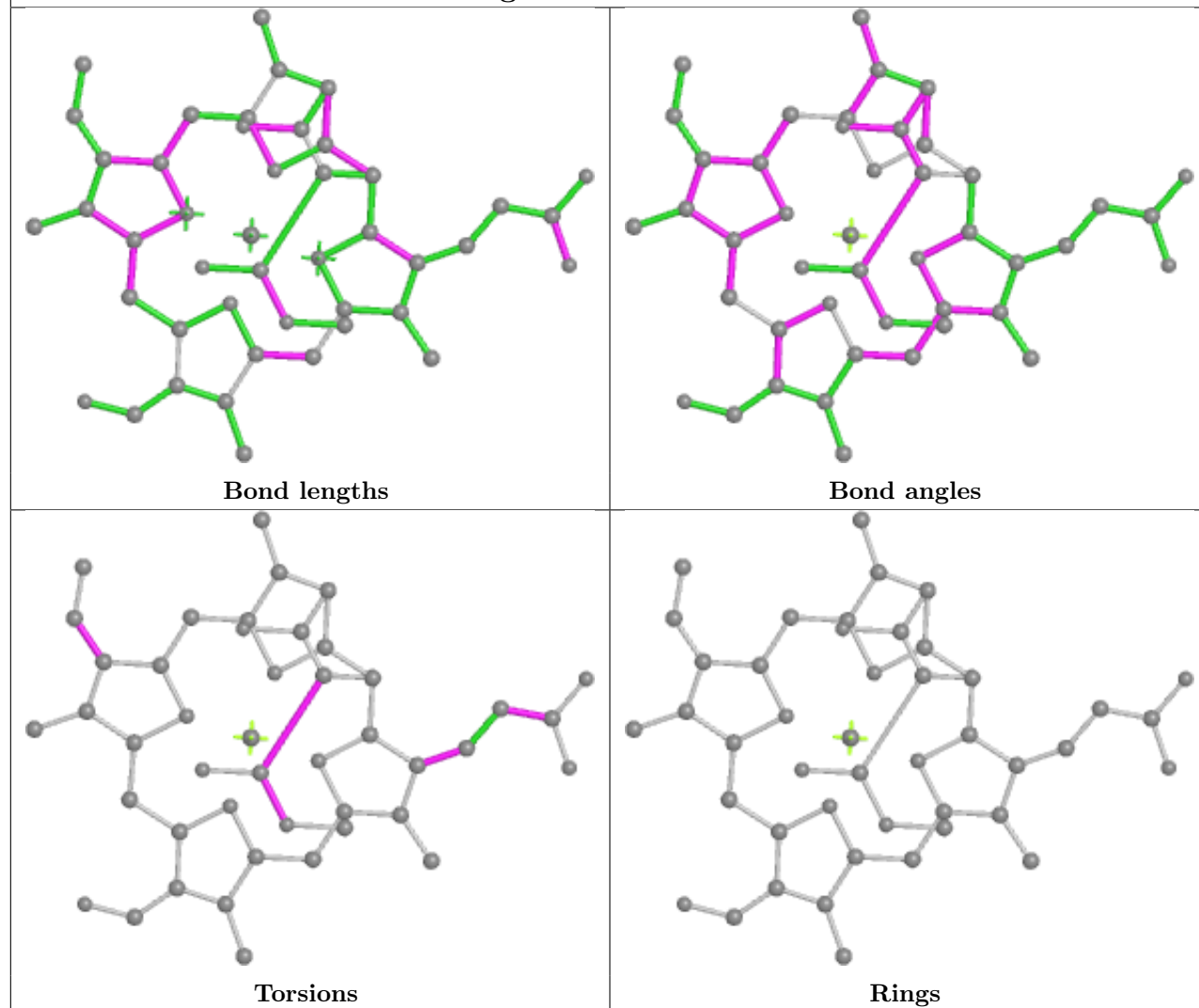




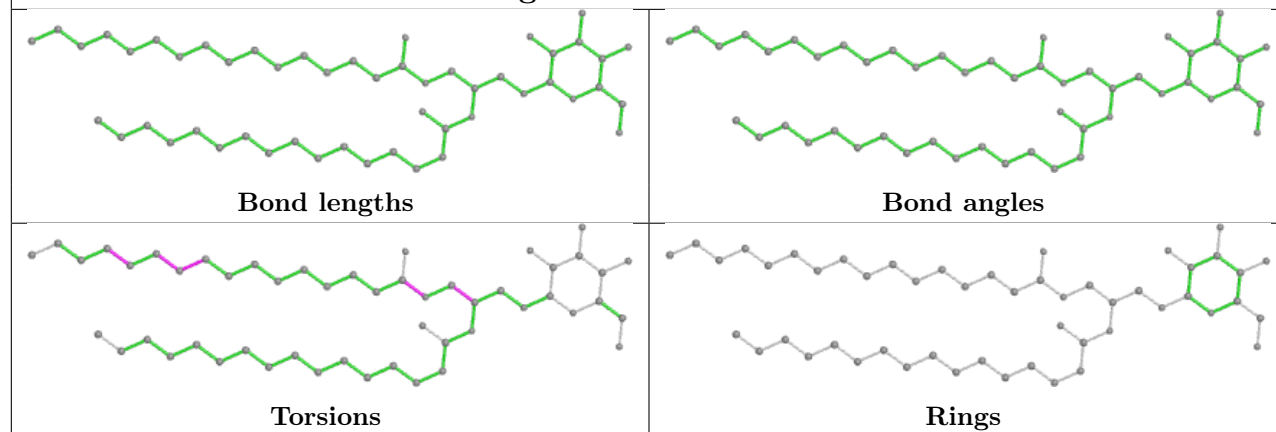


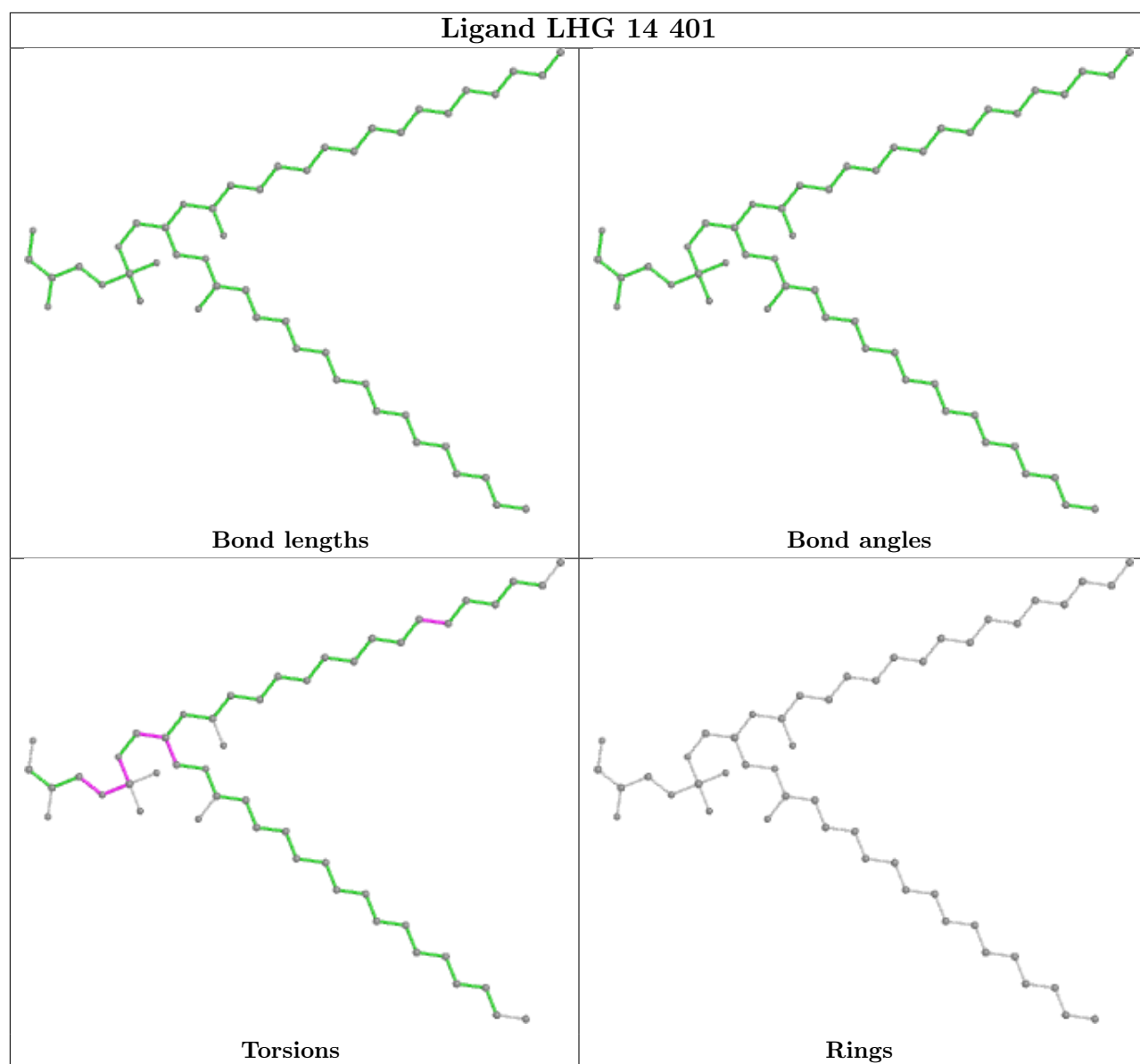


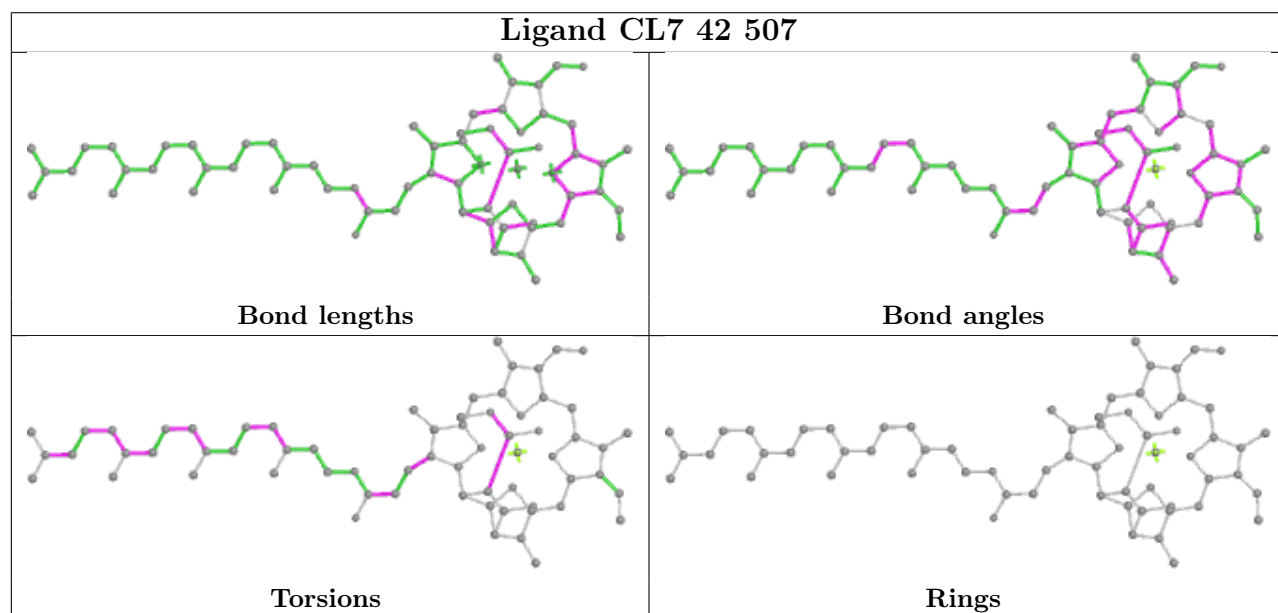
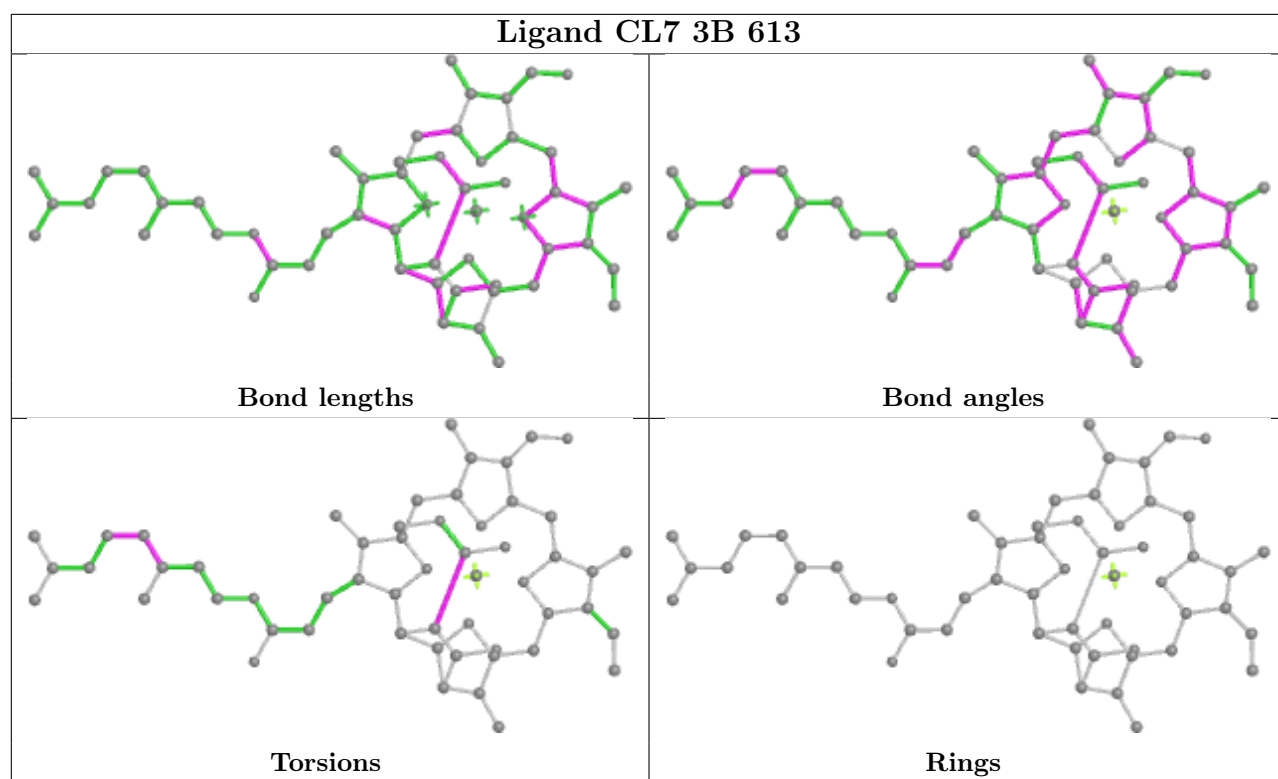
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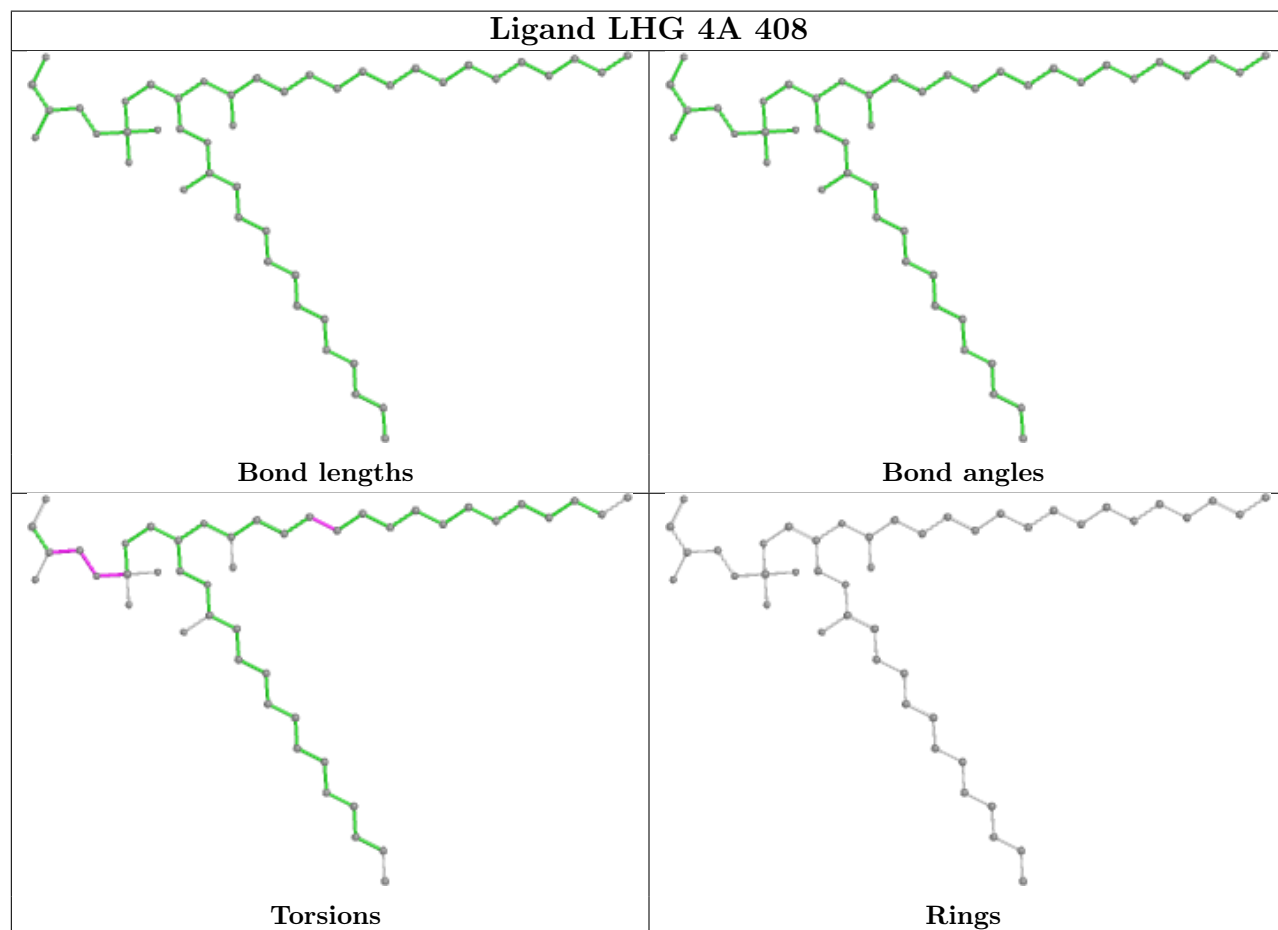
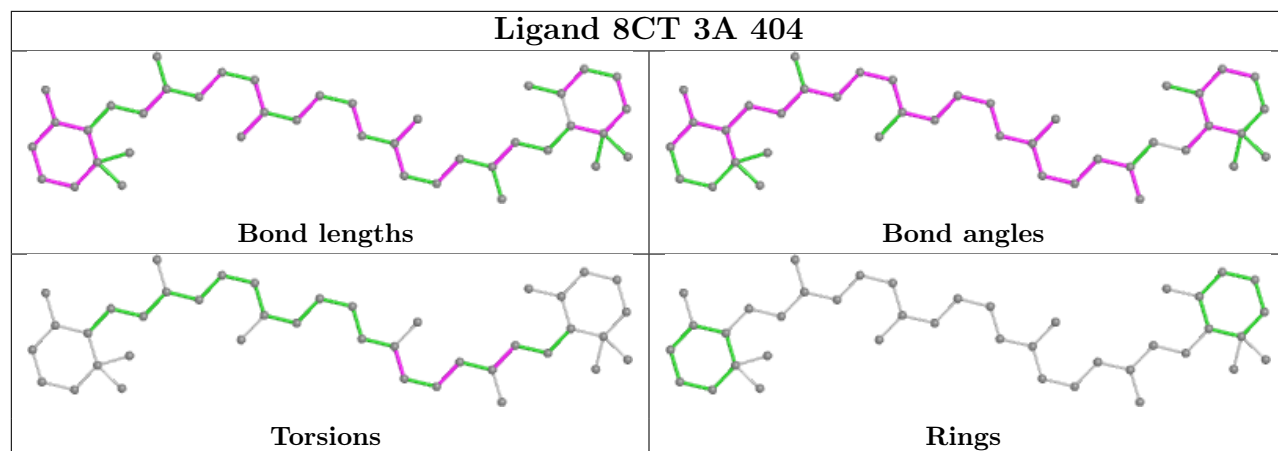


Ligand LMG 4B 622

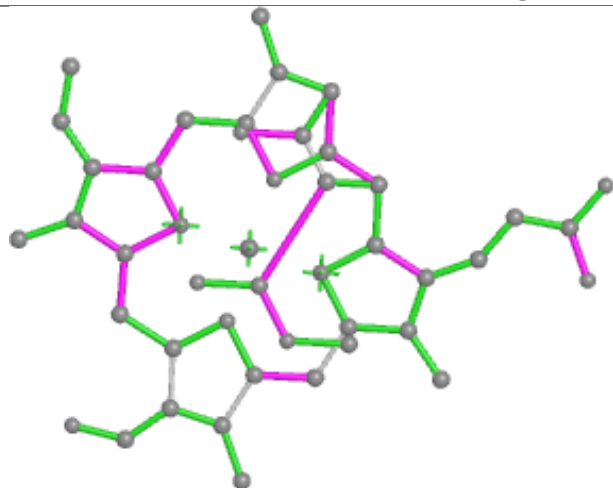




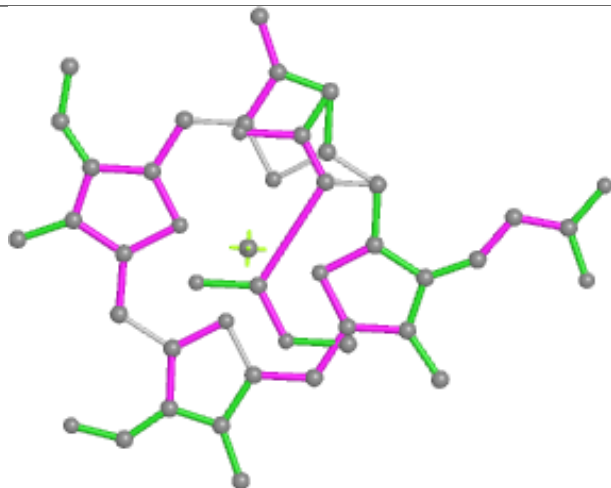




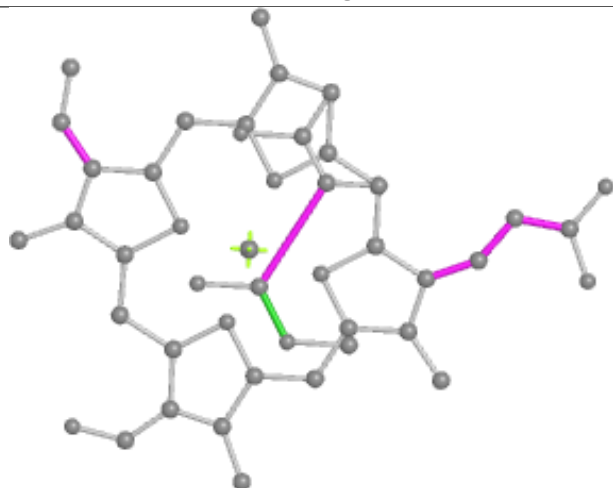
Ligand CL7 43 414



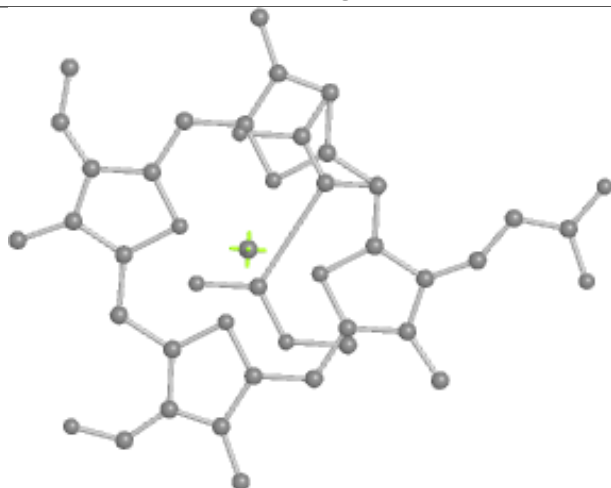
Bond lengths



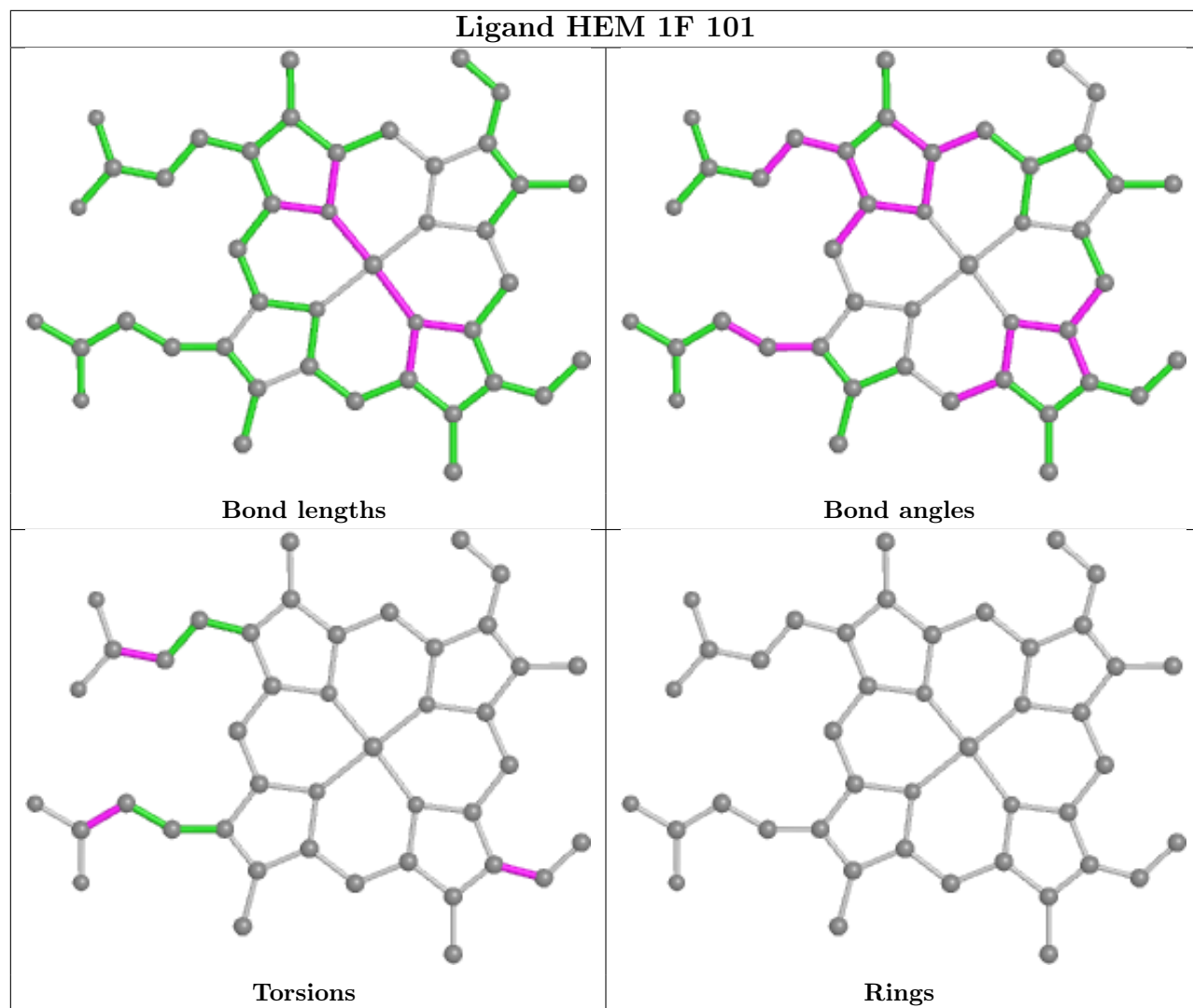
Bond angles



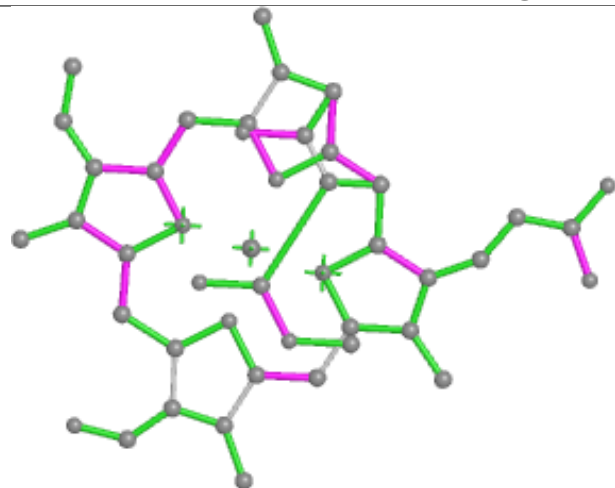
Torsions



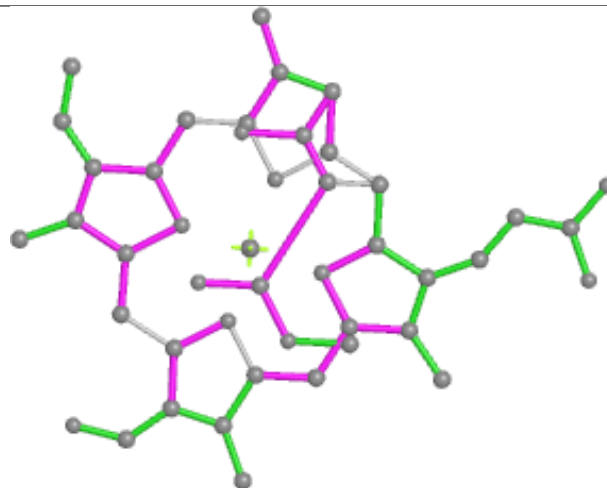
Rings



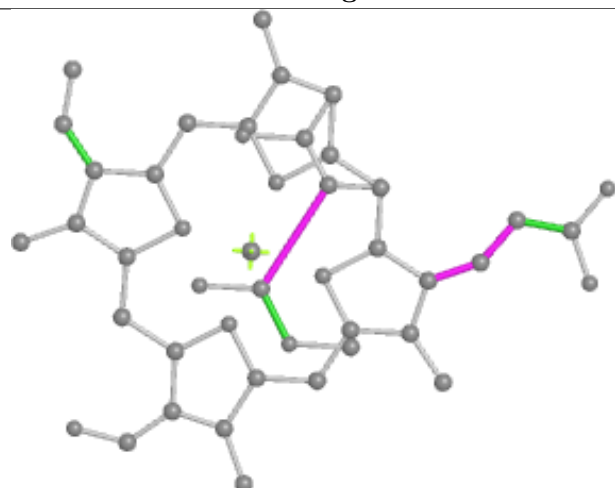
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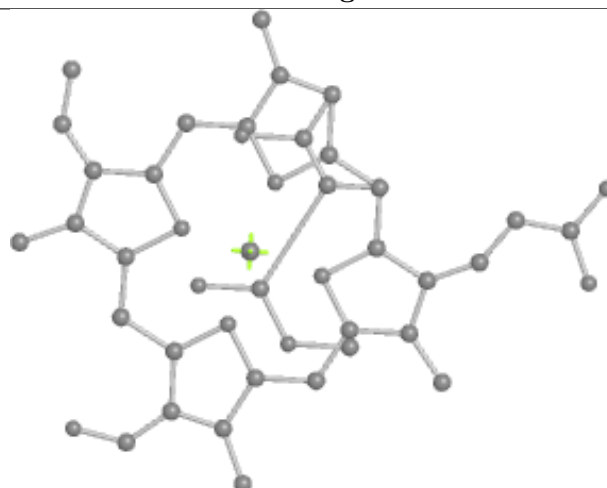
Bond lengths



Bond angles

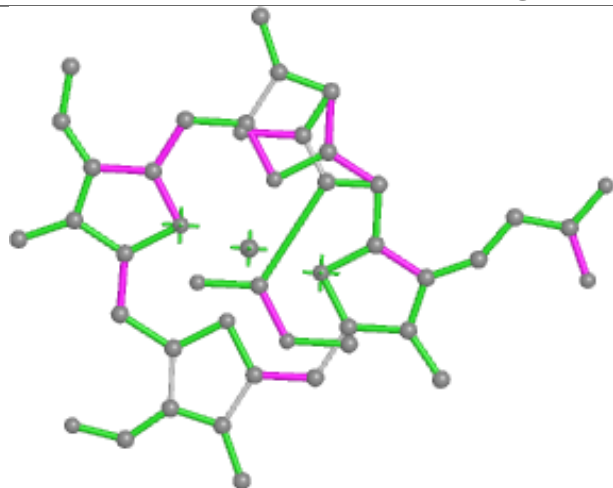


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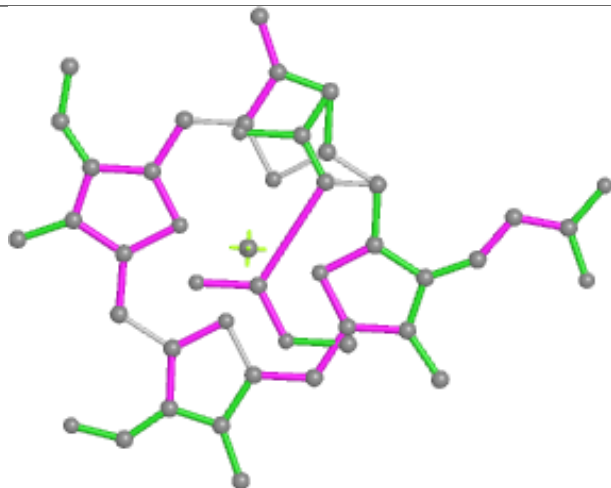


Rings

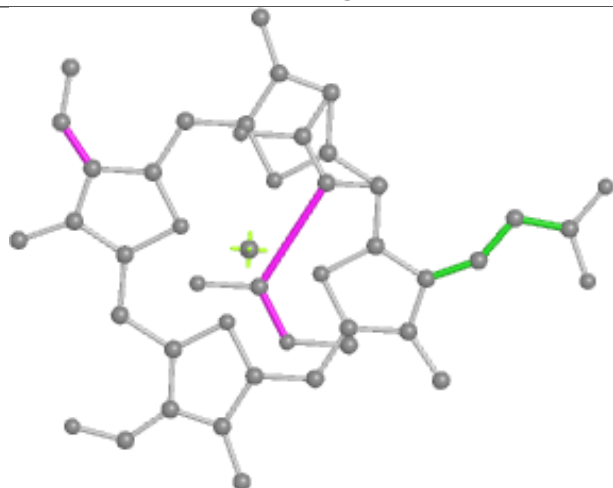
Ligand CL7 31 420



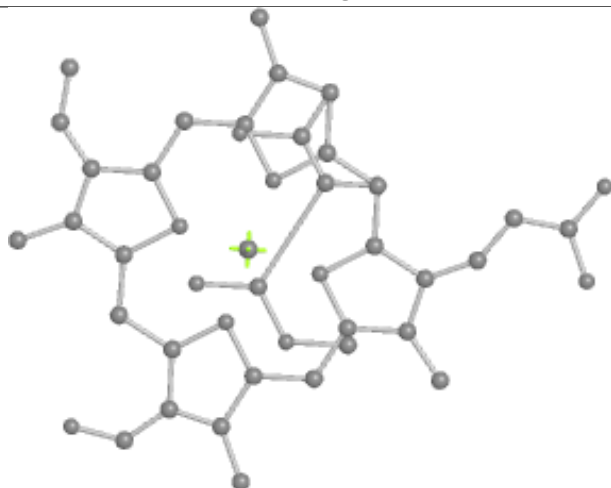
Bond lengths



Bond angles

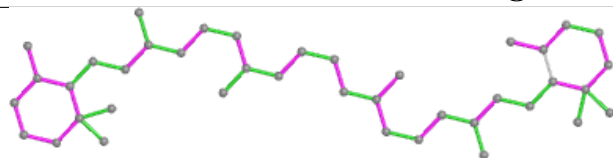


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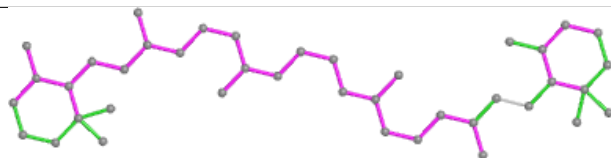


Rings

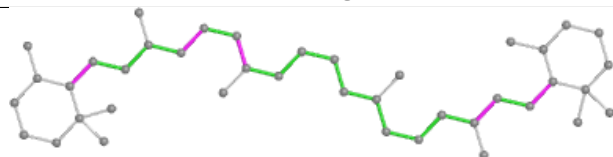
Ligand 8CT 1C 518



Bond lengths



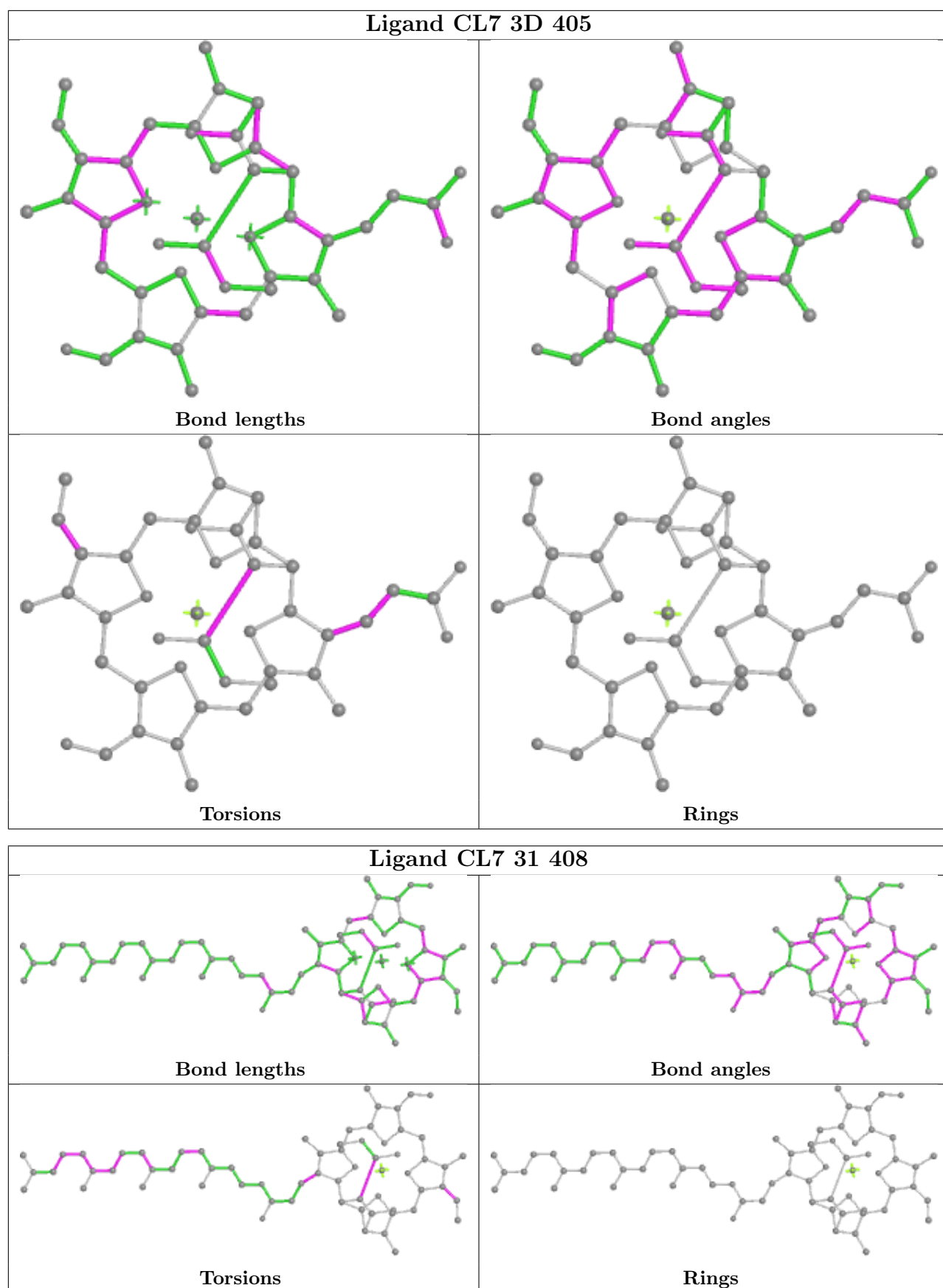
Bond angles

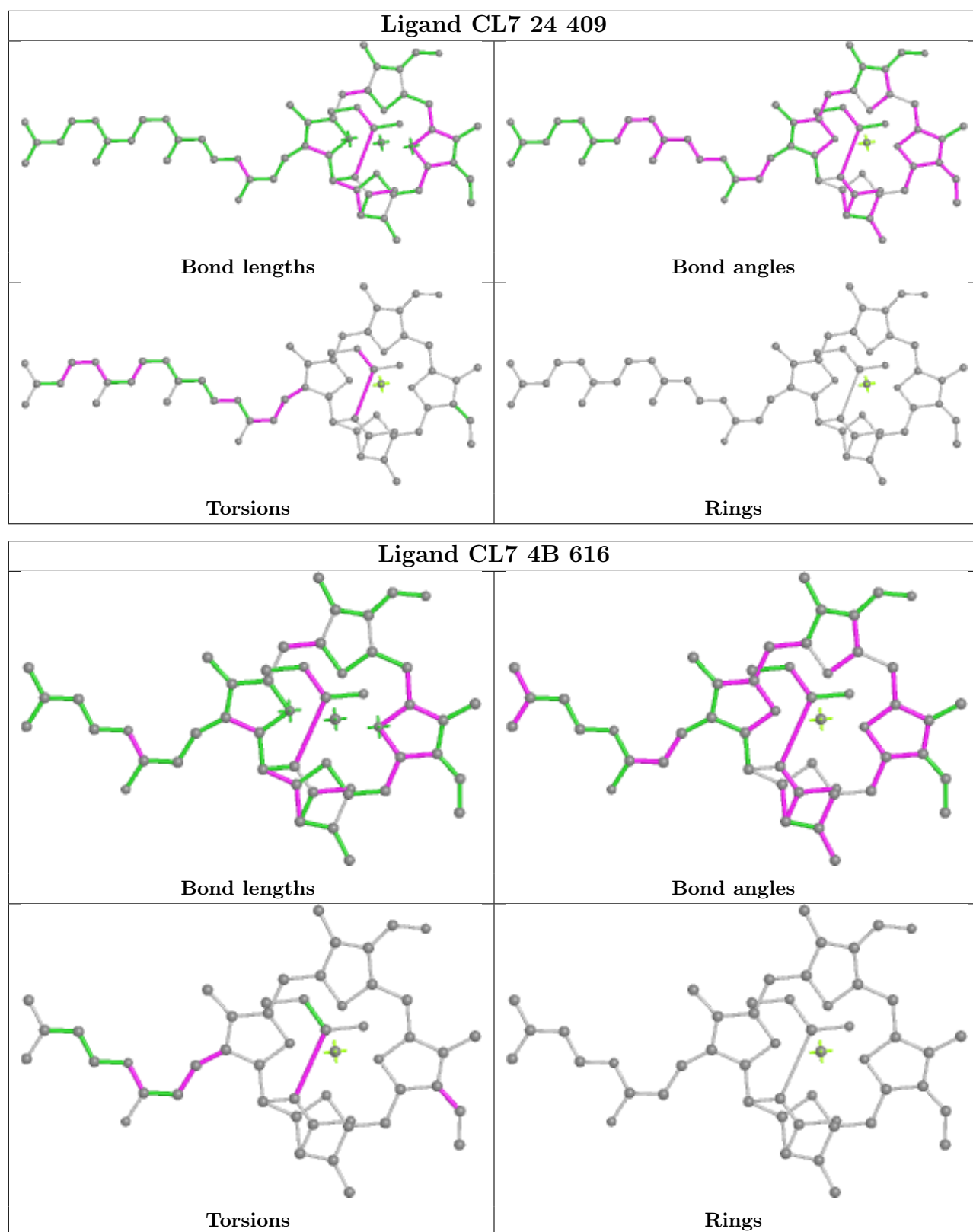


Torsions

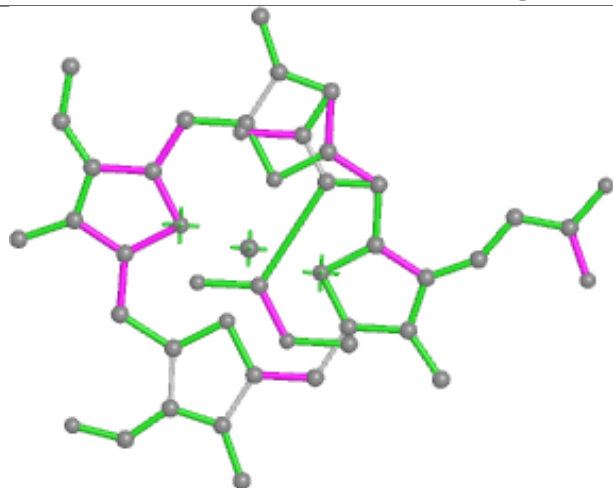


Rings

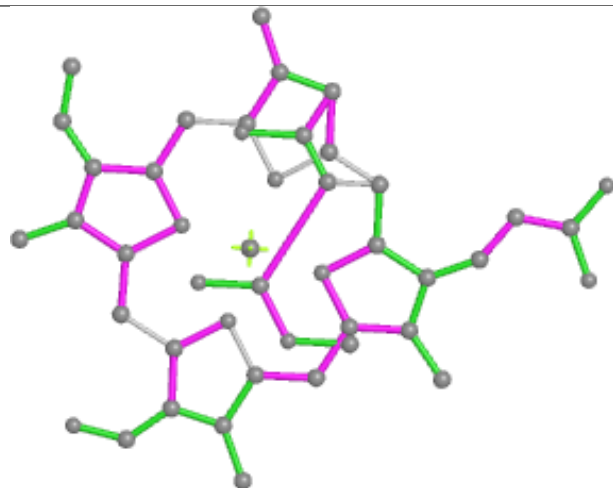




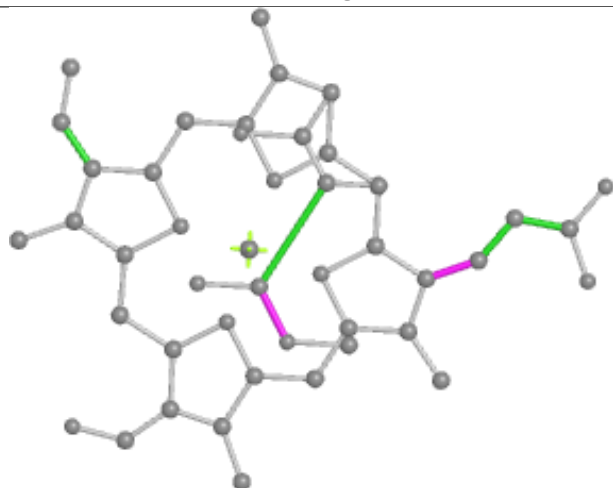
Ligand CL7 12 504



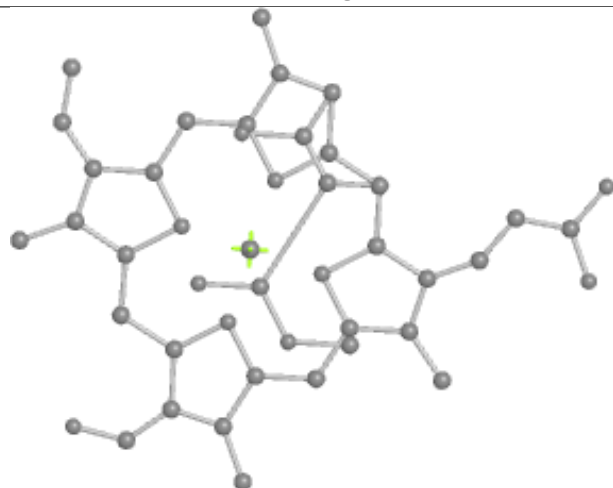
Bond lengths



Bond angles

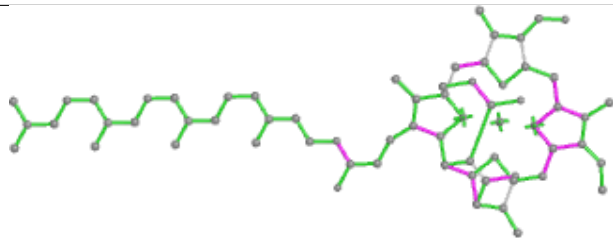


Torsions

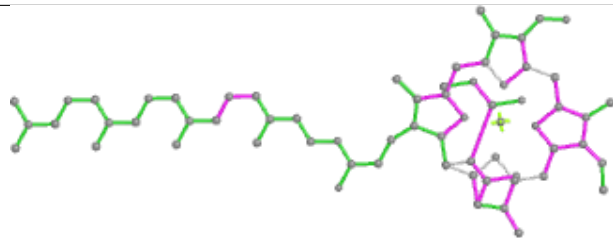


Rings

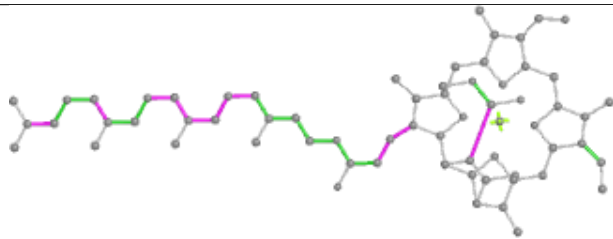
Ligand CL7 14 404



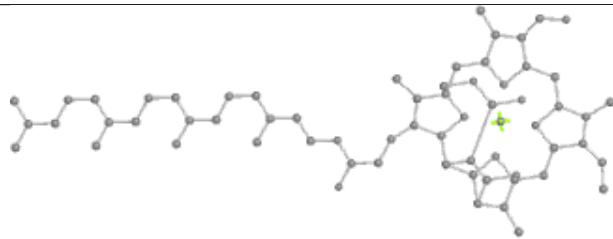
Bond lengths



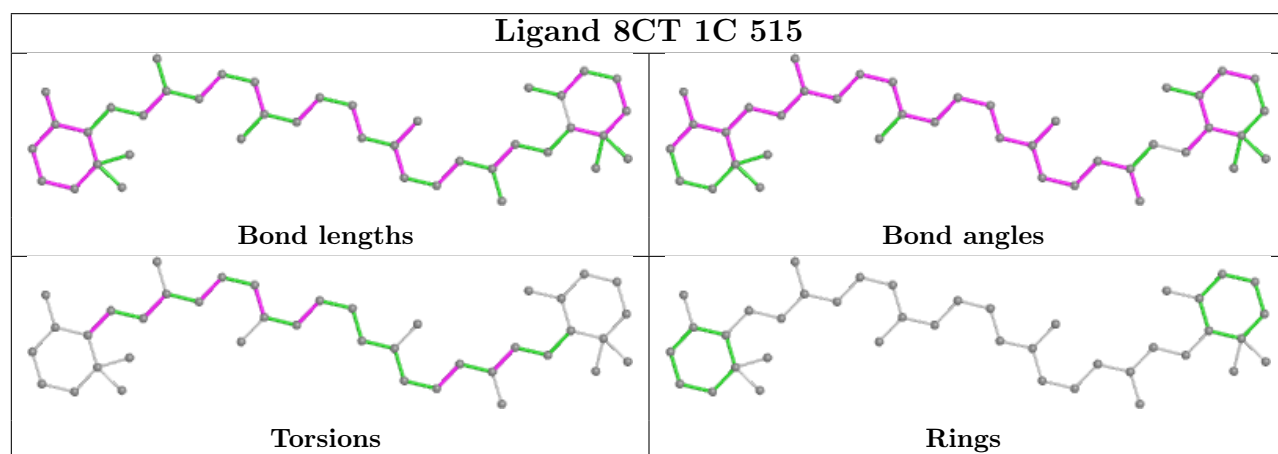
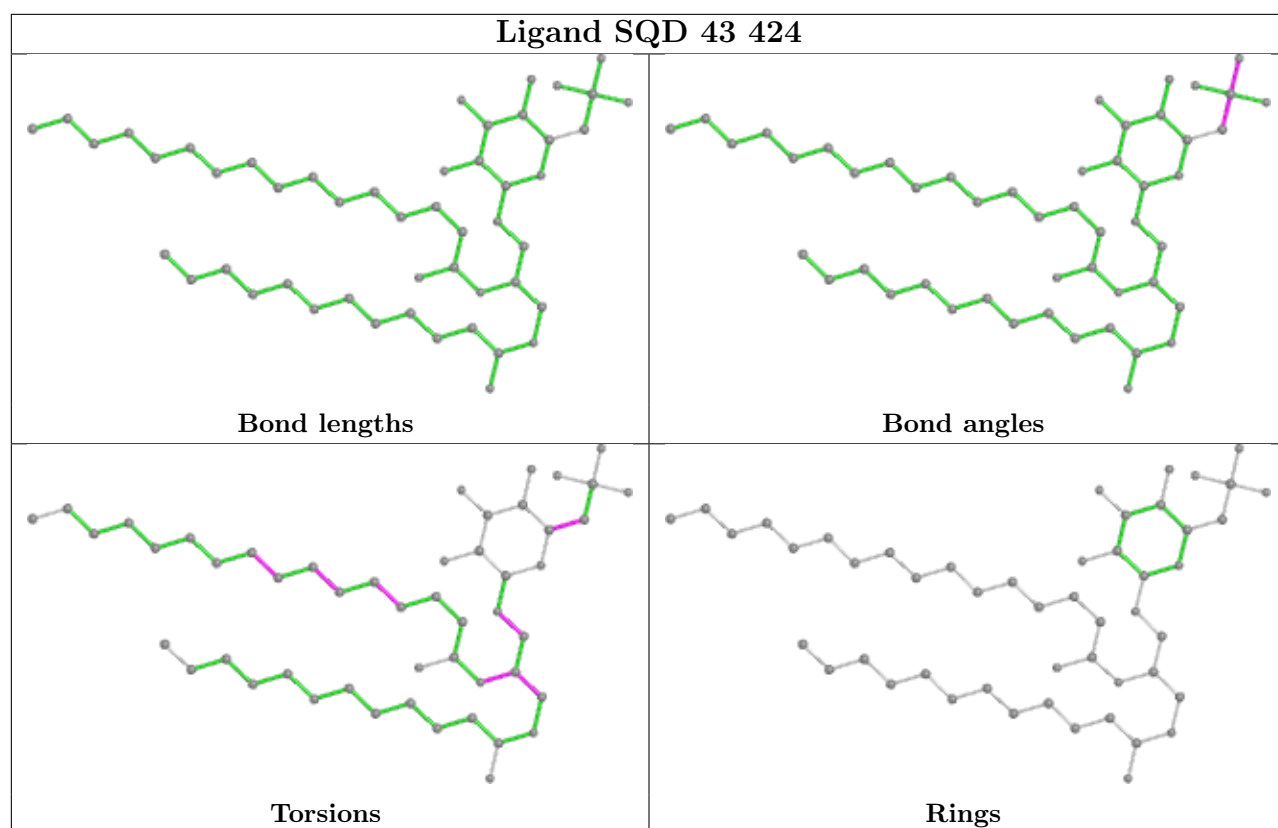
Bond angles

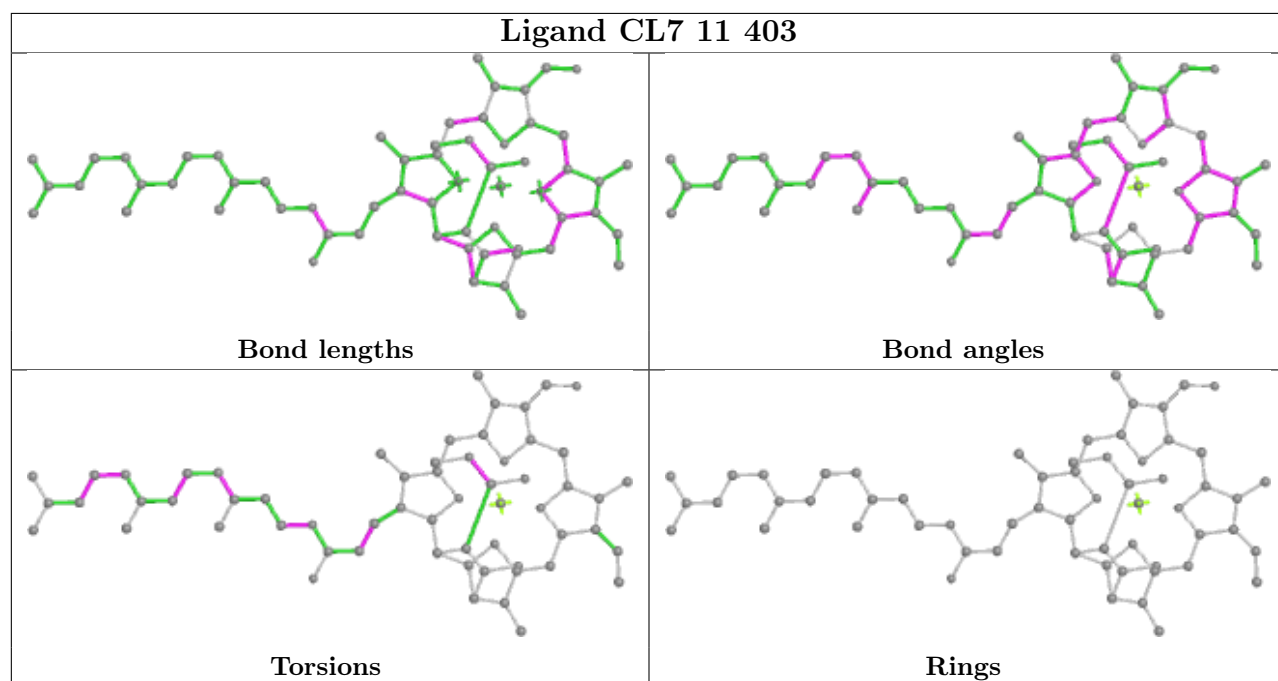
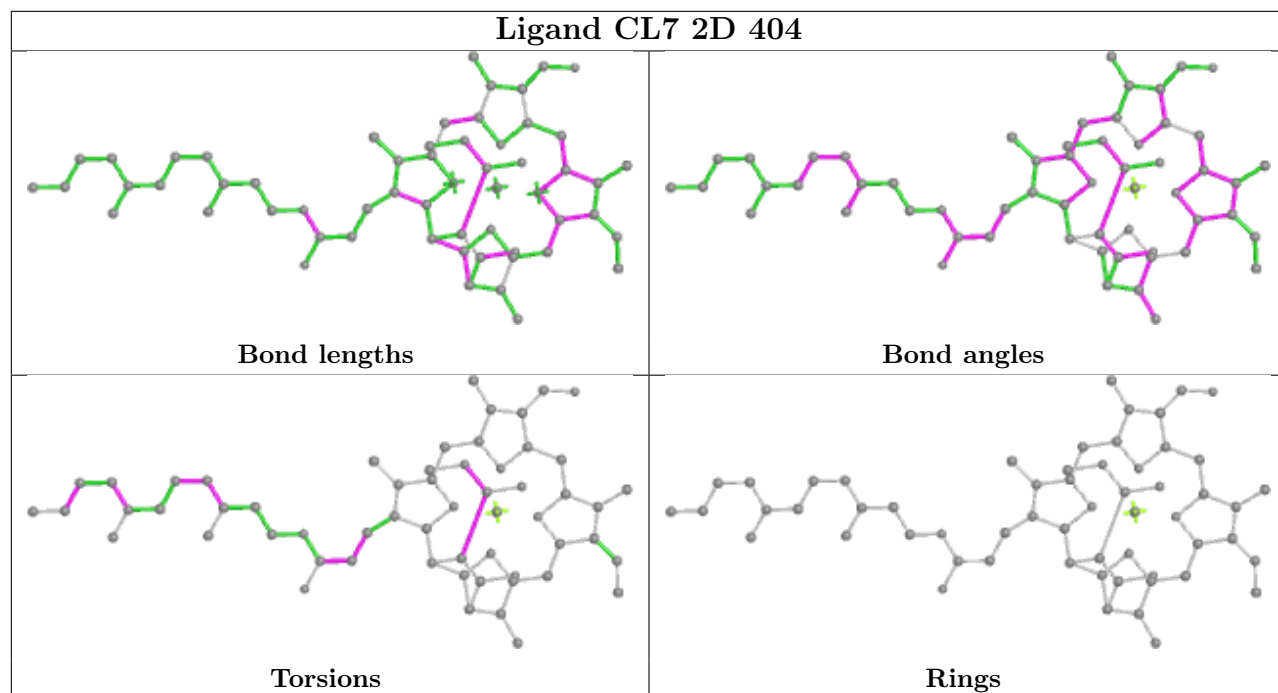


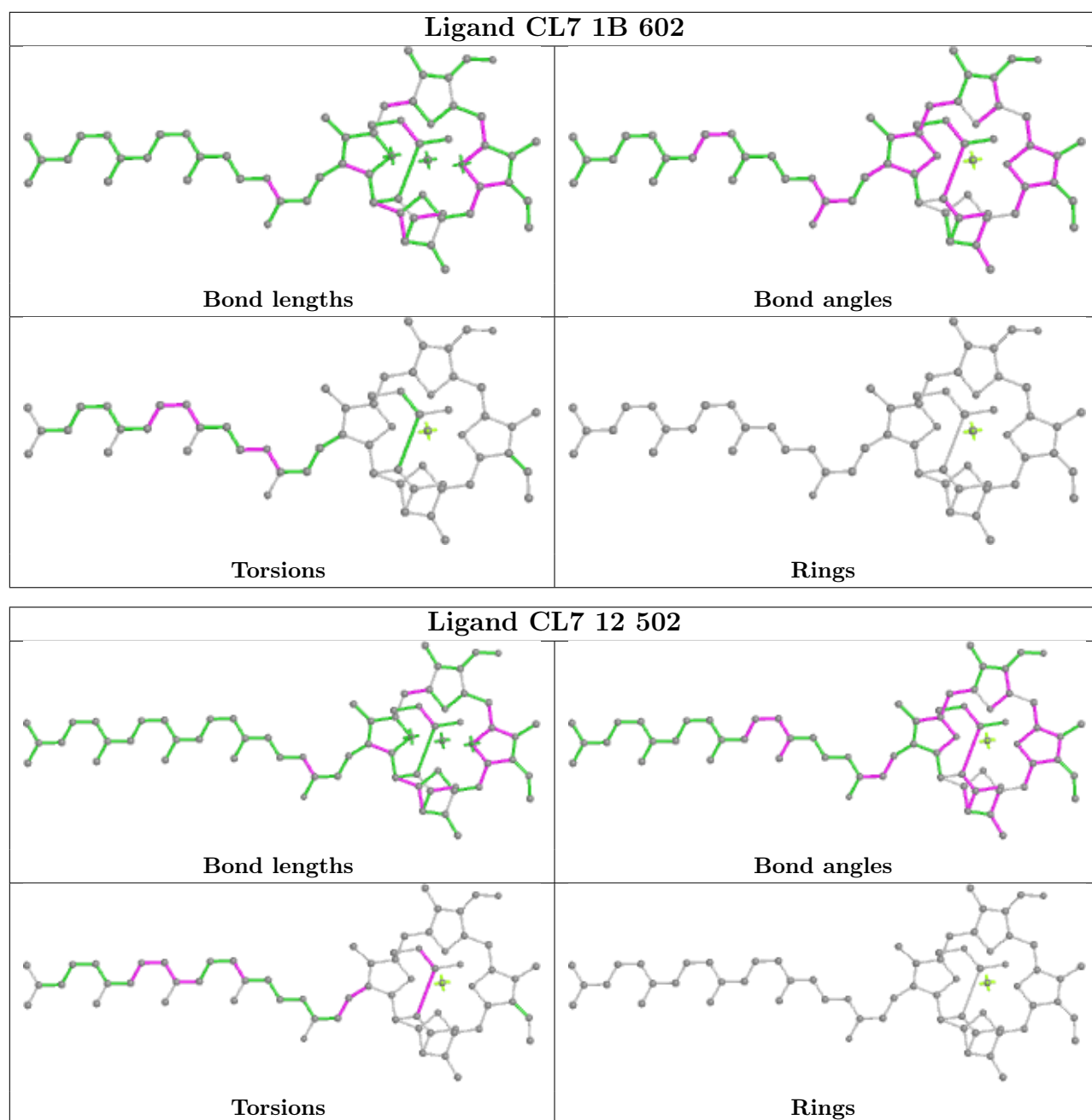
Torsions

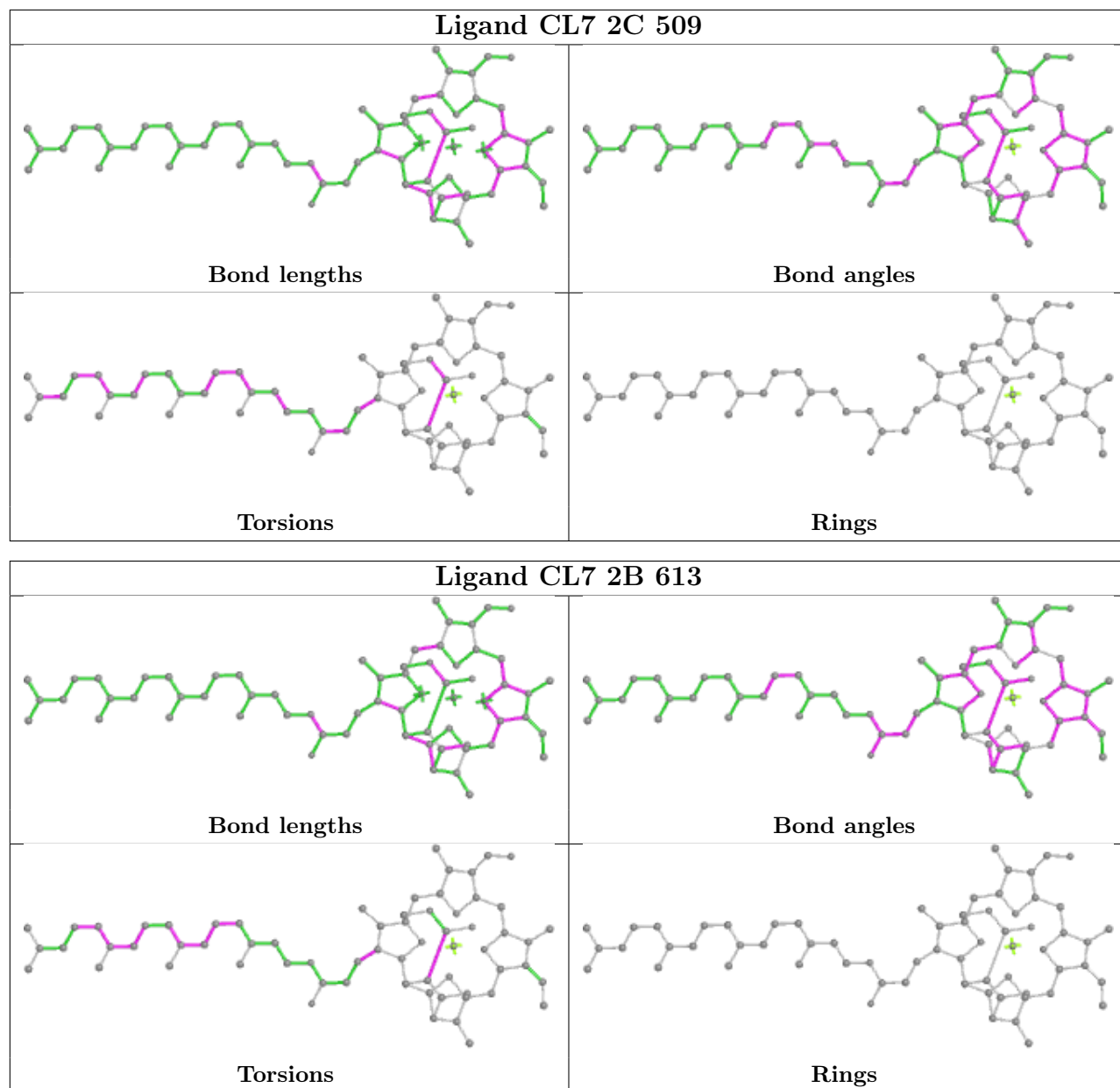


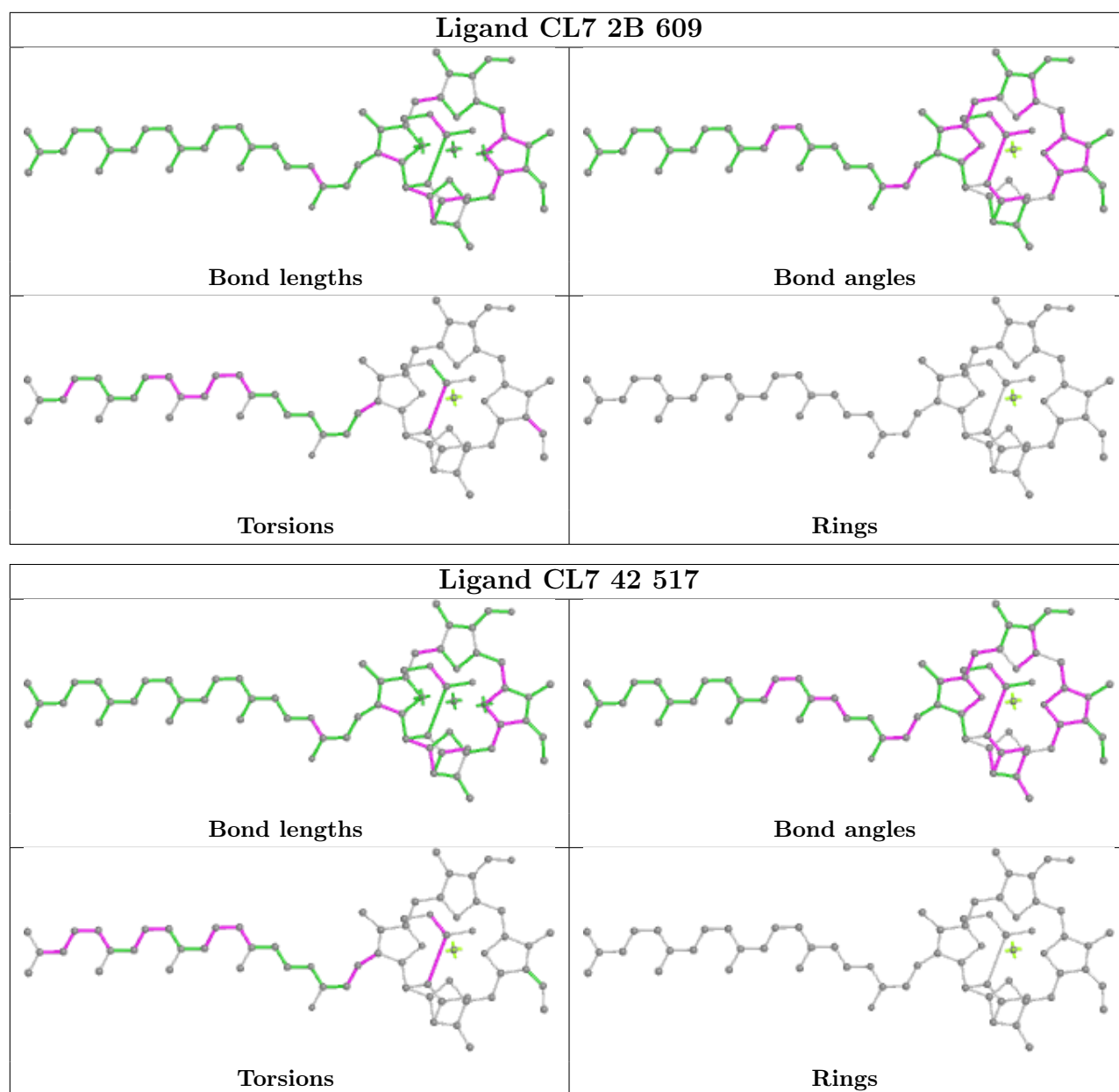
Rings



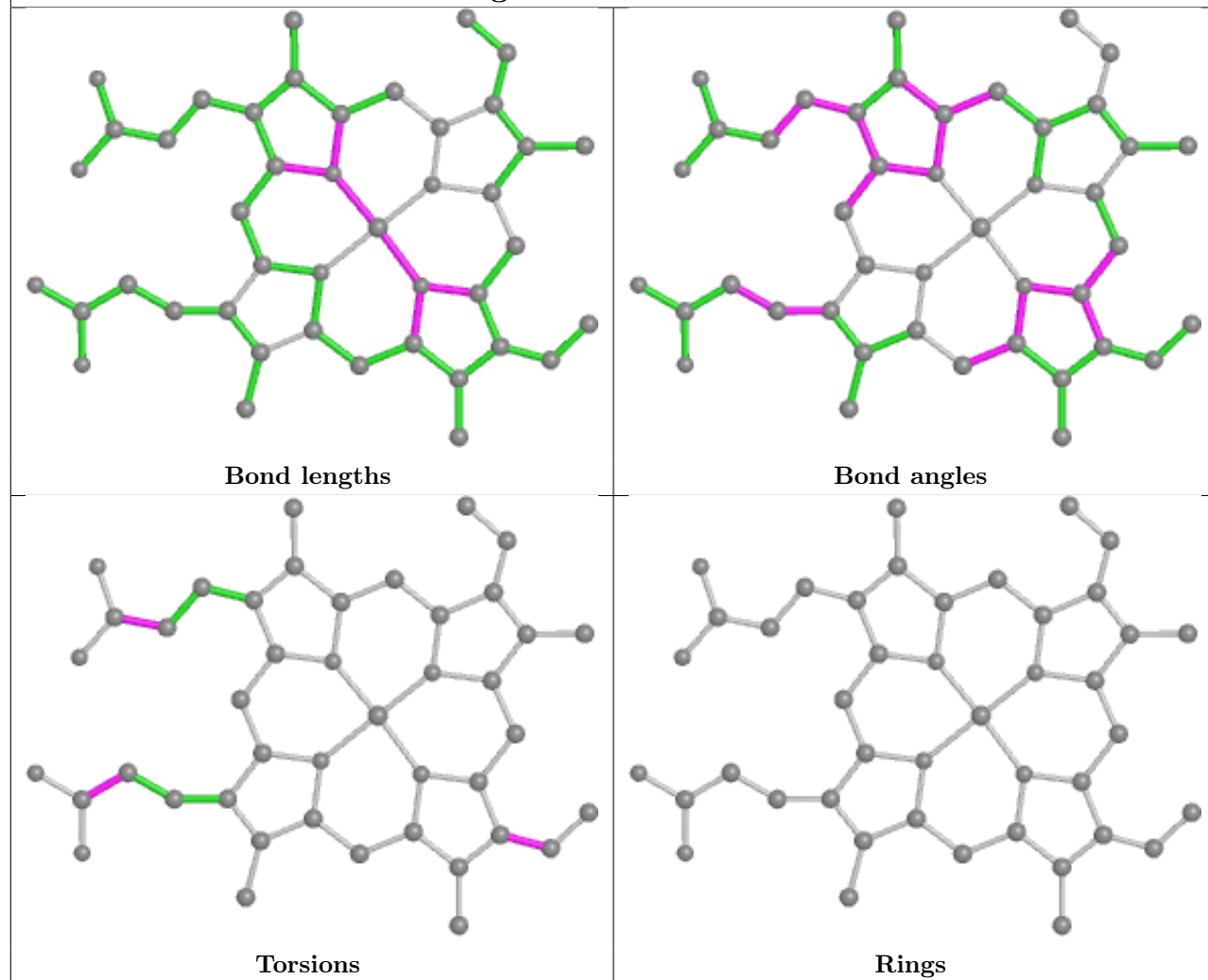




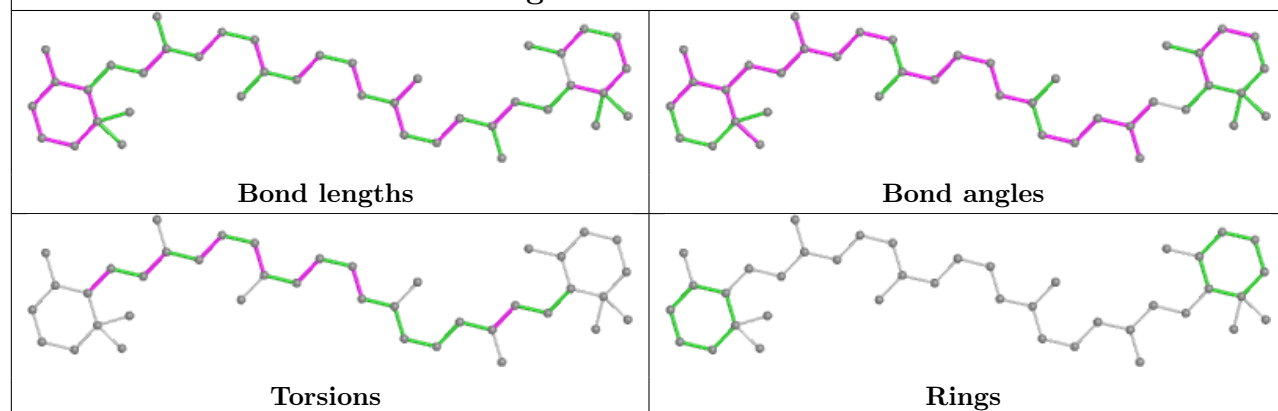


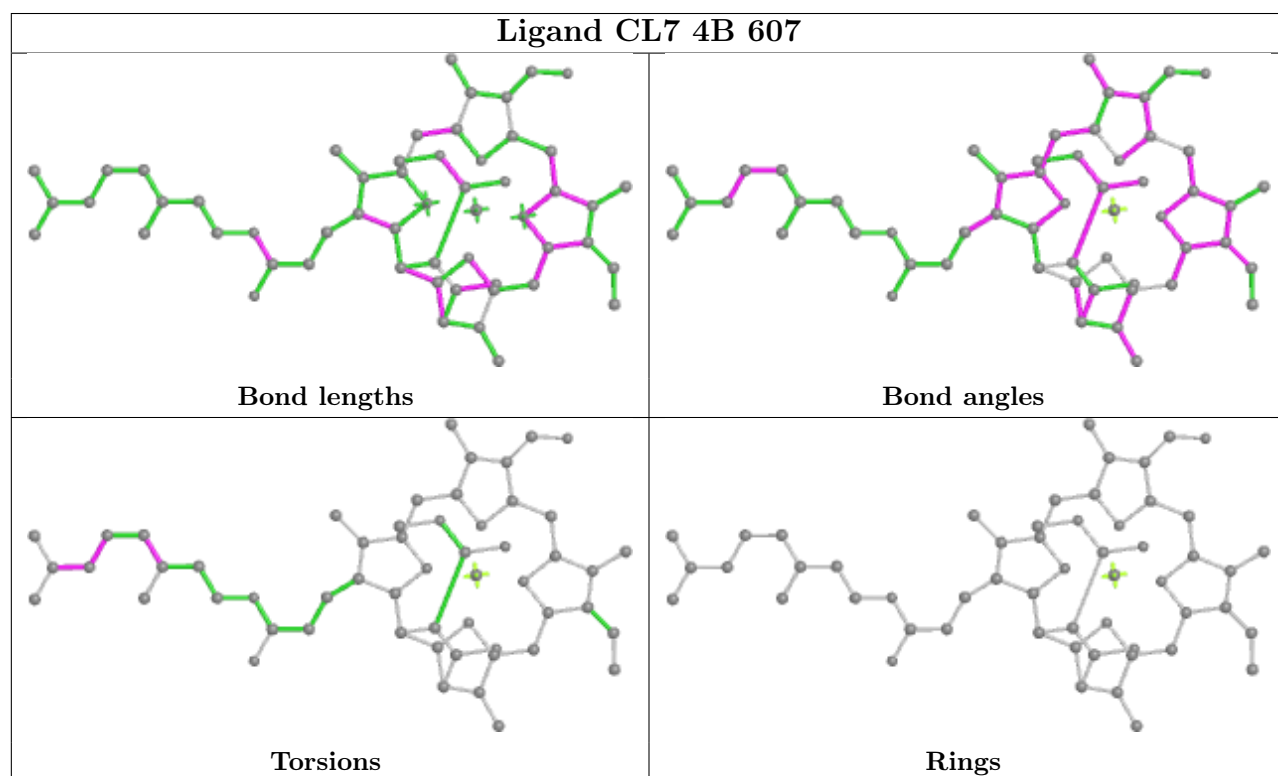
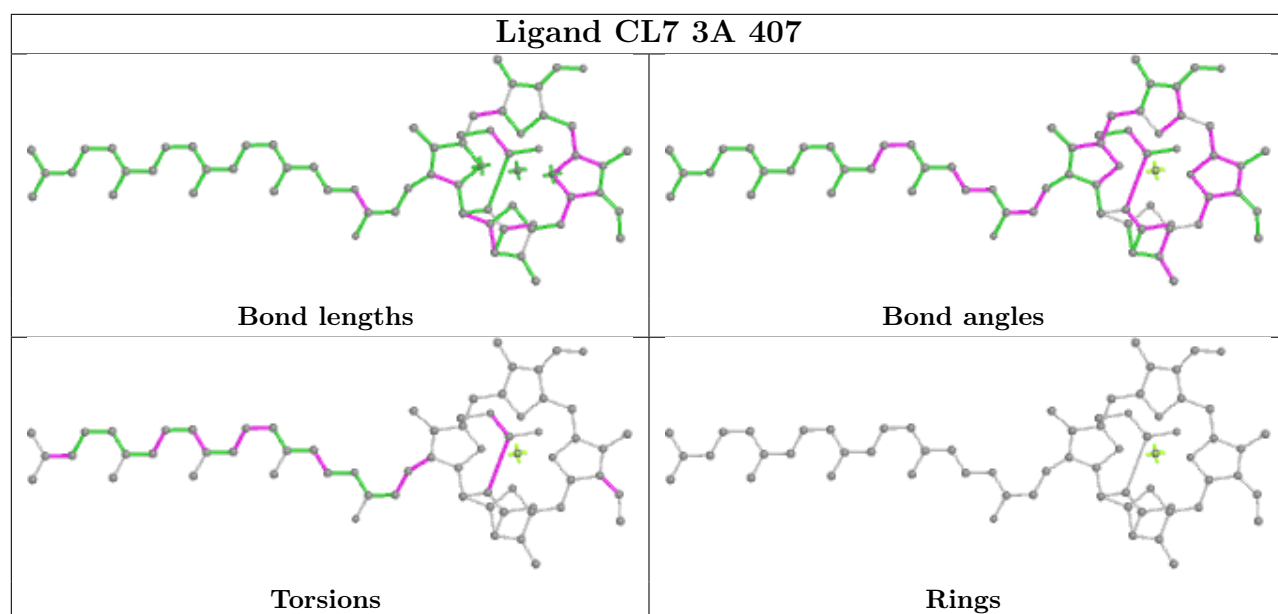


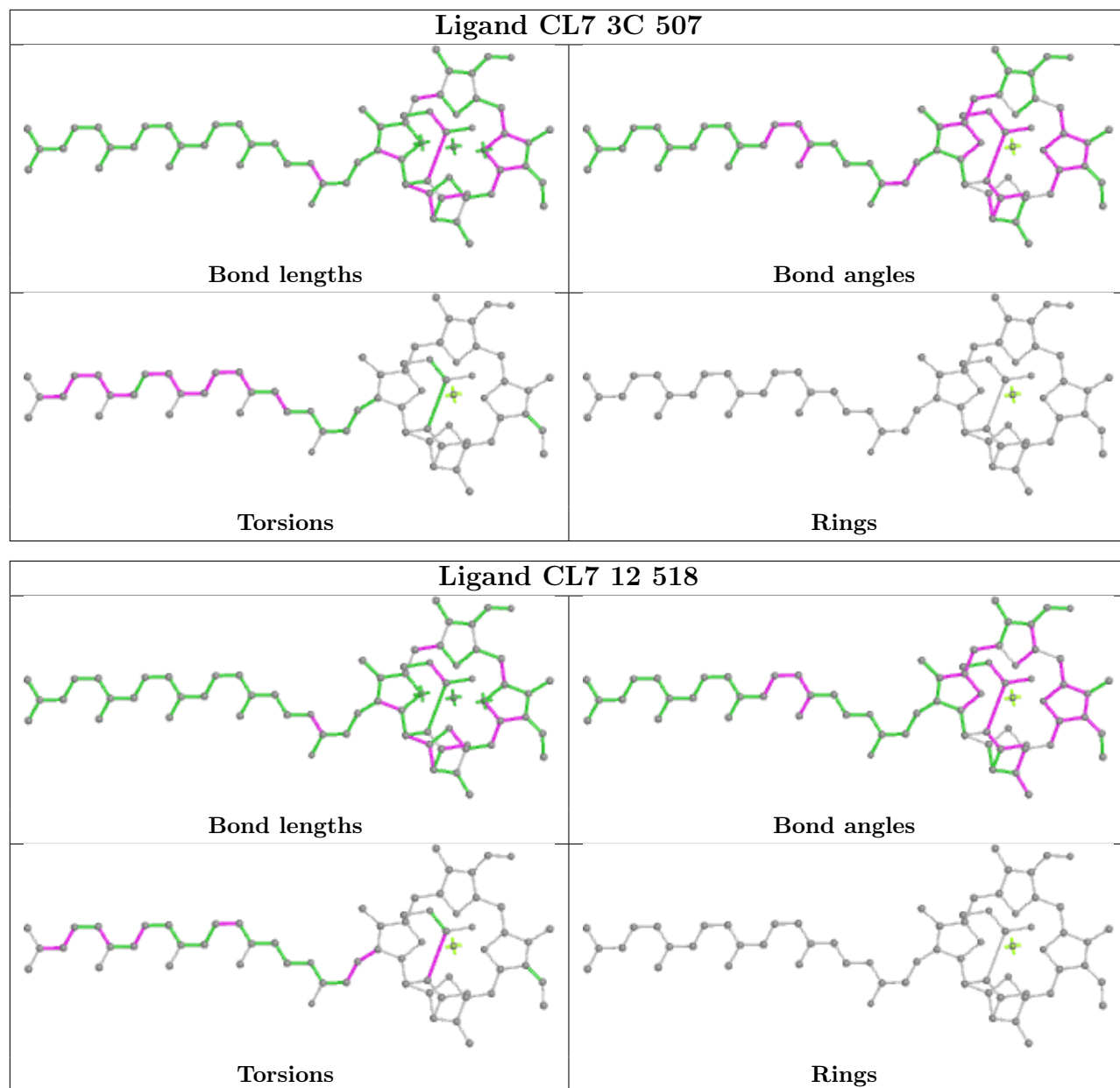
Ligand HEM 2F 101

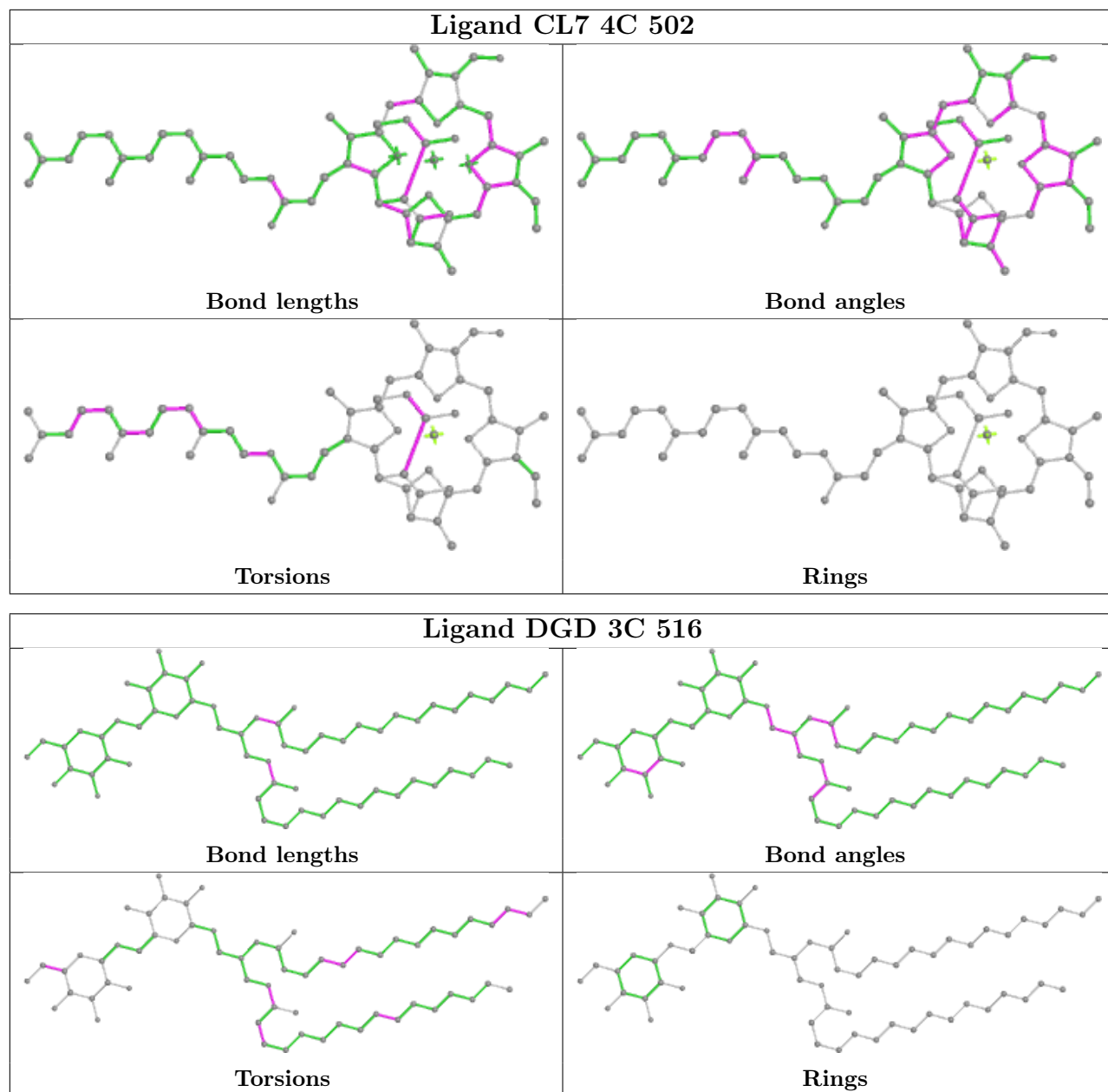


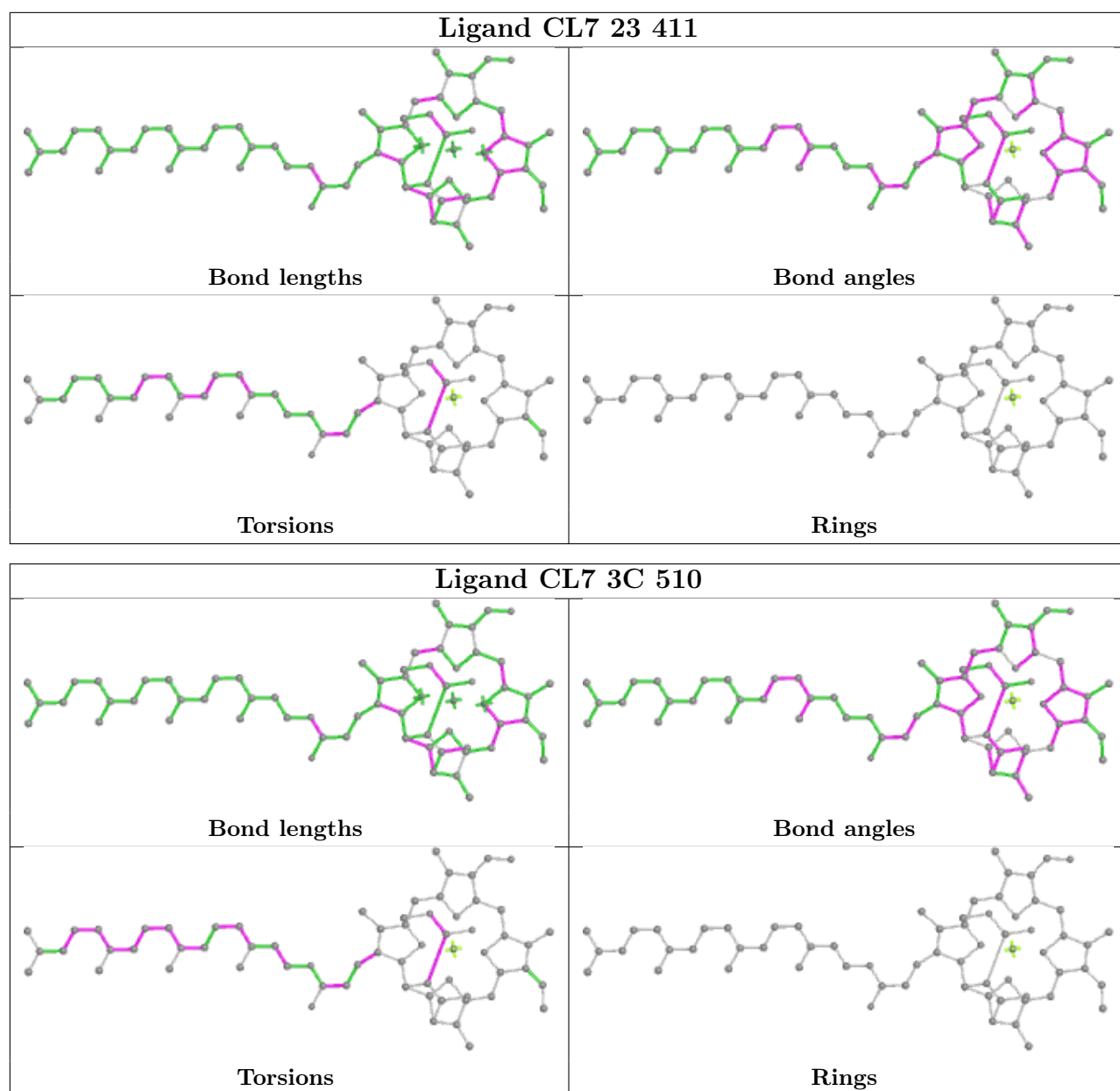
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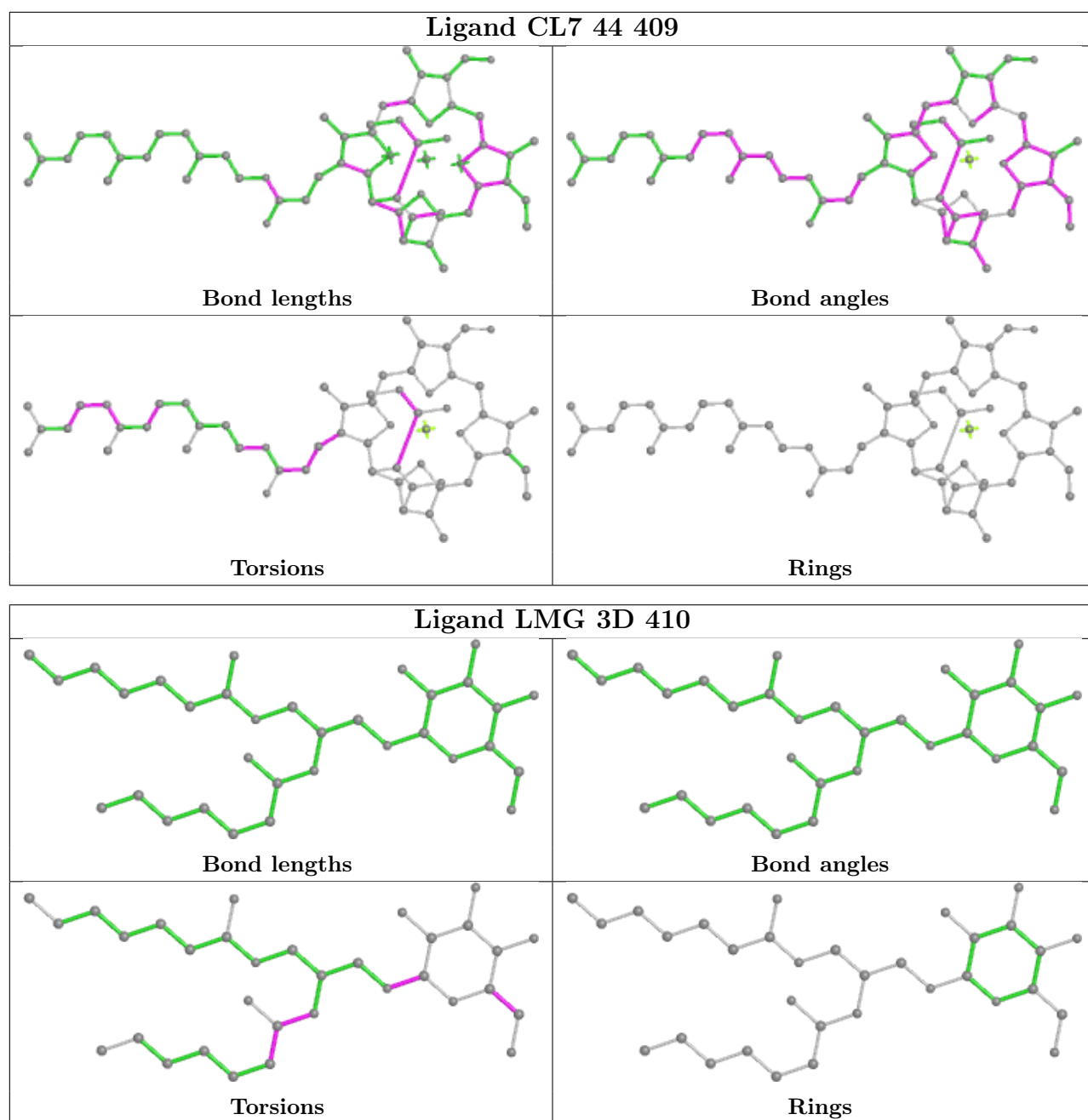


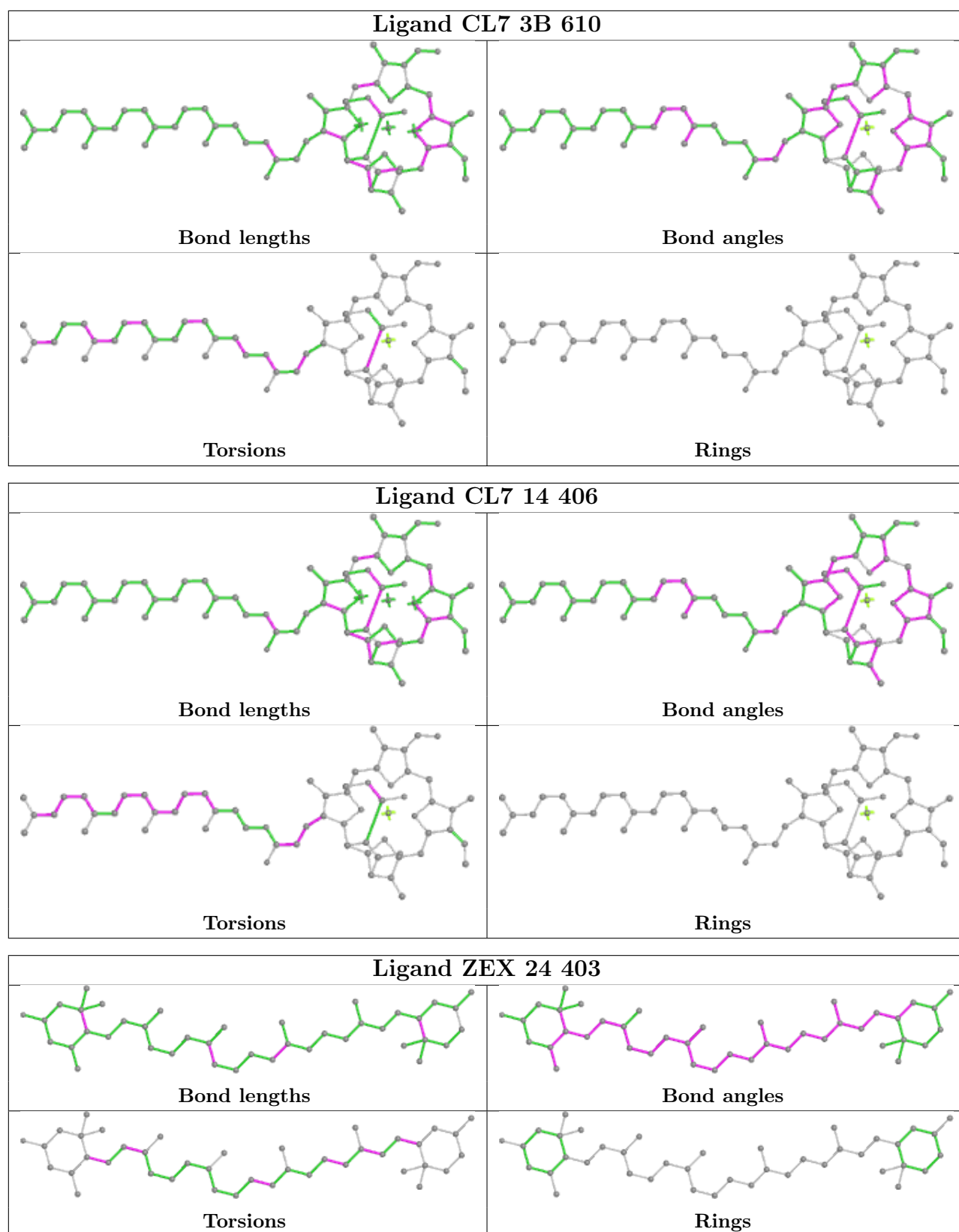




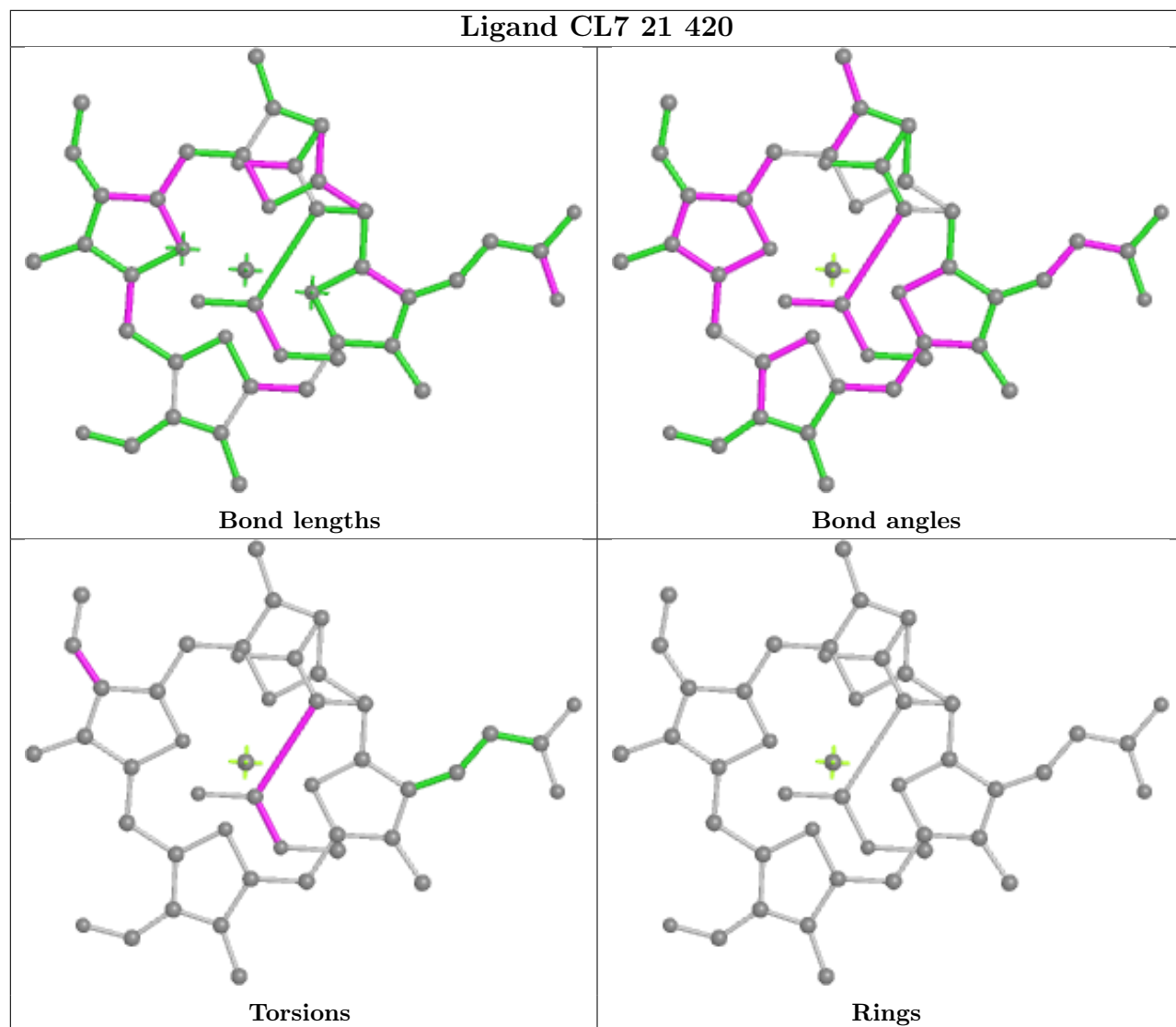


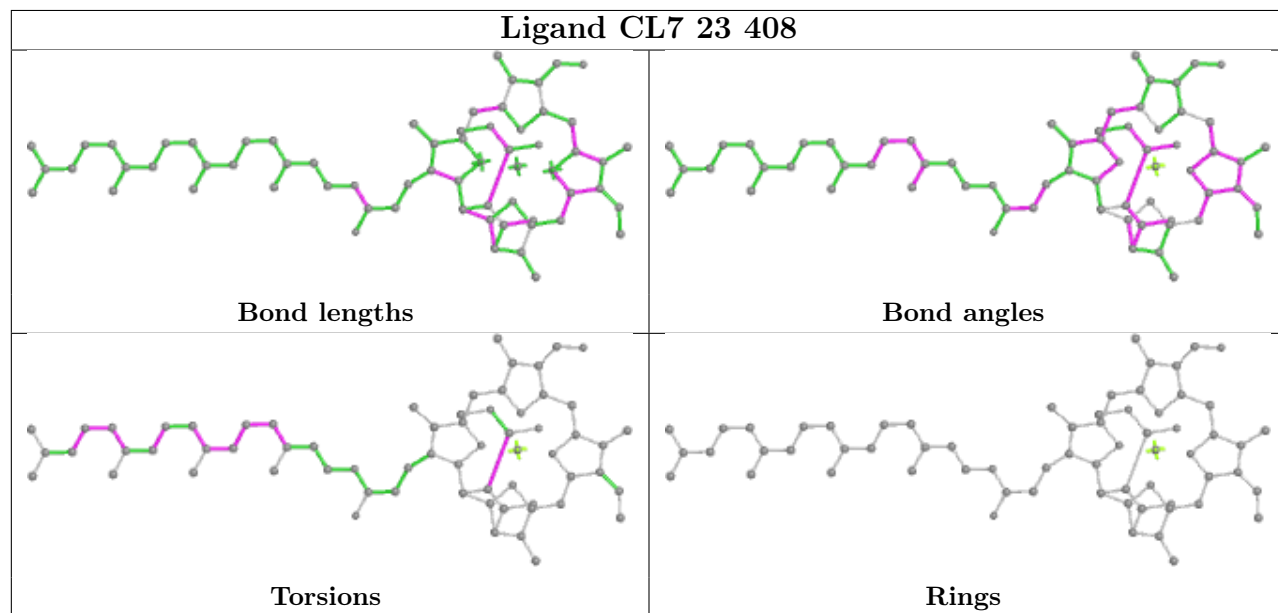
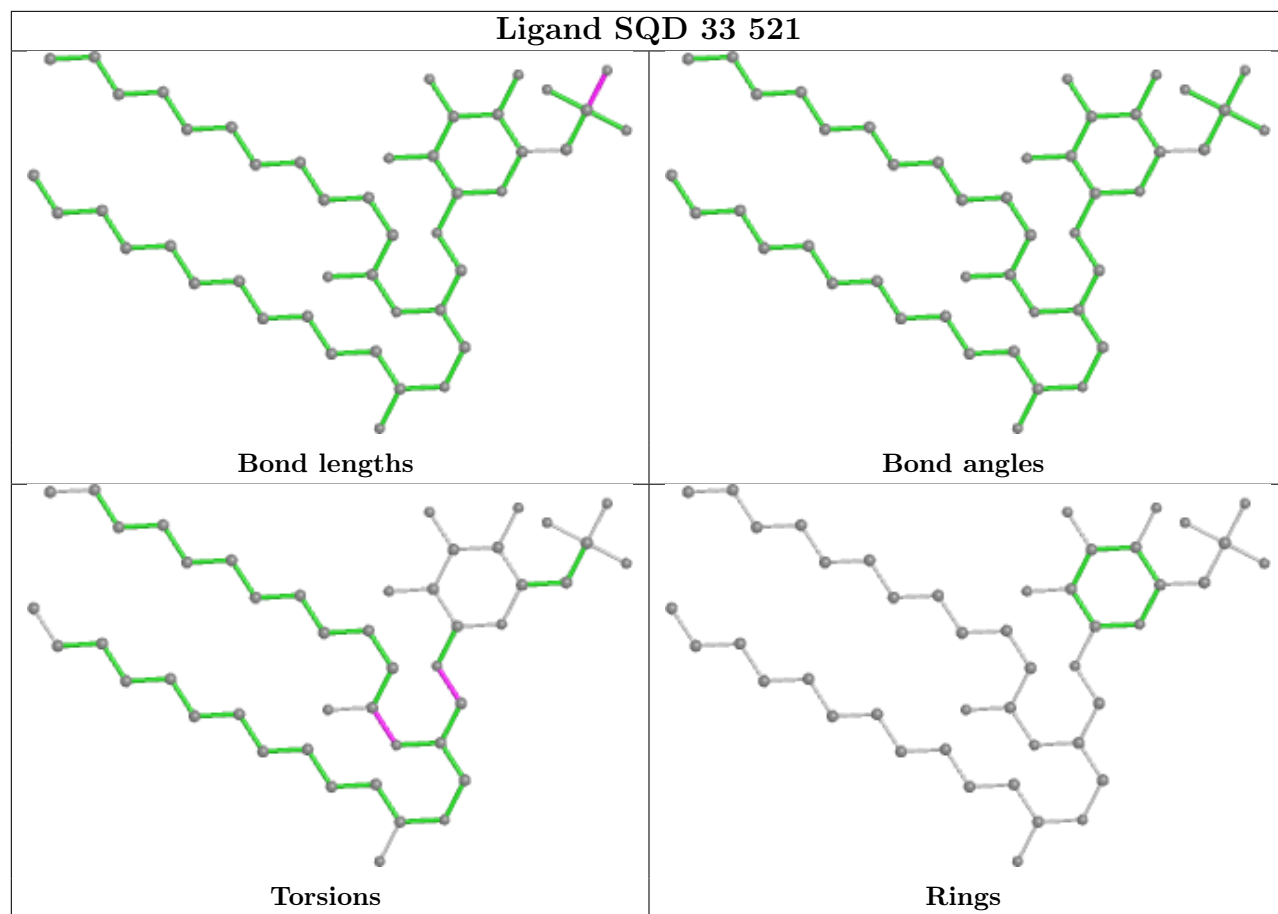


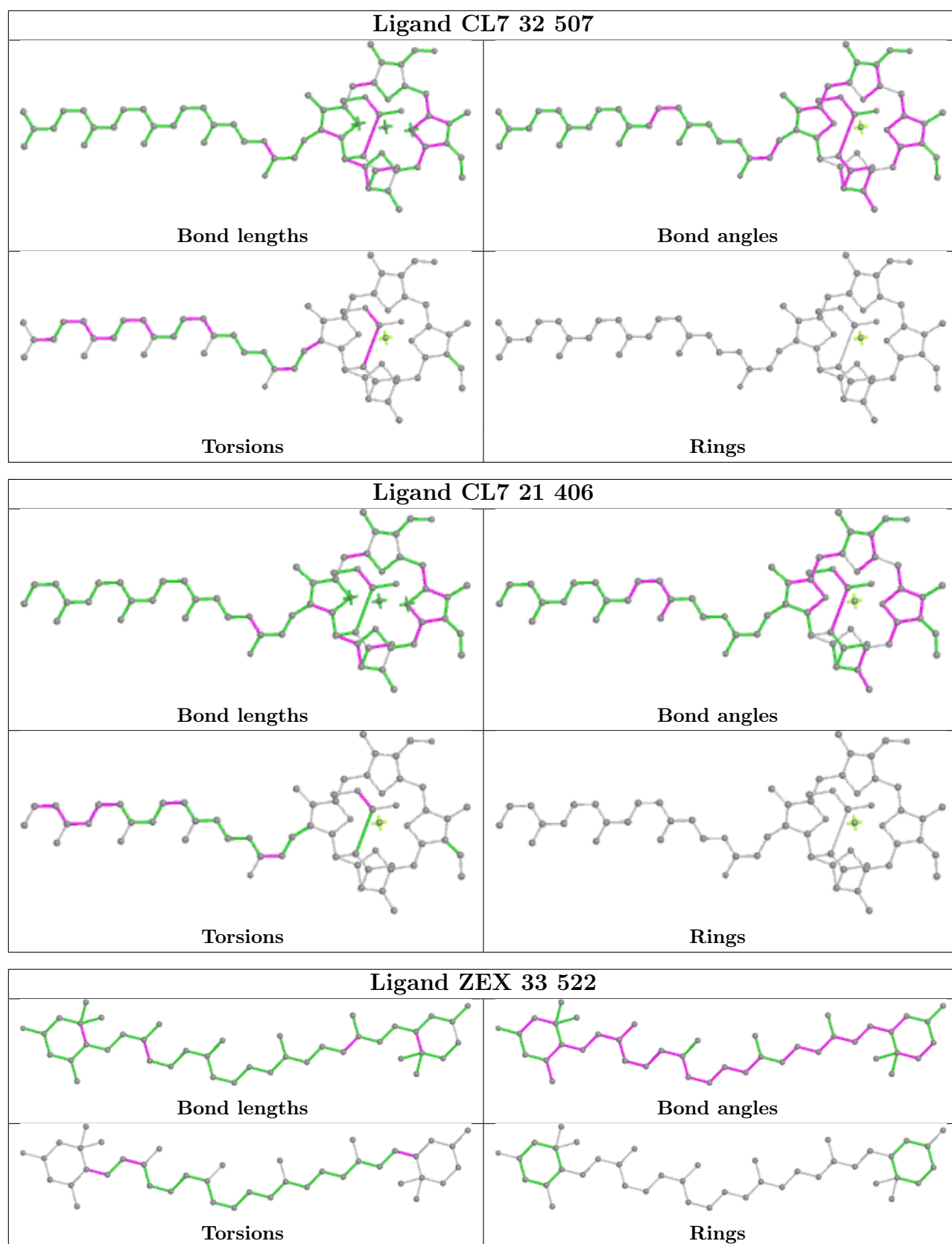




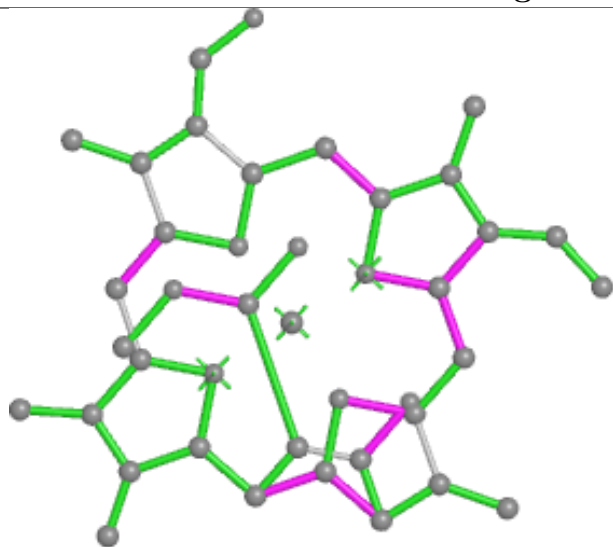
Ligand CL7 21 420



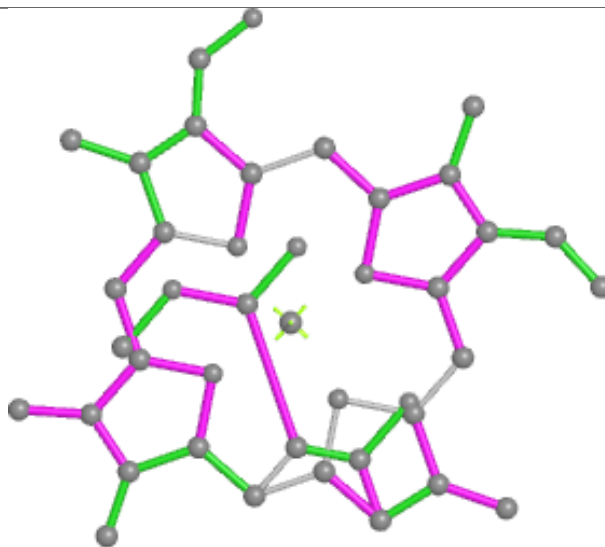




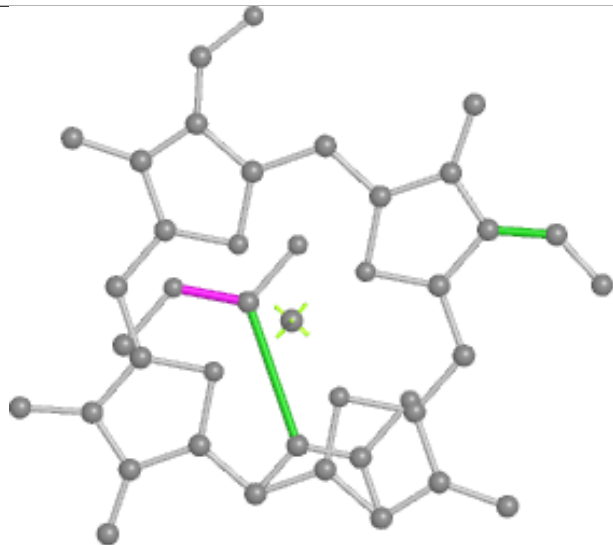
Ligand CL7 11 416



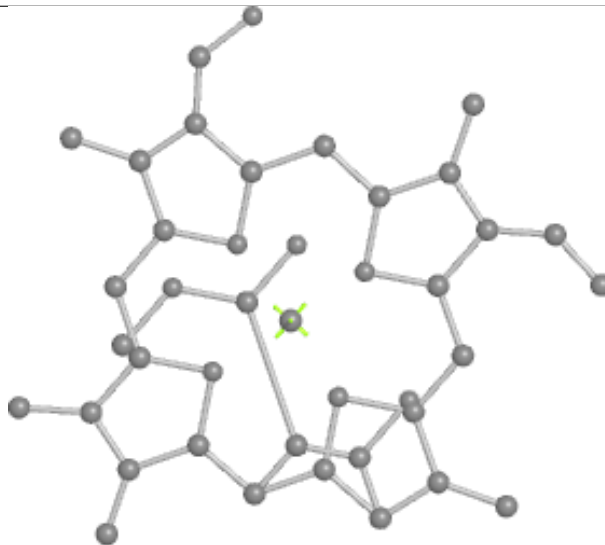
Bond lengths



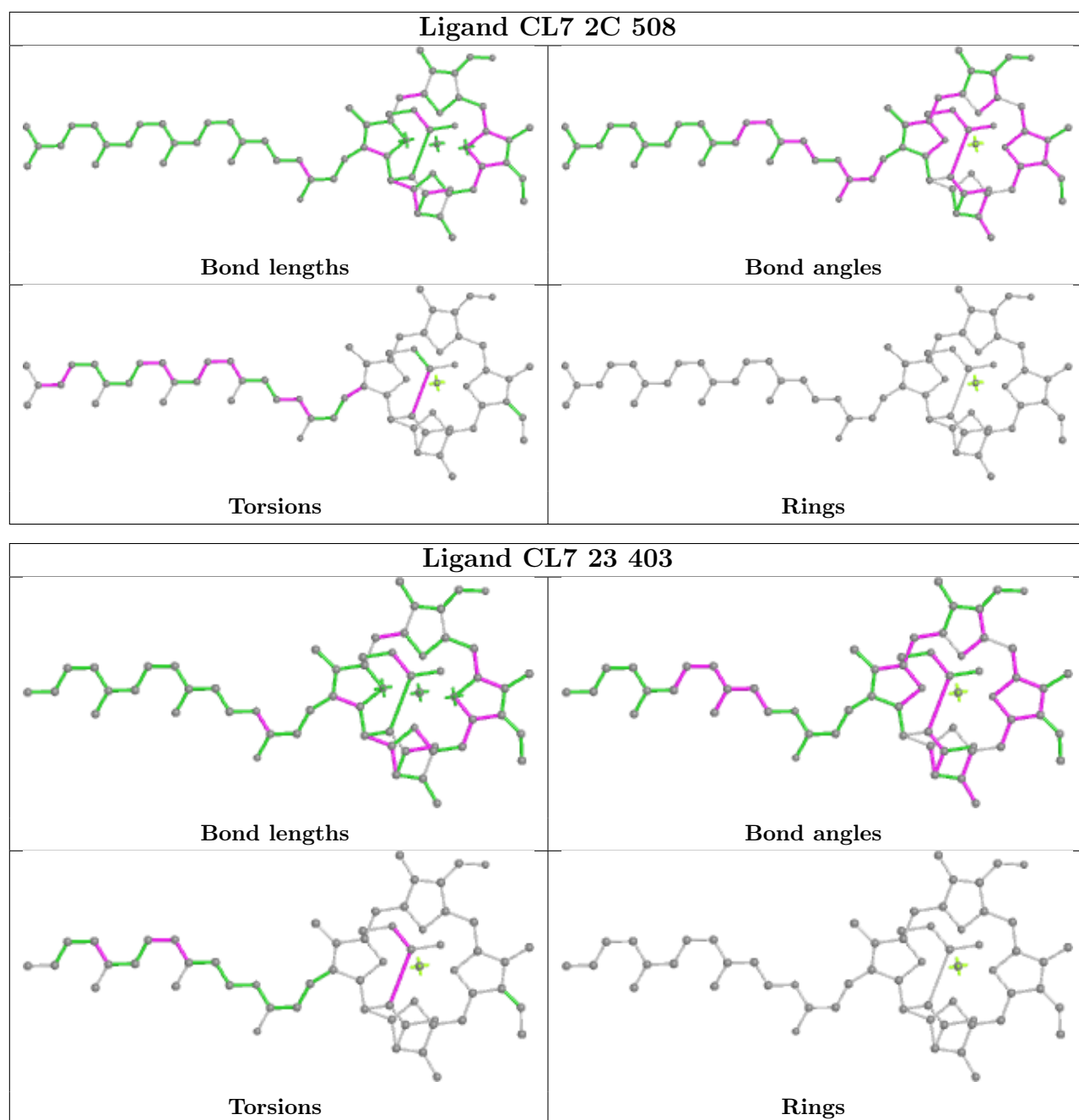
Bond angles



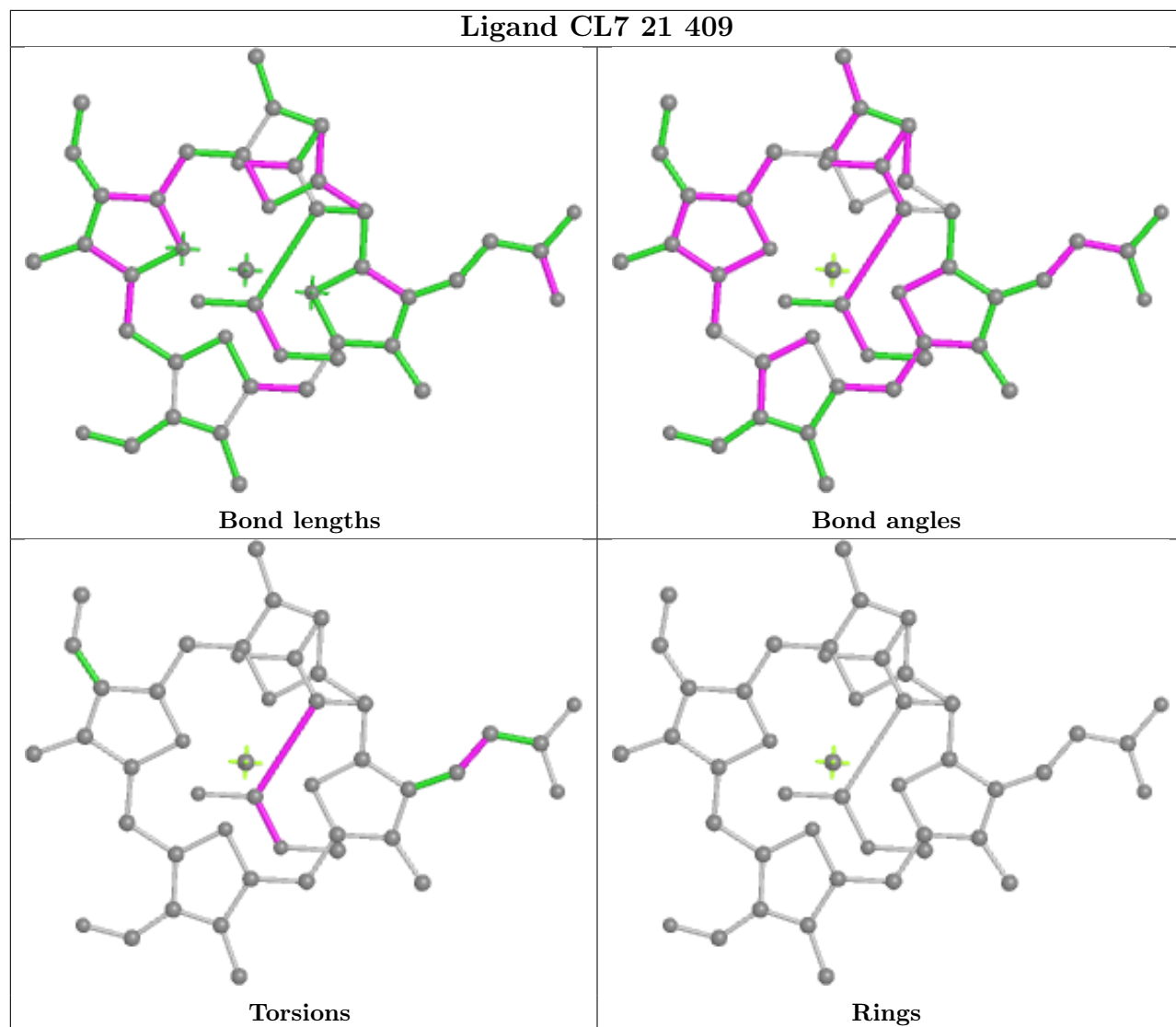
Torsions

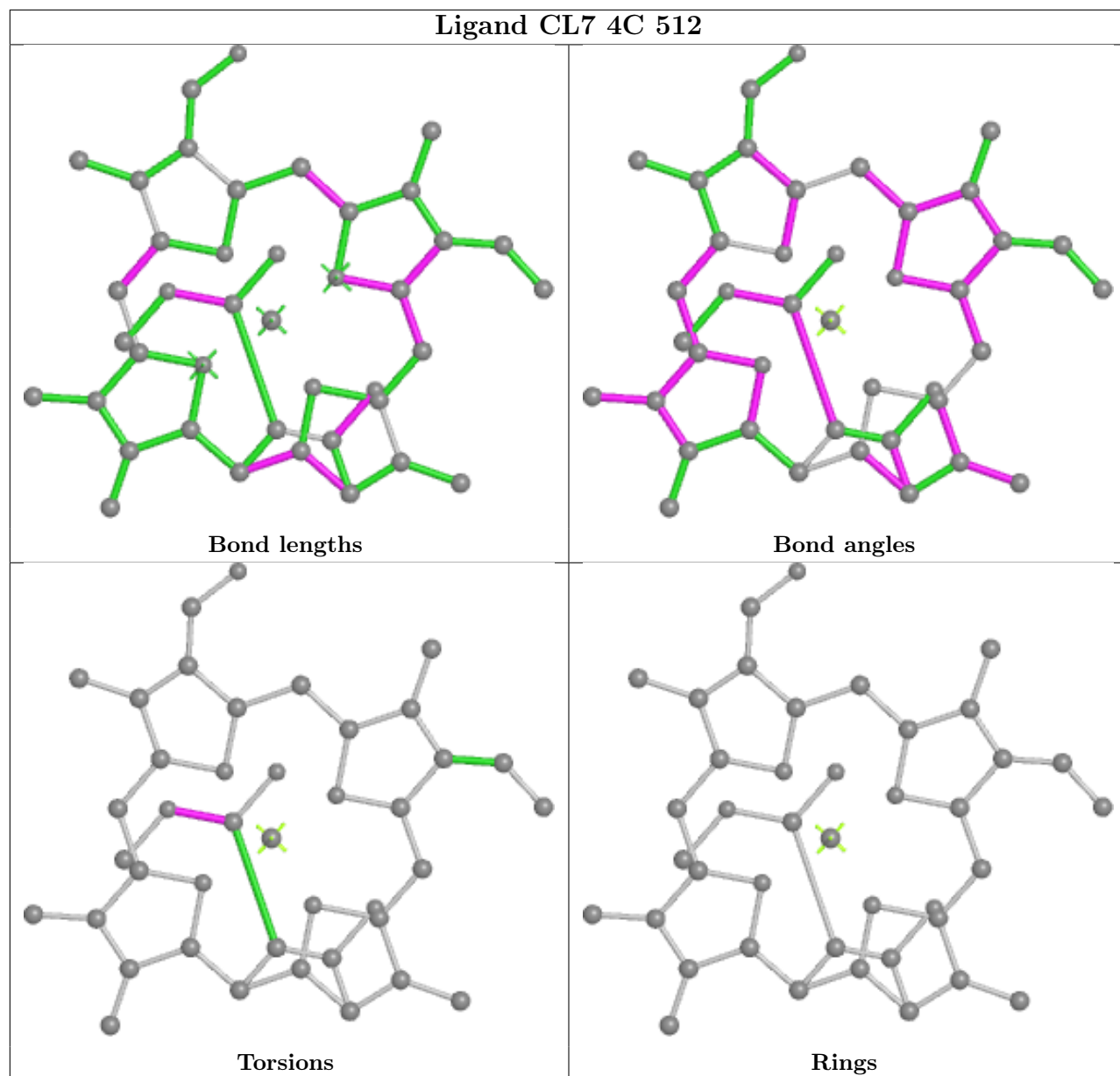


Rings

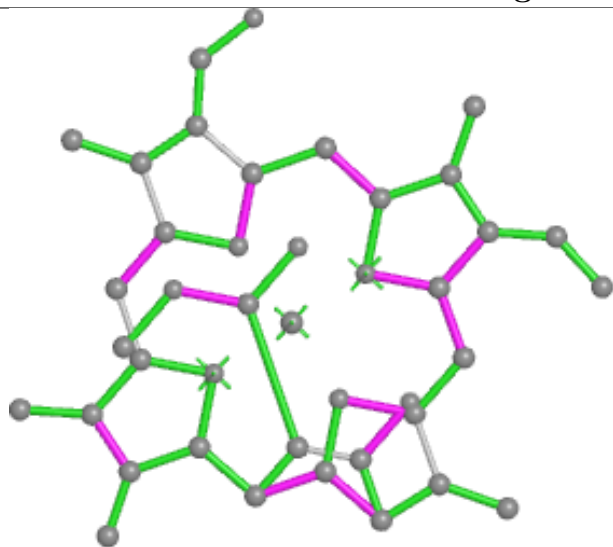


Ligand CL7 21 409

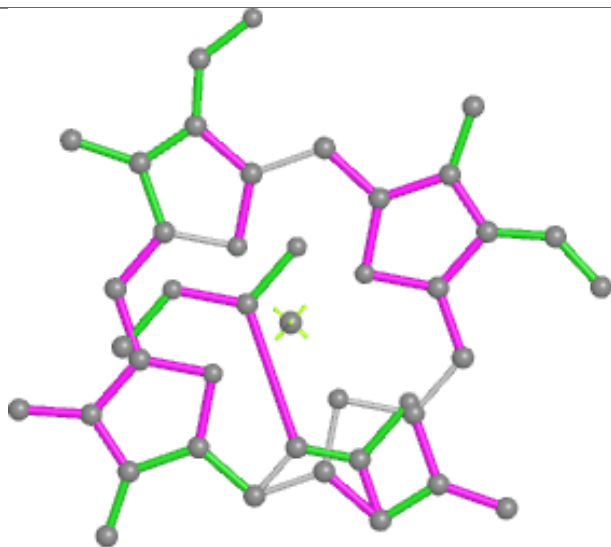




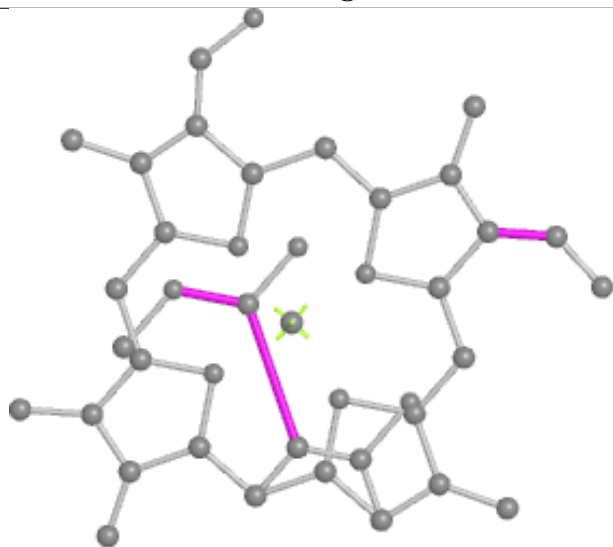
Ligand CL7 31 415



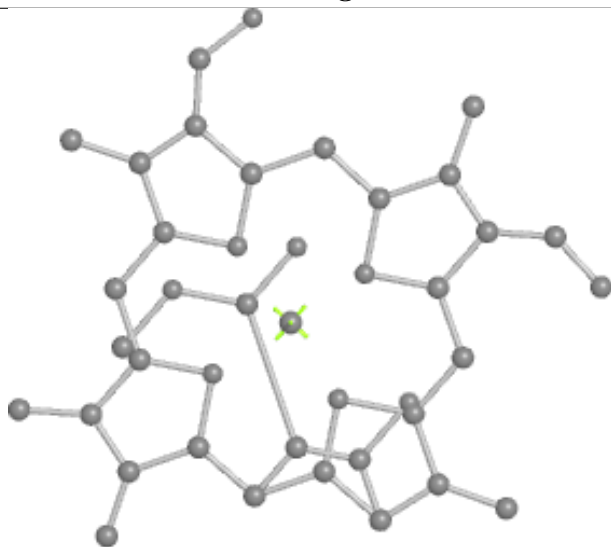
Bond lengths



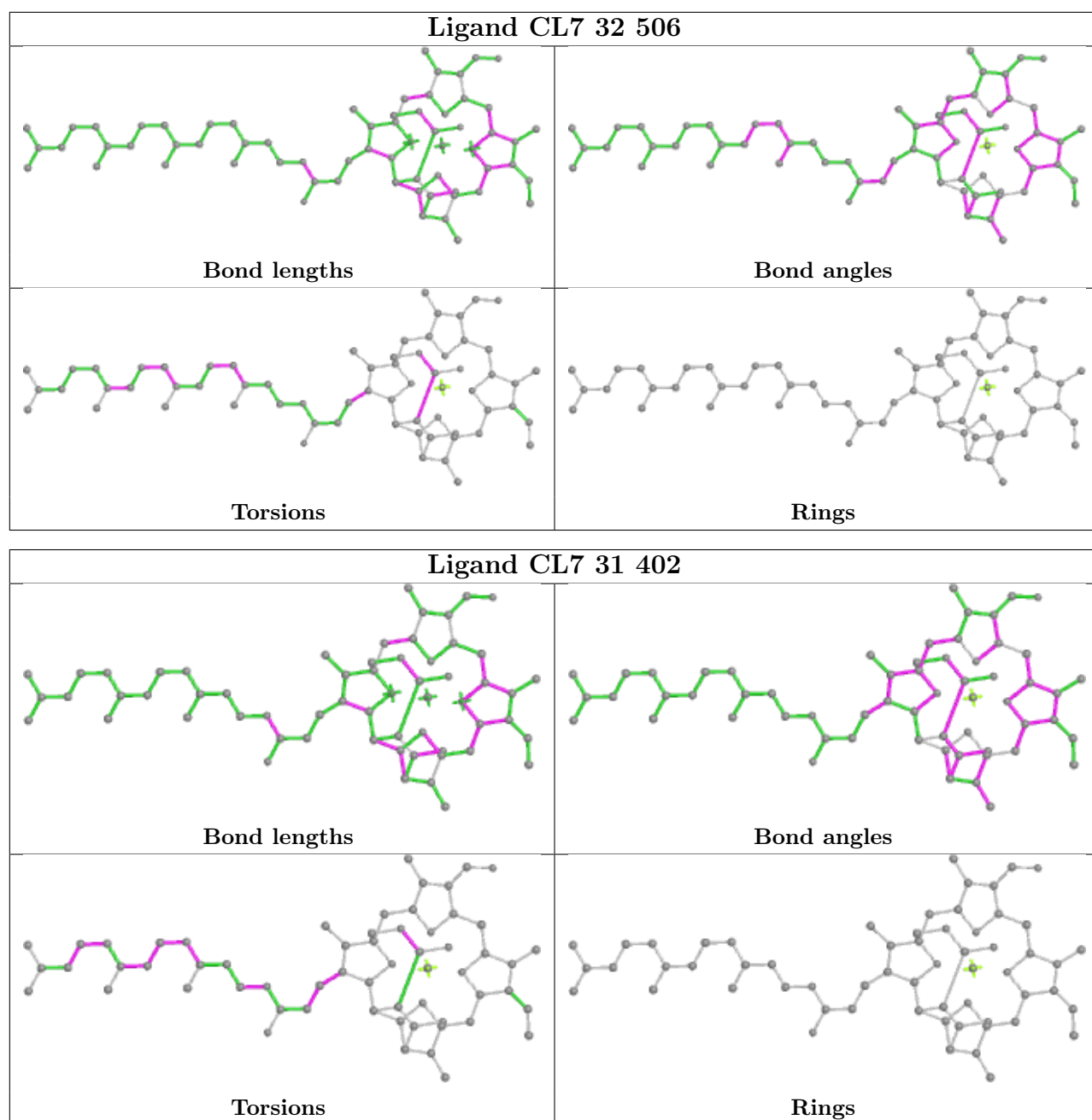
Bond angles



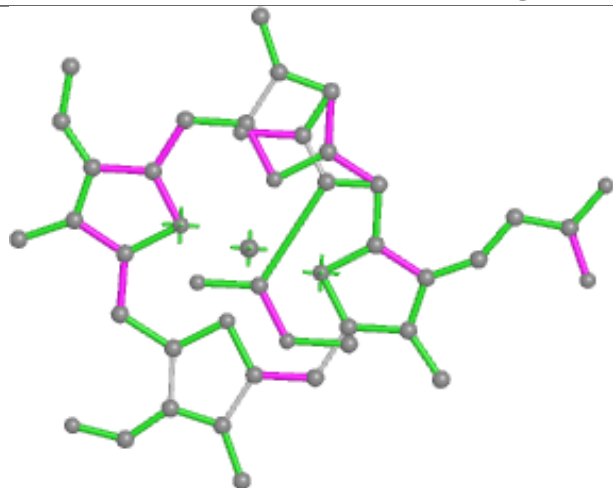
Torsions



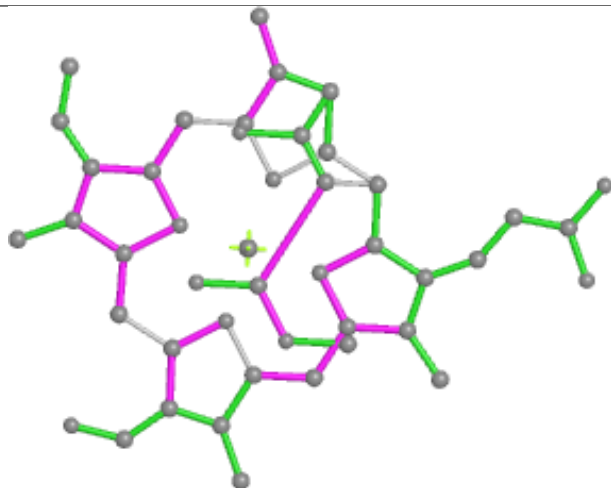
Rings



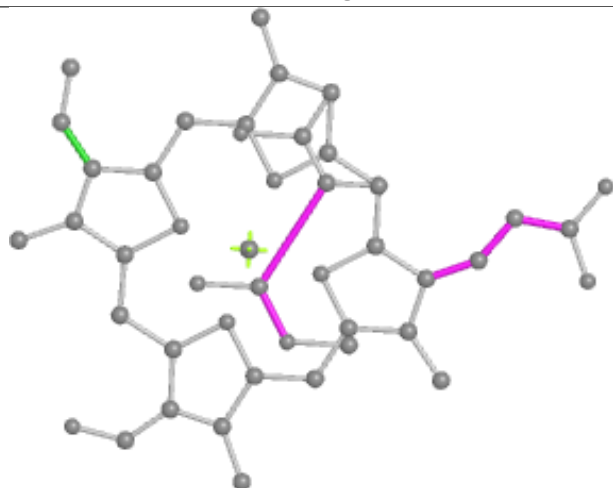
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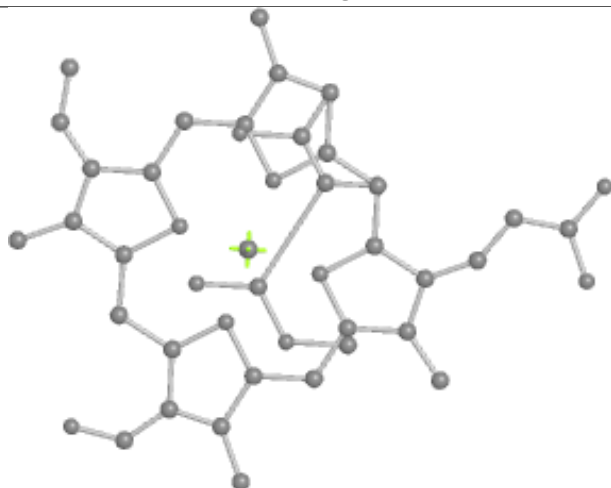
Bond lengths



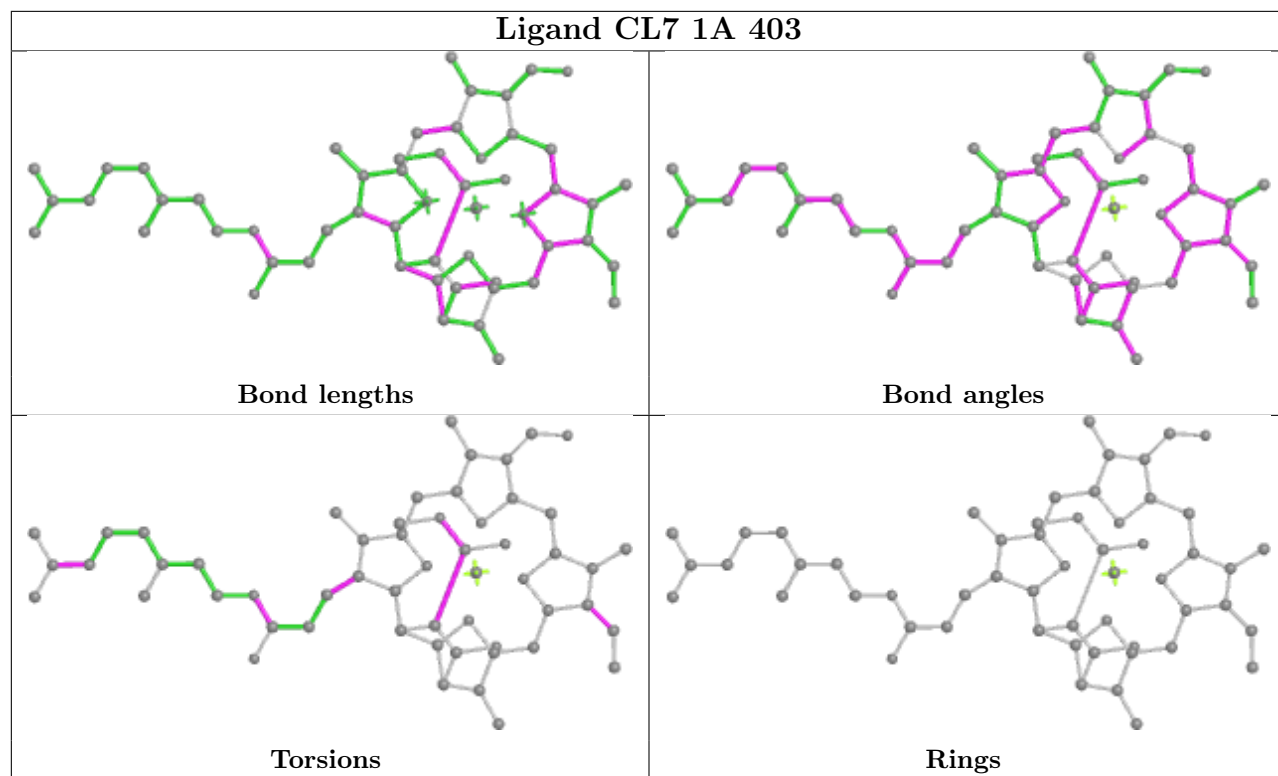
Bond angles

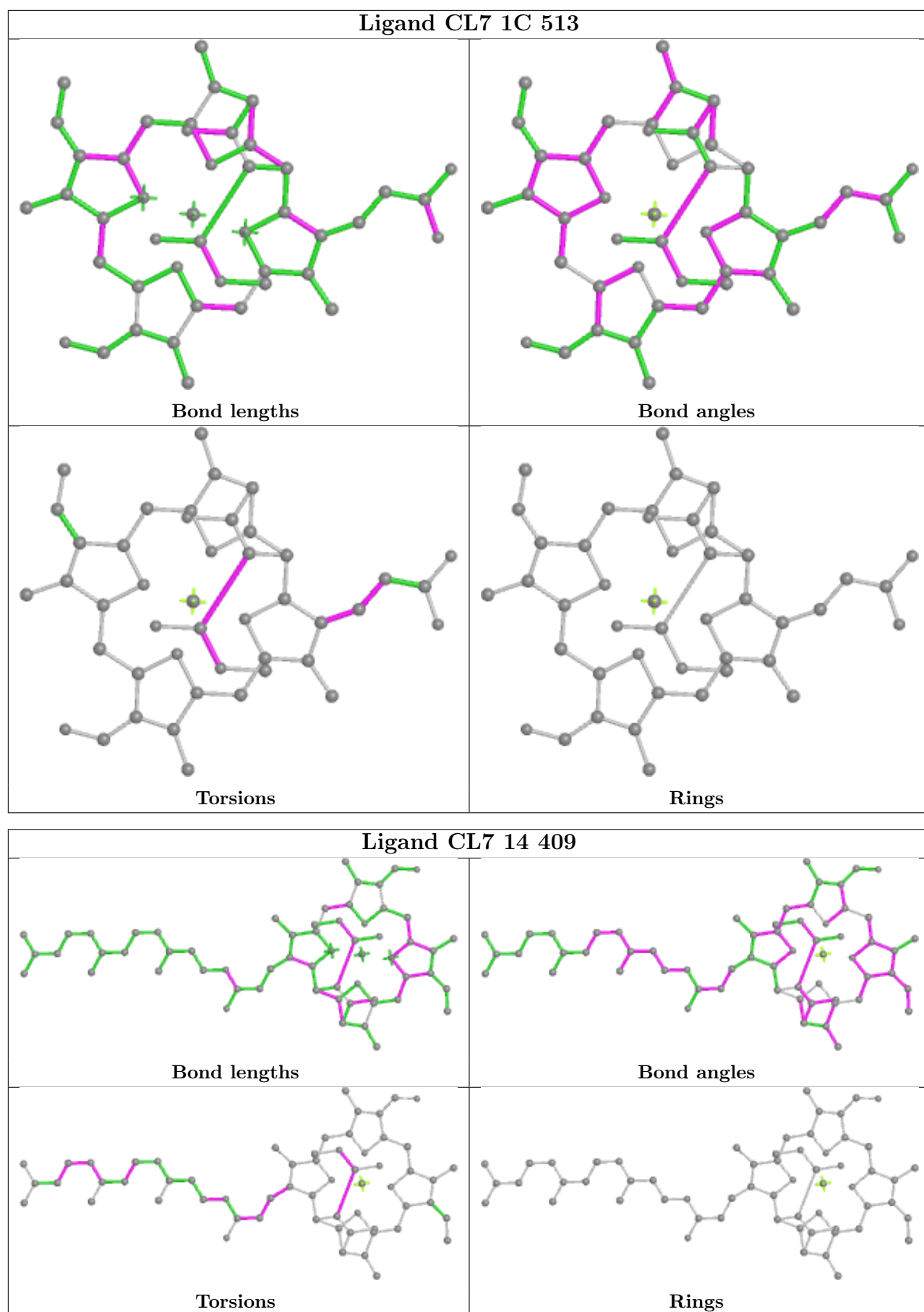


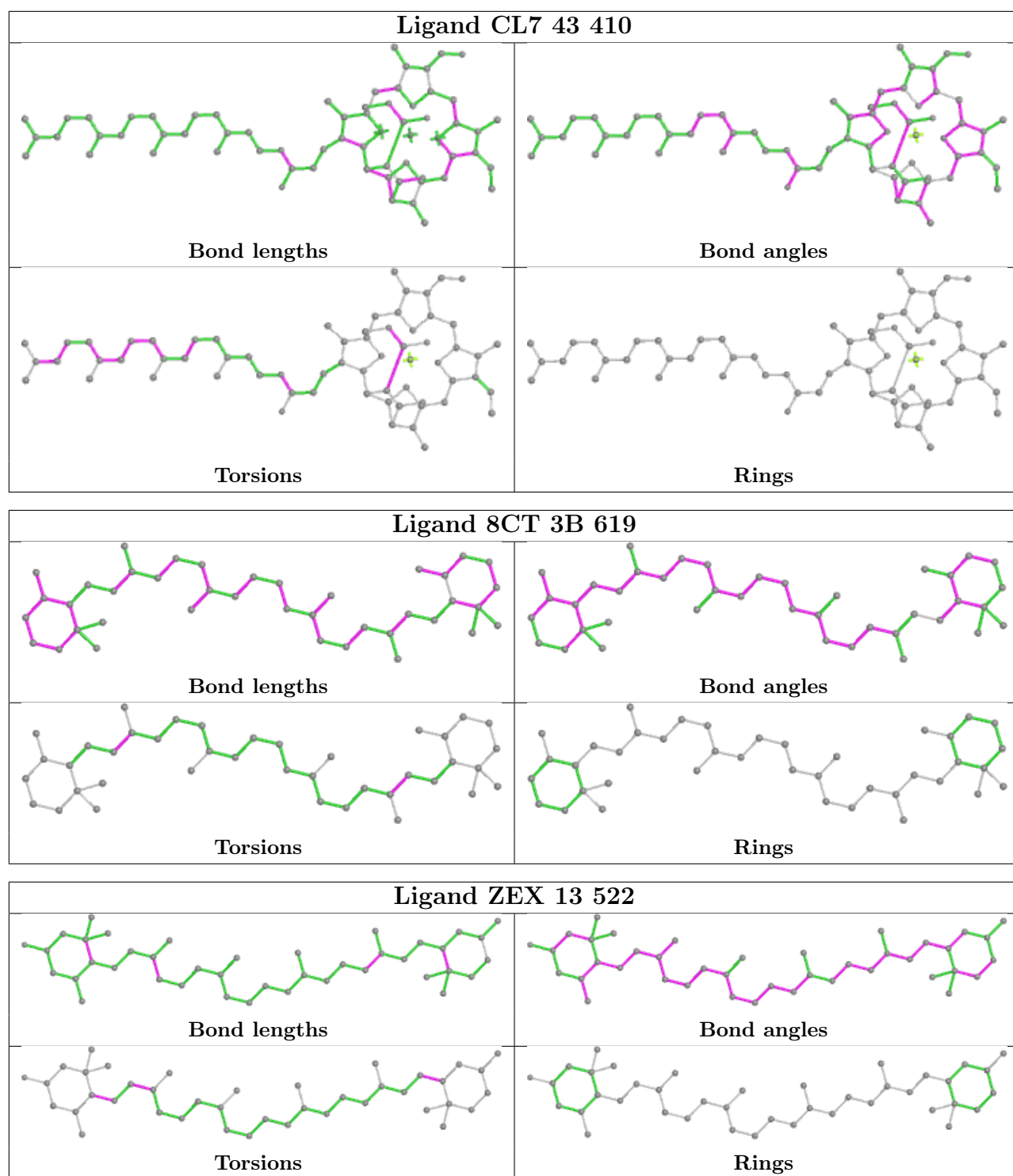
Torsions

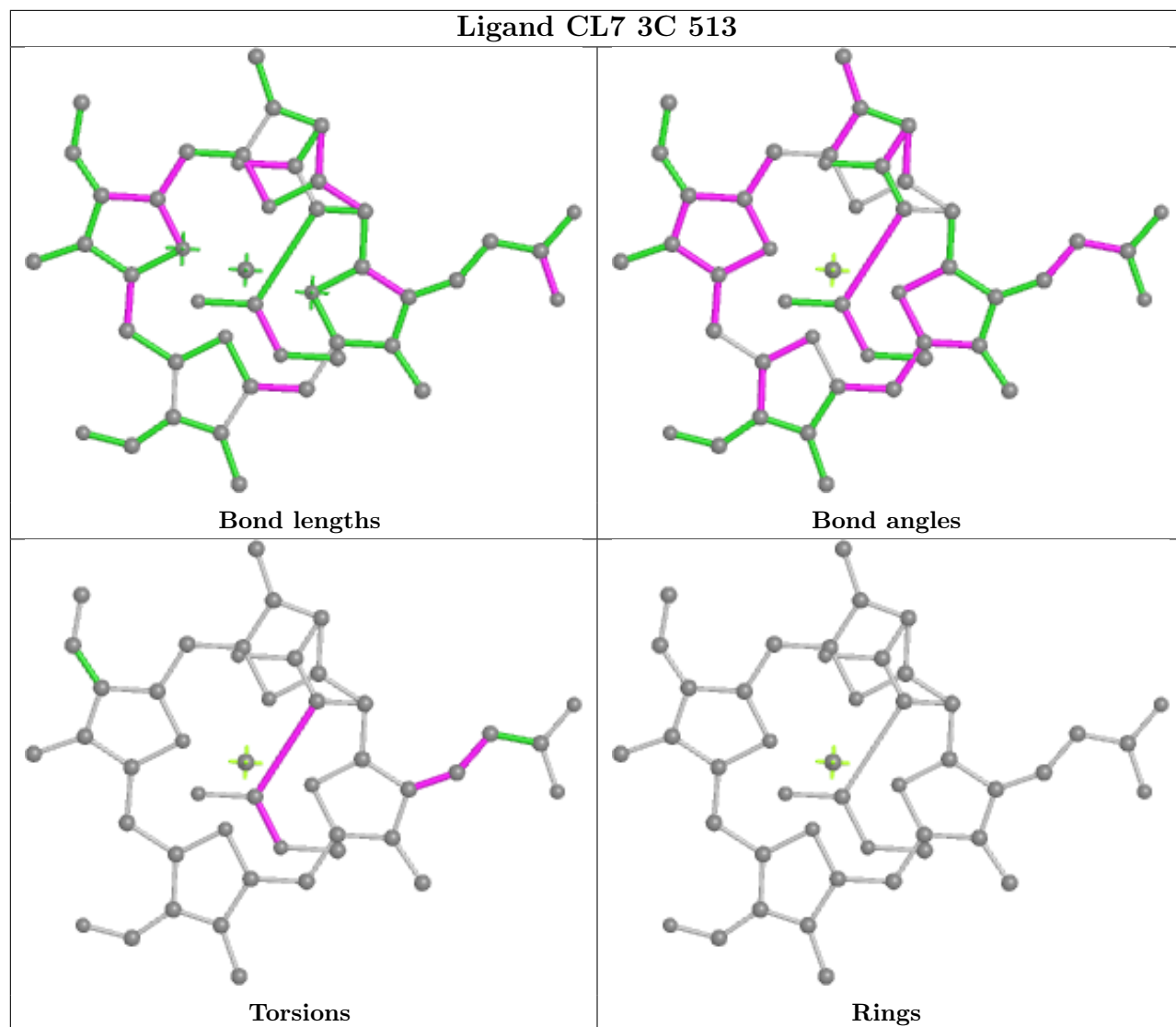


Rings

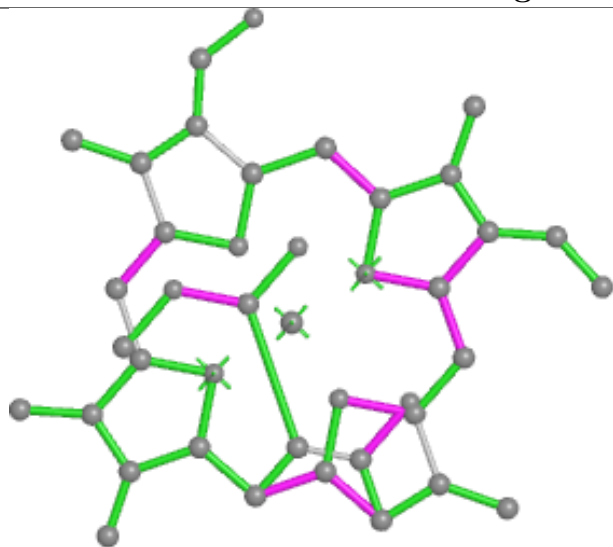




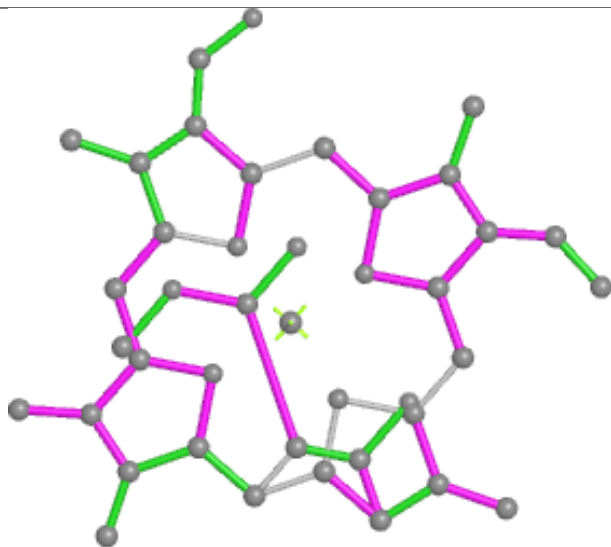




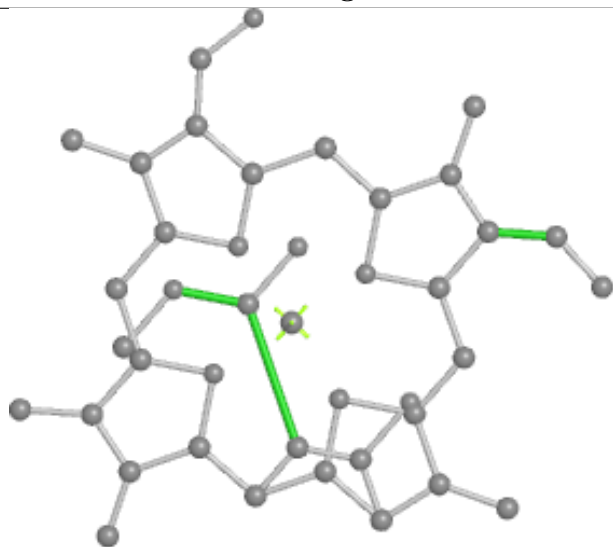
Ligand CL7 43 416



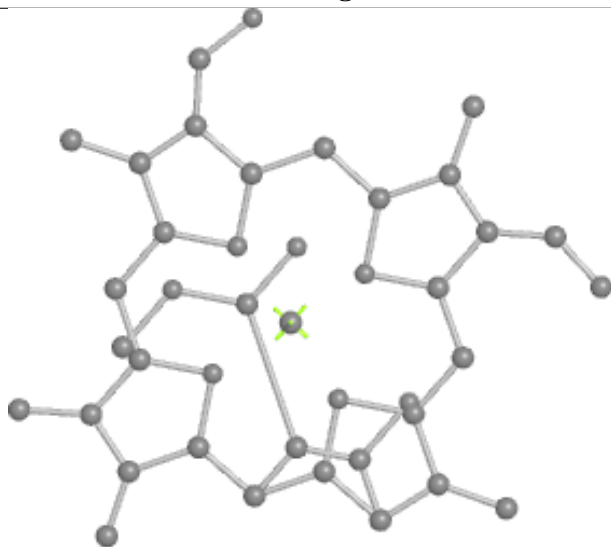
Bond lengths



Bond angles

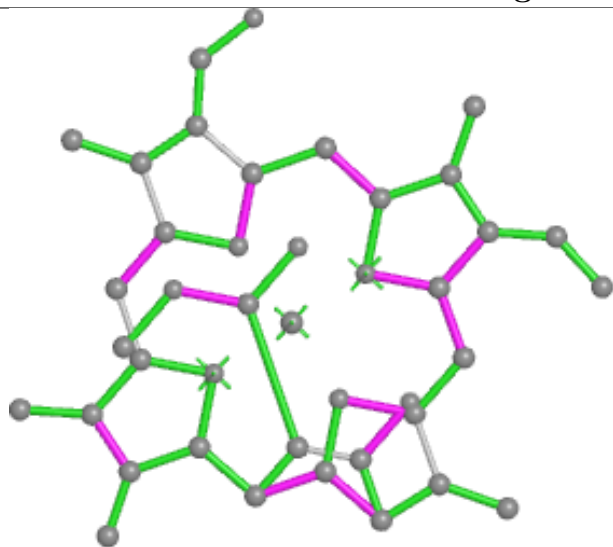


Torsions

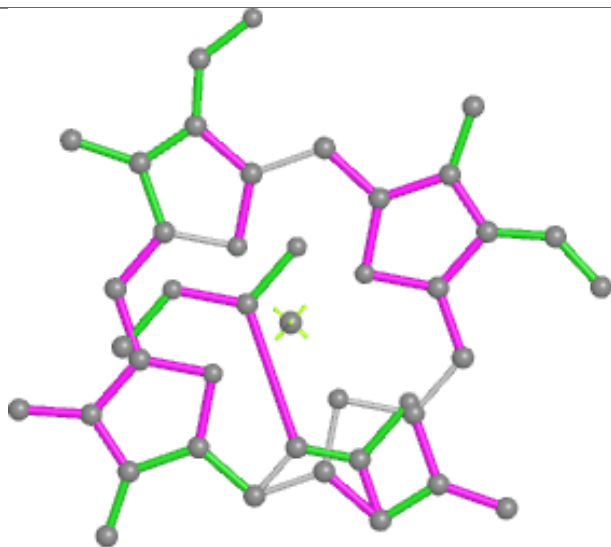


Rings

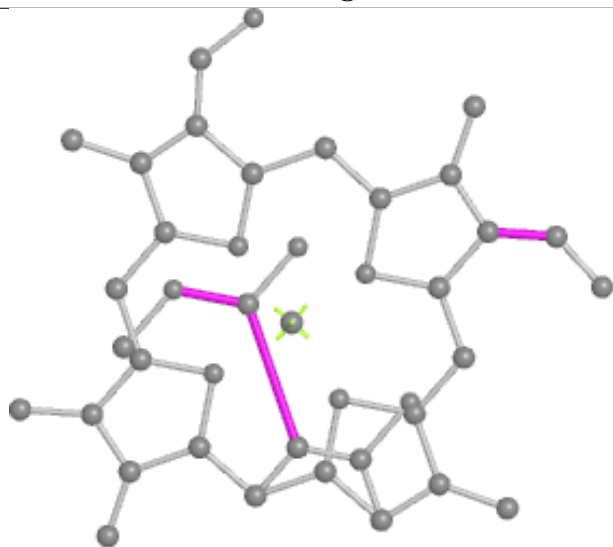
Ligand CL7 11 415



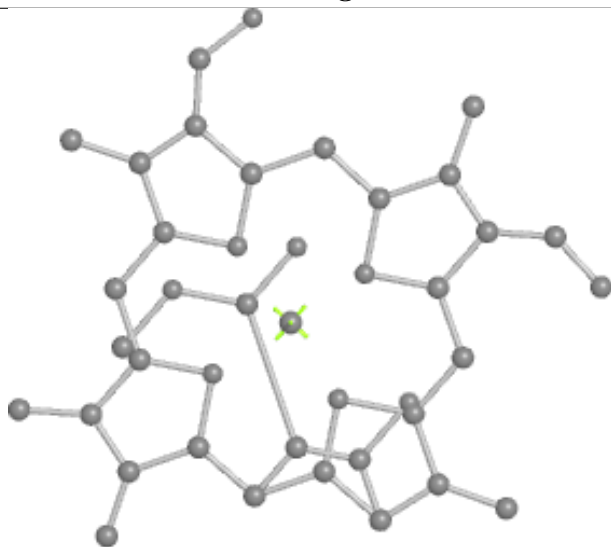
Bond lengths



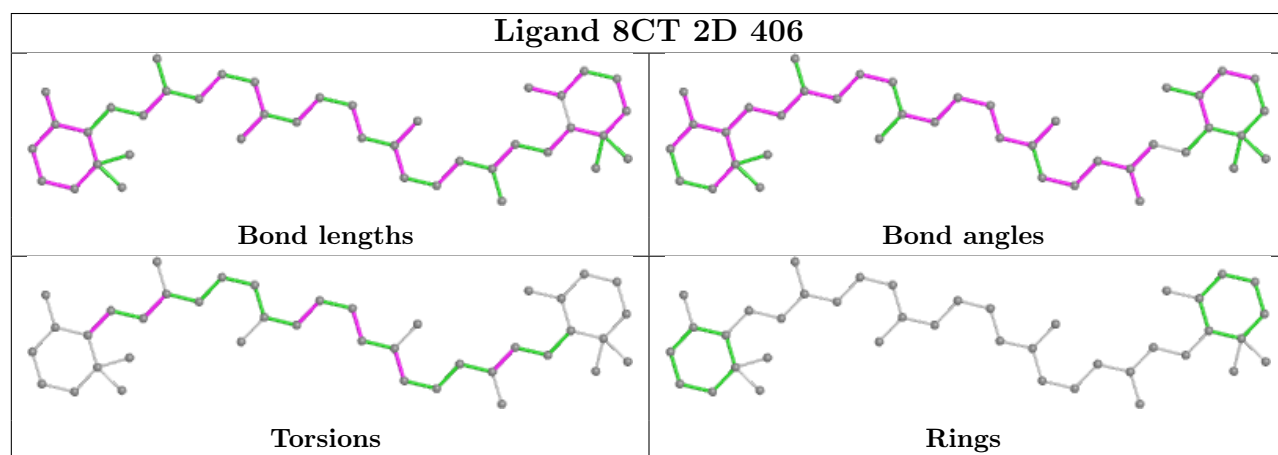
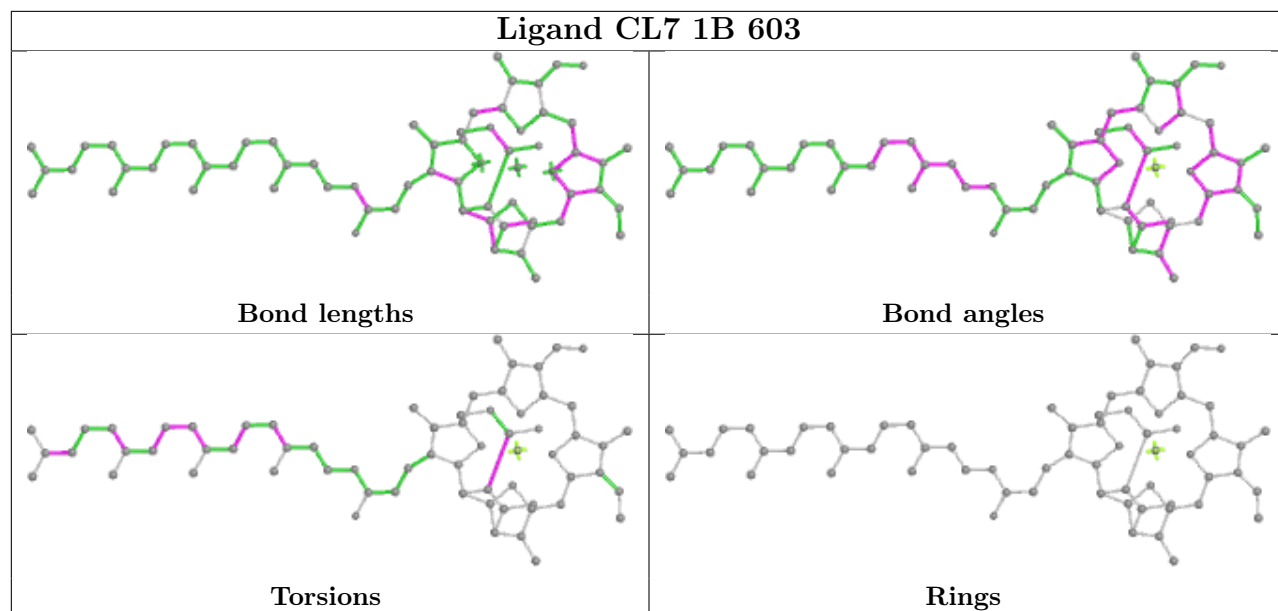
Bond angles



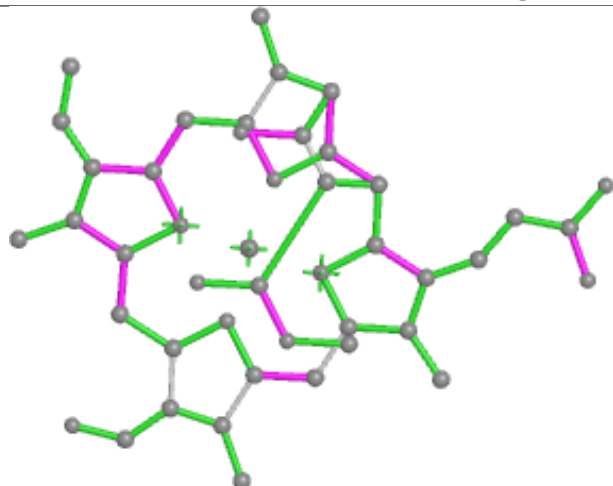
Torsions



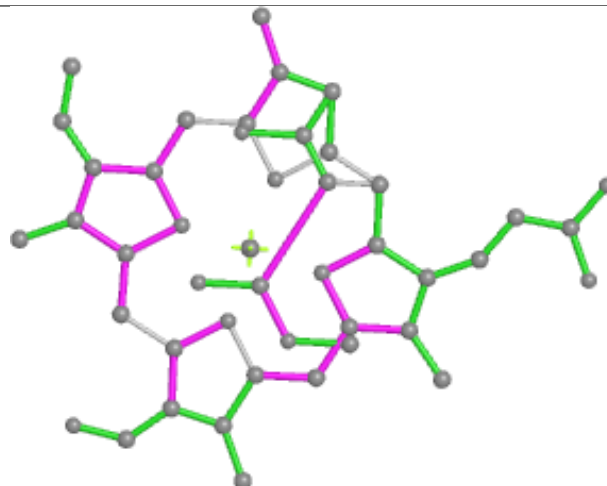
Rings



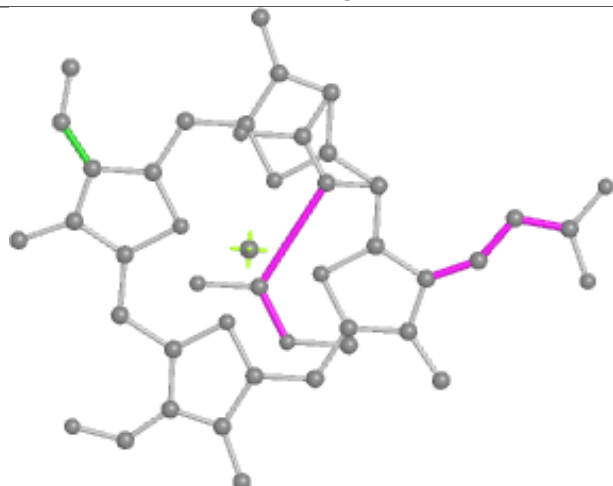
Ligand CL7 41 405



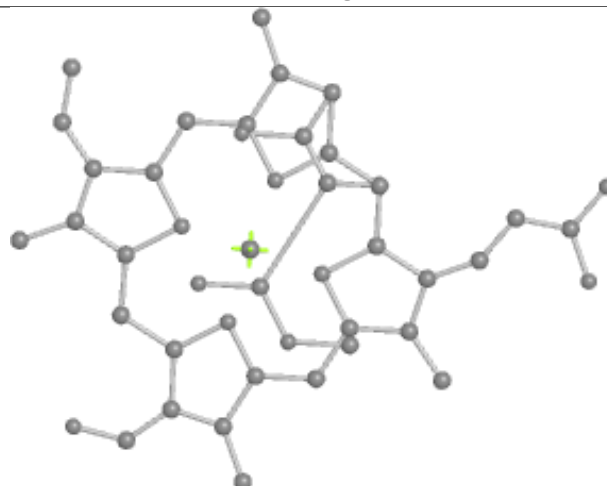
Bond lengths



Bond angles

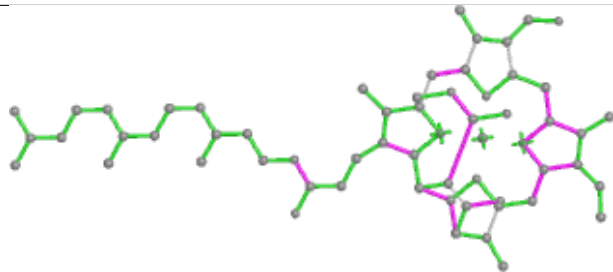


Torsions

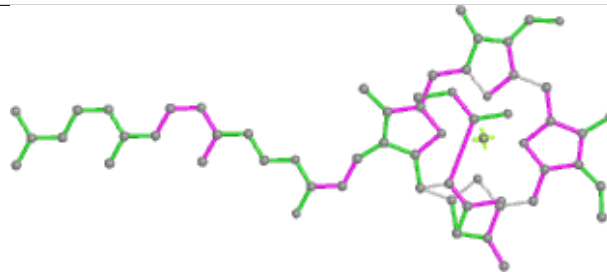


Rings

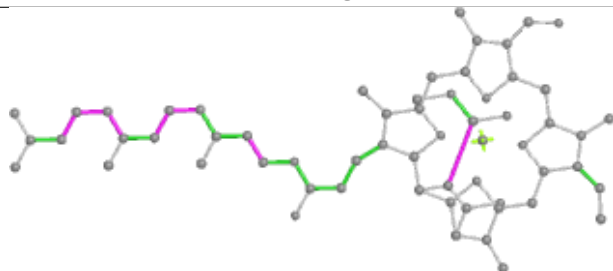
Ligand CL7 14 413



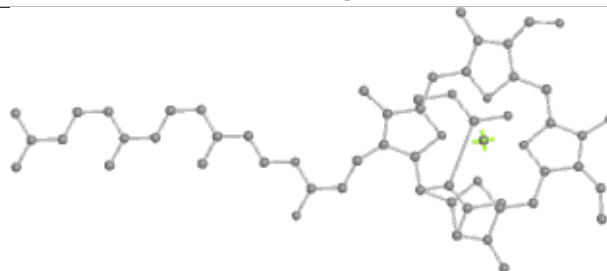
Bond lengths



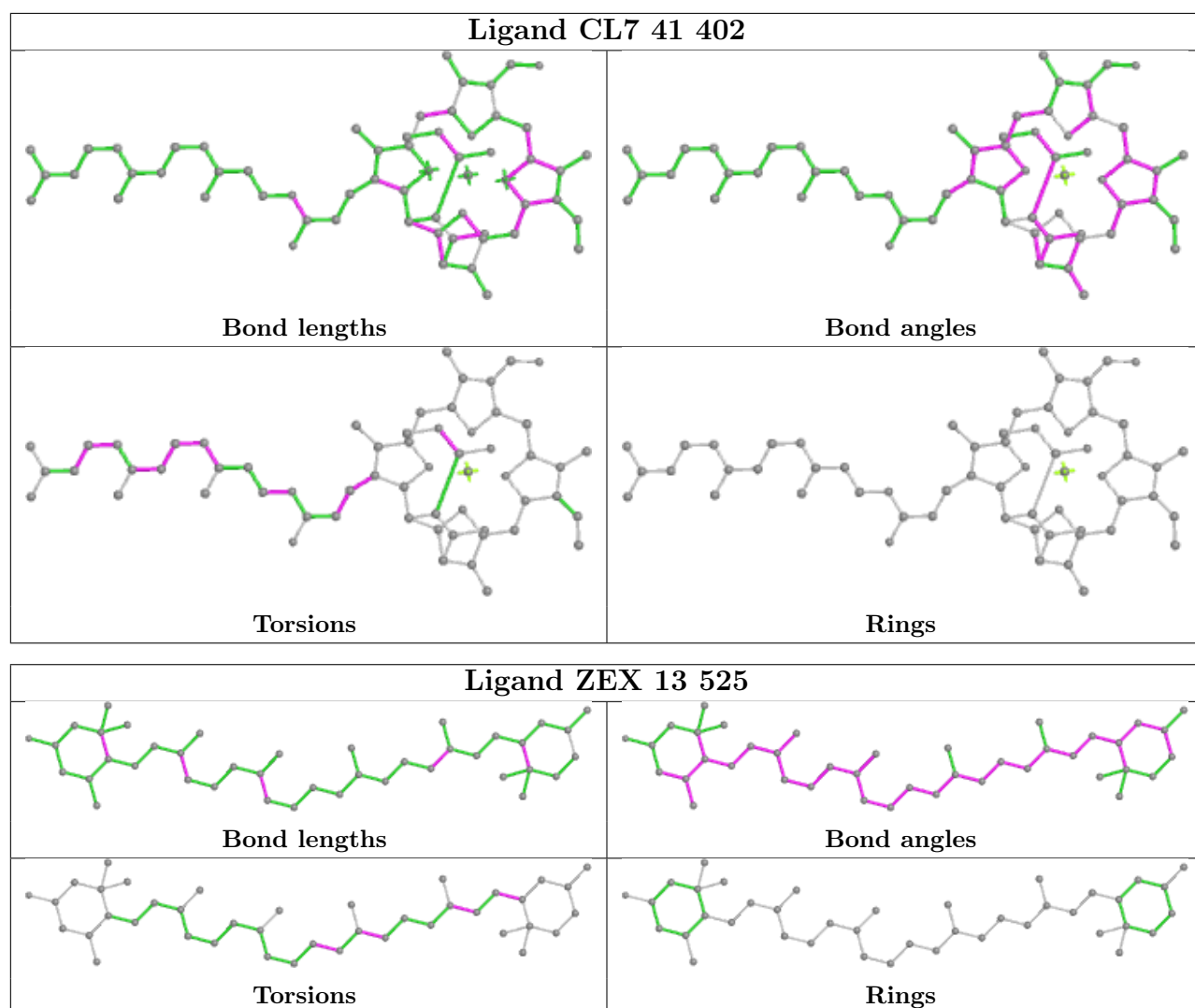
Bond angles



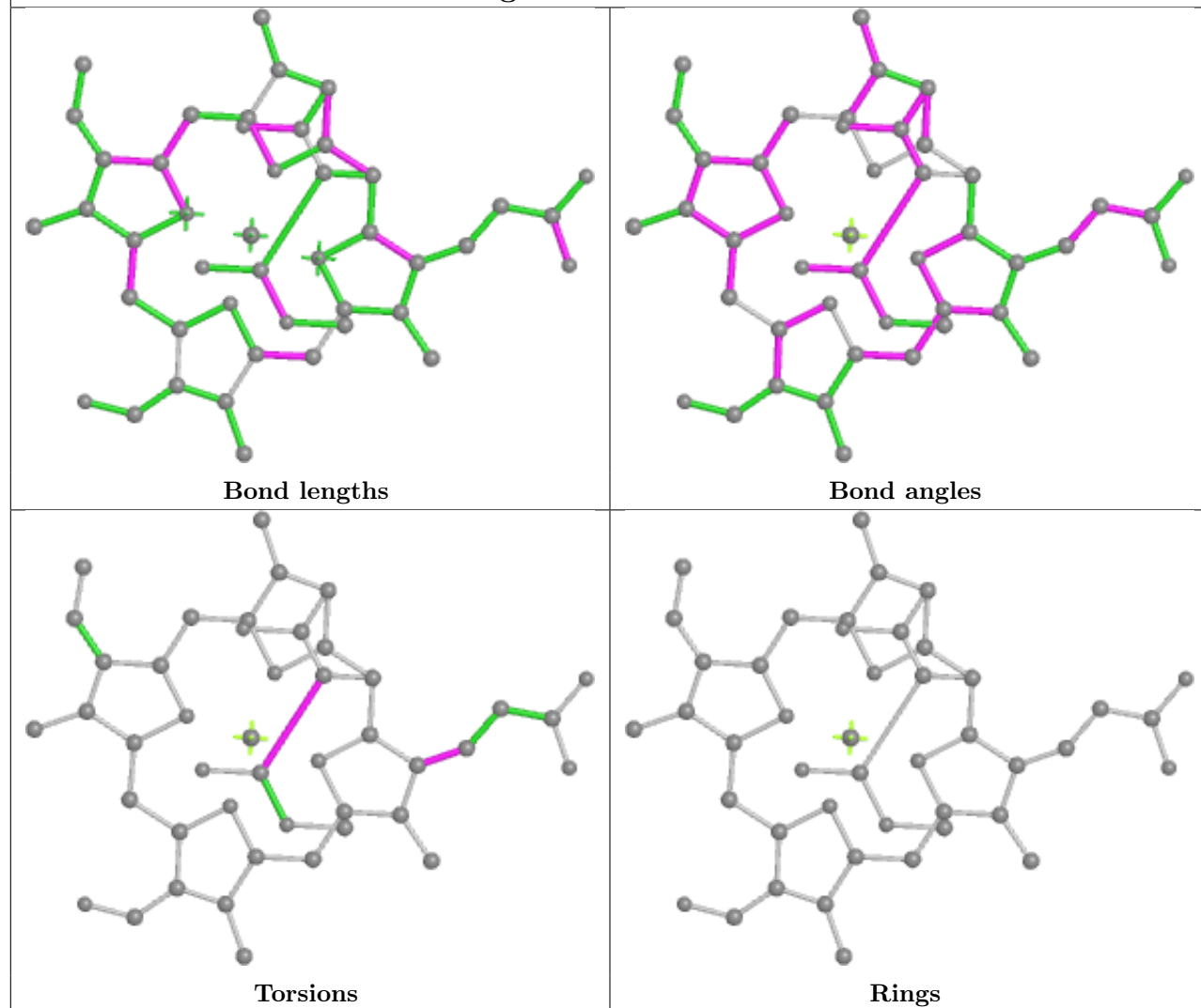
Torsions



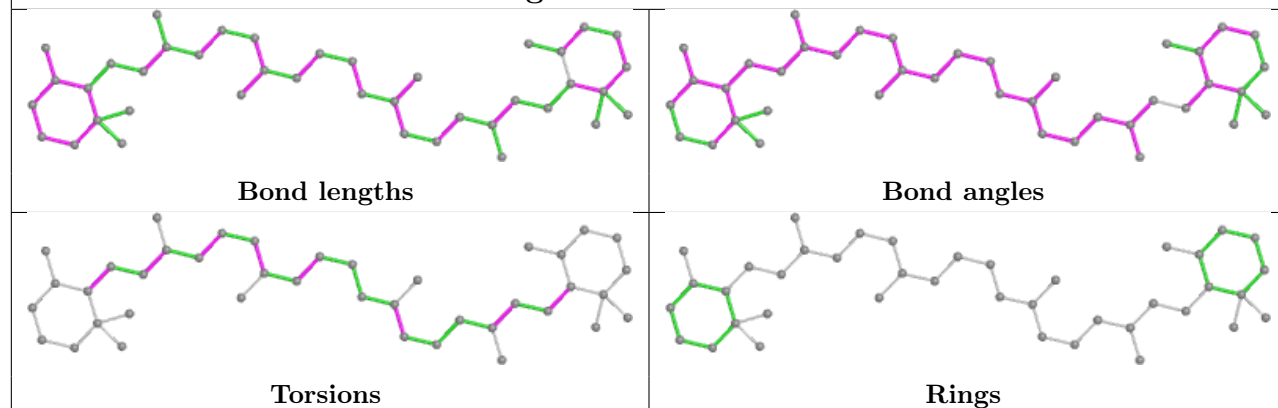
Rings

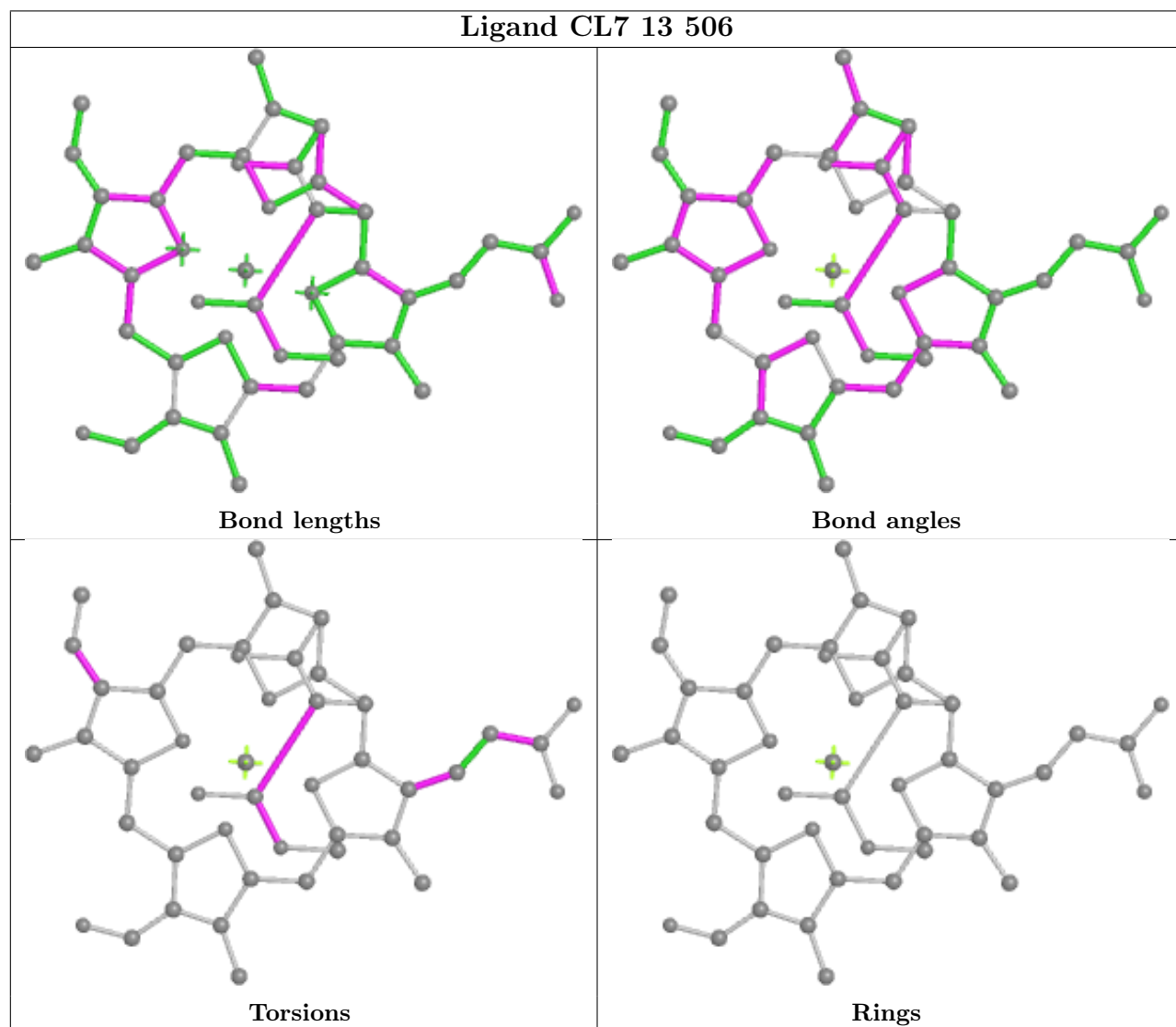
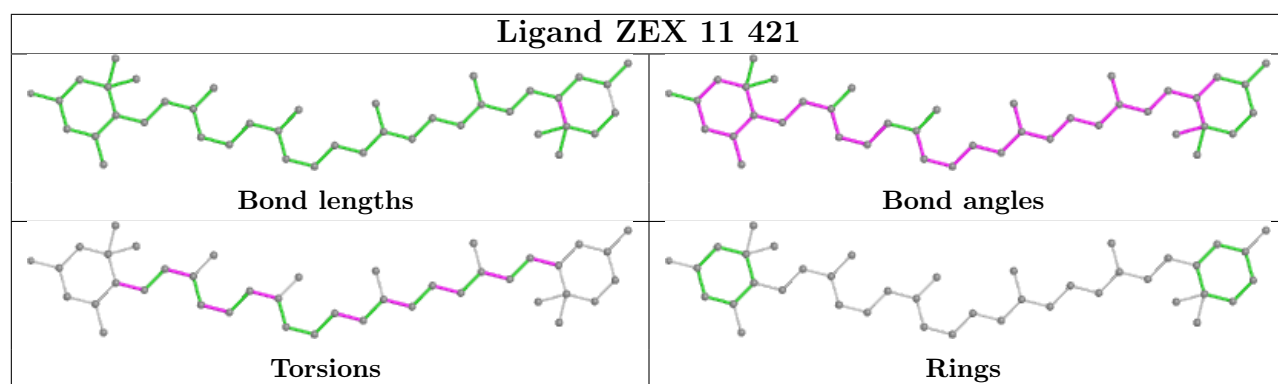


Ligand CL7 22 515

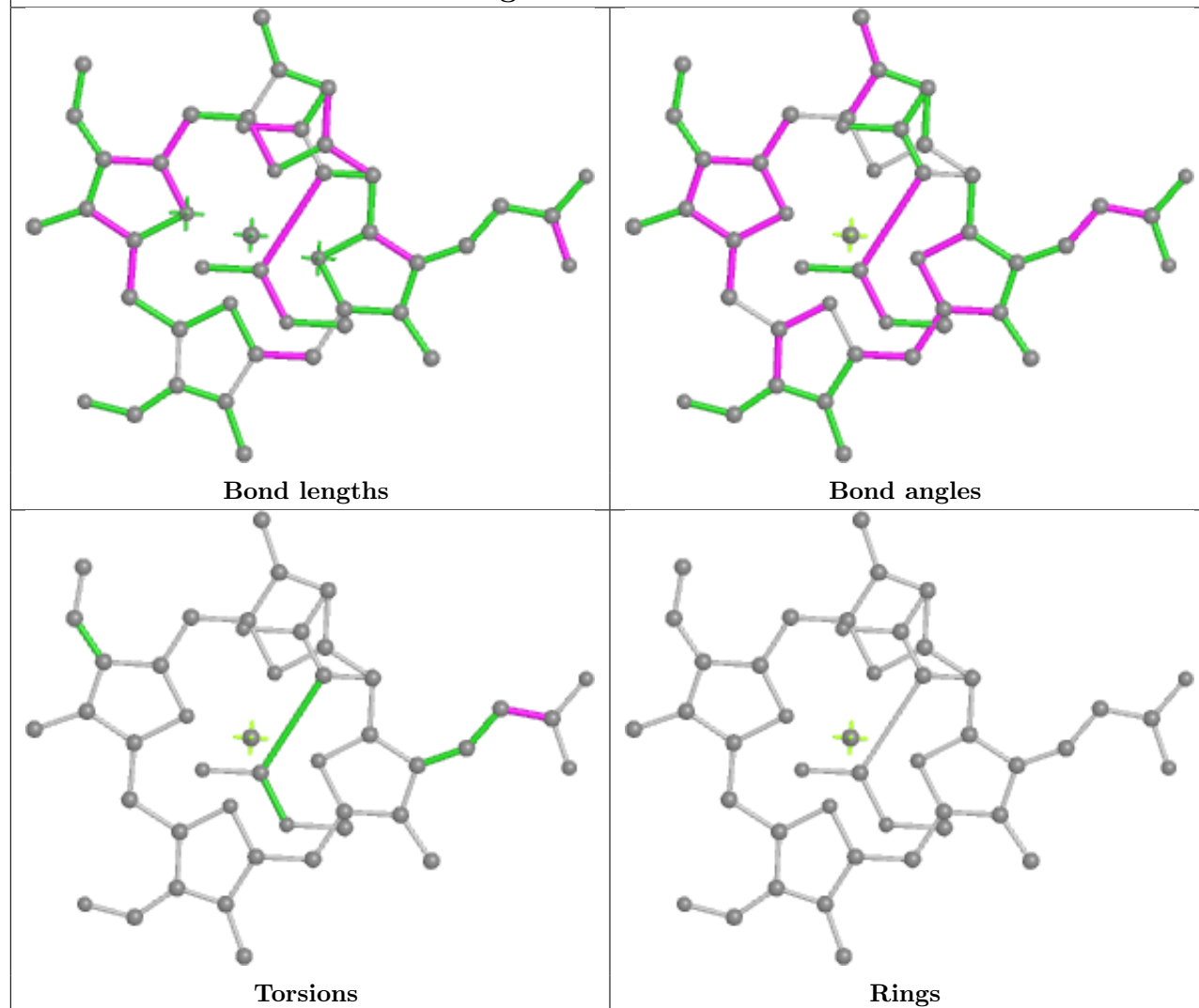


Ligand 8CT 2C 514

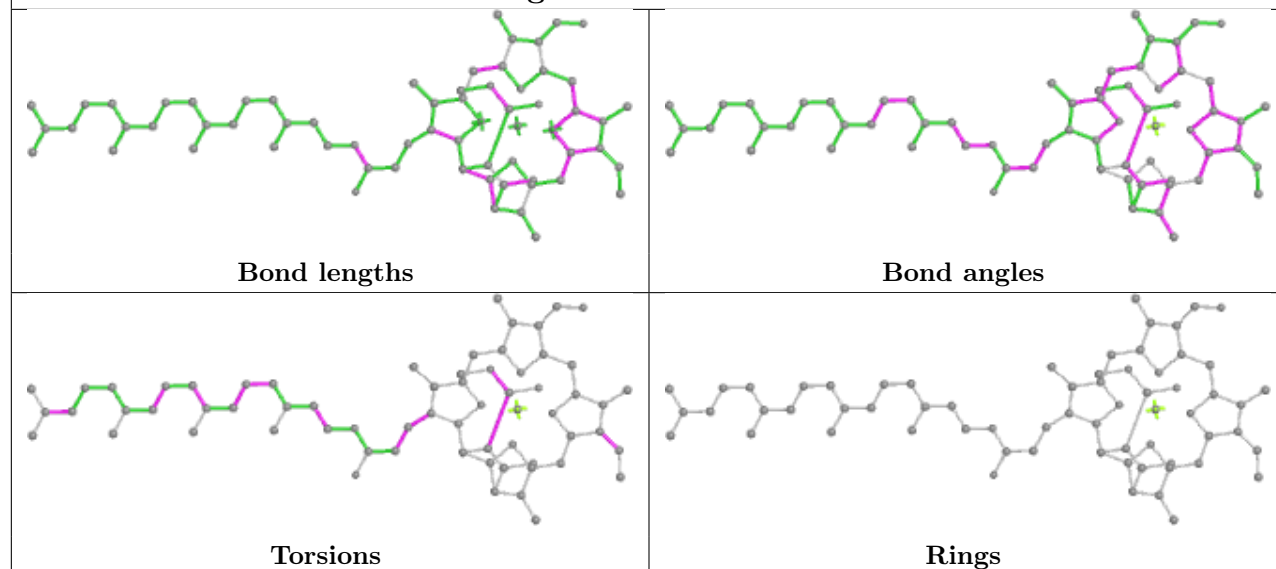


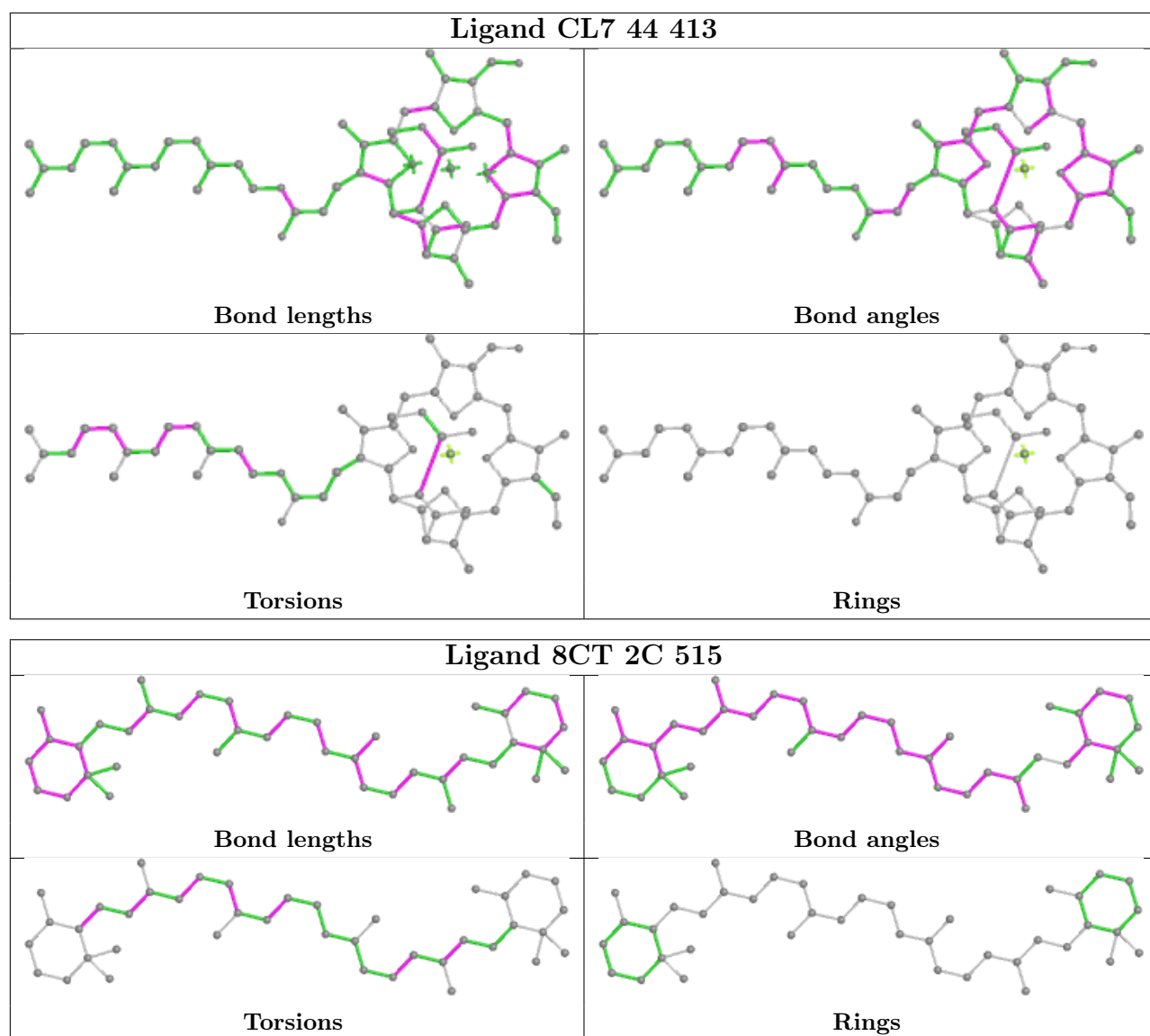


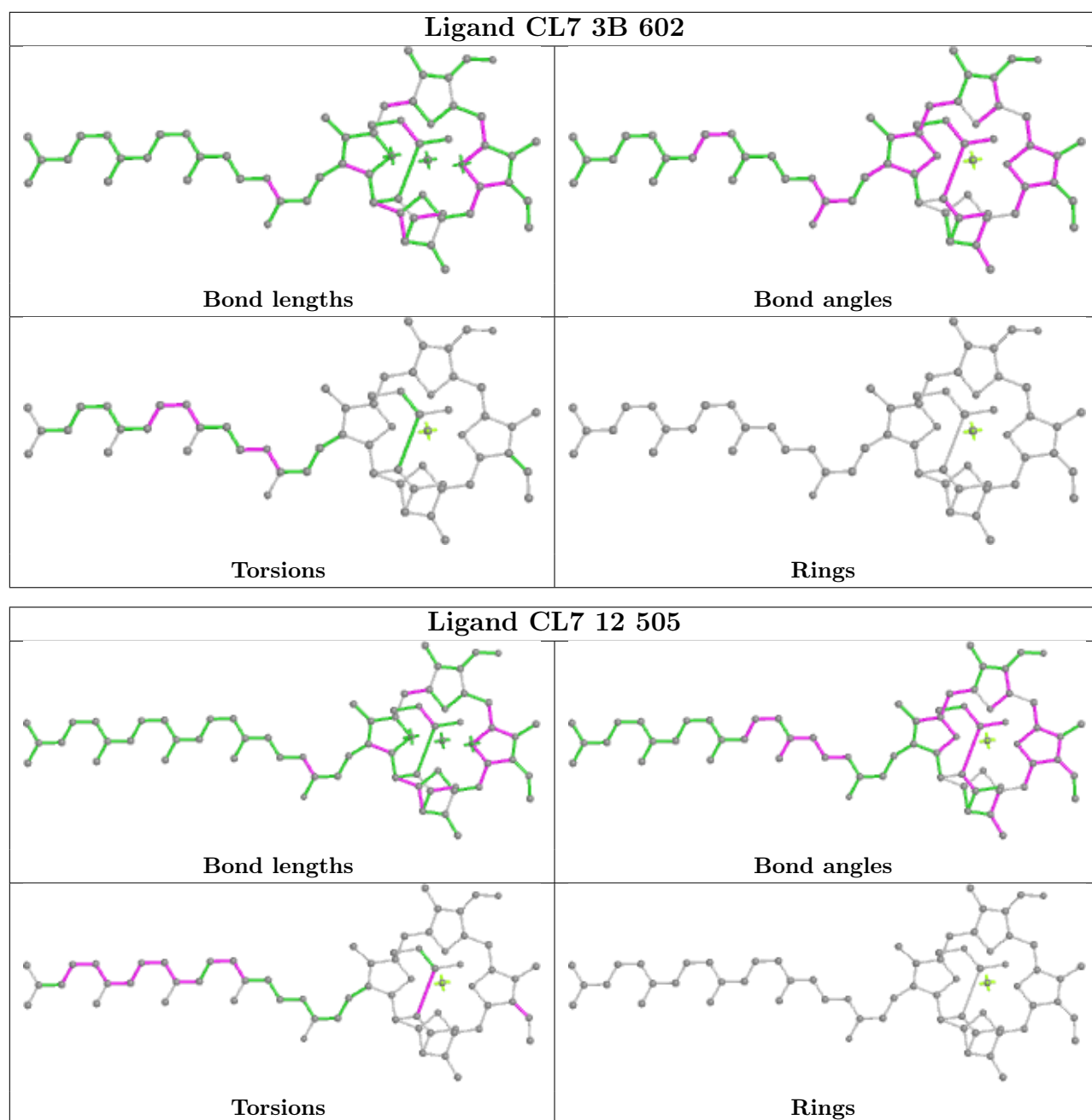
Ligand CL7 24 408

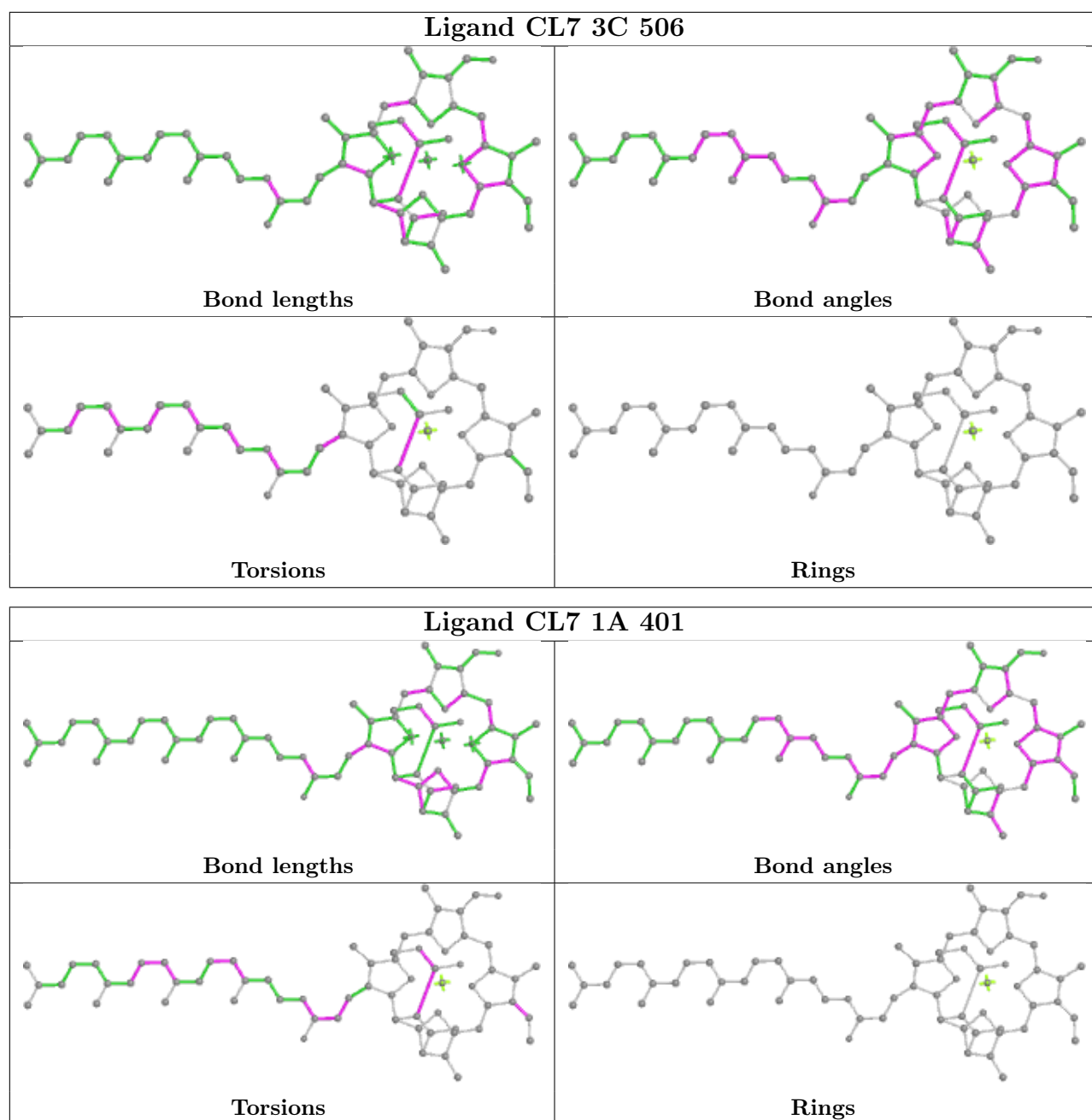


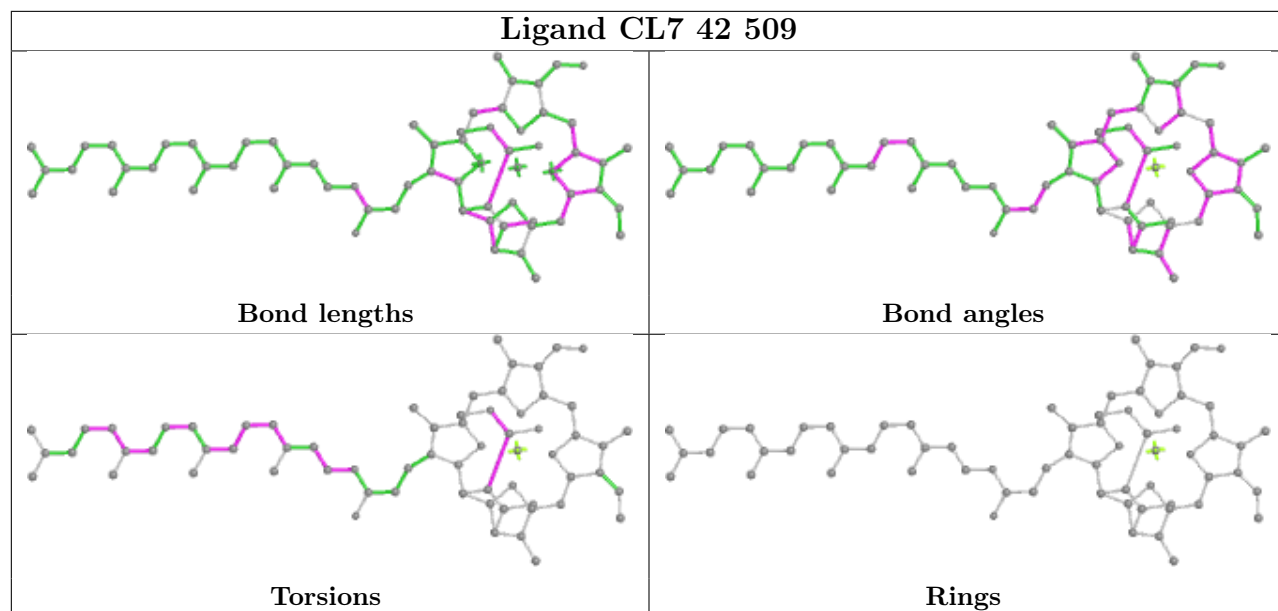
Ligand CL7 1A 407



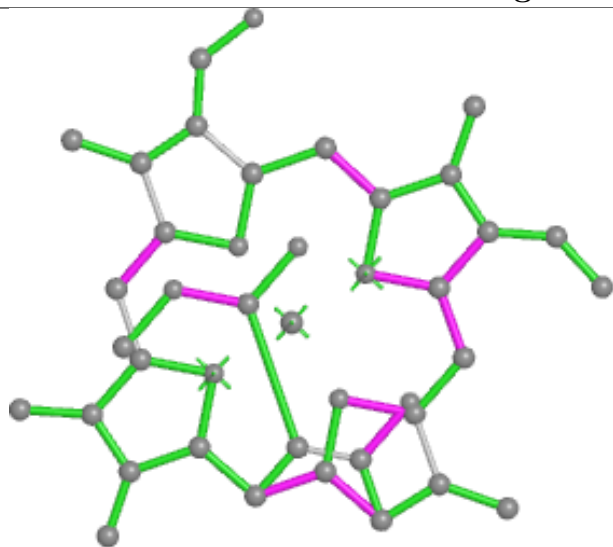




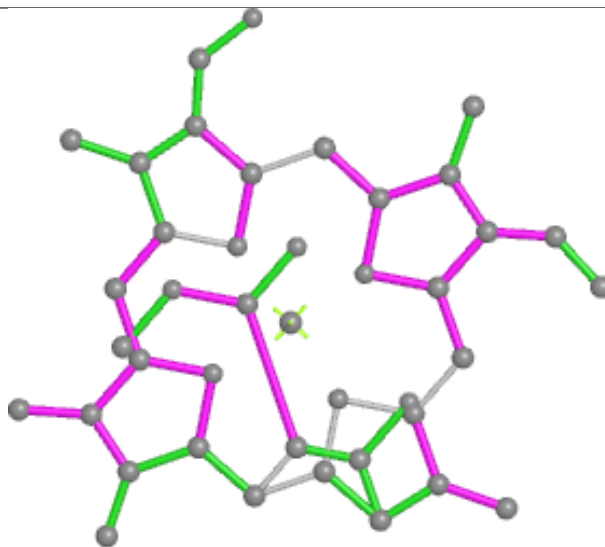




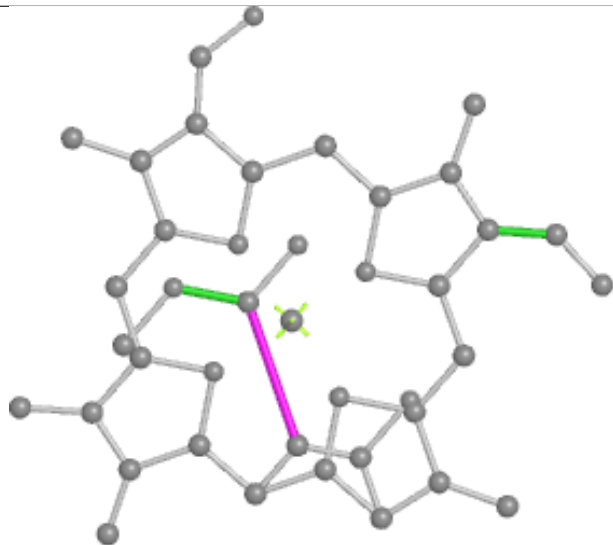
Ligand CL7 24 407



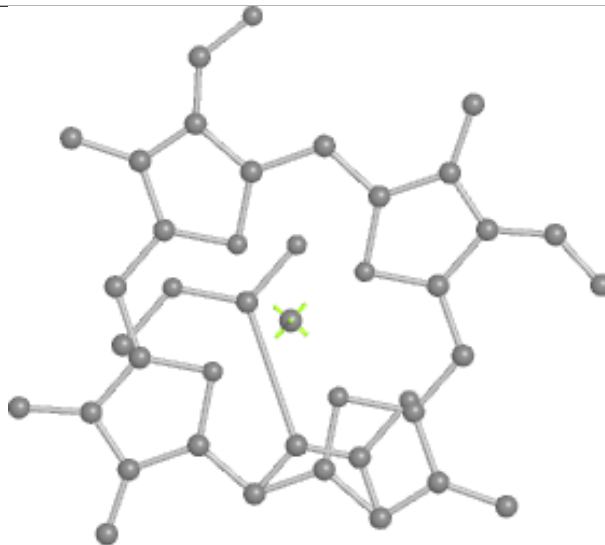
Bond lengths



Bond angles

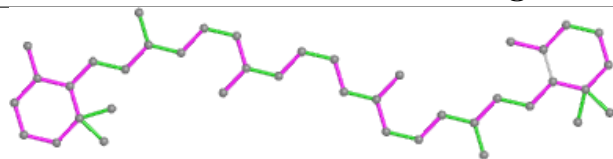


Torsions

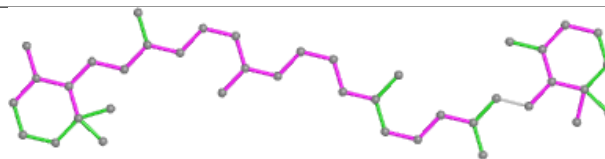


Rings

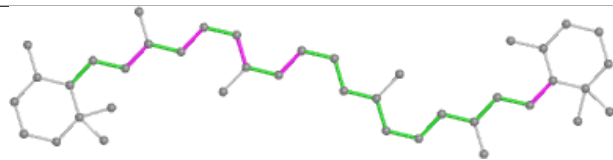
Ligand 8CT 1B 617



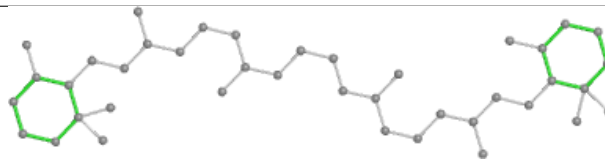
Bond lengths



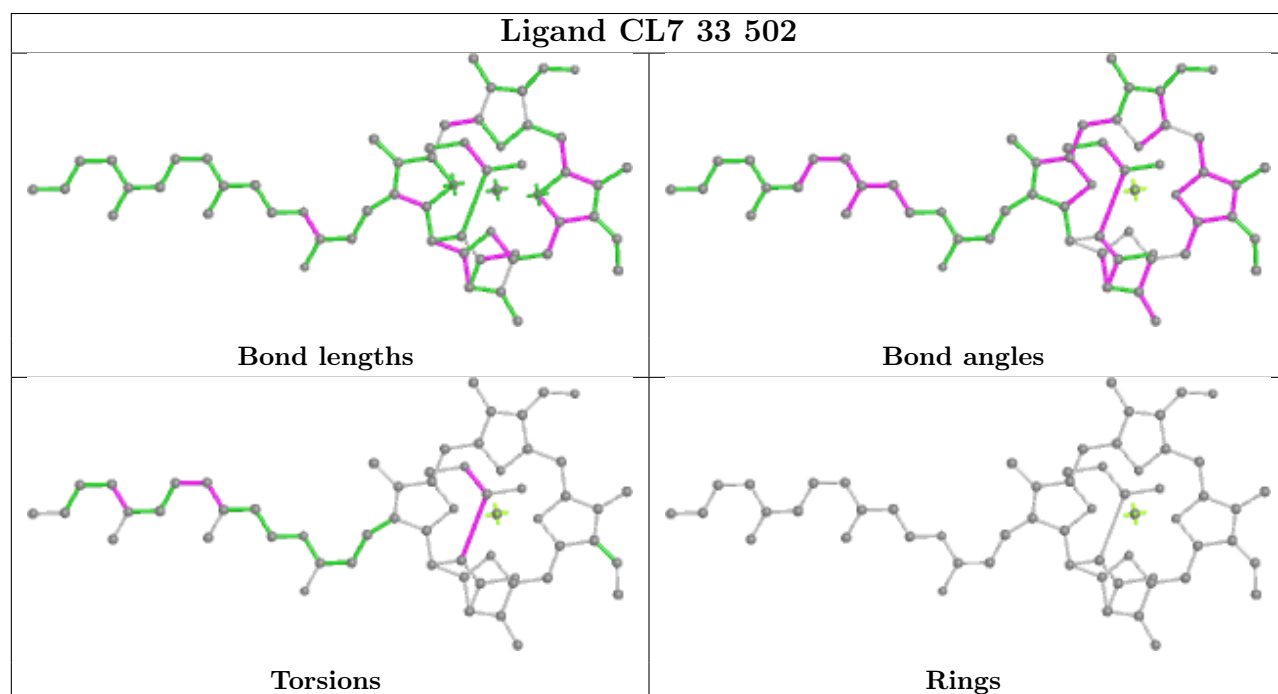
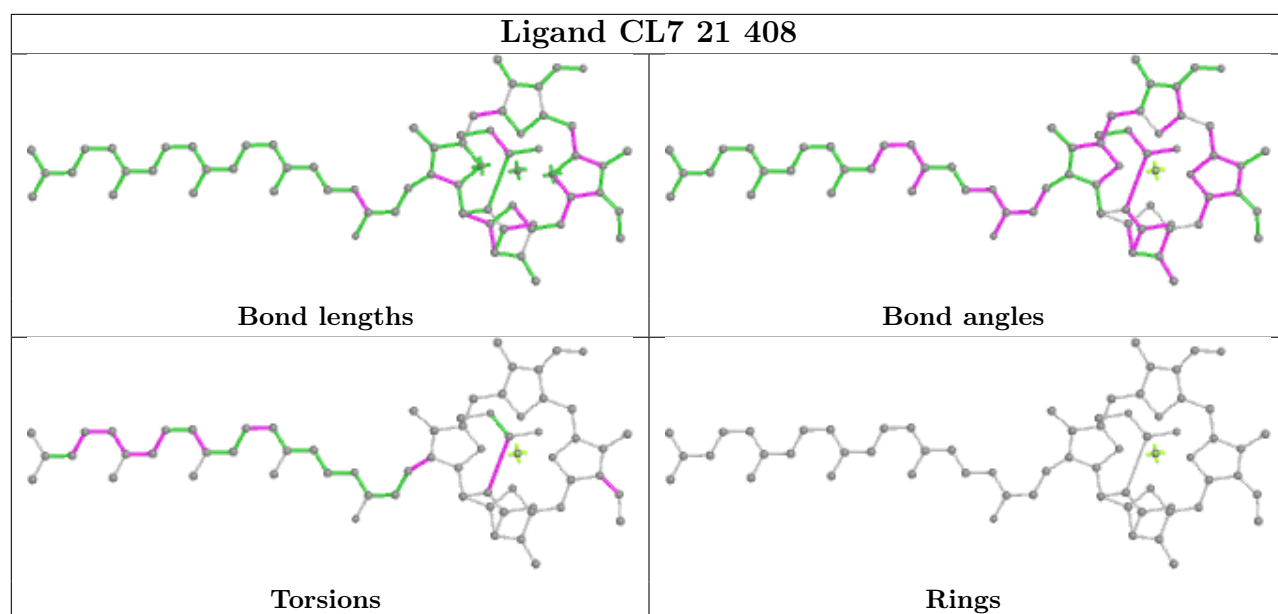
Bond angles

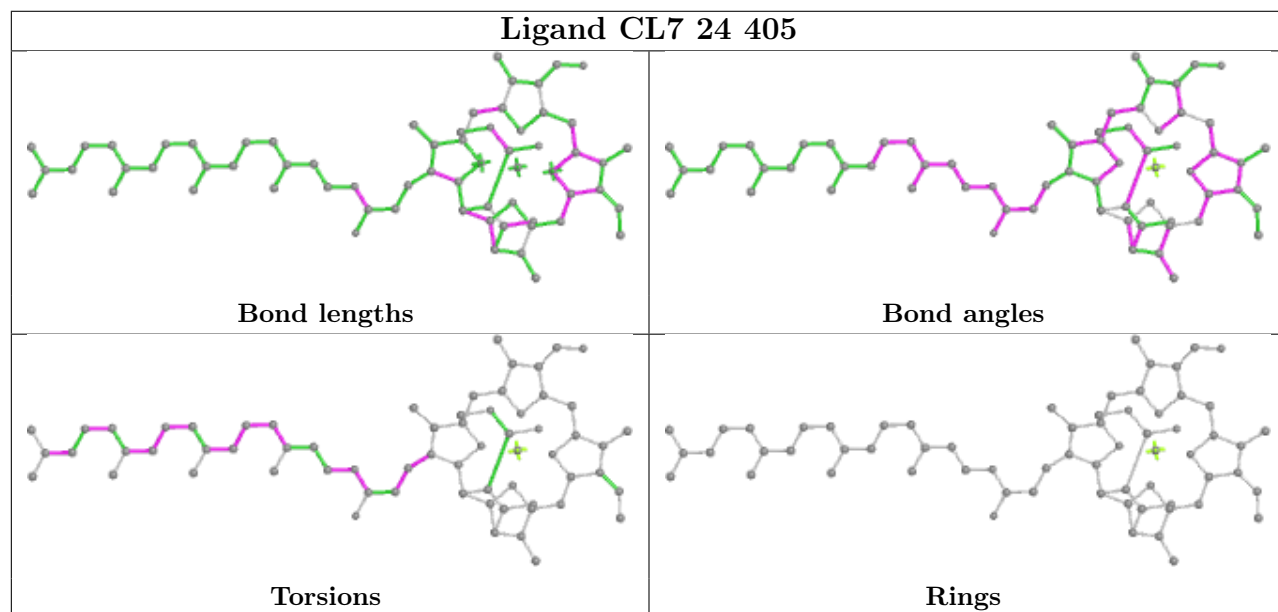
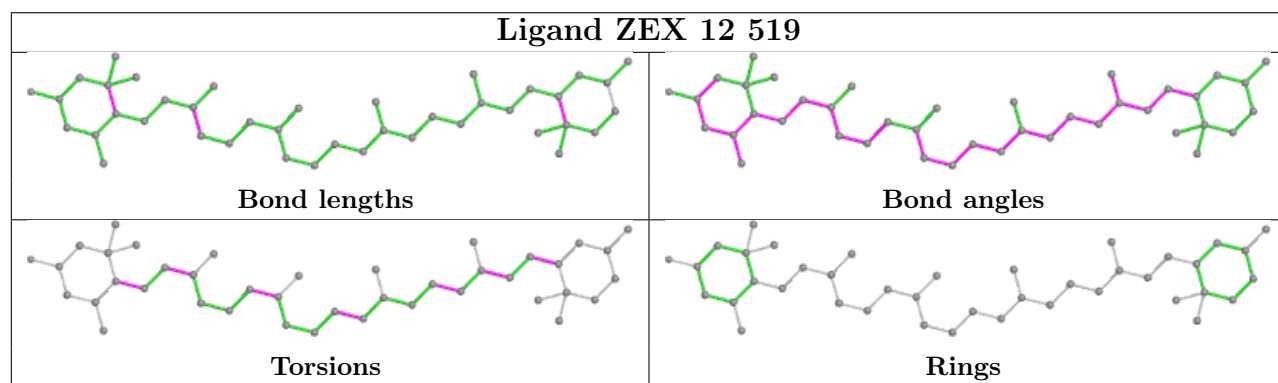
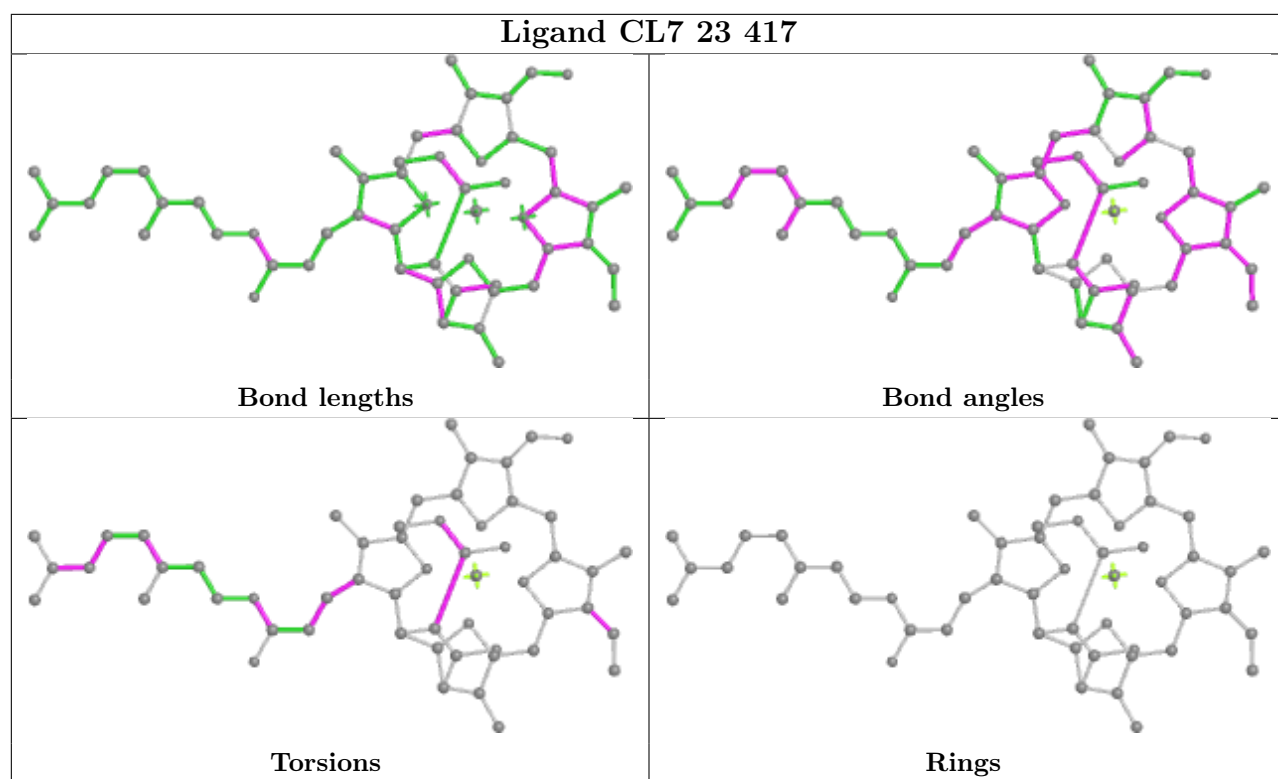


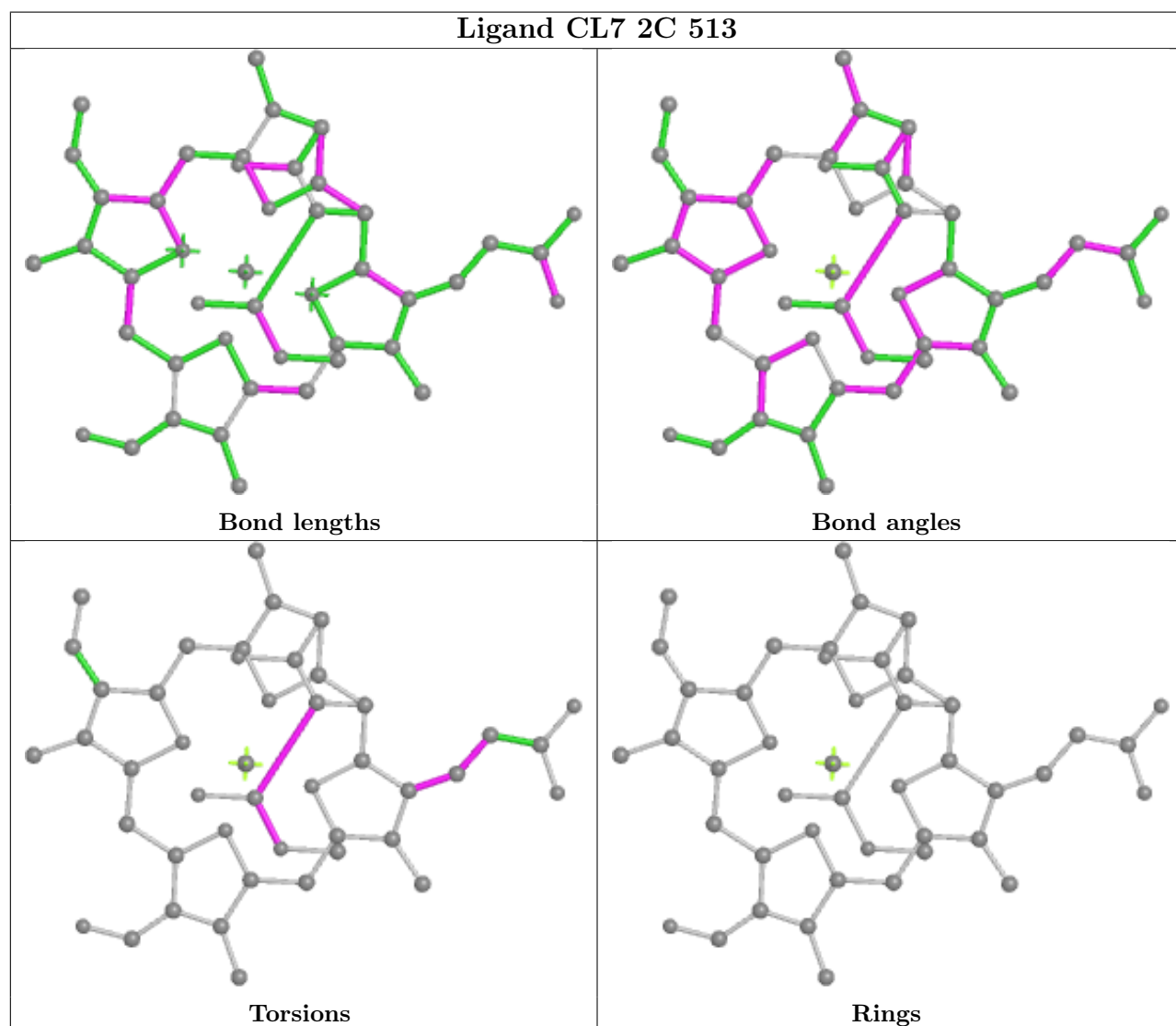
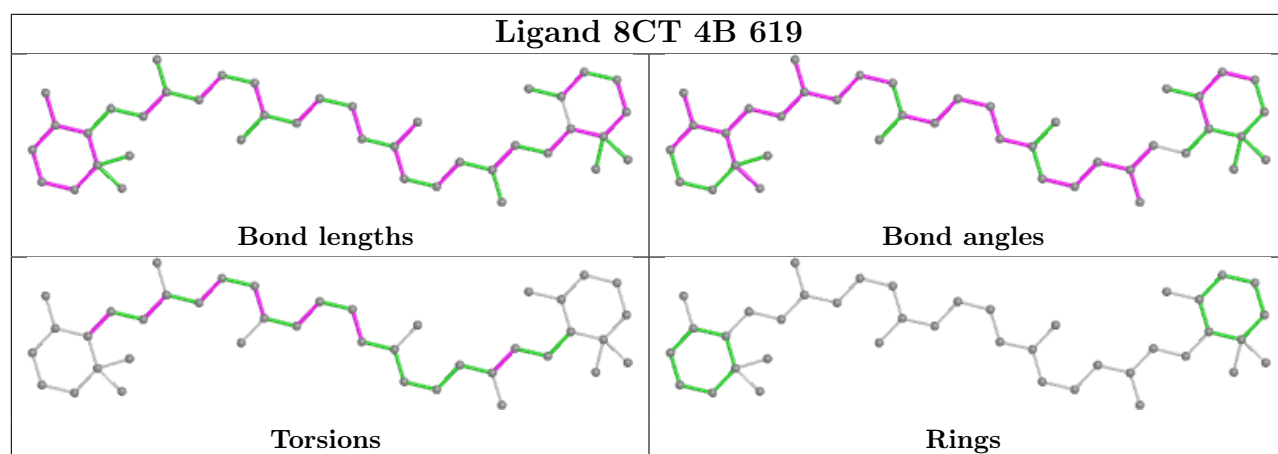
Torsions

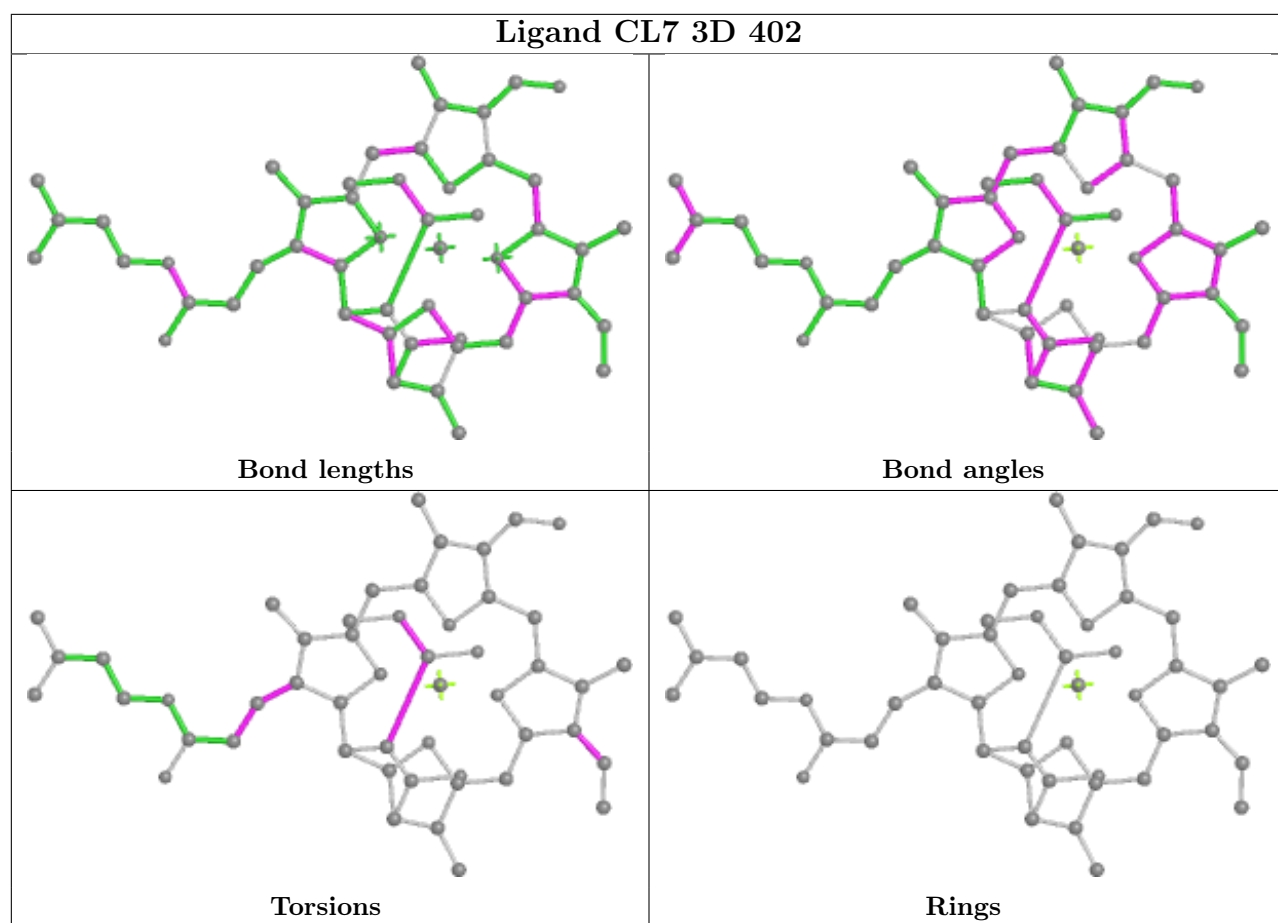


Rings

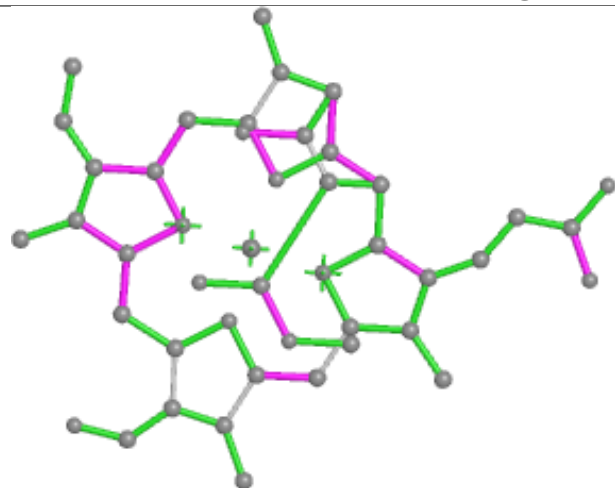




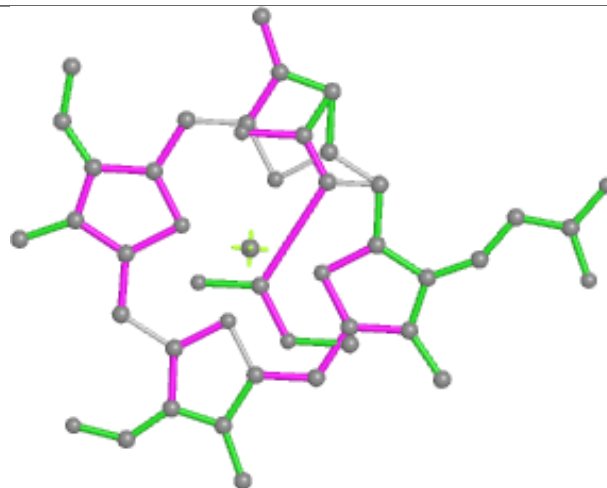




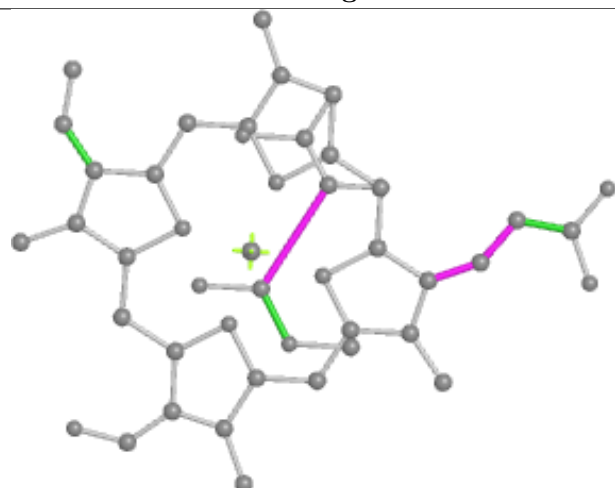
Ligand CL7 12 508



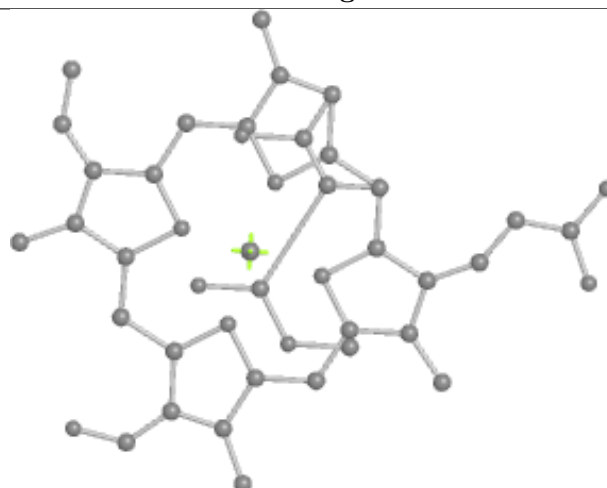
Bond lengths



Bond angles

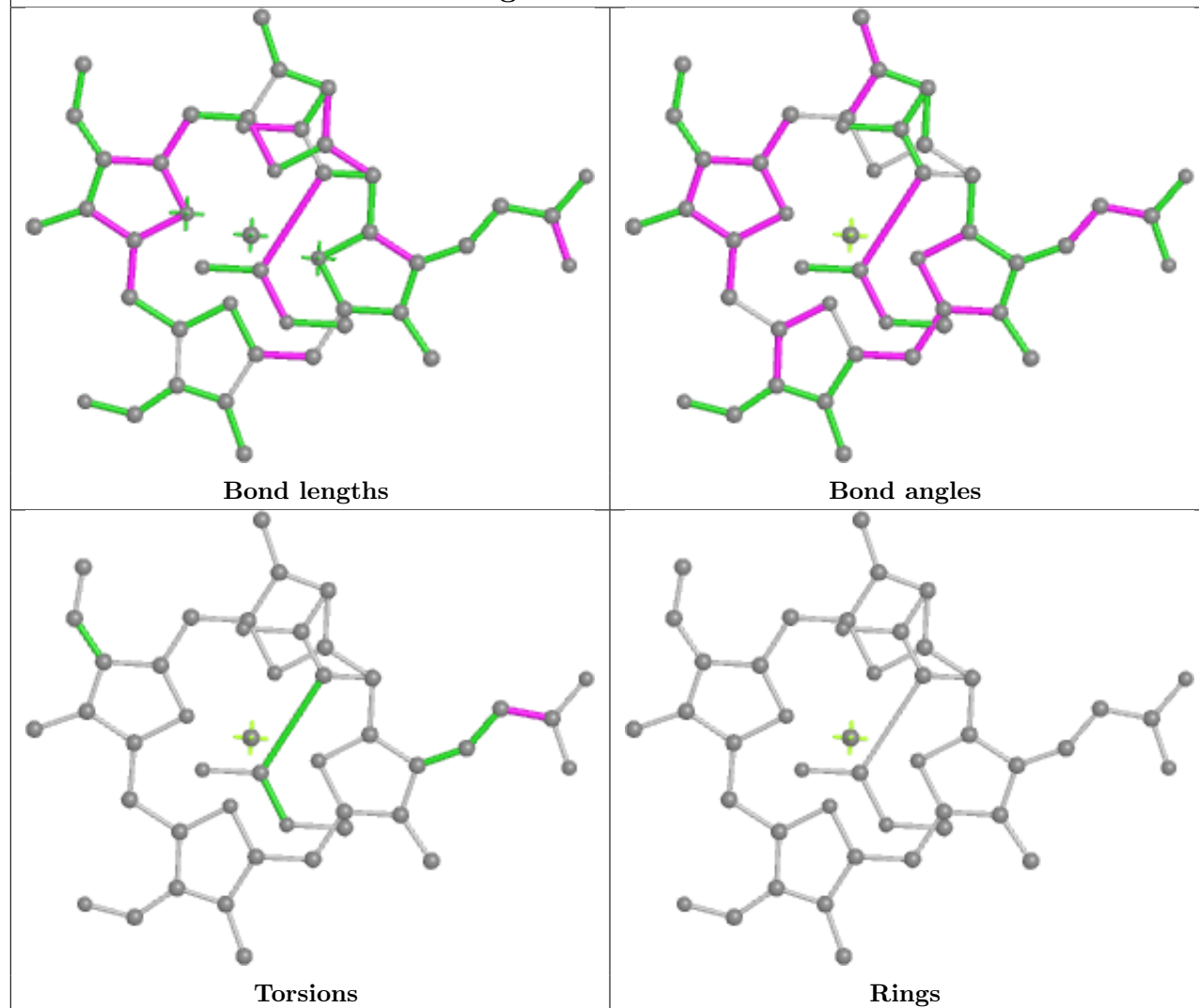


Torsions

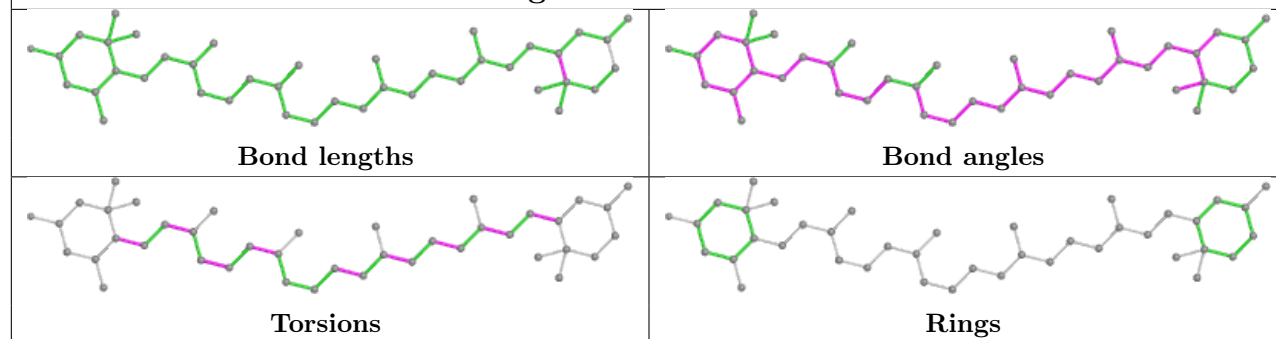


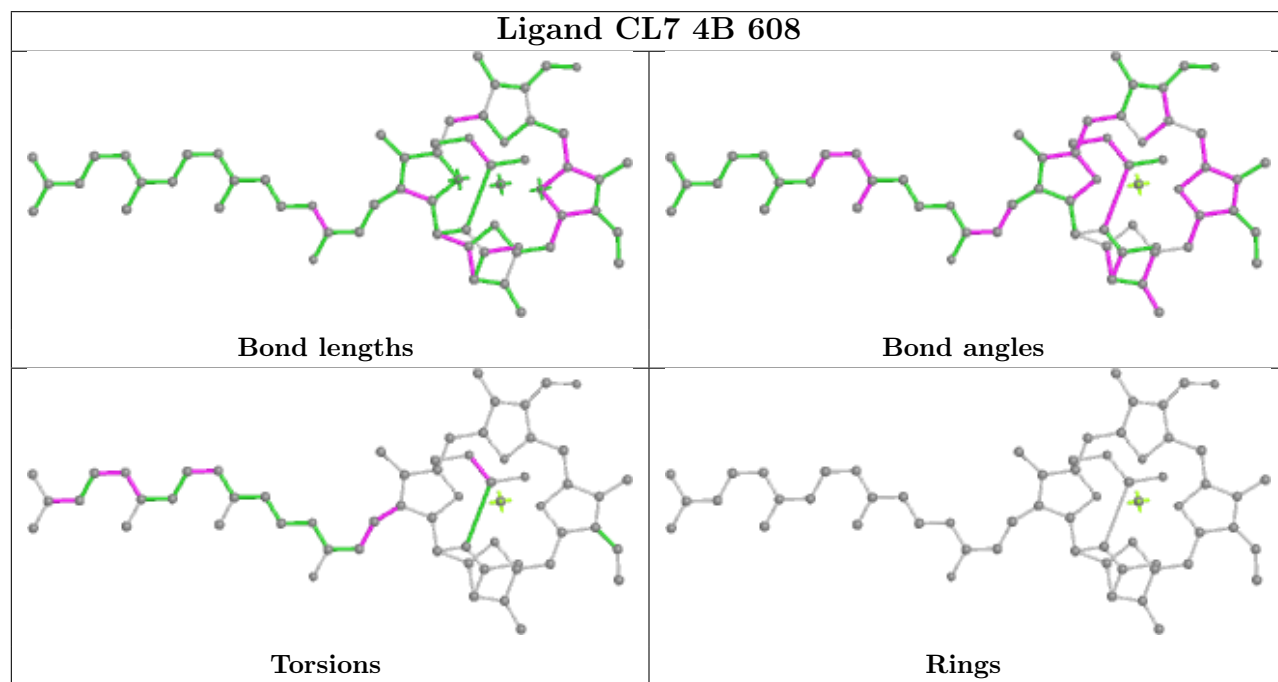
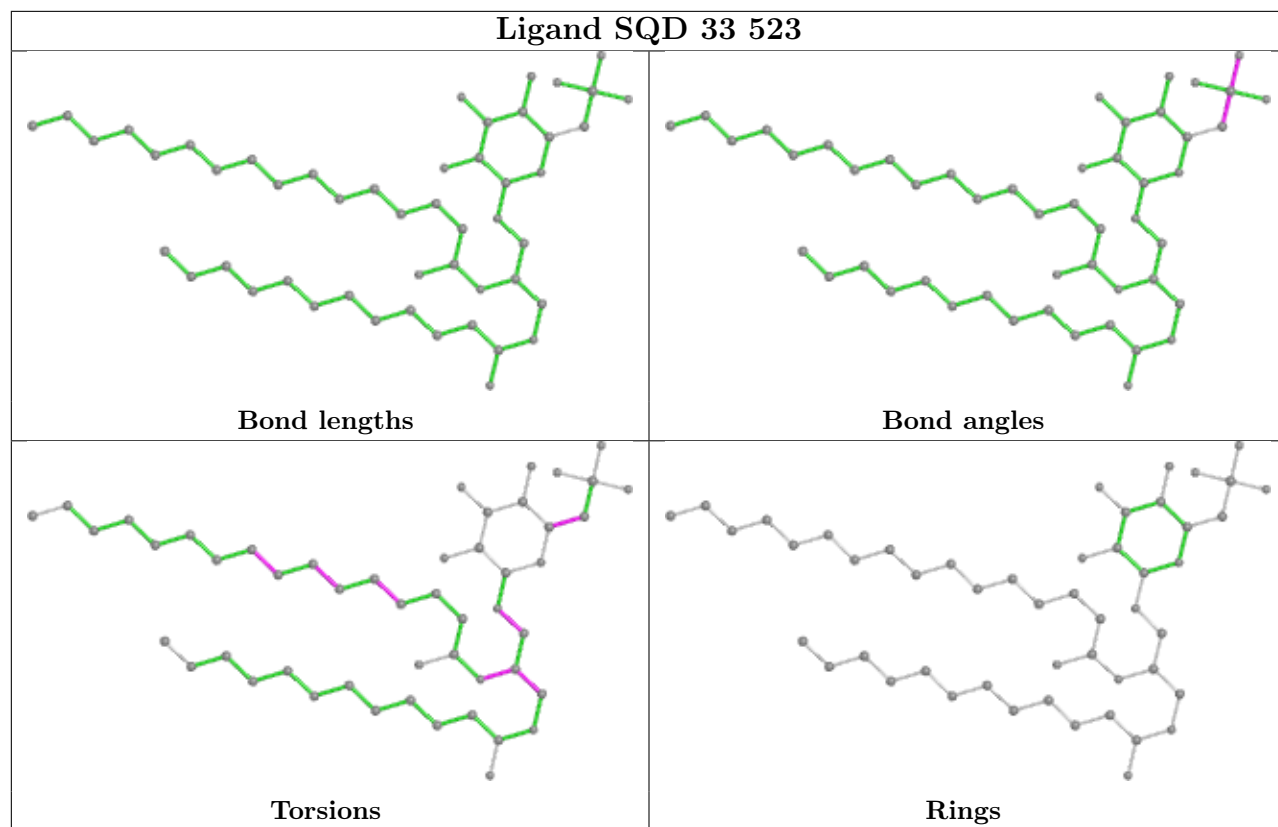
Rings

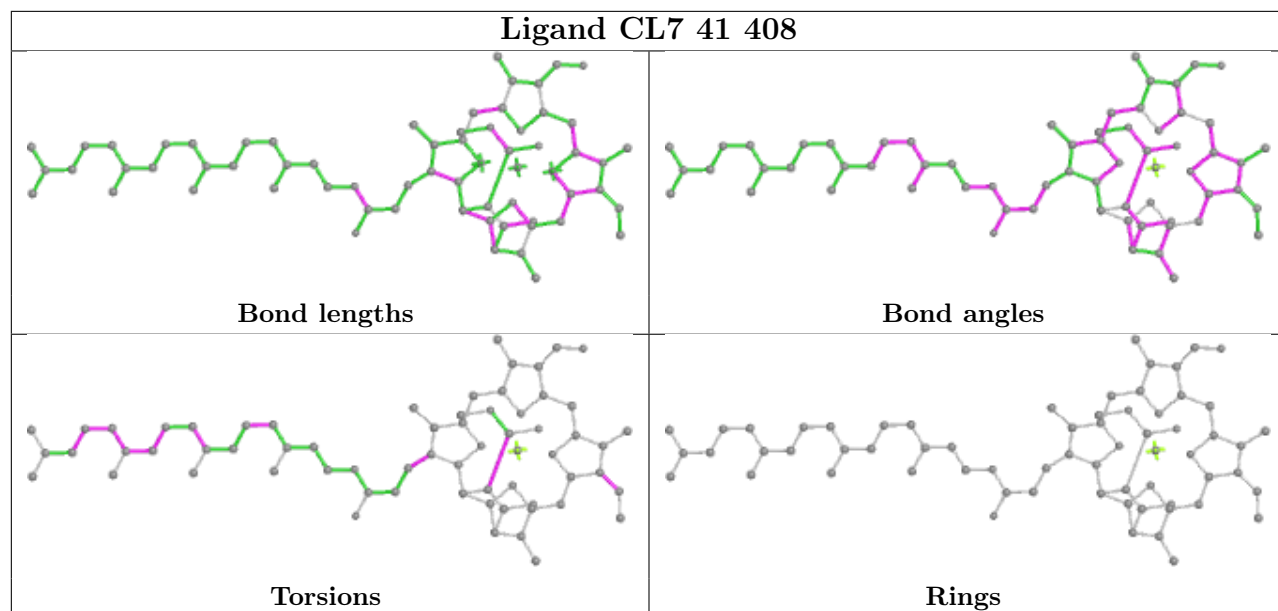
Ligand CL7 14 408



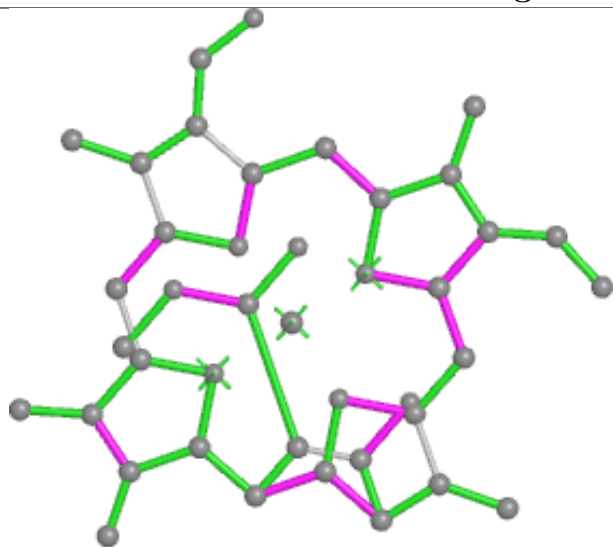
Ligand ZEX 31 421



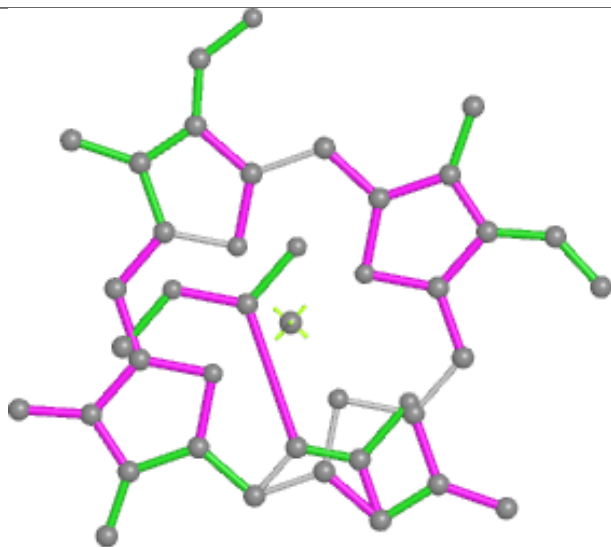




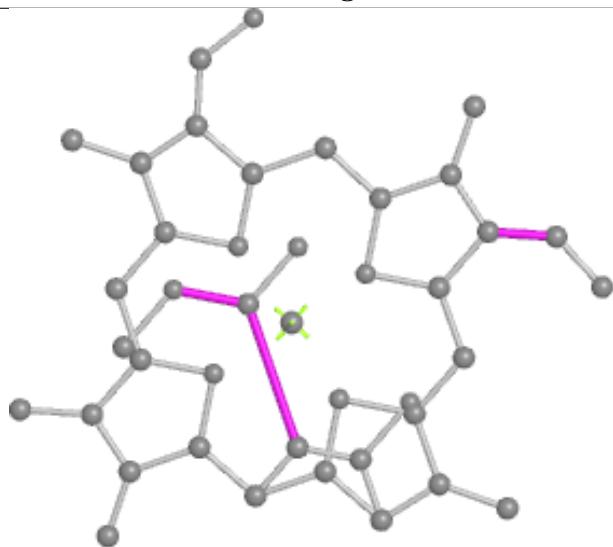
Ligand CL7 41 415



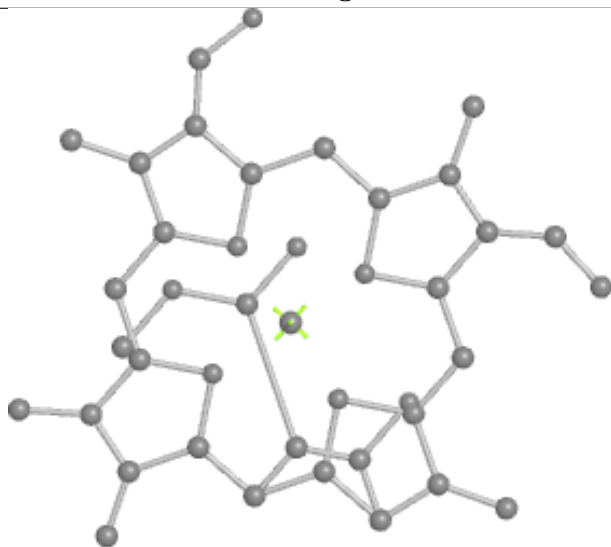
Bond lengths



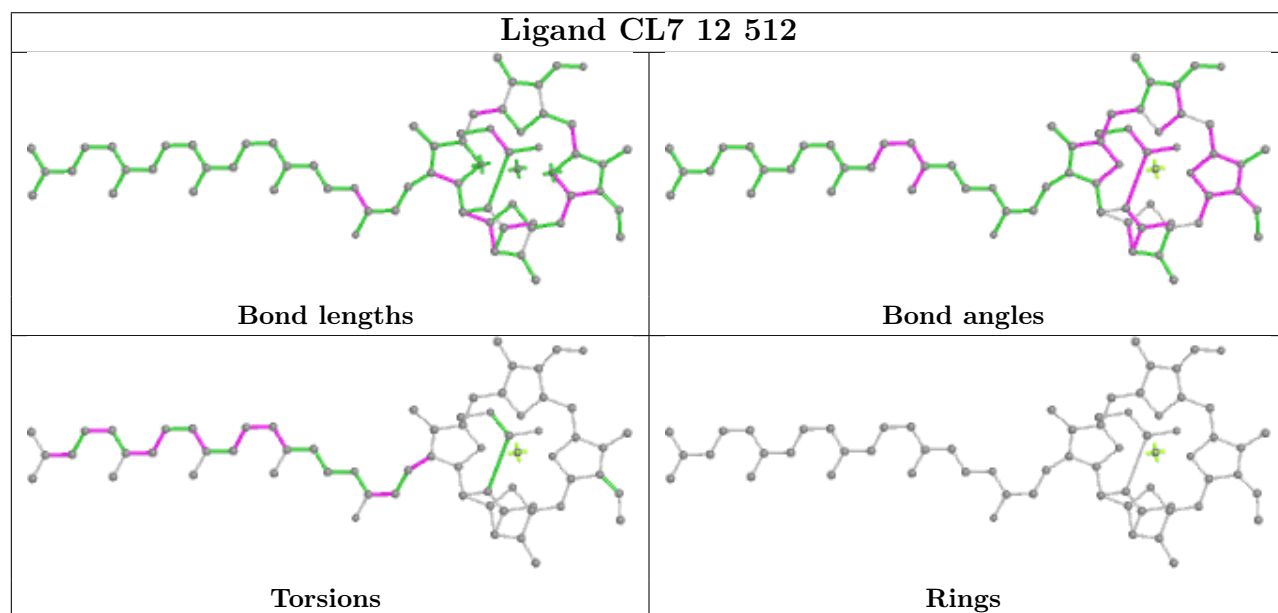
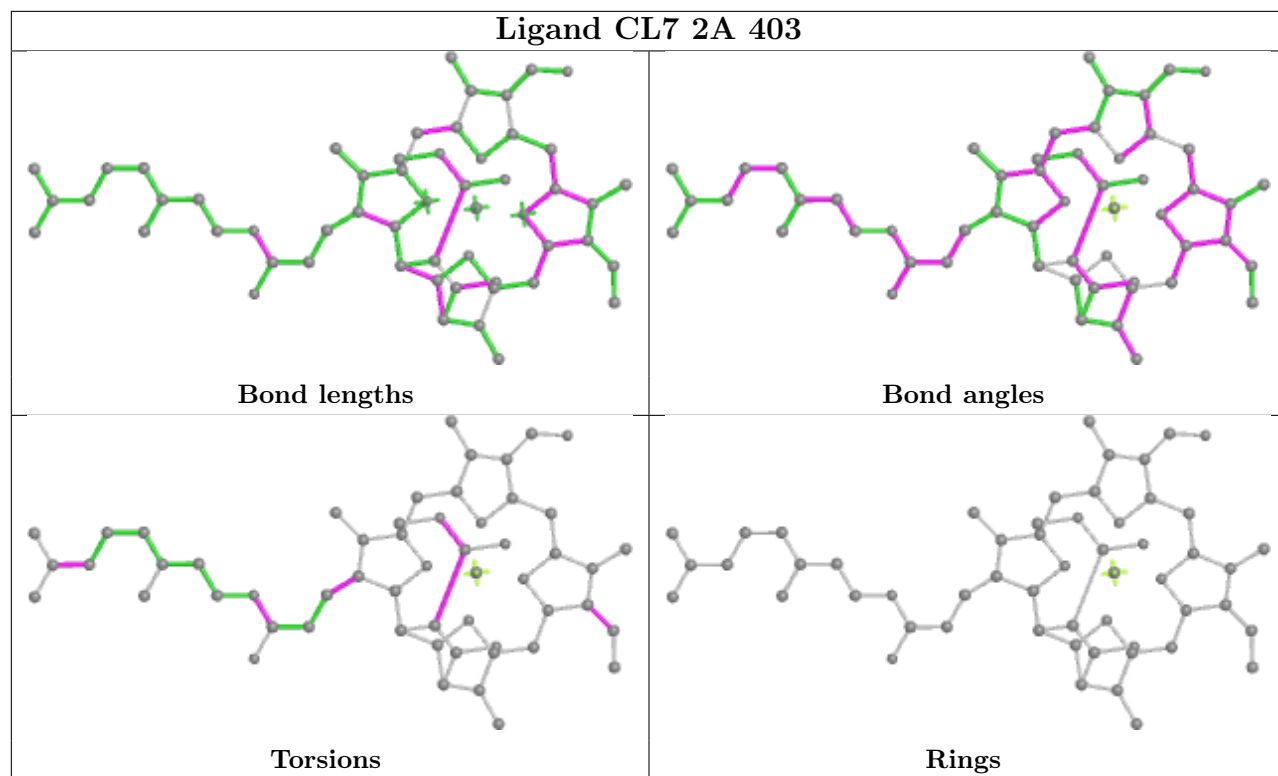
Bond angles



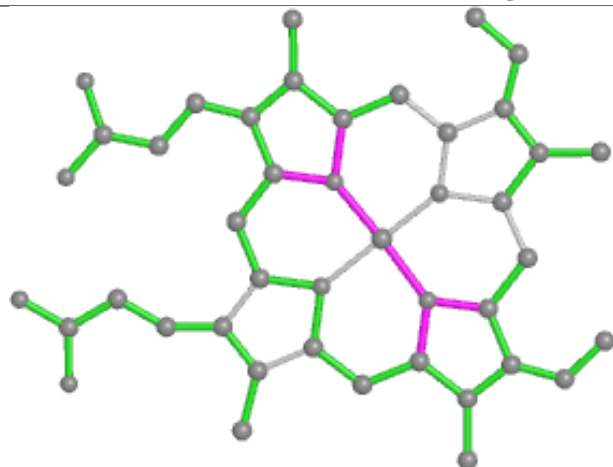
Torsions



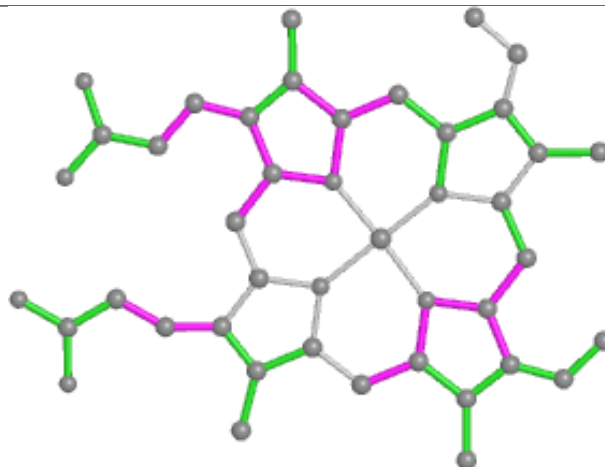
Rings



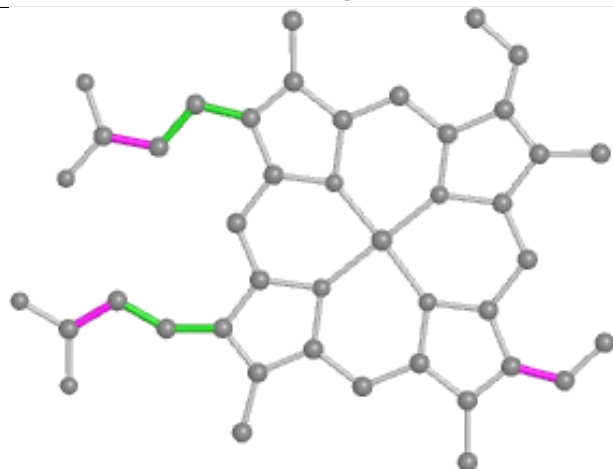
Ligand HEM 3F 101



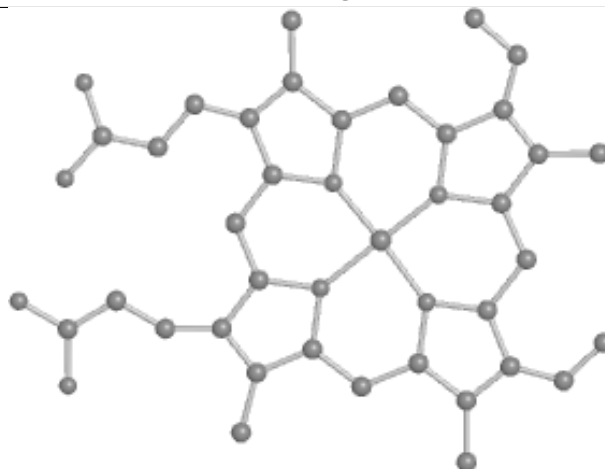
Bond lengths



Bond angles

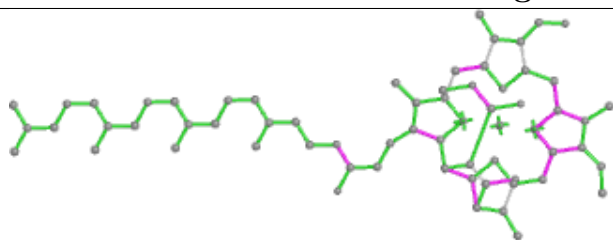


Torsions

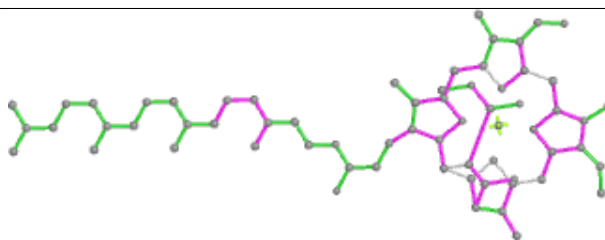


Rings

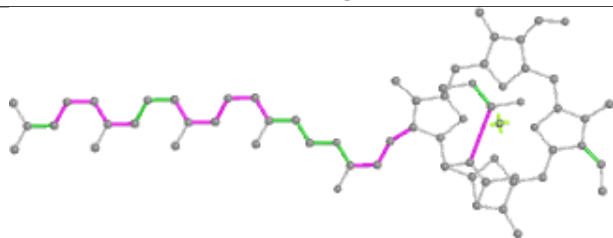
Ligand CL7 13 501



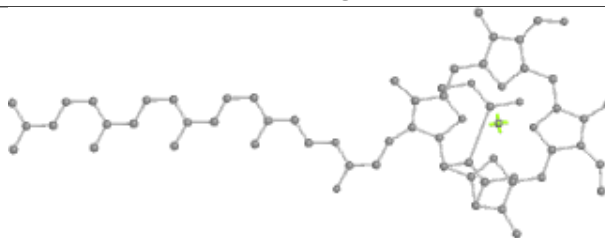
Bond lengths



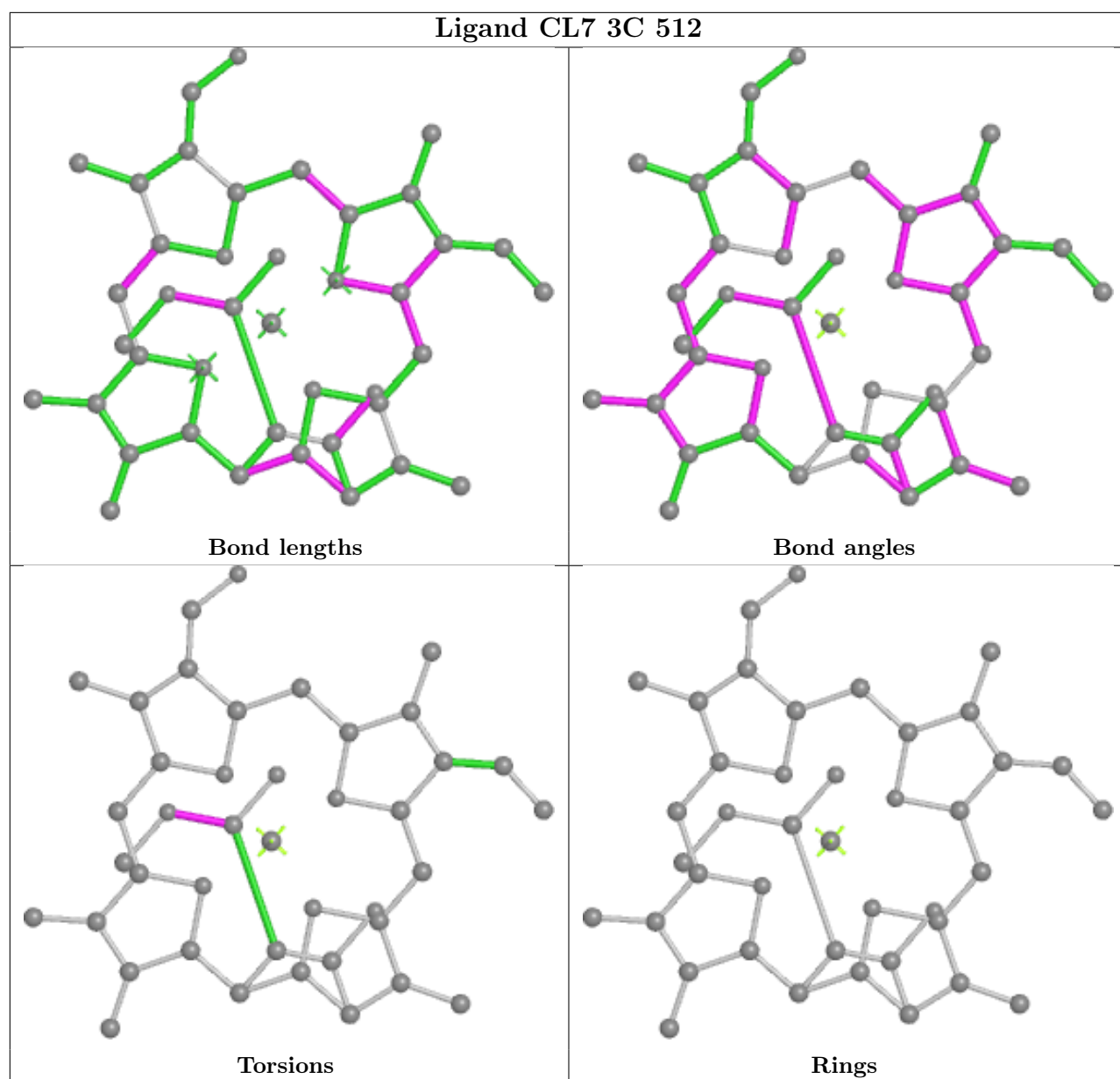
Bond angles

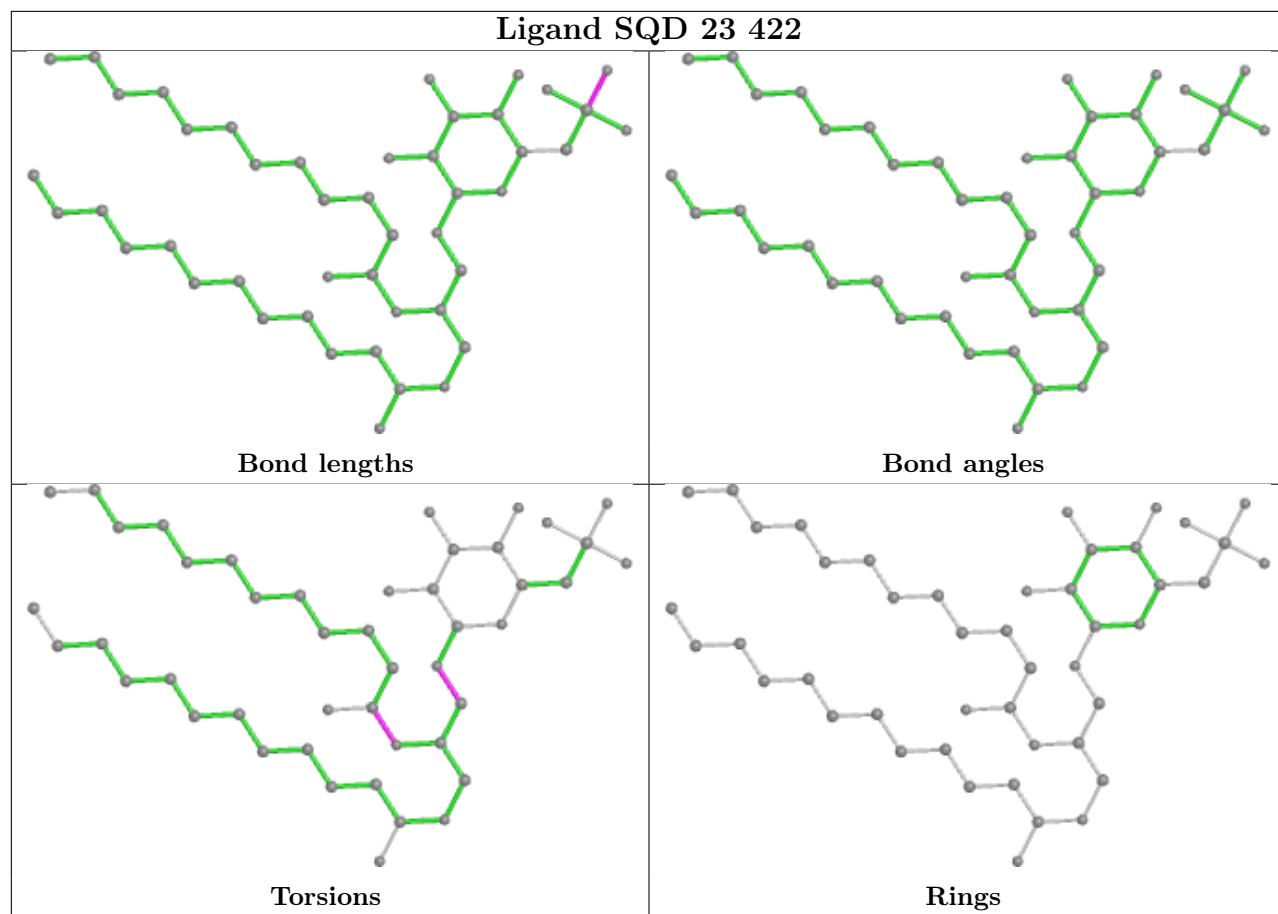


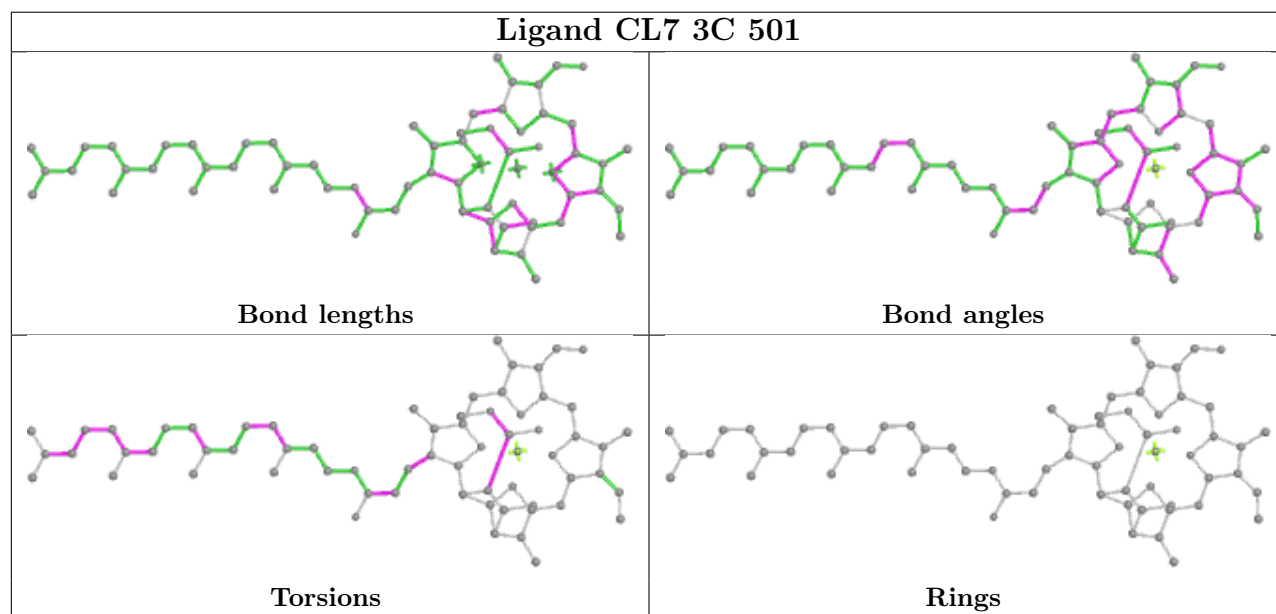
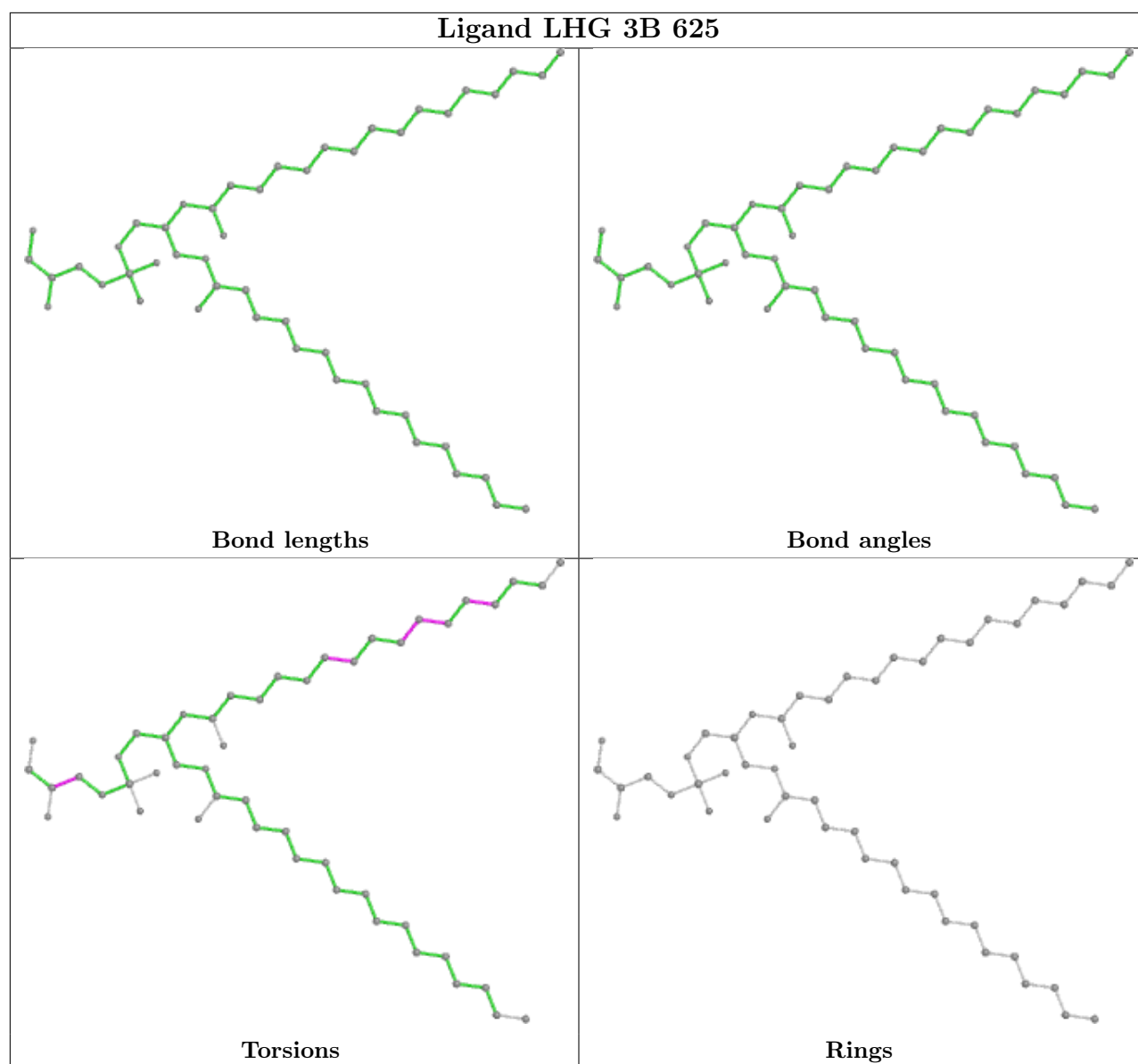
Torsions

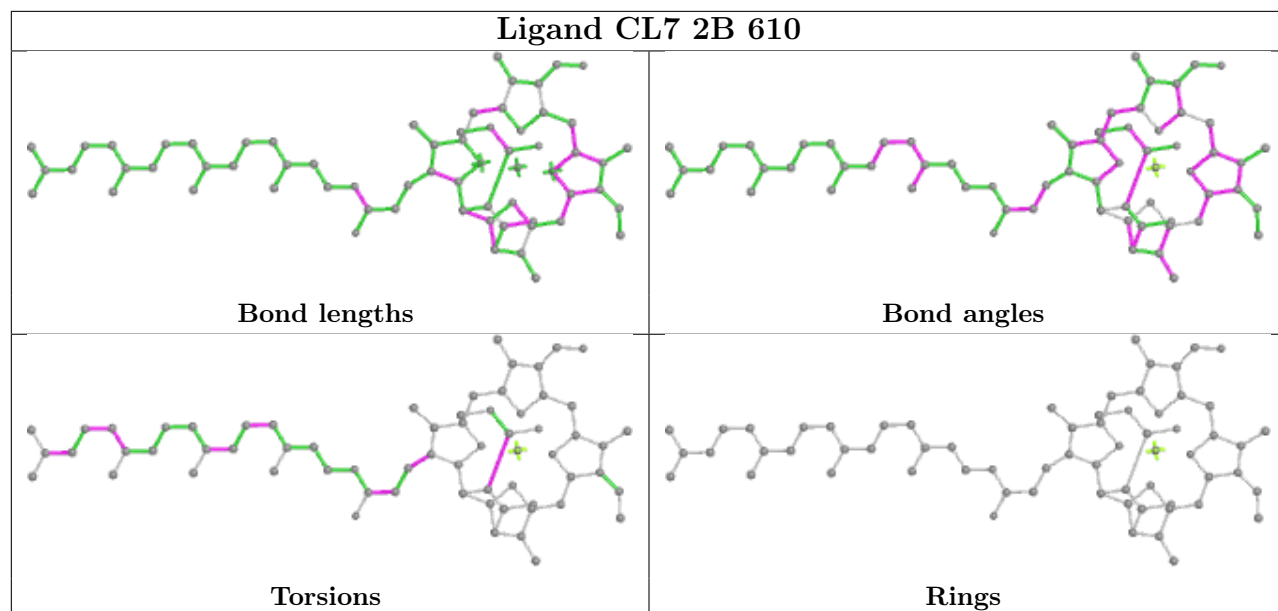


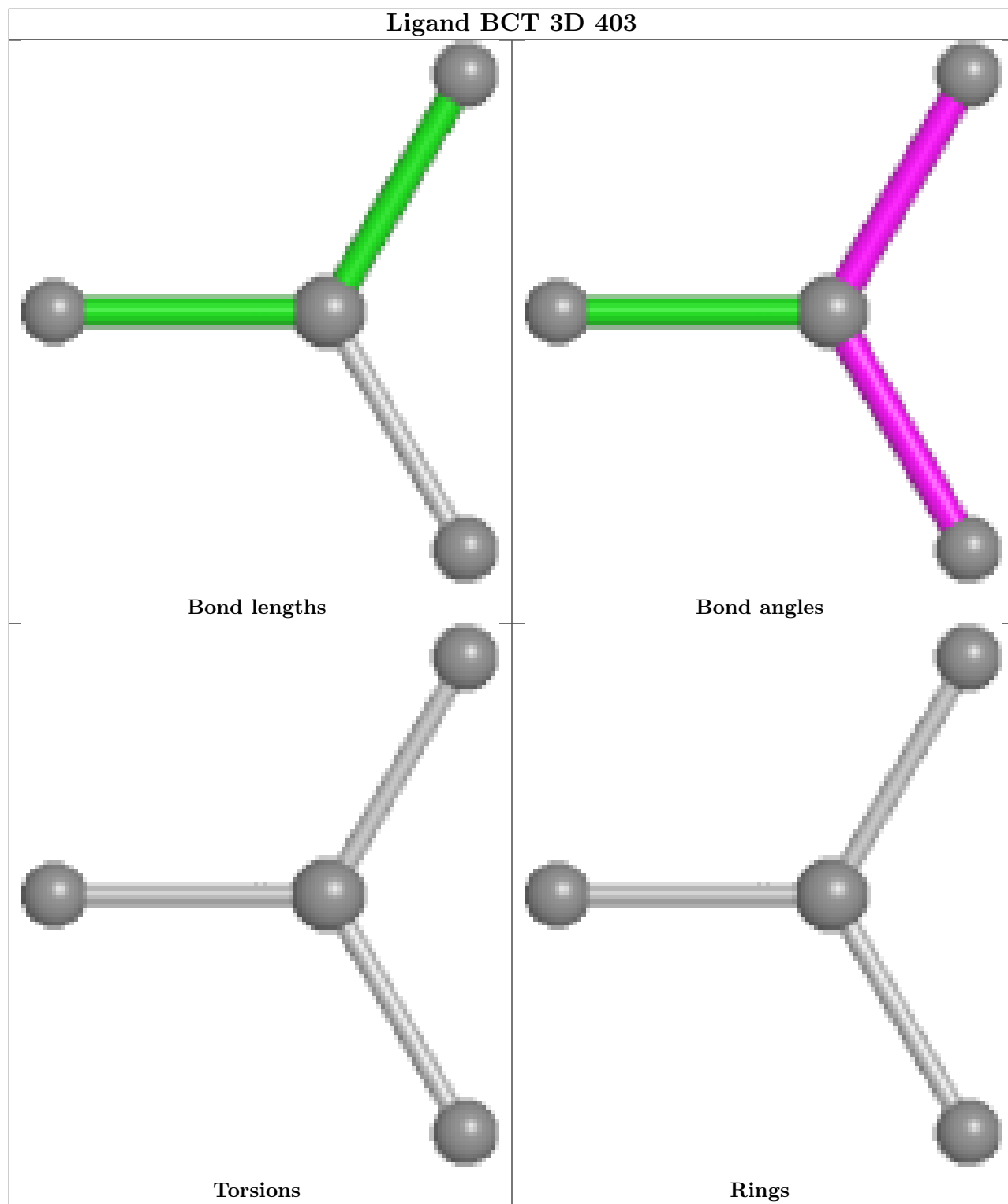
Rings

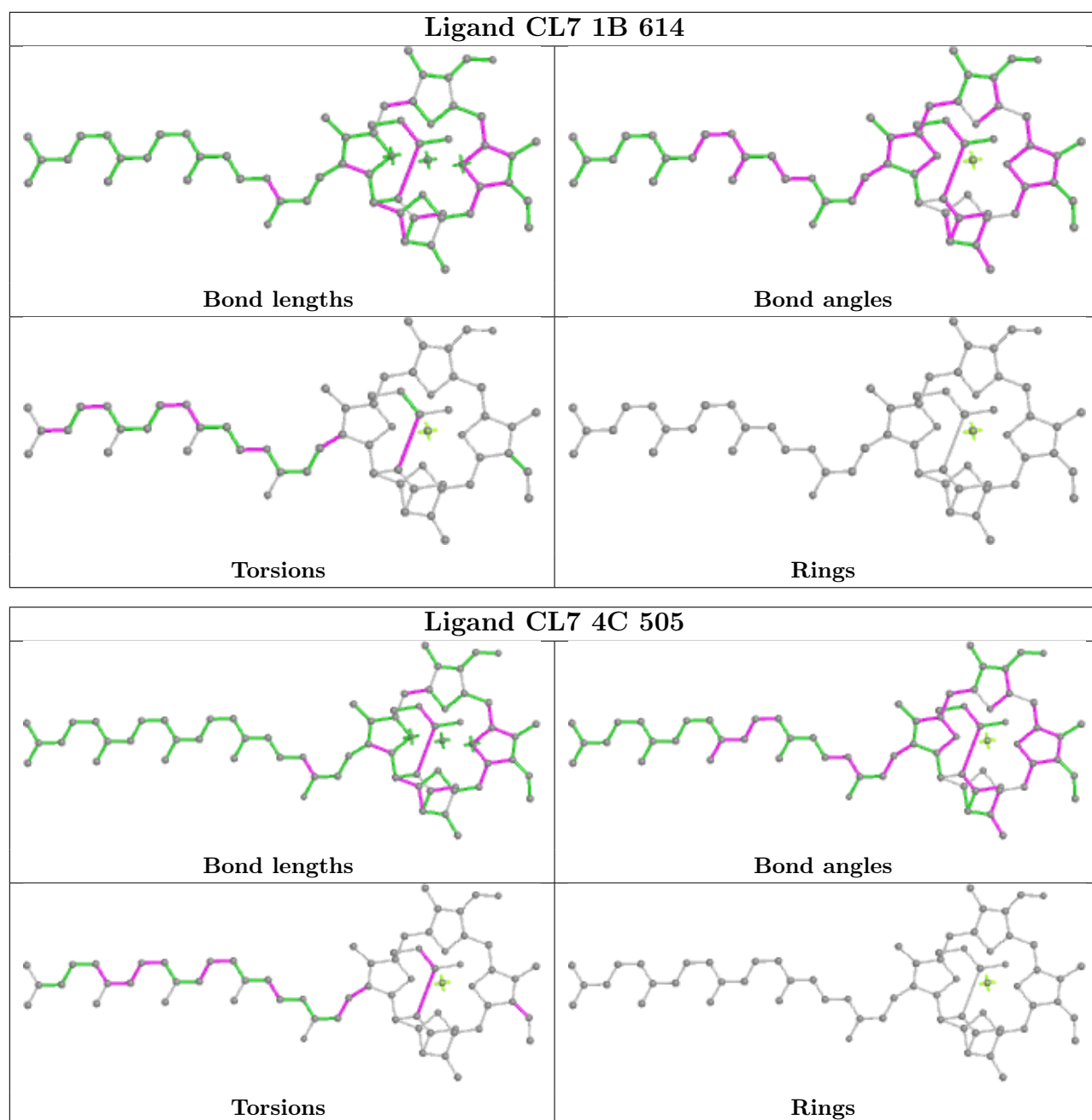




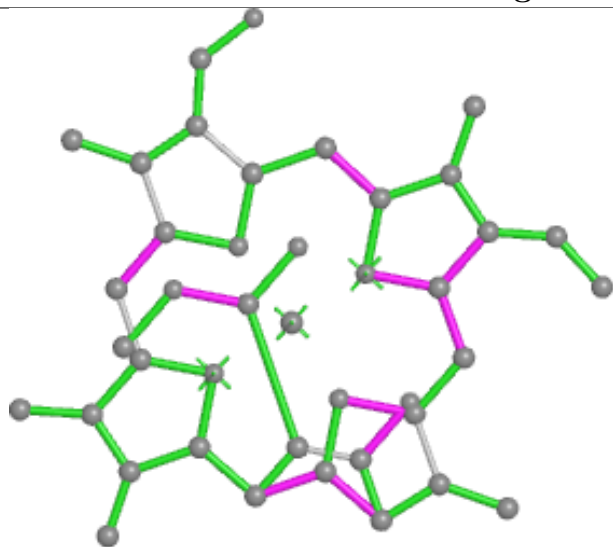




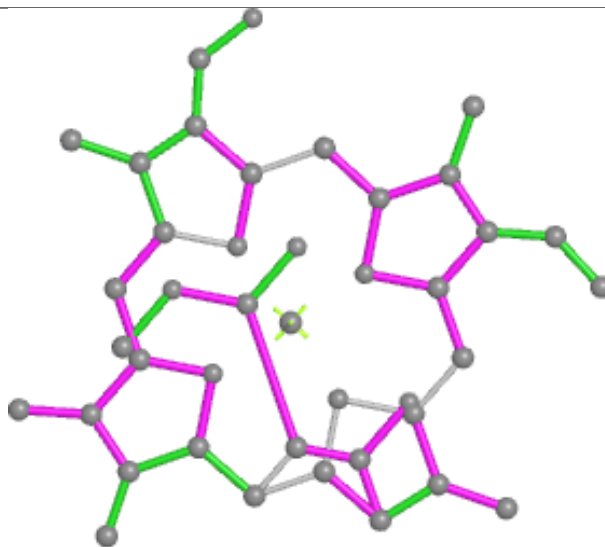




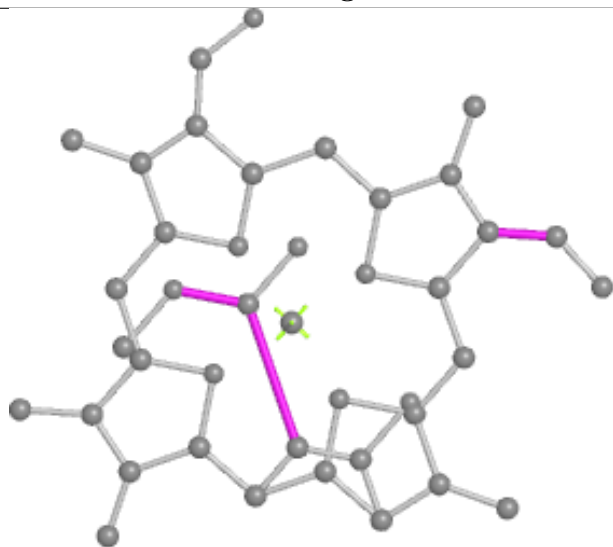
Ligand CL7 24 416



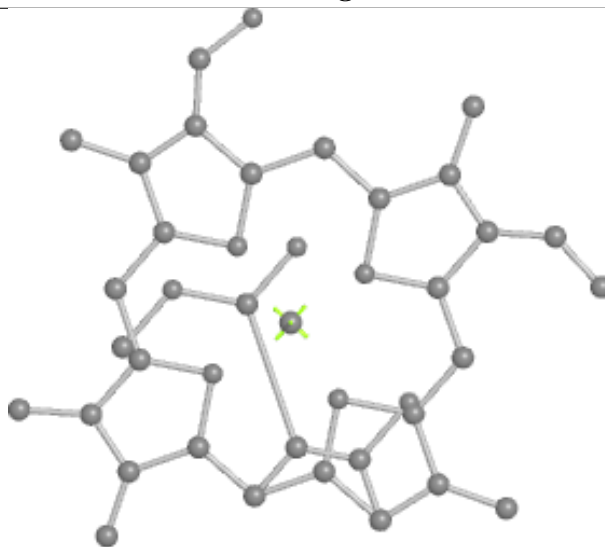
Bond lengths



Bond angles

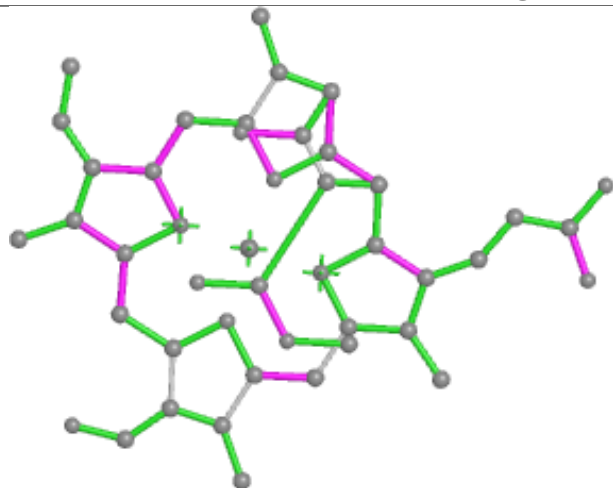


Torsions

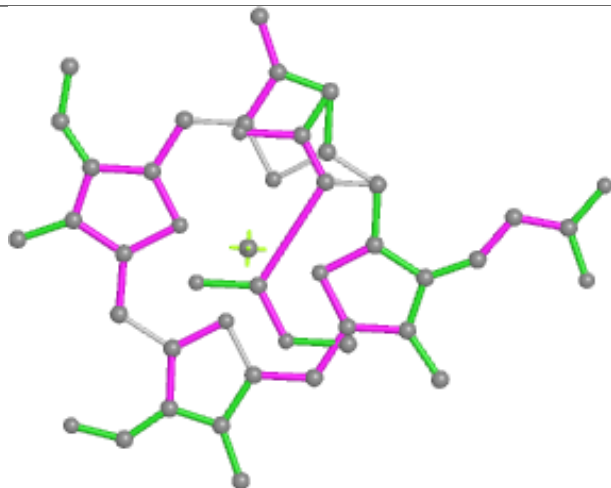


Rings

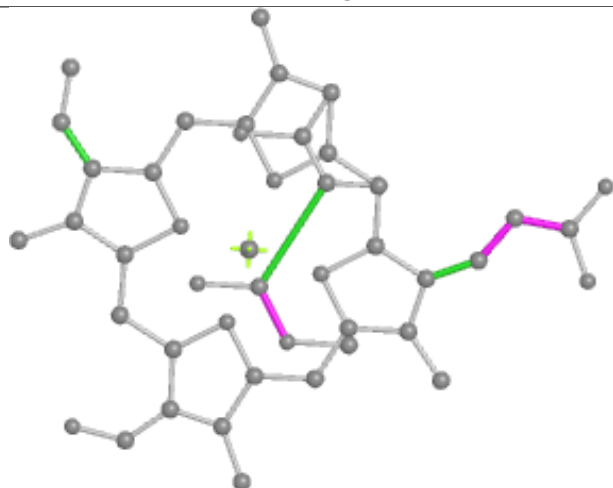
Ligand CL7 43 419



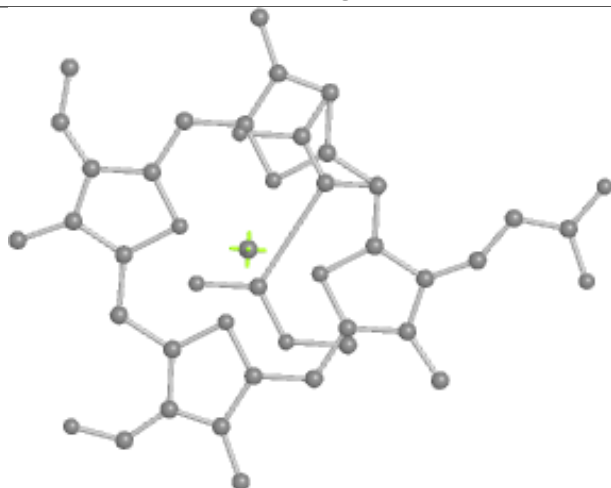
Bond lengths



Bond angles

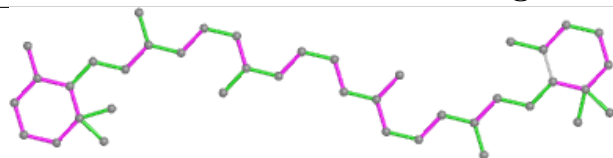


Torsions

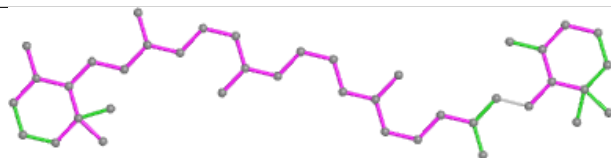


Rings

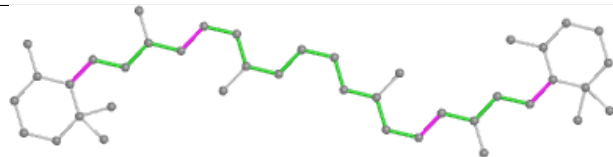
Ligand 8CT 14 402



Bond lengths



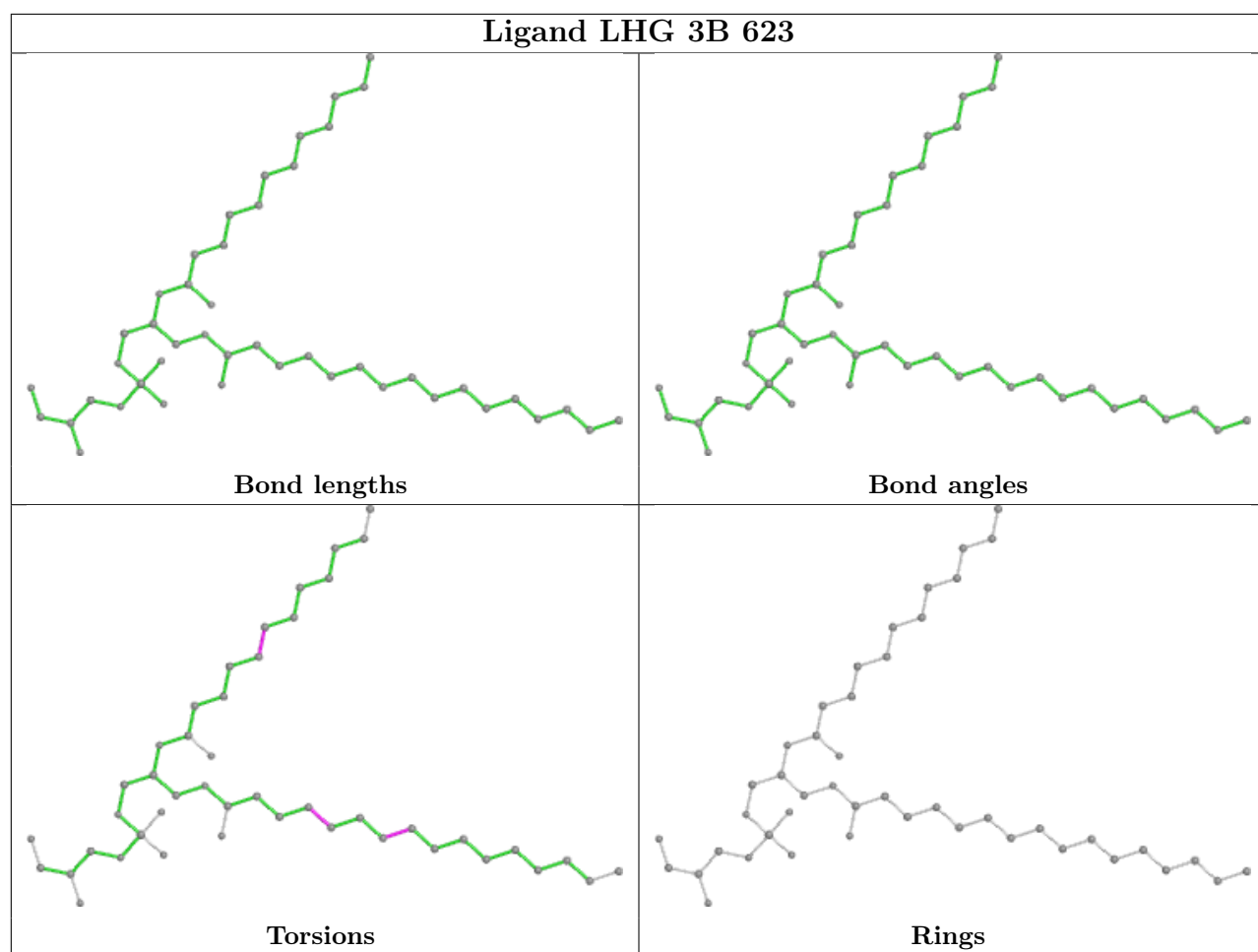
Bond angles



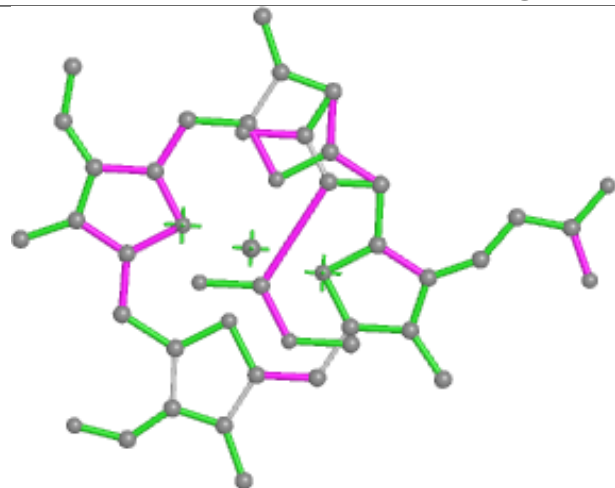
Torsions



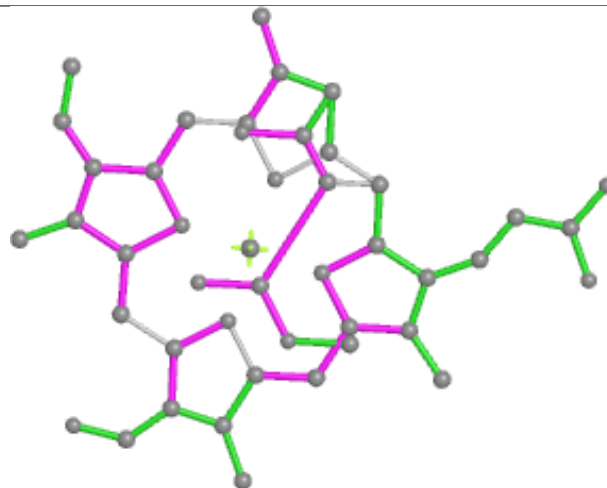
Rings



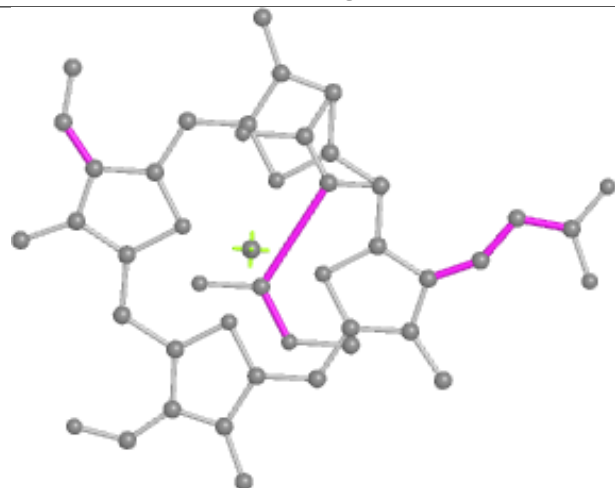
Ligand CL7 24 415



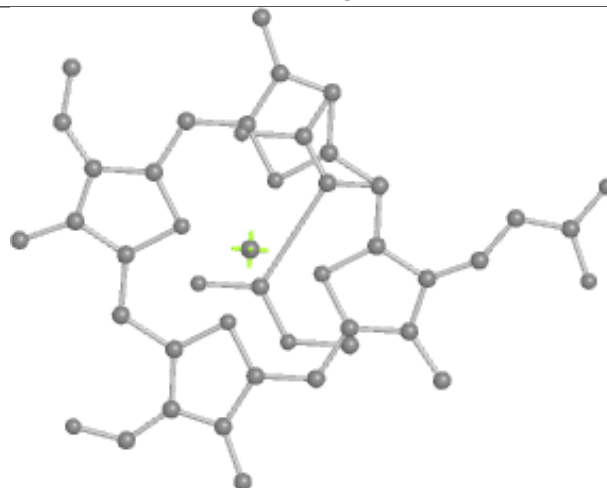
Bond lengths



Bond angles

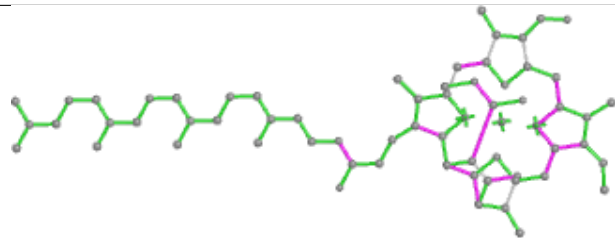


Torsions

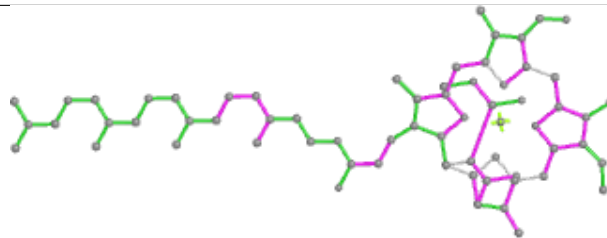


Rings

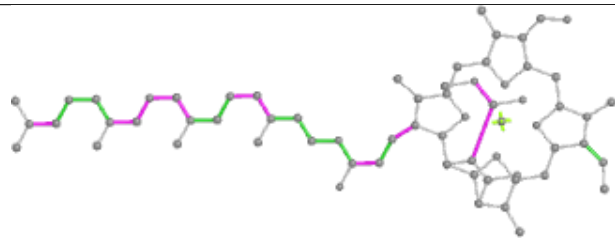
Ligand CL7 1C 503



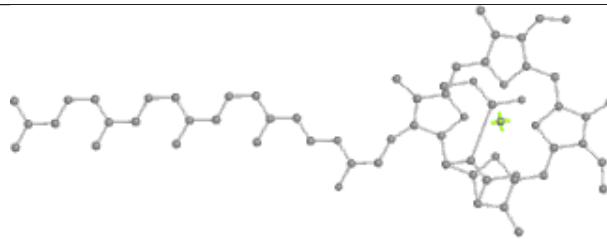
Bond lengths



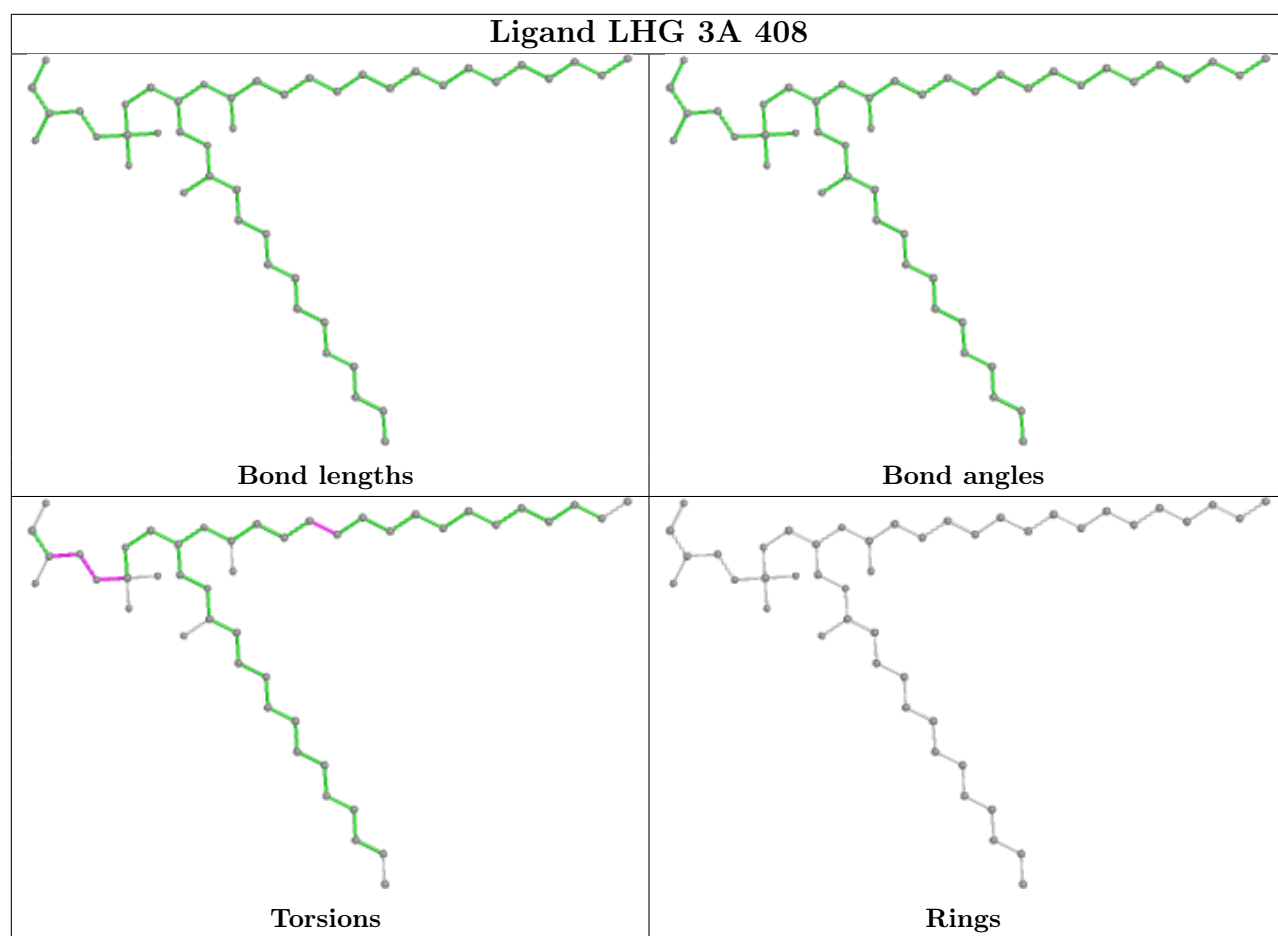
Bond angles

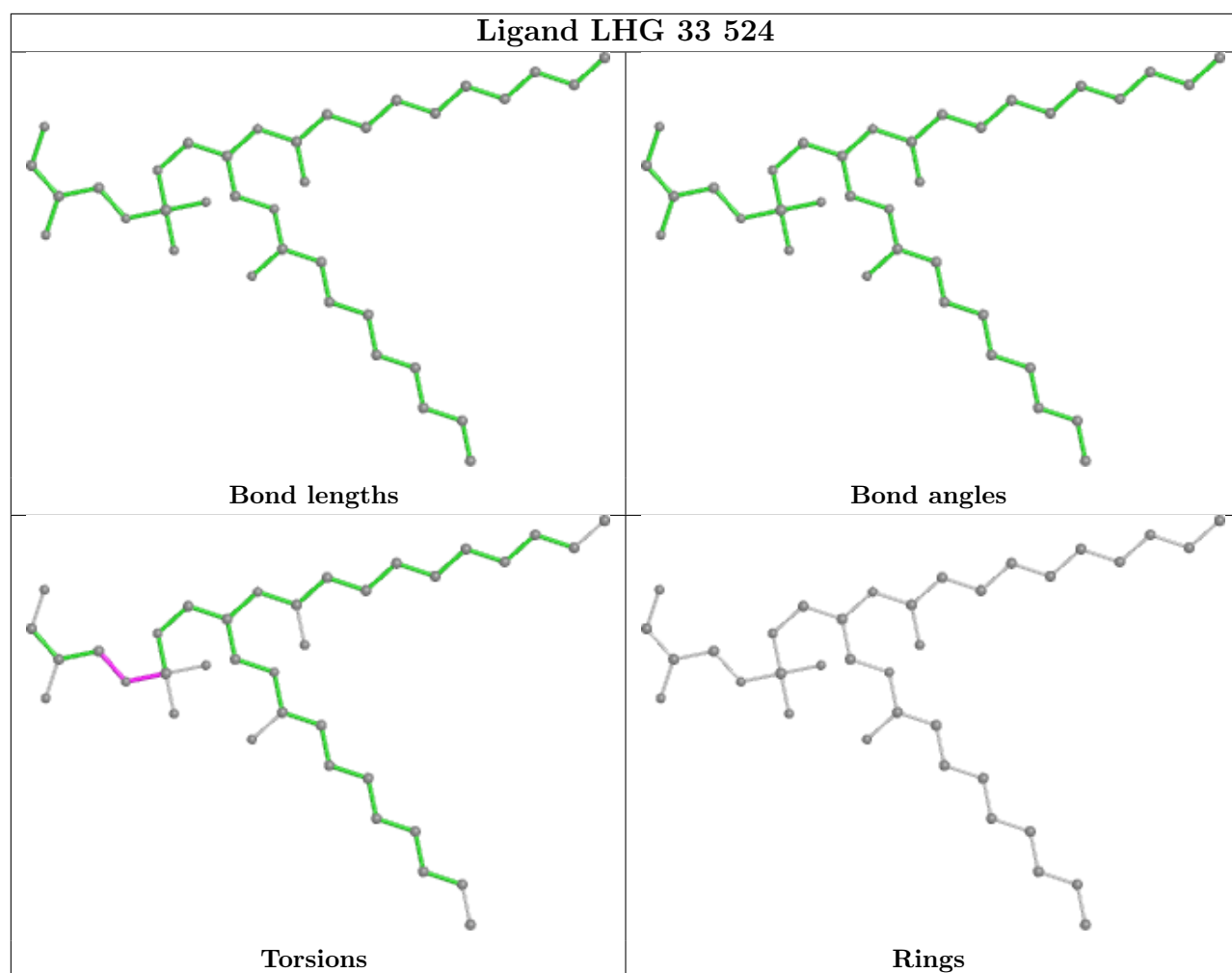


Torsions

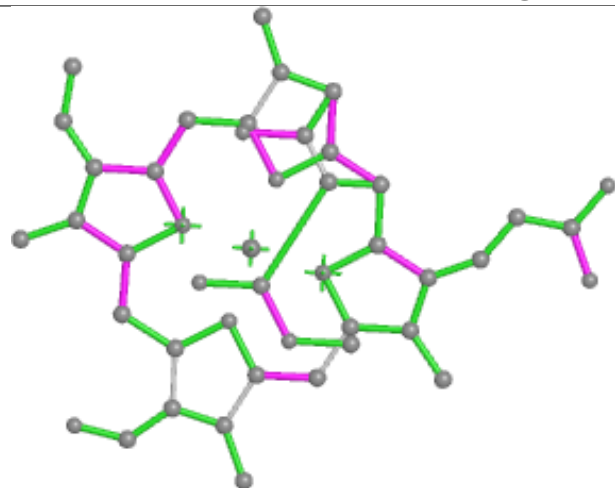


Rings

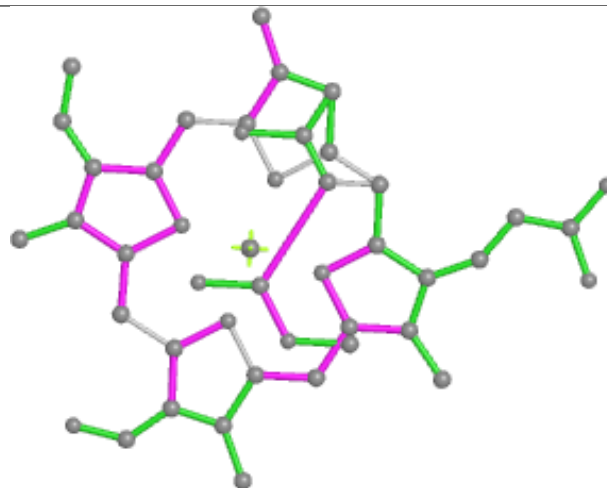




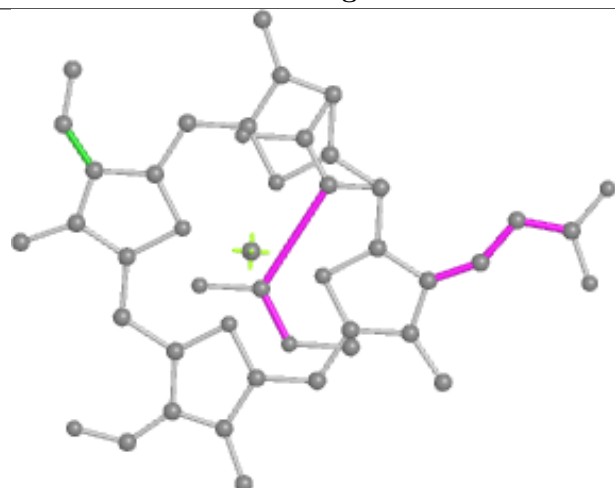
Ligand CL7 11 405



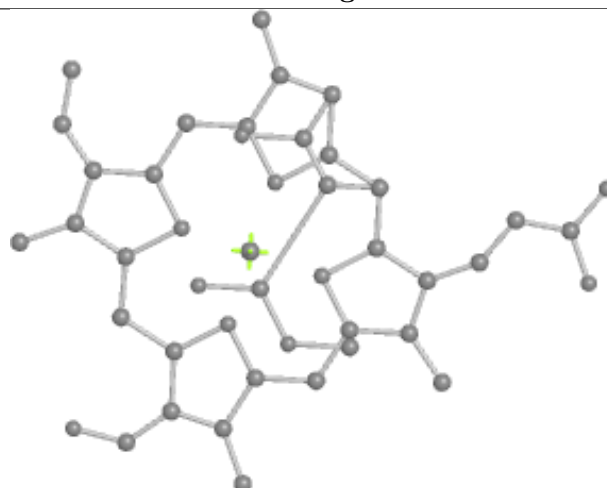
Bond lengths



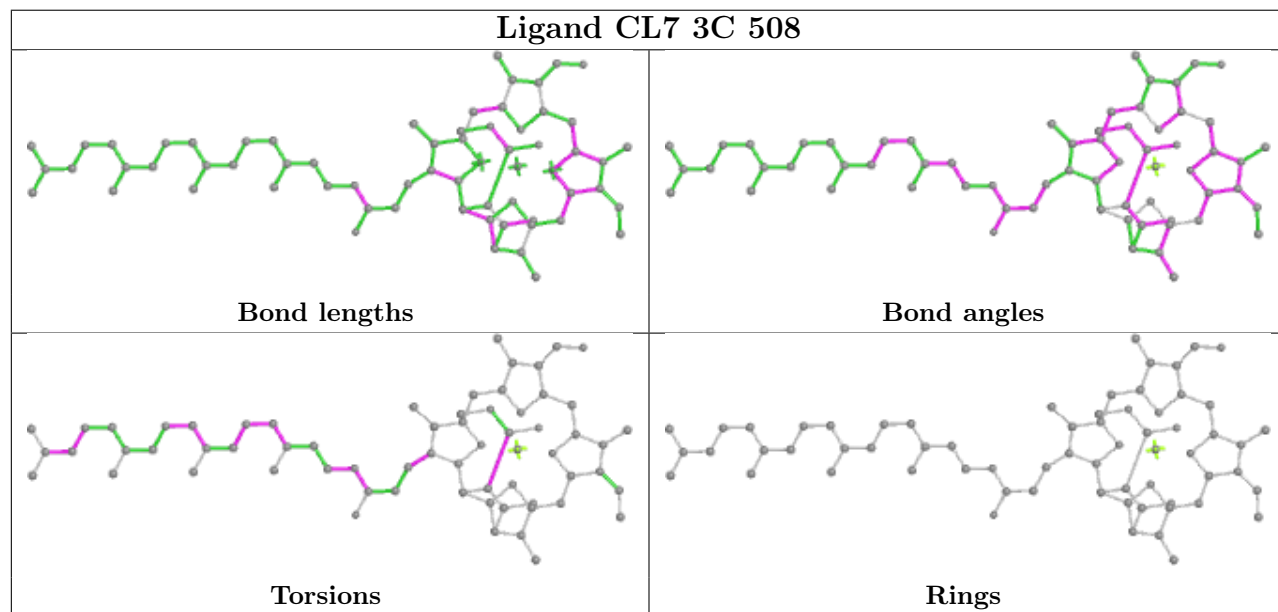
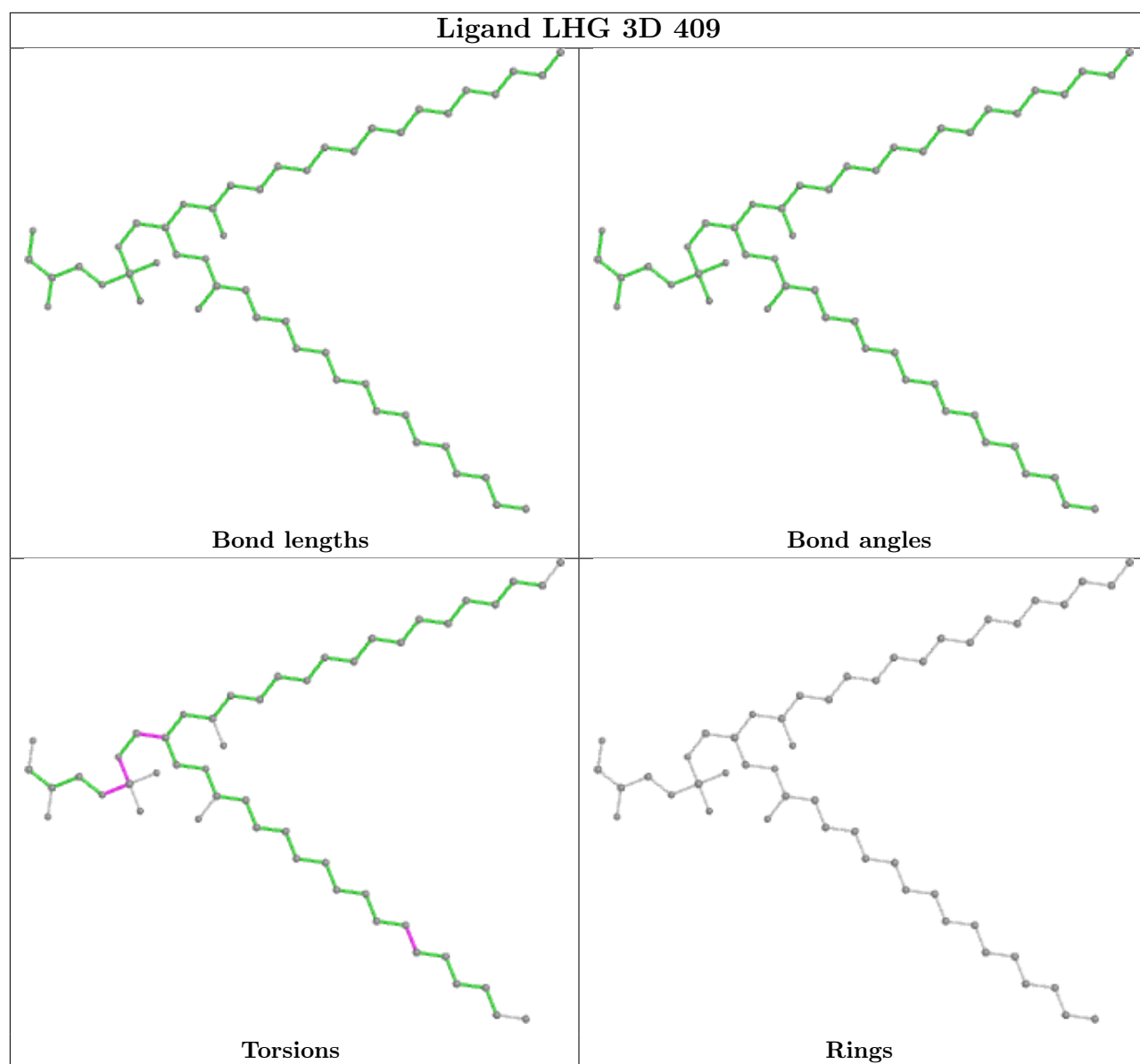
Bond angles

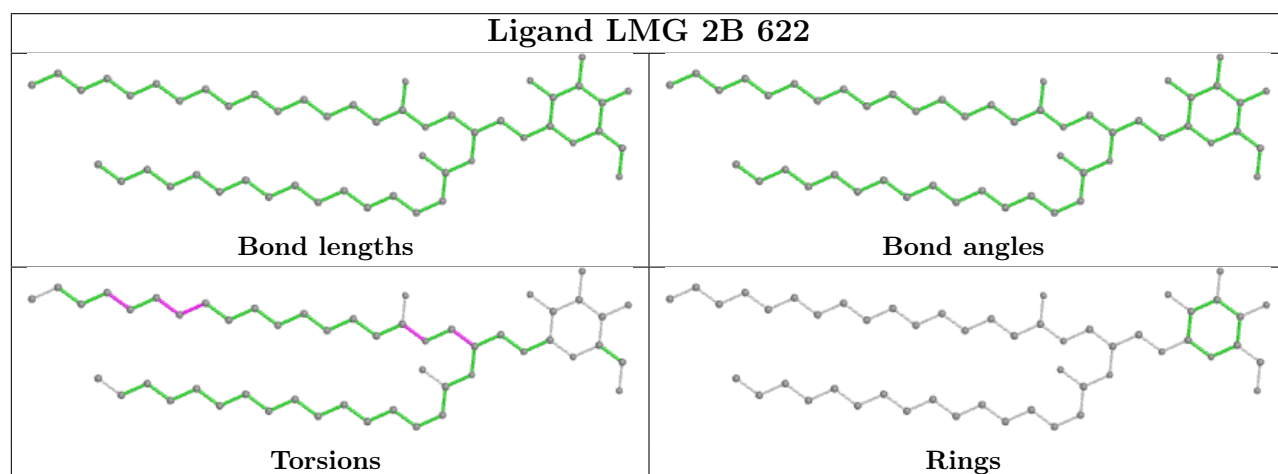
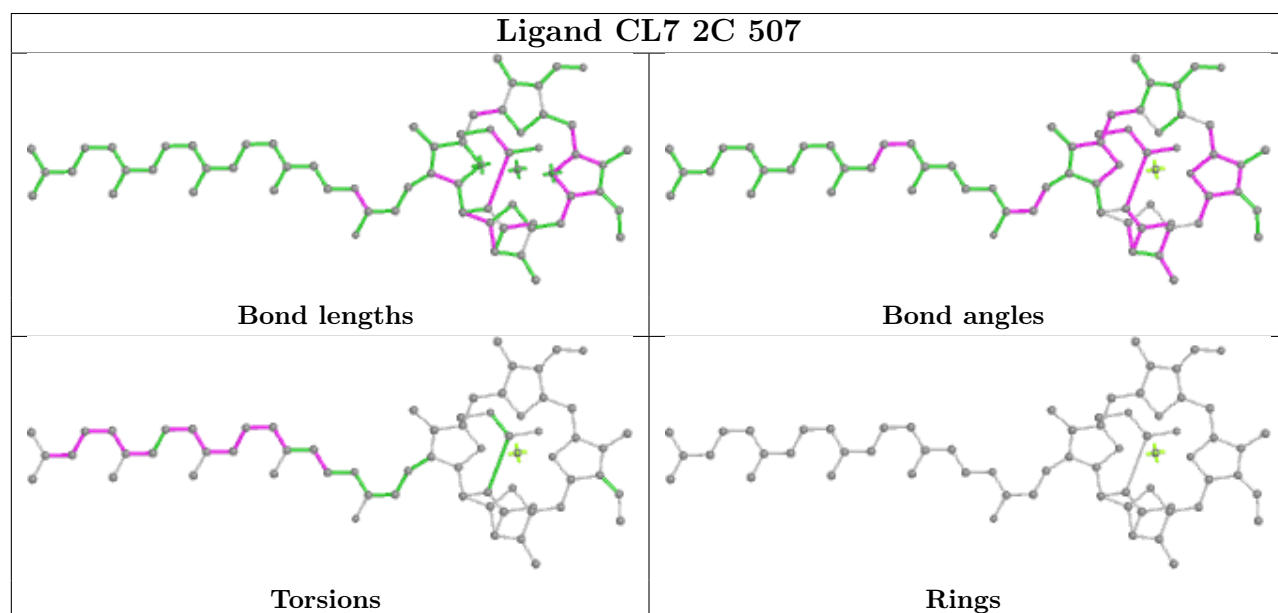
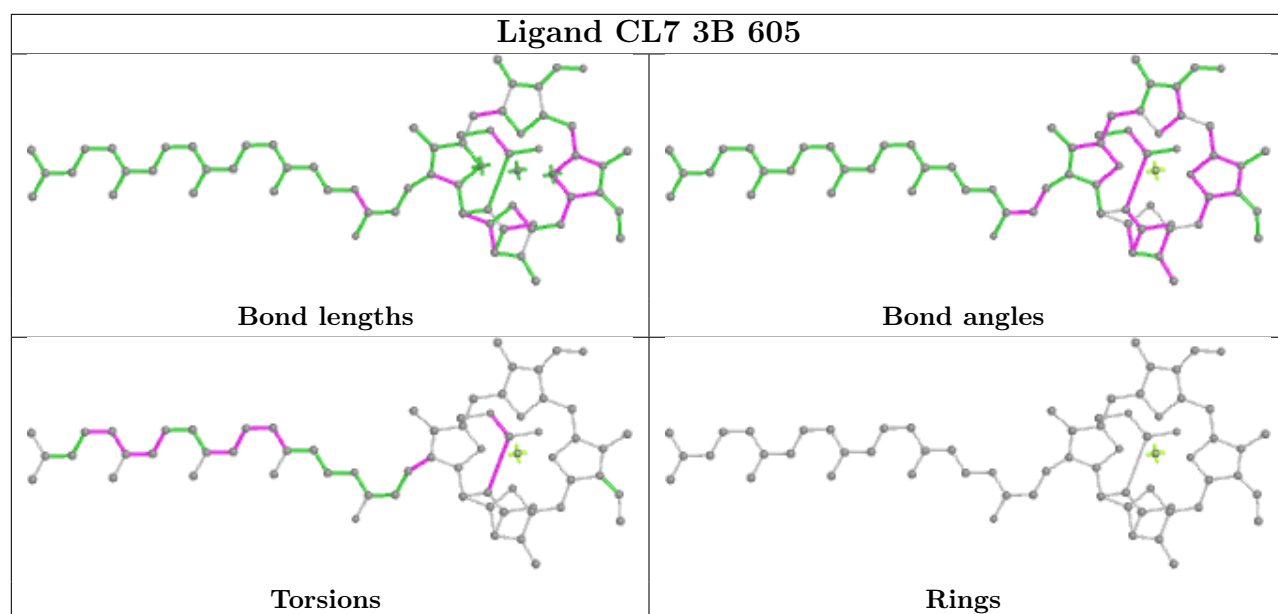


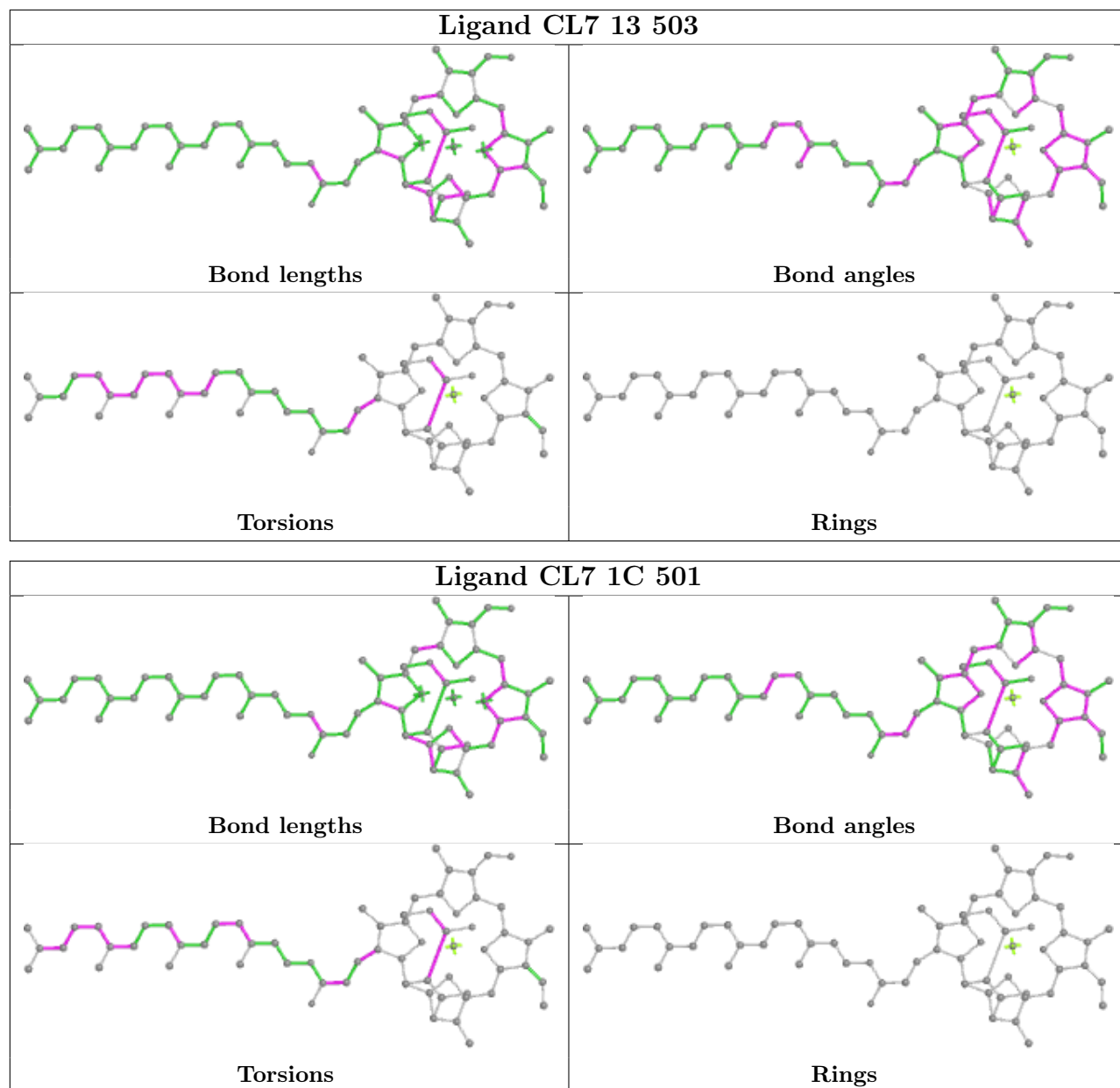
Torsions



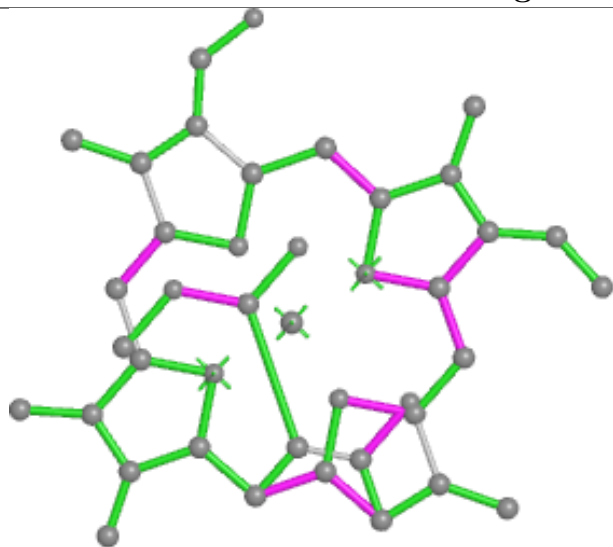
Rings



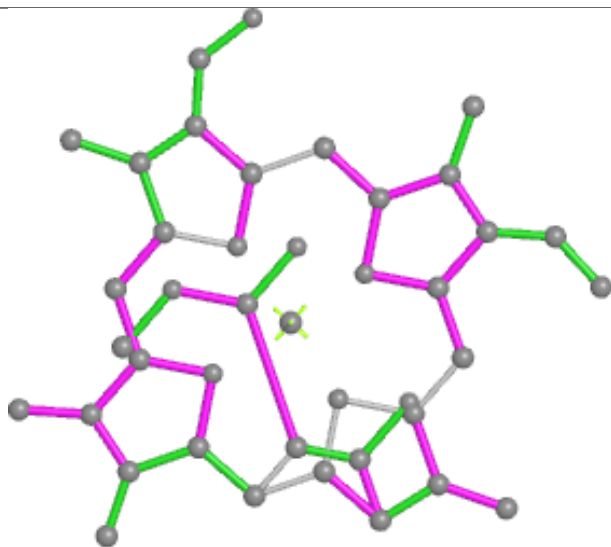




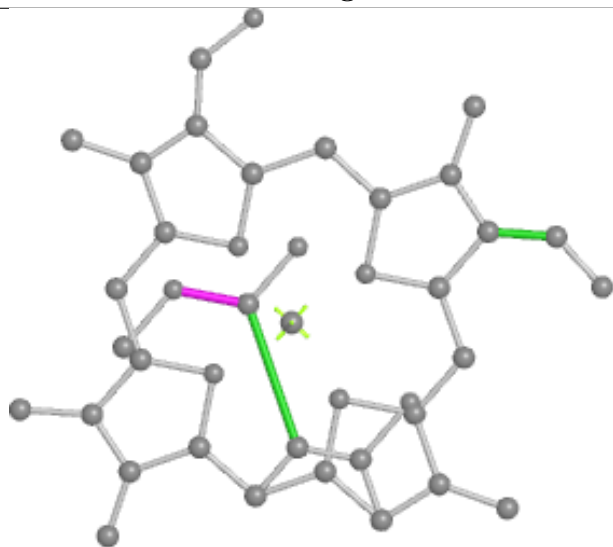
Ligand CL7 41 416



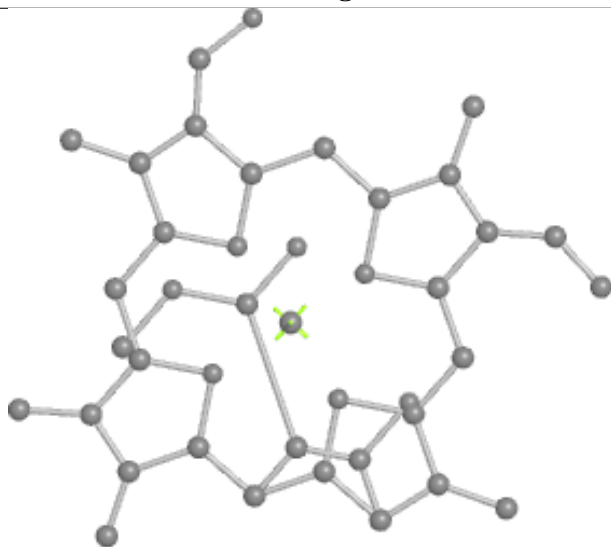
Bond lengths



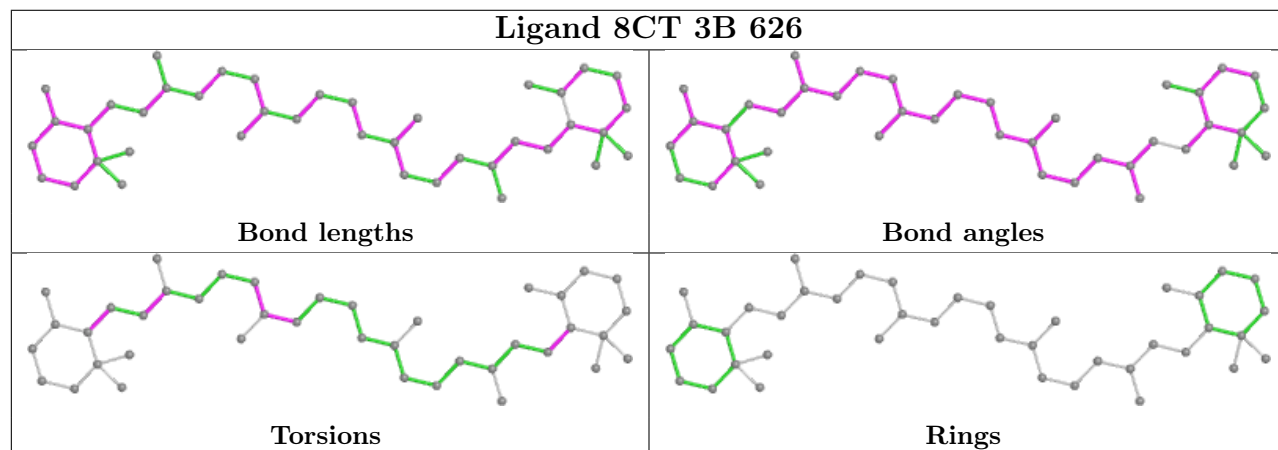
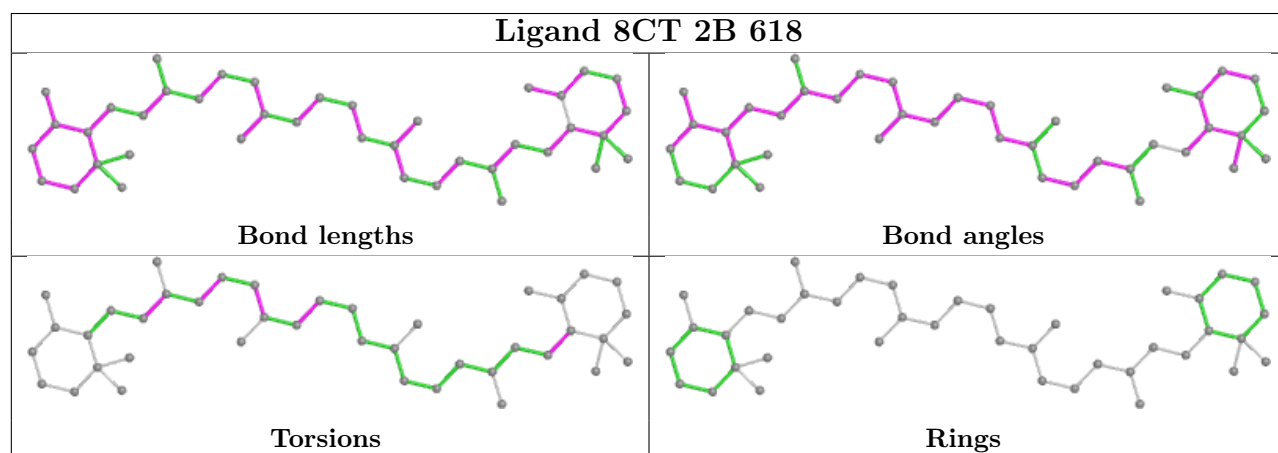
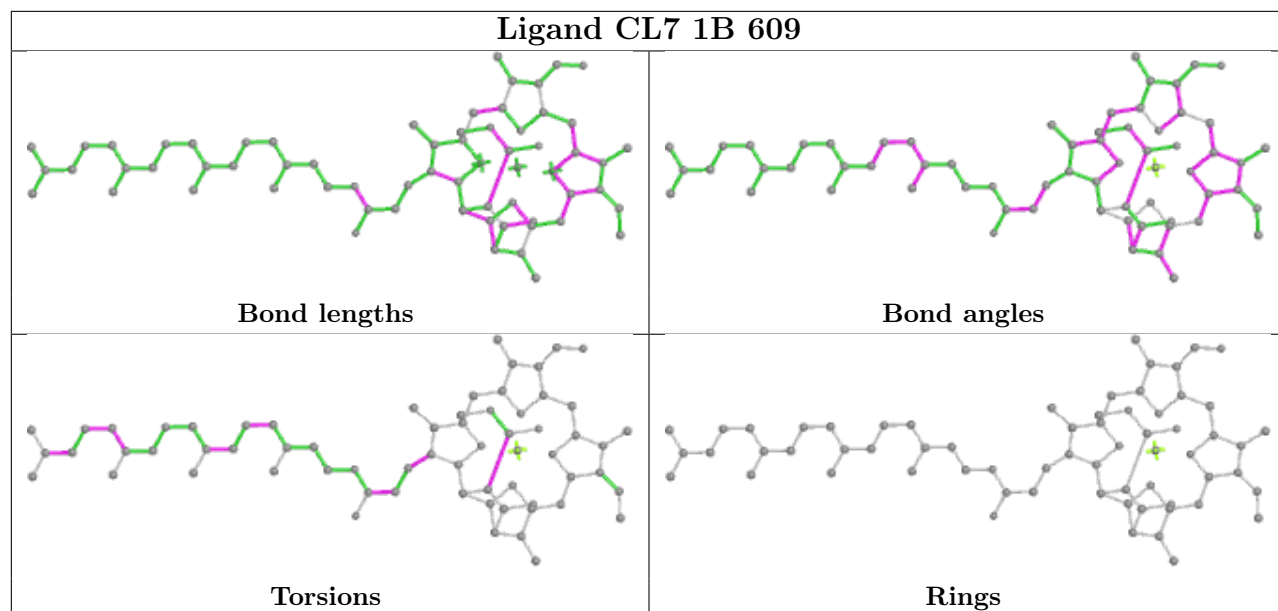
Bond angles

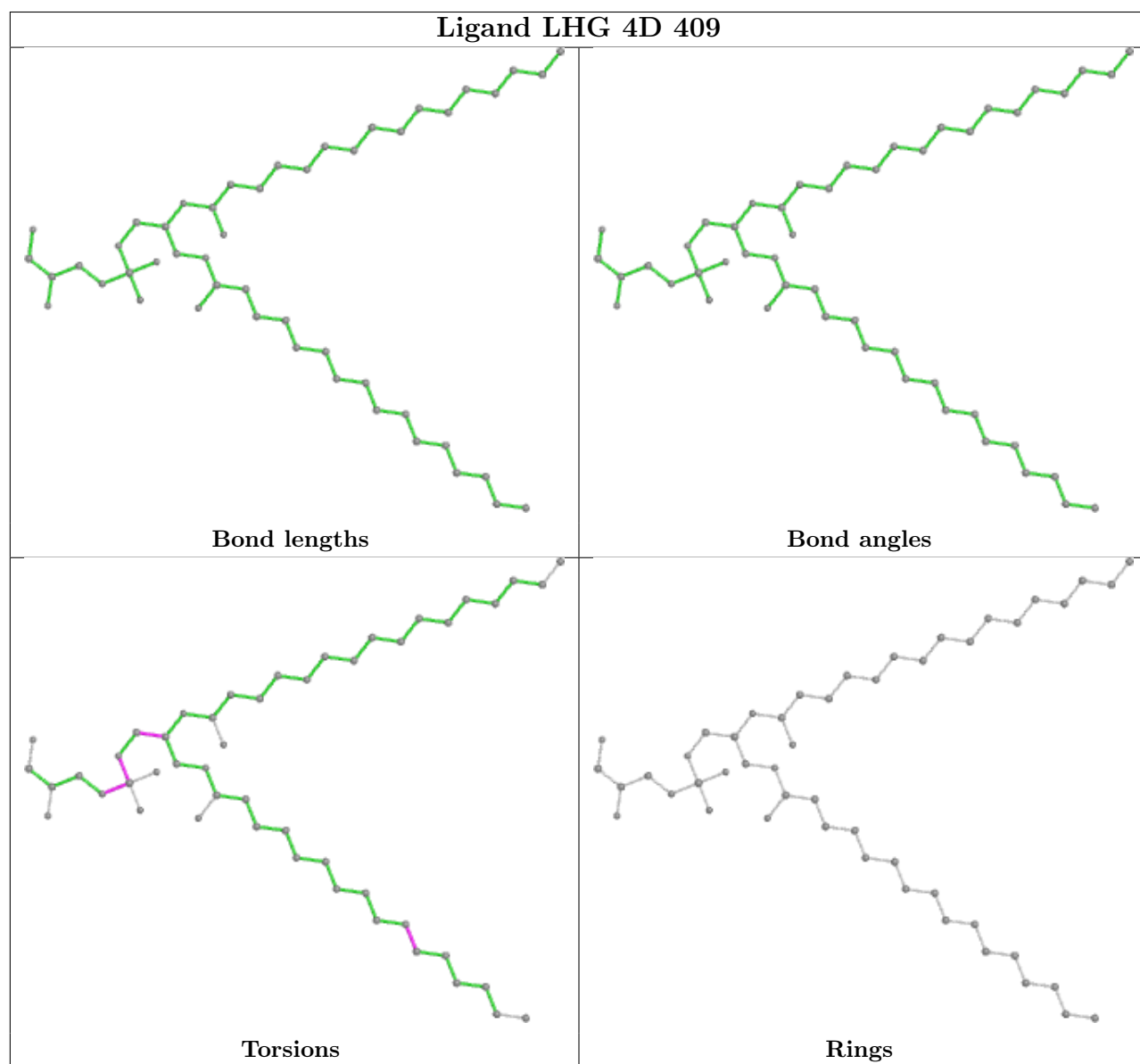
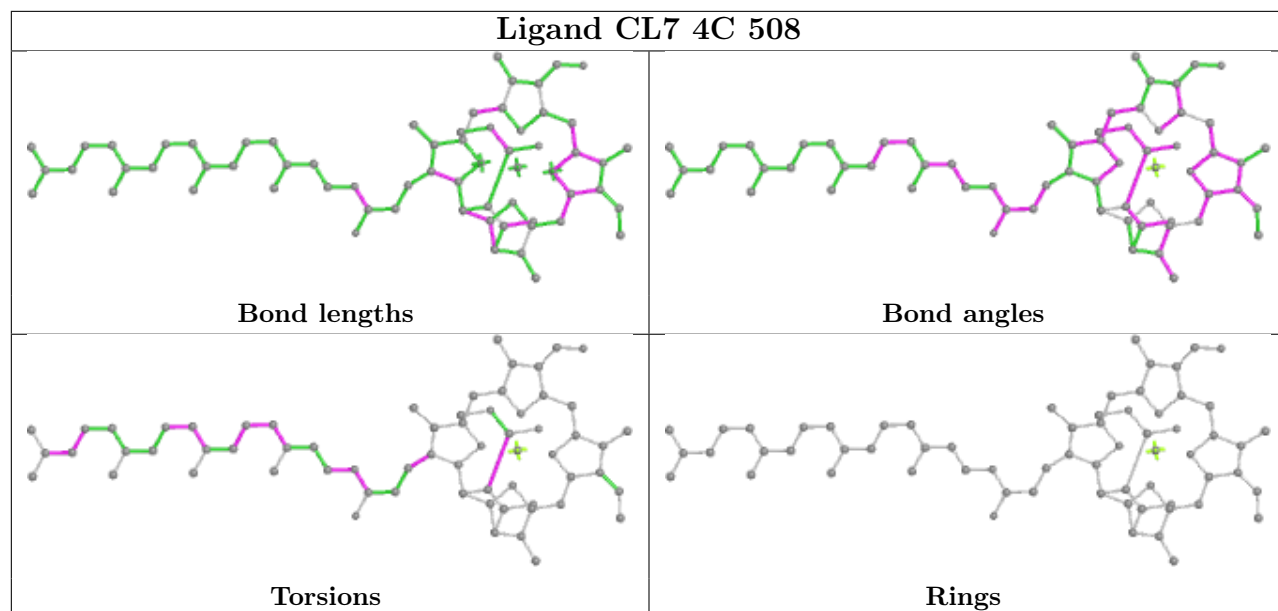


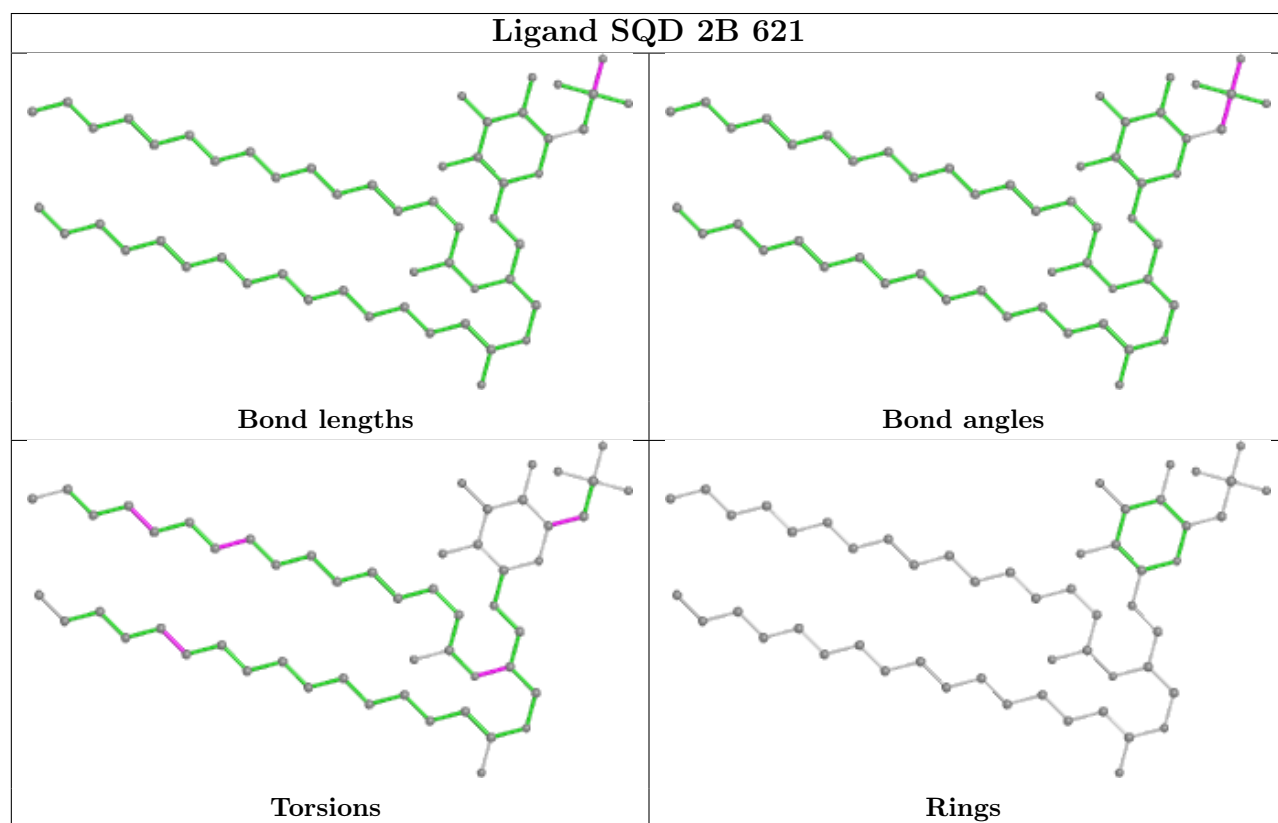
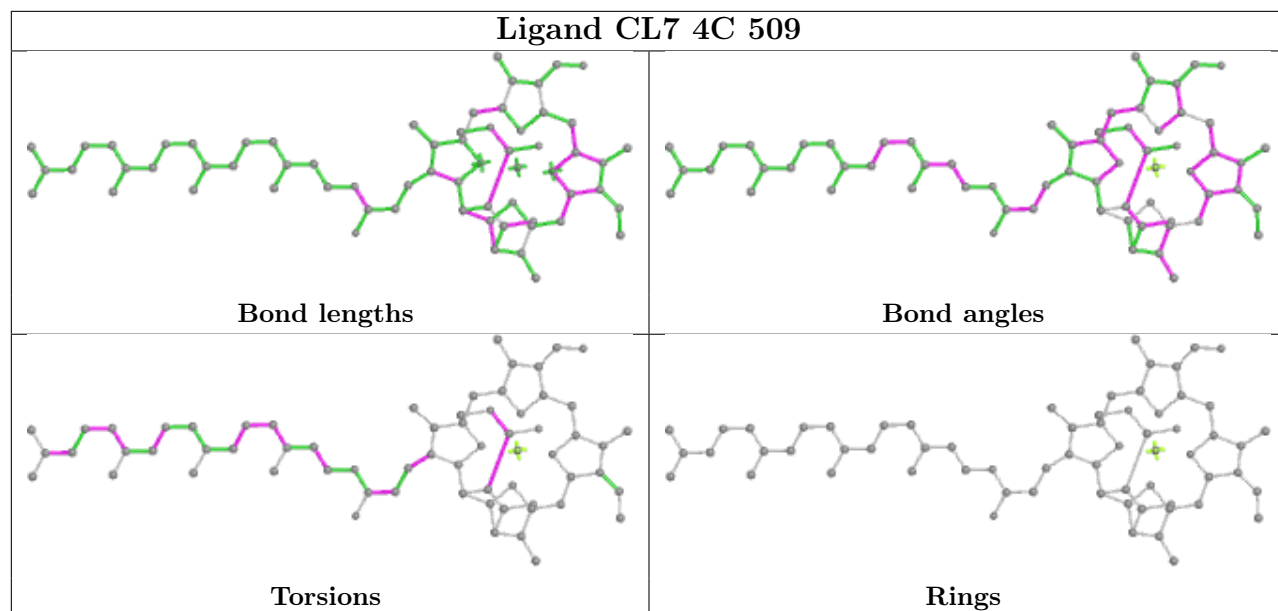
Torsions

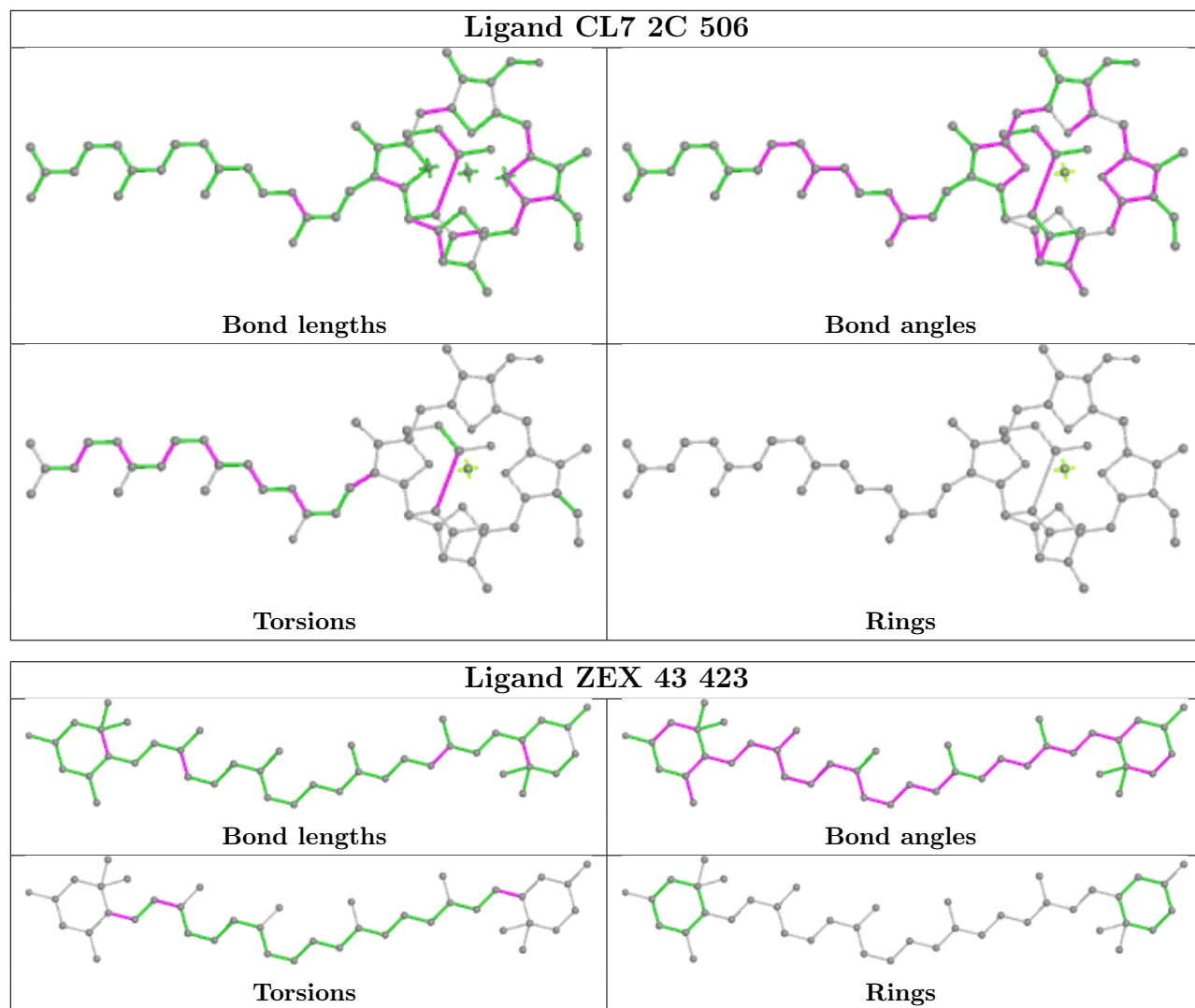


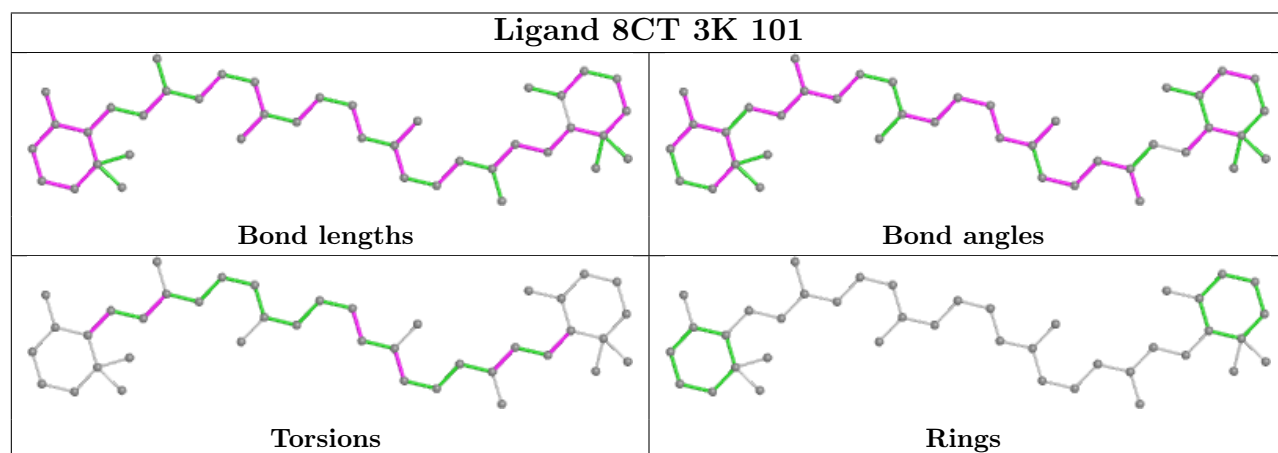
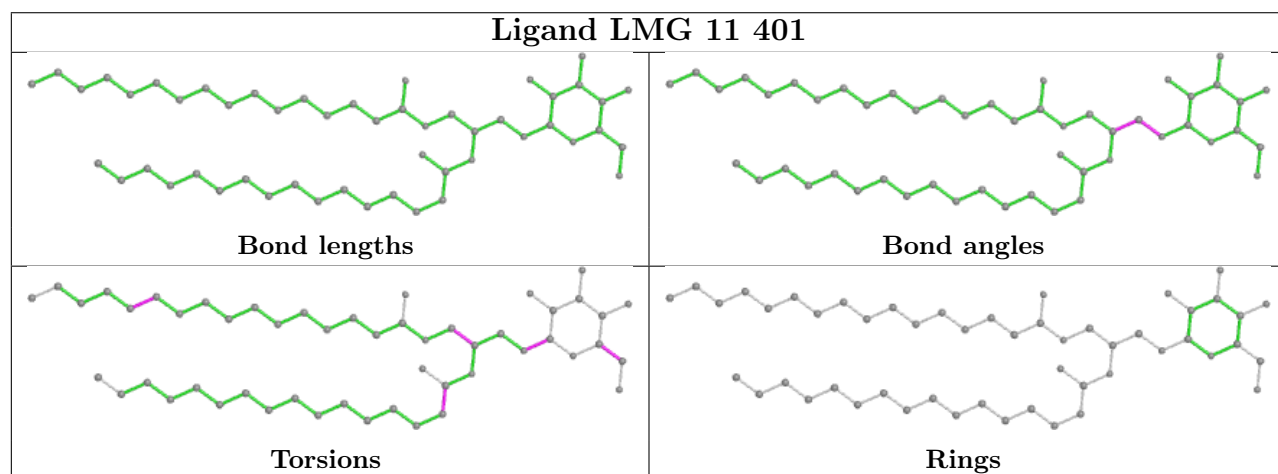
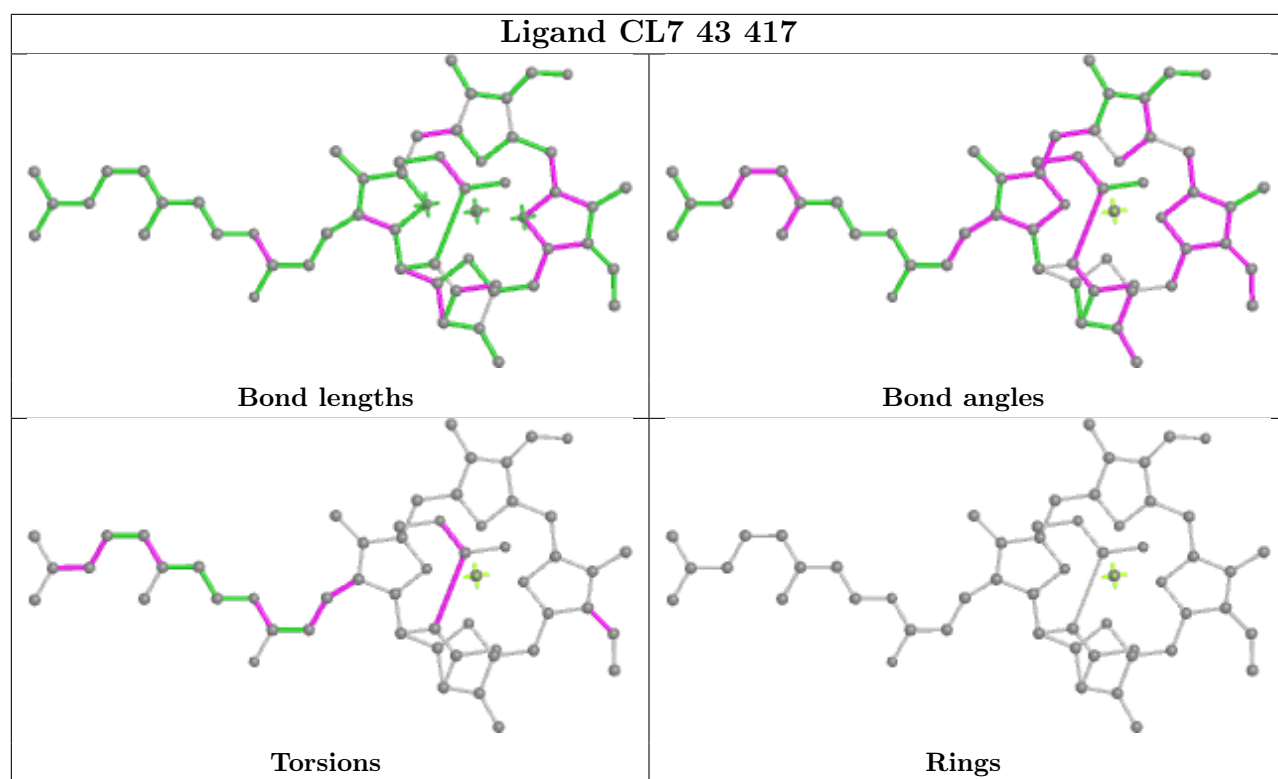
Rings

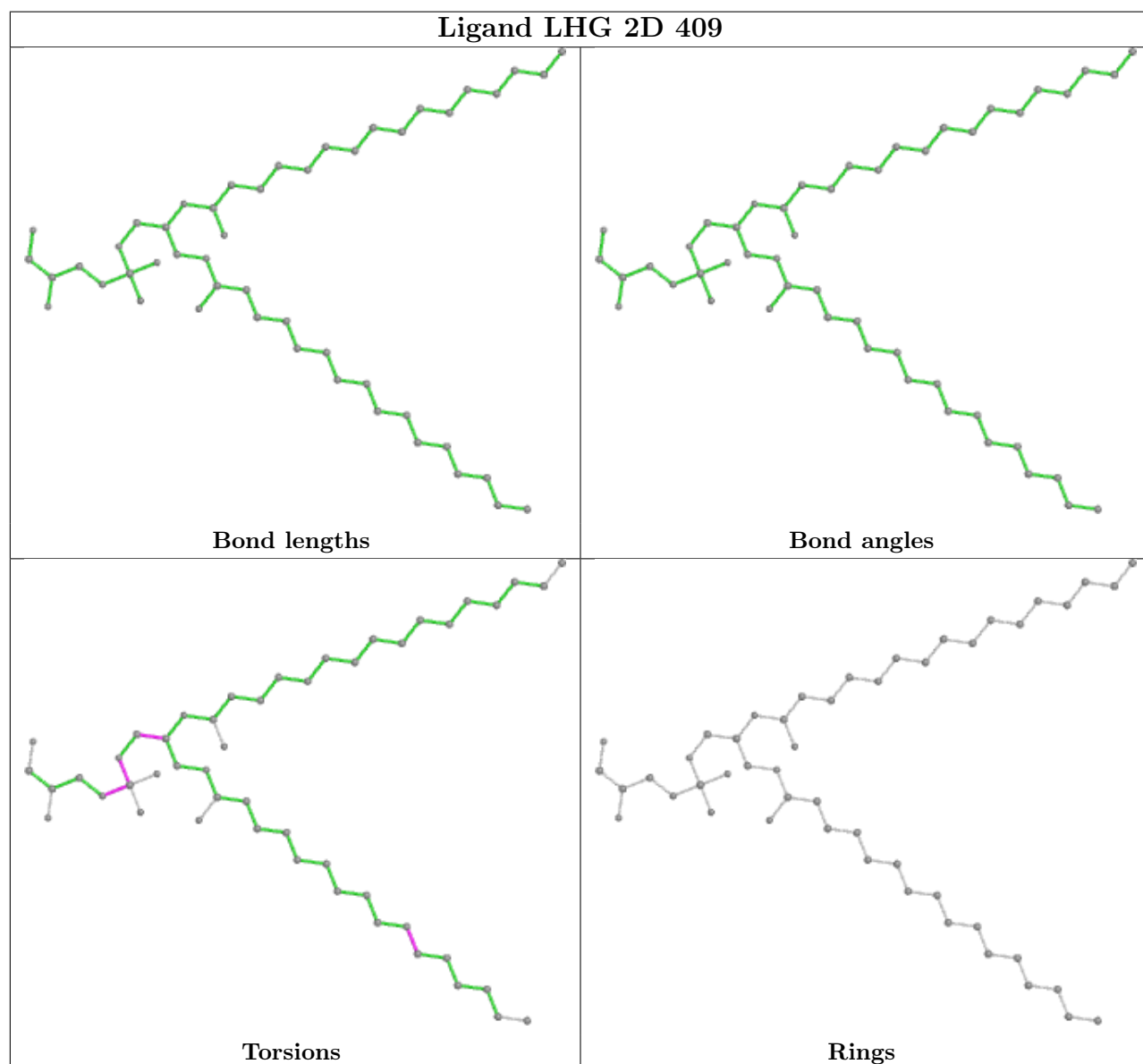
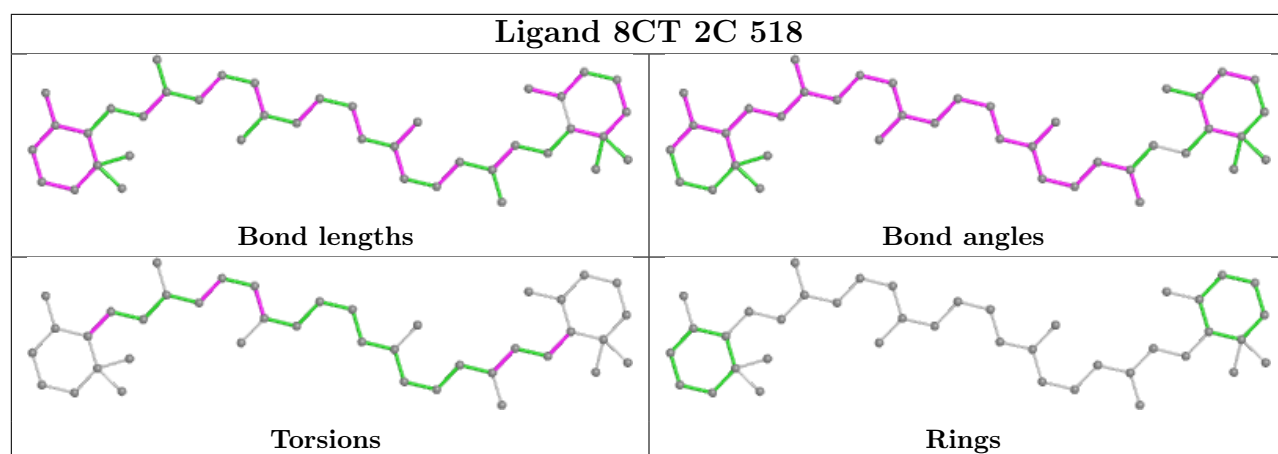


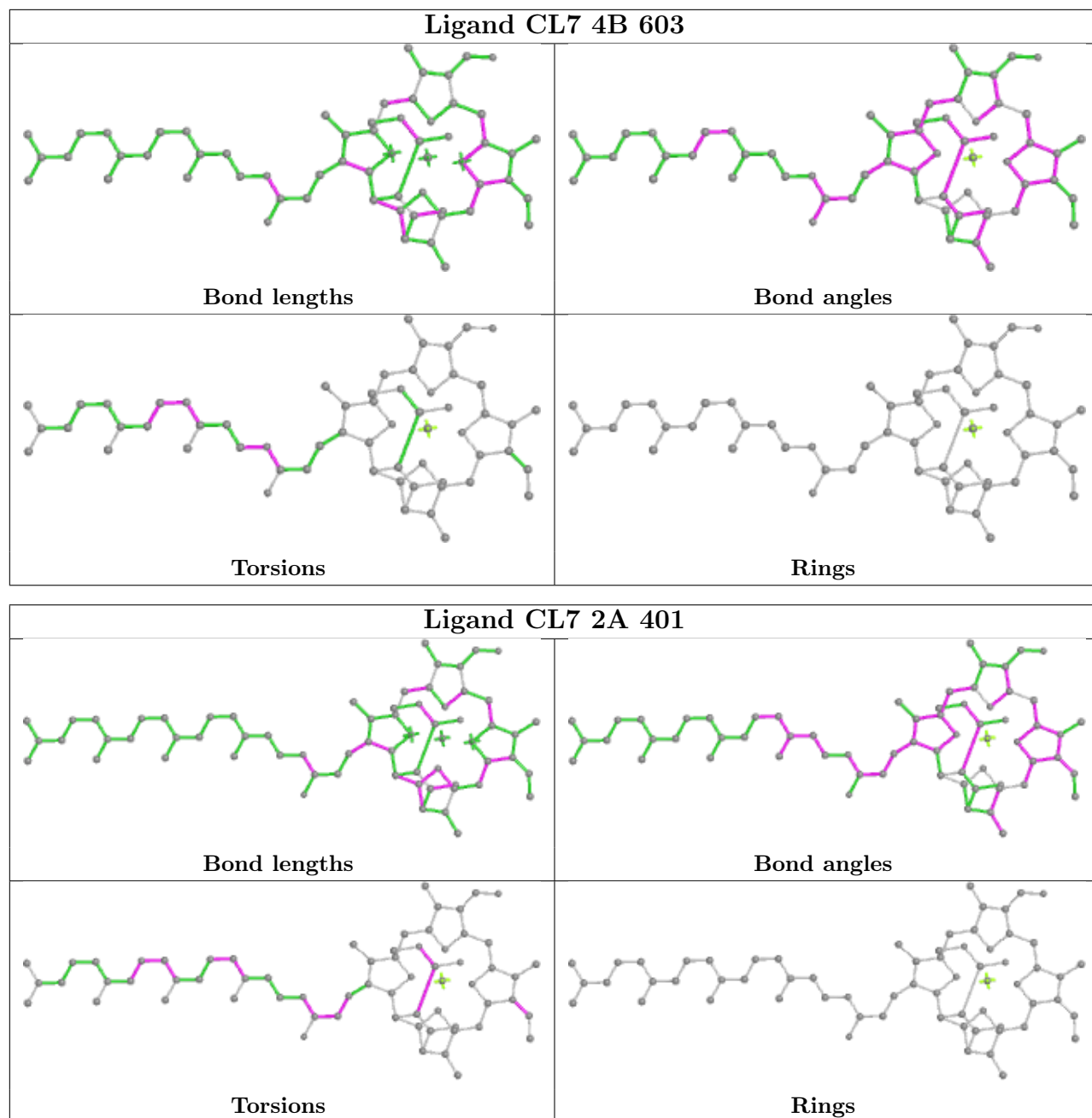


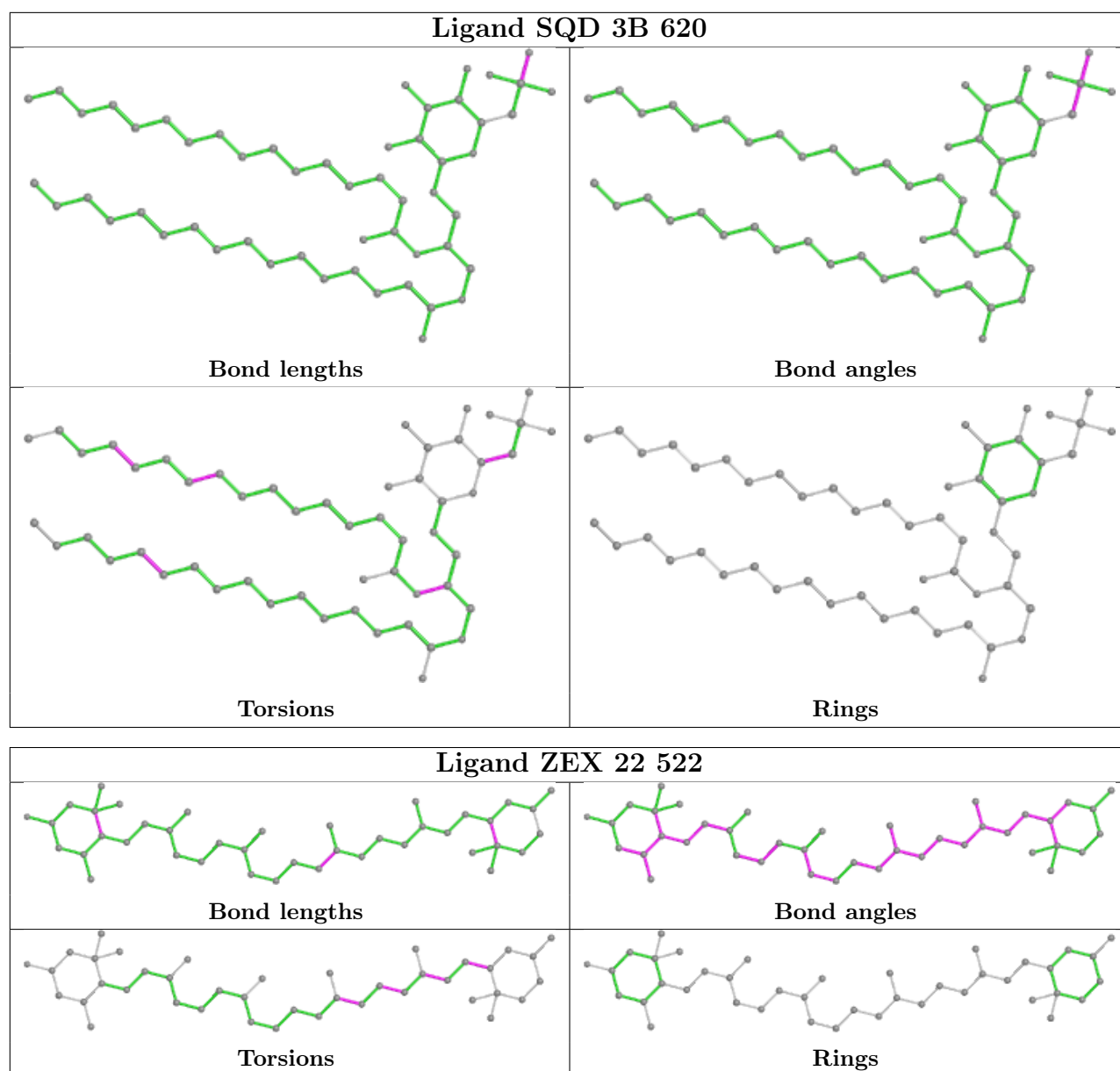




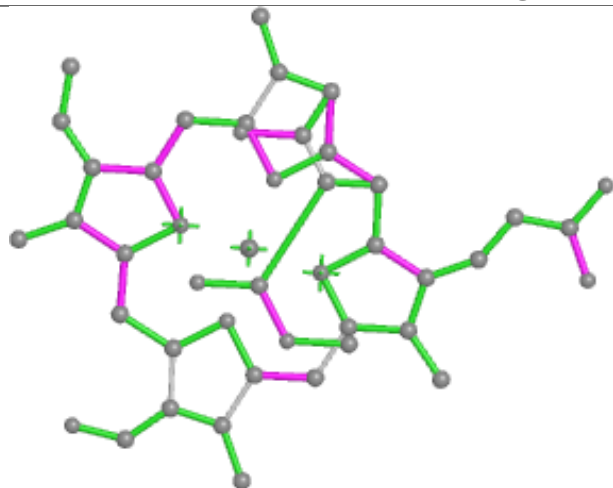




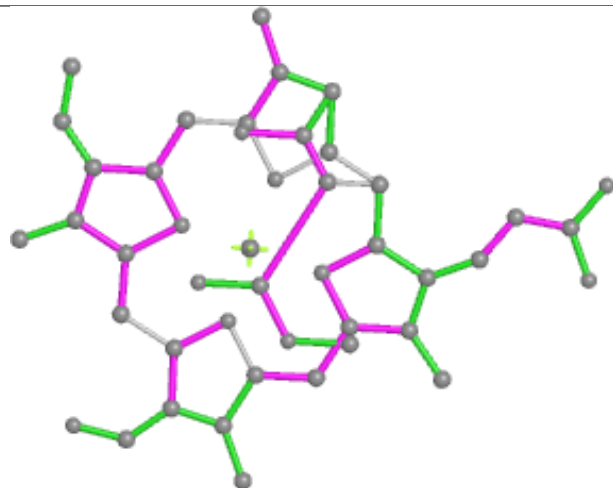




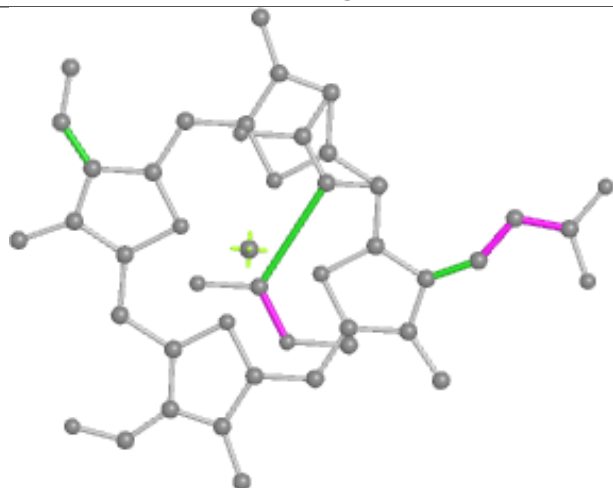
Ligand CL7 23 419



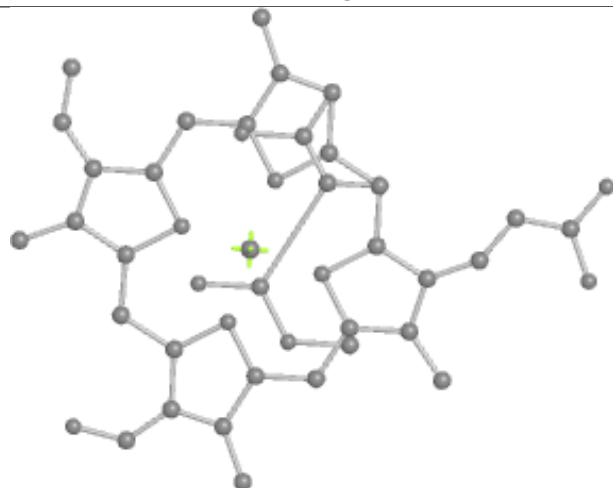
Bond lengths



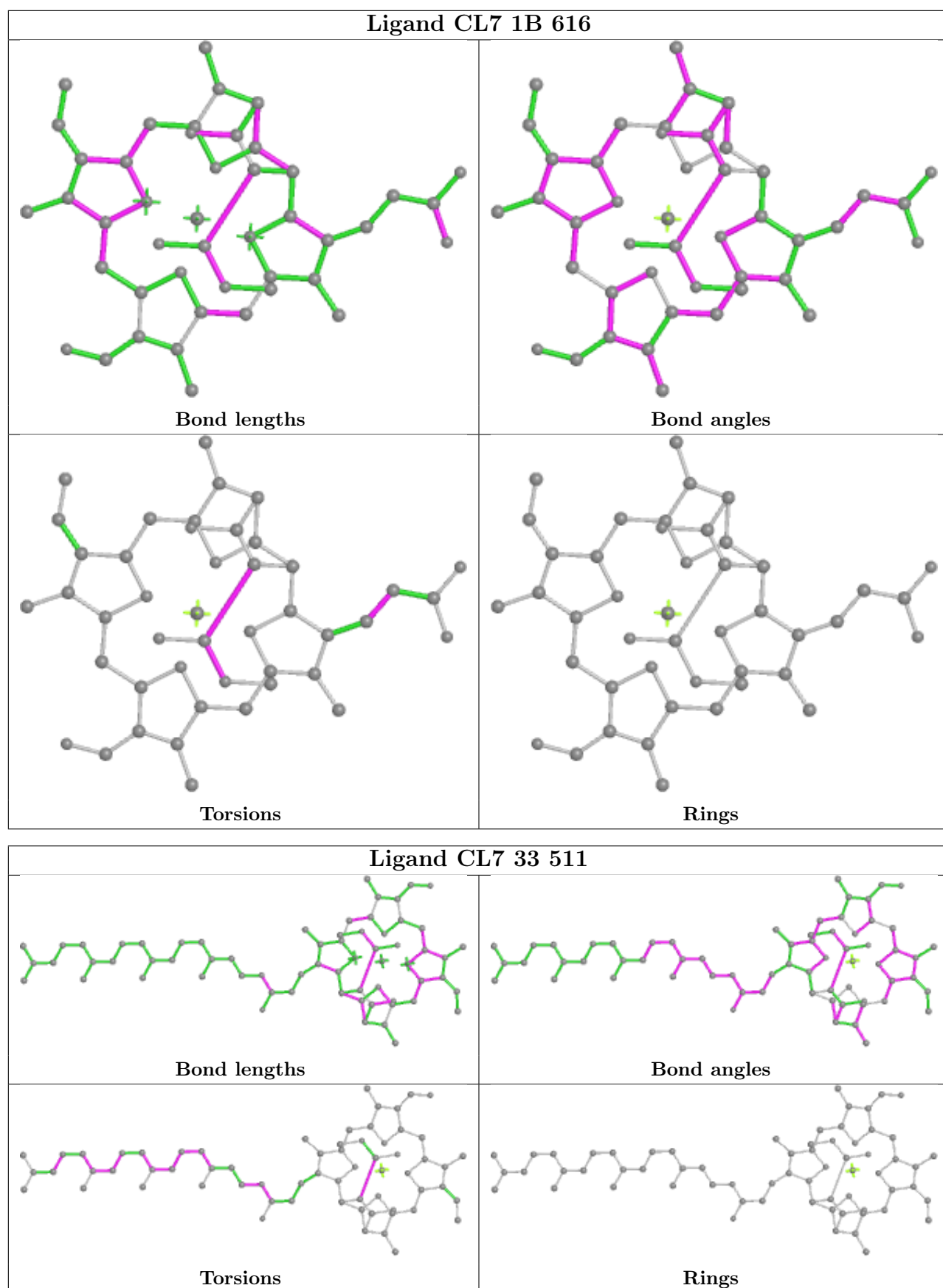
Bond angles



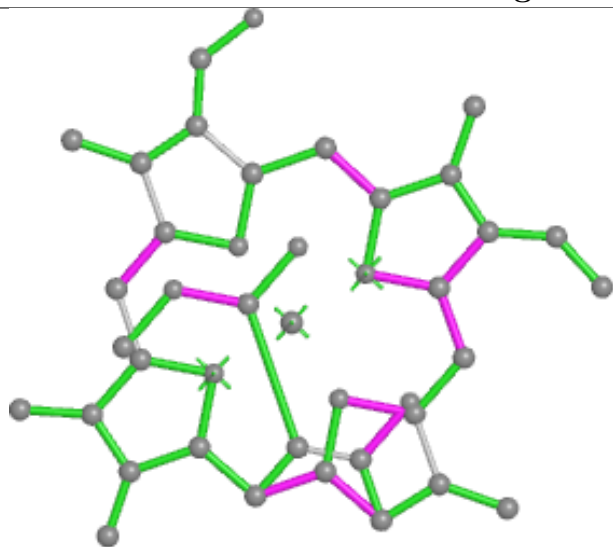
Torsions



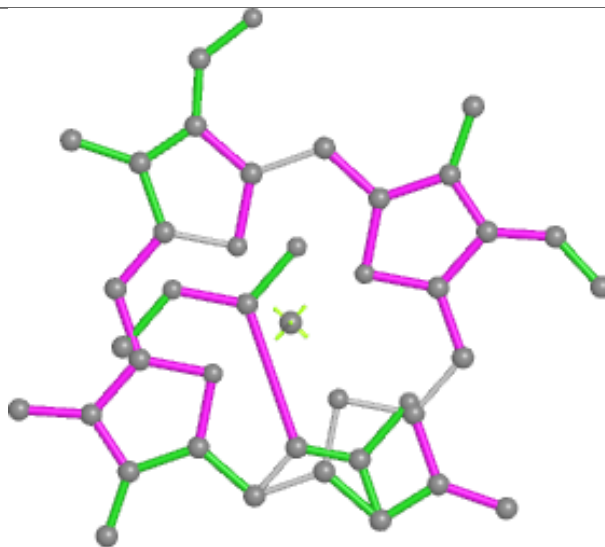
Rings



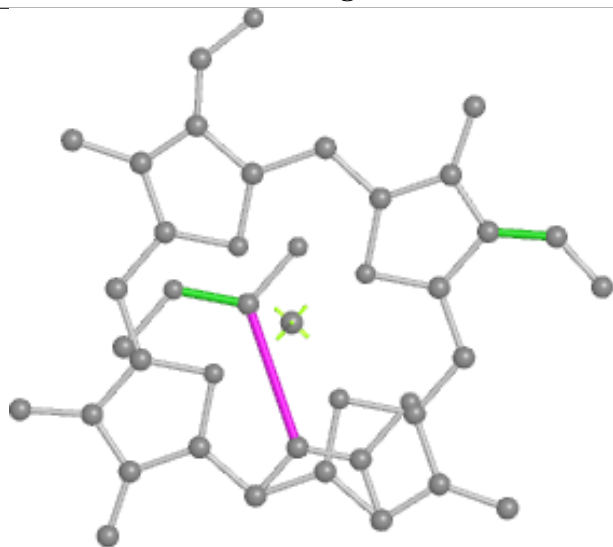
Ligand CL7 44 407



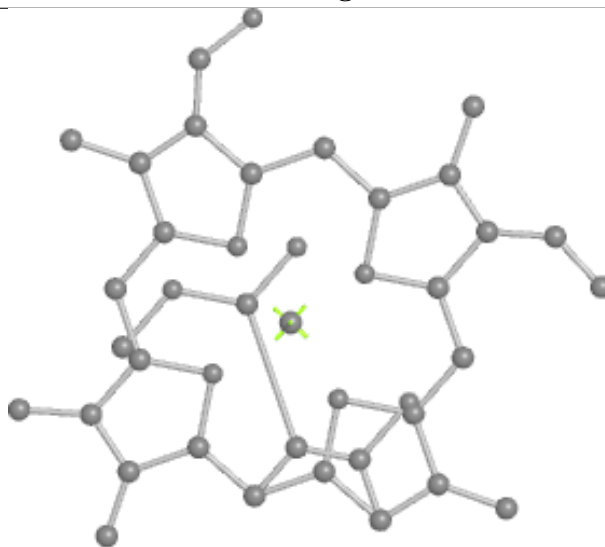
Bond lengths



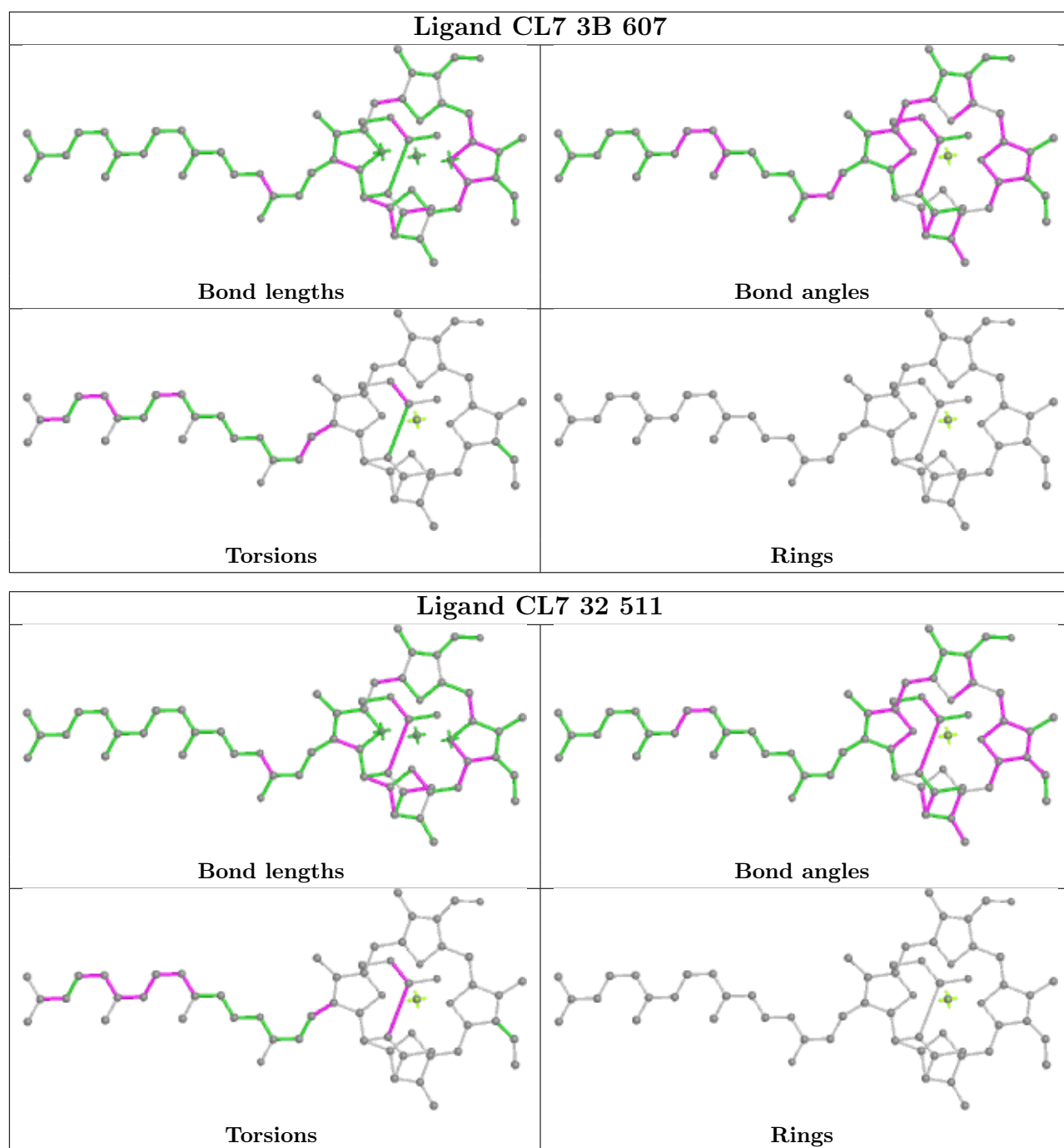
Bond angles



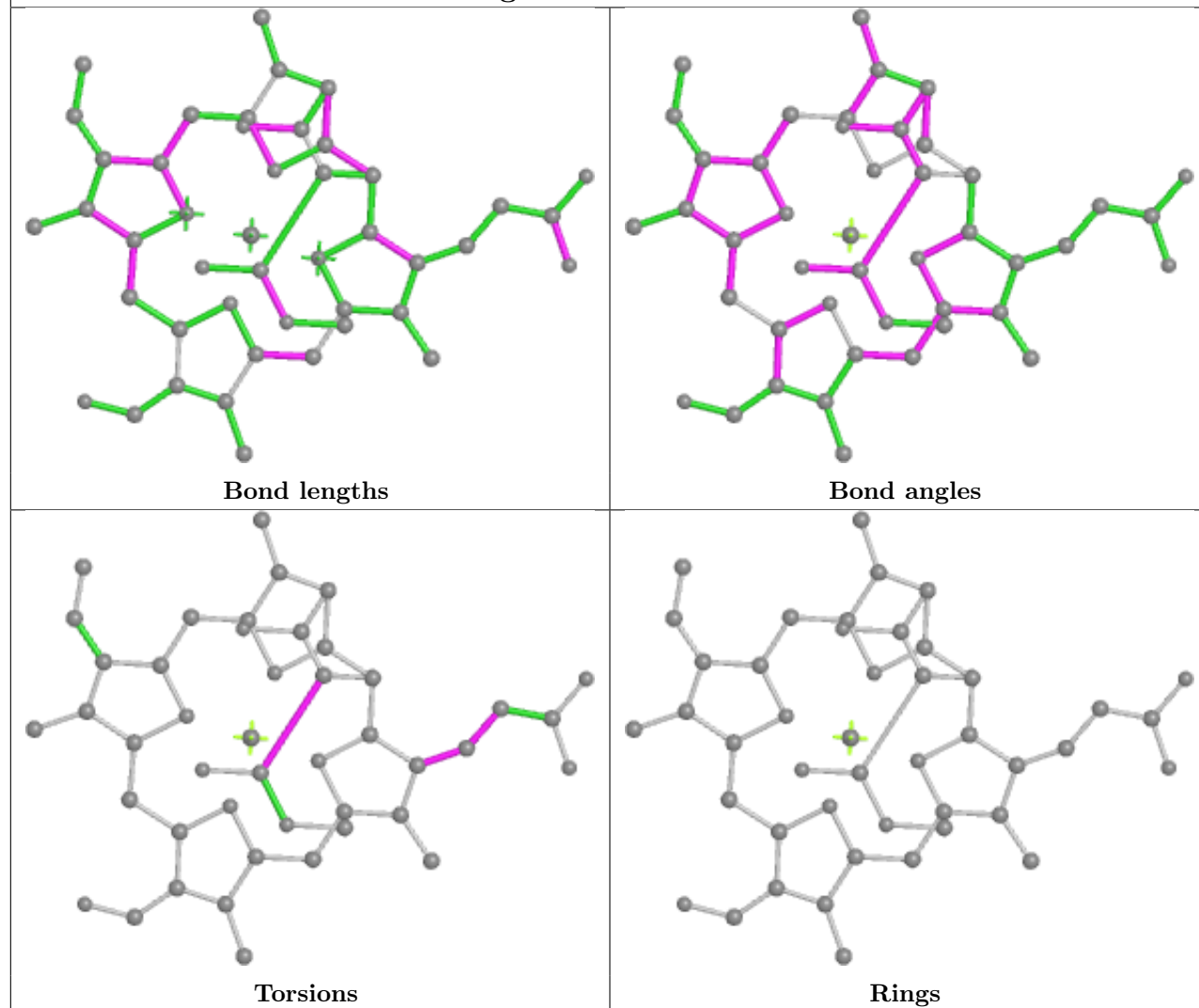
Torsions



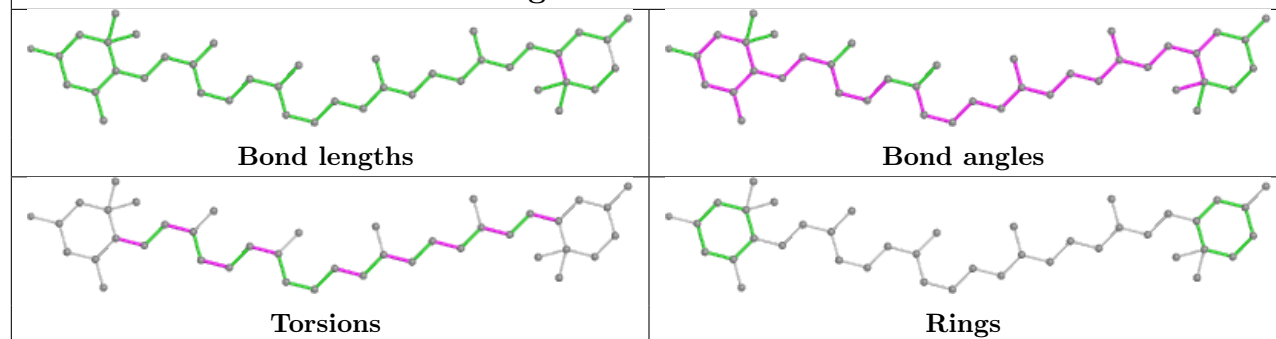
Rings

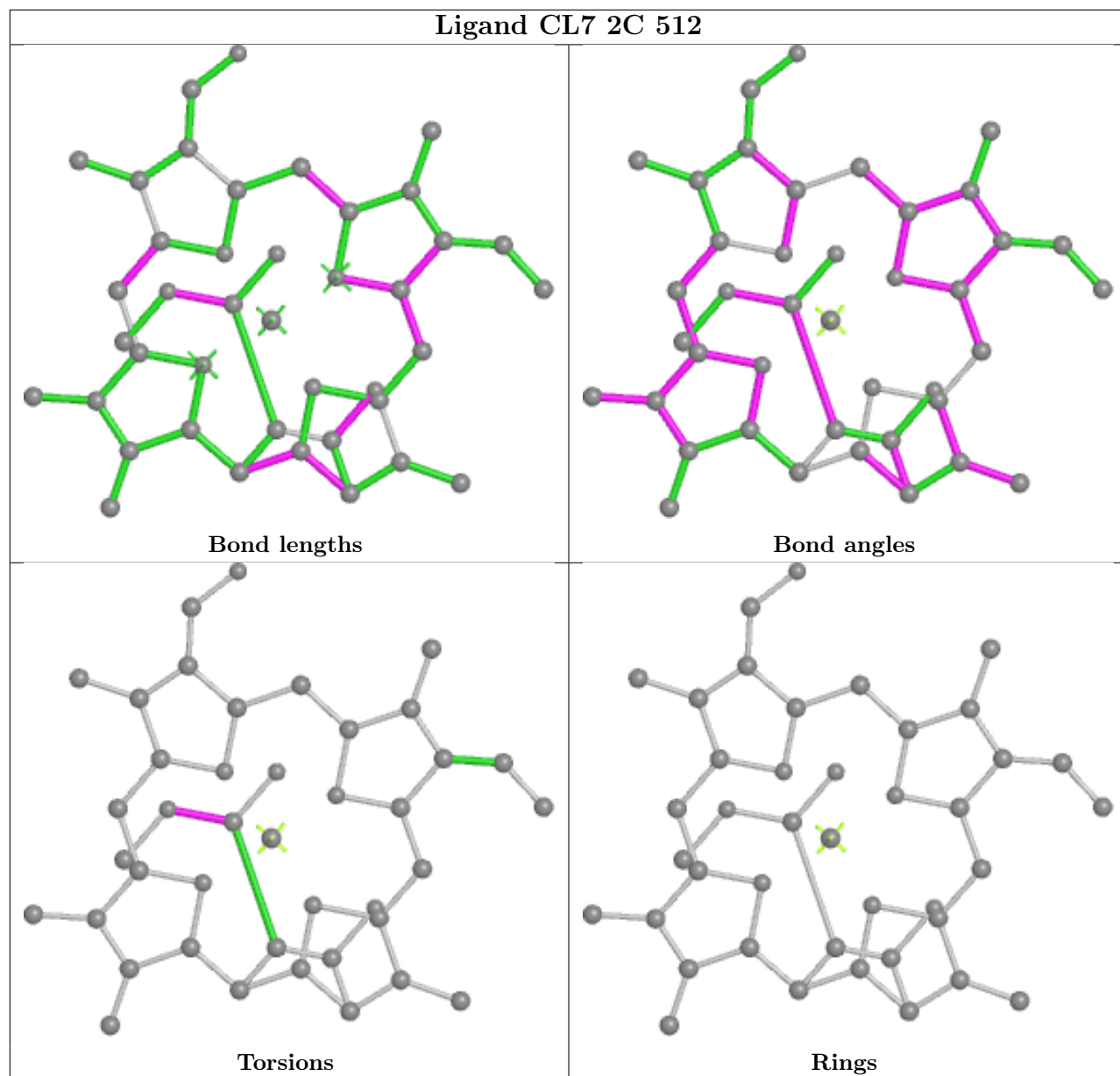


Ligand CL7 42 513

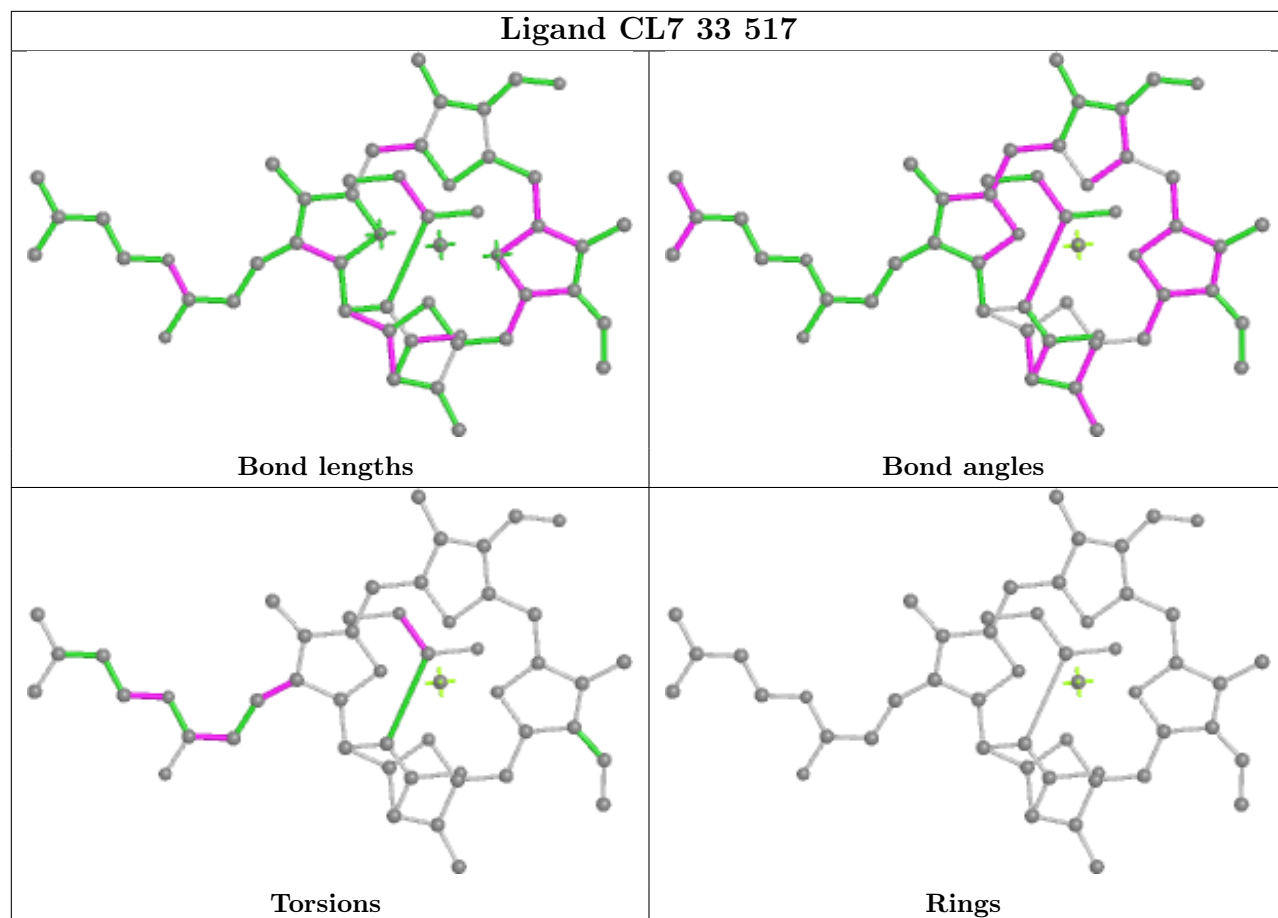


Ligand ZEX 41 421

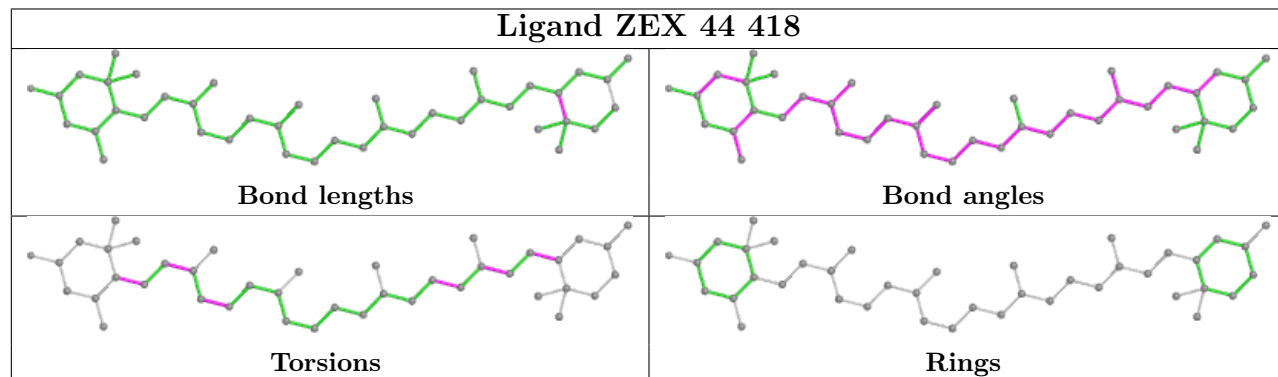


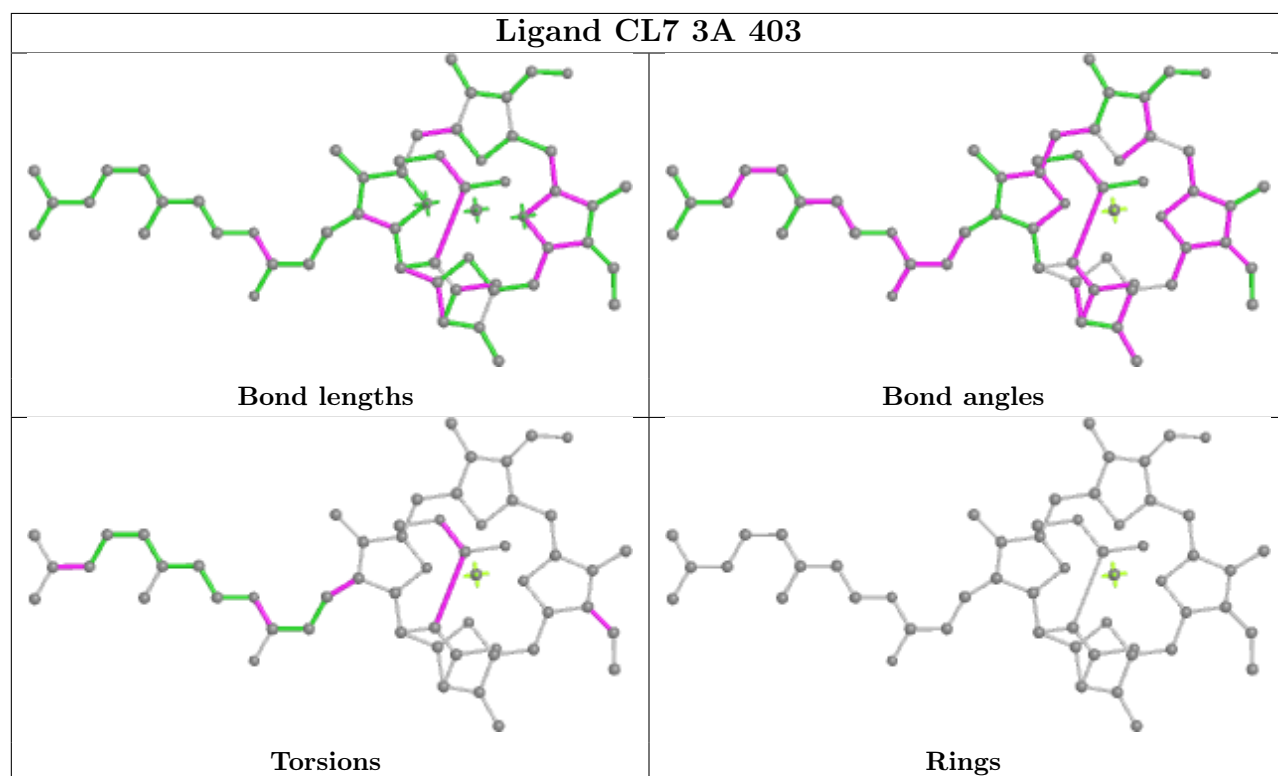
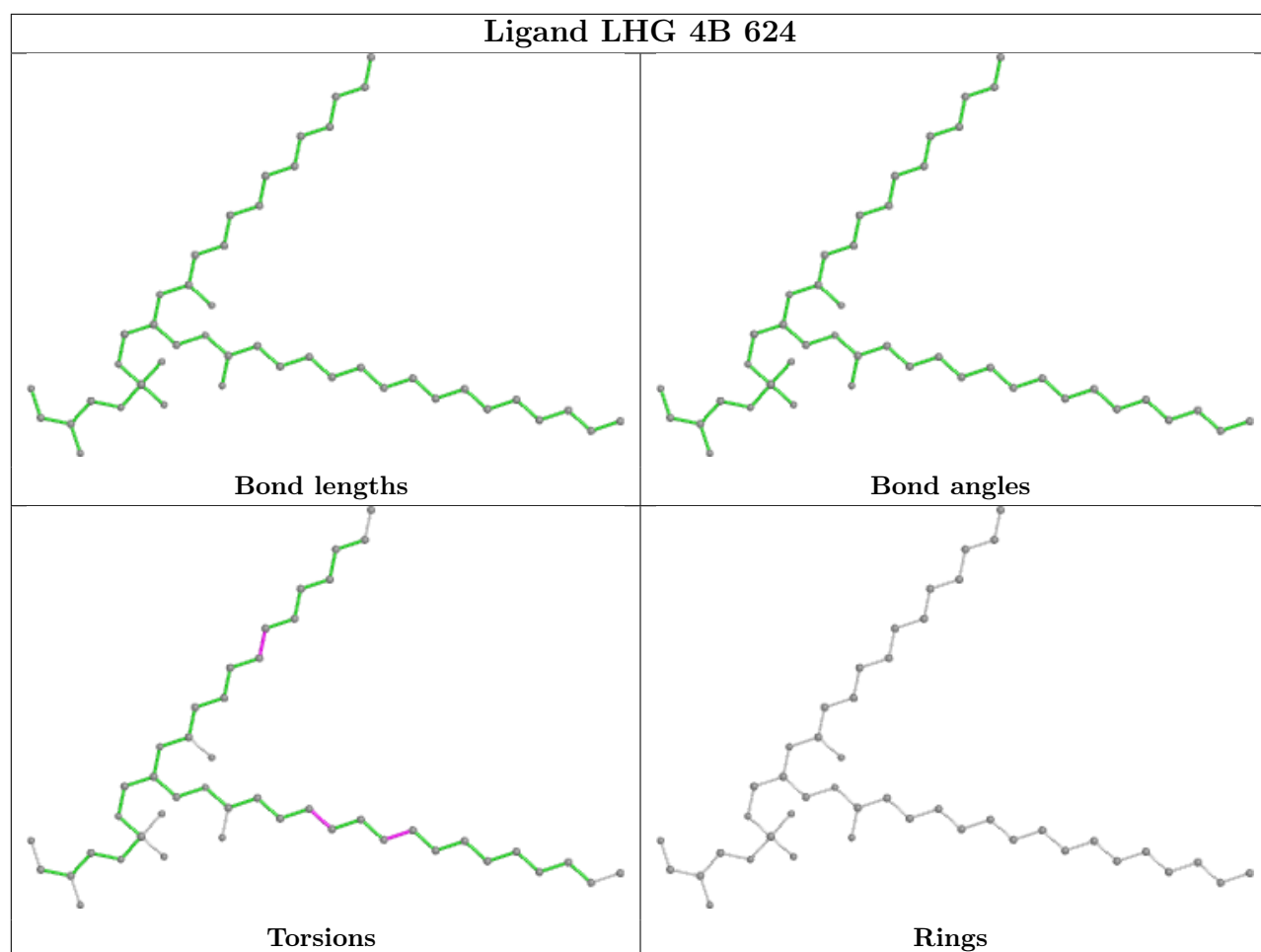


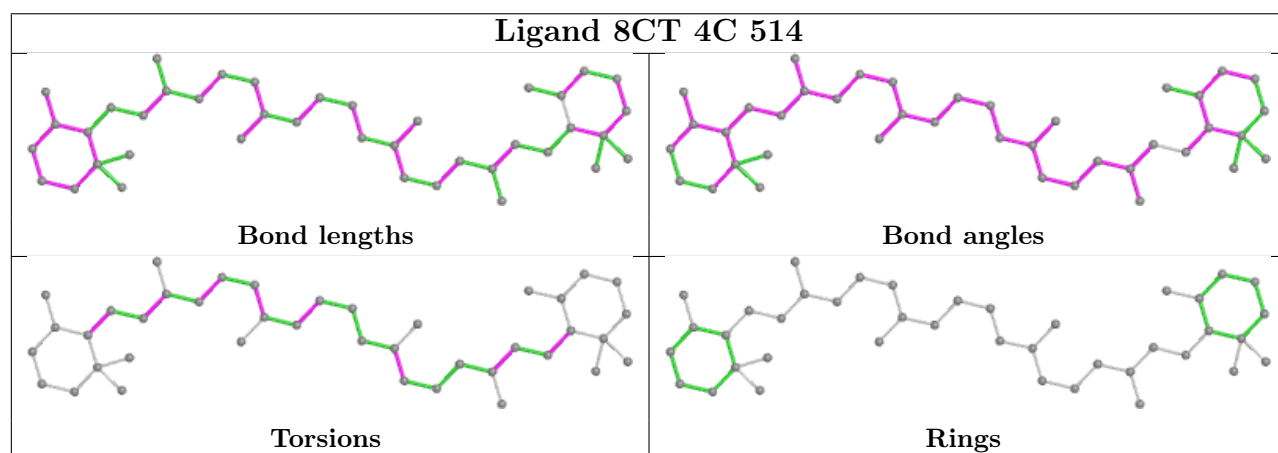
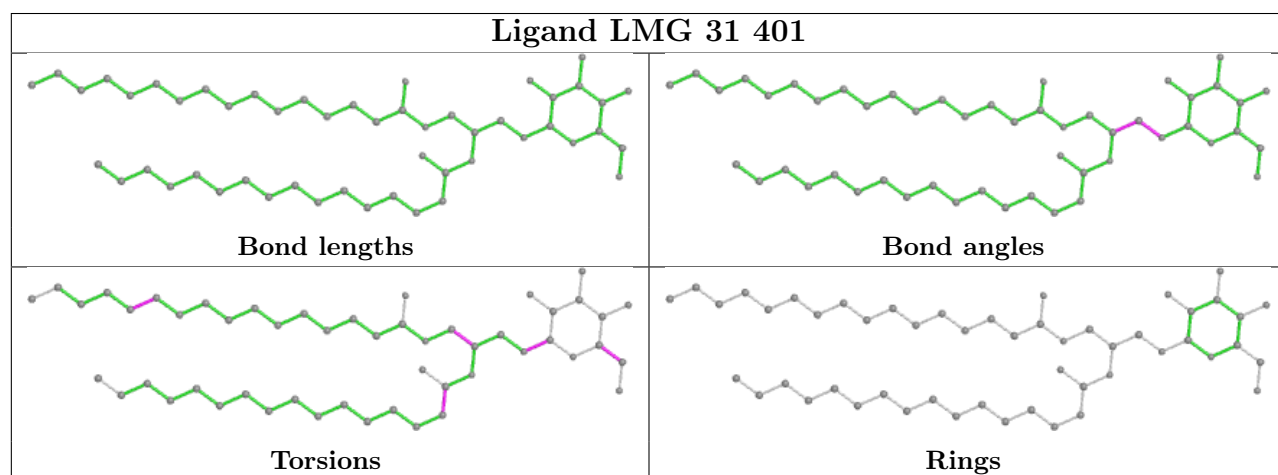
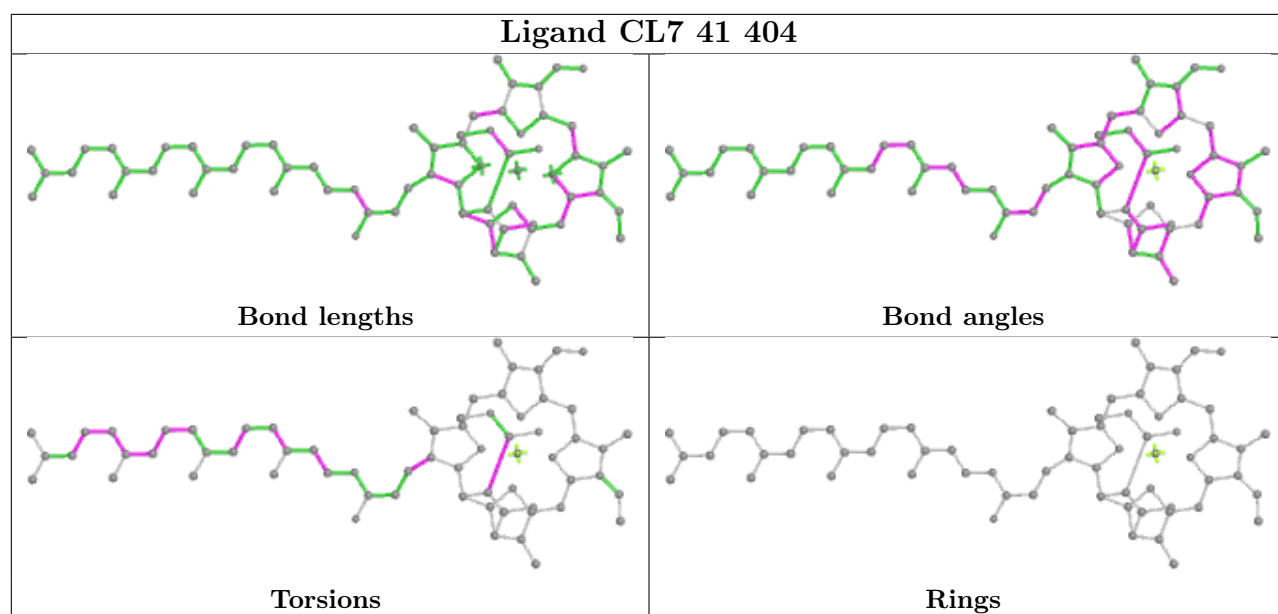
Ligand CL7 33 517

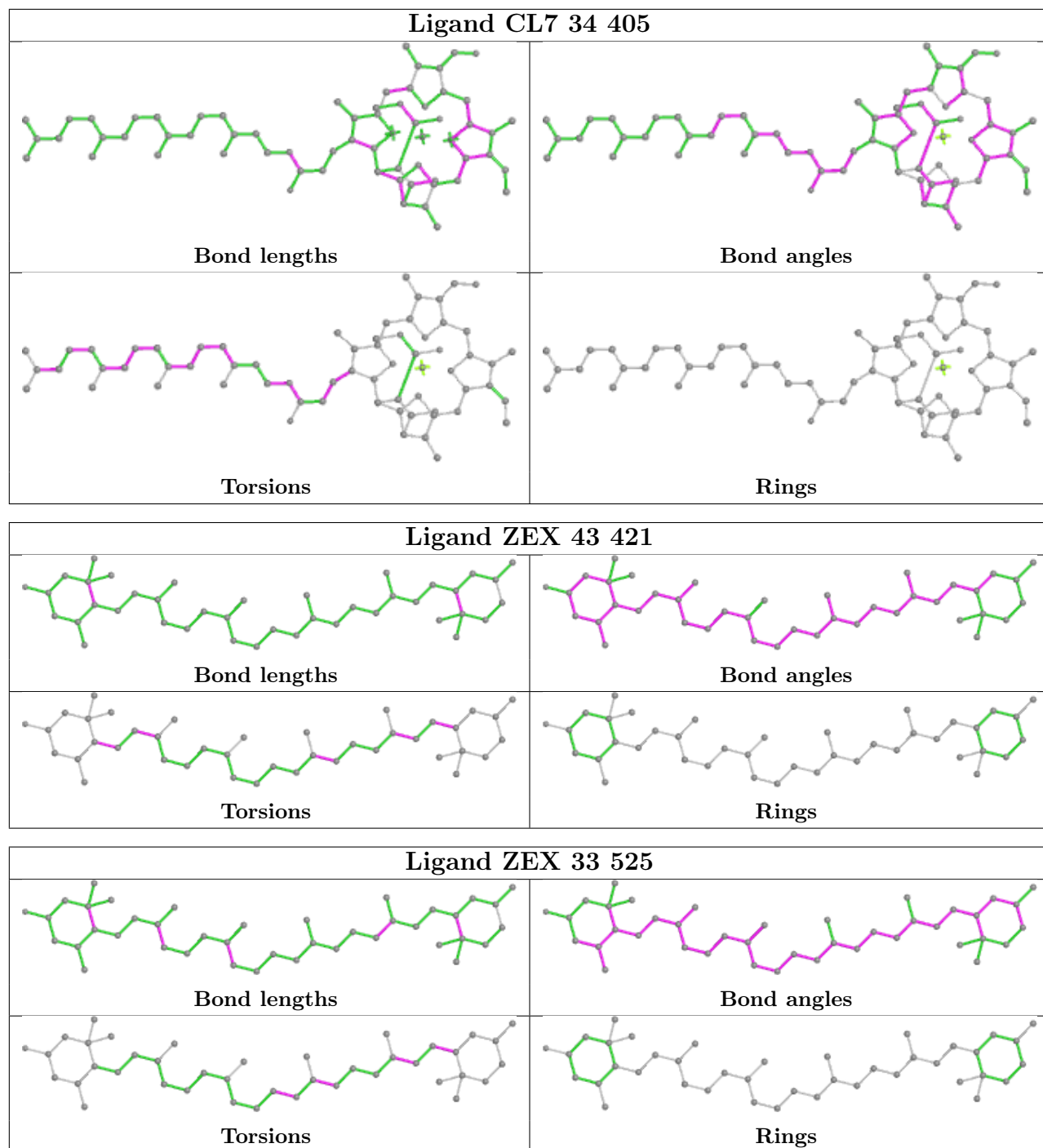


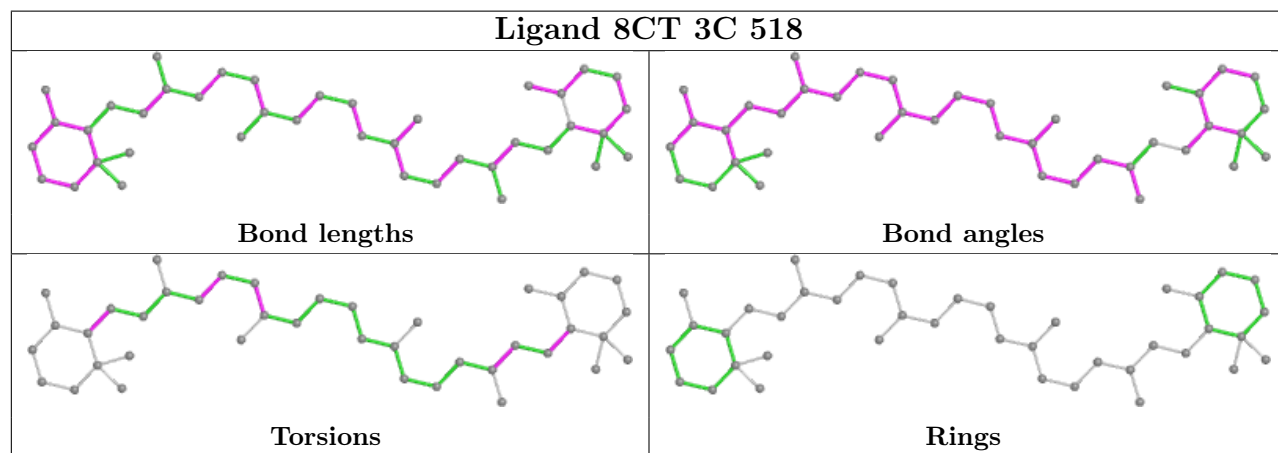
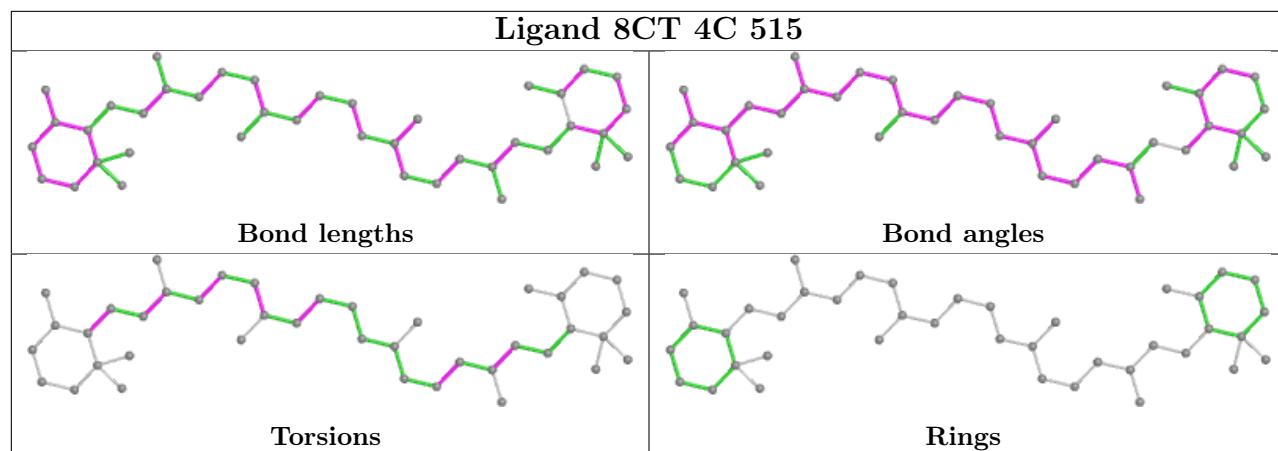
Ligand ZEX 44 418

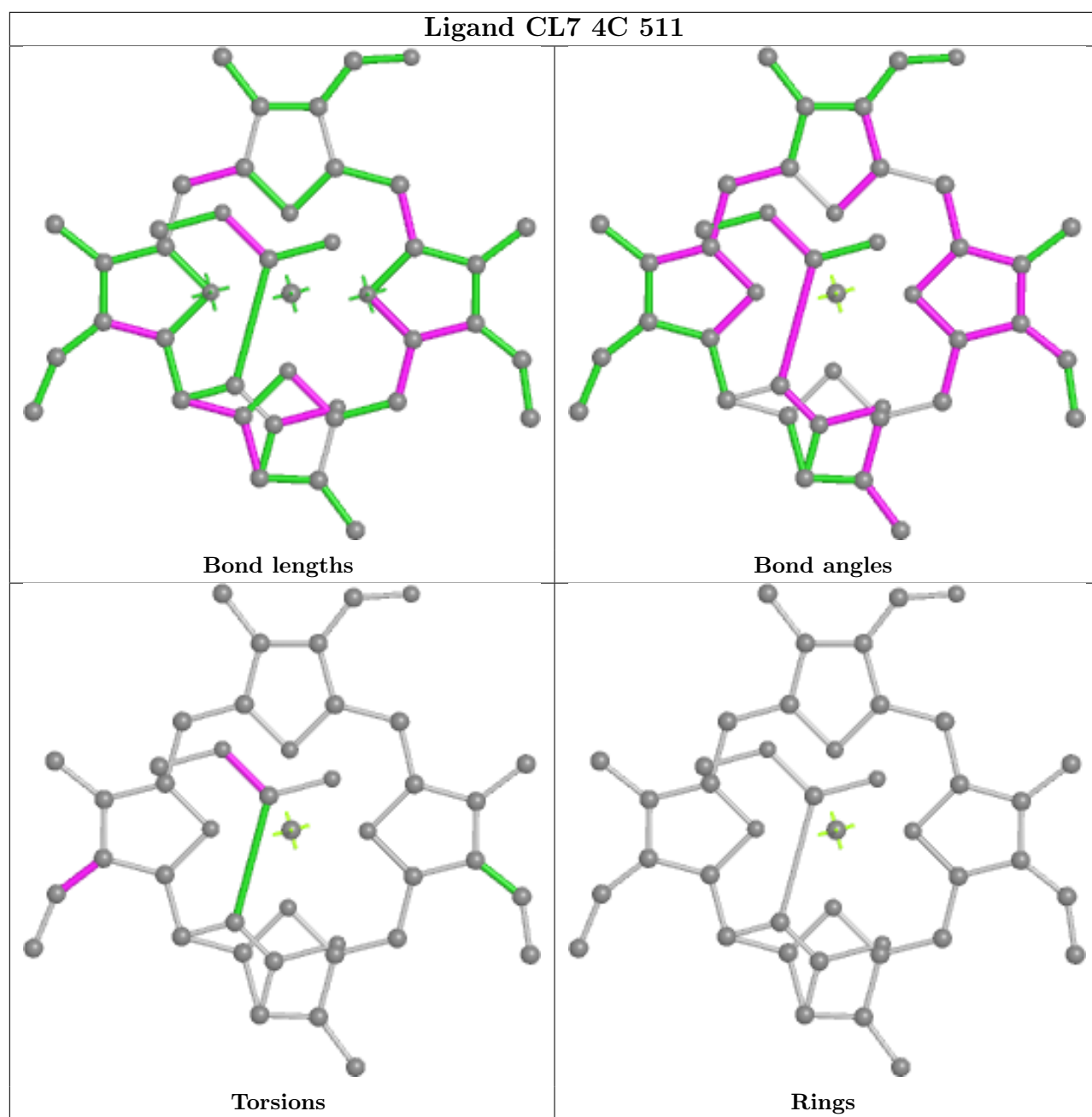




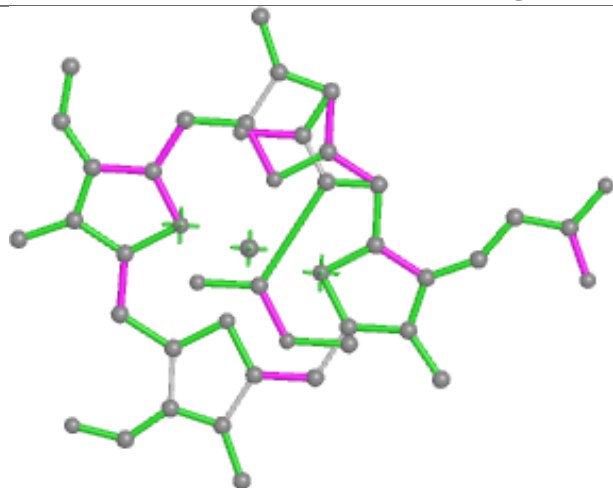




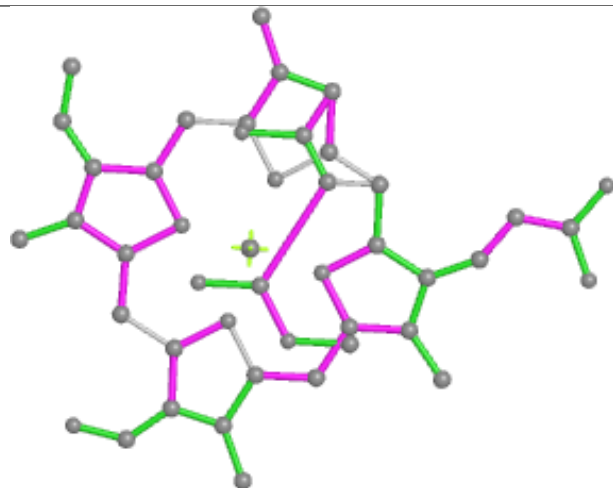




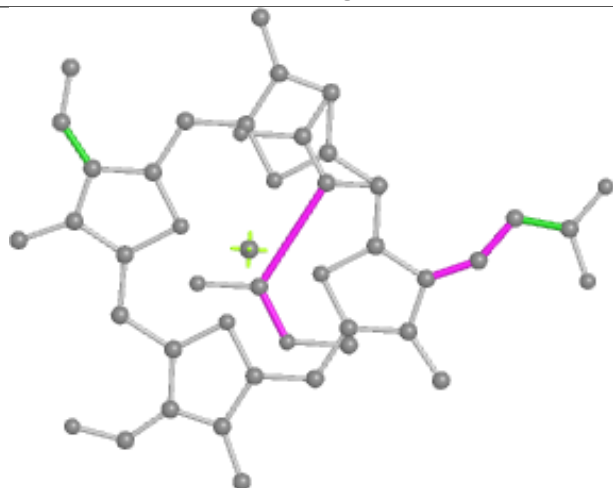
Ligand CL7 4C 513



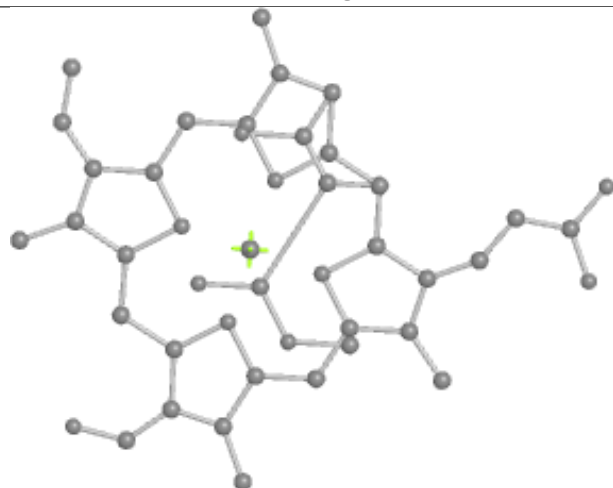
Bond lengths



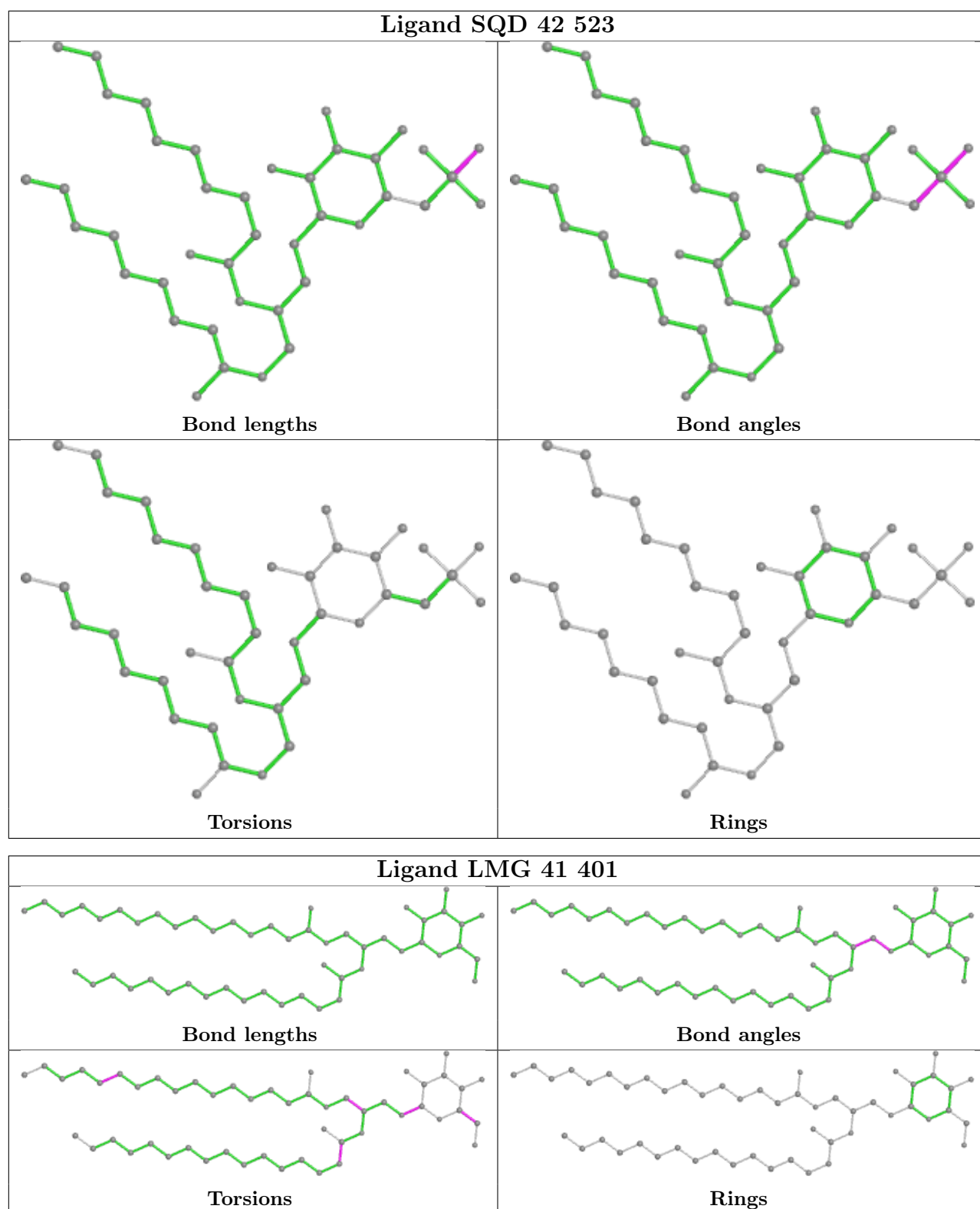
Bond angles

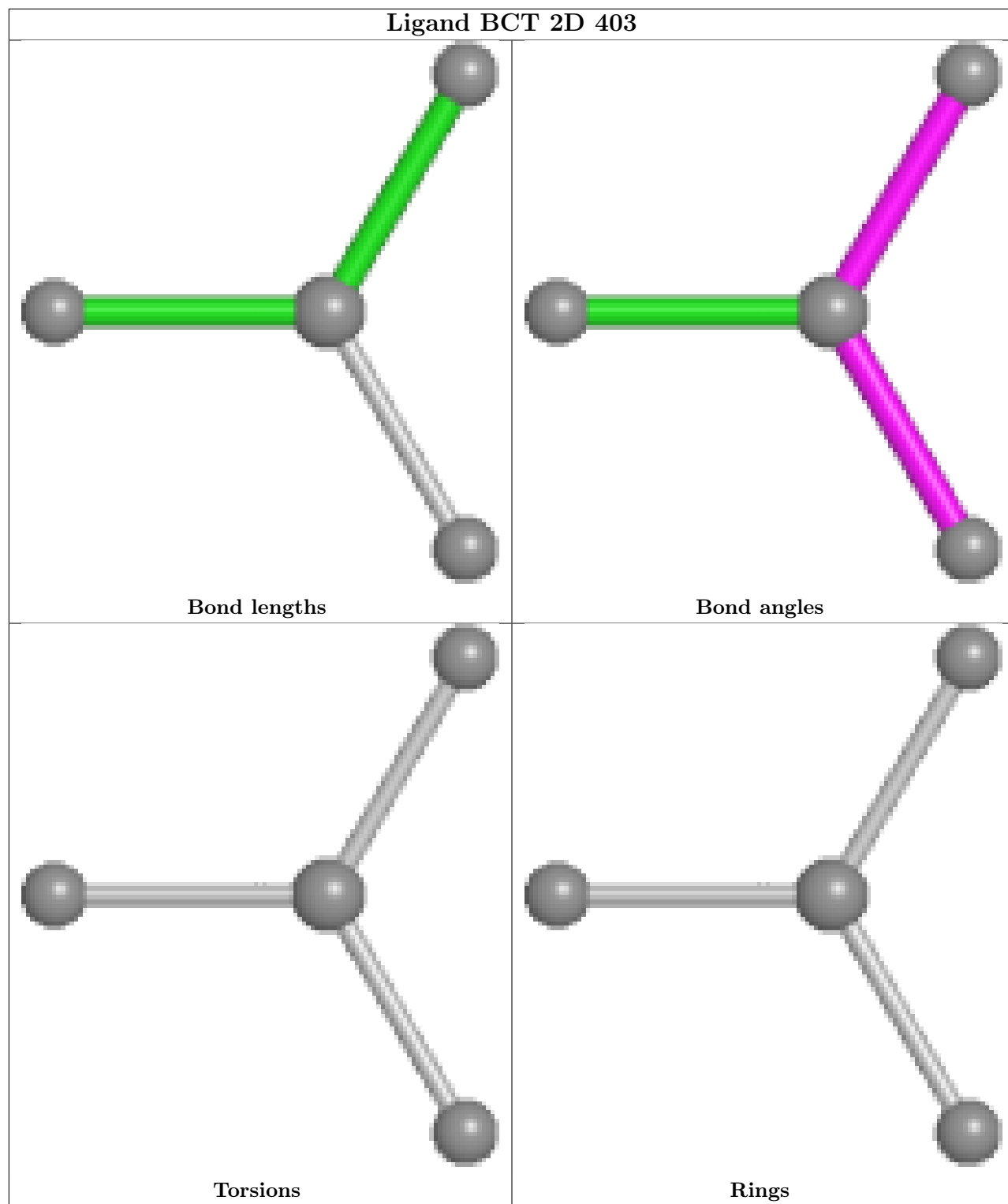


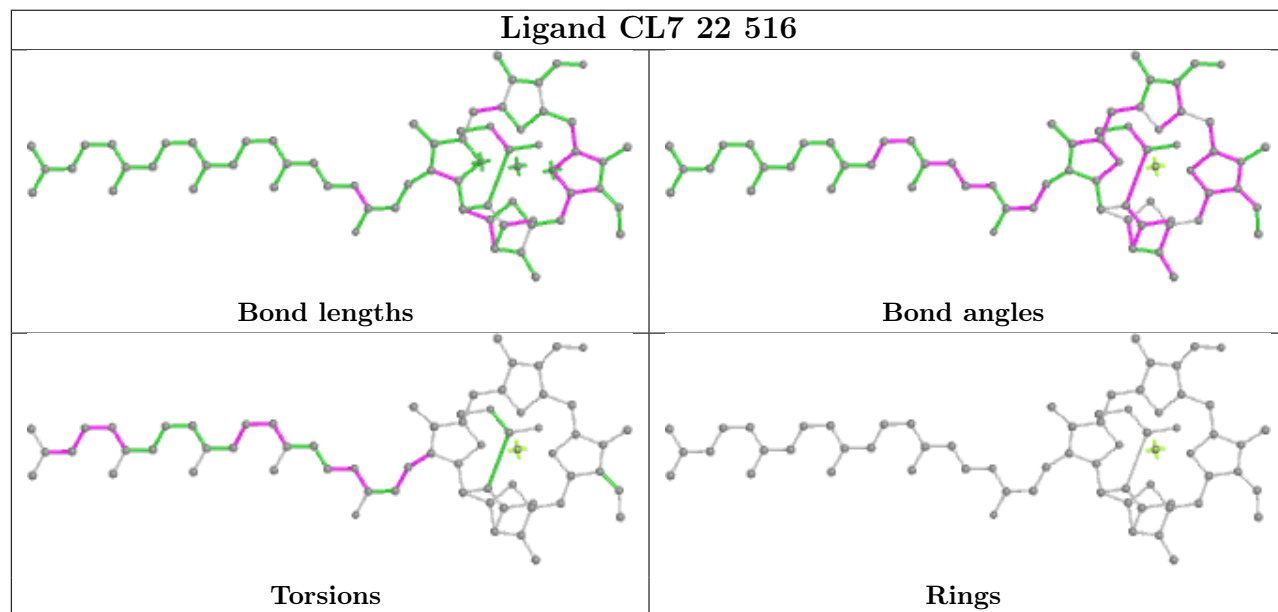
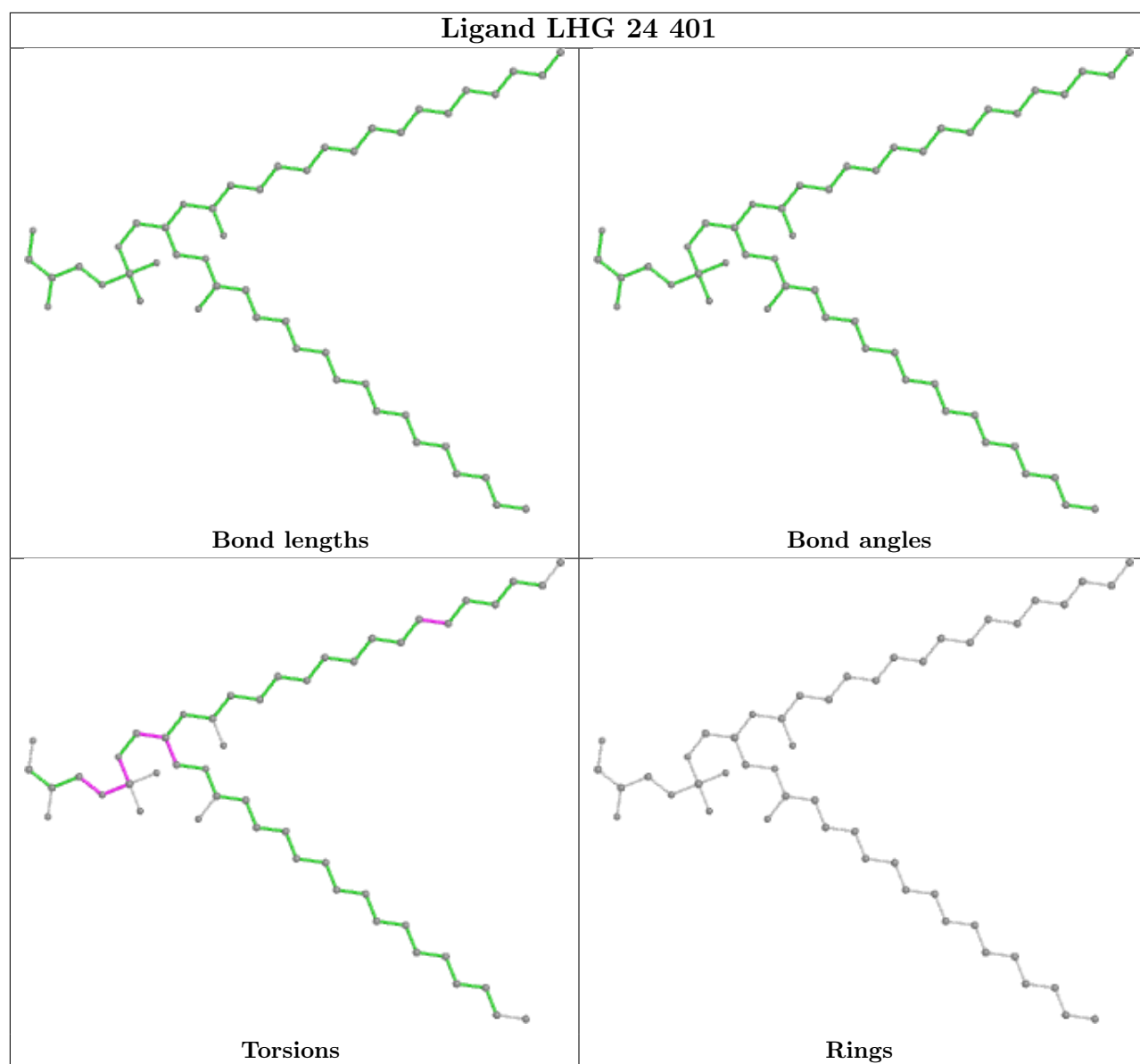
Torsions



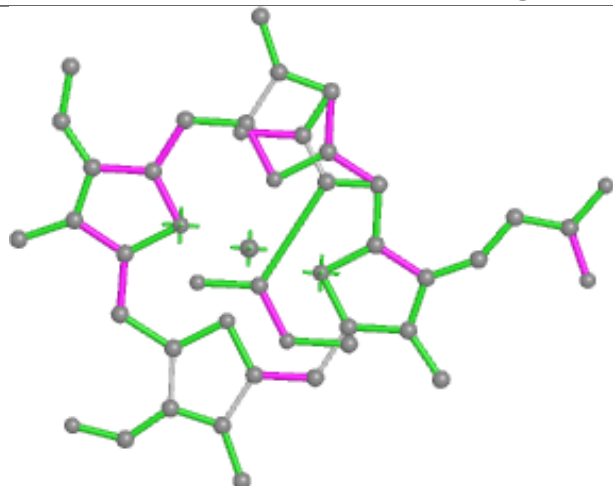
Rings



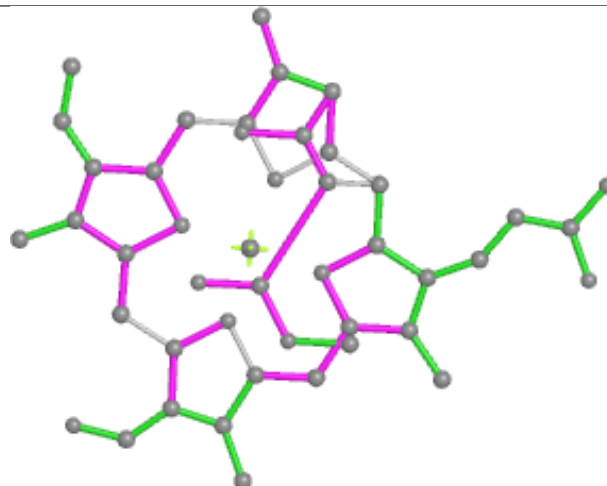




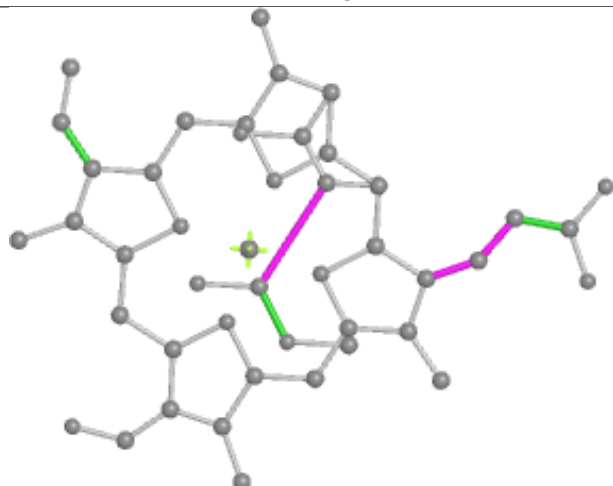
Ligand CL7 12 513



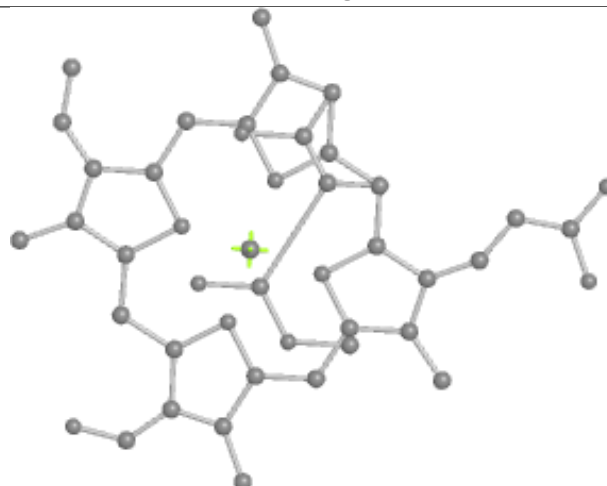
Bond lengths



Bond angles

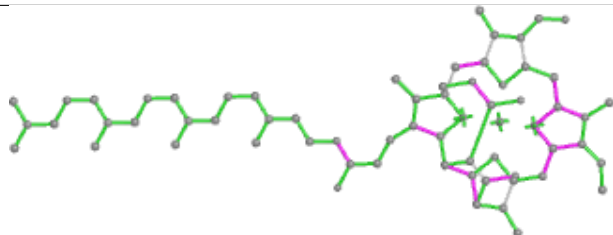


Torsions

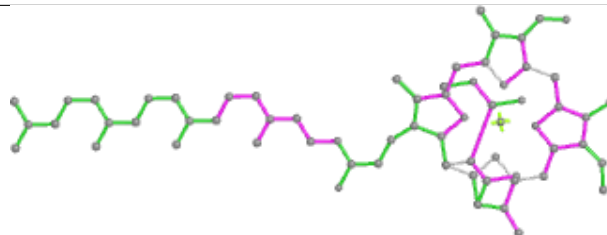


Rings

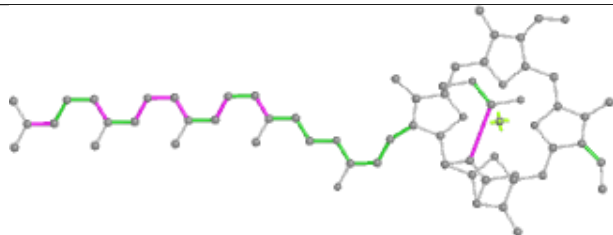
Ligand CL7 4B 604



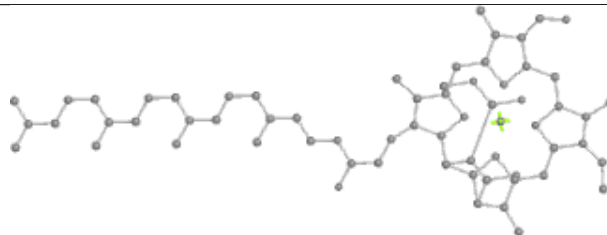
Bond lengths



Bond angles

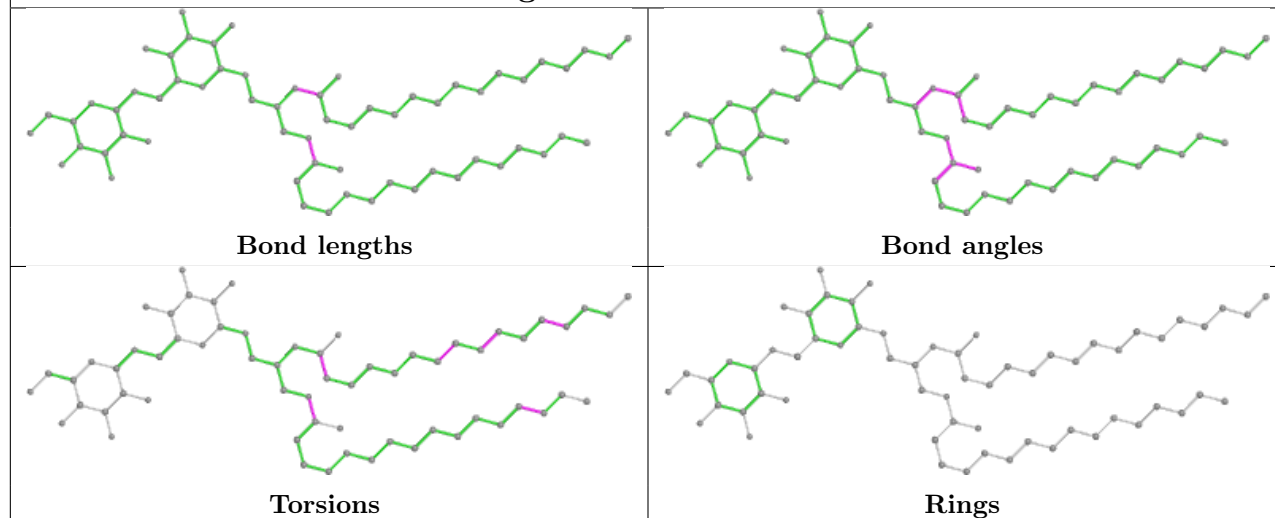


Torsions

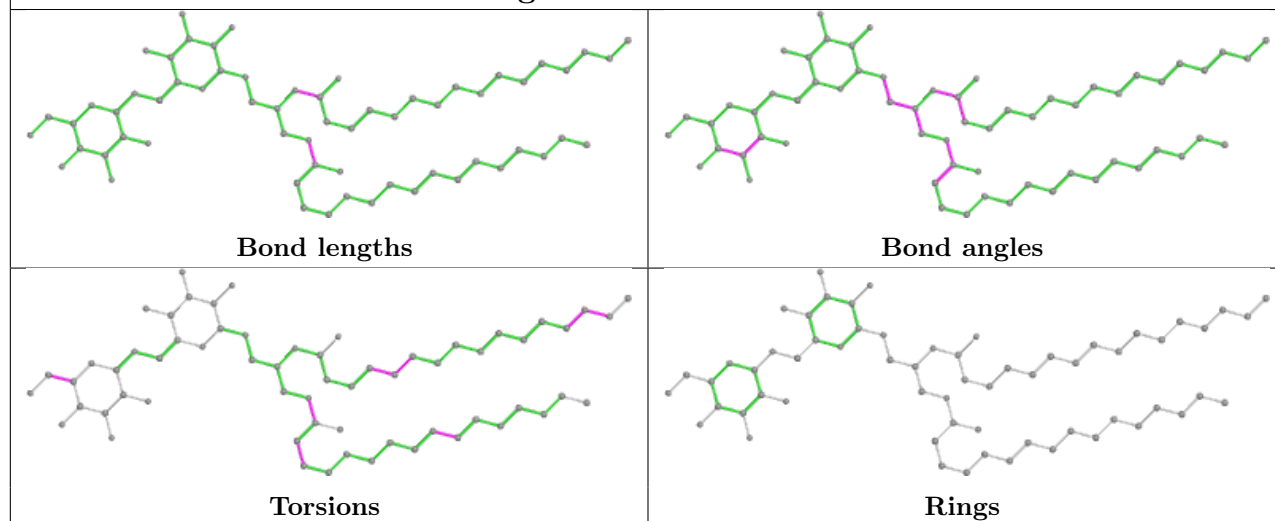


Rings

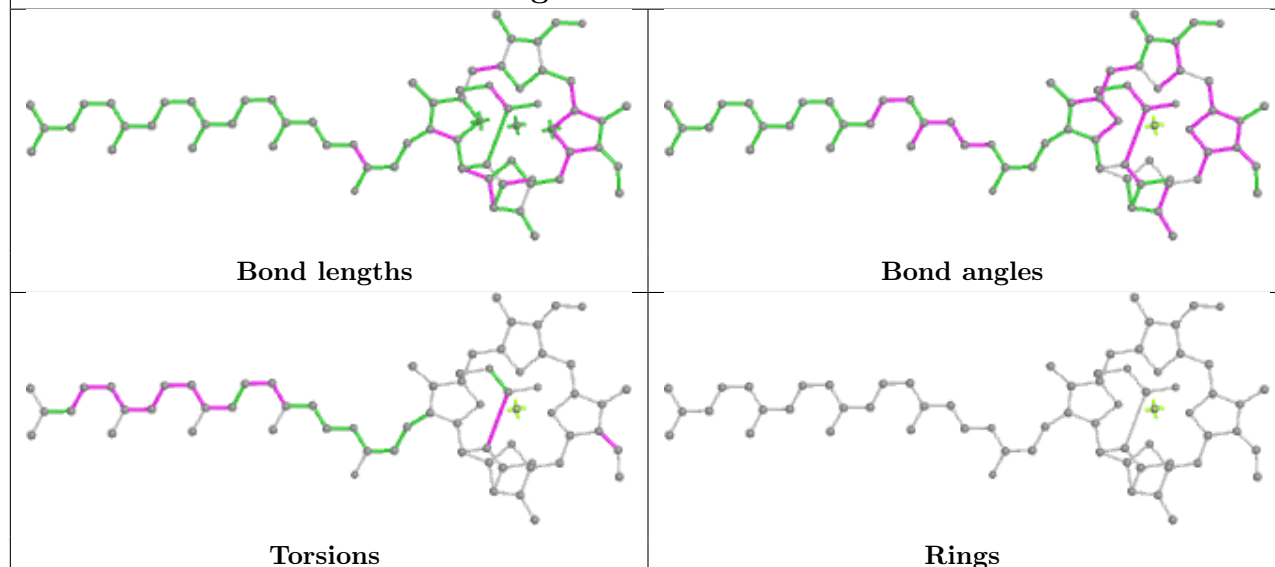
Ligand DGD 2B 625



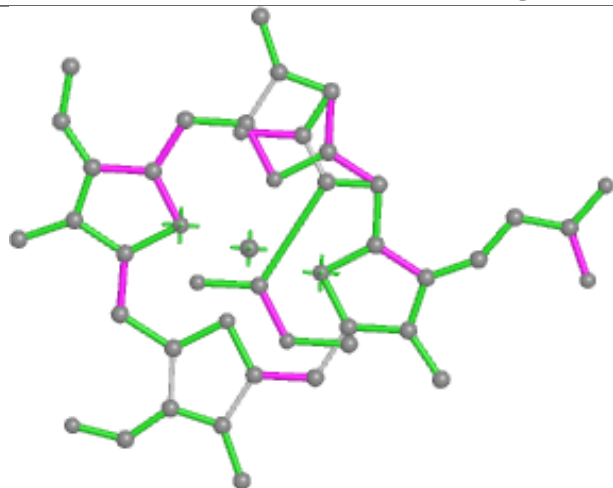
Ligand DGD 4C 516



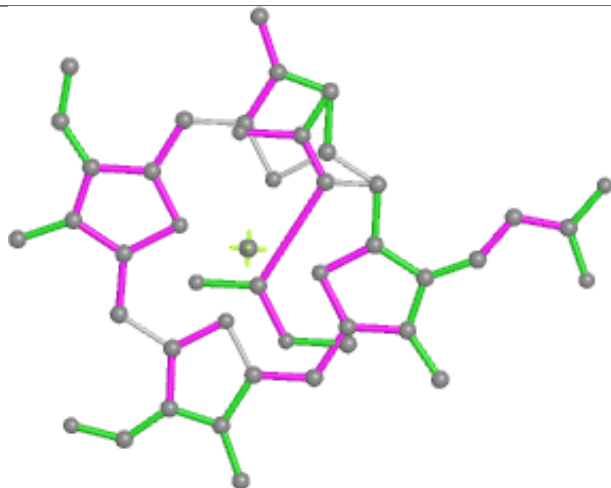
Ligand CL7 22 505



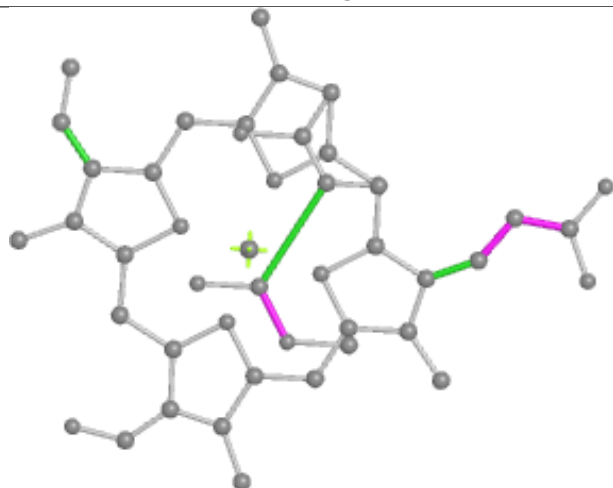
Ligand CL7 33 518



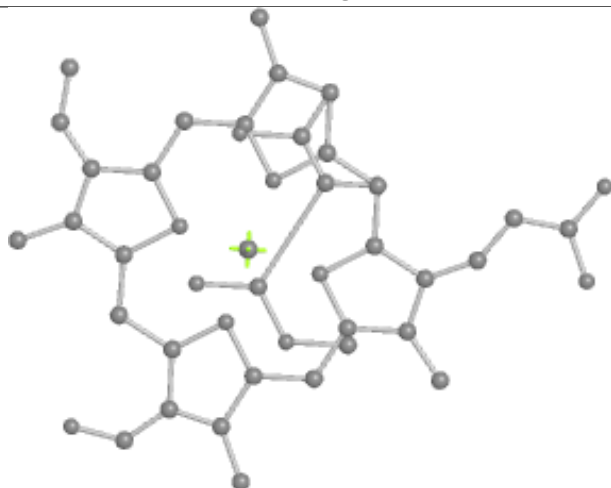
Bond lengths



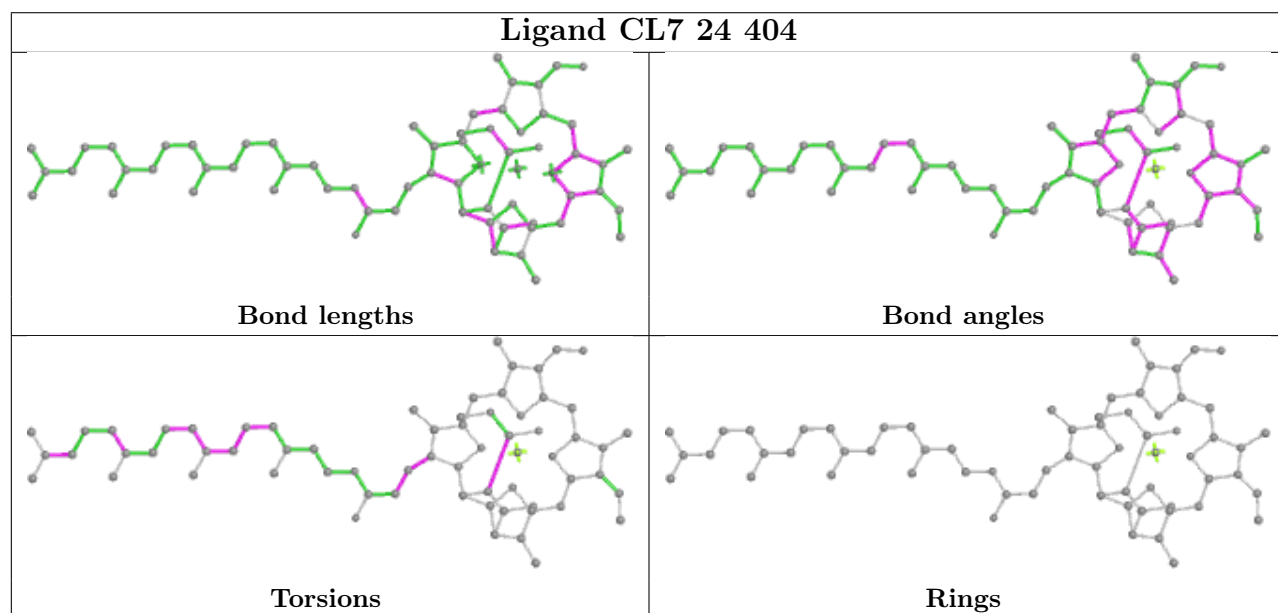
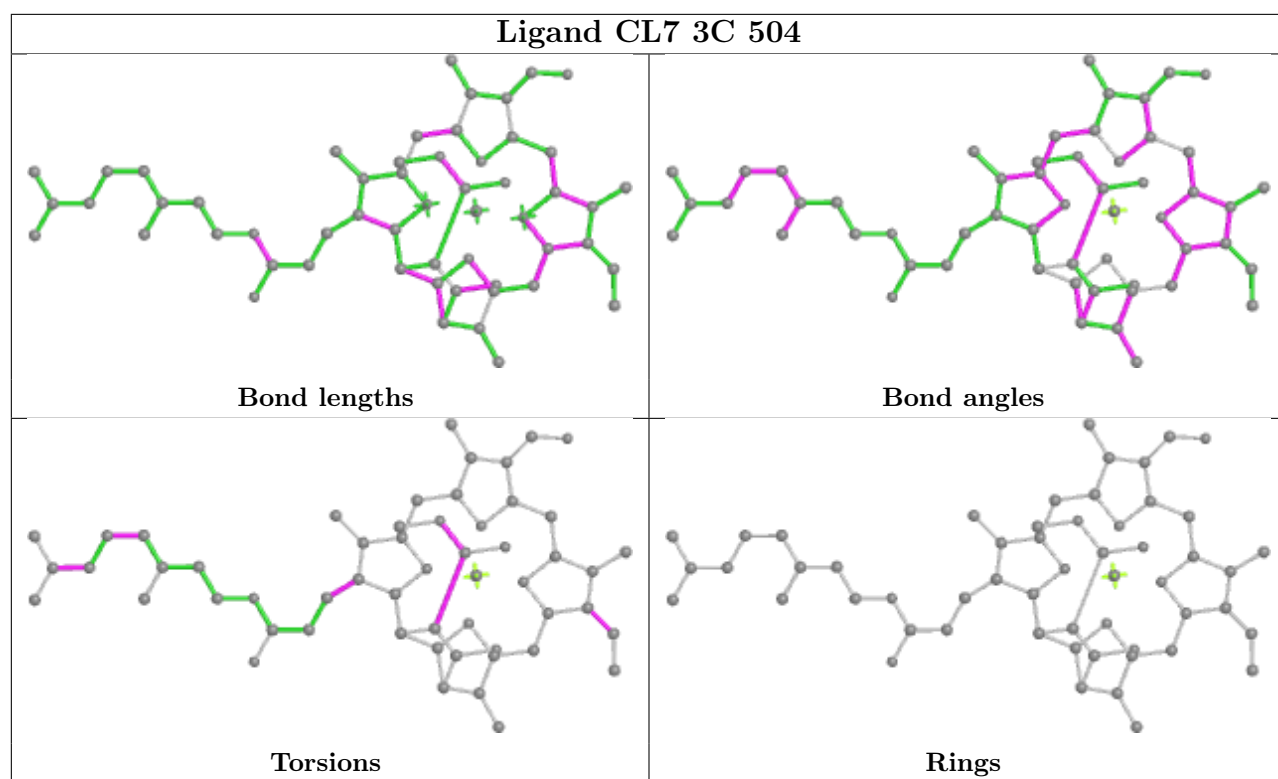
Bond angles

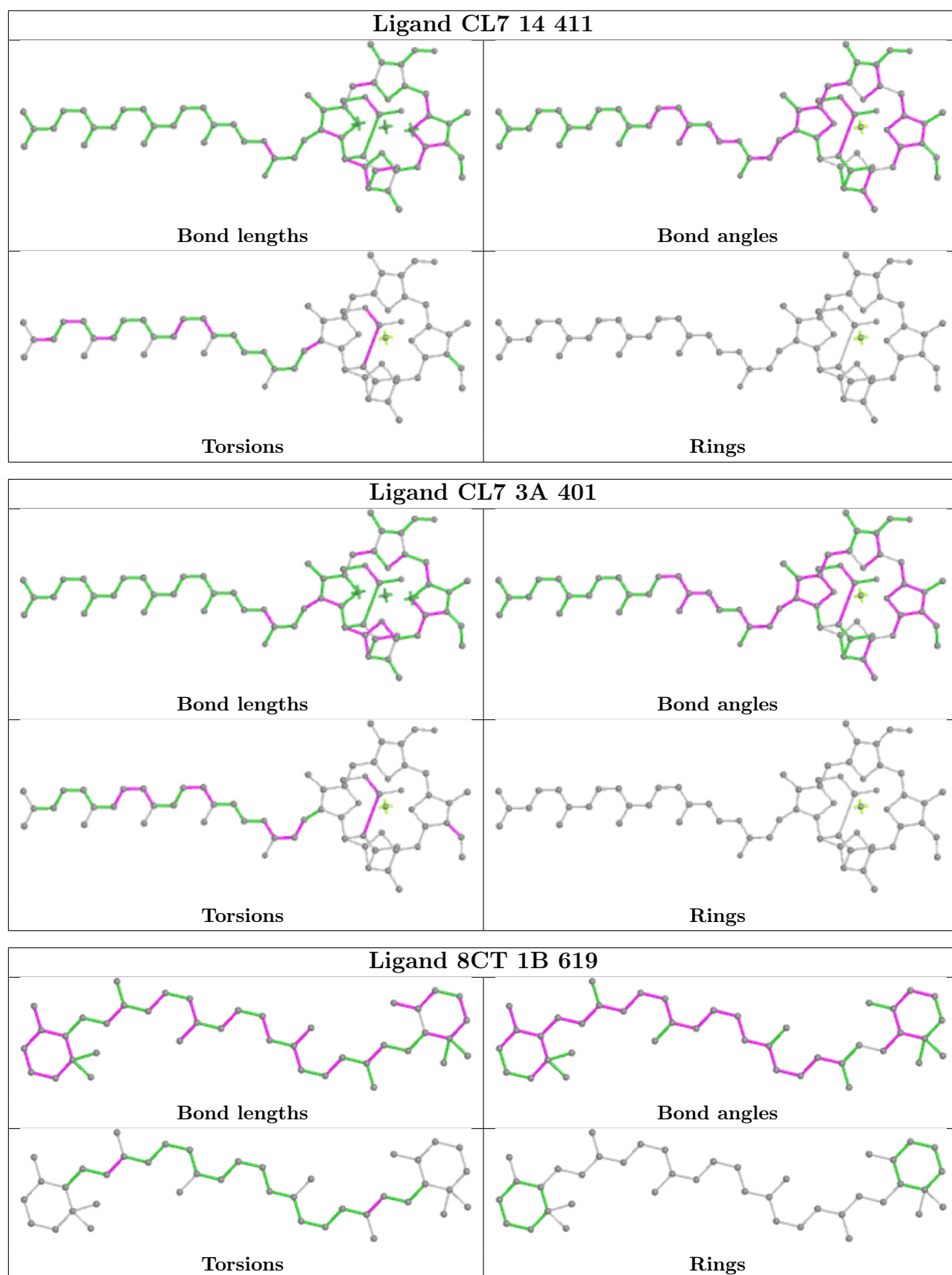


Torsions

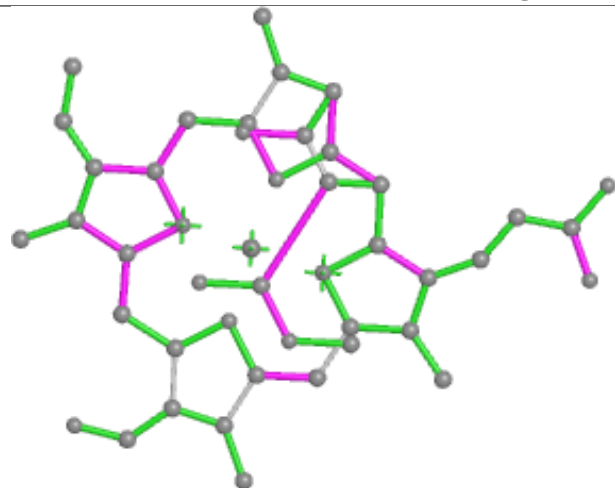


Rings

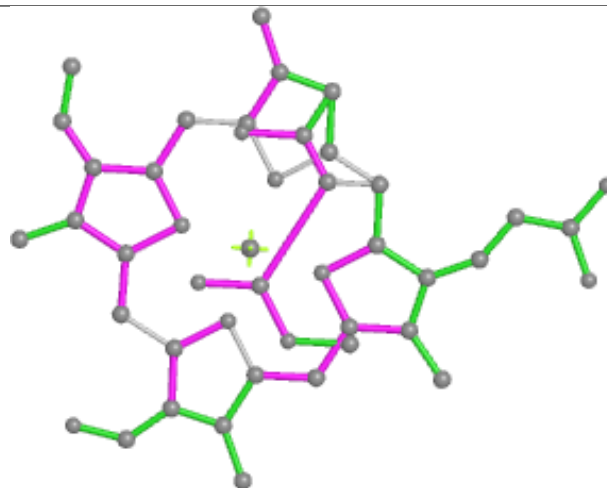




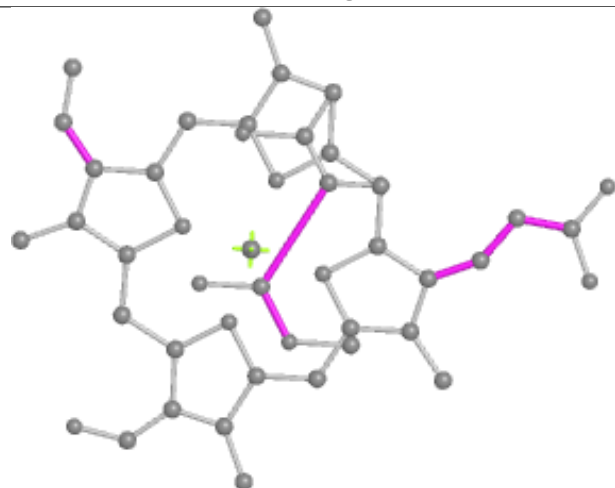
Ligand CL7 34 415



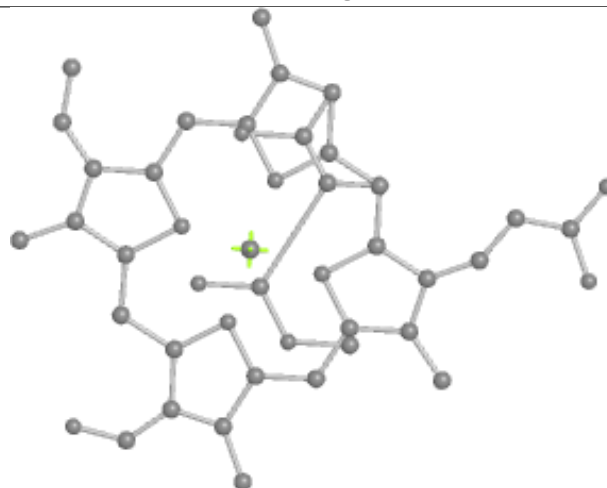
Bond lengths



Bond angles

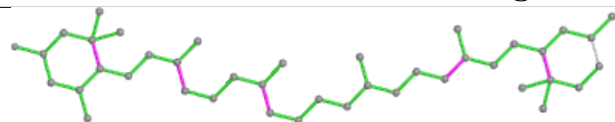


Torsions

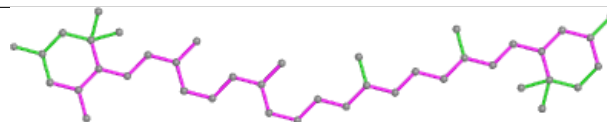


Rings

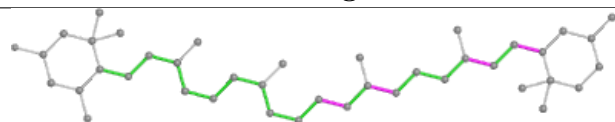
Ligand ZEX 43 401



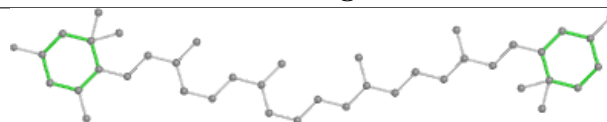
Bond lengths



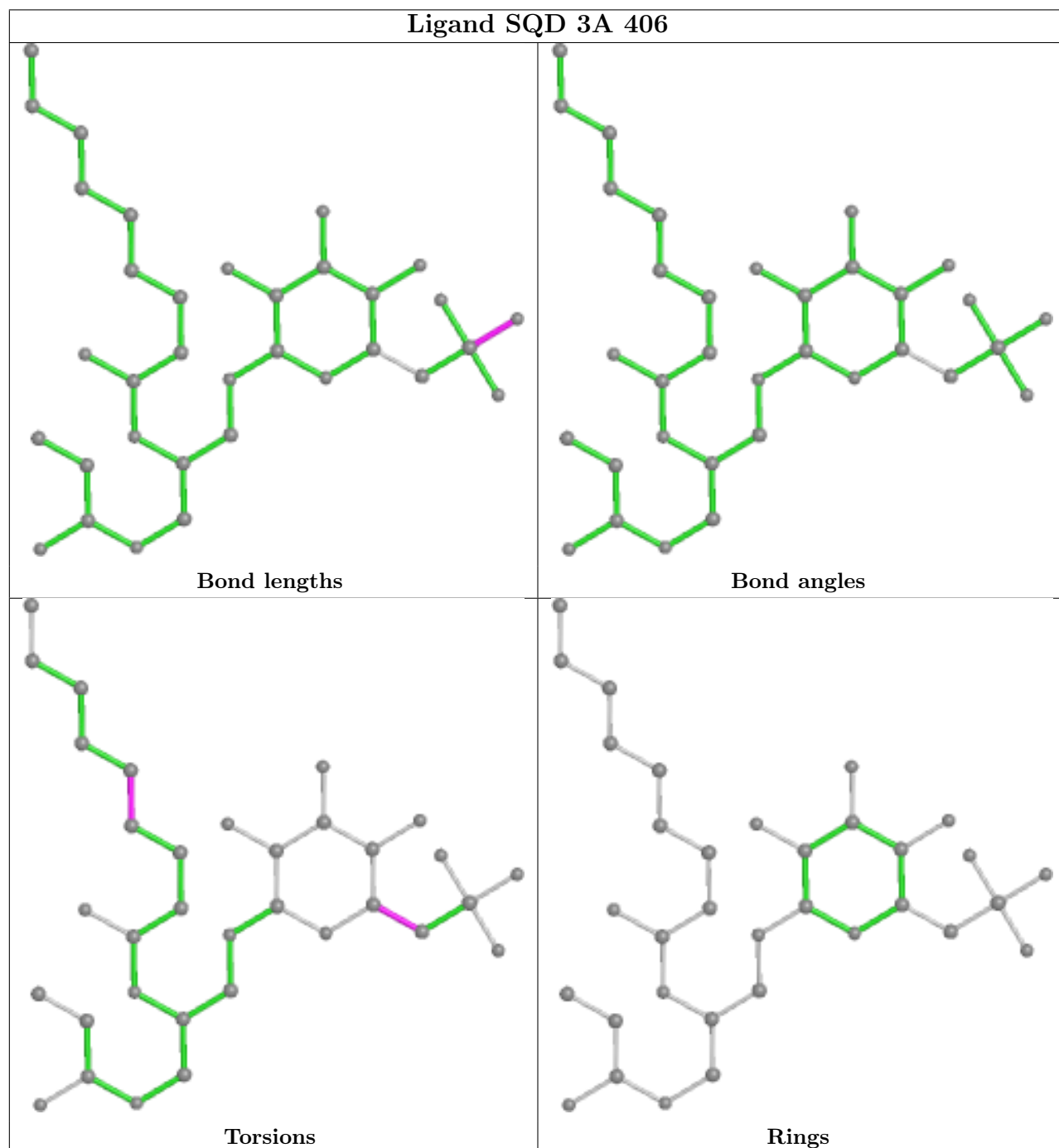
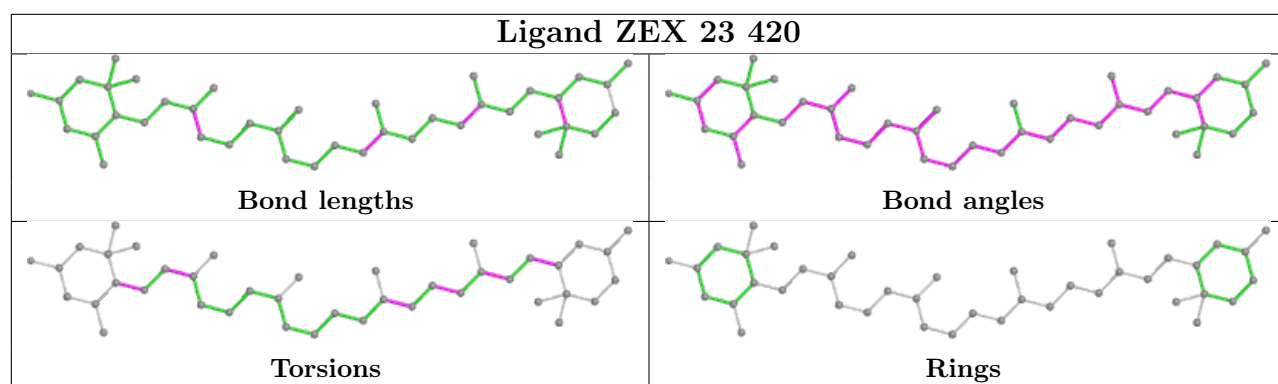
Bond angles



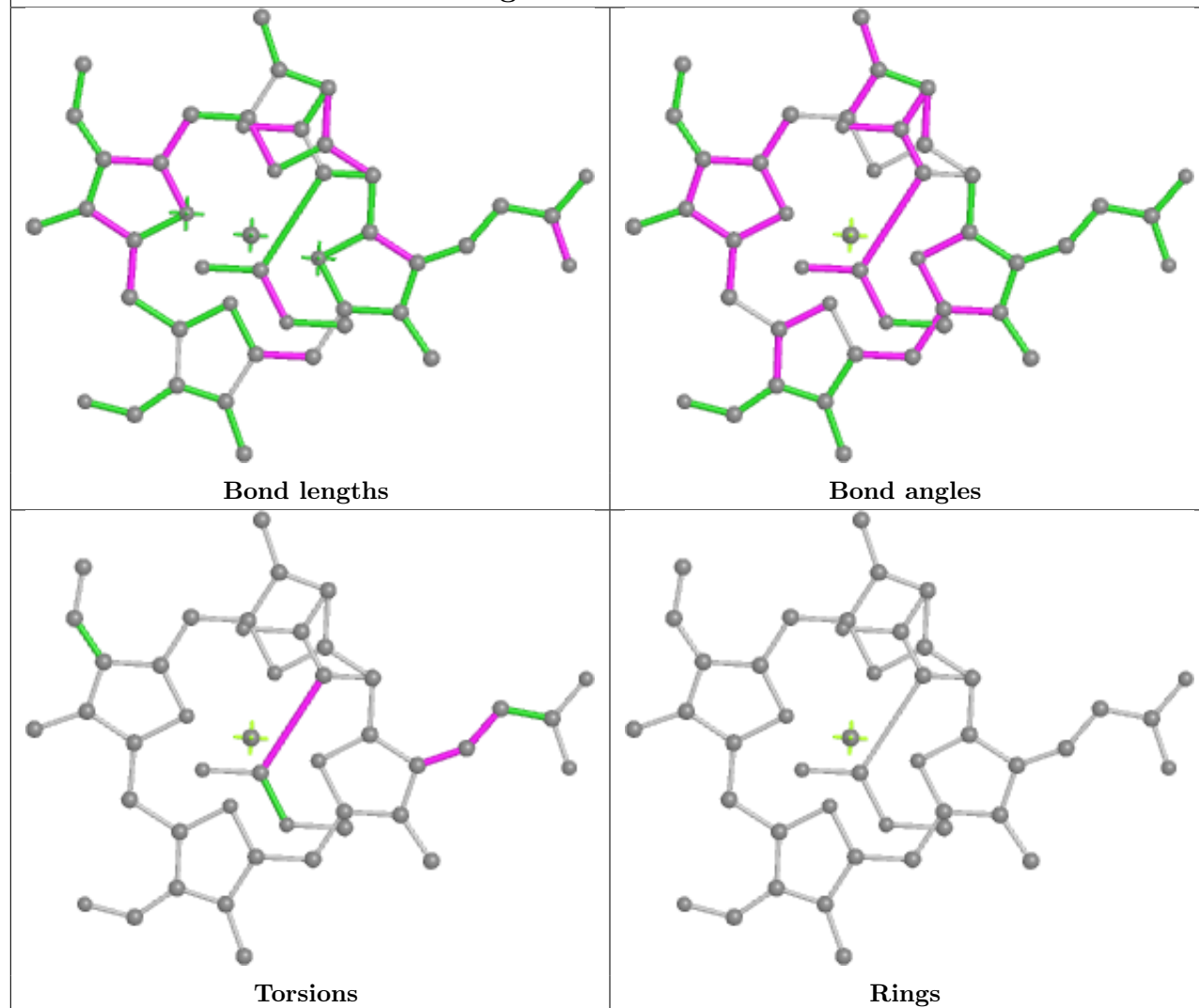
Torsions



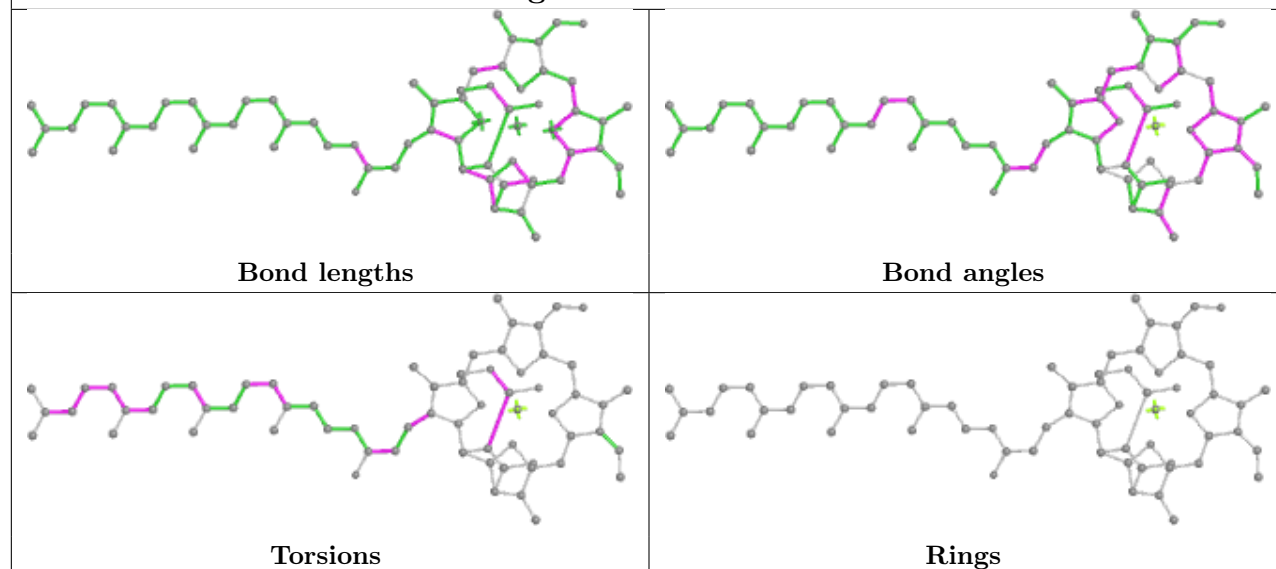
Rings

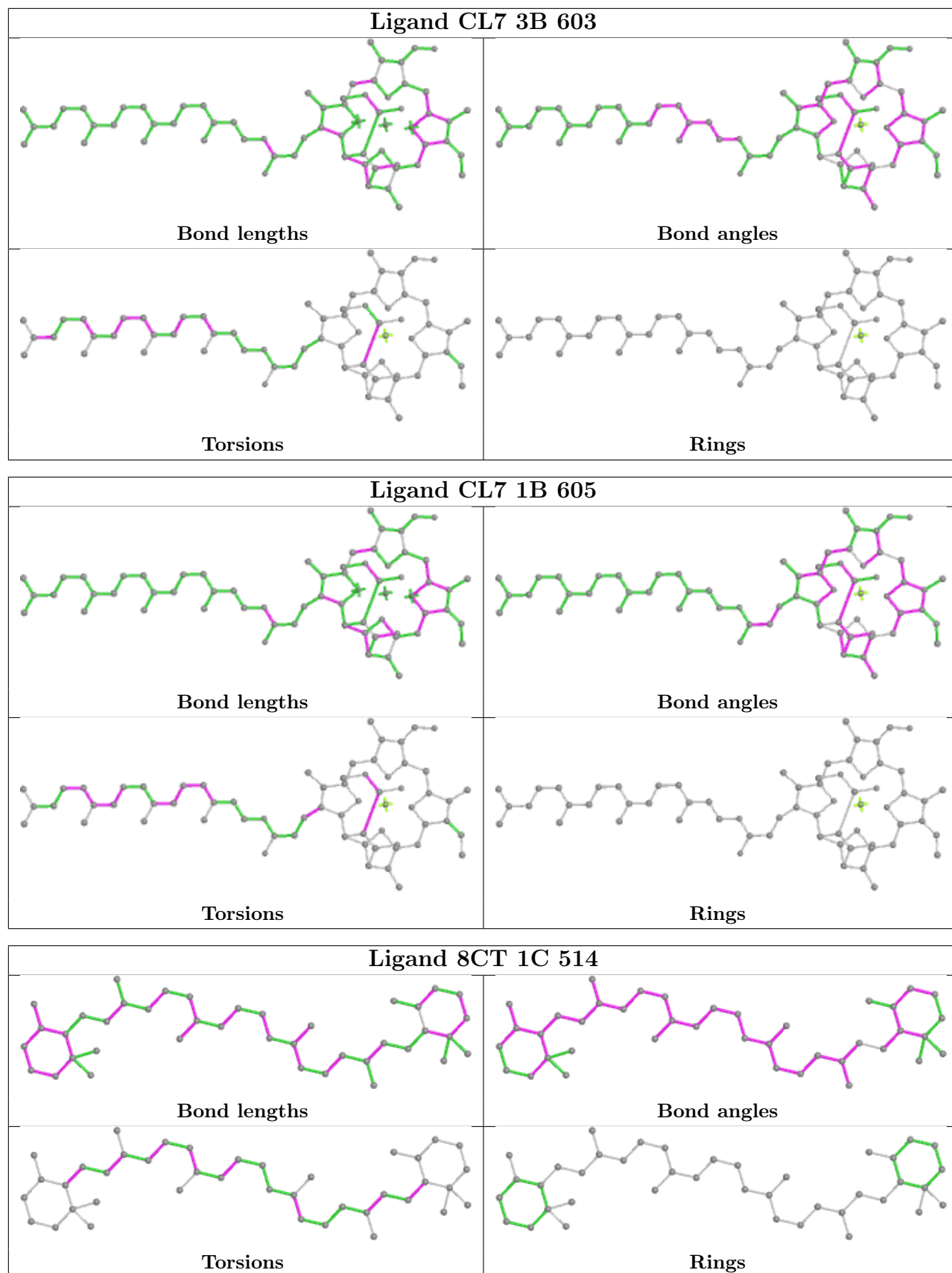


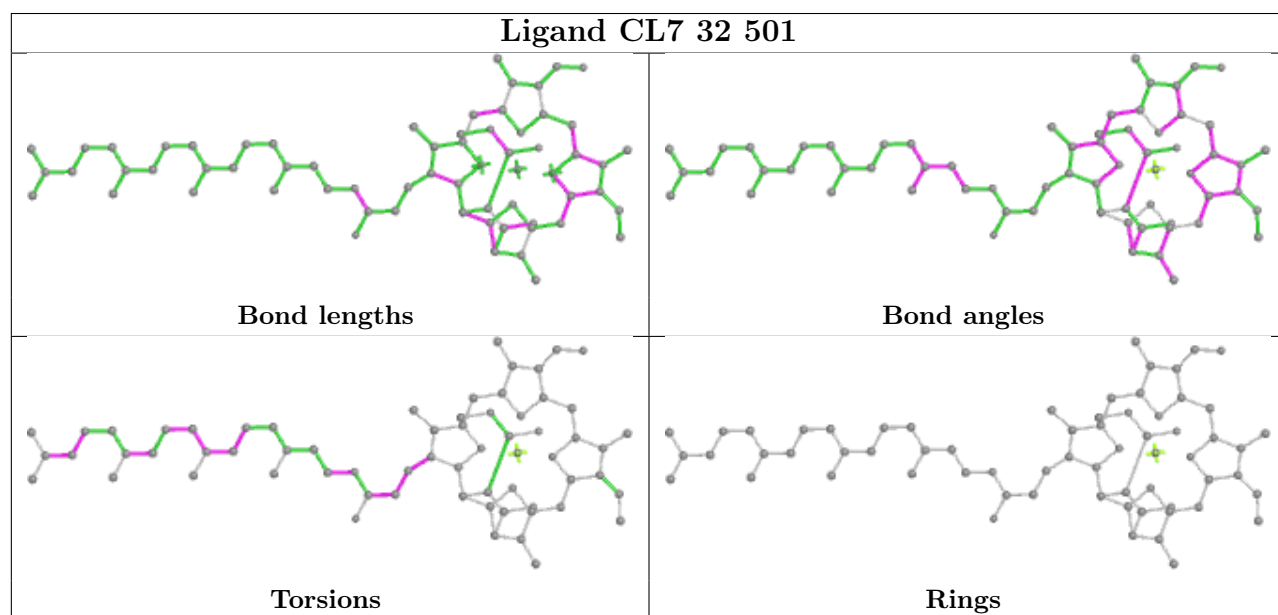
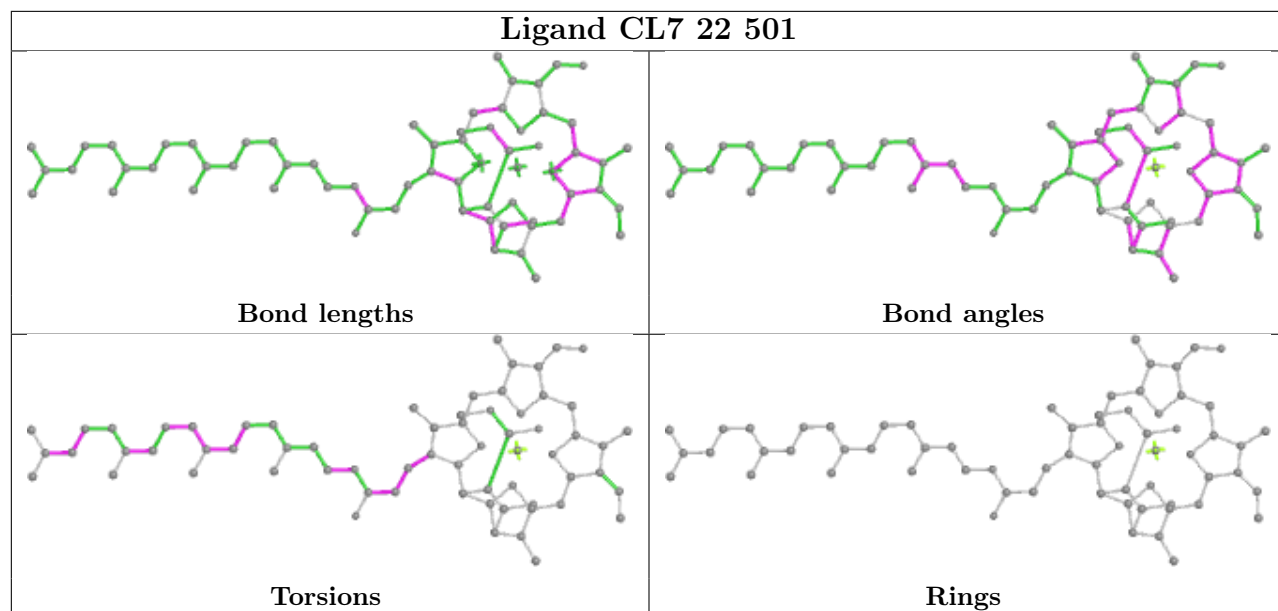
Ligand CL7 22 513

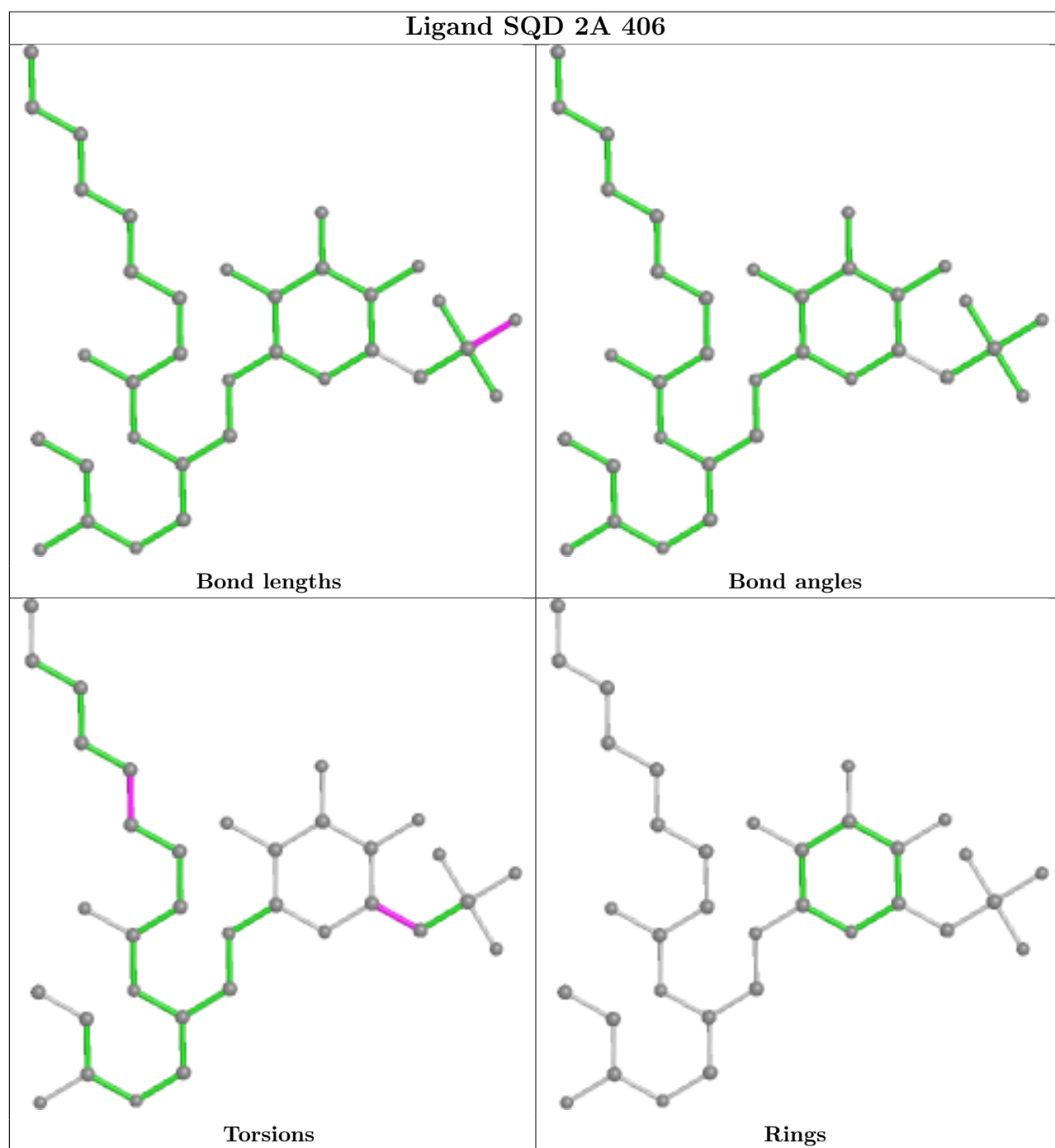


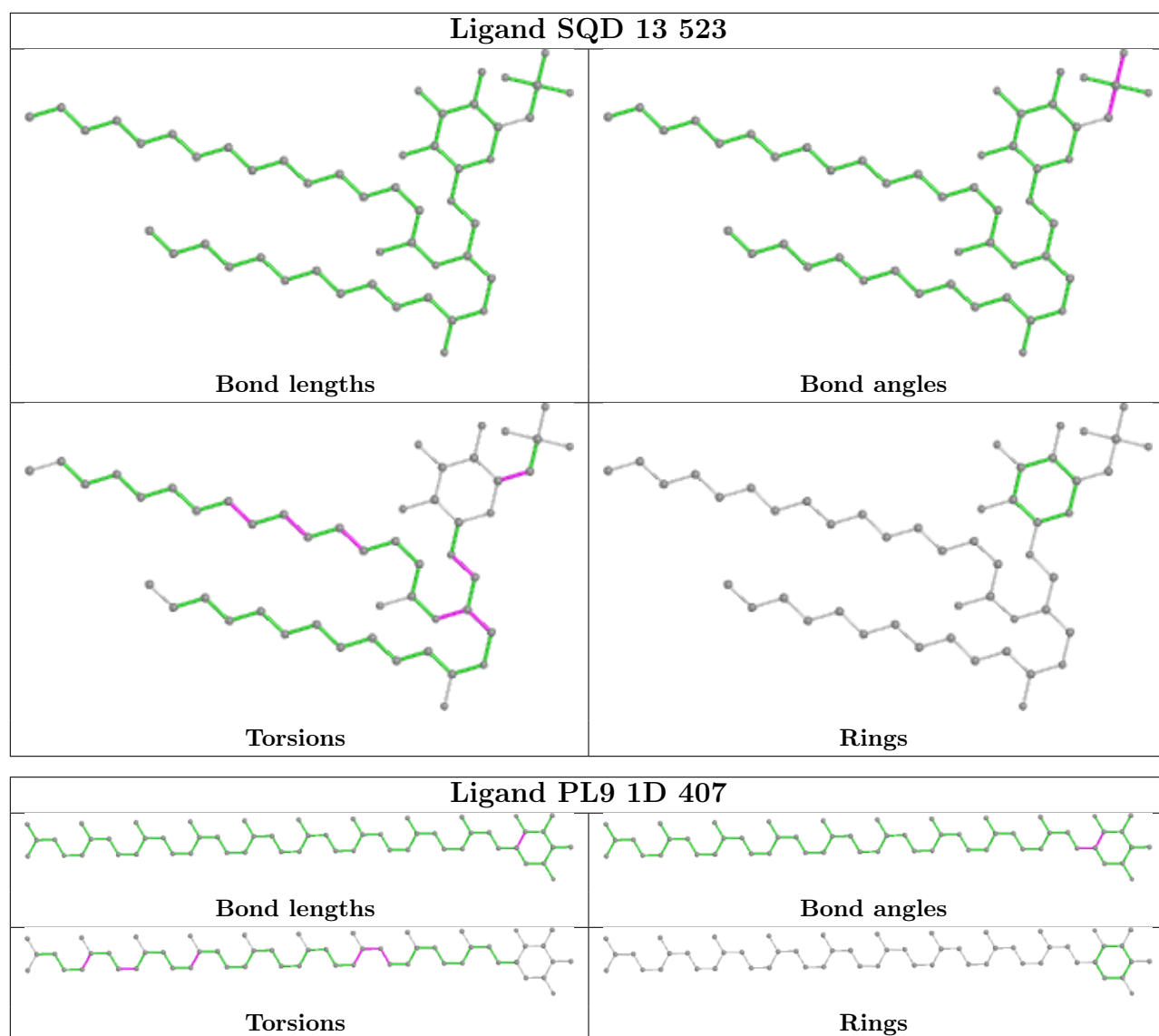
Ligand CL7 2C 501

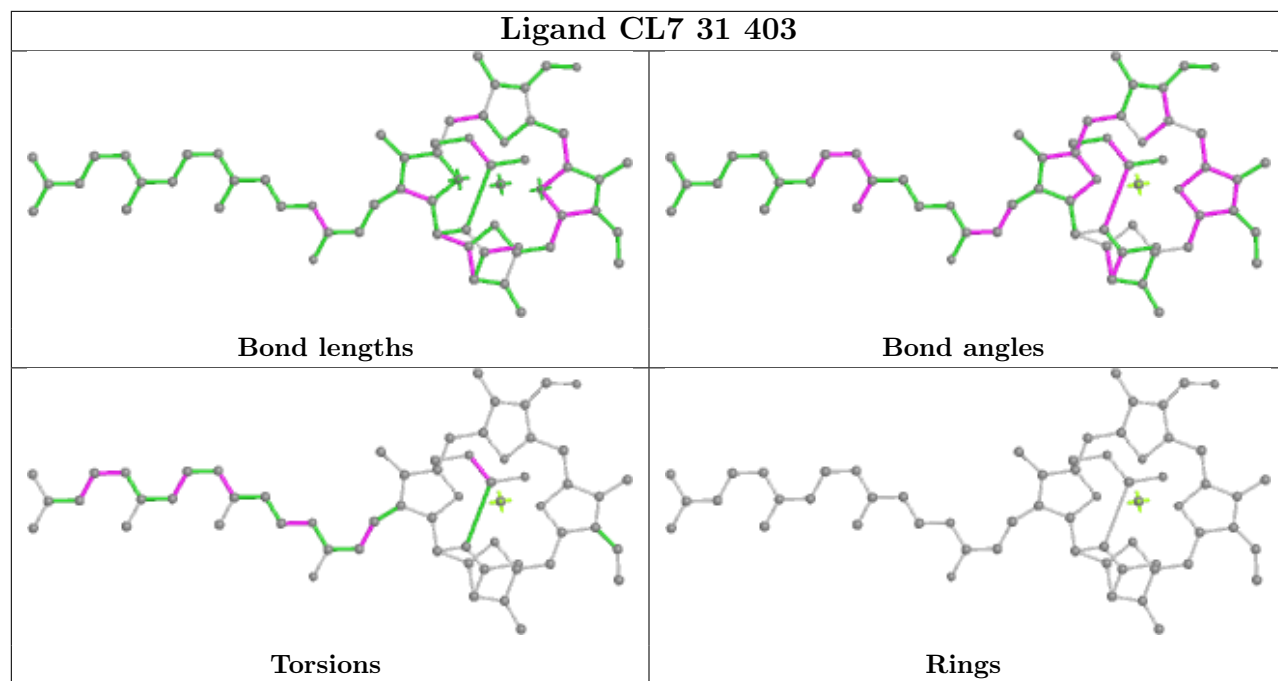


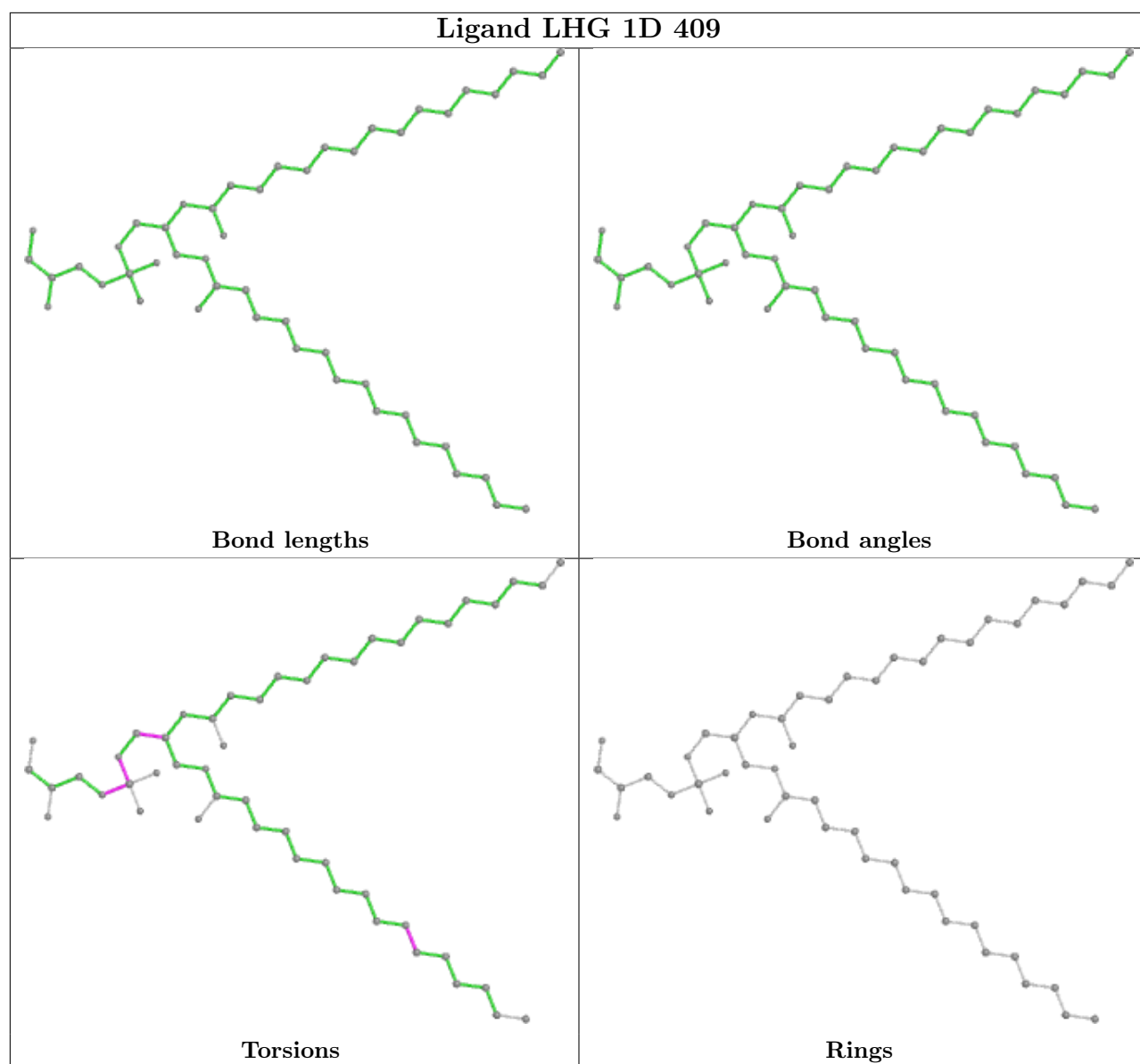




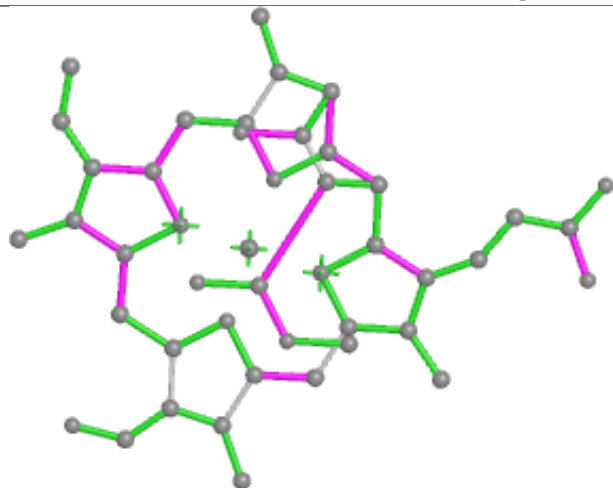




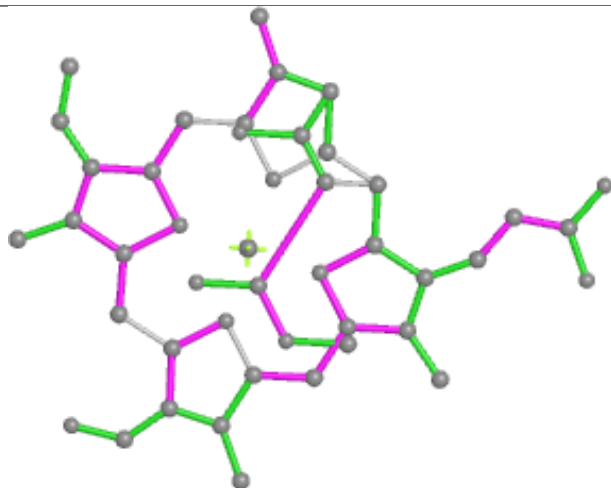




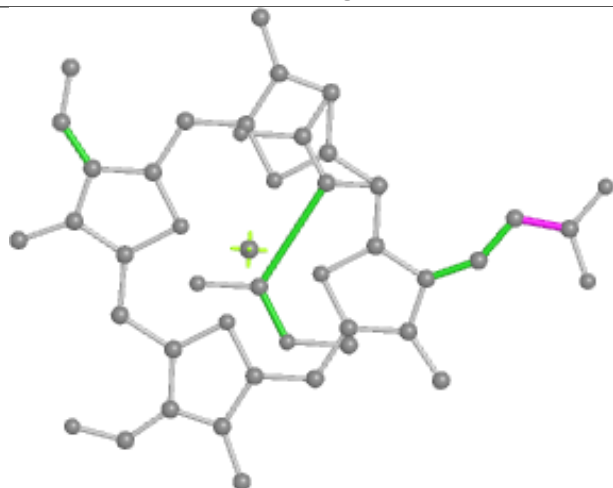
Ligand CL7 44 408



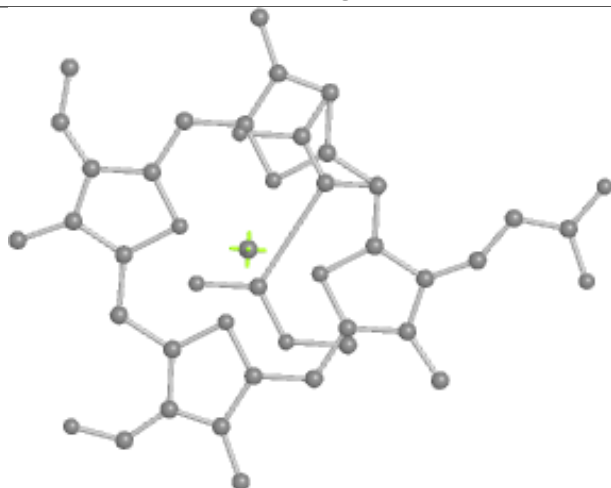
Bond lengths



Bond angles

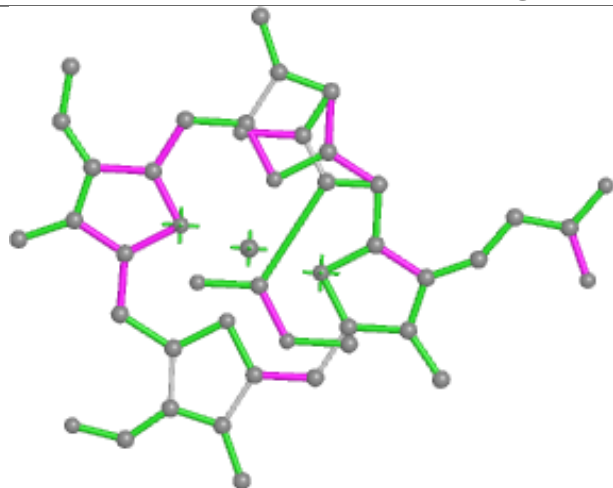


Torsions

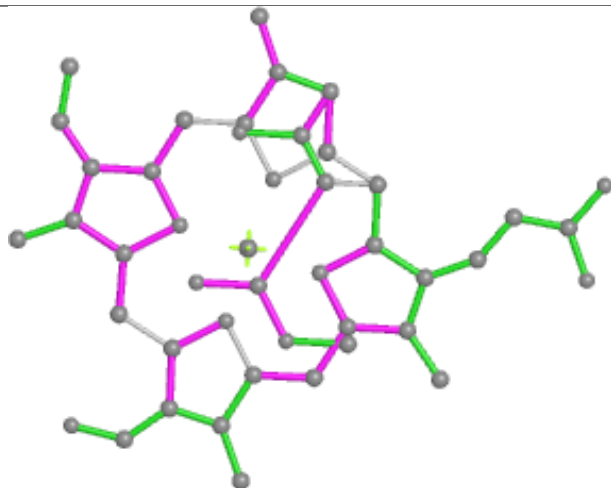


Rings

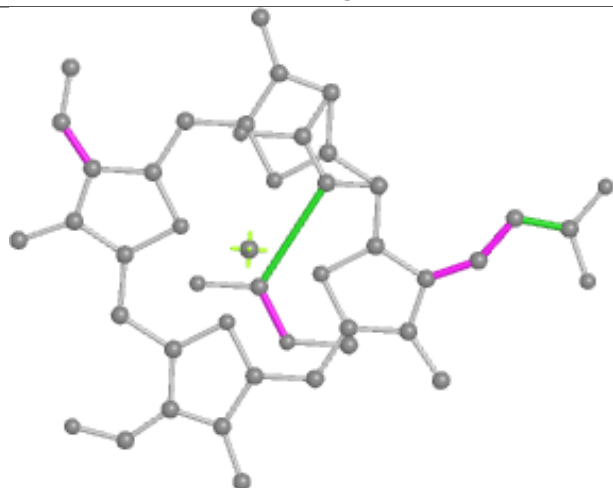
Ligand CL7 13 514



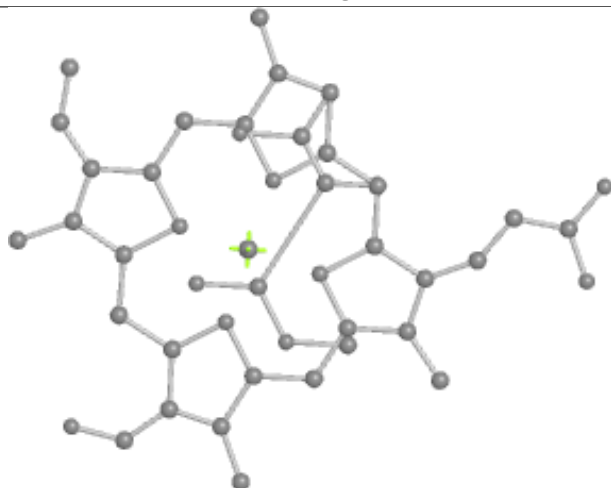
Bond lengths



Bond angles

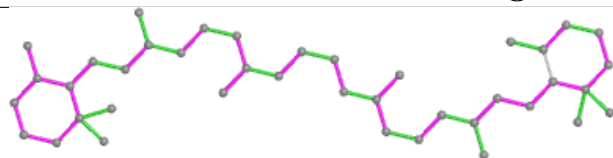


Torsions

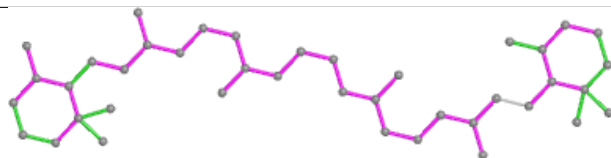


Rings

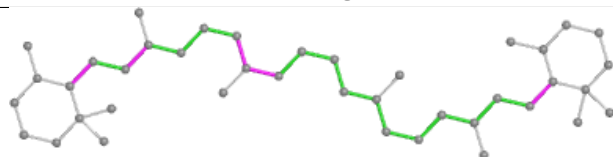
Ligand 8CT 1B 626



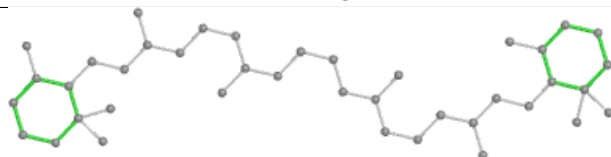
Bond lengths



Bond angles

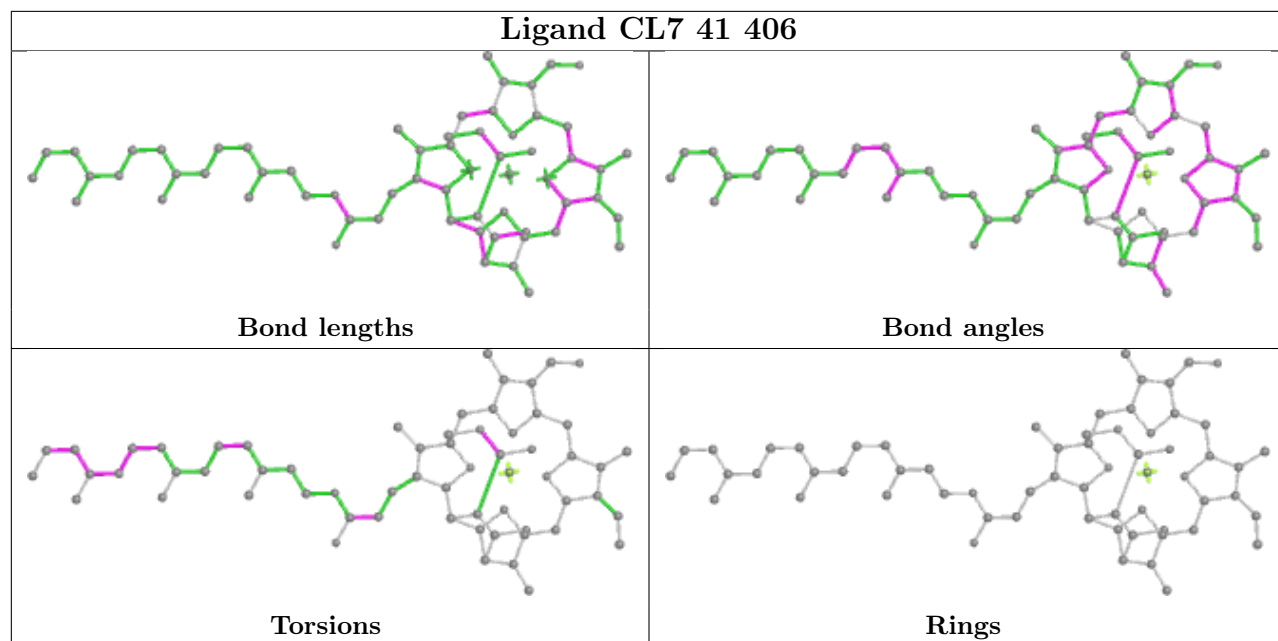


Torsions

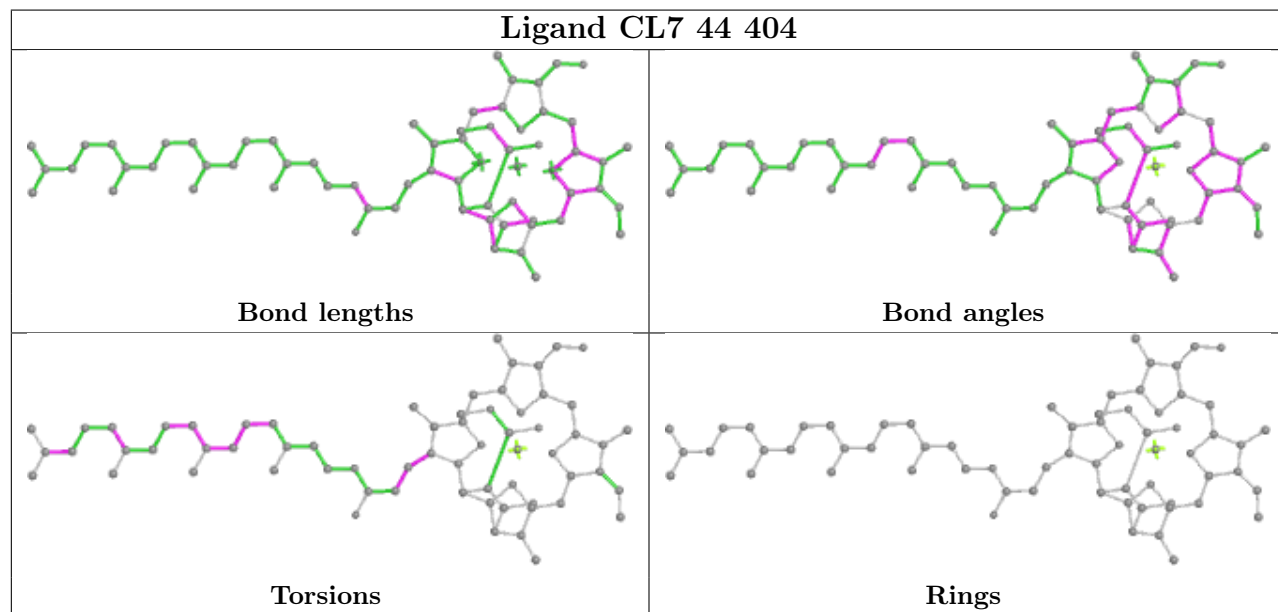


Rings

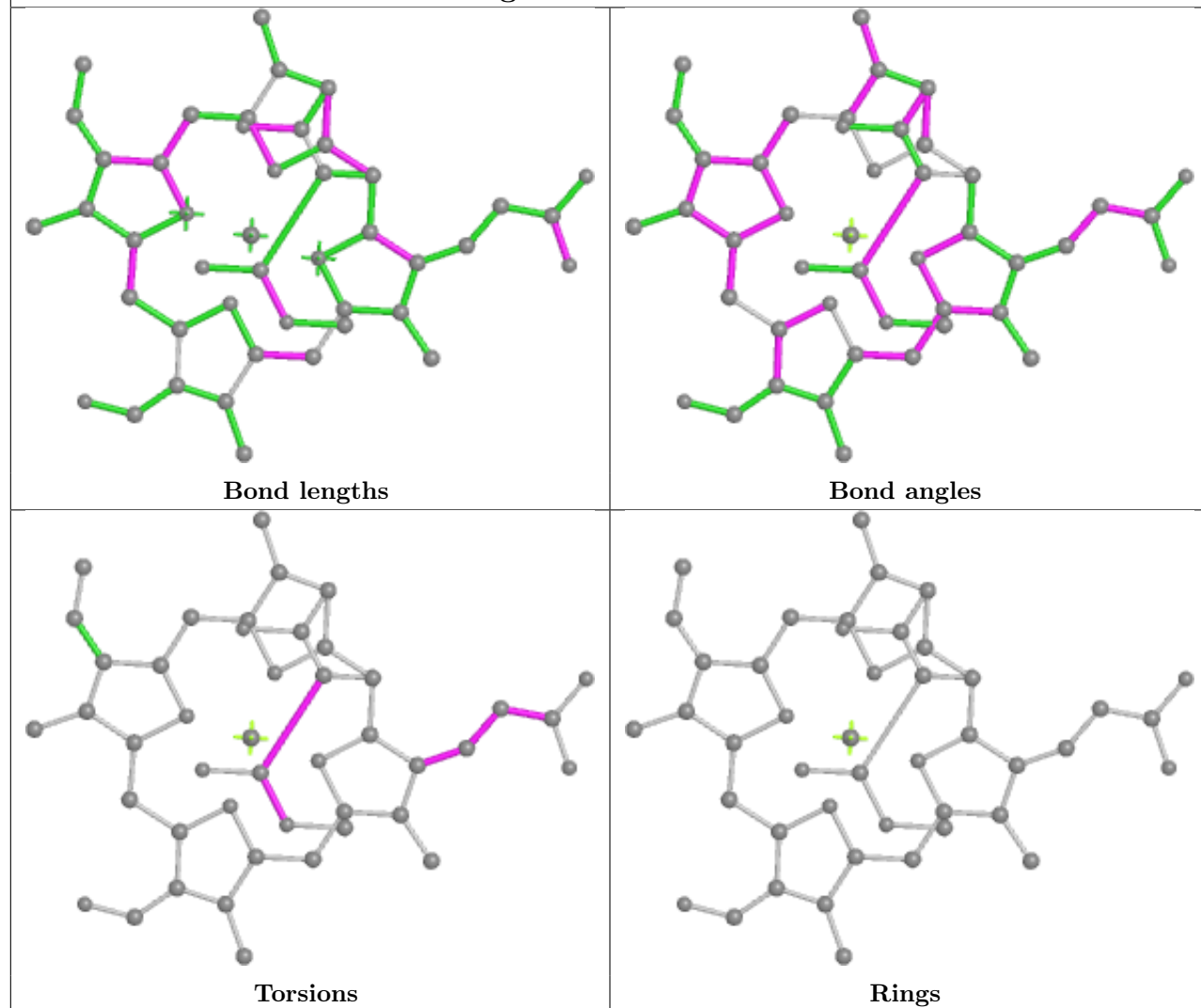
Ligand CL7 41 406



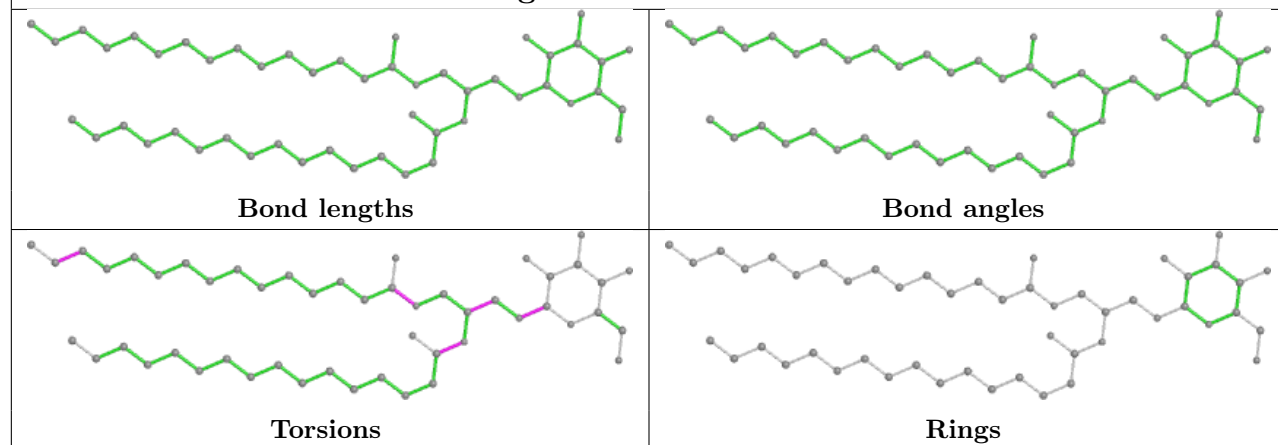
Ligand CL7 44 404



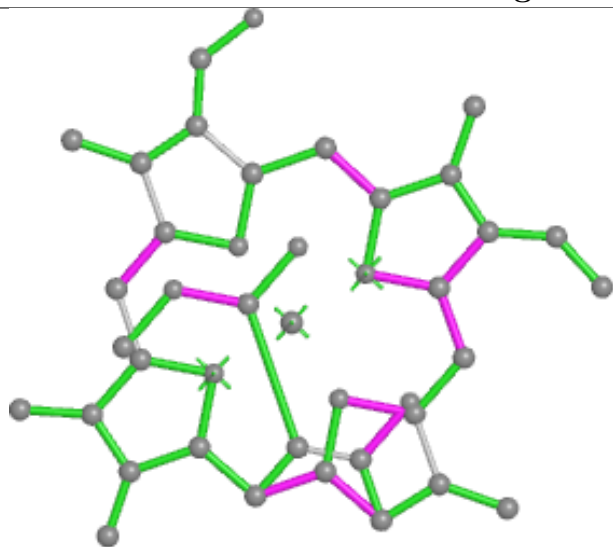
Ligand CL7 11 412



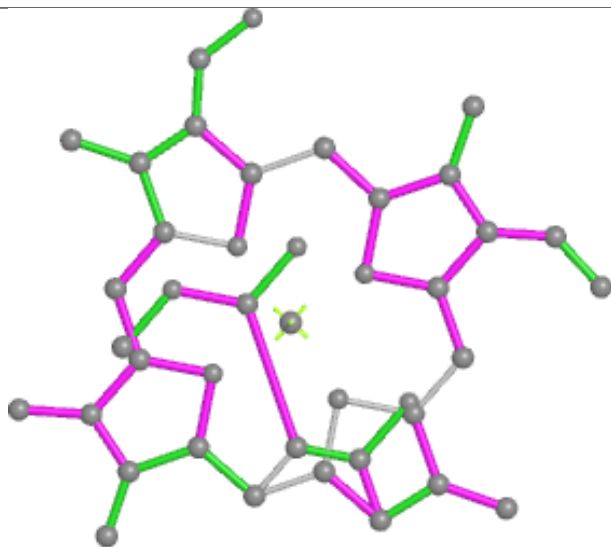
Ligand LMG 1A 405



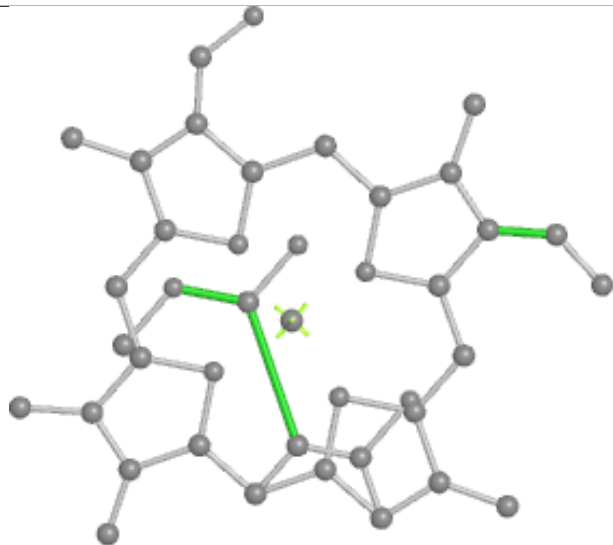
Ligand CL7 13 515



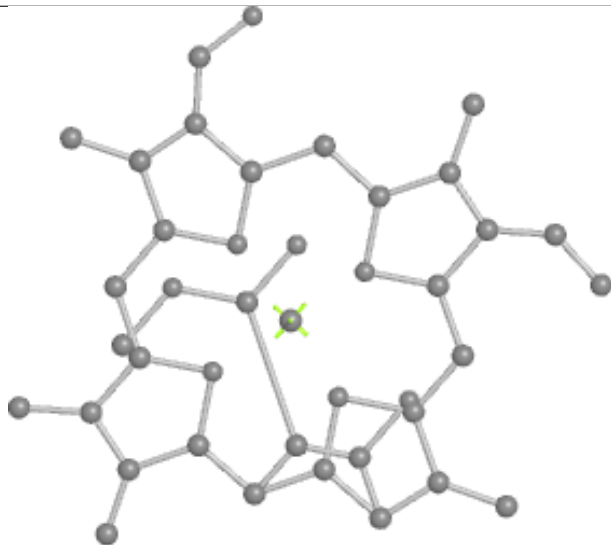
Bond lengths



Bond angles

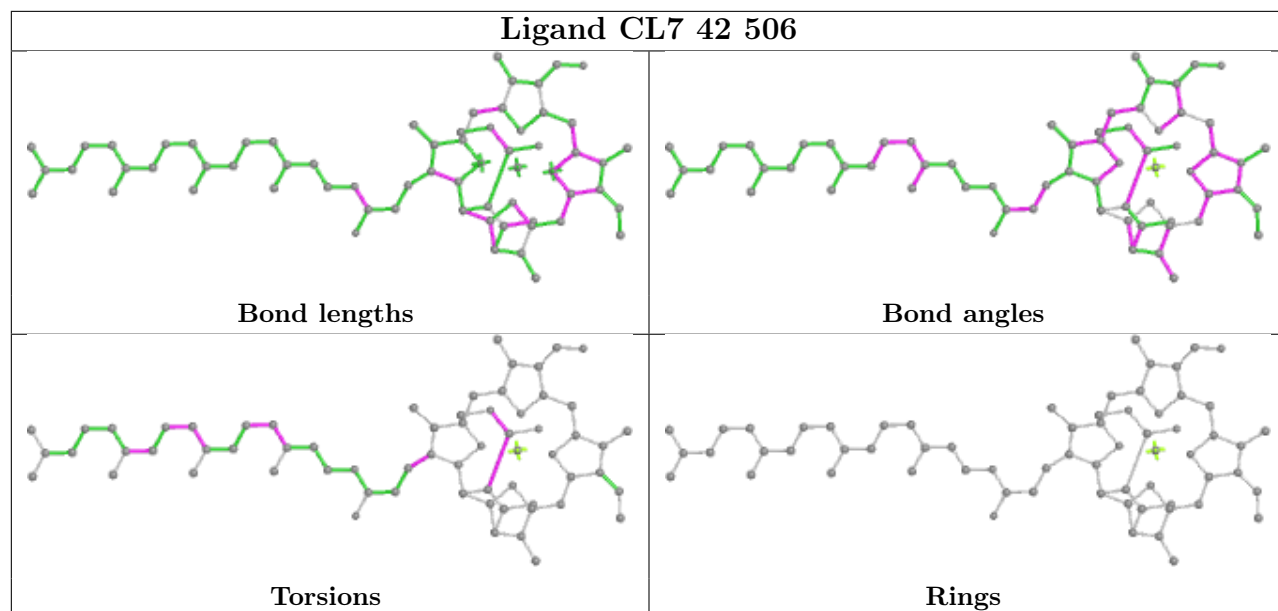


Torsions

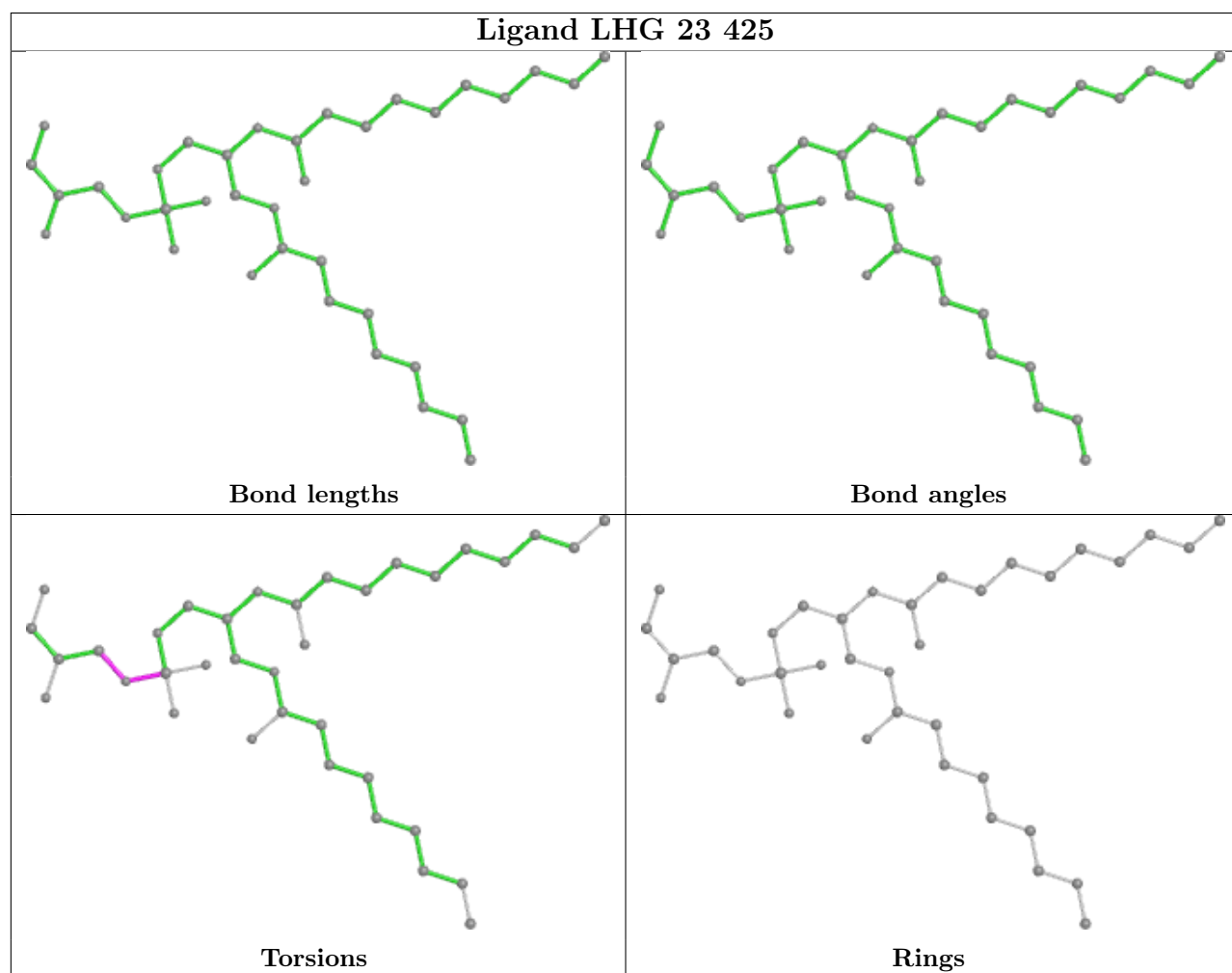


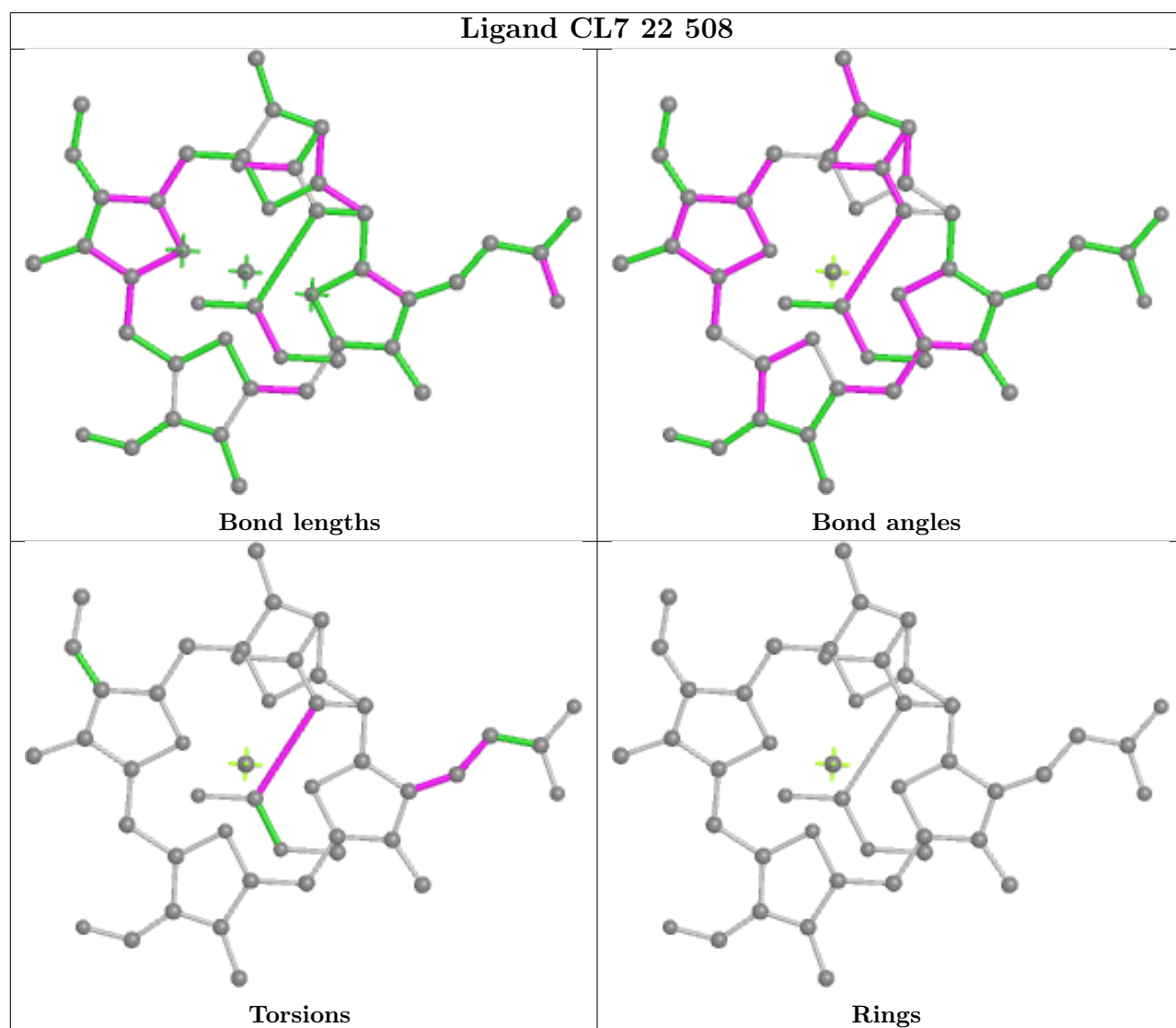
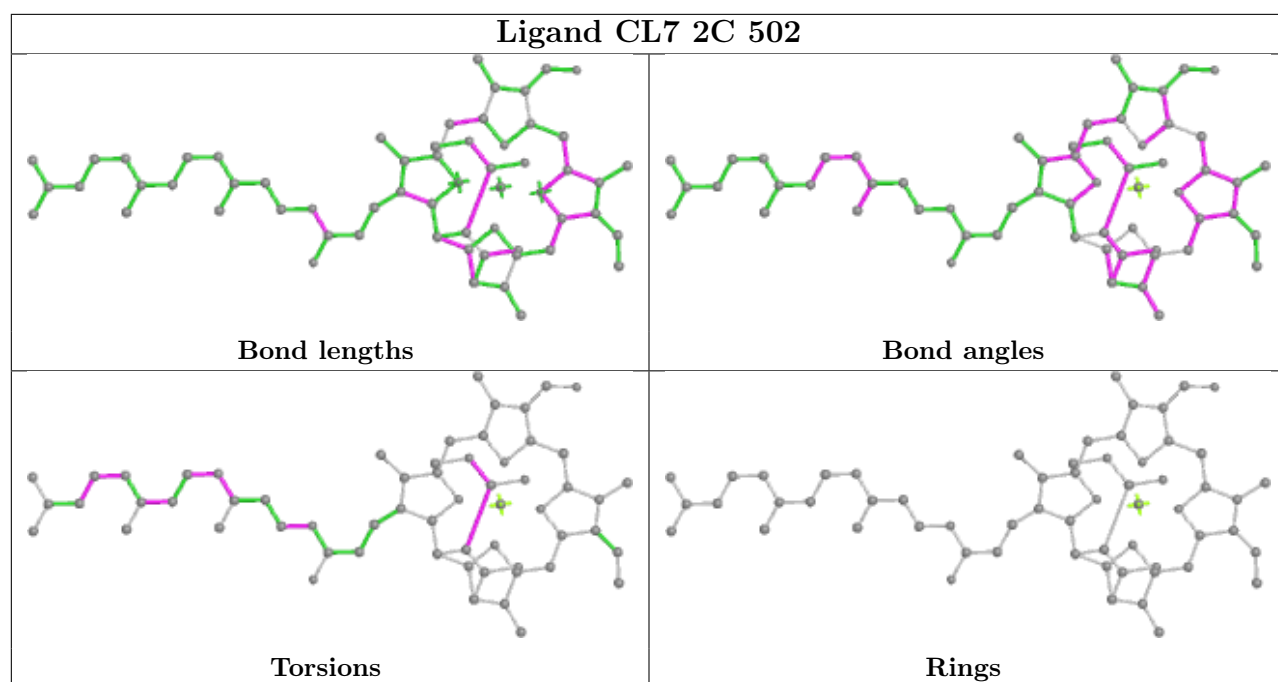
Rings

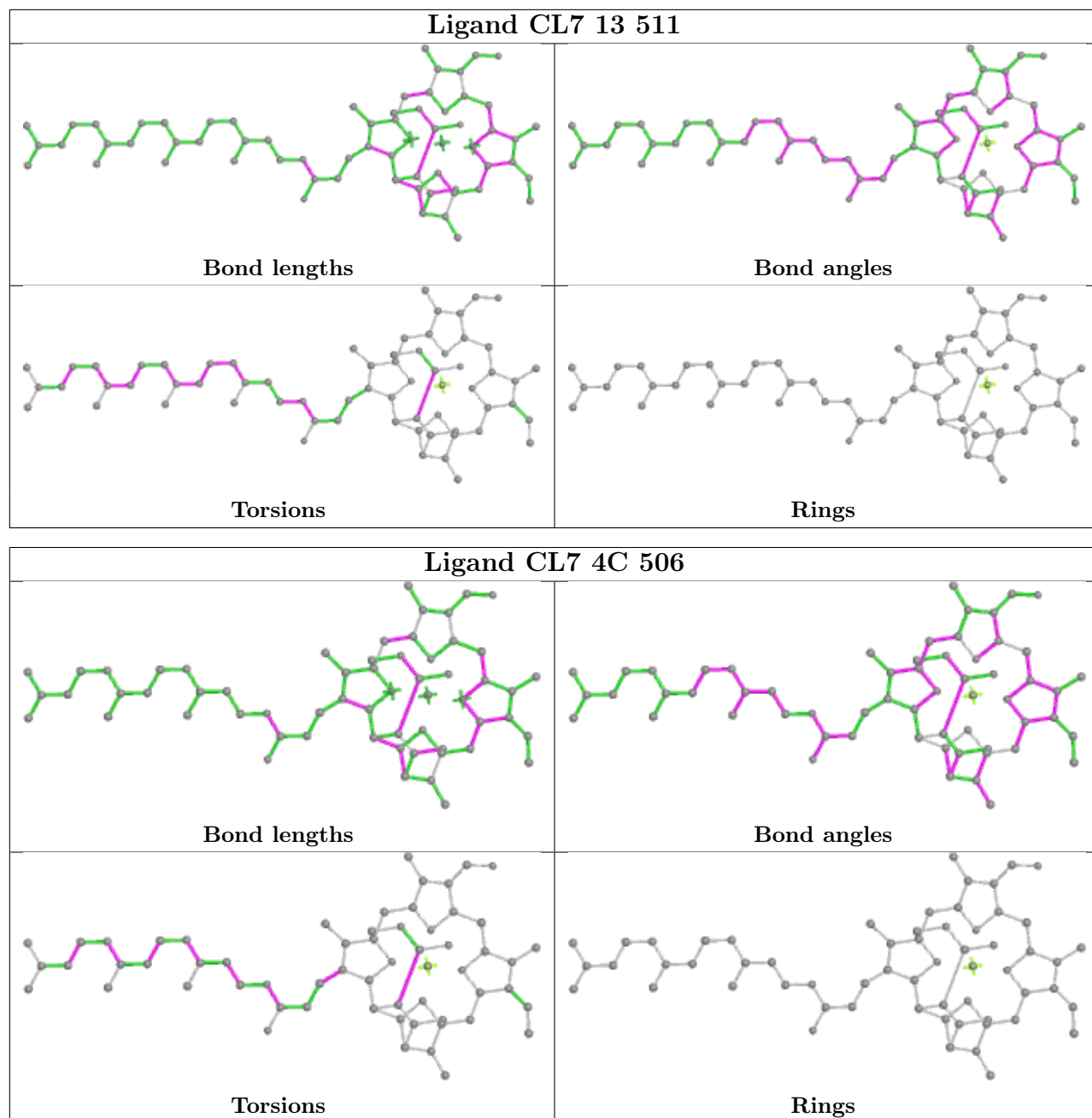
Ligand CL7 42 506

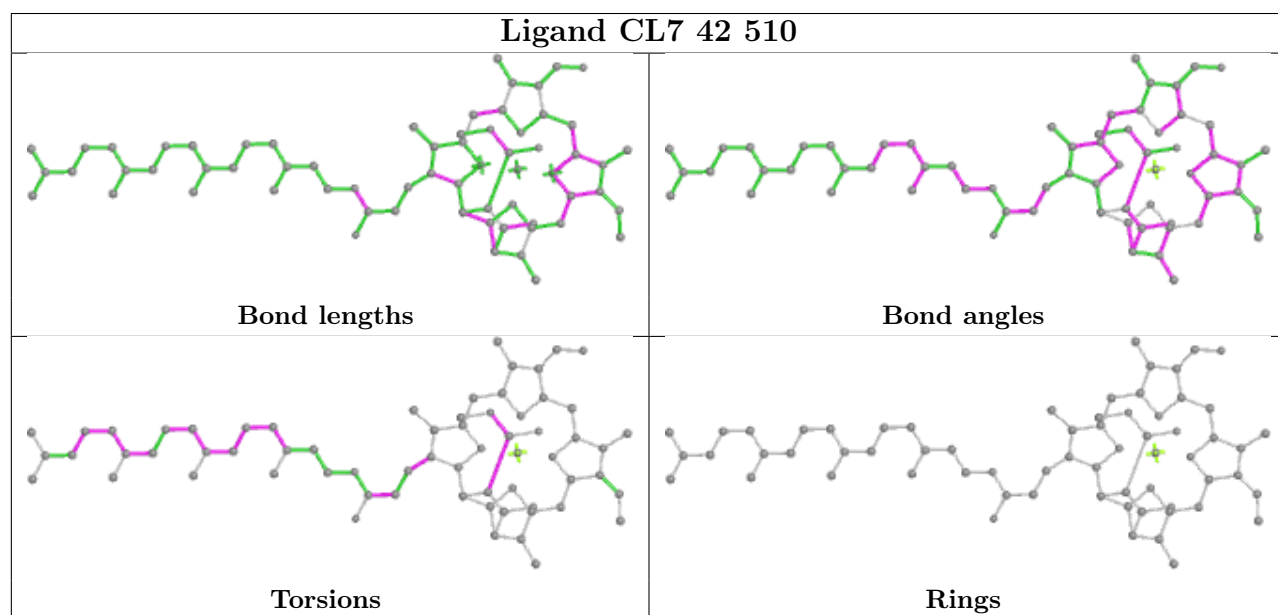
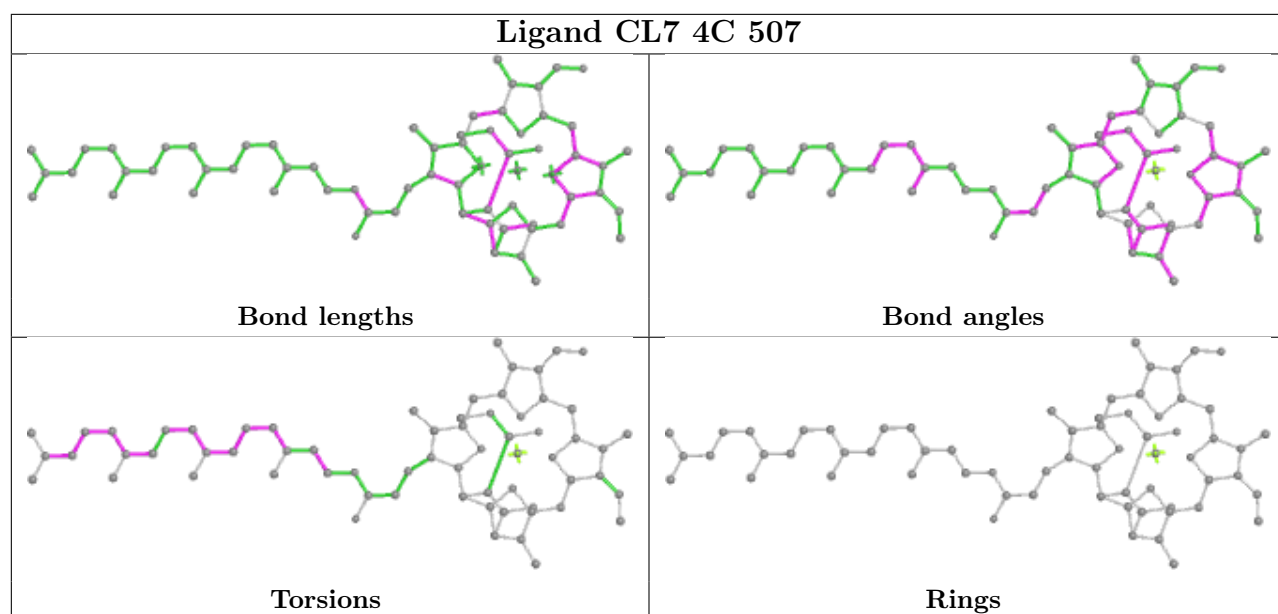


Ligand LHG 23 425

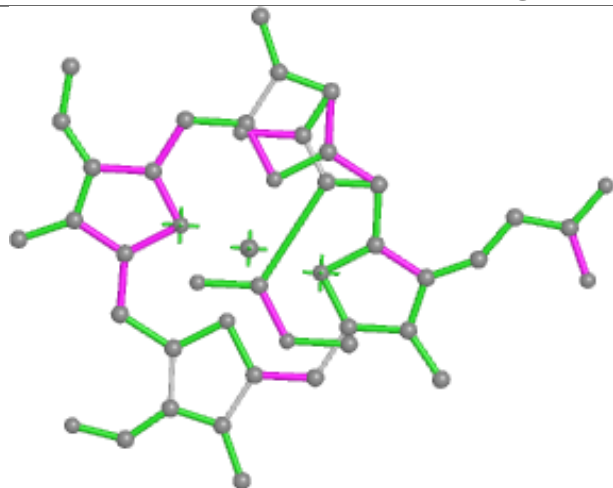




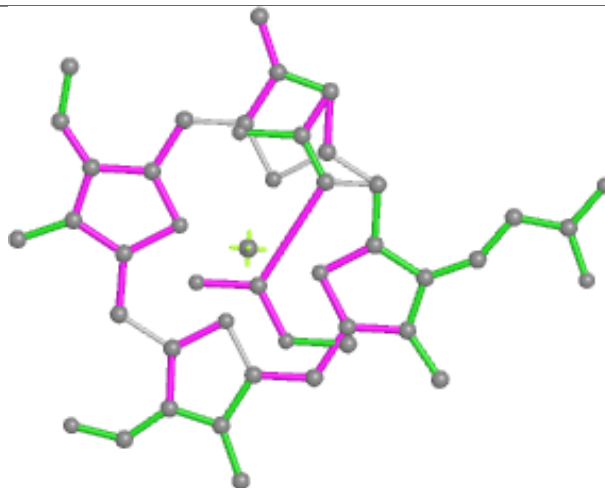




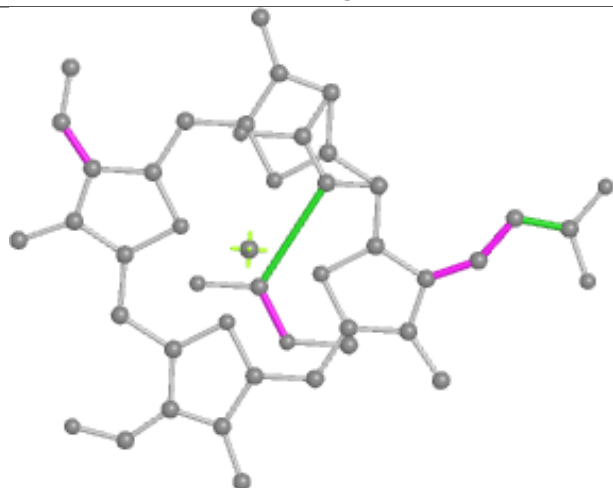
Ligand CL7 43 415



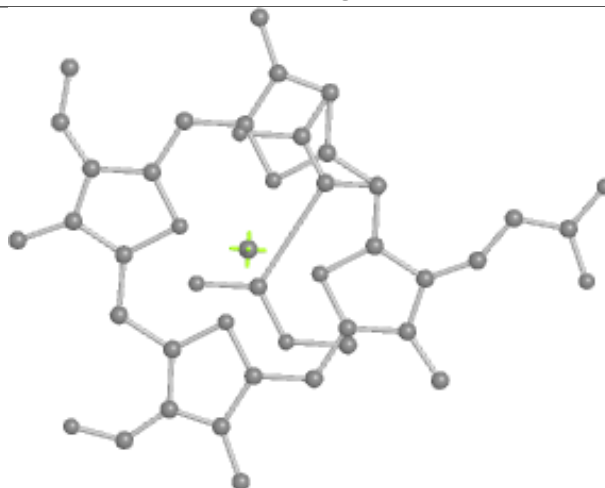
Bond lengths



Bond angles

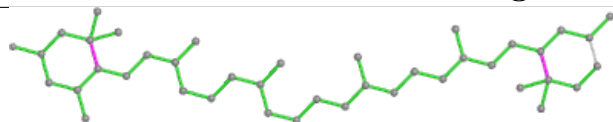


Torsions

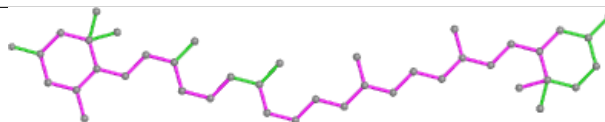


Rings

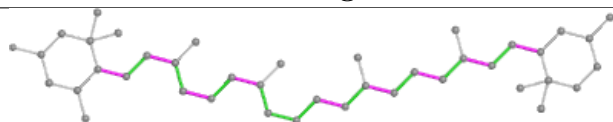
Ligand ZEX 21 421



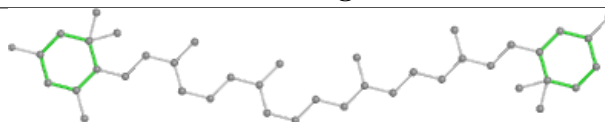
Bond lengths



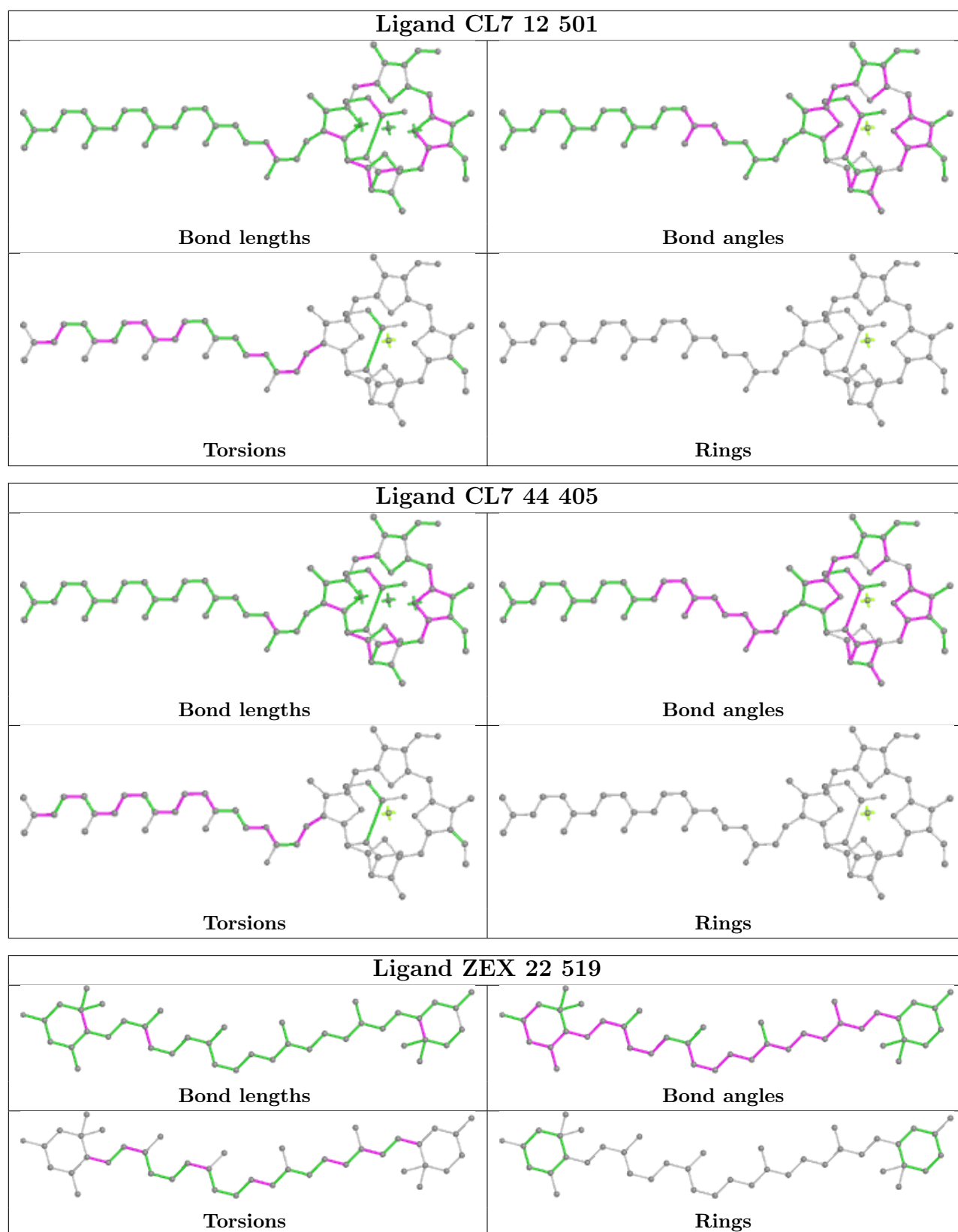
Bond angles



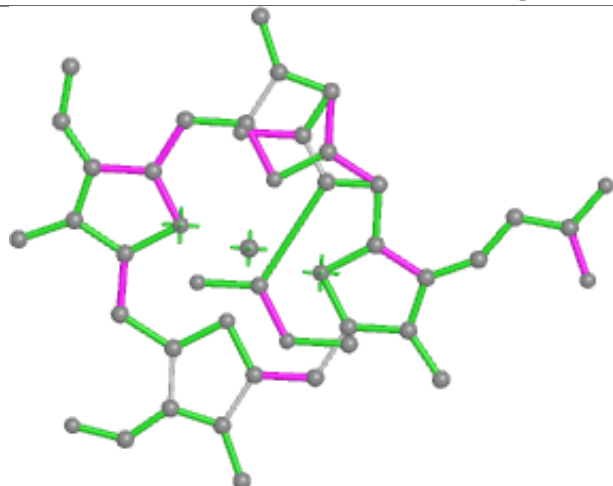
Torsions



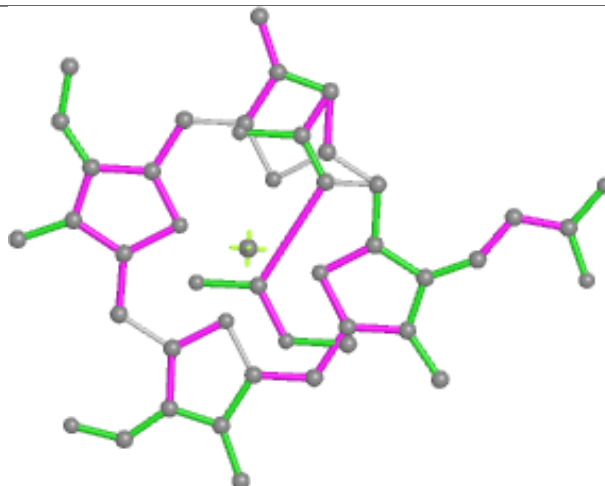
Rings



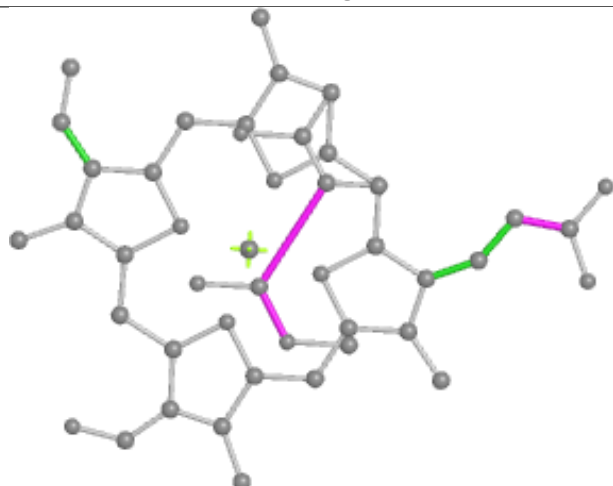
Ligand CL7 11 411



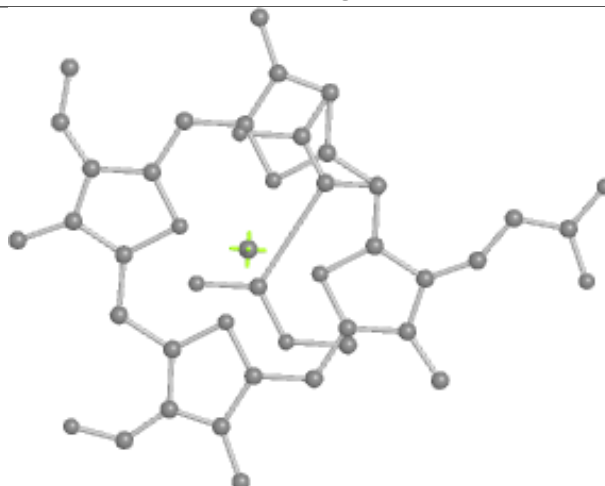
Bond lengths



Bond angles

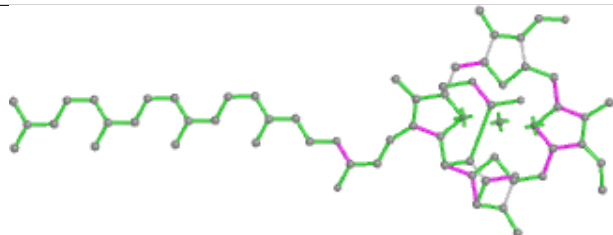


Torsions

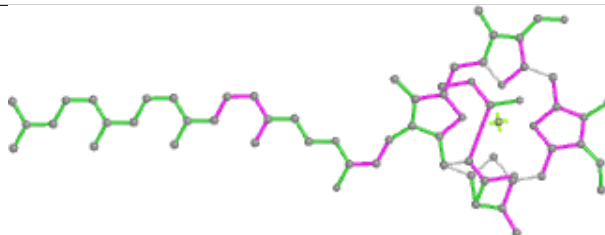


Rings

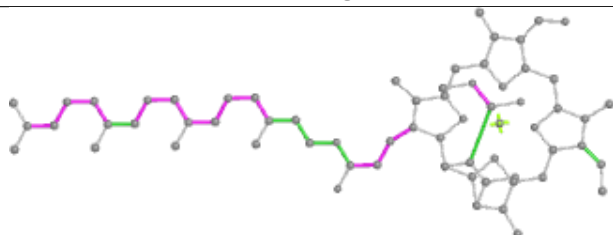
Ligand CL7 34 406



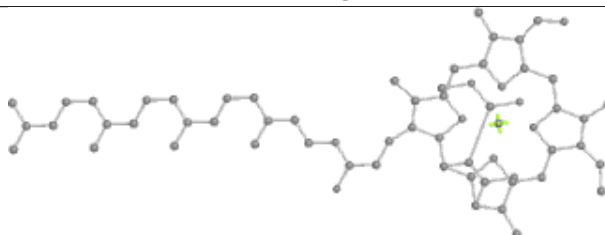
Bond lengths



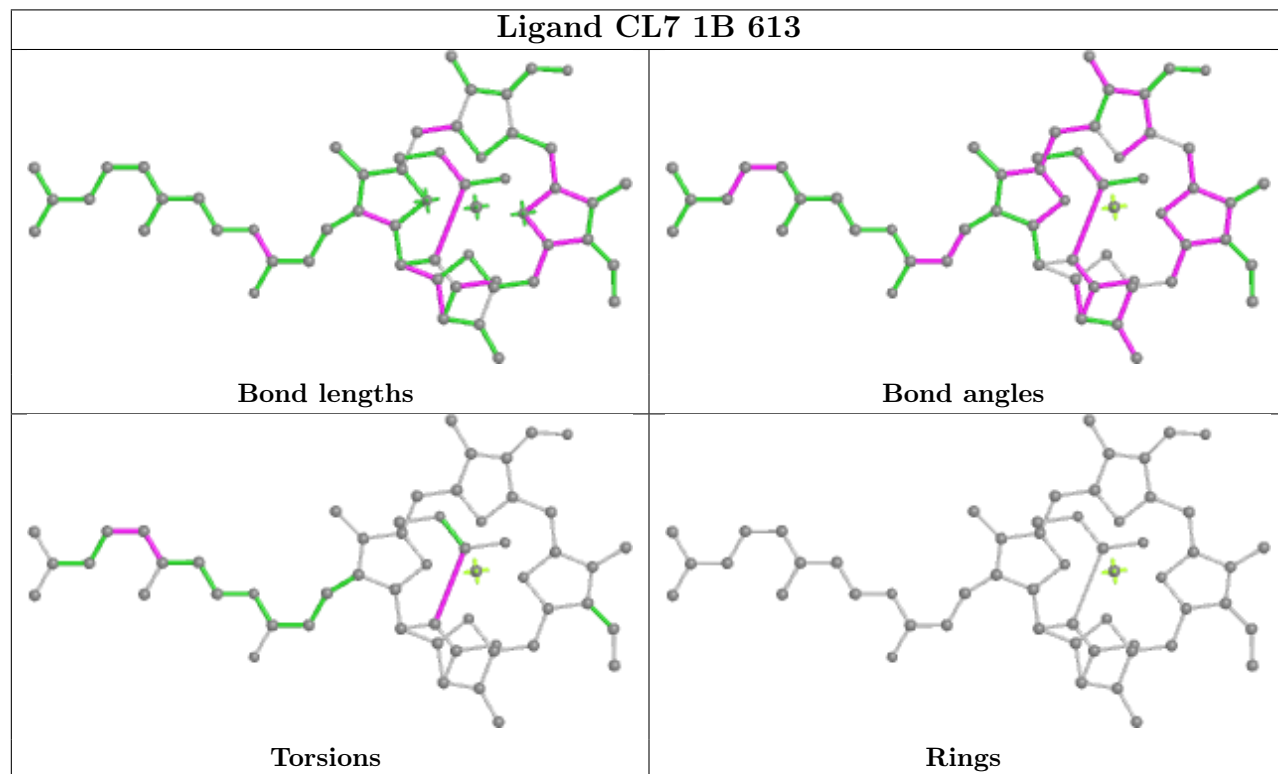
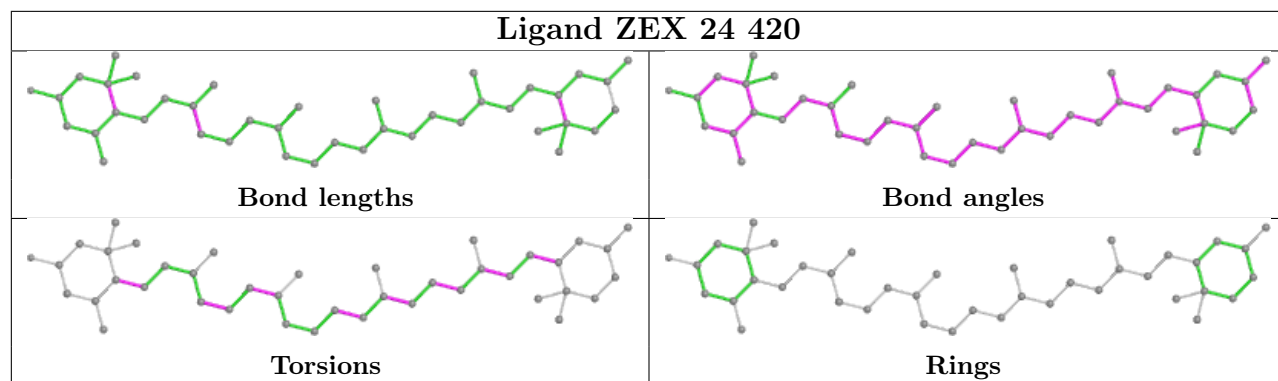
Bond angles

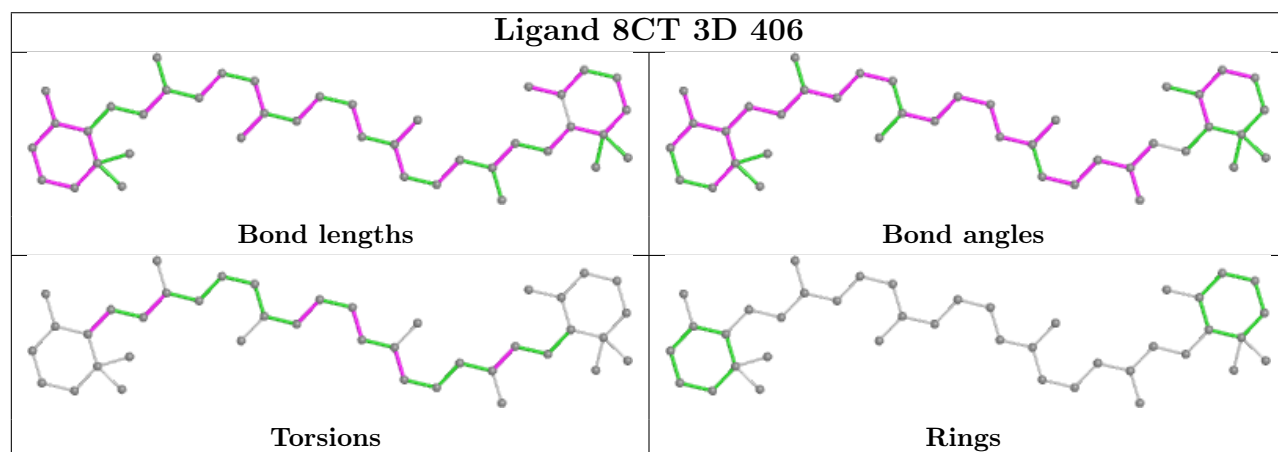
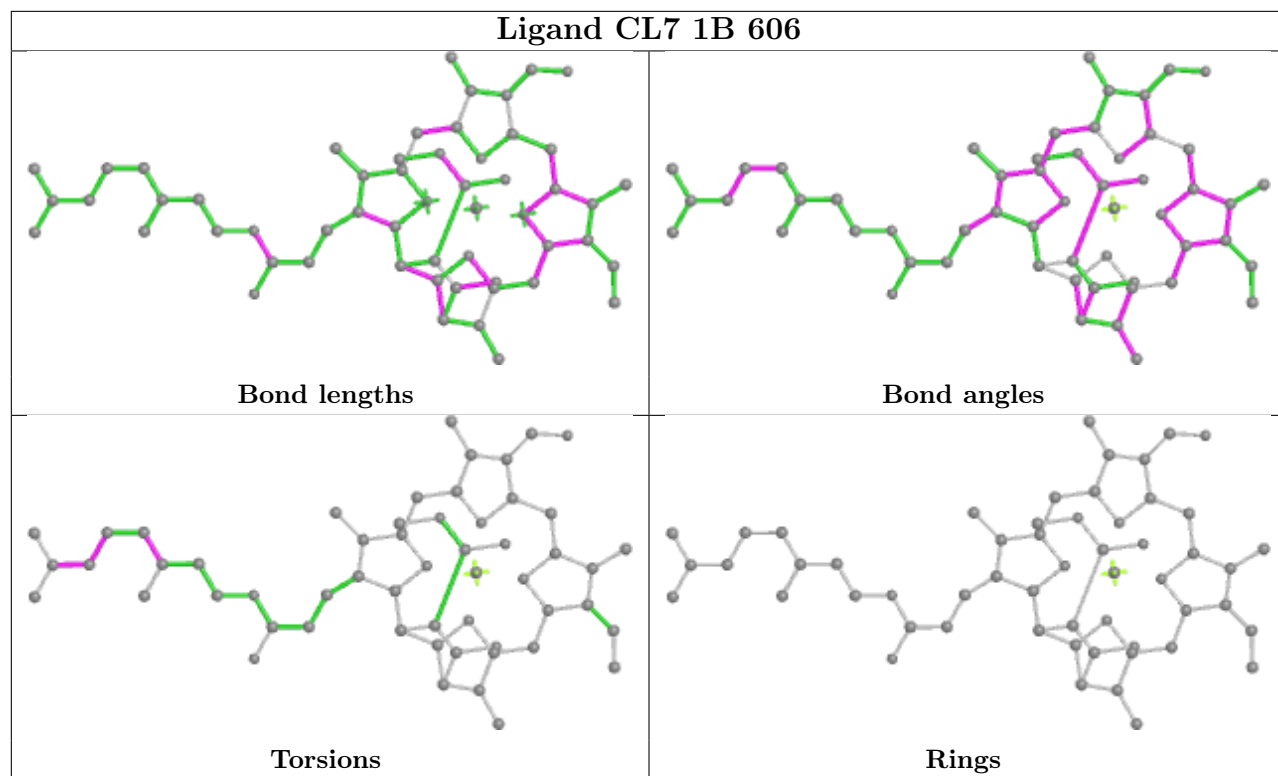


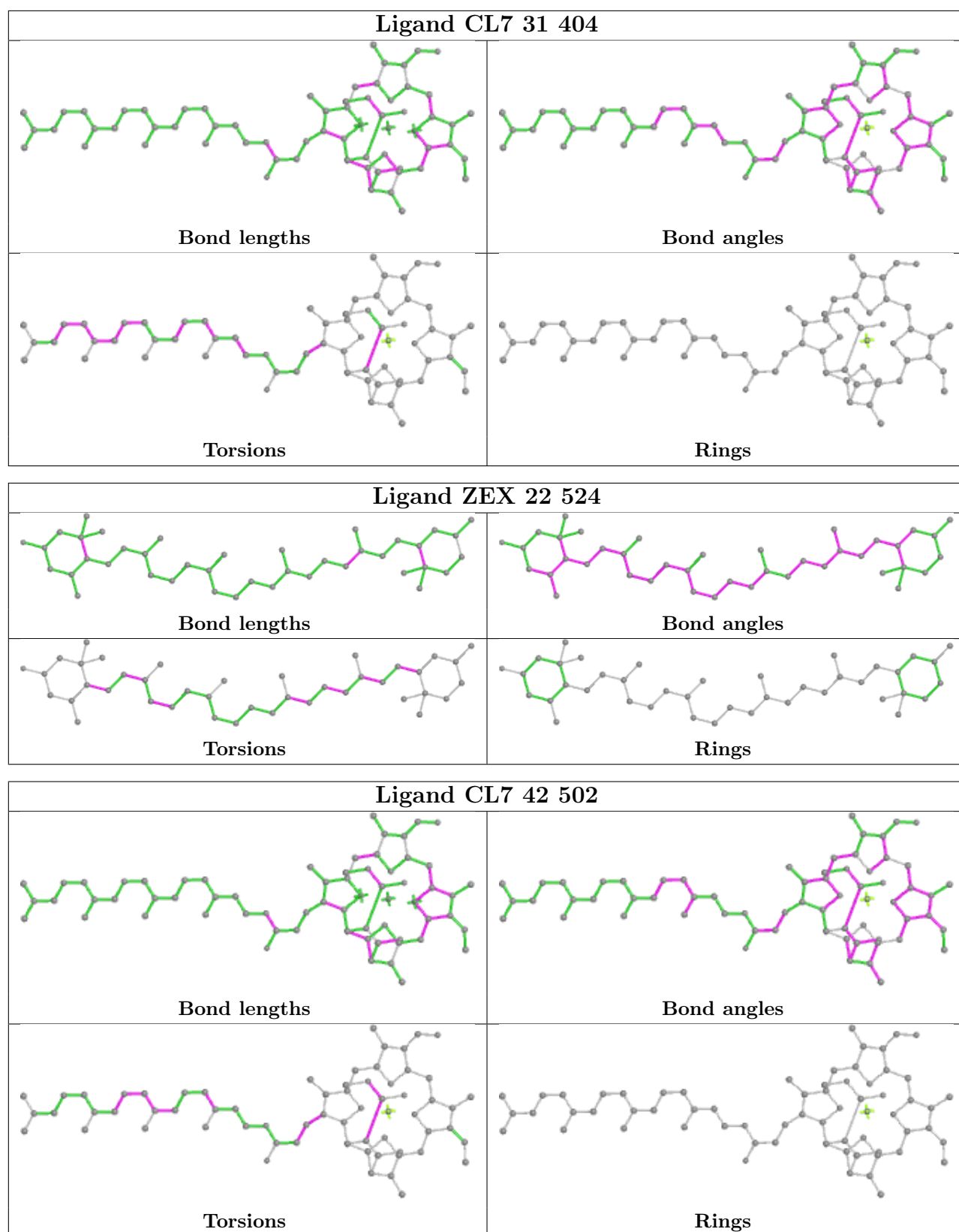
Torsions



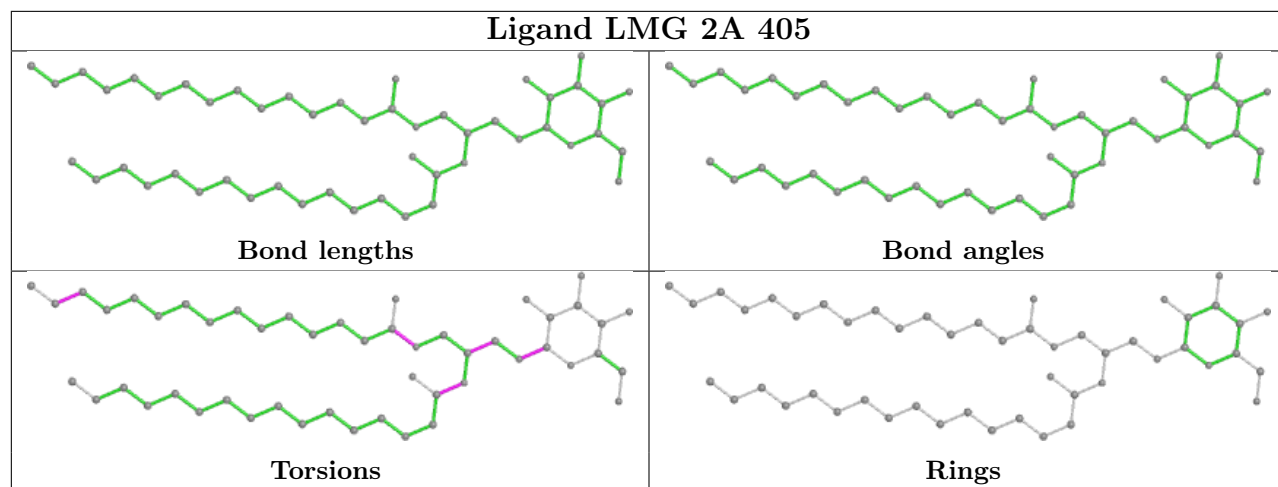
Rings



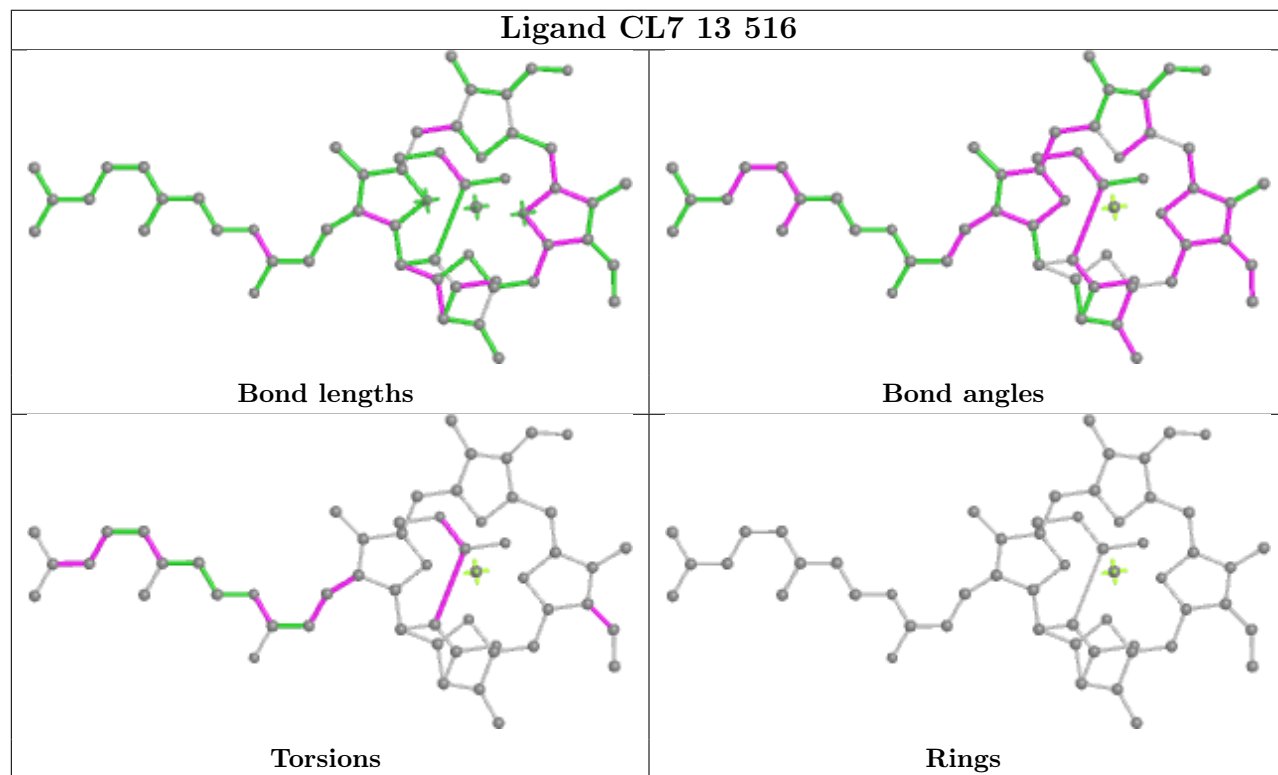




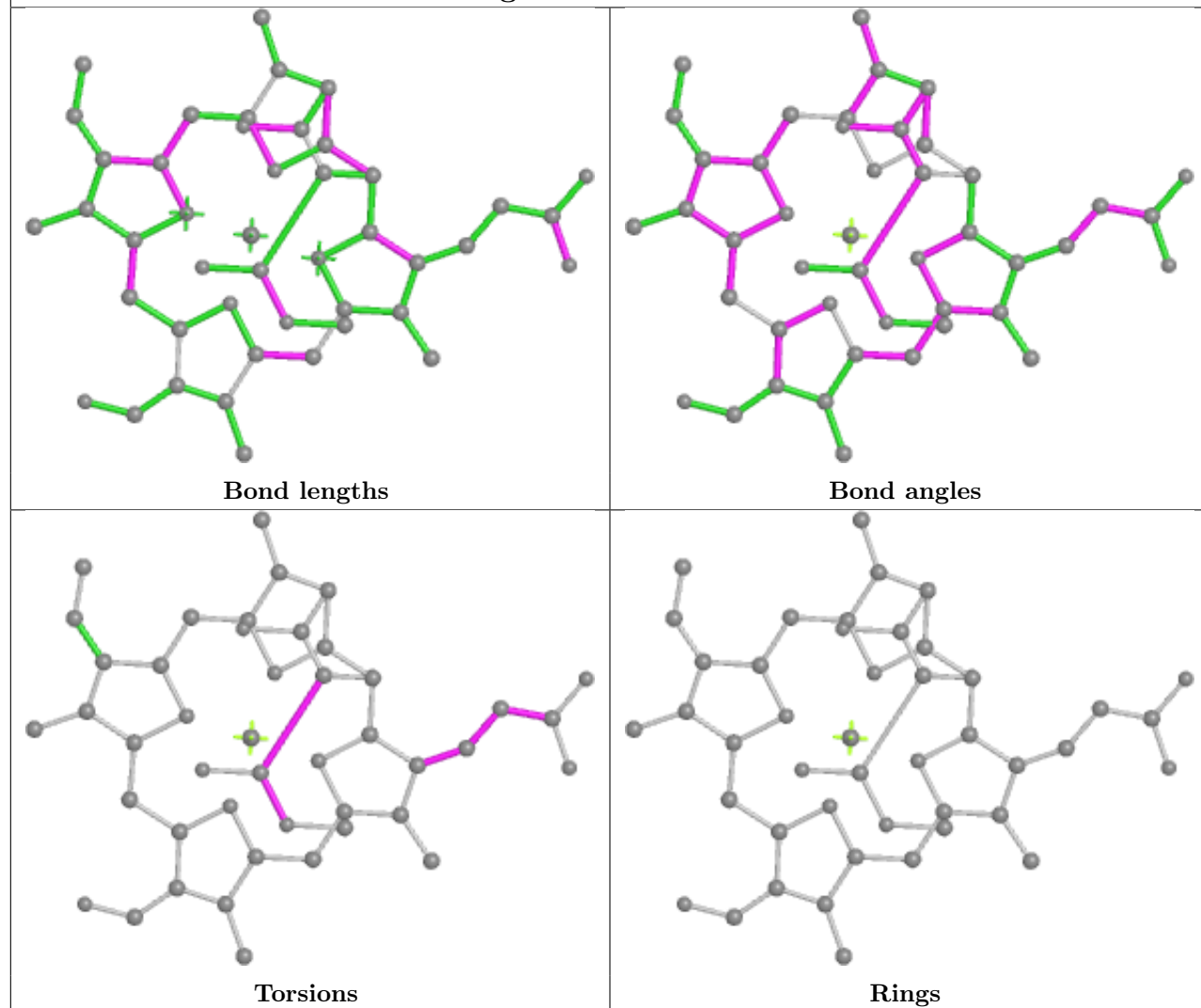
Ligand LMG 2A 405



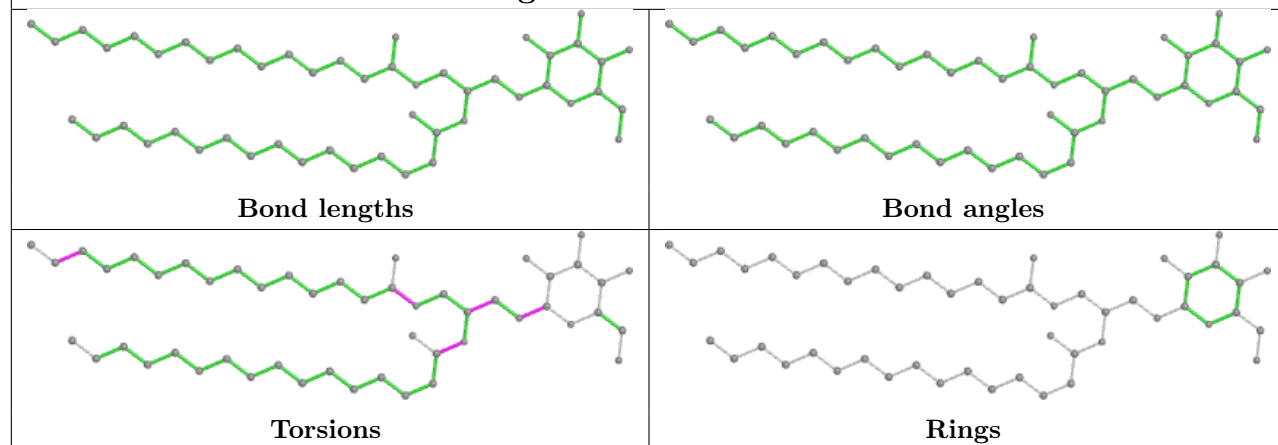
Ligand CL7 13 516

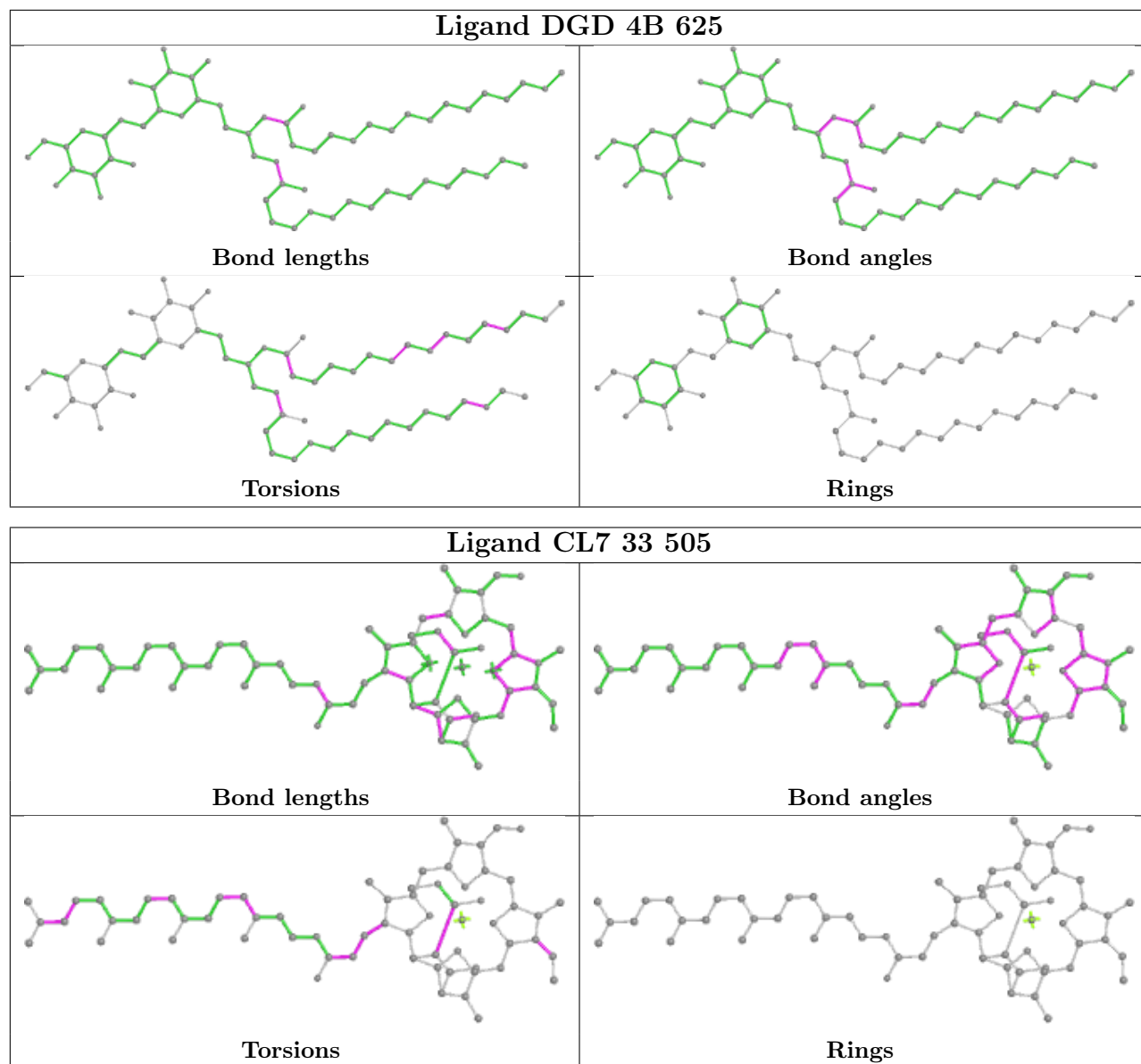


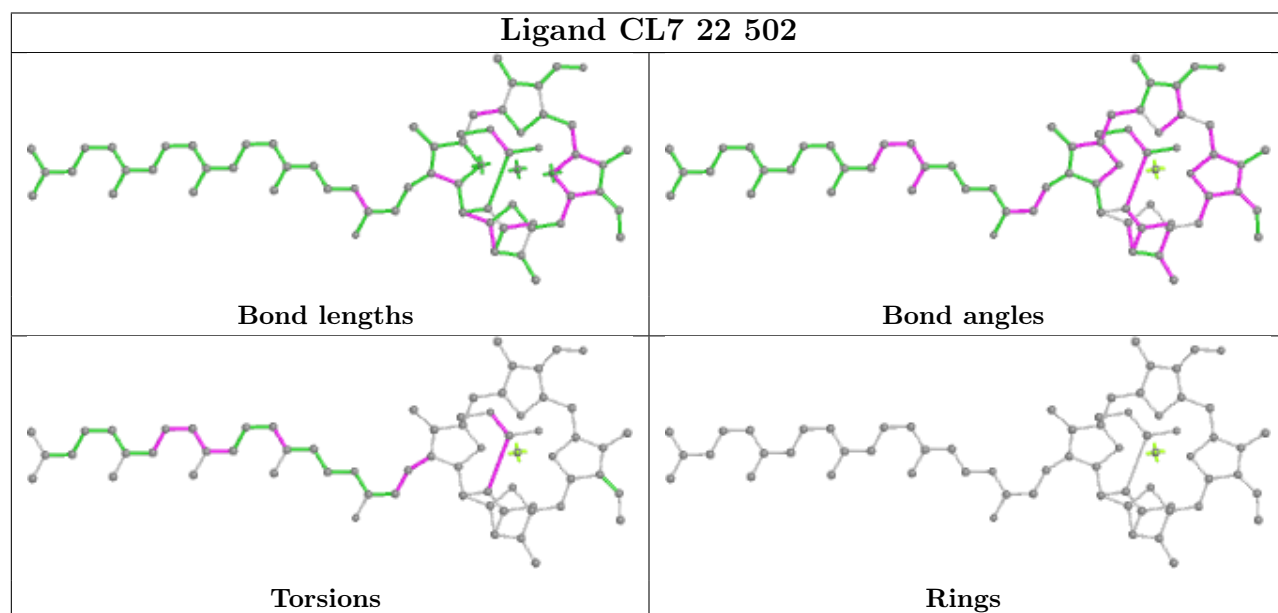
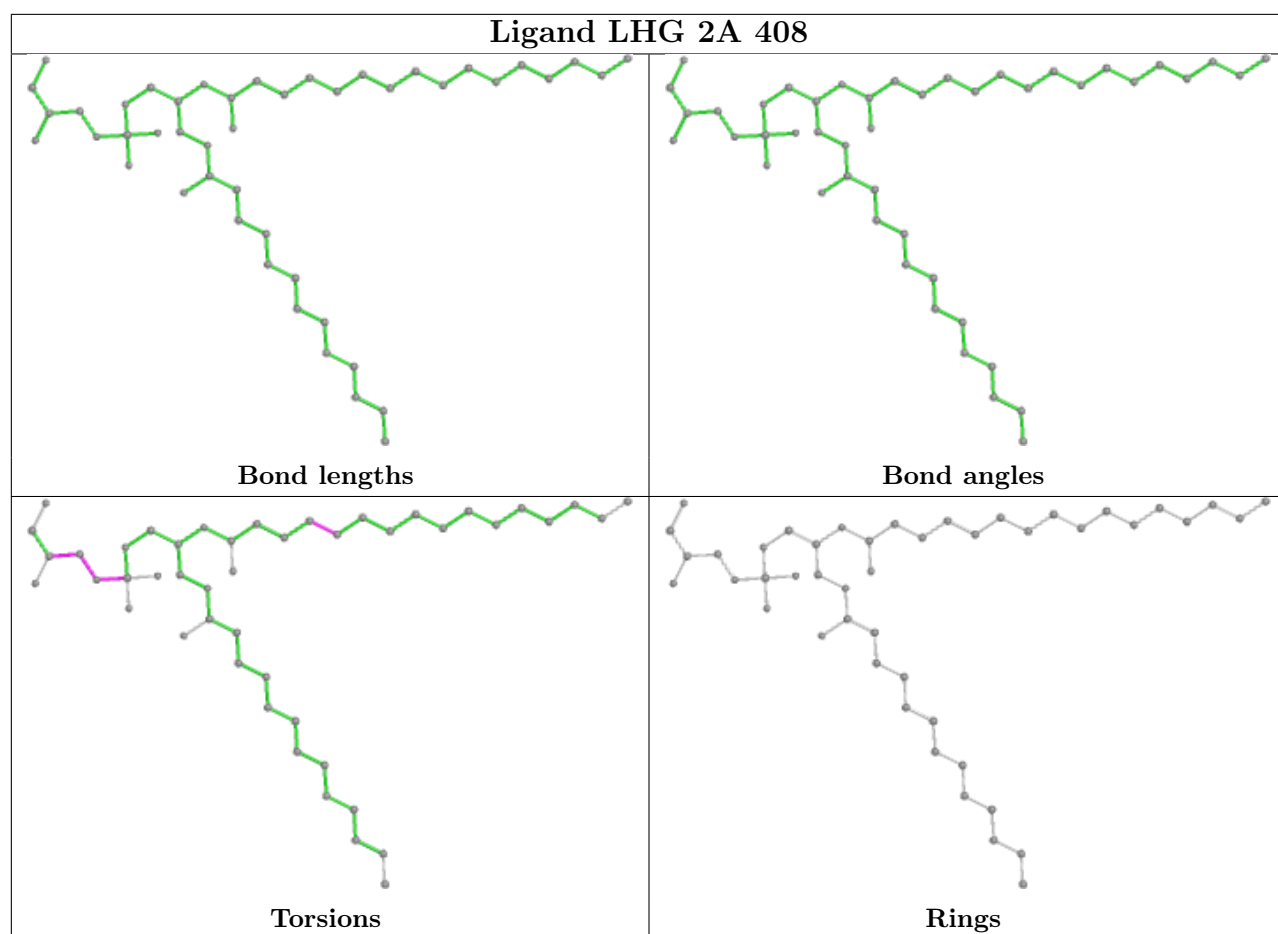
Ligand CL7 4I 412

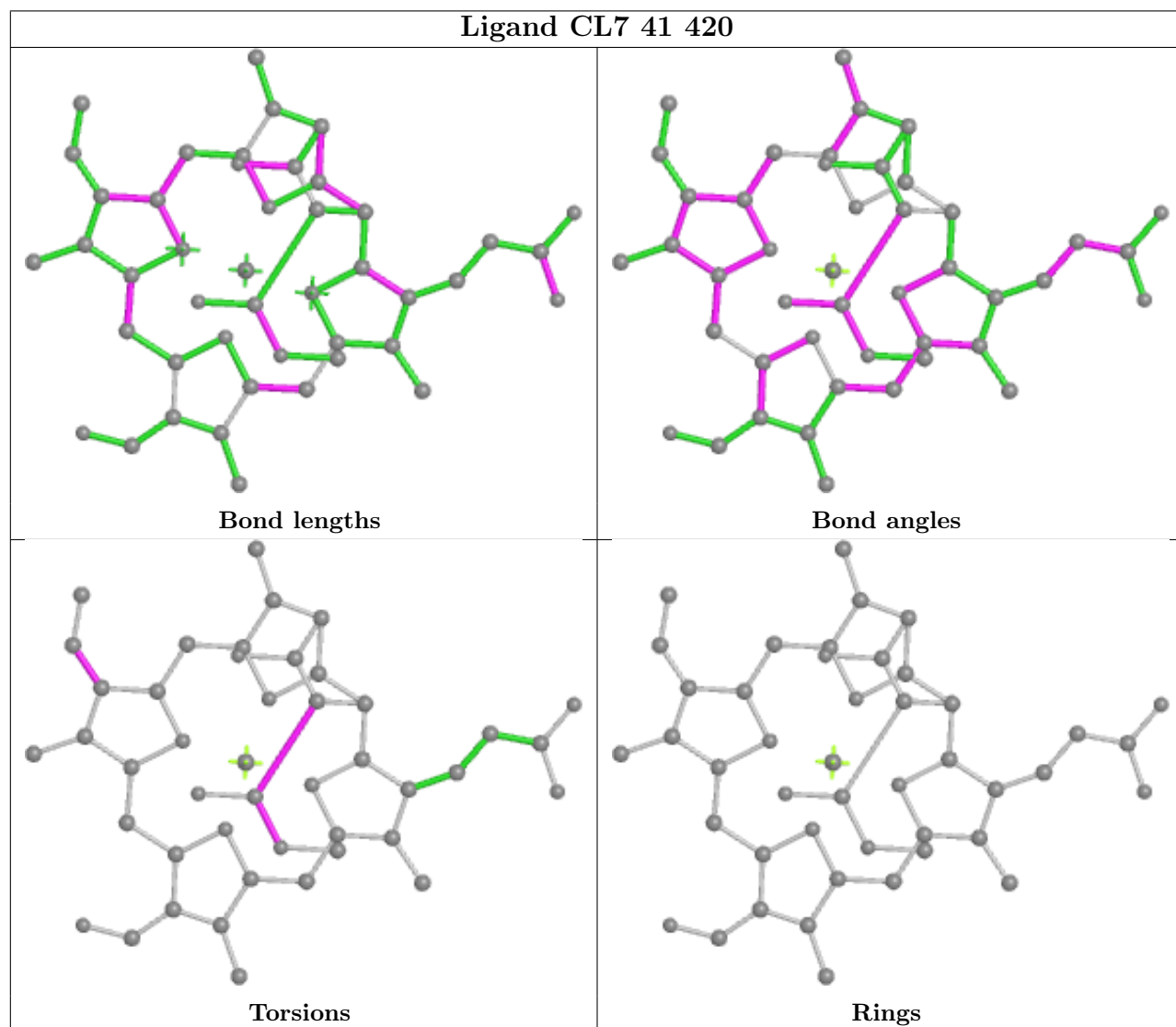
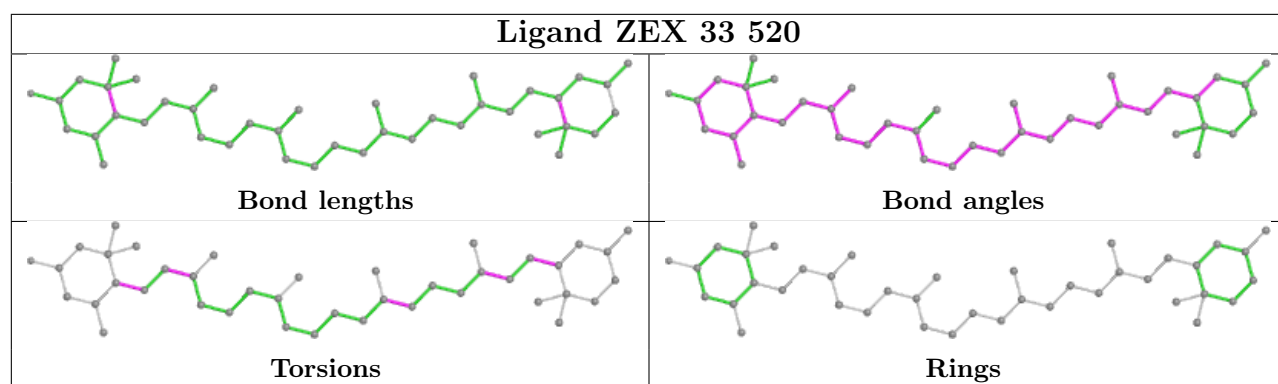


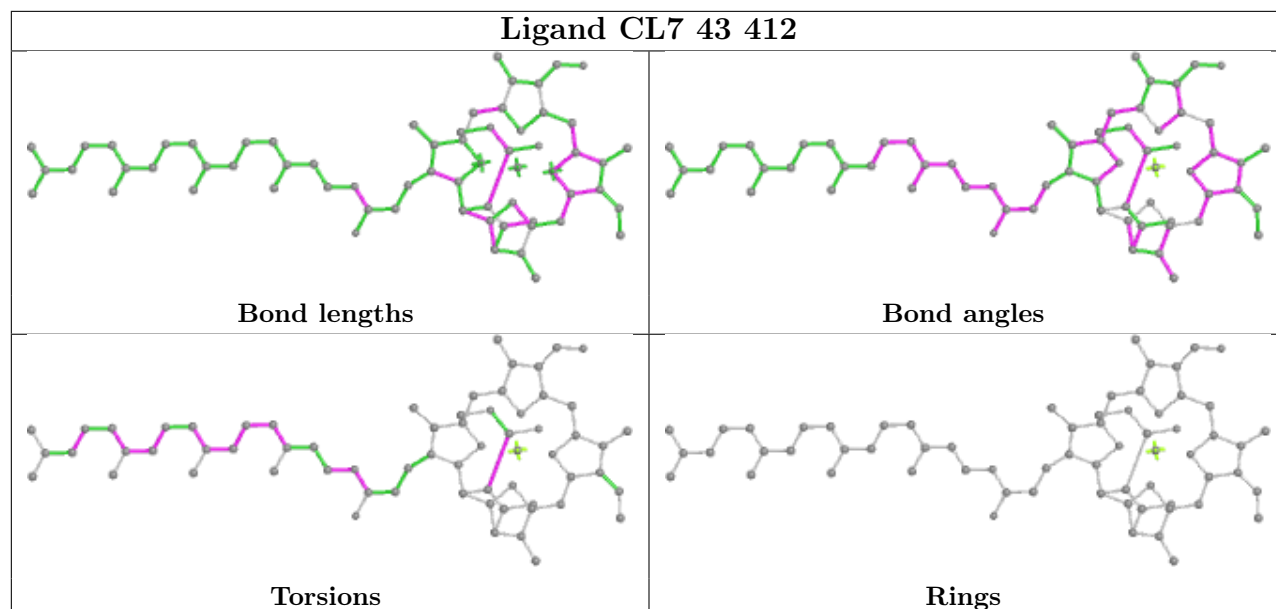
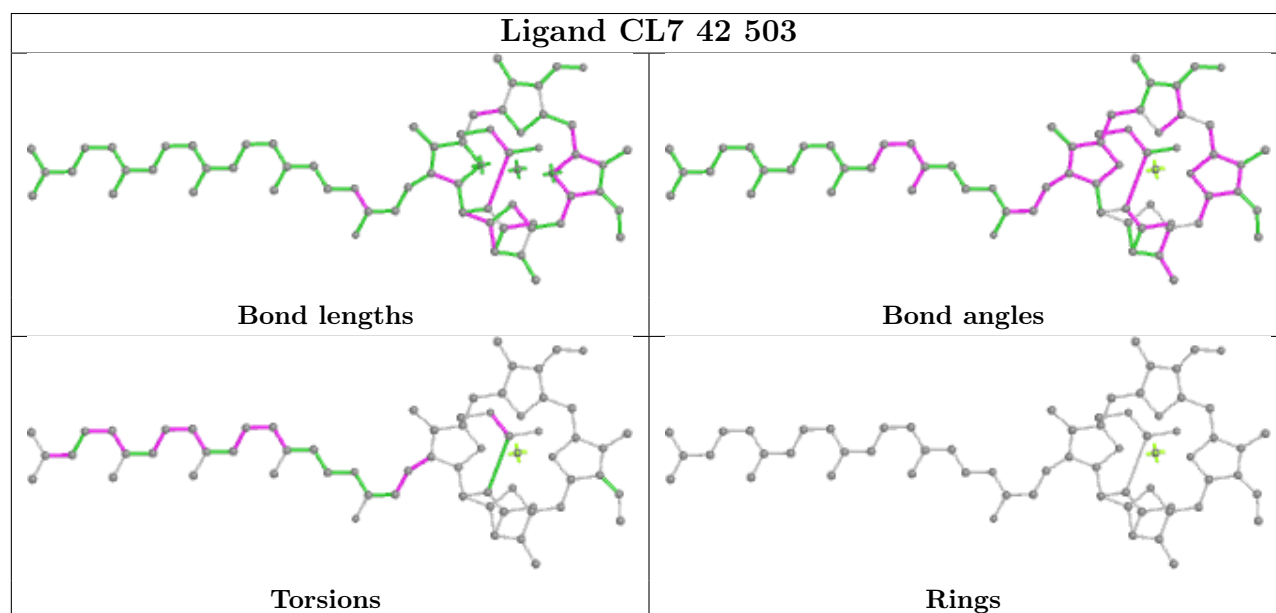
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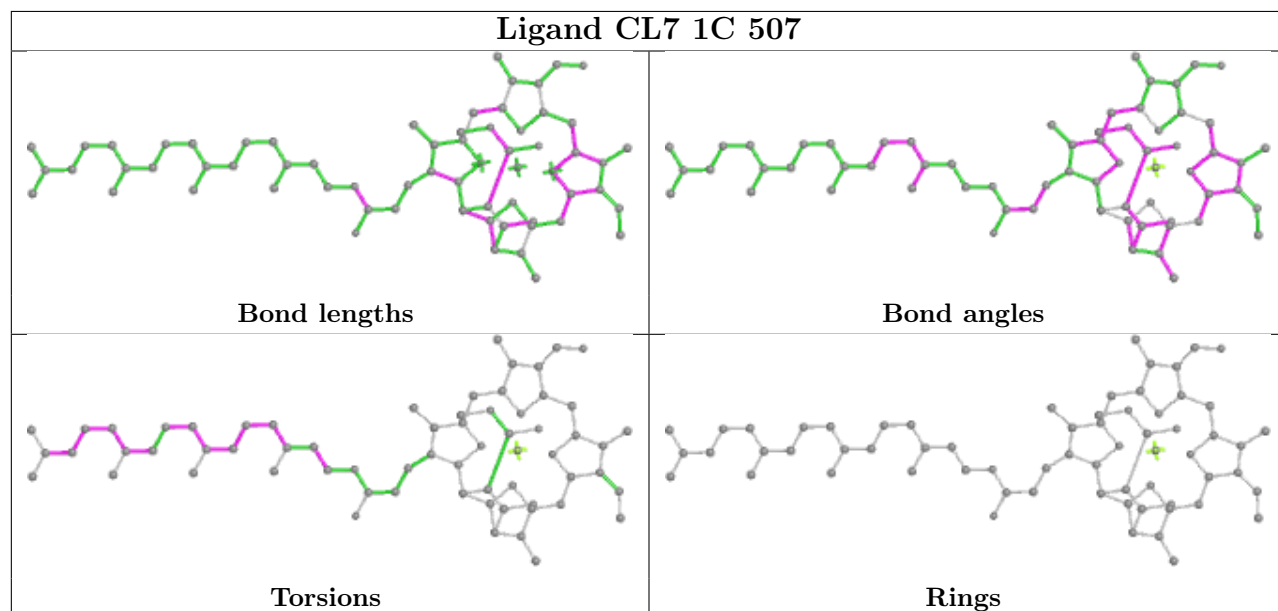
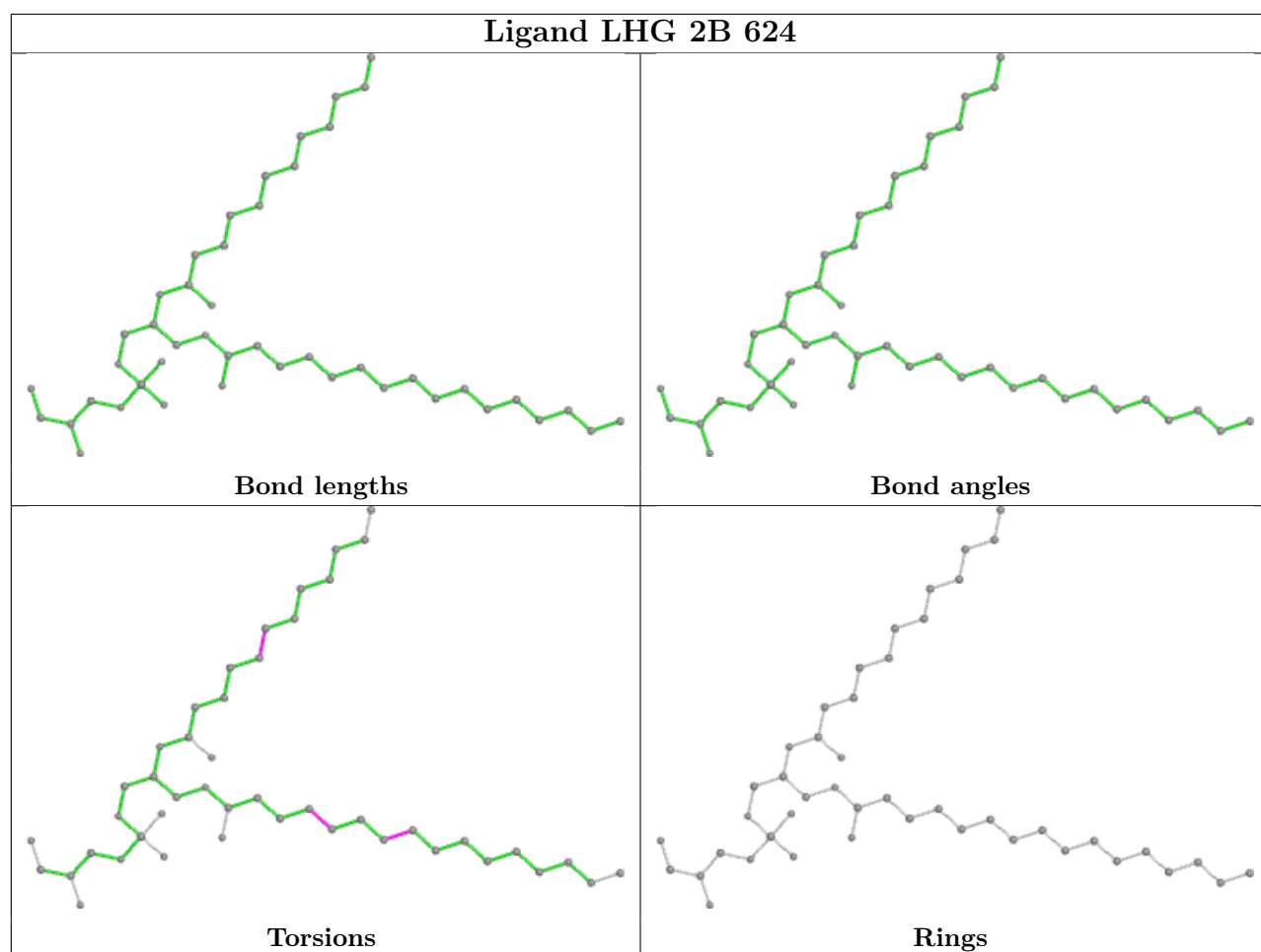




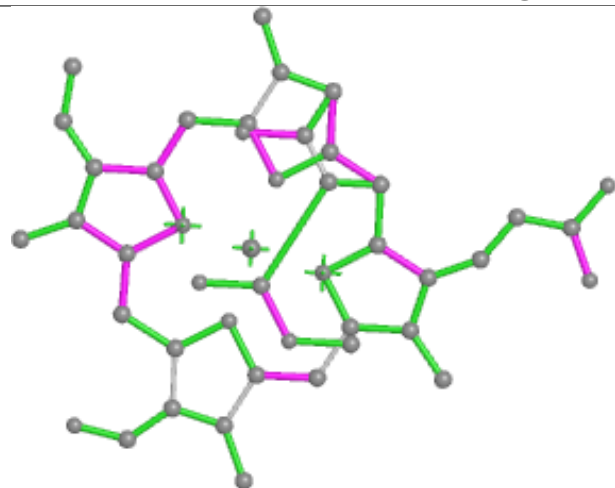




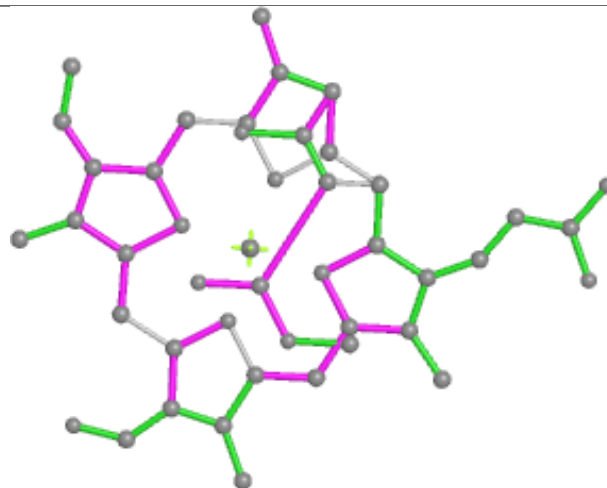
Ligand CL7 43 412**Ligand CL7 42 503**



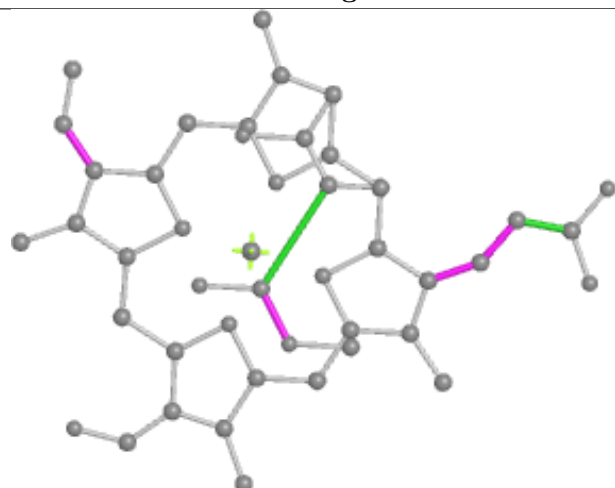
Ligand CL7 23 415



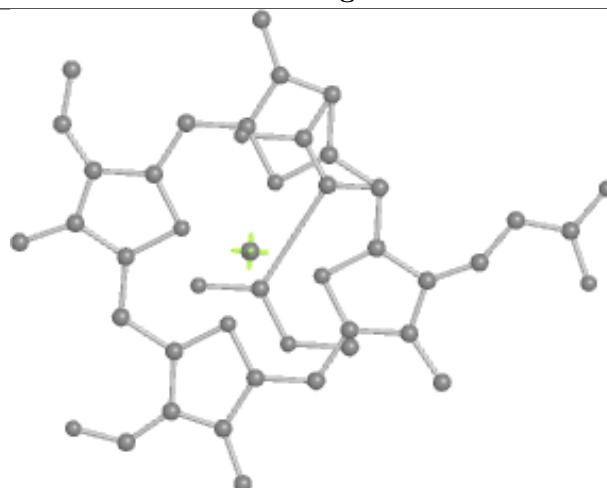
Bond lengths



Bond angles

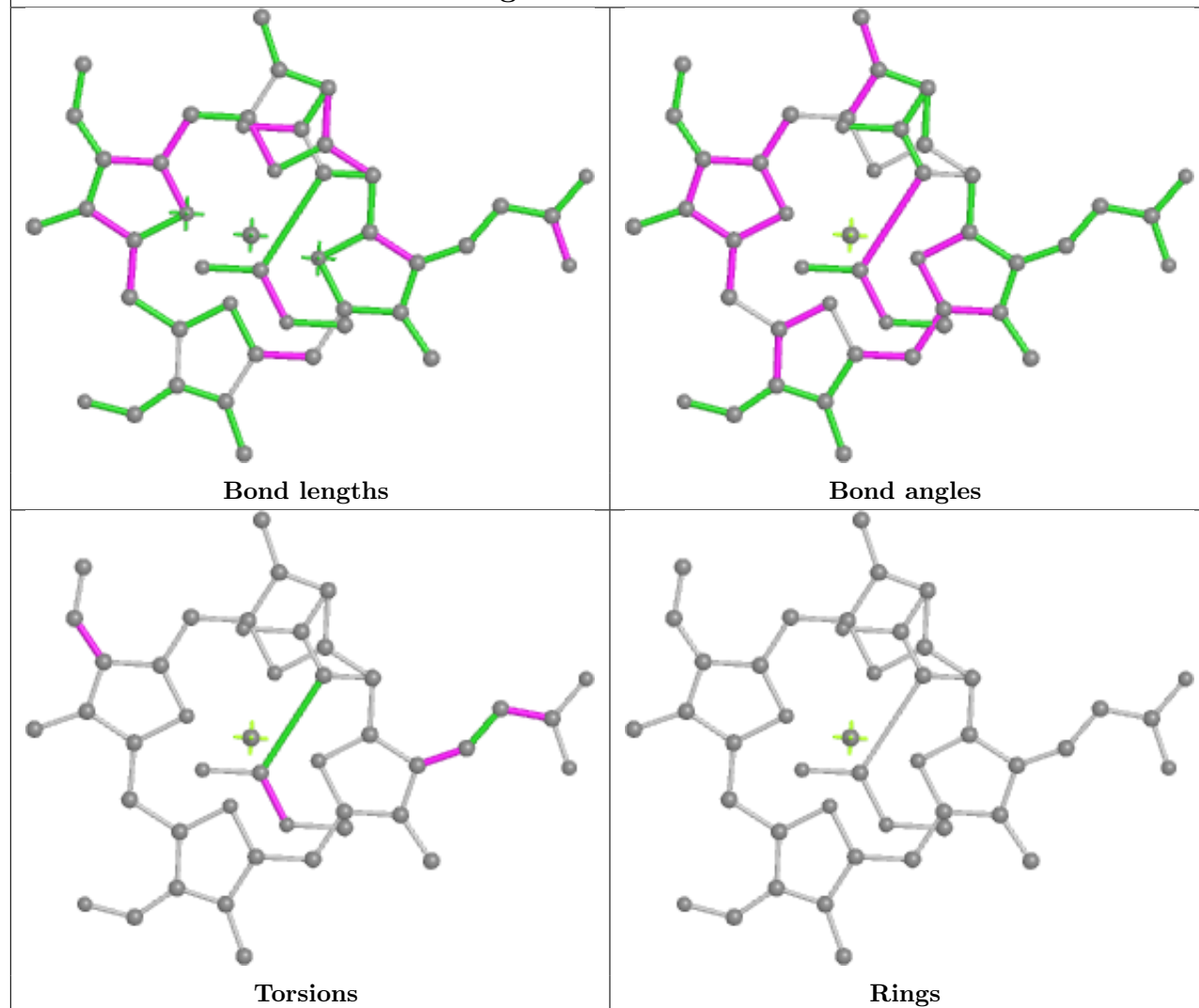


Torsions

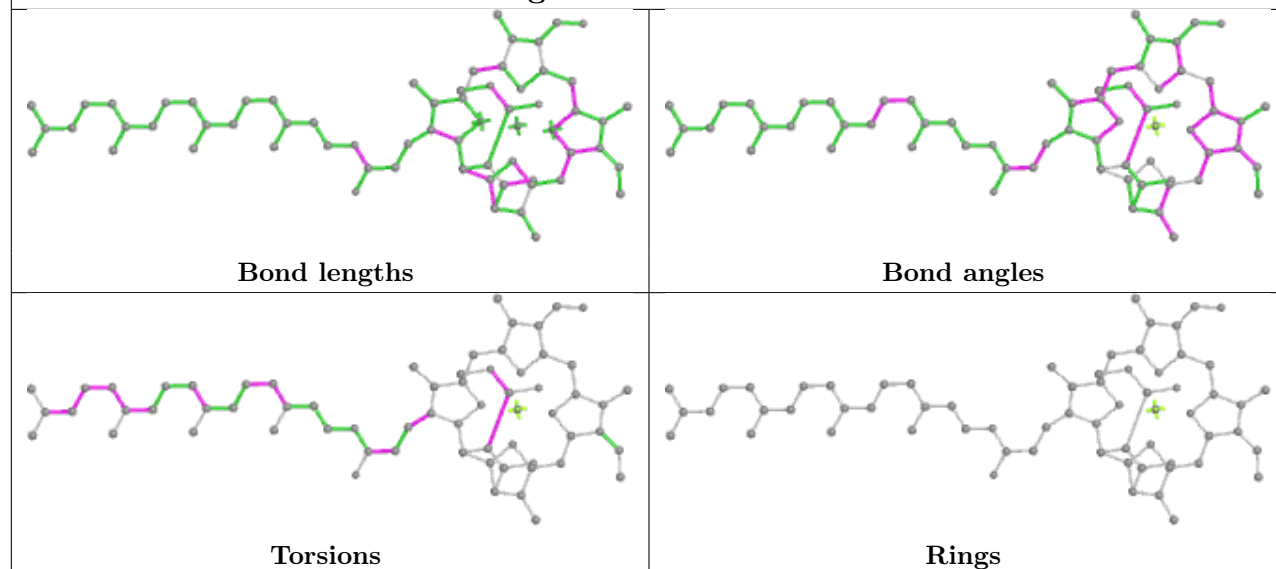


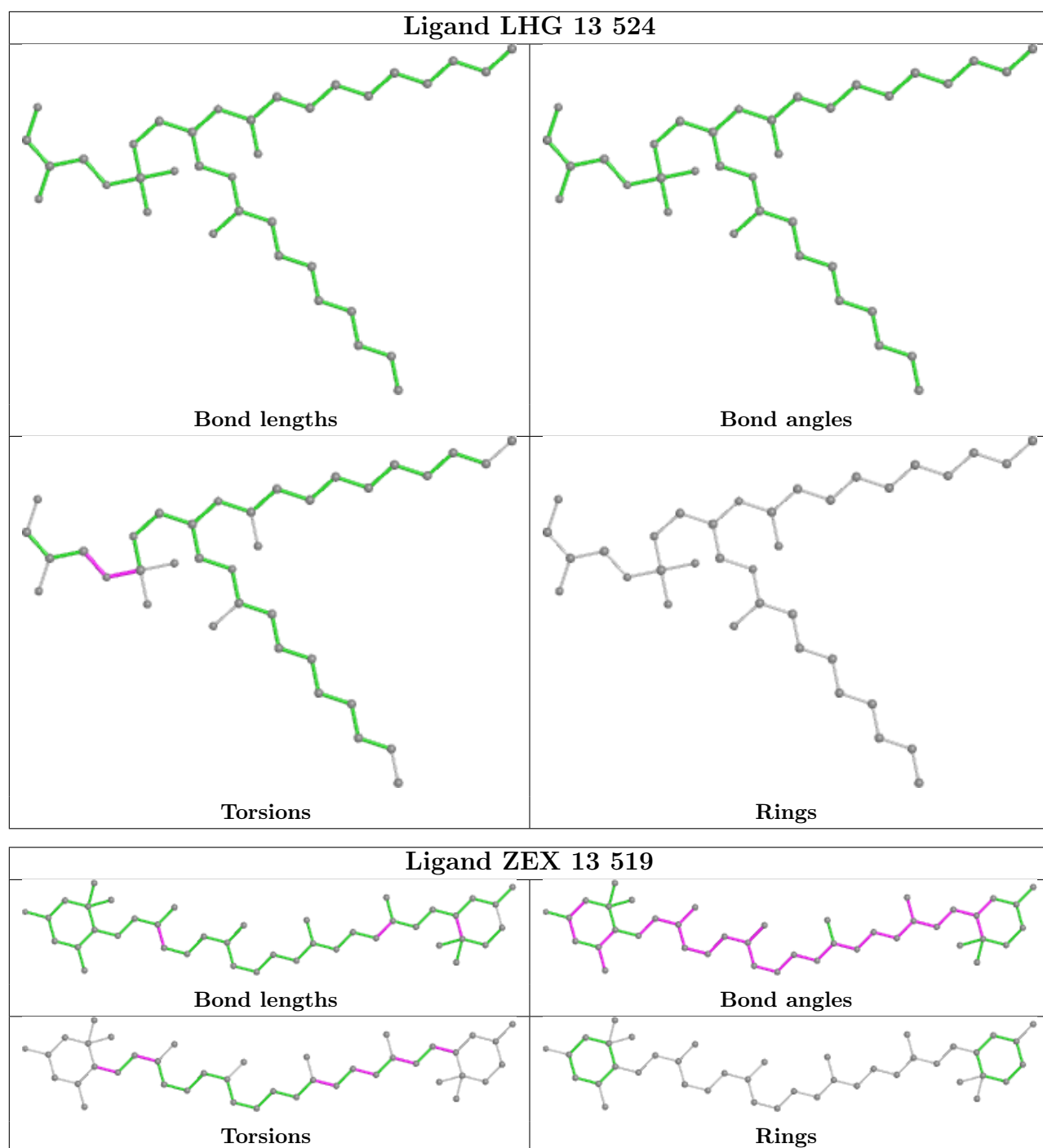
Rings

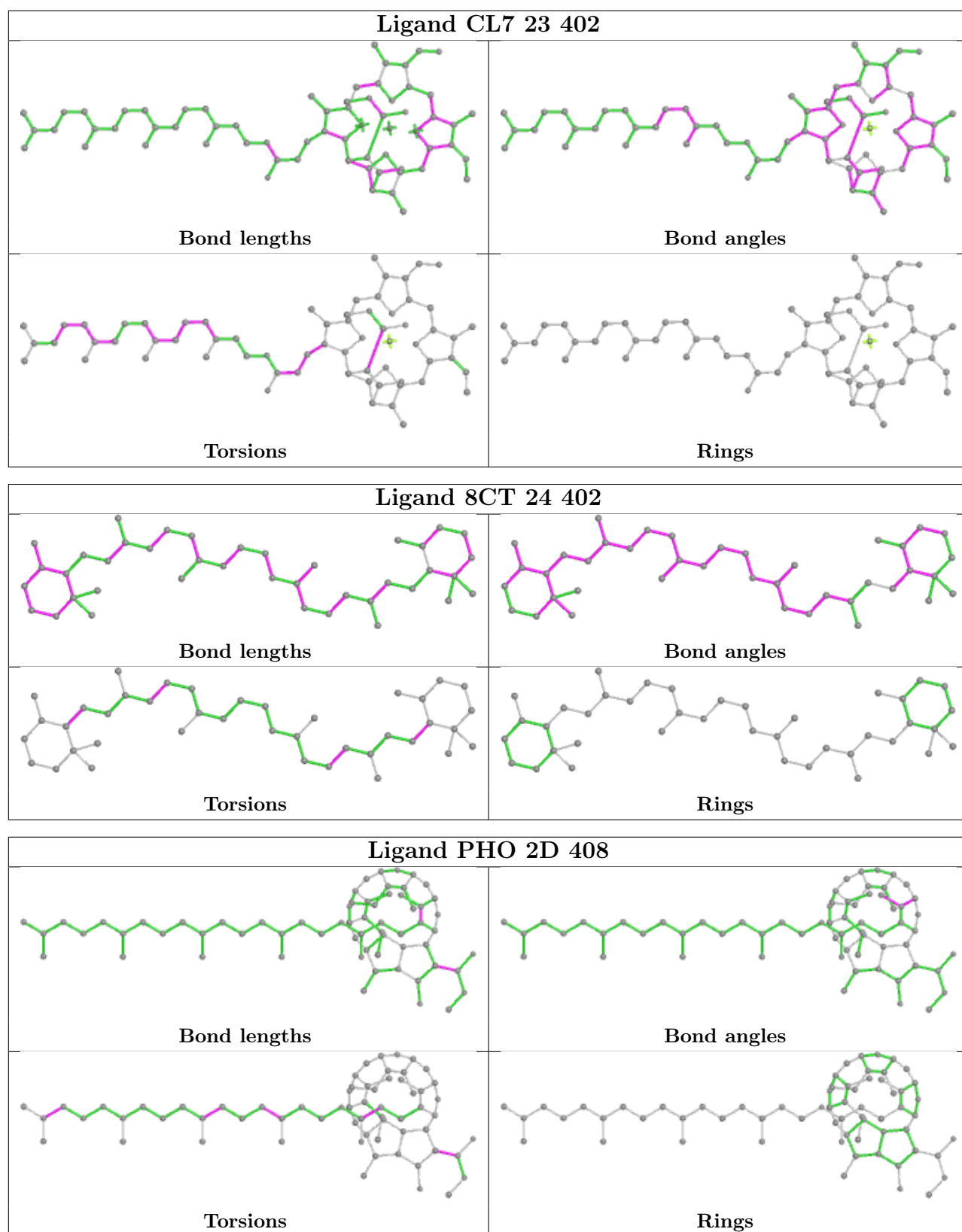
Ligand CL7 22 514

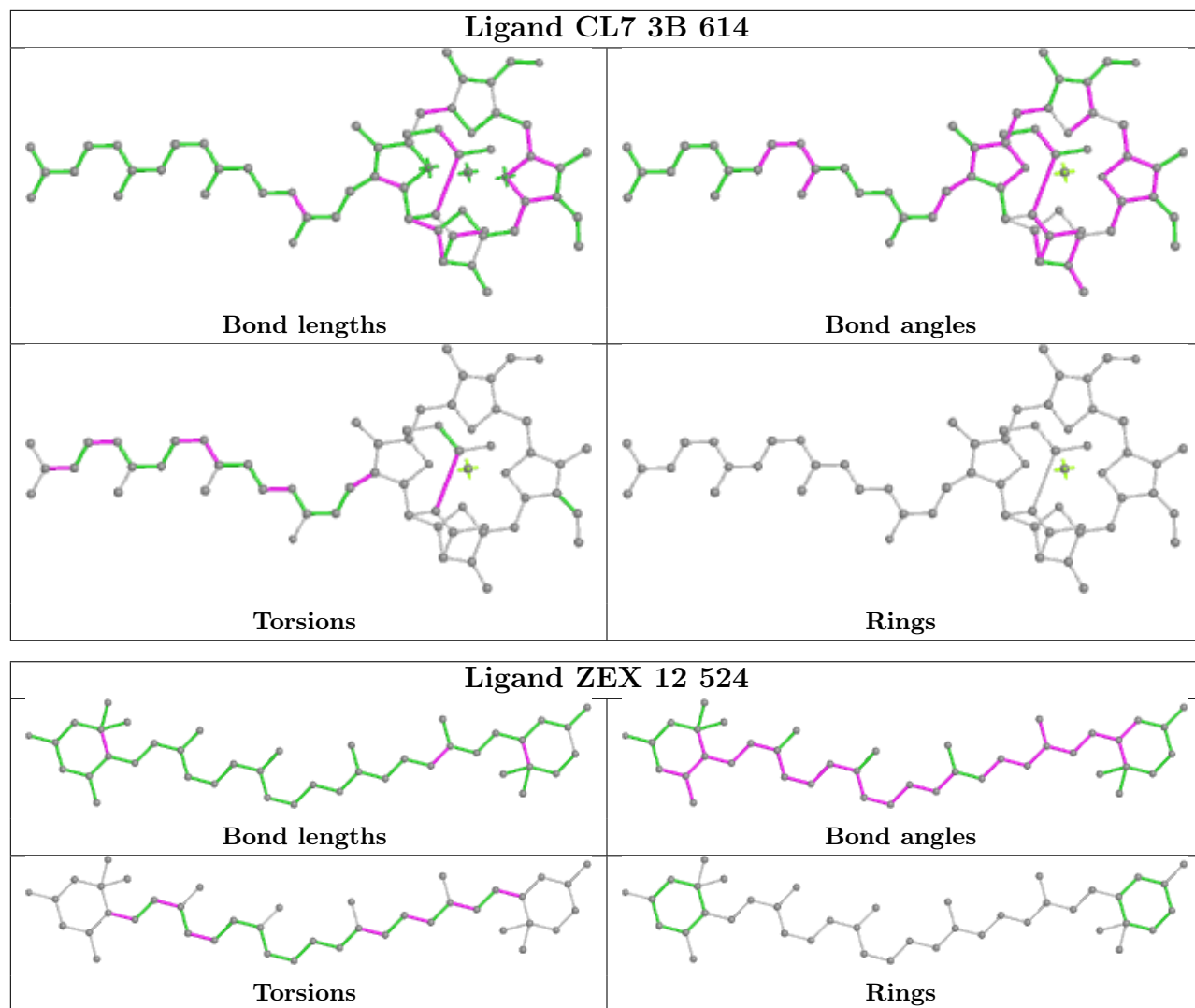


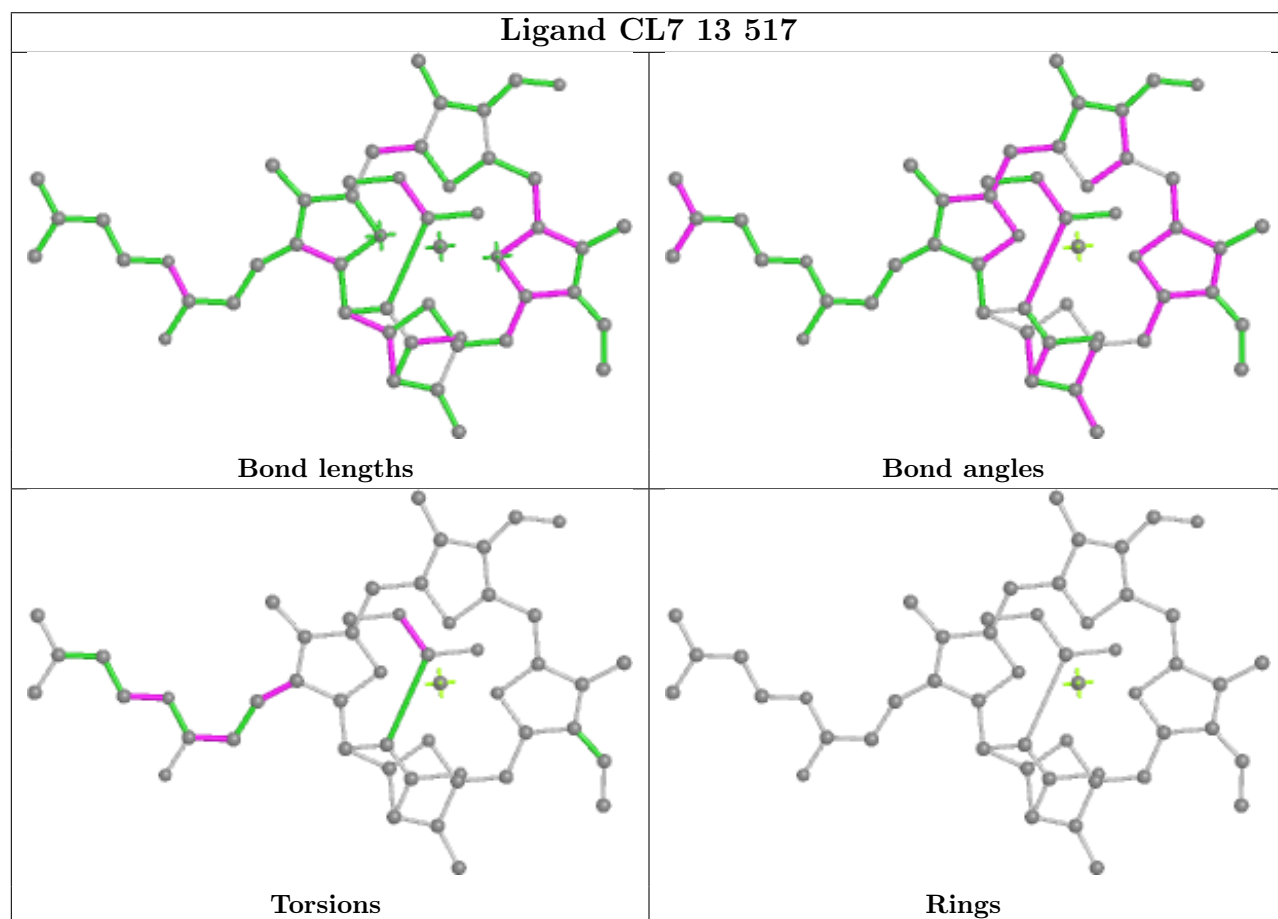
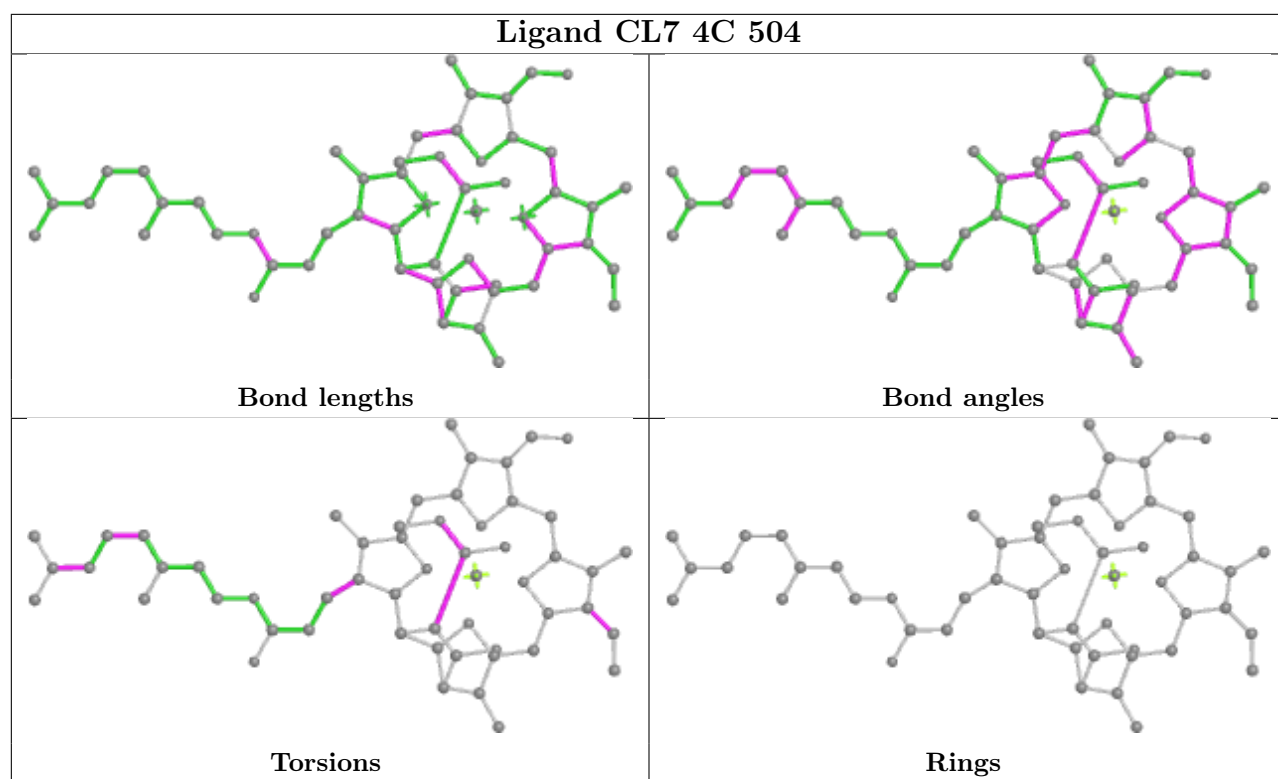
Ligand CL7 4C 501

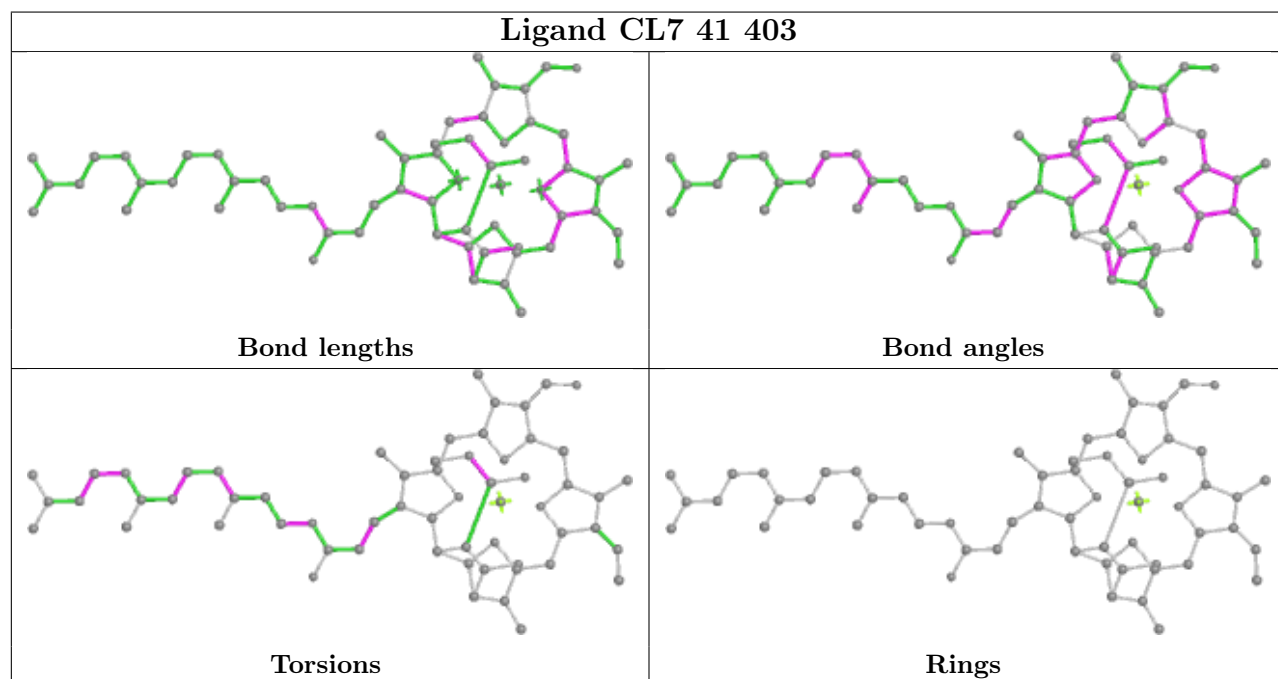
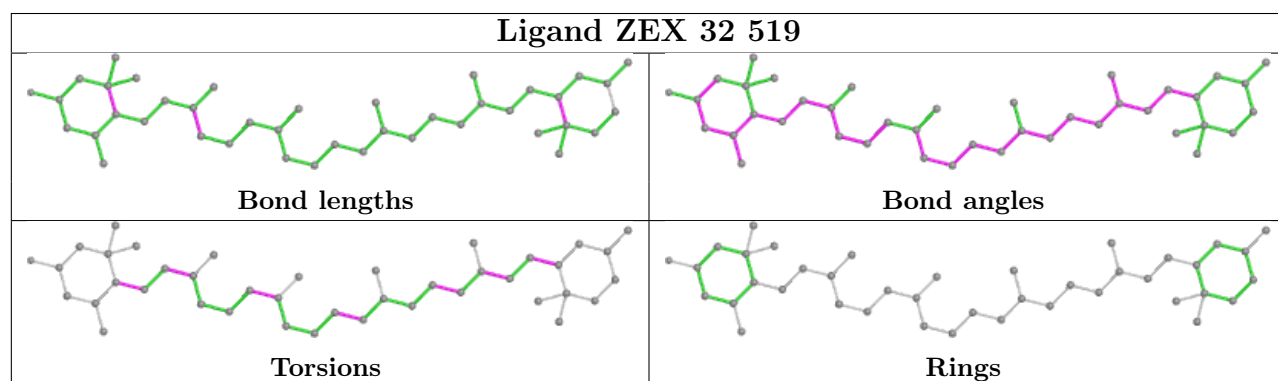
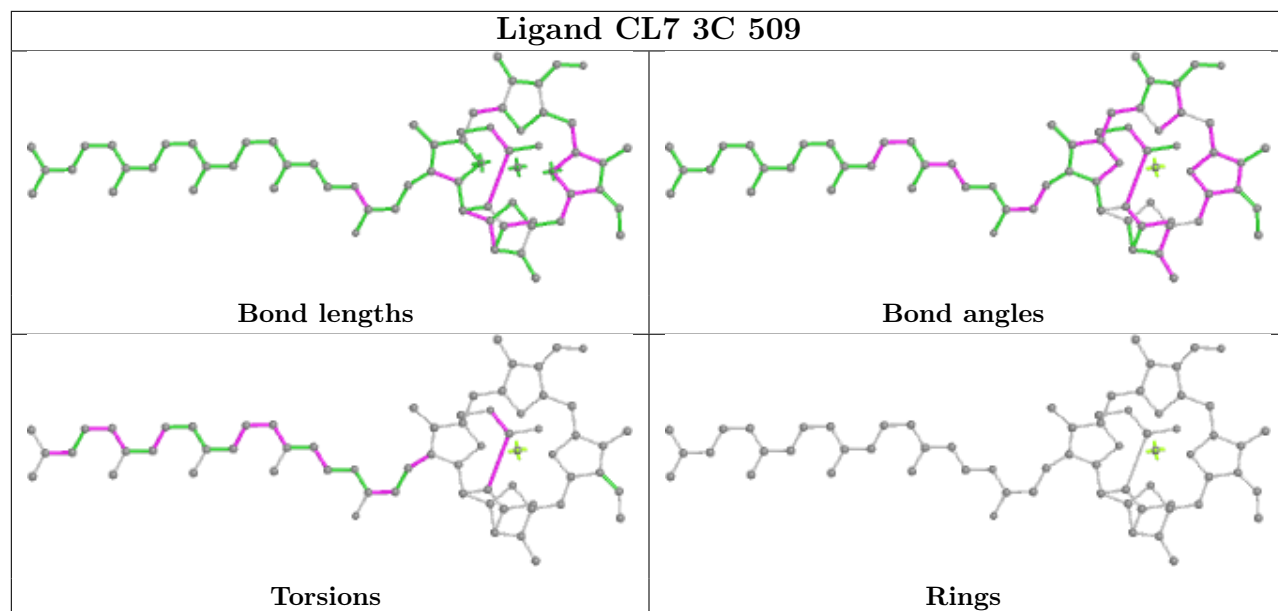


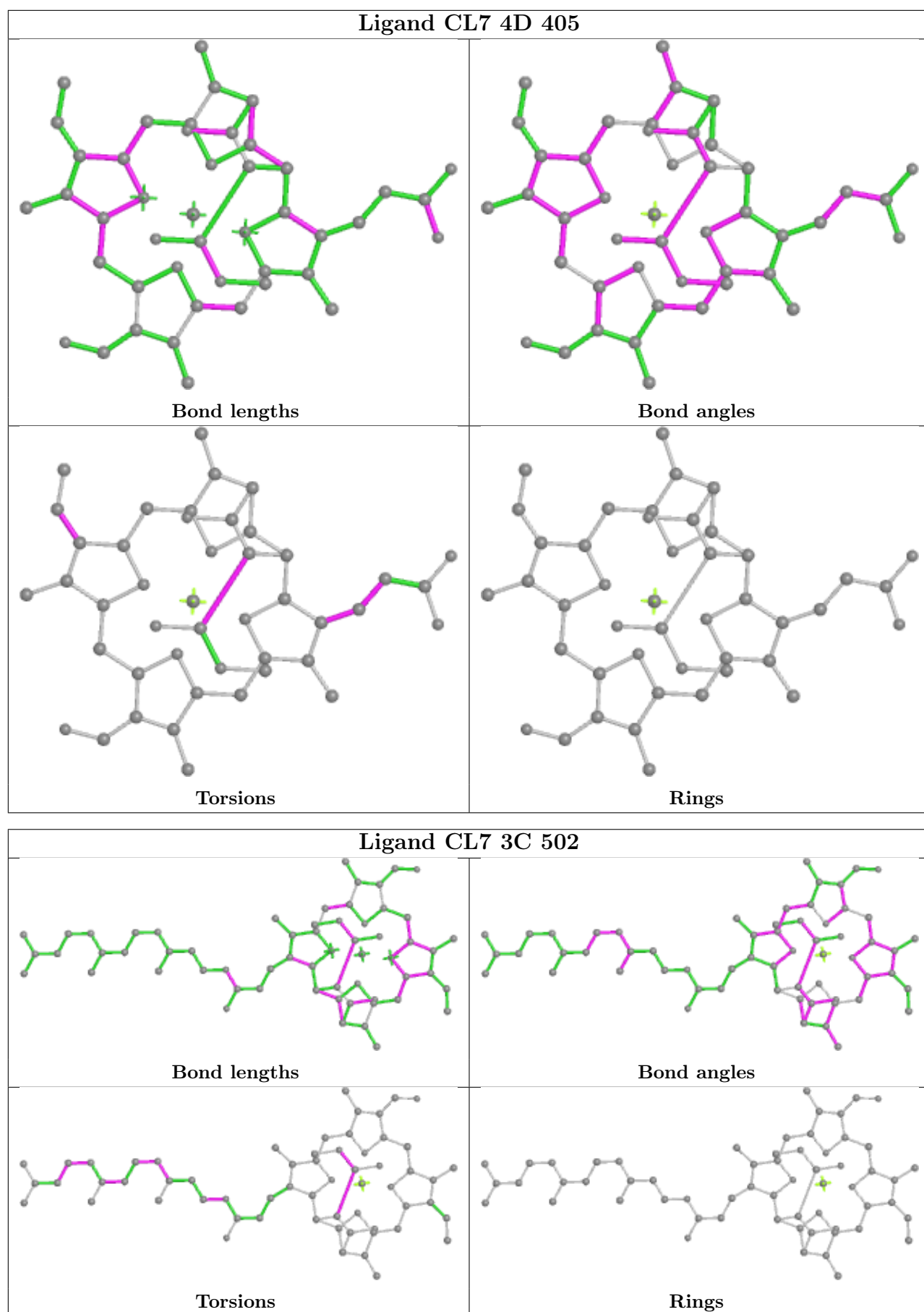




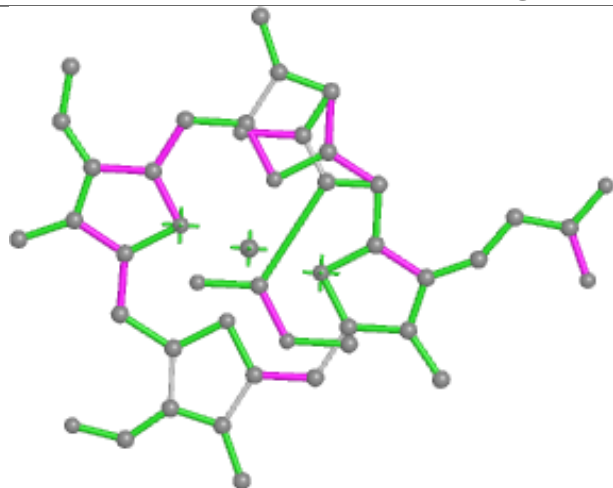




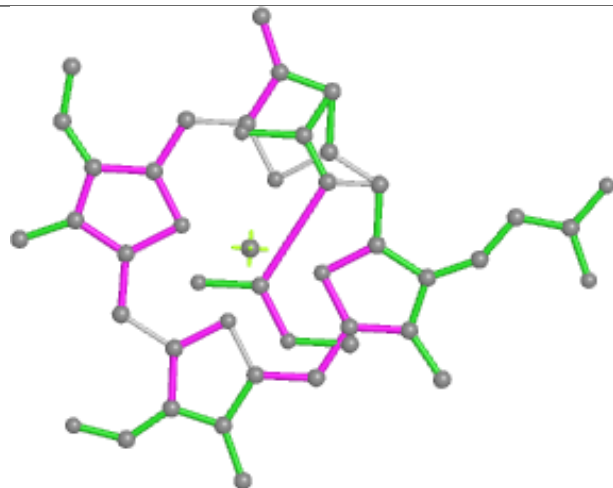




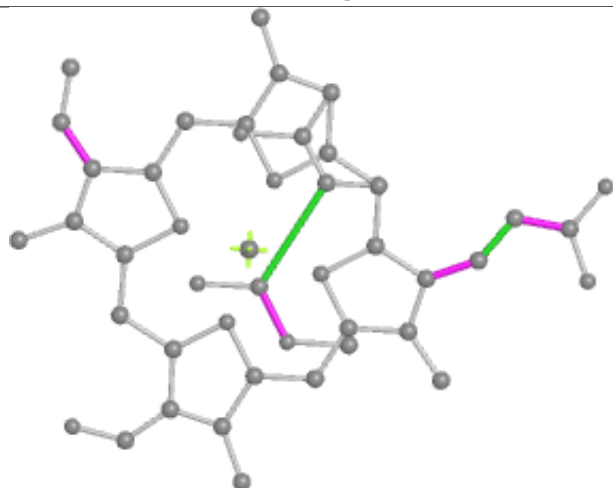
Ligand CL7 32 514



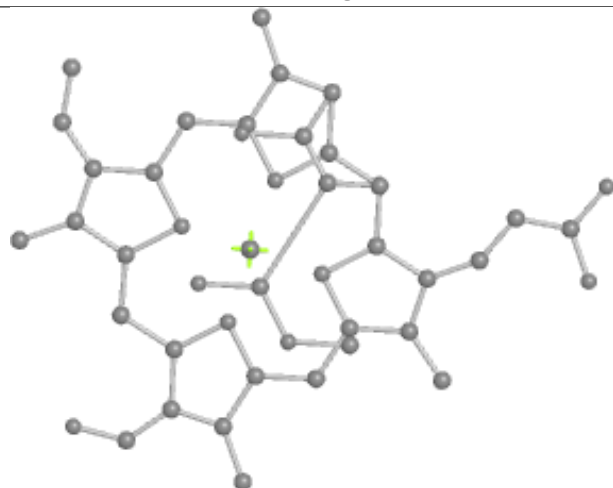
Bond lengths



Bond angles

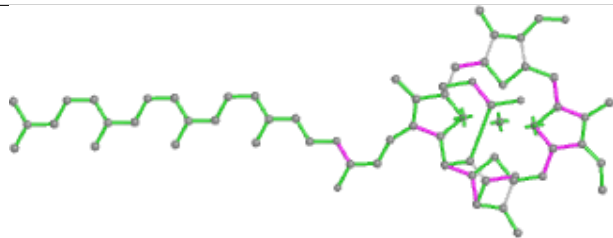


Torsions

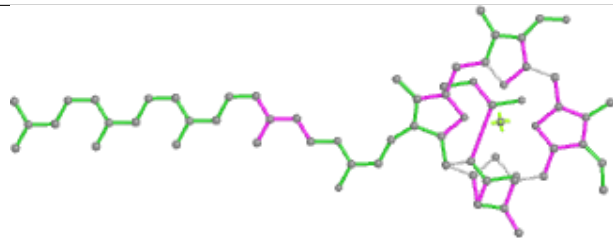


Rings

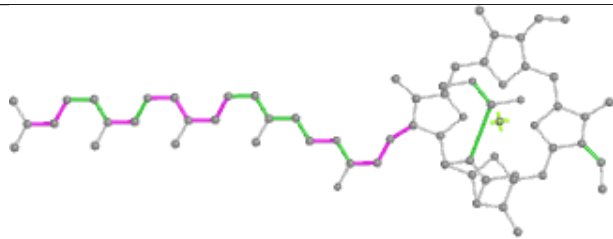
Ligand CL7 42 501



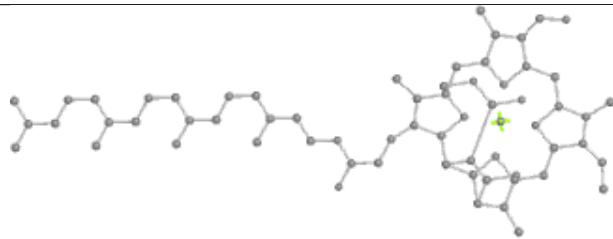
Bond lengths



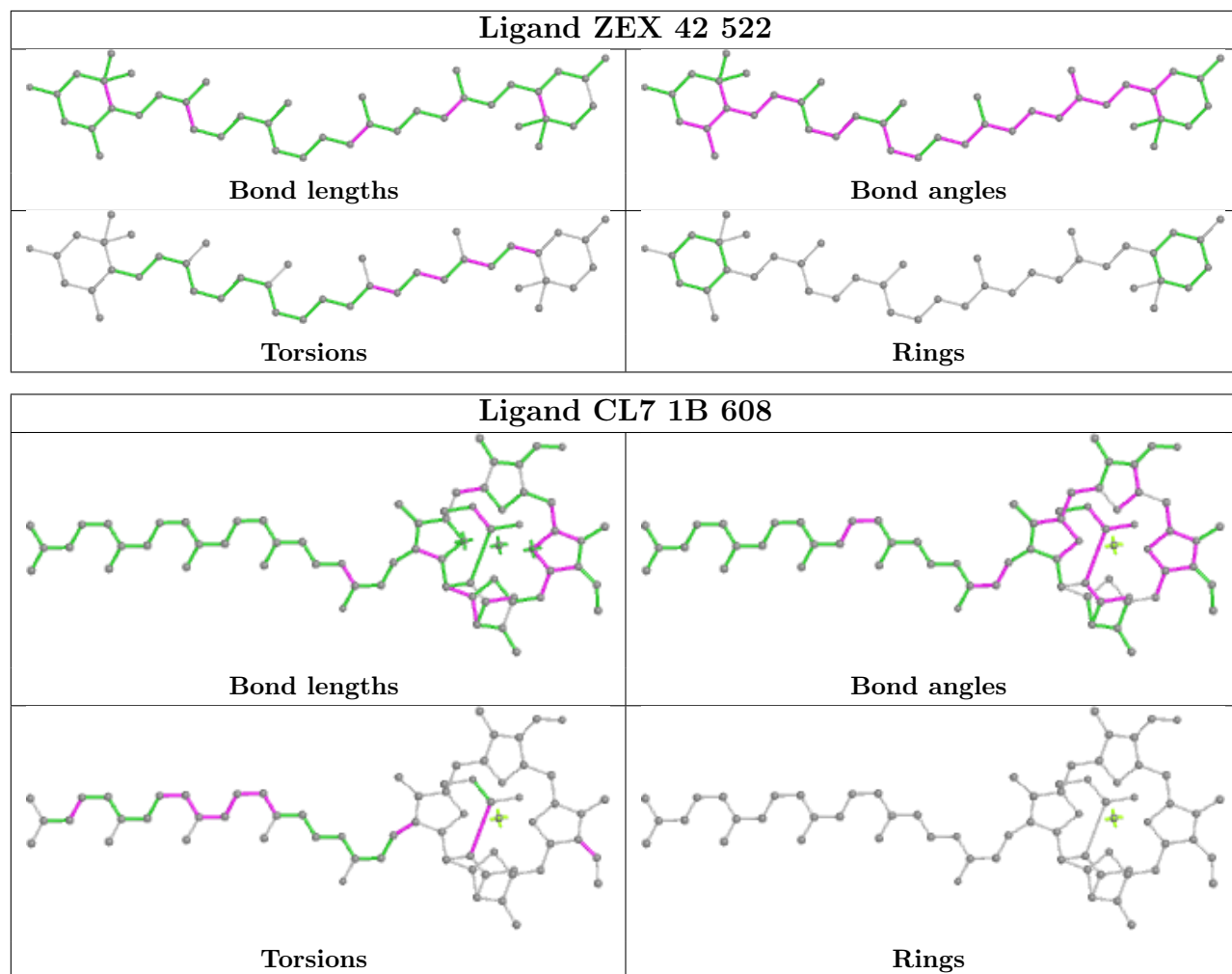
Bond angles



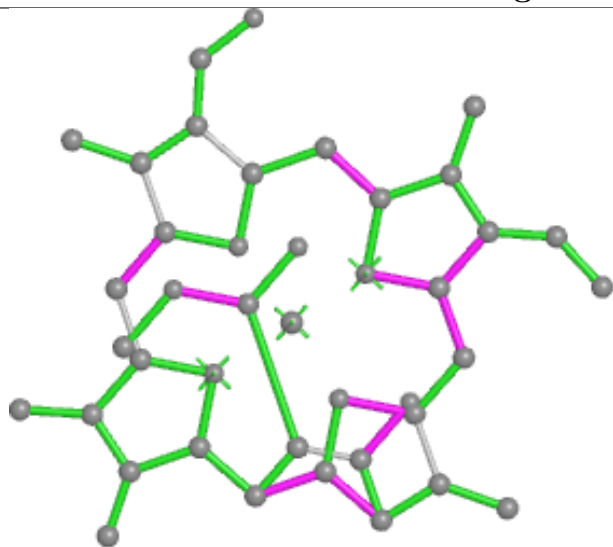
Torsions



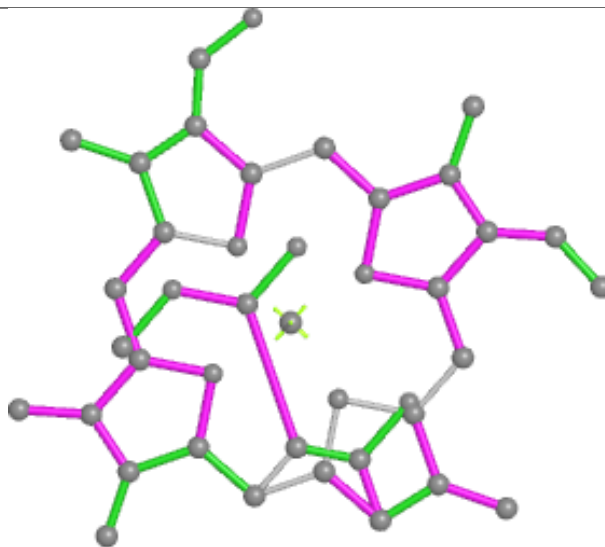
Rings



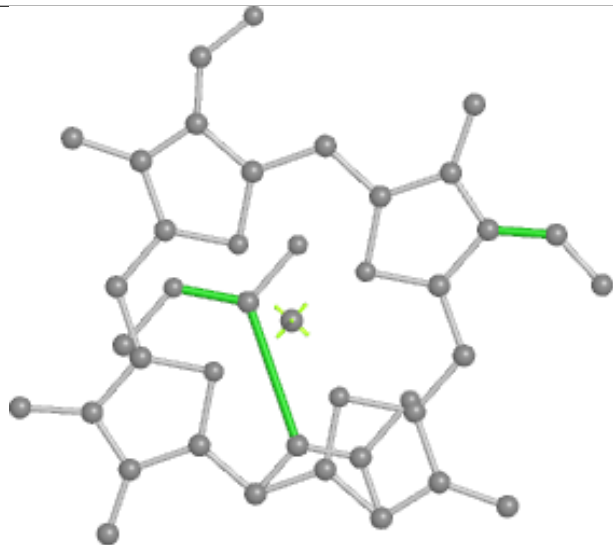
Ligand CL7 33 515



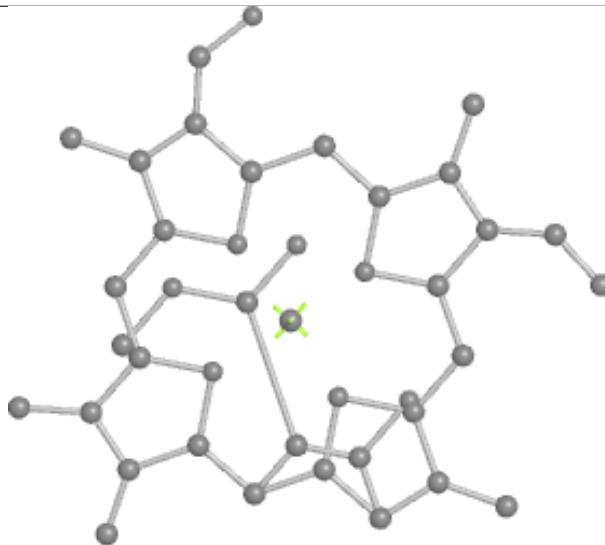
Bond lengths



Bond angles

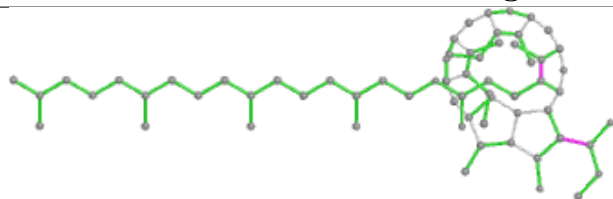


Torsions

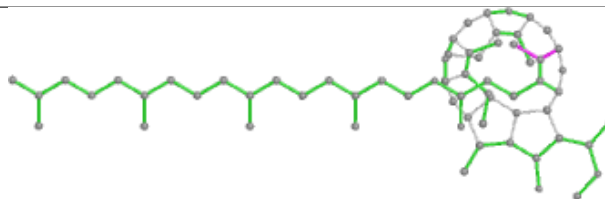


Rings

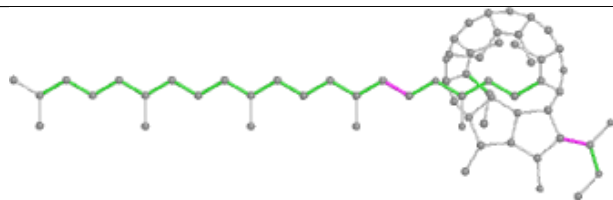
Ligand PHO 1A 402



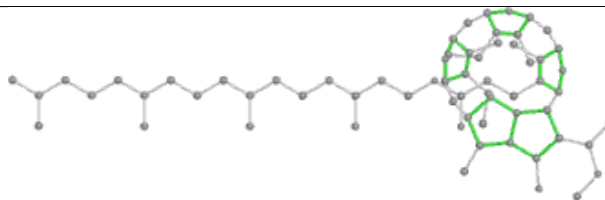
Bond lengths



Bond angles

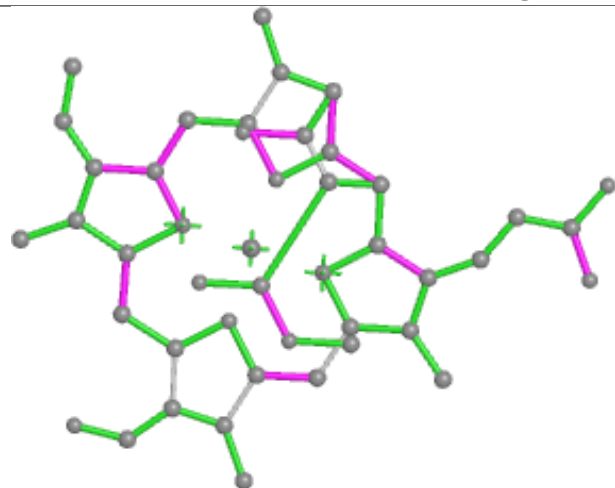


Torsions

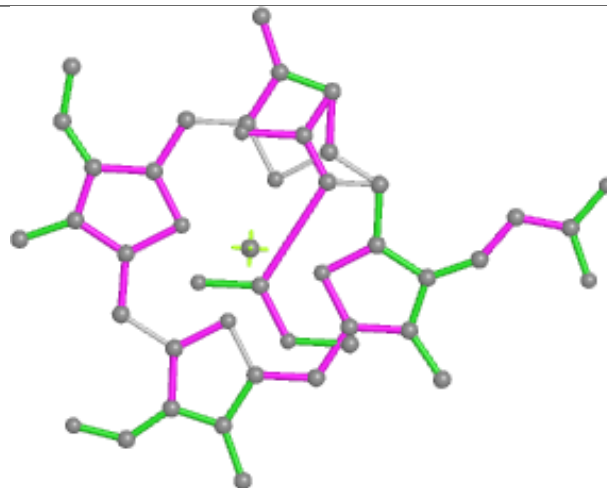


Rings

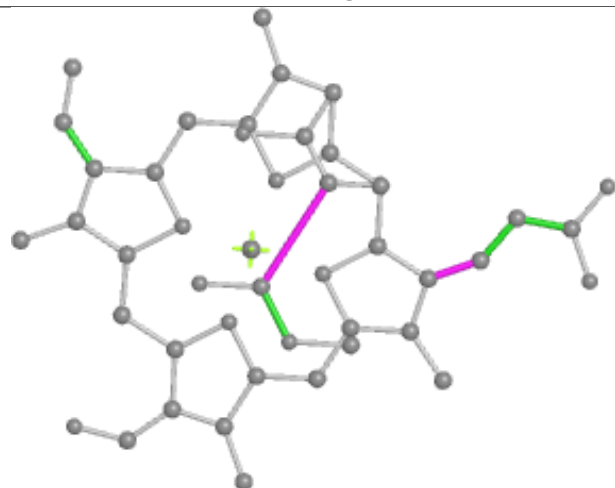
Ligand CL7 32 515



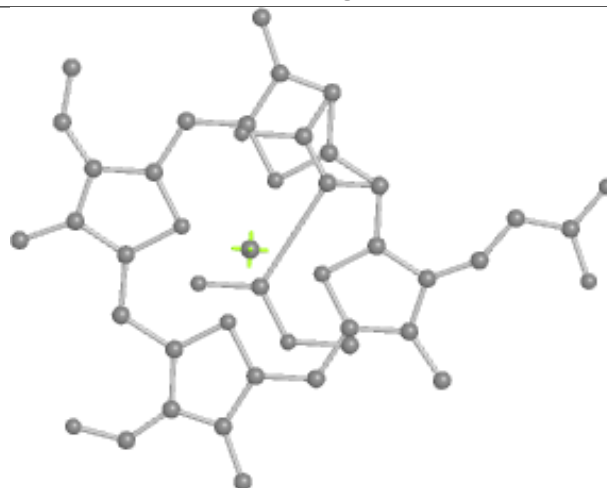
Bond lengths



Bond angles

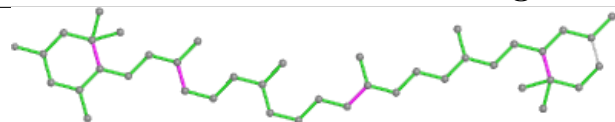


Torsions

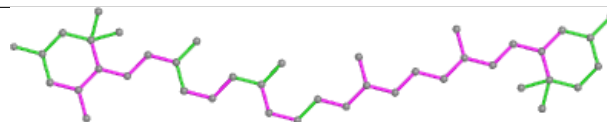


Rings

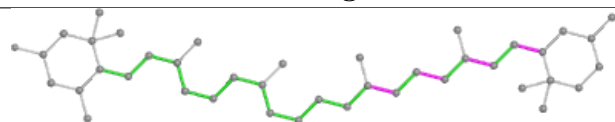
Ligand ZEX 32 522



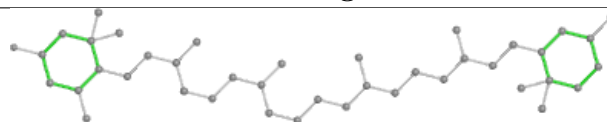
Bond lengths



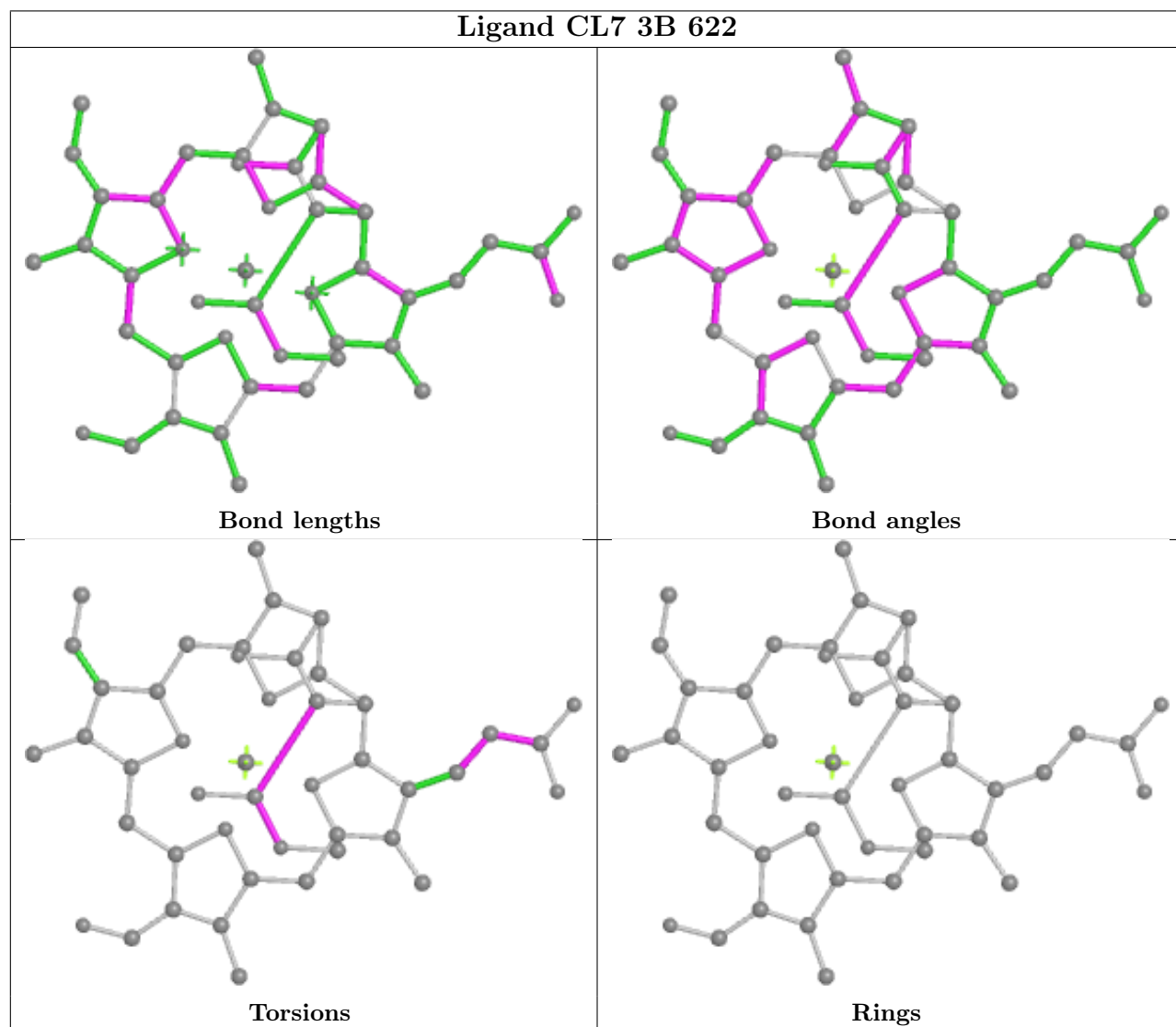
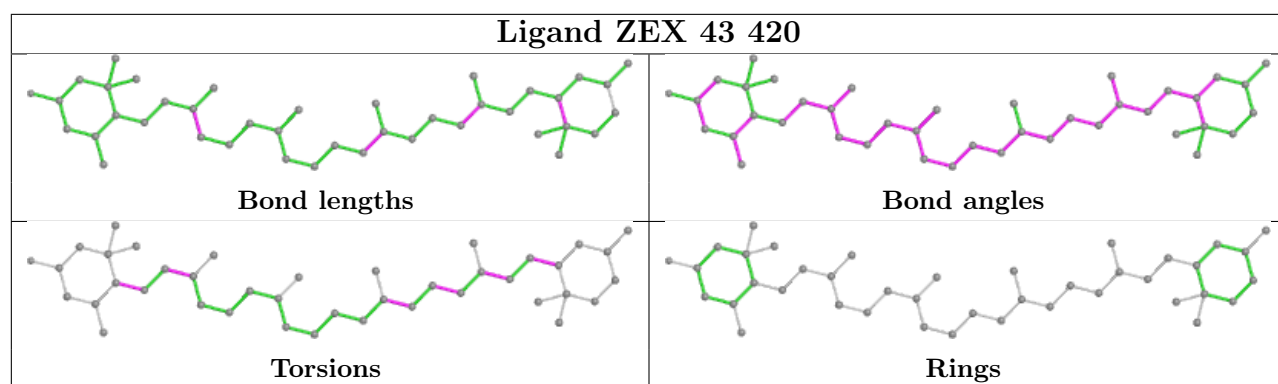
Bond angles

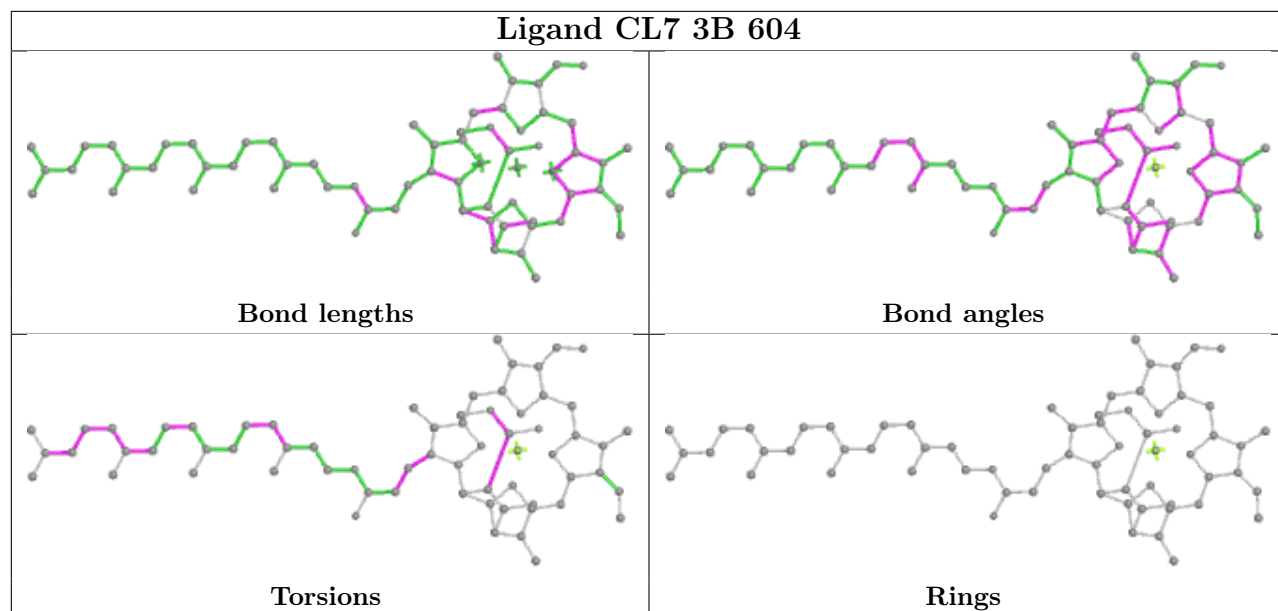


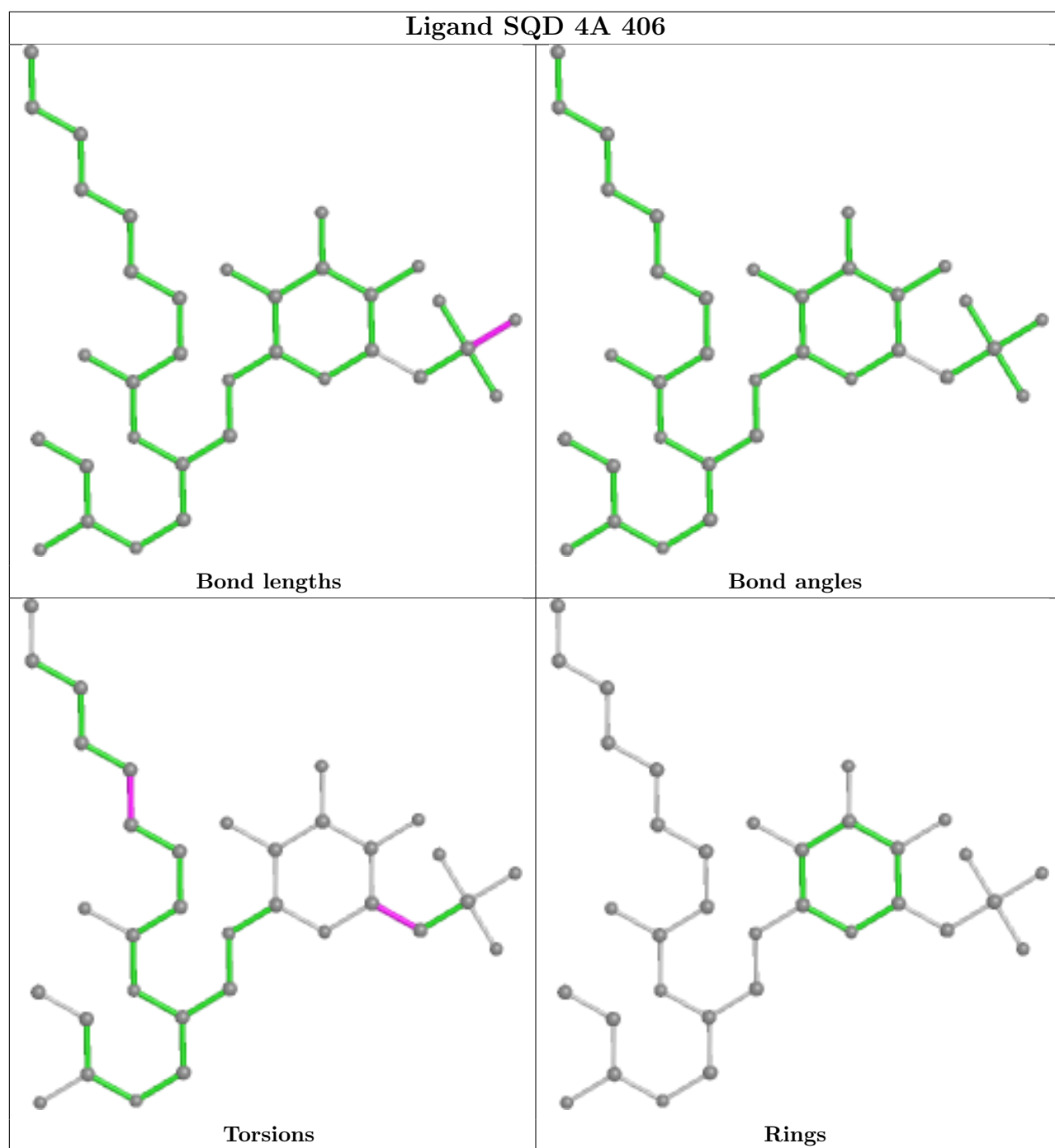
Torsions

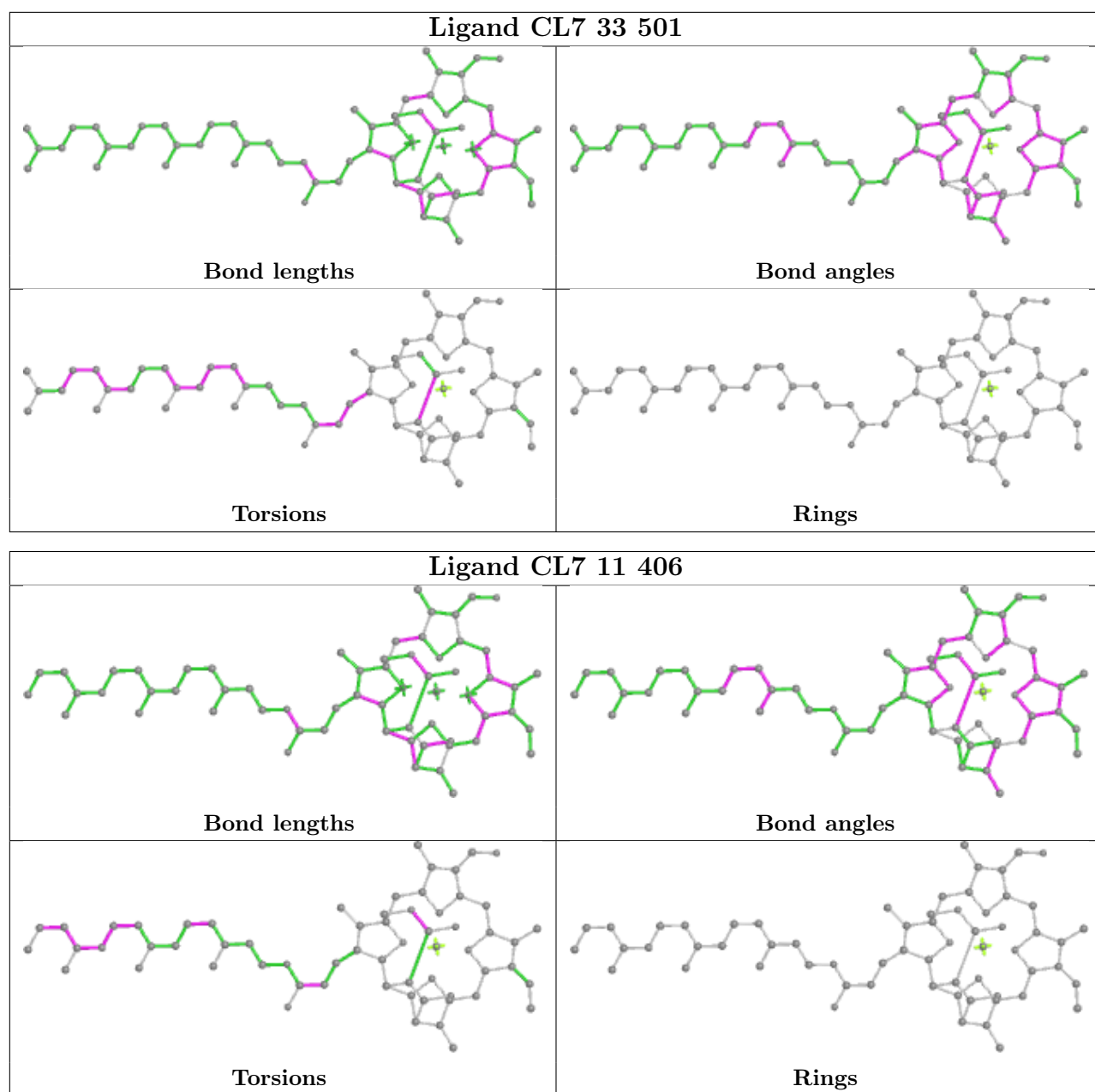


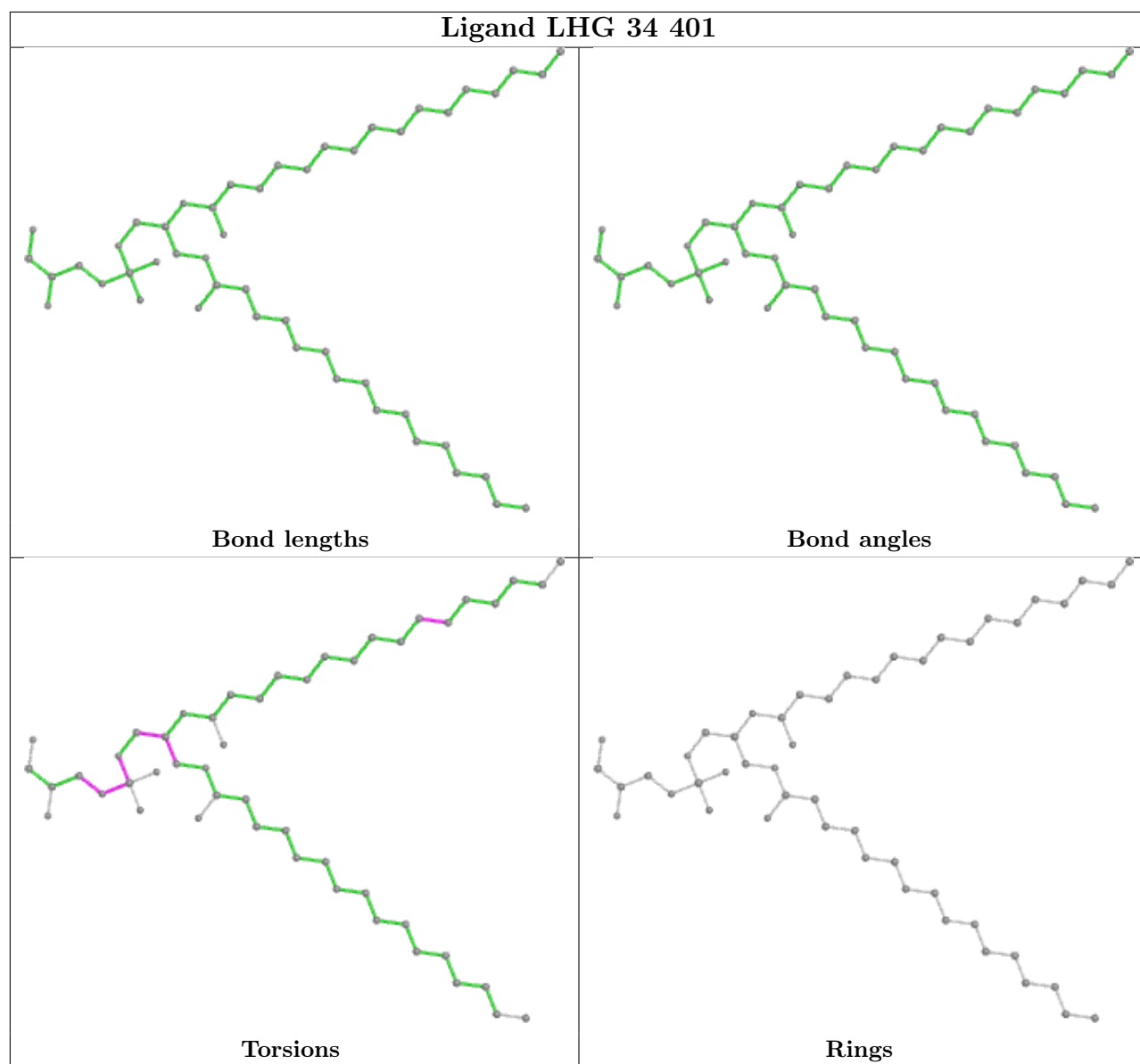
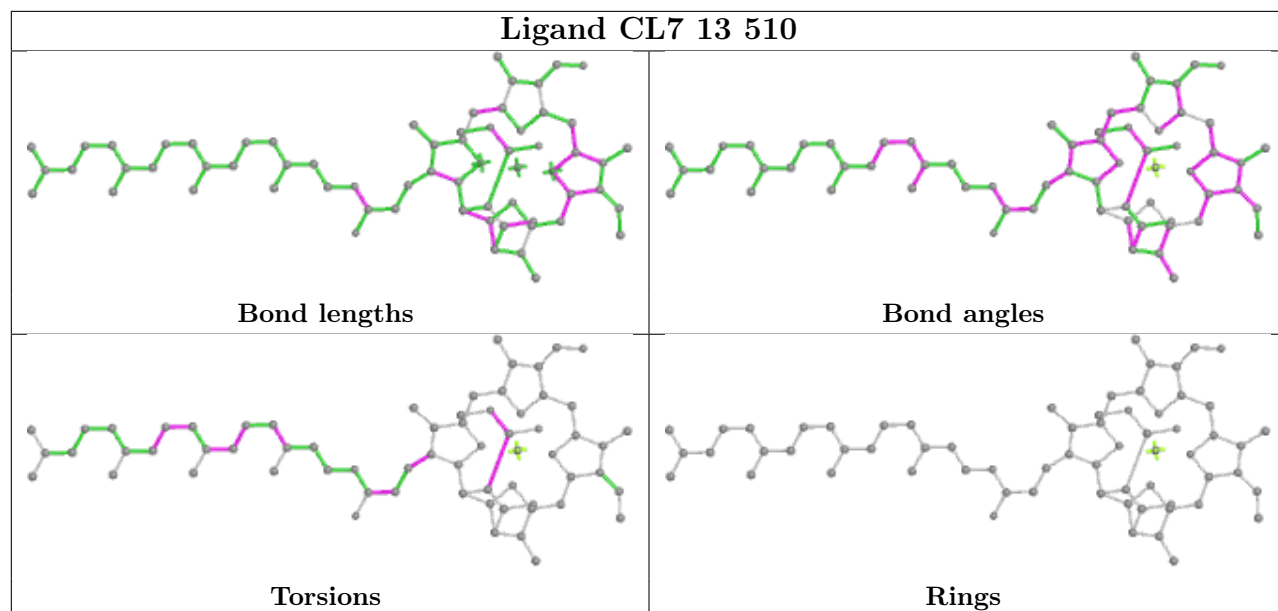
Rings



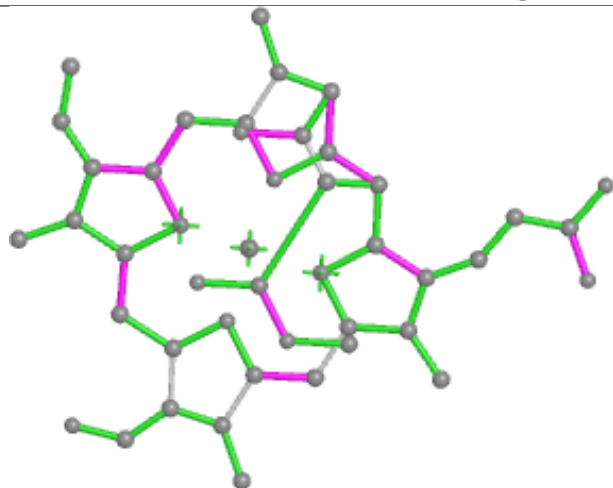




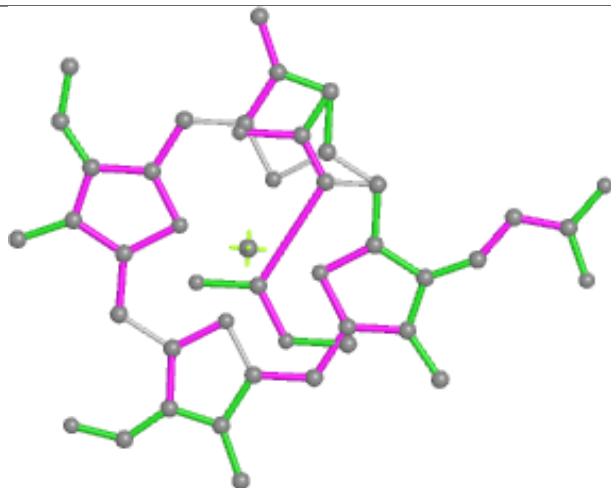




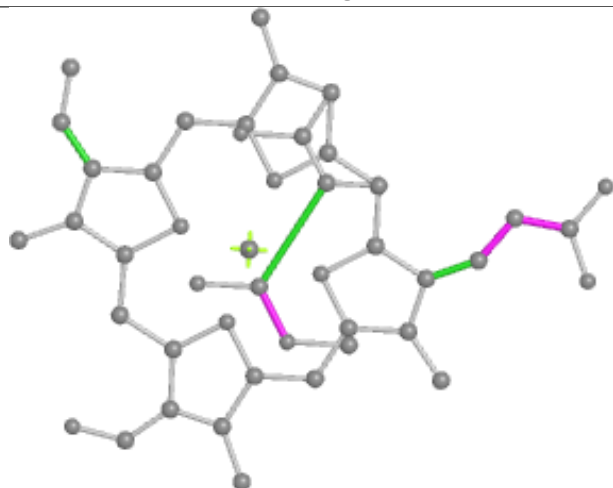
Ligand CL7 13 518



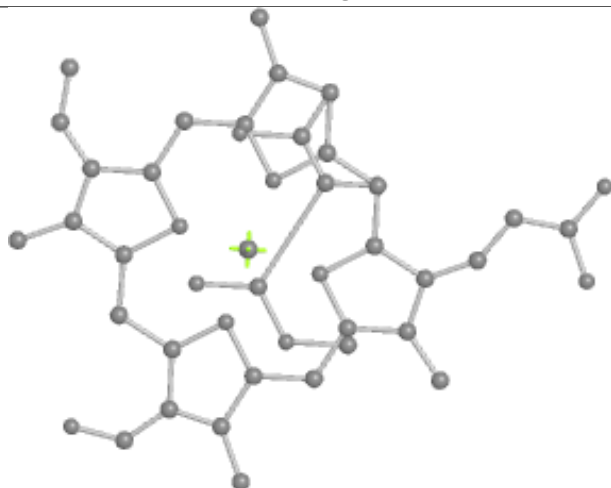
Bond lengths



Bond angles

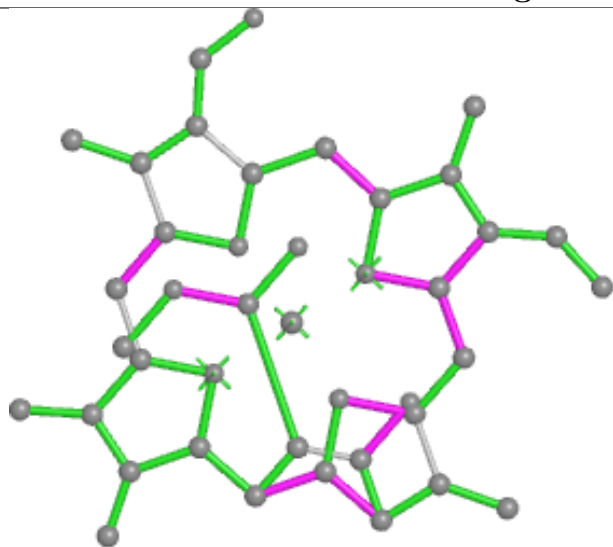


Torsions

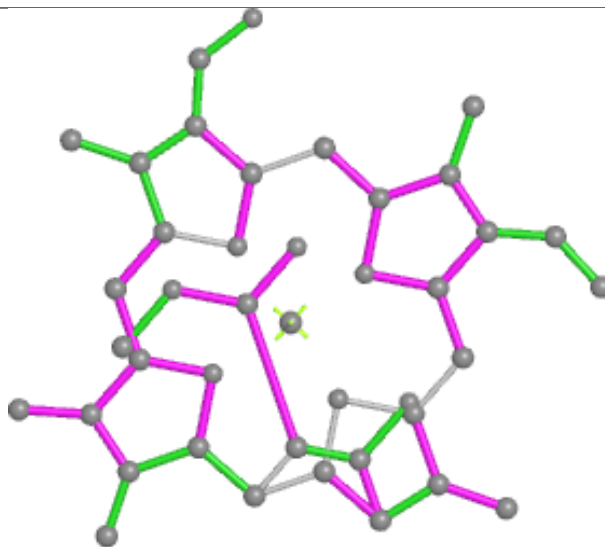


Rings

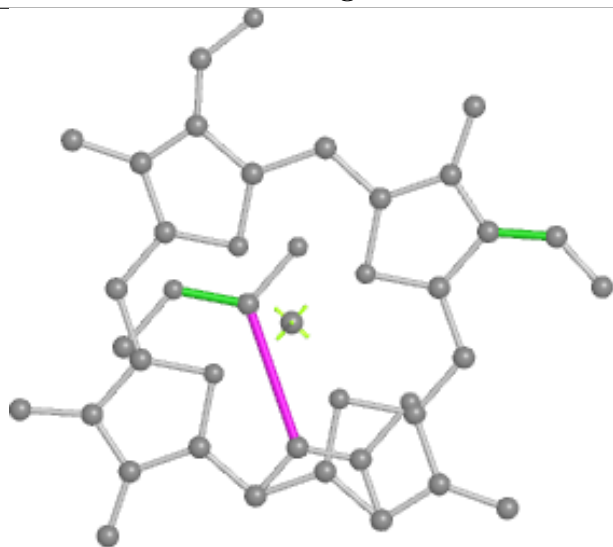
Ligand CL7 31 413



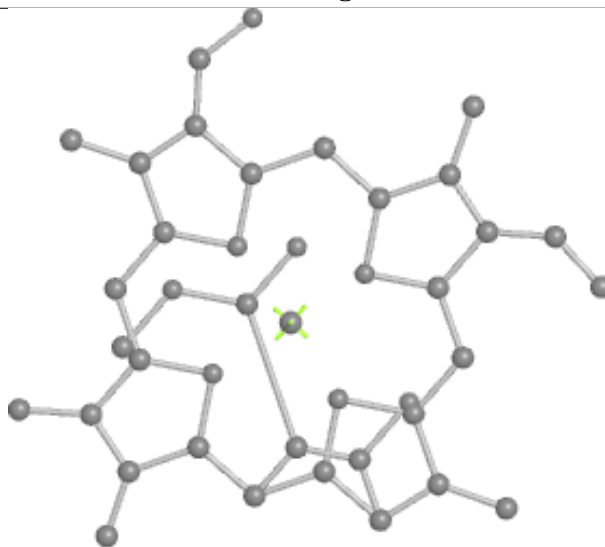
Bond lengths



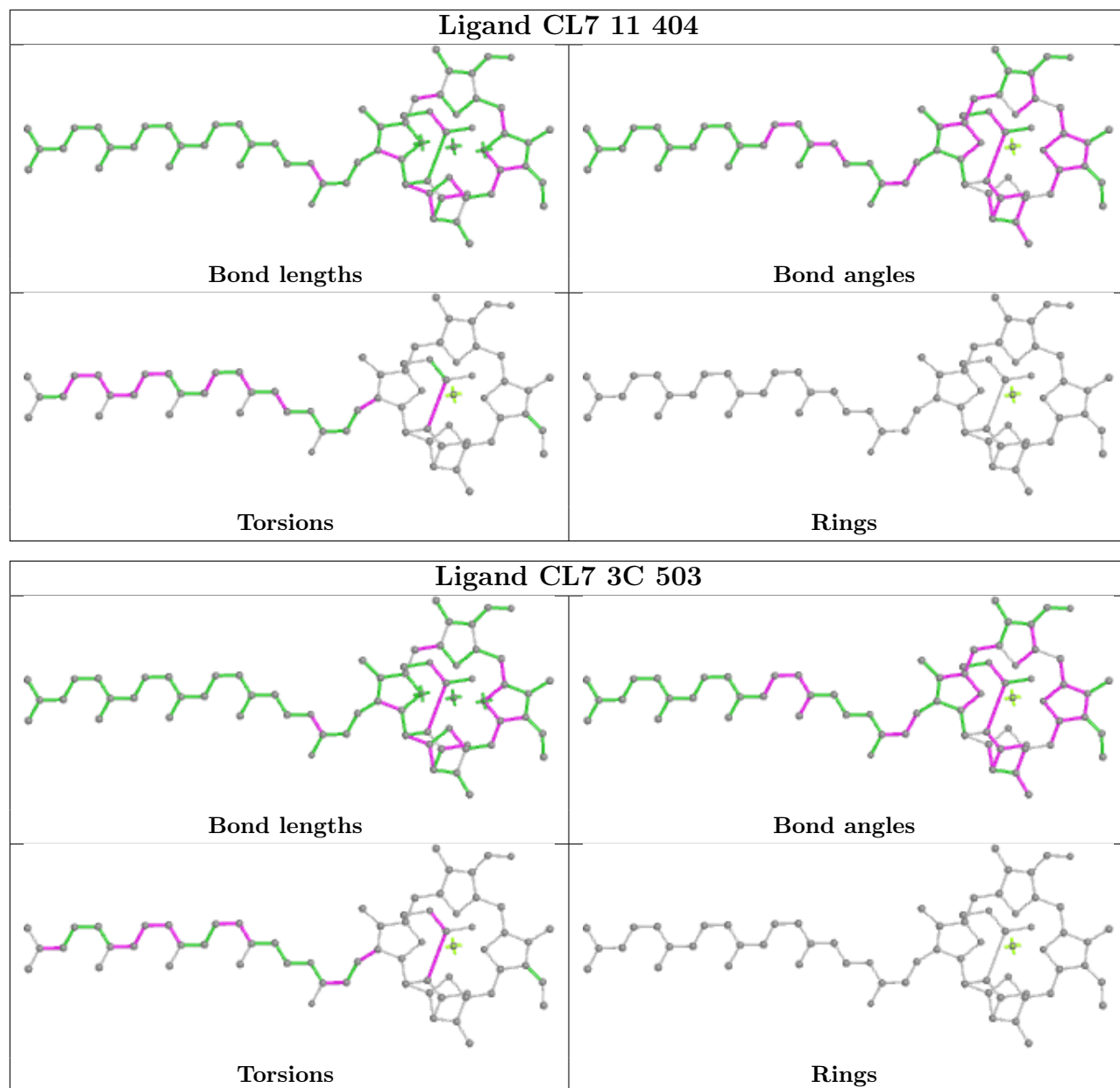
Bond angles

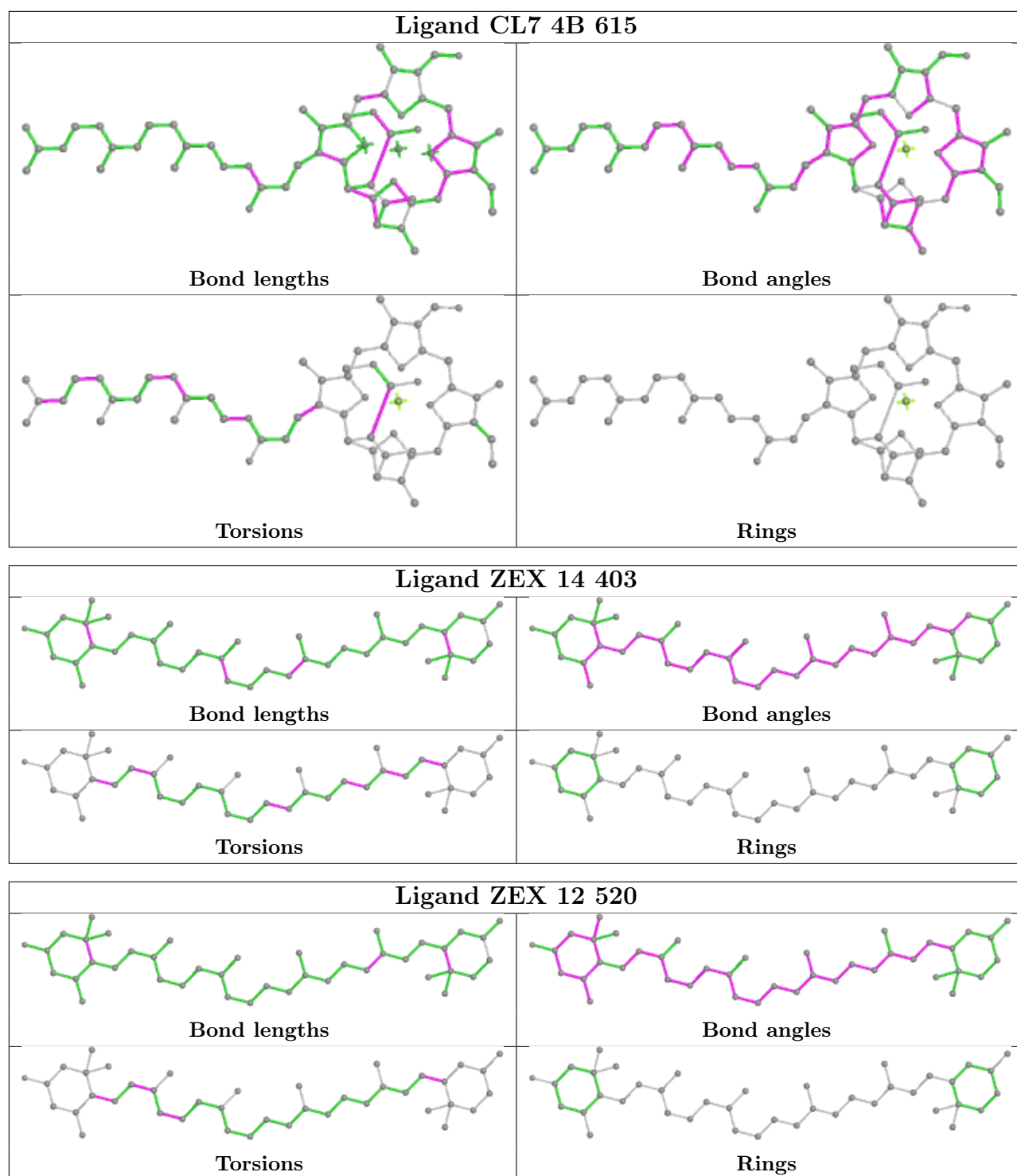


Torsions

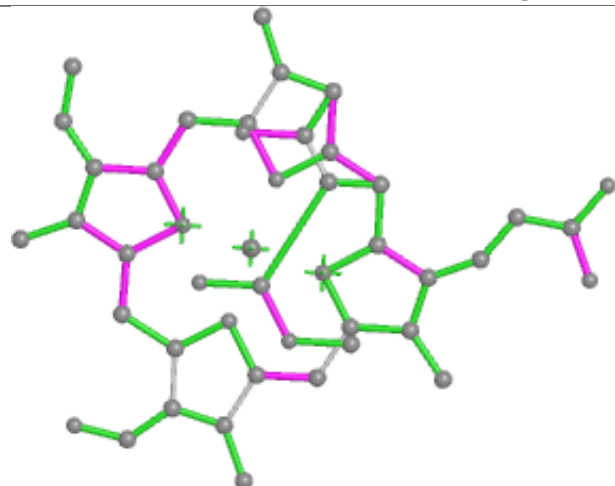


Rings

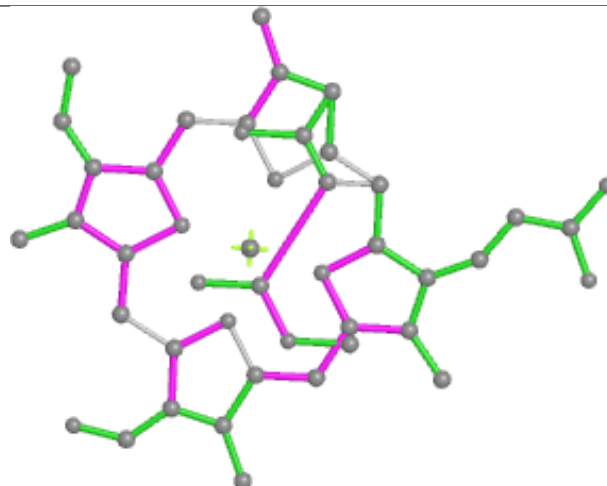




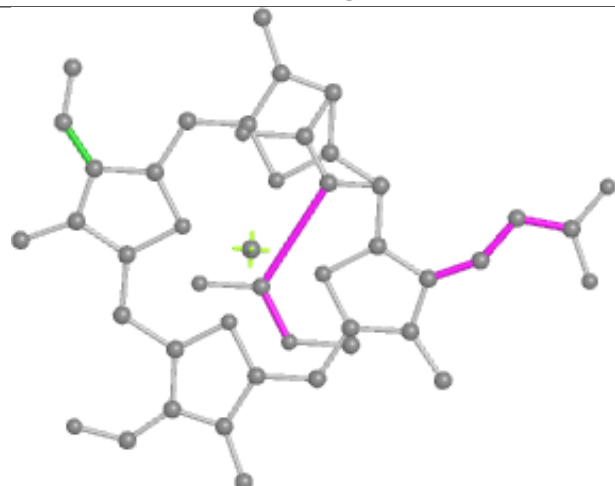
Ligand CL7 21 405



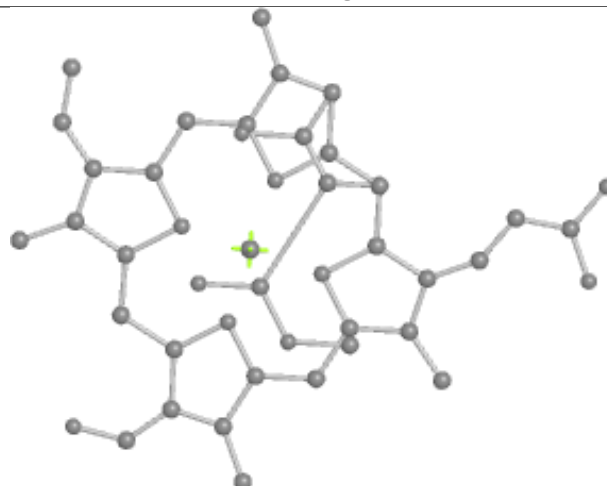
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Bond angles

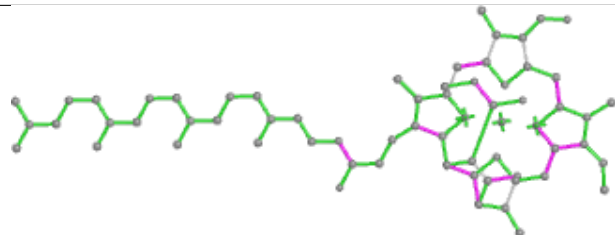


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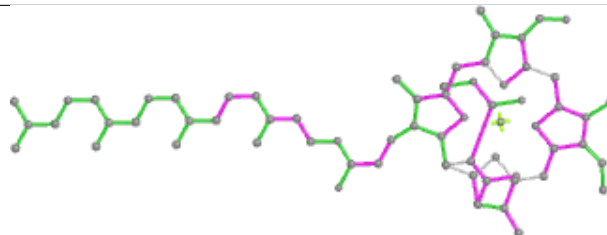


Rings

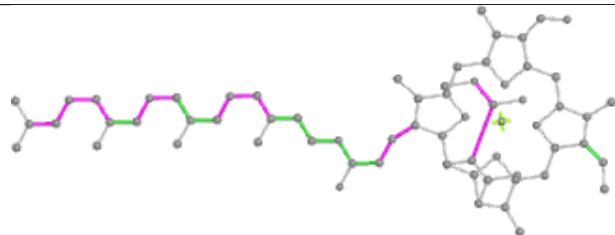
Ligand CL7 12 517



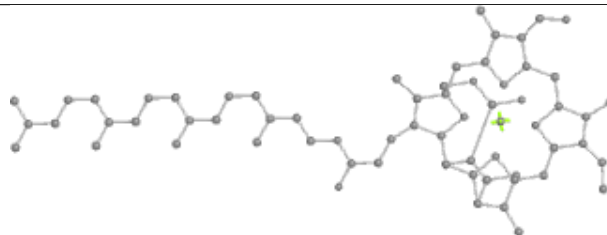
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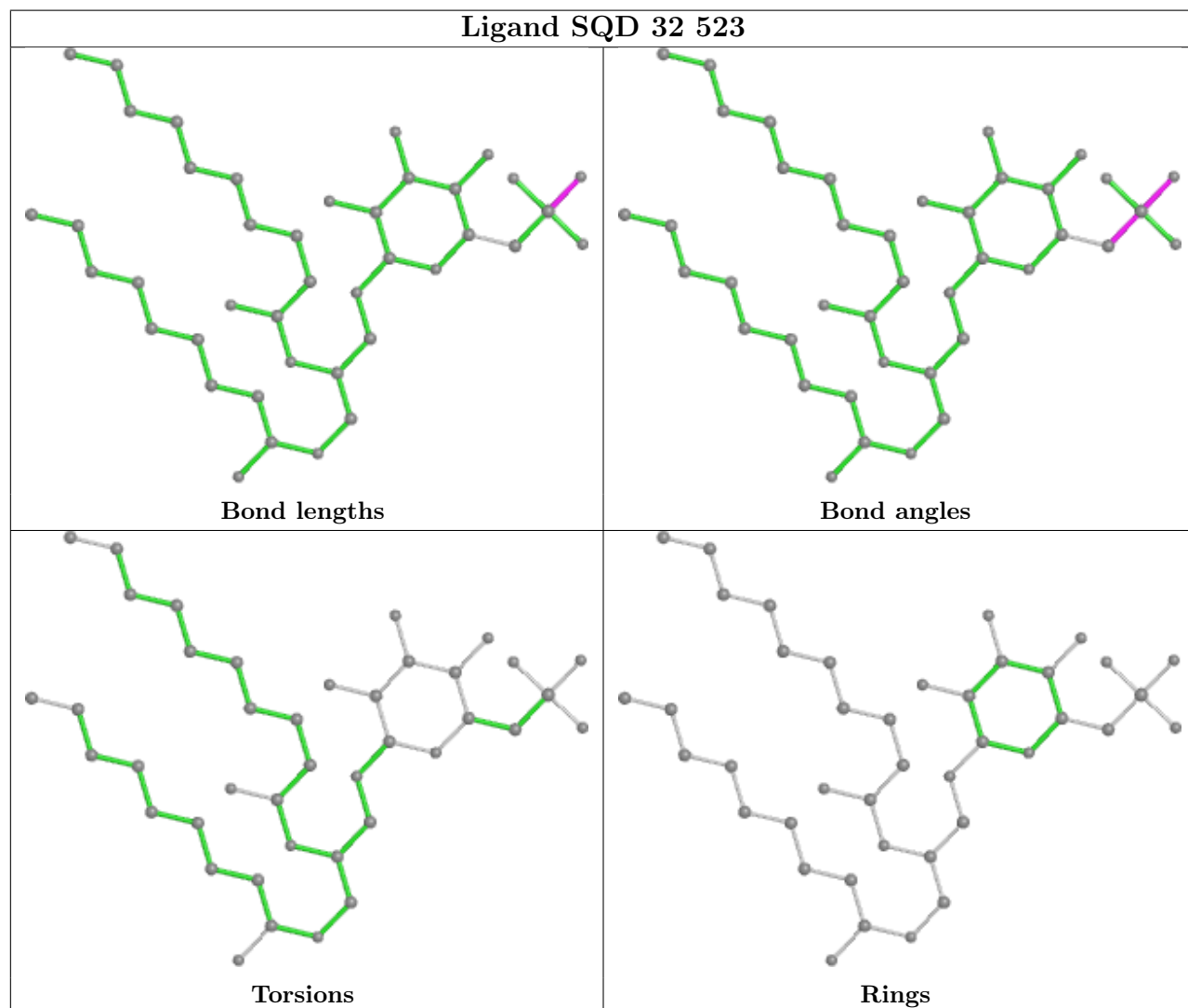
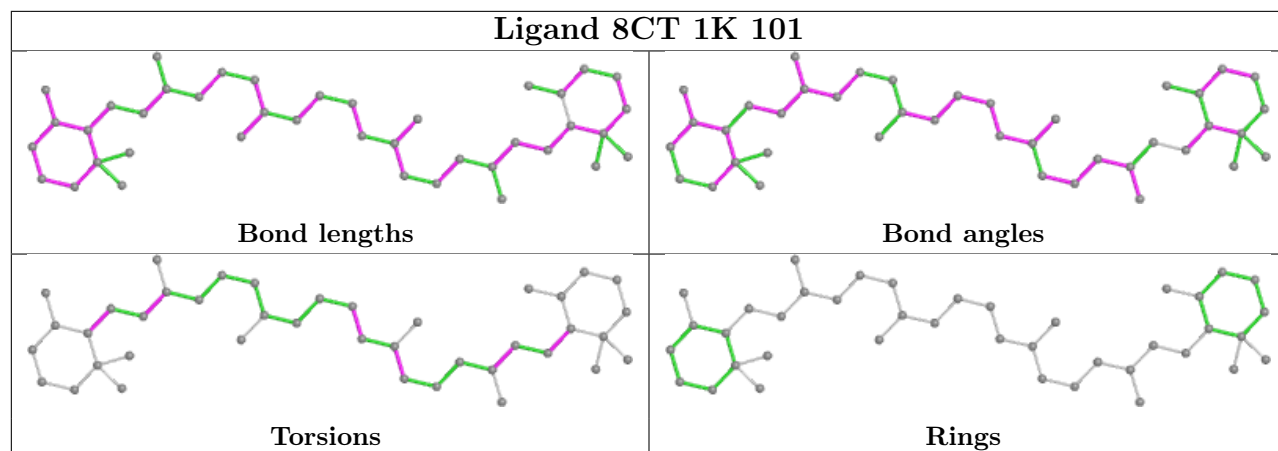
Bond angles



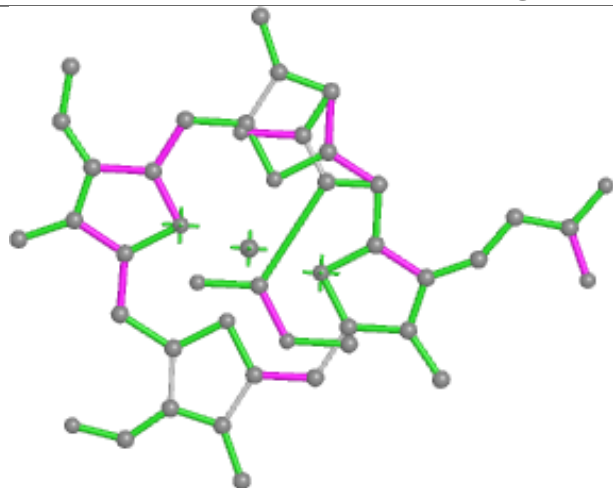
Torsions



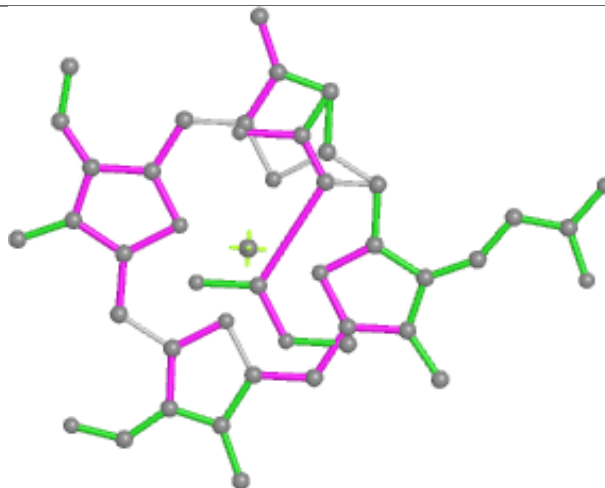
Rings



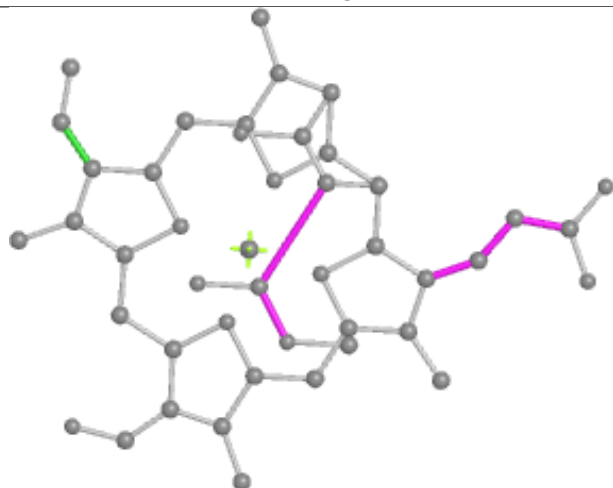
Ligand CL7 24 410



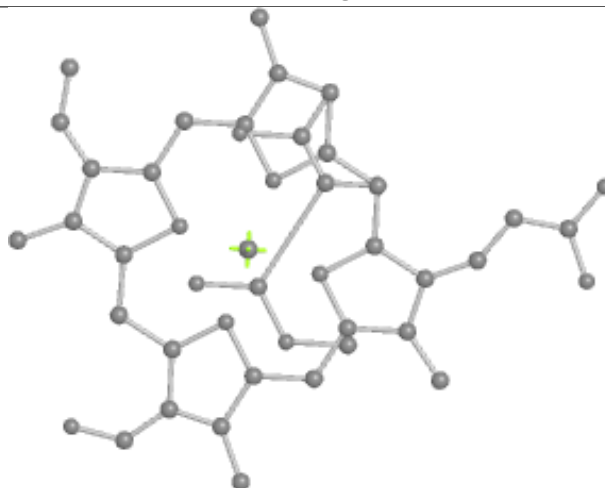
Bond lengths



Bond angles

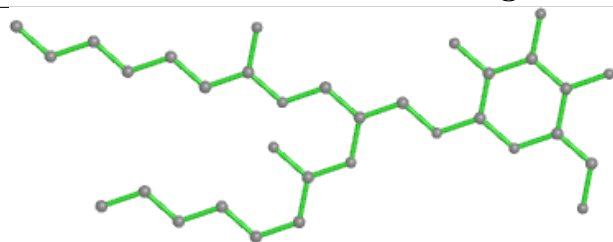


Torsions

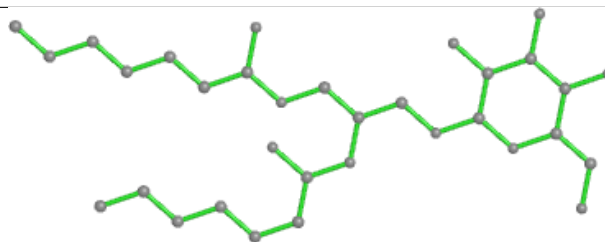


Rings

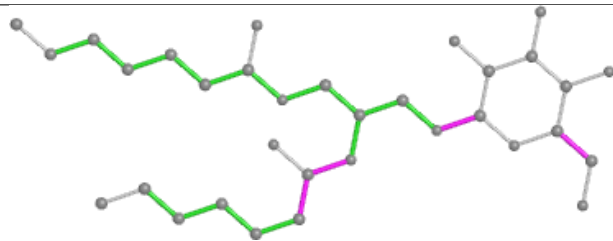
Ligand LMG 4D 410



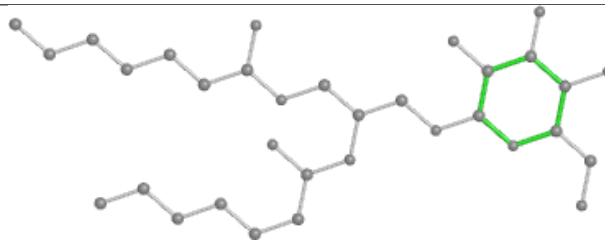
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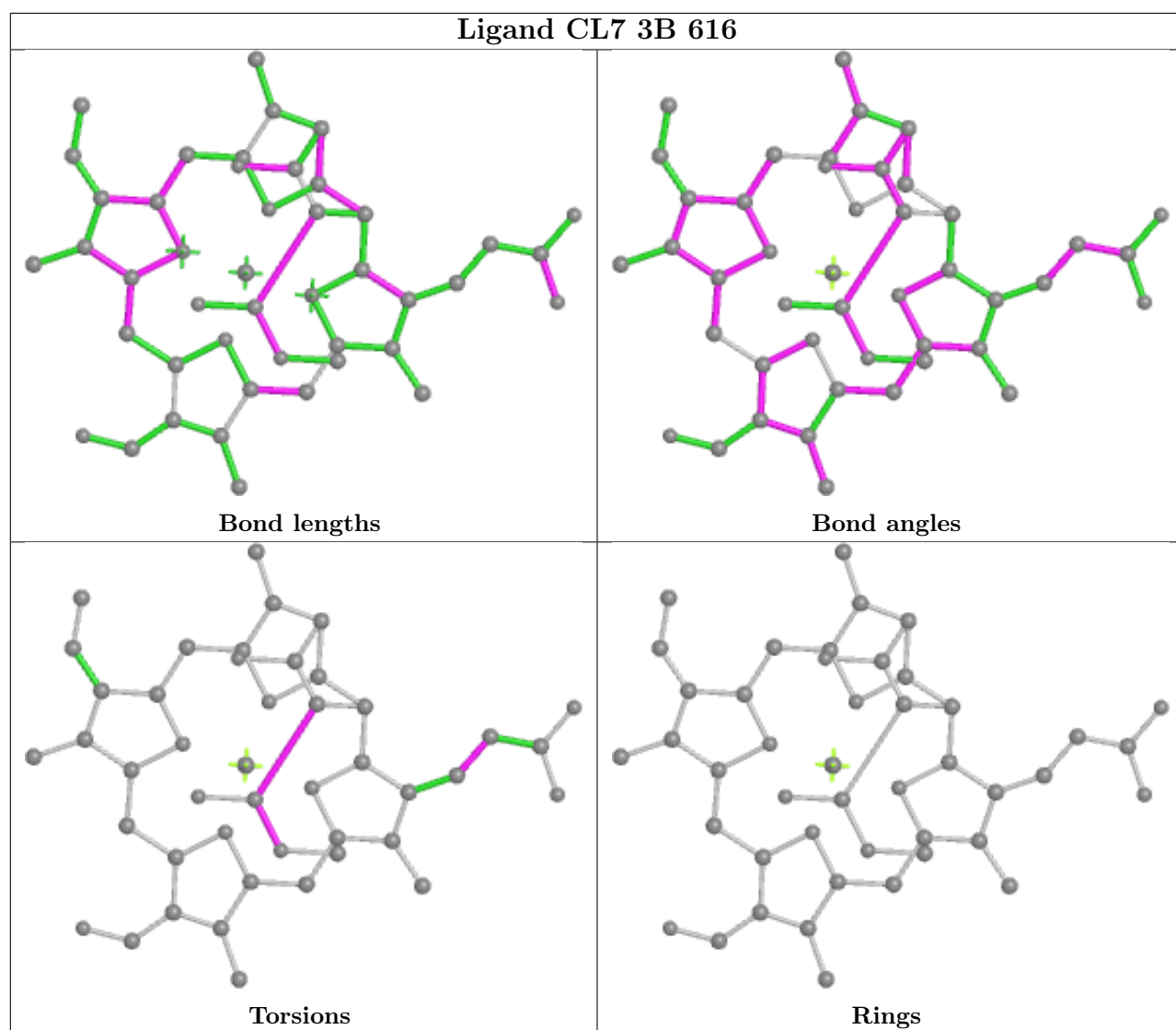
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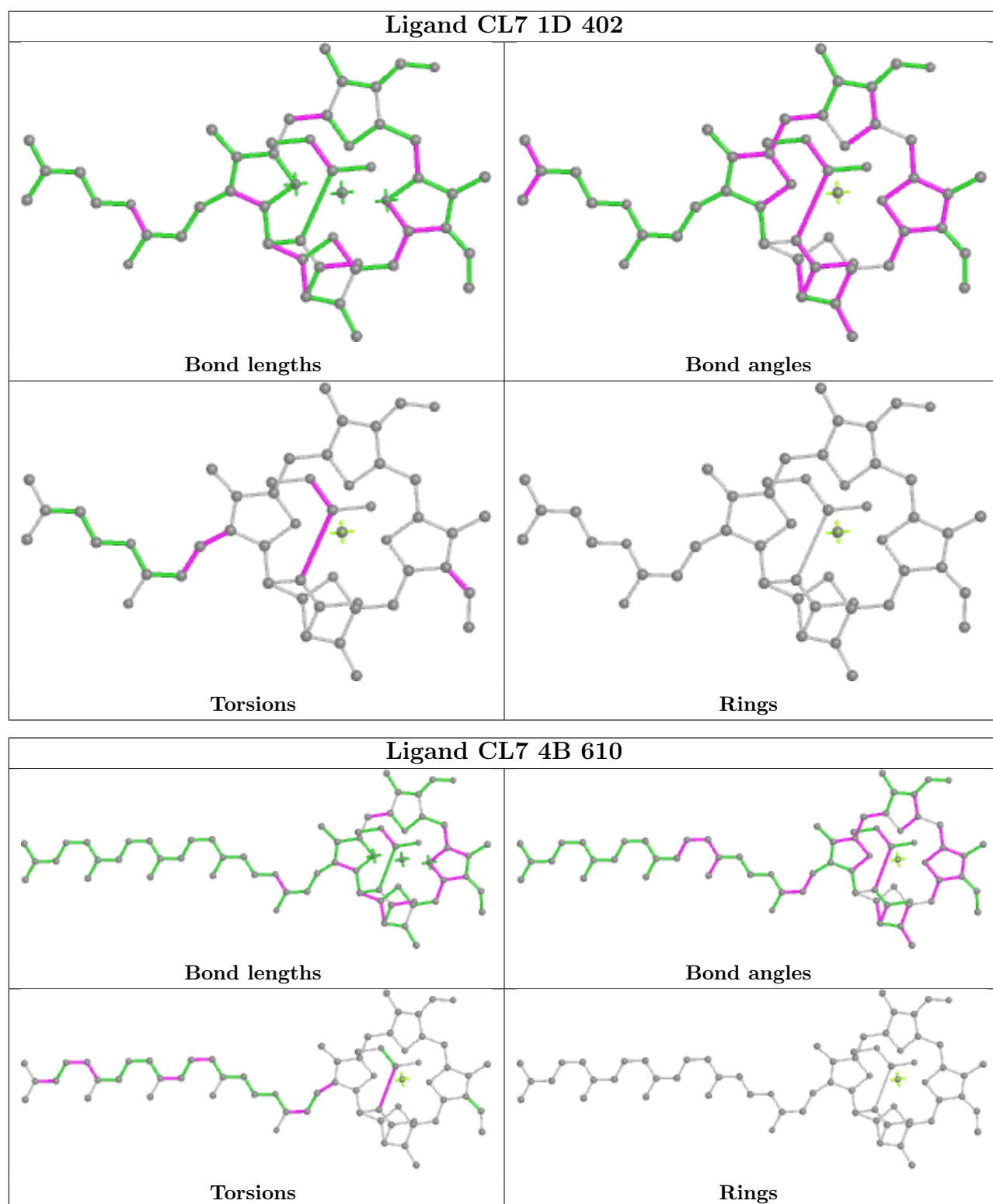


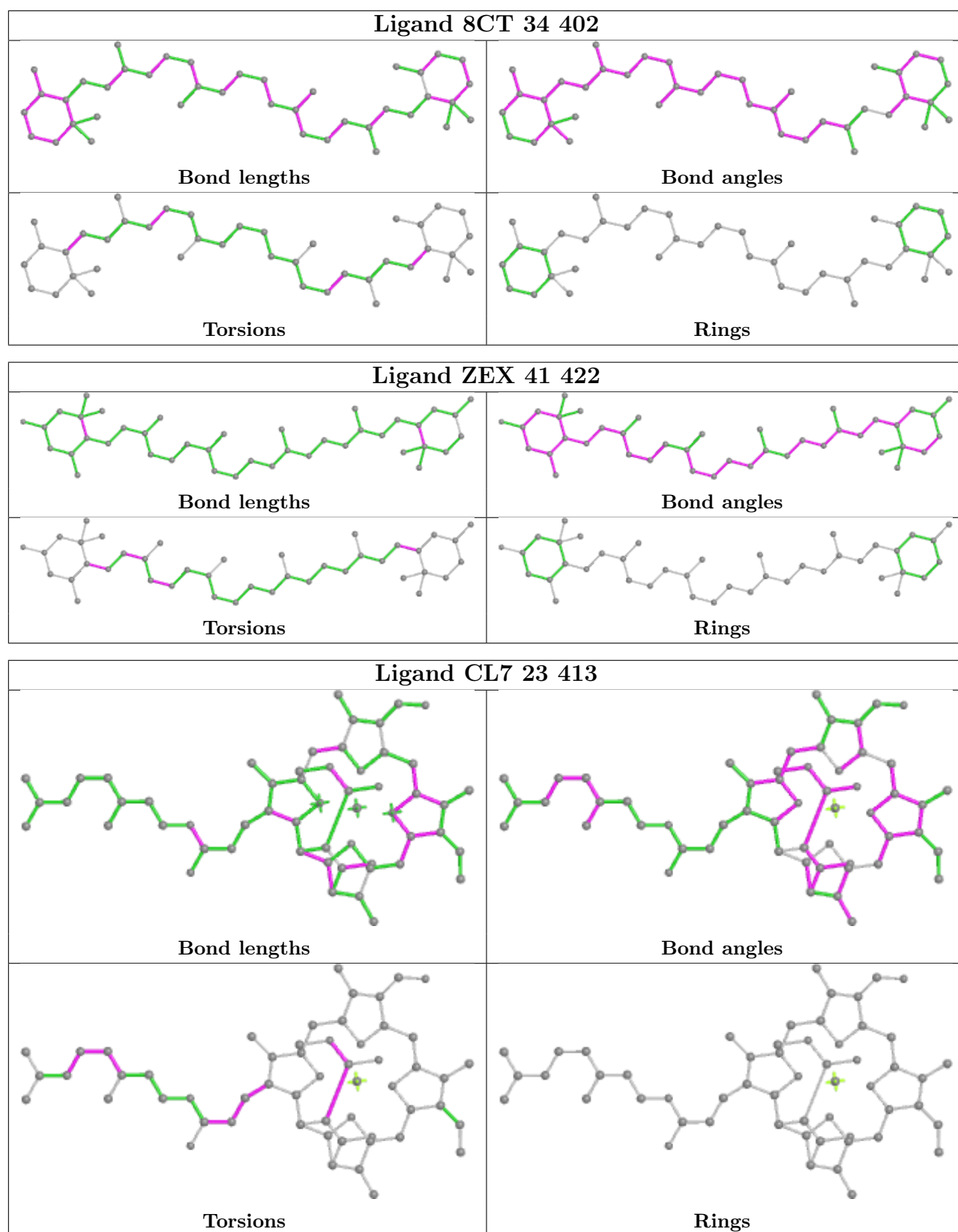
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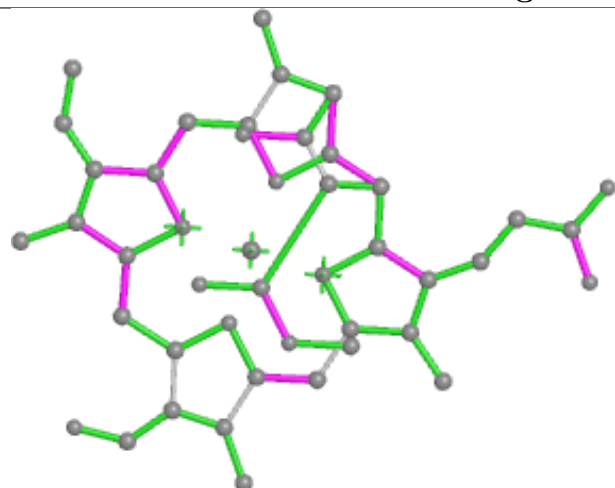
Rings



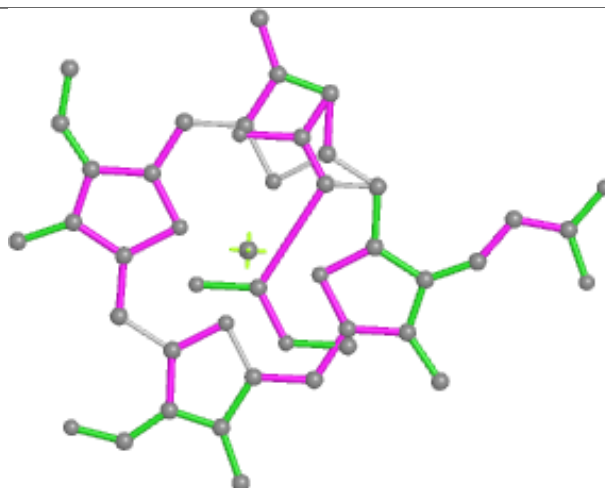




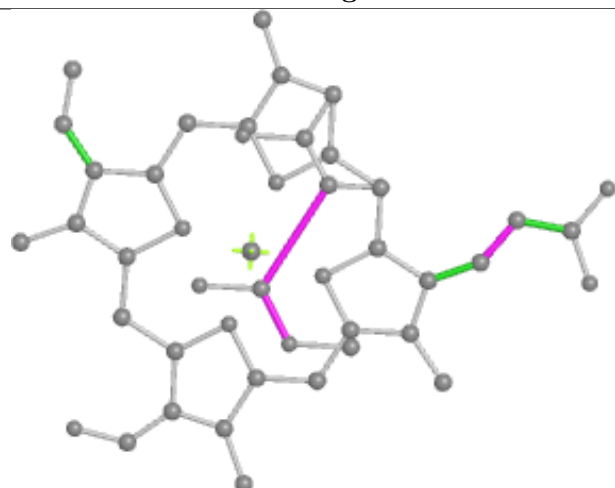
Ligand CL7 11 409



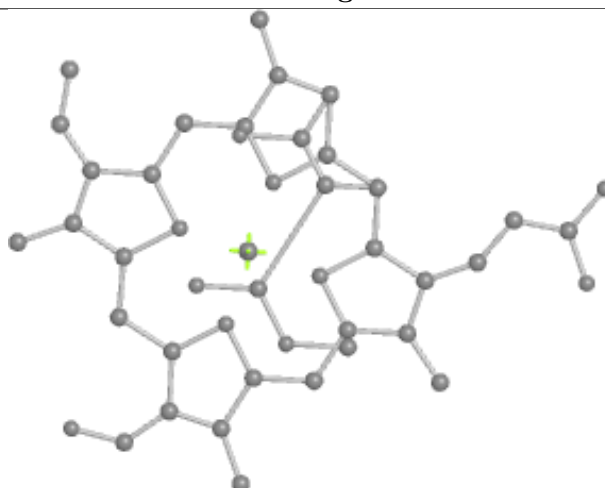
Bond lengths



Bond angles

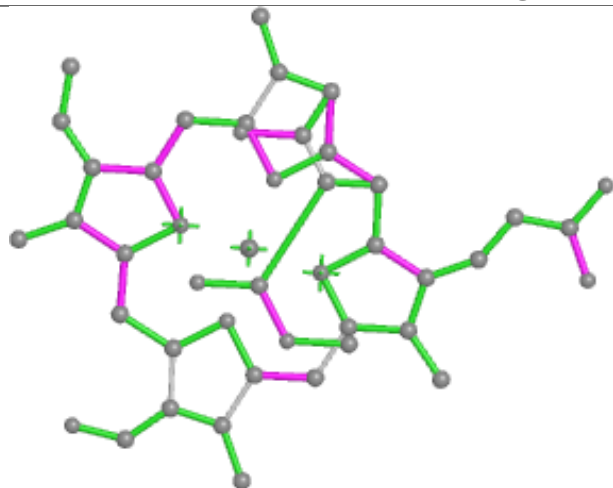


Torsions

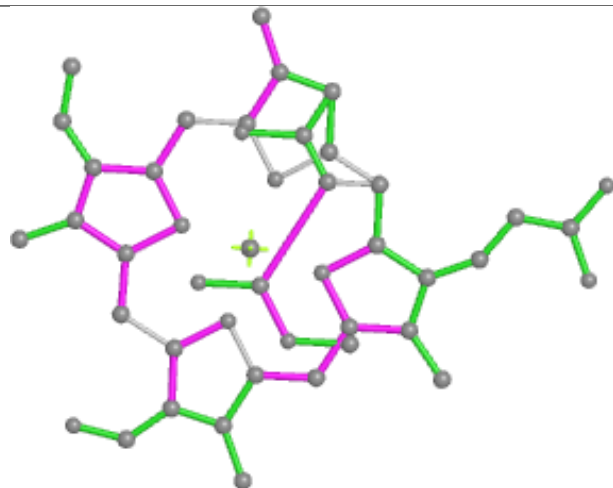


Rings

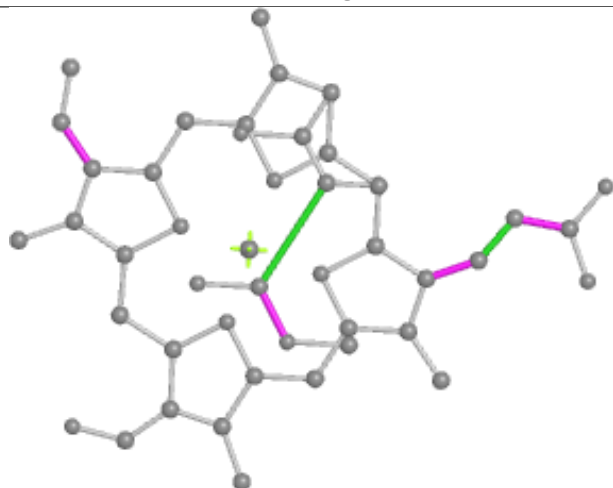
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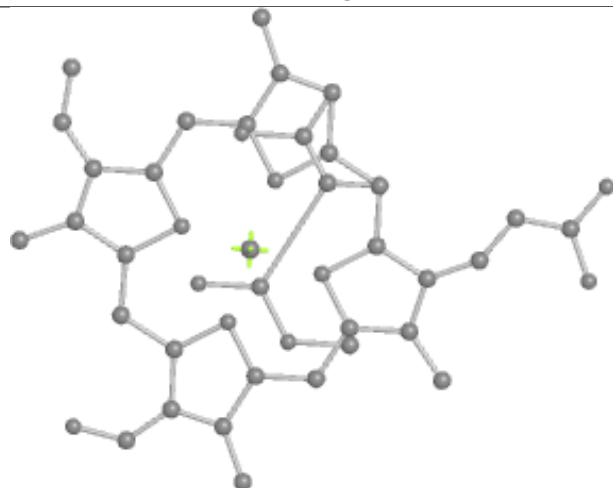
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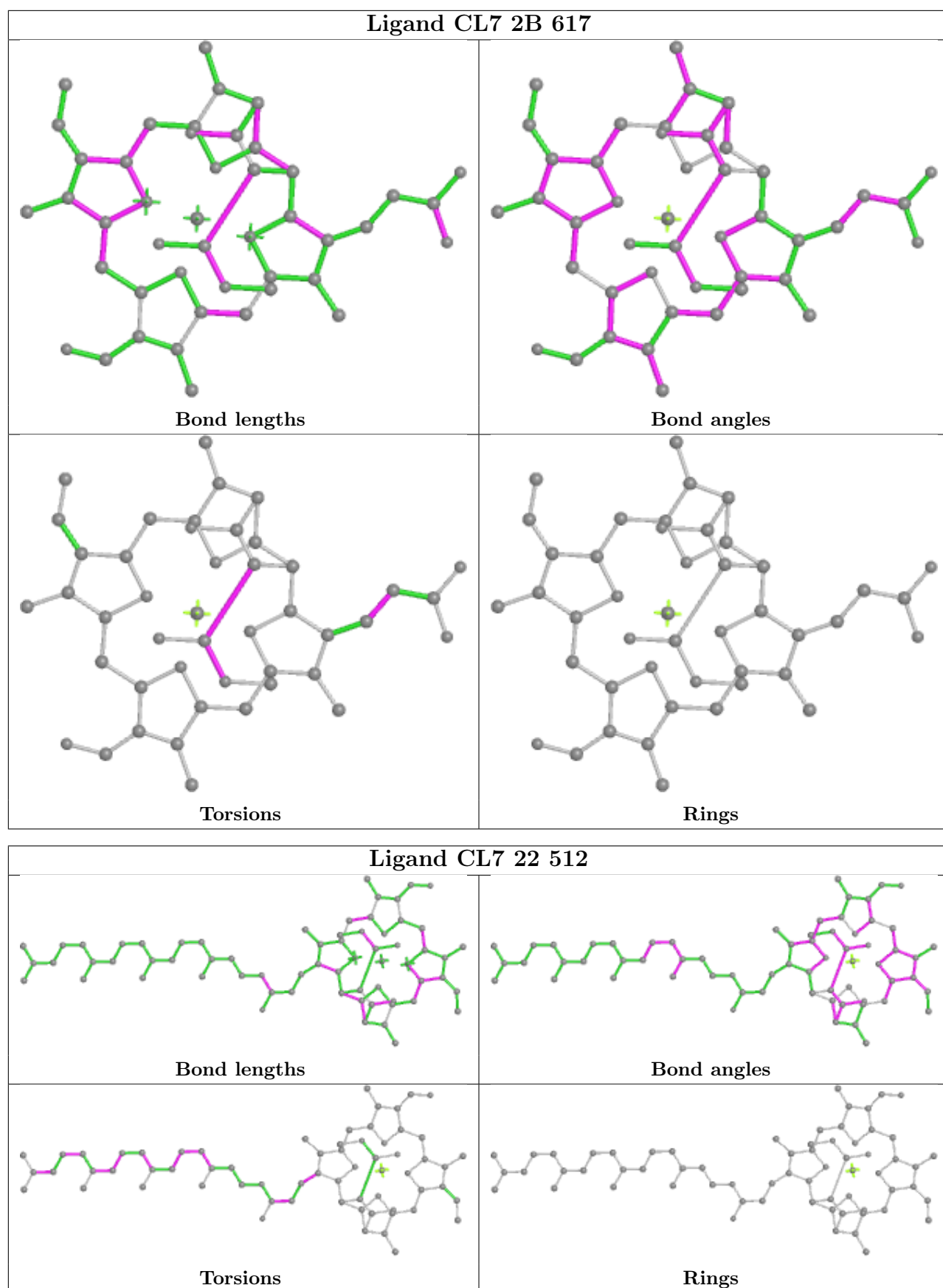
Bond angles

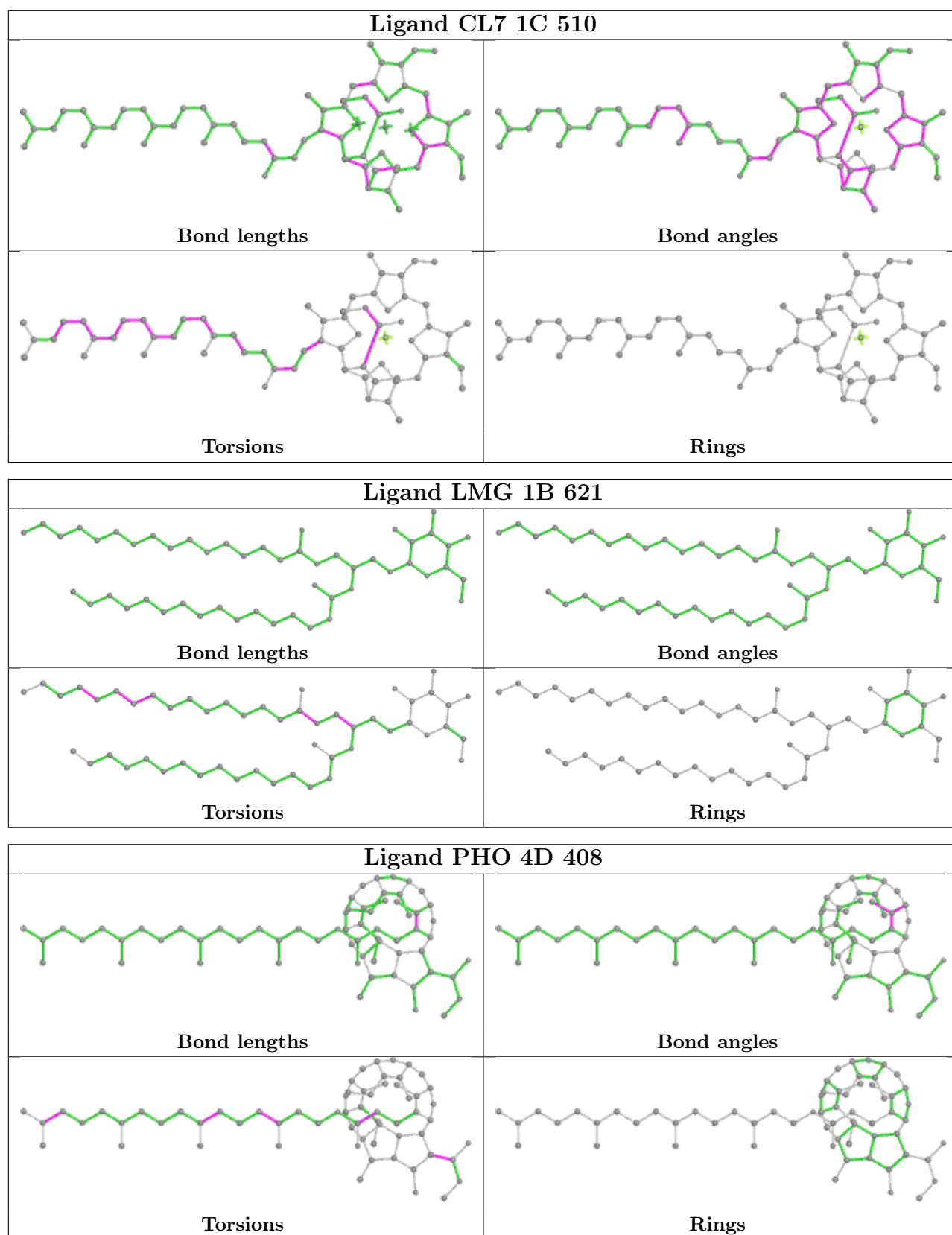


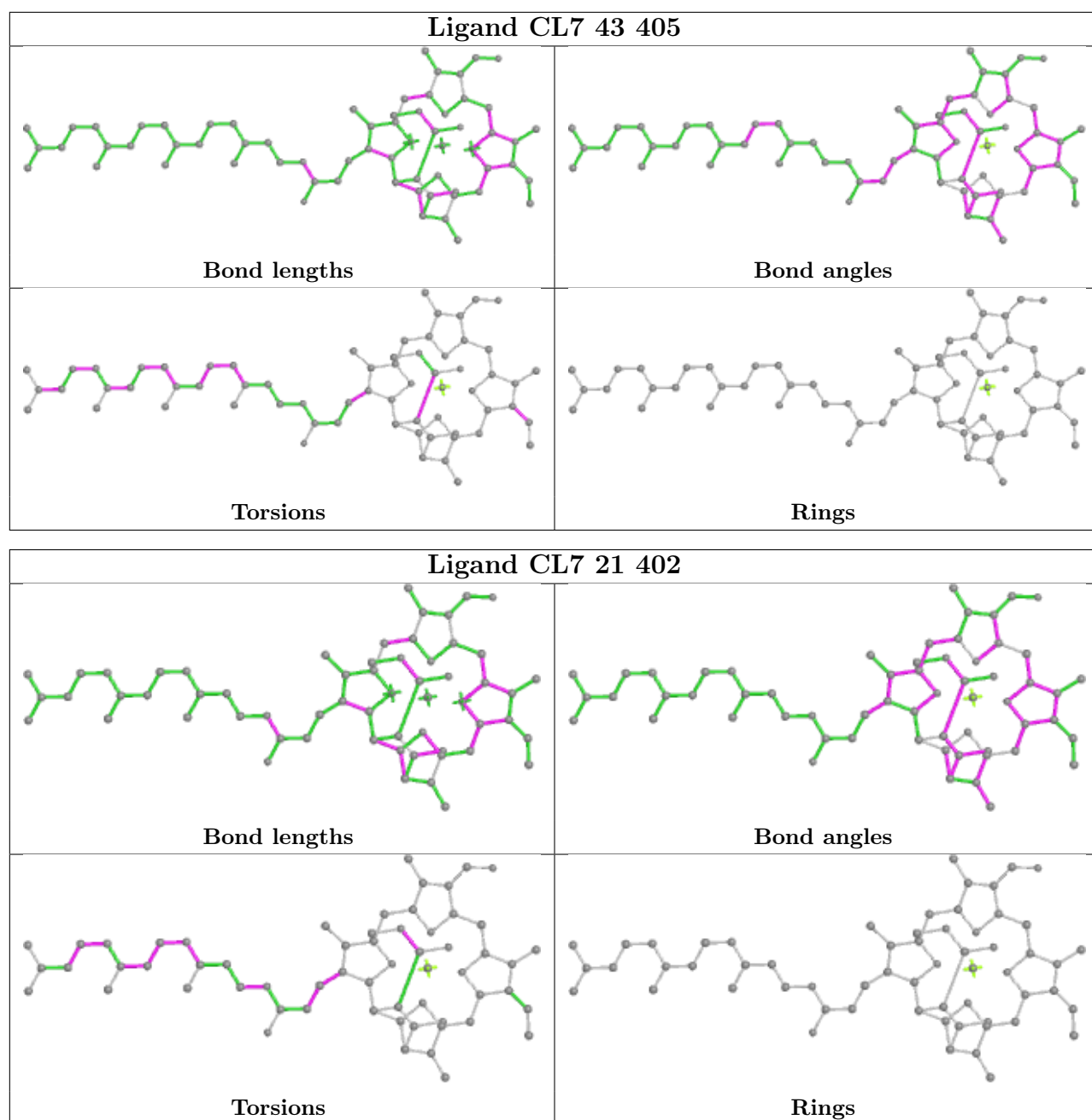
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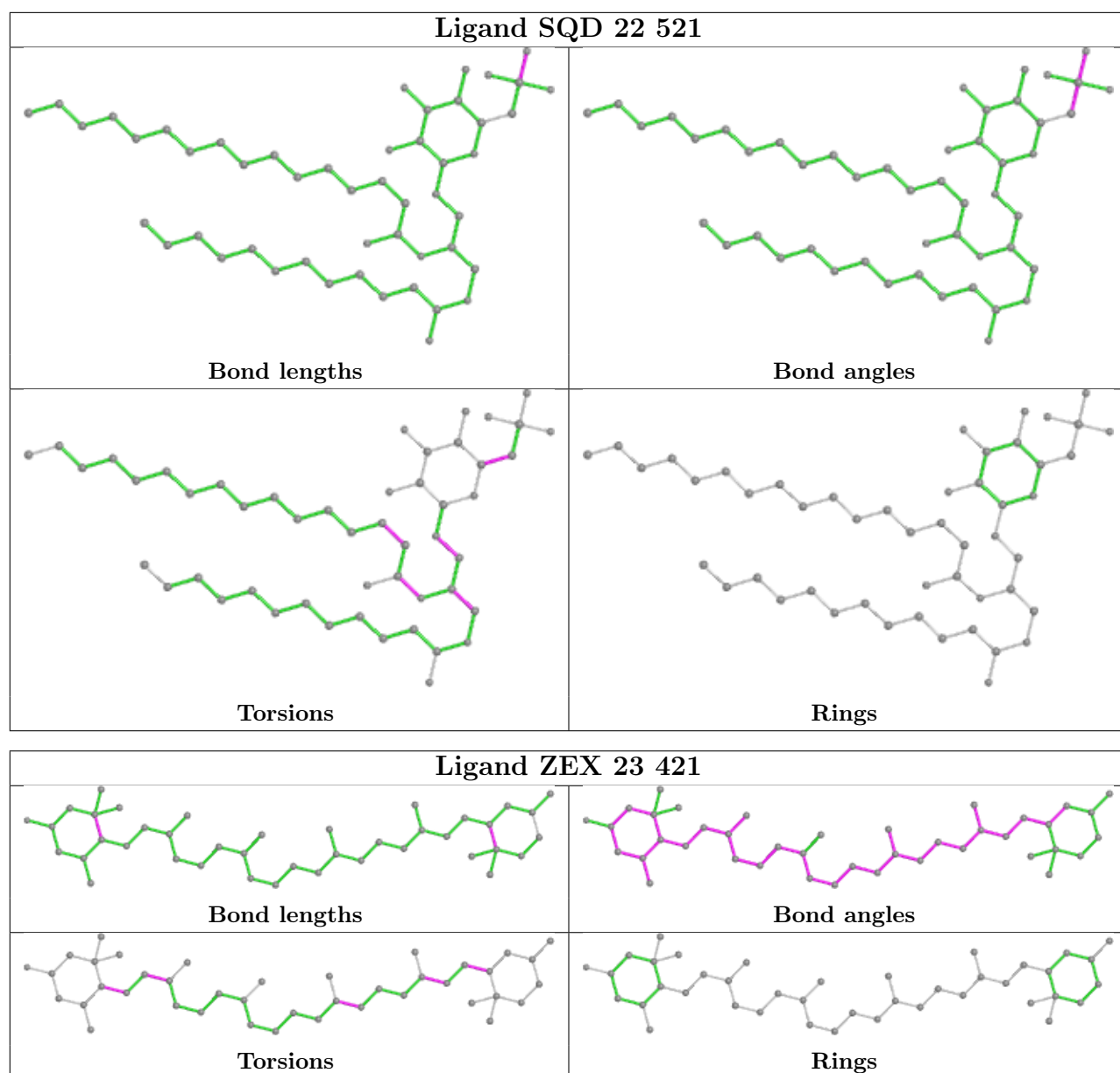


Rings

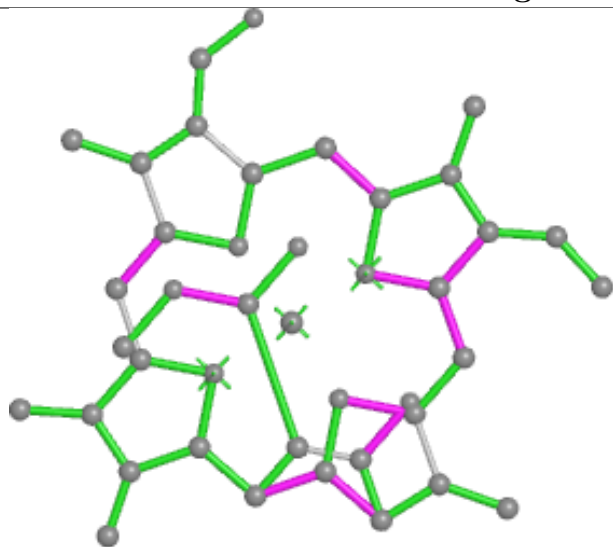




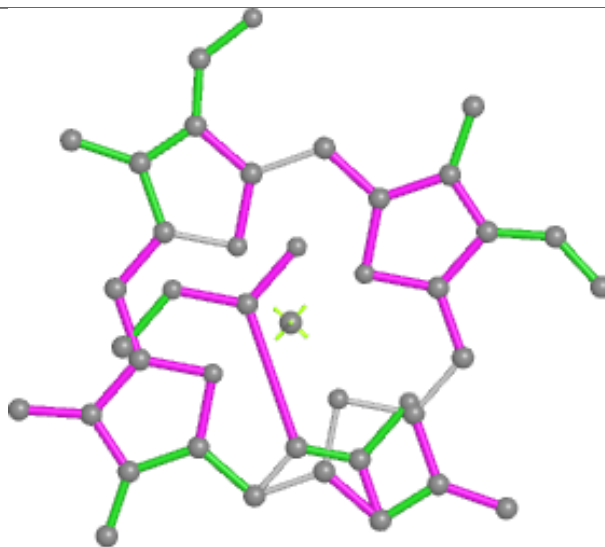




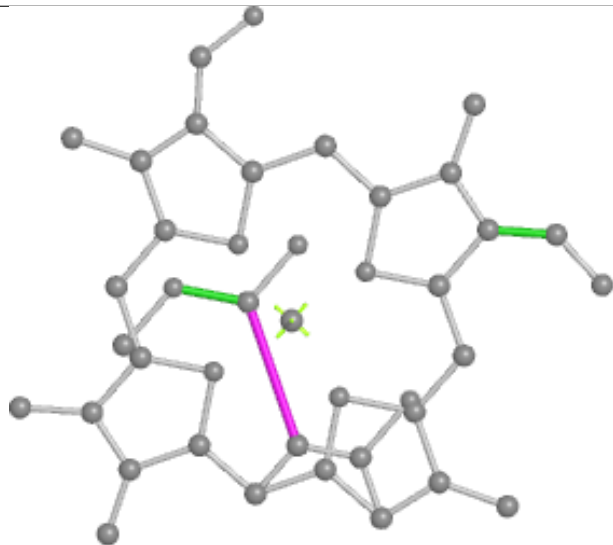
Ligand CL7 11 413



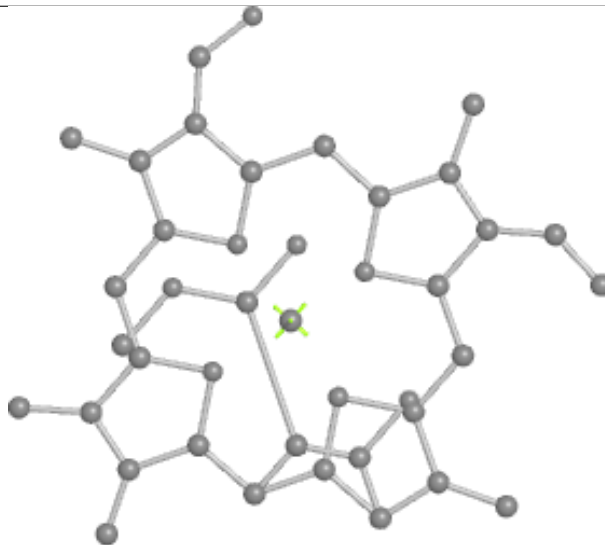
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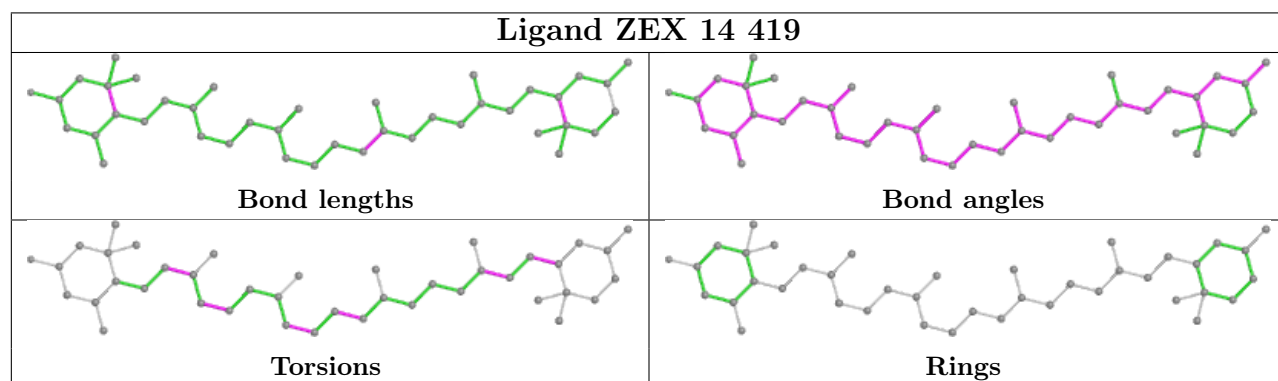
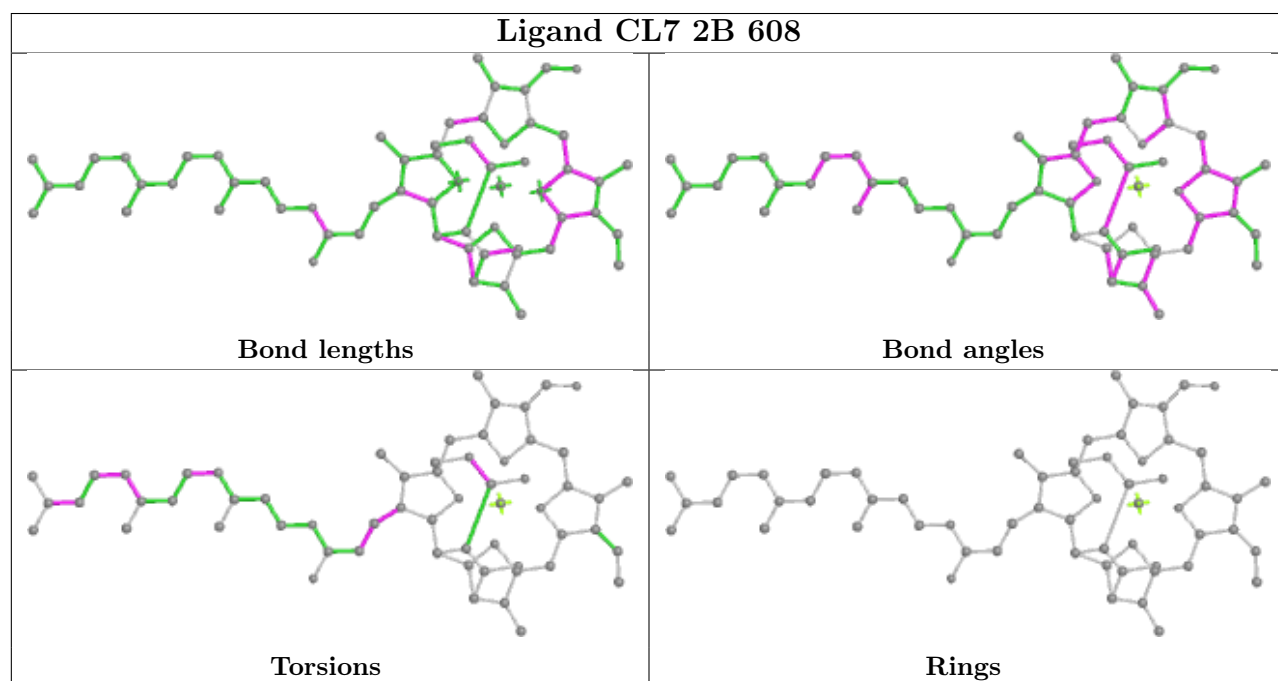
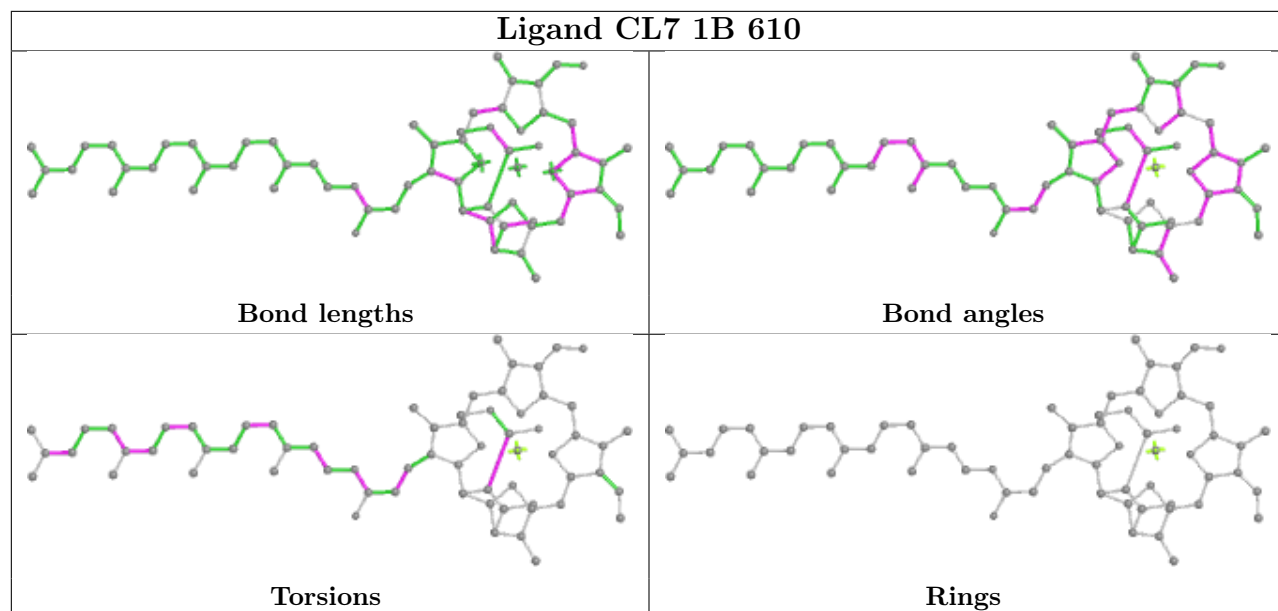
Bond angles

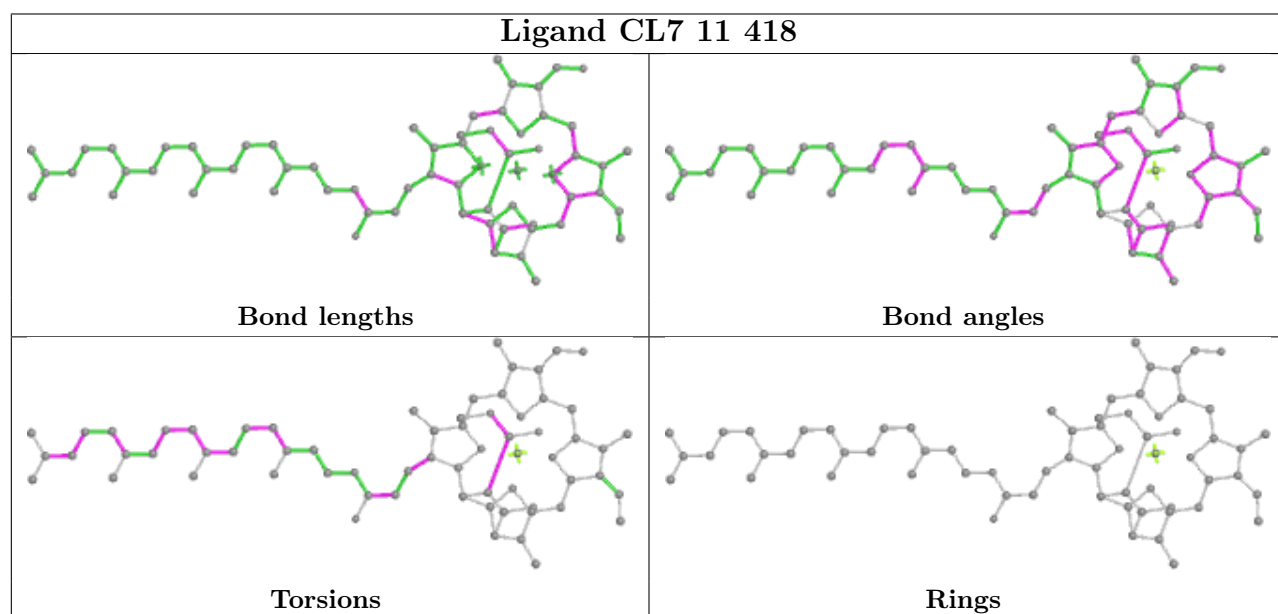
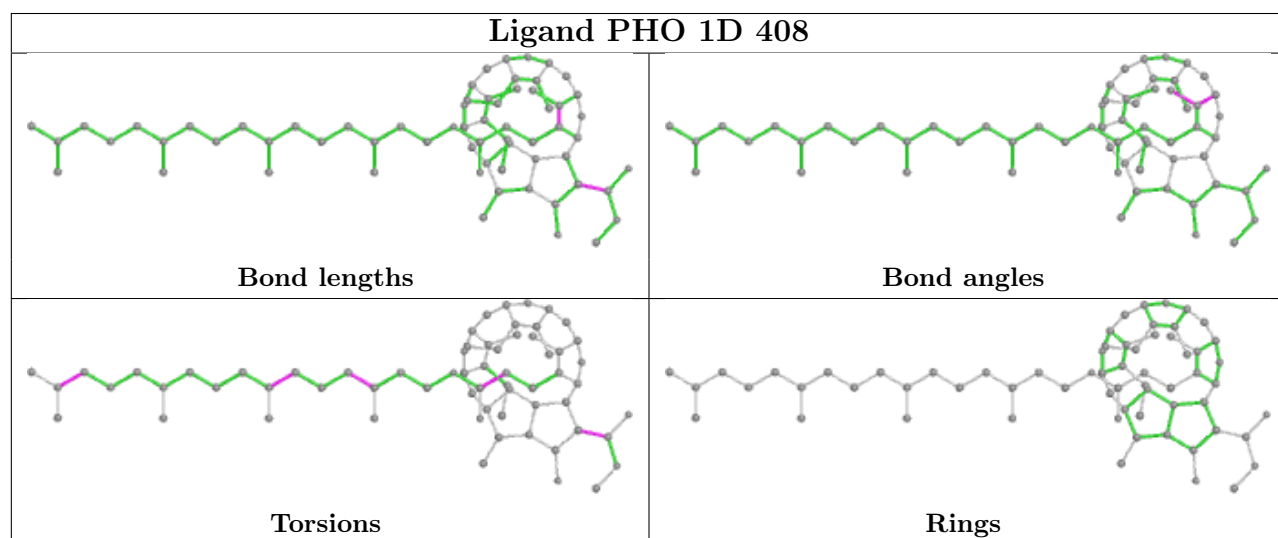
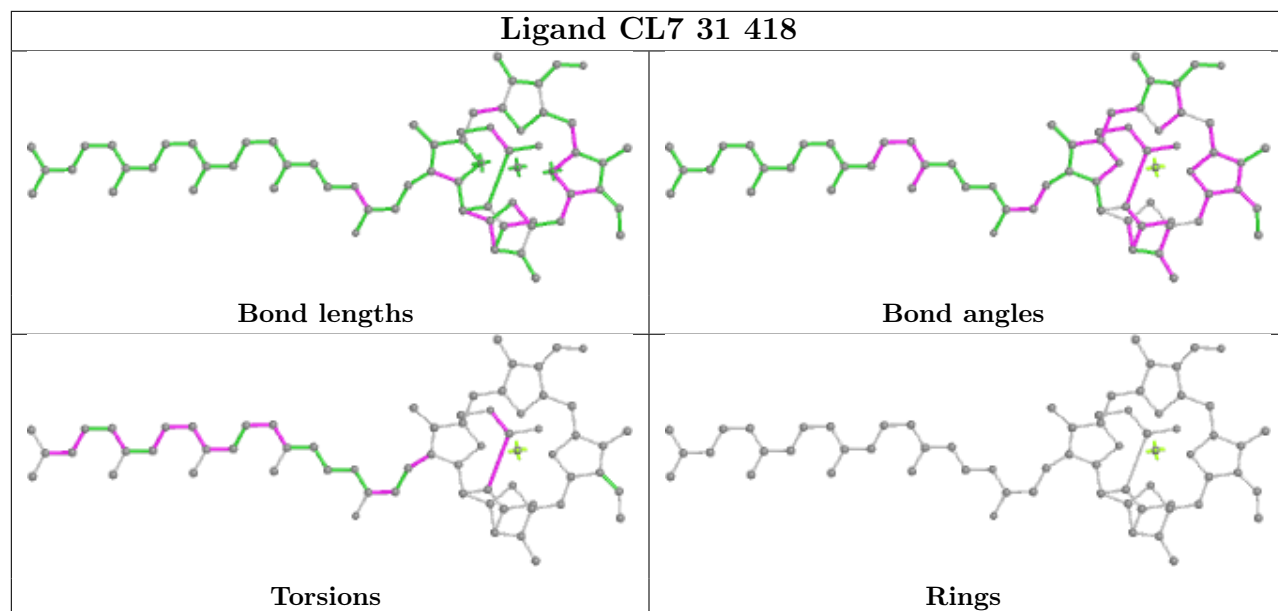


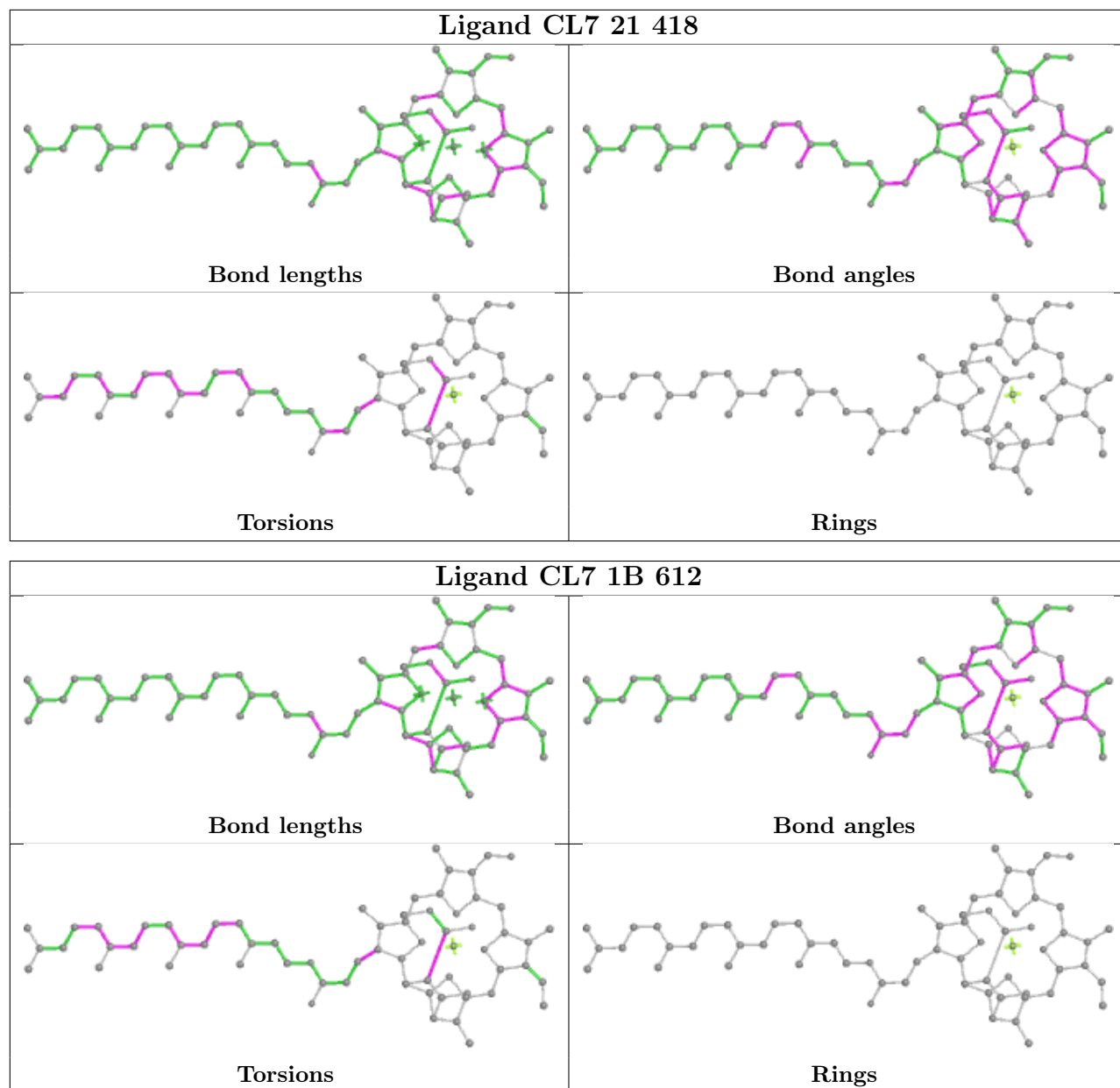
Torsions



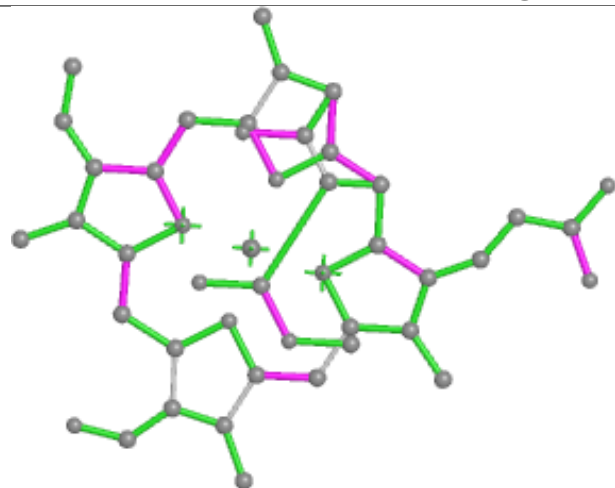
Rings



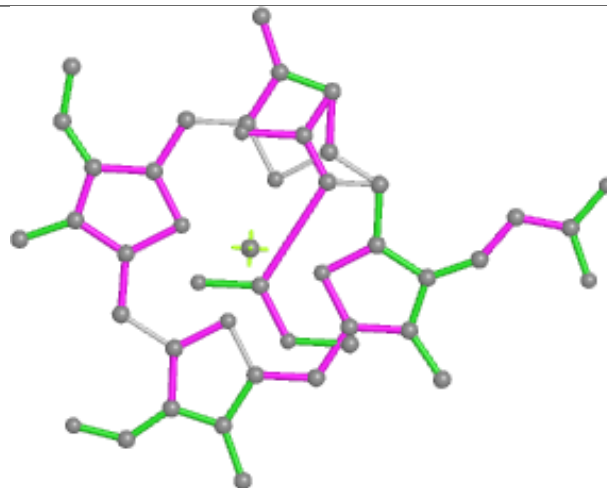




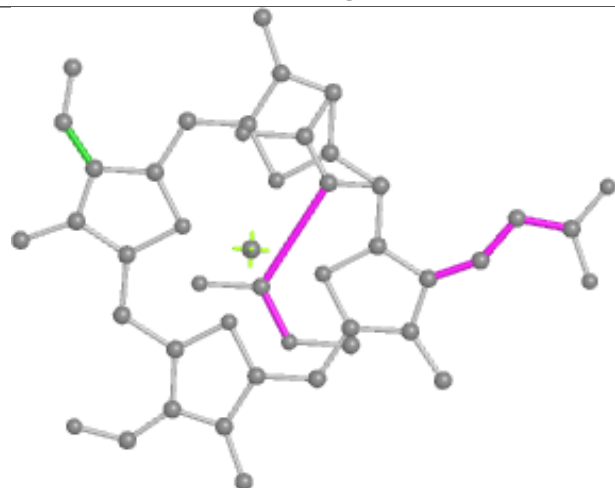
Ligand CL7 21 412



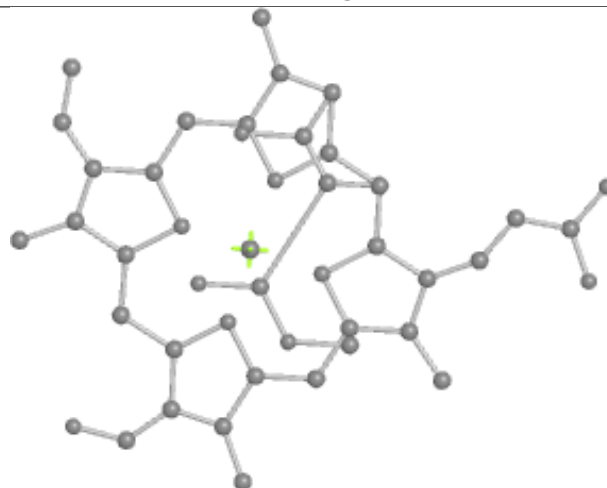
Bond lengths



Bond angles

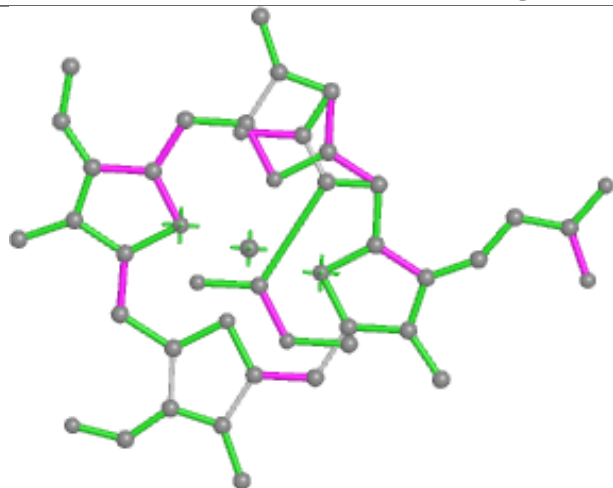


Torsions

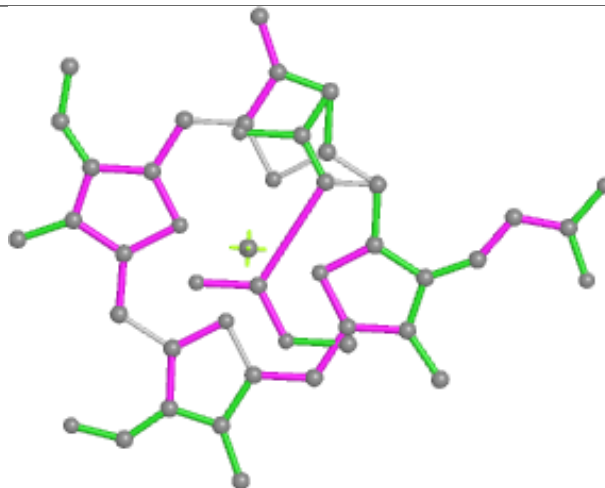


Rings

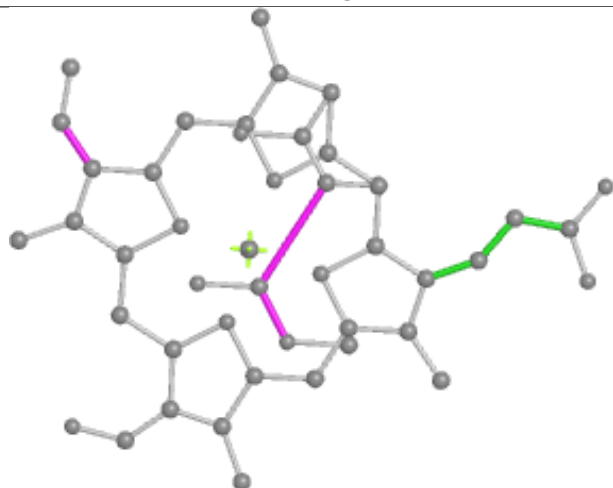
Ligand CL7 11 420



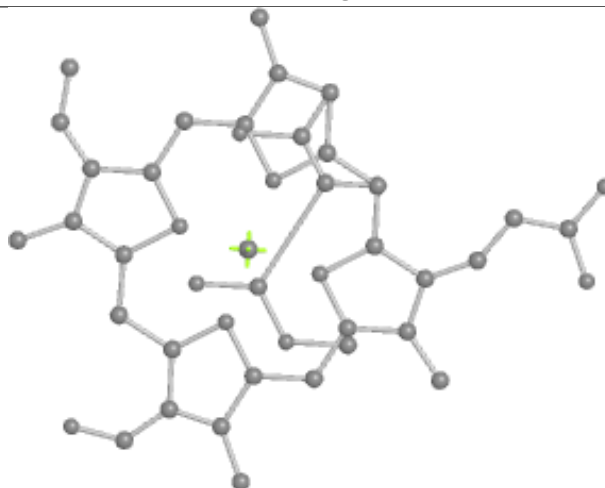
Bond lengths



Bond angles

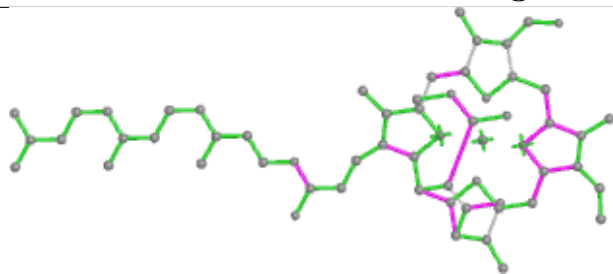


Torsions

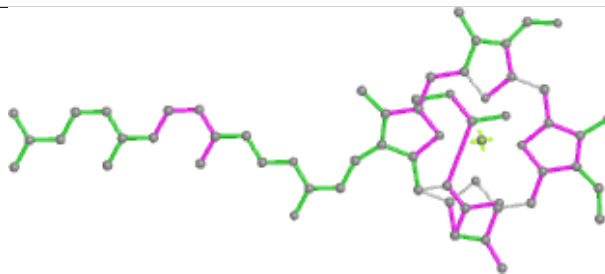


Rings

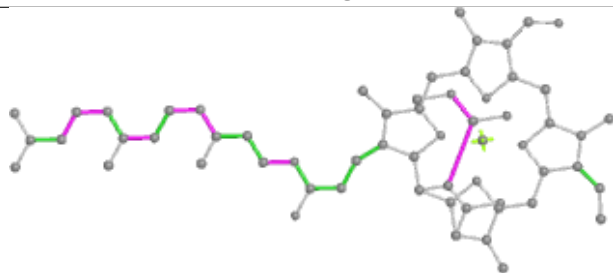
Ligand CL7 1C 502



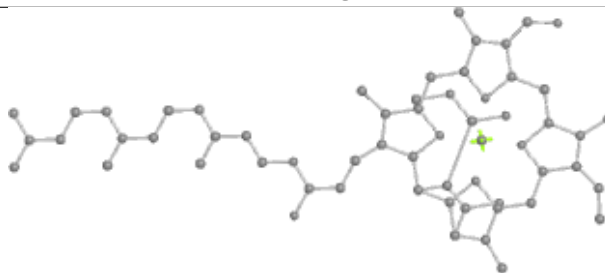
Bond lengths



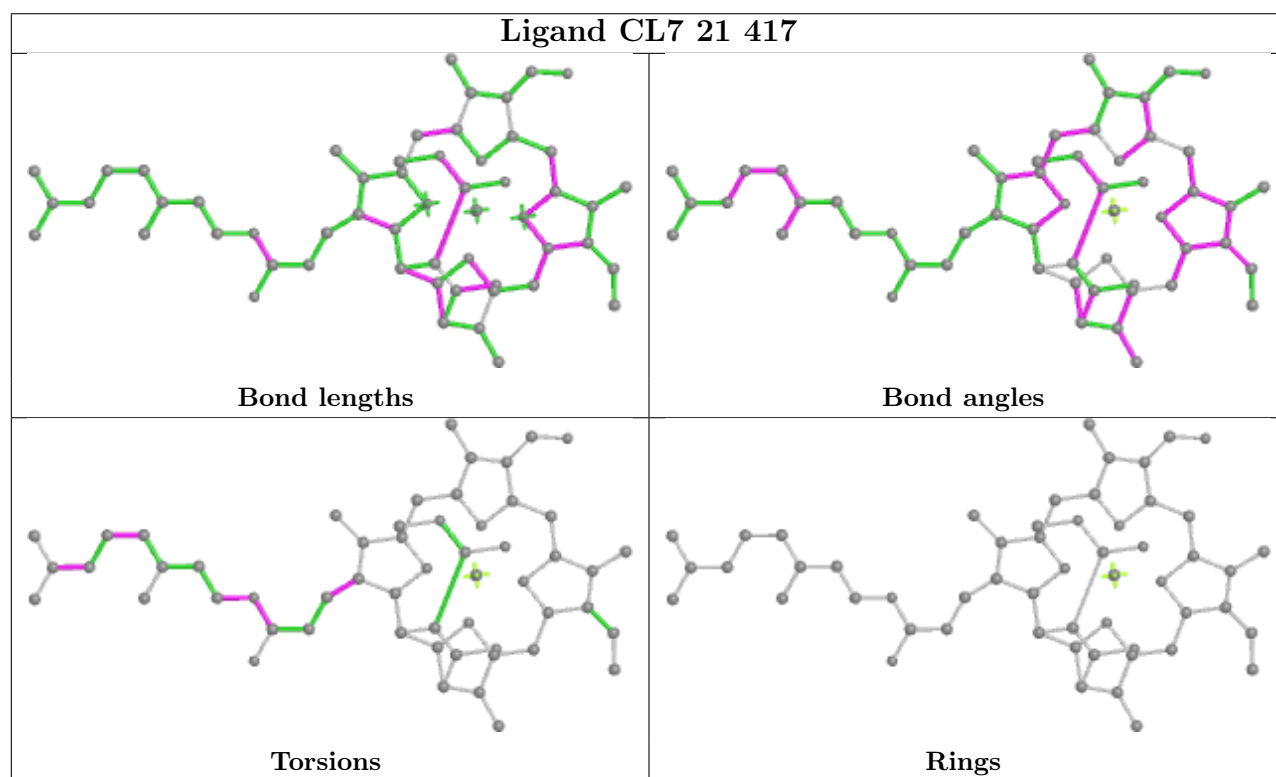
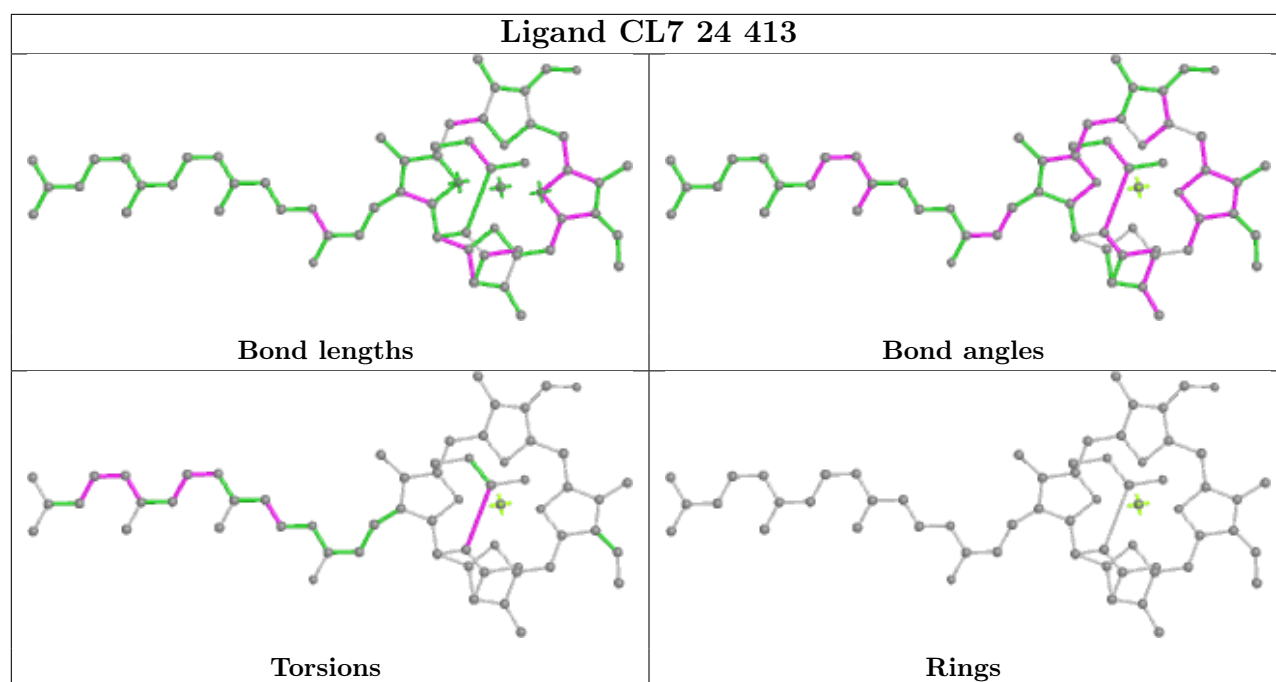
Bond angles

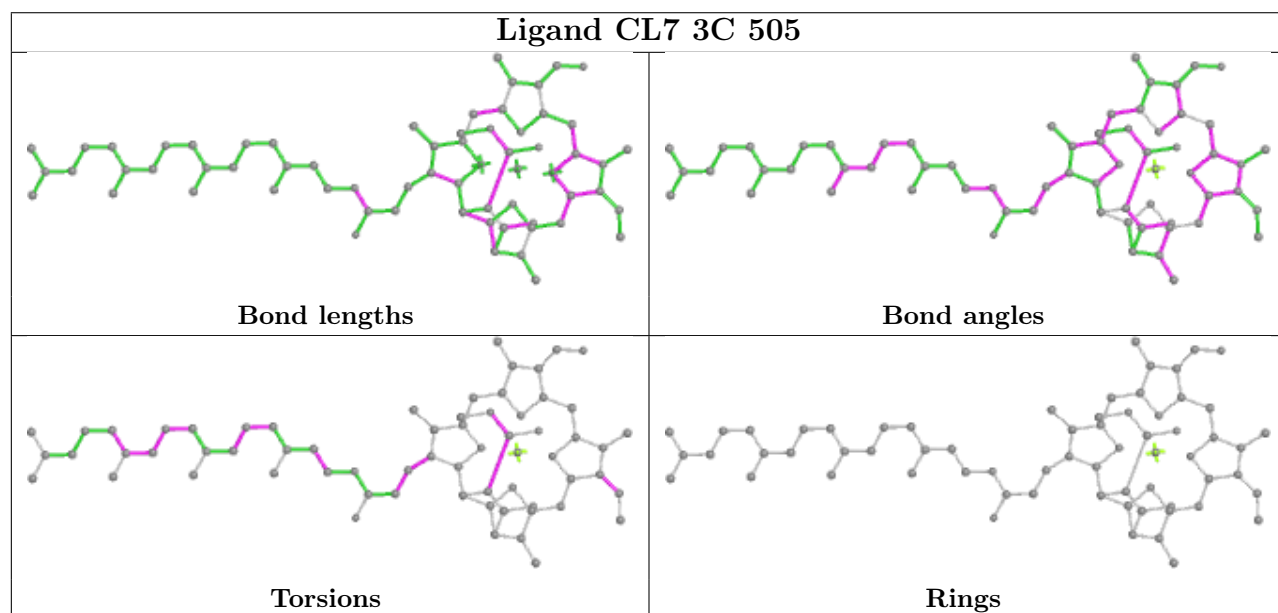
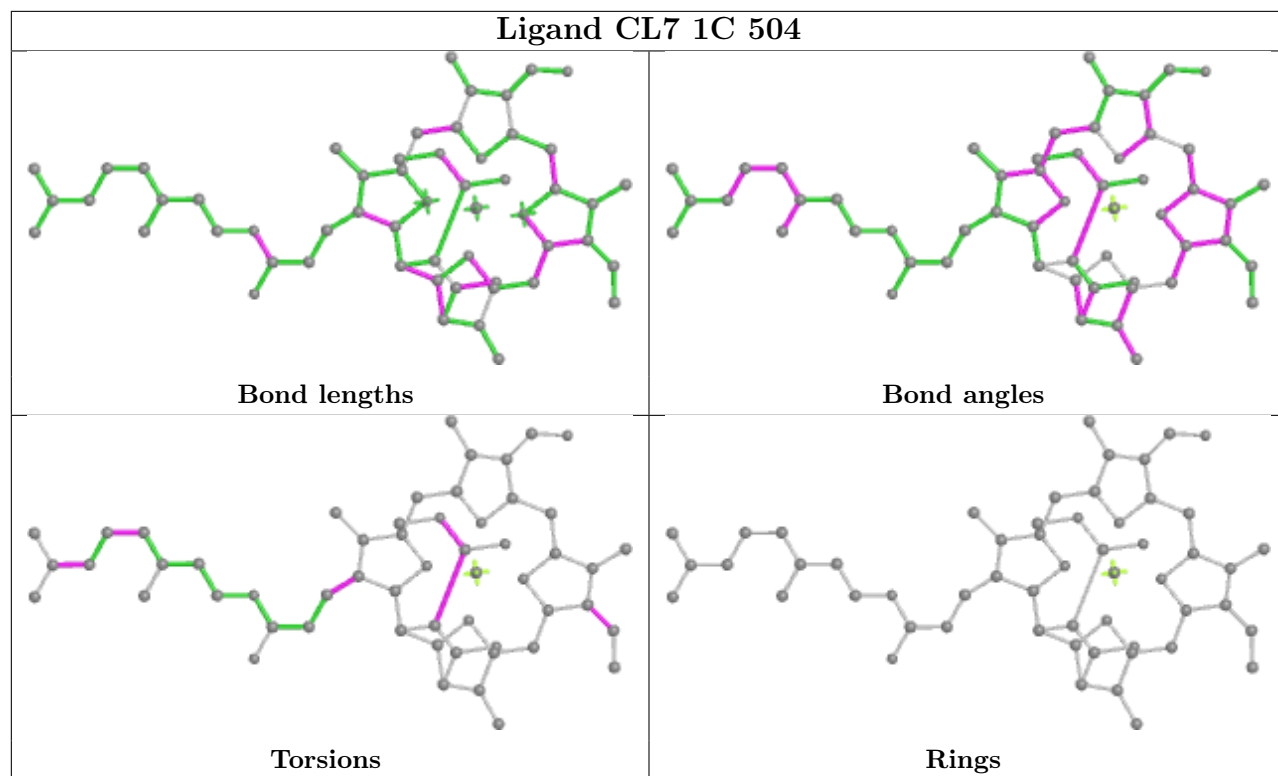


Torsions

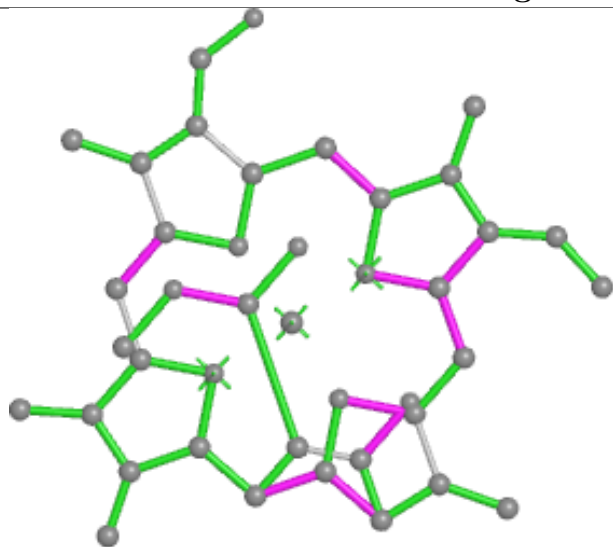


Rings

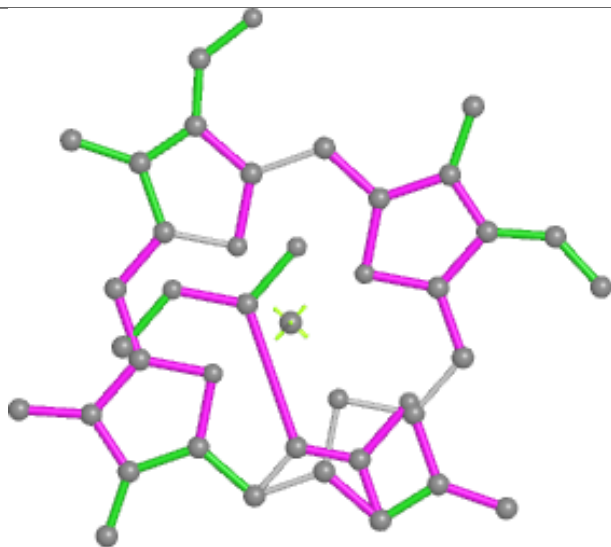




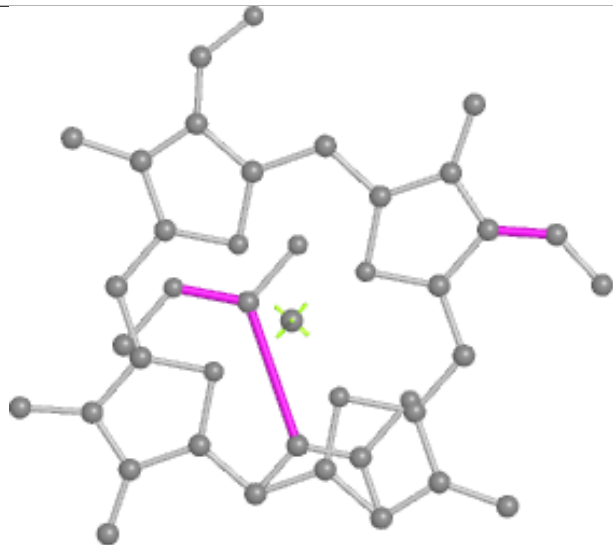
Ligand CL7 44 416



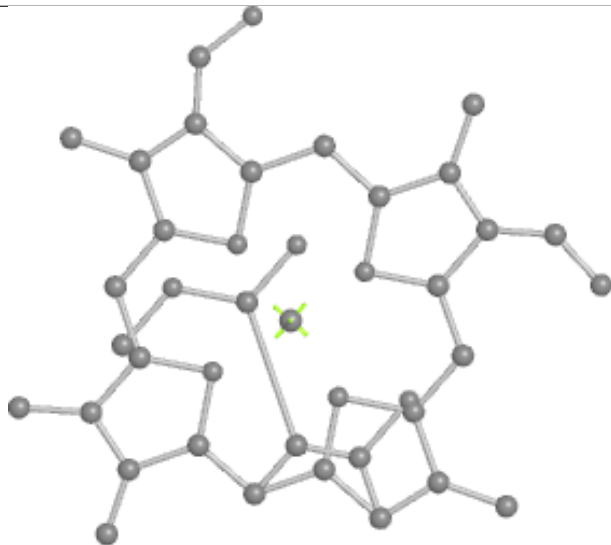
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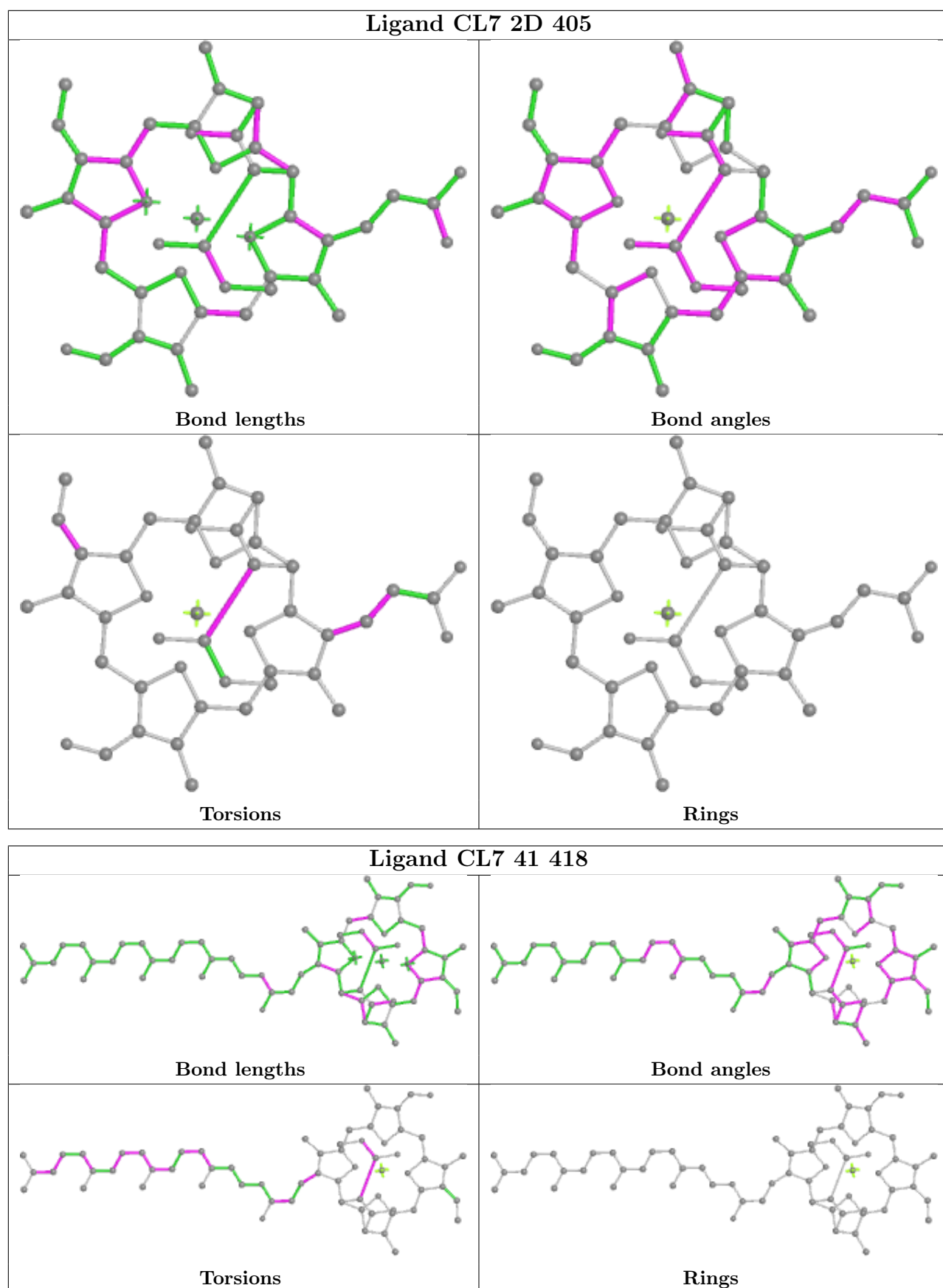
Bond angles

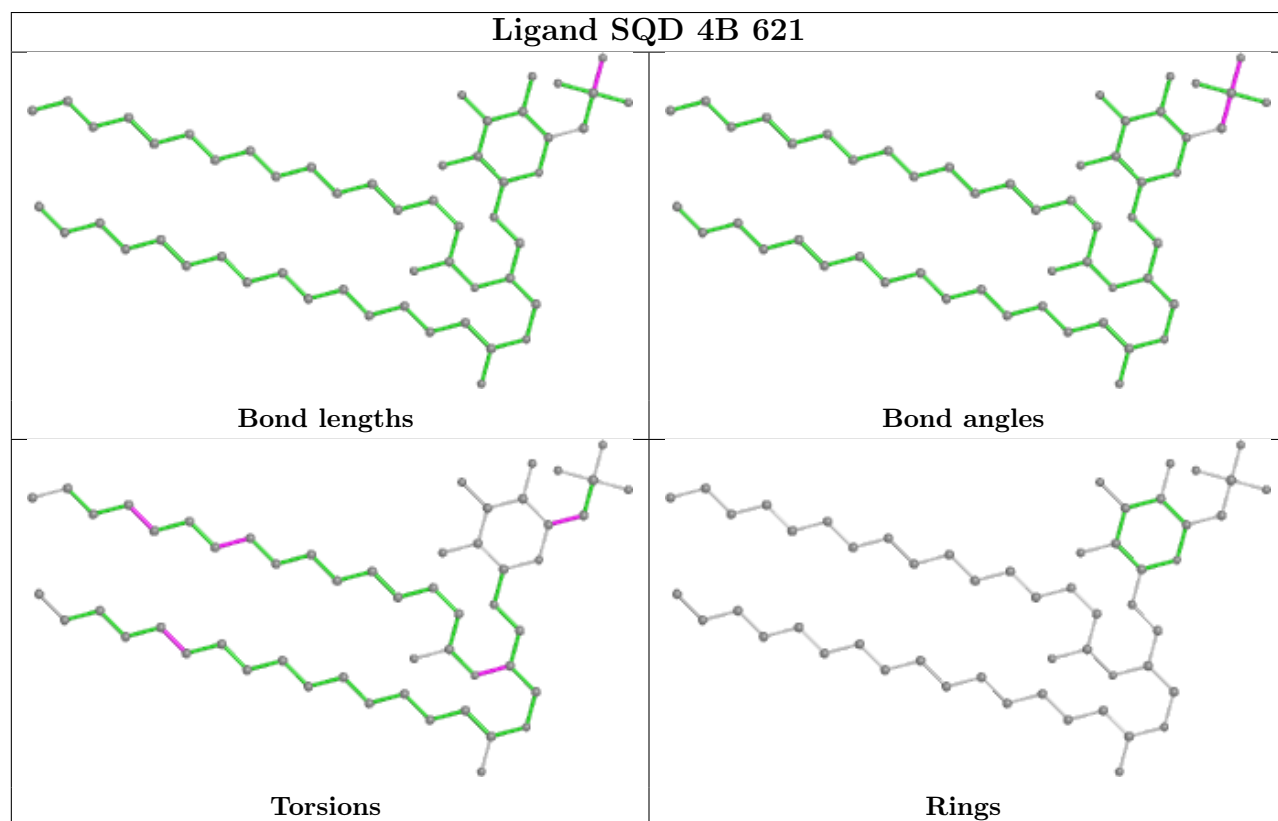
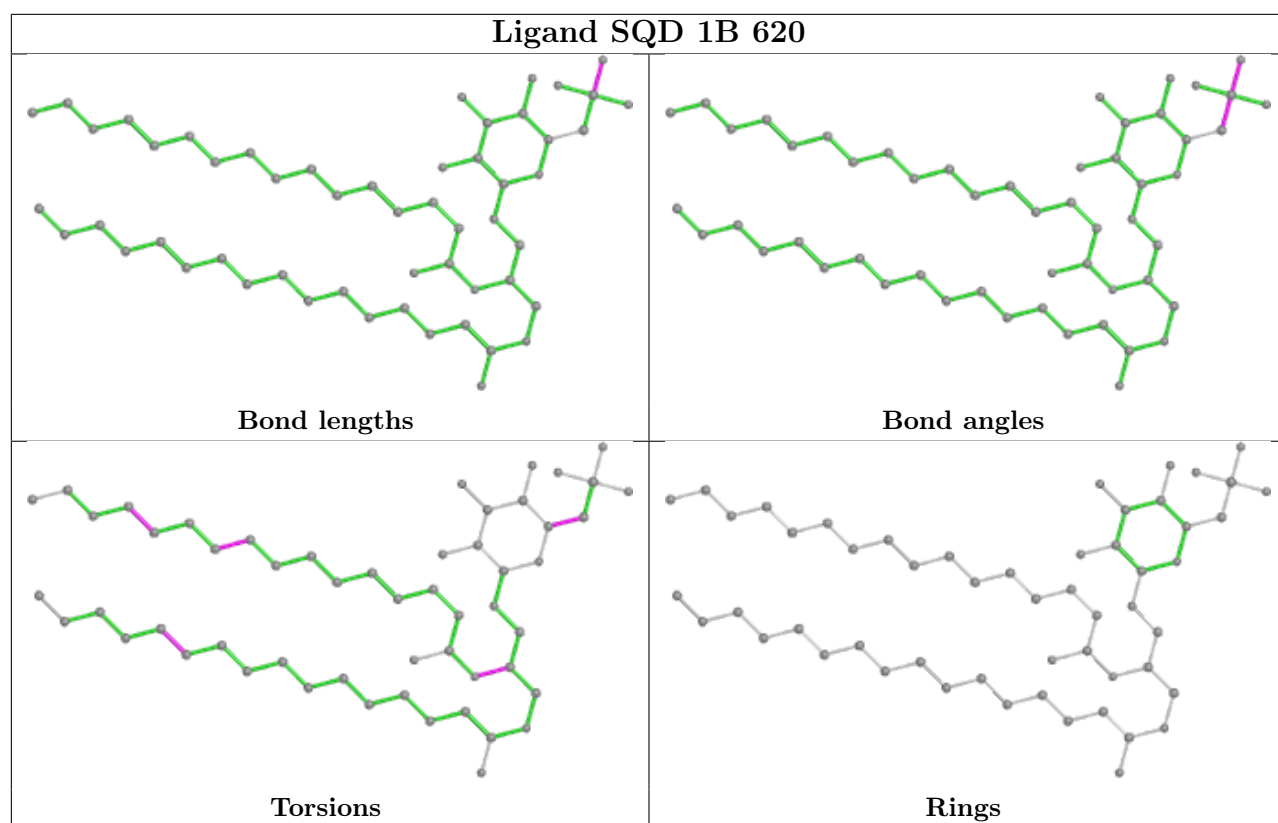


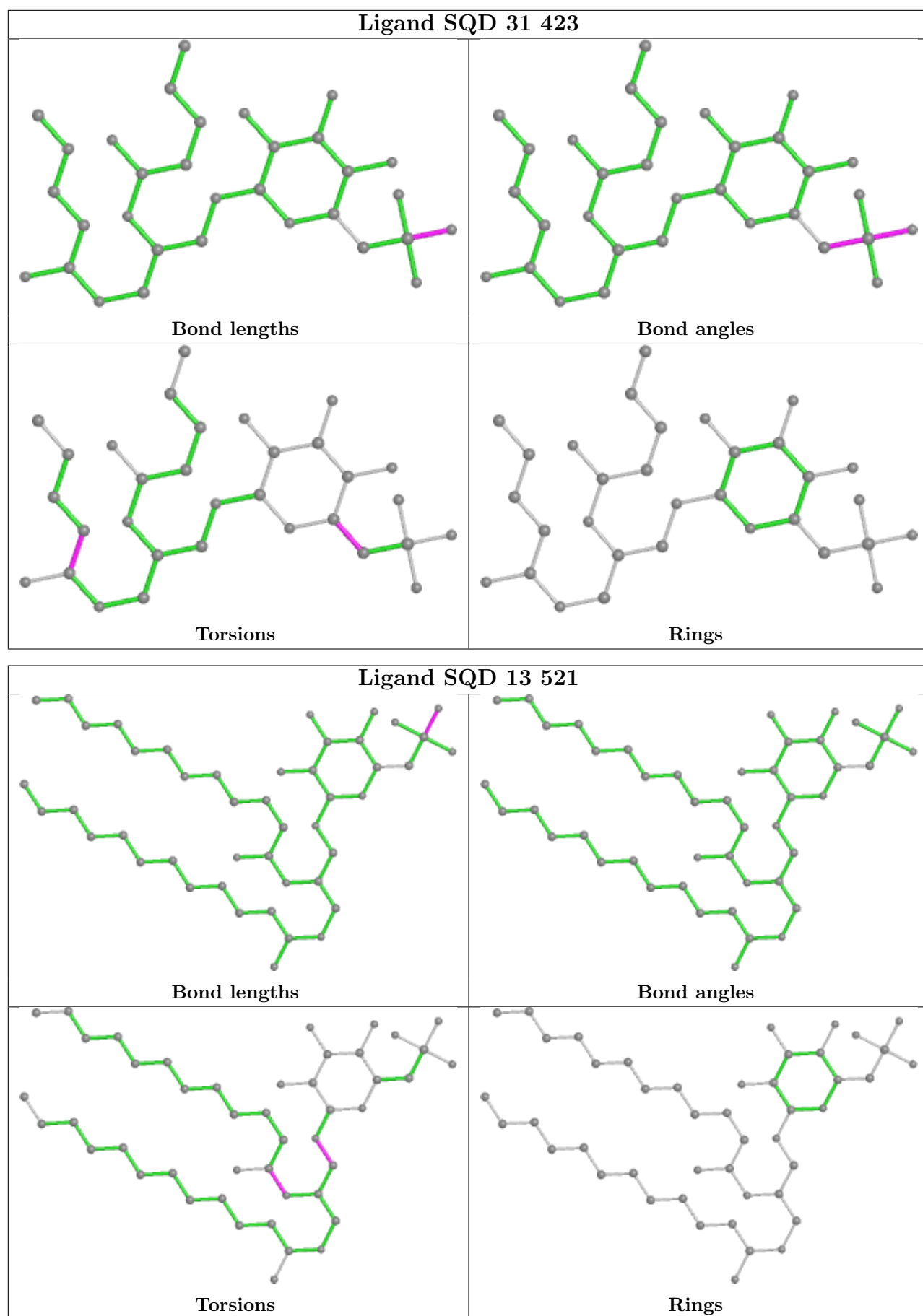
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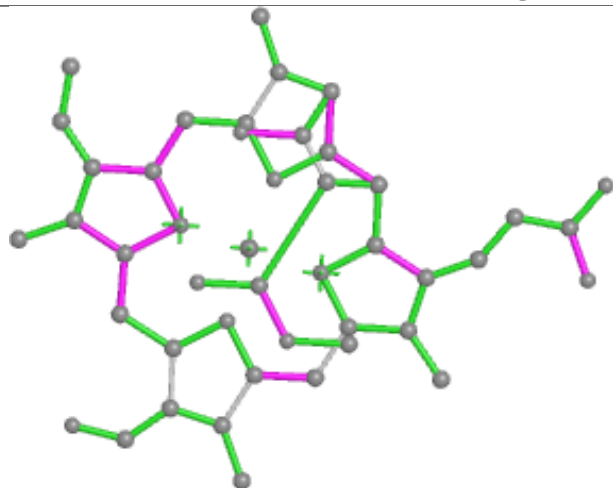
Rings



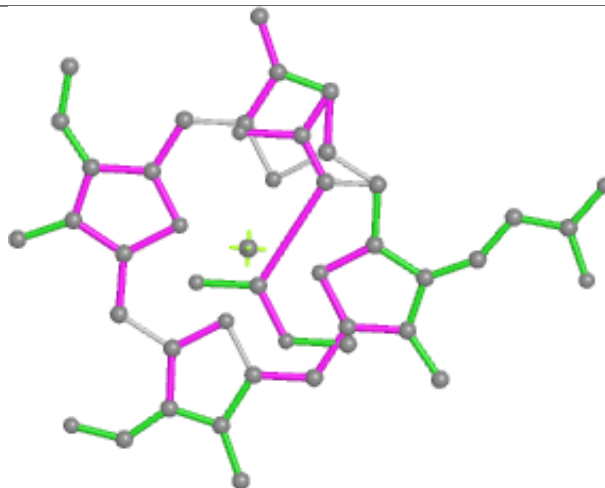




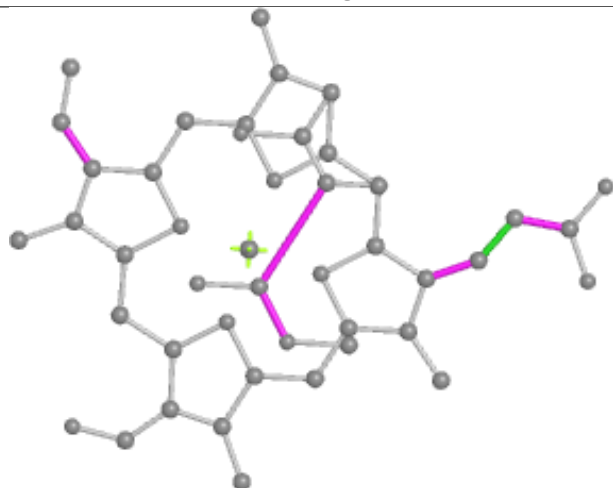
Ligand CL7 33 506



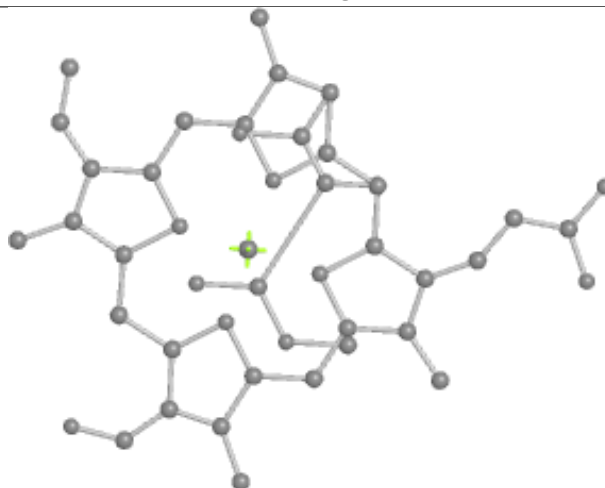
Bond lengths



Bond angles

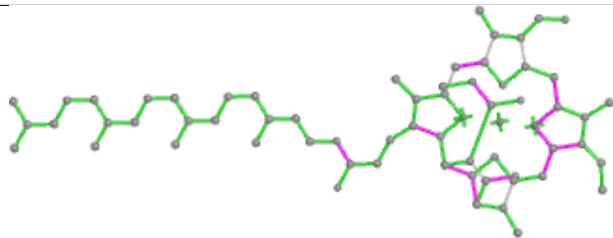


Torsions

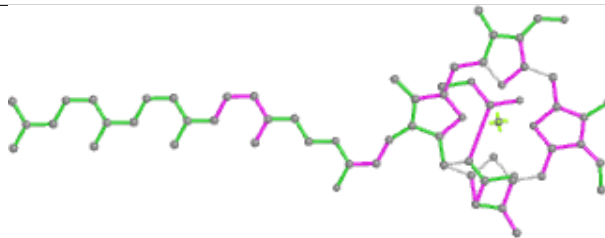


Rings

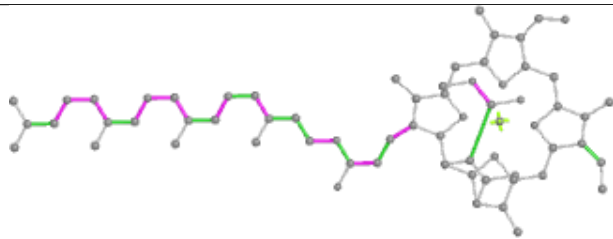
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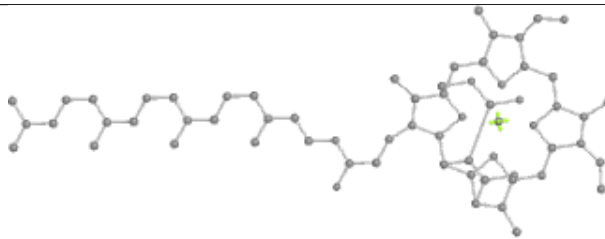
Bond lengths



Bond angles

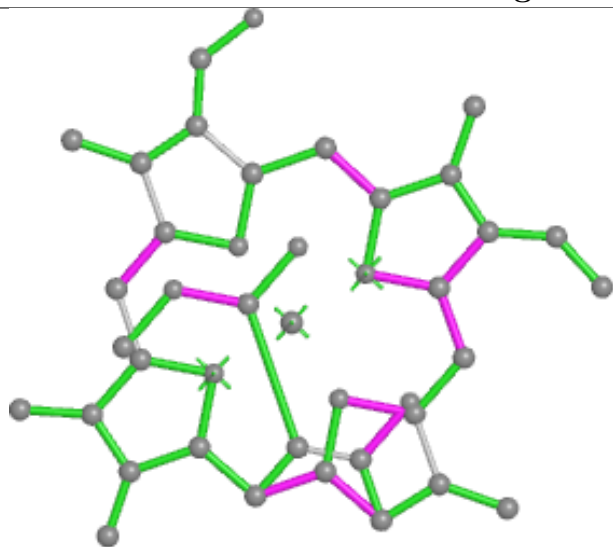


Torsions

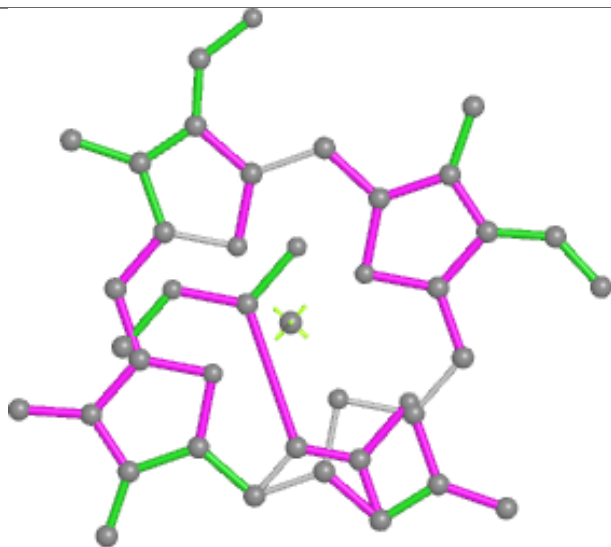


Rings

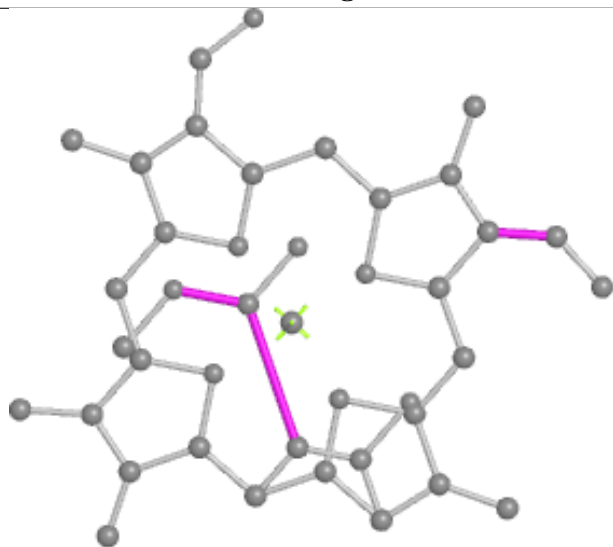
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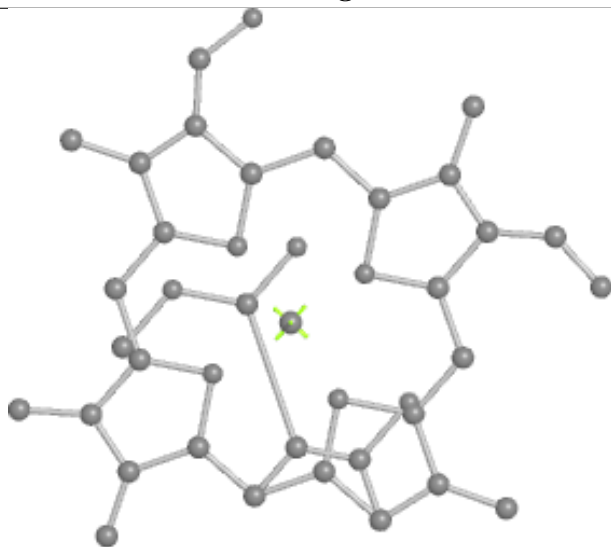
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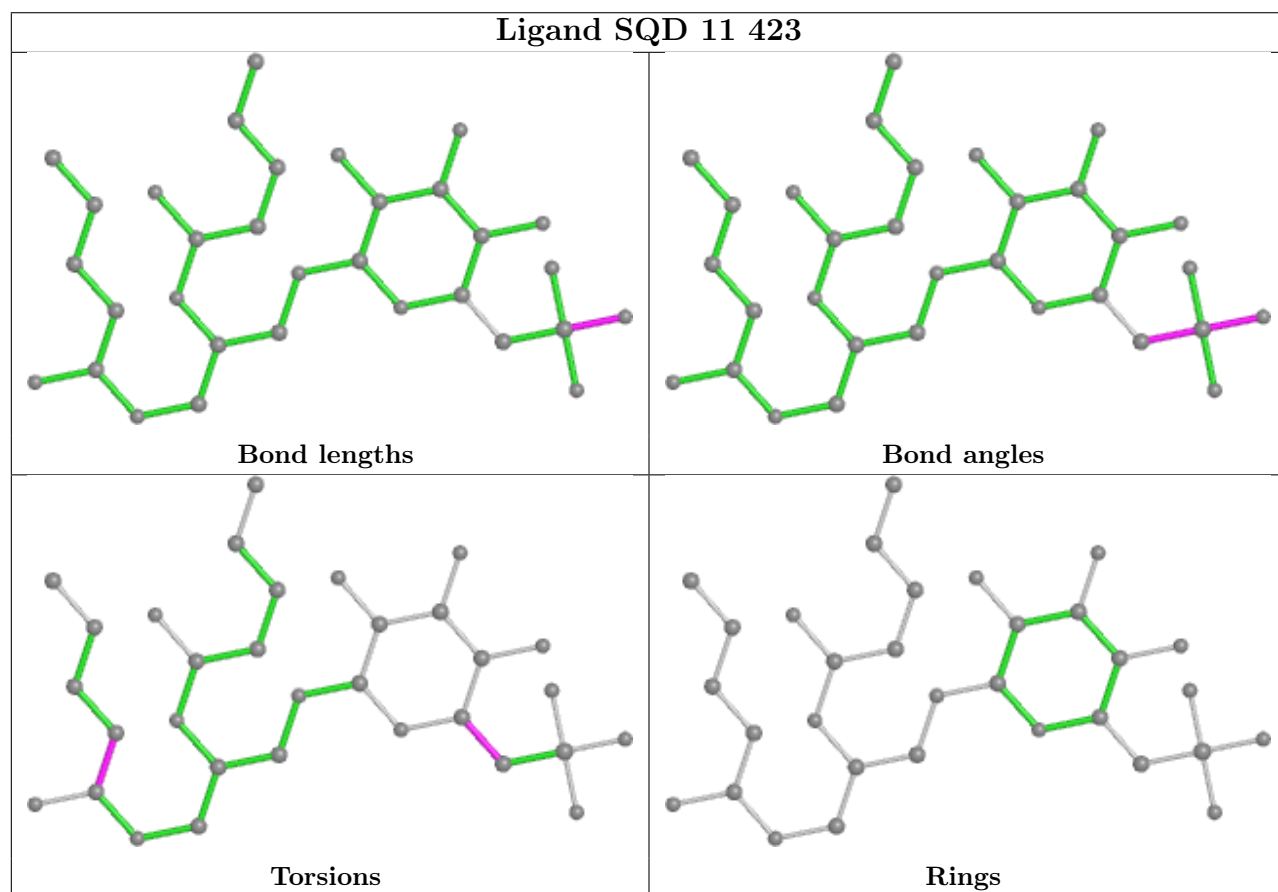
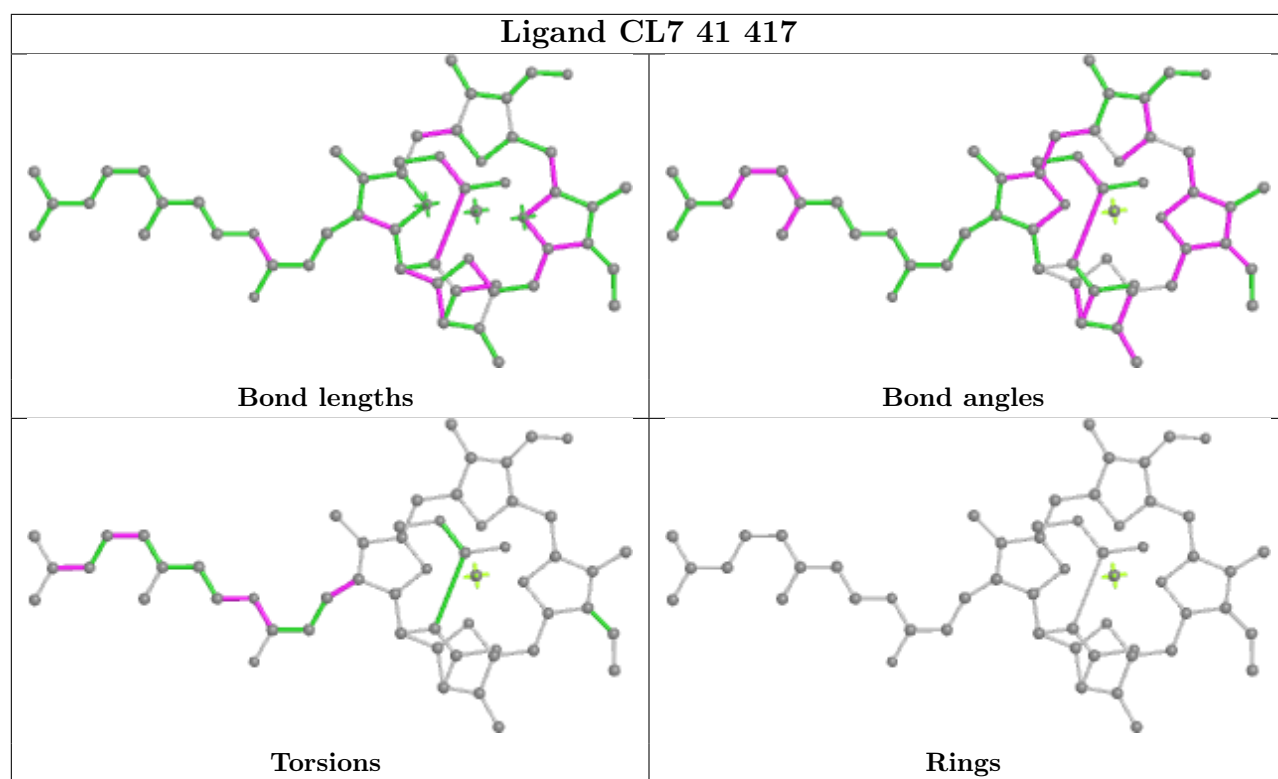
Bond angles

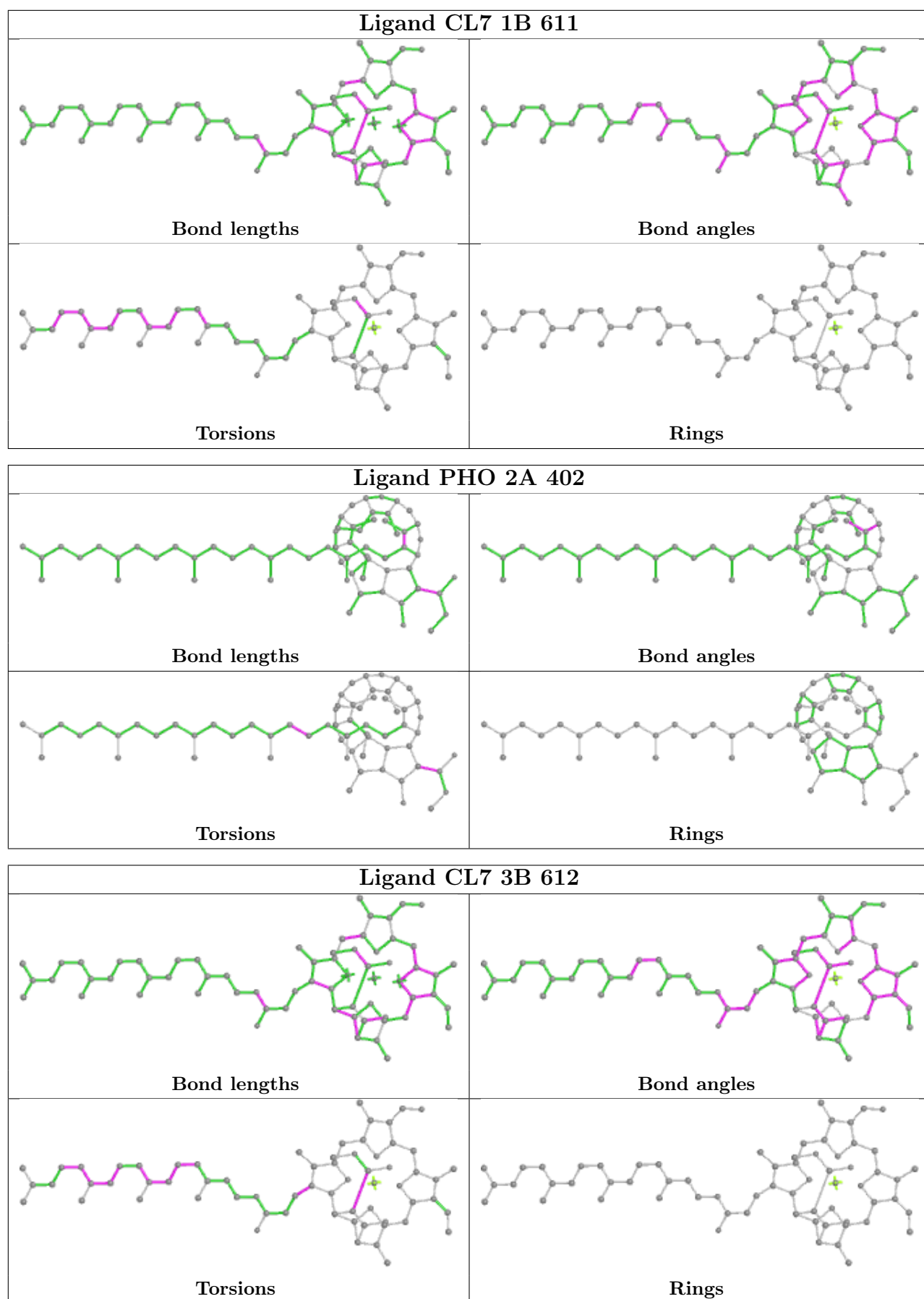


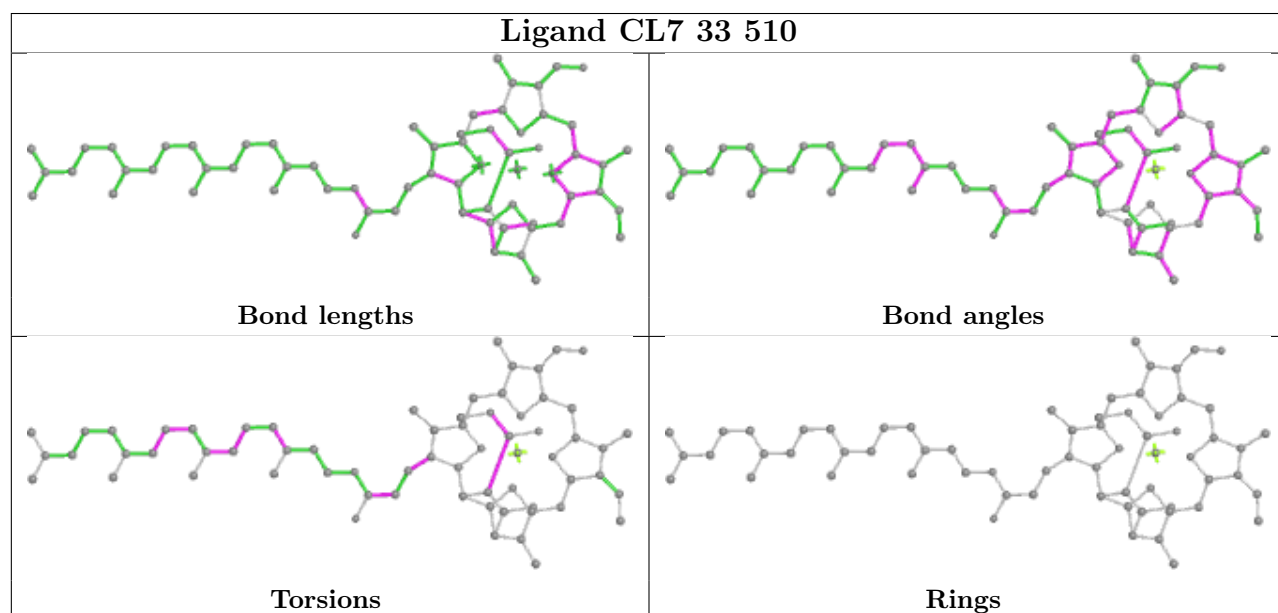
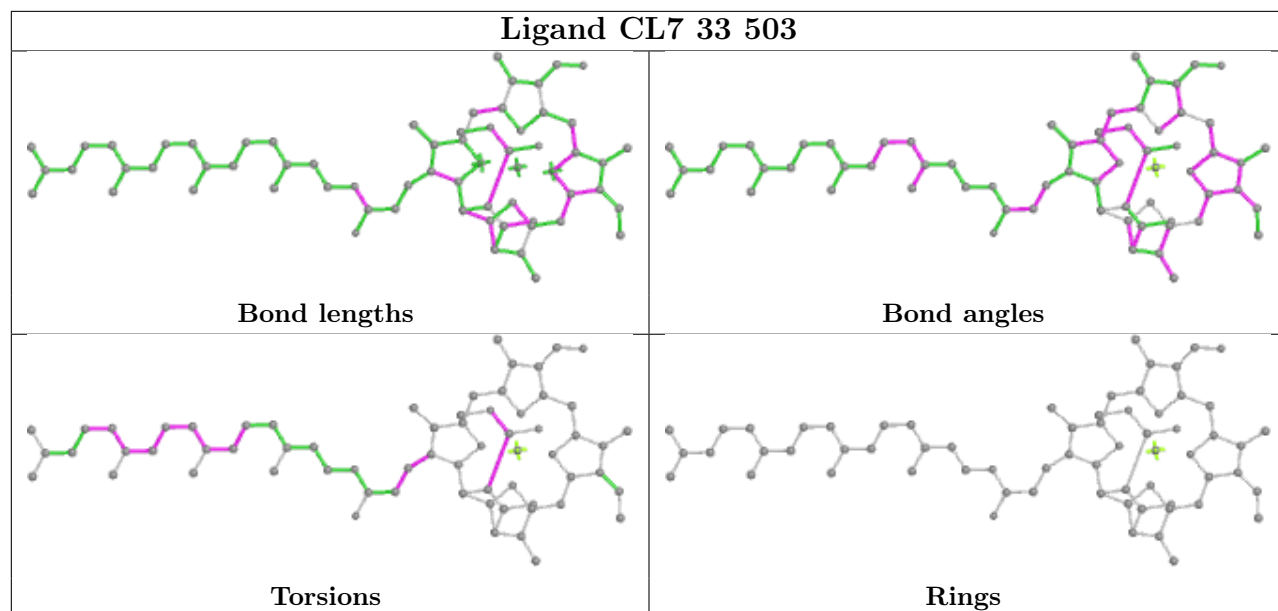
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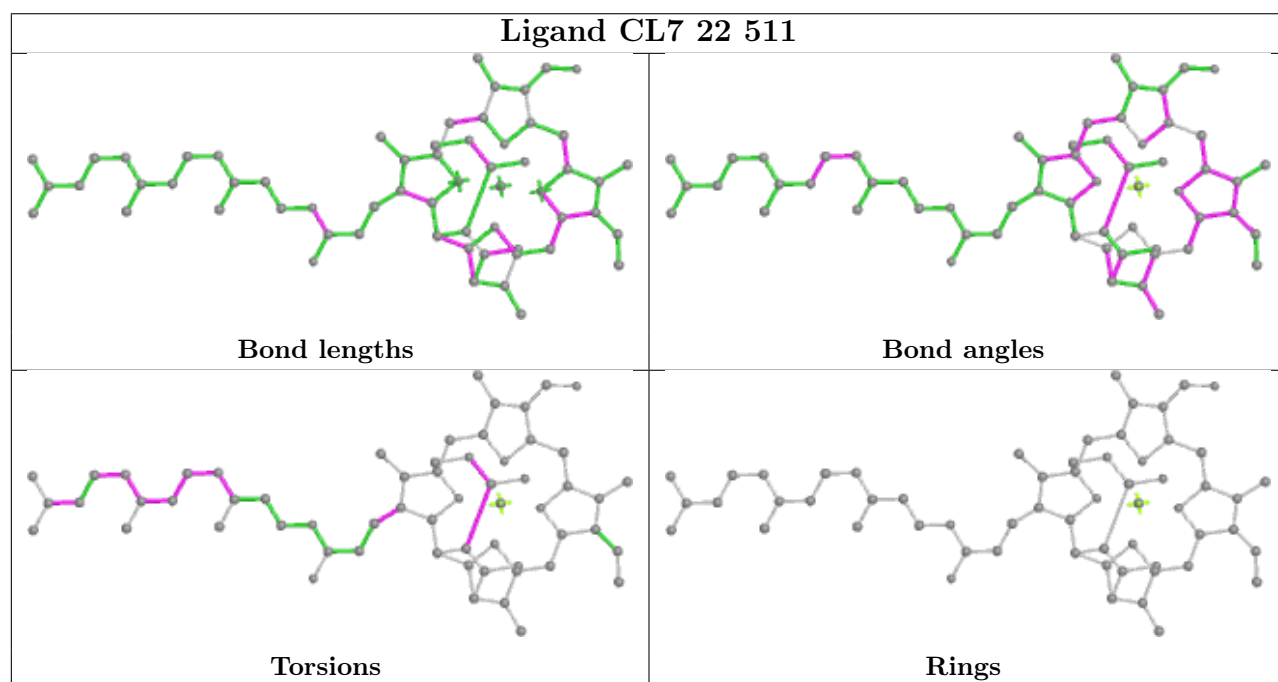
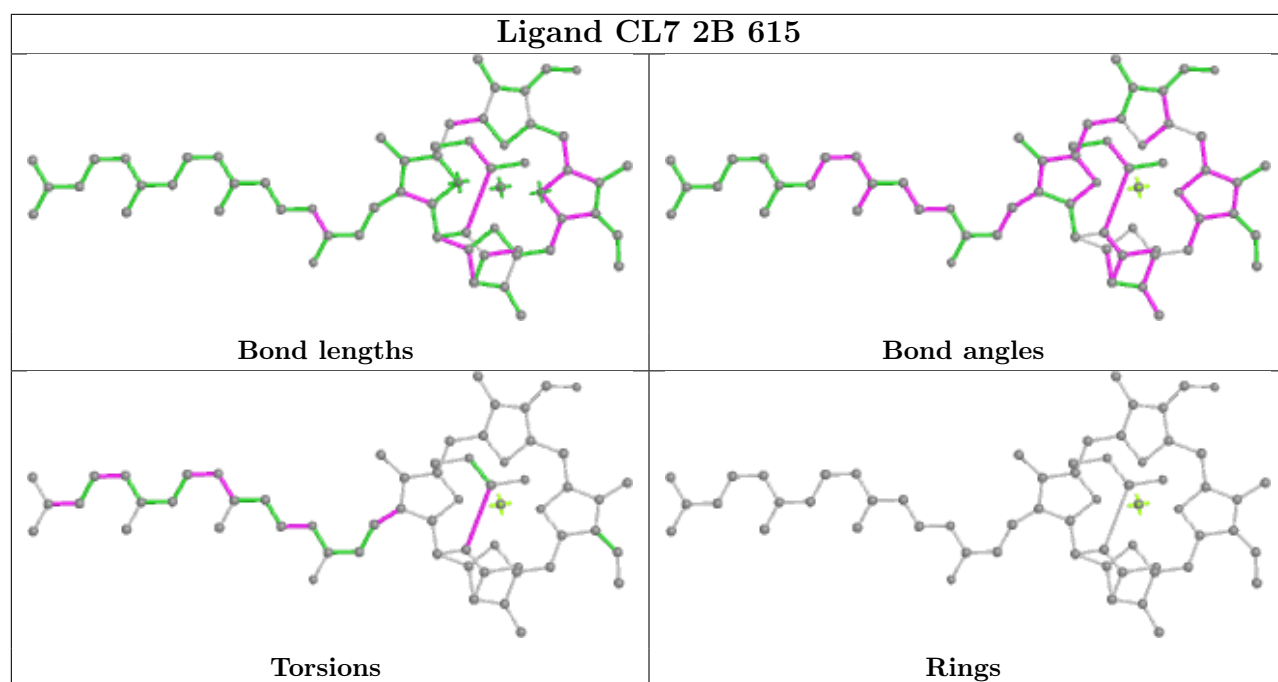


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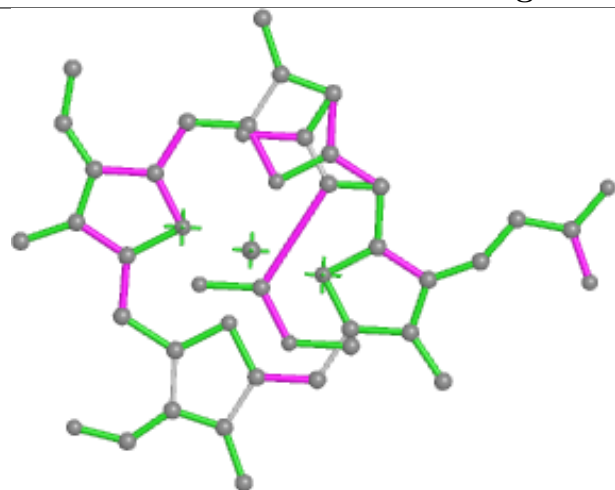




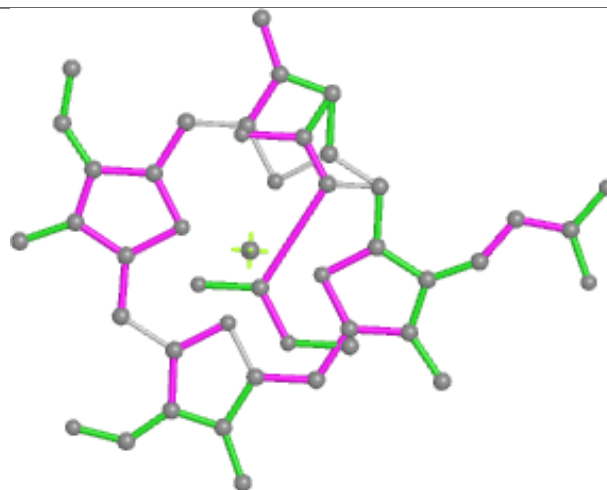




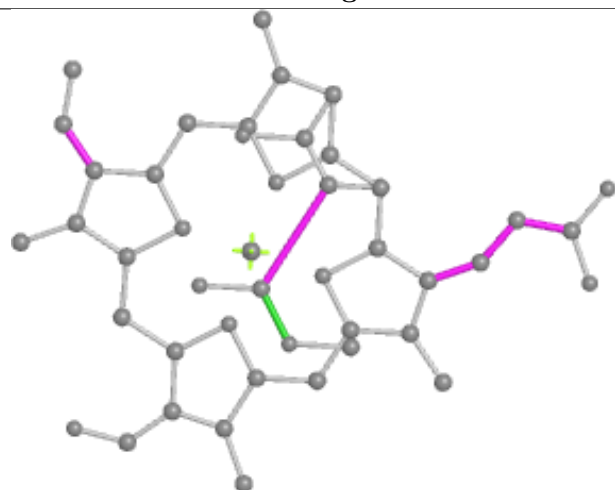
Ligand CL7 23 414



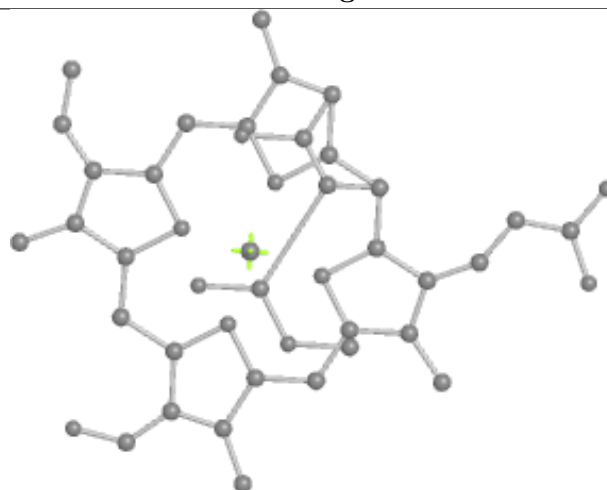
Bond lengths



Bond angles

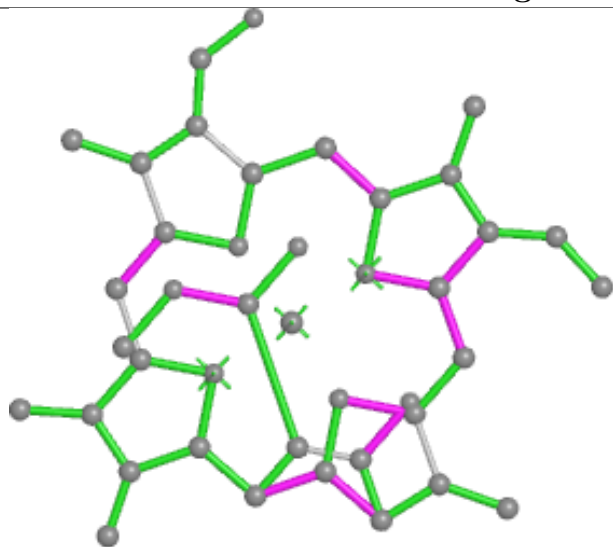


Torsions

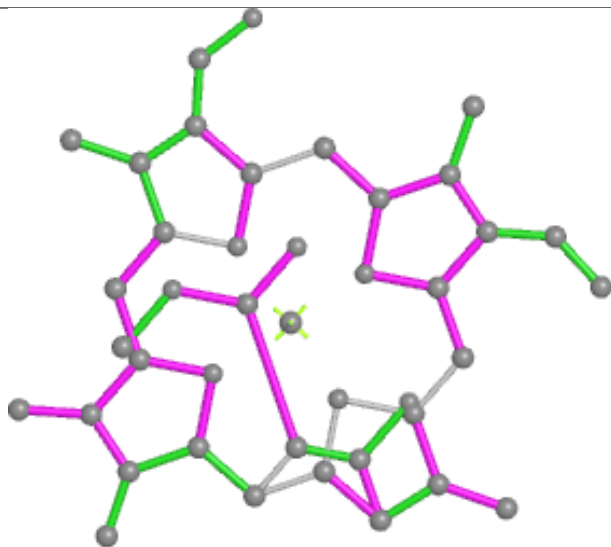


Rings

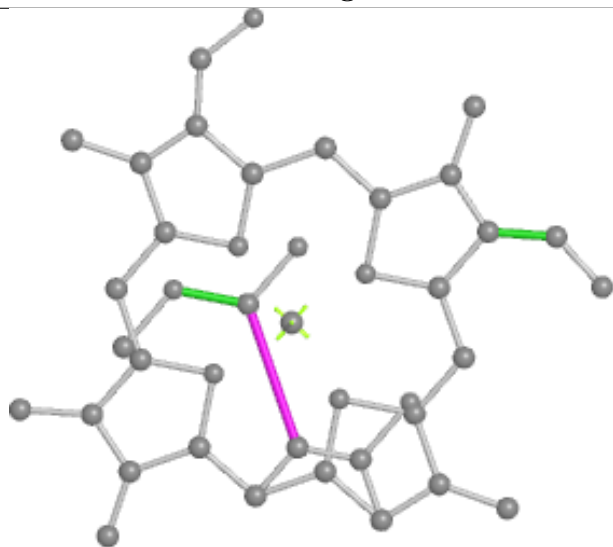
Ligand CL7 41 413



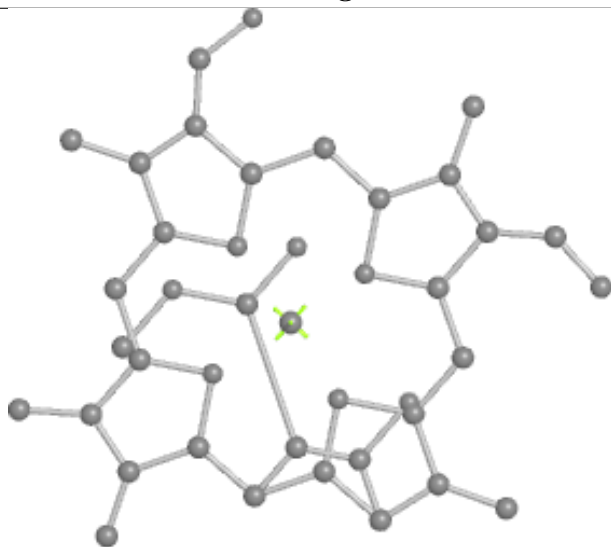
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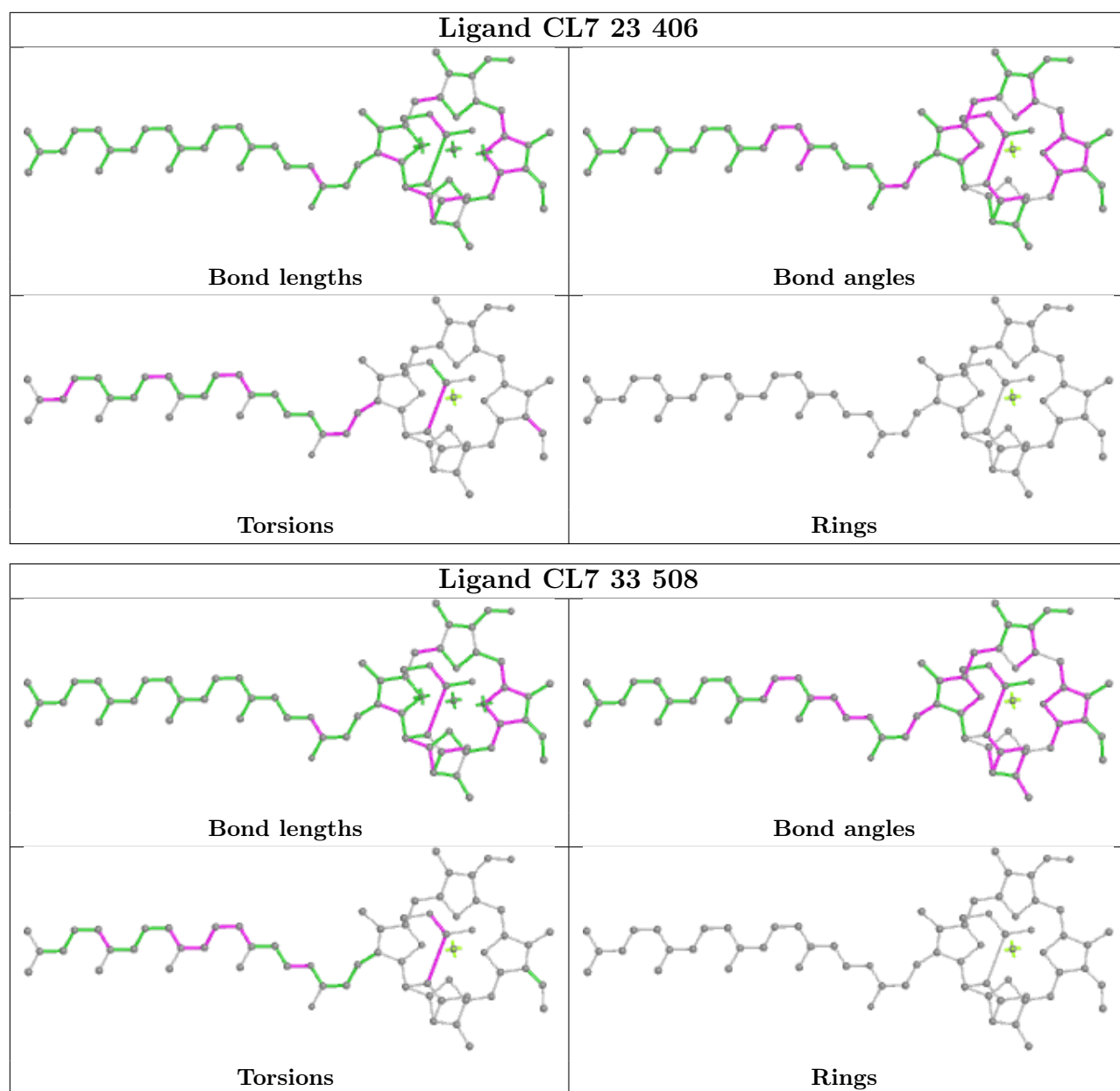
Bond angles

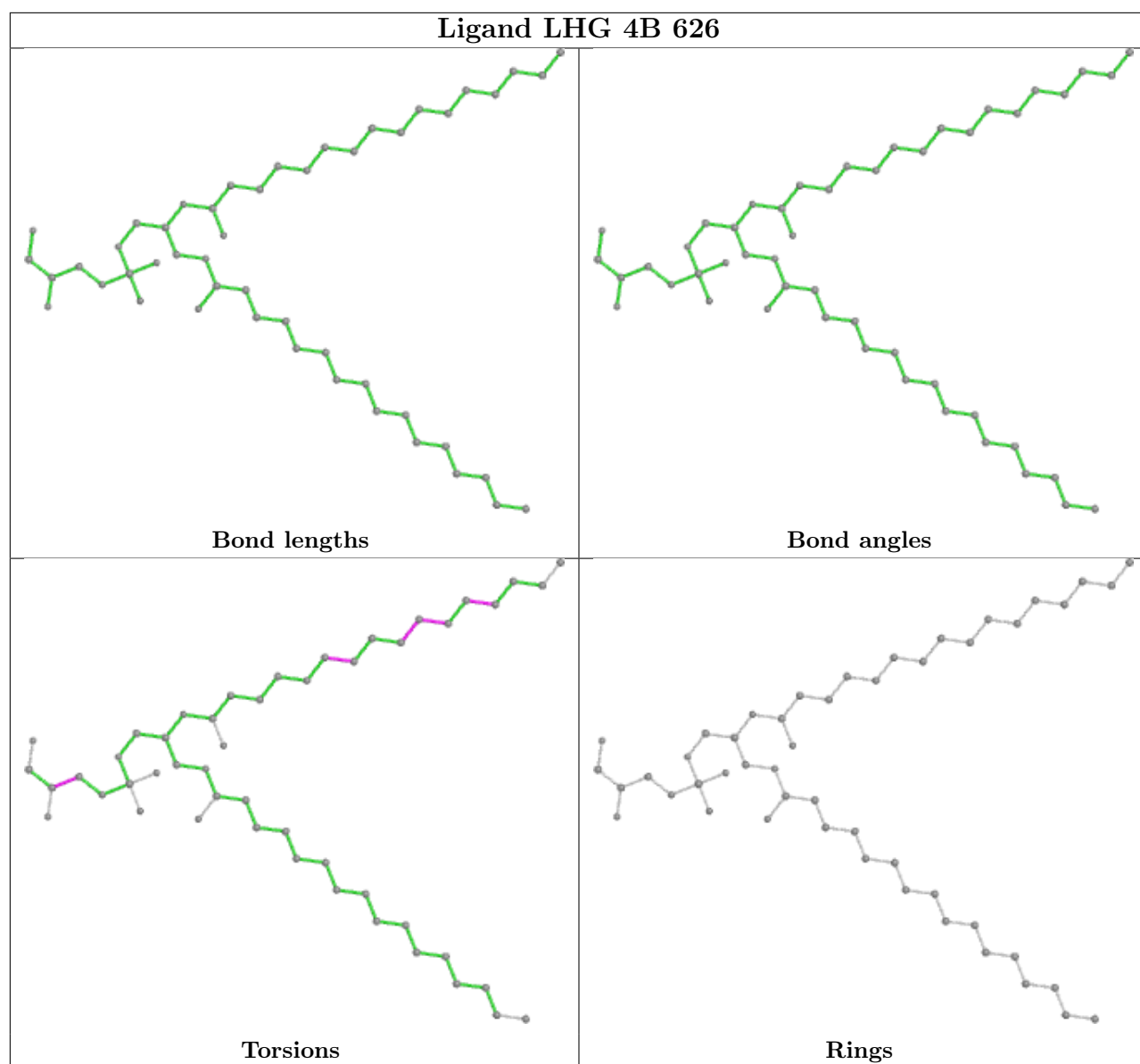


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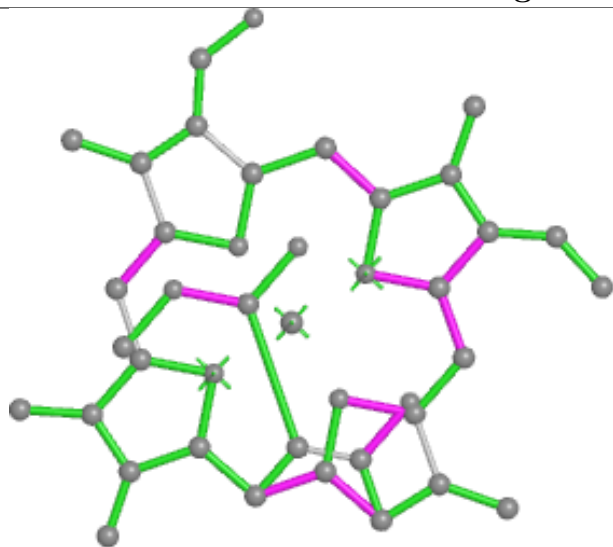


Rings

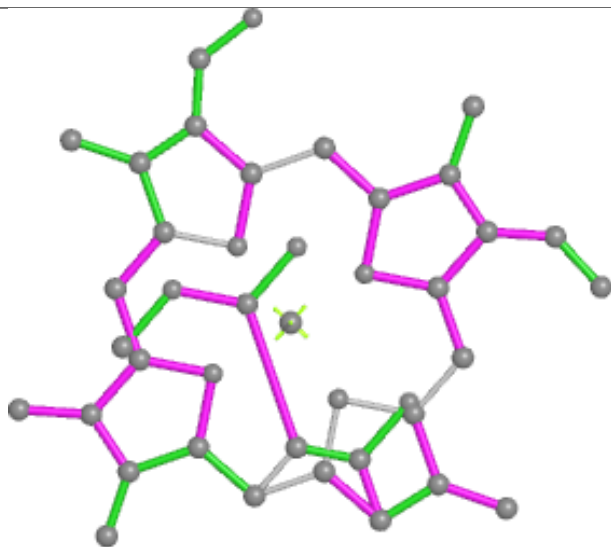




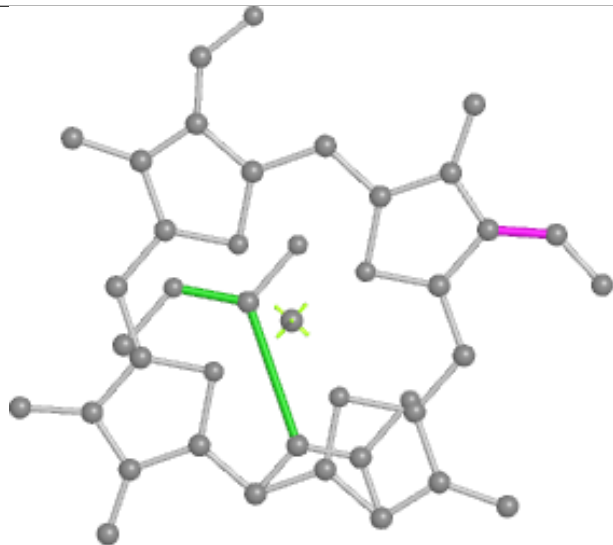
Ligand CL7 21 414



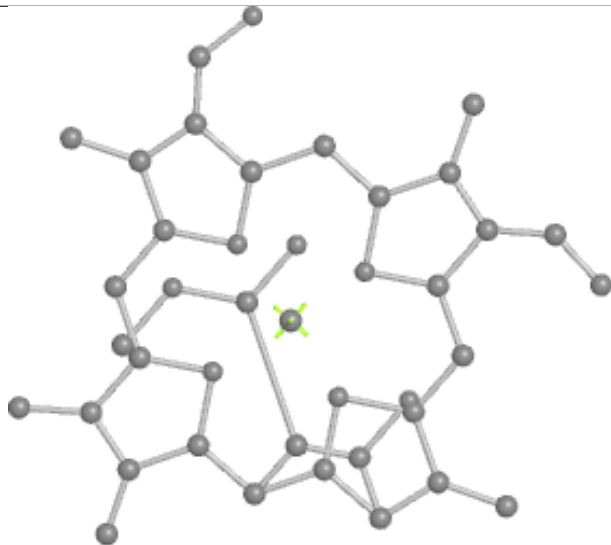
Bond lengths



Bond angles

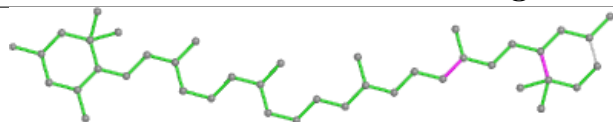


Torsions

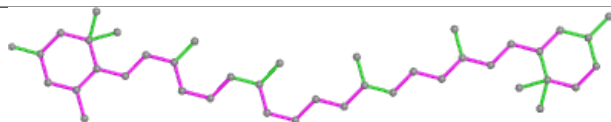


Rings

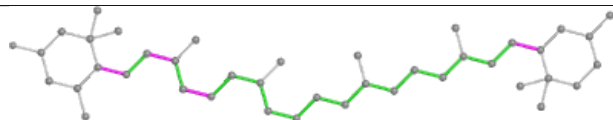
Ligand ZEX 11 422



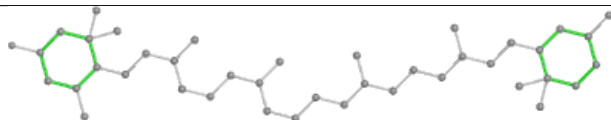
Bond lengths



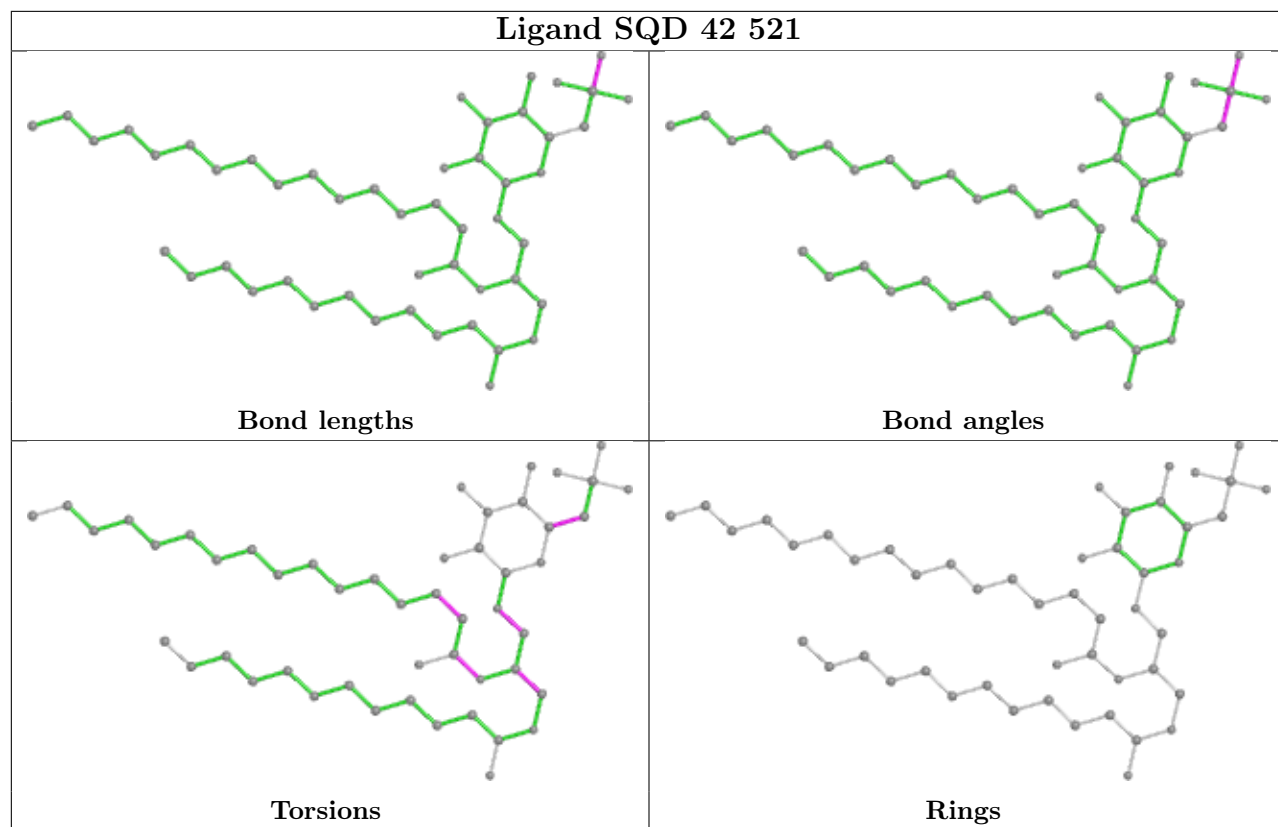
Bond angles



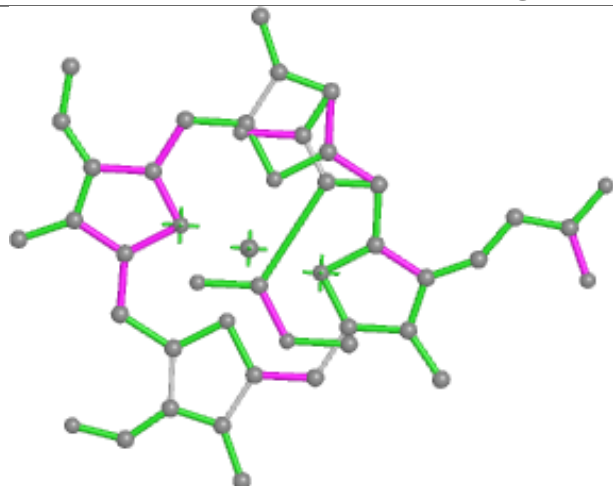
Torsions



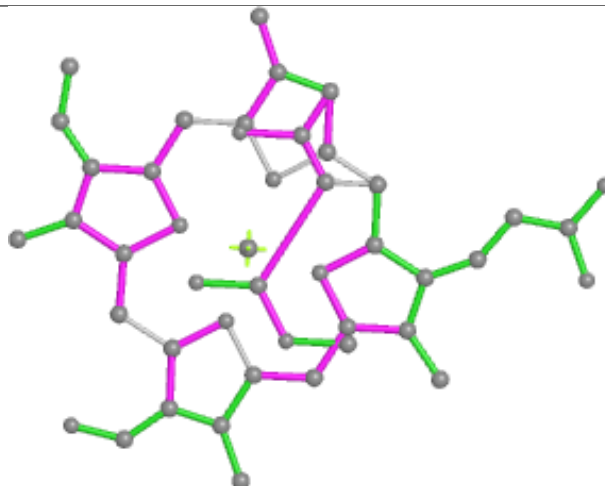
Rings



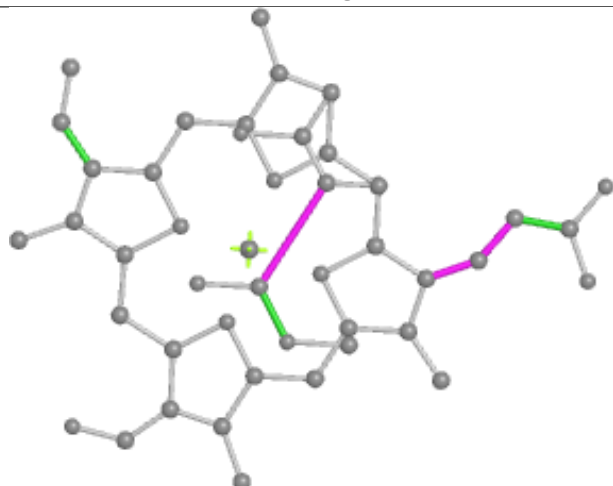
Ligand CL7 32 508



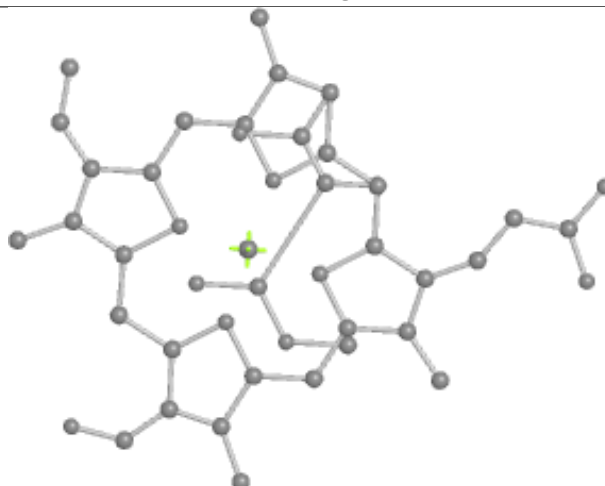
Bond lengths



Bond angles

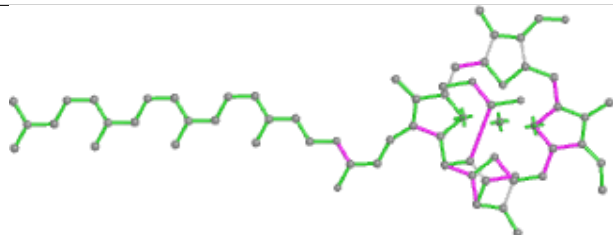


Torsions

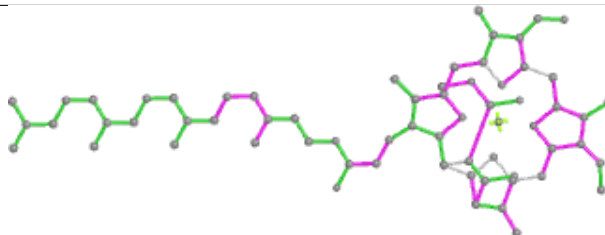


Rings

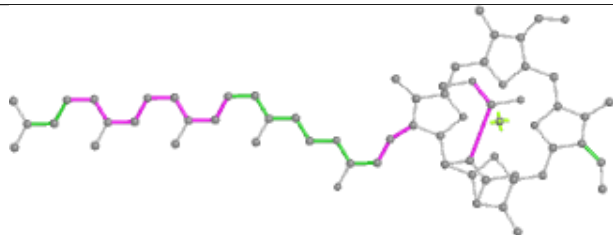
Ligand CL7 23 404



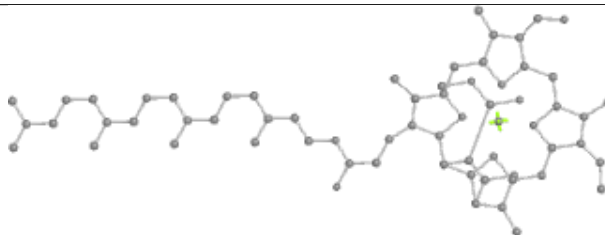
Bond lengths



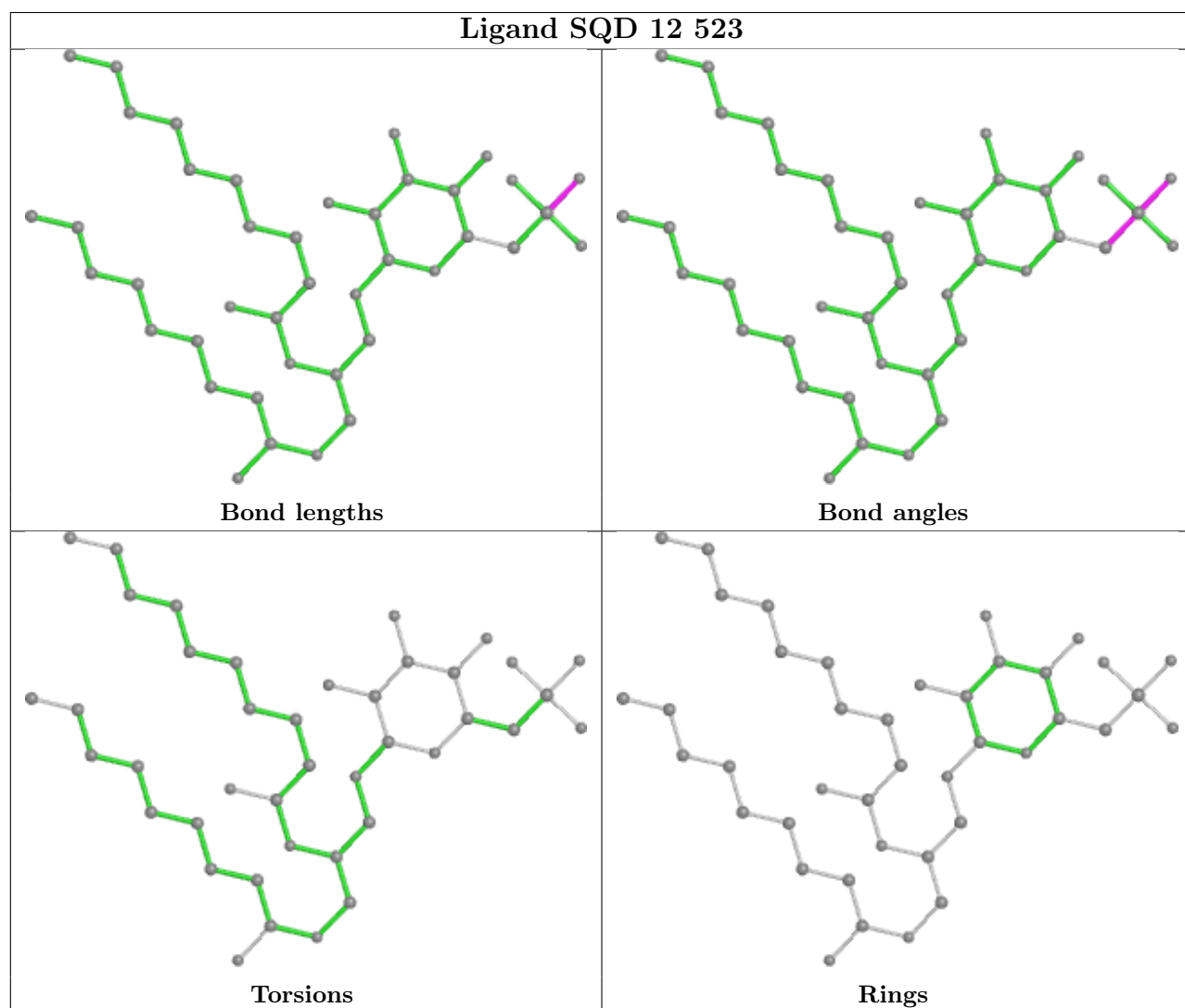
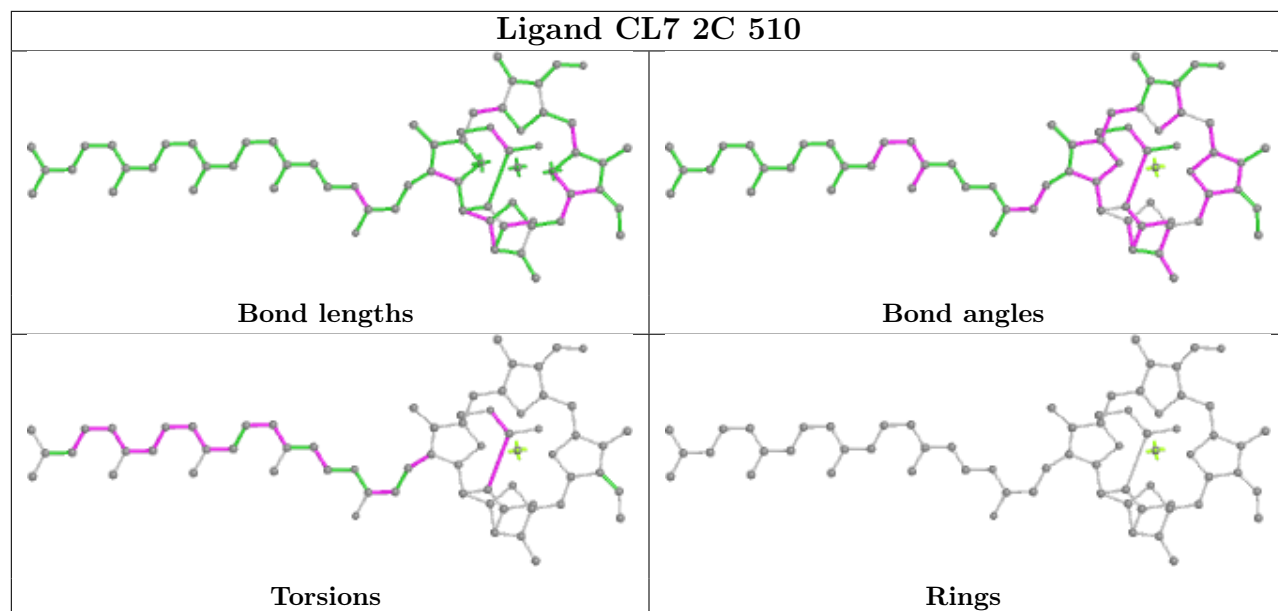
Bond angles

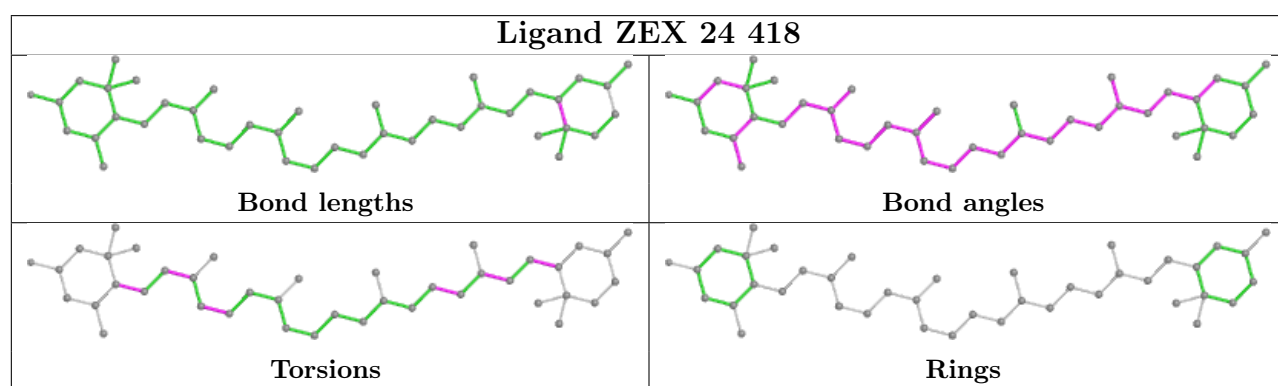
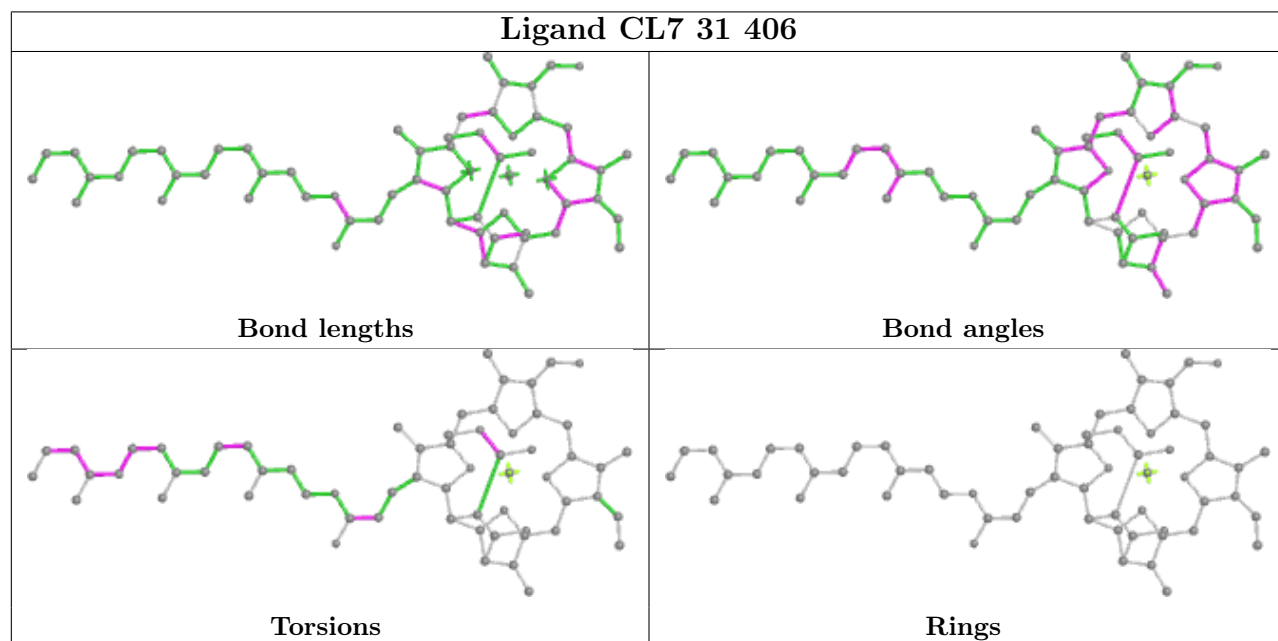
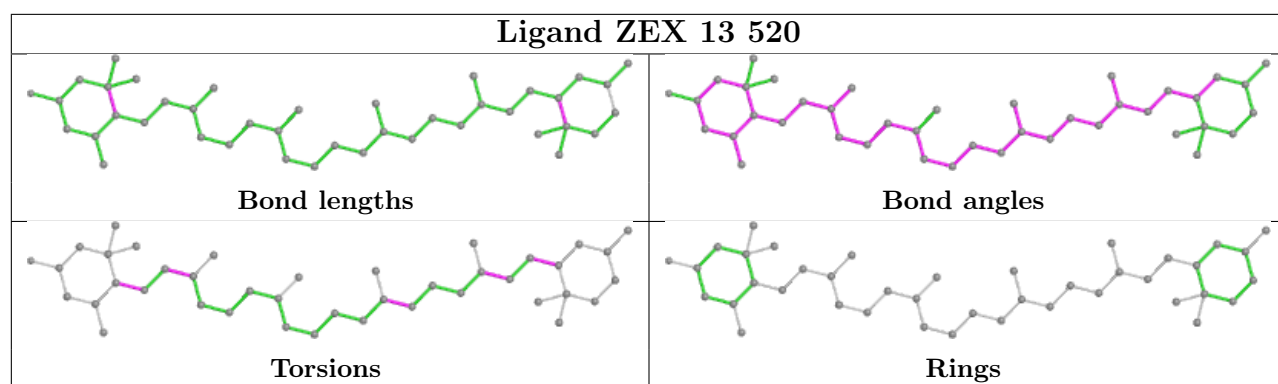


Torsions

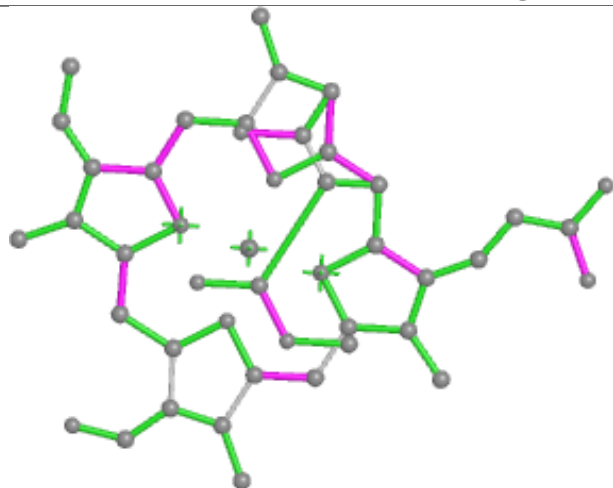


Rings

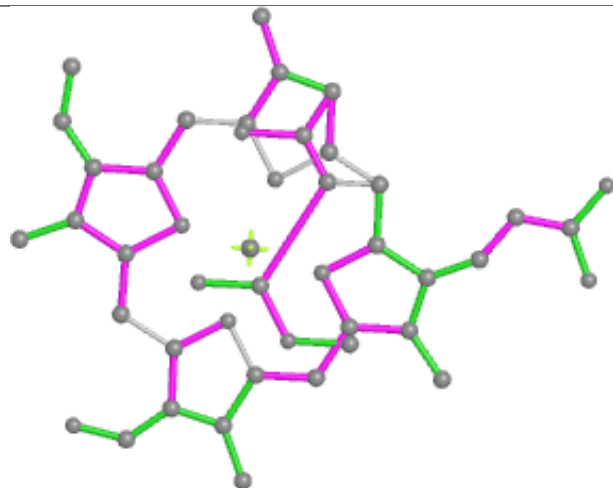




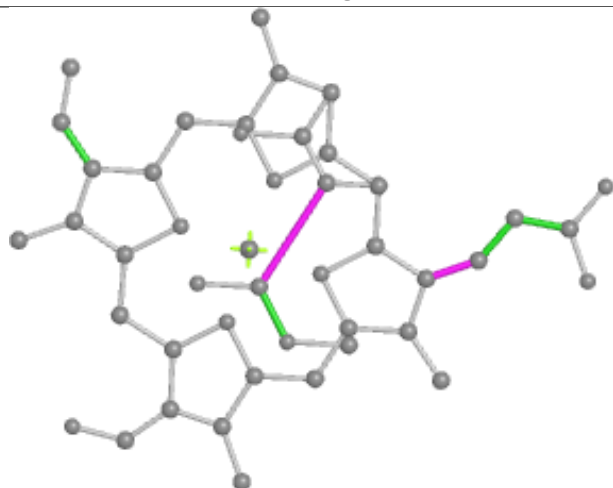
Ligand CL7 42 515



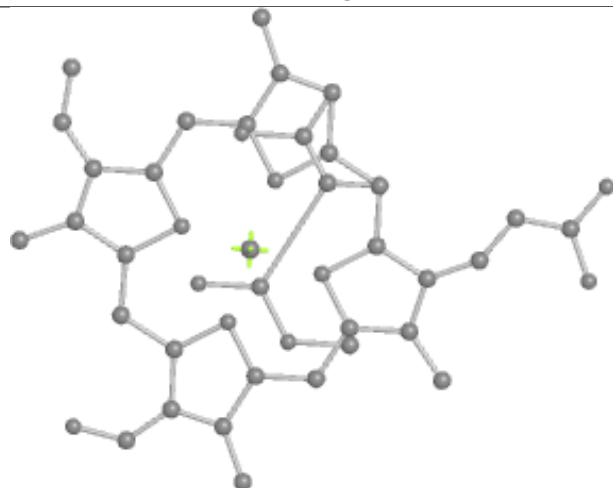
Bond lengths



Bond angles

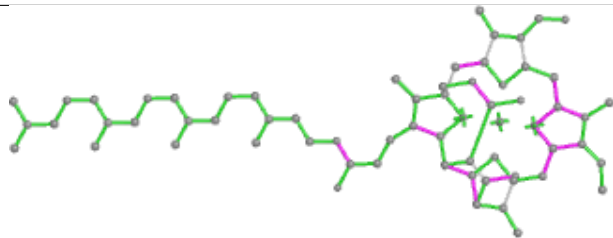


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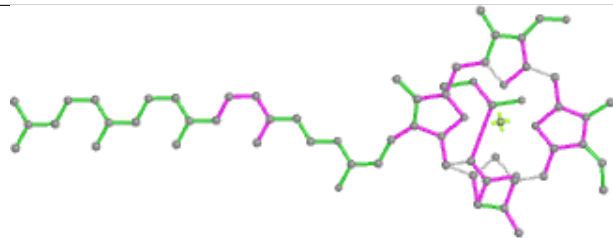


Rings

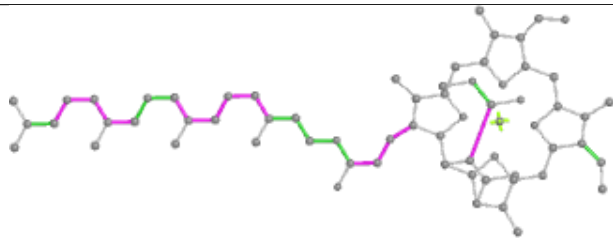
Ligand CL7 43 402



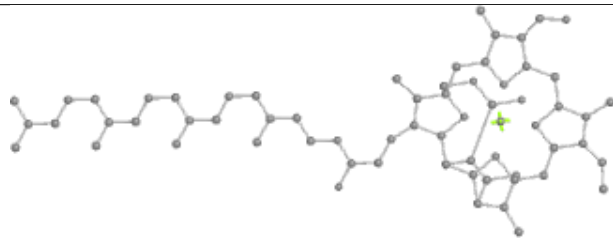
Bond lengths



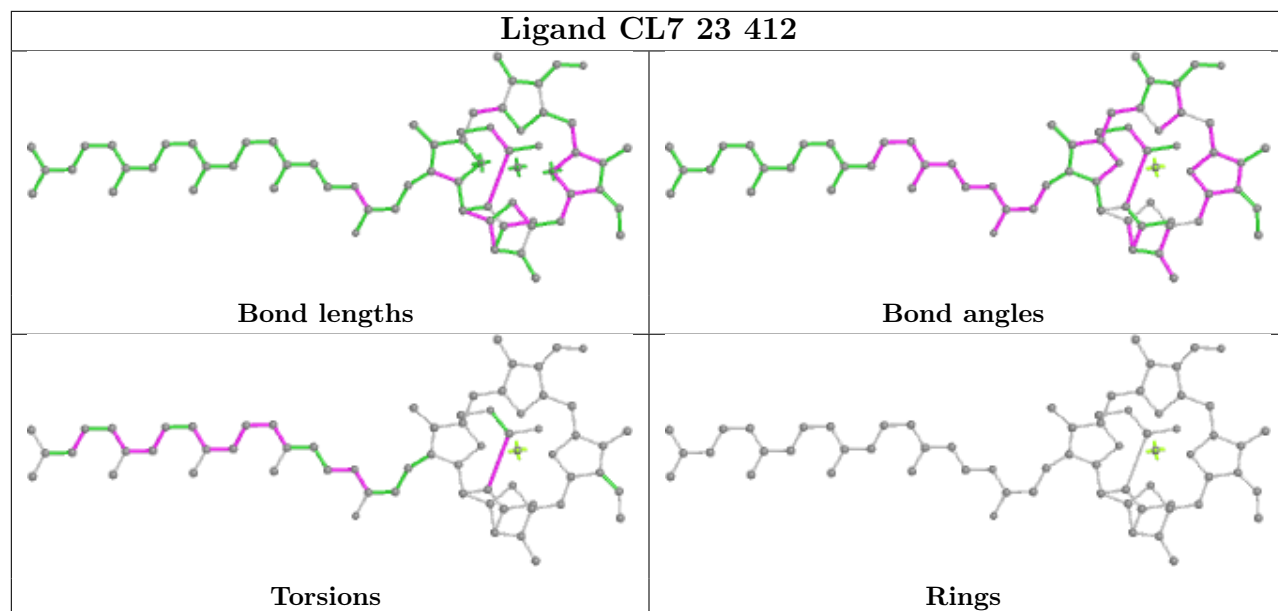
Bond angles



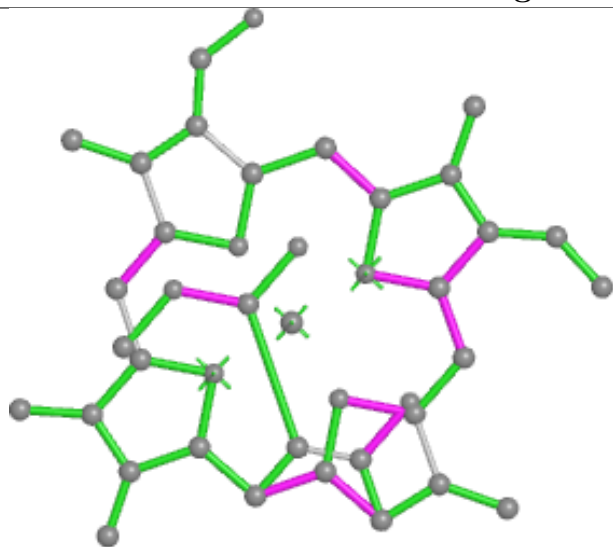
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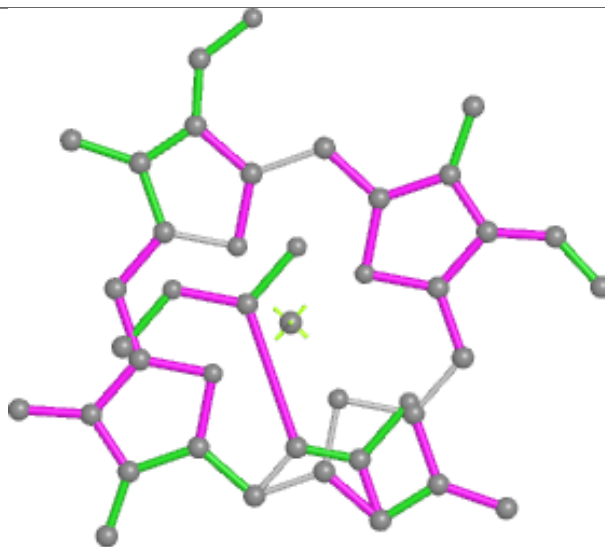
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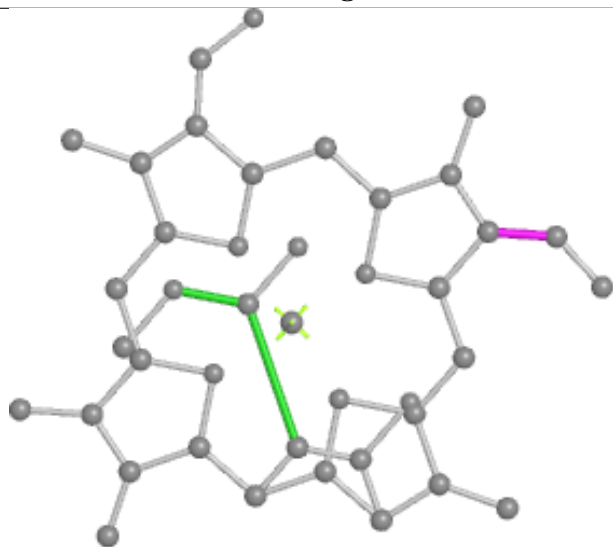
Ligand CL7 41 414



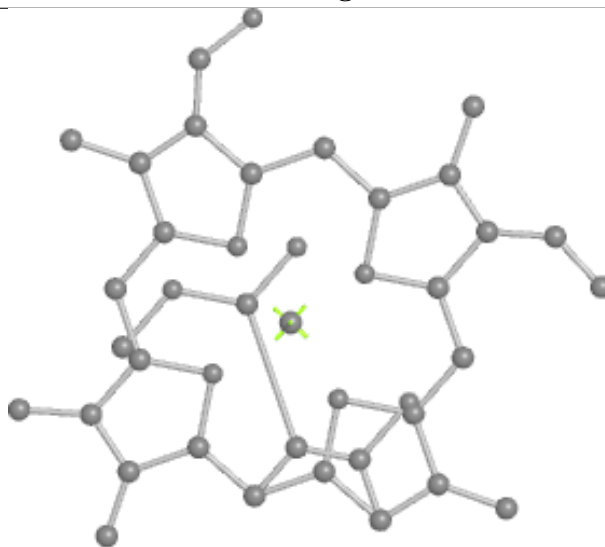
Bond lengths



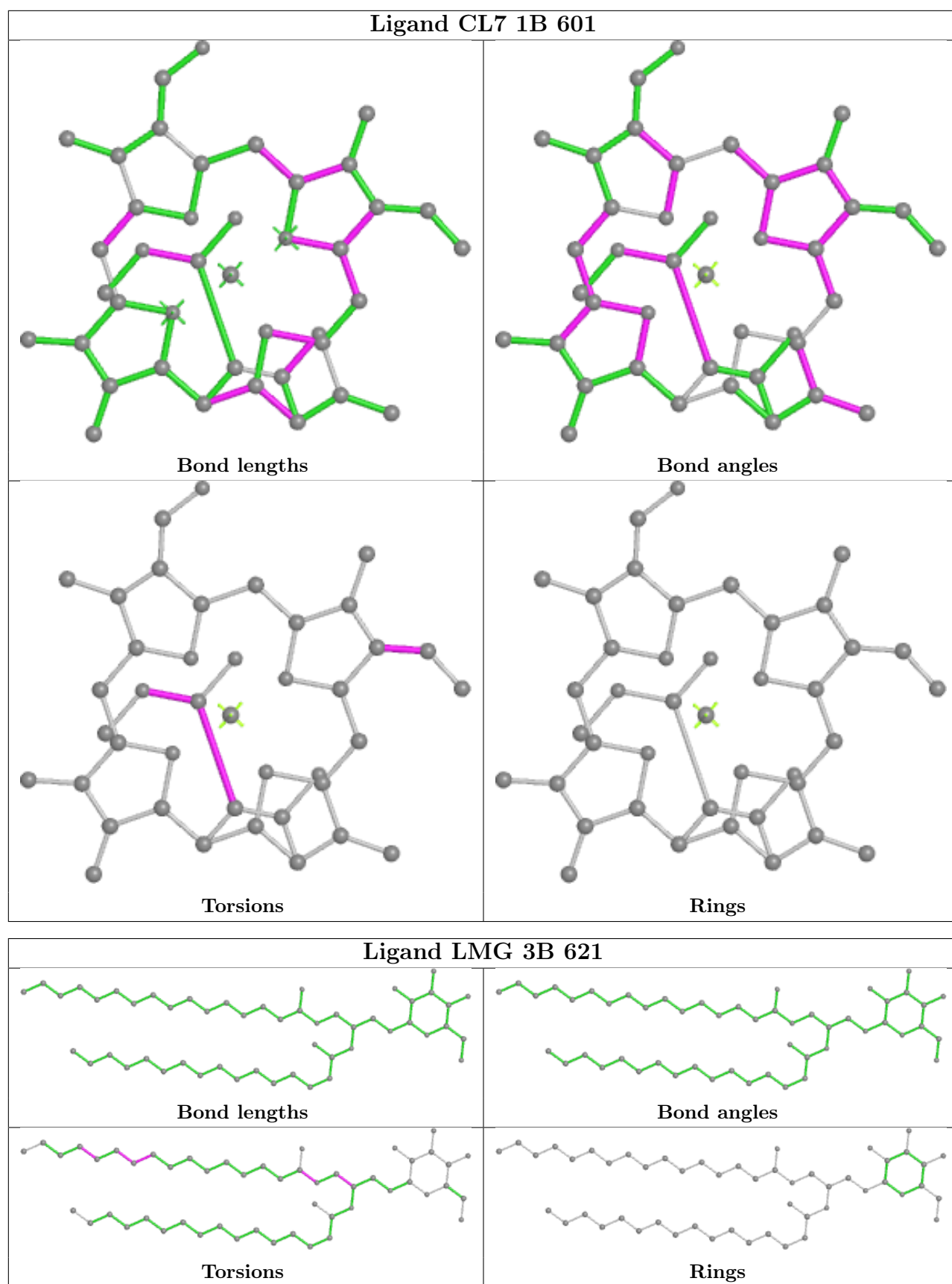
Bond angles



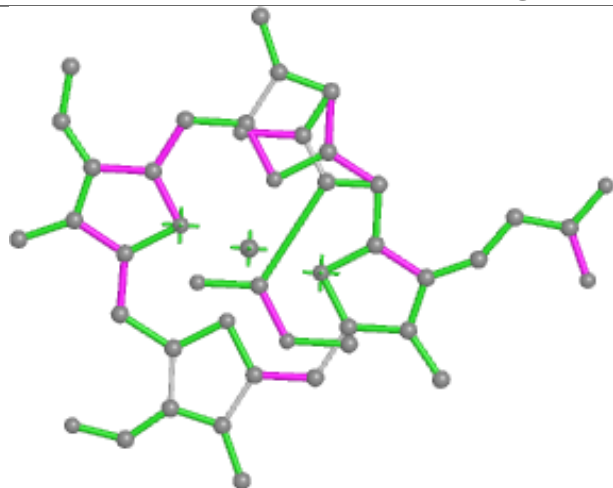
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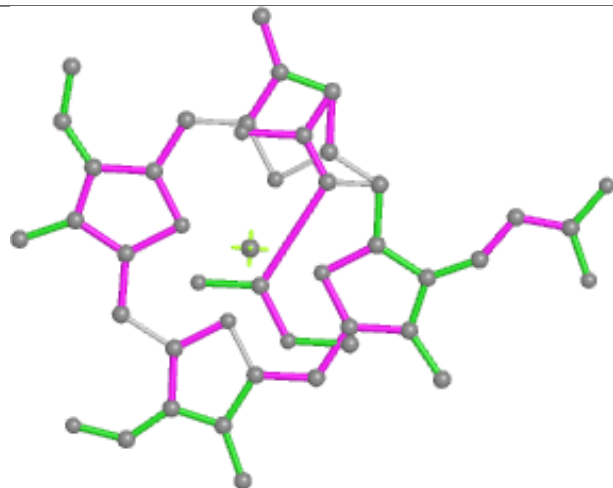
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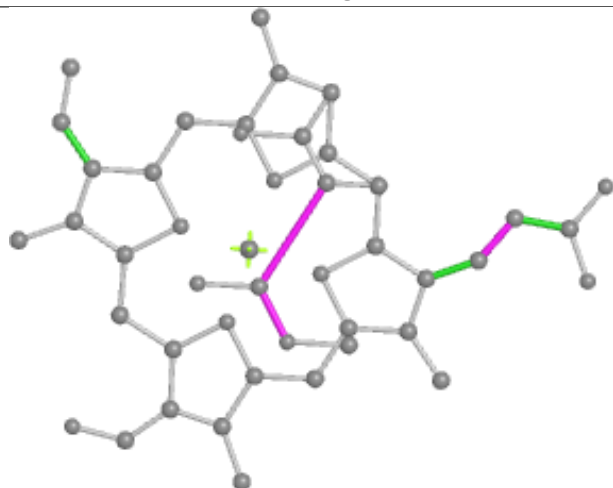
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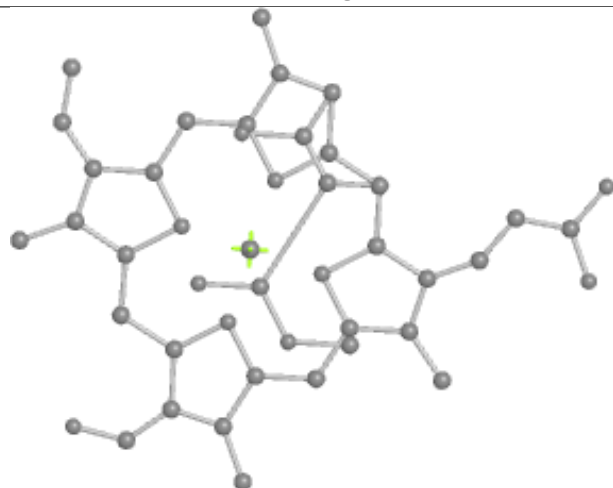
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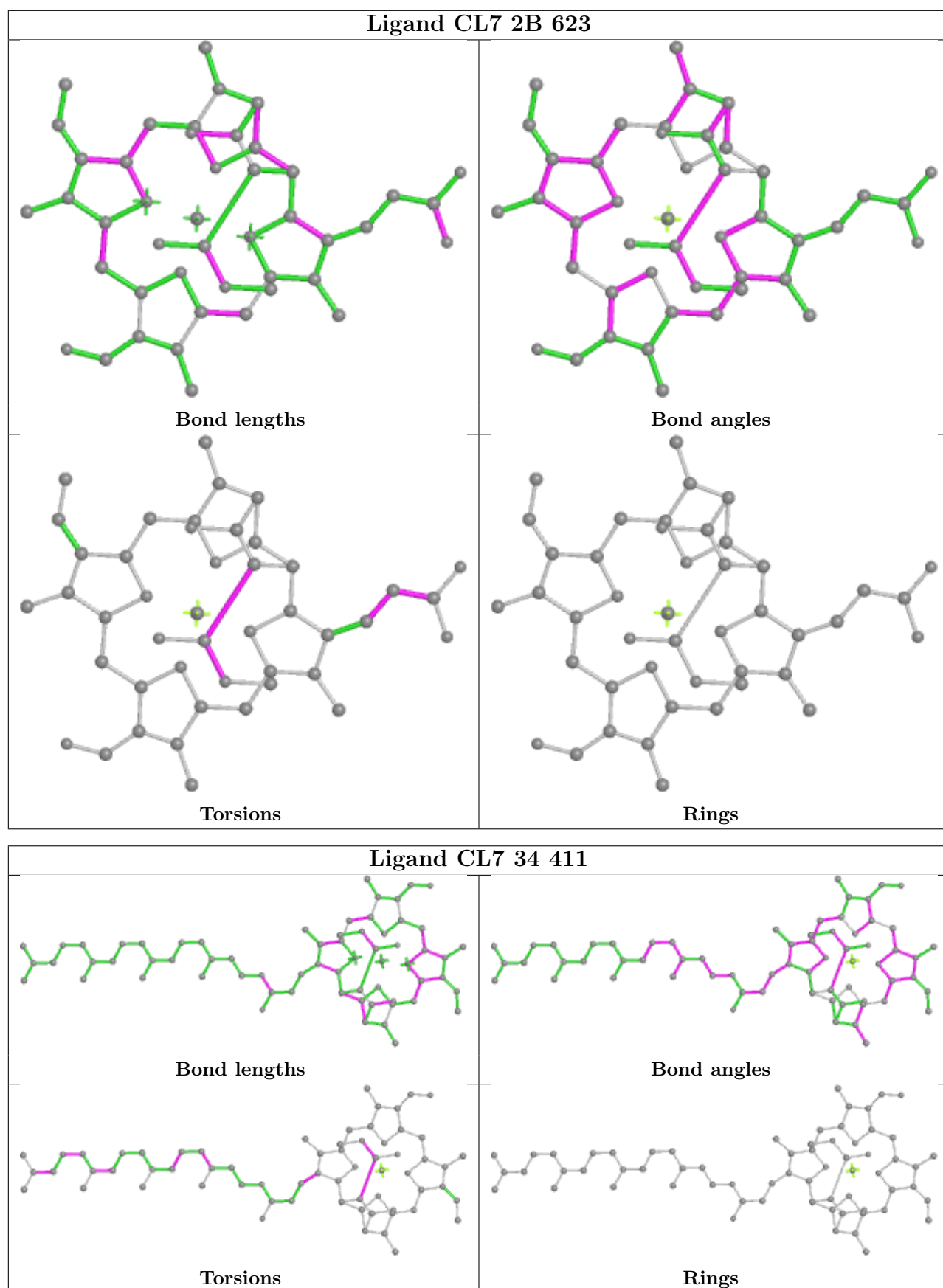
Bond angles

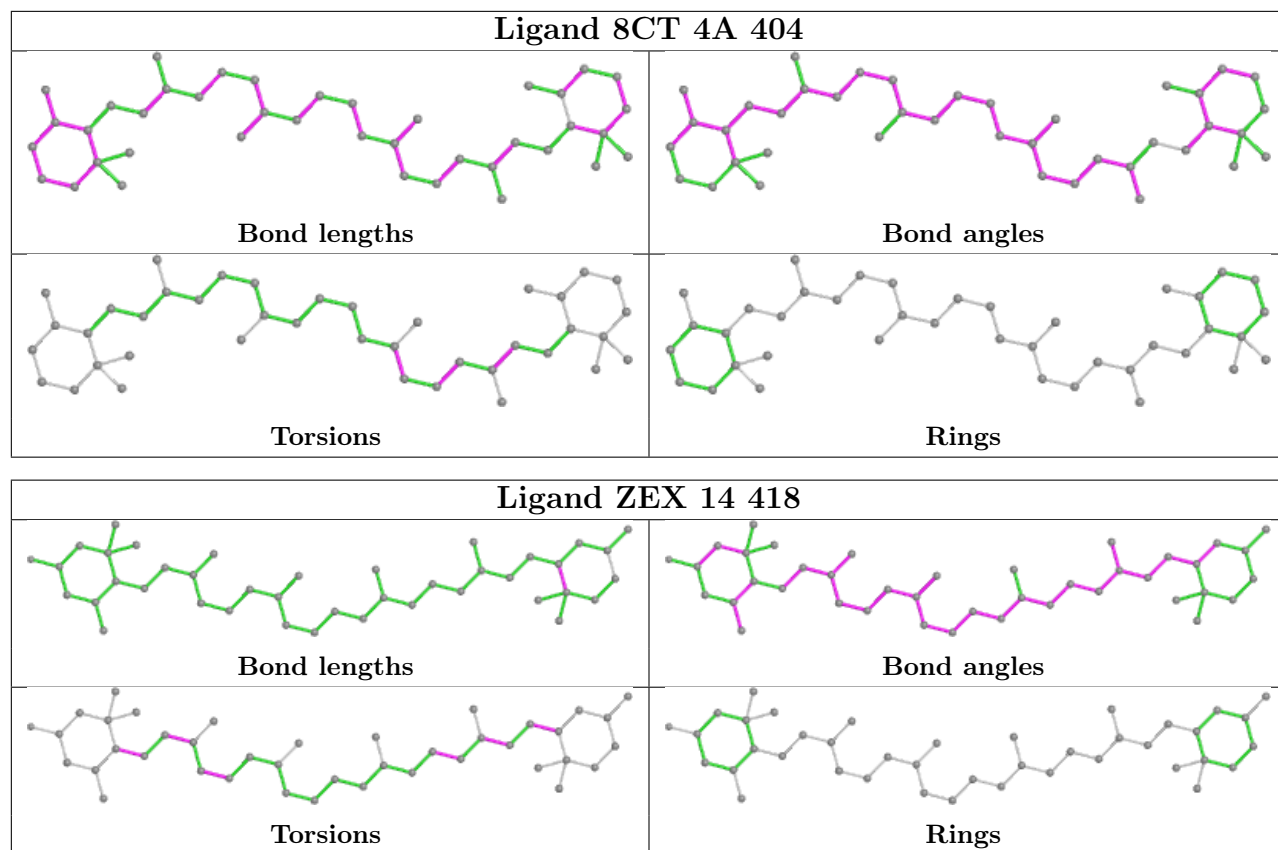


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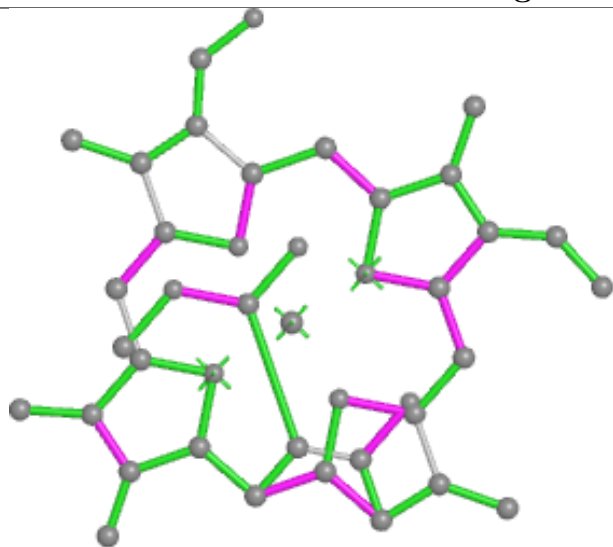


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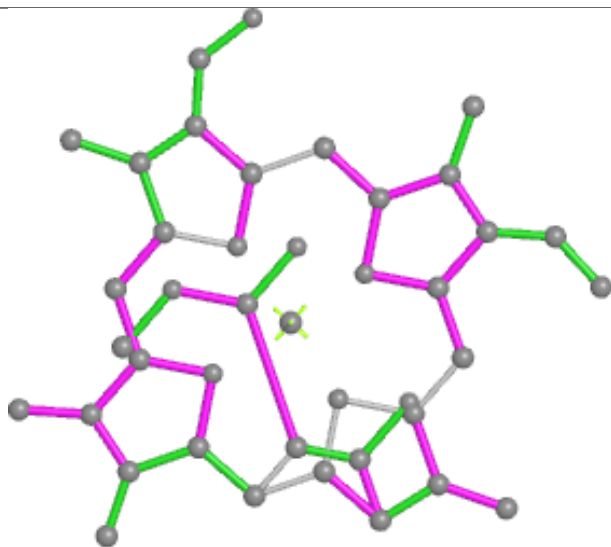




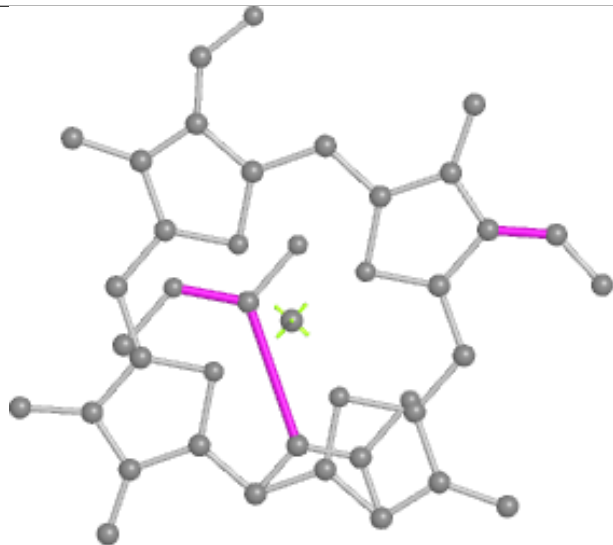
Ligand CL7 21 415



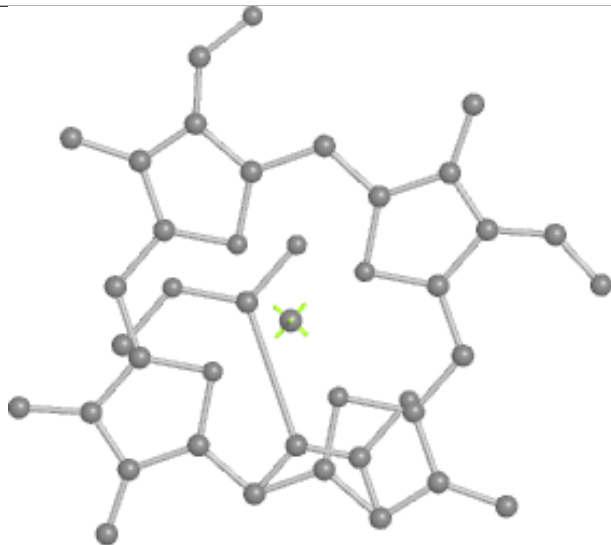
Bond lengths



Bond angles

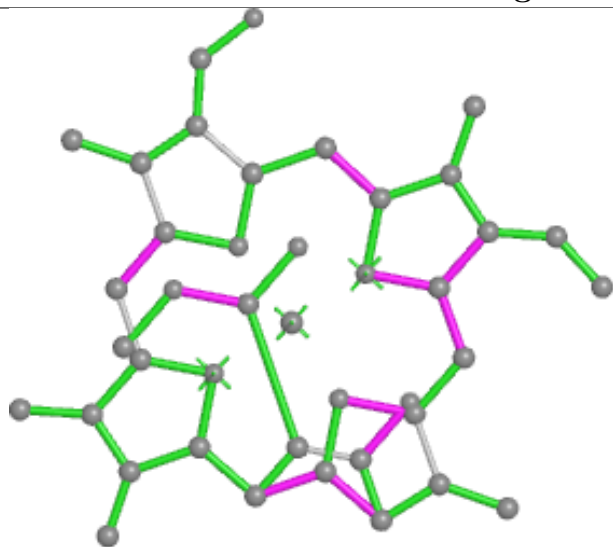


Torsions

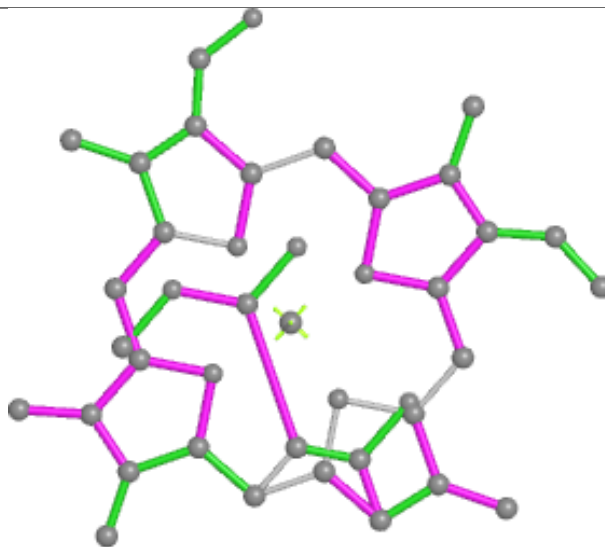


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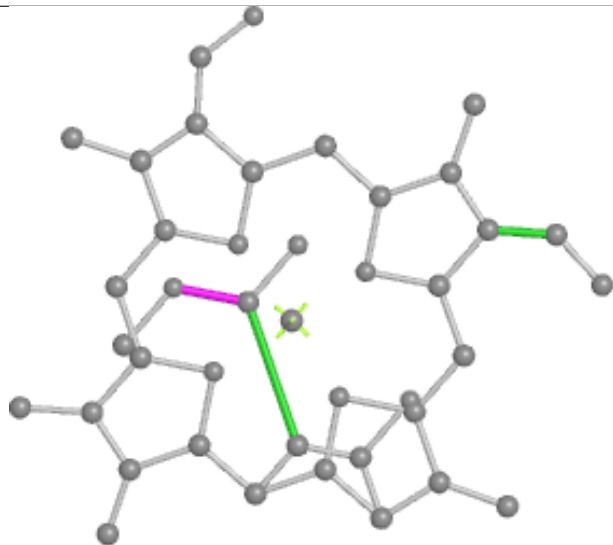
Ligand CL7 31 416



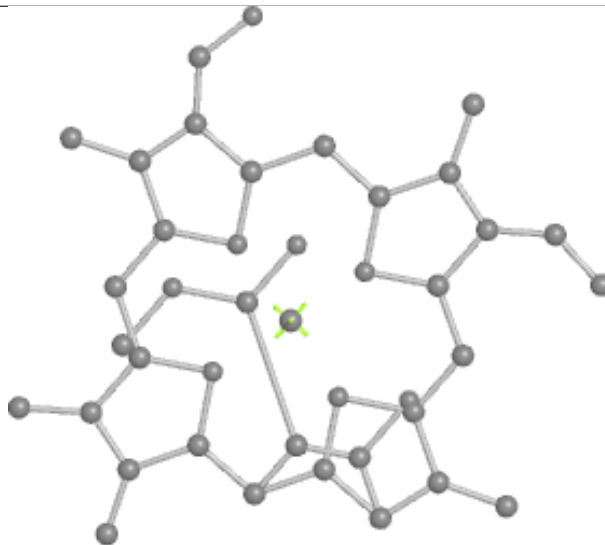
Bond lengths



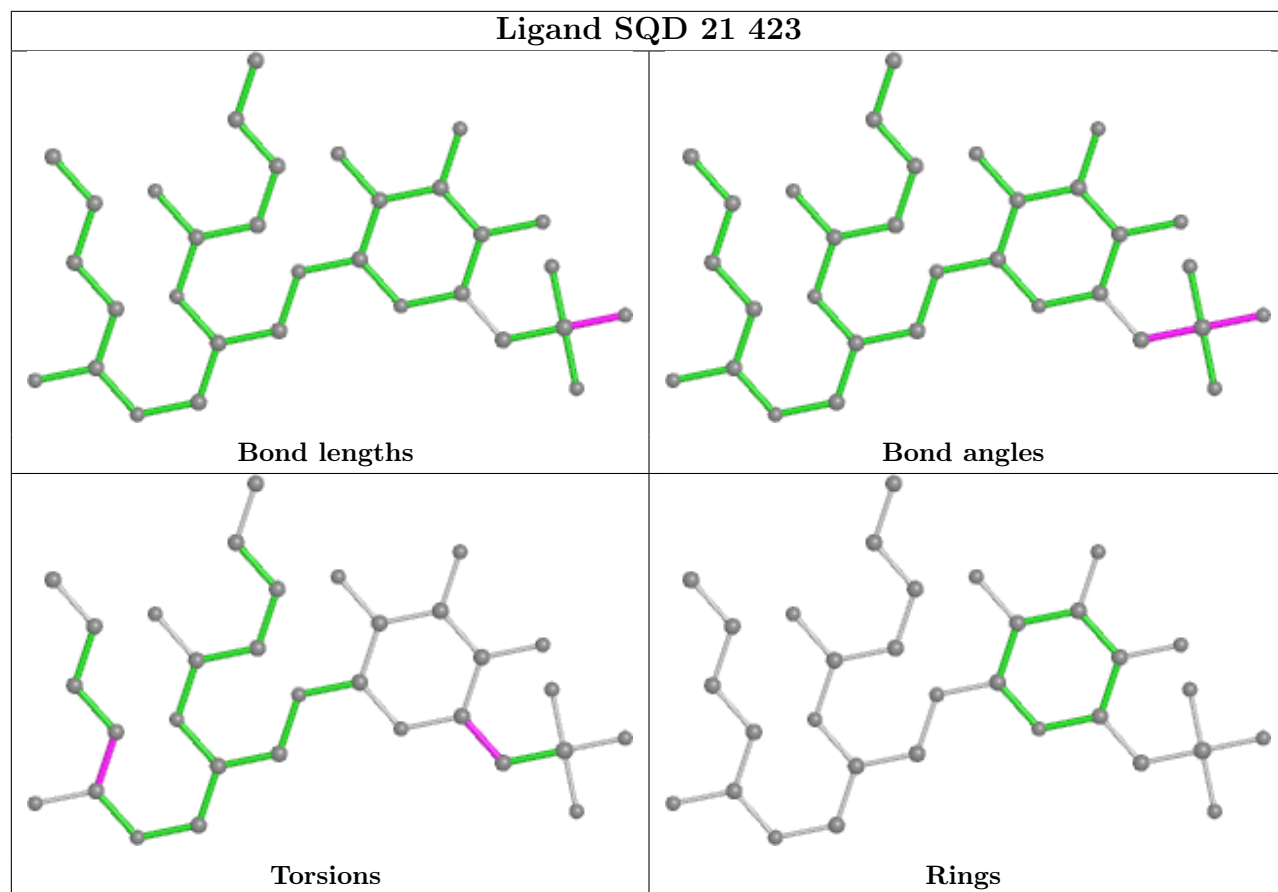
Bond angles

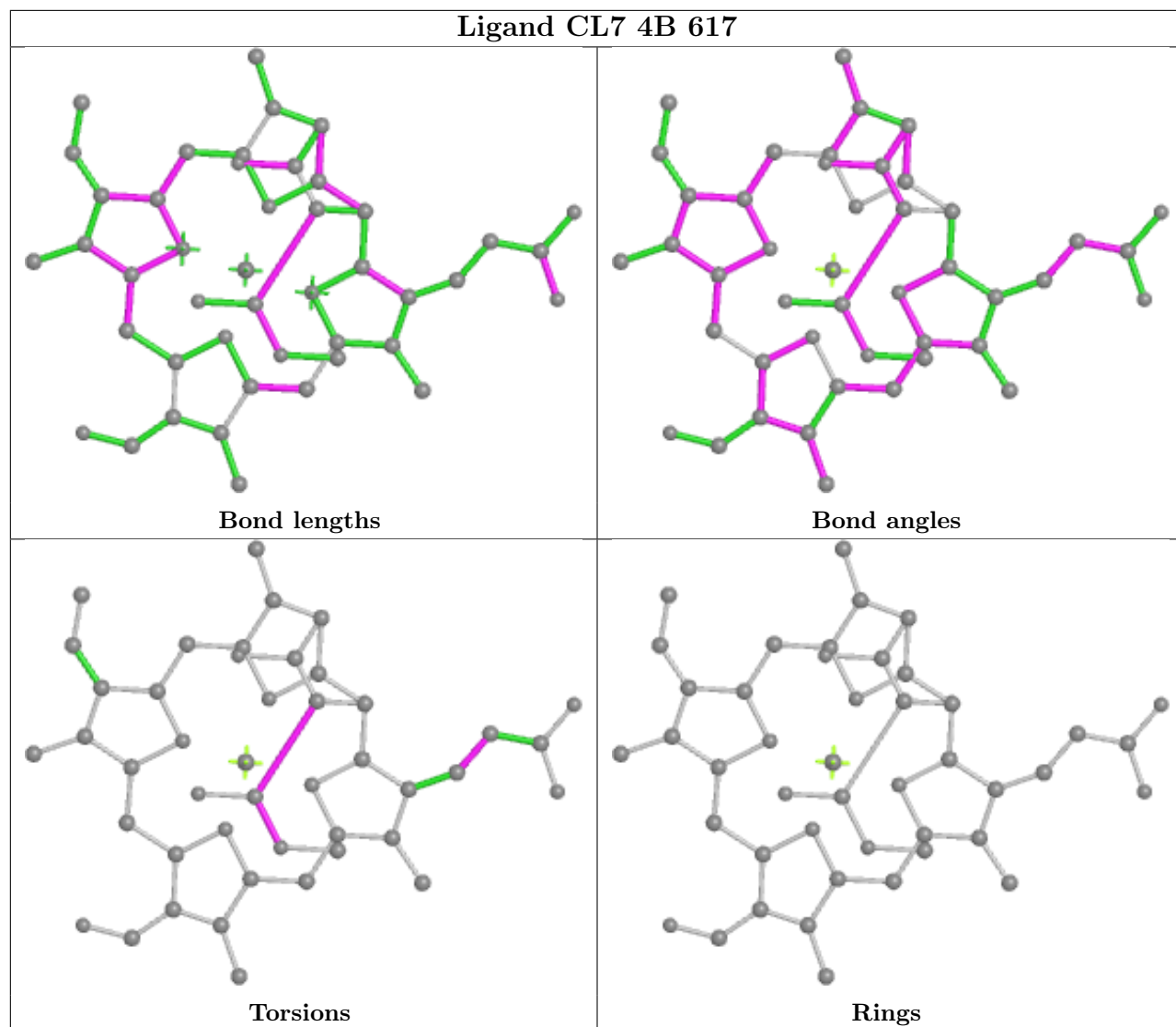


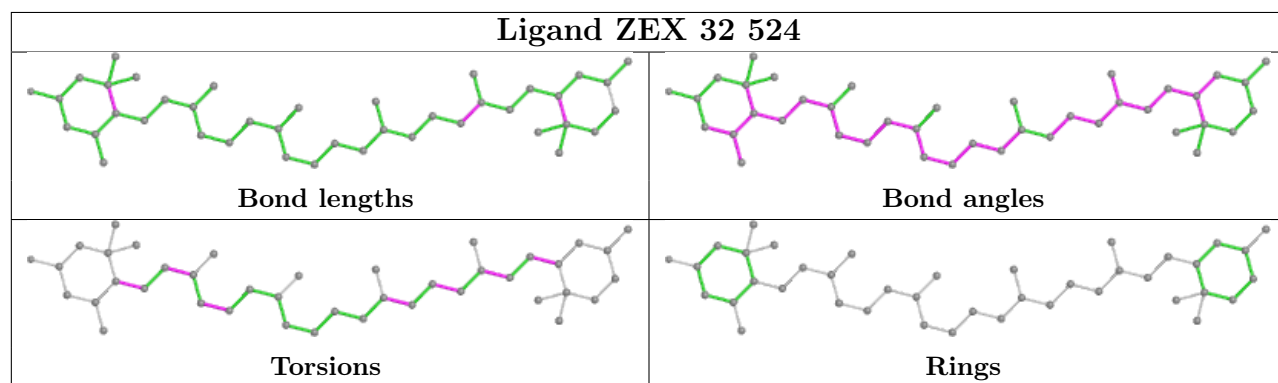
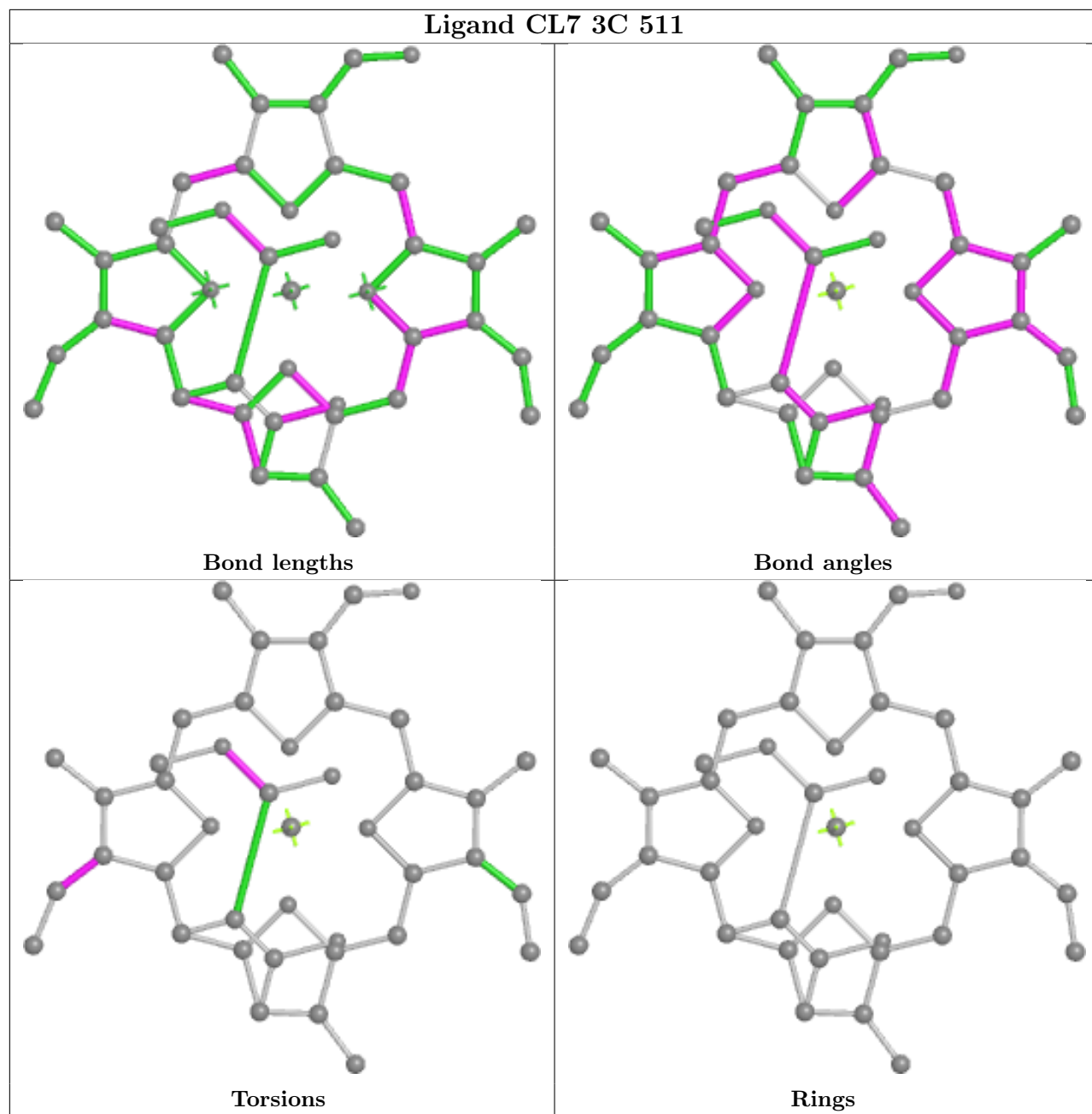
Torsions

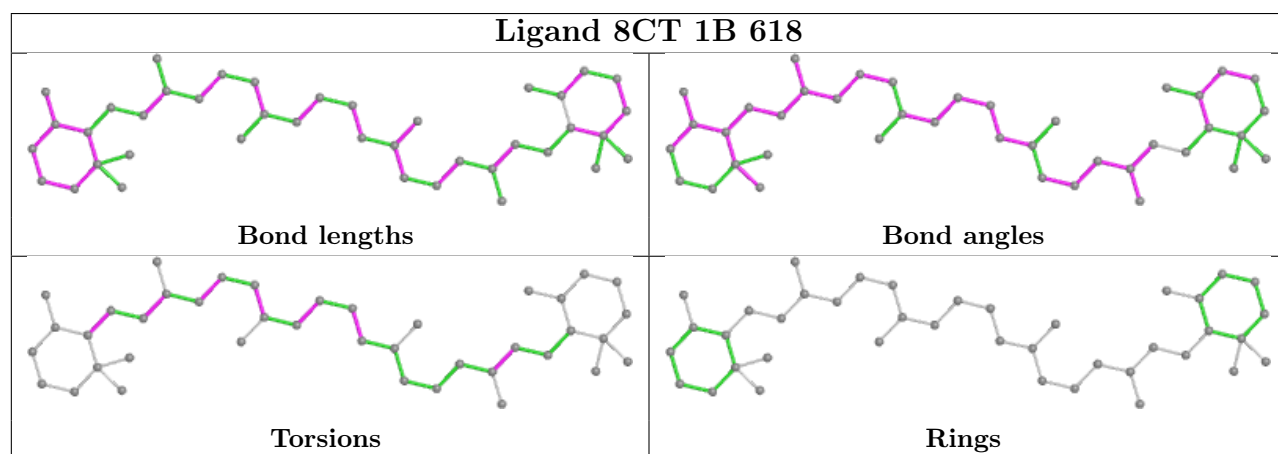
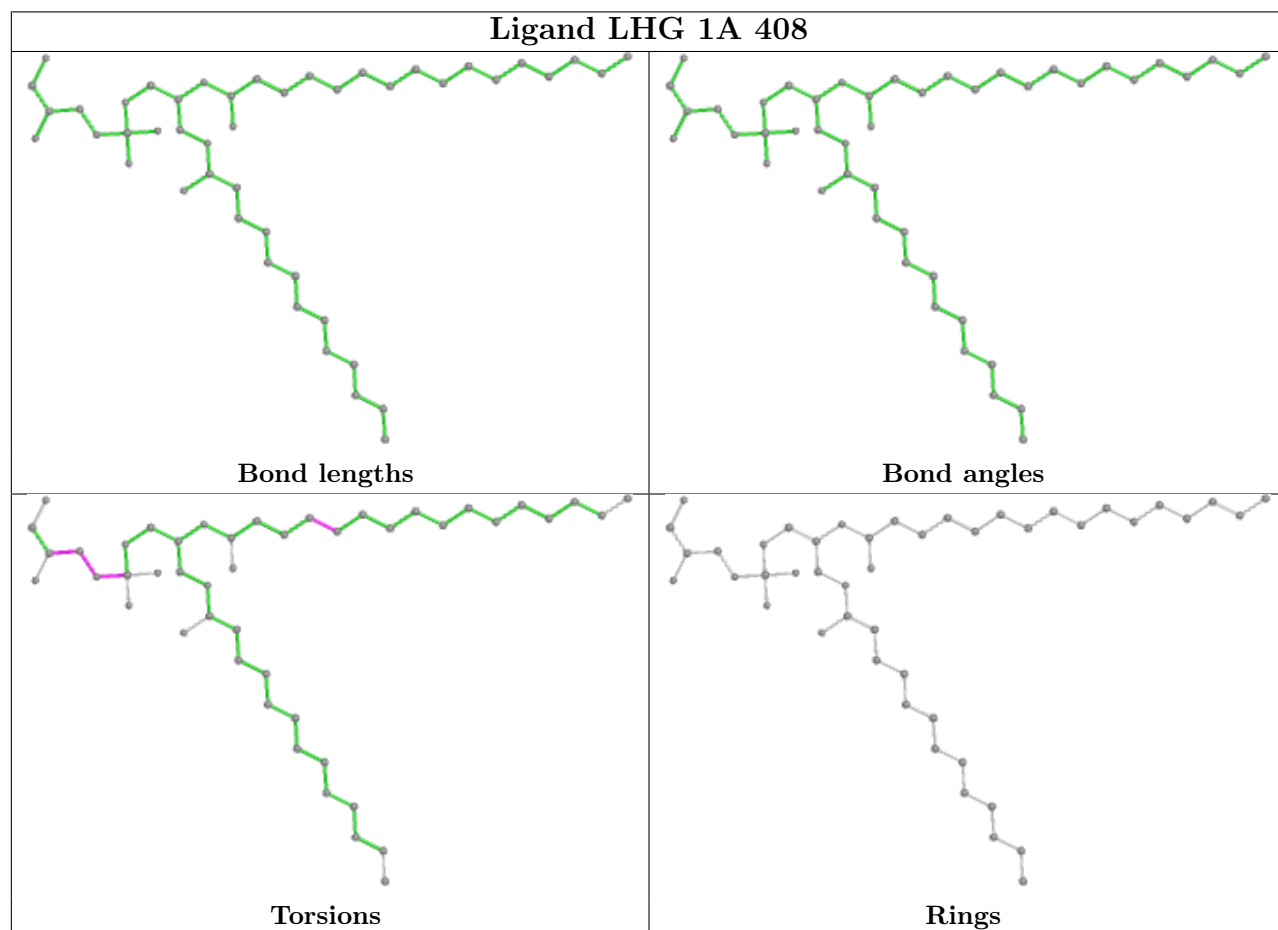
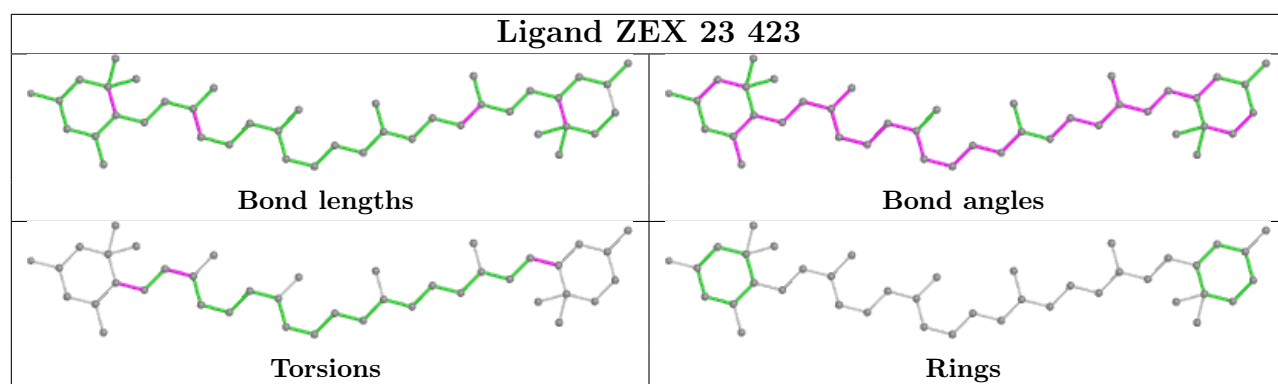


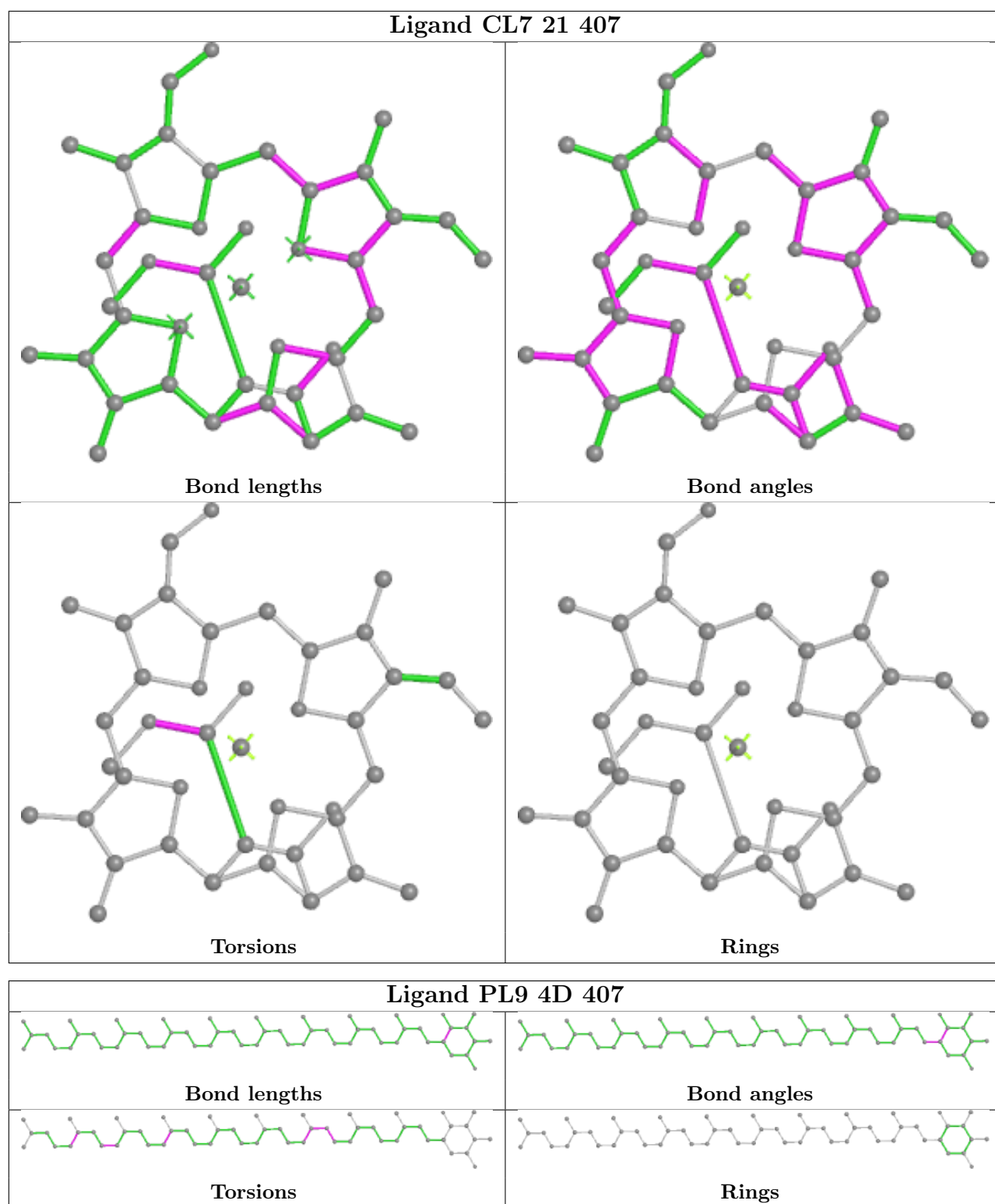
Rings



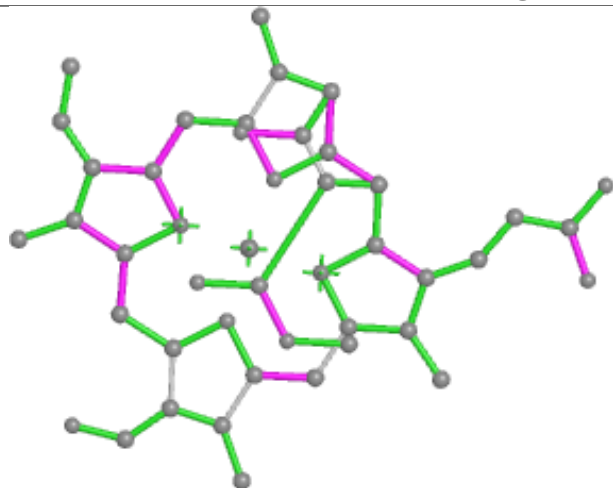




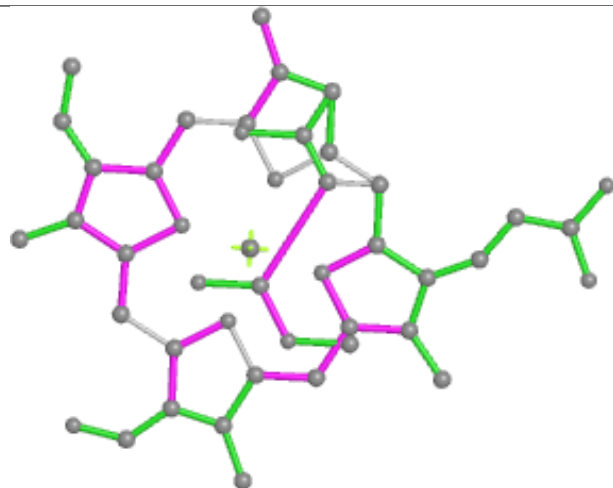




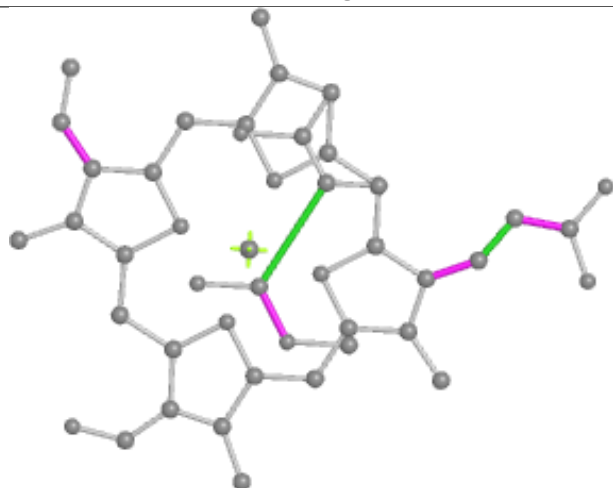
Ligand CL7 42 514



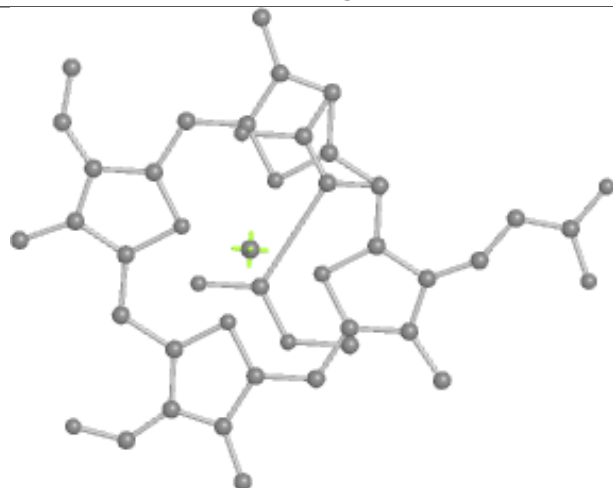
Bond lengths



Bond angles

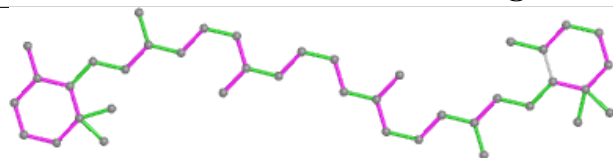


Torsions

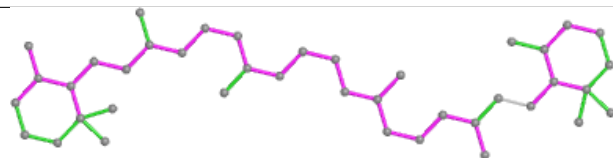


Rings

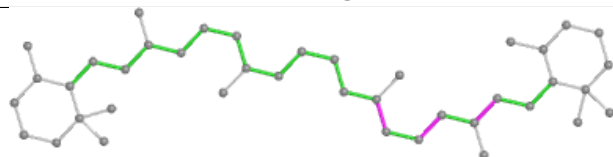
Ligand 8CT 1A 404



Bond lengths



Bond angles

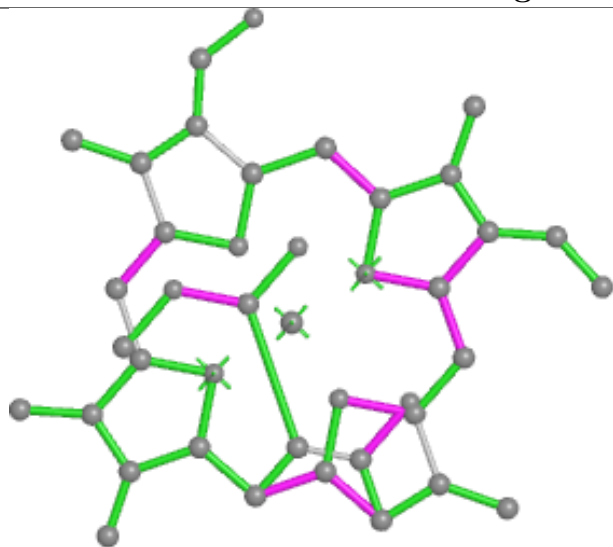


Torsions

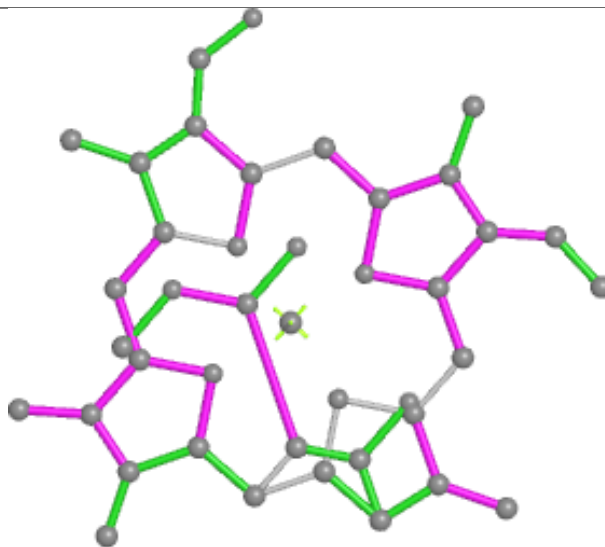


Rings

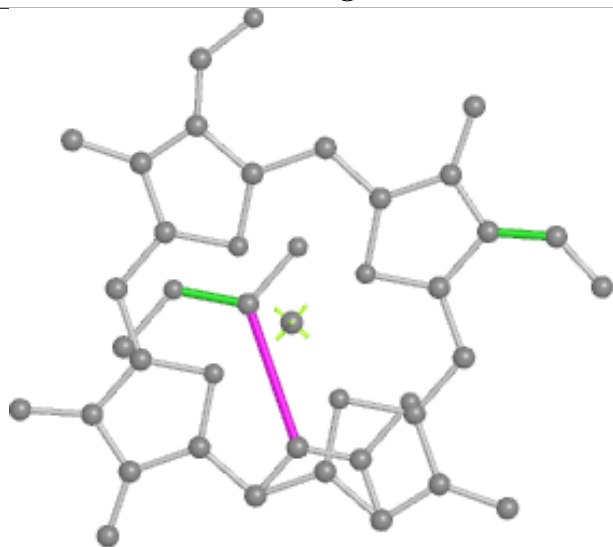
Ligand CL7 34 407



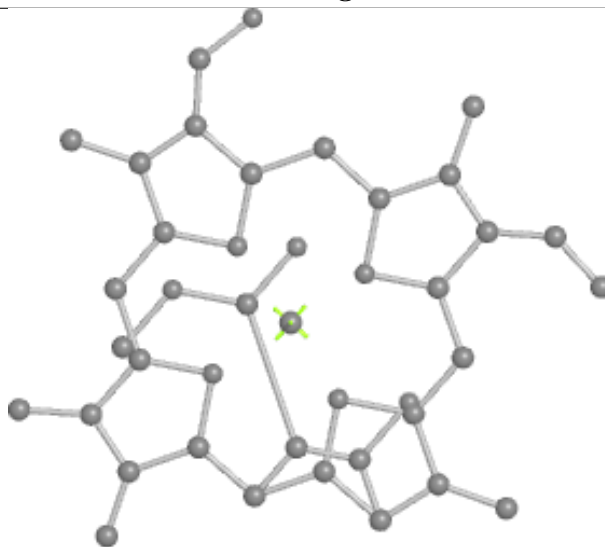
Bond lengths



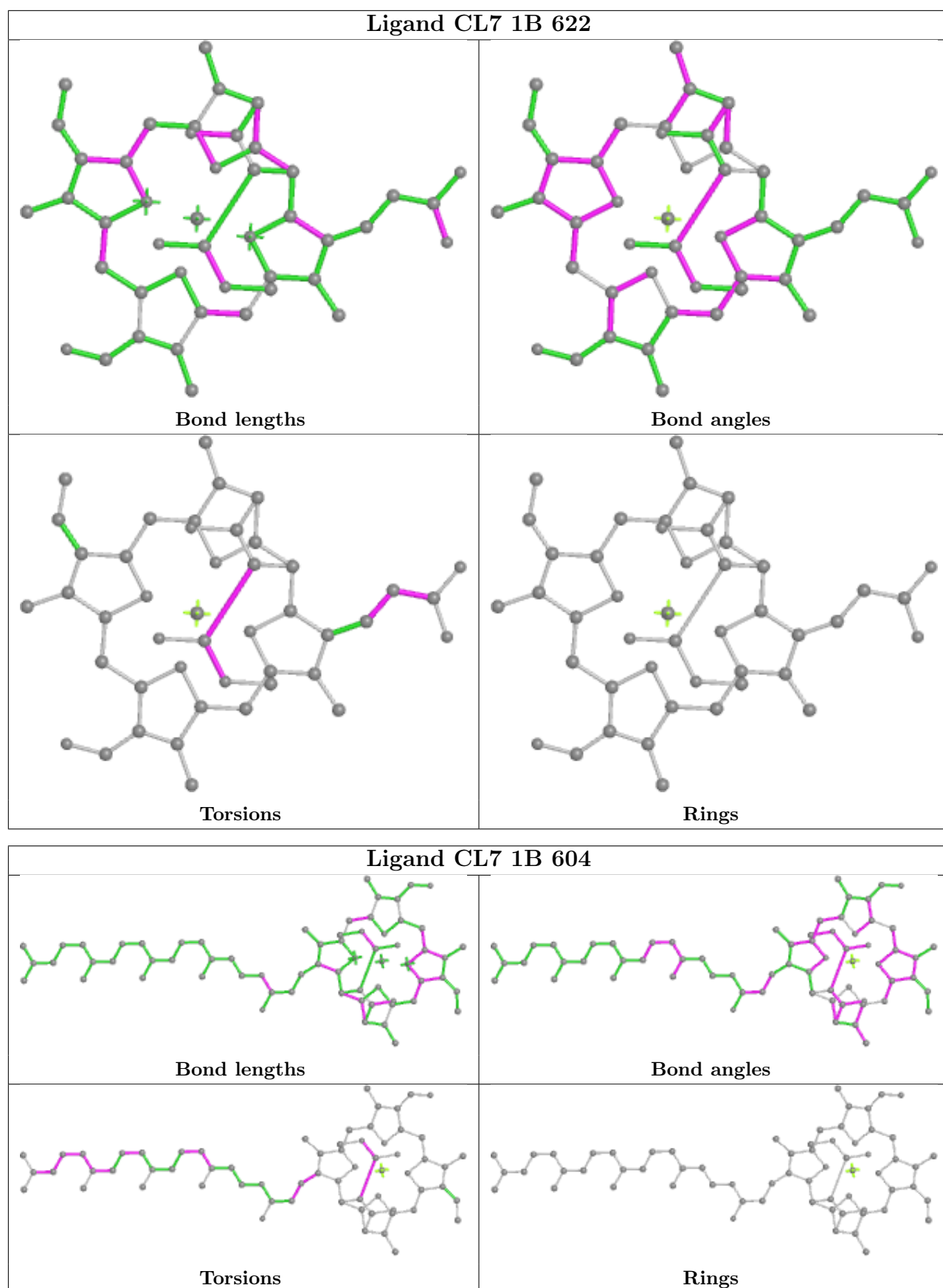
Bond angles

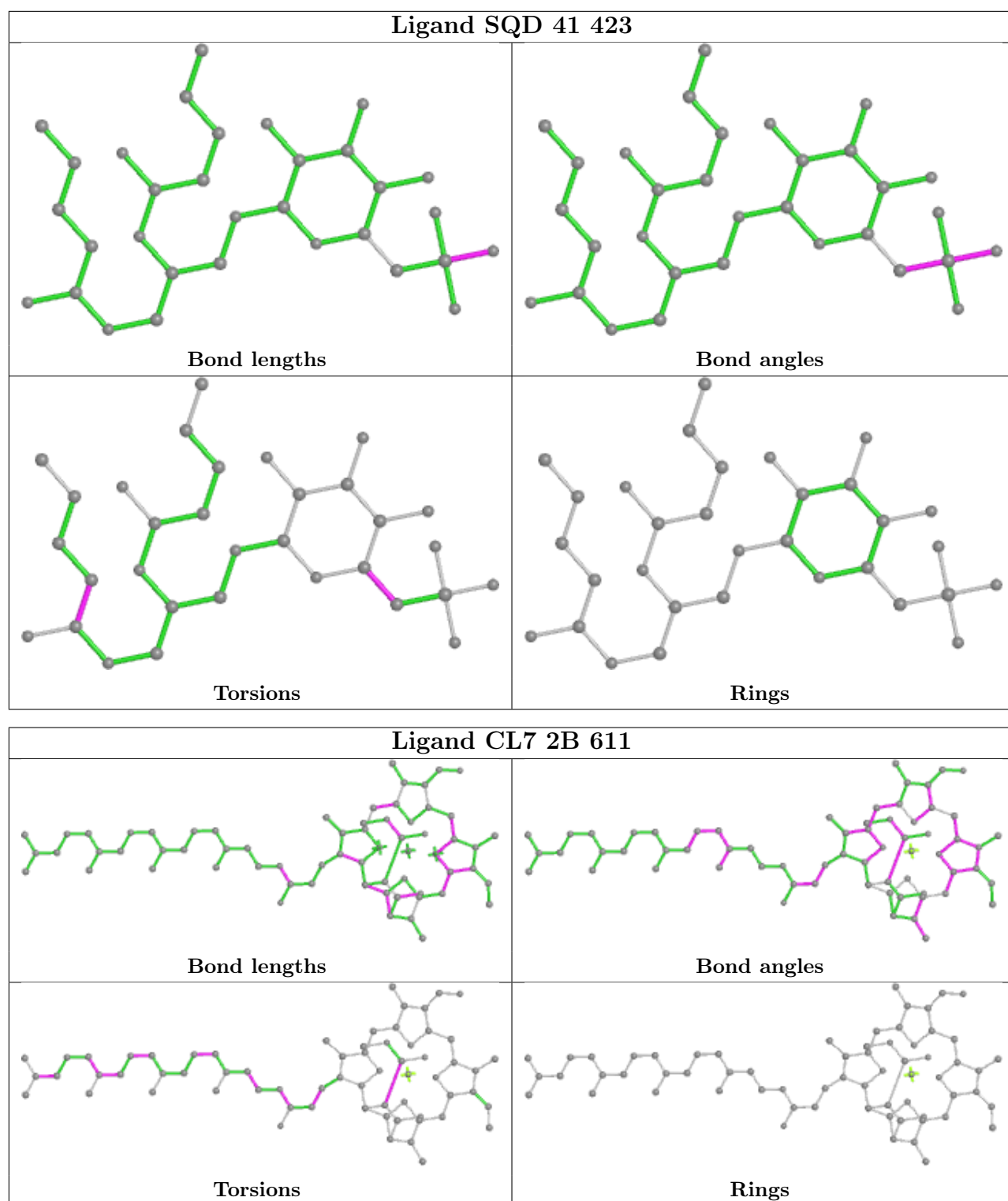


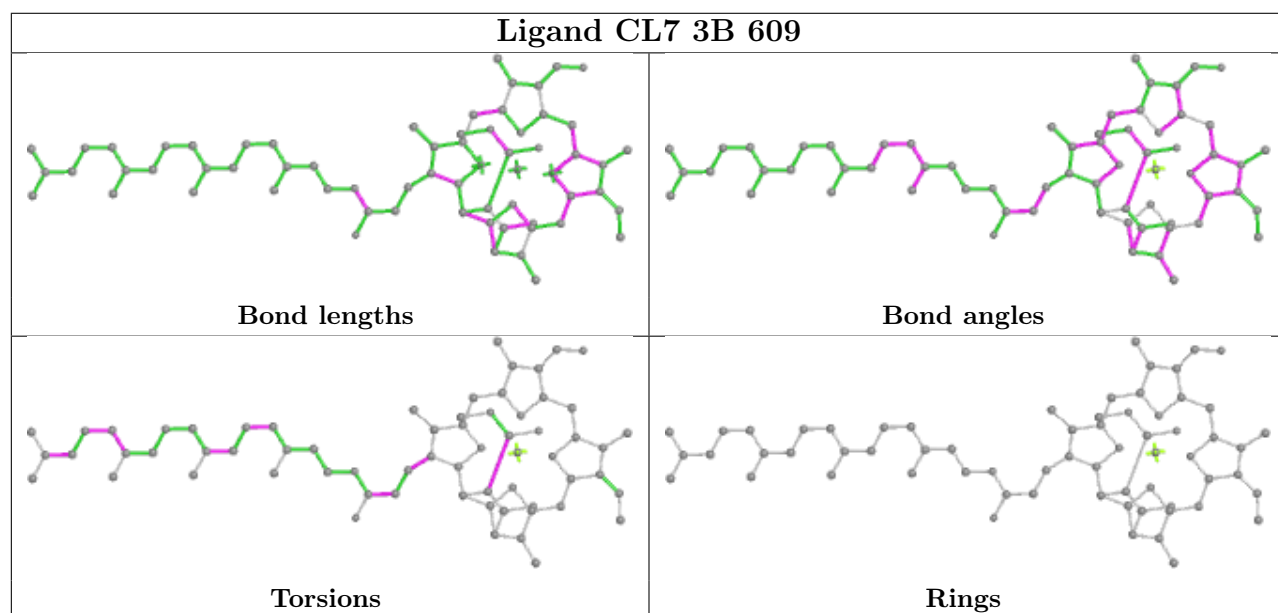
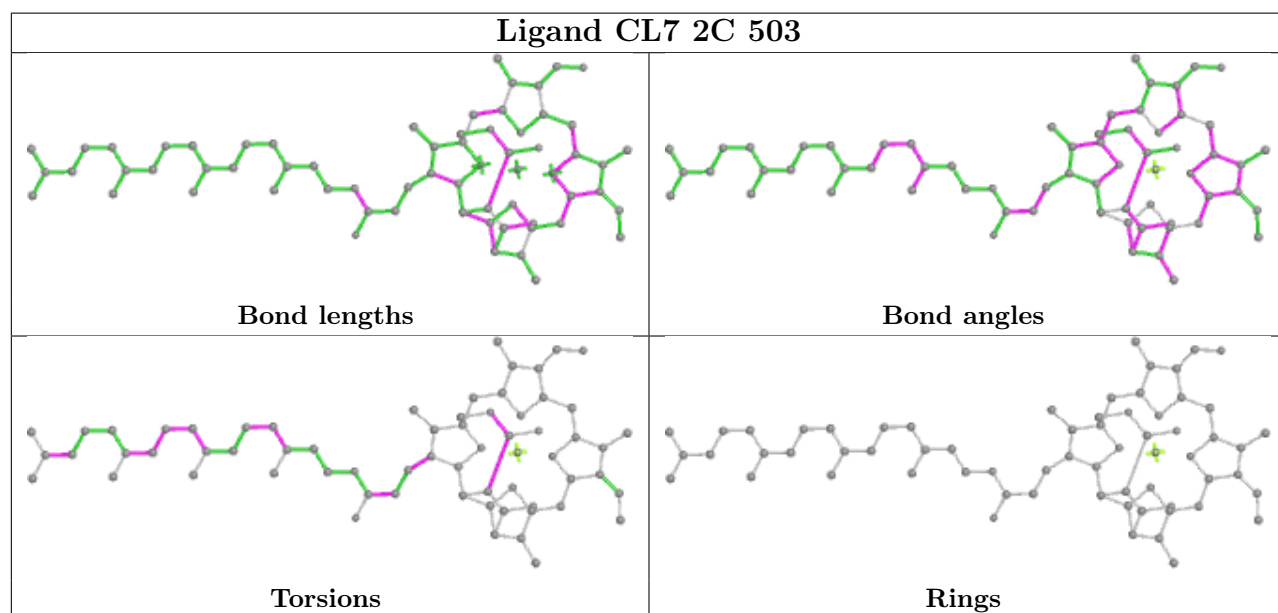
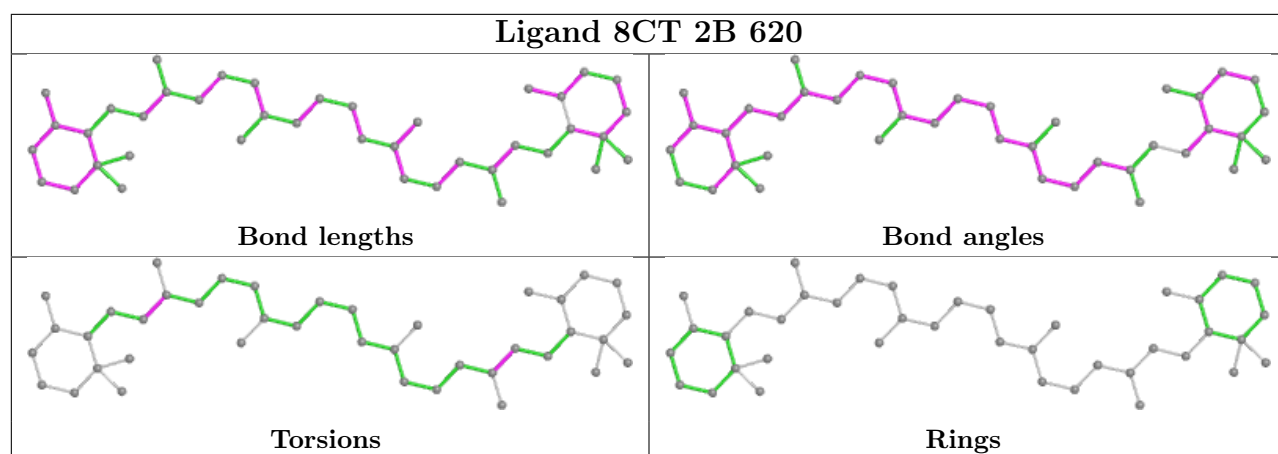
Torsions

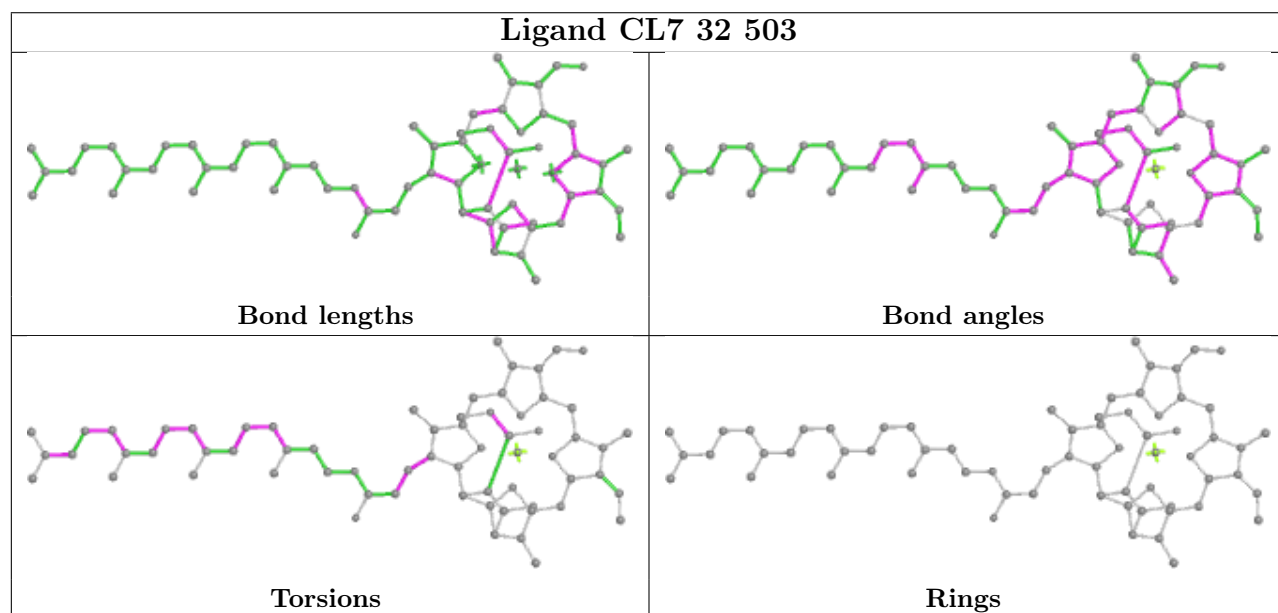
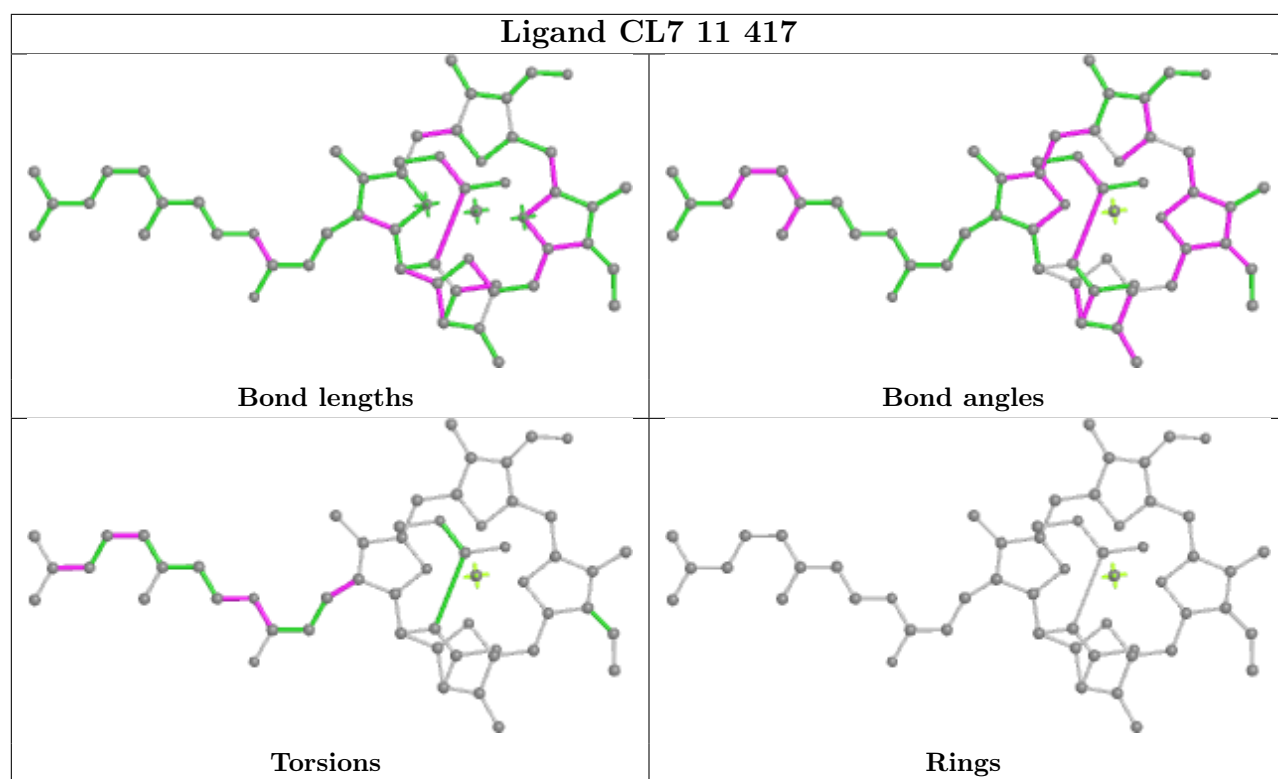


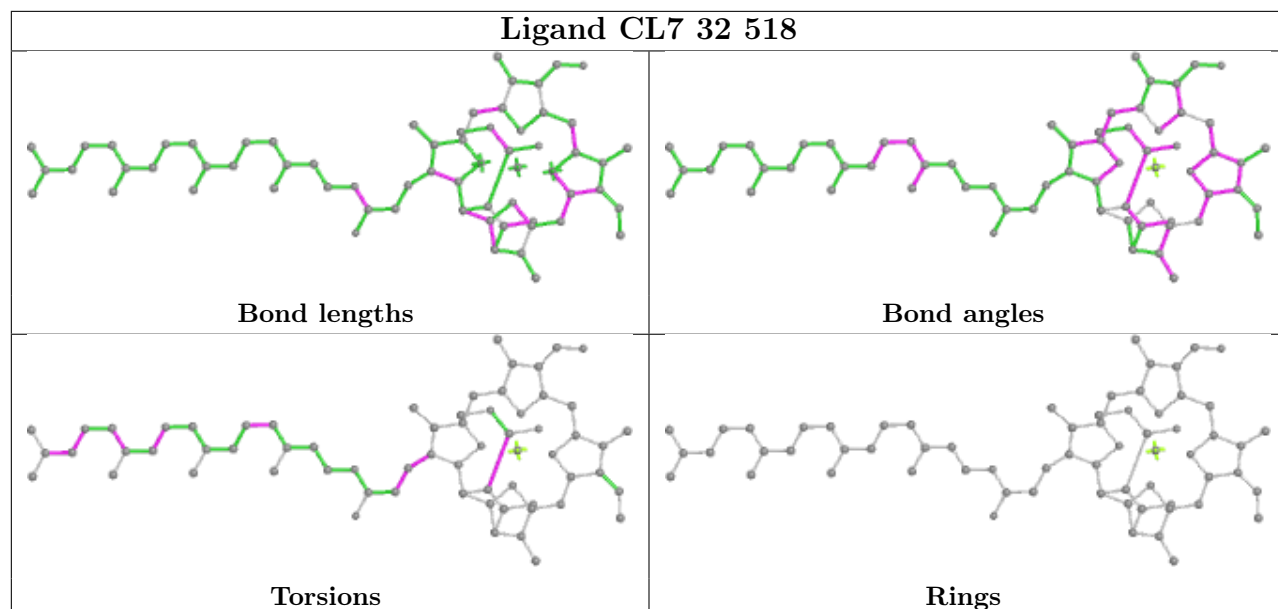
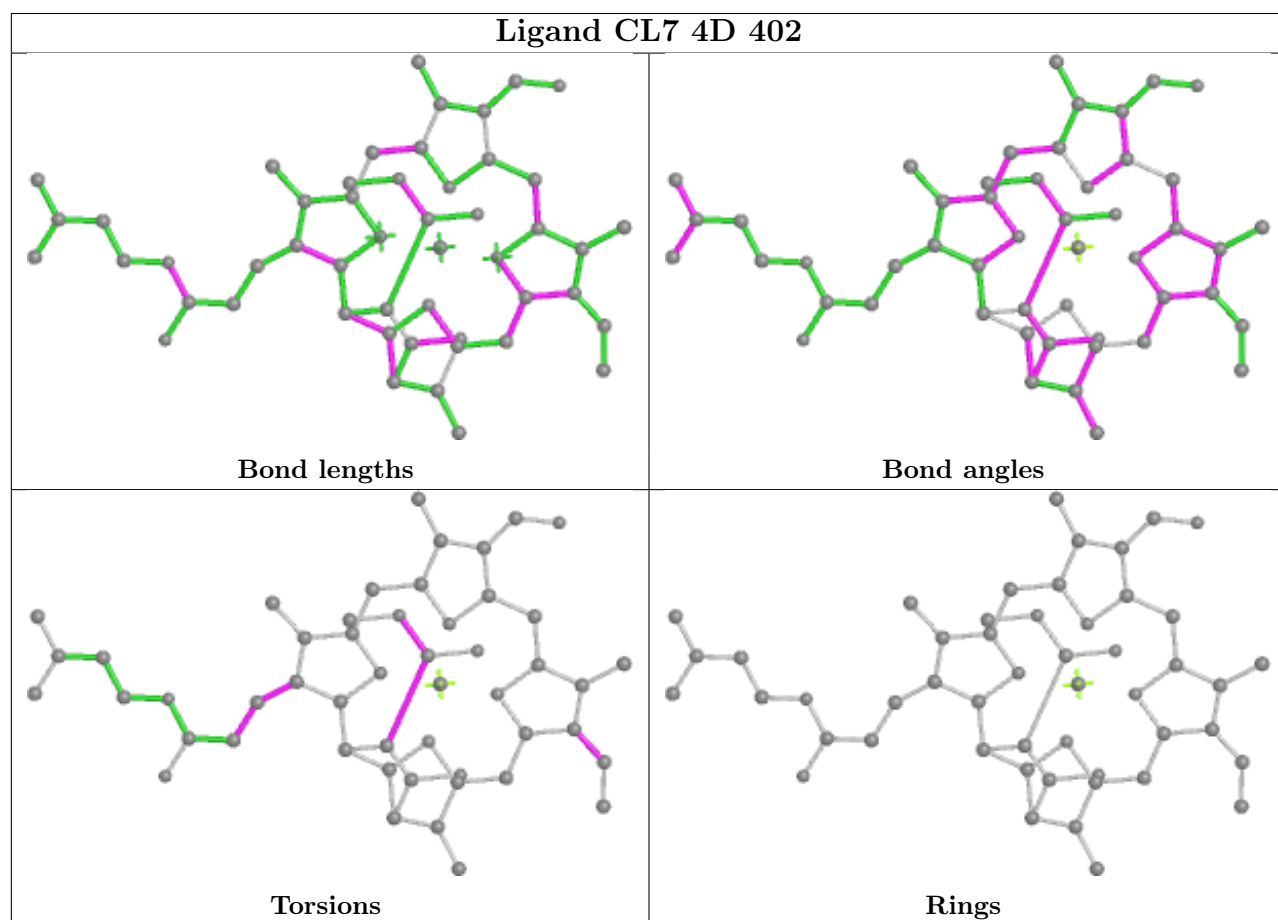
Rings

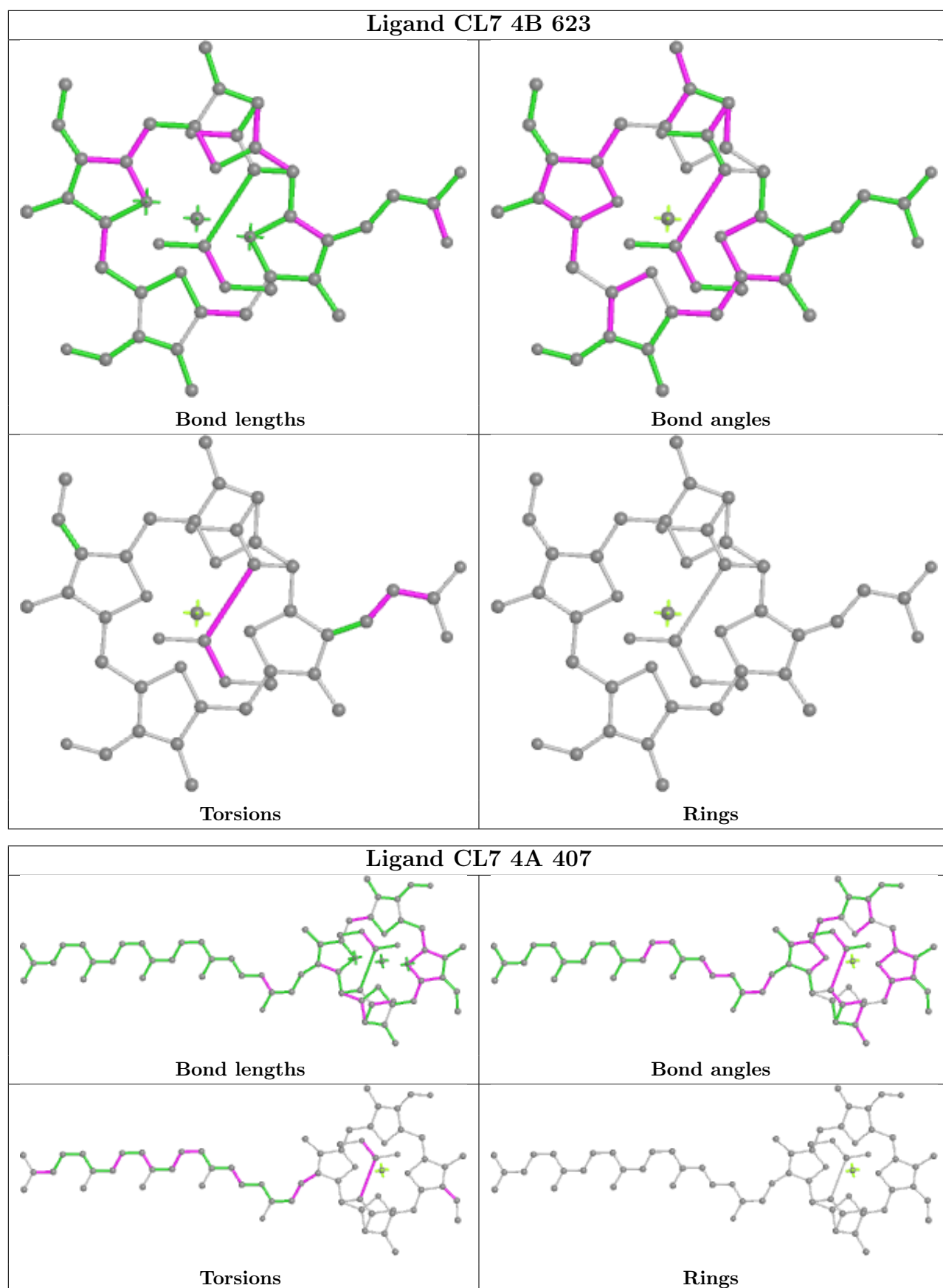




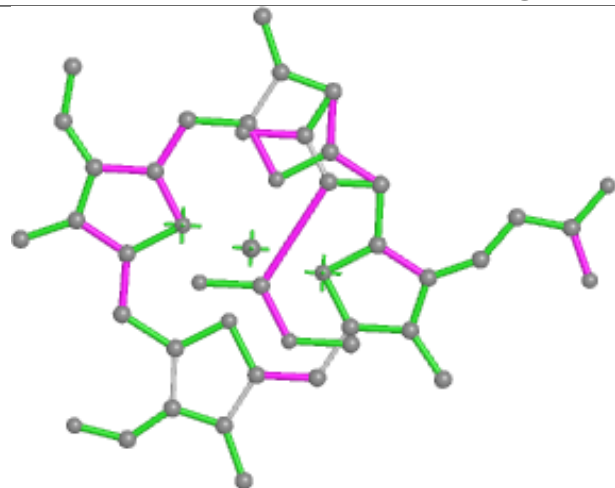




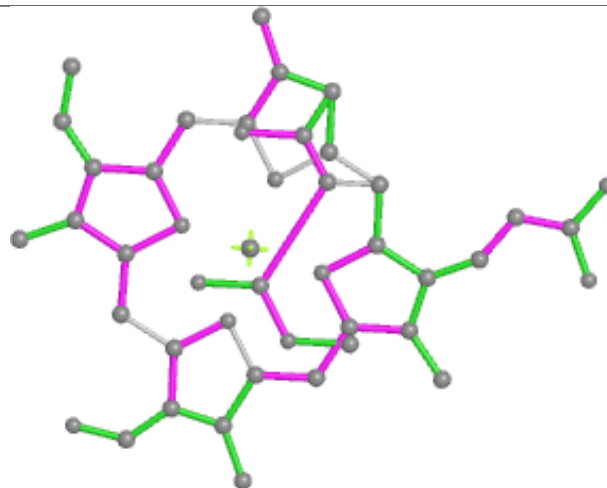
Ligand CL7 32 518**Ligand CL7 4D 402**



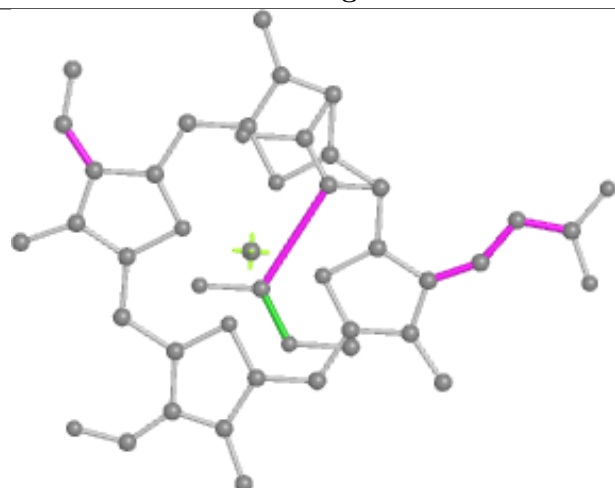
Ligand CL7 33 513



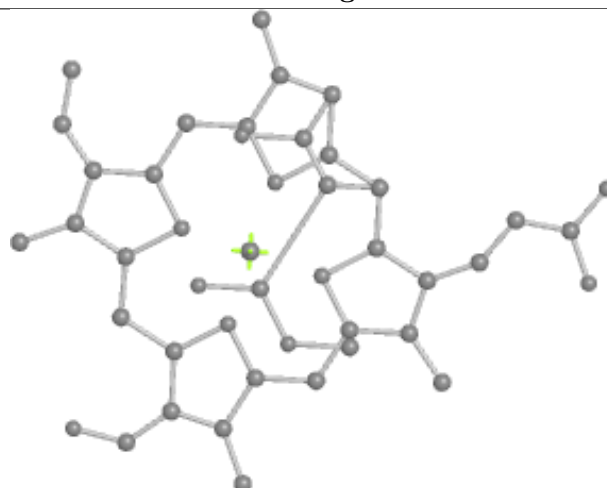
Bond lengths



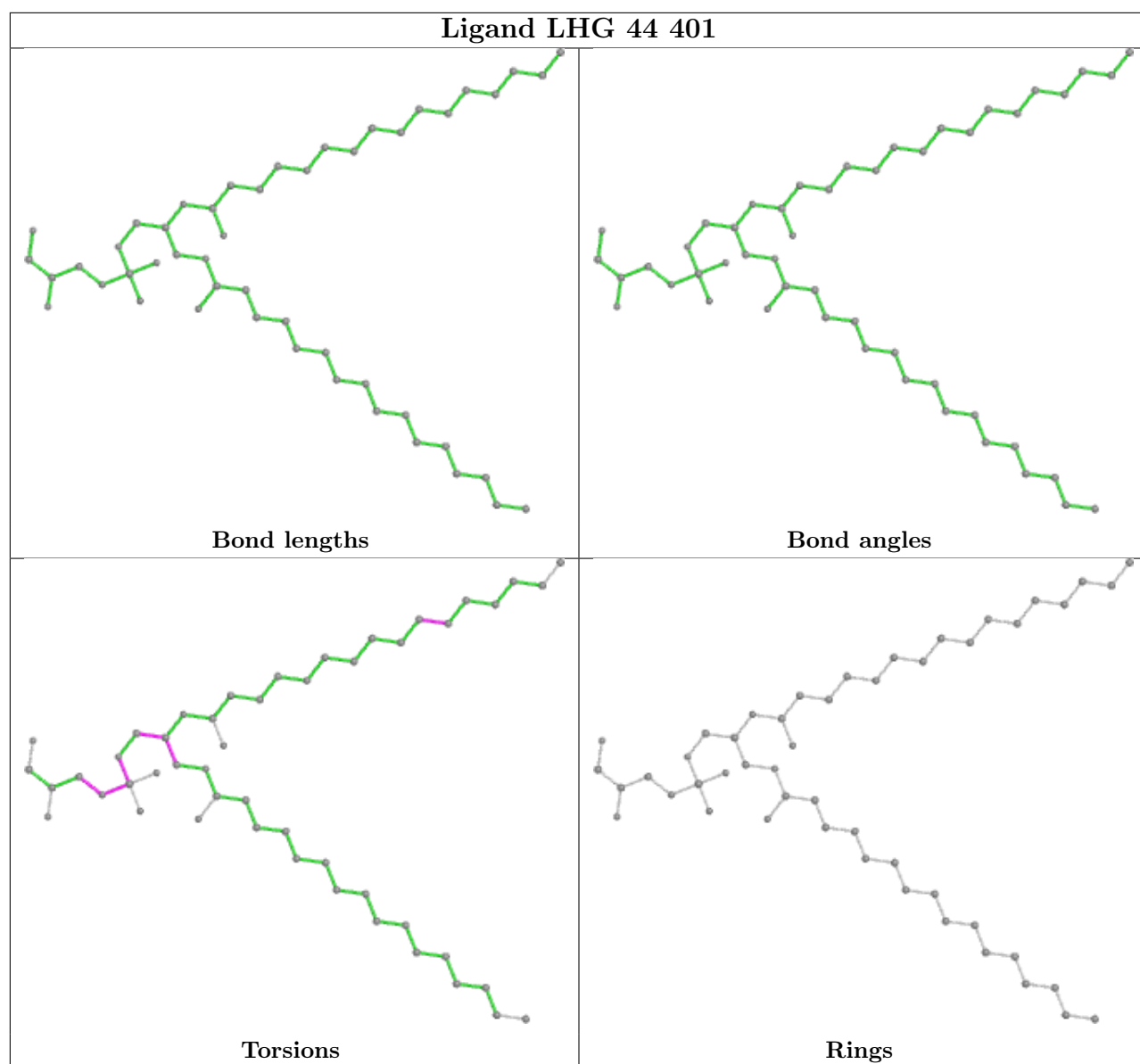
Bond angles

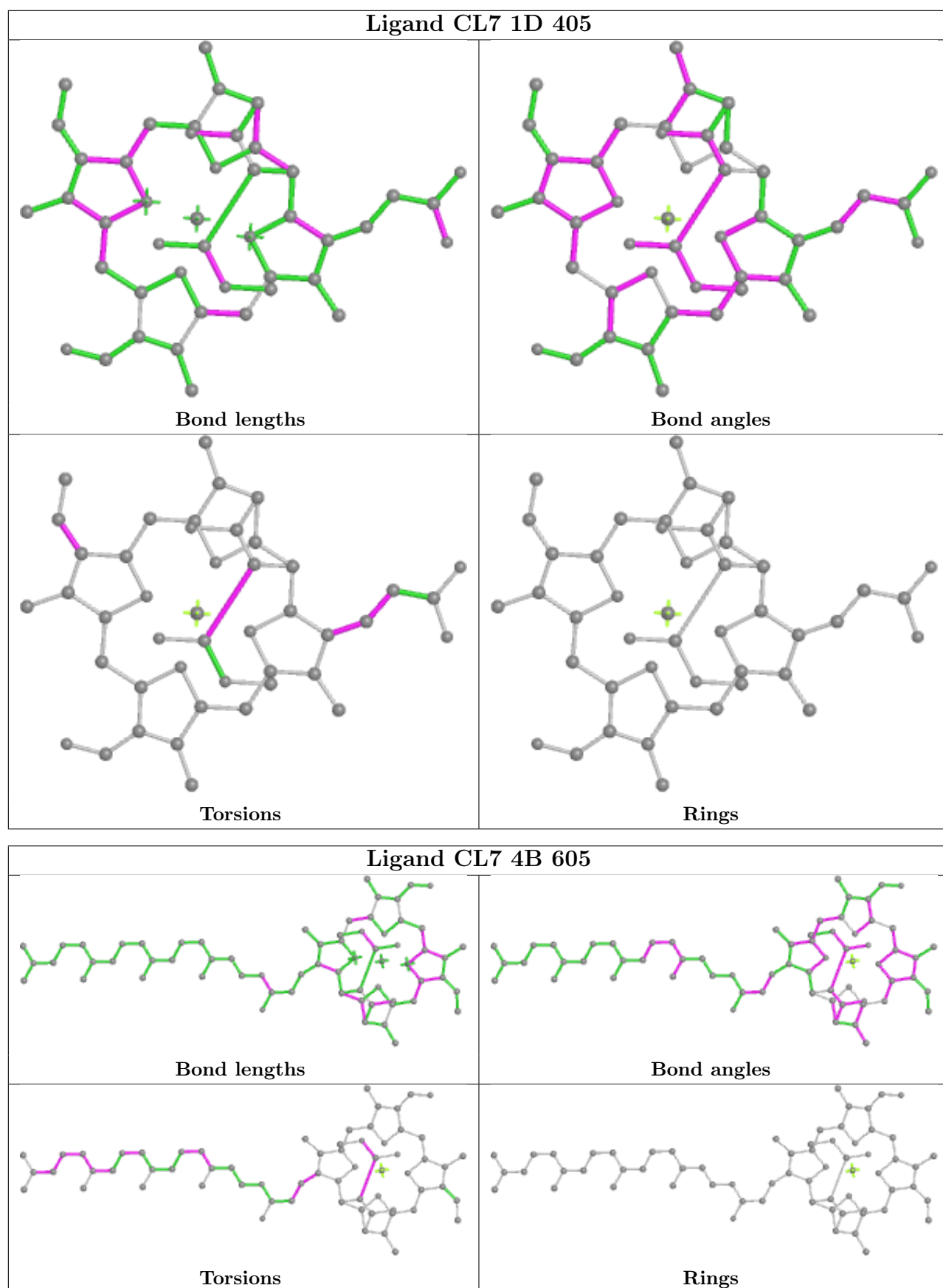


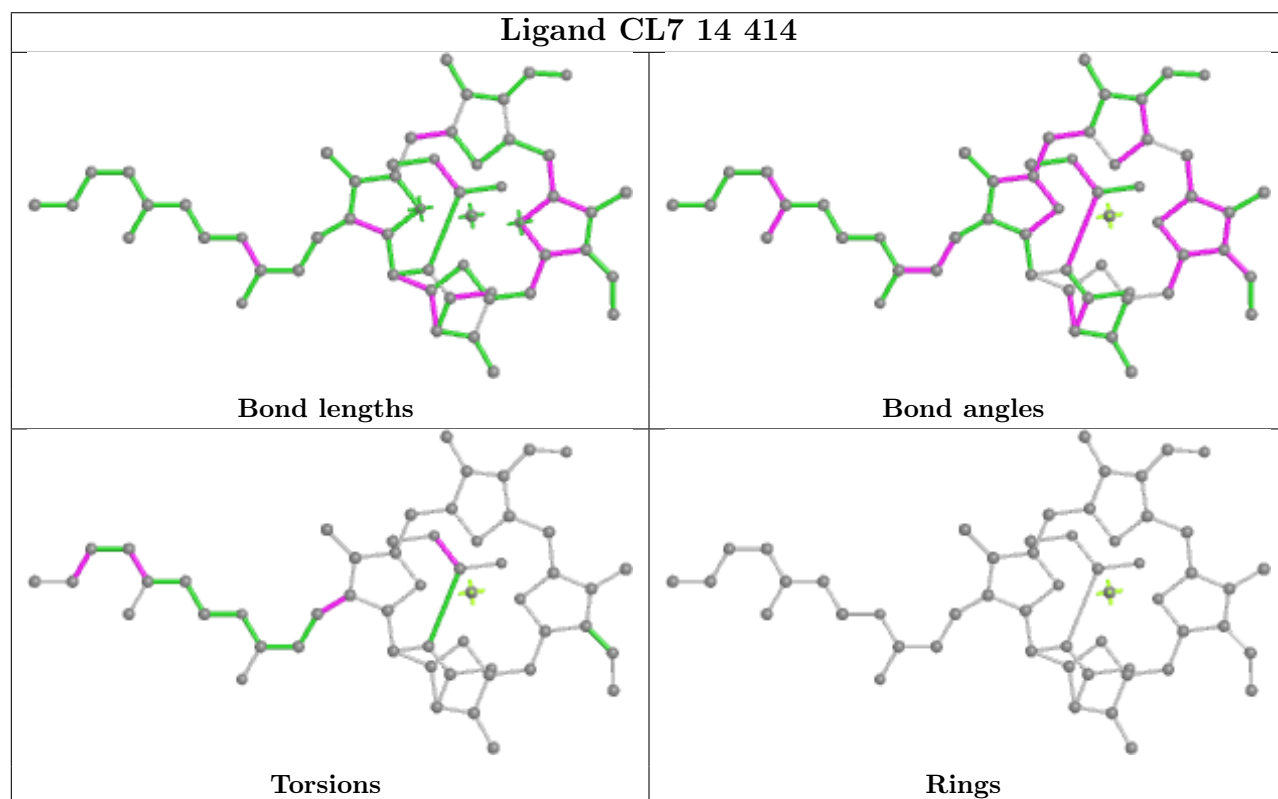
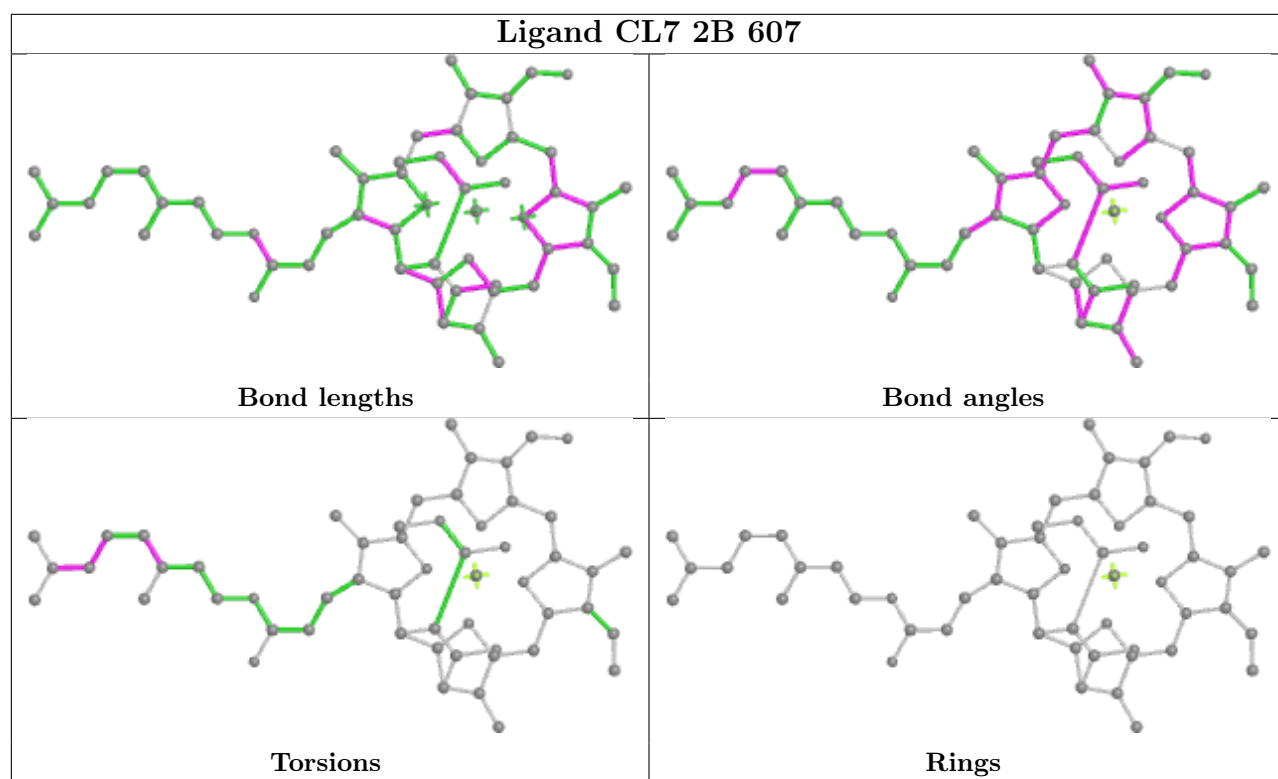
Torsions

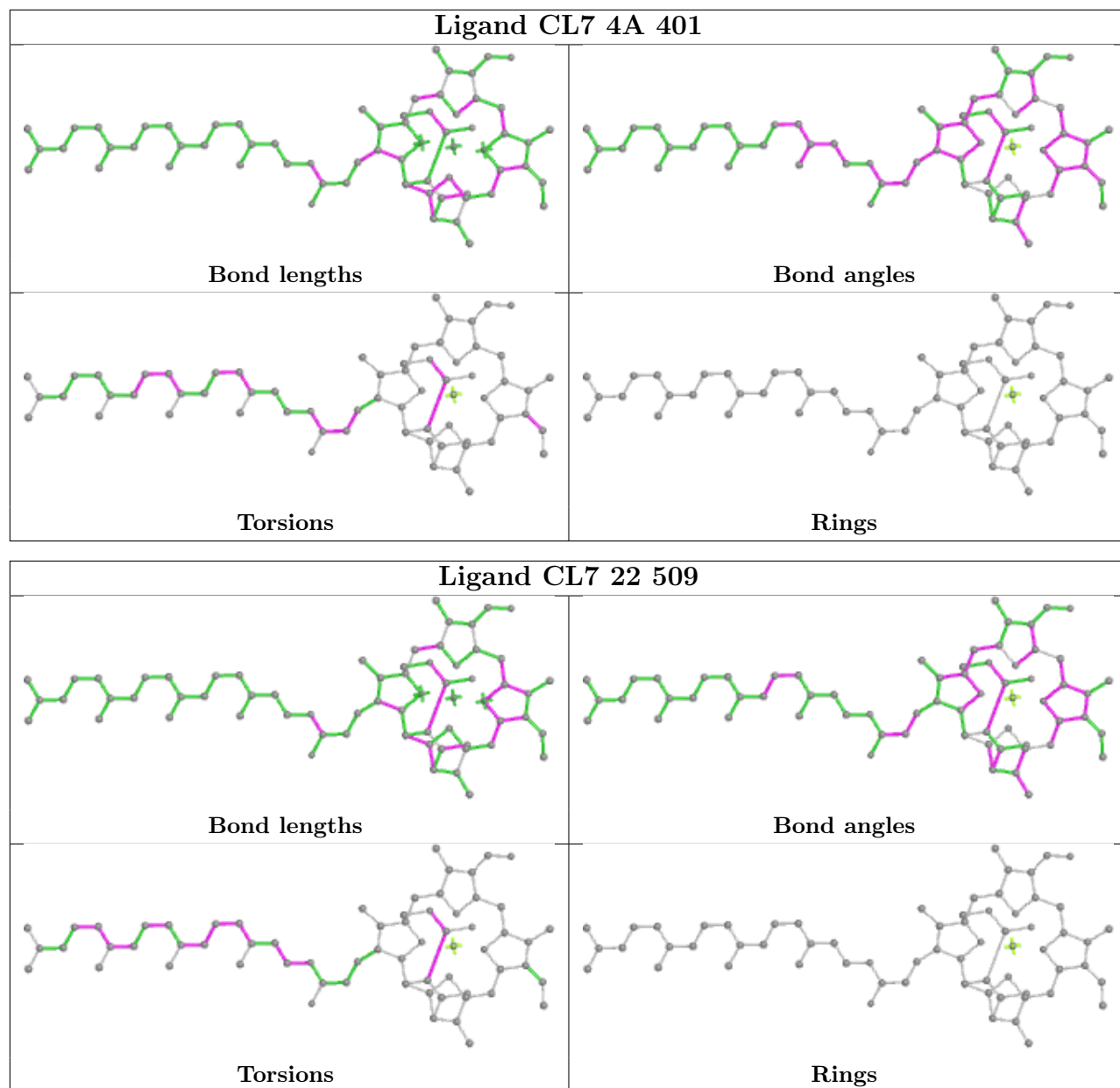


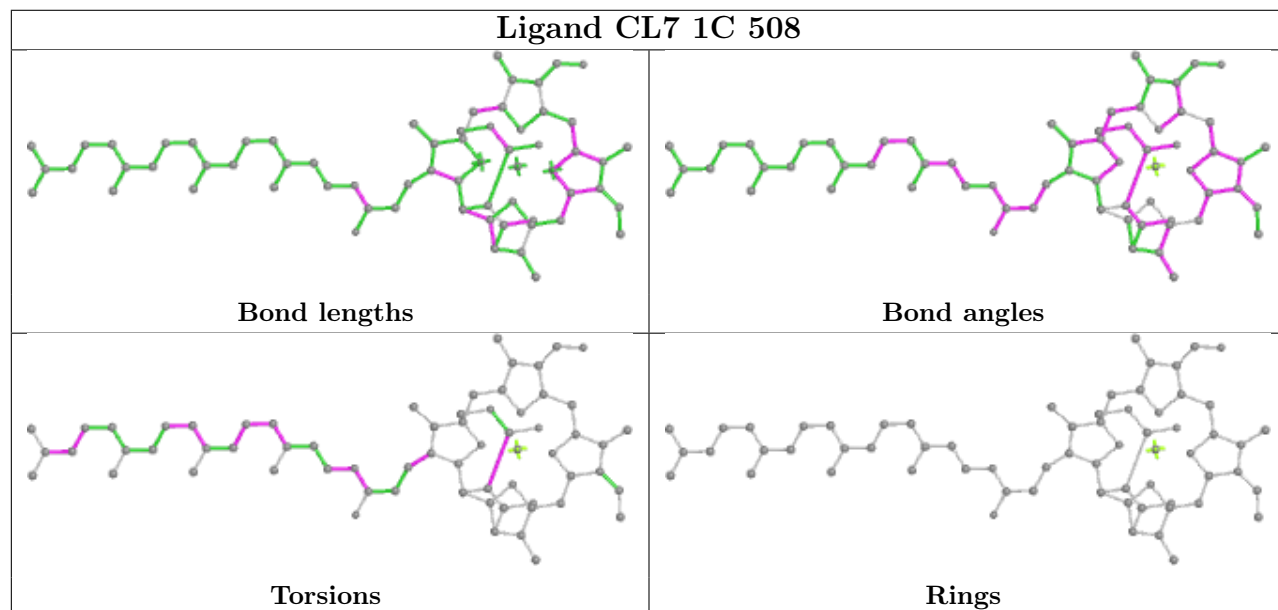
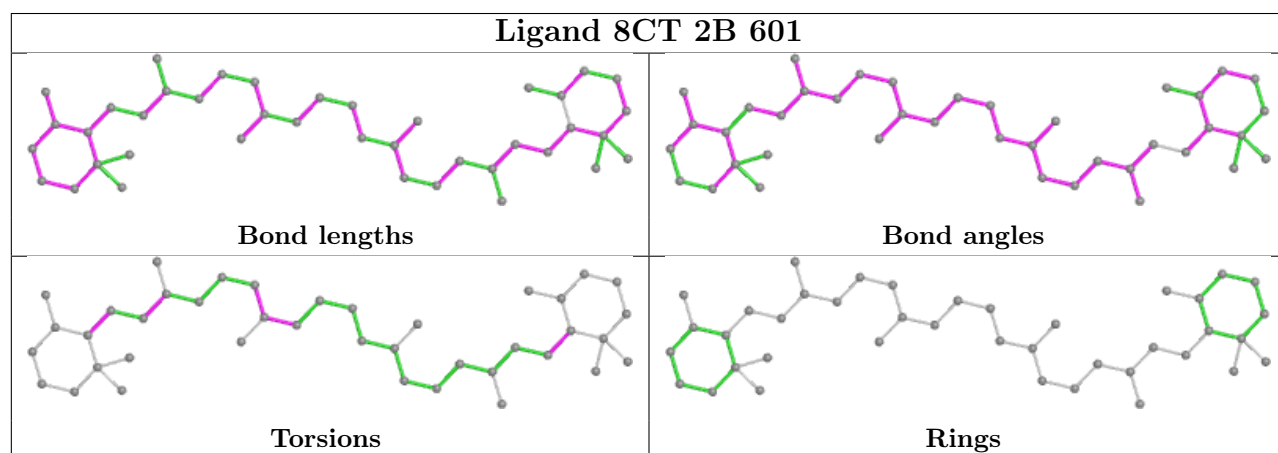
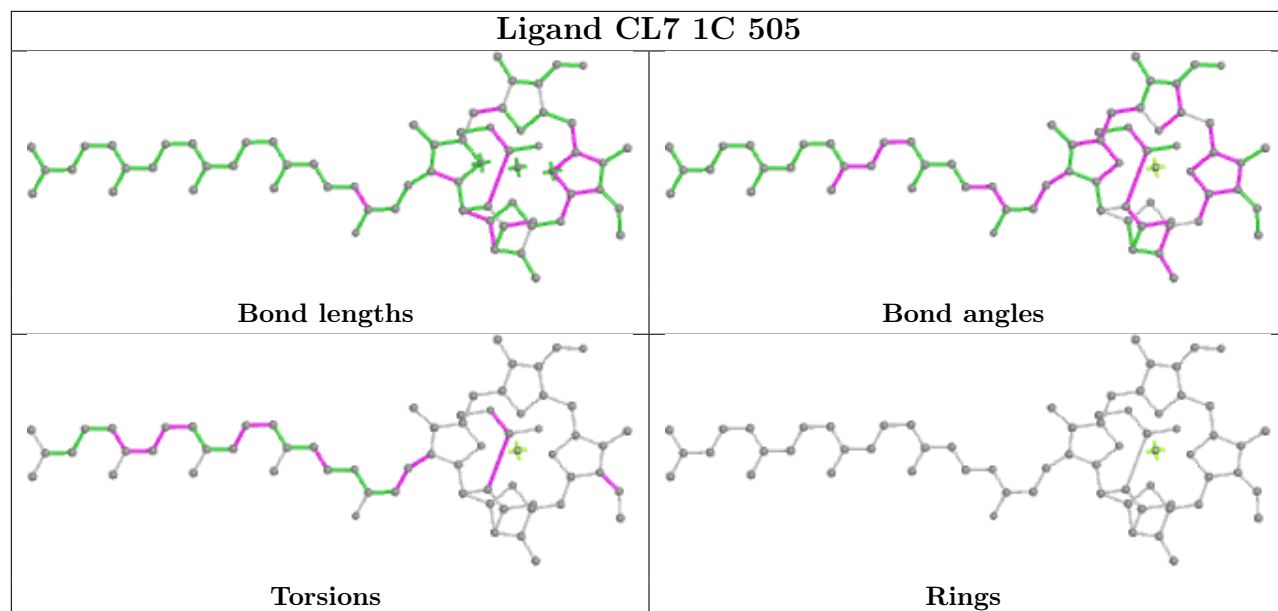
Rings

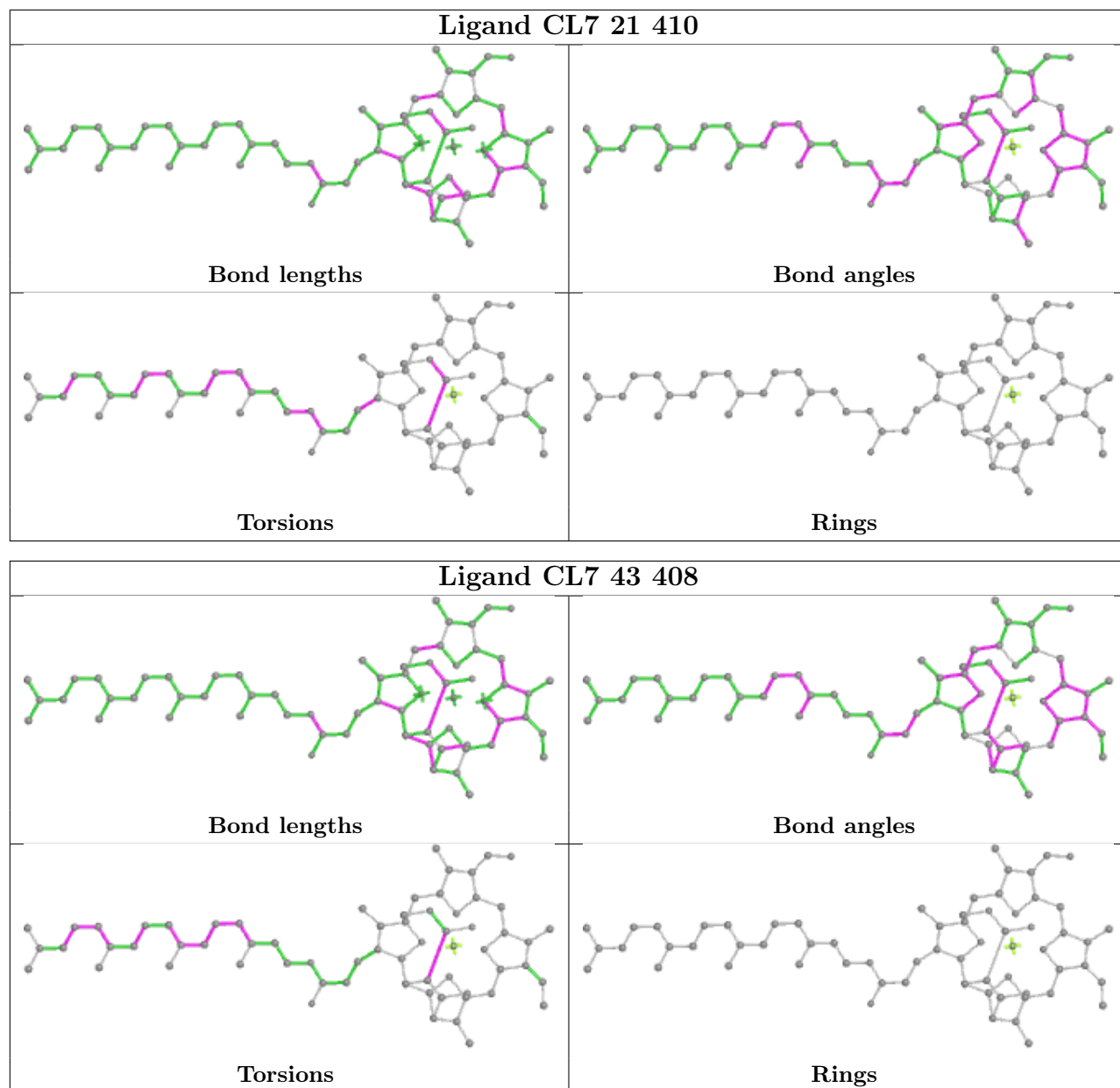




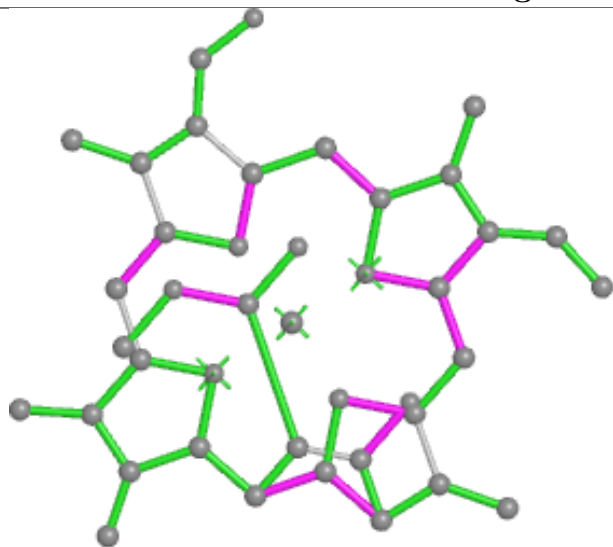




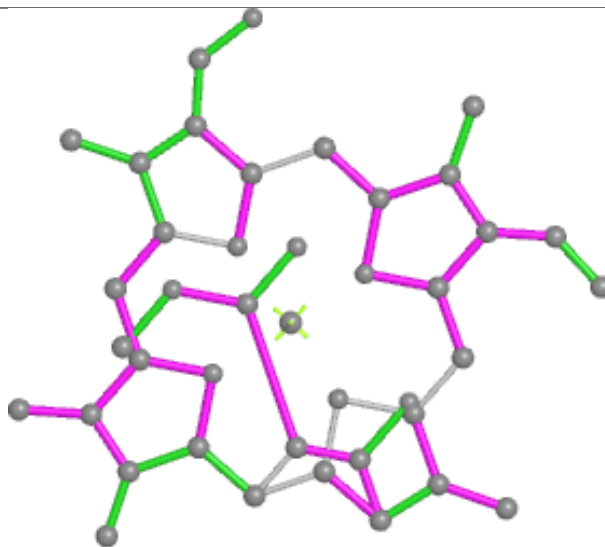




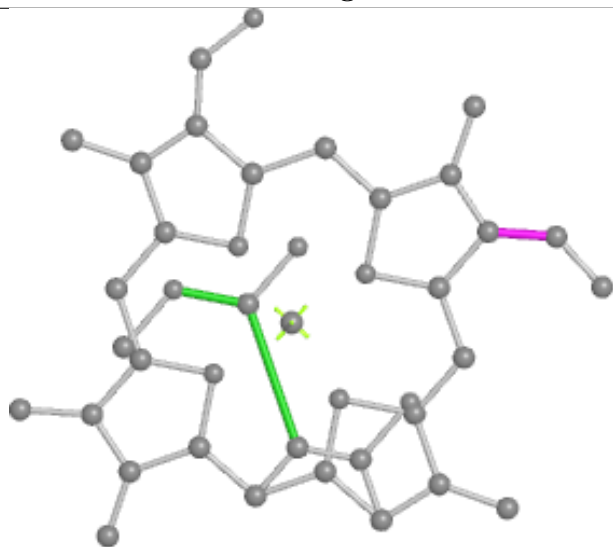
Ligand CL7 11 414



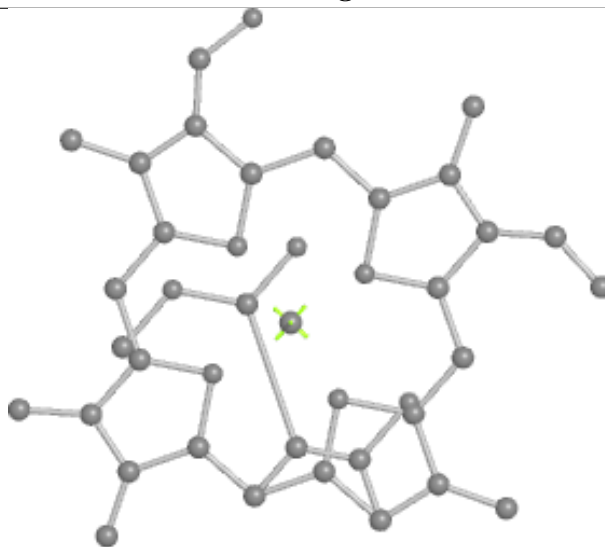
Bond lengths



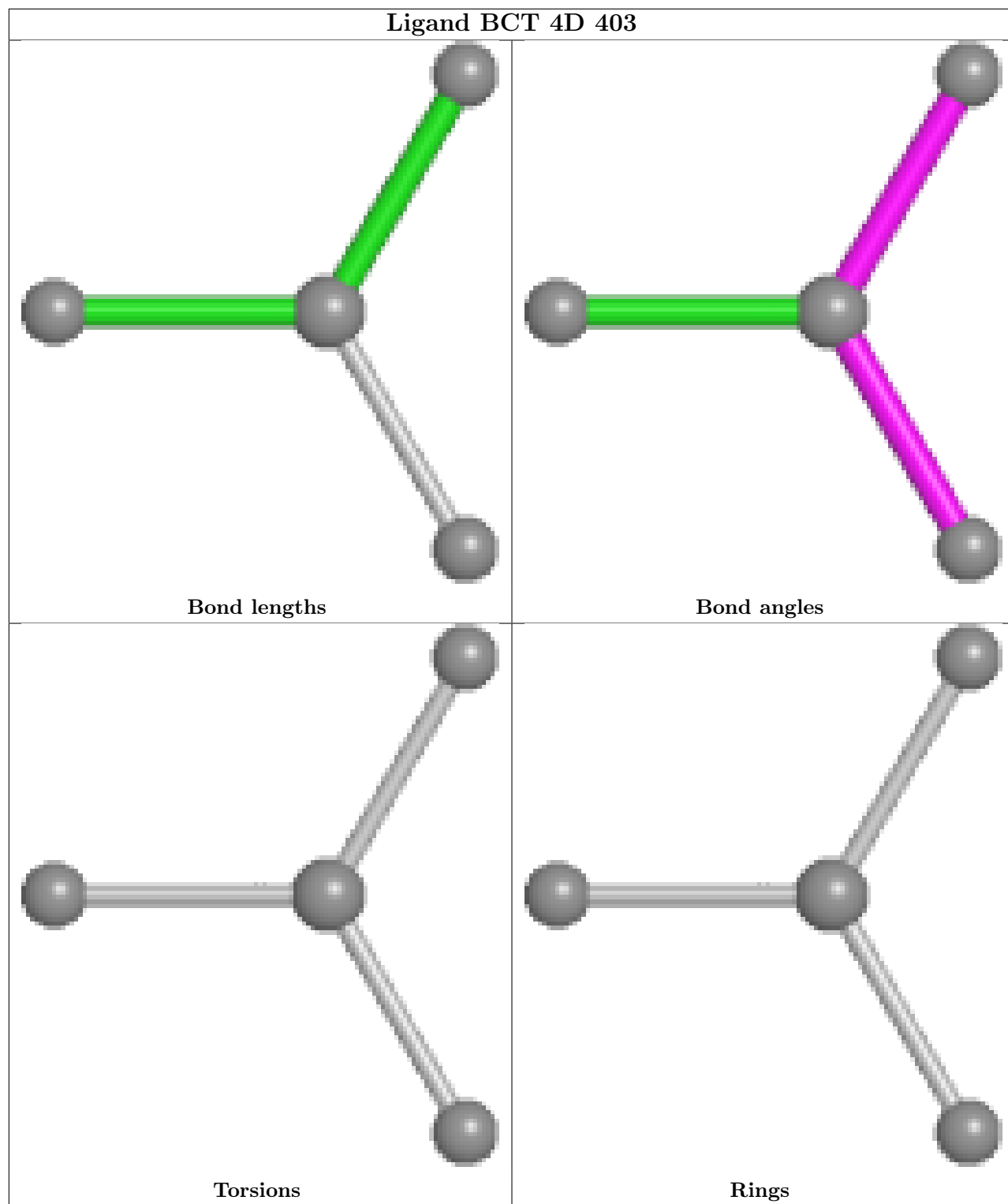
Bond angles



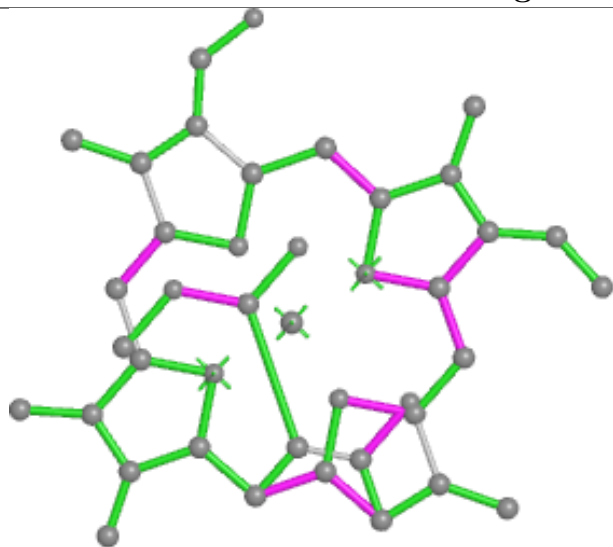
Torsions



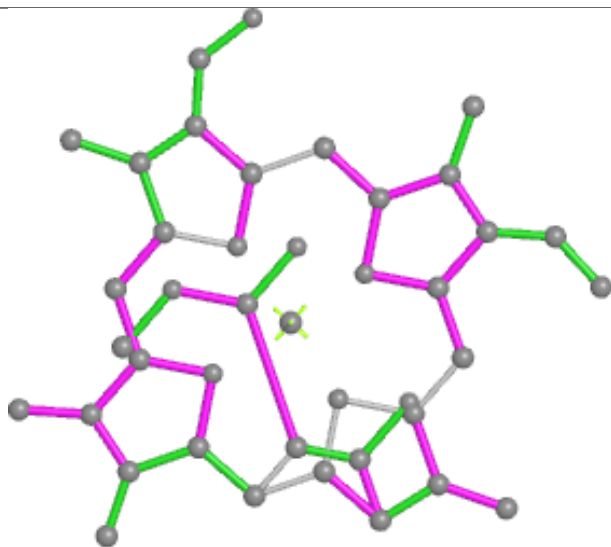
Rings



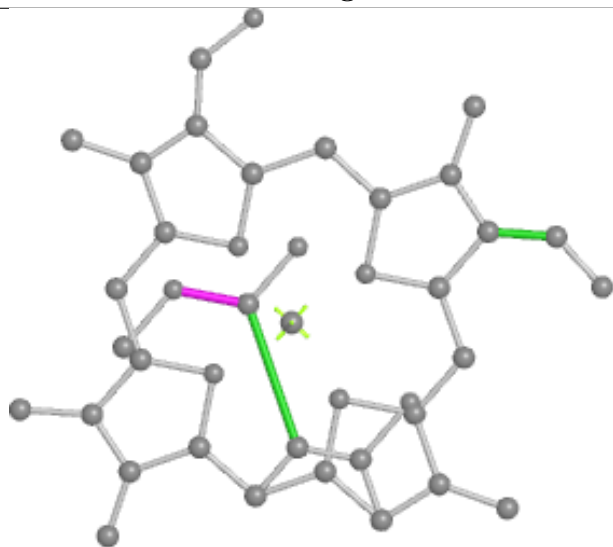
Ligand CL7 21 416



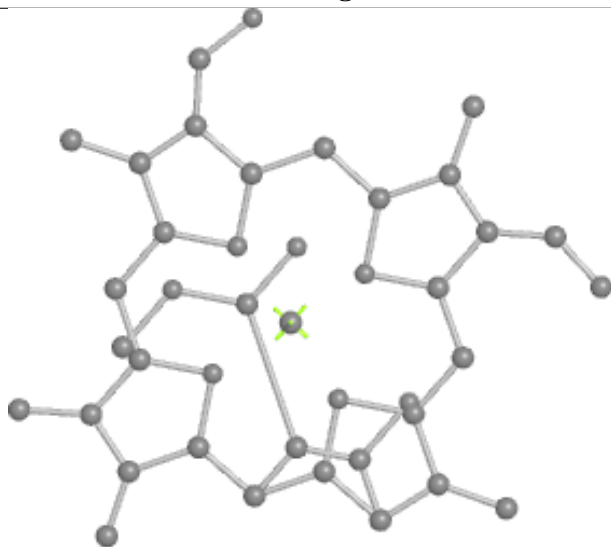
Bond lengths



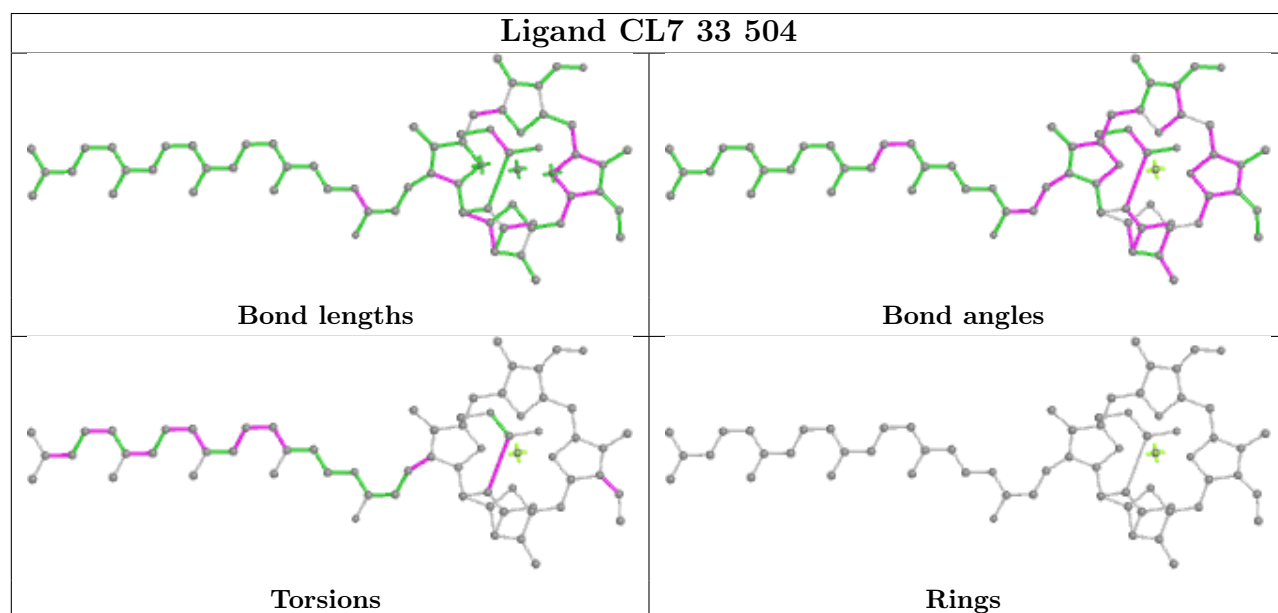
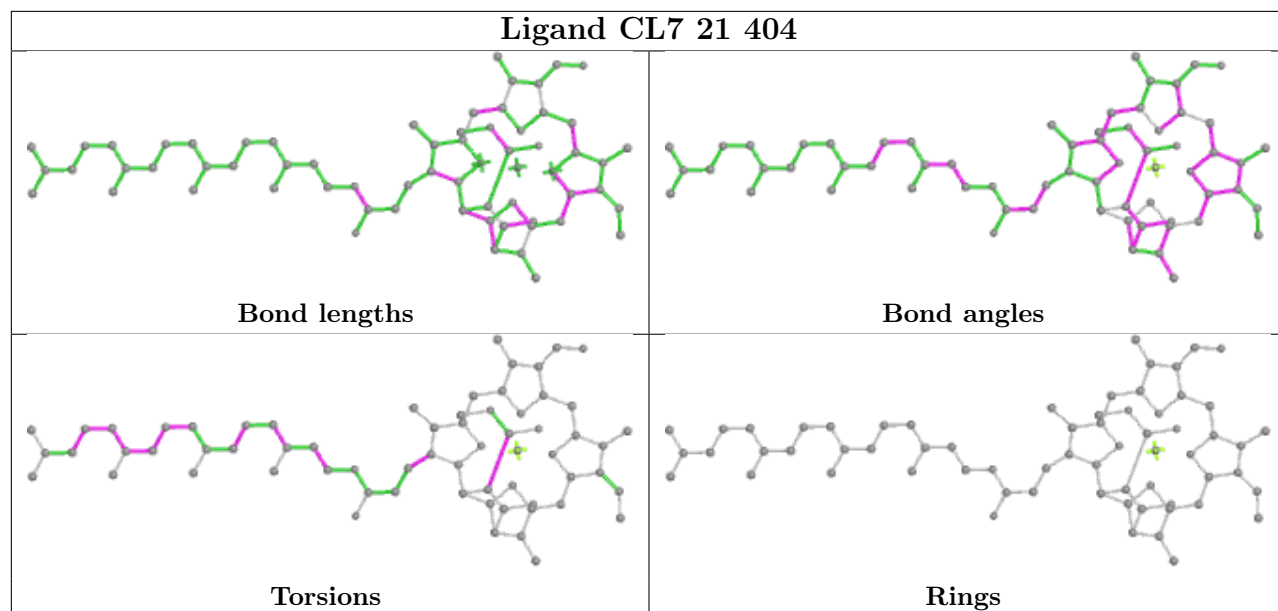
Bond angles

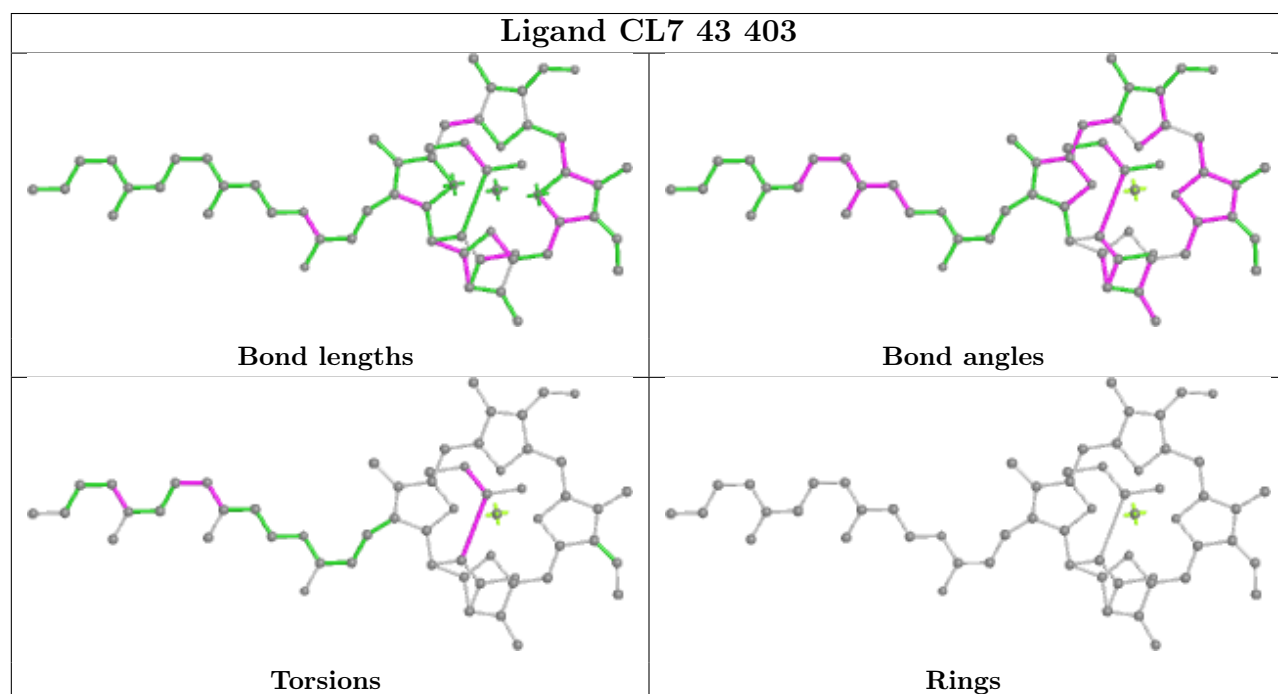
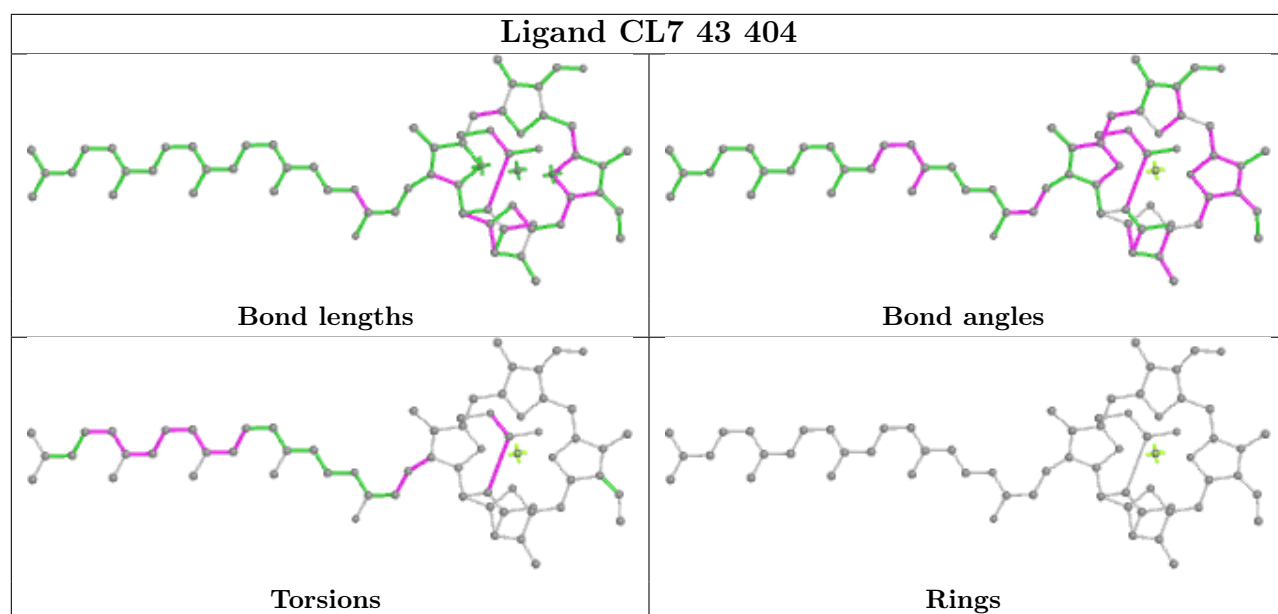


Torsions

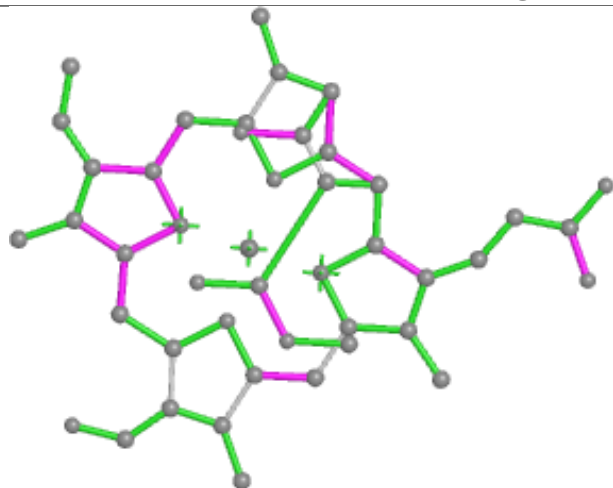


Rings

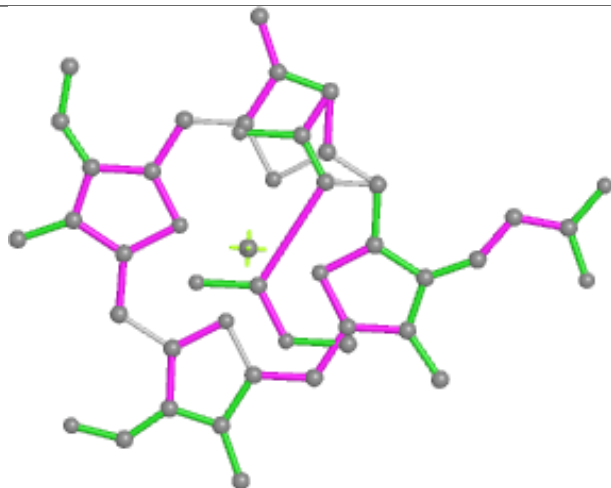




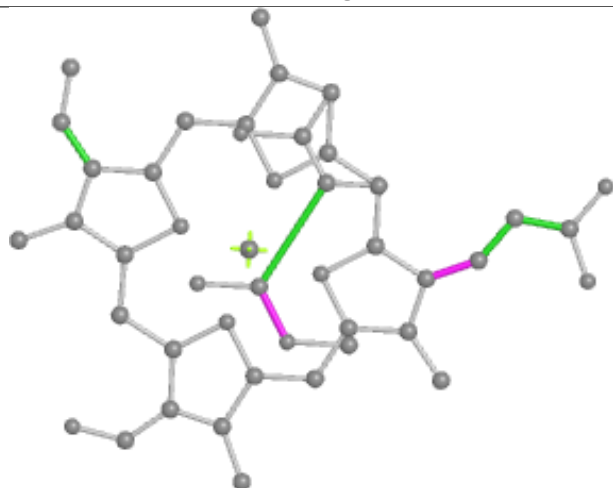
Ligand CL7 22 504



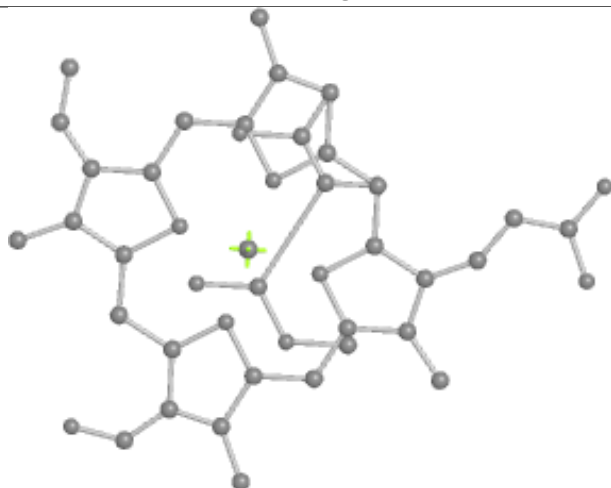
Bond lengths



Bond angles

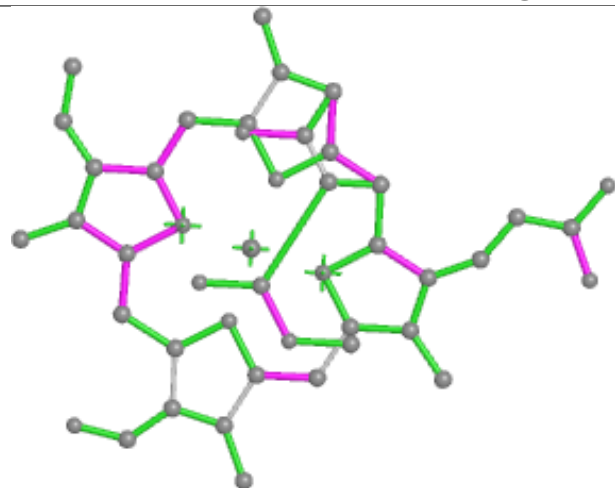


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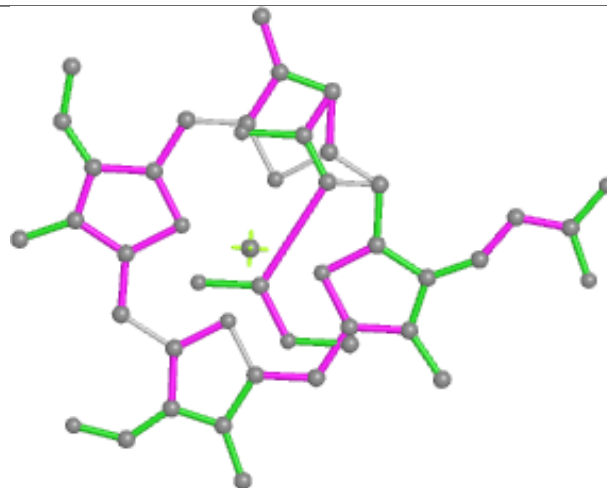


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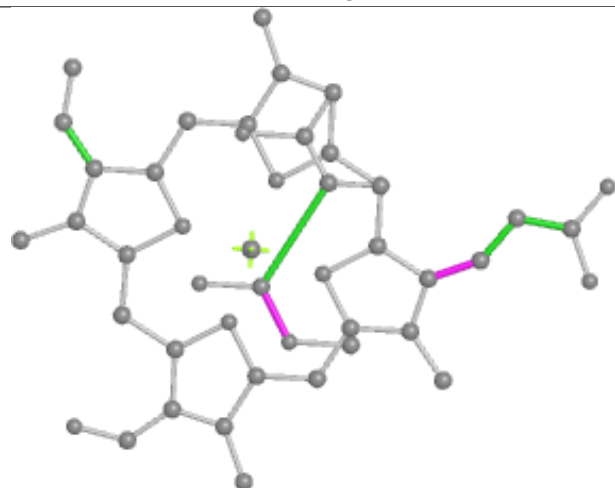
Ligand CL7 32 504



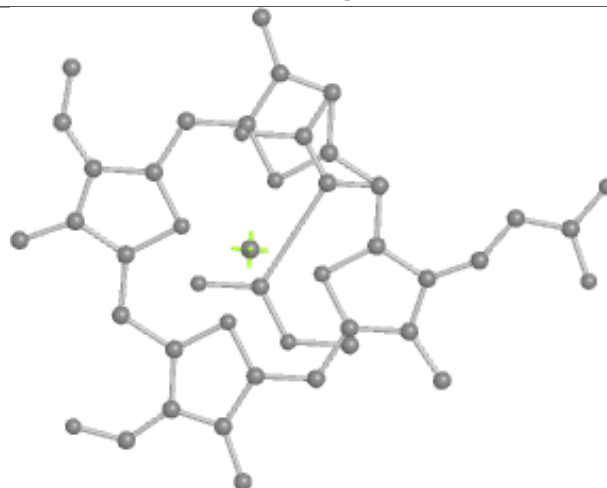
Bond lengths



Bond angles

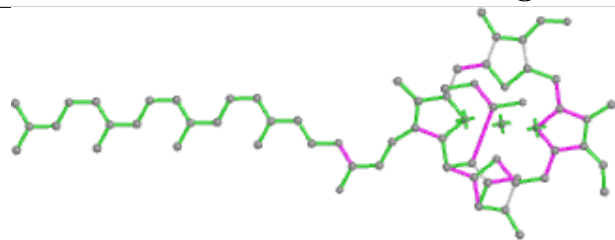


Torsions

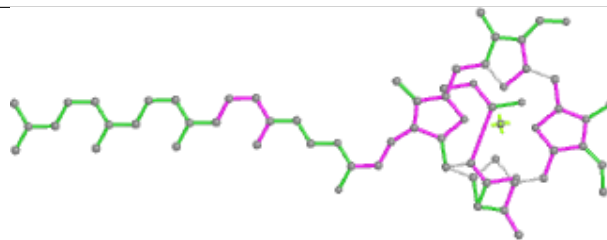


Rings

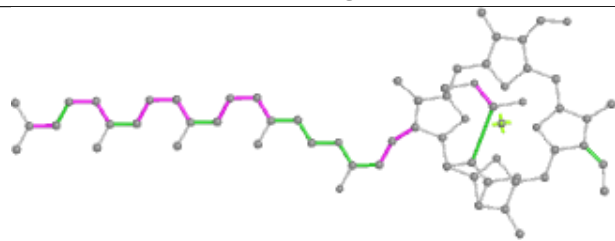
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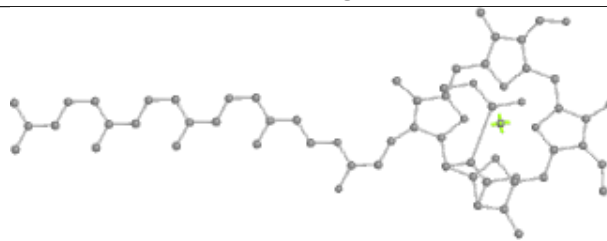
Bond lengths



Bond angles

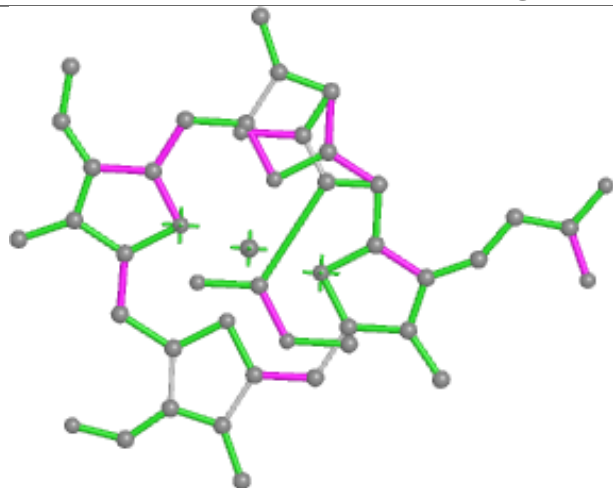


Torsions

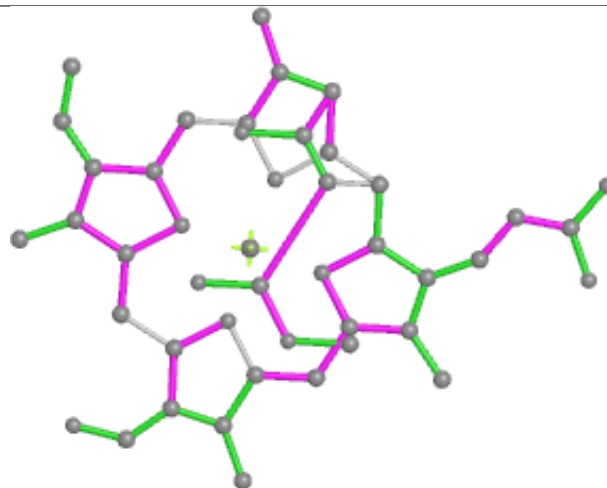


Rings

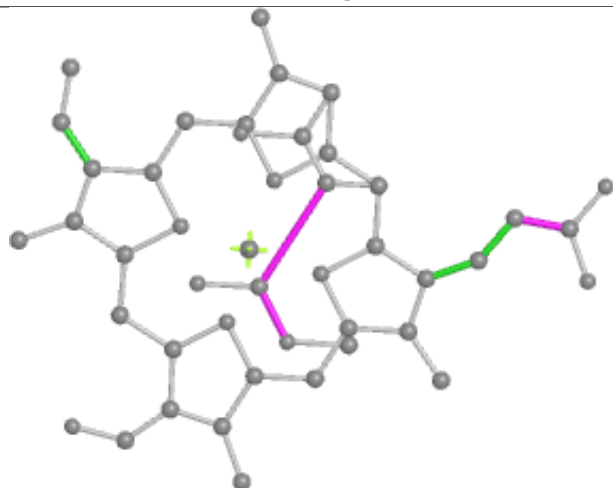
Ligand CL7 31 411



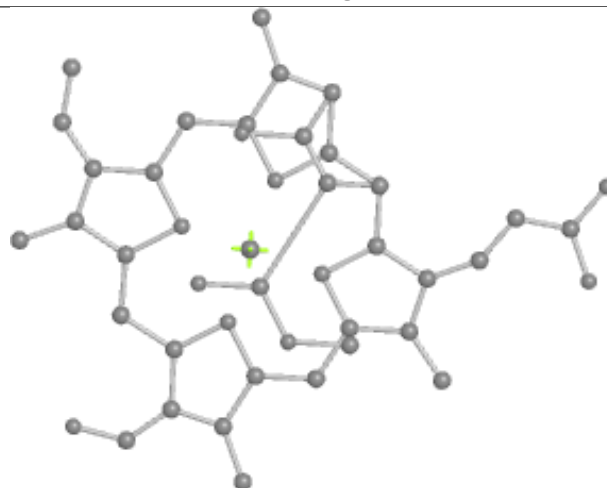
Bond lengths



Bond angles

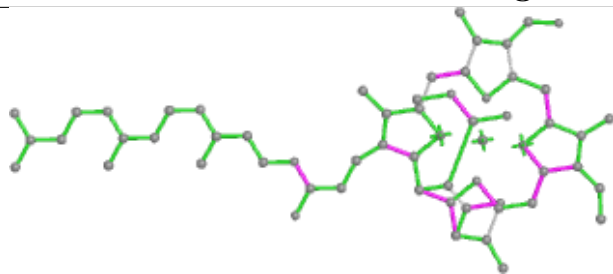


Torsions

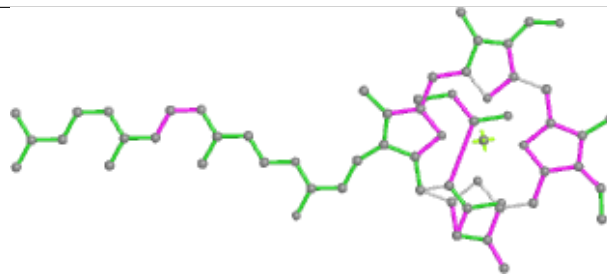


Rings

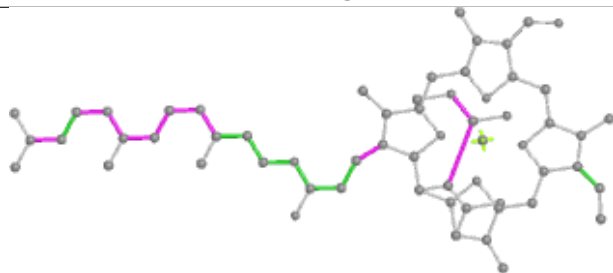
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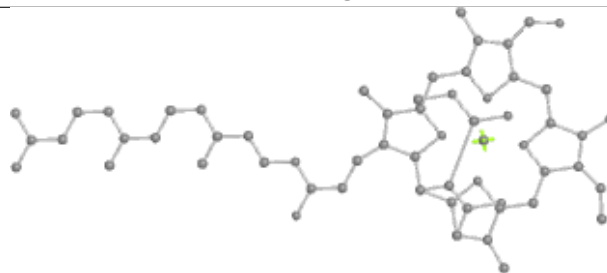
Bond lengths



Bond angles

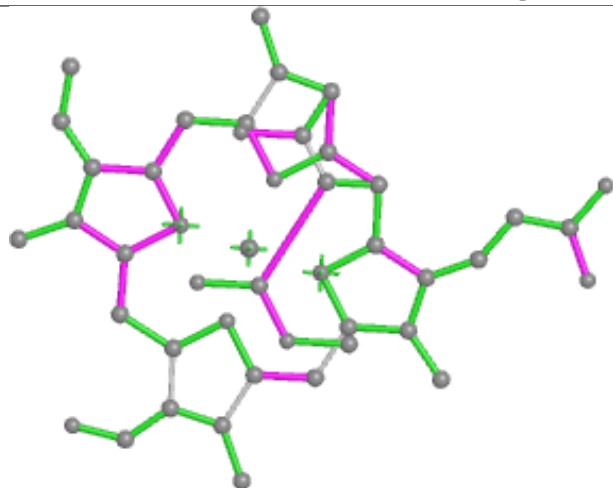


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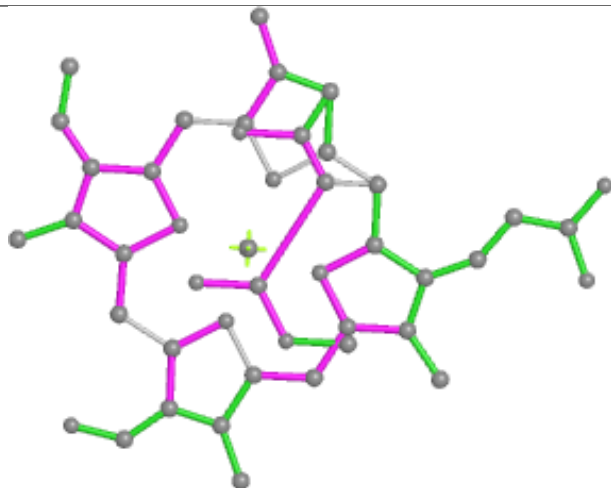


Rings

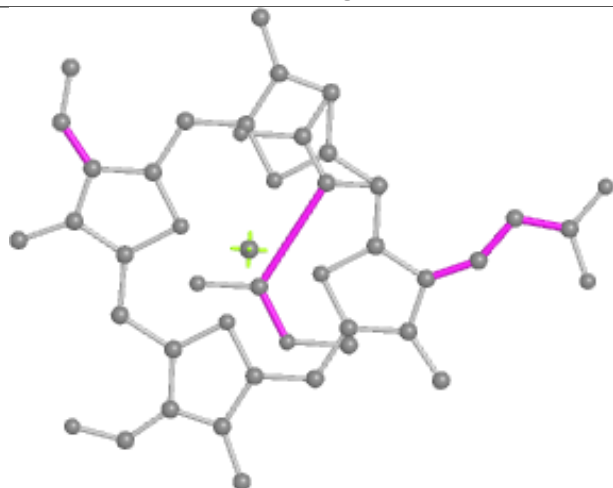
Ligand CL7 14 415



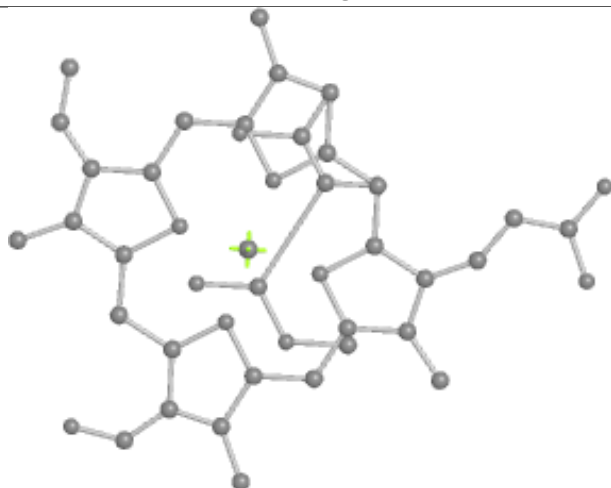
Bond lengths



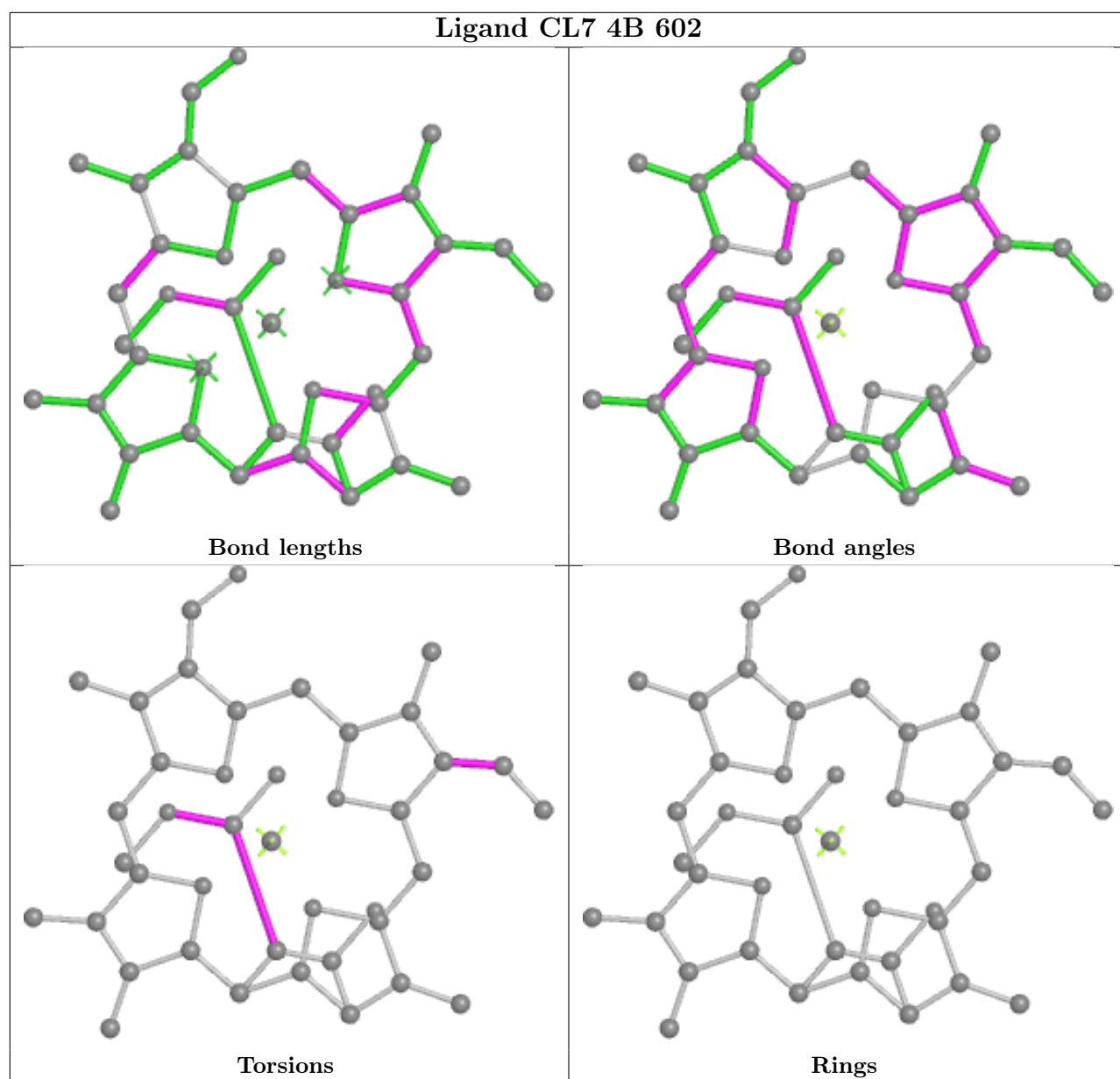
Bond angles



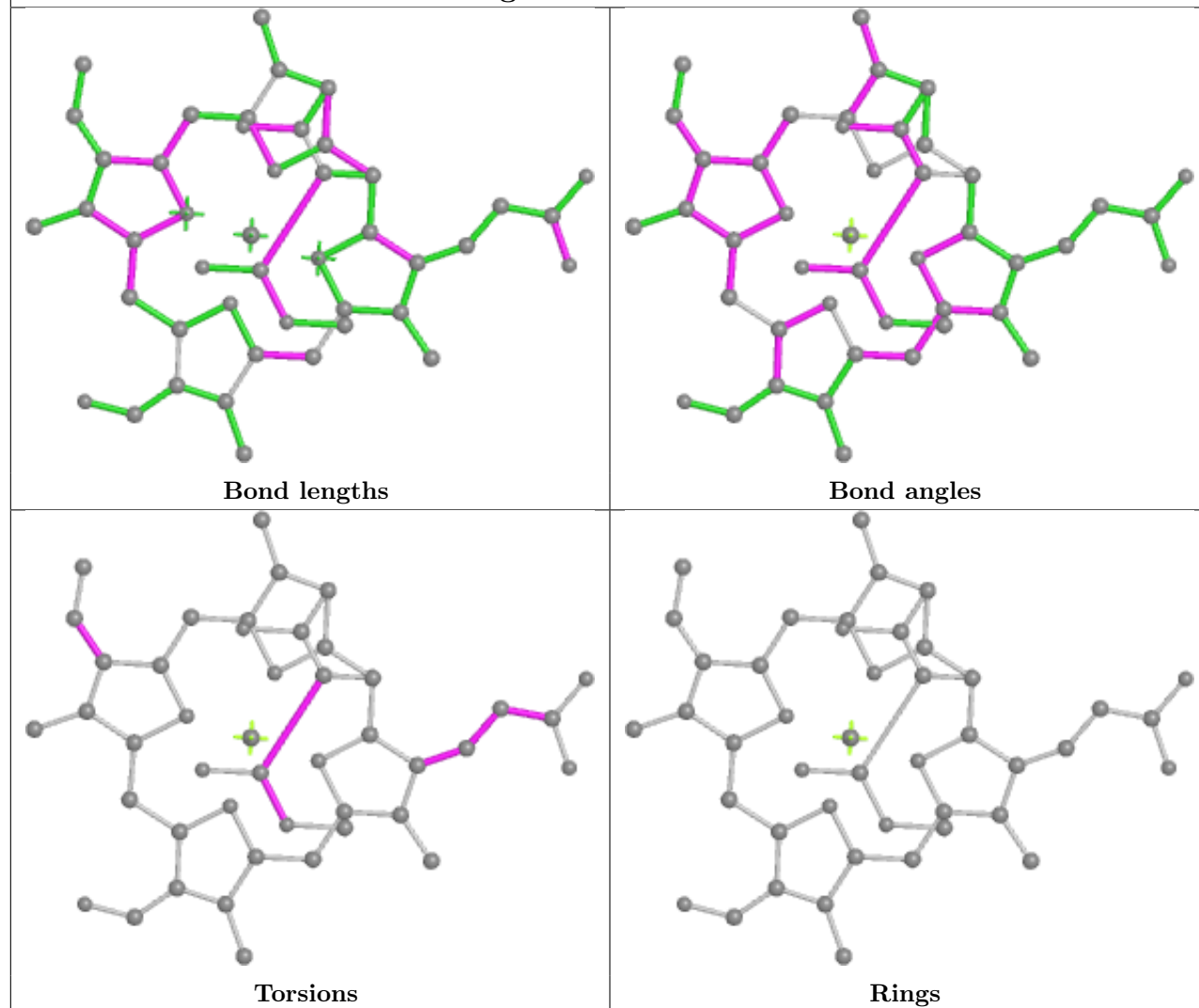
Torsions



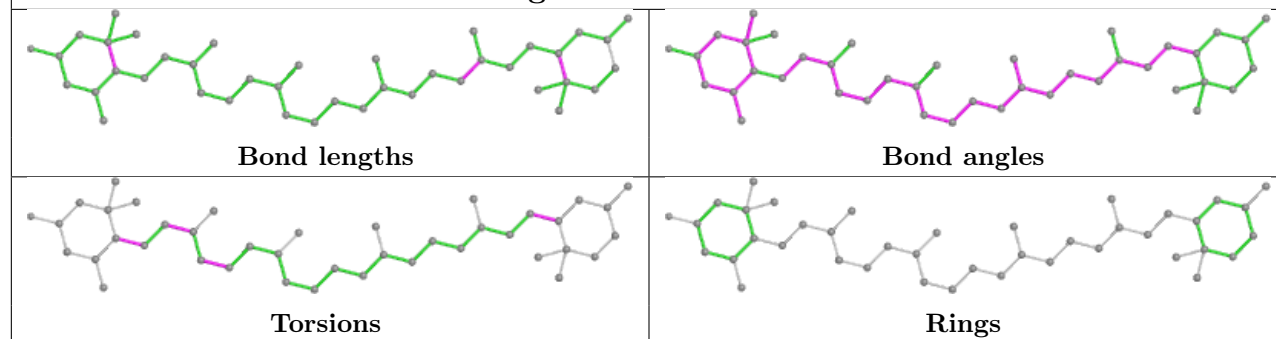
Rings

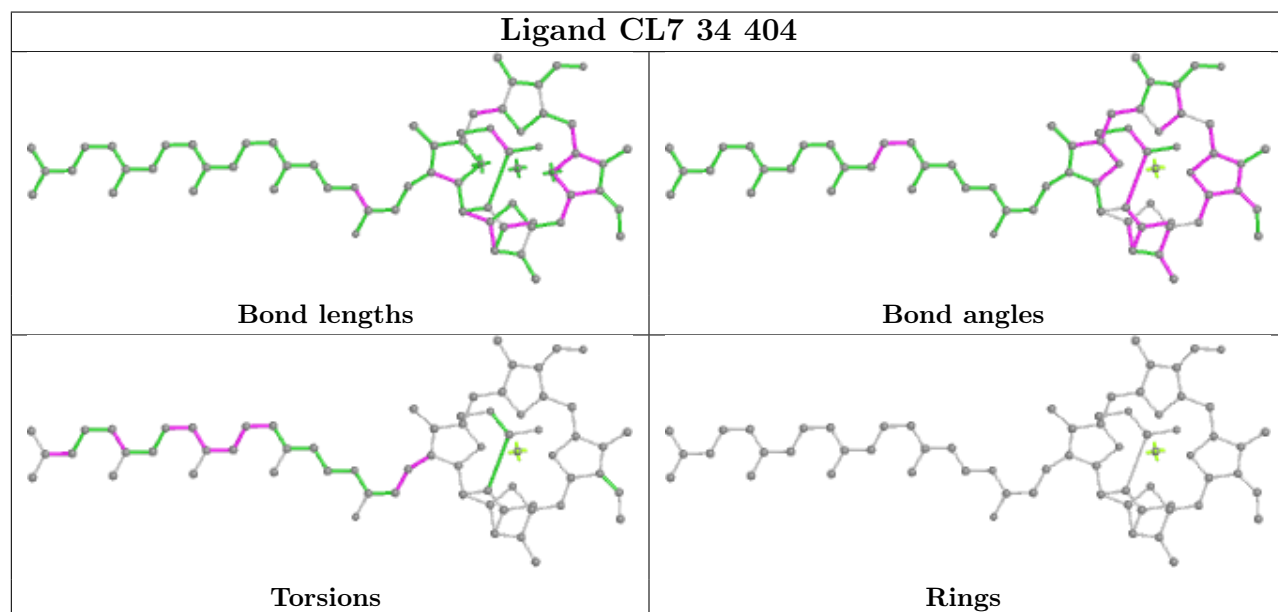
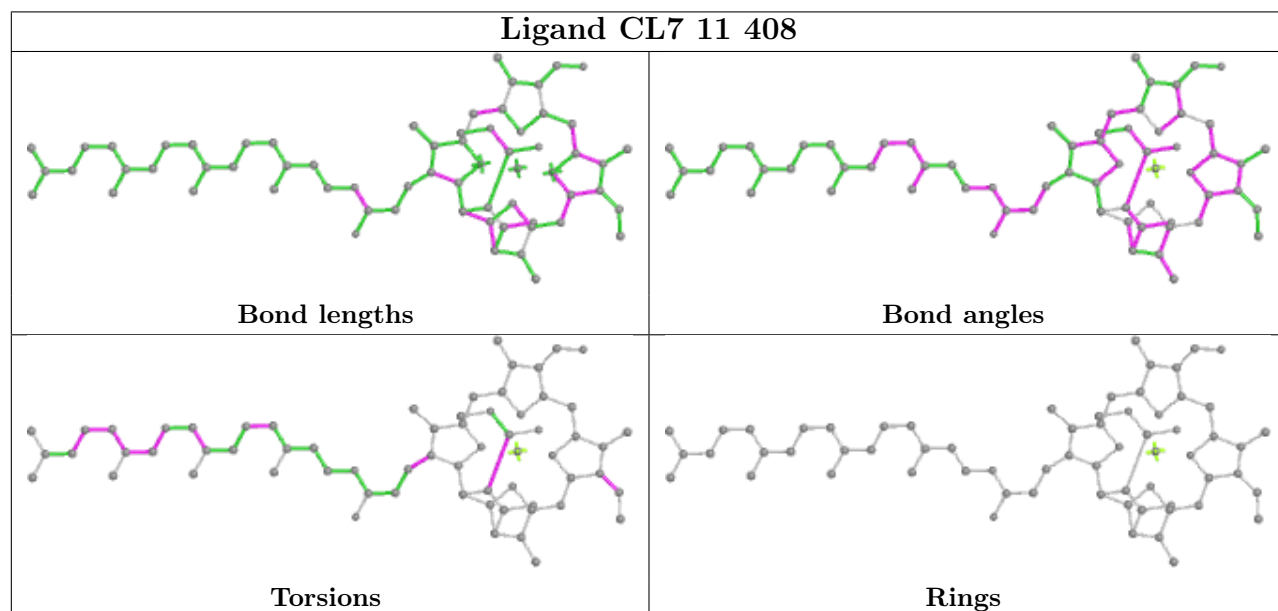
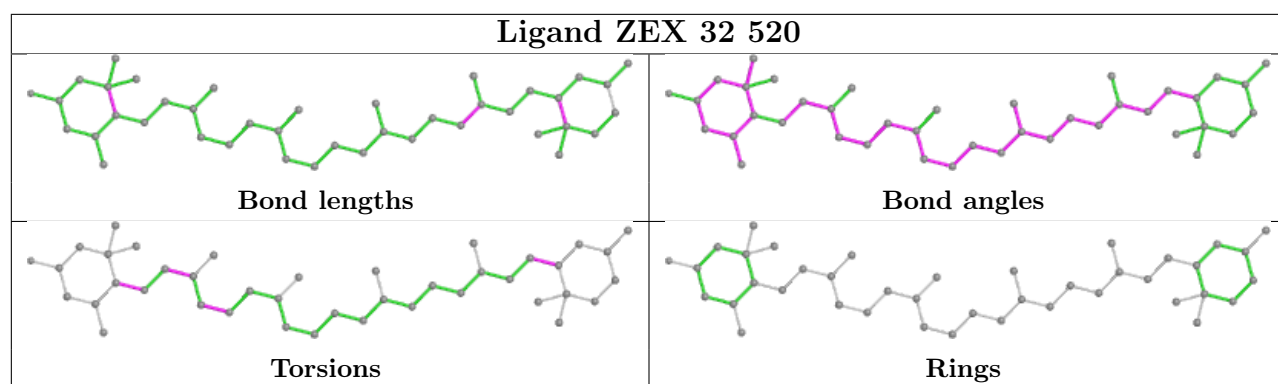


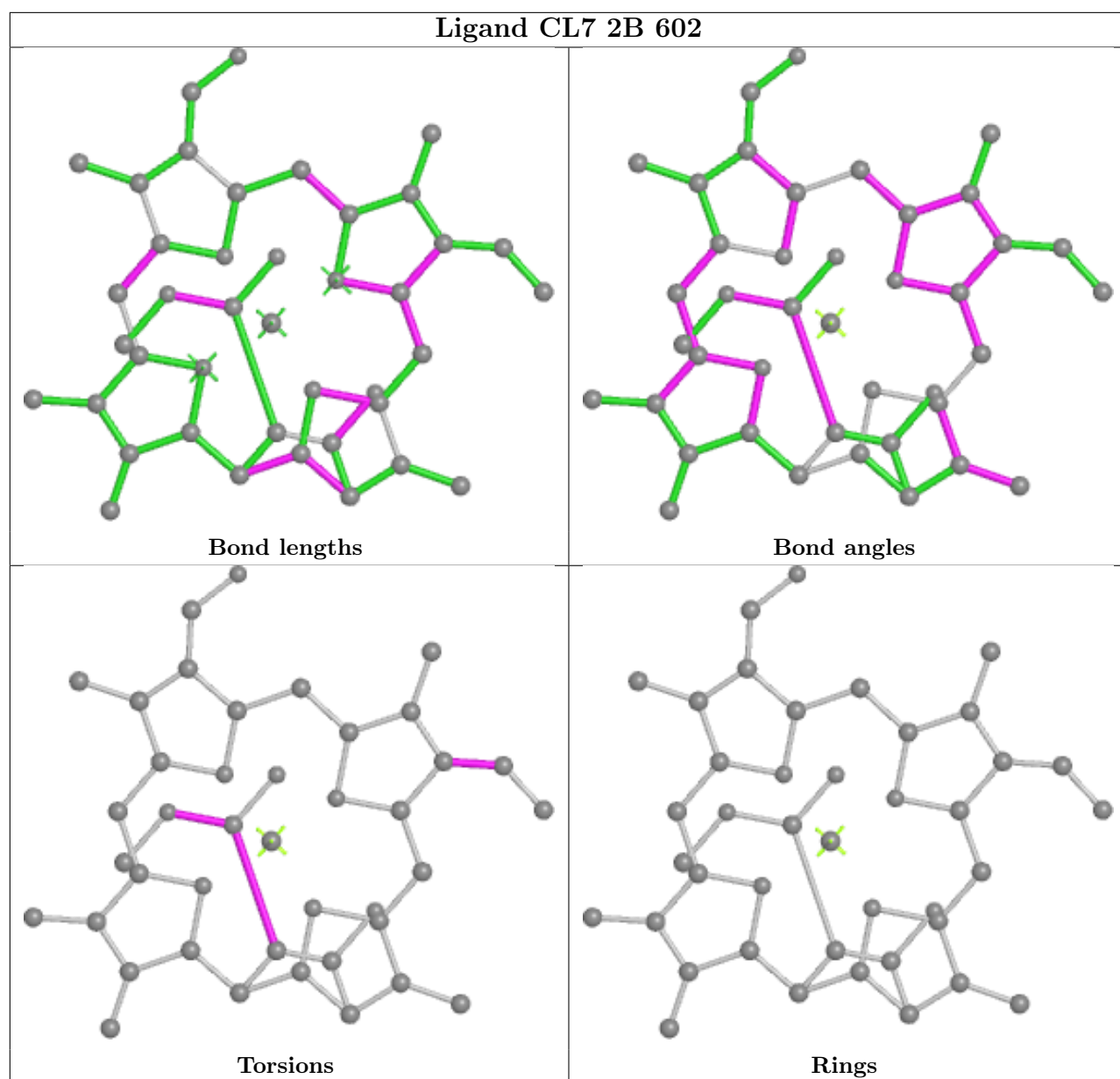
Ligand CL7 44 415

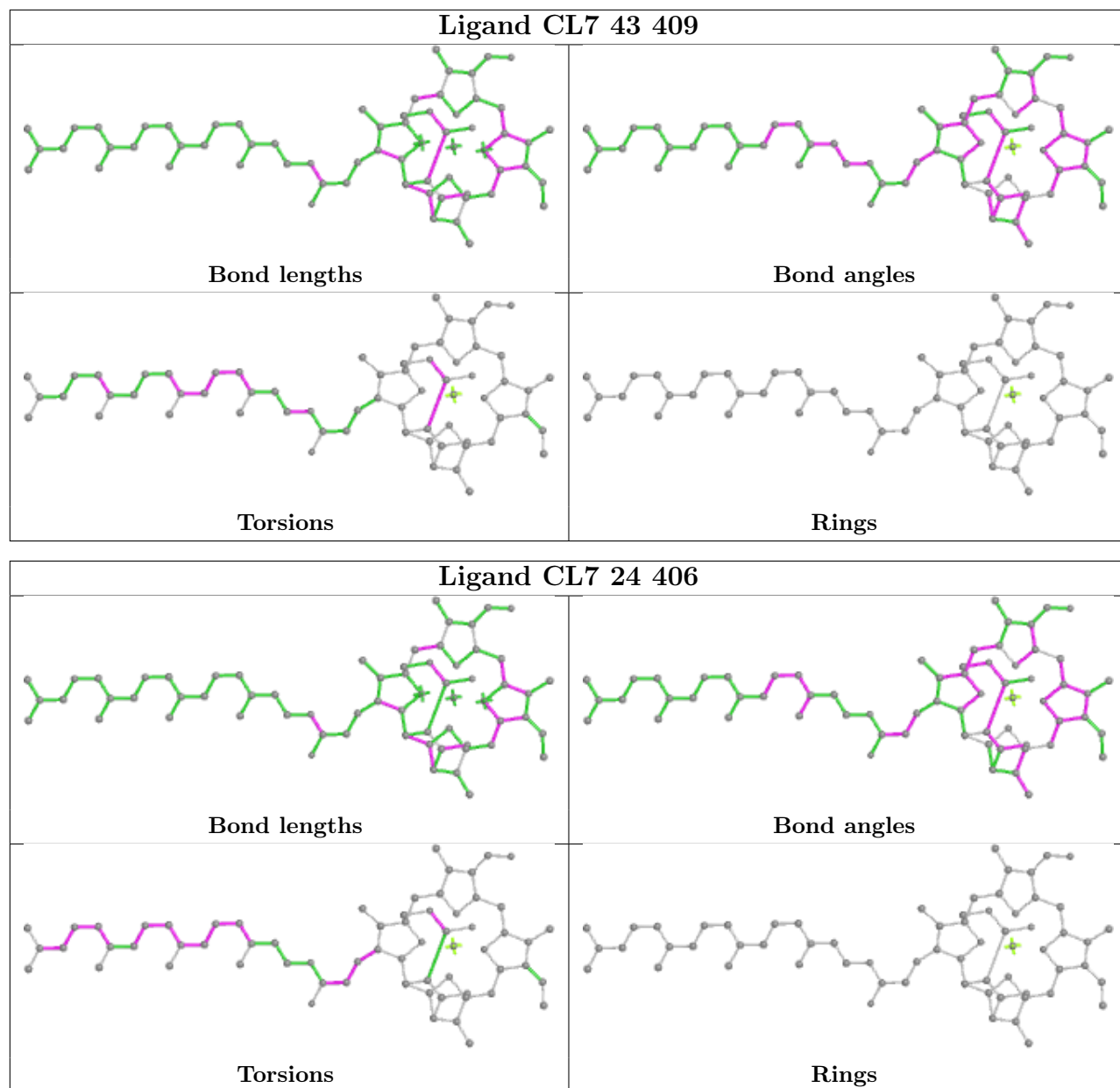


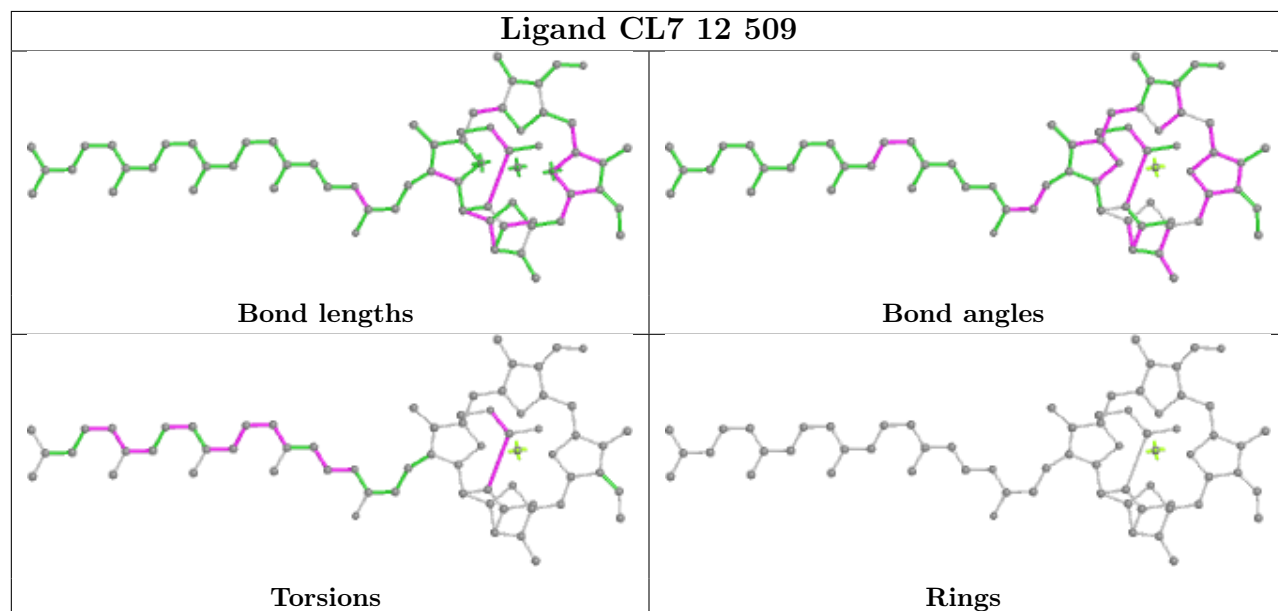
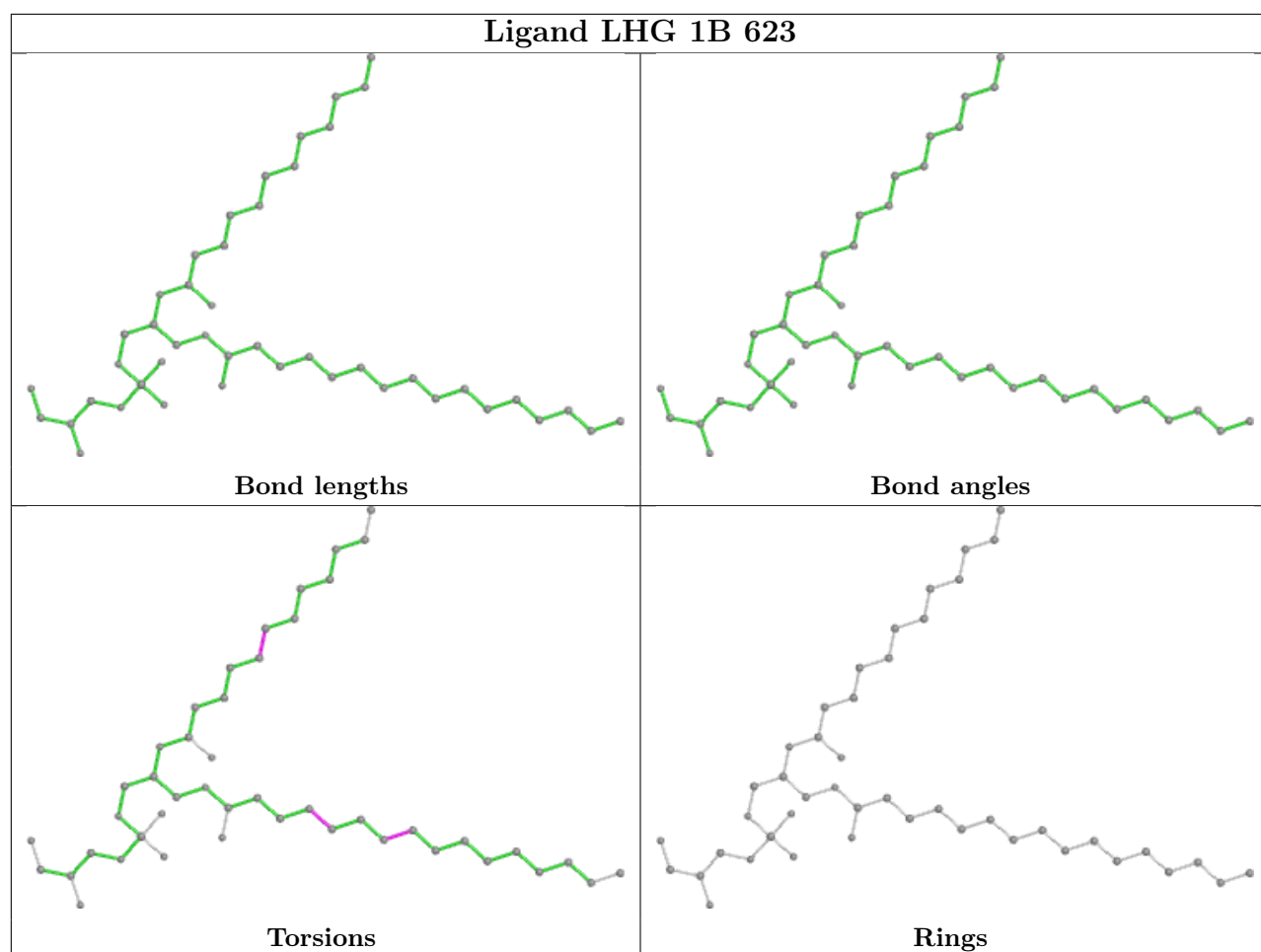
Ligand ZEX 22 520

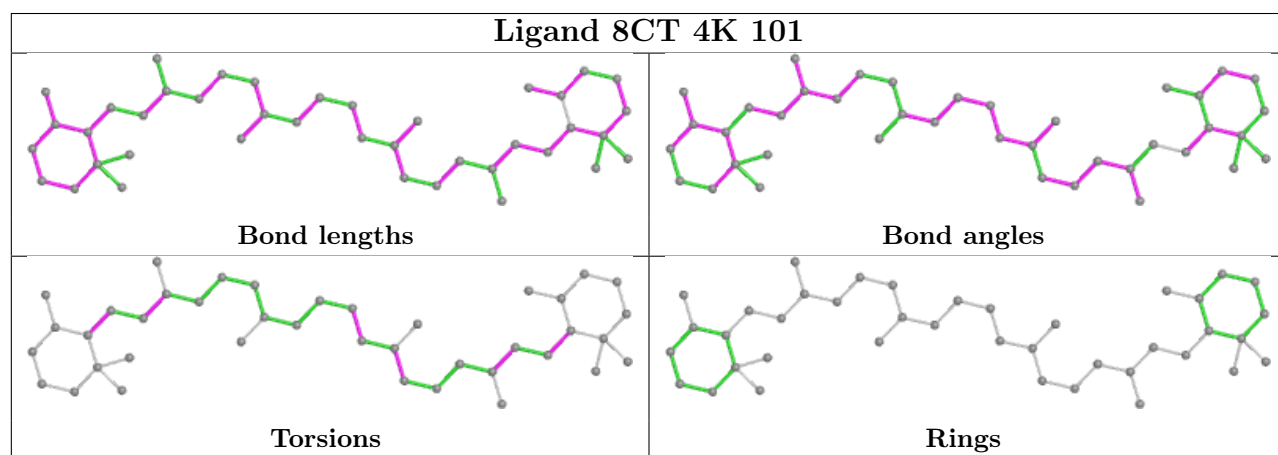
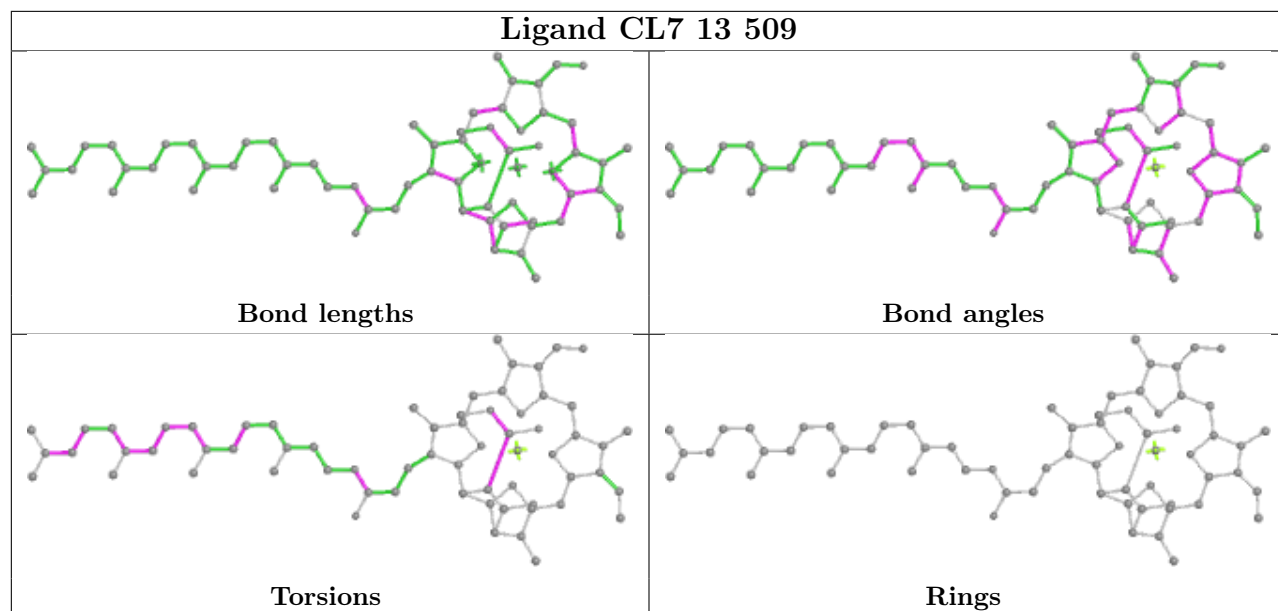


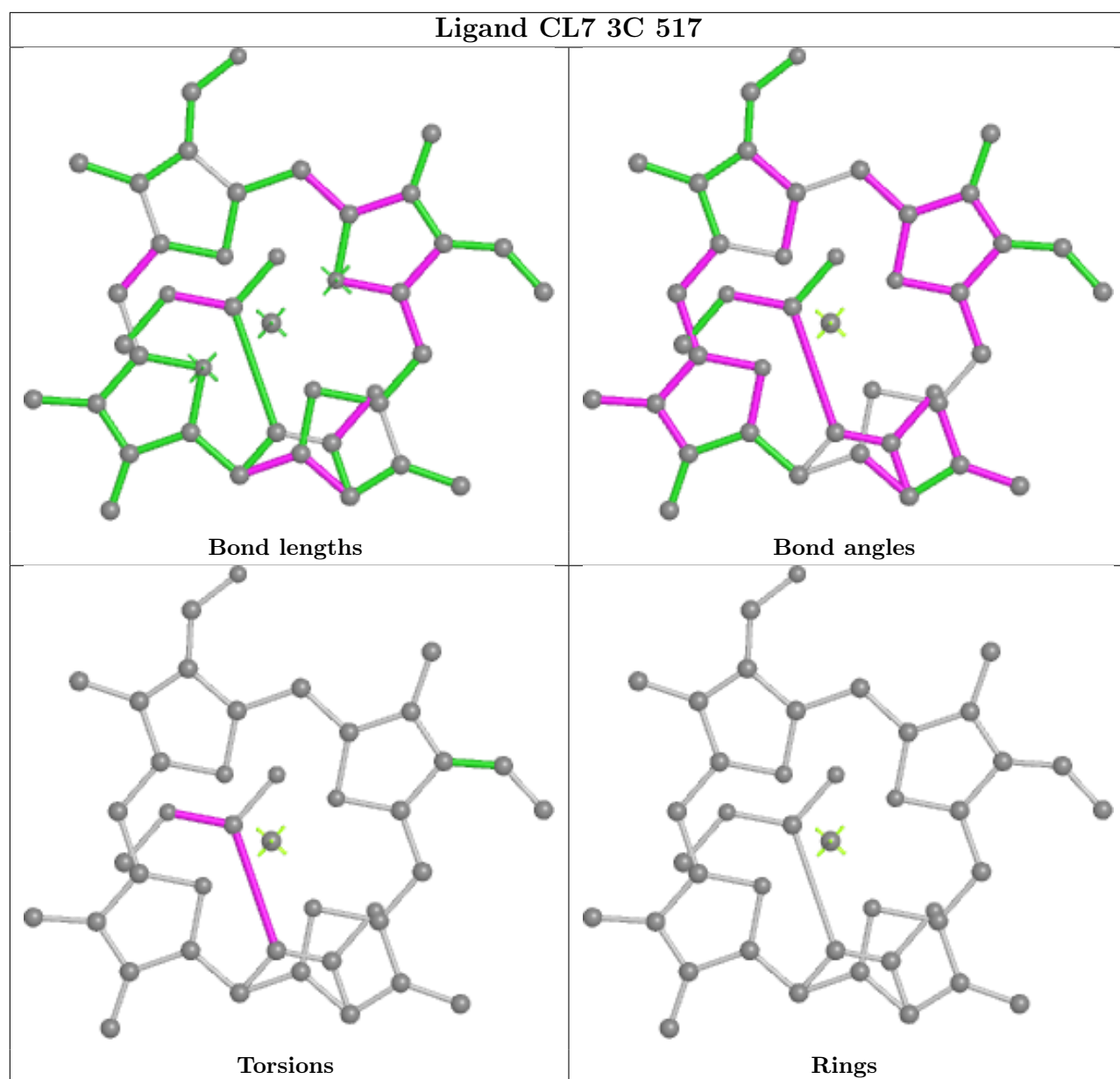




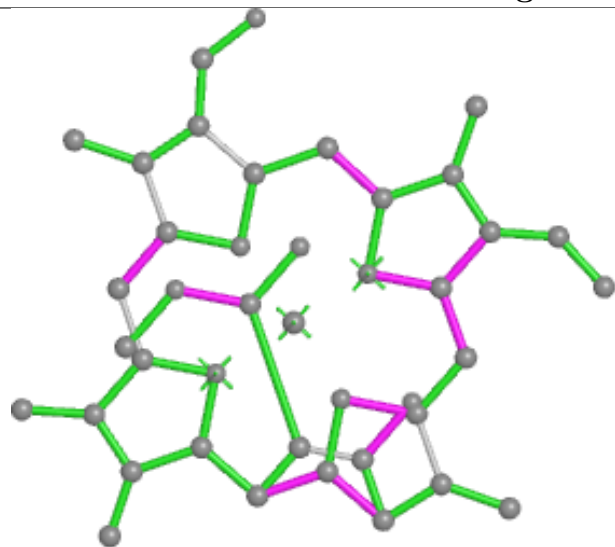




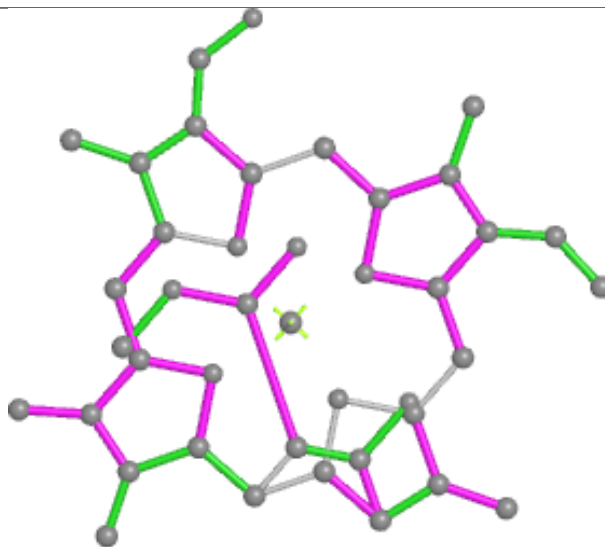




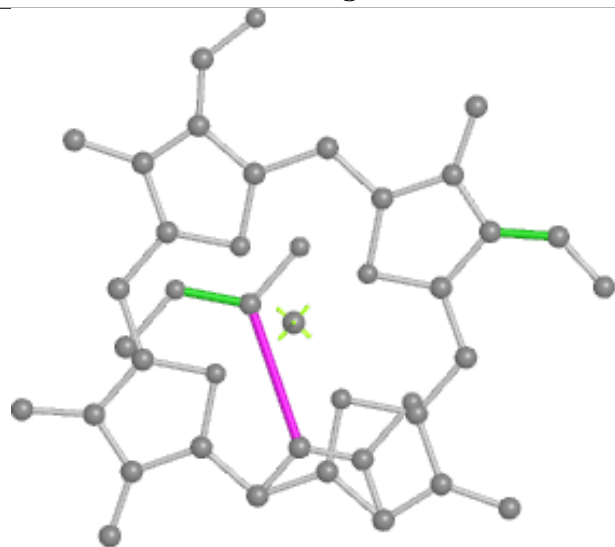
Ligand CL7 21 413



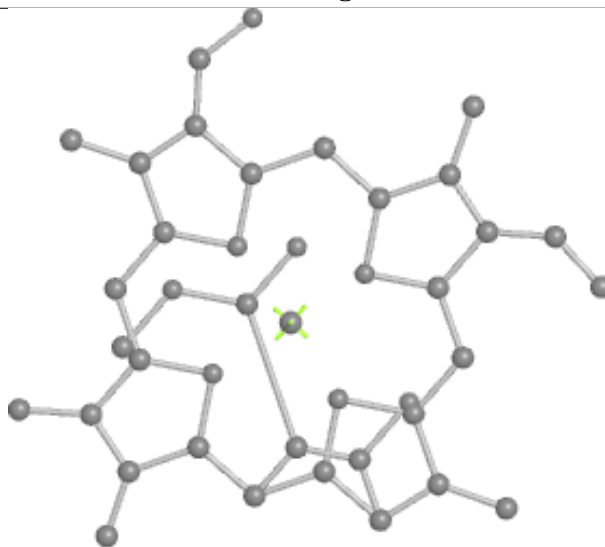
Bond lengths



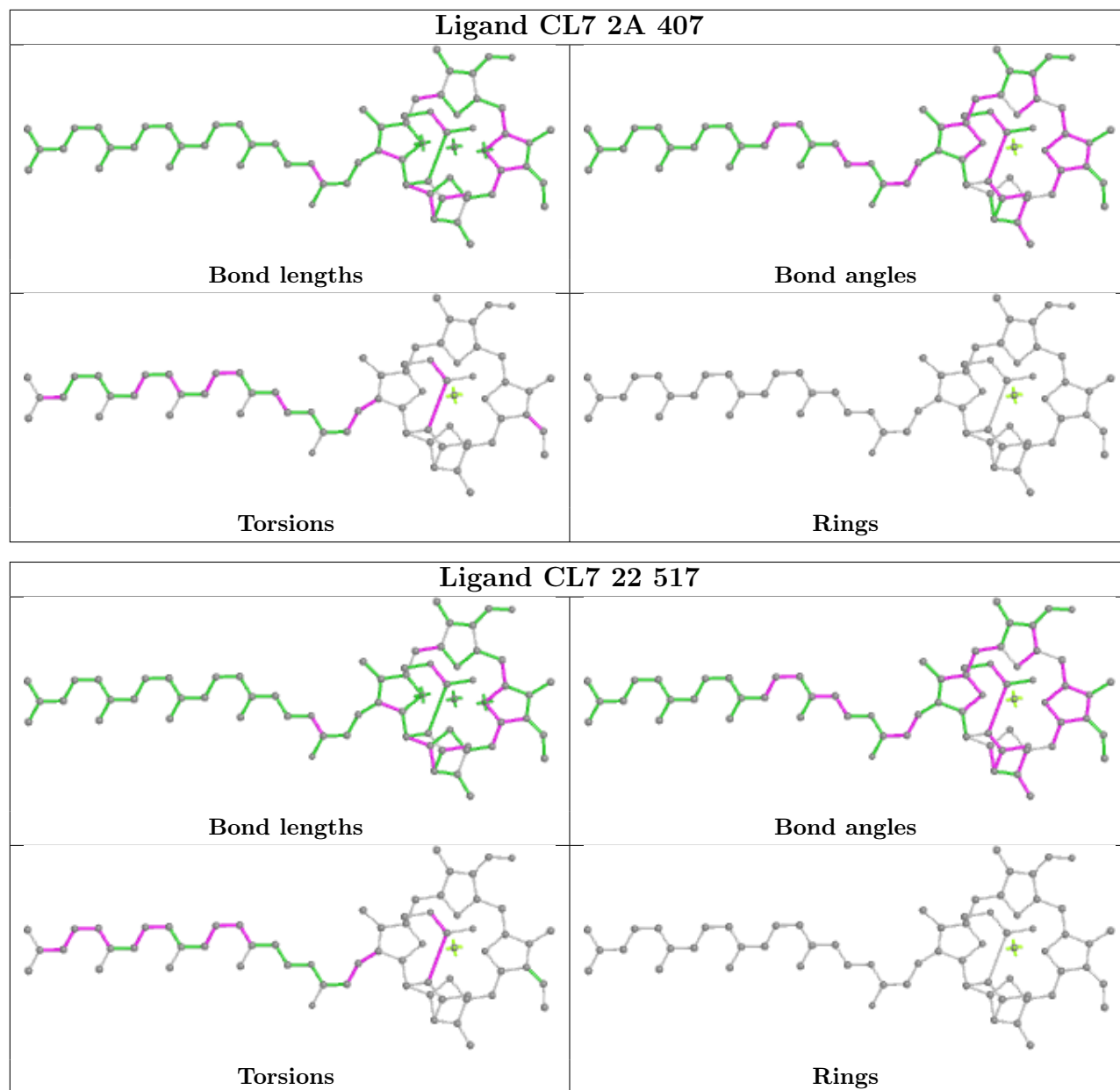
Bond angles

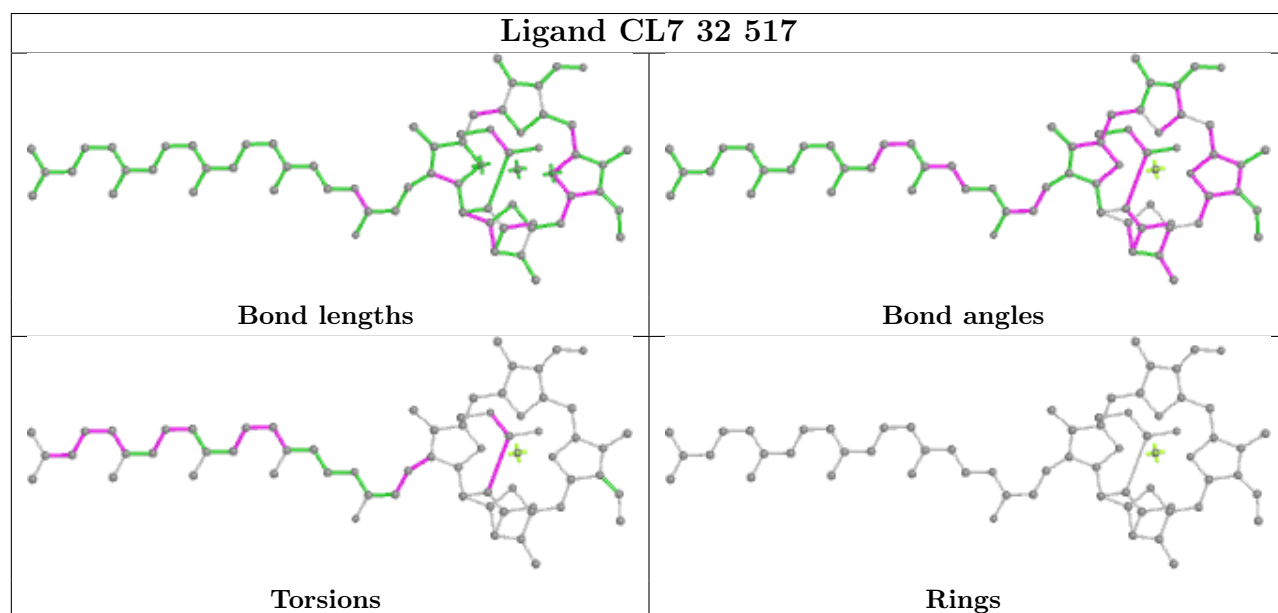
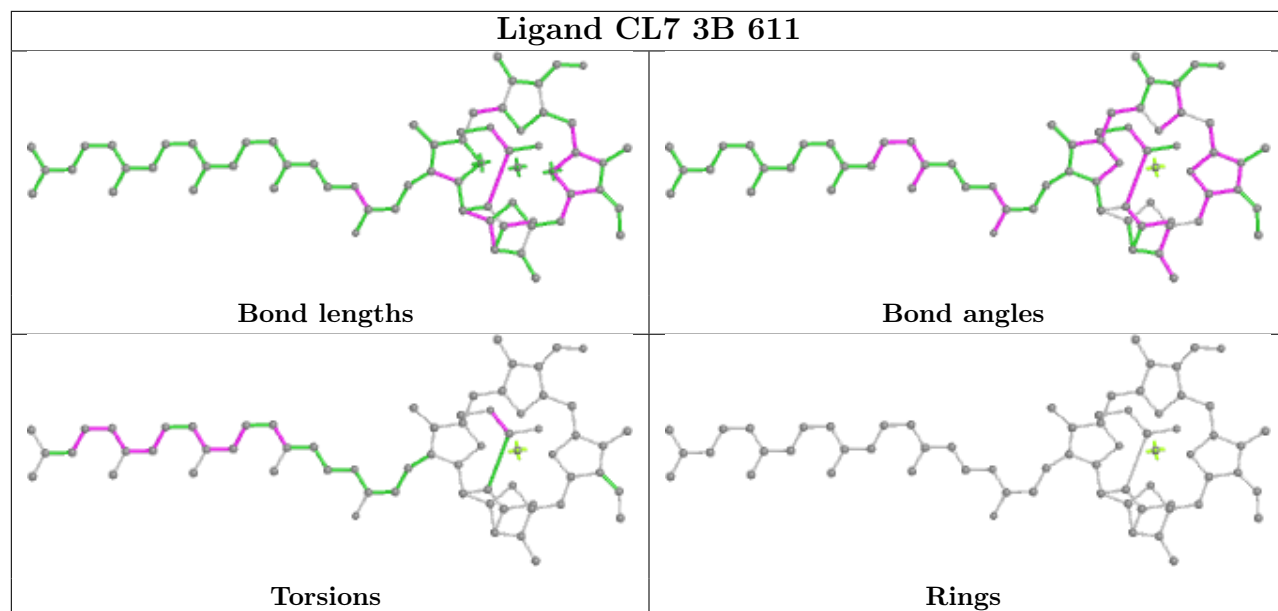


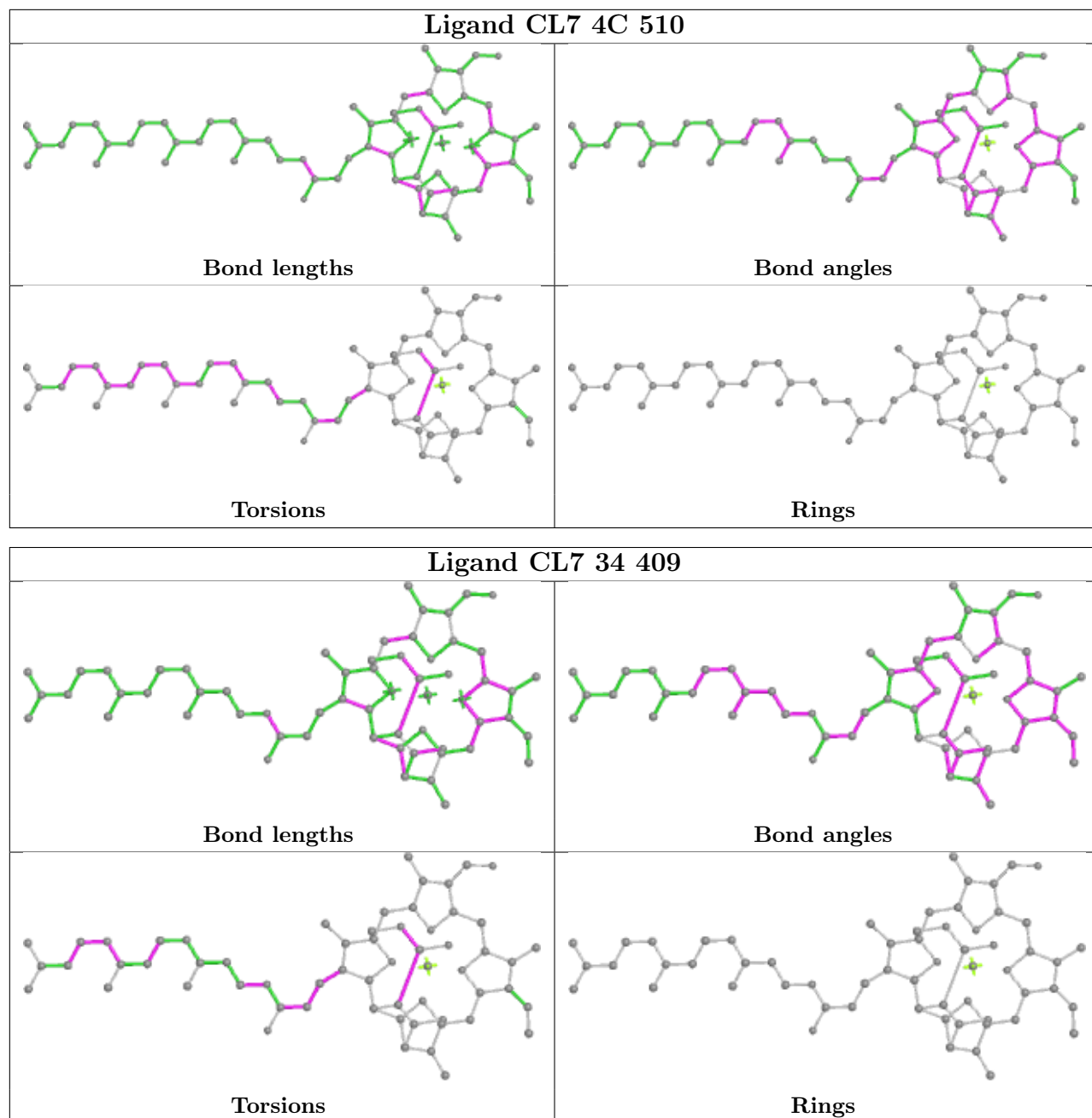
Torsions

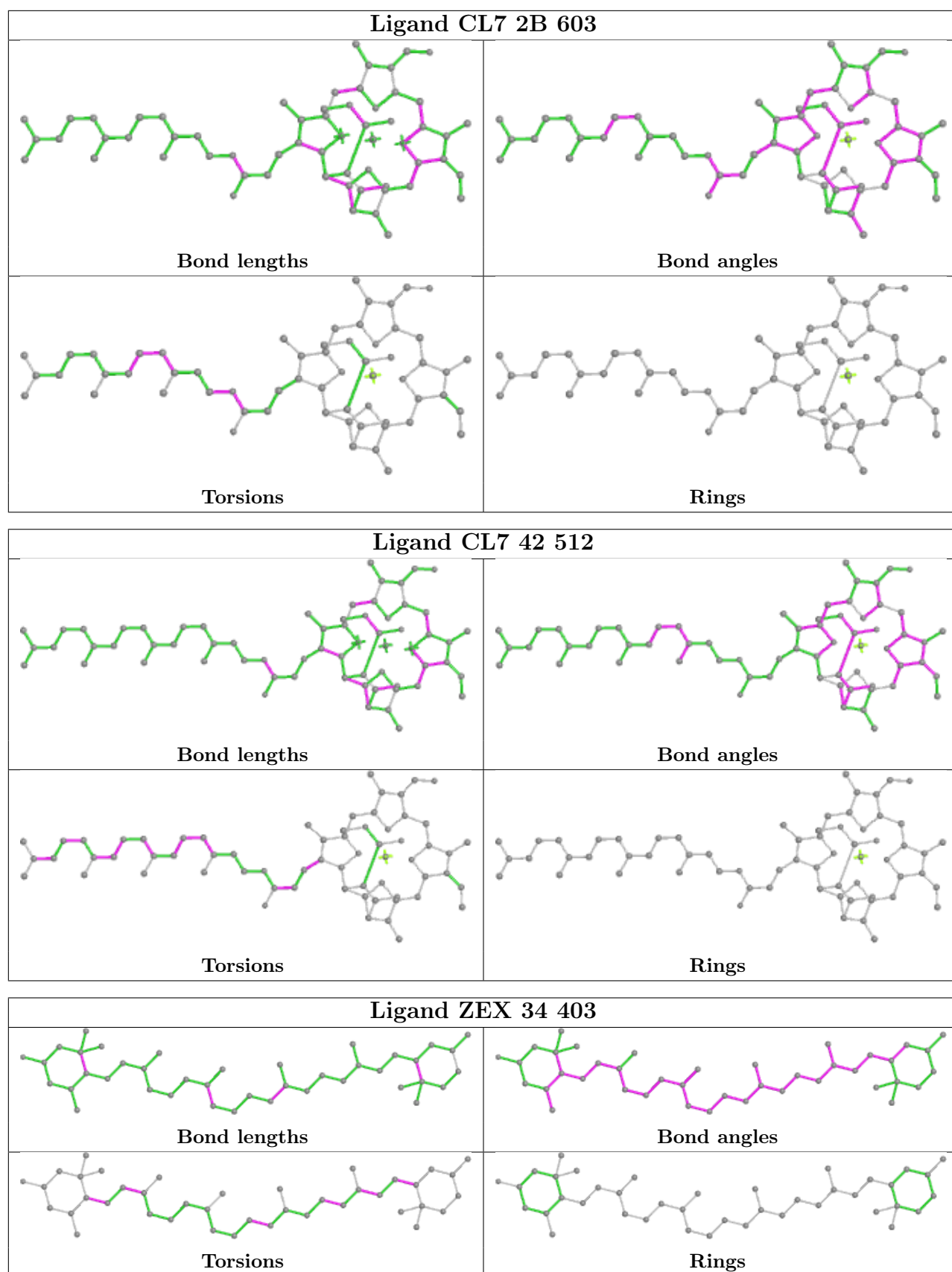


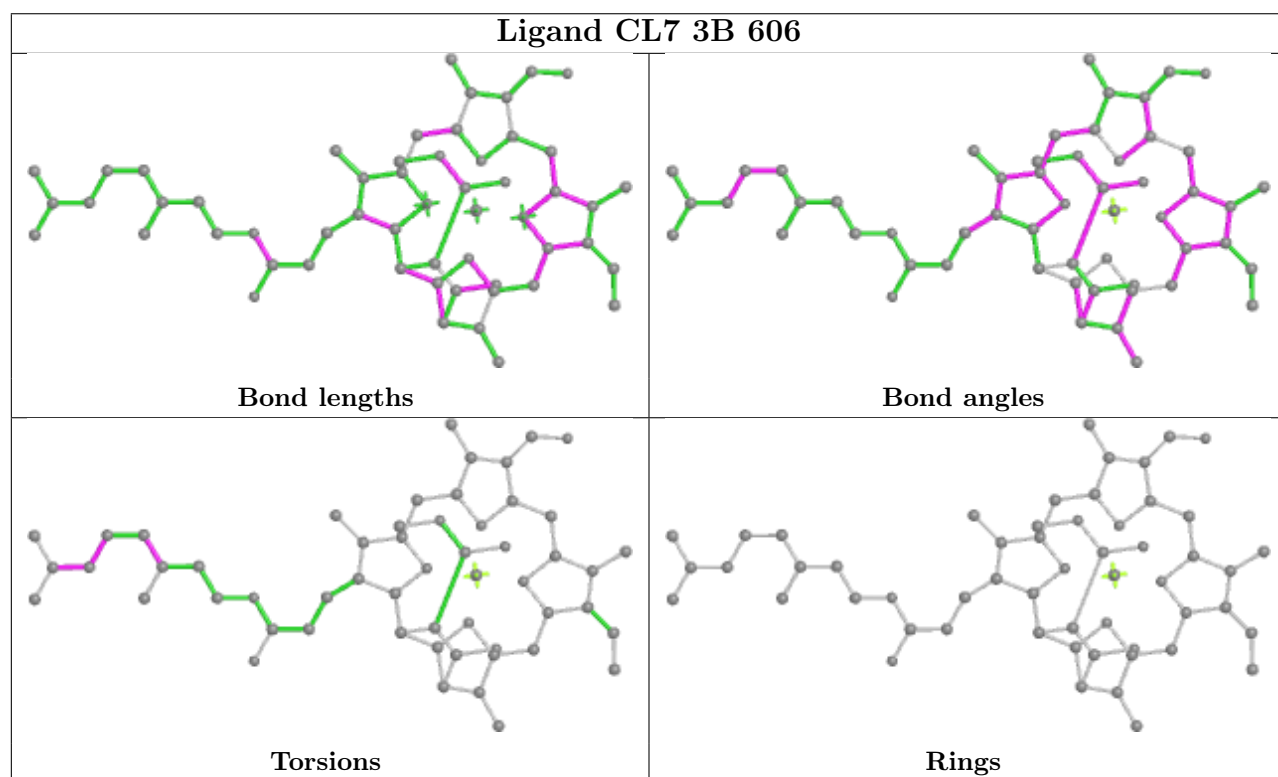
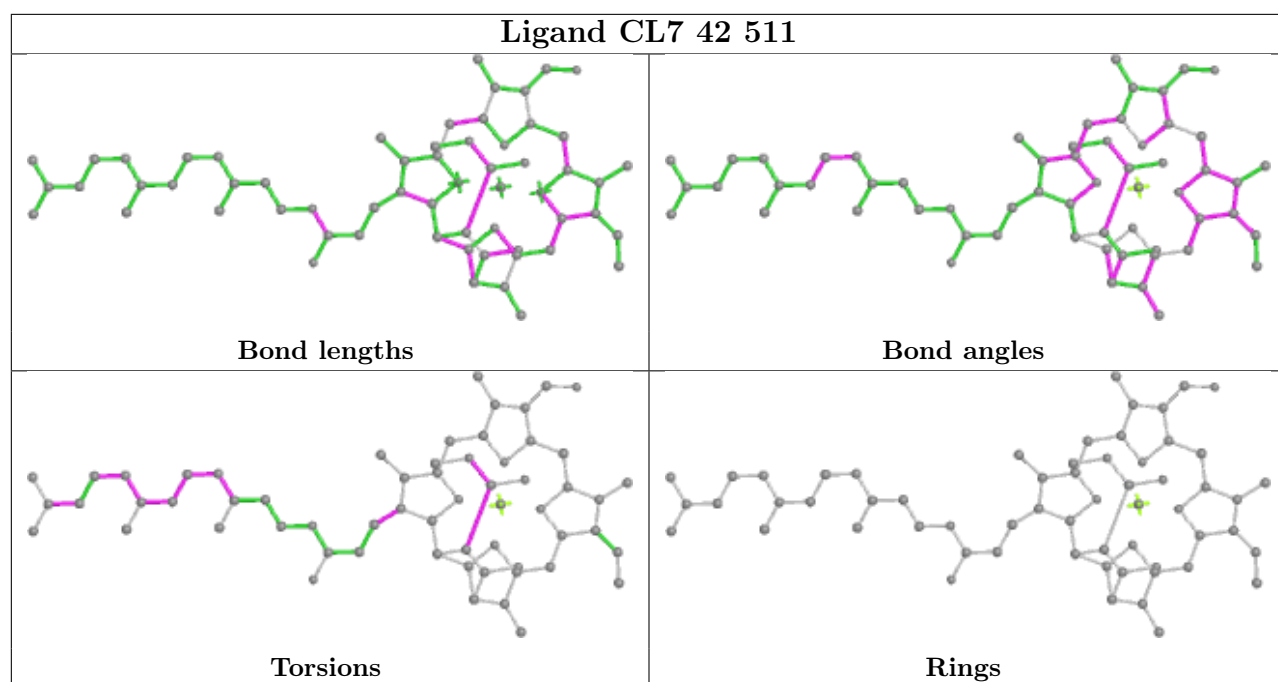
Rings

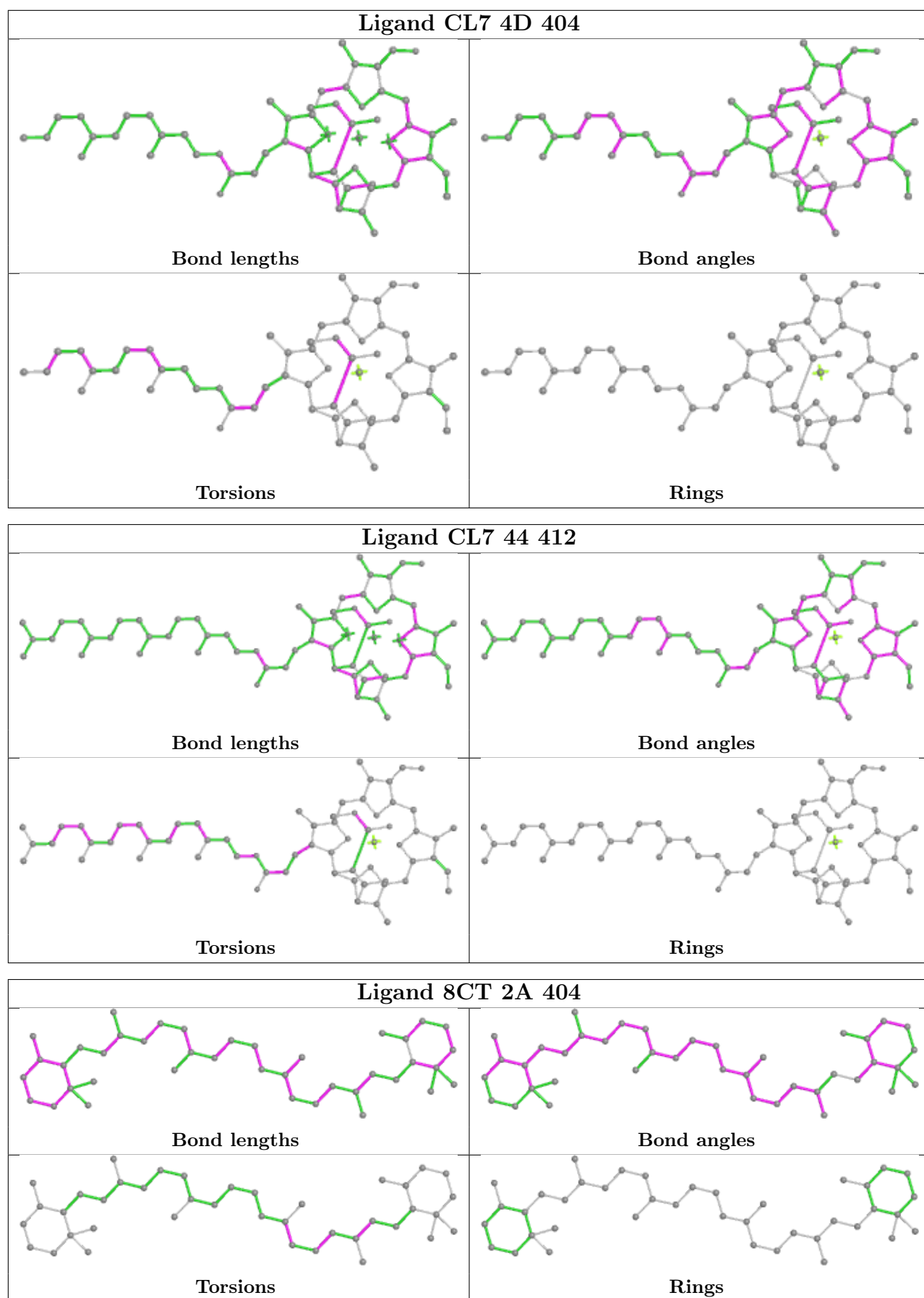


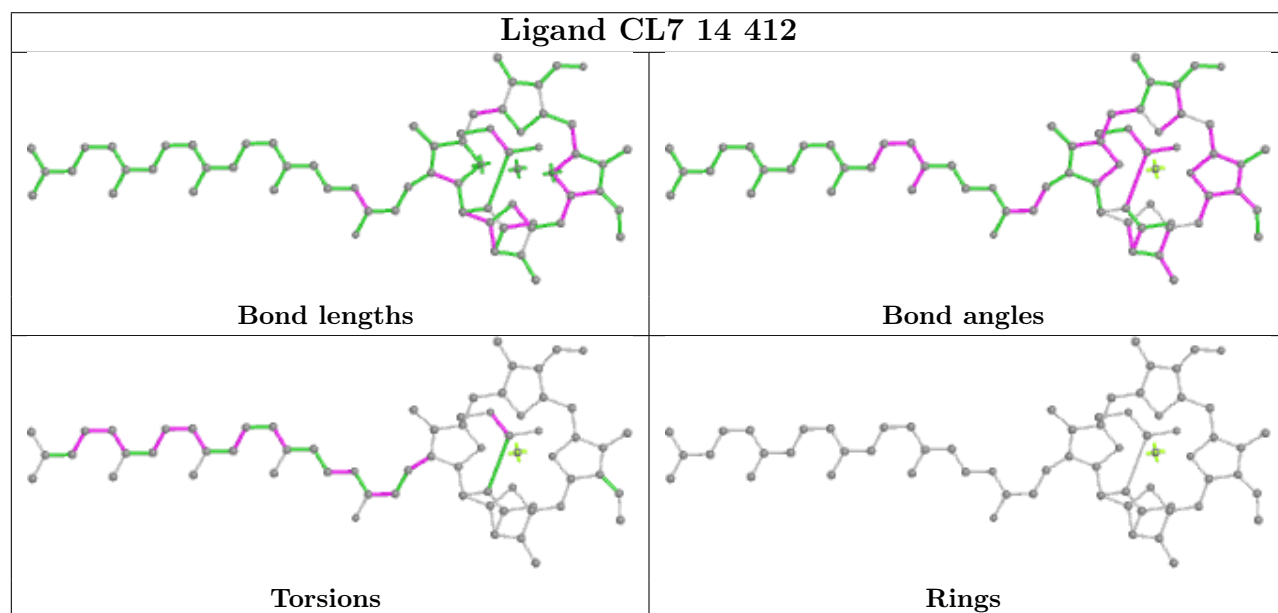
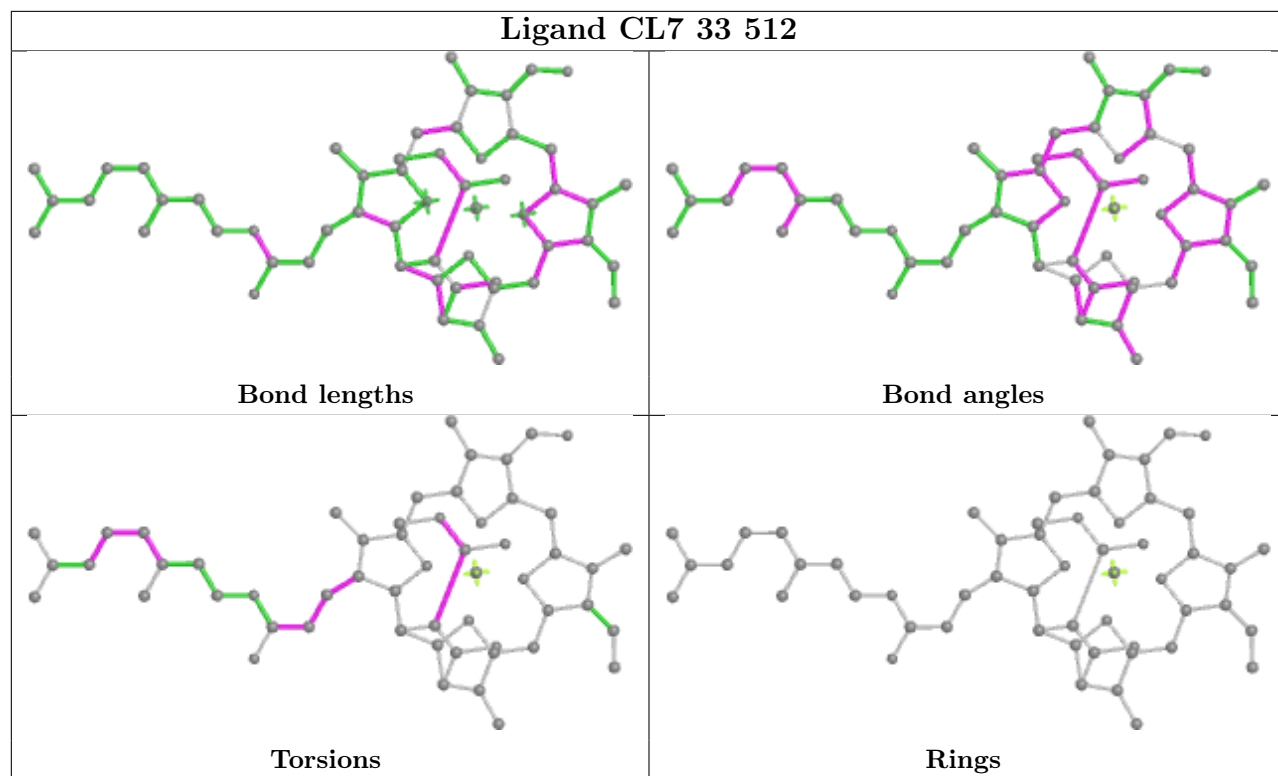




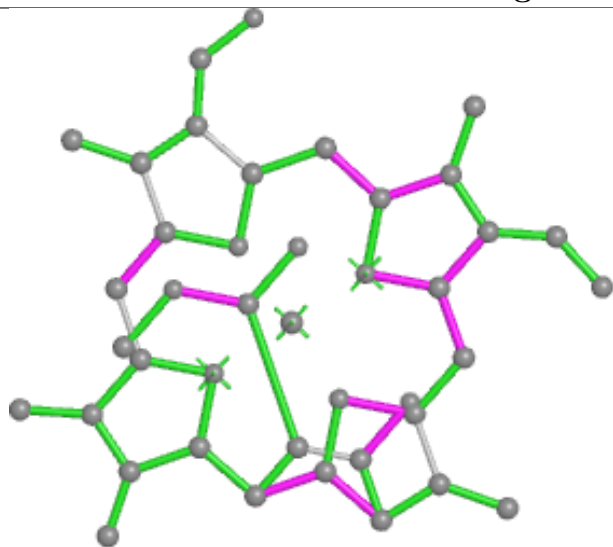




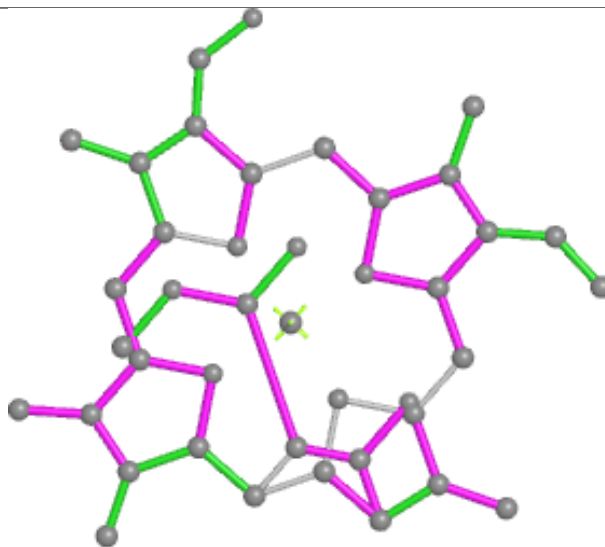




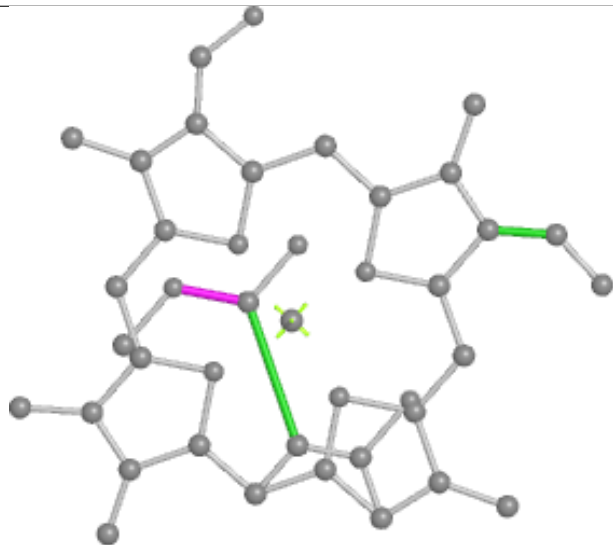
Ligand CL7 11 407



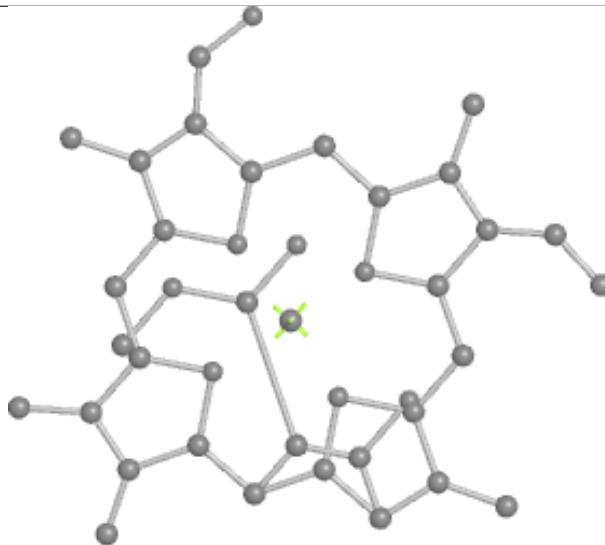
Bond lengths



Bond angles

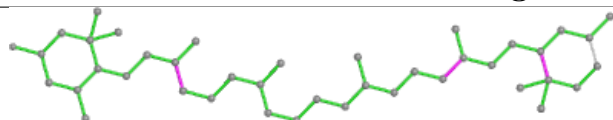


Torsions

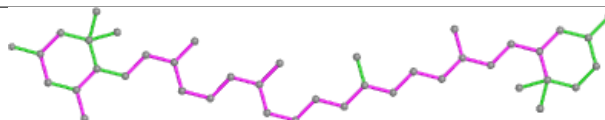


Rings

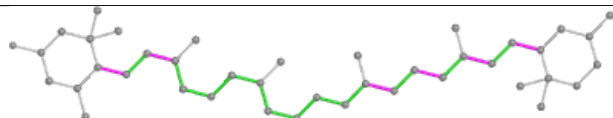
Ligand ZEX 33 519



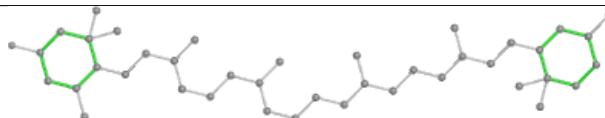
Bond lengths



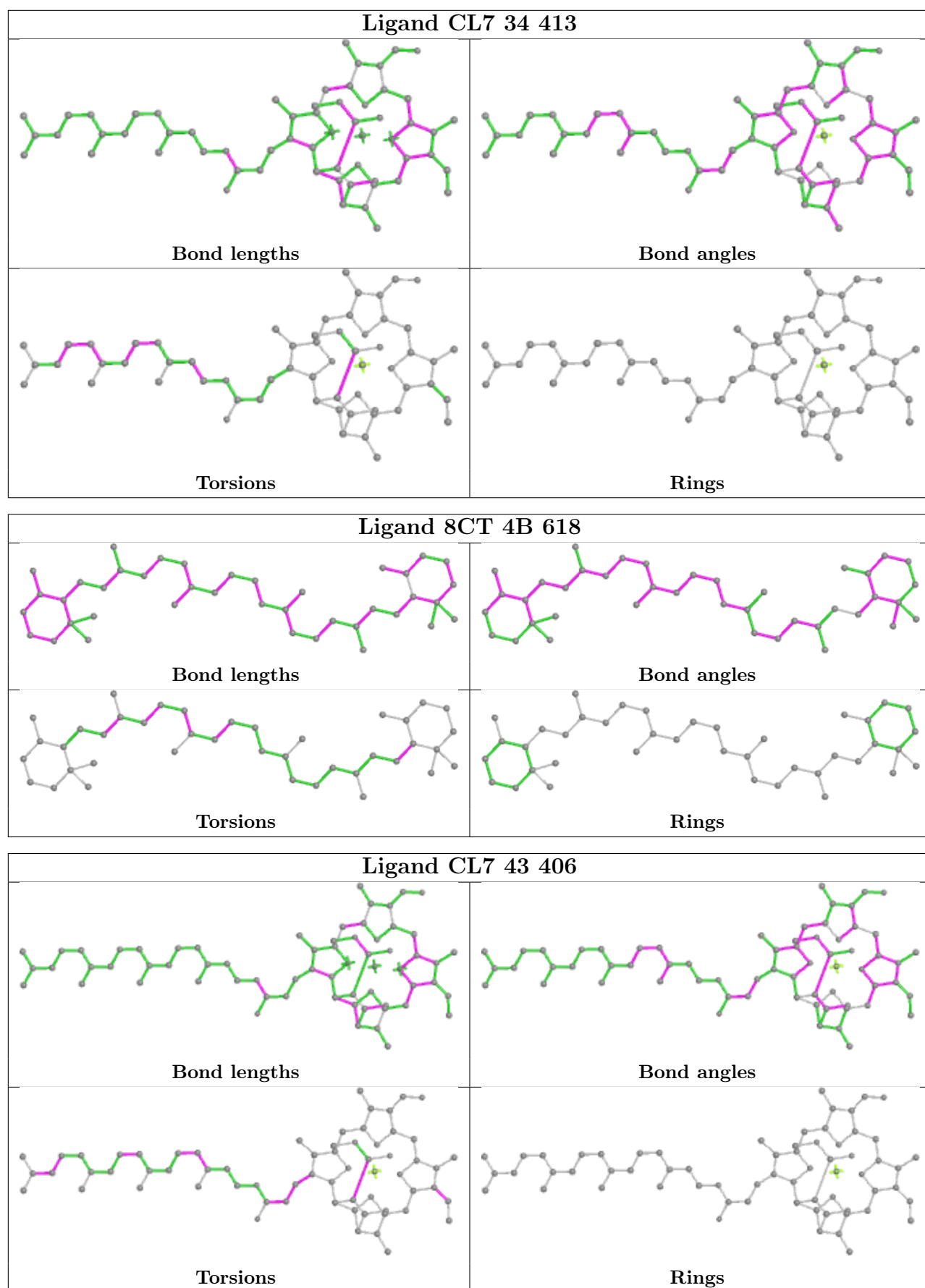
Bond angles



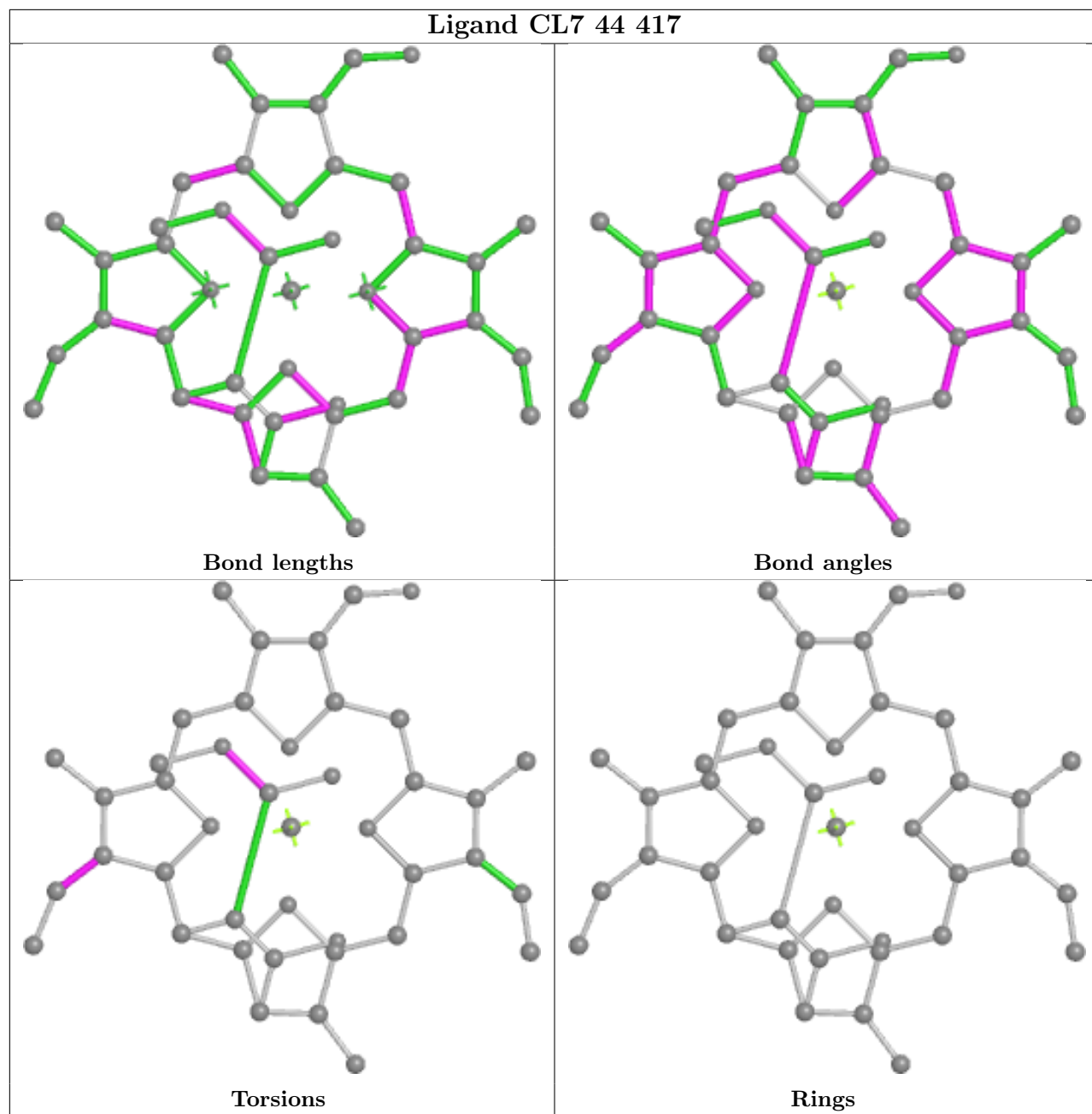
Torsions



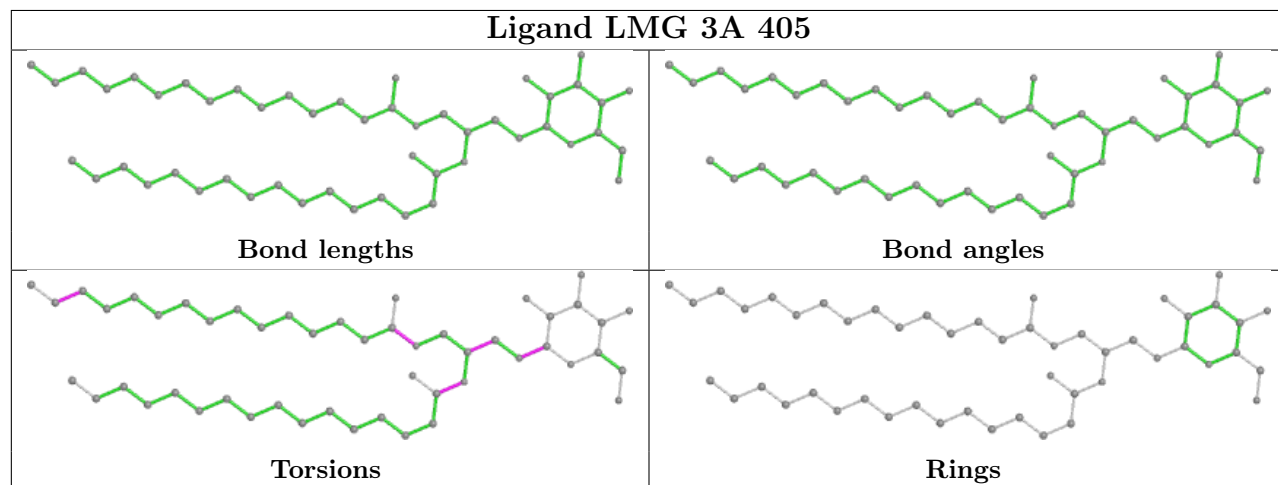
Rings

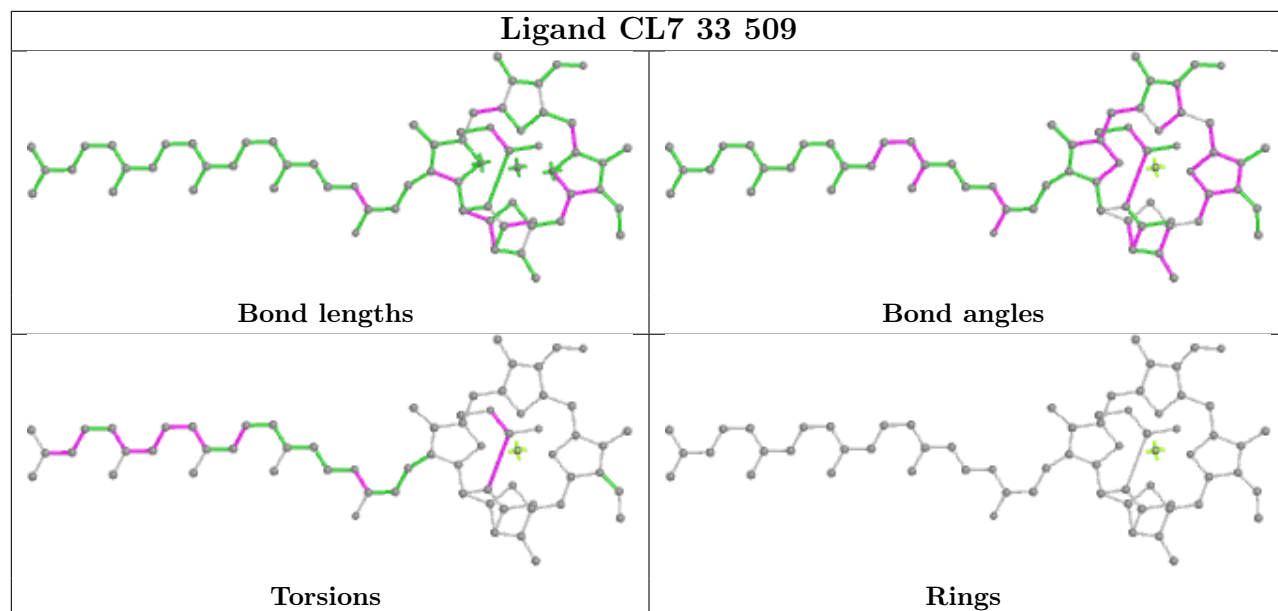
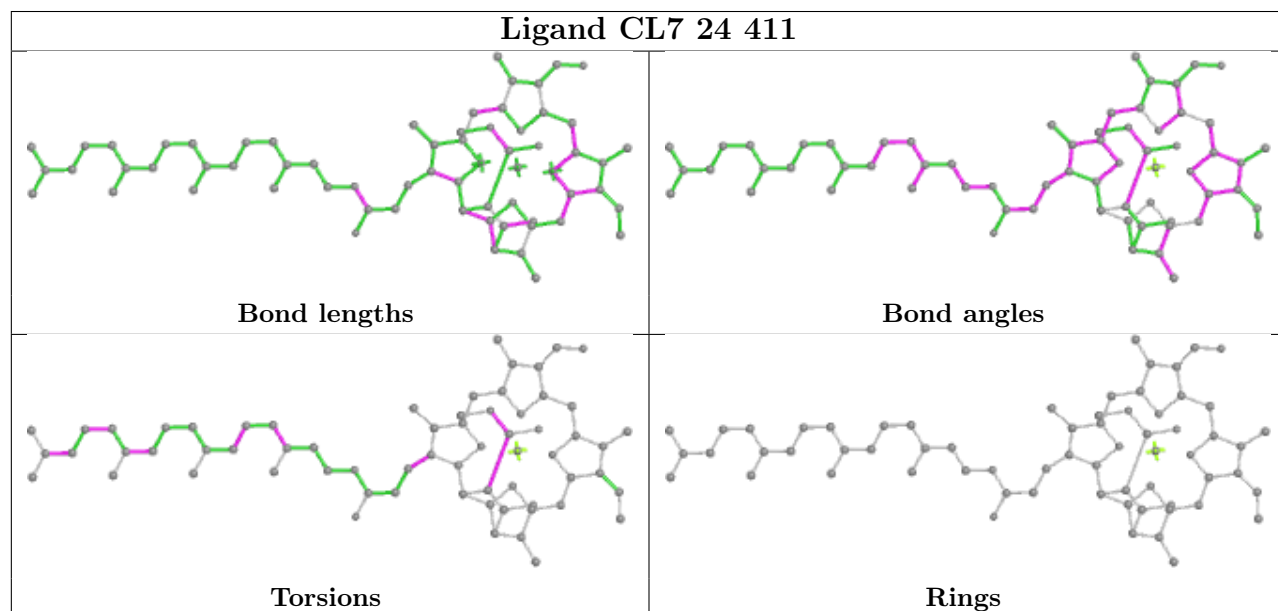


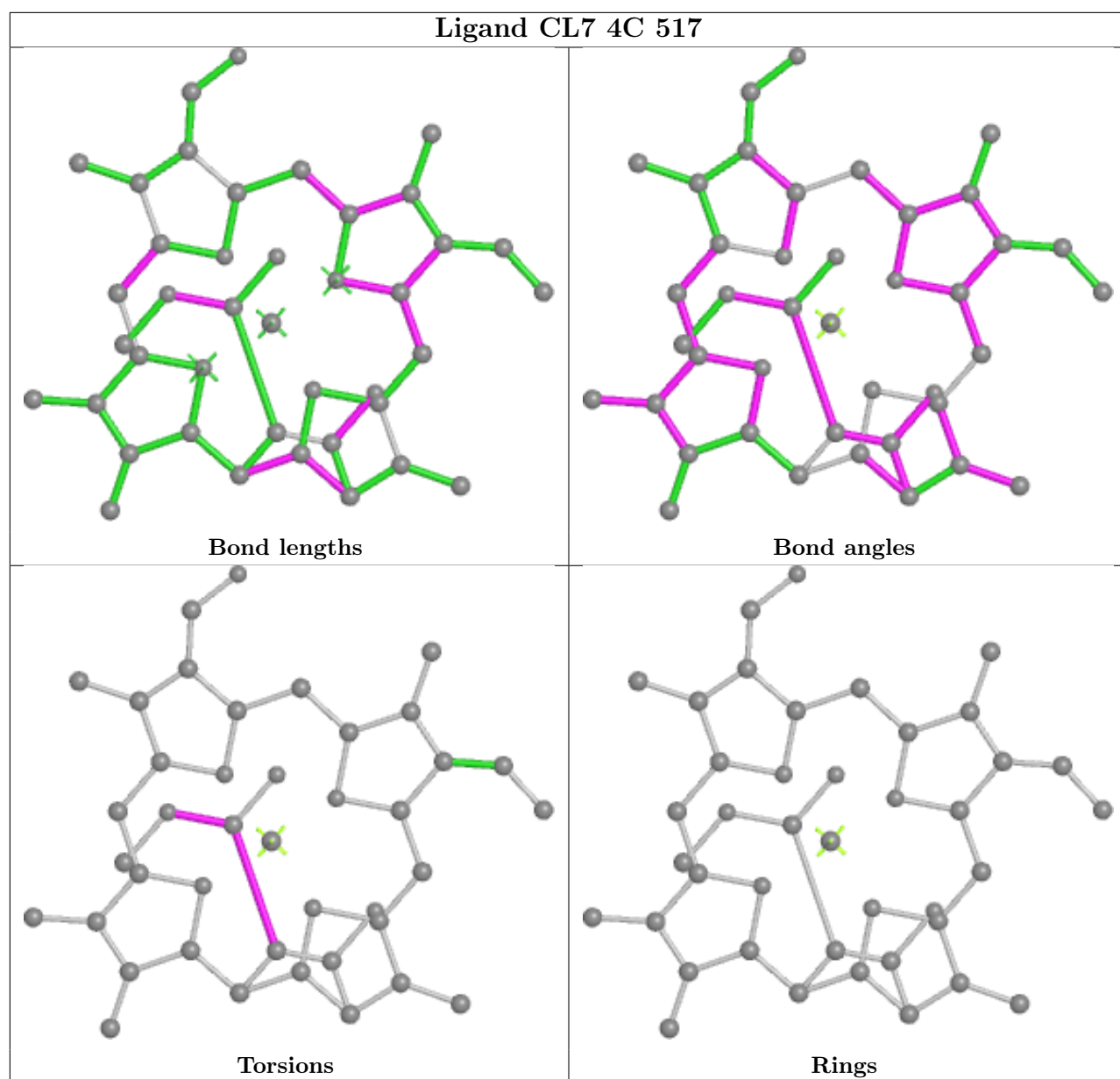
Ligand CL7 44 417

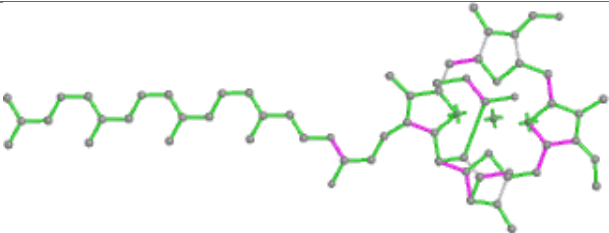
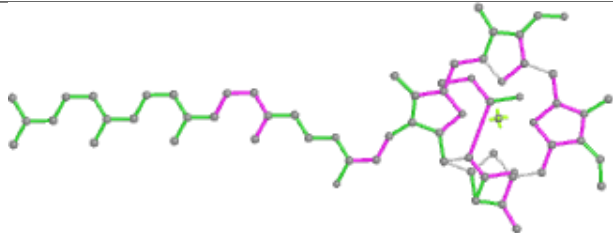
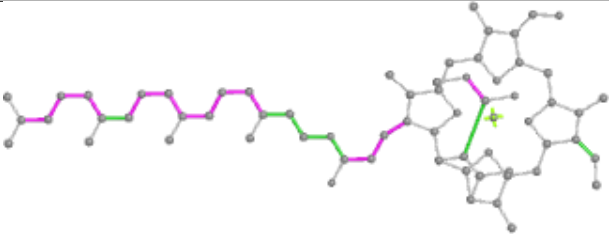
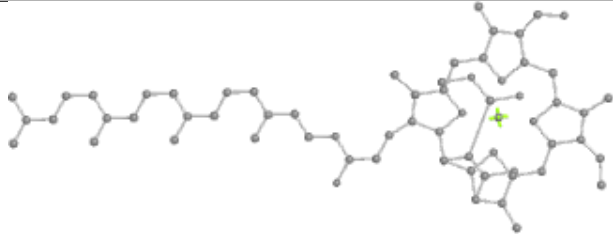


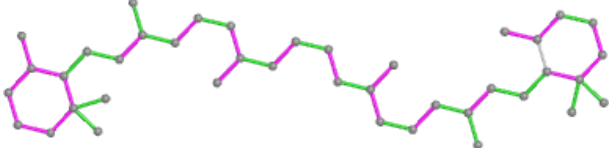
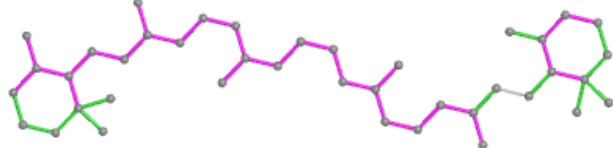
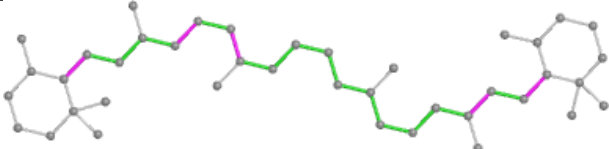
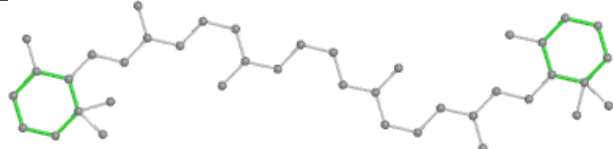
Ligand LMG 3A 405

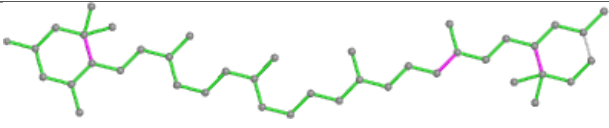
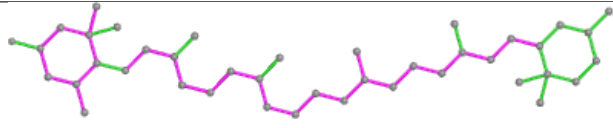
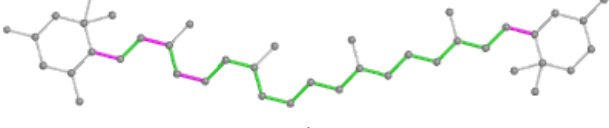
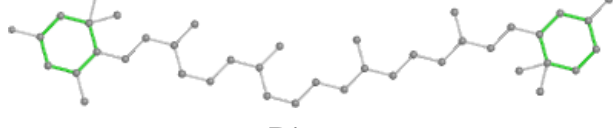


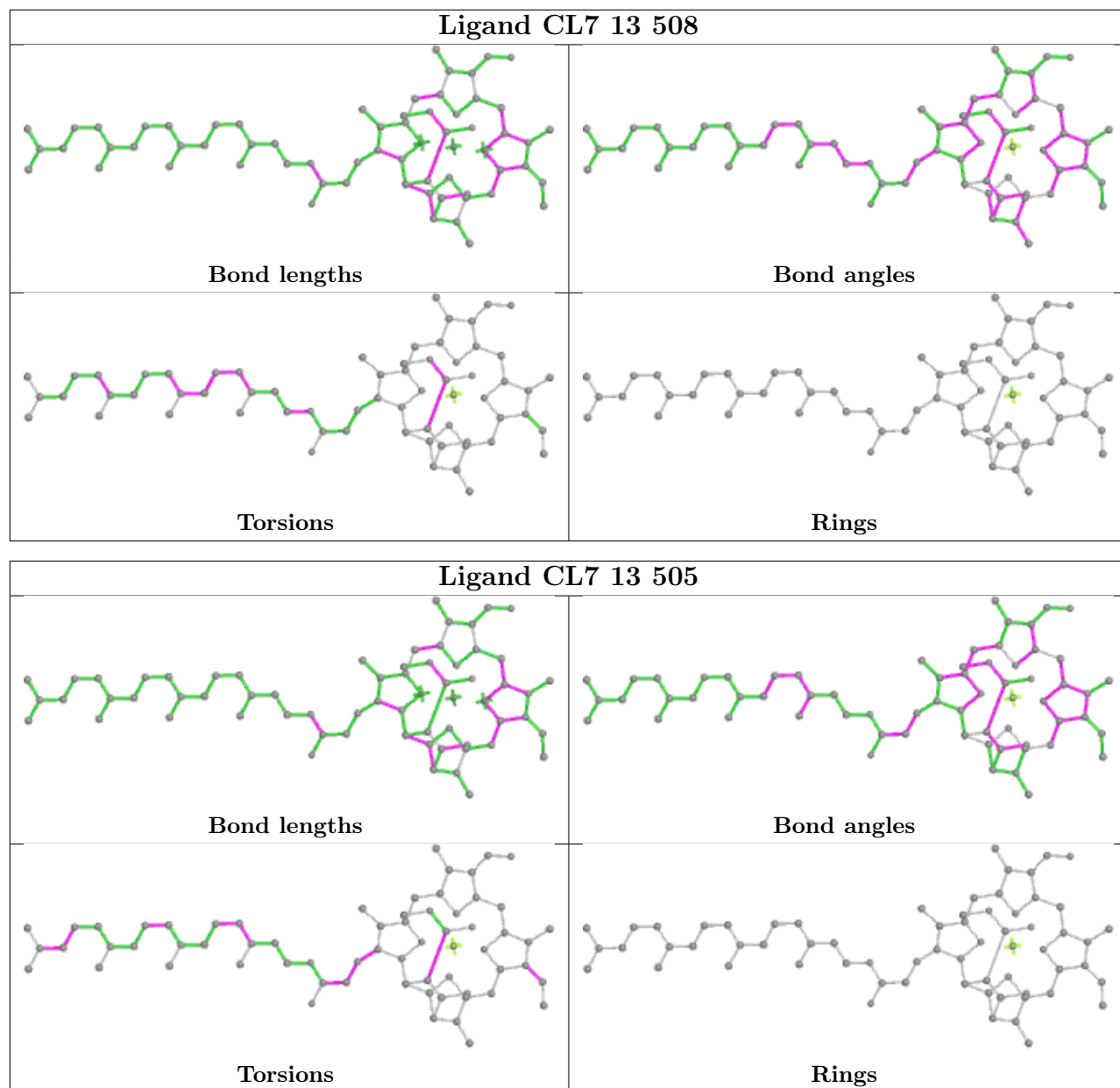
Ligand CL7 33 509**Ligand CL7 24 411**

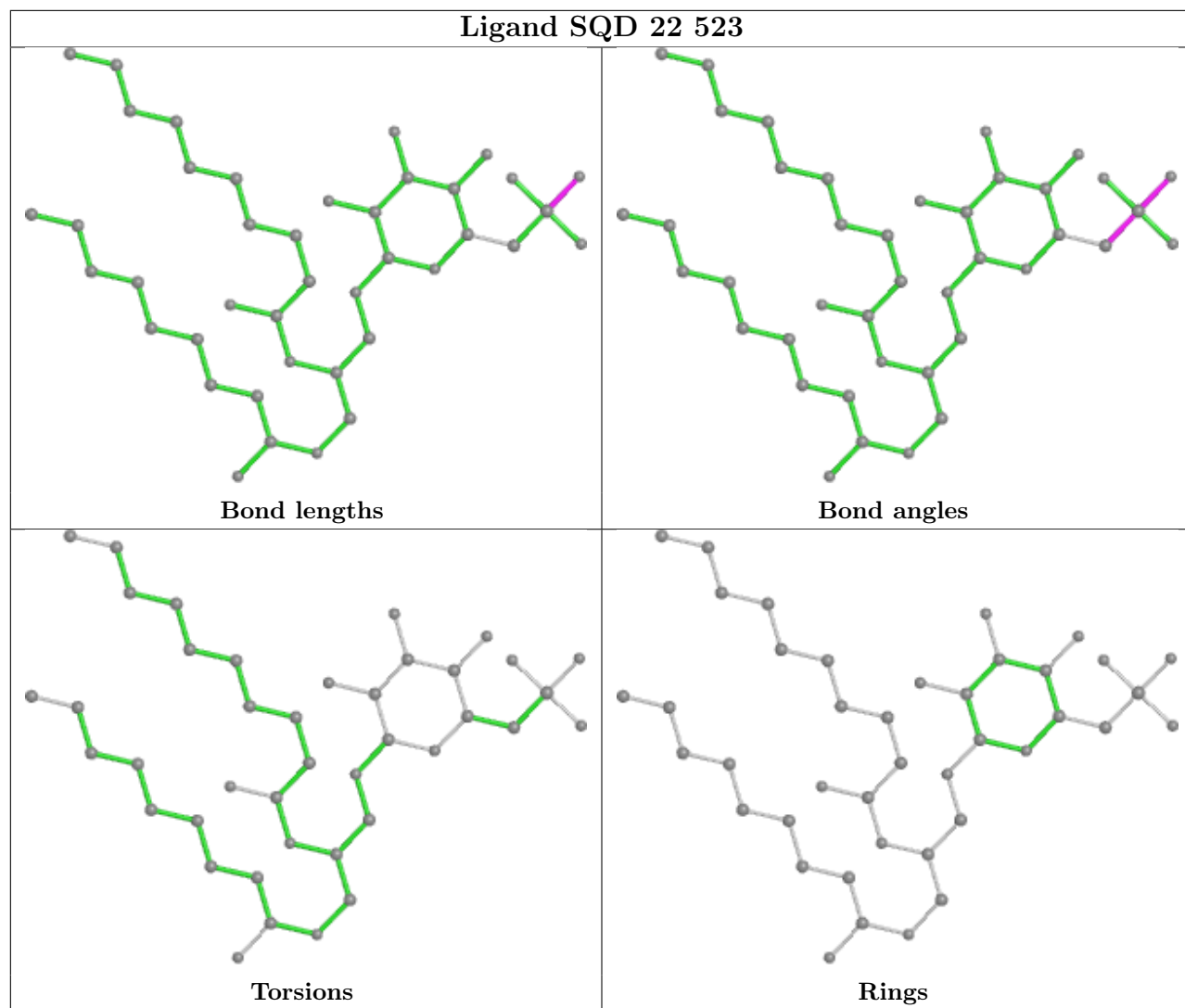


Ligand CL7 44 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

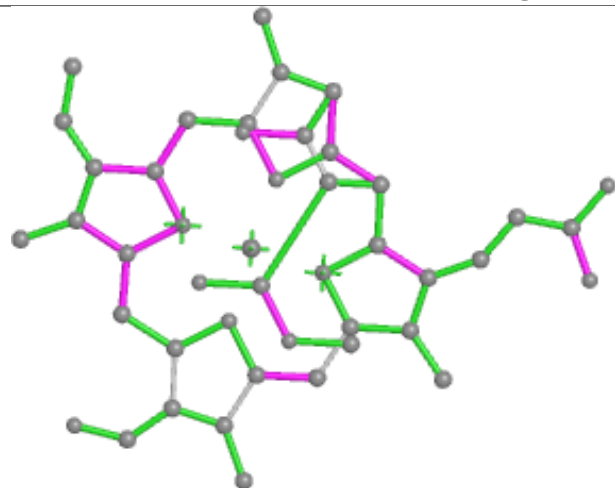
Ligand 8CT 4C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZEX 42 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

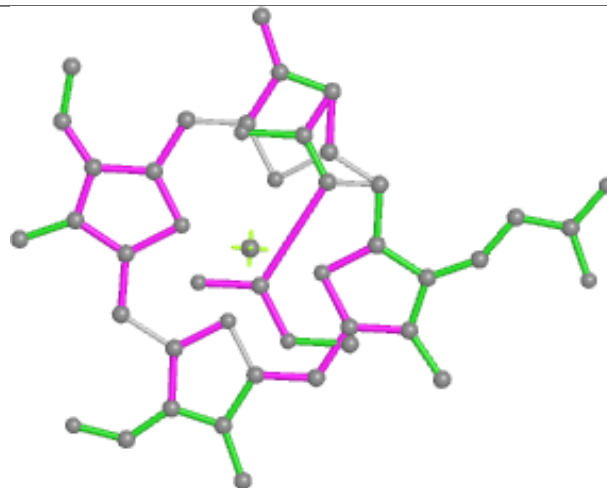




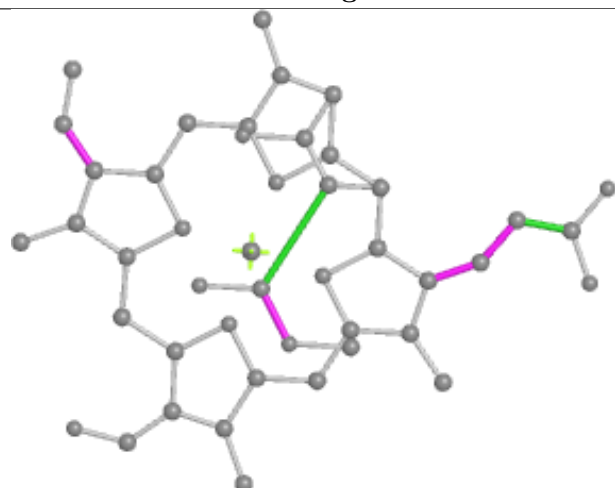
Ligand CL7 33 514



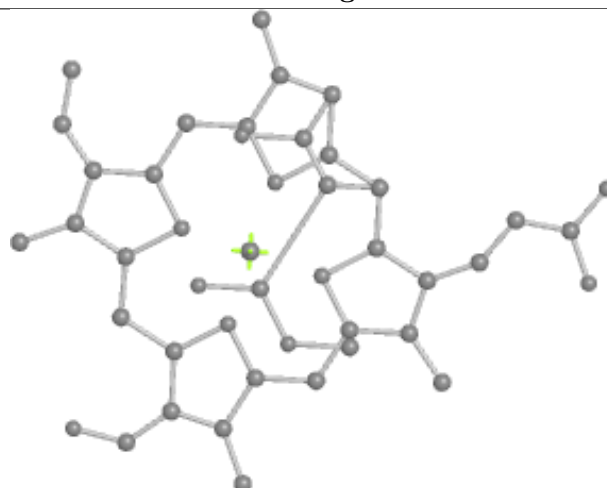
Bond lengths



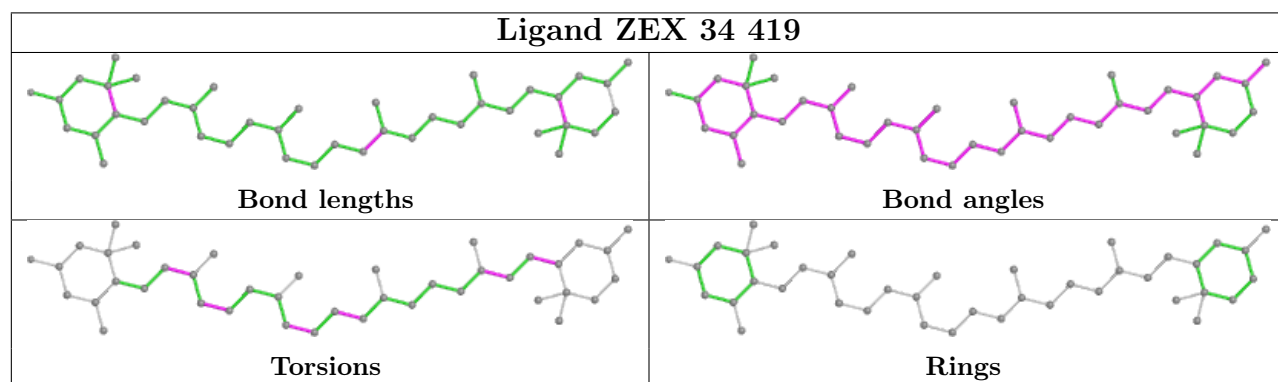
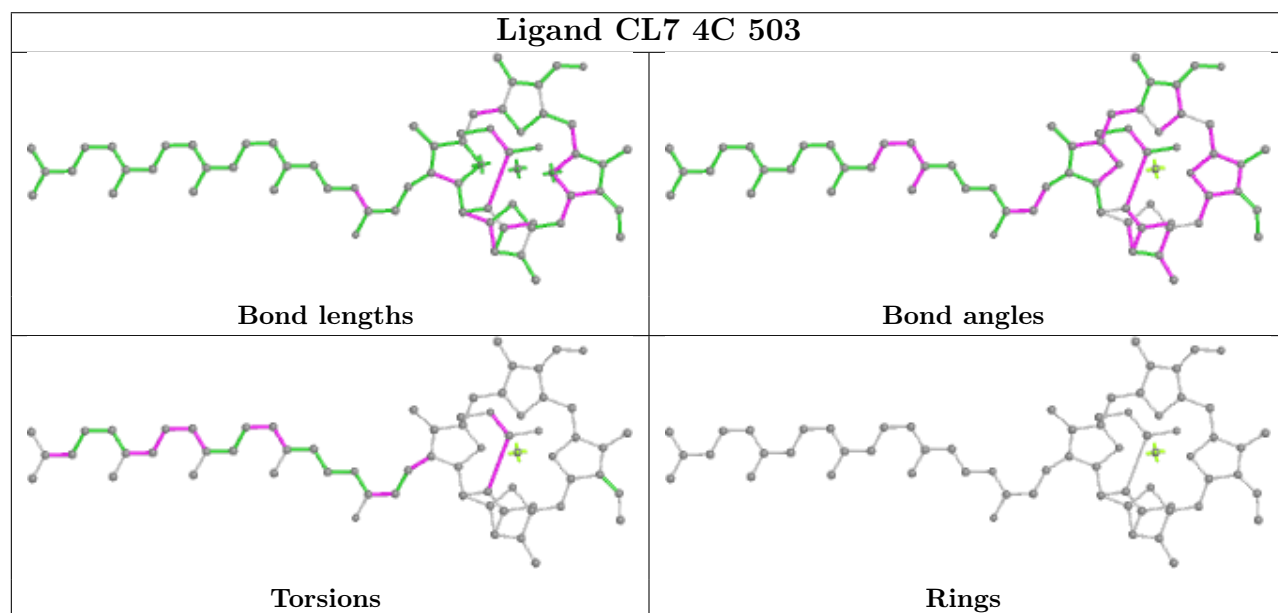
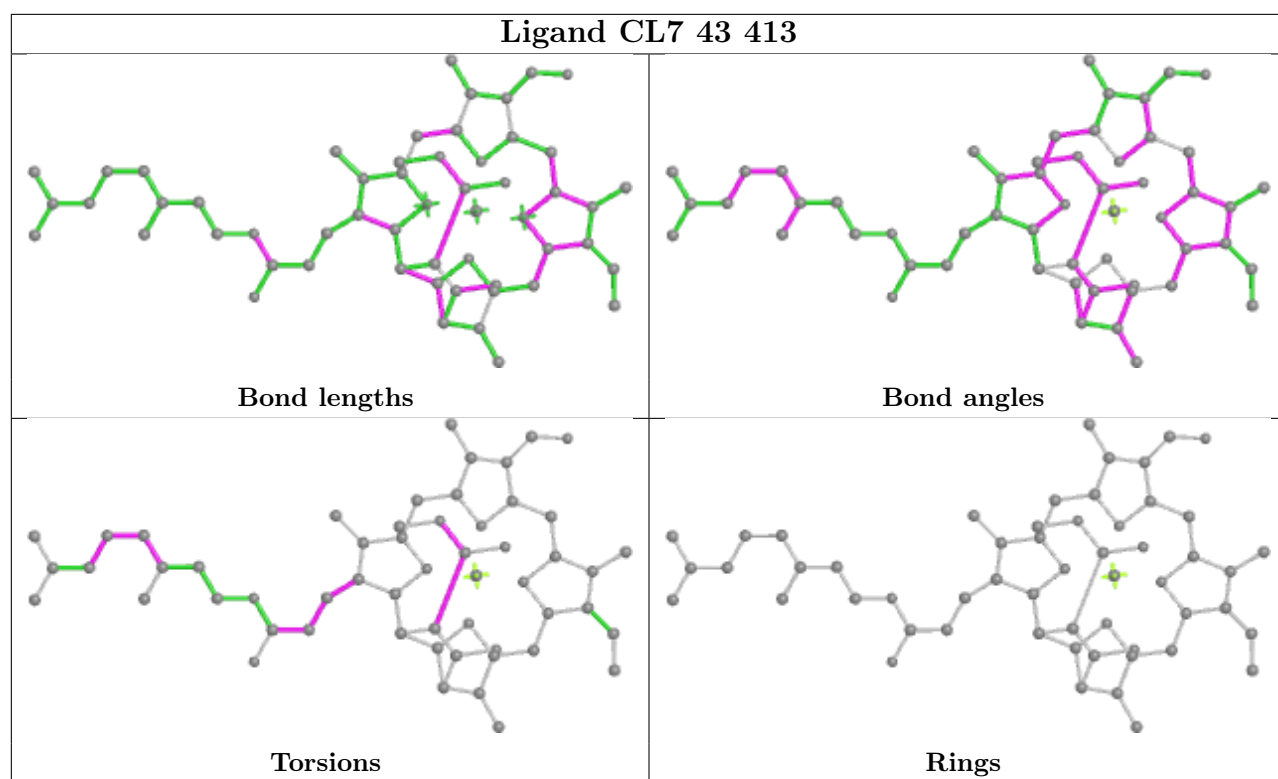
Bond angles



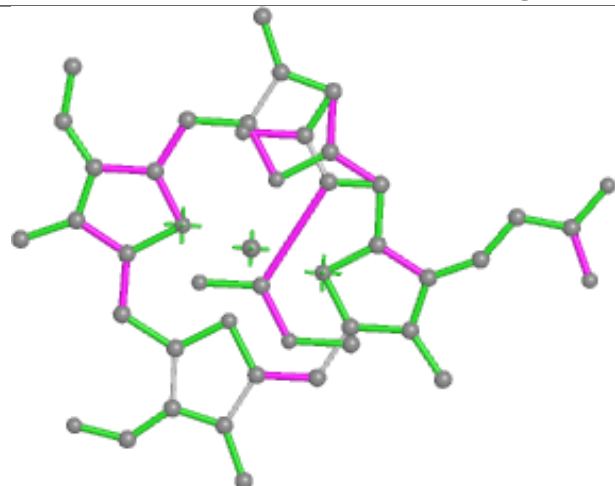
Torsions



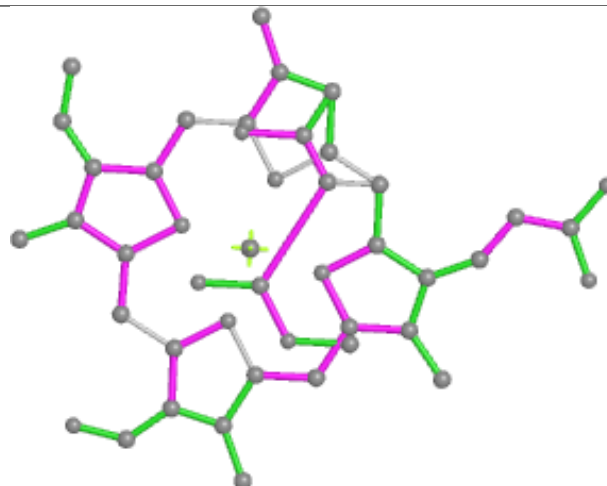
Rings



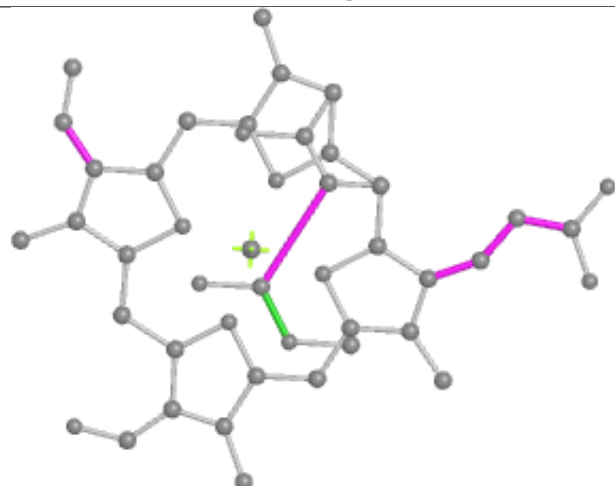
Ligand CL7 13 513



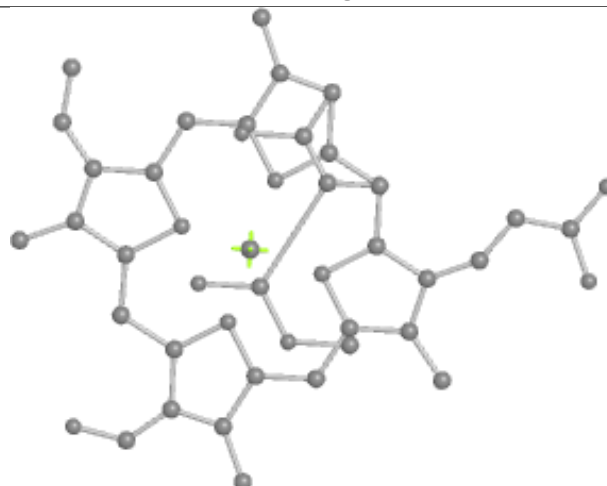
Bond lengths



Bond angles

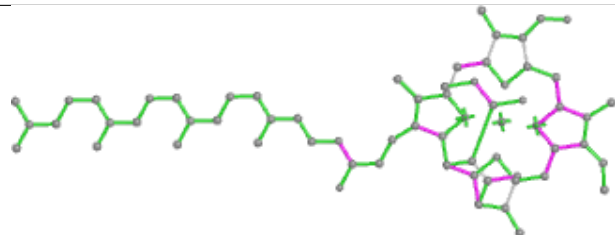


Torsions

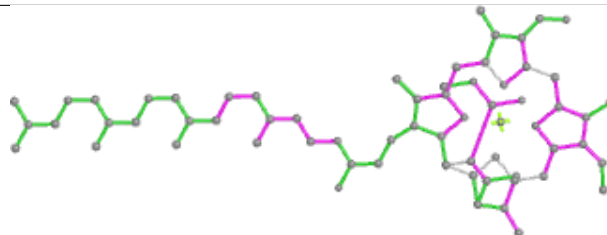


Rings

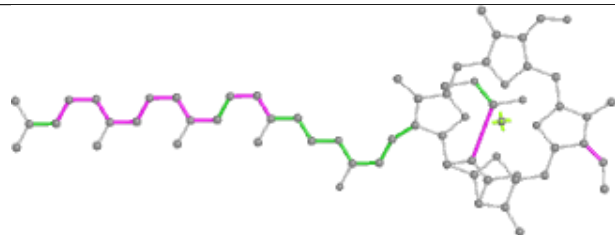
Ligand CL7 32 505



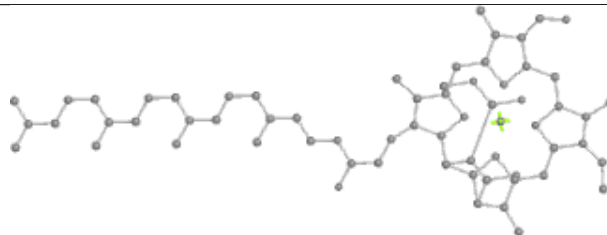
Bond lengths



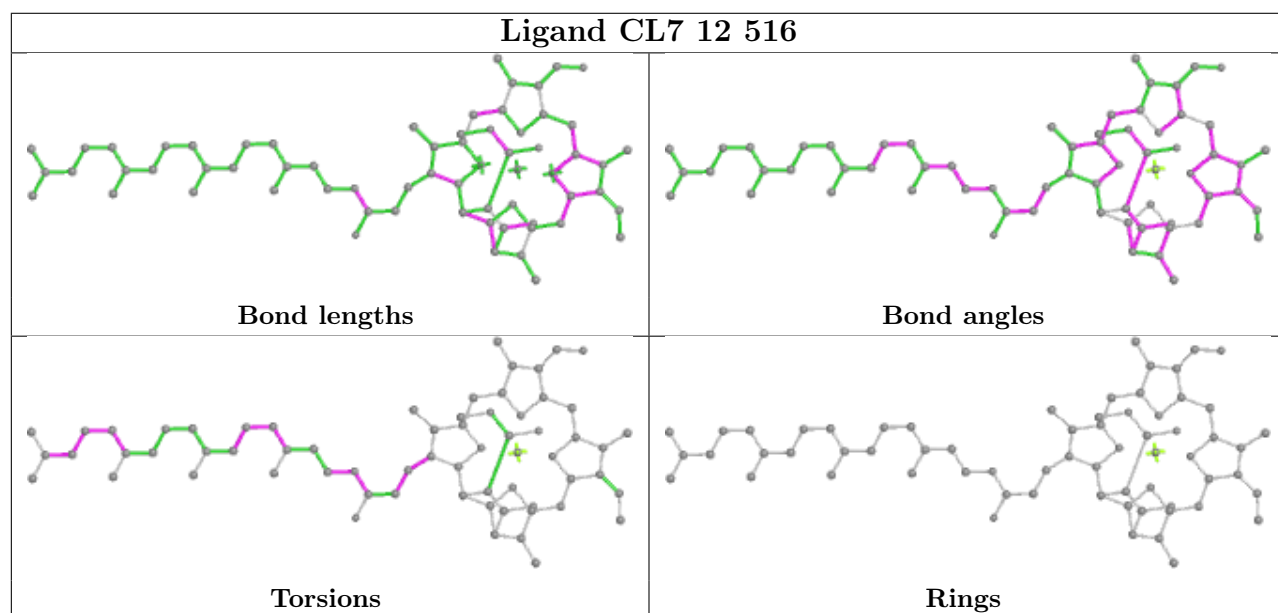
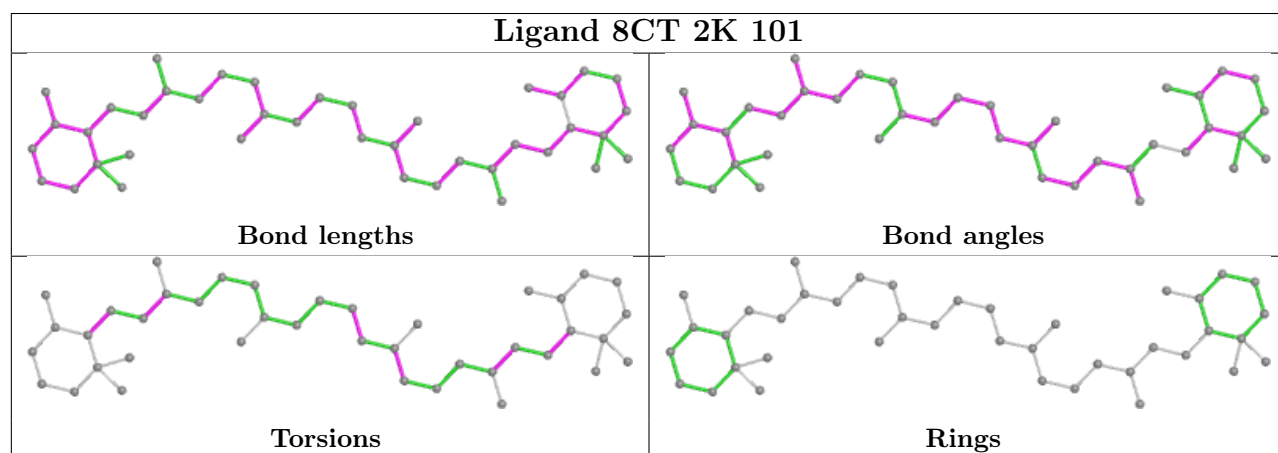
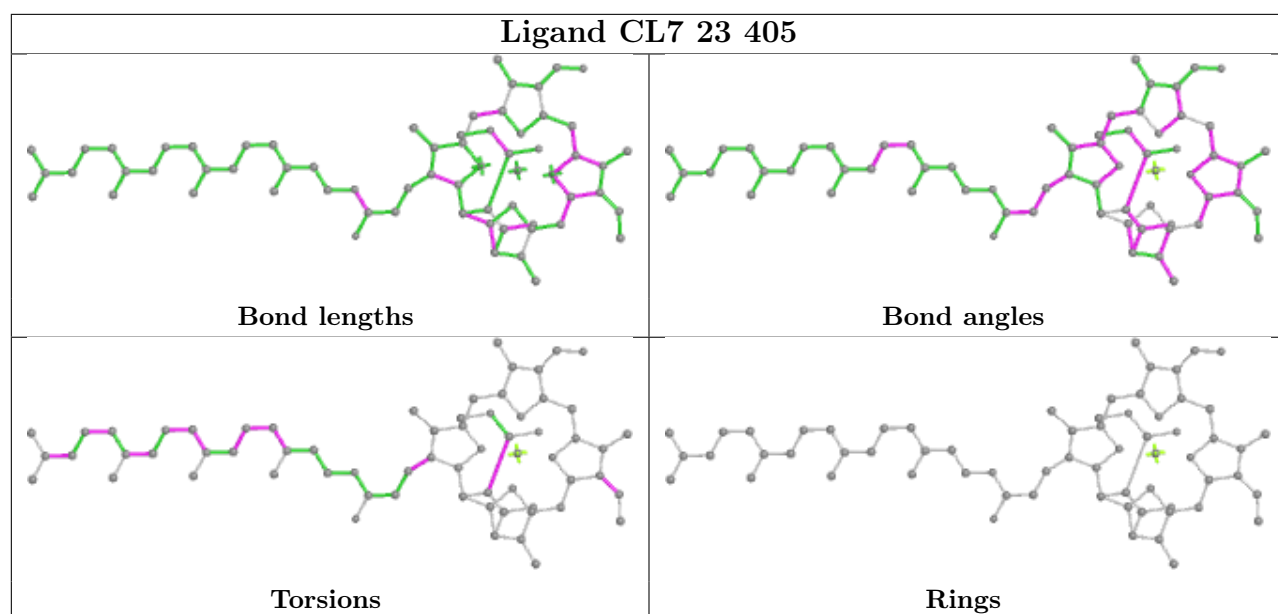
Bond angles

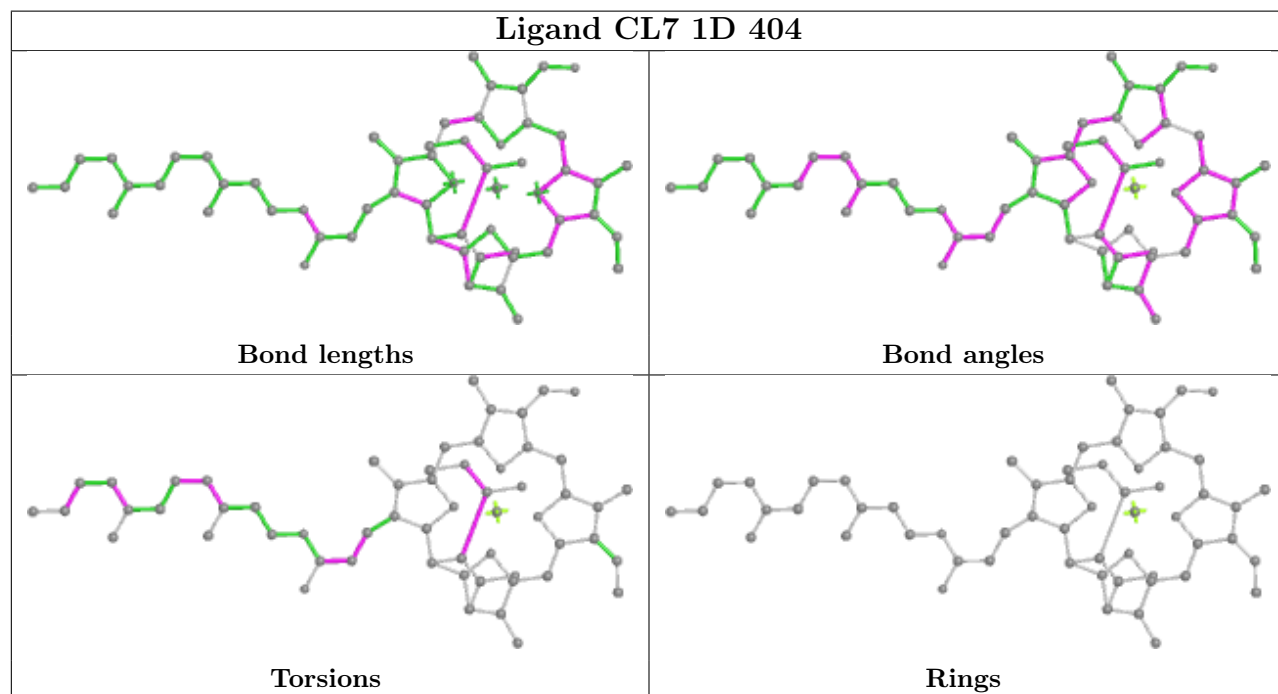
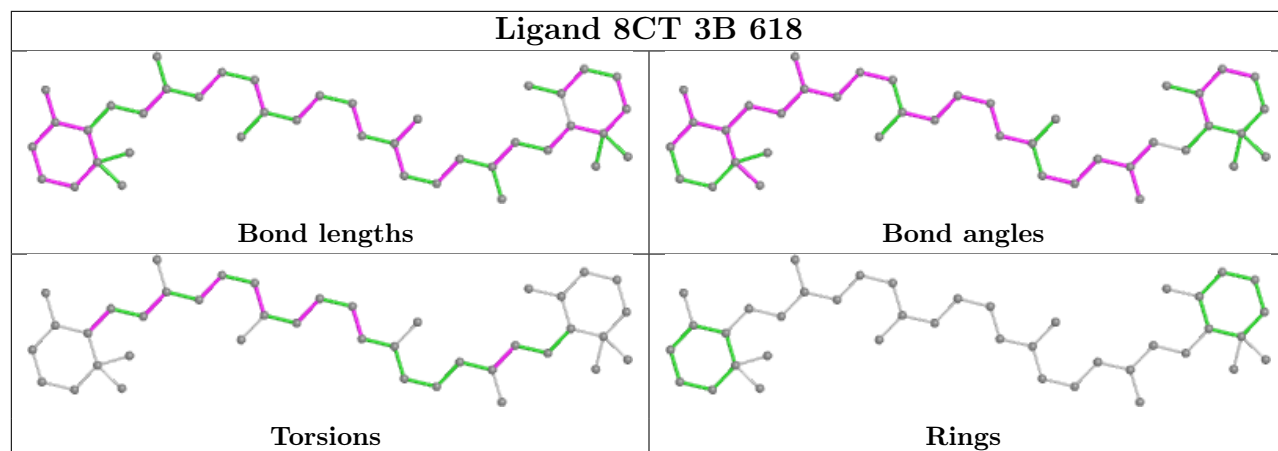


Torsions

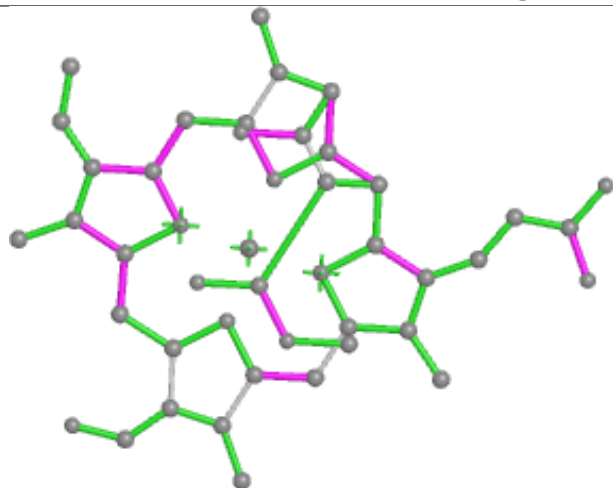


Rings

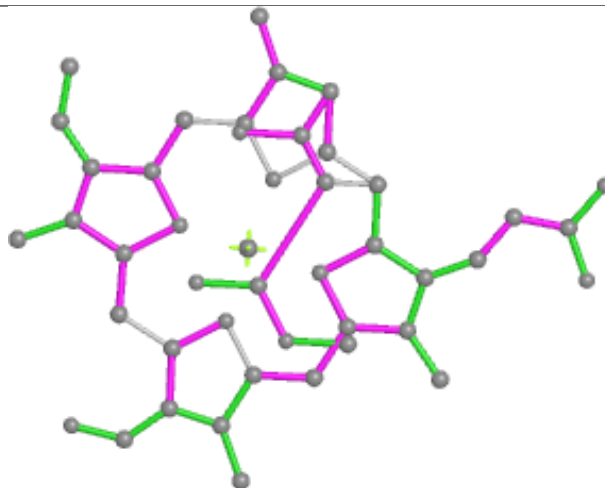




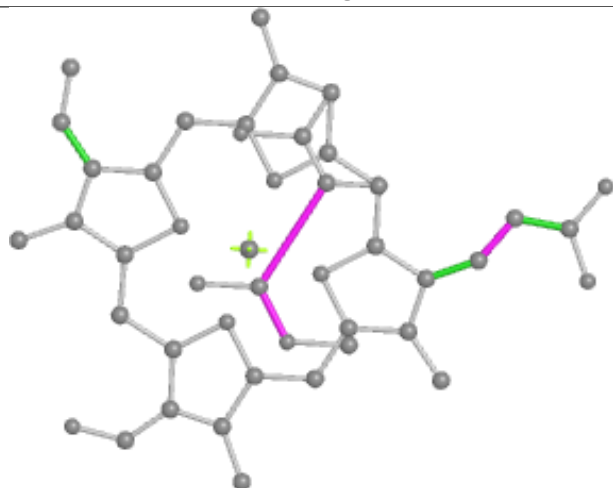
Ligand CL7 4I 409



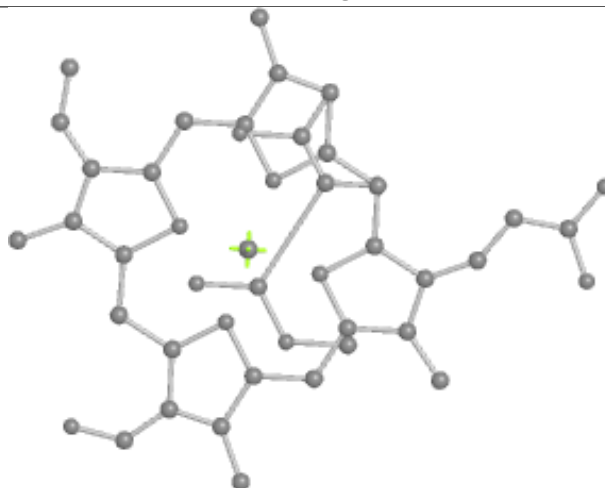
Bond lengths



Bond angles

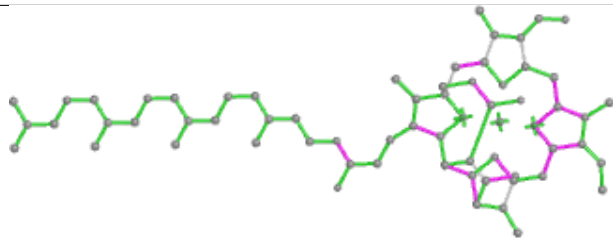


Torsions

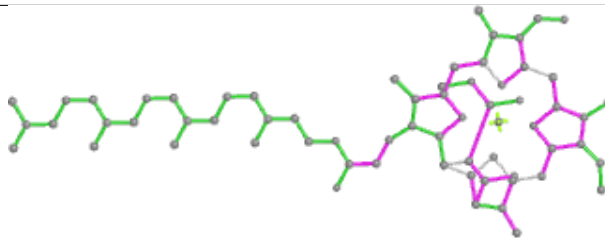


Rings

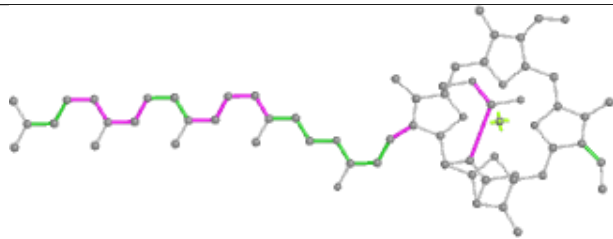
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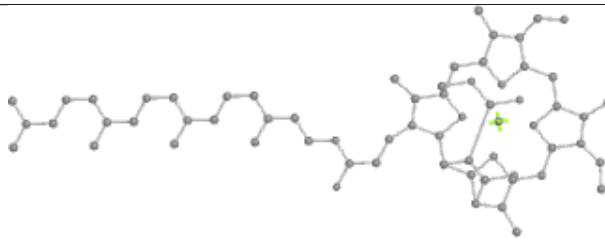
Bond lengths



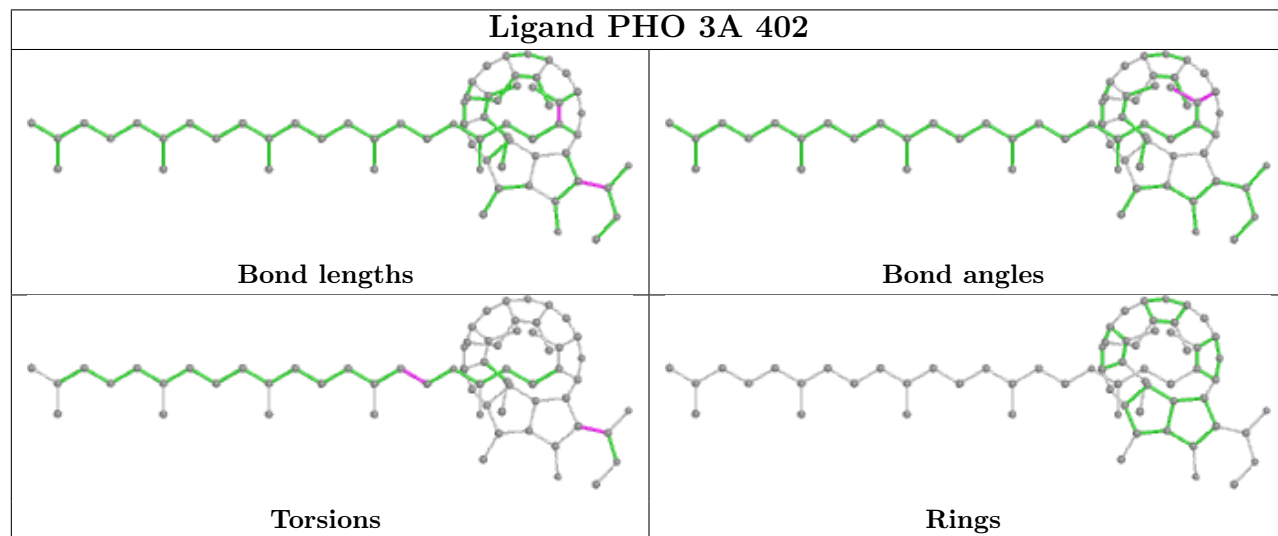
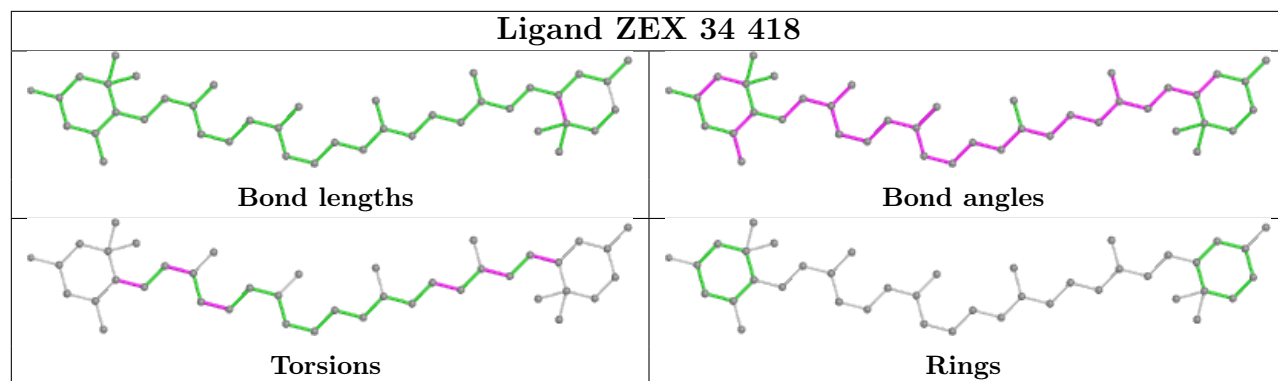
Bond angles

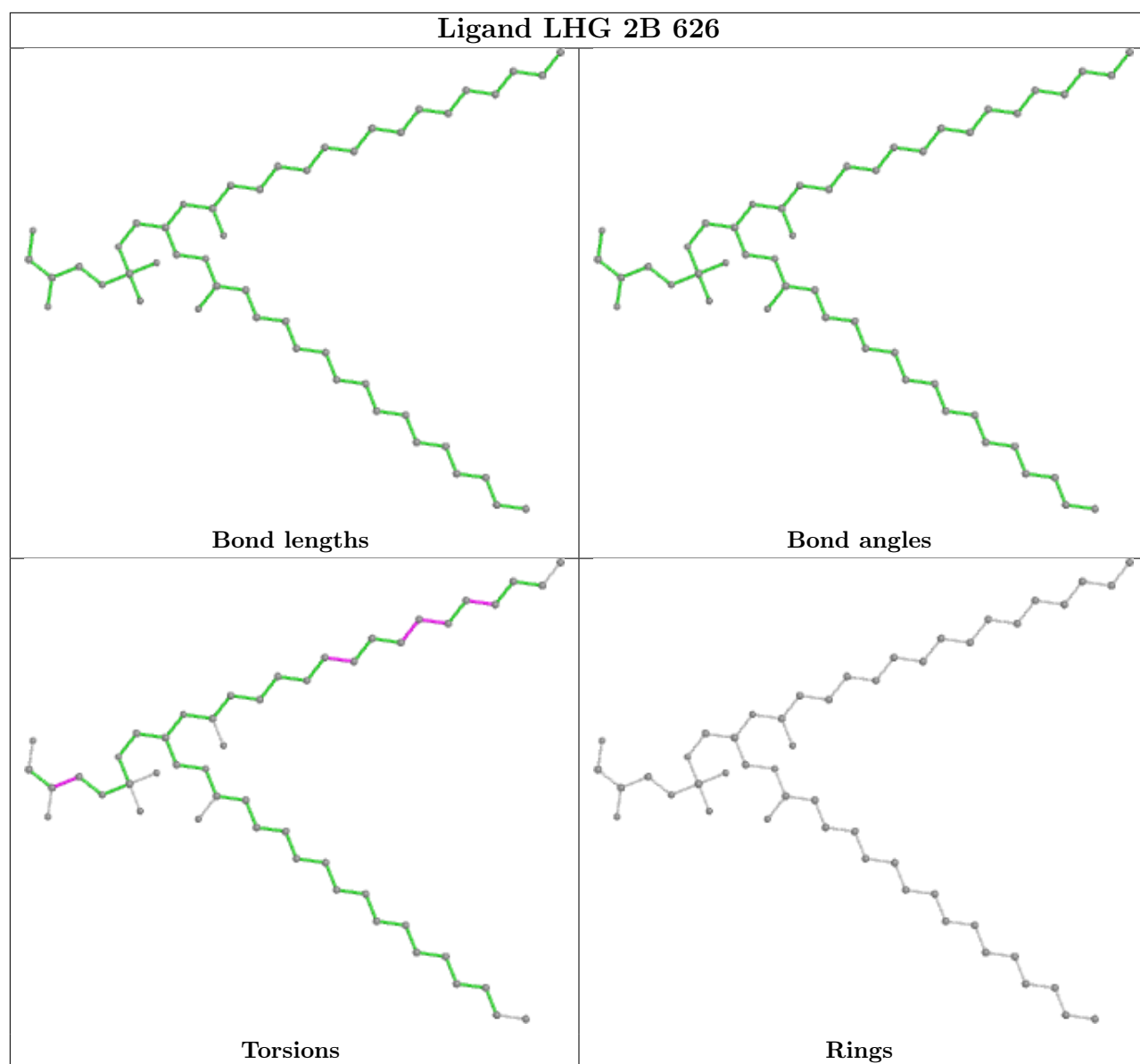


Torsions

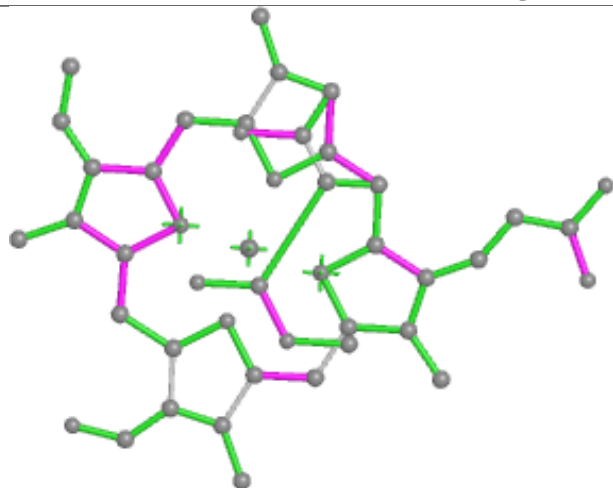


Rings

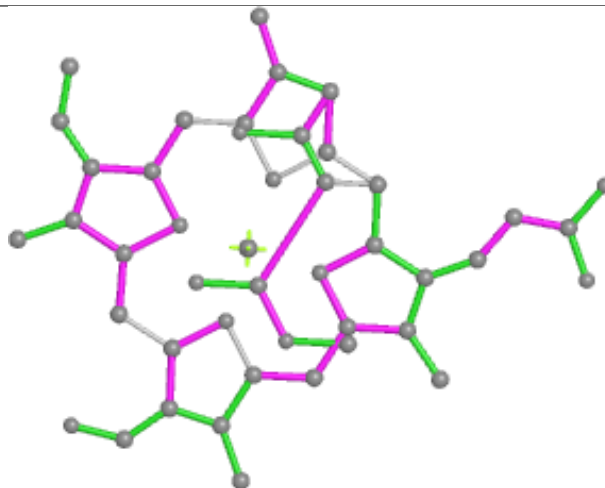




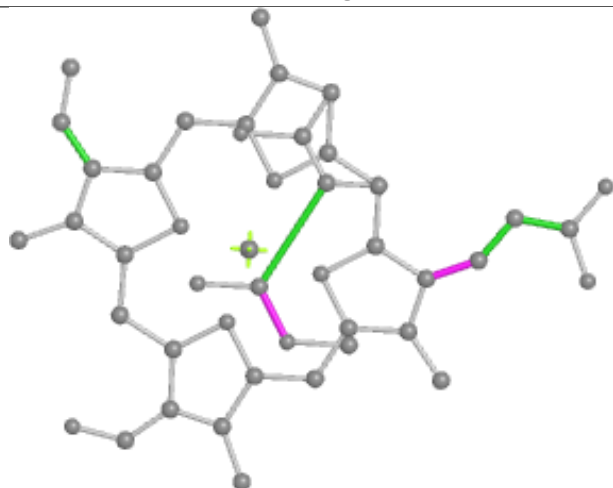
Ligand CL7 42 504



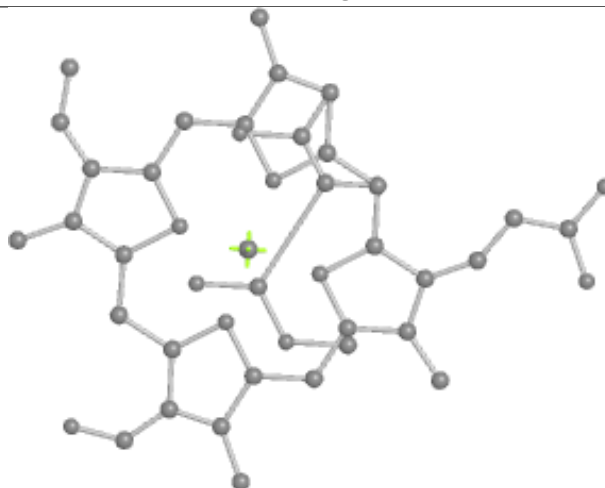
Bond lengths



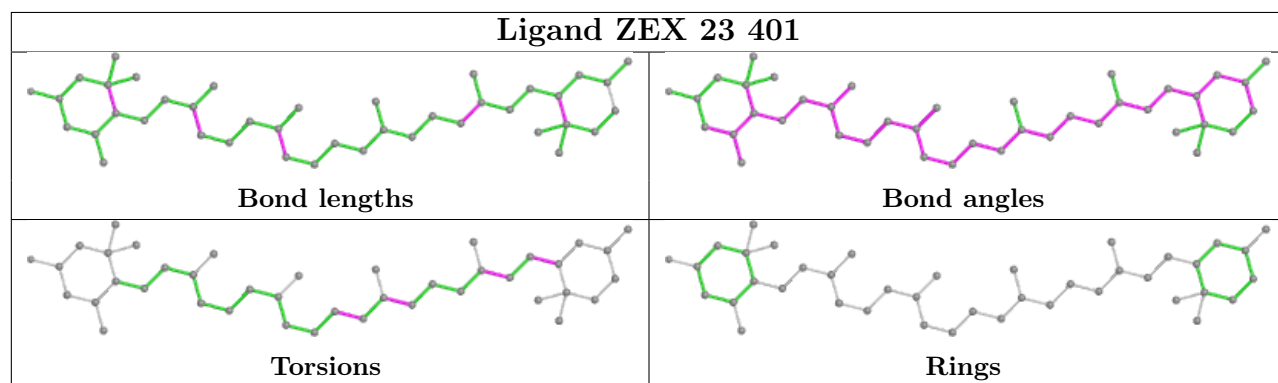
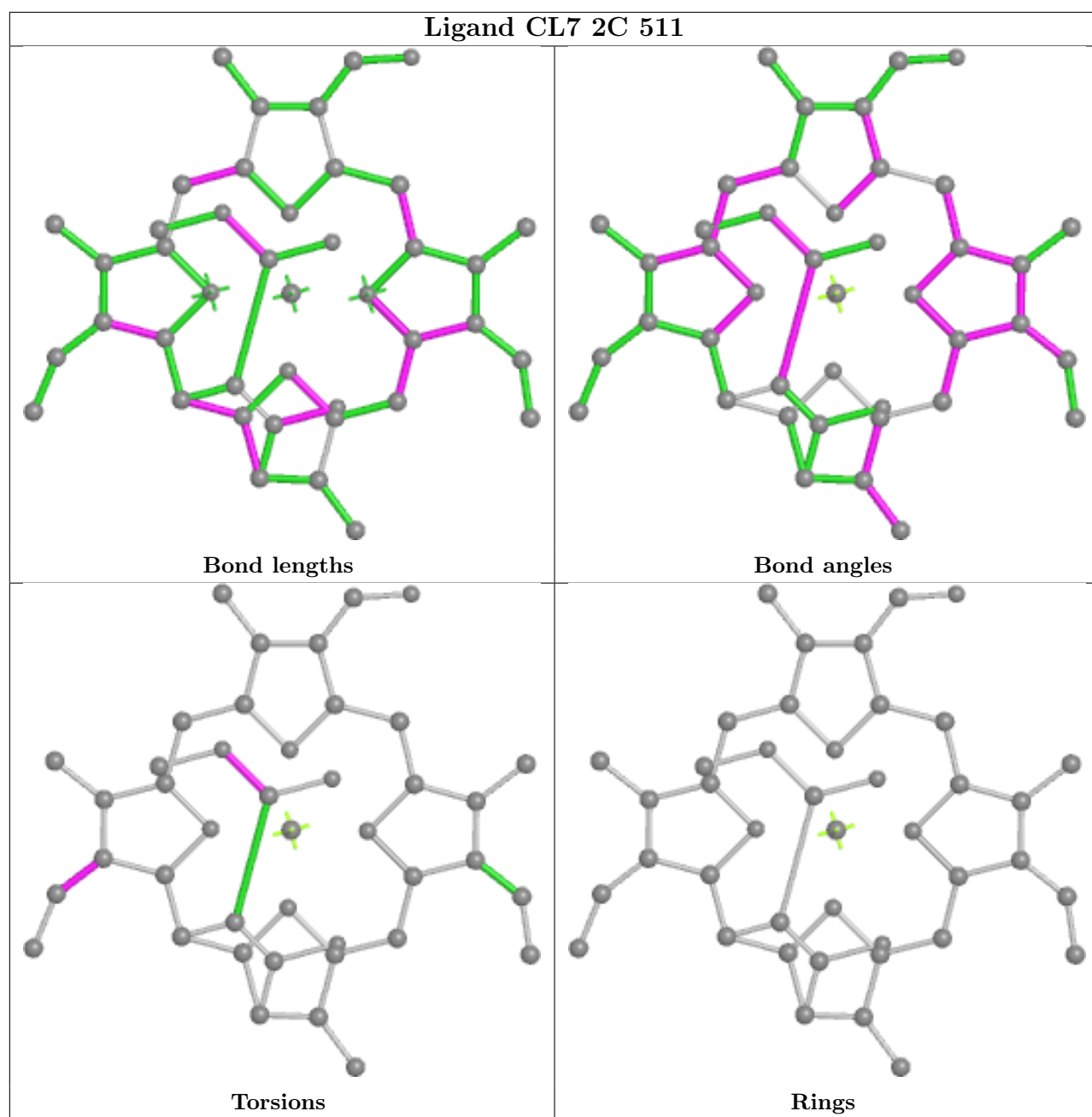
Bond angles

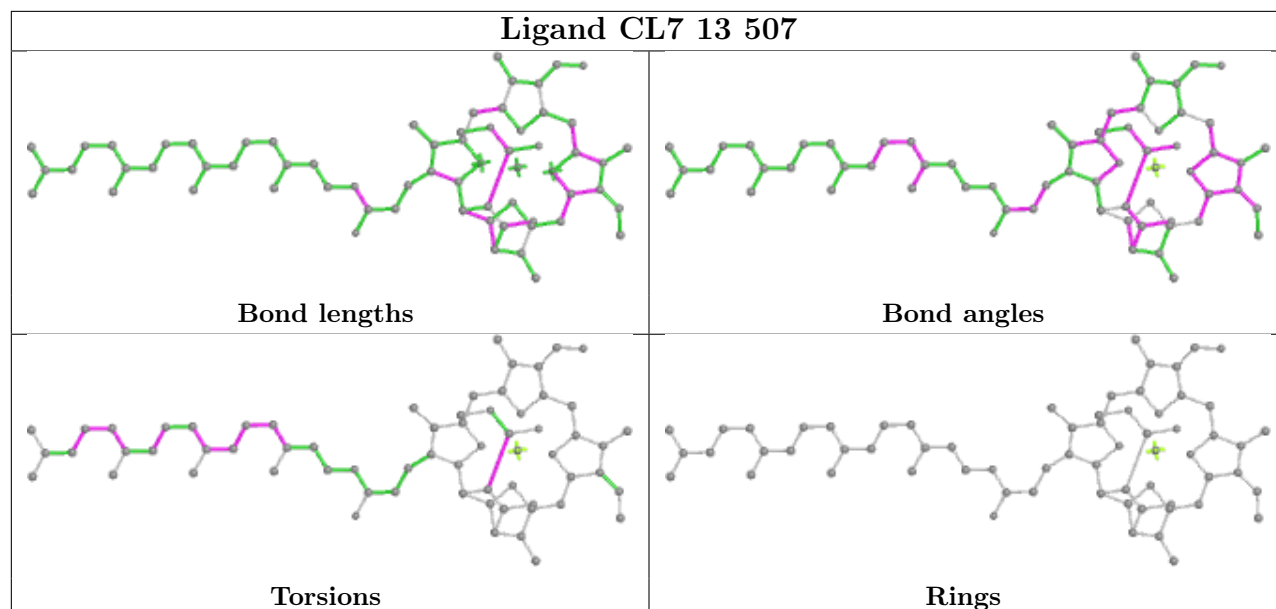
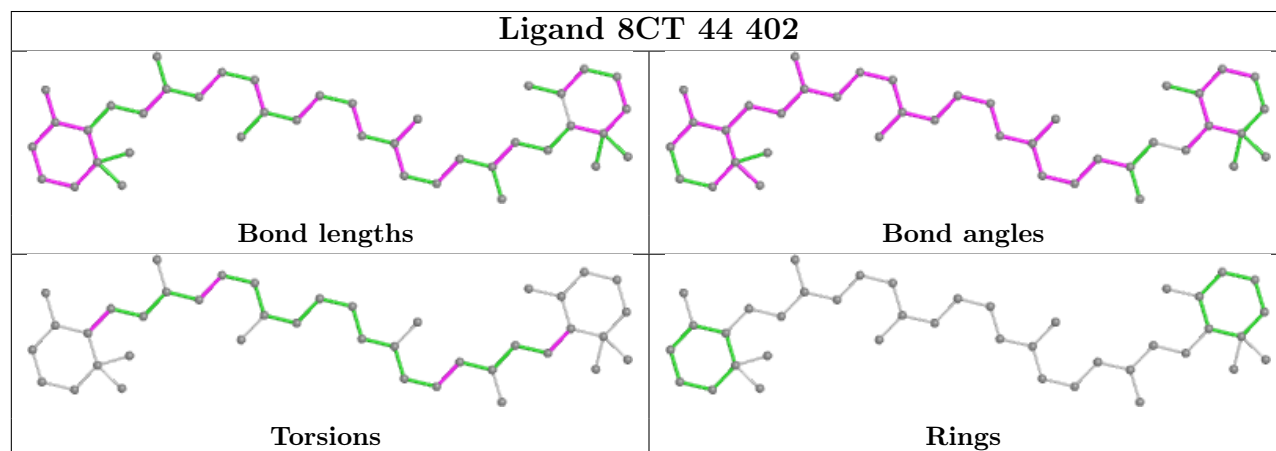
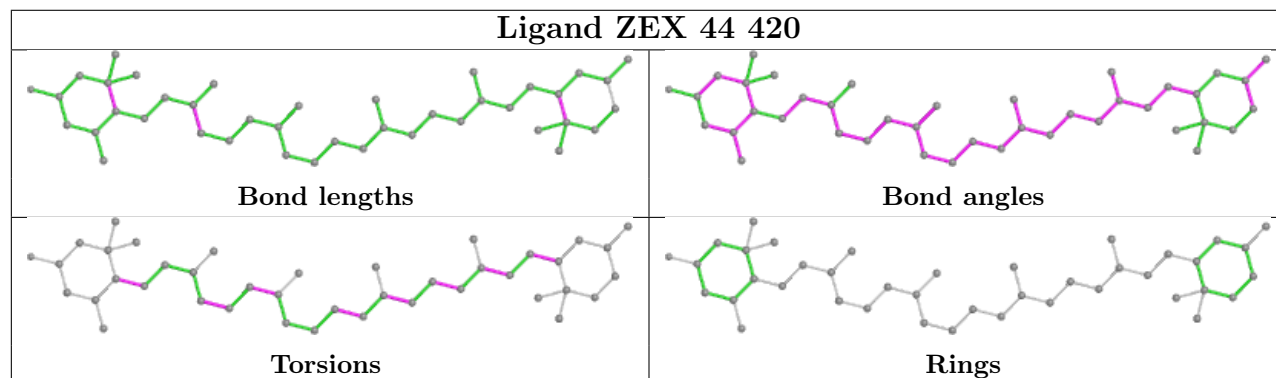


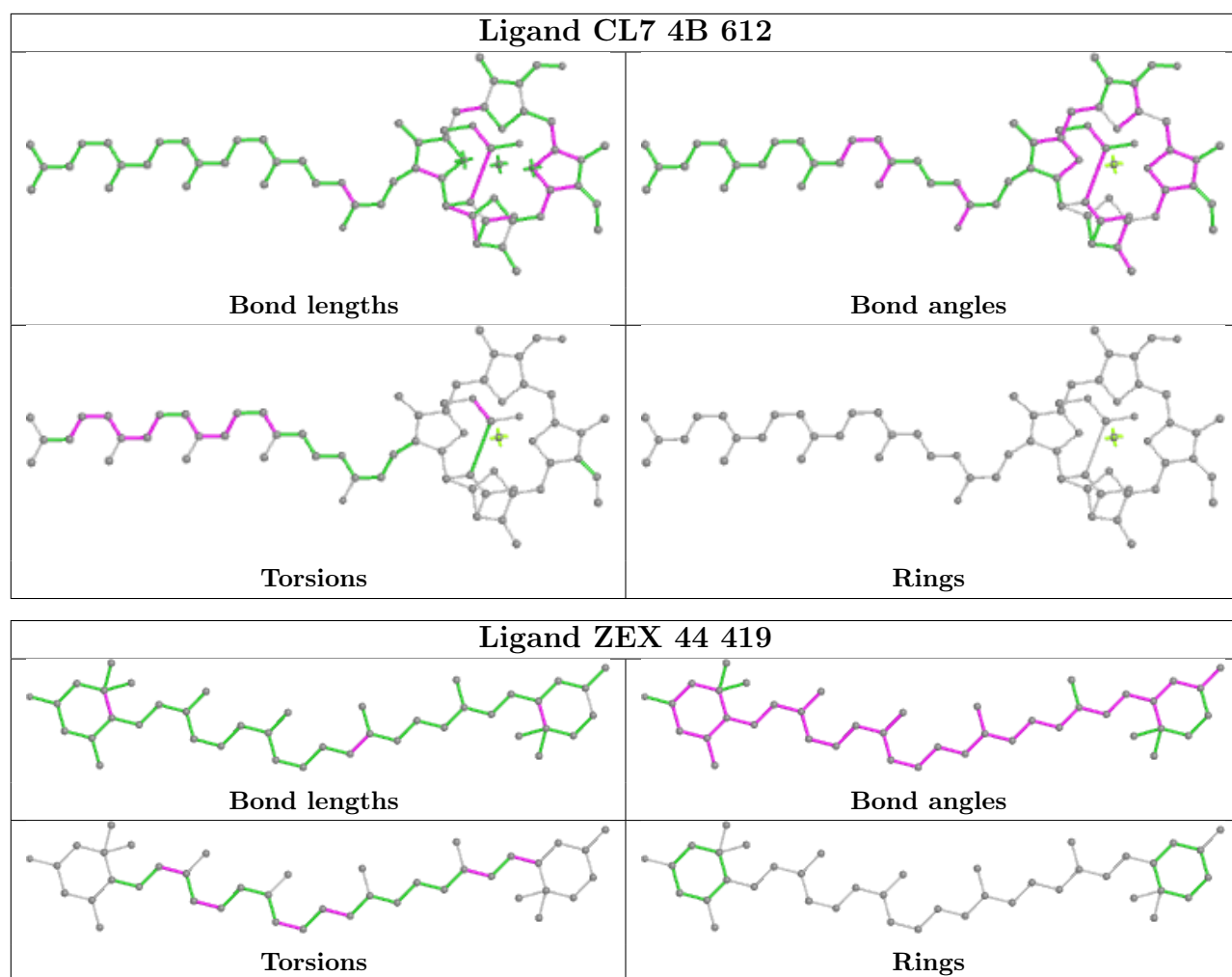
Torsions

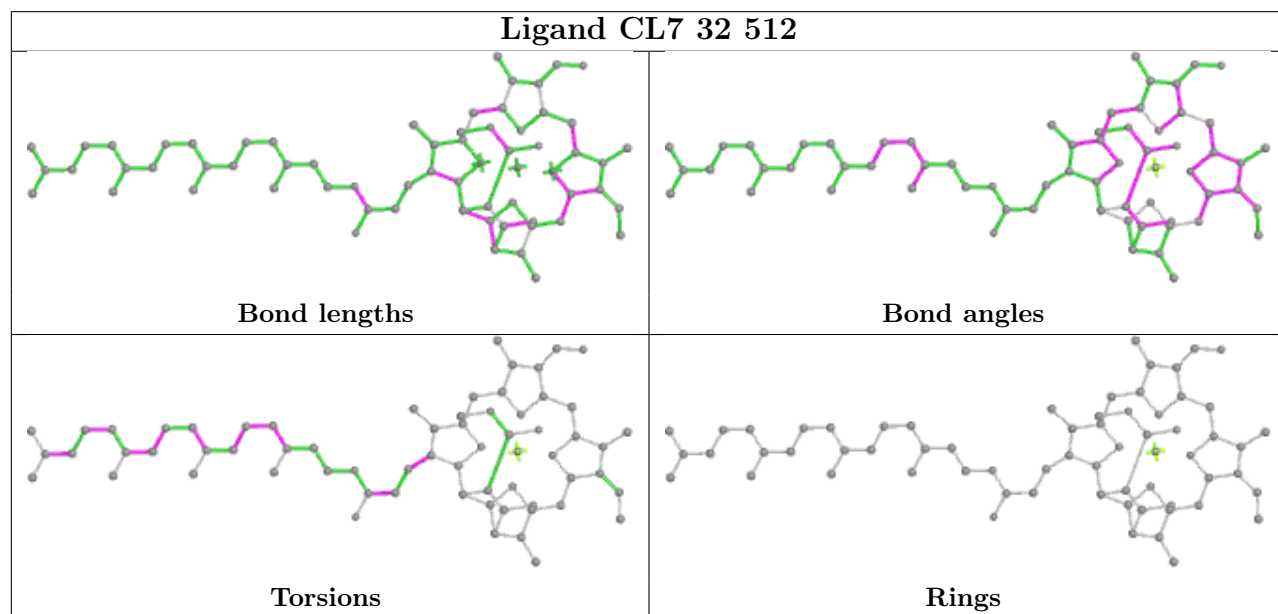
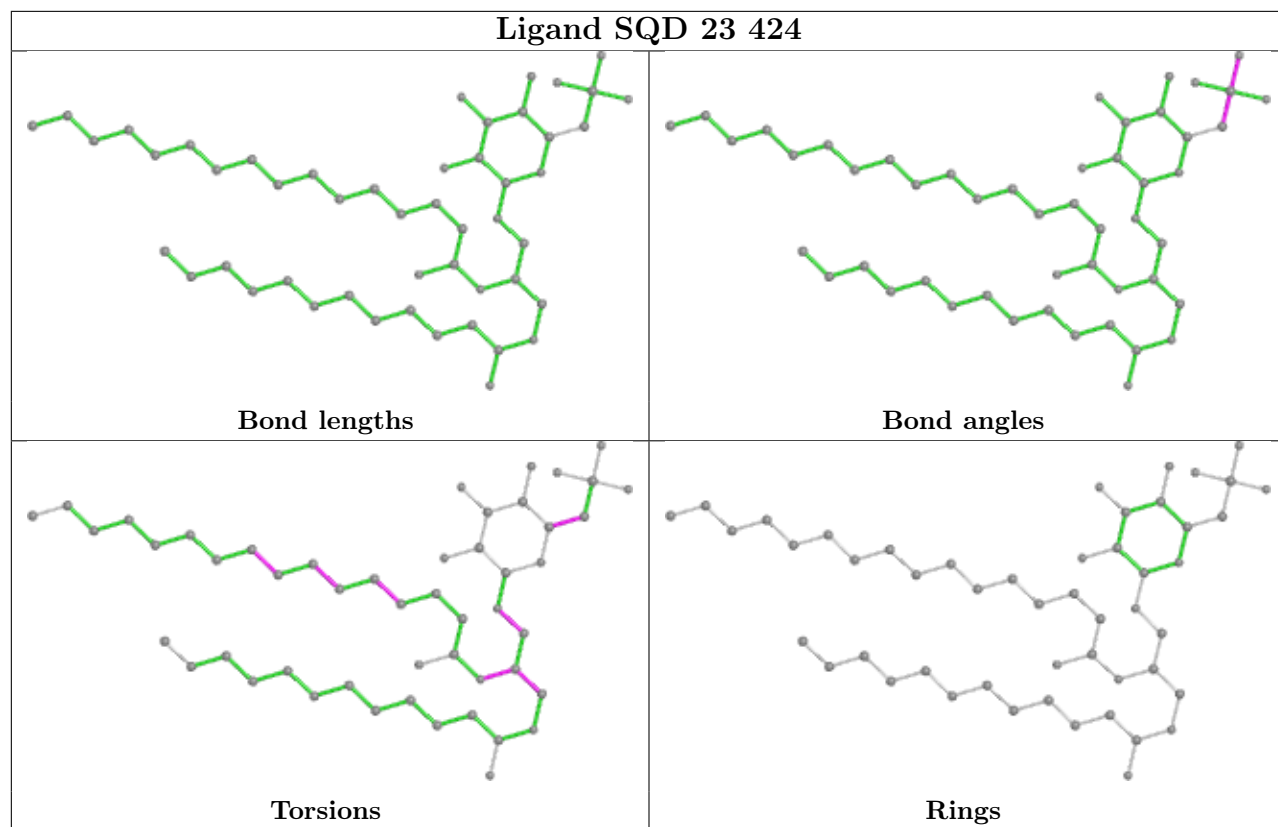


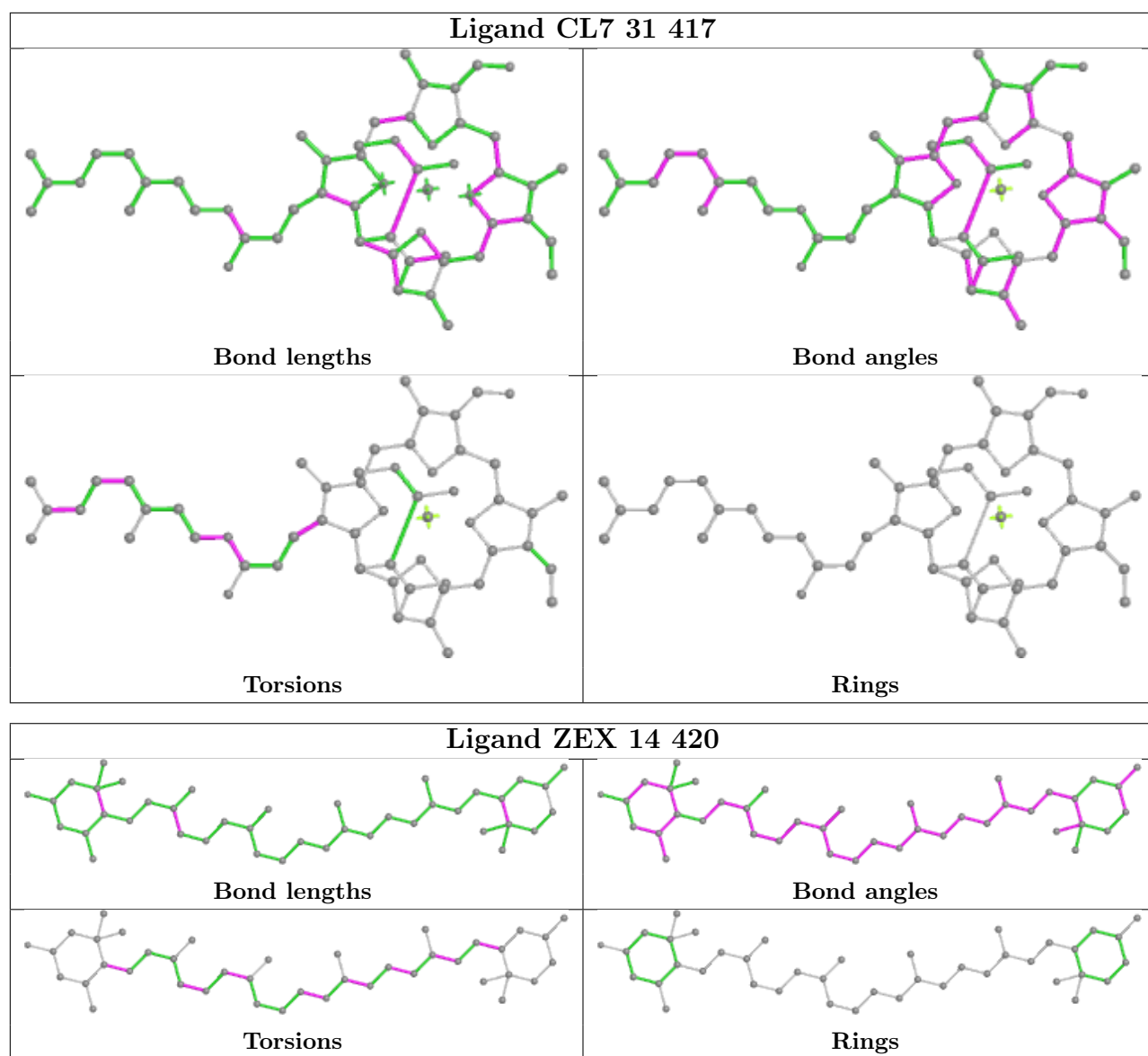
Rings

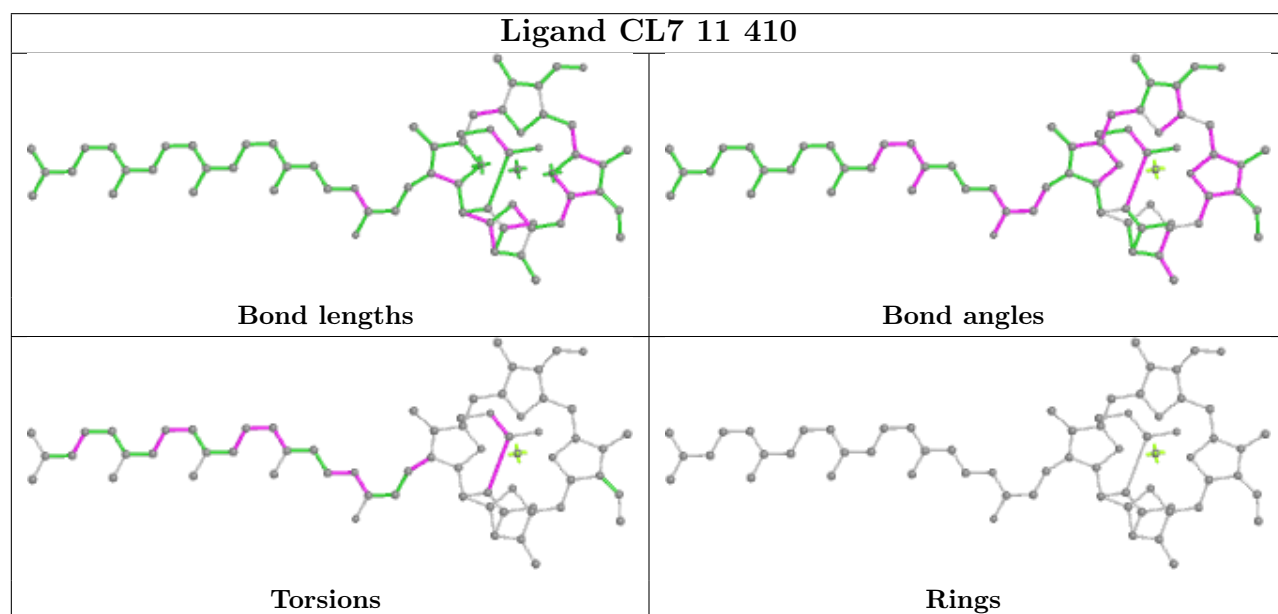
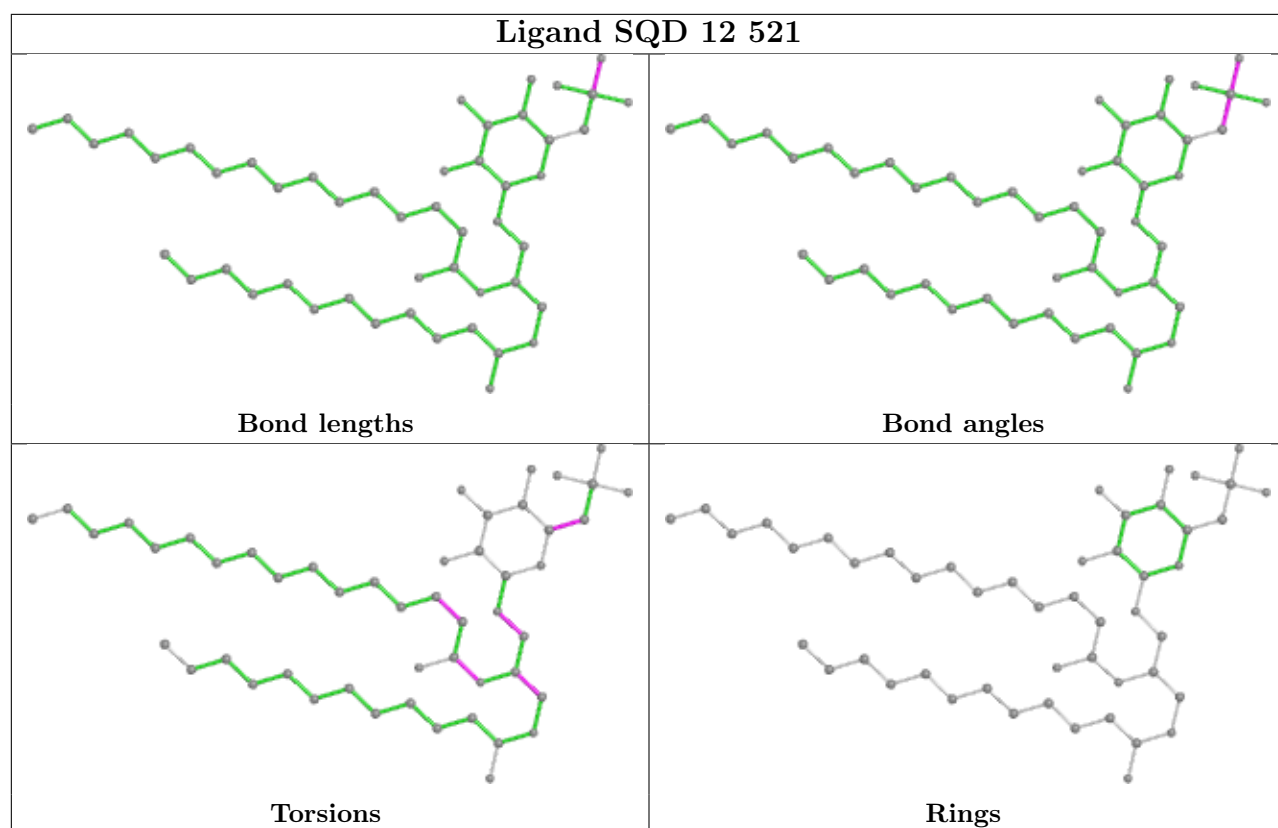


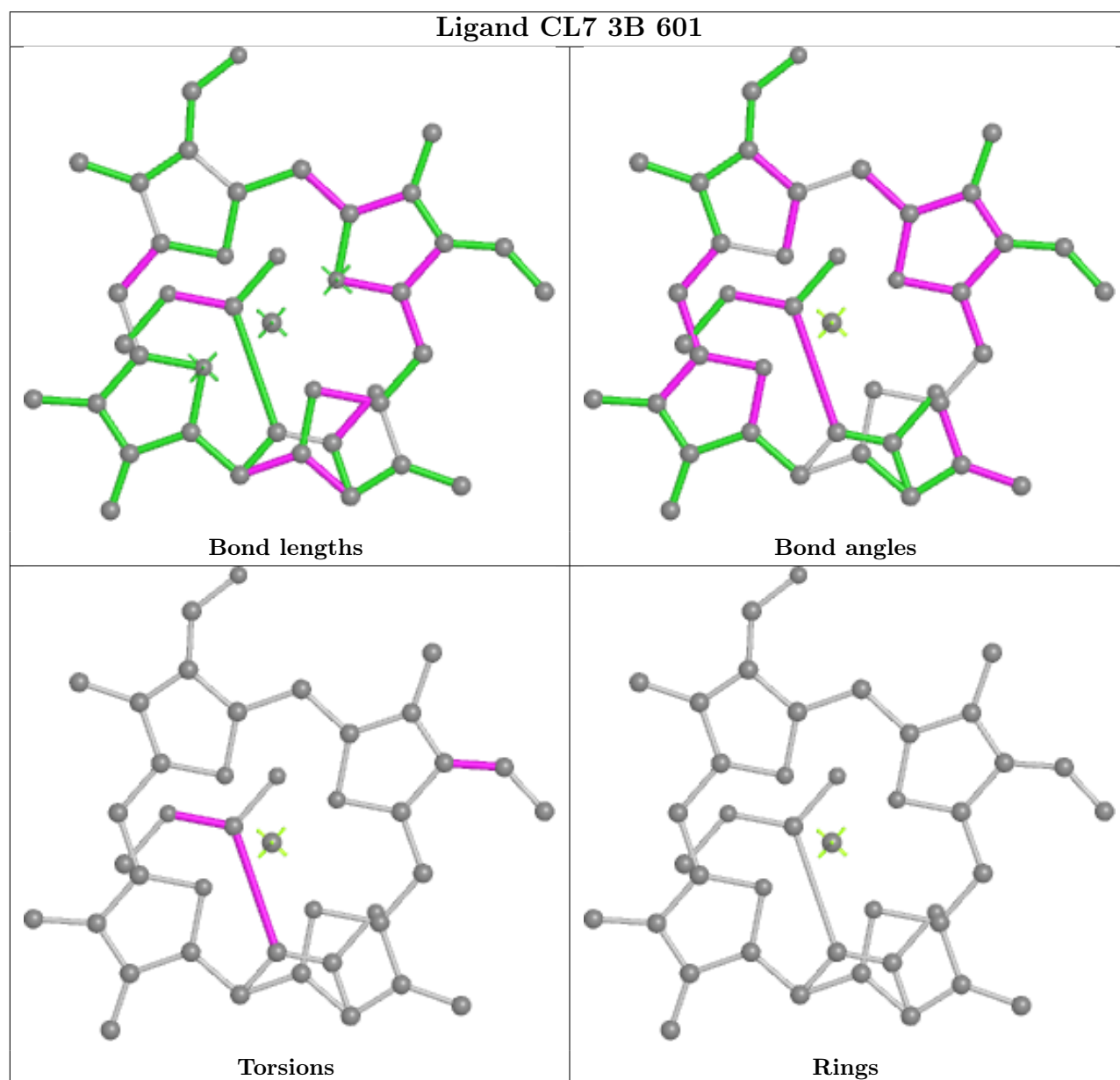
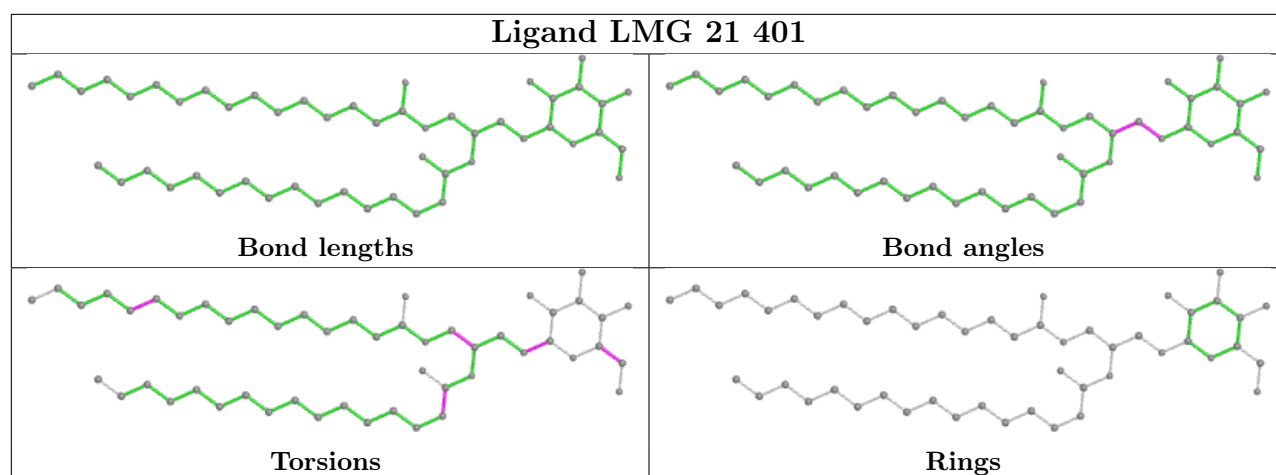
Ligand CL7 13 507**Ligand 8CT 44 402****Ligand ZEX 44 420**



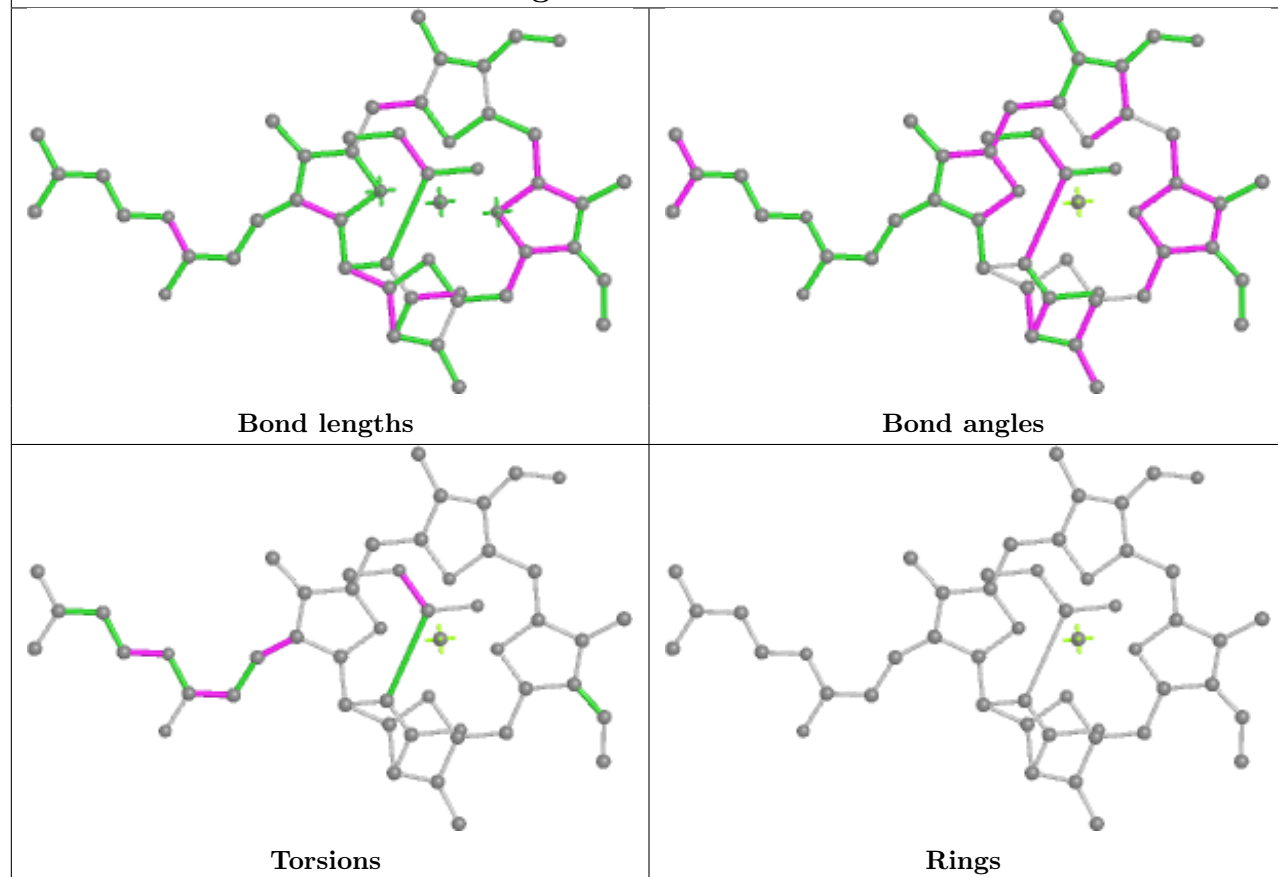




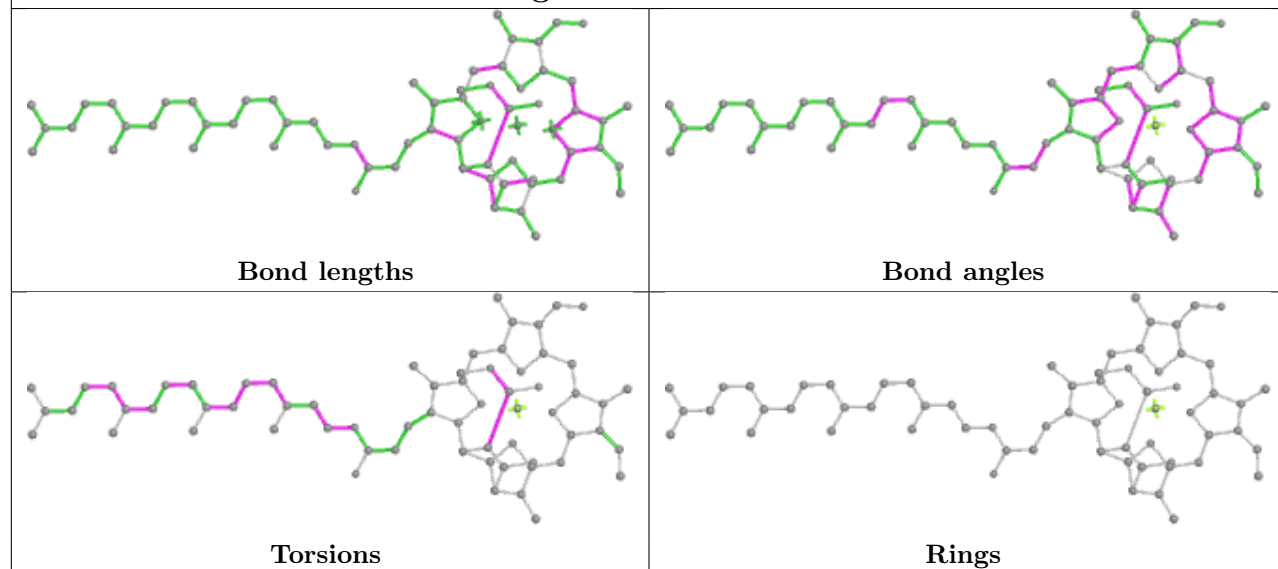


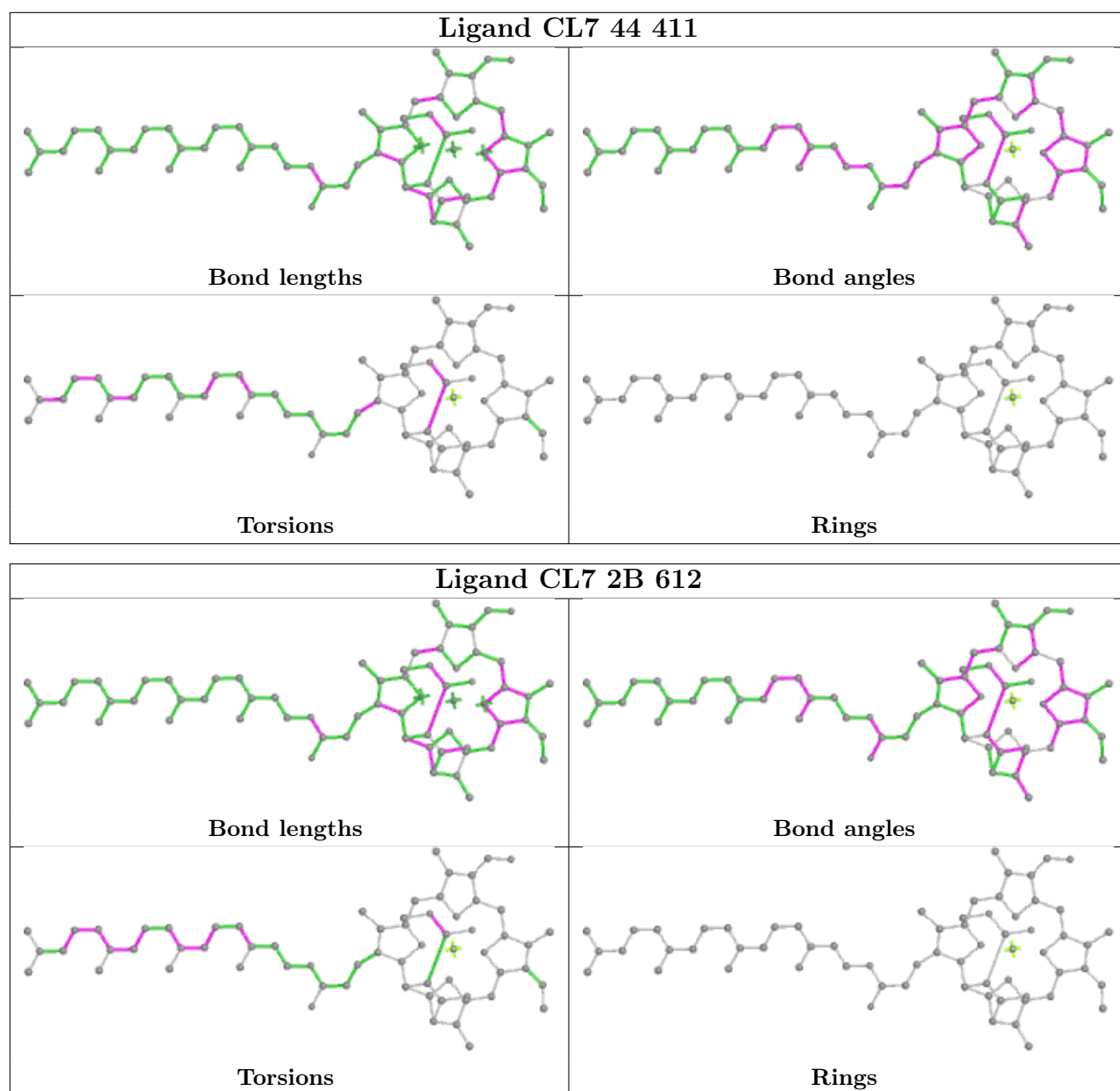


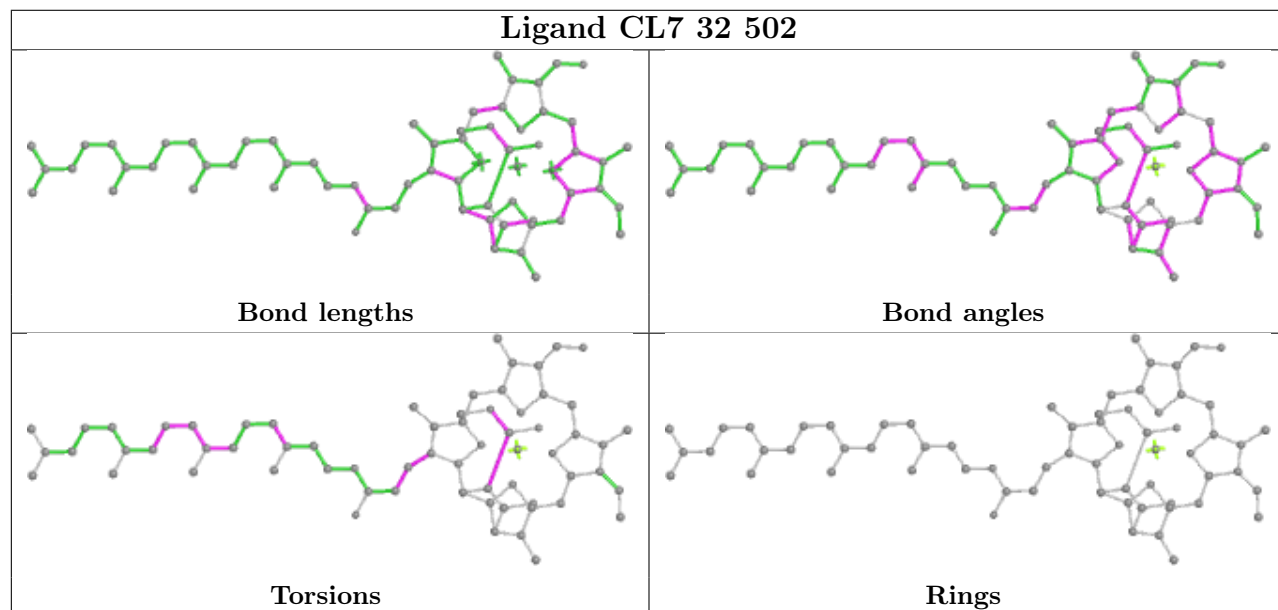
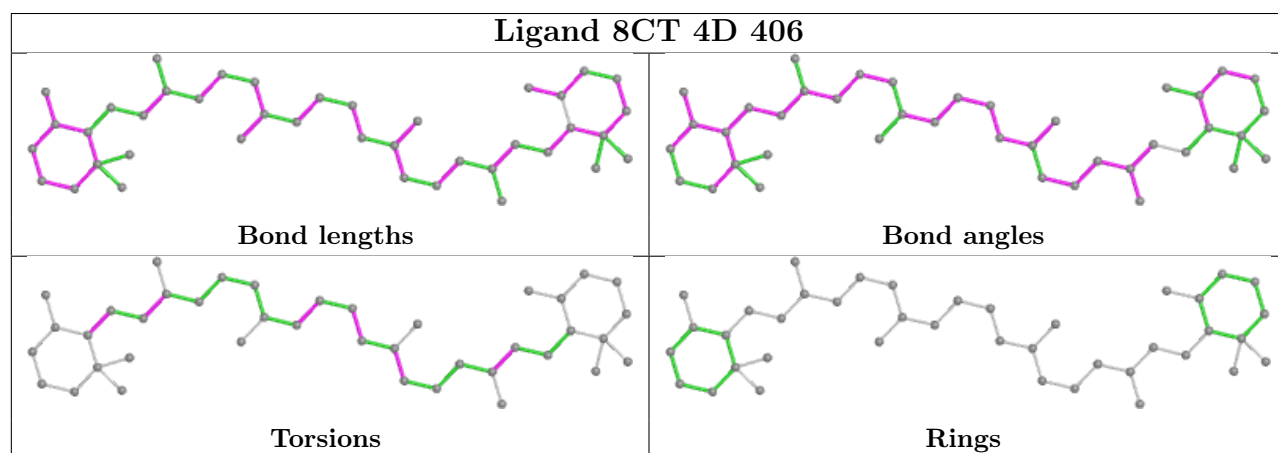
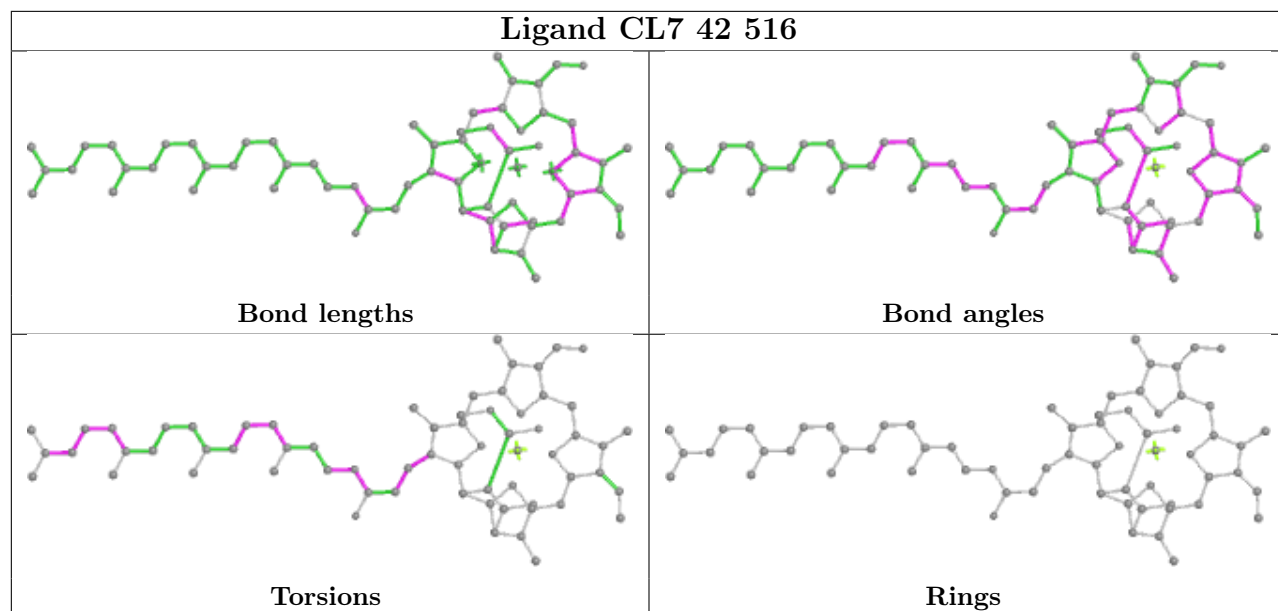
Ligand CL7 43 418

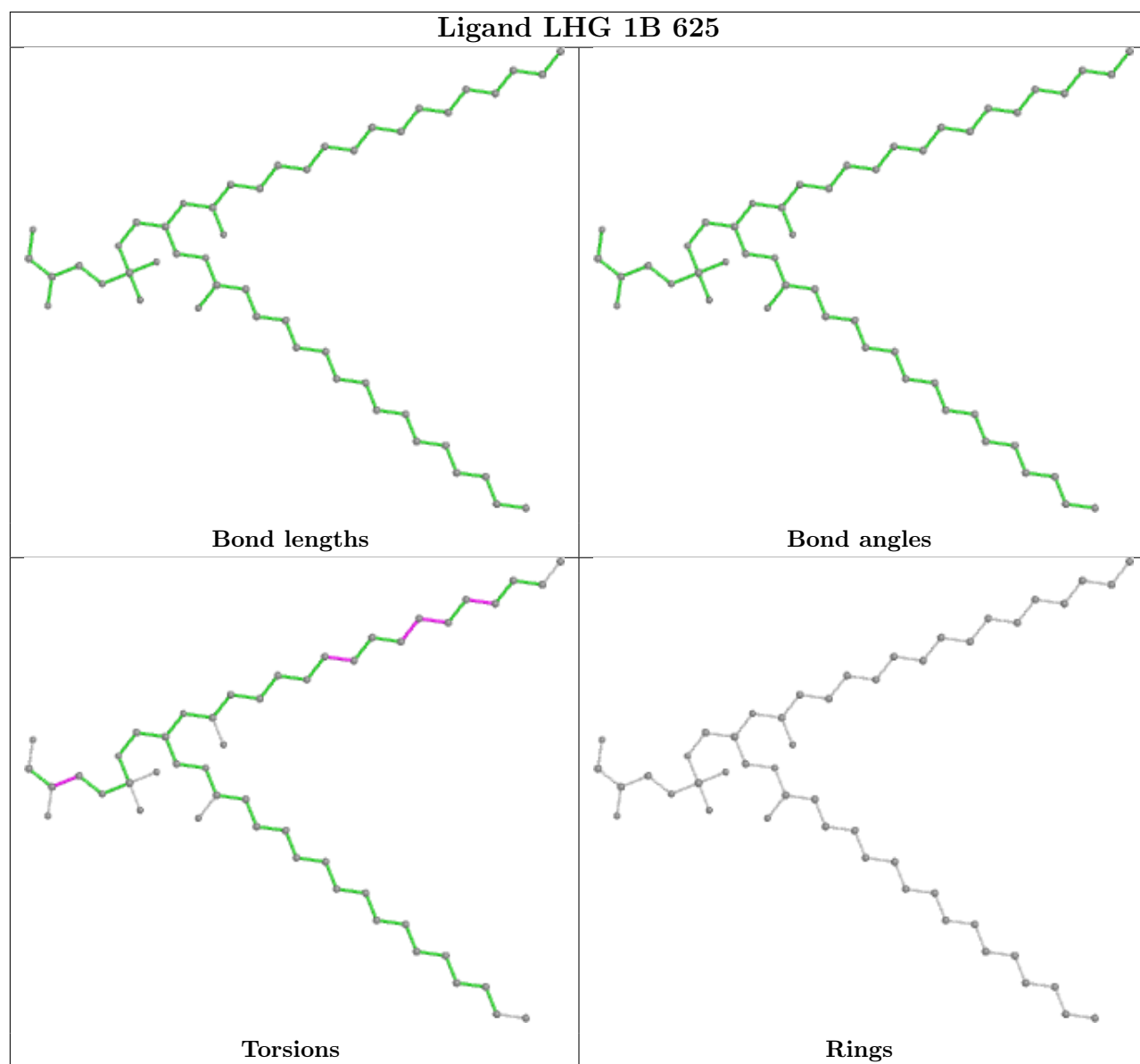
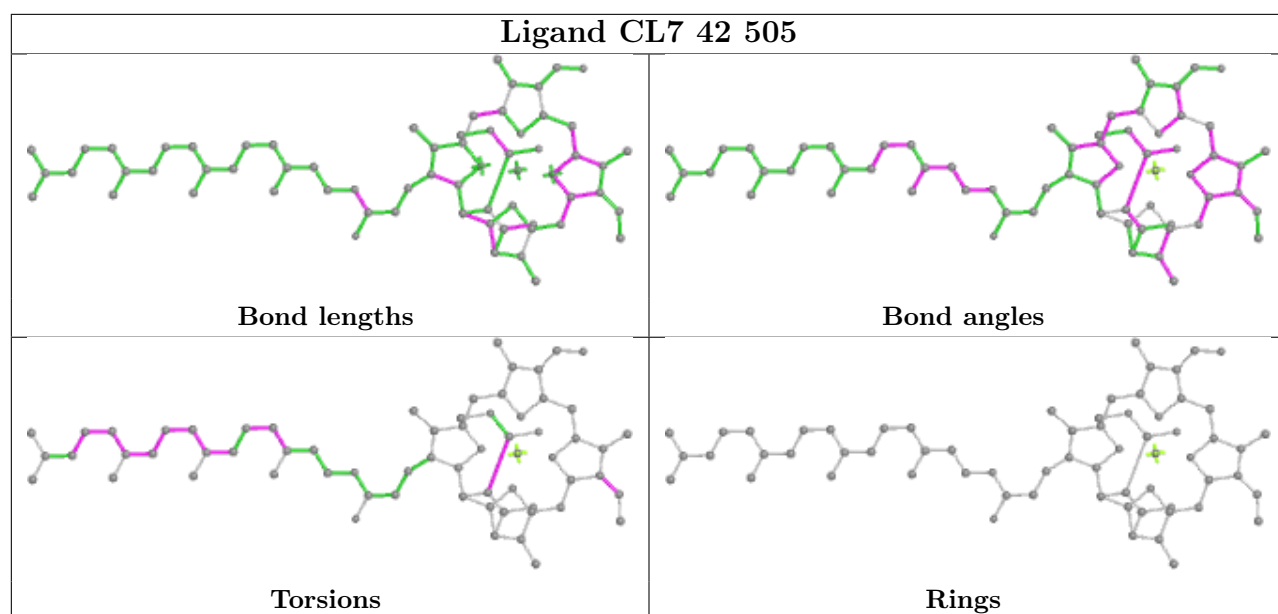


Ligand CL7 32 509

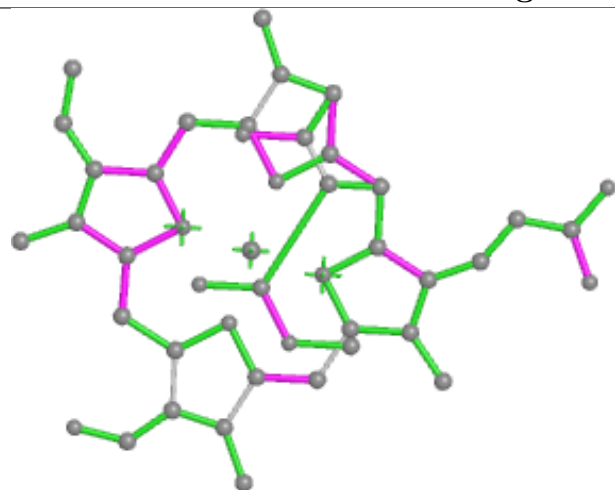




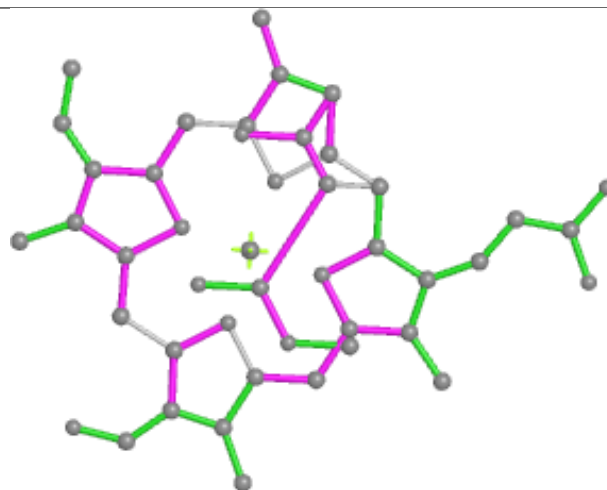




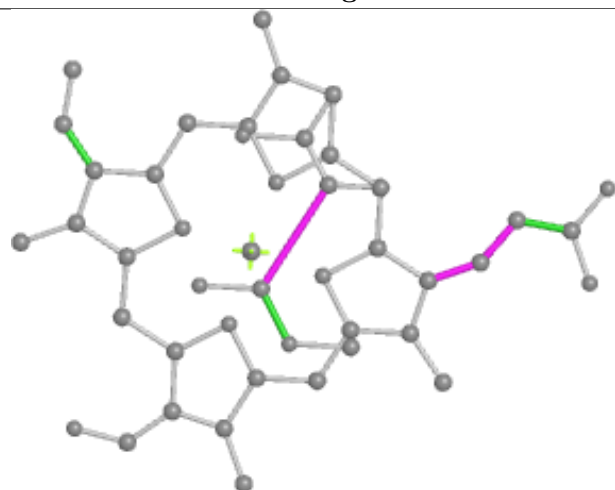
Ligand CL7 42 508



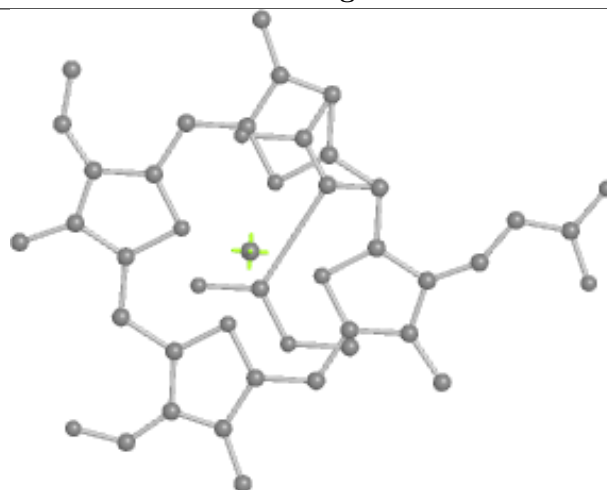
Bond lengths



Bond angles

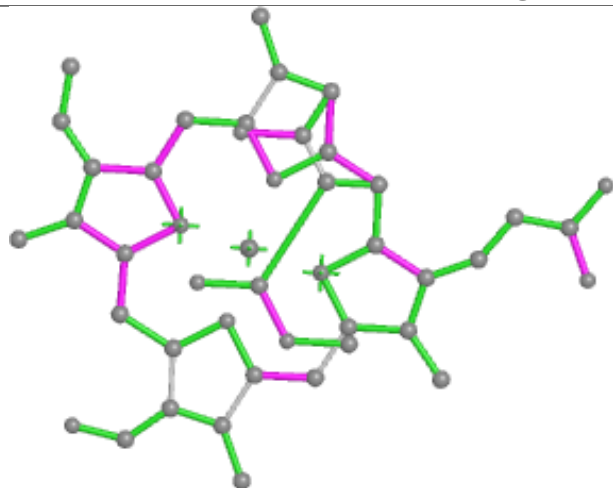


Torsions

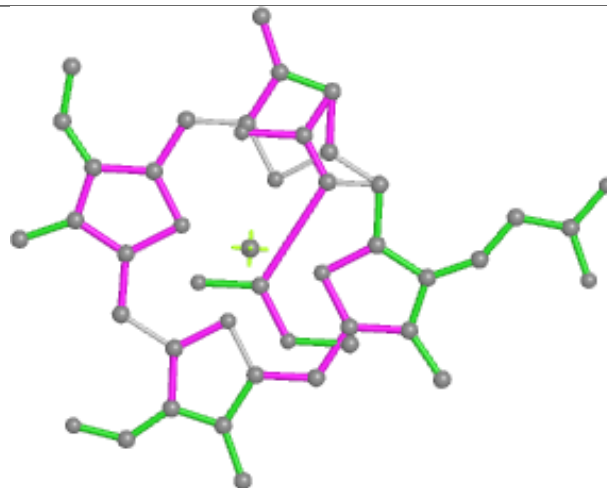


Rings

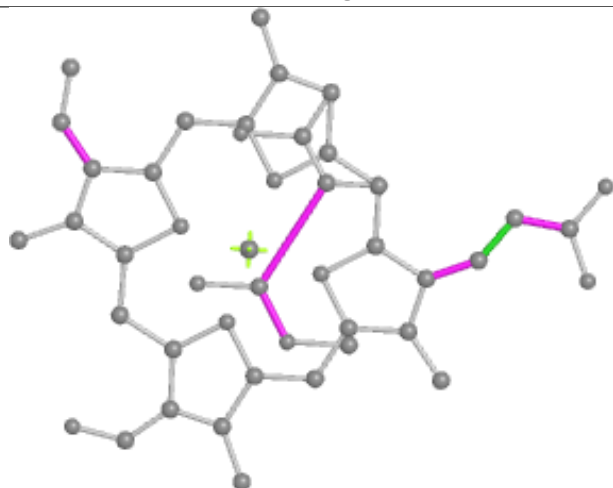
Ligand CL7 23 407



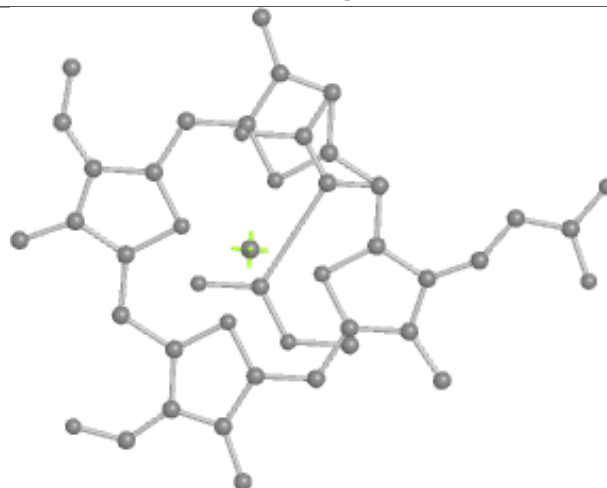
Bond lengths



Bond angles

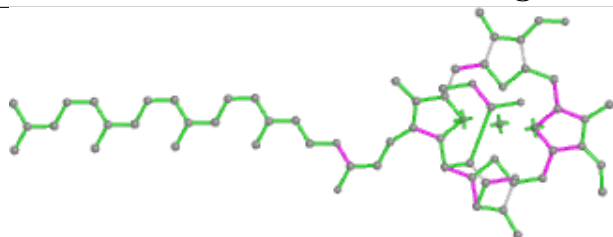


Torsions

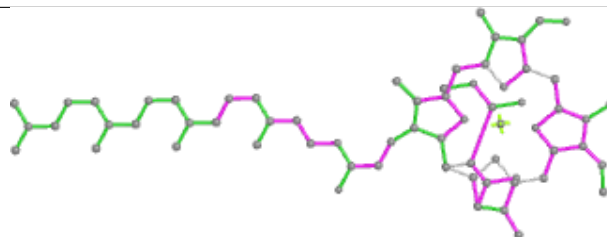


Rings

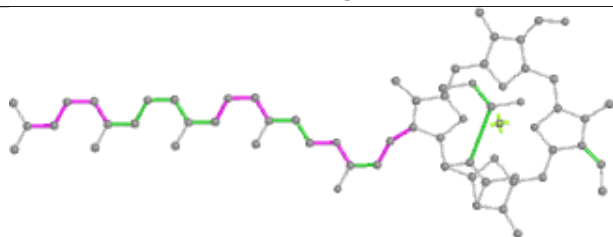
Ligand CL7 32 516



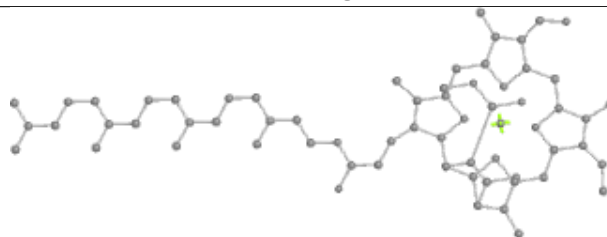
Bond lengths



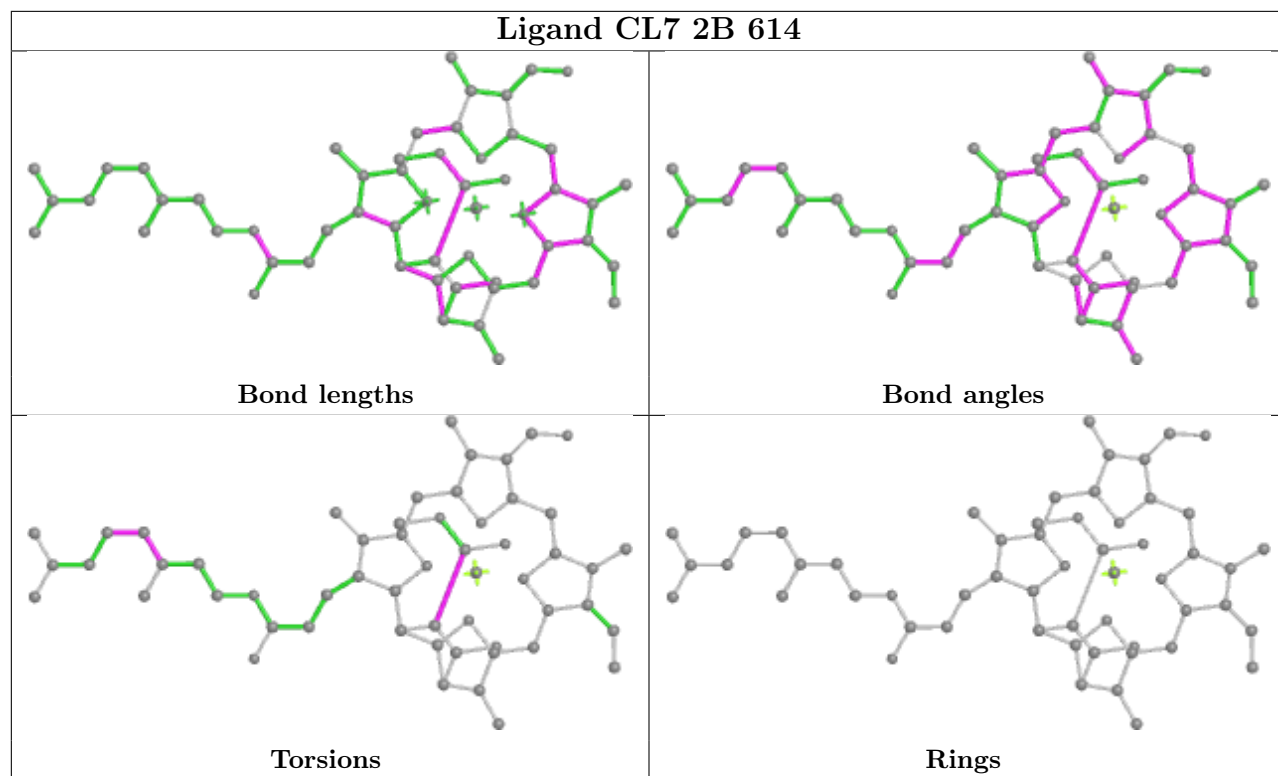
Bond angles



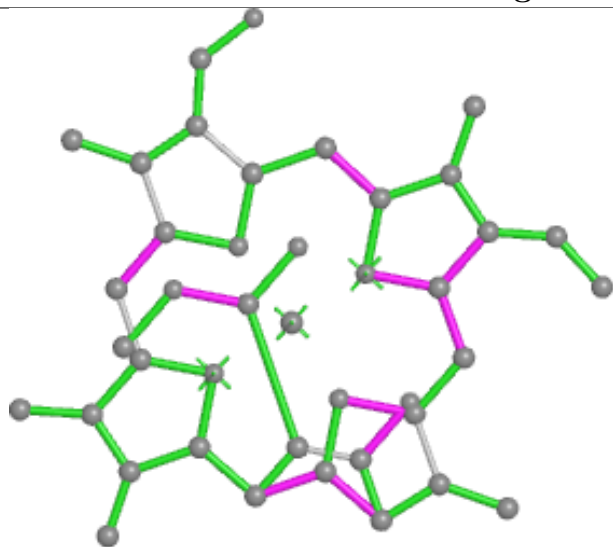
Torsions



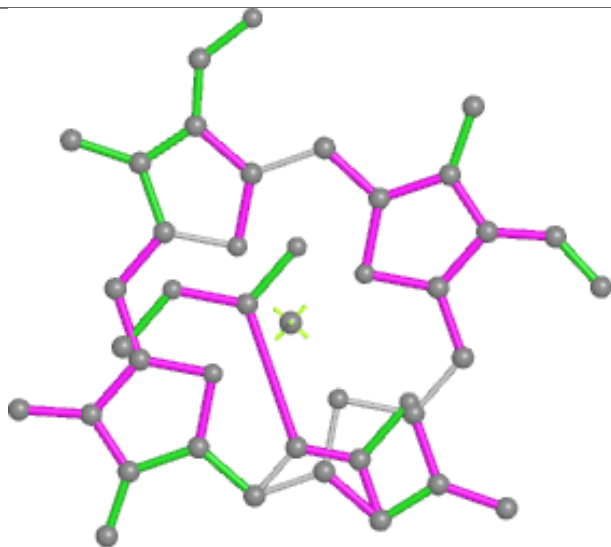
Rings



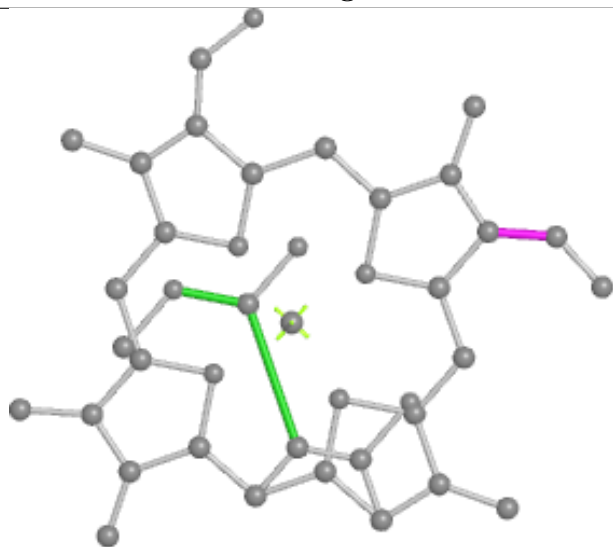
Ligand CL7 31 414



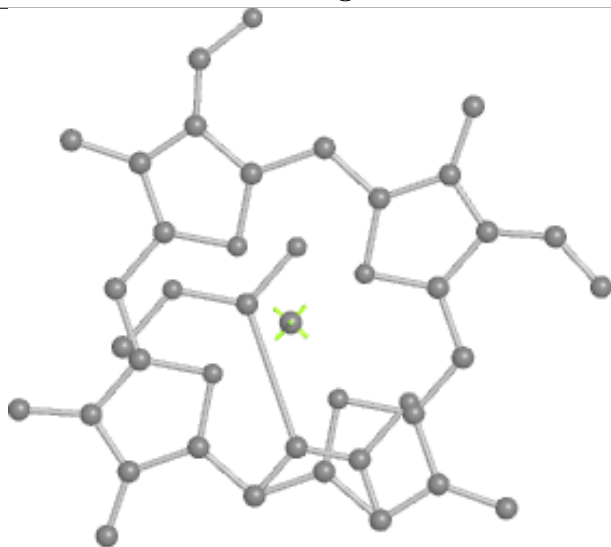
Bond lengths



Bond angles

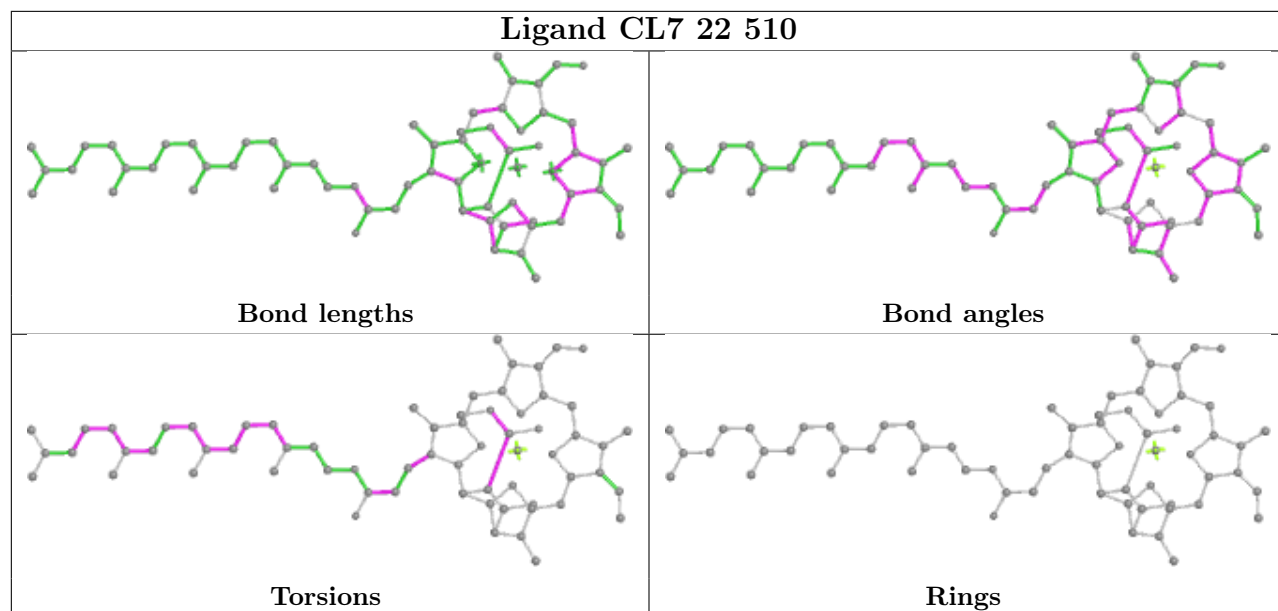


Torsions

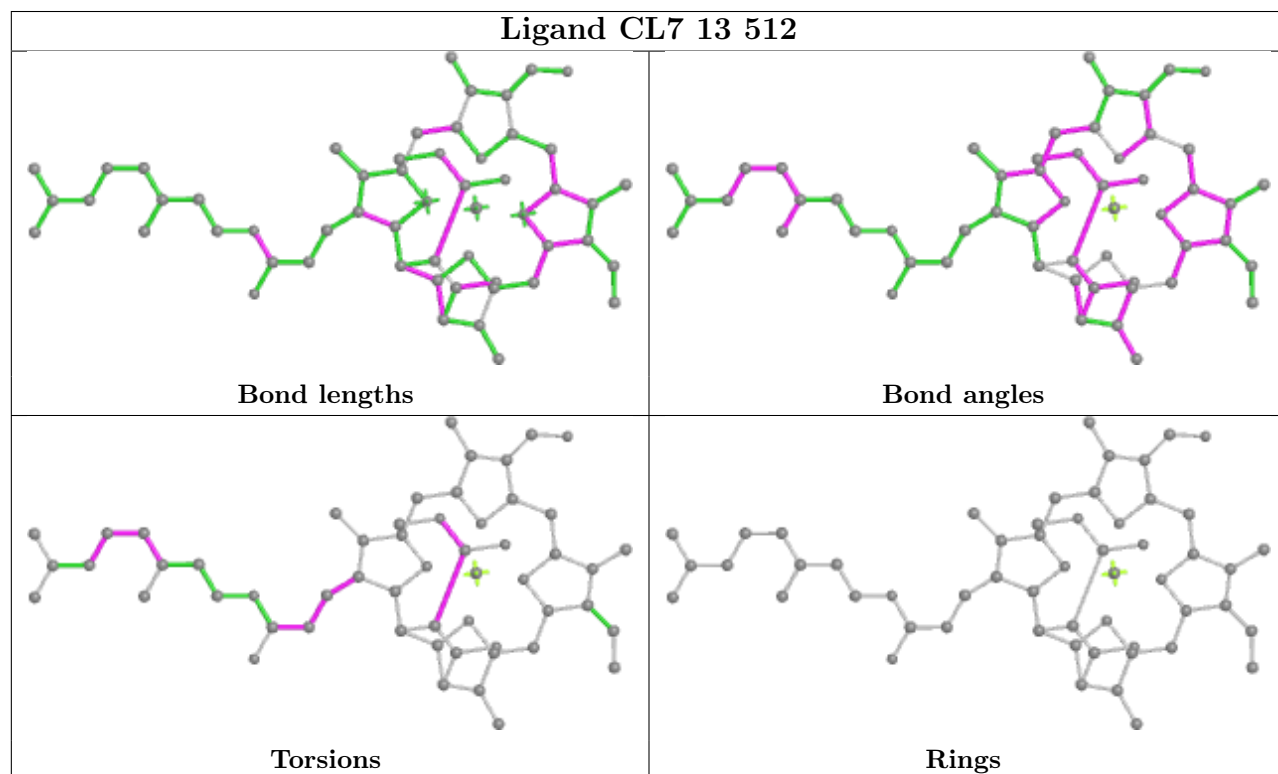


Rings

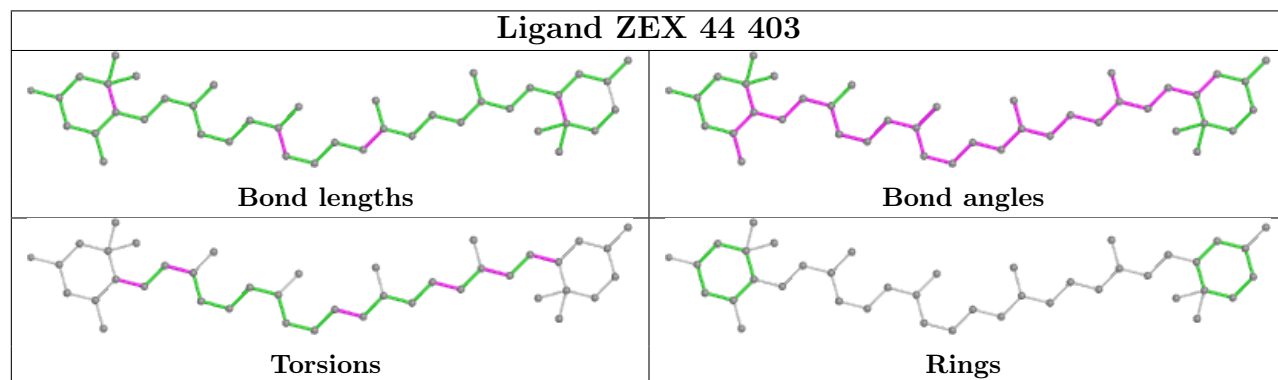
Ligand CL7 22 510



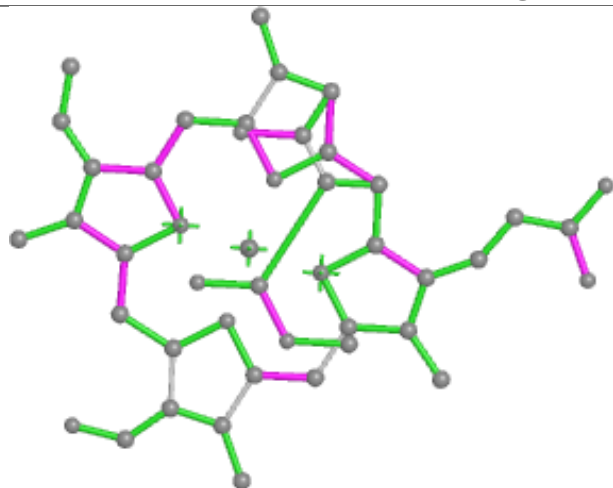
Ligand CL7 13 512



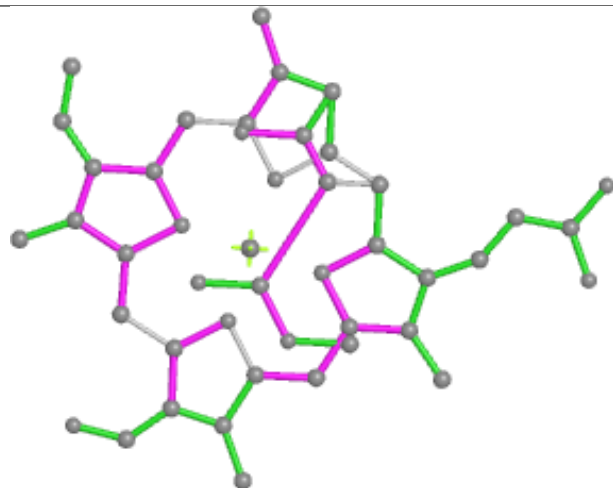
Ligand ZEX 44 403



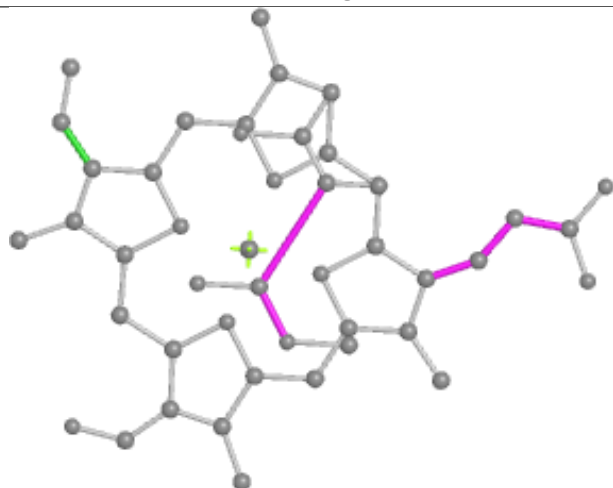
Ligand CL7 34 410



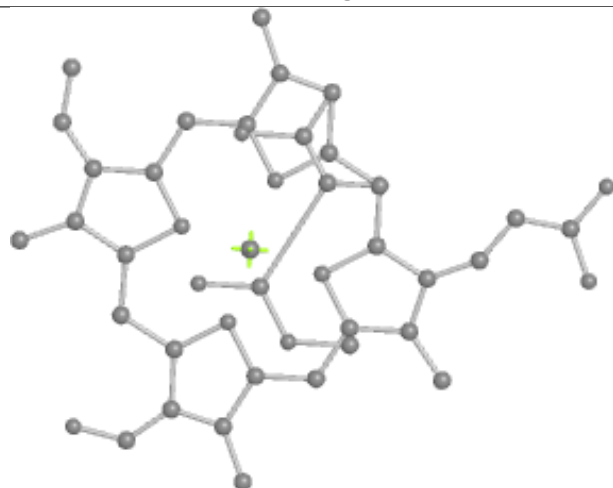
Bond lengths



Bond angles

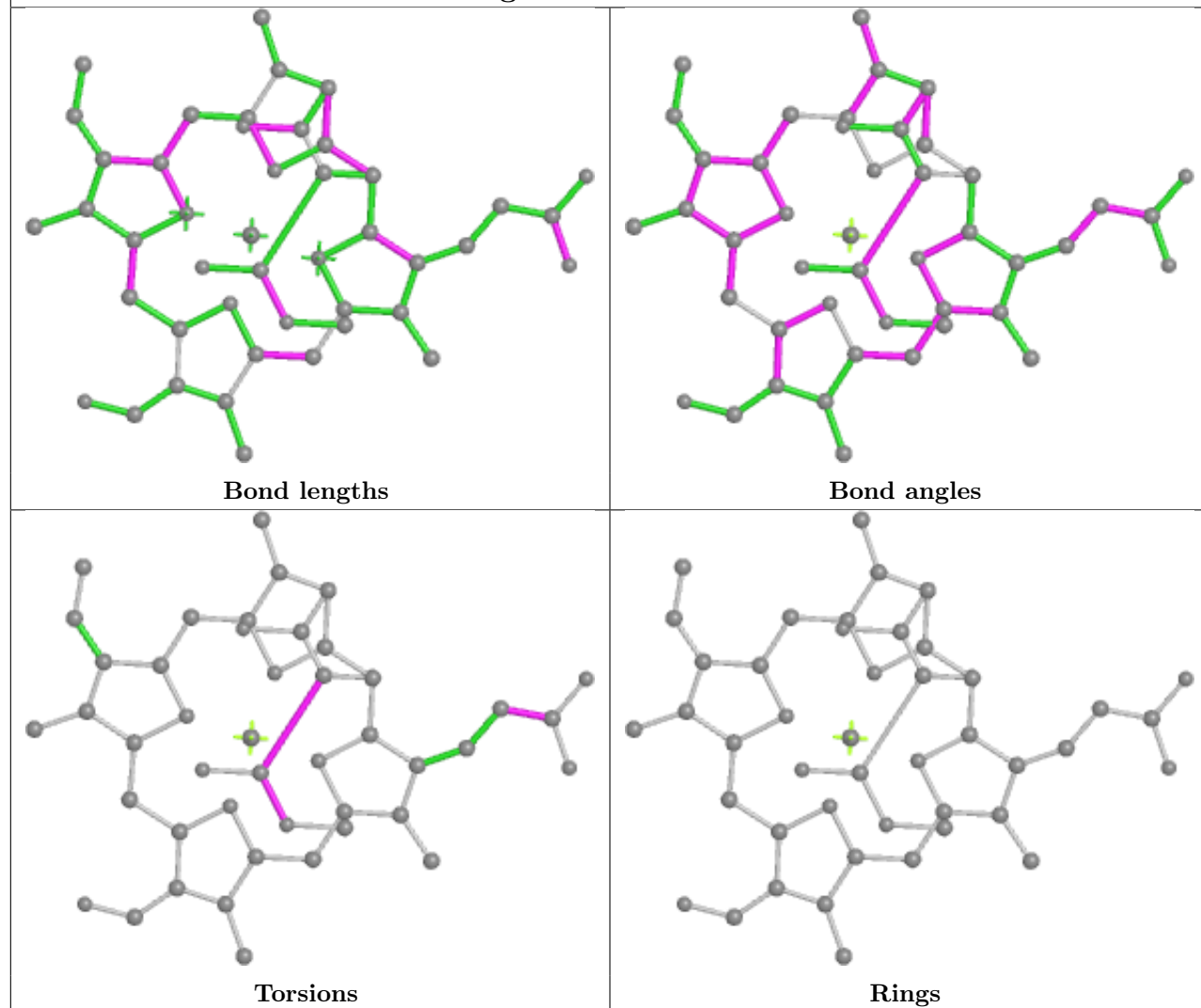


Torsions

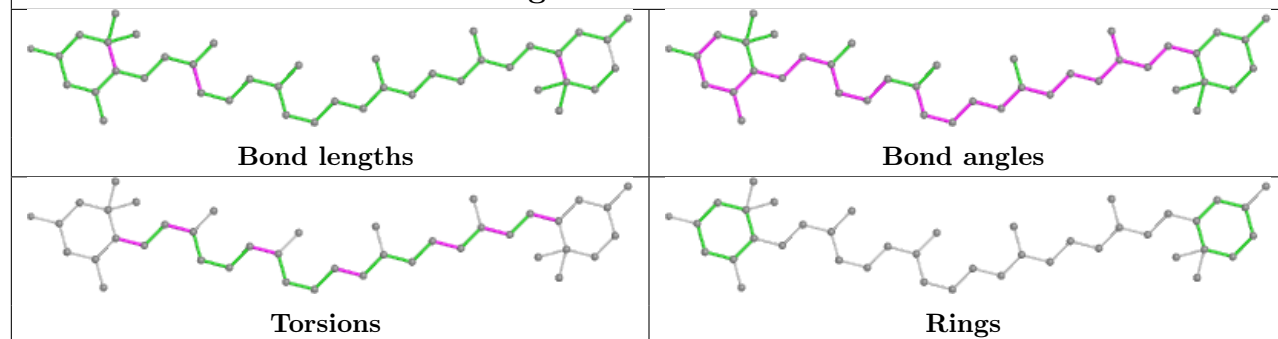


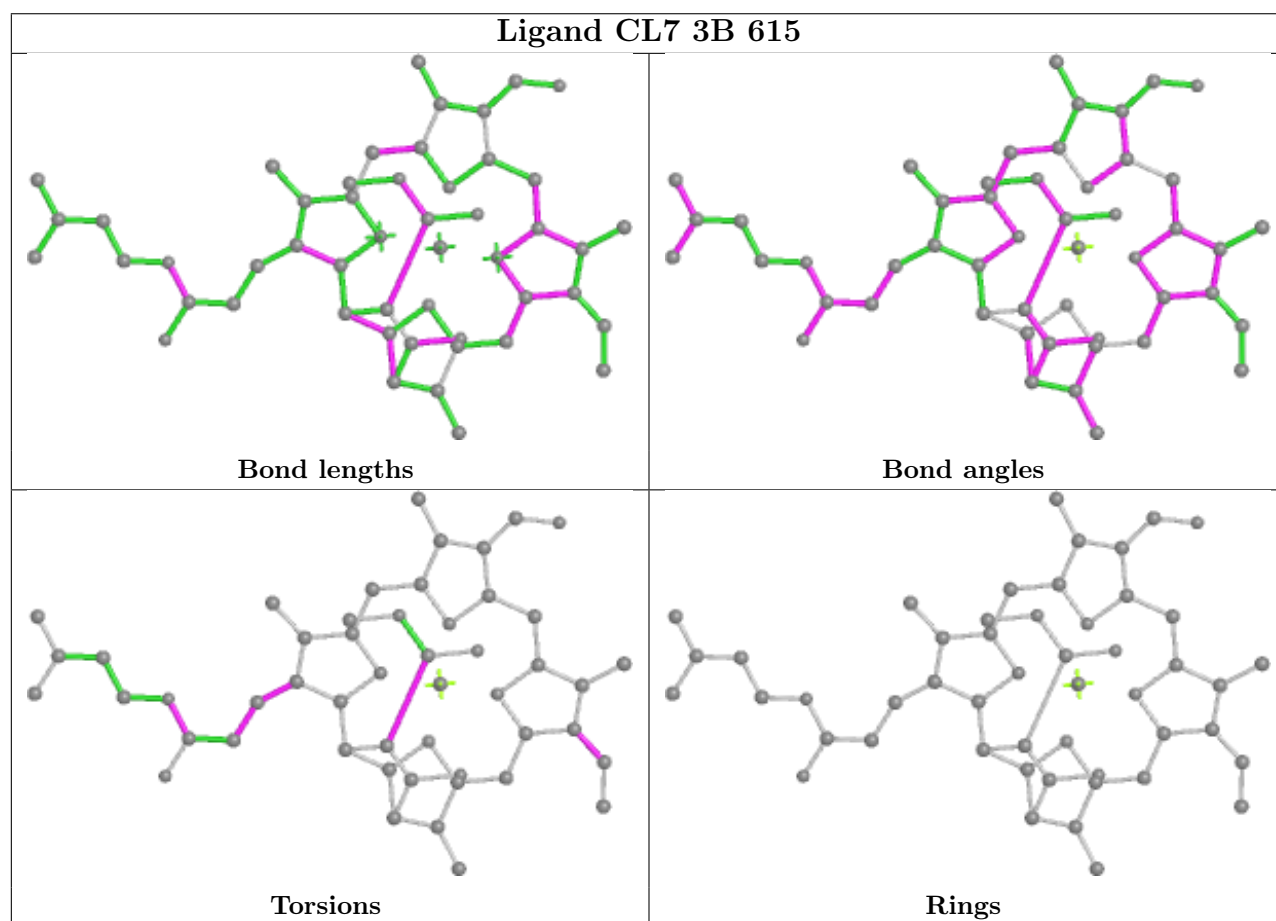
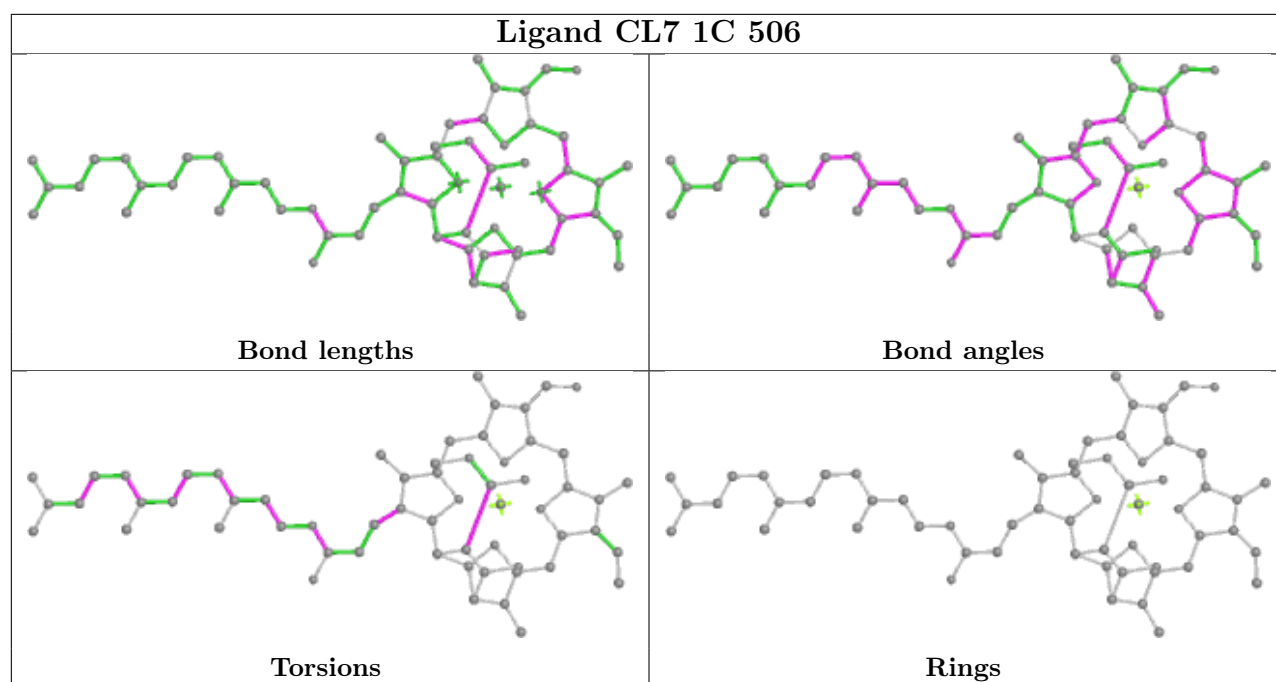
Rings

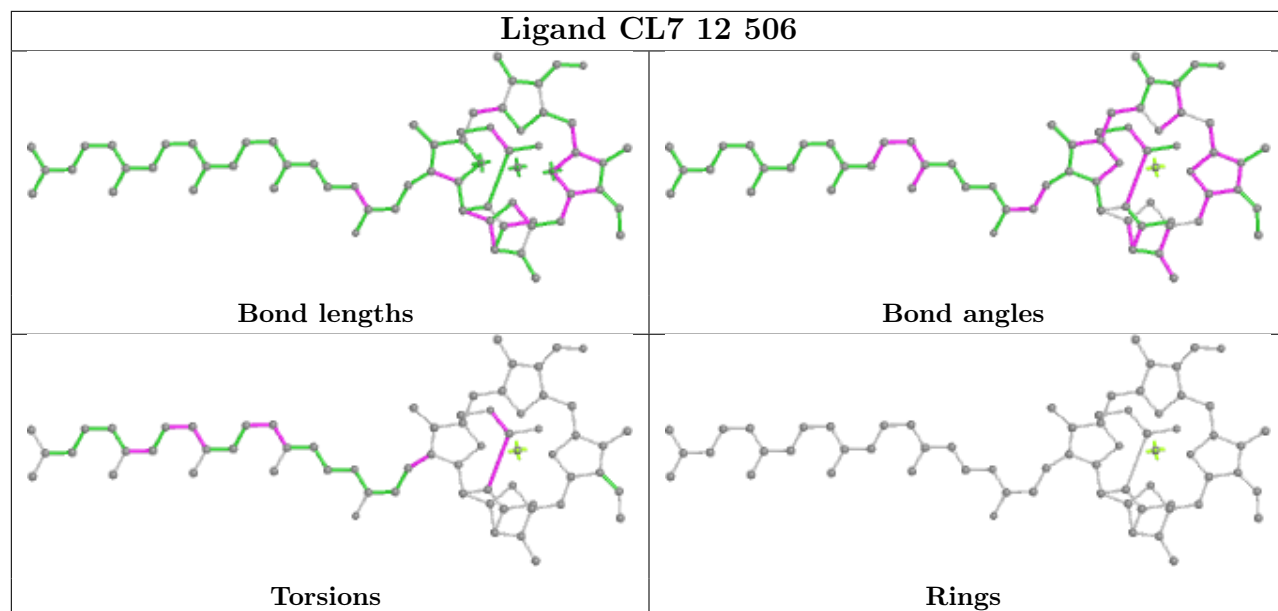
Ligand CL7 21 411



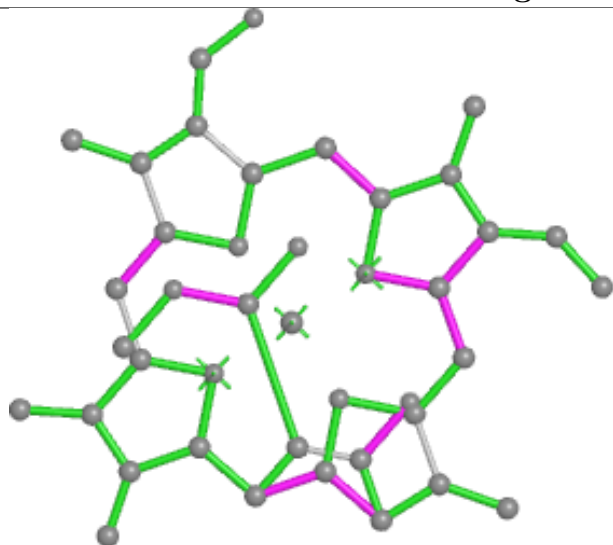
Ligand ZEX 42 519



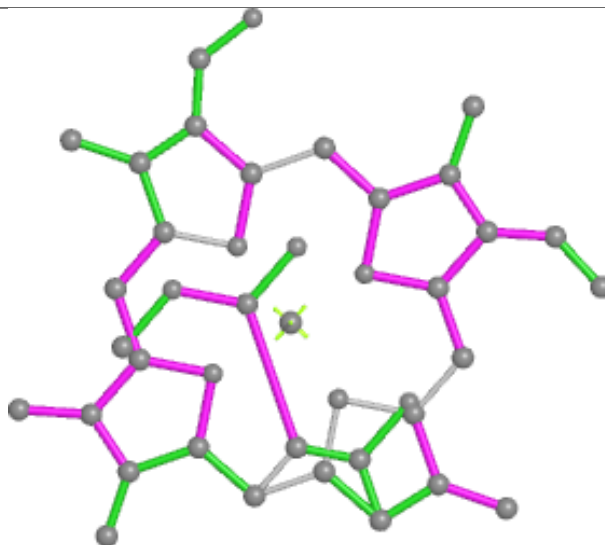




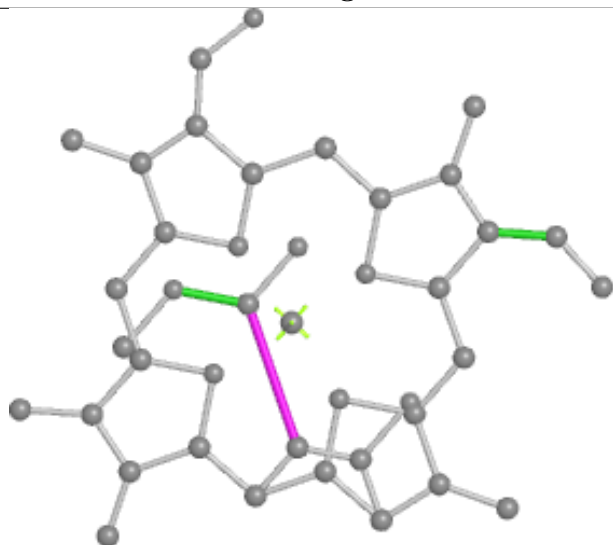
Ligand CL7 14 407



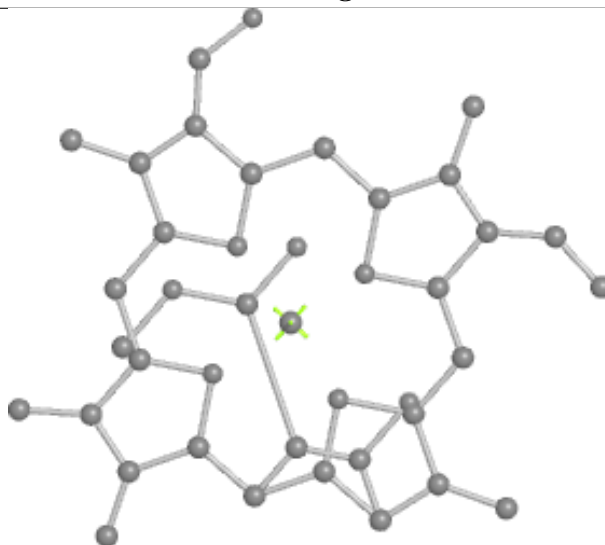
Bond lengths



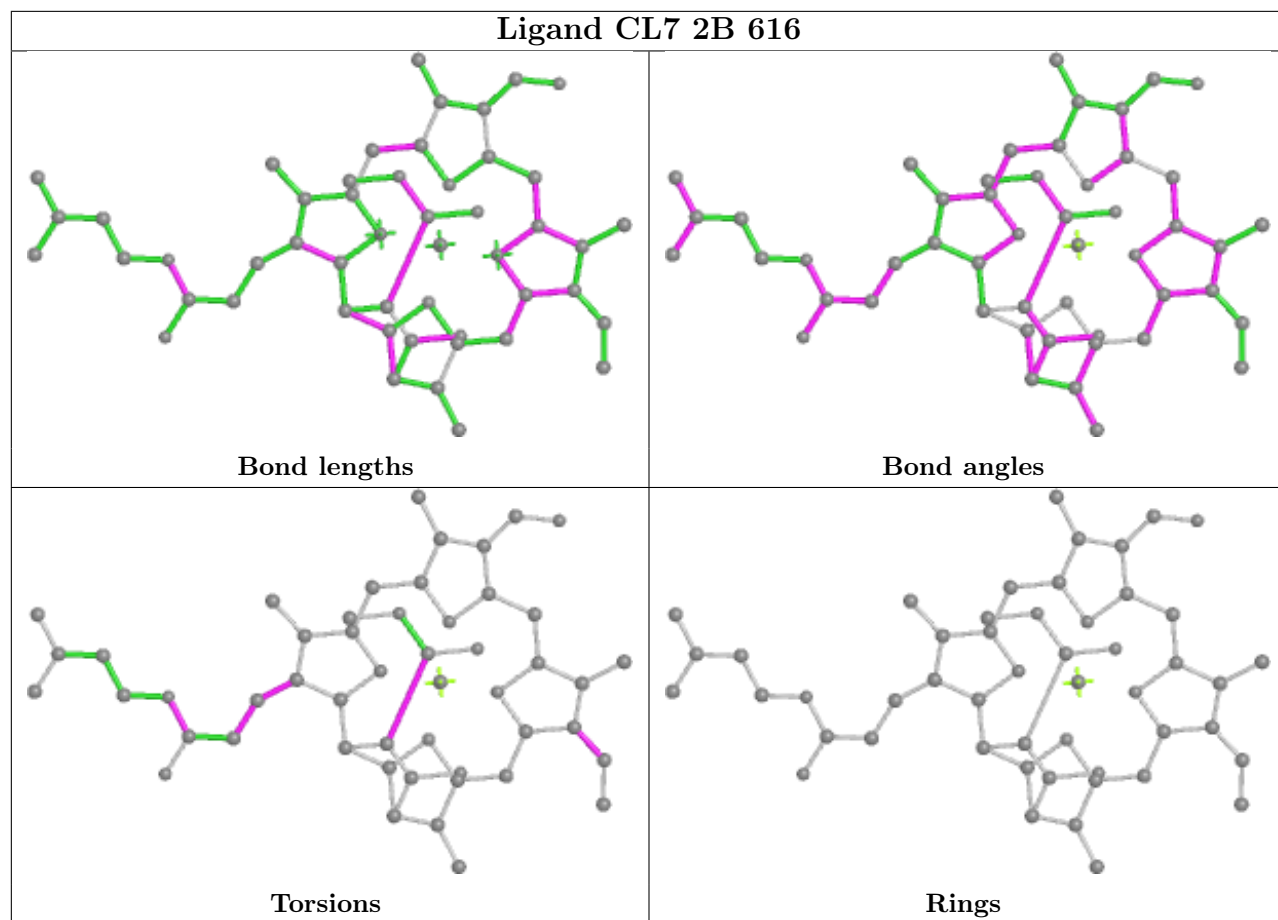
Bond angles



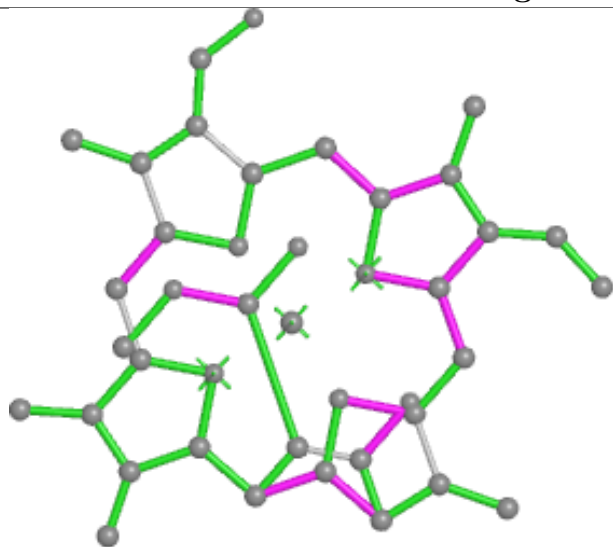
Torsions



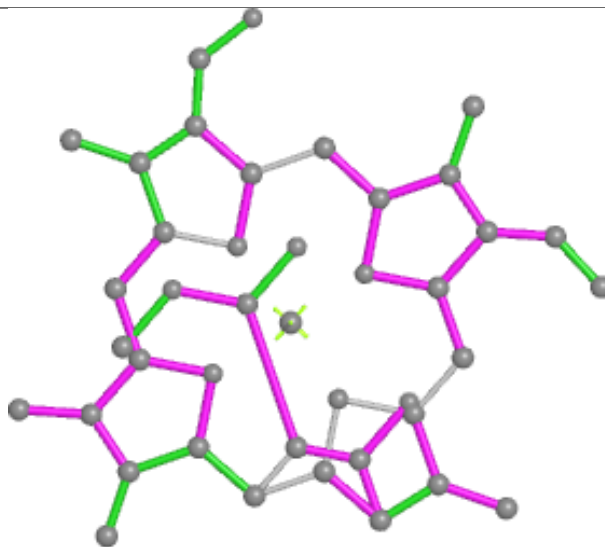
Rings



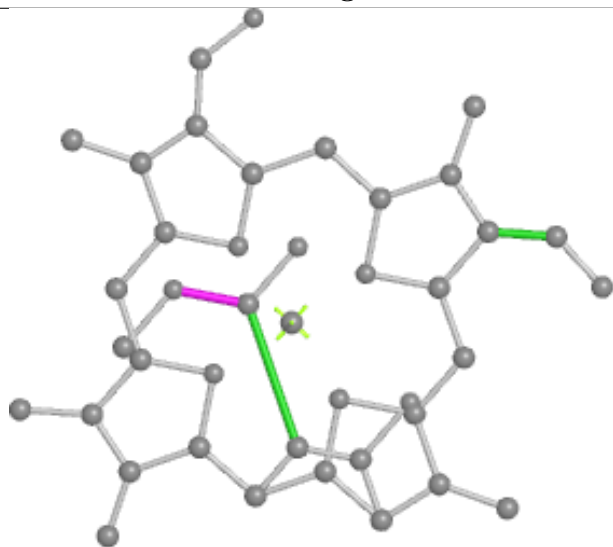
Ligand CL7 41 407



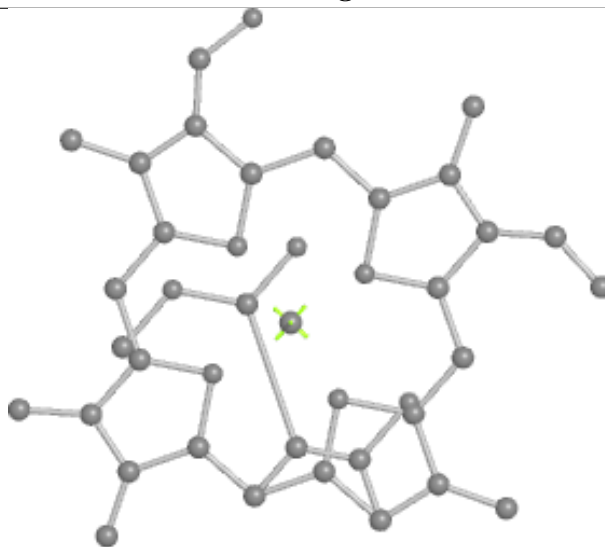
Bond lengths



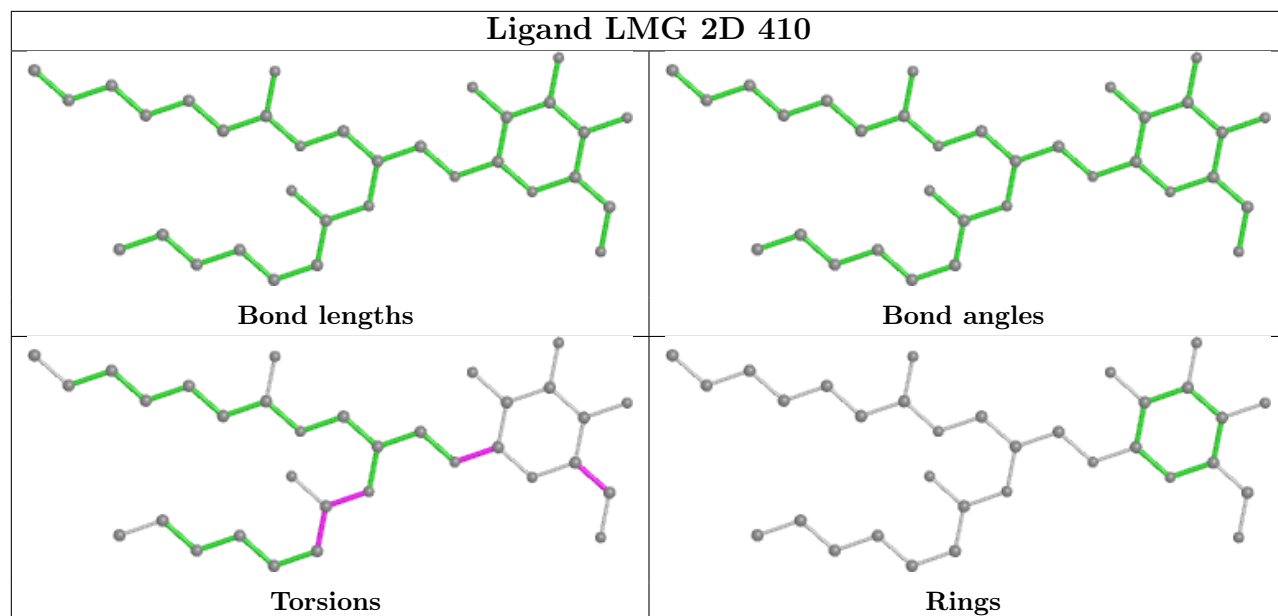
Bond angles



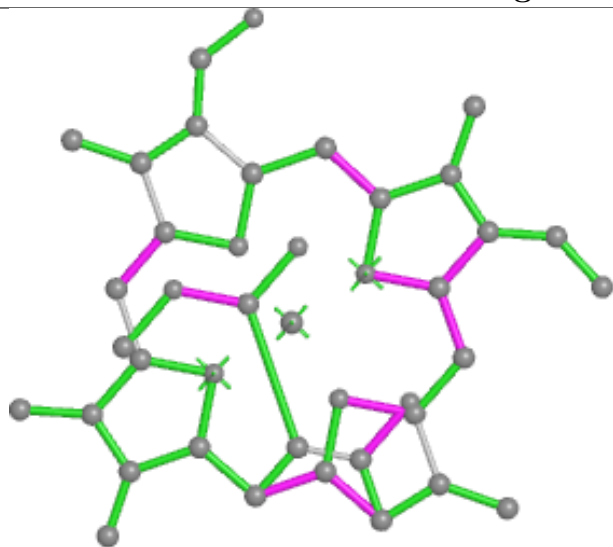
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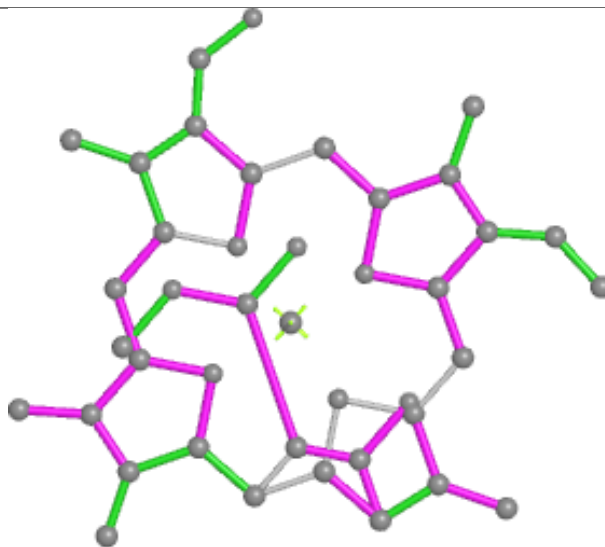
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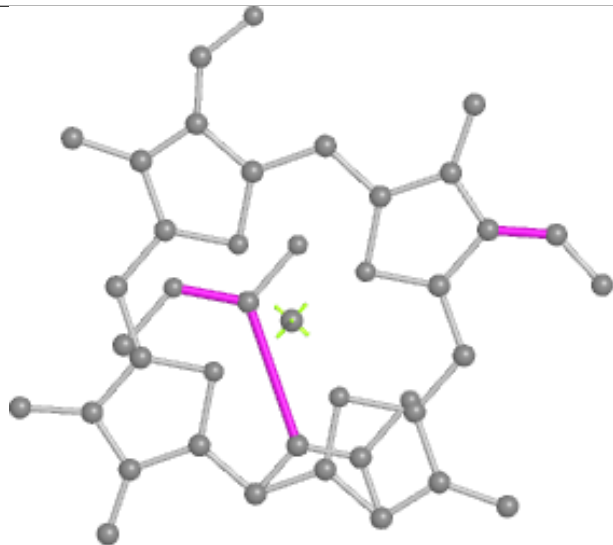
Ligand CL7 34 416



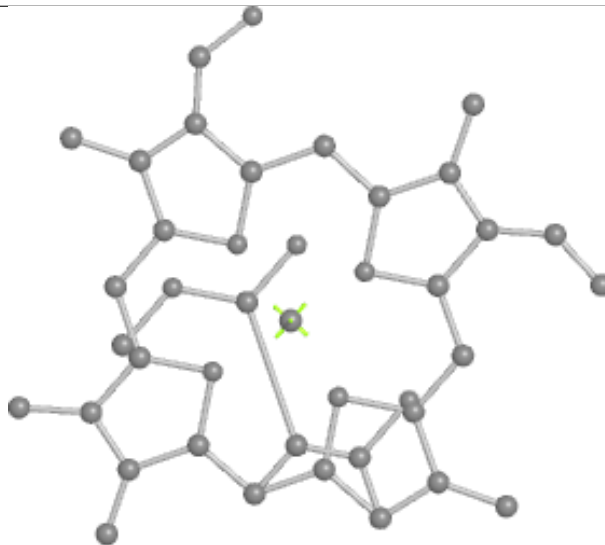
Bond lengths



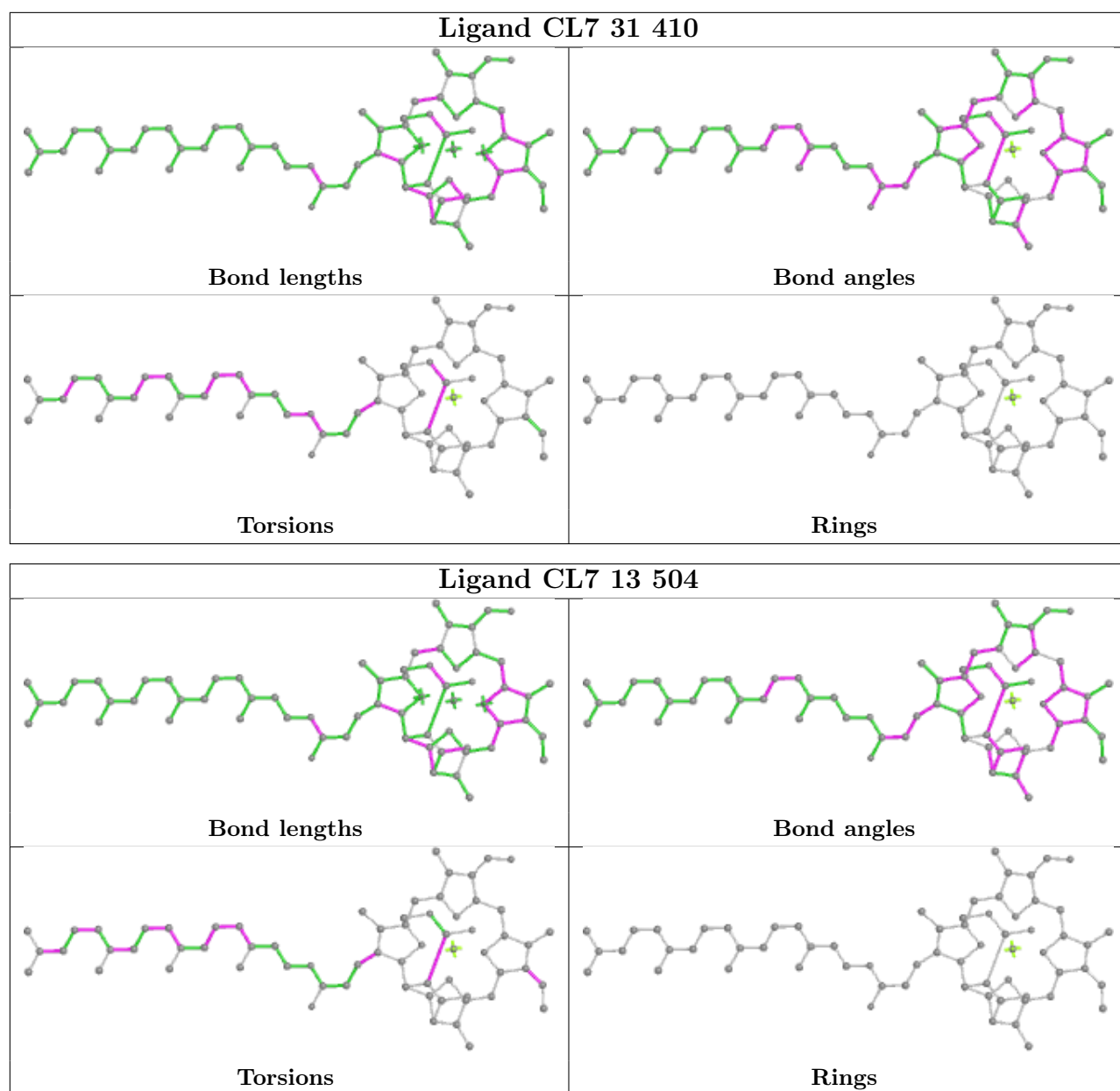
Bond angles



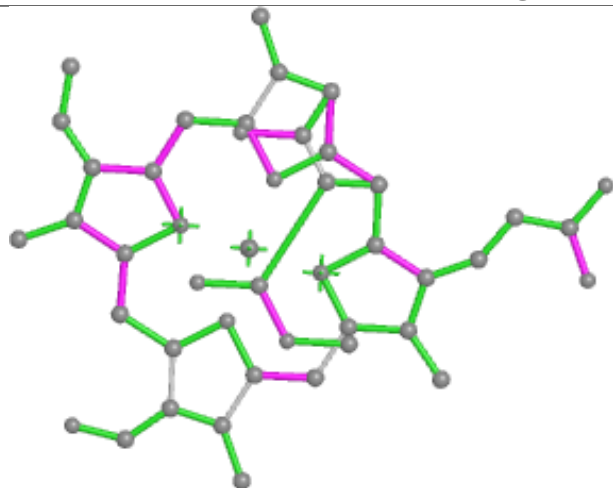
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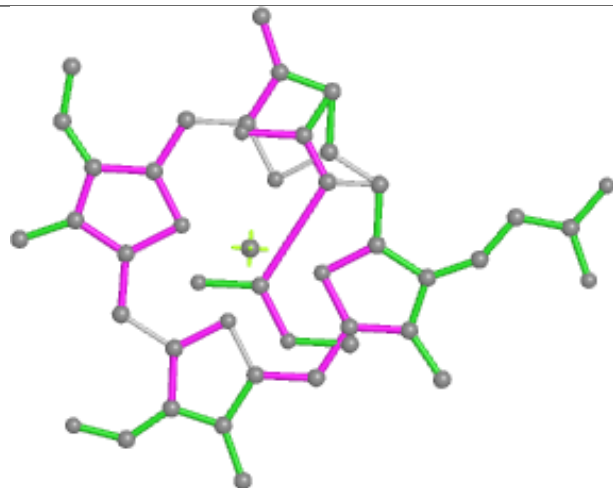
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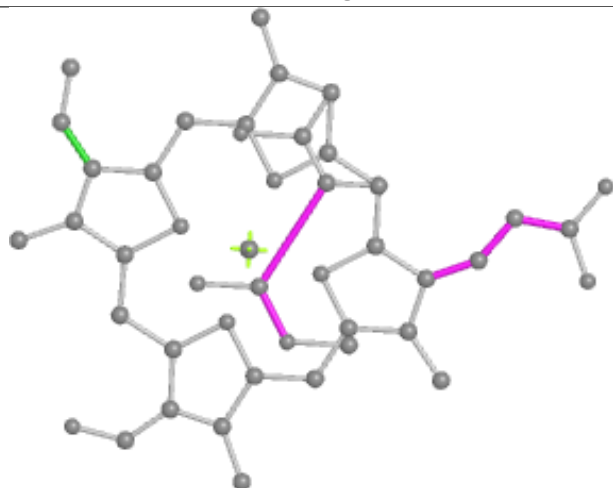
Ligand CL7 14 410



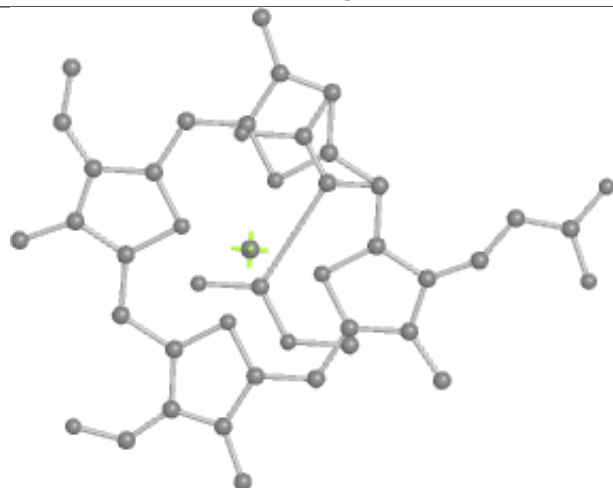
Bond lengths



Bond angles

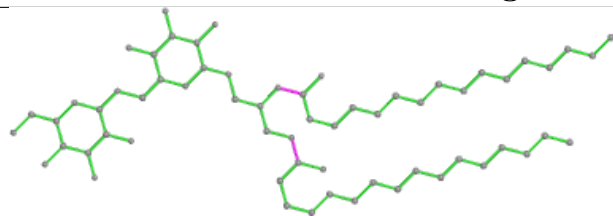


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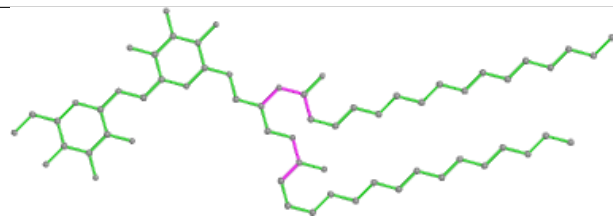


Rings

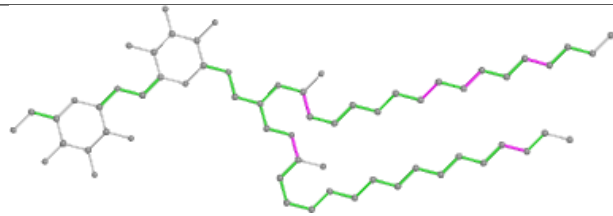
Ligand DGD 1B 624



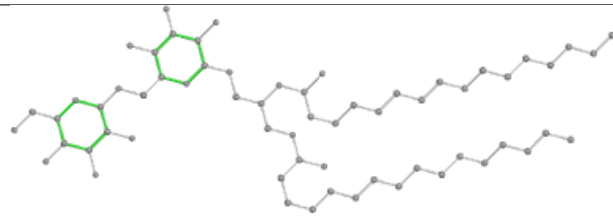
Bond lengths



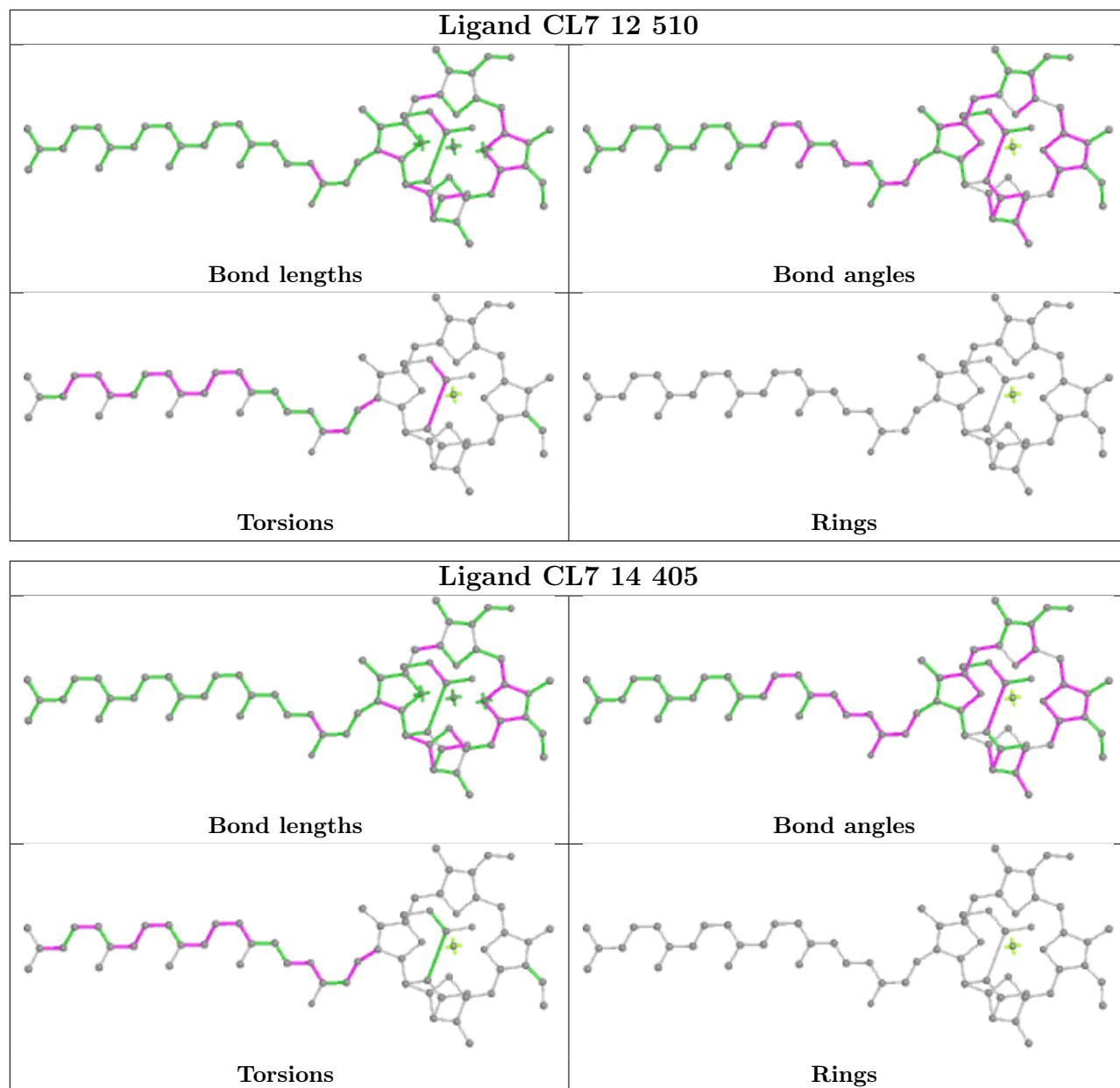
Bond angles



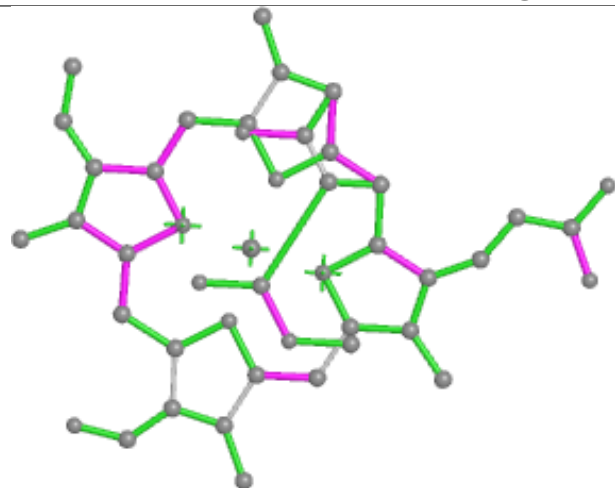
Torsions



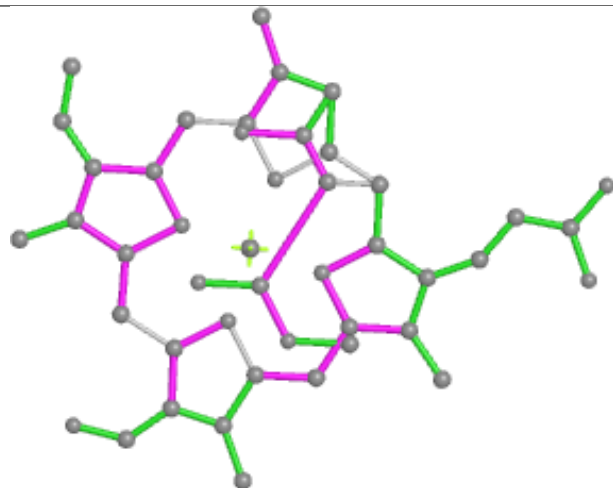
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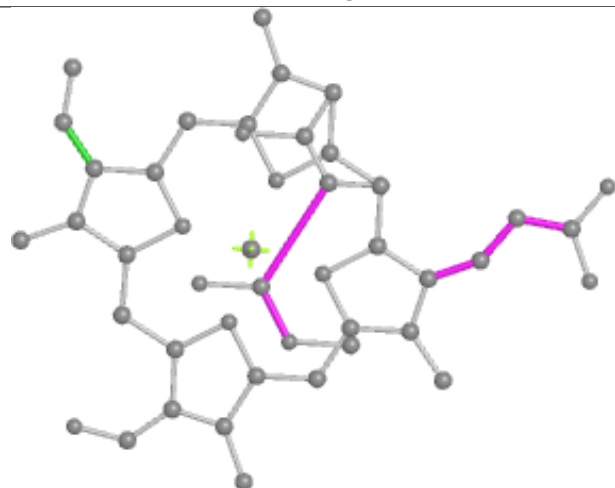
Ligand CL7 44 410



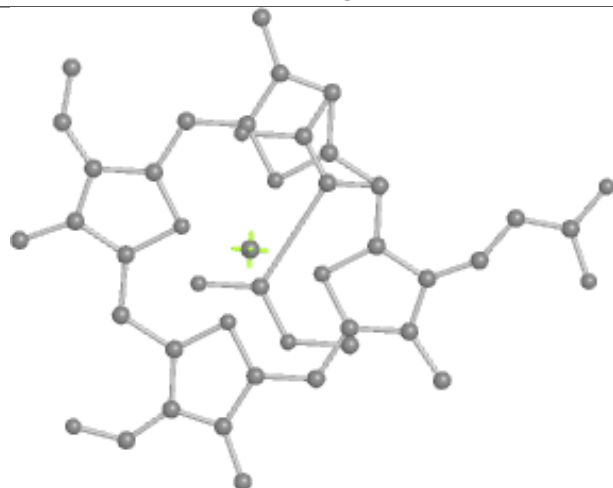
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Bond angles

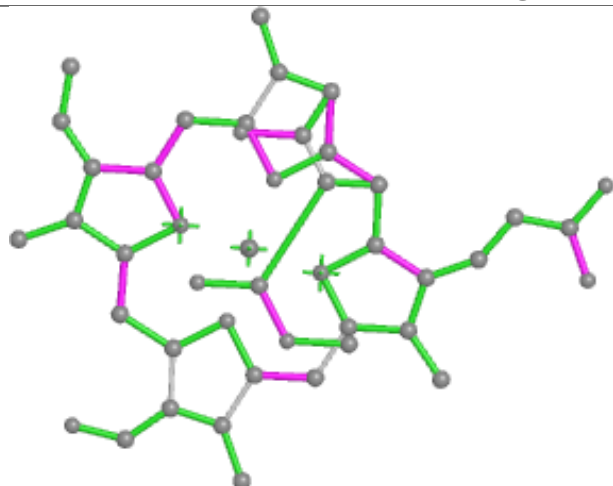


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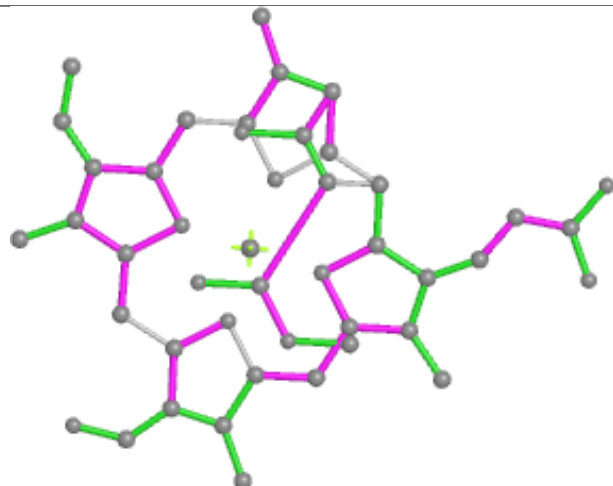


Rings

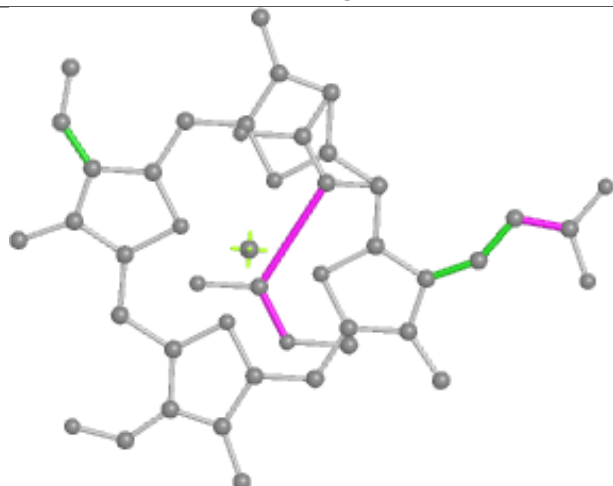
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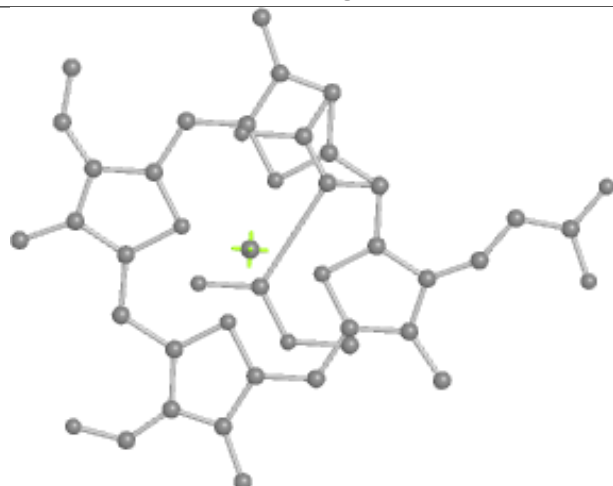
Bond lengths



Bond angles

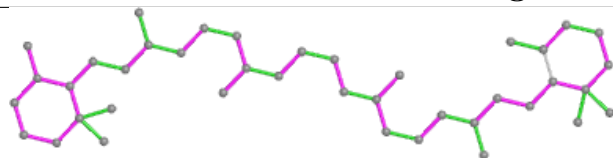


Torsions

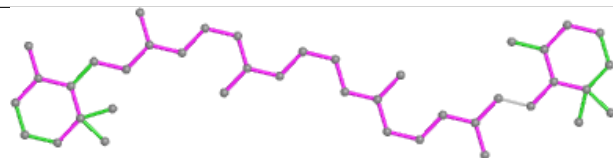


Rings

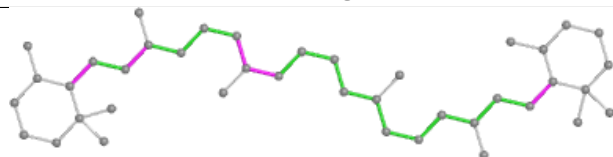
Ligand 8CT 4B 601



Bond lengths



Bond angles

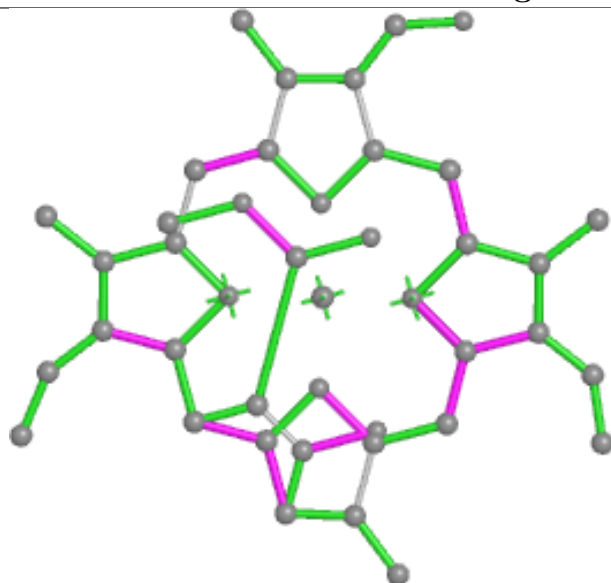


Torsions

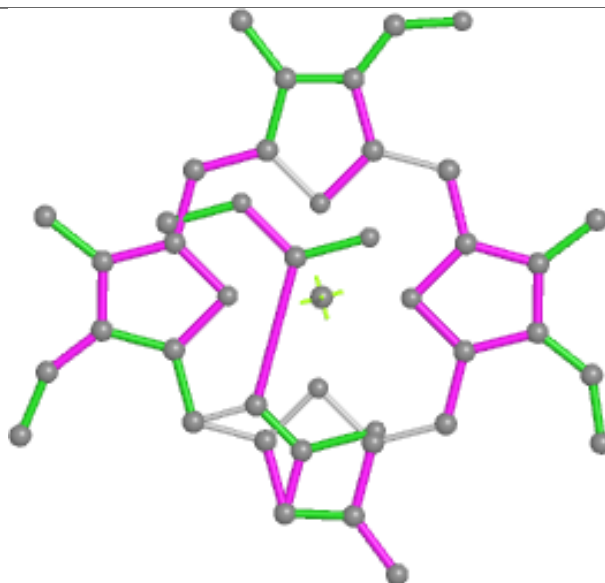


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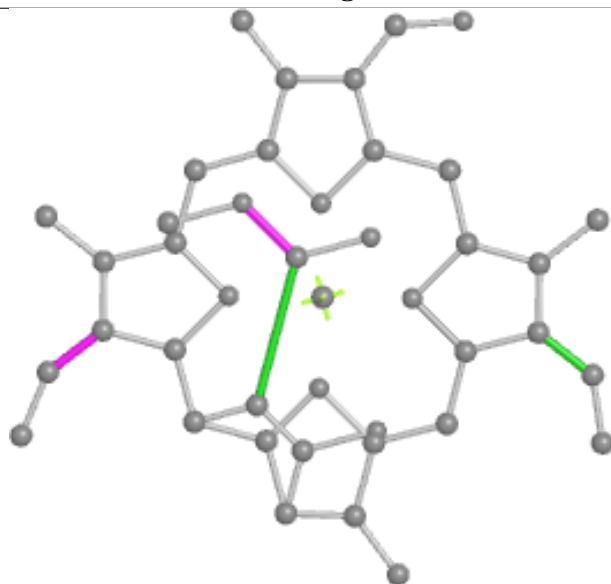
Ligand CL7 24 417



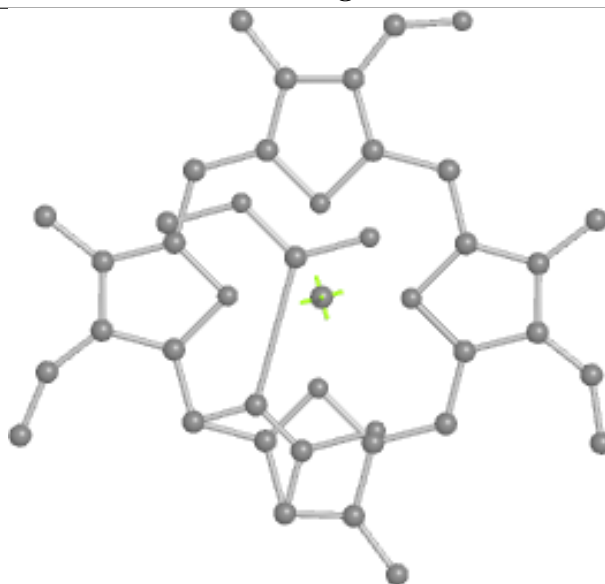
Bond lengths



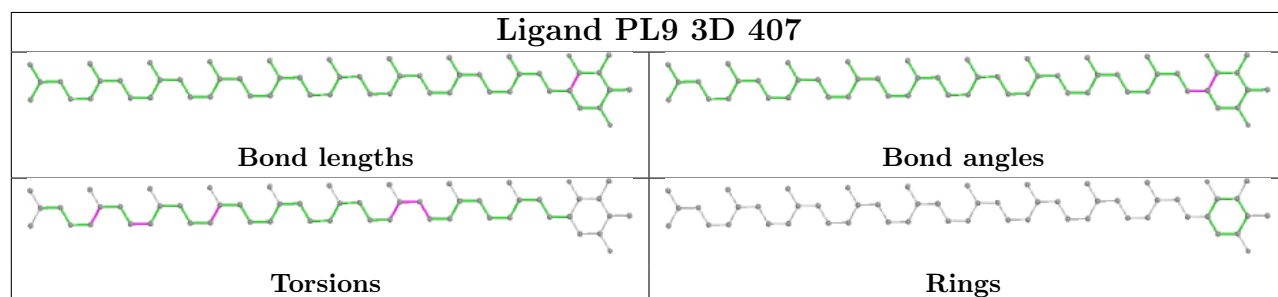
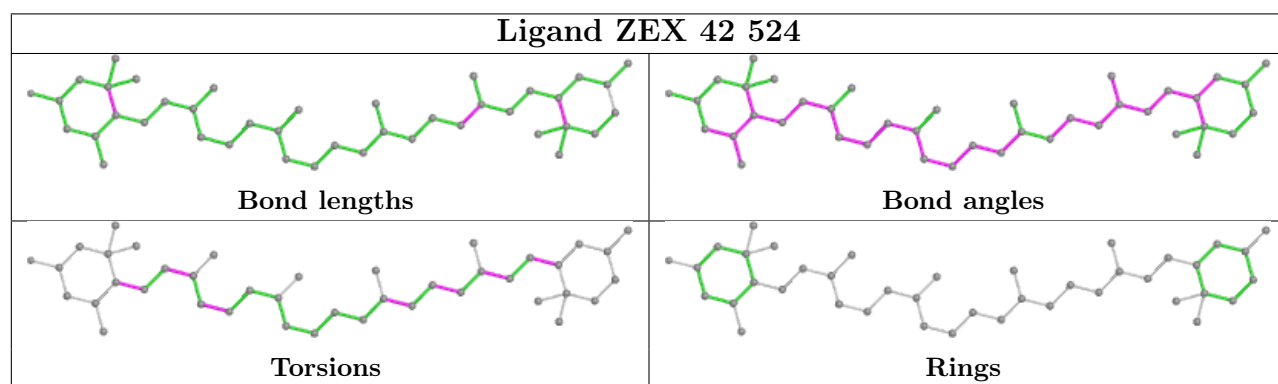
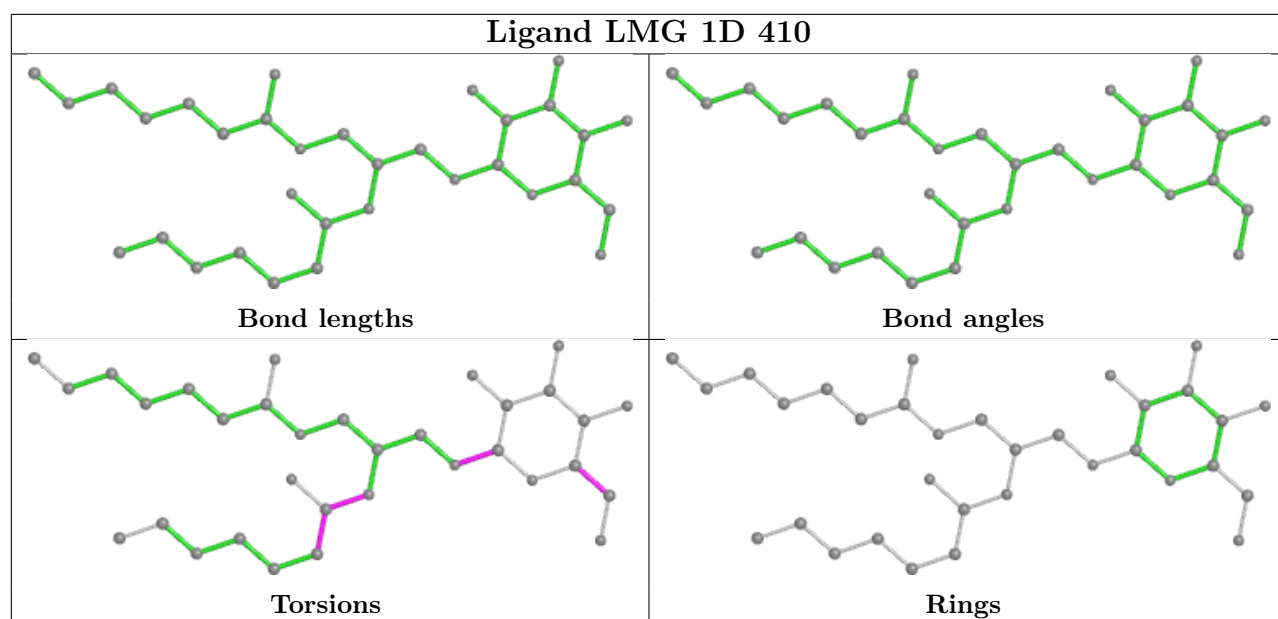
Bond angles



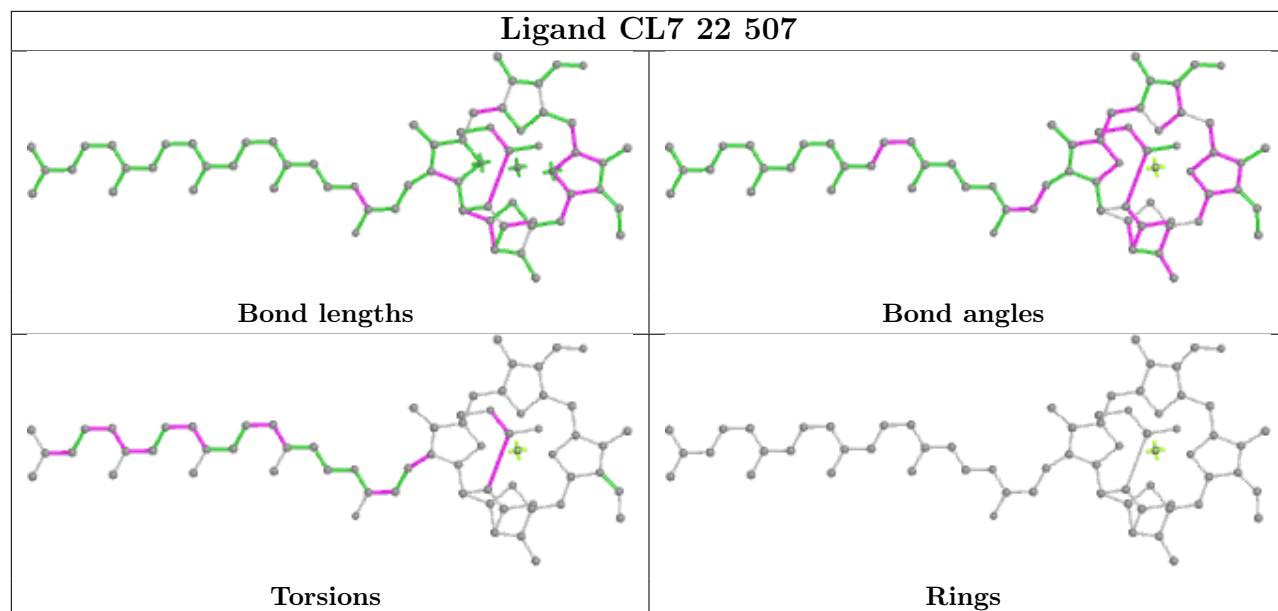
Torsions



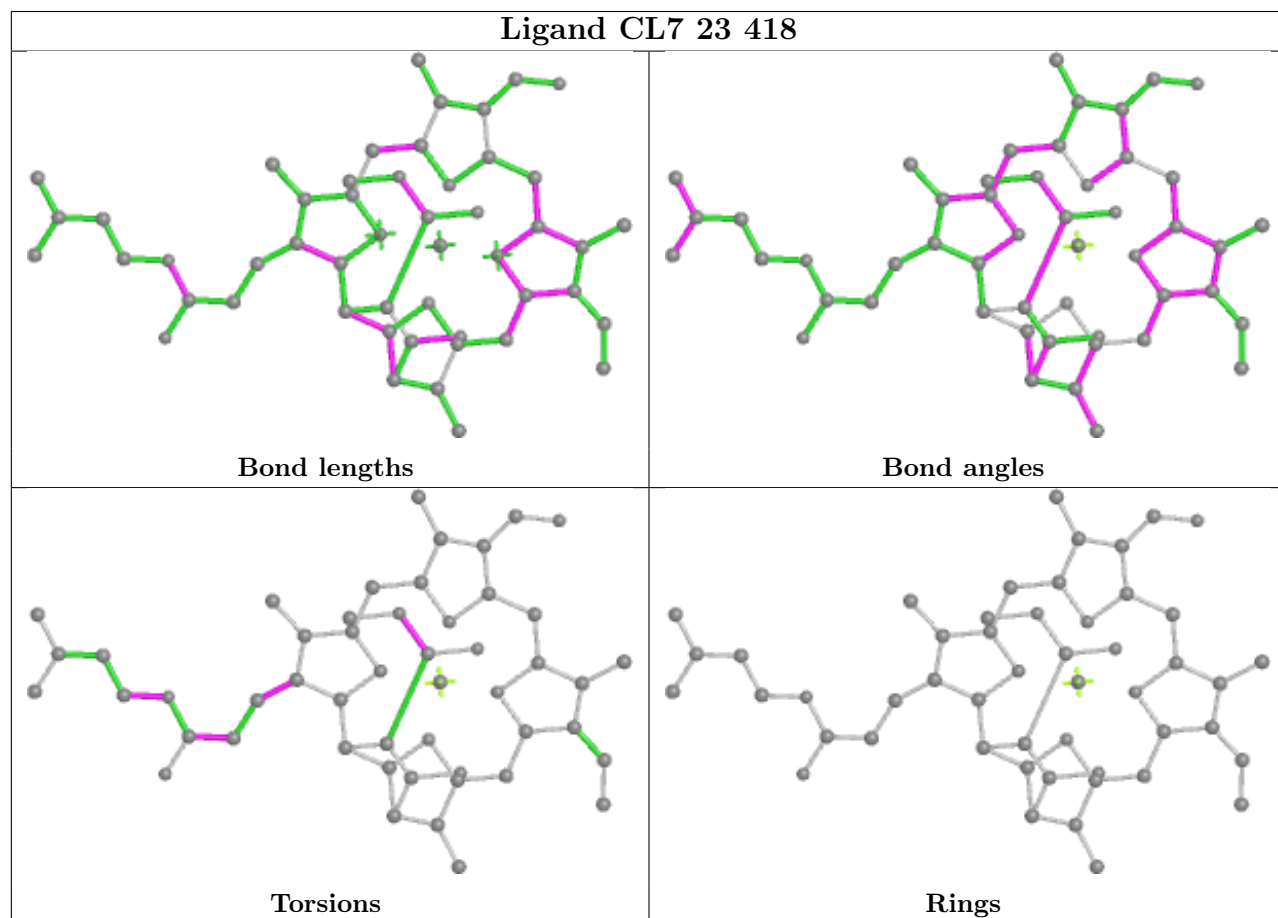
Rings

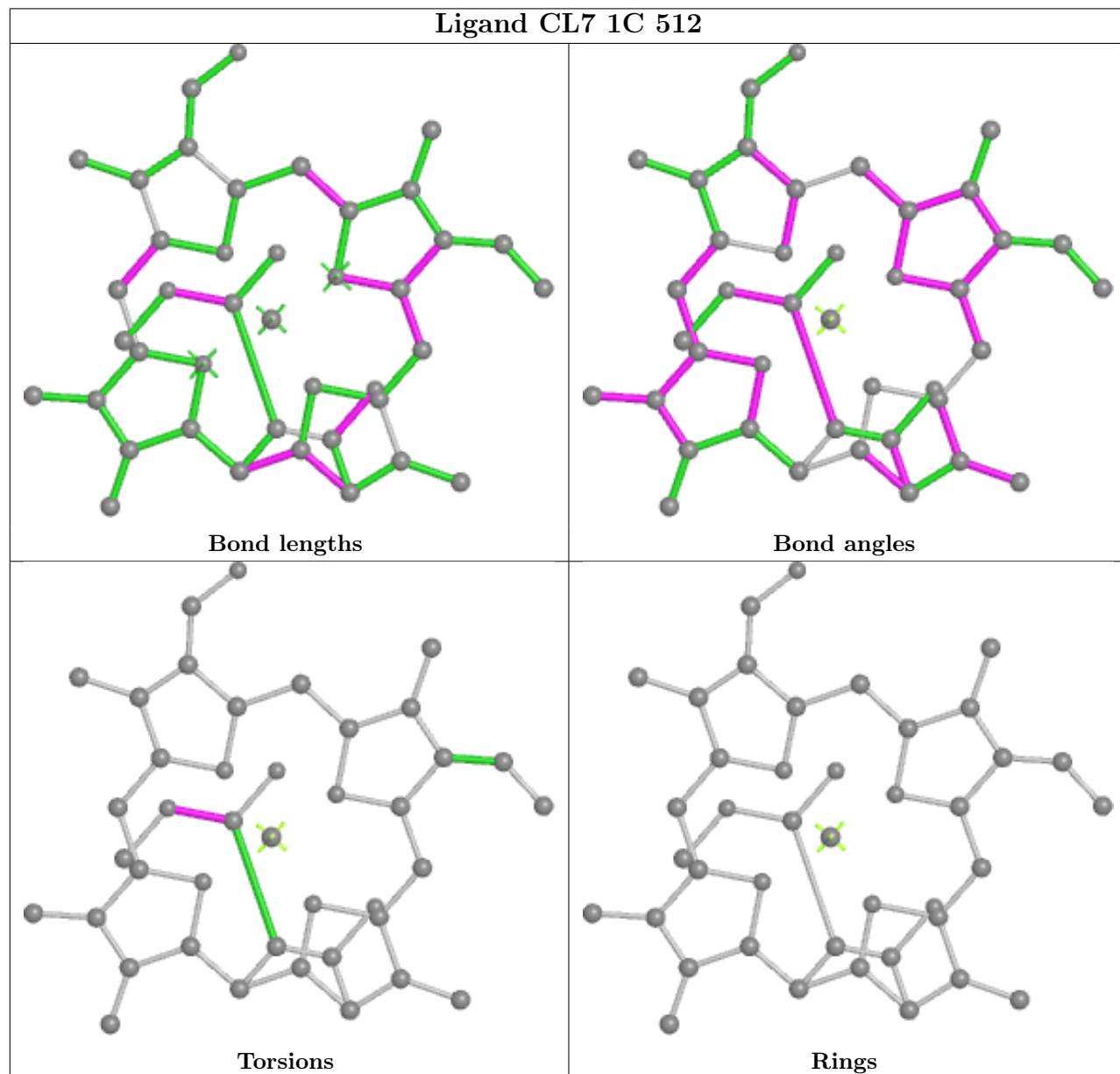
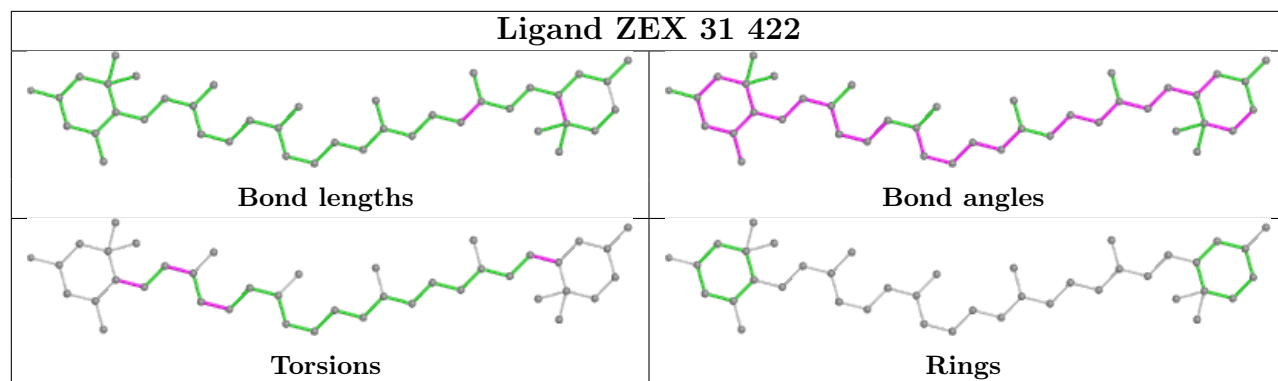


Ligand CL7 22 507

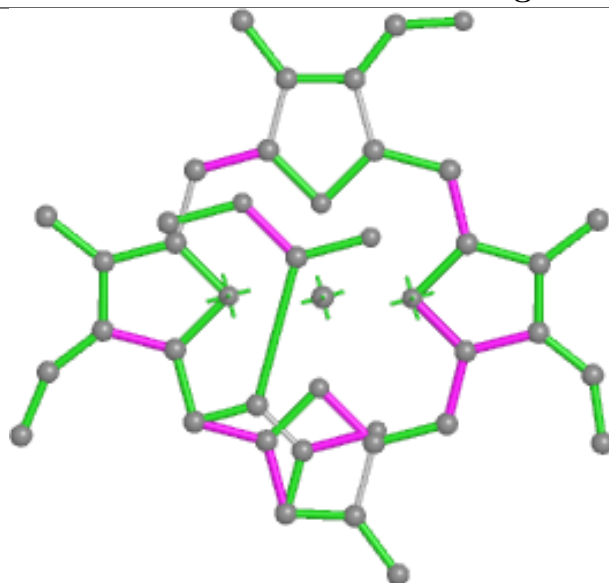


Ligand CL7 23 418

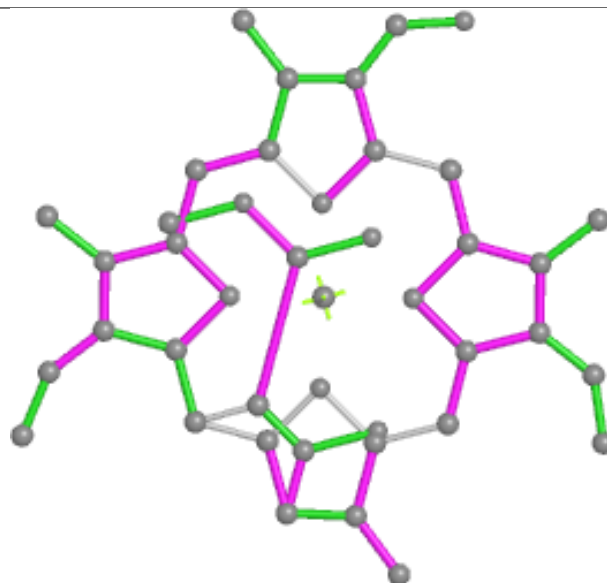




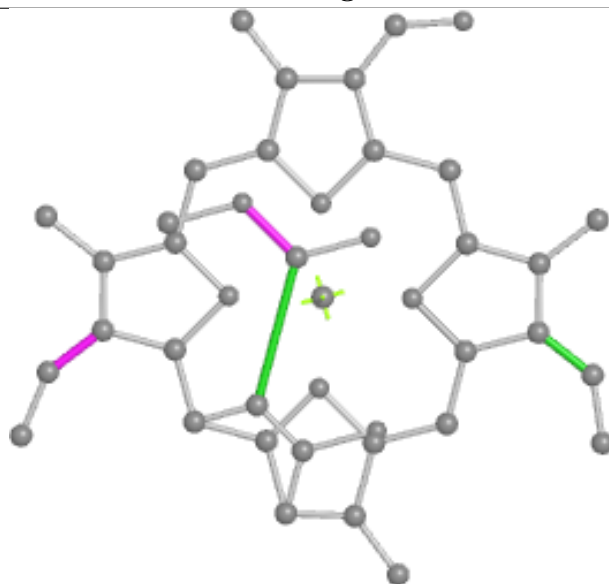
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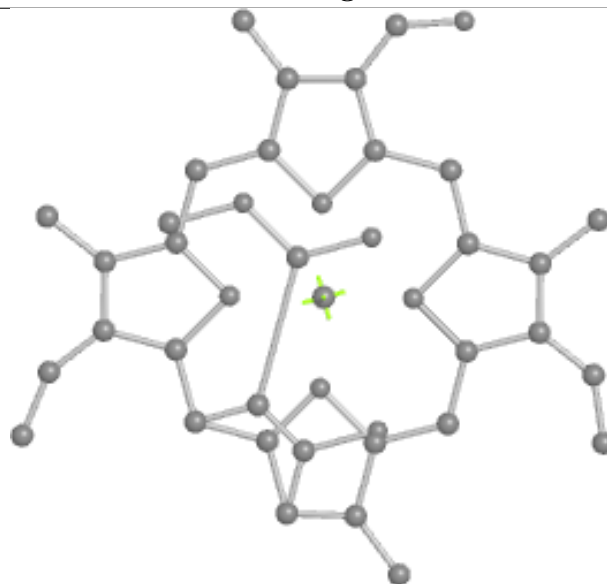
Bond lengths



Bond angles

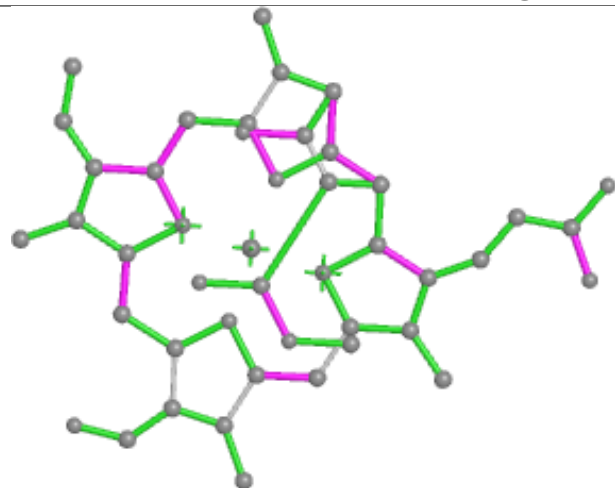


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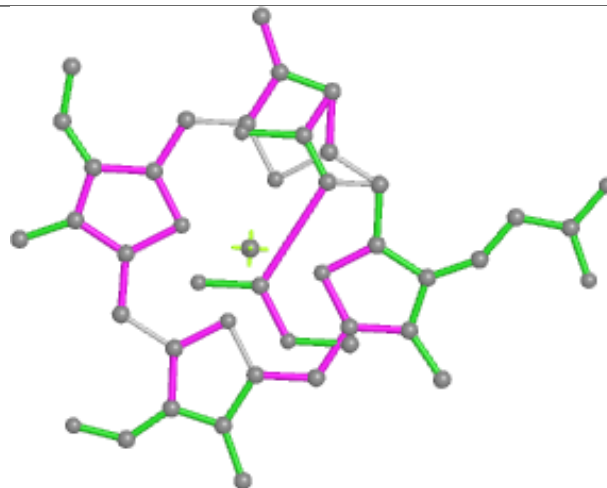


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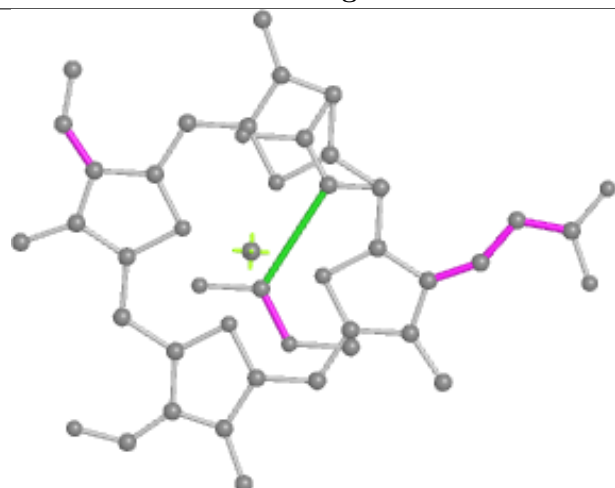
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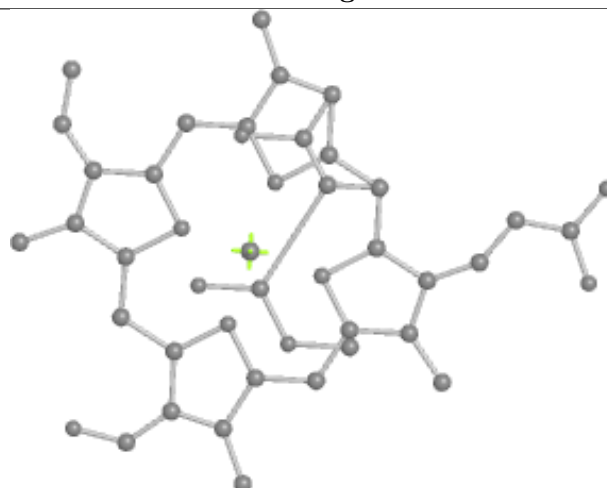
Bond lengths



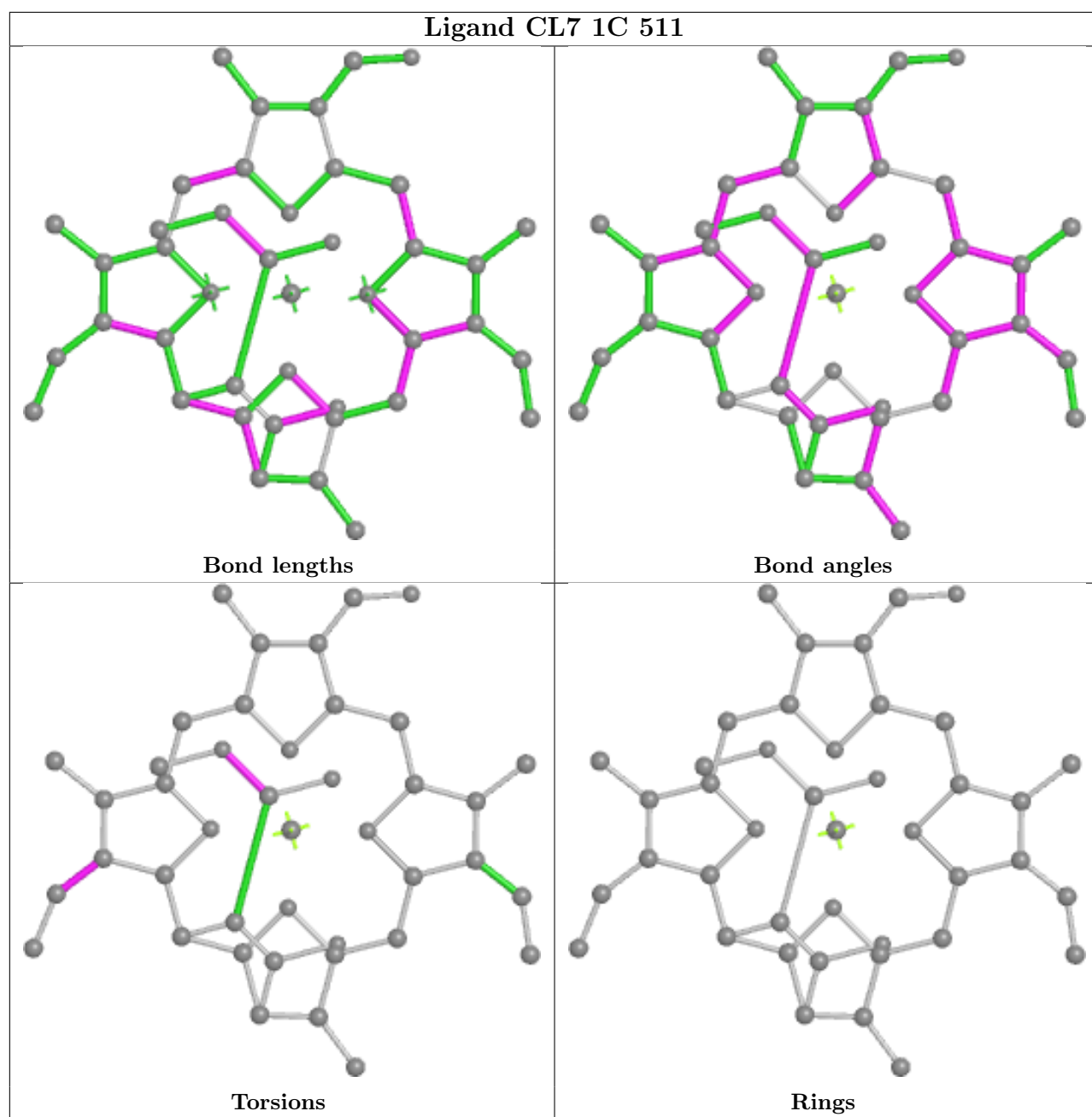
Bond angles

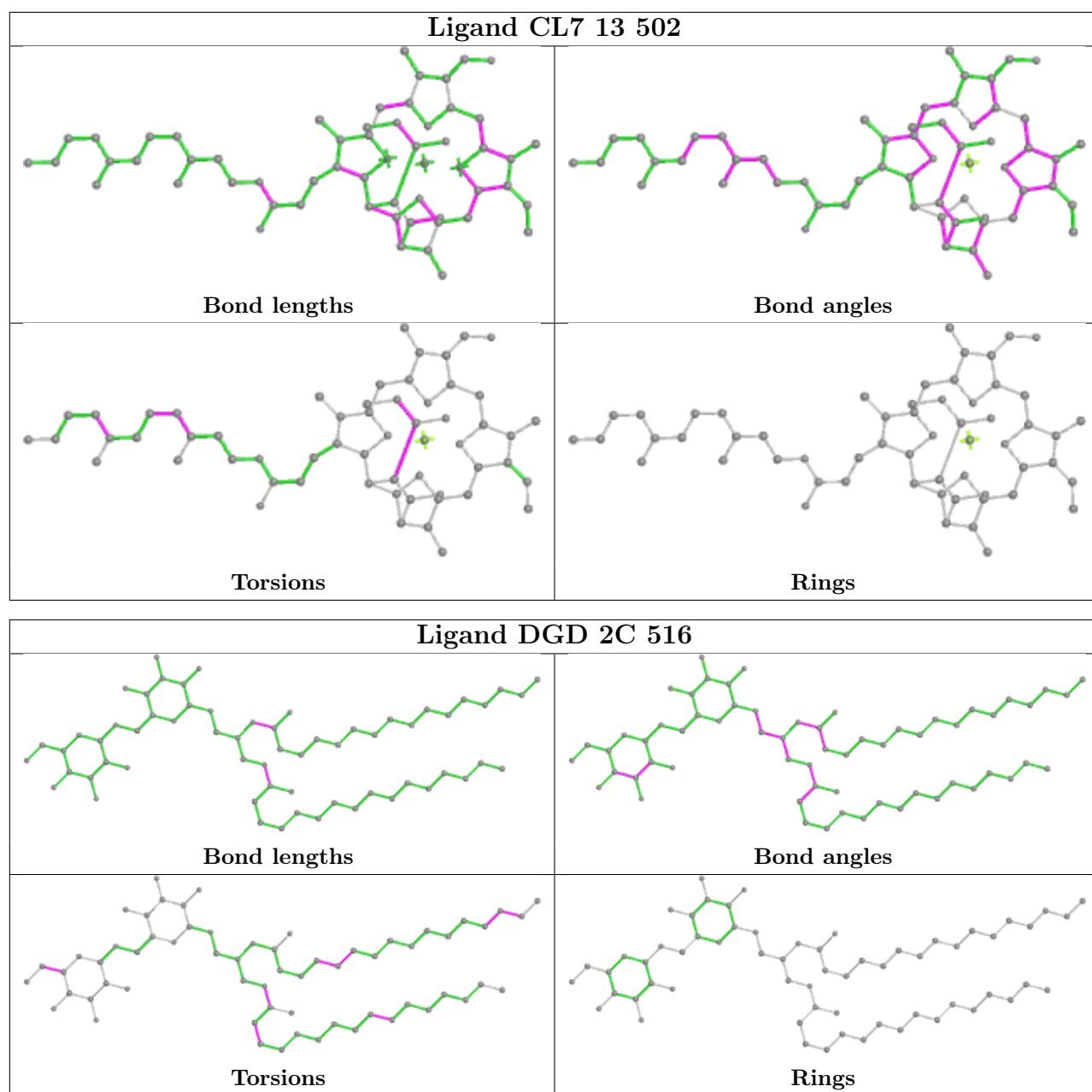


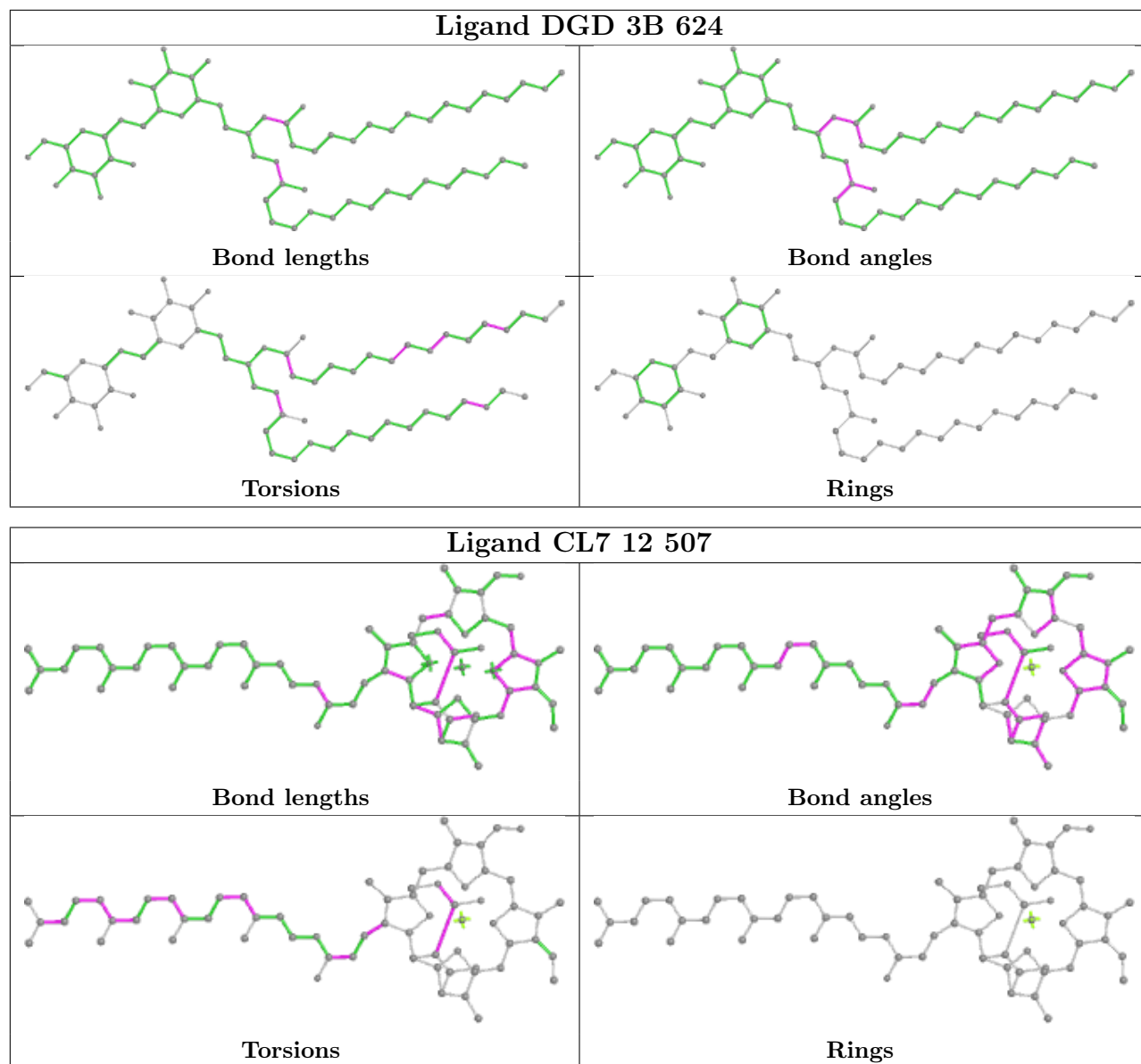
Torsions

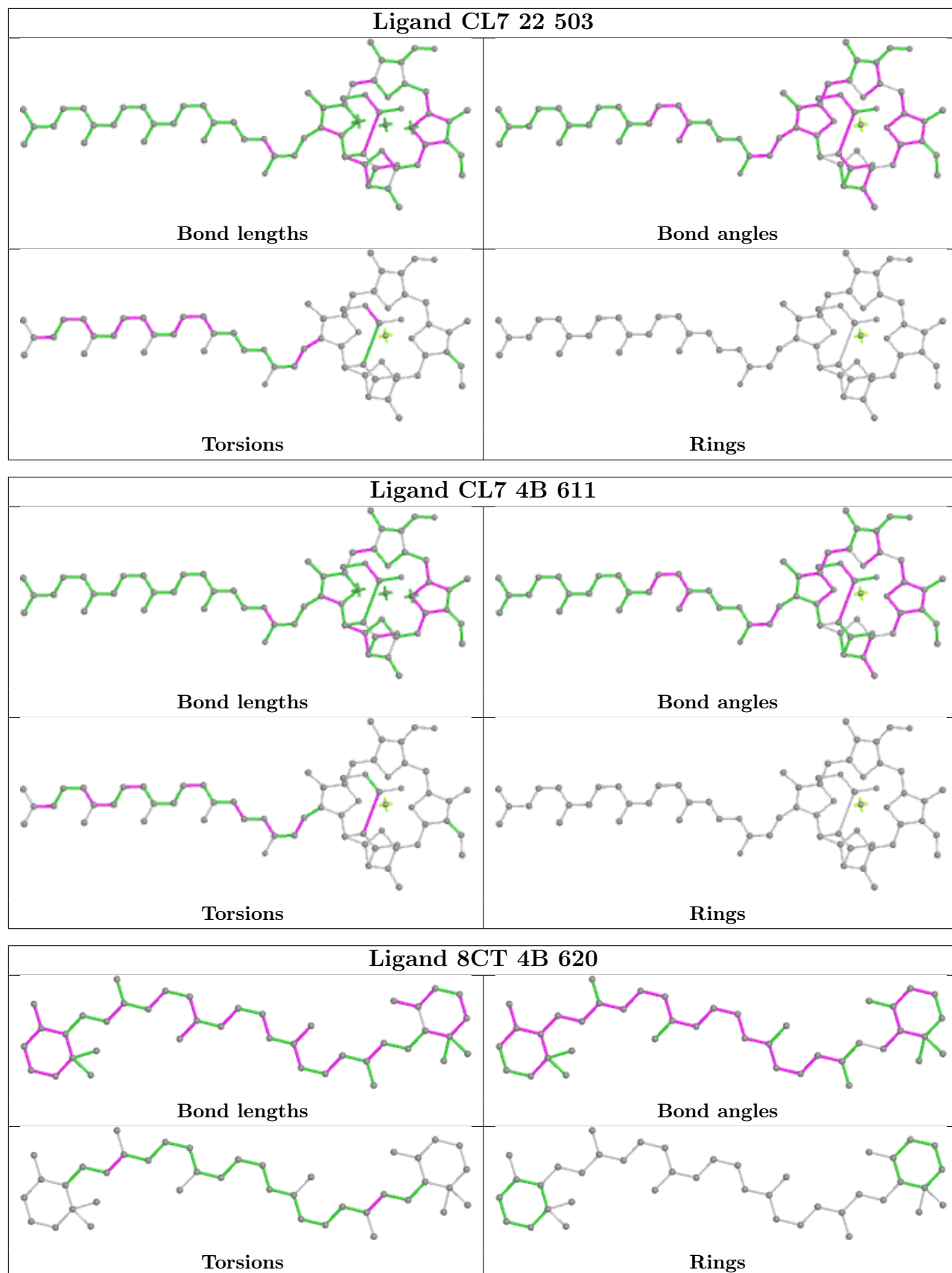


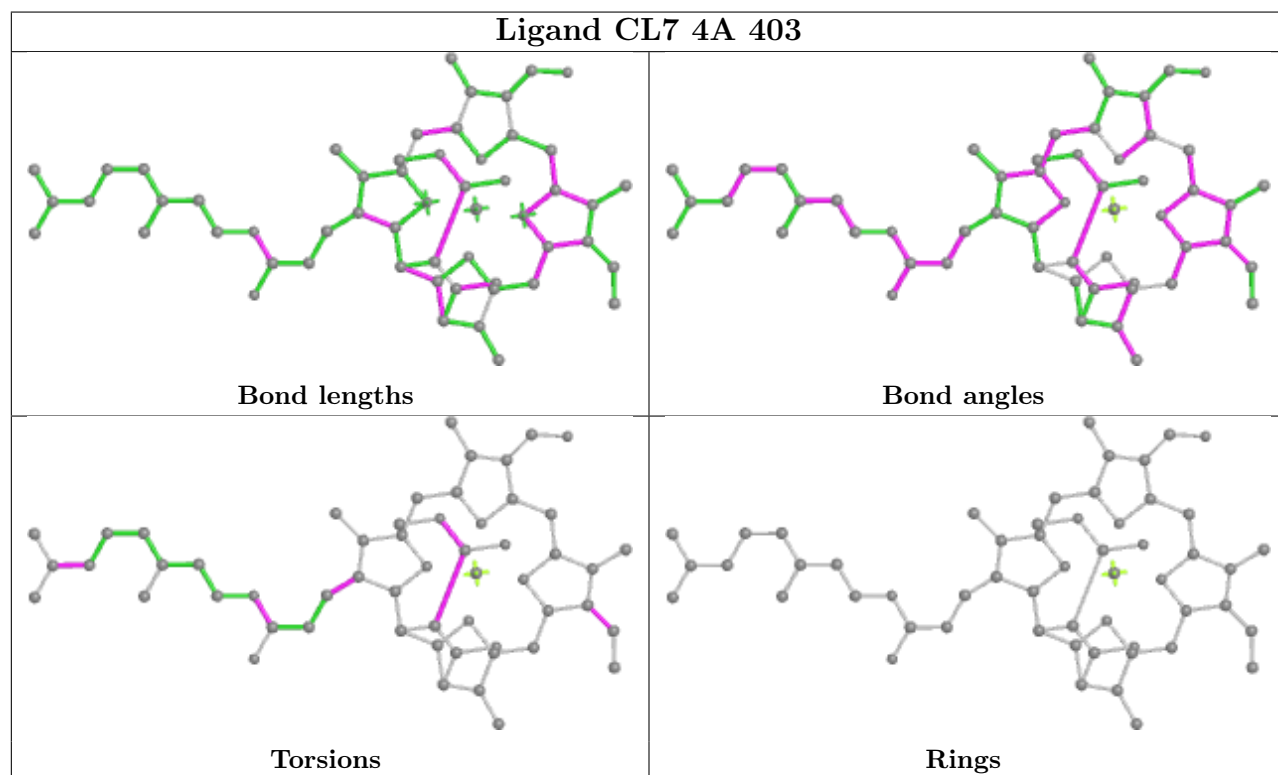
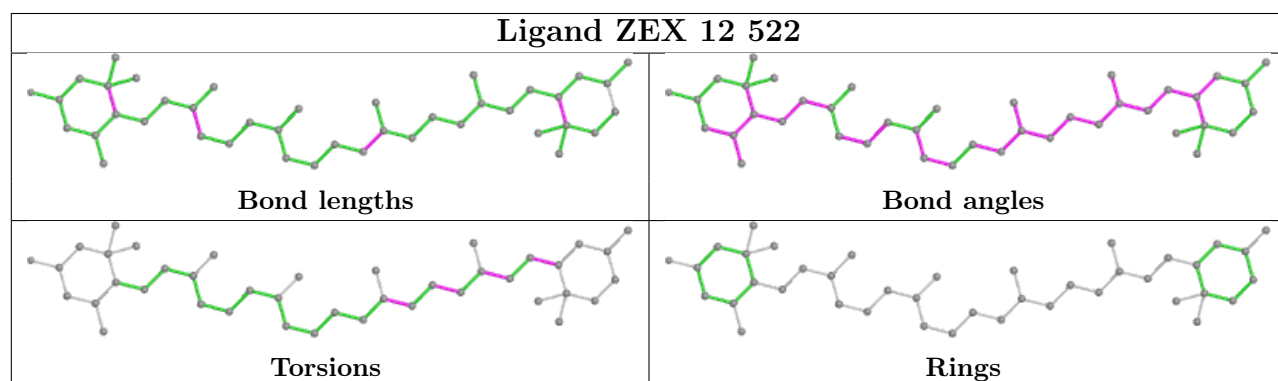
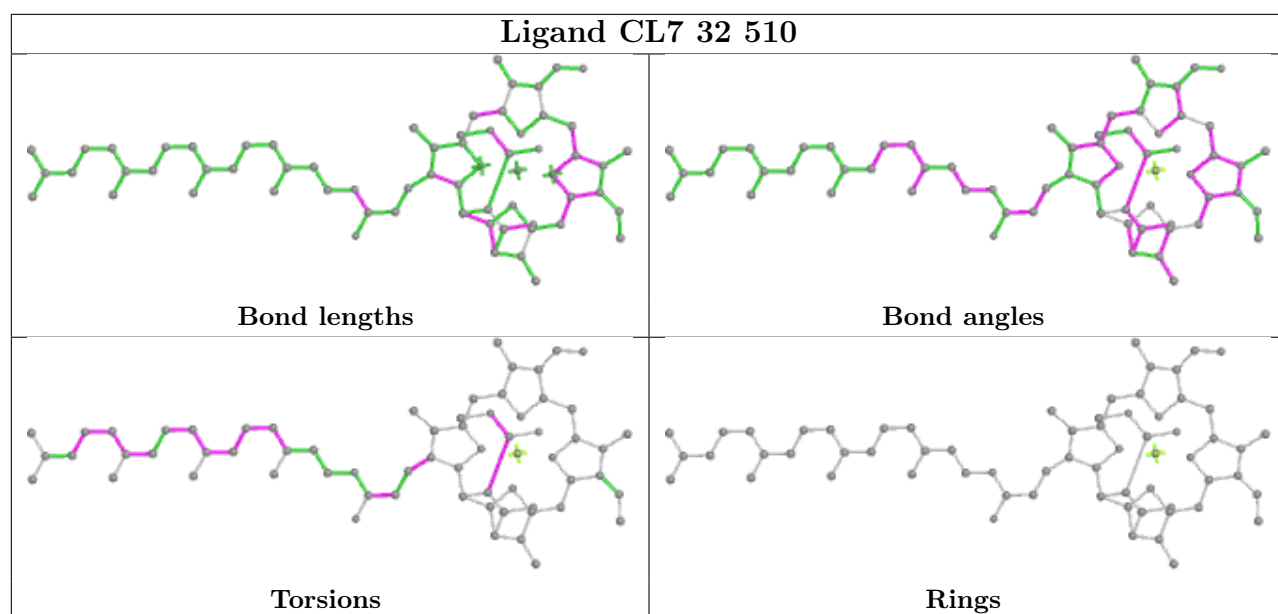
Rings

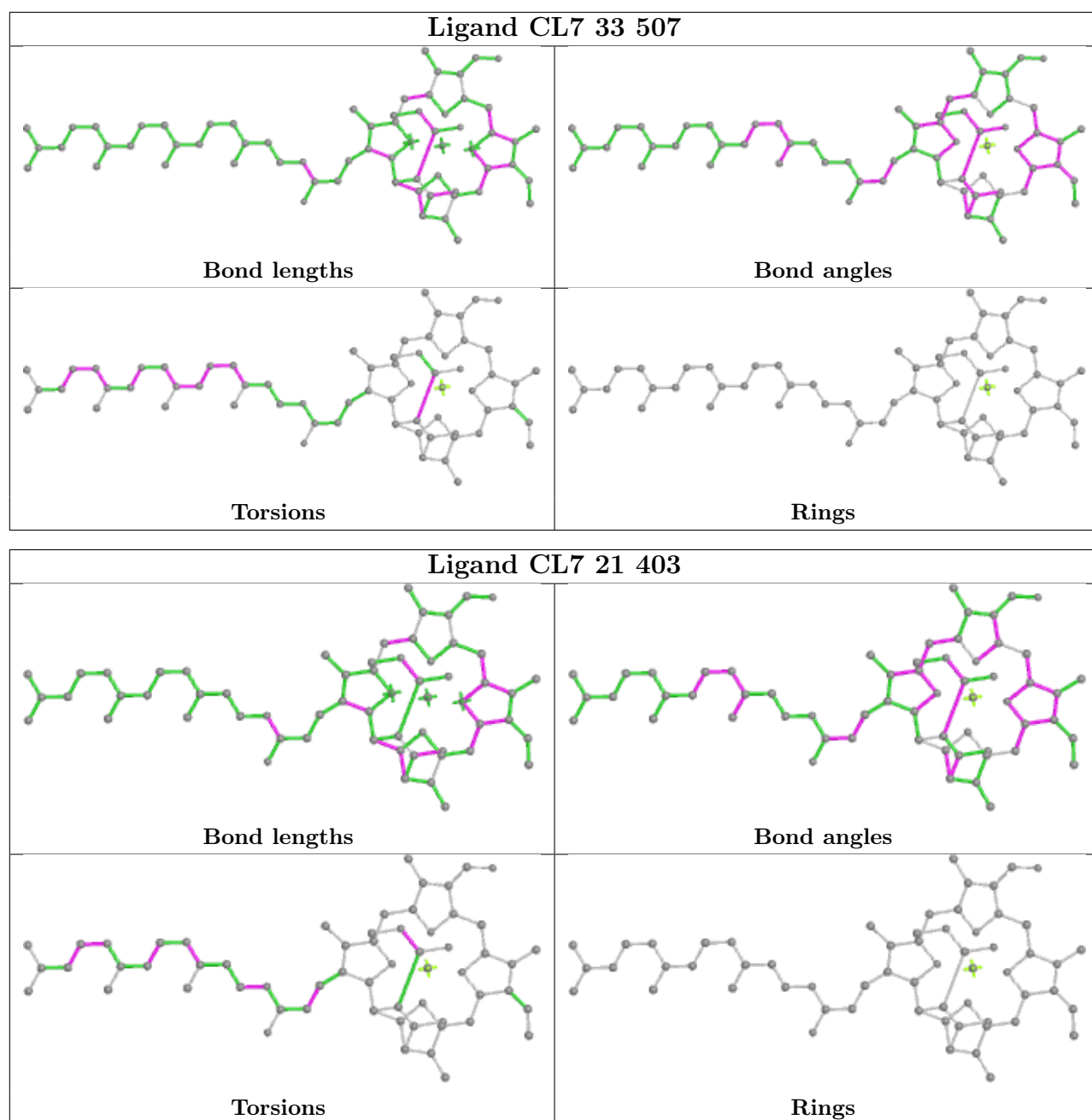




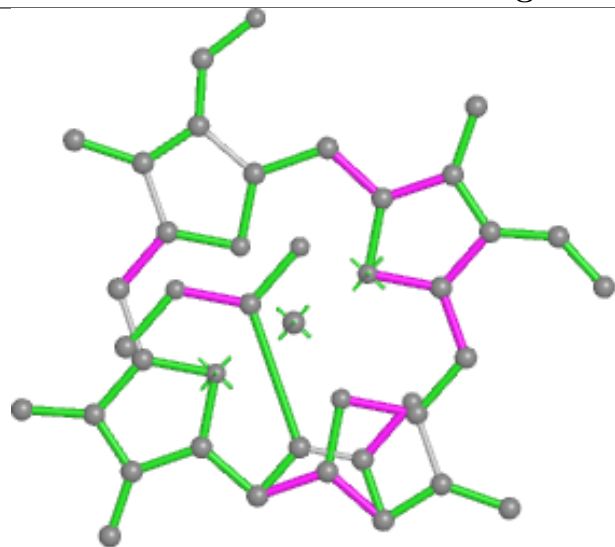




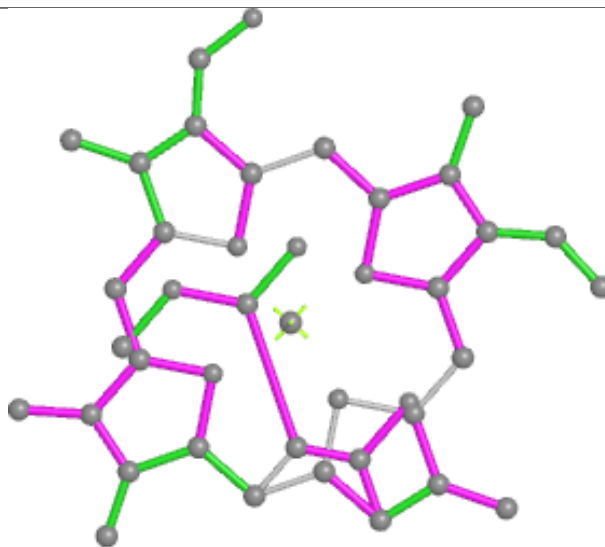




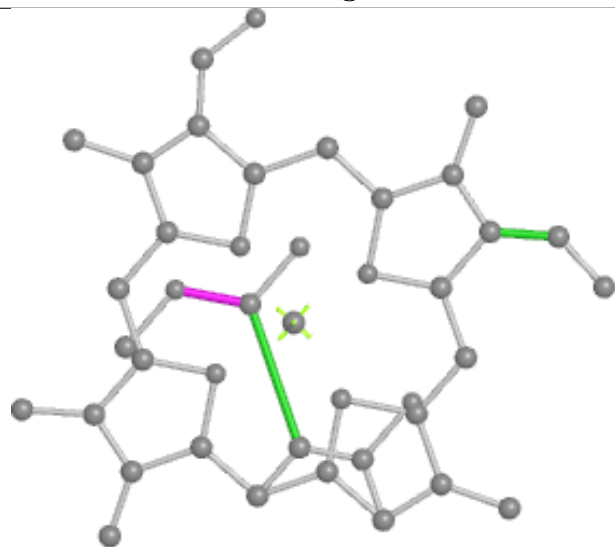
Ligand CL7 31 407



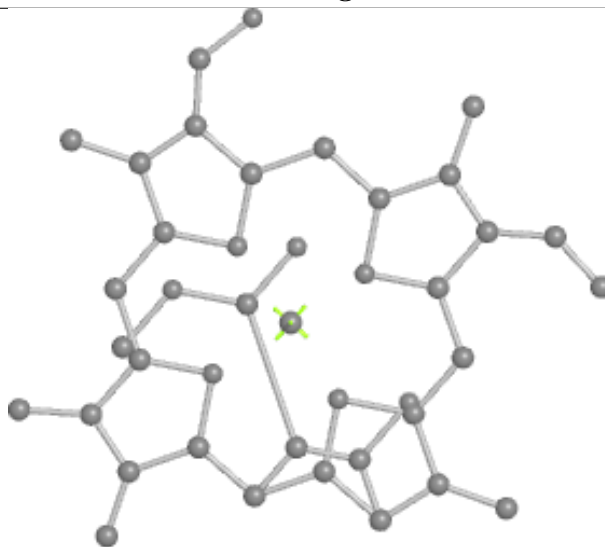
Bond lengths



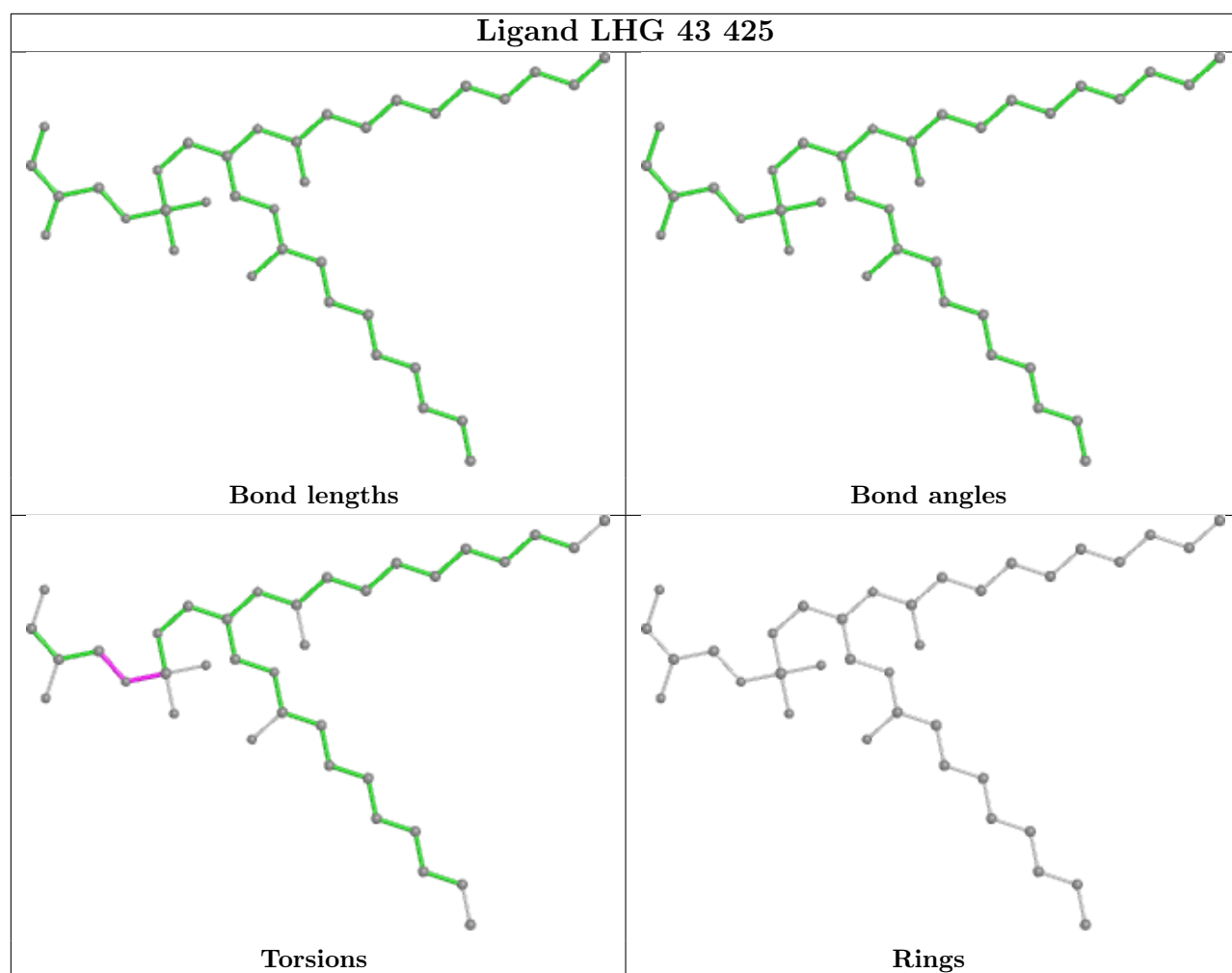
Bond angles

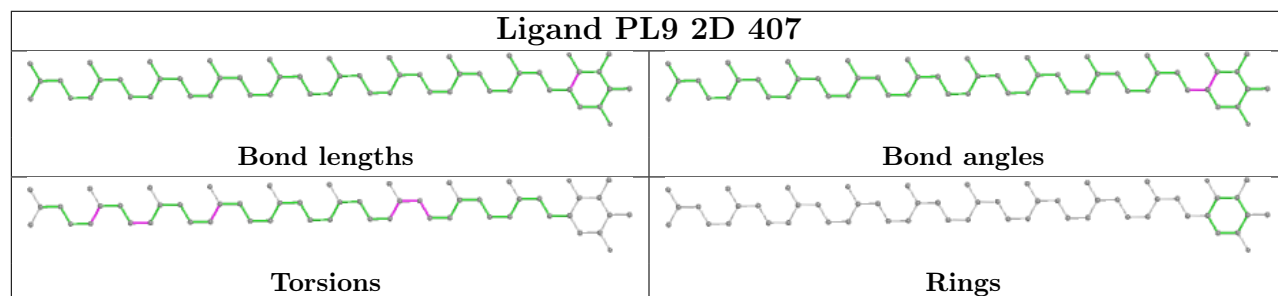
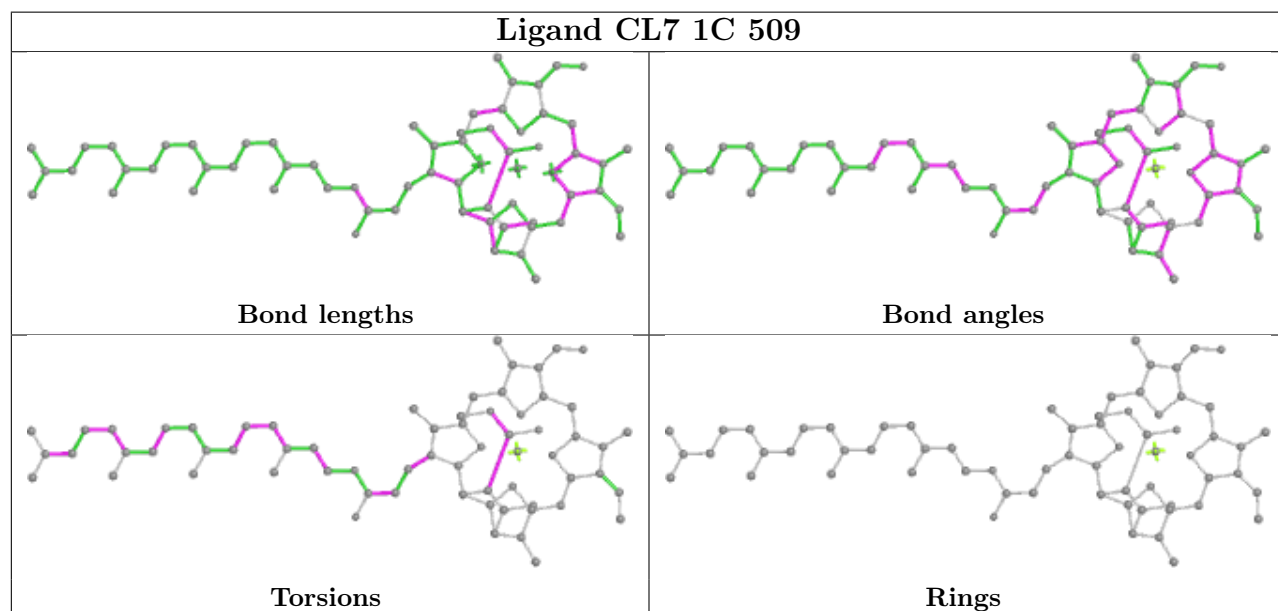
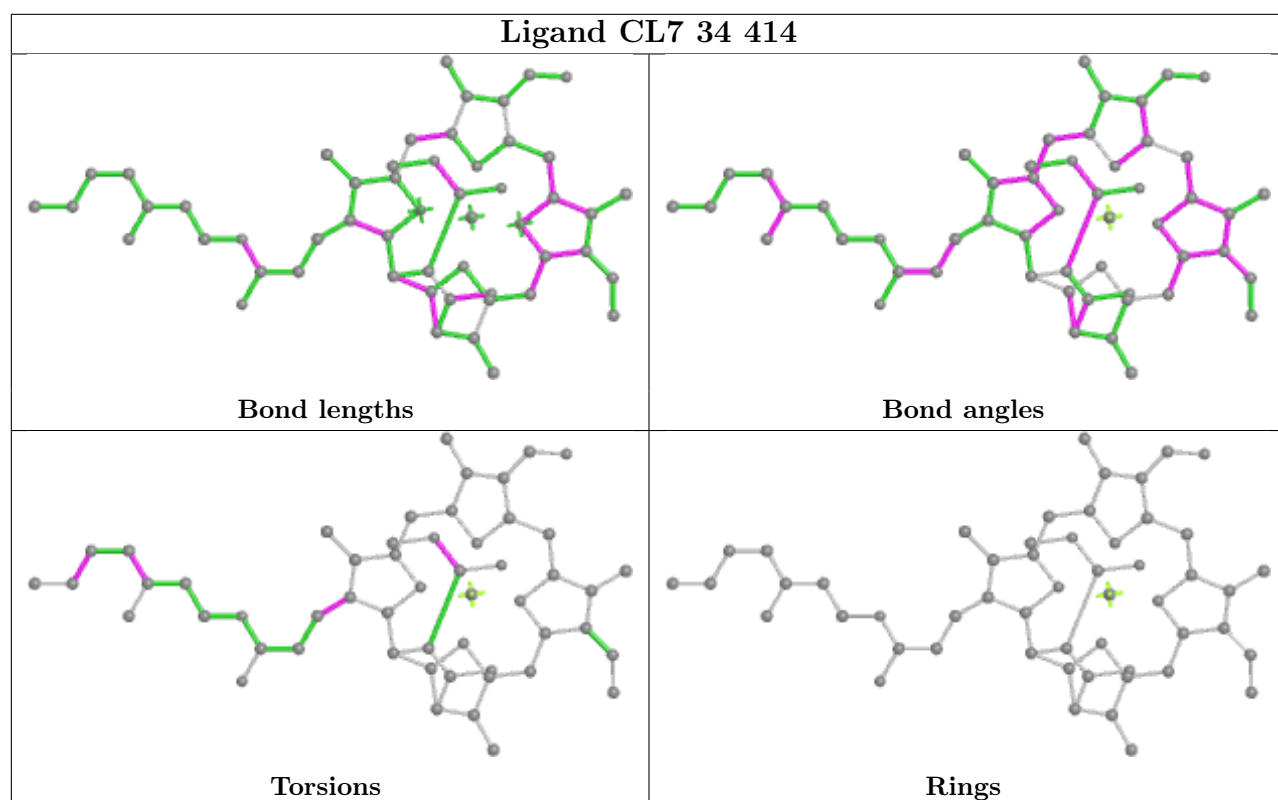


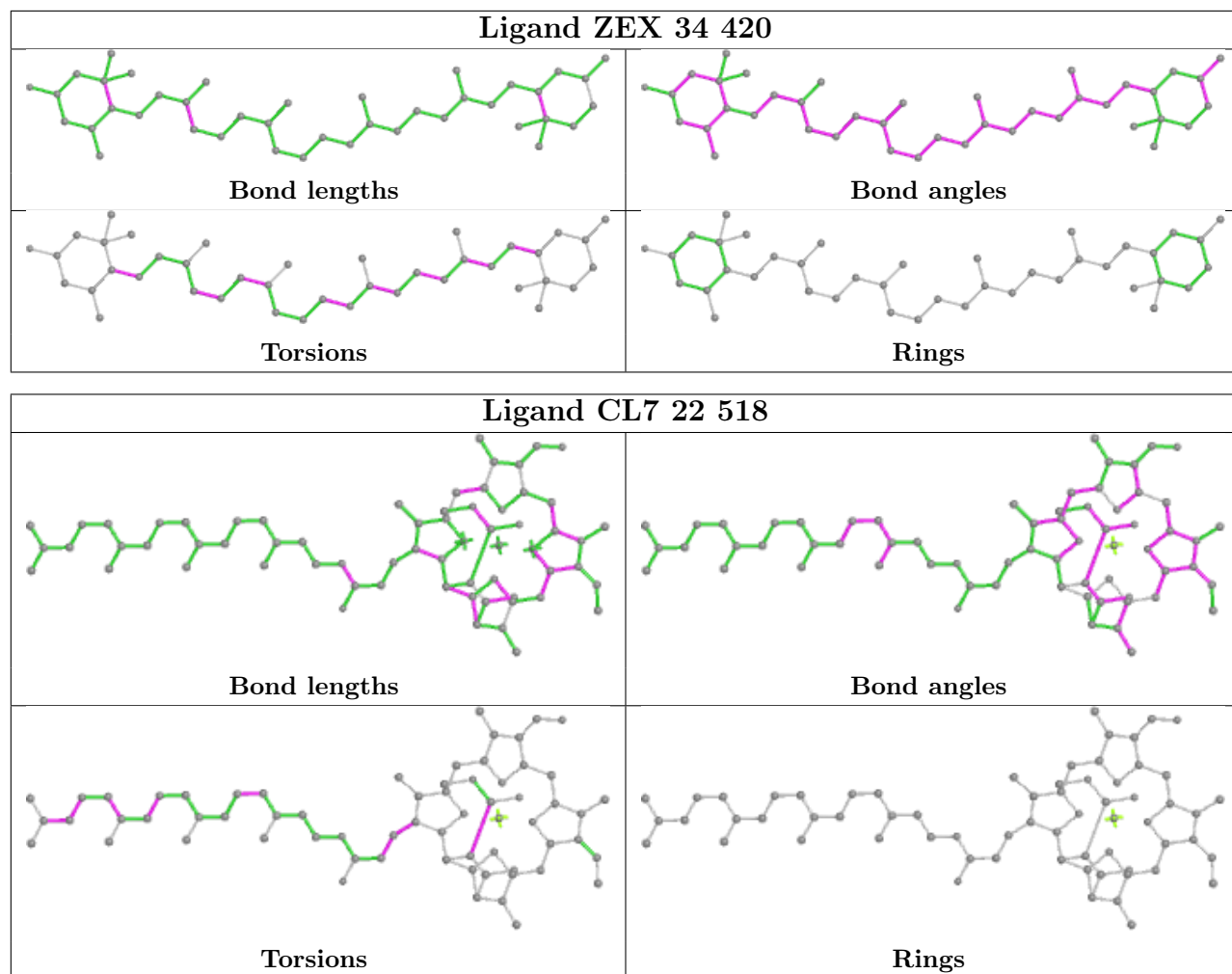
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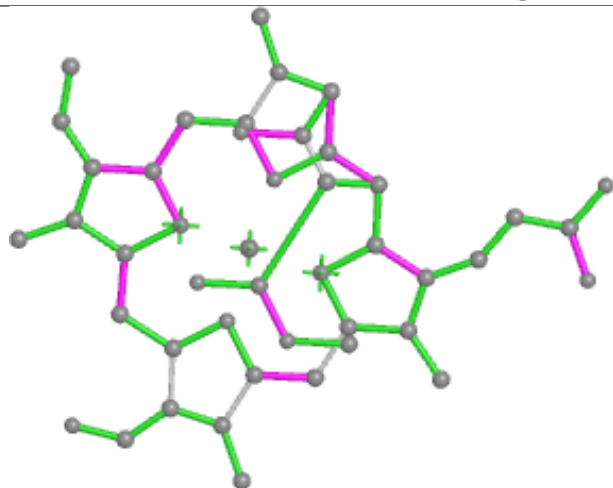
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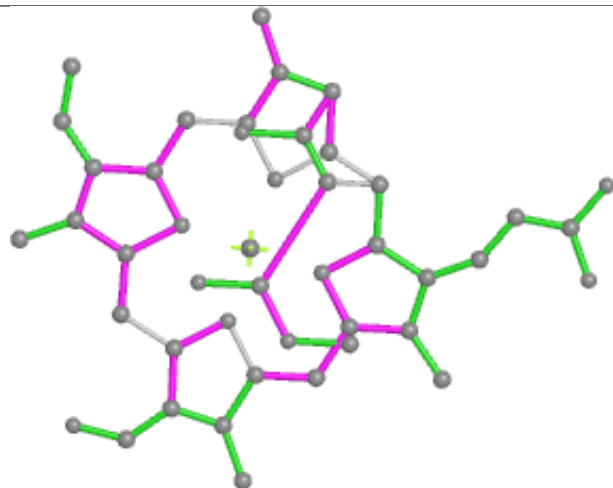




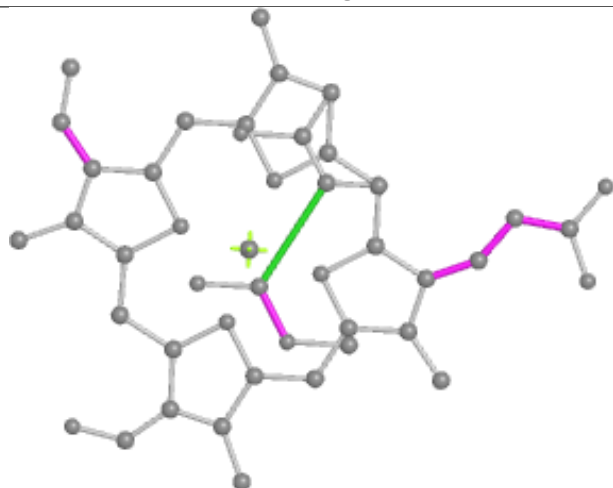
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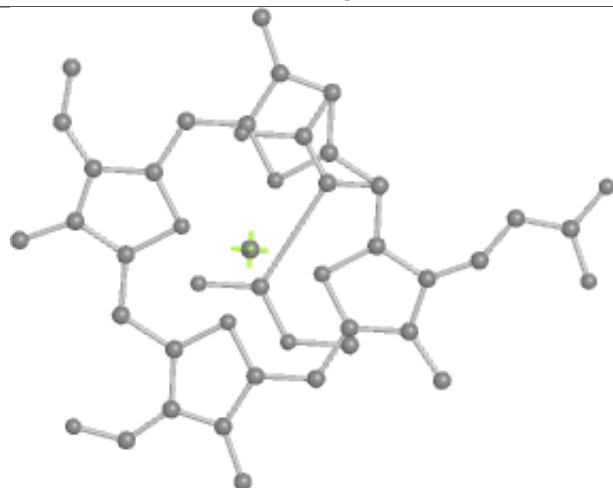
Bond lengths



Bond angles

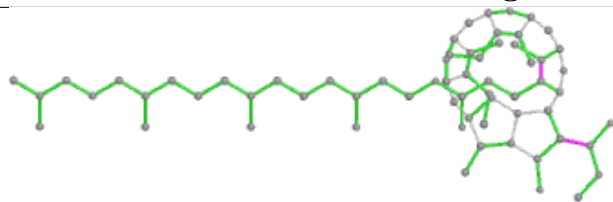


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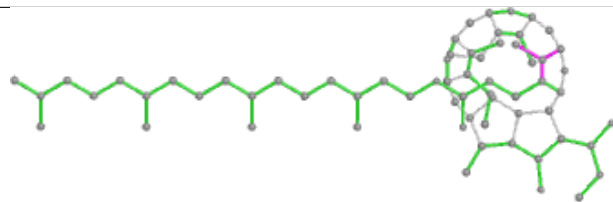


Rings

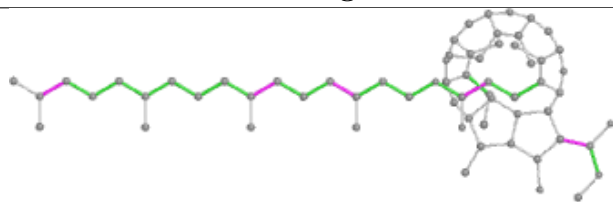
Ligand PHO 3D 408



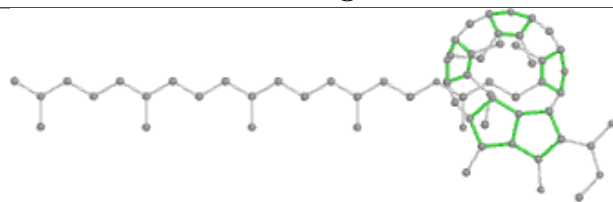
Bond lengths



Bond angles

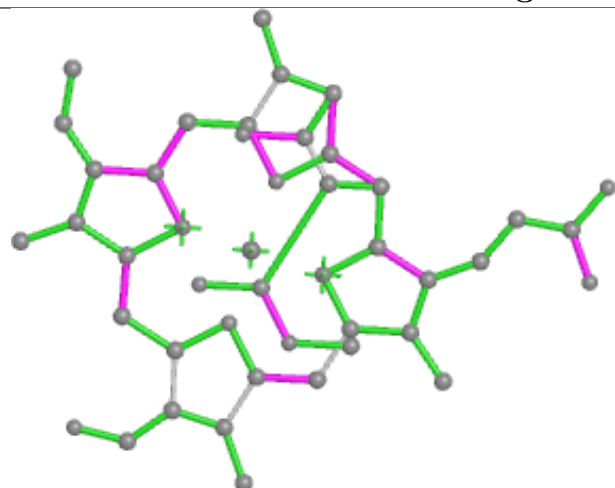


Torsions

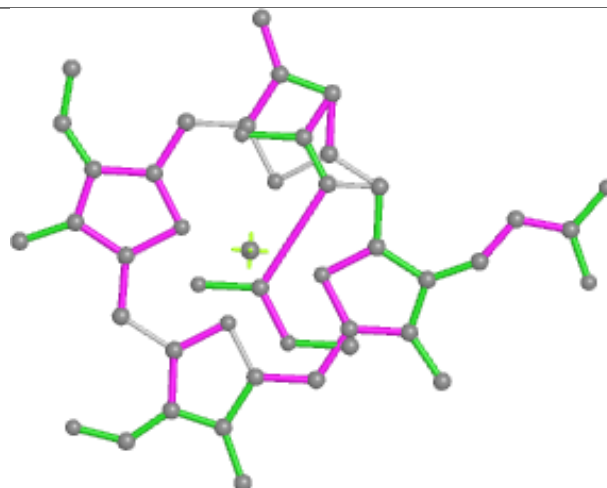


Rings

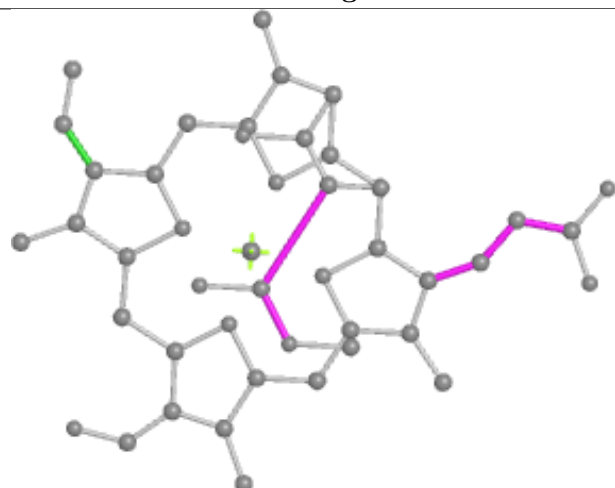
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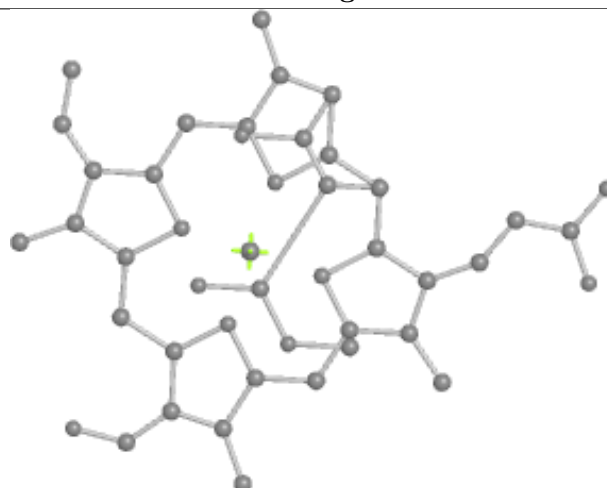
Bond lengths



Bond angles

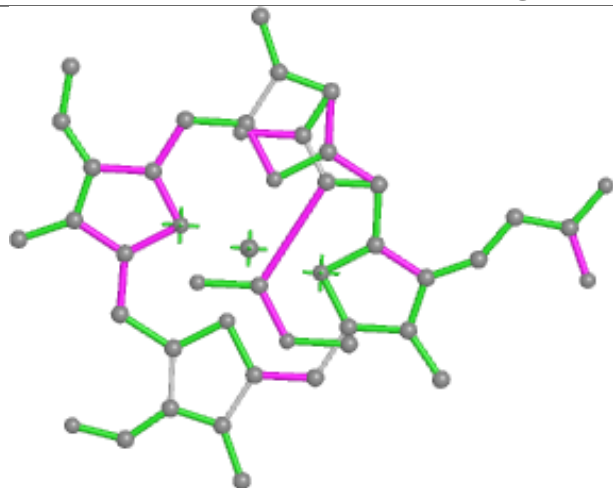


Torsions

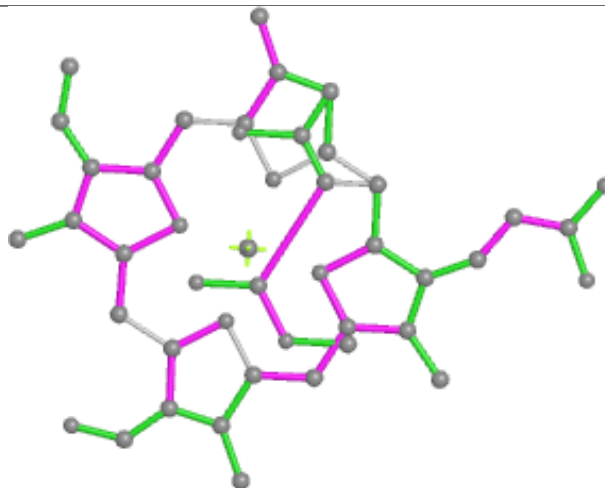


Rings

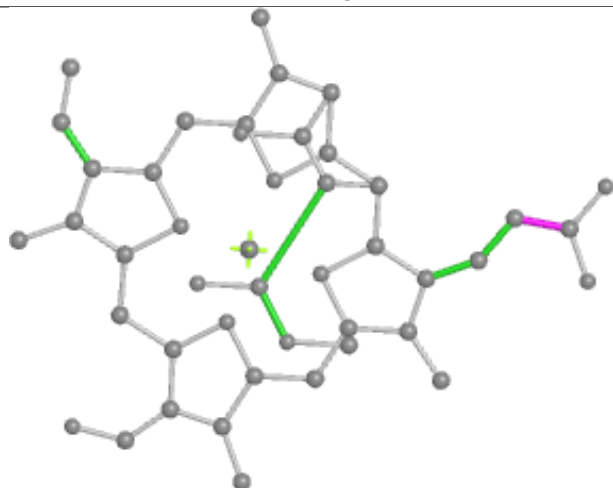
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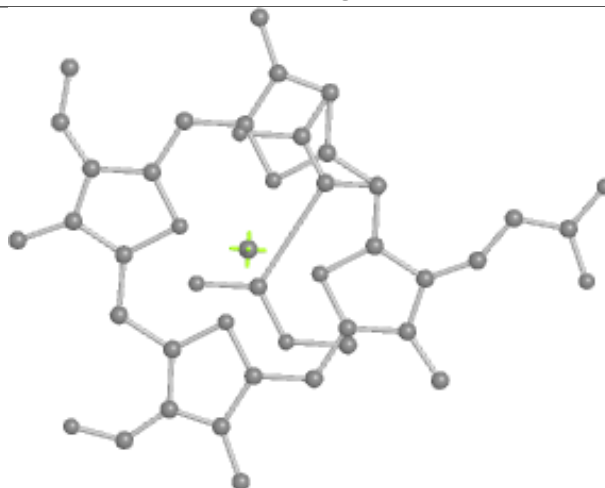
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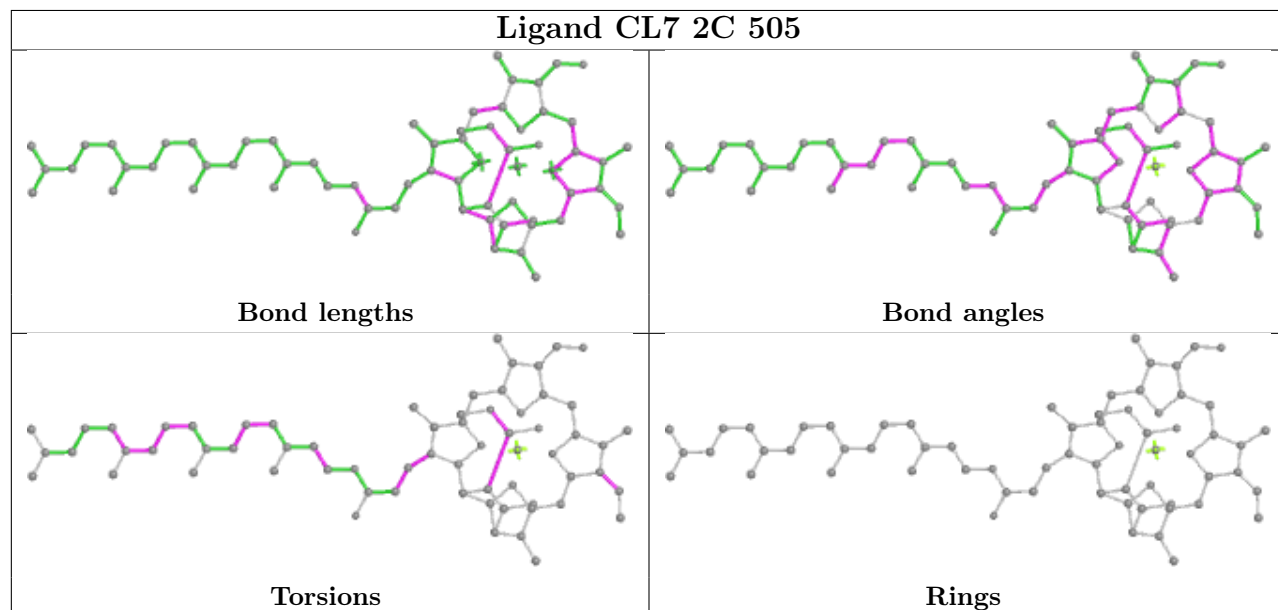
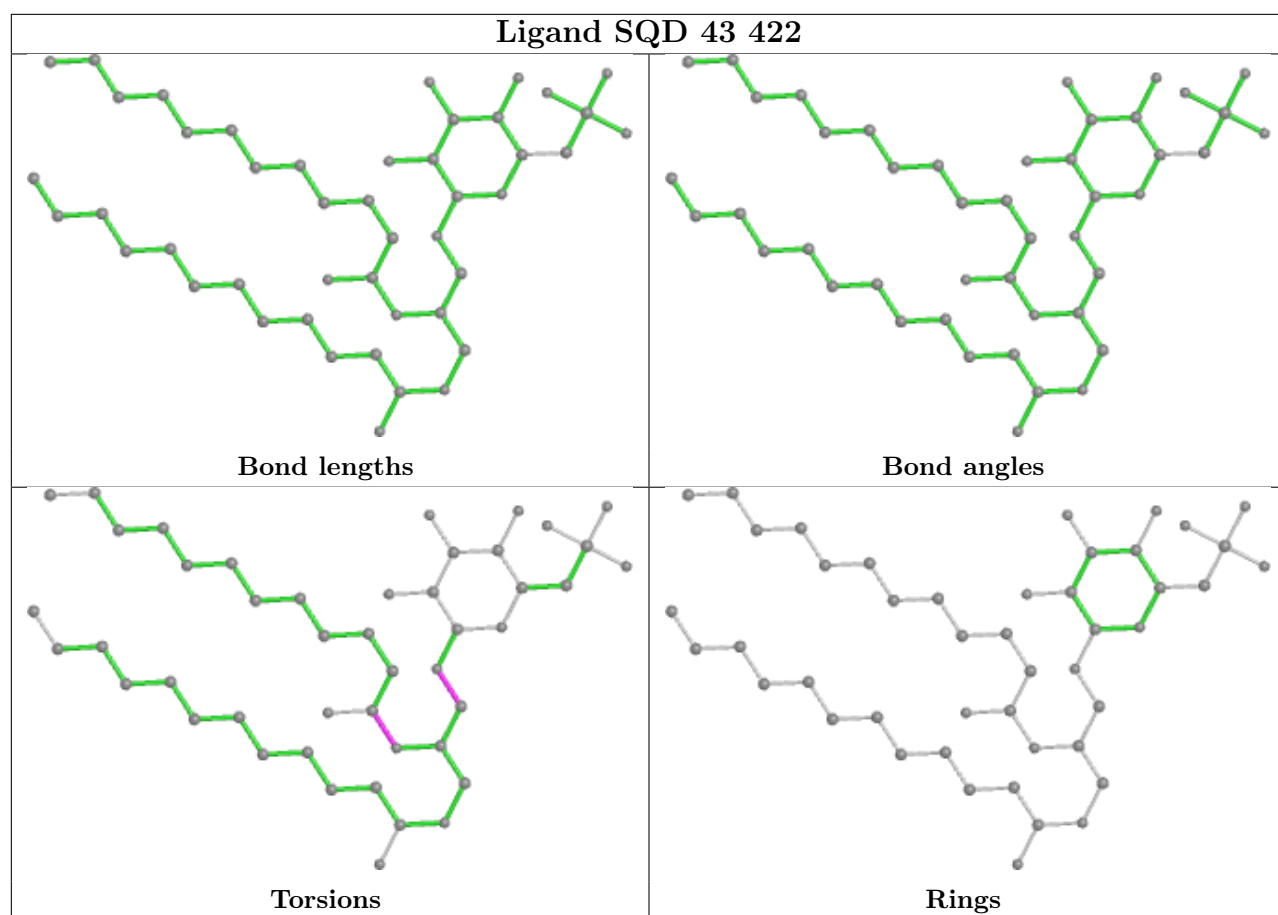
Bond angles

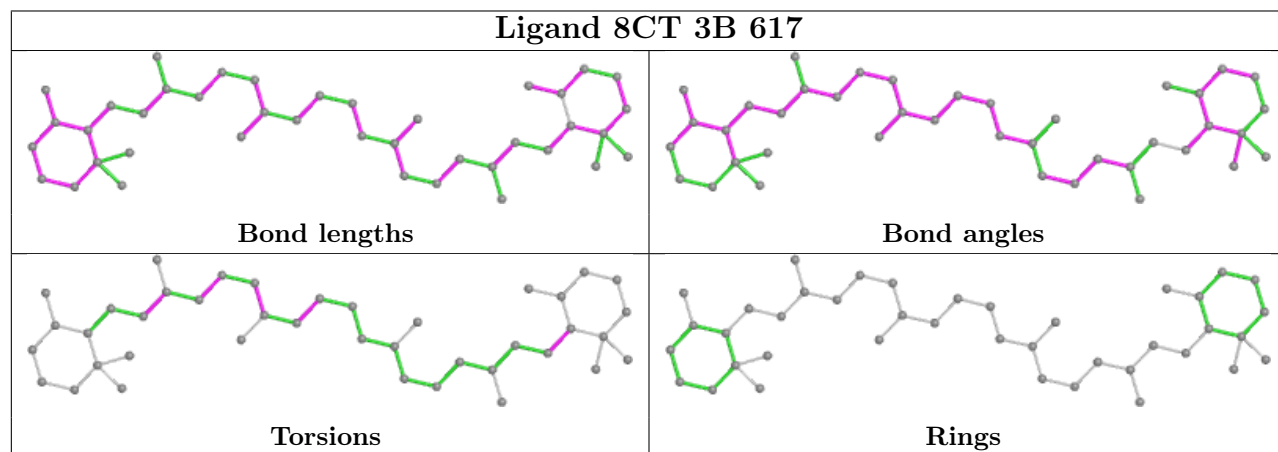
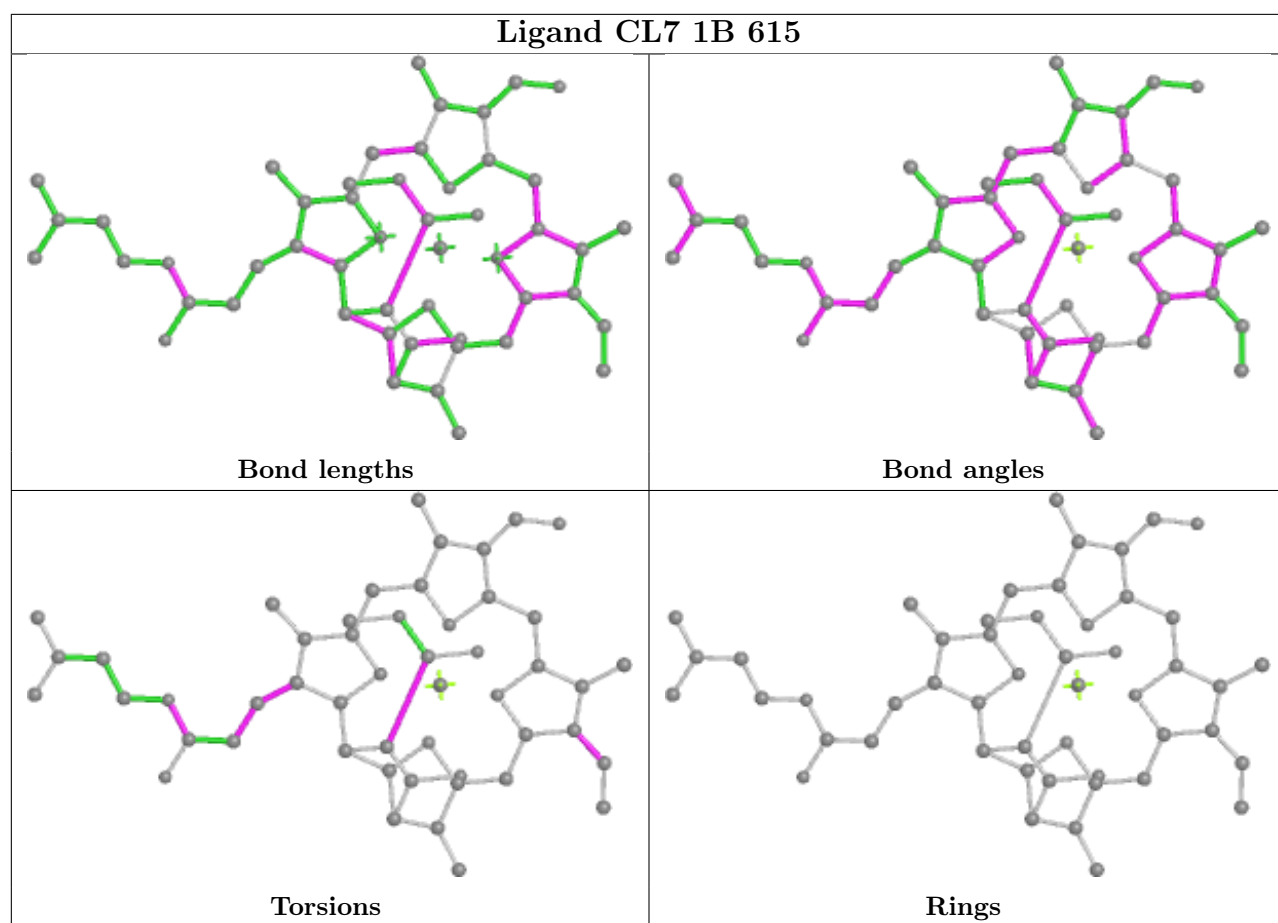


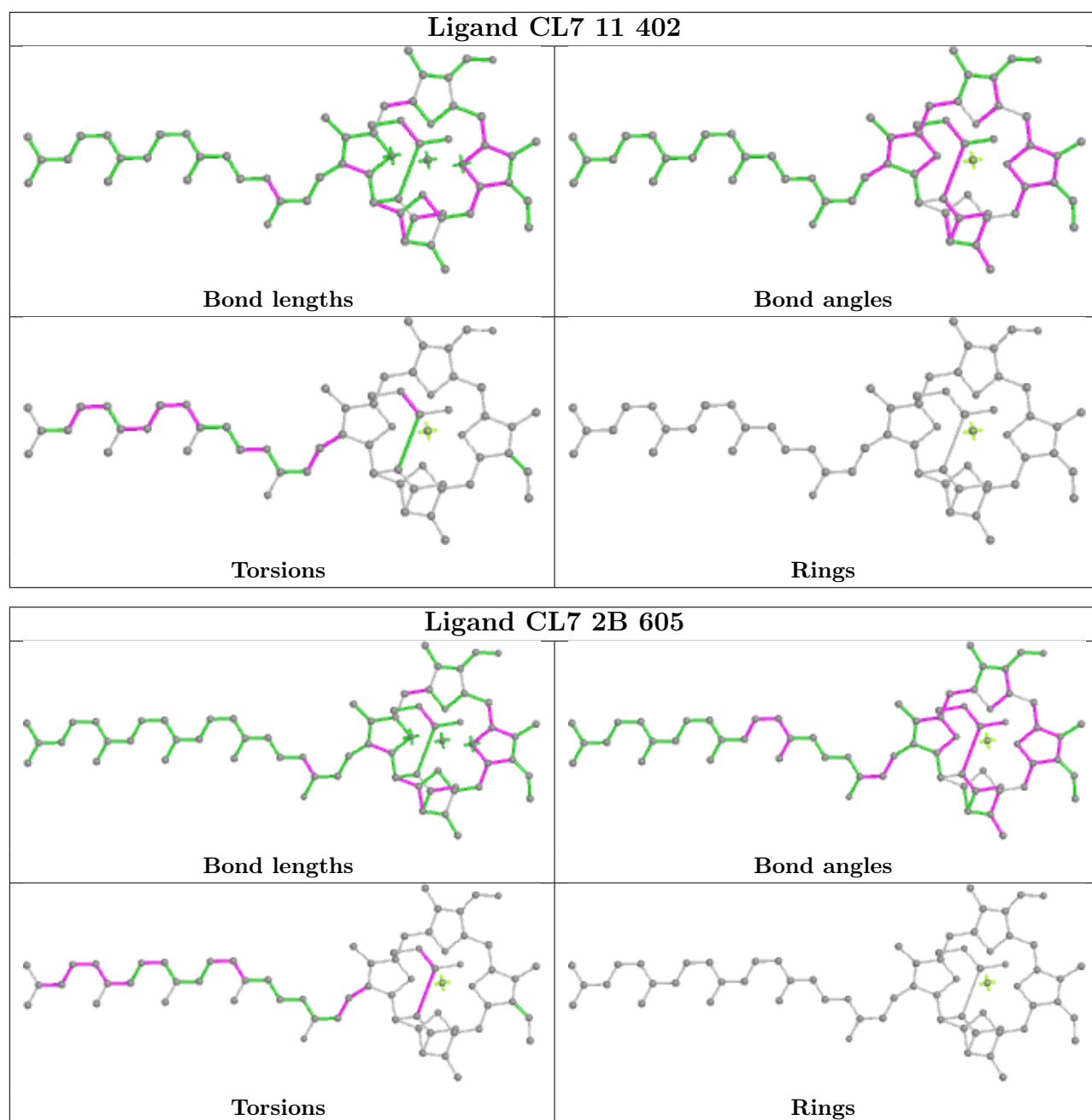
Torsions

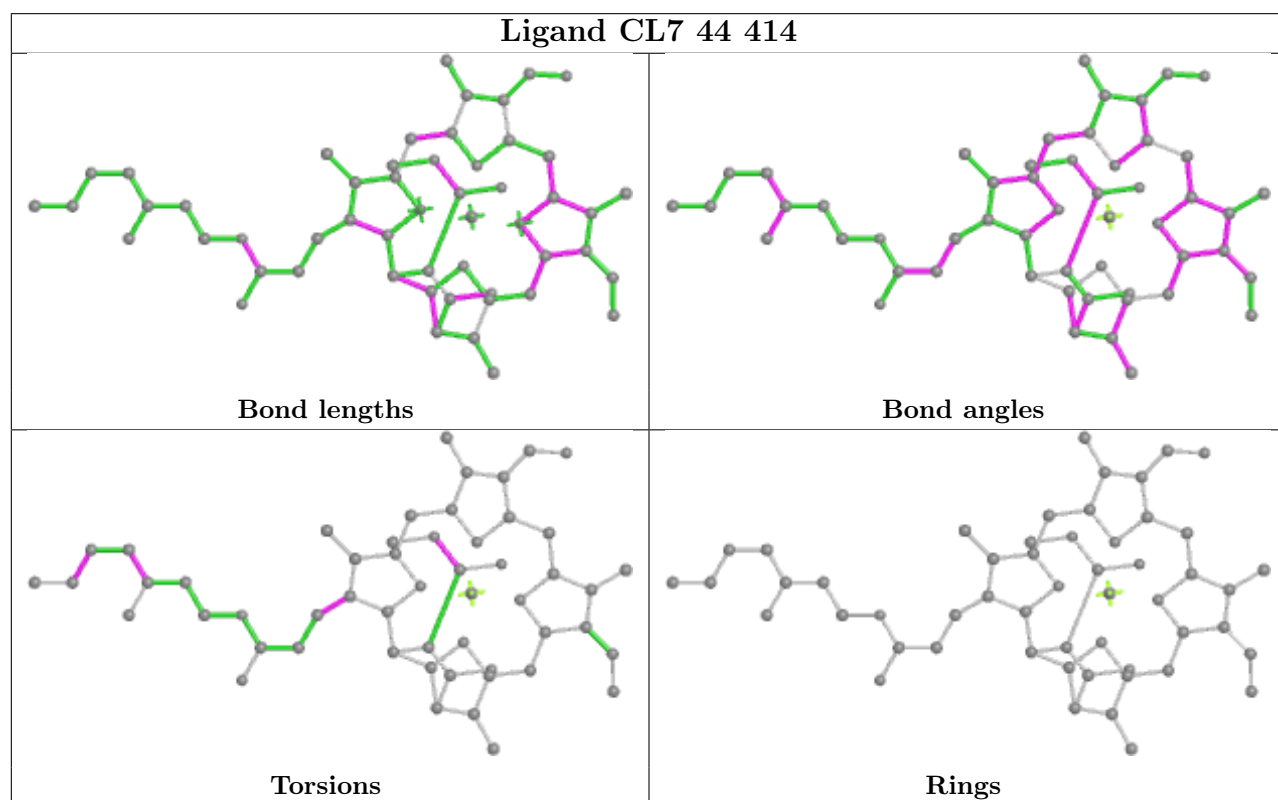
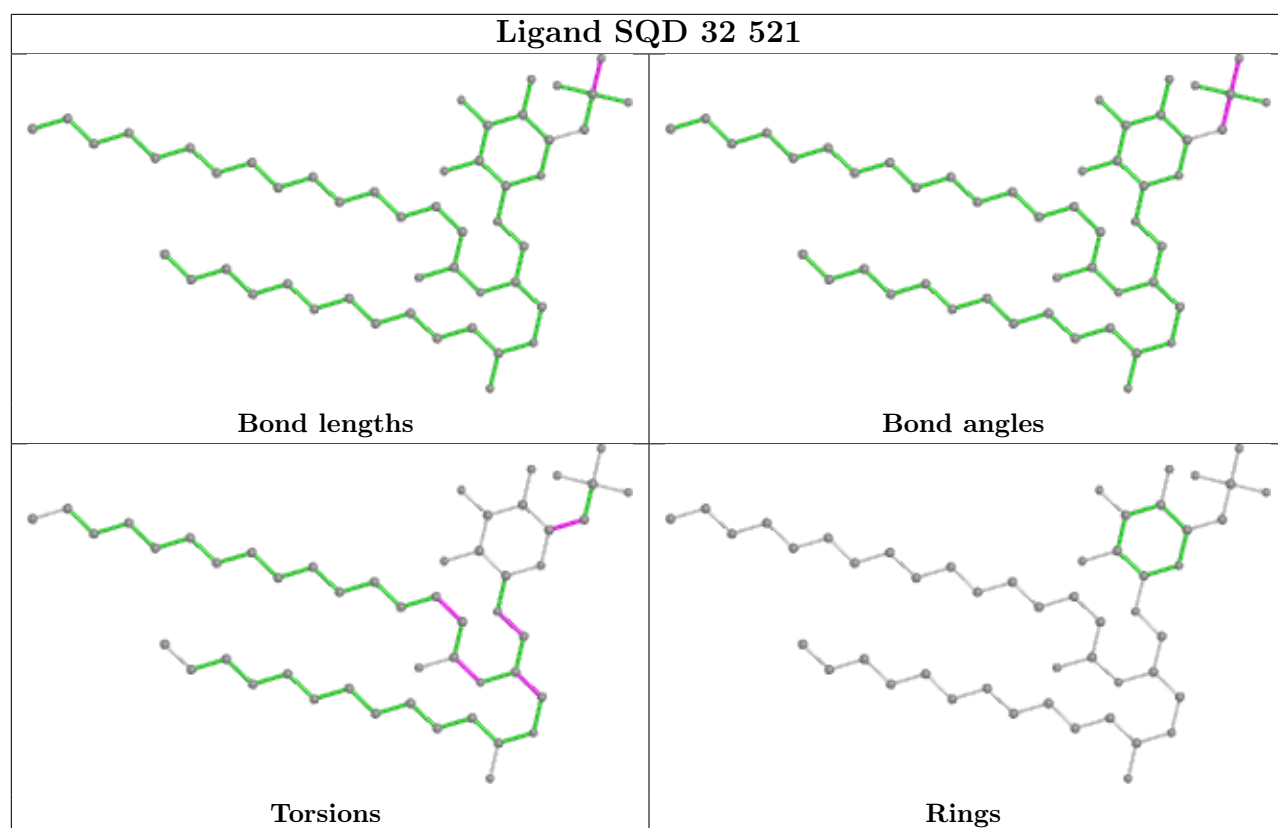


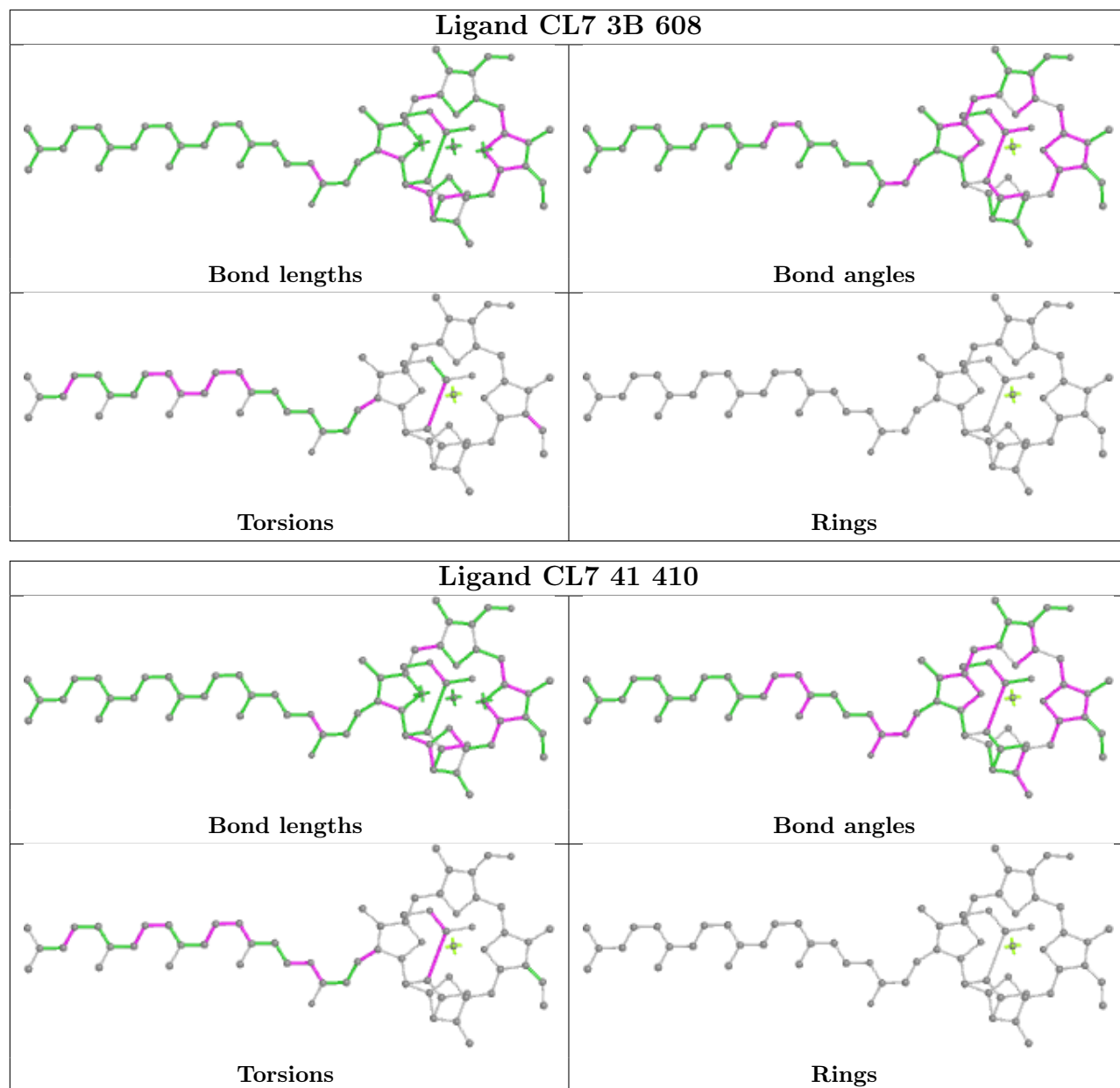
Rings



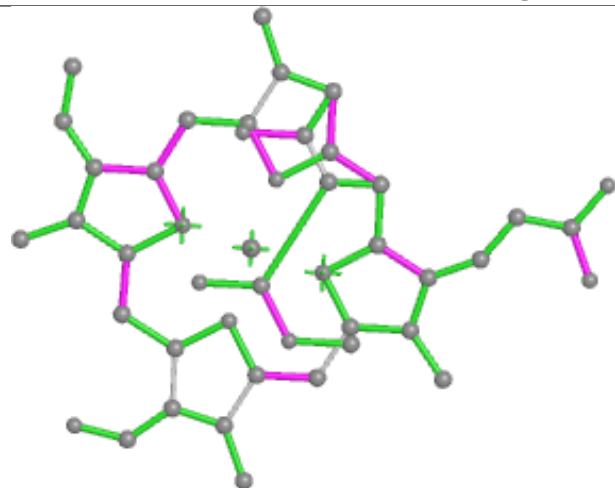




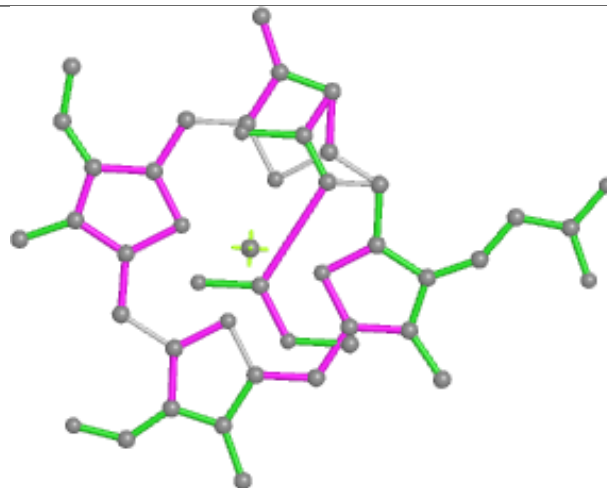




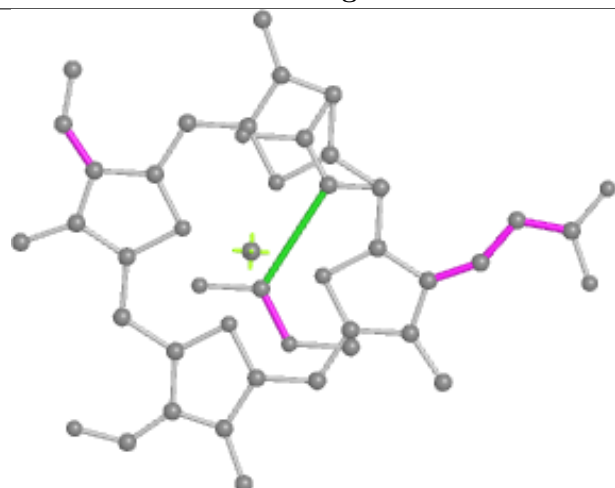
Ligand CL7 41 419



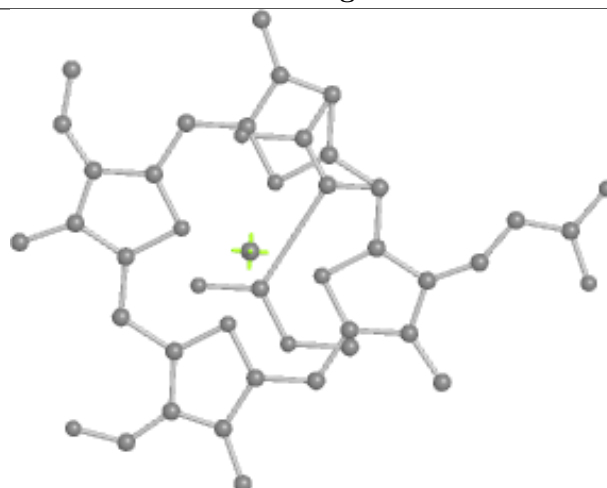
Bond lengths



Bond angles

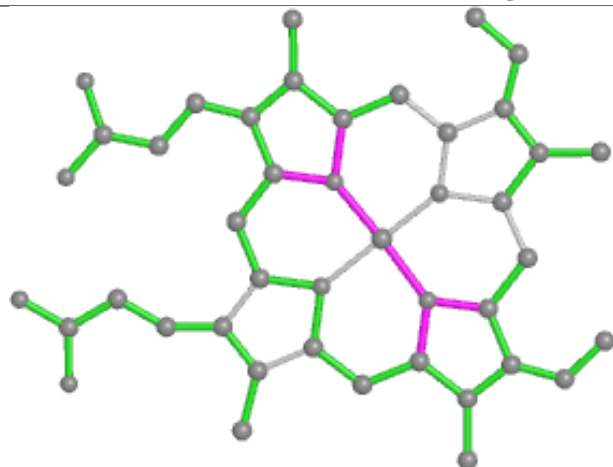


Torsions

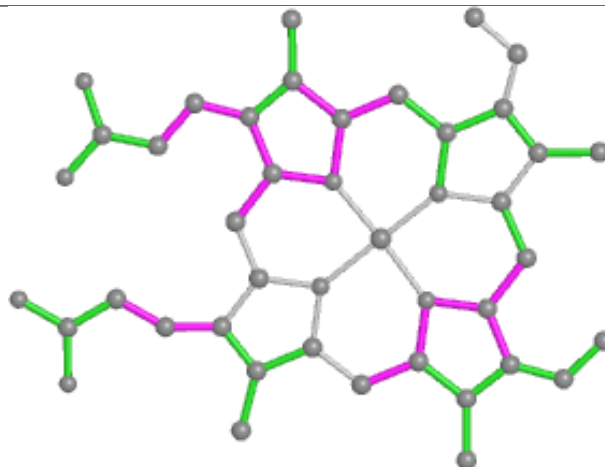


Rings

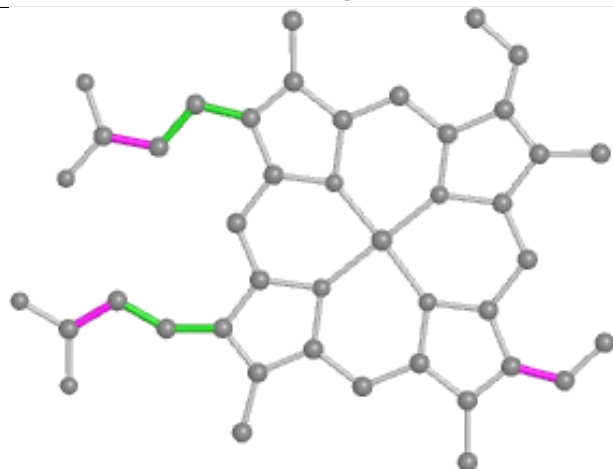
Ligand HEM 4F 101



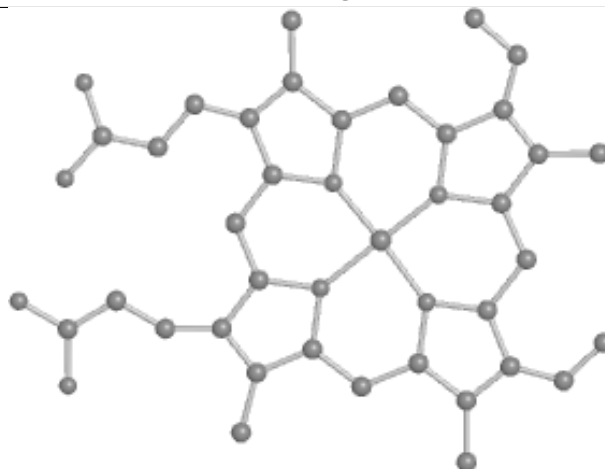
Bond lengths



Bond angles

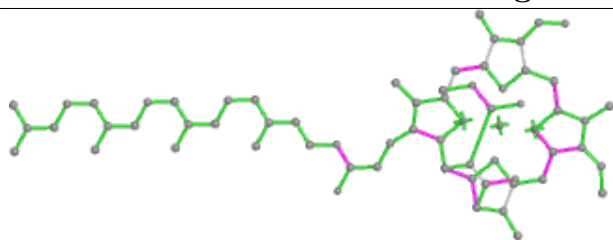


Torsions

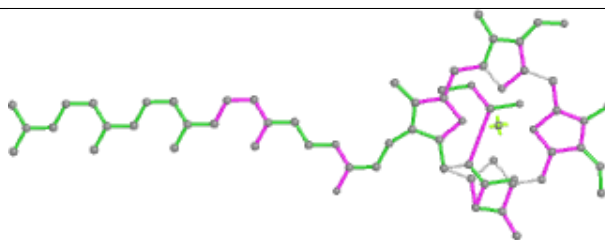


Rings

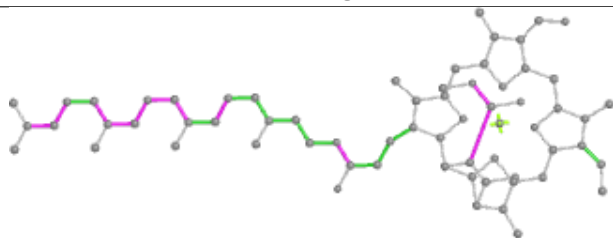
Ligand CL7 23 410



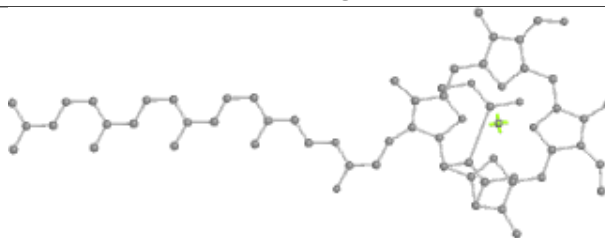
Bond lengths



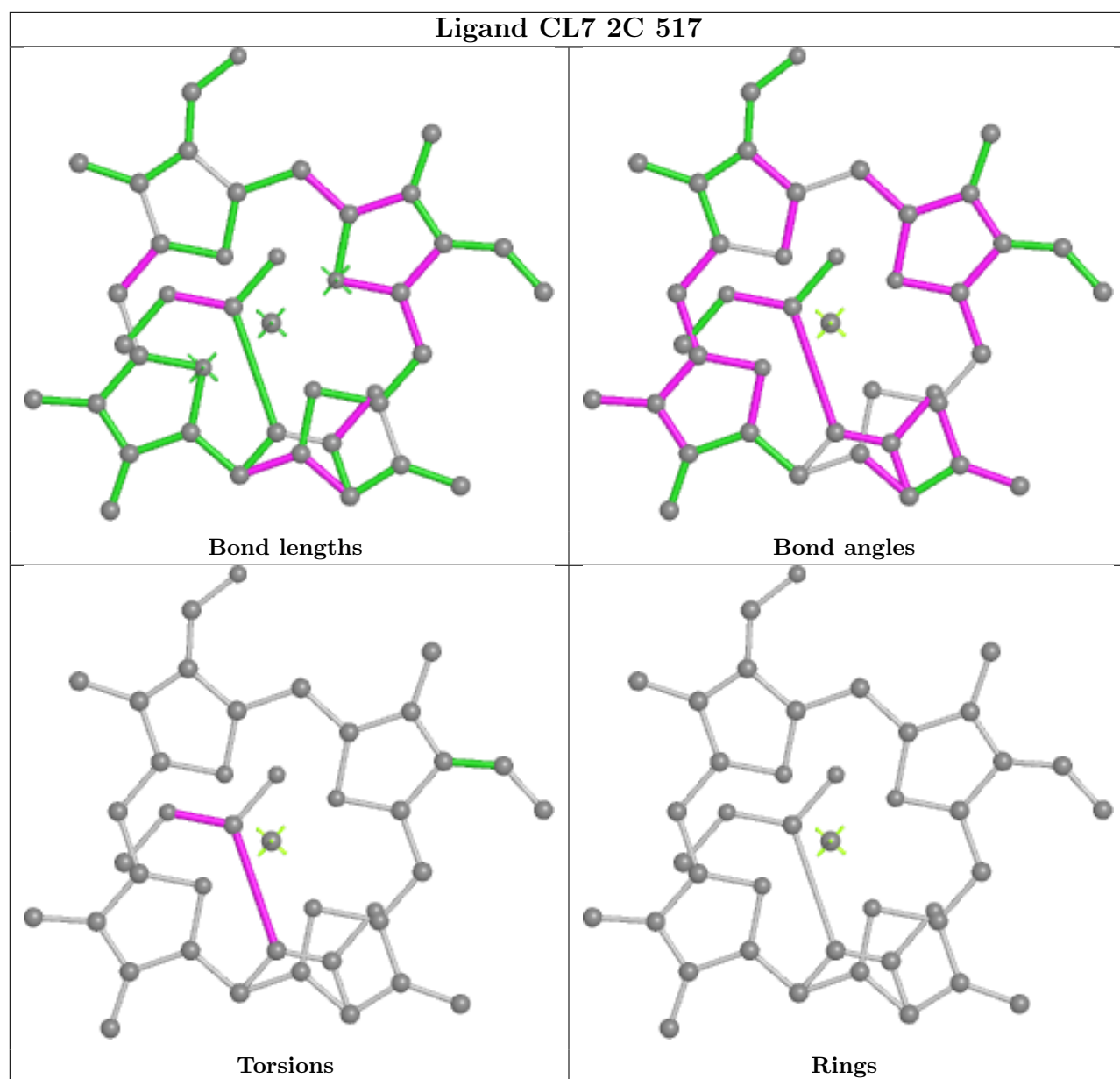
Bond angles

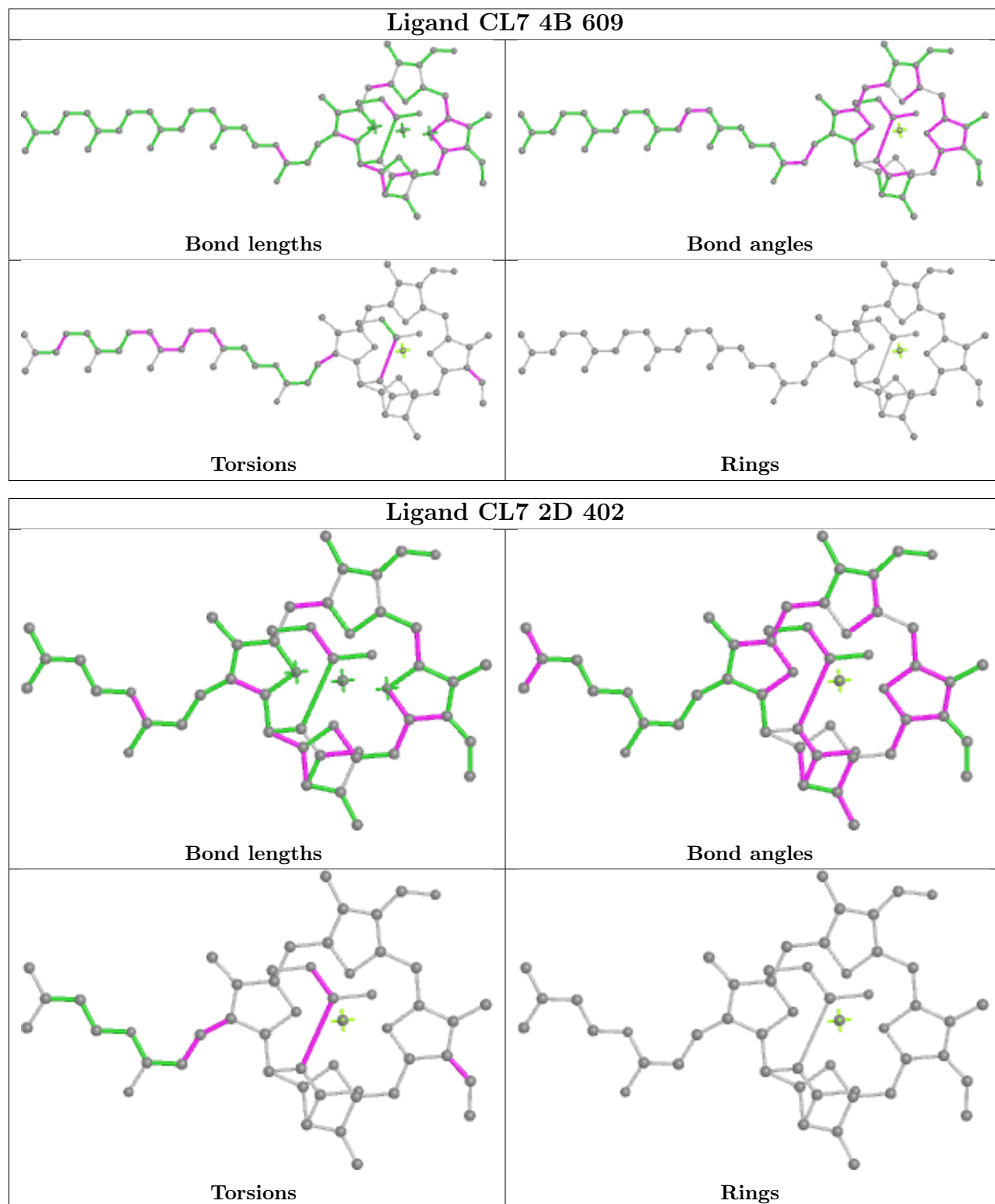


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

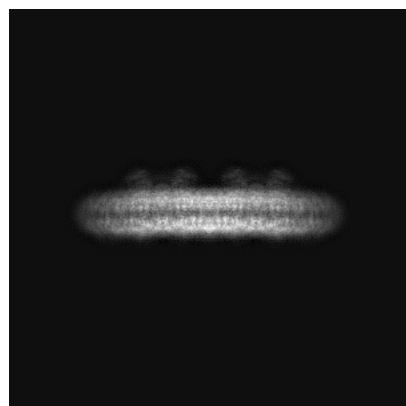
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33933. These allow visual inspection of the internal detail of the map and identification of artifacts.

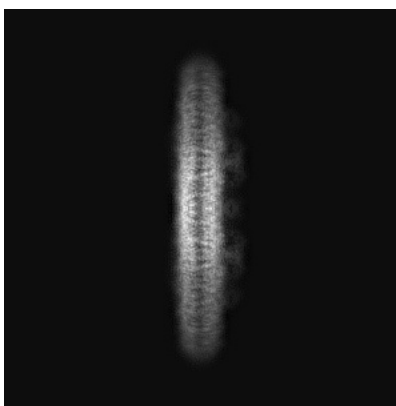
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

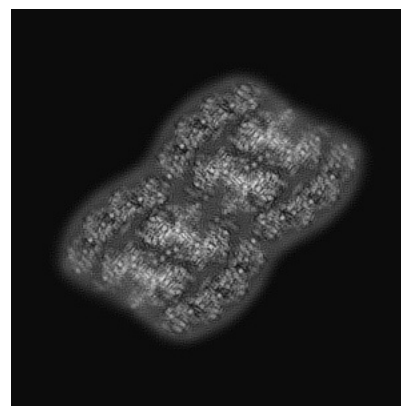
6.1.1 Primary map



X

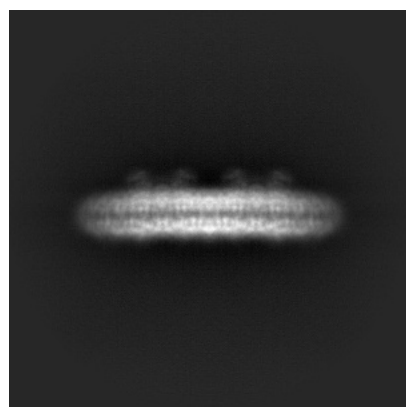


Y

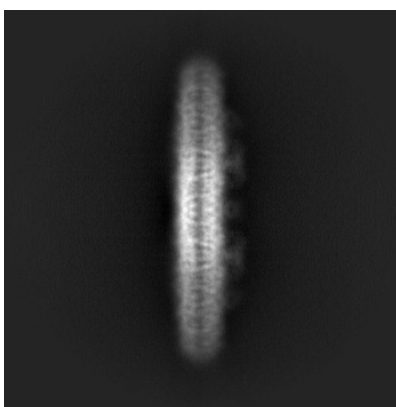


Z

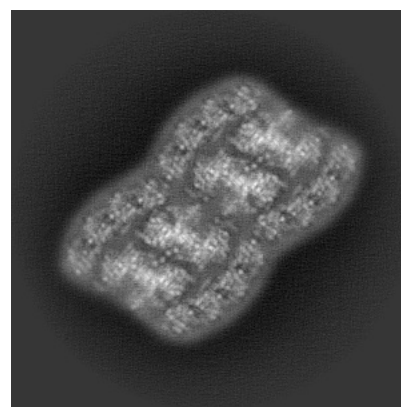
6.1.2 Raw map



X



Y

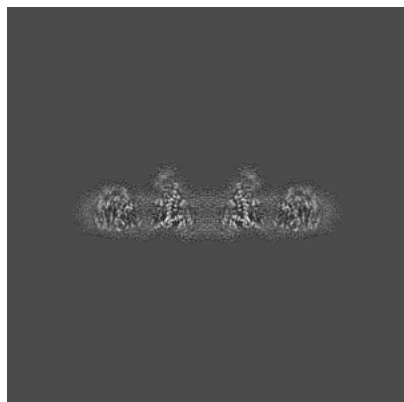


Z

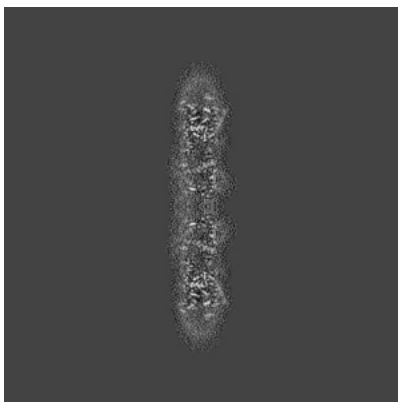
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

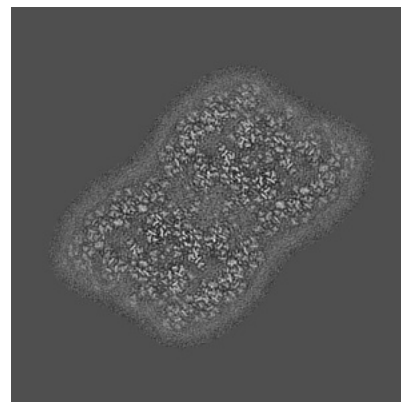
6.2.1 Primary map



X Index: 240

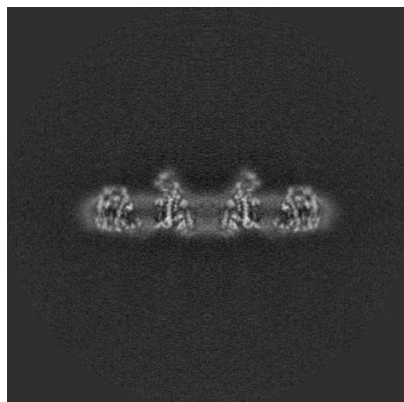


Y Index: 240

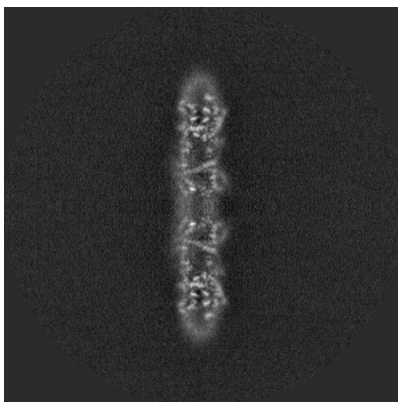


Z Index: 240

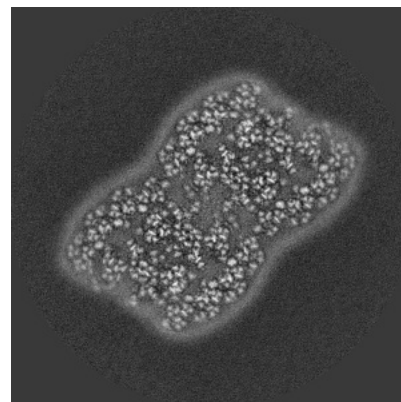
6.2.2 Raw map



X Index: 240



Y Index: 240

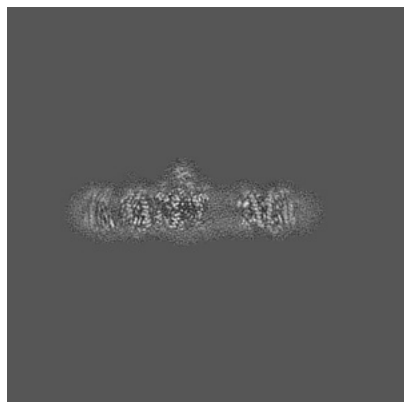


Z Index: 240

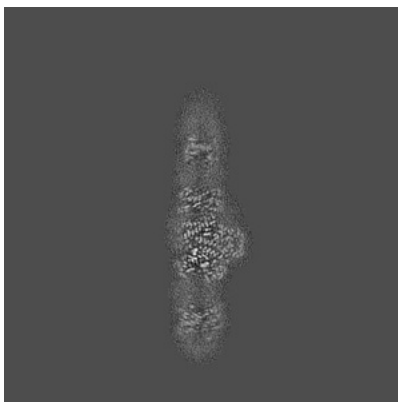
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

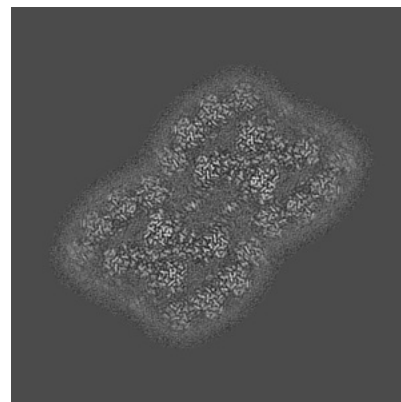
6.3.1 Primary map



X Index: 204

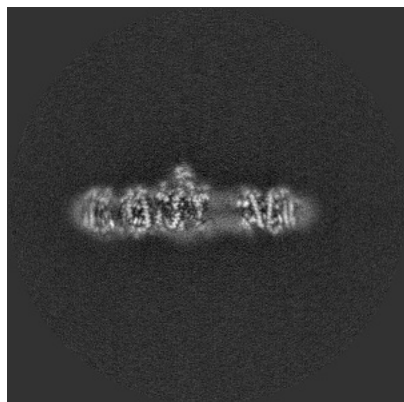


Y Index: 208

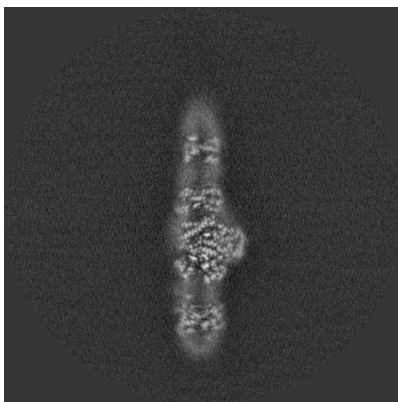


Z Index: 225

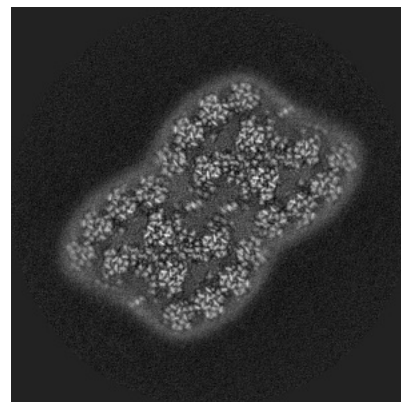
6.3.2 Raw map



X Index: 204



Y Index: 209

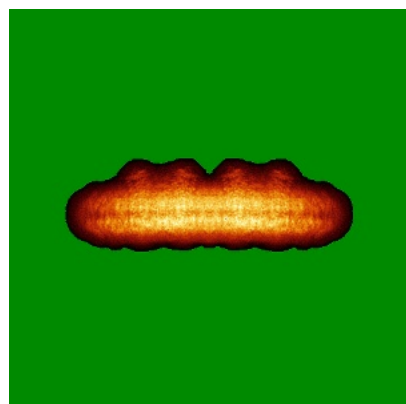


Z Index: 224

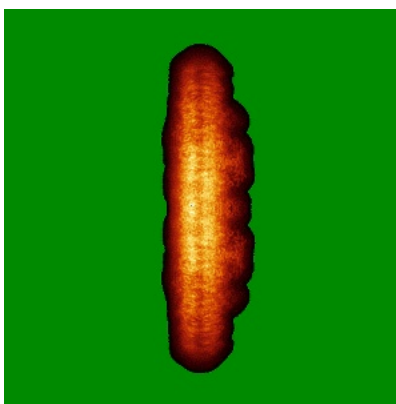
The images above show the largest variance slices of the map in three orthogonal directions.

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

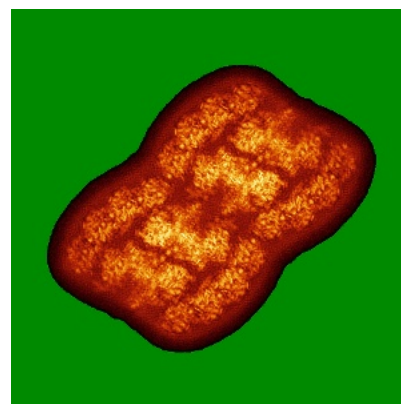
6.4.1 Primary map



X

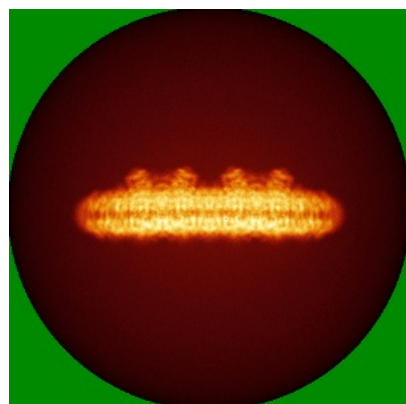


Y

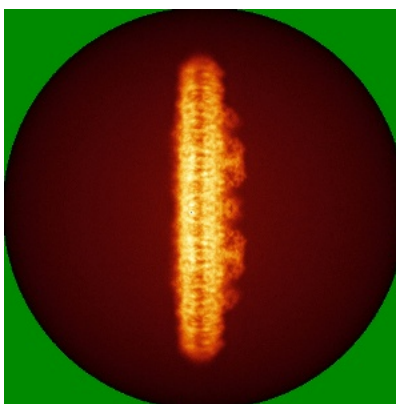


Z

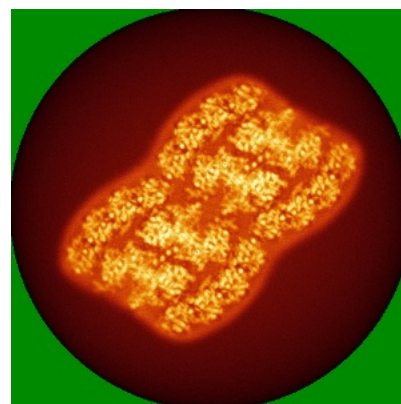
6.4.2 Raw map



X



Y

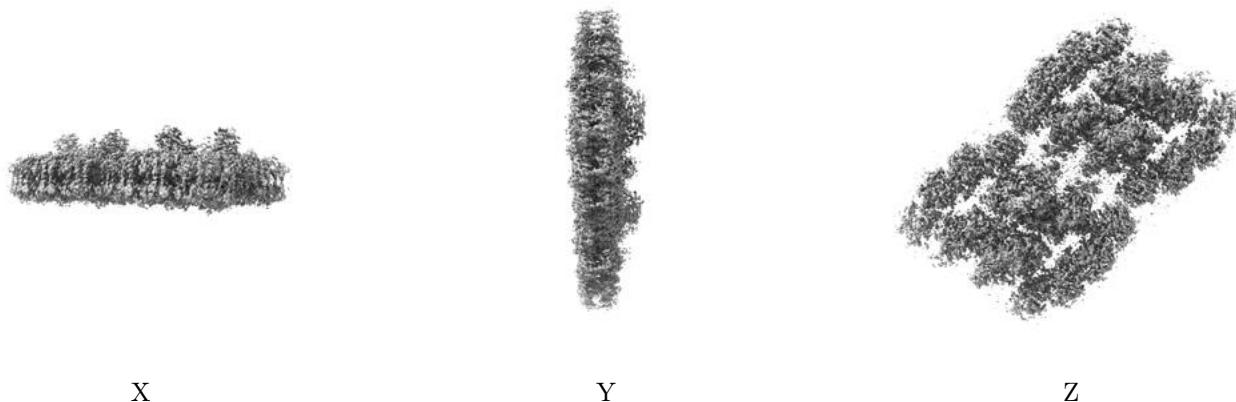


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

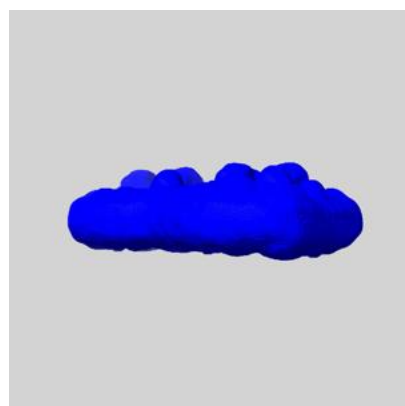
6.6 Mask visualisation [i](#)

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

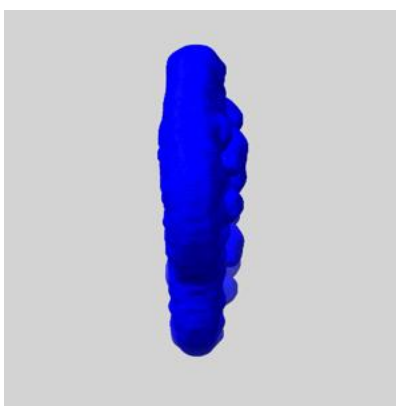
A mask typically either:

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

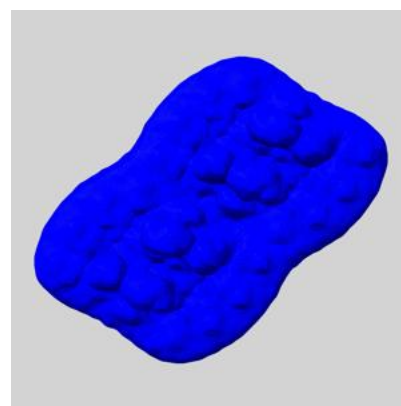
6.6.1 emd_33933_msk_1.map [i](#)



X



Y

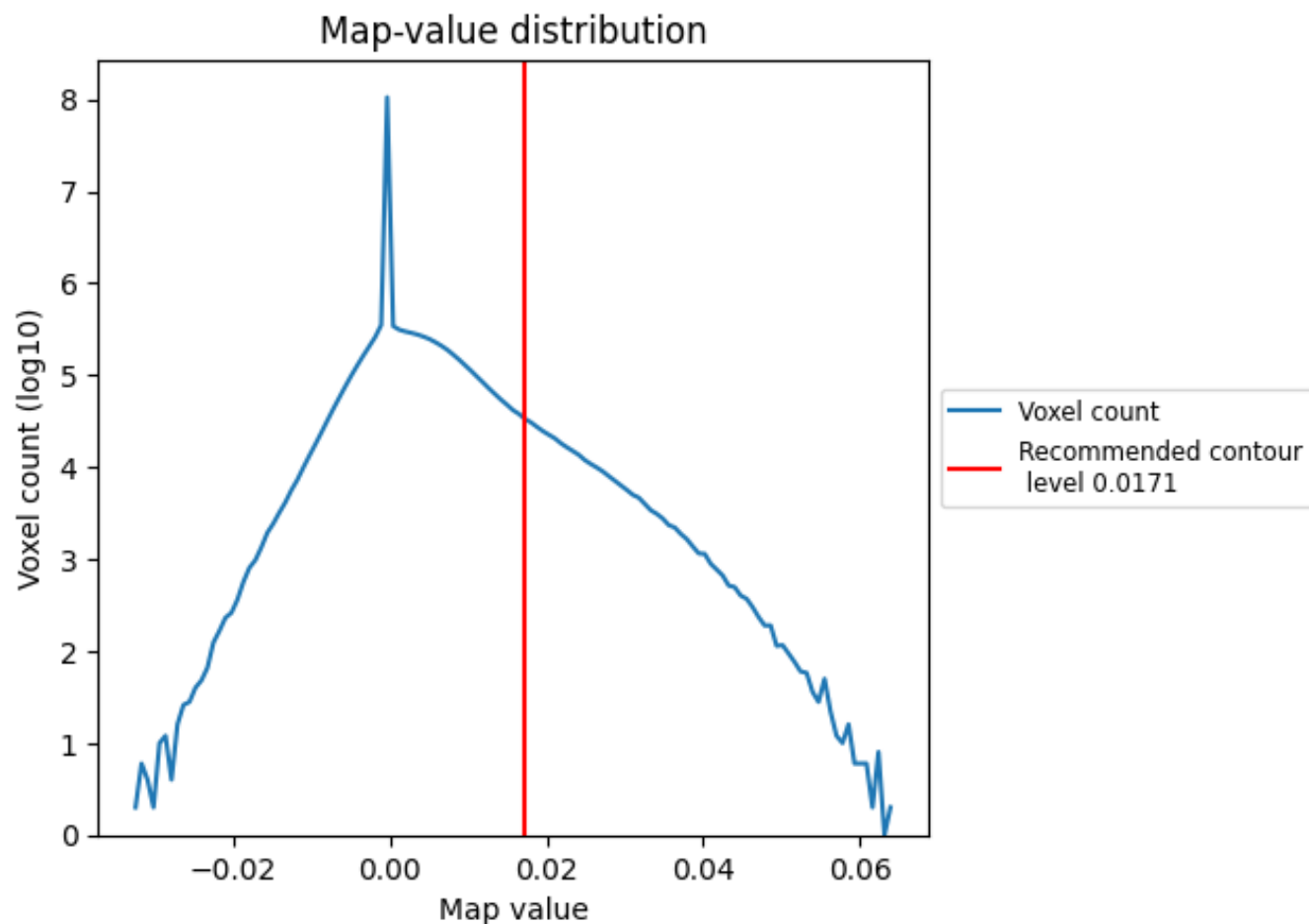


Z

7 Map analysis [i](#)

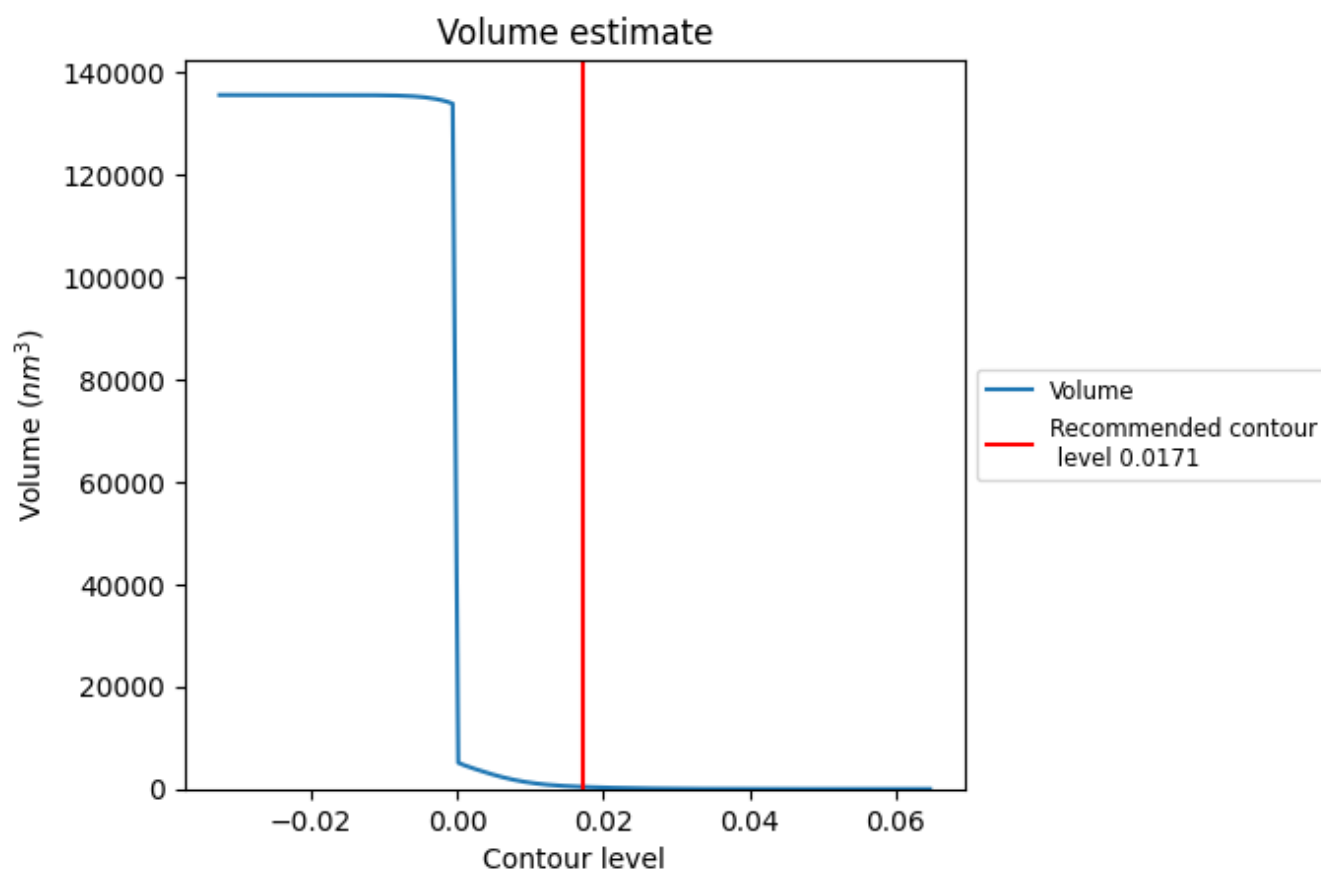
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

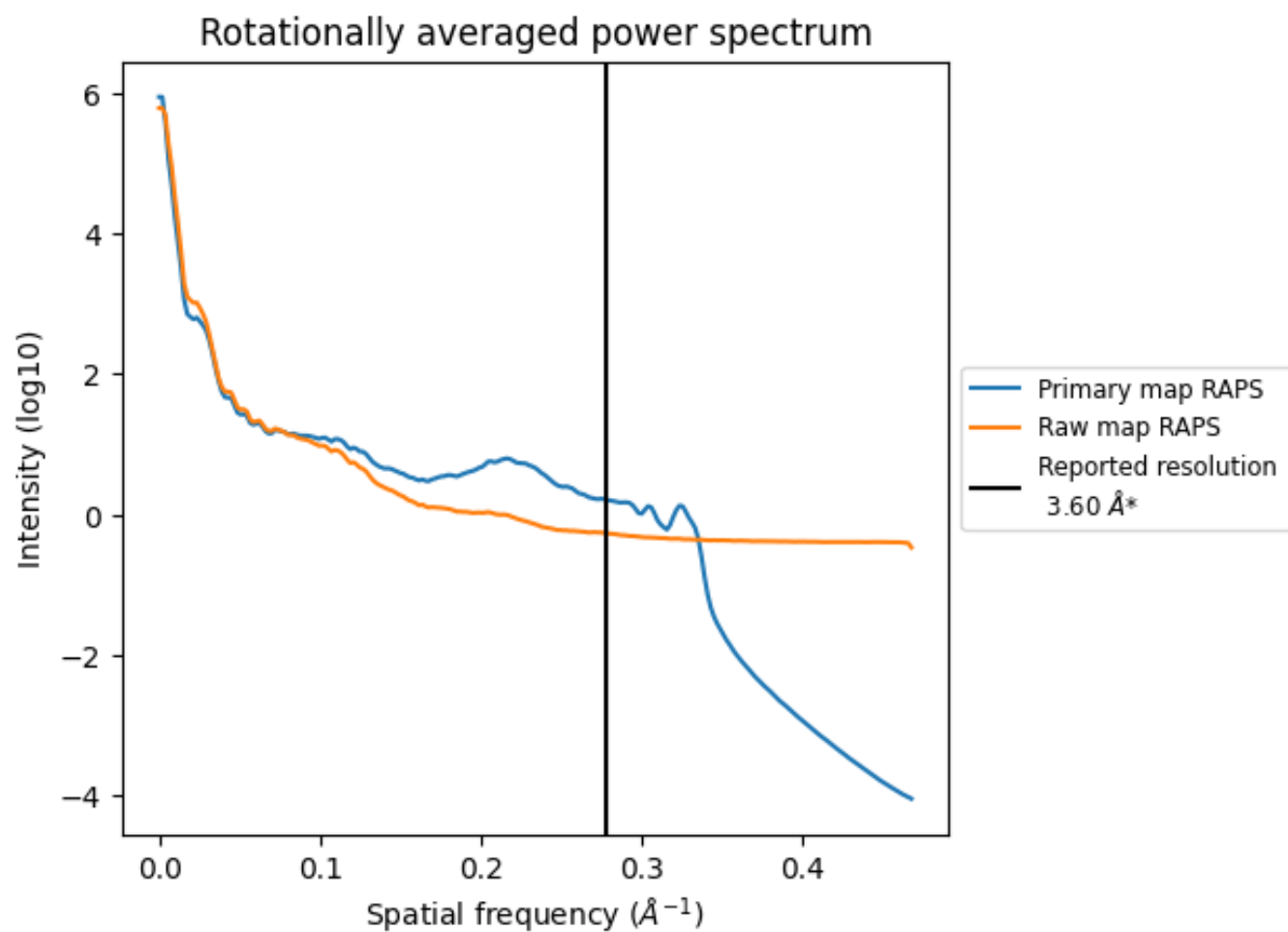
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 416 nm³; this corresponds to an approximate mass of 376 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 ⓘ

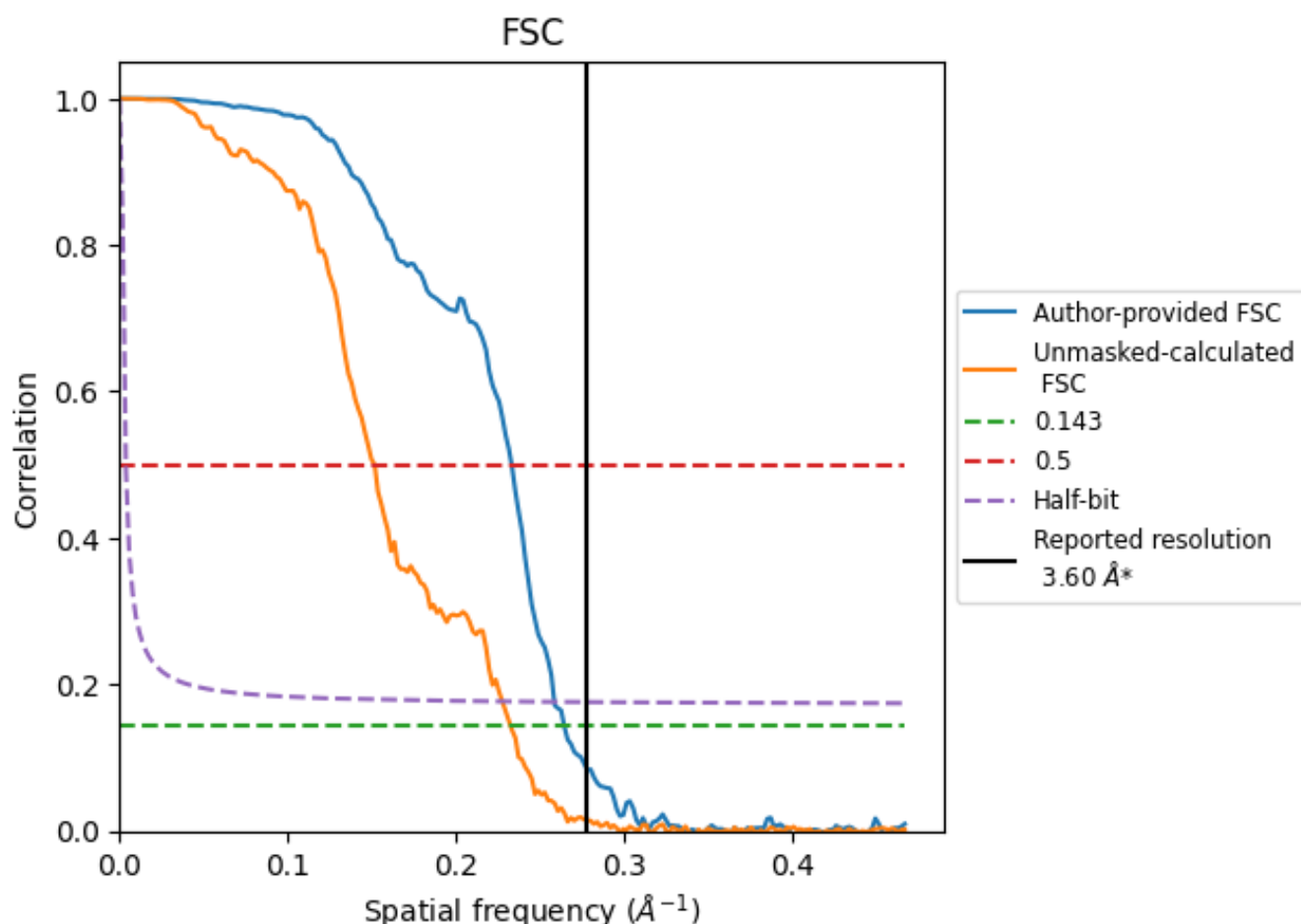


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

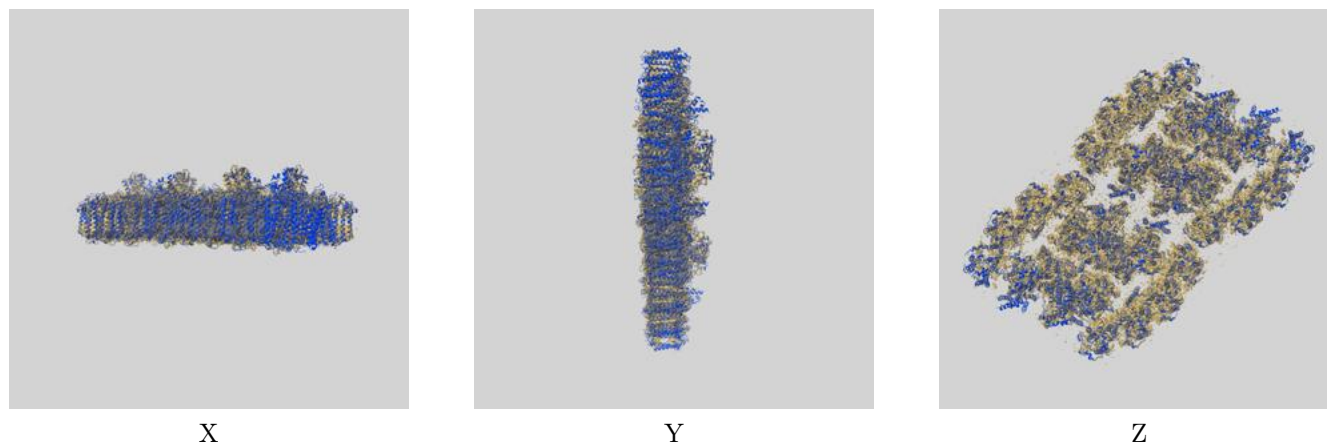
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.78	4.28	3.87
Unmasked-calculated*	4.30	6.59	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

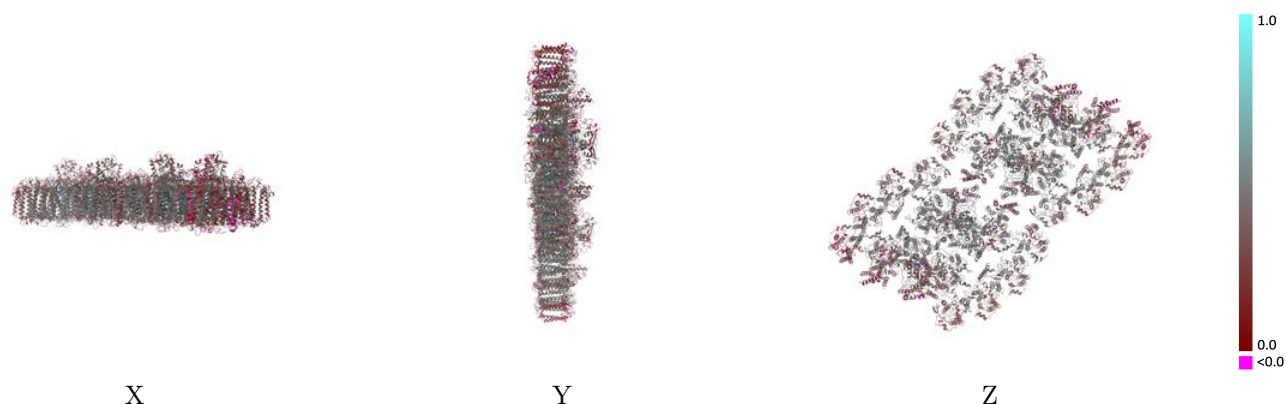
This section contains information regarding the fit between EMDB map EMD-33933 and PDB model 7YMM. Per-residue inclusion information can be found in section 3 on page 59.

9.1 Map-model overlay [i](#)



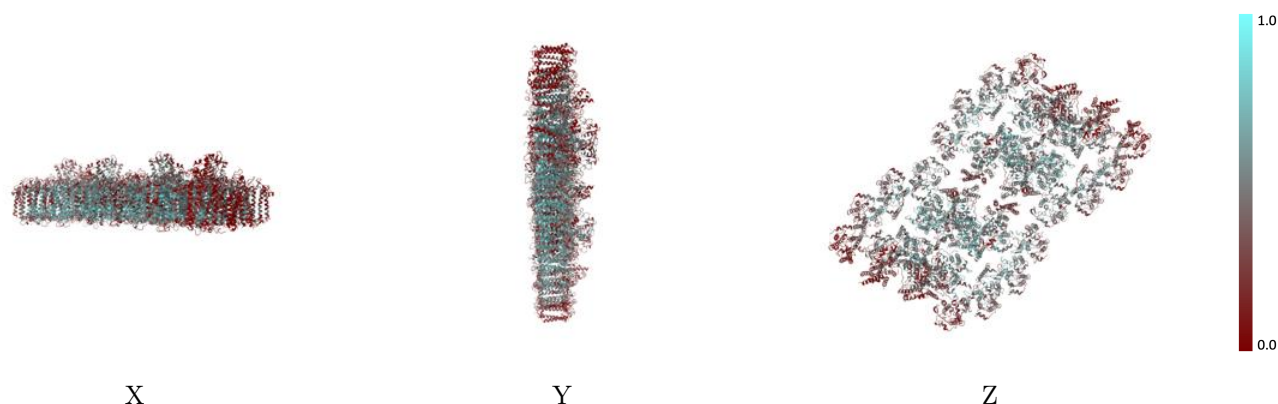
The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



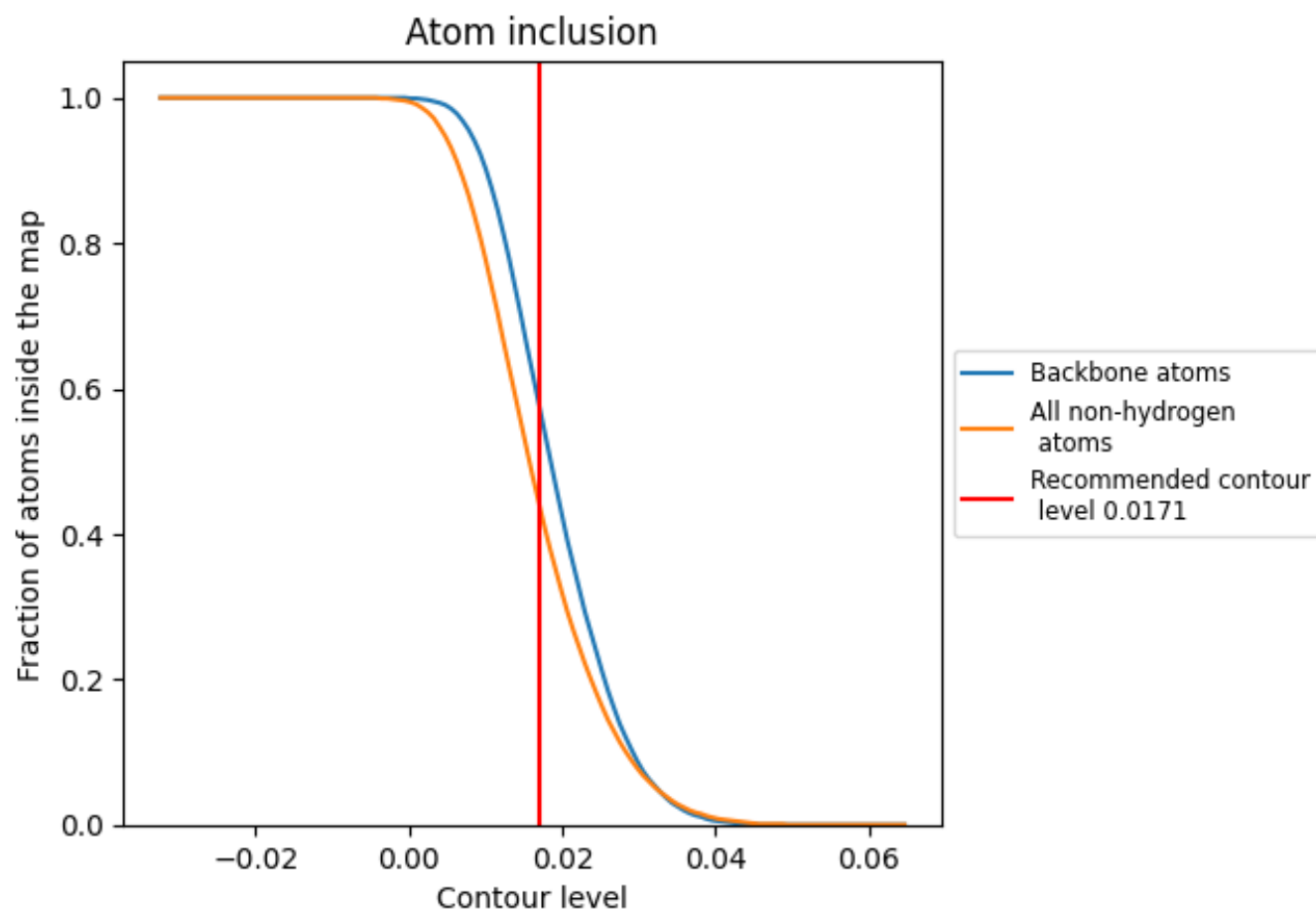
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0171).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 44% 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 (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4360	 0.4150
11	 0.1630	 0.2740
12	 0.3730	 0.4020
13	 0.4540	 0.4310
14	 0.2890	 0.3650
1A	 0.4920	 0.4560
1B	 0.4770	 0.4460
1C	 0.3450	 0.3770
1D	 0.4680	 0.4410
1E	 0.1260	 0.1690
1F	 0.1880	 0.2640
1G	 0.3900	 0.3740
1H	 0.3600	 0.3920
1I	 0.4510	 0.4530
1K	 0.0670	 0.2420
1L	 0.5750	 0.4890
1M	 0.4540	 0.4280
1T	 0.4120	 0.4430
1X	 0.1080	 0.2590
1Y	 0.0000	 0.1200
1Z	 0.0140	 0.1310
21	 0.4480	 0.4060
22	 0.4910	 0.4500
23	 0.4660	 0.4370
24	 0.4680	 0.4210
2A	 0.5940	 0.4900
2B	 0.5820	 0.4800
2C	 0.5220	 0.4400
2D	 0.6000	 0.4840
2E	 0.2790	 0.2920
2F	 0.4420	 0.3740
2G	 0.4240	 0.4160
2H	 0.5190	 0.4680
2I	 0.5920	 0.4840
2K	 0.2630	 0.3470











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Chain	Atom inclusion	Q-score
2L	 0.6180	 0.5080
2M	 0.5020	 0.4500
2T	 0.4870	 0.4680
2X	 0.2610	 0.3470
2Y	 0.1480	 0.2450
2Z	 0.1690	 0.2230
3I	 0.4470	 0.4050
32	 0.4920	 0.4480
33	 0.4660	 0.4380
34	 0.4680	 0.4210
3A	 0.5950	 0.4900
3B	 0.5810	 0.4800
3C	 0.5230	 0.4420
3D	 0.5980	 0.4840
3E	 0.2770	 0.2940
3F	 0.4420	 0.3720
3G	 0.4240	 0.4120
3H	 0.5170	 0.4680
3I	 0.5960	 0.4850
3K	 0.2660	 0.3490
3L	 0.6140	 0.5100
3M	 0.5020	 0.4520
3T	 0.4870	 0.4660
3X	 0.2610	 0.3460
3Y	 0.1480	 0.2410
3Z	 0.1690	 0.2290
4I	 0.1630	 0.2750
42	 0.3730	 0.4020
43	 0.4550	 0.4300
44	 0.2900	 0.3640
4A	 0.4930	 0.4570
4B	 0.4770	 0.4450
4C	 0.3460	 0.3780
4D	 0.4660	 0.4410
4E	 0.1240	 0.1710
4F	 0.1880	 0.2690
4G	 0.3760	 0.3820
4H	 0.3620	 0.3910
4I	 0.4440	 0.4520
4K	 0.0700	 0.2420
4L	 0.5750	 0.4870
4M	 0.4540	 0.4300

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Chain	Atom inclusion	Q-score
4T	 0.4120	 0.4440
4X	 0.1080	 0.2570
4Y	 0.0000	 0.1250
4Z	 0.0160	 0.1280