



Full wwPDB EM Validation Report ⓘ

Feb 18, 2024 – 06:56 PM JST

PDB ID : 8JZE
EMDB ID : EMD-36742
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.99 Å (reported)

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

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

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:

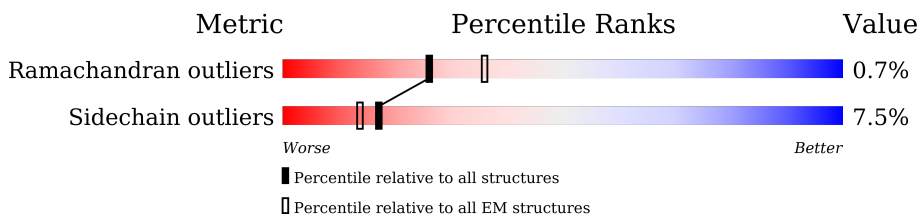
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.99 Å.

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



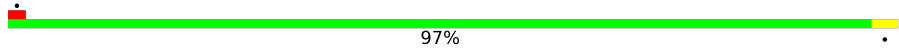
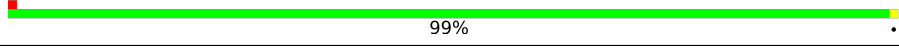
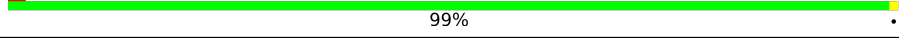
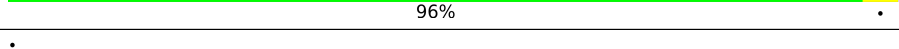
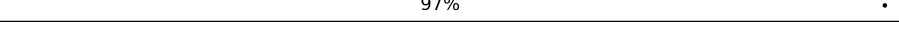
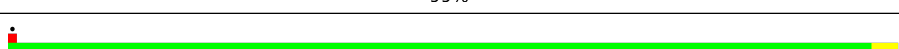
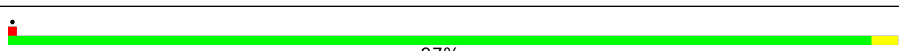
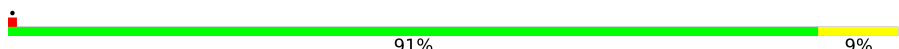


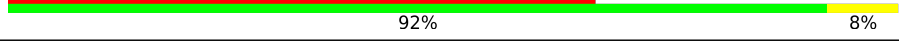
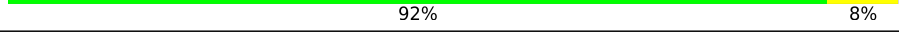
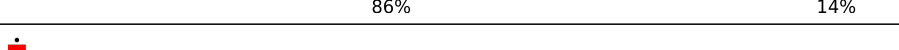
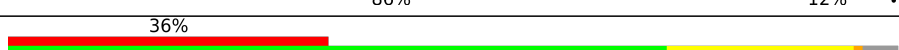
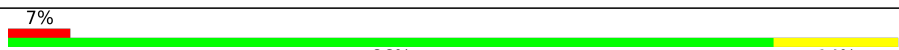


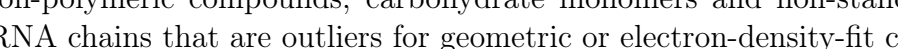
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	I	200	
2	K	177	
3	z	78	
4	y	131	
5	G	224	
6	A	189	
7	c	86	
8	d	218	
9	e	73	

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Mol	Chain	Length	Quality of chain
10	f	184	 97%
11	h	131	 99%
12	i	119	 99%
13	j	98	 96%
14	l	250	 97%
15	m	79	 99%
16	a	670	 97%
17	b	663	 97%
18	B	192	 91% 9%
19	D	165	 82% 15%
20	F	176	 86% 9% 6%
21	H	160	 92% 8% 66%
22	J	220	 92% 8%
23	L	185	 86% 14%
24	M	173	 86% 12%
25	N	160	 74% 21% 36%
26	O	161	 86% 14% 7%
27	P	160	 79% 21%

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
30	CLA	A	307	X	-	-	-
30	CLA	A	308	X	-	-	-
30	CLA	A	309	X	-	-	-
30	CLA	A	310	X	-	-	-
30	CLA	A	311	X	-	-	-
30	CLA	A	312	X	-	-	-
30	CLA	A	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	315	X	-	-	-
30	CLA	A	316	X	-	-	-
30	CLA	A	317	X	-	-	-
30	CLA	A	319	X	-	-	-
30	CLA	A	320	X	-	-	-
30	CLA	B	301	X	-	-	-
30	CLA	B	307	X	-	-	-
30	CLA	B	308	X	-	-	-
30	CLA	B	309	X	-	-	-
30	CLA	B	310	X	-	-	-
30	CLA	B	311	X	-	-	-
30	CLA	B	312	X	-	-	-
30	CLA	B	313	X	-	-	-
30	CLA	B	315	X	-	-	-
30	CLA	B	316	X	-	-	-
30	CLA	B	317	X	-	-	-
30	CLA	D	308	X	-	-	-
30	CLA	D	309	X	-	-	-
30	CLA	D	311	X	-	-	-
30	CLA	D	312	X	-	-	-
30	CLA	D	313	X	-	-	-
30	CLA	D	314	X	-	-	-
30	CLA	D	316	X	-	-	-
30	CLA	F	307	X	-	-	-
30	CLA	F	308	X	-	-	-
30	CLA	F	310	X	-	-	-
30	CLA	F	311	X	-	-	-
30	CLA	F	312	X	-	-	-
30	CLA	F	313	X	-	-	-
30	CLA	F	315	X	-	-	-
30	CLA	G	509	X	-	-	-
30	CLA	G	510	X	-	-	-
30	CLA	G	511	X	-	-	-
30	CLA	G	512	X	-	-	-
30	CLA	G	513	X	-	-	-
30	CLA	G	514	X	-	-	-
30	CLA	G	516	X	-	-	-
30	CLA	G	517	X	-	-	-
30	CLA	G	518	X	-	-	-
30	CLA	G	519	X	-	-	-
30	CLA	G	520	X	-	-	-
30	CLA	H	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	H	305	X	-	-	-
30	CLA	H	307	X	-	-	-
30	CLA	H	308	X	-	-	-
30	CLA	H	309	X	-	-	-
30	CLA	H	312	X	-	-	-
30	CLA	I	306	X	-	-	-
30	CLA	I	307	X	-	-	-
30	CLA	I	308	X	-	-	-
30	CLA	I	309	X	-	-	-
30	CLA	I	310	X	-	-	-
30	CLA	I	311	X	-	-	-
30	CLA	I	312	X	-	-	-
30	CLA	I	313	X	-	-	-
30	CLA	I	315	X	-	-	-
30	CLA	I	316	X	-	-	-
30	CLA	I	319	X	-	-	-
30	CLA	I	321	X	-	-	-
30	CLA	J	301	X	-	-	-
30	CLA	J	306	X	-	-	-
30	CLA	J	307	X	-	-	-
30	CLA	J	308	X	-	-	-
30	CLA	J	309	X	-	-	-
30	CLA	J	310	X	-	-	-
30	CLA	J	311	X	-	-	-
30	CLA	J	312	X	-	-	-
30	CLA	J	314	X	-	-	-
30	CLA	J	315	X	-	-	-
30	CLA	K	306	X	-	-	-
30	CLA	K	307	X	-	-	-
30	CLA	K	308	X	-	-	-
30	CLA	K	309	X	-	-	-
30	CLA	K	310	X	-	-	-
30	CLA	K	311	X	-	-	-
30	CLA	K	312	X	-	-	-
30	CLA	K	313	X	-	-	-
30	CLA	K	315	X	-	-	-
30	CLA	K	316	X	-	-	-
30	CLA	L	308	X	-	-	-
30	CLA	L	309	X	-	-	-
30	CLA	L	310	X	-	-	-
30	CLA	L	311	X	-	-	-
30	CLA	L	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	L	313	X	-	-	-
30	CLA	L	314	X	-	-	-
30	CLA	L	316	X	-	-	-
30	CLA	L	317	X	-	-	-
30	CLA	L	318	X	-	-	-
30	CLA	M	308	X	-	-	-
30	CLA	M	309	X	-	-	-
30	CLA	M	310	X	-	-	-
30	CLA	M	311	X	-	-	-
30	CLA	M	312	X	-	-	-
30	CLA	M	313	X	-	-	-
30	CLA	M	315	X	-	-	-
30	CLA	M	316	X	-	-	-
30	CLA	M	317	X	-	-	-
30	CLA	M	318	X	-	-	-
30	CLA	N	304	X	-	-	-
30	CLA	N	305	X	-	-	-
30	CLA	N	307	X	-	-	-
30	CLA	N	309	X	-	-	-
30	CLA	N	310	X	-	-	-
30	CLA	O	308	X	-	-	-
30	CLA	O	309	X	-	-	-
30	CLA	O	311	X	-	-	-
30	CLA	O	313	X	-	-	-
30	CLA	O	314	X	-	-	-
30	CLA	O	316	X	-	-	-
30	CLA	P	209	X	-	-	-
30	CLA	P	210	X	-	-	-
30	CLA	P	212	X	-	-	-
30	CLA	P	214	X	-	-	-
30	CLA	P	215	X	-	-	-
30	CLA	P	217	X	-	-	-
30	CLA	a	701	X	-	-	-
30	CLA	a	702	X	-	-	-
30	CLA	a	703	X	-	-	-
30	CLA	a	704	X	-	-	-
30	CLA	a	705	X	-	-	-
30	CLA	a	706	X	-	-	-
30	CLA	a	707	X	-	-	-
30	CLA	a	708	X	-	-	-
30	CLA	a	709	X	-	-	-
30	CLA	a	710	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	a	711	X	-	-	-
30	CLA	a	712	X	-	-	-
30	CLA	a	713	X	-	-	-
30	CLA	a	714	X	-	-	-
30	CLA	a	715	X	-	-	-
30	CLA	a	716	X	-	-	-
30	CLA	a	717	X	-	-	-
30	CLA	a	718	X	-	-	-
30	CLA	a	719	X	-	-	-
30	CLA	a	720	X	-	-	-
30	CLA	a	721	X	-	-	-
30	CLA	a	722	X	-	-	-
30	CLA	a	723	X	-	-	-
30	CLA	a	724	X	-	-	-
30	CLA	a	725	X	-	-	-
30	CLA	a	726	X	-	-	-
30	CLA	a	727	X	-	-	-
30	CLA	a	728	X	-	-	-
30	CLA	a	729	X	-	-	-
30	CLA	a	730	X	-	-	-
30	CLA	a	731	X	-	-	-
30	CLA	a	735	X	-	-	-
30	CLA	a	738	X	-	-	-
30	CLA	b	701	X	-	-	-
30	CLA	b	703	X	-	-	-
30	CLA	b	704	X	-	-	-
30	CLA	b	705	X	-	-	-
30	CLA	b	706	X	-	-	-
30	CLA	b	707	X	-	-	-
30	CLA	b	708	X	-	-	-
30	CLA	b	709	X	-	-	-
30	CLA	b	710	X	-	-	-
30	CLA	b	711	X	-	-	-
30	CLA	b	712	X	-	-	-
30	CLA	b	713	X	-	-	-
30	CLA	b	714	X	-	-	-
30	CLA	b	715	X	-	-	-
30	CLA	b	716	X	-	-	-
30	CLA	b	717	X	-	-	-
30	CLA	b	718	X	-	-	-
30	CLA	b	719	X	-	-	-
30	CLA	b	720	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	721	X	-	-	-
30	CLA	b	722	X	-	-	-
30	CLA	b	723	X	-	-	-
30	CLA	b	724	X	-	-	-
30	CLA	b	725	X	-	-	-
30	CLA	b	726	X	-	-	-
30	CLA	b	727	X	-	-	-
30	CLA	b	728	X	-	-	-
30	CLA	f	301	X	-	-	-
30	CLA	f	302	X	-	-	-
30	CLA	f	303	X	-	-	-
30	CLA	h	202	X	-	-	-
30	CLA	j	104	X	-	-	-
30	CLA	j	106	X	-	-	-
30	CLA	l	303	X	-	-	-
30	CLA	l	304	X	-	-	-
30	CLA	l	305	X	-	-	-
30	CLA	l	308	X	-	-	-
30	CLA	l	309	X	-	-	-
30	CLA	l	311	X	-	-	-
30	CLA	l	312	X	-	-	-
30	CLA	l	313	X	-	-	-
30	CLA	m	202	X	-	-	-

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 55927 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 Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	200	1480	961	250	259	10	0	0

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	177	1349	872	227	238	12	0	0

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	z	78	390	234	78	78	0	0

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	y	131	655	393	131	131	0	0

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	217	1572	1004	269	289	10	0	0

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total	C	N	O	0	0
			783	505	125	153		

- Molecule 14 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	250	Total	C	N	O	S	0	0
			1943	1267	312	354	10		

- Molecule 15 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	79	Total	C	N	O	S	0	0
			582	373	100	107	2		

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	670	Total	C	N	O	S	0	0
			5194	3393	875	910	16		

- Molecule 17 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	663	Total	C	N	O	S	0	0
			5199	3408	851	928	12		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	192	Total	C	N	O	S	0	0
			1452	934	241	265	12		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	160	Total	C	N	O	S	0	0
			1158	728	195	228	7		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	F	169	1237	777	209	239	12	0	0

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	H	160	1202	769	198	228	7	0	0

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	J	220	1496	938	261	290	7	0	0

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	L	185	1427	924	239	258	6	0	0

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	M	168	1211	773	208	225	5	0	0

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	N	153	993	607	179	202	5	0	0

- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	161	Total	C	N	O	S	0	0
			1073	670	189	207	7		

- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	159	Total	C	N	O	S	0	0
			1113	693	191	223	6		

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	K	1	Total	C	O	0
			43	40	3	
28	K	1	Total	C	O	0
			43	40	3	

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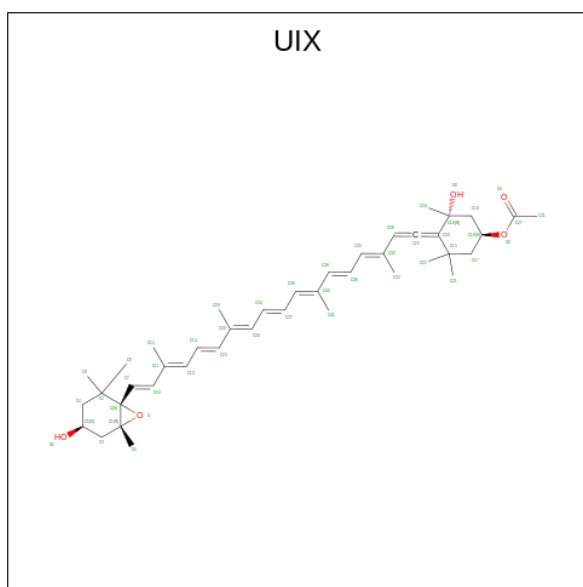
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	K	1	43	40	3	0
28	K	1	43	40	3	0
28	K	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	G	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	A	1	43	40	3	0
28	h	1	43	40	3	0
28	b	1	43	40	3	0
28	B	1	42	39	3	0
28	B	1	43	40	3	0
28	B	1	43	40	3	0
28	B	1	43	40	3	0
28	D	1	43	40	3	0
28	F	1	43	40	3	0
28	F	1	43	40	3	0
28	H	1	43	40	3	0

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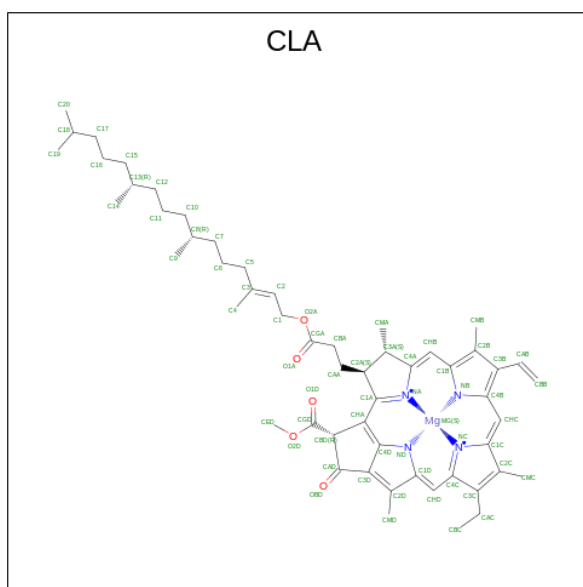
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	J	1	43	40	3	0
28	J	1	43	40	3	0
28	J	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	L	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	M	1	43	40	3	0
28	N	1	43	40	3	0
28	O	1	43	40	3	0
28	P	1	43	40	3	0

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyldene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			47	42	5	
29	K	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	h	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	O	1	Total	C	O	0
			47	42	5	
29	P	1	Total	C	O	0
			47	42	5	

- Molecule 30 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
30	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	K	1	54	44	1	4	5	0
30	K	1	50	40	1	4	5	0
30	K	1	55	45	1	4	5	0
30	K	1	52	42	1	4	5	0
30	K	1	48	38	1	4	5	0
30	K	1	55	45	1	4	5	0
30	K	1	41	33	1	4	3	0
30	K	1	46	36	1	4	5	0
30	G	1	51	41	1	4	5	0
30	G	1	65	55	1	4	5	0
30	G	1	55	45	1	4	5	0
30	G	1	60	50	1	4	5	0
30	G	1	65	55	1	4	5	0
30	G	1	53	43	1	4	5	0
30	G	1	41	33	1	4	3	0
30	G	1	46	36	1	4	5	0
30	G	1	46	36	1	4	5	0
30	G	1	61	51	1	4	5	0
30	G	1	49	39	1	4	5	0
30	A	1	45	35	1	4	5	0
30	A	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	A	1	55	45	1	4	5	0
30	A	1	65	55	1	4	5	0
30	A	1	46	36	1	4	5	0
30	A	1	55	45	1	4	5	0
30	A	1	55	45	1	4	5	0
30	A	1	41	33	1	4	3	0
30	A	1	47	37	1	4	5	0
30	A	1	41	33	1	4	3	0
30	A	1	46	36	1	4	5	0
30	A	1	46	36	1	4	5	0
30	f	1	55	45	1	4	5	0
30	f	1	46	36	1	4	5	0
30	f	1	46	36	1	4	5	0
30	h	1	55	45	1	4	5	0
30	j	1	55	45	1	4	5	0
30	j	1	58	48	1	4	5	0
30	l	1	65	55	1	4	5	0
30	l	1	60	50	1	4	5	0
30	l	1	65	55	1	4	5	0
30	l	1	41	33	1	4	3	0
30	l	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O		
30	l	1	Total 45	C 36	N 4	O 5	0	
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	l	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	b	1	48	38	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	60	50	1	4	5	0
30	b	1	52	42	1	4	5	0
30	b	1	55	45	1	4	5	0
30	b	1	54	44	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	60	50	1	4	5	0
30	b	1	50	40	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	51	41	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	53	43	1	4	5	0
30	b	1	46	36	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	50	40	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	b	1	47	37	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	b	1	65	55	1	4	5	0
30	b	1	65	55	1	4	5	0
30	B	1	60	50	1	4	5	0
30	B	1	49	39	1	4	5	0
30	B	1	45	35	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	55	45	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	51	41	1	4	5	0
30	B	1	65	55	1	4	5	0
30	B	1	41	33	1	4	3	0
30	B	1	46	36	1	4	5	0
30	B	1	45	35	1	4	5	0
30	D	1	47	37	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	45	35	1	4	5	0
30	D	1	46	36	1	4	5	0
30	D	1	41	33	1	4	3	0
30	F	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	46	36	1	4	5	0
30	F	1	41	33	1	4	3	0
30	H	1	47	37	1	4	5	0
30	H	1	65	55	1	4	5	0
30	H	1	51	41	1	4	5	0
30	H	1	46	36	1	4	5	0
30	H	1	47	37	1	4	5	0
30	H	1	41	33	1	4	3	0
30	H	1	46	36	1	4	5	0
30	J	1	60	50	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	65	55	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	56	46	1	4	5	0
30	J	1	46	36	1	4	5	0
30	J	1	47	37	1	4	5	0
30	J	1	53	43	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	J	1	41	33	1	4	3	0
30	J	1	46	36	1	4	5	0
30	J	1	46	36	1	4	5	0
30	L	1	47	39	1	4	3	0
30	L	1	53	43	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	46	36	1	4	5	0
30	L	1	55	45	1	4	5	0
30	L	1	53	43	1	4	5	0
30	L	1	41	33	1	4	3	0
30	L	1	52	42	1	4	5	0
30	L	1	46	36	1	4	5	0
30	M	1	53	43	1	4	5	0
30	M	1	55	45	1	4	5	0
30	M	1	48	38	1	4	5	0
30	M	1	46	36	1	4	5	0
30	M	1	48	38	1	4	5	0
30	M	1	46	36	1	4	5	0
30	M	1	41	33	1	4	3	0
30	M	1	52	42	1	4	5	0

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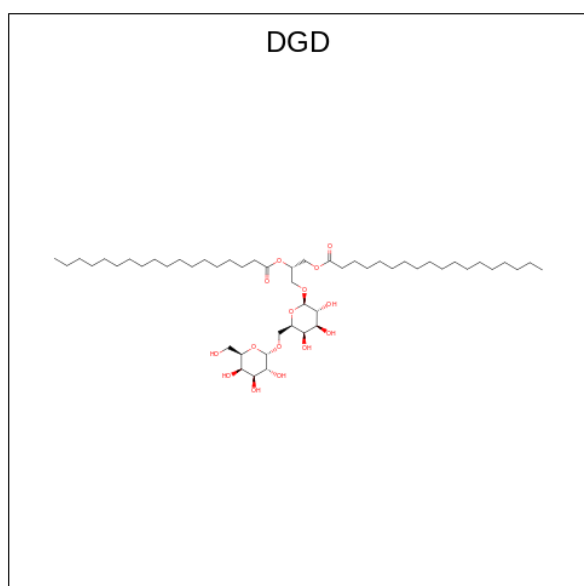
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	M	1	46	36	1	4	5	0
30	M	1	46	36	1	4	5	0
30	N	1	47	37	1	4	5	0
30	N	1	65	55	1	4	5	0
30	N	1	51	41	1	4	5	0
30	N	1	46	36	1	4	5	0
30	N	1	47	37	1	4	5	0
30	O	1	47	37	1	4	5	0
30	O	1	65	55	1	4	5	0
30	O	1	51	41	1	4	5	0
30	O	1	46	36	1	4	5	0
30	O	1	47	37	1	4	5	0
30	O	1	41	33	1	4	3	0
30	P	1	47	37	1	4	5	0
30	P	1	65	55	1	4	5	0
30	P	1	51	41	1	4	5	0
30	P	1	46	36	1	4	5	0
30	P	1	47	37	1	4	5	0
30	P	1	41	33	1	4	3	0

- Molecule 31 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

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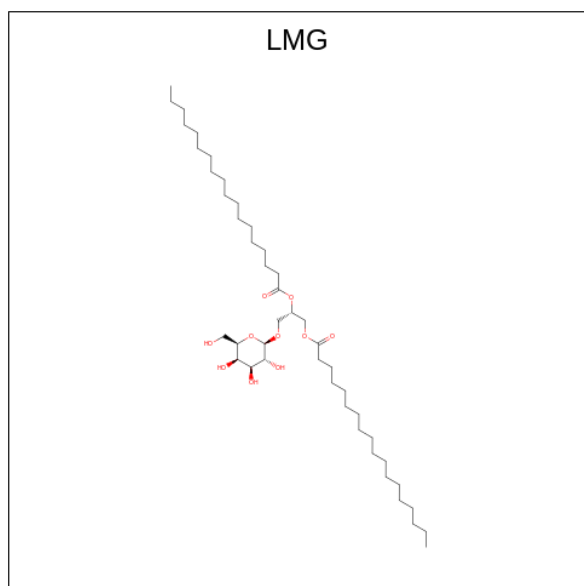
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	P	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 32 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
32	I	1	Total	C	O	0
			39	24	15	
32	y	1	Total	C	O	0
			54	39	15	
32	G	1	Total	C	O	0
			45	30	15	
32	G	1	Total	C	O	0
			44	29	15	
32	j	1	Total	C	O	0
			41	26	15	
32	l	1	Total	C	O	0
			50	35	15	
32	L	1	Total	C	O	0
			38	23	15	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



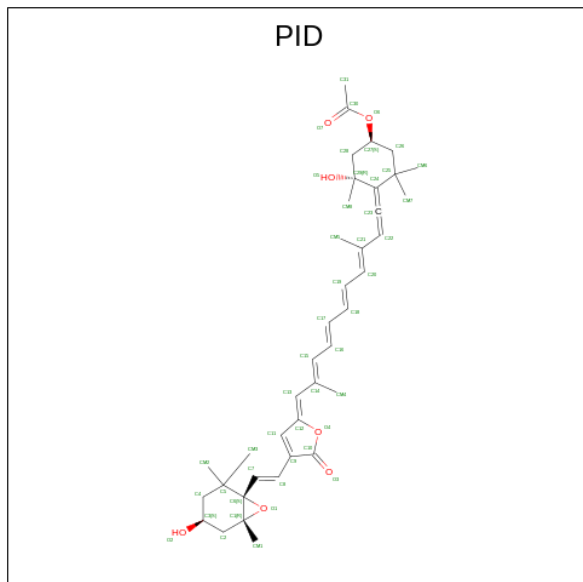
Mol	Chain	Residues	Atoms			AltConf
33	I	1	Total	C	O	0
			36	26	10	
33	I	1	Total	C	O	0
			38	28	10	
33	K	1	Total	C	O	0
			43	33	10	
33	j	1	Total	C	O	0
			35	25	10	

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Mol	Chain	Residues	Atoms			AltConf
33	b	1	Total	C	O	0
			44	34	10	
33	b	1	Total	C	O	0
			31	21	10	
33	B	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			49	39	10	
33	P	1	Total	C	O	0
			27	17	10	

- Molecule 34 is PERIDININ (three-letter code: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	G	1	Total	C	O	0
			46	39	7	
34	G	1	Total	C	O	0
			46	39	7	
34	j	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	

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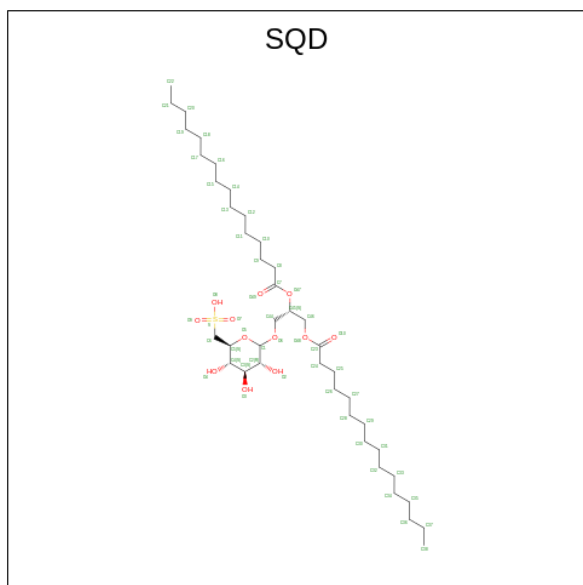
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	D	1	46	39	7	0
34	D	1	46	39	7	0
34	D	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	F	1	46	39	7	0
34	H	1	46	39	7	0
34	H	1	46	39	7	0
34	M	1	46	39	7	0
34	N	1	46	39	7	0
34	N	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	O	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0
34	P	1	46	39	7	0

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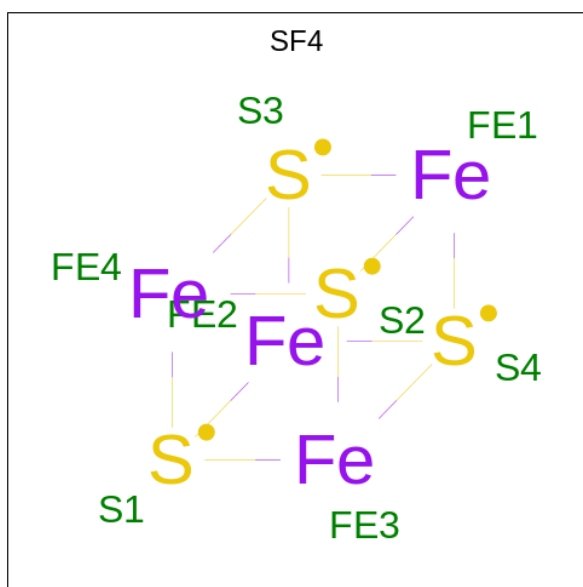
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	P	1	46	39	7	0

- Molecule 35 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).



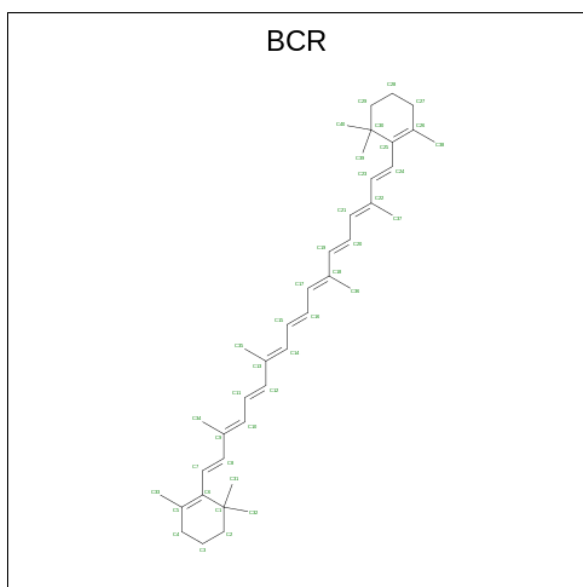
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
35	A	1	50	37	12	1	0

- Molecule 36 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
36	c	1	Total Fe S 8 4 4	0
36	c	1	Total Fe S 8 4 4	0
36	a	1	Total Fe S 8 4 4	0

- Molecule 37 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



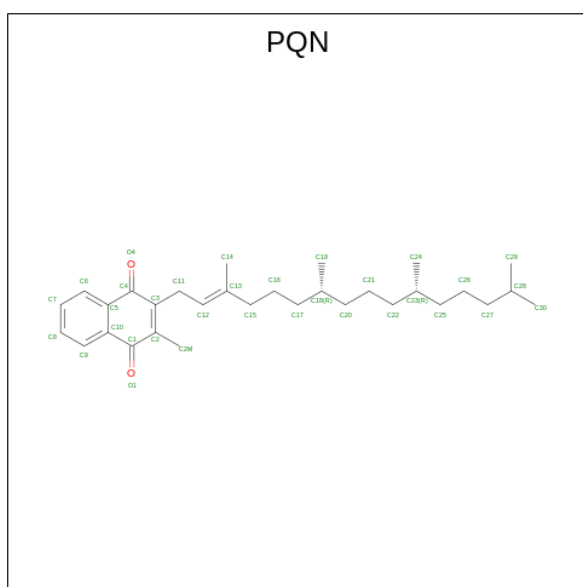
Mol	Chain	Residues	Atoms	AltConf
37	f	1	Total C 40 40	0

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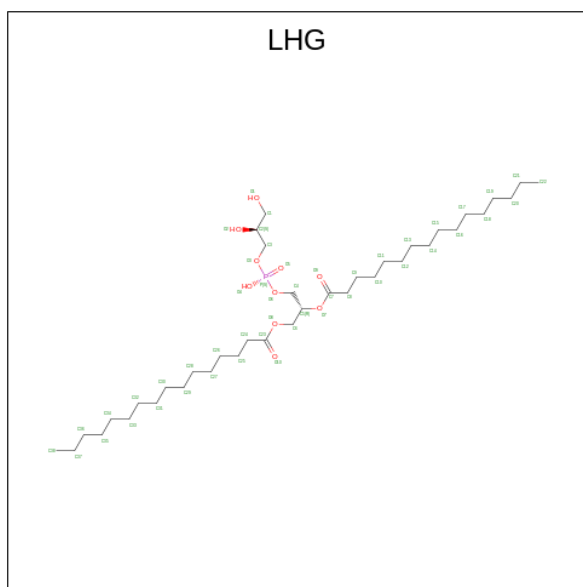
Mol	Chain	Residues	Atoms	AltConf
37	i	1	Total C 40 40	0
37	j	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	m	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0

- Molecule 38 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total	C	O	0
			33	31	2	
38	b	1	Total	C	O	0
			33	31	2	

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

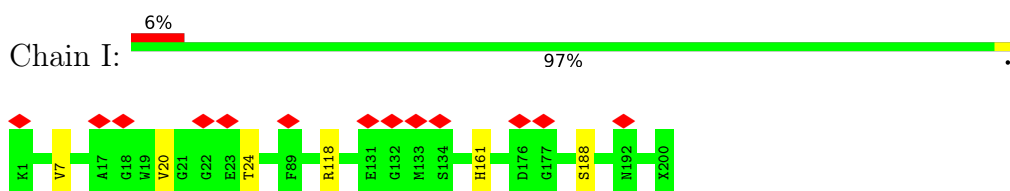


Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total	C	O	P	0
			48	37	10	1	

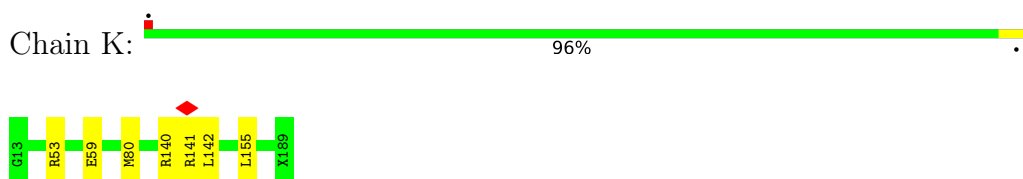
3 Residue-property plots

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

- Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



- Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

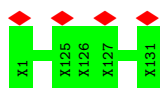


- Molecule 3: Photosystem I unk



There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I unk

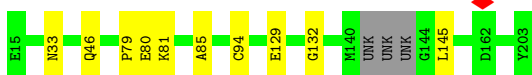


- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



- Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:  93% 5%



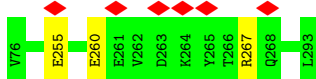
- Molecule 7: Photosystem I PsaC

Chain c:  99%



- Molecule 8: Photosystem I PsaD

Chain d:  99%



- Molecule 9: Photosystem I PsaE

Chain e:  100%

There are no outlier residues recorded for this chain.

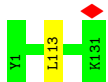
- Molecule 10: Photosystem I PsaF

Chain f:  97%



- Molecule 11: Photosystem I PsaR

Chain h:  99%



- Molecule 12: Photosystem I PsaI

Chain i:  99%



- Molecule 13: Photosystem I PsaJ

Chain j:  96%



- Molecule 14: Photosystem I PsaL

Chain l:  97%



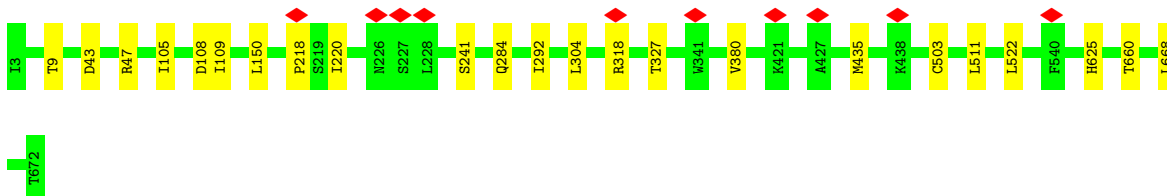
- Molecule 15: Photosystem I PsaM

Chain m:  99%



- Molecule 16: Photosystem I PsaA

Chain a:  97%



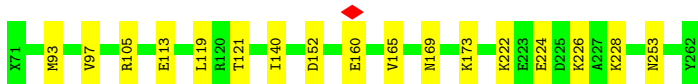
- Molecule 17: Photosystem I PsaB

Chain b:  97%




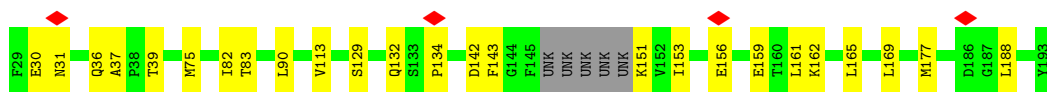
- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

Chain B:  91%

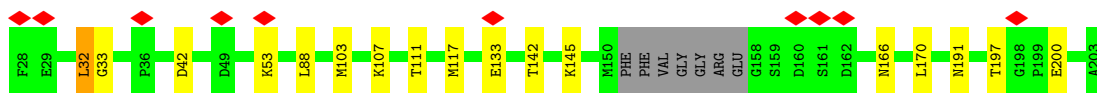
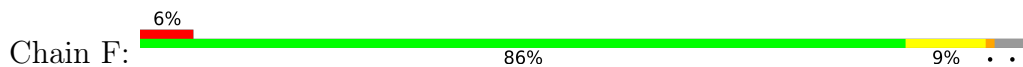


- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

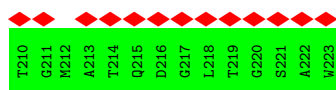
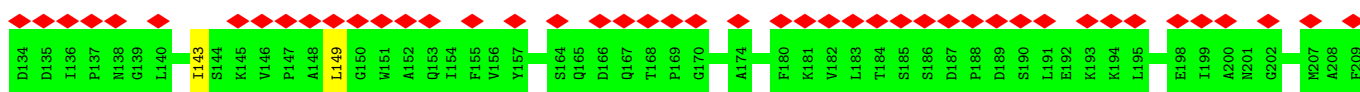
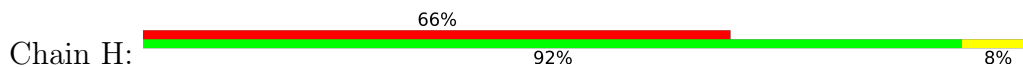
Chain D:  82%



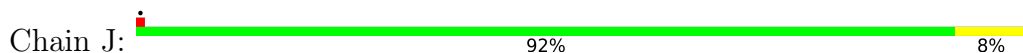
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2



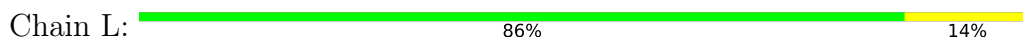
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



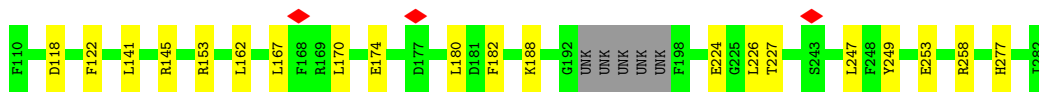
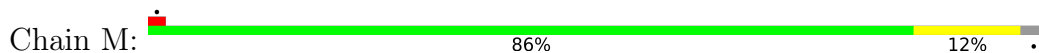
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



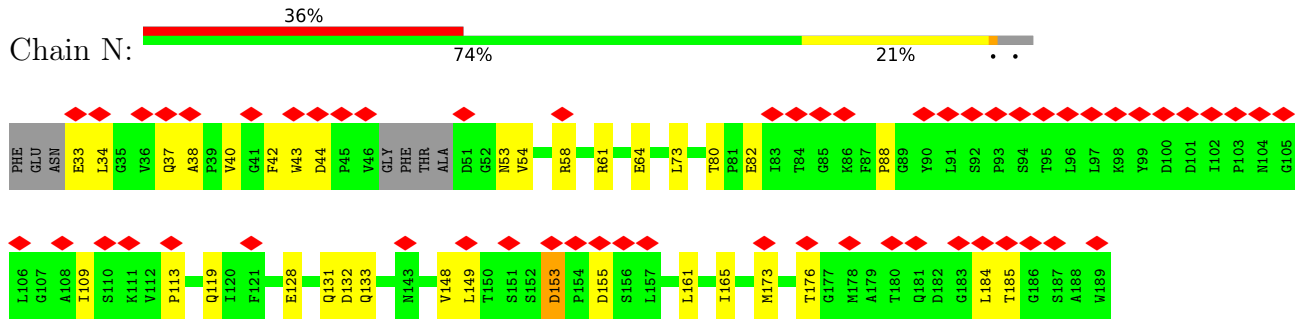
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



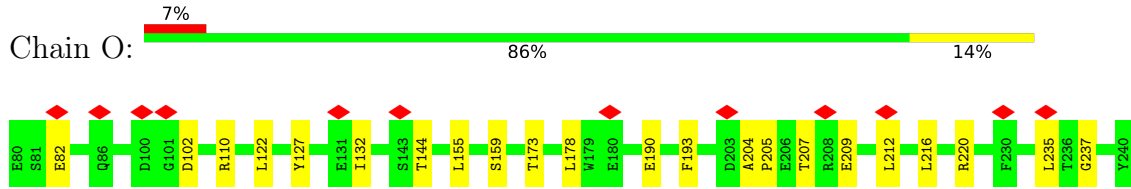
- Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



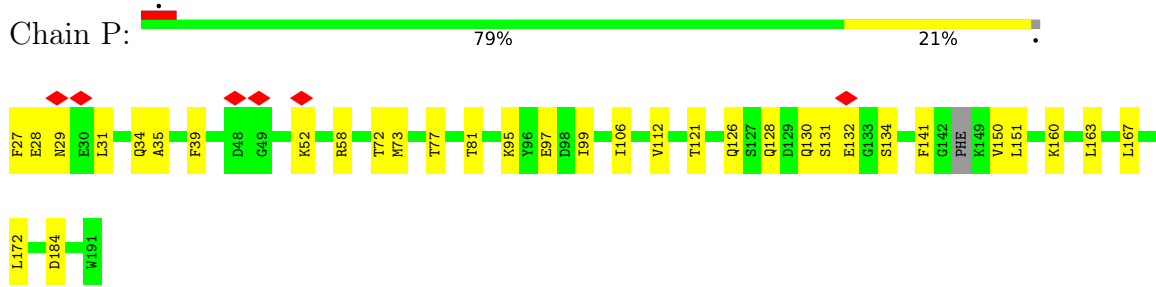
- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



- Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15



- Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46321	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.690	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.235	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LHG, DGD, SF4, BCR, PID, KC1, SQD, DD6, LMG, UIX, CLA

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	I	0.27	0/1484	0.46	0/2019
2	K	0.27	0/1357	0.48	0/1838
5	G	0.32	0/1562	0.48	0/2122
6	A	0.33	0/1276	0.48	0/1725
7	c	0.26	0/663	0.51	0/902
8	d	0.26	0/1767	0.50	0/2375
9	e	0.33	0/608	0.42	0/833
10	f	0.26	0/1489	0.47	0/2016
11	h	0.26	0/1101	0.40	0/1493
12	i	0.26	0/992	0.48	0/1346
13	j	0.26	0/801	0.45	0/1092
14	l	0.28	0/1998	0.45	0/2706
15	m	0.27	0/590	0.48	0/793
16	a	0.30	0/5344	0.47	0/7280
17	b	0.28	0/5362	0.44	0/7335
18	B	0.27	0/1382	0.46	0/1862
19	D	0.29	0/1178	0.50	0/1592
20	F	0.28	0/1263	0.51	0/1708
21	H	0.27	0/1232	0.49	0/1665
22	J	0.27	0/1246	0.45	0/1699
23	L	0.29	0/1462	0.47	0/1985
24	M	0.27	0/1241	0.46	0/1681
25	N	0.27	0/1005	0.53	0/1370
26	O	0.25	0/1091	0.49	0/1491
27	P	0.30	0/1128	0.47	0/1523
All	All	0.28	0/38622	0.47	0/52451

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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	I	191/200 (96%)	163 (85%)	28 (15%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	175 (86%)	27 (13%)	2 (1%)	15	53
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	5	28
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	29	68
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	34	72
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	34	72
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	47	82
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	8	37
19	D	156/165 (94%)	131 (84%)	22 (14%)	3 (2%)	8	36
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	13	48
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	25	64
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	3	17
26	O	159/161 (99%)	130 (82%)	25 (16%)	4 (2%)	5	28
27	P	155/160 (97%)	135 (87%)	19 (12%)	1 (1%)	25	64
All	All	4901/5113 (96%)	4446 (91%)	421 (9%)	34 (1%)	26	60

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG
16	a	218	PRO
19	D	134	PRO
21	H	72	ALA
25	N	88	PRO
25	N	109	ILE
25	N	113	PRO
25	N	153	ASP
26	O	159	SER
26	O	205	PRO
27	P	35	ALA
5	G	76	PHE
21	H	125	LEU
26	O	204	ALA
6	A	79	PRO
10	f	254	GLN
19	D	156	GLU
16	a	220	ILE
18	B	119	LEU
20	F	33	GLY
22	J	74	GLU
18	B	93	MET
20	F	32	LEU
25	N	82	GLU
6	A	33	ASN
17	b	311	LEU

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Mol	Chain	Res	Type
19	D	37	ALA
6	A	132	GLY
18	B	165	VAL
25	N	38	ALA
26	O	237	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	139/155 (90%)	133 (96%)	6 (4%)	29 66
2	K	133/138 (96%)	126 (95%)	7 (5%)	22 58
5	G	147/171 (86%)	140 (95%)	7 (5%)	25 62
6	A	122/129 (95%)	116 (95%)	6 (5%)	25 61
7	c	76/76 (100%)	75 (99%)	1 (1%)	69 89
8	d	182/184 (99%)	179 (98%)	3 (2%)	62 86
9	e	63/63 (100%)	63 (100%)	0	100 100
10	f	148/148 (100%)	144 (97%)	4 (3%)	44 77
11	h	112/114 (98%)	111 (99%)	1 (1%)	78 92
12	i	100/101 (99%)	99 (99%)	1 (1%)	76 91
13	j	88/89 (99%)	84 (96%)	4 (4%)	27 64
14	l	199/201 (99%)	192 (96%)	7 (4%)	36 71
15	m	60/63 (95%)	59 (98%)	1 (2%)	60 85
16	a	540/592 (91%)	520 (96%)	20 (4%)	34 70
17	b	557/581 (96%)	539 (97%)	18 (3%)	39 74
18	B	142/146 (97%)	128 (90%)	14 (10%)	8 30
19	D	116/123 (94%)	94 (81%)	22 (19%)	1 8
20	F	126/140 (90%)	110 (87%)	16 (13%)	4 19
21	H	123/123 (100%)	113 (92%)	10 (8%)	11 40
22	J	124/136 (91%)	108 (87%)	16 (13%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	9
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	8
25	N	80/124 (64%)	51 (64%)	29 (36%)	0	1
26	O	89/124 (72%)	71 (80%)	18 (20%)	1	6
27	P	105/123 (85%)	73 (70%)	32 (30%)	0	1
All	All	3817/4117 (93%)	3529 (92%)	288 (8%)	17	43

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	VAL
1	I	20	VAL
1	I	24	THR
1	I	118	ARG
1	I	161	HIS
1	I	188	SER
2	K	53	ARG
2	K	59	GLU
2	K	80	MET
2	K	140	ARG
2	K	141	ARG
2	K	142	LEU
2	K	155	LEU
5	G	17	VAL
5	G	42	SER
5	G	68	LYS
5	G	81	VAL
5	G	92	GLU
5	G	147	ILE
5	G	220	LEU
6	A	46	GLN
6	A	80	GLU
6	A	81	LYS
6	A	94	CYS
6	A	129	GLU
6	A	145	LEU
7	c	127	VAL
8	d	255	GLU
8	d	260	GLU
8	d	267	ARG

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Mol	Chain	Res	Type
10	f	113	LEU
10	f	156	CYS
10	f	187	ILE
10	f	243	ASN
11	h	113	LEU
12	i	169	HIS
13	j	22	LYS
13	j	33	THR
13	j	57	VAL
13	j	71	VAL
14	l	68	ASN
14	l	71	GLU
14	l	72	ASP
14	l	166	THR
14	l	202	PHE
14	l	252	LYS
14	l	255	ASP
15	m	128	LYS
16	a	9	THR
16	a	43	ASP
16	a	105	ILE
16	a	108	ASP
16	a	109	ILE
16	a	150	LEU
16	a	241	SER
16	a	284	GLN
16	a	292	ILE
16	a	304	LEU
16	a	318	ARG
16	a	327	THR
16	a	380	VAL
16	a	435	MET
16	a	503	CYS
16	a	511	LEU
16	a	522	LEU
16	a	625	HIS
16	a	660	THR
16	a	668	LEU
17	b	36	ARG
17	b	58	ILE
17	b	63	SER
17	b	184	LEU

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Mol	Chain	Res	Type
17	b	188	LEU
17	b	238	ILE
17	b	289	HIS
17	b	325	ILE
17	b	434	ILE
17	b	547	TYR
17	b	557	ASN
17	b	570	THR
17	b	596	LEU
17	b	602	THR
17	b	650	THR
17	b	651	PRO
17	b	662	TYR
17	b	667	LEU
18	B	97	VAL
18	B	105	ARG
18	B	113	GLU
18	B	121	THR
18	B	140	ILE
18	B	152	ASP
18	B	160	GLU
18	B	169	ASN
18	B	173	LYS
18	B	222	LYS
18	B	224	GLU
18	B	226	LYS
18	B	228	LYS
18	B	253	ASN
19	D	30	GLU
19	D	31	ASN
19	D	36	GLN
19	D	39	THR
19	D	75	MET
19	D	82	ILE
19	D	83	THR
19	D	90	LEU
19	D	113	VAL
19	D	129	SER
19	D	132	GLN
19	D	142	ASP
19	D	143	PHE
19	D	151	LYS

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Mol	Chain	Res	Type
19	D	153	ILE
19	D	159	GLU
19	D	161	LEU
19	D	162	LYS
19	D	165	LEU
19	D	169	LEU
19	D	177	MET
19	D	188	LEU
20	F	32	LEU
20	F	42	ASP
20	F	53	LYS
20	F	88	LEU
20	F	103	MET
20	F	107	LYS
20	F	111	THR
20	F	117	MET
20	F	133	GLU
20	F	142	THR
20	F	145	LYS
20	F	166	ASN
20	F	170	LEU
20	F	191	ASN
20	F	197	THR
20	F	200	GLU
21	H	70	VAL
21	H	85	ASP
21	H	89	LYS
21	H	91	PHE
21	H	106	MET
21	H	107	LEU
21	H	110	MET
21	H	130	LEU
21	H	143	ILE
21	H	149	LEU
22	J	73	ARG
22	J	97	THR
22	J	98	ASN
22	J	99	ASN
22	J	134	HIS
22	J	136	LEU
22	J	154	ASN
22	J	156	LEU

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Mol	Chain	Res	Type
22	J	158	LEU
22	J	174	LEU
22	J	188	ASP
22	J	189	VAL
22	J	192	MET
22	J	196	LEU
22	J	197	GLU
22	J	198	GLU
23	L	97	ARG
23	L	98	ARG
23	L	100	LEU
23	L	102	VAL
23	L	116	LYS
23	L	125	GLU
23	L	132	GLU
23	L	173	ARG
23	L	187	VAL
23	L	188	ILE
23	L	189	ASP
23	L	194	LEU
23	L	195	ASN
23	L	218	LYS
23	L	221	GLU
23	L	232	ASN
23	L	237	PHE
23	L	239	GLU
23	L	240	ASP
23	L	241	ASP
23	L	245	LYS
23	L	249	ILE
23	L	270	VAL
23	L	272	THR
23	L	274	LYS
24	M	118	ASP
24	M	122	PHE
24	M	141	LEU
24	M	145	ARG
24	M	153	ARG
24	M	162	LEU
24	M	167	LEU
24	M	170	LEU
24	M	174	GLU

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Mol	Chain	Res	Type
24	M	180	LEU
24	M	182	PHE
24	M	188	LYS
24	M	224	GLU
24	M	226	LEU
24	M	227	THR
24	M	247	LEU
24	M	249	TYR
24	M	253	GLU
24	M	258	ARG
24	M	277	HIS
25	N	33	GLU
25	N	34	LEU
25	N	37	GLN
25	N	40	VAL
25	N	42	PHE
25	N	43	TRP
25	N	44	ASP
25	N	53	ASN
25	N	54	VAL
25	N	58	ARG
25	N	61	ARG
25	N	64	GLU
25	N	73	LEU
25	N	80	THR
25	N	119	GLN
25	N	128	GLU
25	N	131	GLN
25	N	132	ASP
25	N	133	GLN
25	N	148	VAL
25	N	149	LEU
25	N	153	ASP
25	N	155	ASP
25	N	161	LEU
25	N	165	ILE
25	N	173	MET
25	N	176	THR
25	N	184	LEU
25	N	185	THR
26	O	82	GLU
26	O	102	ASP

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Mol	Chain	Res	Type
26	O	110	ARG
26	O	122	LEU
26	O	127	TYR
26	O	132	ILE
26	O	144	THR
26	O	155	LEU
26	O	173	THR
26	O	178	LEU
26	O	190	GLU
26	O	193	PHE
26	O	207	THR
26	O	209	GLU
26	O	212	LEU
26	O	216	LEU
26	O	220	ARG
26	O	235	LEU
27	P	27	PHE
27	P	28	GLU
27	P	29	ASN
27	P	31	LEU
27	P	34	GLN
27	P	39	PHE
27	P	52	LYS
27	P	58	ARG
27	P	72	THR
27	P	73	MET
27	P	77	THR
27	P	81	THR
27	P	95	LYS
27	P	97	GLU
27	P	99	ILE
27	P	106	ILE
27	P	112	VAL
27	P	121	THR
27	P	126	GLN
27	P	128	GLN
27	P	130	GLN
27	P	131	SER
27	P	132	GLU
27	P	134	SER
27	P	141	PHE
27	P	150	VAL

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Mol	Chain	Res	Type
27	P	151	LEU
27	P	160	LYS
27	P	163	LEU
27	P	167	LEU
27	P	172	LEU
27	P	184	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	61	GLN
10	f	247	HIS
13	j	72	ASN
16	a	284	GLN
19	D	55	ASN
20	F	166	ASN
23	L	268	GLN
27	P	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

342 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	G	516	5	41,49,73	1.88	5 (12%)	47,84,113	1.65	7 (14%)
30	CLA	I	319	30	45,53,73	1.77	6 (13%)	52,89,113	1.64	7 (13%)
30	CLA	B	312	-	51,59,73	1.69	5 (9%)	59,96,113	1.48	8 (13%)
30	CLA	j	106	-	58,66,73	1.58	6 (10%)	67,104,113	1.46	8 (11%)
30	CLA	A	320	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	6 (11%)
30	CLA	b	726	-	47,55,73	1.77	5 (10%)	54,91,113	1.51	8 (14%)
34	PID	O	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.31	6 (12%)
29	UIX	B	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.45	16 (30%)
37	BCR	i	201	-	41,41,41	0.82	2 (4%)	56,56,56	2.11	20 (35%)
30	CLA	K	312	-	48,56,73	1.72	7 (14%)	55,92,113	1.53	7 (12%)
30	CLA	A	317	-	41,49,73	1.86	5 (12%)	47,84,113	1.65	9 (19%)
30	CLA	a	726	-	65,73,73	1.51	7 (10%)	76,113,113	1.37	9 (11%)
30	CLA	F	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.59	8 (15%)
28	DD6	D	303	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)
35	SQD	A	318	-	49,50,54	0.40	1 (2%)	58,61,65	0.59	0
30	CLA	A	313	-	55,63,73	1.60	5 (9%)	64,101,113	1.45	9 (14%)
34	PID	P	202	-	41,49,49	1.33	4 (9%)	49,76,76	1.60	7 (14%)
30	CLA	O	314	-	47,55,73	1.74	6 (12%)	54,91,113	1.66	8 (14%)
29	UIX	A	304	-	41,49,49	1.23	3 (7%)	52,74,74	2.44	20 (38%)
30	CLA	a	731	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	9 (11%)
30	CLA	N	307	-	51,59,73	1.73	6 (11%)	59,96,113	1.52	7 (11%)
30	CLA	I	315	-	52,60,73	1.68	5 (9%)	60,97,113	1.50	9 (15%)
28	DD6	H	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.90	12 (23%)
30	CLA	O	311	-	51,59,73	1.67	5 (9%)	59,96,113	1.49	8 (13%)
28	DD6	B	306	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	19 (36%)
30	CLA	l	310	-	44,50,73	1.88	7 (15%)	48,76,113	1.38	8 (16%)
30	CLA	J	311	22	47,55,73	1.73	5 (10%)	54,91,113	1.60	8 (14%)
30	CLA	A	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
31	KC1	O	312	-	48,53,53	1.51	7 (14%)	55,89,89	1.87	12 (21%)
30	CLA	j	104	-	55,63,73	1.65	5 (9%)	64,101,113	1.43	9 (14%)
30	CLA	I	311	1	55,63,73	1.64	5 (9%)	64,101,113	1.46	9 (14%)
30	CLA	h	202	-	55,63,73	1.63	5 (9%)	64,101,113	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	D	309	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)
30	CLA	b	711	-	55,63,73	1.63	5 (9%)	64,101,113	1.43	8 (12%)
30	CLA	a	713	-	60,68,73	1.55	6 (10%)	70,107,113	1.41	9 (12%)
30	CLA	a	728	-	55,63,73	1.60	5 (9%)	64,101,113	1.47	9 (14%)
36	SF4	c	201	7	0,12,12	-	-	-	-	-
30	CLA	I	316	-	55,63,73	1.61	5 (9%)	64,101,113	1.51	9 (14%)
30	CLA	G	514	-	53,61,73	1.64	6 (11%)	61,98,113	1.52	9 (14%)
37	BCR	a	736	-	41,41,41	0.74	0	56,56,56	2.03	18 (32%)
30	CLA	G	518	-	46,54,73	1.79	5 (10%)	53,90,113	1.60	8 (15%)
31	KC1	D	315	19	48,53,53	1.49	7 (14%)	55,89,89	1.85	12 (21%)
30	CLA	B	316	-	46,54,73	1.77	5 (10%)	53,90,113	1.50	7 (13%)
34	PID	O	304	-	41,49,49	1.32	4 (9%)	49,76,76	1.73	8 (16%)
30	CLA	A	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	8 (17%)
30	CLA	B	308	-	45,53,73	1.80	5 (11%)	52,89,113	1.61	8 (15%)
33	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.32	6 (13%)
32	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	3 (5%)
28	DD6	M	302	-	39,45,45	2.17	4 (10%)	52,67,67	2.24	16 (30%)
31	KC1	F	314	20	48,53,53	1.49	7 (14%)	55,89,89	1.88	10 (18%)
28	DD6	b	731	30	39,45,45	2.11	3 (7%)	52,67,67	1.96	15 (28%)
30	CLA	f	301	-	55,63,73	1.62	6 (10%)	64,101,113	1.44	8 (12%)
30	CLA	b	713	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
30	CLA	a	715	-	45,53,73	1.78	6 (13%)	52,89,113	1.61	7 (13%)
33	LMG	j	101	-	35,35,55	0.88	0	43,43,63	1.23	4 (9%)
30	CLA	B	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.45	10 (15%)
30	CLA	G	513	5	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
31	KC1	M	307	30	48,53,53	1.51	7 (14%)	55,89,89	1.88	12 (21%)
30	CLA	P	217	-	41,49,73	1.85	7 (17%)	47,84,113	1.66	7 (14%)
30	CLA	M	318	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	7 (13%)
29	UIX	G	503	-	41,49,49	1.23	3 (7%)	52,74,74	2.34	16 (30%)
30	CLA	G	510	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
30	CLA	J	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	7 (13%)
28	DD6	A	303	-	39,45,45	1.94	2 (5%)	52,67,67	1.87	13 (25%)
31	KC1	P	211	-	48,53,53	1.51	7 (14%)	55,89,89	1.89	11 (20%)
31	KC1	D	310	-	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
30	CLA	a	725	-	61,69,73	1.55	5 (8%)	71,108,113	1.40	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	KC1	O	310	-	48,53,53	1.49	7 (14%)	55,89,89	1.89	11 (20%)
34	PID	G	506	-	41,49,49	1.34	4 (9%)	49,76,76	1.38	6 (12%)
30	CLA	M	310	-	48,56,73	1.73	5 (10%)	55,92,113	1.56	8 (14%)
28	DD6	G	502	-	39,45,45	1.99	2 (5%)	52,67,67	1.94	16 (30%)
30	CLA	a	738	22	46,54,73	1.78	5 (10%)	53,90,113	1.58	7 (13%)
30	CLA	J	316	-	46,54,73	1.78	5 (10%)	53,90,113	1.52	7 (13%)
30	CLA	a	716	-	47,55,73	1.76	5 (10%)	54,91,113	1.54	8 (14%)
30	CLA	I	307	-	46,54,73	1.77	5 (10%)	53,90,113	1.53	6 (11%)
30	CLA	B	317	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
30	CLA	A	308	-	55,63,73	1.60	5 (9%)	64,101,113	1.49	8 (12%)
33	LMG	b	733	-	44,44,55	0.81	1 (2%)	52,52,63	1.30	6 (11%)
30	CLA	O	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.53	8 (14%)
30	CLA	D	314	-	46,54,73	1.80	6 (13%)	53,90,113	1.59	9 (16%)
28	DD6	A	305	31	39,45,45	1.99	2 (5%)	52,67,67	1.96	14 (26%)
32	DGD	y	201	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
30	CLA	a	704	-	65,73,73	1.51	6 (9%)	76,113,113	1.35	6 (7%)
30	CLA	b	701	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
28	DD6	J	302	-	39,45,45	2.02	2 (5%)	52,67,67	2.11	15 (28%)
30	CLA	I	310	-	48,56,73	1.71	5 (10%)	55,92,113	1.61	7 (12%)
28	DD6	K	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.69	10 (19%)
28	DD6	N	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.09	16 (30%)
28	DD6	M	306	-	39,45,45	2.17	3 (7%)	52,67,67	2.24	18 (34%)
37	BCR	a	734	-	41,41,41	0.71	0	56,56,56	2.07	19 (33%)
37	BCR	b	702	-	41,41,41	0.73	0	56,56,56	2.17	17 (30%)
30	CLA	O	313	-	46,54,73	1.72	6 (13%)	53,90,113	1.57	6 (11%)
30	CLA	a	706	16	58,66,73	1.57	6 (10%)	67,104,113	1.47	7 (10%)
29	UIX	I	304	-	41,49,49	1.32	4 (9%)	52,74,74	2.59	14 (26%)
30	CLA	H	309	-	47,55,73	1.75	5 (10%)	54,91,113	1.55	8 (14%)
28	DD6	G	504	-	39,45,45	2.24	5 (12%)	52,67,67	2.19	19 (36%)
30	CLA	B	313	18	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
30	CLA	a	719	-	47,55,73	1.76	7 (14%)	54,91,113	1.51	7 (12%)
31	KC1	A	306	28,30	48,53,53	1.49	7 (14%)	55,89,89	1.81	11 (20%)
28	DD6	B	303	-	39,45,45	2.00	2 (5%)	52,67,67	2.00	17 (32%)
30	CLA	a	707	-	65,73,73	1.52	5 (7%)	76,113,113	1.32	8 (10%)
30	CLA	M	309	24	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	KC1	N	306	-	48,53,53	1.50	7 (14%)	55,89,89	1.84	11 (20%)
31	KC1	P	213	-	48,53,53	1.48	7 (14%)	55,89,89	1.86	12 (21%)
31	KC1	K	314	2	48,53,53	1.50	7 (14%)	55,89,89	1.84	10 (18%)
30	CLA	b	719	-	46,54,73	1.79	5 (10%)	53,90,113	1.61	7 (13%)
31	KC1	P	216	27	48,53,53	1.51	7 (14%)	55,89,89	1.83	10 (18%)
30	CLA	l	309	-	41,49,73	1.85	5 (12%)	47,84,113	1.65	8 (17%)
30	CLA	H	305	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
30	CLA	K	309	-	50,58,73	1.67	5 (10%)	58,95,113	1.57	8 (13%)
30	CLA	J	309	-	56,64,73	1.59	5 (8%)	65,102,113	1.52	9 (13%)
28	DD6	L	303	-	39,45,45	1.98	2 (5%)	52,67,67	1.99	14 (26%)
34	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.58	8 (16%)
30	CLA	L	313	-	55,63,73	1.62	5 (9%)	64,101,113	1.44	8 (12%)
28	DD6	F	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.34	18 (34%)
30	CLA	H	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.51	7 (12%)
30	CLA	l	304	-	60,68,73	1.54	5 (8%)	70,107,113	1.48	6 (8%)
30	CLA	O	316	-	41,49,73	1.86	5 (12%)	47,84,113	1.70	7 (14%)
28	DD6	M	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	14 (26%)
34	PID	F	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.77	7 (14%)
30	CLA	N	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.59	6 (11%)
30	CLA	a	717	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	9 (13%)
30	CLA	a	714	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	7 (13%)
30	CLA	a	708	-	51,59,73	1.69	5 (9%)	59,96,113	1.50	8 (13%)
30	CLA	a	721	-	65,73,73	1.49	5 (7%)	76,113,113	1.35	9 (11%)
37	BCR	b	730	-	41,41,41	0.75	0	56,56,56	2.25	20 (35%)
28	DD6	K	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	13 (25%)
37	BCR	l	307	-	41,41,41	0.72	0	56,56,56	2.01	19 (33%)
30	CLA	l	313	14	65,73,73	1.51	5 (7%)	76,113,113	1.40	8 (10%)
30	CLA	H	308	-	46,54,73	1.77	6 (13%)	53,90,113	1.55	6 (11%)
30	CLA	I	312	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	8 (10%)
30	CLA	B	301	-	60,68,73	1.56	5 (8%)	70,107,113	1.37	8 (11%)
30	CLA	K	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.71	9 (19%)
30	CLA	H	311	-	41,49,73	1.89	6 (14%)	47,84,113	1.63	8 (17%)
33	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
30	CLA	f	302	-	46,54,73	1.75	5 (10%)	53,90,113	1.59	7 (13%)
30	CLA	a	723	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	G	512	-	60,68,73	1.54	6 (10%)	70,107,113	1.44	8 (11%)
29	UIX	P	207	-	41,49,49	1.28	4 (9%)	52,74,74	2.78	20 (38%)
30	CLA	J	301	-	60,68,73	1.55	5 (8%)	70,107,113	1.39	8 (11%)
34	PID	O	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.32	5 (10%)
30	CLA	D	311	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
30	CLA	M	316	-	52,60,73	1.68	6 (11%)	60,97,113	1.47	6 (10%)
34	PID	D	302	-	41,49,49	1.35	4 (9%)	49,76,76	1.44	7 (14%)
30	CLA	J	310	-	46,54,73	1.81	6 (13%)	53,90,113	1.56	6 (11%)
30	CLA	M	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.76	9 (19%)
34	PID	P	205	-	41,49,49	1.32	4 (9%)	49,76,76	1.70	6 (12%)
31	KC1	F	309	20	48,53,53	1.50	7 (14%)	55,89,89	1.92	12 (21%)
33	LMG	b	734	-	31,31,55	0.99	0	39,39,63	1.17	3 (7%)
30	CLA	l	303	14	65,73,73	1.53	5 (7%)	76,113,113	1.38	9 (11%)
30	CLA	a	724	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
30	CLA	b	714	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)
30	CLA	b	720	-	53,61,73	1.63	5 (9%)	61,98,113	1.50	8 (13%)
30	CLA	l	305	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
28	DD6	B	302	-	38,44,45	2.18	3 (7%)	50,65,67	2.12	20 (40%)
31	KC1	N	311	25	48,53,53	1.49	6 (12%)	55,89,89	1.85	11 (20%)
39	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
34	PID	F	302	-	41,49,49	1.33	4 (9%)	49,76,76	1.66	6 (12%)
30	CLA	H	307	-	51,59,73	1.68	5 (9%)	59,96,113	1.53	8 (13%)
30	CLA	P	215	-	47,55,73	1.74	5 (10%)	54,91,113	1.68	8 (14%)
30	CLA	F	308	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
30	CLA	K	313	-	55,63,73	1.61	5 (9%)	64,101,113	1.51	8 (12%)
28	DD6	G	508	-	39,45,45	2.04	3 (7%)	52,67,67	2.02	13 (25%)
30	CLA	l	308	-	41,49,73	1.86	5 (12%)	47,84,113	1.64	8 (17%)
30	CLA	b	716	-	50,58,73	1.70	5 (10%)	58,95,113	1.56	8 (13%)
30	CLA	K	310	-	55,63,73	1.62	6 (10%)	64,101,113	1.46	8 (12%)
30	CLA	A	311	6	46,54,73	1.77	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	a	709	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
30	CLA	I	313	-	55,63,73	1.60	5 (9%)	64,101,113	1.51	8 (12%)
30	CLA	a	703	-	55,63,73	1.56	10 (18%)	64,101,113	1.59	9 (14%)
30	CLA	b	723	-	50,58,73	1.70	5 (10%)	58,95,113	1.51	10 (17%)
30	CLA	L	308	31	46,55,73	1.75	5 (10%)	55,91,113	1.53	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	D	313	19	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
28	DD6	M	303	-	39,45,45	2.20	4 (10%)	52,67,67	2.20	19 (36%)
28	DD6	O	303	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	14 (26%)
34	PID	P	203	-	41,49,49	1.33	4 (9%)	49,76,76	1.37	5 (10%)
34	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.53	5 (10%)
31	KC1	J	313	-	48,53,53	1.50	7 (14%)	55,89,89	1.83	9 (16%)
30	CLA	I	306	1	49,57,73	1.71	5 (10%)	55,93,113	1.57	8 (14%)
30	CLA	b	704	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	9 (11%)
30	CLA	D	312	19	46,54,73	1.77	5 (10%)	53,90,113	1.49	6 (11%)
33	LMG	I	318	-	36,36,55	0.90	1 (2%)	44,44,63	1.24	3 (6%)
30	CLA	L	309	-	53,61,73	1.66	5 (9%)	61,98,113	1.51	9 (14%)
30	CLA	b	728	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
31	KC1	M	314	24	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
30	CLA	b	727	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
33	LMG	P	201	-	27,27,55	1.00	0	35,35,63	1.19	4 (11%)
30	CLA	A	307	31	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
30	CLA	b	707	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	9 (11%)
29	UIX	h	201	-	41,49,49	1.28	3 (7%)	52,74,74	2.48	19 (36%)
31	KC1	H	306	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
34	PID	P	206	-	41,49,49	1.33	4 (9%)	49,76,76	1.86	9 (18%)
30	CLA	D	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.65	8 (17%)
30	CLA	F	312	-	46,54,73	1.69	10 (21%)	53,90,113	1.51	6 (11%)
38	PQN	b	729	-	34,34,34	1.55	2 (5%)	42,45,45	1.23	4 (9%)
28	DD6	L	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.95	12 (23%)
30	CLA	K	307	-	46,54,73	1.71	5 (10%)	53,90,113	1.60	6 (11%)
30	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.72	8 (17%)
30	CLA	b	708	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
31	KC1	L	315	-	48,53,53	1.50	7 (14%)	55,89,89	1.90	11 (20%)
34	PID	M	301	-	41,49,49	1.33	4 (9%)	49,76,76	1.74	8 (16%)
30	CLA	b	715	-	60,68,73	1.55	5 (8%)	70,107,113	1.43	8 (11%)
30	CLA	F	313	-	46,54,73	1.75	6 (13%)	53,90,113	1.64	7 (13%)
29	UIX	J	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.46	17 (32%)
30	CLA	J	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.67	8 (17%)
30	CLA	G	517	-	46,54,73	1.76	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	b	706	-	48,56,73	1.74	5 (10%)	55,92,113	1.57	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	N	310	-	47,55,73	1.75	5 (10%)	54,91,113	1.65	8 (14%)
30	CLA	f	303	10	46,54,73	1.75	5 (10%)	53,90,113	1.55	7 (13%)
31	KC1	A	314	6	48,53,53	1.52	7 (14%)	55,89,89	1.88	12 (21%)
30	CLA	a	730	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
28	DD6	G	505	-	39,45,45	2.26	4 (10%)	52,67,67	2.31	21 (40%)
30	CLA	B	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.70	7 (14%)
30	CLA	B	307	18	49,57,73	1.74	5 (10%)	55,93,113	1.52	8 (14%)
30	CLA	P	214	-	46,54,73	1.72	6 (13%)	53,90,113	1.55	6 (11%)
34	PID	D	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.78	7 (14%)
37	BCR	f	304	-	41,41,41	0.72	0	56,56,56	2.07	17 (30%)
30	CLA	A	309	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
30	CLA	A	319	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
30	CLA	G	520	-	49,57,73	1.69	6 (12%)	55,93,113	1.54	8 (14%)
34	PID	N	301	-	41,49,49	1.35	4 (9%)	49,76,76	1.50	6 (12%)
30	CLA	A	312	-	55,63,73	1.62	5 (9%)	64,101,113	1.47	7 (10%)
30	CLA	K	316	-	46,54,73	1.78	5 (10%)	53,90,113	1.56	8 (15%)
30	CLA	b	717	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
30	CLA	a	705	30	55,63,73	1.63	5 (9%)	64,101,113	1.53	9 (14%)
30	CLA	F	310	-	46,54,73	1.76	6 (13%)	53,90,113	1.63	8 (15%)
28	DD6	I	303	-	39,45,45	2.22	5 (12%)	52,67,67	2.03	17 (32%)
30	CLA	I	308	-	60,68,73	1.56	5 (8%)	70,107,113	1.42	10 (14%)
34	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.68	9 (18%)
30	CLA	b	724	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
30	CLA	A	316	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
34	PID	F	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.49	5 (10%)
33	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
30	CLA	I	309	-	55,63,73	1.64	5 (9%)	64,101,113	1.45	8 (12%)
28	DD6	K	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	13 (25%)
36	SF4	c	202	7	0,12,12	-	-	-	-	-
30	CLA	P	210	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
30	CLA	K	308	2	54,62,73	1.63	5 (9%)	62,99,113	1.49	8 (12%)
30	CLA	F	307	-	46,54,73	1.76	6 (13%)	53,90,113	1.60	7 (13%)
30	CLA	b	718	-	51,59,73	1.71	5 (9%)	59,96,113	1.54	7 (11%)
28	DD6	F	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.01	14 (26%)
30	CLA	K	306	2	49,57,73	1.72	5 (10%)	55,93,113	1.55	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	J	306	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	6 (11%)
30	CLA	M	311	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
28	DD6	J	303	-	39,45,45	2.31	4 (10%)	52,67,67	2.44	18 (34%)
30	CLA	b	712	-	54,62,73	1.69	7 (12%)	67,100,113	1.55	11 (16%)
28	DD6	L	302	-	39,45,45	1.94	2 (5%)	52,67,67	2.00	14 (26%)
30	CLA	L	314	-	53,61,73	1.63	5 (9%)	61,98,113	1.51	9 (14%)
30	CLA	b	721	28	46,54,73	1.76	6 (13%)	53,90,113	1.51	6 (11%)
30	CLA	b	705	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
34	PID	D	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.51	6 (12%)
30	CLA	l	311	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
32	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
30	CLA	a	720	-	62,70,73	1.52	5 (8%)	72,109,113	1.41	8 (11%)
30	CLA	I	321	30	52,60,73	1.67	5 (9%)	60,97,113	1.61	9 (15%)
30	CLA	L	317	-	52,60,73	1.69	6 (11%)	60,97,113	1.51	9 (15%)
30	CLA	D	308	-	47,55,73	1.75	5 (10%)	54,91,113	1.51	7 (12%)
30	CLA	b	710	-	52,60,73	1.70	6 (11%)	60,97,113	1.50	8 (13%)
34	PID	D	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.41	5 (10%)
30	CLA	b	722	-	65,73,73	1.51	6 (9%)	76,113,113	1.45	9 (11%)
30	CLA	G	519	-	59,67,73	1.56	5 (8%)	68,105,113	1.44	7 (10%)
30	CLA	P	212	-	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
30	CLA	M	313	-	46,54,73	1.78	5 (10%)	53,90,113	1.55	7 (13%)
30	CLA	B	309	18	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
37	BCR	b	732	-	41,41,41	0.80	0	56,56,56	1.88	20 (35%)
36	SF4	a	737	16,17	0,12,12	-	-	-	-	-
28	DD6	A	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.13	16 (30%)
34	PID	F	305	-	41,49,49	1.38	5 (12%)	49,76,76	1.87	9 (18%)
28	DD6	I	305	-	39,45,45	2.28	6 (15%)	52,67,67	2.29	17 (32%)
30	CLA	L	318	-	46,54,73	1.76	7 (15%)	53,90,113	1.58	7 (13%)
30	CLA	K	311	-	52,60,73	1.68	6 (11%)	60,97,113	1.49	7 (11%)
28	DD6	h	203	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
29	UIX	K	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.71	23 (44%)
30	CLA	a	727	-	46,54,73	1.79	6 (13%)	53,90,113	1.52	7 (13%)
28	DD6	L	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.82	12 (23%)
28	DD6	A	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.13	14 (26%)
32	DGD	l	301	-	51,51,67	0.95	2 (3%)	65,65,81	0.89	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	KC1	G	515	5	48,53,53	1.50	7 (14%)	55,89,89	1.81	12 (21%)
28	DD6	L	306	-	39,45,45	2.00	3 (7%)	52,67,67	2.04	15 (28%)
37	BCR	l	302	-	41,41,41	0.73	0	56,56,56	2.19	21 (37%)
30	CLA	b	709	-	60,68,73	1.57	6 (10%)	70,107,113	1.43	9 (12%)
34	PID	H	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.37	6 (12%)
30	CLA	L	310	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
30	CLA	b	703	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	8 (10%)
32	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.02	4 (7%)
30	CLA	B	311	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
30	CLA	a	701	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
32	DGD	L	301	-	39,39,67	0.95	2 (5%)	53,53,81	0.98	2 (3%)
33	LMG	K	317	-	43,43,55	0.81	1 (2%)	51,51,63	1.31	6 (11%)
31	KC1	N	308	-	48,53,53	1.52	7 (14%)	55,89,89	2.13	13 (23%)
37	BCR	j	102	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
34	PID	j	105	-	41,49,49	1.41	4 (9%)	49,76,76	1.48	10 (20%)
31	KC1	H	310	-	48,53,53	1.49	7 (14%)	55,89,89	1.86	9 (16%)
30	CLA	L	316	-	41,49,73	1.87	5 (12%)	47,84,113	1.65	8 (17%)
30	CLA	l	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.52	7 (13%)
30	CLA	a	735	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
30	CLA	a	729	-	56,64,73	1.59	6 (10%)	65,102,113	1.42	8 (12%)
34	PID	P	208	-	41,49,49	1.34	4 (9%)	49,76,76	1.46	6 (12%)
30	CLA	M	317	-	46,54,73	1.75	5 (10%)	53,90,113	1.58	7 (13%)
30	CLA	a	711	-	45,53,73	1.77	6 (13%)	52,89,113	1.65	8 (15%)
34	PID	G	507	-	41,49,49	1.33	4 (9%)	49,76,76	1.40	7 (14%)
28	DD6	P	204	-	39,45,45	2.00	3 (7%)	52,67,67	2.06	14 (26%)
34	PID	D	306	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	5 (10%)
34	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.65	6 (12%)
30	CLA	J	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	6 (7%)
30	CLA	O	309	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	9 (11%)
30	CLA	G	511	-	55,63,73	1.62	6 (10%)	64,101,113	1.47	7 (10%)
30	CLA	J	308	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	7 (13%)
28	DD6	I	302	-	39,45,45	2.05	3 (7%)	52,67,67	2.16	17 (32%)
28	DD6	I	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.20	20 (38%)
30	CLA	P	209	-	47,55,73	1.76	6 (12%)	54,91,113	1.53	8 (14%)
30	CLA	L	312	-	46,54,73	1.76	5 (10%)	53,90,113	1.55	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	a	718	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
30	CLA	H	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
28	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	15 (28%)
28	DD6	J	304	-	39,45,45	2.20	5 (12%)	52,67,67	2.12	18 (34%)
38	PQN	a	732	-	34,34,34	1.58	2 (5%)	42,45,45	1.10	4 (9%)
30	CLA	a	712	30	60,68,73	1.55	5 (8%)	70,107,113	1.41	8 (11%)
31	KC1	L	307	30	48,53,53	1.51	7 (14%)	55,89,89	1.89	14 (25%)
30	CLA	a	702	-	65,73,73	1.47	10 (15%)	76,113,113	1.42	7 (9%)
31	KC1	O	315	26	48,53,53	1.50	6 (12%)	55,89,89	1.79	10 (18%)
30	CLA	N	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.54	8 (14%)
34	PID	D	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.46	7 (14%)
30	CLA	b	725	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
30	CLA	L	311	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	8 (12%)
31	KC1	B	314	18	48,53,53	1.51	7 (14%)	55,89,89	1.83	11 (20%)
30	CLA	m	202	-	60,68,73	1.55	5 (8%)	70,107,113	1.49	7 (10%)
28	DD6	M	304	-	39,45,45	2.04	3 (7%)	52,67,67	1.91	14 (26%)
30	CLA	a	710	16	55,63,73	1.64	6 (10%)	64,101,113	1.47	9 (14%)
30	CLA	G	509	5	51,59,73	1.68	5 (9%)	59,96,113	1.52	8 (13%)
30	CLA	a	722	-	58,66,73	1.57	6 (10%)	67,104,113	1.48	8 (11%)
30	CLA	J	312	-	53,61,73	1.64	6 (11%)	61,98,113	1.56	9 (14%)
37	BCR	l	306	-	41,41,41	0.73	0	56,56,56	1.91	13 (23%)
28	DD6	B	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.89	11 (21%)
37	BCR	m	201	-	41,41,41	0.71	0	56,56,56	2.33	16 (28%)
29	UIX	O	306	-	41,49,49	1.28	3 (7%)	52,74,74	2.86	23 (44%)
28	DD6	K	318	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
31	KC1	I	314	1	48,53,53	1.50	7 (14%)	55,89,89	1.88	13 (23%)
30	CLA	N	305	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
30	CLA	M	312	-	48,56,73	1.74	5 (10%)	55,92,113	1.56	8 (14%)
30	CLA	M	308	31	53,61,73	1.65	5 (9%)	61,98,113	1.52	8 (13%)
32	DGD	j	103	-	42,42,67	1.05	2 (4%)	56,56,81	1.00	3 (5%)

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
30	CLA	G	516	5	1/1/10/20	4/8/86/115	-
30	CLA	I	319	30	1/1/11/20	8/13/91/115	-
30	CLA	B	312	-	1/1/12/20	2/21/99/115	-
30	CLA	j	106	-	1/1/13/20	12/29/107/115	-
30	CLA	A	320	-	1/1/11/20	6/15/93/115	-
30	CLA	b	726	-	1/1/11/20	1/16/94/115	-
34	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	UIX	B	305	-	-	2/31/87/87	0/3/3/3
37	BCR	i	201	-	-	8/29/63/63	0/2/2/2
30	CLA	K	312	-	1/1/11/20	4/17/95/115	-
30	CLA	A	317	-	1/1/10/20	0/8/86/115	-
30	CLA	a	726	-	1/1/15/20	11/37/115/115	-
30	CLA	F	311	-	1/1/11/20	4/15/93/115	-
28	DD6	D	303	-	-	6/26/80/80	0/3/3/3
35	SQD	A	318	-	-	6/45/65/69	0/1/1/1
30	CLA	A	313	-	1/1/13/20	10/25/103/115	-
34	PID	P	202	-	-	3/24/93/93	0/4/4/4
30	CLA	O	314	-	1/1/11/20	9/16/94/115	-
29	UIX	A	304	-	-	0/31/87/87	0/3/3/3
30	CLA	a	731	-	1/1/15/20	13/37/115/115	-
30	CLA	N	307	-	1/1/12/20	7/21/99/115	-
30	CLA	I	315	-	1/1/12/20	7/22/100/115	-
28	DD6	H	303	-	-	1/26/80/80	0/3/3/3
30	CLA	O	311	-	1/1/12/20	5/21/99/115	-
28	DD6	B	306	-	-	2/26/80/80	0/3/3/3
30	CLA	l	310	-	-	9/26/65/115	0/5/5/9
30	CLA	J	311	22	1/1/11/20	8/16/94/115	-
30	CLA	A	310	-	1/1/15/20	15/37/115/115	-
31	KC1	O	312	-	-	8/15/71/71	-
30	CLA	j	104	-	1/1/13/20	6/25/103/115	-
30	CLA	I	311	1	1/1/13/20	10/25/103/115	-
30	CLA	h	202	-	1/1/13/20	7/25/103/115	-
30	CLA	D	309	-	1/1/11/20	7/15/93/115	-
30	CLA	b	711	-	1/1/13/20	11/25/103/115	-
30	CLA	a	713	-	1/1/14/20	10/31/109/115	-
30	CLA	a	728	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SF4	c	201	7	-	-	0/6/5/5
30	CLA	I	316	-	1/1/13/20	14/25/103/115	-
30	CLA	G	514	-	1/1/12/20	11/23/101/115	-
37	BCR	a	736	-	-	3/29/63/63	0/2/2/2
30	CLA	G	518	-	1/1/11/20	7/15/93/115	-
31	KC1	D	315	19	-	3/15/71/71	-
30	CLA	B	316	-	1/1/11/20	7/15/93/115	-
34	PID	O	304	-	-	3/24/93/93	0/4/4/4
30	CLA	A	315	-	1/1/10/20	6/8/86/115	-
30	CLA	B	308	-	1/1/11/20	5/13/91/115	-
33	LMG	B	318	-	-	15/32/52/70	0/1/1/1
32	DGD	G	501	-	-	10/34/74/95	0/2/2/2
28	DD6	M	302	-	-	3/26/80/80	0/3/3/3
31	KC1	F	314	20	-	8/15/71/71	-
28	DD6	b	731	30	-	3/26/80/80	0/3/3/3
30	CLA	f	301	-	1/1/13/20	9/25/103/115	-
30	CLA	b	713	-	1/1/15/20	11/37/115/115	-
30	CLA	a	715	-	1/1/11/20	5/13/91/115	-
33	LMG	j	101	-	-	14/30/50/70	0/1/1/1
30	CLA	B	310	-	1/1/13/20	8/25/103/115	-
30	CLA	G	513	5	1/1/15/20	10/37/115/115	-
31	KC1	M	307	30	-	7/15/71/71	-
30	CLA	P	217	-	1/1/10/20	5/8/86/115	-
30	CLA	M	318	-	1/1/11/20	9/15/93/115	-
29	UIX	G	503	-	-	4/31/87/87	0/3/3/3
30	CLA	G	510	-	1/1/15/20	14/37/115/115	-
30	CLA	J	315	-	1/1/11/20	4/15/93/115	-
28	DD6	A	303	-	-	1/26/80/80	0/3/3/3
31	KC1	P	211	-	-	11/15/71/71	-
31	KC1	D	310	-	-	10/15/71/71	-
30	CLA	a	725	-	1/1/14/20	11/33/111/115	-
31	KC1	O	310	-	-	8/15/71/71	-
34	PID	G	506	-	-	3/24/93/93	0/4/4/4
30	CLA	M	310	-	1/1/11/20	7/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	G	502	-	-	6/26/80/80	0/3/3/3
30	CLA	a	738	22	1/1/11/20	2/15/93/115	-
30	CLA	J	316	-	-	2/15/93/115	-
30	CLA	a	716	-	1/1/11/20	4/16/94/115	-
30	CLA	I	307	-	1/1/11/20	6/15/93/115	-
30	CLA	B	317	-	1/1/11/20	5/13/91/115	-
30	CLA	A	308	-	1/1/13/20	5/25/103/115	-
33	LMG	b	733	-	-	19/39/59/70	0/1/1/1
30	CLA	O	308	-	1/1/11/20	5/16/94/115	-
30	CLA	D	314	-	1/1/11/20	6/15/93/115	-
28	DD6	A	305	31	-	1/26/80/80	0/3/3/3
32	DGD	y	201	-	-	7/43/83/95	0/2/2/2
30	CLA	a	704	-	1/1/15/20	6/37/115/115	-
30	CLA	b	701	-	1/1/15/20	15/37/115/115	-
28	DD6	J	302	-	-	3/26/80/80	0/3/3/3
30	CLA	I	310	-	1/1/11/20	10/17/95/115	-
28	DD6	K	303	-	-	0/26/80/80	0/3/3/3
28	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	DD6	M	306	-	-	5/26/80/80	0/3/3/3
37	BCR	a	734	-	-	4/29/63/63	0/2/2/2
37	BCR	b	702	-	-	2/29/63/63	0/2/2/2
30	CLA	O	313	-	1/1/11/20	4/15/93/115	-
30	CLA	a	706	16	1/1/13/20	17/29/107/115	-
29	UIX	I	304	-	-	4/31/87/87	0/3/3/3
30	CLA	H	309	-	1/1/11/20	7/16/94/115	-
28	DD6	G	504	-	-	5/26/80/80	0/3/3/3
30	CLA	B	313	18	1/1/15/20	11/37/115/115	-
30	CLA	a	719	-	1/1/11/20	4/16/94/115	-
31	KC1	A	306	28,30	-	6/15/71/71	-
28	DD6	B	303	-	-	2/26/80/80	0/3/3/3
30	CLA	a	707	-	1/1/15/20	16/37/115/115	-
30	CLA	M	309	24	1/1/13/20	5/25/103/115	-
31	KC1	N	306	-	-	6/15/71/71	-
31	KC1	P	213	-	-	8/15/71/71	-
31	KC1	K	314	2	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	719	-	1/1/11/20	11/15/93/115	-
31	KC1	P	216	27	-	8/15/71/71	-
30	CLA	l	309	-	1/1/10/20	4/8/86/115	-
30	CLA	H	305	-	1/1/15/20	8/37/115/115	-
30	CLA	K	309	-	1/1/12/20	2/19/97/115	-
30	CLA	J	309	-	1/1/13/20	8/27/105/115	-
28	DD6	L	303	-	-	0/26/80/80	0/3/3/3
34	PID	O	305	-	-	16/24/93/93	0/4/4/4
30	CLA	L	313	-	1/1/13/20	11/25/103/115	-
28	DD6	F	301	-	-	2/26/80/80	0/3/3/3
30	CLA	H	304	-	1/1/11/20	6/16/94/115	-
30	CLA	l	304	-	1/1/14/20	11/31/109/115	-
30	CLA	O	316	-	1/1/10/20	4/8/86/115	-
28	DD6	M	305	-	-	1/26/80/80	0/3/3/3
34	PID	F	304	-	-	3/24/93/93	0/4/4/4
30	CLA	N	309	25	1/1/11/20	3/15/93/115	-
30	CLA	a	717	-	1/1/13/20	13/28/106/115	-
30	CLA	a	714	-	1/1/11/20	4/13/91/115	-
30	CLA	a	708	-	1/1/12/20	4/21/99/115	-
30	CLA	a	721	-	1/1/15/20	18/37/115/115	-
37	BCR	b	730	-	-	8/29/63/63	0/2/2/2
28	DD6	K	305	-	-	4/26/80/80	0/3/3/3
37	BCR	l	307	-	-	0/29/63/63	0/2/2/2
30	CLA	l	313	14	1/1/15/20	19/37/115/115	-
30	CLA	H	308	-	1/1/11/20	4/15/93/115	-
30	CLA	I	312	-	1/1/15/20	14/37/115/115	-
30	CLA	B	301	-	1/1/14/20	11/31/109/115	-
30	CLA	K	315	-	1/1/10/20	3/8/86/115	-
30	CLA	H	311	-	-	6/8/86/115	-
33	LMG	D	317	-	-	17/41/61/70	0/1/1/1
30	CLA	f	302	-	1/1/11/20	6/15/93/115	-
30	CLA	a	723	-	1/1/15/20	16/37/115/115	-
30	CLA	G	512	-	1/1/14/20	13/31/109/115	-
29	UIX	P	207	-	-	8/31/87/87	0/3/3/3
30	CLA	J	301	-	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	O	307	-	-	3/24/93/93	0/4/4/4
30	CLA	D	311	-	1/1/11/20	4/15/93/115	-
30	CLA	M	316	-	1/1/12/20	11/22/100/115	-
34	PID	D	302	-	-	2/24/93/93	0/4/4/4
30	CLA	J	310	-	1/1/11/20	6/15/93/115	-
30	CLA	M	315	-	1/1/10/20	5/8/86/115	-
34	PID	P	205	-	-	2/24/93/93	0/4/4/4
31	KC1	F	309	20	-	8/15/71/71	-
33	LMG	b	734	-	-	12/26/46/70	0/1/1/1
30	CLA	l	303	14	1/1/15/20	14/37/115/115	-
30	CLA	a	724	-	1/1/15/20	15/37/115/115	-
30	CLA	b	714	-	1/1/11/20	5/15/93/115	-
30	CLA	b	720	-	1/1/12/20	9/23/101/115	-
30	CLA	l	305	-	1/1/15/20	13/37/115/115	-
28	DD6	B	302	-	-	3/24/78/80	0/3/3/3
31	KC1	N	311	25	-	7/15/71/71	-
39	LHG	a	733	-	-	18/52/52/53	-
34	PID	F	302	-	-	2/24/93/93	0/4/4/4
30	CLA	H	307	-	1/1/12/20	7/21/99/115	-
30	CLA	P	215	-	1/1/11/20	7/16/94/115	-
30	CLA	F	308	-	1/1/11/20	1/15/93/115	-
30	CLA	K	313	-	1/1/13/20	7/25/103/115	-
28	DD6	G	508	-	-	1/26/80/80	0/3/3/3
30	CLA	l	308	-	1/1/10/20	2/8/86/115	-
30	CLA	b	716	-	1/1/12/20	7/19/97/115	-
30	CLA	K	310	-	1/1/13/20	6/25/103/115	-
30	CLA	A	311	6	1/1/11/20	5/15/93/115	-
30	CLA	a	709	-	1/1/15/20	17/37/115/115	-
30	CLA	I	313	-	1/1/13/20	12/25/103/115	-
30	CLA	a	703	-	1/1/13/20	9/25/103/115	-
30	CLA	b	723	-	1/1/12/20	7/19/97/115	-
30	CLA	L	308	31	1/1/11/20	7/13/91/115	-
30	CLA	D	313	19	1/1/11/20	3/13/91/115	-
28	DD6	M	303	-	-	2/26/80/80	0/3/3/3
28	DD6	O	303	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	P	203	-	-	2/24/93/93	0/4/4/4
34	PID	O	301	-	-	4/24/93/93	0/4/4/4
31	KC1	J	313	-	-	6/15/71/71	-
30	CLA	I	306	1	1/1/11/20	7/18/96/115	-
30	CLA	b	704	-	1/1/15/20	19/37/115/115	-
30	CLA	D	312	19	1/1/11/20	6/15/93/115	-
33	LMG	I	318	-	-	21/31/51/70	0/1/1/1
30	CLA	L	309	-	1/1/12/20	11/23/101/115	-
30	CLA	b	728	-	1/1/15/20	7/37/115/115	-
31	KC1	M	314	24	-	9/15/71/71	-
30	CLA	b	727	-	1/1/15/20	10/37/115/115	-
33	LMG	P	201	-	-	8/22/42/70	0/1/1/1
30	CLA	A	307	31	1/1/11/20	2/13/91/115	-
30	CLA	b	707	-	1/1/15/20	17/37/115/115	-
29	UIX	h	201	-	-	2/31/87/87	0/3/3/3
31	KC1	H	306	-	-	4/15/71/71	-
34	PID	P	206	-	-	2/24/93/93	0/4/4/4
30	CLA	D	316	-	1/1/10/20	0/8/86/115	-
30	CLA	F	312	-	1/1/11/20	4/15/93/115	-
38	PQN	b	729	-	-	4/23/43/43	0/2/2/2
30	CLA	K	307	-	1/1/11/20	0/15/93/115	-
28	DD6	L	305	-	-	3/26/80/80	0/3/3/3
30	CLA	F	315	-	1/1/10/20	4/8/86/115	-
30	CLA	b	708	-	1/1/15/20	11/37/115/115	-
31	KC1	L	315	-	-	8/15/71/71	-
34	PID	M	301	-	-	1/24/93/93	0/4/4/4
30	CLA	b	715	-	1/1/14/20	14/31/109/115	-
30	CLA	F	313	-	1/1/11/20	5/15/93/115	-
30	CLA	J	314	-	1/1/10/20	4/8/86/115	-
29	UIX	J	305	-	-	11/31/87/87	0/3/3/3
30	CLA	G	517	-	1/1/11/20	4/15/93/115	-
30	CLA	b	706	-	1/1/11/20	4/17/95/115	-
30	CLA	N	310	-	1/1/11/20	9/16/94/115	-
30	CLA	f	303	10	1/1/11/20	10/15/93/115	-
31	KC1	A	314	6	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	a	730	-	1/1/15/20	4/37/115/115	-
28	DD6	G	505	-	-	4/26/80/80	0/3/3/3
30	CLA	B	315	-	1/1/10/20	6/8/86/115	-
30	CLA	B	307	18	1/1/11/20	3/18/96/115	-
30	CLA	P	214	-	1/1/11/20	3/15/93/115	-
34	PID	D	304	-	-	3/24/93/93	0/4/4/4
37	BCR	f	304	-	-	3/29/63/63	0/2/2/2
30	CLA	A	309	-	1/1/13/20	7/25/103/115	-
30	CLA	A	319	-	1/1/11/20	8/15/93/115	-
30	CLA	G	520	-	1/1/11/20	6/18/96/115	-
34	PID	N	301	-	-	6/24/93/93	0/4/4/4
30	CLA	A	312	-	1/1/13/20	6/25/103/115	-
30	CLA	K	316	-	1/1/11/20	2/15/93/115	-
30	CLA	b	717	-	1/1/15/20	18/37/115/115	-
30	CLA	a	705	30	1/1/13/20	9/25/103/115	-
30	CLA	F	310	-	1/1/11/20	8/15/93/115	-
28	DD6	I	303	-	-	2/26/80/80	0/3/3/3
30	CLA	I	308	-	1/1/14/20	12/31/109/115	-
34	PID	N	302	-	-	2/24/93/93	0/4/4/4
30	CLA	b	724	-	1/1/15/20	14/37/115/115	-
30	CLA	A	316	-	1/1/11/20	3/16/94/115	-
34	PID	F	306	-	-	0/24/93/93	0/4/4/4
33	LMG	I	320	-	-	14/33/53/70	0/1/1/1
30	CLA	I	309	-	1/1/13/20	8/25/103/115	-
28	DD6	K	301	-	-	5/26/80/80	0/3/3/3
36	SF4	c	202	7	-	-	0/6/5/5
30	CLA	P	210	-	1/1/15/20	14/37/115/115	-
30	CLA	K	308	2	1/1/12/20	13/24/102/115	-
30	CLA	F	307	-	1/1/11/20	5/15/93/115	-
30	CLA	b	718	-	1/1/12/20	1/21/99/115	-
28	DD6	F	303	-	-	2/26/80/80	0/3/3/3
30	CLA	K	306	2	1/1/11/20	4/18/96/115	-
30	CLA	J	306	-	1/1/11/20	4/15/93/115	-
30	CLA	M	311	-	1/1/11/20	6/15/93/115	-
28	DD6	J	303	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	712	-	1/1/13/20	9/25/101/115	-
28	DD6	L	302	-	-	4/26/80/80	0/3/3/3
30	CLA	L	314	-	1/1/12/20	6/23/101/115	-
30	CLA	b	721	28	1/1/11/20	5/15/93/115	-
30	CLA	b	705	-	1/1/15/20	14/37/115/115	-
34	PID	D	301	-	-	2/24/93/93	0/4/4/4
30	CLA	l	311	-	1/1/15/20	17/37/115/115	-
32	DGD	G	521	-	-	18/33/73/95	0/2/2/2
30	CLA	a	720	-	1/1/14/20	6/34/112/115	-
30	CLA	I	321	30	1/1/12/20	9/22/100/115	-
30	CLA	L	317	-	1/1/12/20	11/22/100/115	-
30	CLA	D	308	-	1/1/11/20	4/16/94/115	-
30	CLA	b	710	-	1/1/12/20	6/22/100/115	-
34	PID	D	307	-	-	4/24/93/93	0/4/4/4
30	CLA	b	722	-	1/1/15/20	8/37/115/115	-
30	CLA	G	519	-	1/1/13/20	13/30/108/115	-
30	CLA	P	212	-	1/1/12/20	9/21/99/115	-
30	CLA	M	313	-	1/1/11/20	4/15/93/115	-
30	CLA	B	309	18	1/1/15/20	22/37/115/115	-
37	BCR	b	732	-	-	2/29/63/63	0/2/2/2
36	SF4	a	737	16,17	-	-	0/6/5/5
28	DD6	A	302	-	-	3/26/80/80	0/3/3/3
34	PID	F	305	-	-	8/24/93/93	0/4/4/4
28	DD6	I	305	-	-	5/26/80/80	0/3/3/3
30	CLA	L	318	-	1/1/11/20	8/15/93/115	-
30	CLA	K	311	-	1/1/12/20	9/22/100/115	-
28	DD6	h	203	-	-	1/26/80/80	0/3/3/3
30	CLA	a	727	-	1/1/11/20	8/15/93/115	-
29	UIX	K	302	-	-	4/31/87/87	0/3/3/3
28	DD6	L	304	-	-	0/26/80/80	0/3/3/3
28	DD6	A	301	-	-	3/26/80/80	0/3/3/3
32	DGD	l	301	-	-	7/39/79/95	0/2/2/2
31	KC1	G	515	5	-	8/15/71/71	-
28	DD6	L	306	-	-	3/26/80/80	0/3/3/3
37	BCR	l	302	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	709	-	1/1/14/20	8/31/109/115	-
34	PID	H	302	-	-	2/24/93/93	0/4/4/4
30	CLA	L	310	-	1/1/13/20	2/25/103/115	-
30	CLA	b	703	-	1/1/15/20	12/37/115/115	-
32	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	CLA	B	311	-	1/1/15/20	21/37/115/115	-
30	CLA	a	701	-	1/1/11/20	0/13/91/115	-
32	DGD	L	301	-	-	2/26/66/95	0/2/2/2
33	LMG	K	317	-	-	18/38/58/70	0/1/1/1
31	KC1	N	308	-	-	8/15/71/71	-
37	BCR	j	102	-	-	6/29/63/63	0/2/2/2
34	PID	j	105	-	-	4/24/93/93	0/4/4/4
31	KC1	H	310	-	-	6/15/71/71	-
30	CLA	L	316	-	1/1/10/20	4/8/86/115	-
30	CLA	l	312	-	1/1/11/20	8/15/93/115	-
30	CLA	a	735	-	1/1/15/20	20/37/115/115	-
30	CLA	a	729	-	1/1/13/20	9/27/105/115	-
34	PID	P	208	-	-	2/24/93/93	0/4/4/4
30	CLA	M	317	-	1/1/11/20	6/15/93/115	-
30	CLA	a	711	-	1/1/11/20	6/13/91/115	-
34	PID	G	507	-	-	0/24/93/93	1/4/4/4
28	DD6	P	204	-	-	1/26/80/80	0/3/3/3
34	PID	D	306	-	-	8/24/93/93	0/4/4/4
34	PID	H	301	-	-	4/24/93/93	0/4/4/4
30	CLA	J	307	-	1/1/15/20	21/37/115/115	-
30	CLA	O	309	-	1/1/15/20	2/37/115/115	-
30	CLA	G	511	-	1/1/13/20	4/25/103/115	-
30	CLA	J	308	-	1/1/11/20	9/15/93/115	-
28	DD6	I	302	-	-	5/26/80/80	0/3/3/3
28	DD6	I	301	-	-	3/26/80/80	0/3/3/3
30	CLA	P	209	-	1/1/11/20	4/16/94/115	-
30	CLA	L	312	-	1/1/11/20	5/15/93/115	-
30	CLA	a	718	-	1/1/11/20	8/15/93/115	-
30	CLA	H	312	-	1/1/11/20	10/15/93/115	-
28	DD6	K	304	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	J	304	-	-	2/26/80/80	0/3/3/3
38	PQN	a	732	-	-	8/23/43/43	0/2/2/2
30	CLA	a	712	30	1/1/14/20	8/31/109/115	-
31	KC1	L	307	30	-	6/15/71/71	-
30	CLA	a	702	-	1/1/15/20	12/37/115/115	-
31	KC1	O	315	26	-	5/15/71/71	-
30	CLA	N	304	-	1/1/11/20	3/16/94/115	-
34	PID	D	305	-	-	2/24/93/93	0/4/4/4
30	CLA	b	725	-	1/1/15/20	13/37/115/115	-
30	CLA	L	311	-	1/1/13/20	4/25/103/115	-
31	KC1	B	314	18	-	7/15/71/71	-
30	CLA	m	202	-	1/1/14/20	10/31/109/115	-
28	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	CLA	a	710	16	1/1/13/20	4/25/103/115	-
30	CLA	G	509	5	1/1/12/20	4/21/99/115	-
30	CLA	a	722	-	1/1/13/20	10/29/107/115	-
30	CLA	J	312	-	1/1/12/20	8/23/101/115	-
37	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	DD6	B	304	-	-	0/26/80/80	0/3/3/3
37	BCR	m	201	-	-	5/29/63/63	0/2/2/2
29	UIX	O	306	-	-	4/31/87/87	0/3/3/3
28	DD6	K	318	-	-	4/26/80/80	0/3/3/3
31	KC1	I	314	1	-	8/15/71/71	-
30	CLA	N	305	-	1/1/15/20	11/37/115/115	-
30	CLA	M	312	-	1/1/11/20	4/17/95/115	-
30	CLA	M	308	31	1/1/12/20	8/23/101/115	-
32	DGD	j	103	-	-	7/30/70/95	0/2/2/2

All (1591) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	310	CLA	CHC-C1C	9.35	1.42	1.35
28	I	305	DD6	C29-C27	-9.13	1.25	1.42
28	J	303	DD6	C29-C27	-9.10	1.25	1.42
28	M	303	DD6	C29-C27	-9.07	1.25	1.42
28	b	731	DD6	C29-C27	-9.03	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	505	DD6	C29-C27	-9.01	1.25	1.42
28	M	306	DD6	C29-C27	-9.01	1.25	1.42
28	I	303	DD6	C29-C27	-8.92	1.25	1.42
28	G	504	DD6	C29-C27	-8.87	1.25	1.42
28	M	304	DD6	C29-C27	-8.85	1.25	1.42
28	I	301	DD6	C29-C27	-8.85	1.25	1.42
28	B	302	DD6	C29-C27	-8.79	1.25	1.42
28	F	303	DD6	C29-C27	-8.78	1.25	1.42
28	G	508	DD6	C29-C27	-8.76	1.25	1.42
28	B	306	DD6	C29-C27	-8.74	1.25	1.42
28	I	302	DD6	C29-C27	-8.71	1.25	1.42
28	J	304	DD6	C29-C27	-8.71	1.25	1.42
28	J	302	DD6	C29-C27	-8.70	1.25	1.42
28	B	303	DD6	C29-C27	-8.70	1.25	1.42
28	M	302	DD6	C29-C27	-8.69	1.25	1.42
28	h	203	DD6	C29-C27	-8.69	1.25	1.42
28	K	318	DD6	C29-C27	-8.69	1.25	1.42
28	N	303	DD6	C29-C27	-8.68	1.25	1.42
28	M	305	DD6	C29-C27	-8.67	1.25	1.42
28	K	304	DD6	C29-C27	-8.64	1.25	1.42
28	B	304	DD6	C29-C27	-8.60	1.26	1.42
28	K	301	DD6	C29-C27	-8.59	1.26	1.42
28	K	305	DD6	C29-C27	-8.58	1.26	1.42
28	L	306	DD6	C29-C27	-8.58	1.26	1.42
28	A	301	DD6	C29-C27	-8.58	1.26	1.42
28	L	303	DD6	C29-C27	-8.58	1.26	1.42
28	P	204	DD6	C29-C27	-8.56	1.26	1.42
28	A	305	DD6	C29-C27	-8.55	1.26	1.42
28	L	305	DD6	C29-C27	-8.53	1.26	1.42
28	L	304	DD6	C29-C27	-8.53	1.26	1.42
28	D	303	DD6	C29-C27	-8.53	1.26	1.42
28	F	301	DD6	C29-C27	-8.53	1.26	1.42
28	G	502	DD6	C29-C27	-8.52	1.26	1.42
28	H	303	DD6	C29-C27	-8.48	1.26	1.42
28	O	303	DD6	C29-C27	-8.47	1.26	1.42
28	A	302	DD6	C29-C27	-8.46	1.26	1.42
28	A	303	DD6	C29-C27	-8.33	1.26	1.42
28	L	302	DD6	C29-C27	-8.31	1.26	1.42
28	K	303	DD6	C29-C27	-8.30	1.26	1.42
28	J	303	DD6	C30-C31	-8.30	1.25	1.42
28	I	305	DD6	C30-C31	-8.30	1.25	1.42
28	G	505	DD6	C30-C31	-8.28	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	306	DD6	C30-C31	-8.28	1.25	1.42
28	M	303	DD6	C30-C31	-8.21	1.25	1.42
28	b	731	DD6	C30-C31	-8.12	1.25	1.42
28	G	504	DD6	C30-C31	-8.11	1.25	1.42
28	I	303	DD6	C30-C31	-8.08	1.25	1.42
28	B	302	DD6	C30-C31	-8.07	1.25	1.42
28	J	304	DD6	C30-C31	-8.05	1.25	1.42
28	M	302	DD6	C30-C31	-8.05	1.25	1.42
28	O	303	DD6	C30-C31	-7.94	1.25	1.42
28	h	203	DD6	C30-C31	-7.88	1.25	1.42
28	N	303	DD6	C30-C31	-7.88	1.25	1.42
28	B	306	DD6	C30-C31	-7.87	1.25	1.42
28	I	301	DD6	C30-C31	-7.85	1.26	1.42
28	M	304	DD6	C30-C31	-7.85	1.26	1.42
30	A	320	CLA	C4B-NB	7.85	1.42	1.35
30	I	311	CLA	C4B-NB	7.81	1.42	1.35
28	A	302	DD6	C30-C31	-7.81	1.26	1.42
28	K	304	DD6	C30-C31	-7.81	1.26	1.42
28	G	508	DD6	C30-C31	-7.80	1.26	1.42
30	B	307	CLA	C4B-NB	7.80	1.42	1.35
30	j	104	CLA	C4B-NB	7.79	1.42	1.35
30	l	303	CLA	C4B-NB	7.79	1.42	1.35
28	I	302	DD6	C30-C31	-7.79	1.26	1.42
28	G	502	DD6	C30-C31	-7.79	1.26	1.42
30	b	719	CLA	C4B-NB	7.78	1.42	1.35
28	P	204	DD6	C30-C31	-7.77	1.26	1.42
30	b	709	CLA	C4B-NB	7.77	1.42	1.35
28	K	303	DD6	C30-C31	-7.76	1.26	1.42
30	G	518	CLA	C4B-NB	7.75	1.42	1.35
28	K	318	DD6	C30-C31	-7.75	1.26	1.42
30	b	718	CLA	C4B-NB	7.75	1.42	1.35
28	B	303	DD6	C30-C31	-7.75	1.26	1.42
28	F	303	DD6	C30-C31	-7.75	1.26	1.42
28	M	305	DD6	C30-C31	-7.75	1.26	1.42
28	A	301	DD6	C30-C31	-7.74	1.26	1.42
30	a	727	CLA	C4B-NB	7.74	1.42	1.35
30	N	307	CLA	C4B-NB	7.73	1.42	1.35
28	F	301	DD6	C30-C31	-7.73	1.26	1.42
28	L	306	DD6	C30-C31	-7.72	1.26	1.42
28	L	305	DD6	C30-C31	-7.71	1.26	1.42
30	A	307	CLA	C4B-NB	7.71	1.42	1.35
30	a	707	CLA	C4B-NB	7.70	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	310	CLA	C4B-NB	7.69	1.42	1.35
28	A	305	DD6	C30-C31	-7.68	1.26	1.42
30	G	516	CLA	C4B-NB	7.68	1.42	1.35
30	a	735	CLA	C4B-NB	7.68	1.42	1.35
30	a	731	CLA	C4B-NB	7.66	1.42	1.35
30	H	311	CLA	C4B-NB	7.66	1.42	1.35
28	K	305	DD6	C30-C31	-7.66	1.26	1.42
30	L	316	CLA	C4B-NB	7.65	1.42	1.35
30	L	309	CLA	C4B-NB	7.65	1.42	1.35
28	B	304	DD6	C30-C31	-7.64	1.26	1.42
30	K	316	CLA	C4B-NB	7.64	1.42	1.35
30	b	706	CLA	C4B-NB	7.64	1.42	1.35
30	b	726	CLA	C4B-NB	7.64	1.42	1.35
30	O	308	CLA	C4B-NB	7.62	1.42	1.35
28	L	304	DD6	C30-C31	-7.62	1.26	1.42
30	I	307	CLA	C4B-NB	7.62	1.42	1.35
30	a	738	CLA	C4B-NB	7.62	1.42	1.35
30	b	728	CLA	C4B-NB	7.62	1.42	1.35
30	M	313	CLA	C4B-NB	7.62	1.42	1.35
28	D	303	DD6	C30-C31	-7.62	1.26	1.42
30	N	304	CLA	C4B-NB	7.62	1.42	1.35
30	b	723	CLA	C4B-NB	7.62	1.42	1.35
30	D	308	CLA	C4B-NB	7.62	1.42	1.35
30	B	308	CLA	C4B-NB	7.61	1.42	1.35
30	L	317	CLA	C4B-NB	7.61	1.42	1.35
30	M	316	CLA	C4B-NB	7.61	1.42	1.35
28	J	302	DD6	C30-C31	-7.61	1.26	1.42
30	a	716	CLA	C4B-NB	7.61	1.42	1.35
28	H	303	DD6	C30-C31	-7.60	1.26	1.42
30	l	308	CLA	C4B-NB	7.59	1.42	1.35
30	F	311	CLA	C4B-NB	7.59	1.42	1.35
30	M	318	CLA	C4B-NB	7.59	1.42	1.35
30	A	319	CLA	C4B-NB	7.59	1.42	1.35
30	a	724	CLA	C4B-NB	7.59	1.42	1.35
30	b	710	CLA	C4B-NB	7.59	1.42	1.35
28	L	303	DD6	C30-C31	-7.59	1.26	1.42
30	l	309	CLA	C4B-NB	7.58	1.42	1.35
28	A	303	DD6	C30-C31	-7.58	1.26	1.42
30	b	711	CLA	C4B-NB	7.58	1.42	1.35
30	a	719	CLA	C4B-NB	7.58	1.42	1.35
30	A	317	CLA	C4B-NB	7.58	1.42	1.35
30	H	312	CLA	C4B-NB	7.58	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	311	CLA	C4B-NB	7.58	1.42	1.35
30	I	321	CLA	C4B-NB	7.57	1.42	1.35
30	a	710	CLA	C4B-NB	7.57	1.42	1.35
30	a	718	CLA	C4B-NB	7.57	1.42	1.35
30	a	714	CLA	C4B-NB	7.57	1.42	1.35
30	H	304	CLA	C4B-NB	7.57	1.42	1.35
30	M	310	CLA	C4B-NB	7.57	1.42	1.35
28	K	301	DD6	C30-C31	-7.57	1.26	1.42
30	A	316	CLA	C4B-NB	7.57	1.42	1.35
30	J	316	CLA	C4B-NB	7.57	1.42	1.35
30	a	704	CLA	C4B-NB	7.56	1.42	1.35
30	b	721	CLA	C4B-NB	7.56	1.42	1.35
30	B	317	CLA	C4B-NB	7.56	1.42	1.35
30	I	315	CLA	C4B-NB	7.55	1.41	1.35
30	l	311	CLA	C4B-NB	7.55	1.41	1.35
30	H	308	CLA	C4B-NB	7.55	1.41	1.35
30	l	304	CLA	C4B-NB	7.55	1.41	1.35
30	b	712	CLA	C4B-NB	7.55	1.41	1.35
30	J	306	CLA	C4B-NB	7.55	1.41	1.35
30	P	217	CLA	C4B-NB	7.55	1.41	1.35
30	b	722	CLA	C4B-NB	7.55	1.41	1.35
30	L	311	CLA	C4B-NB	7.54	1.41	1.35
38	a	732	PQN	C3-C2	7.54	1.49	1.35
30	a	709	CLA	C4B-NB	7.54	1.41	1.35
30	I	309	CLA	C4B-NB	7.54	1.41	1.35
30	F	310	CLA	C4B-NB	7.54	1.41	1.35
30	P	210	CLA	C4B-NB	7.53	1.41	1.35
30	D	314	CLA	C4B-NB	7.53	1.41	1.35
30	D	316	CLA	C4B-NB	7.53	1.41	1.35
30	B	301	CLA	C4B-NB	7.53	1.41	1.35
30	b	716	CLA	C4B-NB	7.53	1.41	1.35
30	D	312	CLA	C4B-NB	7.53	1.41	1.35
30	K	306	CLA	C4B-NB	7.53	1.41	1.35
30	O	316	CLA	C4B-NB	7.52	1.41	1.35
30	D	311	CLA	C4B-NB	7.52	1.41	1.35
30	I	308	CLA	C4B-NB	7.52	1.41	1.35
30	j	106	CLA	C4B-NB	7.52	1.41	1.35
30	b	701	CLA	C4B-NB	7.52	1.41	1.35
30	A	311	CLA	C4B-NB	7.52	1.41	1.35
30	G	511	CLA	C4B-NB	7.52	1.41	1.35
30	m	202	CLA	C4B-NB	7.52	1.41	1.35
30	l	312	CLA	C4B-NB	7.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	J	314	CLA	C4B-NB	7.52	1.41	1.35
30	B	316	CLA	C4B-NB	7.52	1.41	1.35
30	P	209	CLA	C4B-NB	7.51	1.41	1.35
30	a	712	CLA	C4B-NB	7.51	1.41	1.35
30	h	202	CLA	C4B-NB	7.51	1.41	1.35
30	G	519	CLA	C4B-NB	7.51	1.41	1.35
30	a	717	CLA	C4B-NB	7.51	1.41	1.35
30	M	315	CLA	C4B-NB	7.50	1.41	1.35
30	J	315	CLA	C4B-NB	7.50	1.41	1.35
30	H	309	CLA	C4B-NB	7.50	1.41	1.35
30	a	705	CLA	C4B-NB	7.50	1.41	1.35
30	a	708	CLA	C4B-NB	7.50	1.41	1.35
30	L	308	CLA	C4B-NB	7.50	1.41	1.35
30	I	306	CLA	C4B-NB	7.49	1.41	1.35
30	B	315	CLA	C4B-NB	7.49	1.41	1.35
30	J	312	CLA	C4B-NB	7.49	1.41	1.35
30	M	308	CLA	C4B-NB	7.49	1.41	1.35
30	K	311	CLA	C4B-NB	7.49	1.41	1.35
30	b	713	CLA	C4B-NB	7.49	1.41	1.35
30	l	305	CLA	C4B-NB	7.49	1.41	1.35
30	B	311	CLA	C4B-NB	7.49	1.41	1.35
30	K	315	CLA	C4B-NB	7.49	1.41	1.35
30	O	314	CLA	C4B-NB	7.48	1.41	1.35
30	F	315	CLA	C4B-NB	7.48	1.41	1.35
30	l	313	CLA	C4B-NB	7.48	1.41	1.35
30	F	307	CLA	C4B-NB	7.48	1.41	1.35
28	L	302	DD6	C30-C31	-7.48	1.26	1.42
30	J	308	CLA	C4B-NB	7.48	1.41	1.35
30	B	310	CLA	C4B-NB	7.47	1.41	1.35
30	L	312	CLA	C4B-NB	7.47	1.41	1.35
30	b	707	CLA	C4B-NB	7.47	1.41	1.35
30	L	310	CLA	C4B-NB	7.47	1.41	1.35
30	a	713	CLA	C4B-NB	7.47	1.41	1.35
30	I	316	CLA	C4B-NB	7.47	1.41	1.35
30	K	310	CLA	C4B-NB	7.47	1.41	1.35
30	b	714	CLA	C4B-NB	7.46	1.41	1.35
30	b	715	CLA	C4B-NB	7.46	1.41	1.35
30	b	724	CLA	C4B-NB	7.46	1.41	1.35
30	I	319	CLA	C4B-NB	7.46	1.41	1.35
30	J	307	CLA	C4B-NB	7.46	1.41	1.35
30	A	315	CLA	C4B-NB	7.46	1.41	1.35
30	A	308	CLA	C4B-NB	7.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	305	CLA	C4B-NB	7.45	1.41	1.35
30	b	727	CLA	C4B-NB	7.45	1.41	1.35
30	I	312	CLA	C4B-NB	7.45	1.41	1.35
30	D	309	CLA	C4B-NB	7.45	1.41	1.35
30	I	313	CLA	C4B-NB	7.44	1.41	1.35
30	a	701	CLA	C4B-NB	7.44	1.41	1.35
30	M	309	CLA	C4B-NB	7.44	1.41	1.35
30	b	703	CLA	C4B-NB	7.44	1.41	1.35
30	J	301	CLA	C4B-NB	7.44	1.41	1.35
30	a	722	CLA	C4B-NB	7.44	1.41	1.35
30	a	725	CLA	C4B-NB	7.44	1.41	1.35
30	f	301	CLA	C4B-NB	7.43	1.41	1.35
30	b	725	CLA	C4B-NB	7.43	1.41	1.35
30	G	509	CLA	C4B-NB	7.43	1.41	1.35
30	A	312	CLA	C4B-NB	7.42	1.41	1.35
30	M	317	CLA	C4B-NB	7.42	1.41	1.35
30	a	715	CLA	C4B-NB	7.42	1.41	1.35
30	K	313	CLA	C4B-NB	7.42	1.41	1.35
30	P	212	CLA	C4B-NB	7.41	1.41	1.35
30	K	308	CLA	C4B-NB	7.41	1.41	1.35
30	O	309	CLA	C4B-NB	7.41	1.41	1.35
30	H	307	CLA	C4B-NB	7.41	1.41	1.35
30	B	312	CLA	C4B-NB	7.40	1.41	1.35
30	G	517	CLA	C4B-NB	7.40	1.41	1.35
30	a	706	CLA	C4B-NB	7.40	1.41	1.35
30	f	303	CLA	C4B-NB	7.40	1.41	1.35
30	I	310	CLA	C4B-NB	7.39	1.41	1.35
30	G	514	CLA	C4B-NB	7.39	1.41	1.35
30	a	711	CLA	C4B-NB	7.39	1.41	1.35
30	f	302	CLA	C4B-NB	7.39	1.41	1.35
30	O	311	CLA	C4B-NB	7.39	1.41	1.35
30	B	309	CLA	C4B-NB	7.39	1.41	1.35
30	a	723	CLA	C4B-NB	7.38	1.41	1.35
30	N	310	CLA	C4B-NB	7.38	1.41	1.35
30	b	717	CLA	C4B-NB	7.38	1.41	1.35
30	G	520	CLA	C4B-NB	7.38	1.41	1.35
30	a	720	CLA	C4B-NB	7.38	1.41	1.35
30	F	308	CLA	C4B-NB	7.37	1.41	1.35
30	G	512	CLA	C4B-NB	7.37	1.41	1.35
30	A	309	CLA	C4B-NB	7.37	1.41	1.35
30	P	215	CLA	C4B-NB	7.37	1.41	1.35
30	L	318	CLA	C4B-NB	7.37	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	305	CLA	C4B-NB	7.37	1.41	1.35
30	M	312	CLA	C4B-NB	7.35	1.41	1.35
30	J	311	CLA	C4B-NB	7.35	1.41	1.35
30	L	313	CLA	C4B-NB	7.35	1.41	1.35
30	L	314	CLA	C4B-NB	7.34	1.41	1.35
30	J	309	CLA	C4B-NB	7.34	1.41	1.35
30	K	312	CLA	C4B-NB	7.34	1.41	1.35
38	b	729	PQN	C3-C2	7.34	1.48	1.35
30	K	309	CLA	C4B-NB	7.33	1.41	1.35
30	a	721	CLA	C4B-NB	7.33	1.41	1.35
30	A	310	CLA	C4B-NB	7.33	1.41	1.35
30	b	720	CLA	C4B-NB	7.33	1.41	1.35
30	B	313	CLA	C4B-NB	7.33	1.41	1.35
30	a	729	CLA	C4B-NB	7.32	1.41	1.35
30	a	726	CLA	C4B-NB	7.32	1.41	1.35
30	G	510	CLA	C4B-NB	7.31	1.41	1.35
30	A	313	CLA	C4B-NB	7.30	1.41	1.35
30	D	313	CLA	C4B-NB	7.30	1.41	1.35
30	P	214	CLA	C4B-NB	7.30	1.41	1.35
30	b	708	CLA	C4B-NB	7.30	1.41	1.35
30	b	705	CLA	C4B-NB	7.28	1.41	1.35
30	F	313	CLA	C4B-NB	7.26	1.41	1.35
30	a	728	CLA	C4B-NB	7.26	1.41	1.35
30	a	730	CLA	C4B-NB	7.24	1.41	1.35
30	O	313	CLA	C4B-NB	7.24	1.41	1.35
30	N	309	CLA	C4B-NB	7.23	1.41	1.35
30	G	513	CLA	C4B-NB	7.17	1.41	1.35
30	K	307	CLA	C4B-NB	7.02	1.41	1.35
31	H	306	KC1	C4D-CHA	-6.90	1.36	1.45
31	A	314	KC1	C4D-CHA	-6.76	1.36	1.45
31	L	307	KC1	C4D-CHA	-6.74	1.36	1.45
31	B	314	KC1	C4D-CHA	-6.69	1.36	1.45
31	M	314	KC1	C4D-CHA	-6.65	1.36	1.45
31	O	312	KC1	C4D-CHA	-6.65	1.36	1.45
31	P	216	KC1	C4D-CHA	-6.64	1.36	1.45
31	I	314	KC1	C4D-CHA	-6.61	1.36	1.45
31	K	314	KC1	C4D-CHA	-6.61	1.36	1.45
31	P	211	KC1	C4D-CHA	-6.60	1.36	1.45
31	L	315	KC1	C4D-CHA	-6.60	1.36	1.45
31	N	311	KC1	C4D-CHA	-6.58	1.36	1.45
31	N	306	KC1	C4D-CHA	-6.57	1.36	1.45
31	D	315	KC1	C4D-CHA	-6.56	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	O	310	KC1	C4D-CHA	-6.55	1.36	1.45
31	J	313	KC1	C4D-CHA	-6.52	1.36	1.45
31	M	307	KC1	C4D-CHA	-6.48	1.37	1.45
31	O	315	KC1	C4D-CHA	-6.48	1.37	1.45
31	D	310	KC1	C4D-CHA	-6.48	1.37	1.45
31	F	309	KC1	C4D-CHA	-6.47	1.37	1.45
31	G	515	KC1	C4D-CHA	-6.45	1.37	1.45
31	F	314	KC1	C4D-CHA	-6.40	1.37	1.45
31	A	306	KC1	C4D-CHA	-6.38	1.37	1.45
30	F	312	CLA	C4B-NB	6.38	1.40	1.35
31	H	310	KC1	C4D-CHA	-6.37	1.37	1.45
31	P	213	KC1	C4D-CHA	-6.26	1.37	1.45
30	b	704	CLA	C4B-NB	6.16	1.40	1.35
30	a	703	CLA	C4B-NB	6.14	1.40	1.35
30	a	702	CLA	C4B-NB	6.09	1.40	1.35
34	N	302	PID	C13-C14	-6.00	1.33	1.45
31	N	308	KC1	C4D-CHA	-5.77	1.37	1.45
34	H	302	PID	C13-C14	-5.75	1.34	1.45
34	G	506	PID	C13-C14	-5.74	1.34	1.45
34	O	302	PID	C13-C14	-5.67	1.34	1.45
34	P	203	PID	C13-C14	-5.66	1.34	1.45
34	O	307	PID	C13-C14	-5.58	1.34	1.45
34	D	302	PID	C13-C14	-5.56	1.34	1.45
34	O	305	PID	C13-C14	-5.55	1.34	1.45
34	D	305	PID	C13-C14	-5.54	1.34	1.45
34	D	306	PID	C13-C14	-5.50	1.34	1.45
34	D	301	PID	C13-C14	-5.48	1.35	1.45
34	j	105	PID	C13-C14	-5.47	1.35	1.45
34	G	507	PID	C13-C14	-5.47	1.35	1.45
34	N	301	PID	C13-C14	-5.43	1.35	1.45
34	O	301	PID	C13-C14	-5.39	1.35	1.45
34	P	208	PID	C13-C14	-5.39	1.35	1.45
34	F	306	PID	C13-C14	-5.37	1.35	1.45
34	H	301	PID	C13-C14	-5.35	1.35	1.45
34	P	205	PID	C13-C14	-5.34	1.35	1.45
34	F	304	PID	C13-C14	-5.25	1.35	1.45
34	P	202	PID	C13-C14	-5.23	1.35	1.45
34	F	302	PID	C13-C14	-5.21	1.35	1.45
34	F	305	PID	C13-C14	-5.21	1.35	1.45
34	P	206	PID	C13-C14	-5.19	1.35	1.45
34	D	307	PID	C13-C14	-5.18	1.35	1.45
34	O	304	PID	C13-C14	-5.16	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	304	PID	C13-C14	-5.11	1.35	1.45
34	M	301	PID	C13-C14	-5.10	1.35	1.45
29	B	305	UIX	O2-C27	4.91	1.46	1.35
38	b	729	PQN	C10-C5	4.83	1.48	1.40
29	J	305	UIX	O2-C27	4.80	1.46	1.35
29	h	201	UIX	O2-C27	4.78	1.46	1.35
38	a	732	PQN	C10-C5	4.78	1.48	1.40
29	O	306	UIX	O2-C27	4.77	1.46	1.35
29	P	207	UIX	O2-C27	4.75	1.45	1.35
29	G	503	UIX	O2-C27	4.73	1.45	1.35
31	M	307	KC1	MG-NB	-4.72	1.96	2.05
29	A	304	UIX	O2-C27	4.71	1.45	1.35
29	K	302	UIX	O2-C27	4.70	1.45	1.35
31	P	211	KC1	MG-NB	-4.68	1.96	2.05
31	H	310	KC1	MG-NB	-4.68	1.96	2.05
31	F	314	KC1	MG-NB	-4.67	1.96	2.05
31	O	315	KC1	MG-NB	-4.65	1.96	2.05
31	D	310	KC1	MG-NB	-4.65	1.96	2.05
31	M	314	KC1	MG-NB	-4.64	1.96	2.05
31	N	311	KC1	MG-NB	-4.63	1.96	2.05
31	F	309	KC1	MG-NB	-4.63	1.96	2.05
31	P	216	KC1	MG-NB	-4.62	1.96	2.05
31	N	308	KC1	MG-NB	-4.62	1.96	2.05
31	N	306	KC1	MG-NB	-4.62	1.96	2.05
31	H	306	KC1	MG-NB	-4.60	1.96	2.05
31	J	313	KC1	MG-NB	-4.59	1.96	2.05
31	O	310	KC1	MG-NB	-4.58	1.96	2.05
31	A	306	KC1	MG-NB	-4.57	1.96	2.05
31	I	314	KC1	MG-NB	-4.57	1.96	2.05
31	L	315	KC1	MG-NB	-4.57	1.96	2.05
31	A	314	KC1	MG-NB	-4.57	1.96	2.05
31	B	314	KC1	MG-NB	-4.55	1.96	2.05
31	L	307	KC1	MG-NB	-4.55	1.96	2.05
31	O	312	KC1	MG-NB	-4.54	1.96	2.05
31	G	515	KC1	MG-NB	-4.54	1.96	2.05
31	K	314	KC1	MG-NB	-4.53	1.96	2.05
31	P	213	KC1	MG-NB	-4.50	1.96	2.05
31	D	315	KC1	MG-NB	-4.49	1.96	2.05
32	I	317	DGD	O1G-C1A	4.26	1.45	1.33
32	G	501	DGD	O1G-C1A	4.25	1.45	1.33
29	I	304	UIX	O2-C27	4.24	1.44	1.35
32	l	301	DGD	O1G-C1A	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	j	103	DGD	O1G-C1A	4.21	1.45	1.33
32	G	521	DGD	O2G-C1B	4.19	1.46	1.34
32	y	201	DGD	O1G-C1A	4.19	1.45	1.33
28	J	303	DD6	C19-C20	4.15	1.58	1.52
32	G	501	DGD	O2G-C1B	4.14	1.46	1.34
32	l	301	DGD	O2G-C1B	4.11	1.45	1.34
32	j	103	DGD	O2G-C1B	4.11	1.45	1.34
30	L	317	CLA	C1D-ND	4.08	1.42	1.37
30	J	316	CLA	C1D-ND	4.07	1.42	1.37
30	a	702	CLA	C4D-ND	-4.07	1.32	1.37
32	y	201	DGD	O2G-C1B	4.06	1.45	1.34
30	b	718	CLA	C1D-ND	4.04	1.42	1.37
30	H	311	CLA	C1D-ND	4.04	1.42	1.37
32	I	317	DGD	O2G-C1B	4.04	1.45	1.34
30	M	318	CLA	C1D-ND	4.04	1.42	1.37
30	N	310	CLA	C1D-ND	4.04	1.42	1.37
32	L	301	DGD	O2G-C1B	4.03	1.45	1.34
30	N	307	CLA	C1D-ND	4.03	1.42	1.37
30	O	316	CLA	C1D-ND	4.02	1.42	1.37
32	G	521	DGD	O1G-C1A	4.00	1.45	1.33
30	H	308	CLA	C1D-ND	4.00	1.42	1.37
30	a	703	CLA	C4D-ND	-3.99	1.32	1.37
30	a	738	CLA	C1D-ND	3.99	1.42	1.37
30	H	304	CLA	C1D-ND	3.98	1.42	1.37
30	b	704	CLA	C4D-ND	-3.98	1.32	1.37
30	G	516	CLA	C1D-ND	3.98	1.42	1.37
30	J	311	CLA	C1D-ND	3.98	1.42	1.37
30	G	518	CLA	C1D-ND	3.97	1.42	1.37
30	A	307	CLA	C1D-ND	3.97	1.42	1.37
30	a	717	CLA	C1D-ND	3.97	1.42	1.37
30	F	315	CLA	C1D-ND	3.97	1.42	1.37
30	K	306	CLA	C1D-ND	3.97	1.42	1.37
30	K	316	CLA	C1D-ND	3.95	1.42	1.37
30	B	316	CLA	C1D-ND	3.94	1.42	1.37
34	j	105	PID	C20-C21	3.94	1.41	1.35
30	b	726	CLA	C1D-ND	3.94	1.42	1.37
30	H	312	CLA	C1D-ND	3.94	1.42	1.37
30	a	726	CLA	C1D-ND	3.94	1.42	1.37
30	B	307	CLA	C1D-ND	3.94	1.42	1.37
30	a	728	CLA	C1D-ND	3.94	1.42	1.37
30	J	308	CLA	C1D-ND	3.94	1.42	1.37
30	P	209	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	312	CLA	C1D-ND	3.93	1.42	1.37
30	G	512	CLA	C1D-ND	3.93	1.42	1.37
30	b	708	CLA	C1D-ND	3.93	1.42	1.37
30	P	215	CLA	C1D-ND	3.93	1.42	1.37
30	J	314	CLA	C1D-ND	3.93	1.42	1.37
30	A	316	CLA	C1D-ND	3.92	1.42	1.37
30	h	202	CLA	C1D-ND	3.92	1.42	1.37
30	L	313	CLA	C1D-ND	3.91	1.42	1.37
30	b	711	CLA	C1D-ND	3.91	1.42	1.37
30	M	308	CLA	C1D-ND	3.91	1.42	1.37
30	j	104	CLA	C1D-ND	3.91	1.42	1.37
30	b	705	CLA	C1D-ND	3.91	1.42	1.37
30	b	707	CLA	C1D-ND	3.91	1.42	1.37
30	b	717	CLA	C1D-ND	3.91	1.42	1.37
30	F	313	CLA	C1D-ND	3.91	1.42	1.37
30	M	309	CLA	C1D-ND	3.91	1.42	1.37
30	I	311	CLA	C1D-ND	3.91	1.42	1.37
30	L	318	CLA	C1D-ND	3.90	1.42	1.37
30	I	315	CLA	C1D-ND	3.90	1.42	1.37
30	l	309	CLA	C1D-ND	3.90	1.42	1.37
30	L	316	CLA	C1D-ND	3.90	1.42	1.37
30	M	315	CLA	C1D-ND	3.90	1.42	1.37
30	F	310	CLA	C1D-ND	3.90	1.42	1.37
30	l	303	CLA	C1D-ND	3.90	1.42	1.37
30	a	721	CLA	C1D-ND	3.89	1.42	1.37
30	B	312	CLA	C1D-ND	3.89	1.42	1.37
30	A	311	CLA	C1D-ND	3.89	1.42	1.37
30	m	202	CLA	C1D-ND	3.89	1.42	1.37
30	b	706	CLA	C1D-ND	3.89	1.42	1.37
30	K	307	CLA	C1D-ND	3.89	1.42	1.37
30	O	314	CLA	C1D-ND	3.89	1.42	1.37
30	a	705	CLA	C1D-ND	3.89	1.42	1.37
30	A	312	CLA	C1D-ND	3.89	1.42	1.37
30	O	308	CLA	C1D-ND	3.89	1.42	1.37
30	G	509	CLA	C1D-ND	3.88	1.42	1.37
30	l	305	CLA	C1D-ND	3.88	1.42	1.37
30	K	310	CLA	C1D-ND	3.88	1.42	1.37
30	F	311	CLA	C1D-ND	3.88	1.42	1.37
30	D	314	CLA	C1D-ND	3.88	1.42	1.37
30	H	307	CLA	C1D-ND	3.88	1.42	1.37
30	f	301	CLA	C1D-ND	3.88	1.42	1.37
30	a	731	CLA	C1D-ND	3.88	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	513	CLA	C1D-ND	3.88	1.42	1.37
30	I	308	CLA	C1D-ND	3.88	1.42	1.37
30	N	304	CLA	C1D-ND	3.88	1.42	1.37
30	G	511	CLA	C1D-ND	3.88	1.42	1.37
30	a	714	CLA	C1D-ND	3.88	1.42	1.37
30	H	305	CLA	C1D-ND	3.88	1.42	1.37
30	a	715	CLA	C1D-ND	3.88	1.42	1.37
30	N	305	CLA	C1D-ND	3.87	1.42	1.37
30	a	707	CLA	C1D-ND	3.87	1.42	1.37
30	I	307	CLA	C1D-ND	3.87	1.42	1.37
30	F	307	CLA	C1D-ND	3.87	1.42	1.37
30	f	302	CLA	C1D-ND	3.87	1.42	1.37
30	M	311	CLA	C1D-ND	3.87	1.42	1.37
30	a	720	CLA	C1D-ND	3.87	1.42	1.37
30	D	316	CLA	C1D-ND	3.87	1.42	1.37
30	A	315	CLA	C1D-ND	3.86	1.42	1.37
30	D	311	CLA	C1D-ND	3.86	1.42	1.37
30	I	306	CLA	C1D-ND	3.86	1.42	1.37
30	A	309	CLA	C1D-ND	3.86	1.42	1.37
30	D	309	CLA	C1D-ND	3.86	1.42	1.37
30	I	311	CLA	C1D-ND	3.86	1.42	1.37
30	a	716	CLA	C1D-ND	3.86	1.42	1.37
30	b	714	CLA	C1D-ND	3.86	1.42	1.37
30	a	722	CLA	C1D-ND	3.86	1.42	1.37
30	b	715	CLA	C1D-ND	3.86	1.42	1.37
30	b	716	CLA	C1D-ND	3.86	1.42	1.37
30	O	309	CLA	C1D-ND	3.86	1.42	1.37
30	P	217	CLA	C1D-ND	3.86	1.42	1.37
30	G	517	CLA	C1D-ND	3.85	1.42	1.37
30	b	719	CLA	C1D-ND	3.85	1.42	1.37
30	G	510	CLA	C1D-ND	3.85	1.42	1.37
30	A	317	CLA	C1D-ND	3.85	1.42	1.37
30	B	308	CLA	C1D-ND	3.85	1.42	1.37
30	B	313	CLA	C1D-ND	3.85	1.42	1.37
30	L	311	CLA	C1D-ND	3.85	1.42	1.37
30	K	311	CLA	C1D-ND	3.85	1.42	1.37
30	a	723	CLA	C1D-ND	3.85	1.42	1.37
30	b	701	CLA	C1D-ND	3.84	1.42	1.37
30	M	310	CLA	C1D-ND	3.84	1.42	1.37
30	O	311	CLA	C1D-ND	3.84	1.42	1.37
30	I	310	CLA	C1D-ND	3.84	1.42	1.37
30	J	315	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	709	CLA	C1D-ND	3.84	1.42	1.37
30	B	301	CLA	C1D-ND	3.84	1.42	1.37
30	b	728	CLA	C1D-ND	3.84	1.42	1.37
30	J	301	CLA	C1D-ND	3.84	1.42	1.37
30	I	312	CLA	C1D-ND	3.83	1.42	1.37
30	M	313	CLA	C1D-ND	3.83	1.42	1.37
30	b	724	CLA	C1D-ND	3.83	1.42	1.37
30	K	315	CLA	C1D-ND	3.83	1.42	1.37
30	a	708	CLA	C1D-ND	3.83	1.42	1.37
30	N	309	CLA	C1D-ND	3.83	1.42	1.37
30	D	312	CLA	C1D-ND	3.83	1.42	1.37
30	H	309	CLA	C1D-ND	3.83	1.42	1.37
30	f	303	CLA	C1D-ND	3.83	1.42	1.37
30	b	720	CLA	C1D-ND	3.83	1.42	1.37
30	J	310	CLA	C1D-ND	3.82	1.42	1.37
30	j	106	CLA	C1D-ND	3.82	1.42	1.37
30	l	313	CLA	C1D-ND	3.82	1.42	1.37
30	B	317	CLA	C1D-ND	3.82	1.42	1.37
30	P	212	CLA	C1D-ND	3.82	1.42	1.37
30	a	718	CLA	C1D-ND	3.82	1.42	1.37
30	M	317	CLA	C1D-ND	3.82	1.42	1.37
30	B	310	CLA	C1D-ND	3.82	1.42	1.37
30	B	309	CLA	C1D-ND	3.81	1.42	1.37
30	a	704	CLA	C1D-ND	3.81	1.42	1.37
30	A	319	CLA	C1D-ND	3.81	1.42	1.37
34	F	305	PID	C20-C21	3.81	1.40	1.35
30	a	729	CLA	C1D-ND	3.81	1.42	1.37
30	L	314	CLA	C1D-ND	3.81	1.42	1.37
30	L	310	CLA	C1D-ND	3.80	1.42	1.37
30	I	308	CLA	C1D-ND	3.80	1.42	1.37
30	a	706	CLA	C1D-ND	3.80	1.42	1.37
30	D	313	CLA	C1D-ND	3.80	1.42	1.37
30	A	313	CLA	C1D-ND	3.80	1.42	1.37
30	L	308	CLA	C1D-ND	3.80	1.42	1.37
30	J	306	CLA	C1D-ND	3.79	1.42	1.37
28	G	505	DD6	C19-C20	3.79	1.57	1.52
30	a	711	CLA	C1D-ND	3.79	1.42	1.37
30	b	727	CLA	C1D-ND	3.79	1.42	1.37
30	L	309	CLA	C1D-ND	3.79	1.42	1.37
30	D	308	CLA	C1D-ND	3.79	1.42	1.37
30	I	309	CLA	C1D-ND	3.79	1.42	1.37
30	I	319	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	312	CLA	C1D-ND	3.78	1.42	1.37
30	a	725	CLA	C1D-ND	3.78	1.42	1.37
30	P	210	CLA	C1D-ND	3.78	1.42	1.37
29	h	201	UIX	C25-C28	-3.78	1.25	1.32
30	b	723	CLA	C1D-ND	3.78	1.42	1.37
30	a	727	CLA	C1D-ND	3.78	1.42	1.37
30	K	309	CLA	C1D-ND	3.77	1.42	1.37
30	a	701	CLA	C1D-ND	3.77	1.42	1.37
30	b	710	CLA	C1D-ND	3.77	1.42	1.37
30	K	308	CLA	C1D-ND	3.77	1.42	1.37
30	b	725	CLA	C1D-ND	3.77	1.42	1.37
30	b	713	CLA	C1D-ND	3.77	1.42	1.37
30	M	316	CLA	C1D-ND	3.77	1.42	1.37
30	l	304	CLA	C1D-ND	3.76	1.42	1.37
30	F	308	CLA	C1D-ND	3.76	1.42	1.37
30	M	312	CLA	C1D-ND	3.76	1.42	1.37
30	I	316	CLA	C1D-ND	3.76	1.42	1.37
30	G	519	CLA	C1D-ND	3.76	1.42	1.37
30	A	308	CLA	C1D-ND	3.75	1.42	1.37
30	J	309	CLA	C1D-ND	3.75	1.42	1.37
30	A	310	CLA	C1D-ND	3.74	1.42	1.37
30	a	735	CLA	C1D-ND	3.74	1.42	1.37
29	I	304	UIX	C25-C28	-3.74	1.25	1.32
30	I	321	CLA	C1D-ND	3.73	1.42	1.37
30	K	313	CLA	C1D-ND	3.73	1.42	1.37
30	b	712	CLA	C1D-ND	3.73	1.42	1.37
30	b	722	CLA	C1D-ND	3.73	1.42	1.37
30	G	520	CLA	C1D-ND	3.73	1.42	1.37
30	I	313	CLA	C1D-ND	3.73	1.42	1.37
30	l	312	CLA	C1D-ND	3.73	1.42	1.37
30	G	514	CLA	C1D-ND	3.72	1.42	1.37
30	B	315	CLA	C1D-ND	3.71	1.42	1.37
30	b	703	CLA	C1D-ND	3.70	1.42	1.37
30	J	307	CLA	C1D-ND	3.70	1.42	1.37
30	a	719	CLA	C1D-ND	3.70	1.42	1.37
30	a	730	CLA	C1D-ND	3.70	1.42	1.37
30	a	710	CLA	C1D-ND	3.69	1.42	1.37
29	K	302	UIX	C25-C28	-3.69	1.25	1.32
30	b	709	CLA	C1D-ND	3.69	1.42	1.37
30	J	312	CLA	C1D-ND	3.68	1.42	1.37
30	O	313	CLA	C1D-ND	3.68	1.42	1.37
30	a	724	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	713	CLA	C1D-ND	3.67	1.42	1.37
30	a	712	CLA	C1D-ND	3.66	1.42	1.37
29	A	304	UIX	C25-C28	-3.64	1.25	1.32
30	A	320	CLA	C1D-ND	3.64	1.42	1.37
30	b	721	CLA	C1D-ND	3.63	1.42	1.37
30	P	214	CLA	C1D-ND	3.61	1.42	1.37
34	D	307	PID	C20-C21	3.61	1.40	1.35
30	B	311	CLA	C1D-ND	3.60	1.42	1.37
28	G	504	DD6	C19-C20	3.58	1.57	1.52
29	B	305	UIX	C25-C28	-3.56	1.26	1.32
29	O	306	UIX	C25-C28	-3.53	1.26	1.32
30	F	312	CLA	C4D-ND	-3.53	1.32	1.37
29	P	207	UIX	C25-C28	-3.52	1.26	1.32
30	b	712	CLA	CAB-C3B	-3.51	1.44	1.51
34	D	304	PID	C20-C21	3.43	1.40	1.35
34	M	301	PID	C20-C21	3.41	1.40	1.35
34	N	301	PID	C20-C21	3.38	1.40	1.35
30	a	726	CLA	CHC-C1C	3.37	1.43	1.35
29	G	503	UIX	C25-C28	-3.36	1.26	1.32
30	a	735	CLA	CHC-C1C	3.35	1.43	1.35
34	F	304	PID	C20-C21	3.33	1.40	1.35
30	a	705	CLA	CHC-C1C	3.33	1.43	1.35
30	M	313	CLA	CHC-C1C	3.33	1.43	1.35
34	O	305	PID	C20-C21	3.30	1.40	1.35
29	J	305	UIX	C25-C28	-3.30	1.26	1.32
30	I	316	CLA	CHC-C1C	3.29	1.43	1.35
34	F	302	PID	C20-C21	3.28	1.40	1.35
30	I	308	CLA	CHC-C1C	3.28	1.43	1.35
30	I	309	CLA	CHC-C1C	3.28	1.43	1.35
30	b	725	CLA	CHC-C1C	3.27	1.43	1.35
30	A	311	CLA	CHC-C1C	3.27	1.43	1.35
30	L	316	CLA	CHC-C1C	3.27	1.43	1.35
30	L	313	CLA	CHC-C1C	3.27	1.43	1.35
30	b	715	CLA	CHC-C1C	3.27	1.43	1.35
30	D	314	CLA	CHC-C1C	3.26	1.43	1.35
30	A	319	CLA	CHC-C1C	3.26	1.43	1.35
30	K	309	CLA	CHC-C1C	3.26	1.43	1.35
30	a	701	CLA	CHC-C1C	3.26	1.43	1.35
30	a	709	CLA	CHC-C1C	3.25	1.43	1.35
34	P	202	PID	C20-C21	3.25	1.40	1.35
34	P	208	PID	C20-C21	3.25	1.40	1.35
30	O	311	CLA	CHC-C1C	3.25	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	306	PID	C20-C21	3.25	1.40	1.35
30	a	711	CLA	CHC-C1C	3.25	1.43	1.35
30	L	310	CLA	CHC-C1C	3.25	1.43	1.35
30	b	714	CLA	CHC-C1C	3.25	1.43	1.35
30	F	310	CLA	CHC-C1C	3.24	1.43	1.35
30	J	301	CLA	CHC-C1C	3.24	1.43	1.35
30	N	309	CLA	CHC-C1C	3.24	1.43	1.35
34	H	301	PID	C20-C21	3.24	1.40	1.35
34	D	301	PID	C20-C21	3.24	1.40	1.35
30	J	312	CLA	CHC-C1C	3.24	1.43	1.35
30	I	313	CLA	CHC-C1C	3.24	1.43	1.35
34	H	302	PID	C20-C21	3.24	1.40	1.35
30	A	309	CLA	CHC-C1C	3.24	1.43	1.35
30	K	313	CLA	CHC-C1C	3.24	1.43	1.35
30	a	704	CLA	CHC-C1C	3.23	1.43	1.35
30	A	313	CLA	CHC-C1C	3.23	1.43	1.35
30	b	727	CLA	CHC-C1C	3.23	1.43	1.35
30	K	308	CLA	CHC-C1C	3.23	1.43	1.35
30	L	314	CLA	CHC-C1C	3.23	1.43	1.35
30	A	315	CLA	CHC-C1C	3.23	1.43	1.35
30	I	321	CLA	CHC-C1C	3.23	1.43	1.35
30	f	303	CLA	CHC-C1C	3.23	1.43	1.35
30	I	319	CLA	CHC-C1C	3.22	1.43	1.35
30	b	724	CLA	CHC-C1C	3.22	1.43	1.35
30	b	703	CLA	CHC-C1C	3.22	1.43	1.35
30	a	706	CLA	CHC-C1C	3.22	1.43	1.35
30	G	510	CLA	CHC-C1C	3.22	1.43	1.35
30	B	312	CLA	CHC-C1C	3.22	1.43	1.35
30	J	311	CLA	CHC-C1C	3.22	1.43	1.35
30	J	314	CLA	CHC-C1C	3.22	1.43	1.35
34	O	304	PID	C20-C21	3.22	1.40	1.35
30	j	104	CLA	CHC-C1C	3.22	1.43	1.35
30	l	312	CLA	CHC-C1C	3.22	1.43	1.35
30	H	305	CLA	CHC-C1C	3.22	1.43	1.35
30	J	315	CLA	CHC-C1C	3.22	1.43	1.35
30	P	212	CLA	CHC-C1C	3.22	1.43	1.35
30	a	719	CLA	CHC-C1C	3.22	1.43	1.35
30	K	310	CLA	CHC-C1C	3.22	1.43	1.35
30	H	307	CLA	CHC-C1C	3.22	1.43	1.35
30	M	318	CLA	CHC-C1C	3.22	1.43	1.35
30	D	316	CLA	CHC-C1C	3.21	1.43	1.35
30	G	520	CLA	CHC-C1C	3.21	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	312	CLA	CHC-C1C	3.21	1.43	1.35
30	l	309	CLA	CHC-C1C	3.21	1.43	1.35
30	a	714	CLA	CHC-C1C	3.21	1.43	1.35
30	a	717	CLA	CHC-C1C	3.21	1.43	1.35
30	l	308	CLA	CHC-C1C	3.21	1.43	1.35
30	M	311	CLA	CHC-C1C	3.21	1.43	1.35
30	L	309	CLA	CHC-C1C	3.20	1.43	1.35
30	b	707	CLA	CHC-C1C	3.20	1.43	1.35
34	P	206	PID	C20-C21	3.20	1.40	1.35
30	B	317	CLA	CHC-C1C	3.20	1.43	1.35
30	A	317	CLA	CHC-C1C	3.20	1.43	1.35
30	D	311	CLA	CHC-C1C	3.20	1.43	1.35
30	M	310	CLA	CHC-C1C	3.20	1.43	1.35
30	f	301	CLA	CHC-C1C	3.20	1.43	1.35
30	a	722	CLA	CHC-C1C	3.20	1.43	1.35
34	D	305	PID	C20-C21	3.20	1.40	1.35
30	b	706	CLA	CHC-C1C	3.20	1.43	1.35
30	B	309	CLA	CHC-C1C	3.20	1.43	1.35
30	l	313	CLA	CHC-C1C	3.20	1.43	1.35
30	a	708	CLA	CHC-C1C	3.20	1.43	1.35
30	L	311	CLA	CHC-C1C	3.19	1.43	1.35
30	M	315	CLA	CHC-C1C	3.19	1.43	1.35
30	F	315	CLA	CHC-C1C	3.19	1.43	1.35
30	O	316	CLA	CHC-C1C	3.19	1.43	1.35
30	B	310	CLA	CHC-C1C	3.19	1.43	1.35
30	a	727	CLA	CHC-C1C	3.19	1.43	1.35
30	b	716	CLA	CHC-C1C	3.19	1.43	1.35
30	a	723	CLA	CHC-C1C	3.19	1.43	1.35
30	a	725	CLA	CHC-C1C	3.19	1.43	1.35
30	G	513	CLA	CHC-C1C	3.19	1.43	1.35
30	G	519	CLA	CHC-C1C	3.19	1.43	1.35
30	D	308	CLA	CHC-C1C	3.19	1.43	1.35
30	L	308	CLA	CHC-C1C	3.19	1.43	1.35
30	f	302	CLA	CHC-C1C	3.19	1.43	1.35
30	a	729	CLA	CHC-C1C	3.19	1.43	1.35
30	a	707	CLA	CHC-C1C	3.19	1.43	1.35
30	L	312	CLA	CHC-C1C	3.19	1.43	1.35
30	M	309	CLA	CHC-C1C	3.19	1.43	1.35
30	a	730	CLA	CHC-C1C	3.19	1.43	1.35
34	D	306	PID	C20-C21	3.18	1.40	1.35
30	l	304	CLA	CHC-C1C	3.18	1.43	1.35
30	b	723	CLA	CHC-C1C	3.18	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	315	CLA	CHC-C1C	3.18	1.43	1.35
30	l	305	CLA	CHC-C1C	3.18	1.43	1.35
30	j	106	CLA	CHC-C1C	3.18	1.43	1.35
30	b	726	CLA	CHC-C1C	3.18	1.43	1.35
30	P	217	CLA	CHC-C1C	3.18	1.43	1.35
30	N	307	CLA	CHC-C1C	3.18	1.43	1.35
30	G	514	CLA	CHC-C1C	3.18	1.43	1.35
30	b	705	CLA	CHC-C1C	3.18	1.43	1.35
30	D	312	CLA	CHC-C1C	3.18	1.43	1.35
30	H	308	CLA	CHC-C1C	3.18	1.43	1.35
30	M	317	CLA	CHC-C1C	3.18	1.43	1.35
30	K	312	CLA	CHC-C1C	3.18	1.43	1.35
30	D	309	CLA	CHC-C1C	3.17	1.43	1.35
30	a	716	CLA	CHC-C1C	3.17	1.43	1.35
30	A	308	CLA	CHC-C1C	3.17	1.43	1.35
30	a	713	CLA	CHC-C1C	3.17	1.43	1.35
30	I	312	CLA	CHC-C1C	3.17	1.43	1.35
30	B	311	CLA	CHC-C1C	3.17	1.43	1.35
30	a	718	CLA	CHC-C1C	3.17	1.43	1.35
30	A	320	CLA	CHC-C1C	3.17	1.43	1.35
30	O	313	CLA	CHC-C1C	3.17	1.43	1.35
30	G	517	CLA	CHC-C1C	3.17	1.43	1.35
30	M	316	CLA	CHC-C1C	3.17	1.43	1.35
30	F	311	CLA	CHC-C1C	3.16	1.43	1.35
30	a	710	CLA	CHC-C1C	3.16	1.43	1.35
28	M	302	DD6	C19-C20	3.16	1.56	1.52
30	b	713	CLA	CHC-C1C	3.16	1.43	1.35
30	H	312	CLA	CHC-C1C	3.16	1.43	1.35
30	a	731	CLA	CHC-C1C	3.16	1.43	1.35
30	b	712	CLA	CHC-C1C	3.16	1.43	1.35
30	a	712	CLA	CHC-C1C	3.16	1.43	1.35
30	b	720	CLA	CHC-C1C	3.16	1.43	1.35
30	B	308	CLA	CHC-C1C	3.16	1.43	1.35
30	b	728	CLA	CHC-C1C	3.16	1.43	1.35
30	M	308	CLA	CHC-C1C	3.16	1.43	1.35
30	G	516	CLA	CHC-C1C	3.16	1.43	1.35
30	a	720	CLA	CHC-C1C	3.16	1.43	1.35
30	h	202	CLA	CHC-C1C	3.16	1.43	1.35
30	H	311	CLA	CHC-C1C	3.16	1.43	1.35
30	L	318	CLA	CHC-C1C	3.15	1.43	1.35
30	A	310	CLA	CHC-C1C	3.15	1.43	1.35
30	K	311	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	701	CLA	CHC-C1C	3.15	1.43	1.35
30	B	315	CLA	CHC-C1C	3.15	1.43	1.35
30	G	511	CLA	CHC-C1C	3.15	1.43	1.35
30	b	709	CLA	CHC-C1C	3.15	1.43	1.35
30	l	303	CLA	CHC-C1C	3.15	1.43	1.35
30	a	721	CLA	CHC-C1C	3.15	1.43	1.35
30	a	728	CLA	CHC-C1C	3.15	1.43	1.35
30	B	313	CLA	CHC-C1C	3.15	1.43	1.35
30	B	316	CLA	CHC-C1C	3.15	1.43	1.35
30	J	308	CLA	CHC-C1C	3.15	1.43	1.35
30	I	310	CLA	CHC-C1C	3.14	1.43	1.35
30	a	738	CLA	CHC-C1C	3.14	1.43	1.35
30	G	518	CLA	CHC-C1C	3.14	1.43	1.35
30	H	309	CLA	CHC-C1C	3.14	1.43	1.35
30	O	308	CLA	CHC-C1C	3.14	1.43	1.35
30	l	311	CLA	CHC-C1C	3.14	1.43	1.35
30	b	711	CLA	CHC-C1C	3.14	1.43	1.35
30	a	715	CLA	CHC-C1C	3.14	1.43	1.35
30	N	304	CLA	CHC-C1C	3.14	1.43	1.35
30	I	315	CLA	CHC-C1C	3.13	1.43	1.35
34	D	302	PID	C20-C21	3.13	1.39	1.35
30	A	307	CLA	CHC-C1C	3.13	1.43	1.35
30	I	307	CLA	CHC-C1C	3.13	1.43	1.35
30	B	301	CLA	CHC-C1C	3.13	1.43	1.35
30	B	307	CLA	CHC-C1C	3.13	1.43	1.35
34	G	507	PID	C20-C21	3.13	1.39	1.35
30	N	305	CLA	CHC-C1C	3.13	1.43	1.35
30	K	306	CLA	CHC-C1C	3.13	1.43	1.35
30	m	202	CLA	CHC-C1C	3.12	1.43	1.35
30	O	309	CLA	CHC-C1C	3.12	1.43	1.35
30	H	304	CLA	CHC-C1C	3.12	1.43	1.35
30	J	307	CLA	CHC-C1C	3.12	1.43	1.35
30	G	509	CLA	CHC-C1C	3.12	1.43	1.35
30	M	312	CLA	CHC-C1C	3.12	1.43	1.35
30	b	710	CLA	CHC-C1C	3.12	1.43	1.35
30	J	316	CLA	CHC-C1C	3.12	1.43	1.35
30	b	708	CLA	CHC-C1C	3.11	1.42	1.35
30	P	209	CLA	CHC-C1C	3.11	1.42	1.35
30	N	307	CLA	C4D-ND	-3.11	1.33	1.37
30	b	721	CLA	CHC-C1C	3.11	1.42	1.35
30	b	719	CLA	CHC-C1C	3.11	1.42	1.35
30	P	210	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	P	214	CLA	CHC-C1C	3.10	1.42	1.35
30	I	311	CLA	CHC-C1C	3.10	1.42	1.35
30	J	306	CLA	CHC-C1C	3.10	1.42	1.35
30	a	724	CLA	CHC-C1C	3.10	1.42	1.35
30	K	313	CLA	C4D-ND	-3.09	1.33	1.37
30	D	313	CLA	CHC-C1C	3.08	1.42	1.35
30	I	306	CLA	CHC-C1C	3.08	1.42	1.35
30	b	717	CLA	CHC-C1C	3.08	1.42	1.35
34	O	307	PID	C20-C21	3.07	1.39	1.35
30	F	307	CLA	CHC-C1C	3.06	1.42	1.35
30	G	512	CLA	CHC-C1C	3.06	1.42	1.35
30	P	215	CLA	CHC-C1C	3.06	1.42	1.35
30	F	308	CLA	CHC-C1C	3.06	1.42	1.35
30	J	309	CLA	CHC-C1C	3.06	1.42	1.35
30	L	317	CLA	CHC-C1C	3.06	1.42	1.35
30	b	718	CLA	CHC-C1C	3.06	1.42	1.35
30	A	316	CLA	CHC-C1C	3.05	1.42	1.35
34	O	301	PID	C20-C21	3.04	1.39	1.35
30	O	314	CLA	CHC-C1C	3.04	1.42	1.35
30	F	313	CLA	CHC-C1C	3.04	1.42	1.35
30	K	316	CLA	CHC-C1C	3.04	1.42	1.35
30	J	310	CLA	CHC-C1C	3.04	1.42	1.35
30	a	706	CLA	C4D-ND	-3.04	1.33	1.37
34	P	205	PID	C20-C21	3.03	1.39	1.35
28	J	303	DD6	O1-C20	-3.02	1.41	1.46
30	N	310	CLA	CHC-C1C	3.02	1.42	1.35
30	a	725	CLA	C4D-ND	-3.02	1.33	1.37
30	G	510	CLA	C4D-ND	-3.02	1.33	1.37
30	B	311	CLA	C4D-ND	-3.01	1.33	1.37
30	a	705	CLA	C4D-ND	-3.01	1.33	1.37
30	K	307	CLA	C4D-ND	-3.00	1.33	1.37
30	I	309	CLA	C4D-ND	-2.99	1.33	1.37
30	M	312	CLA	C4D-ND	-2.99	1.33	1.37
30	A	308	CLA	C4D-ND	-2.99	1.33	1.37
30	b	713	CLA	C4D-ND	-2.98	1.33	1.37
30	B	310	CLA	C4D-ND	-2.98	1.33	1.37
30	A	312	CLA	C4D-ND	-2.98	1.33	1.37
30	a	704	CLA	C4D-ND	-2.98	1.33	1.37
30	B	313	CLA	C4D-ND	-2.98	1.33	1.37
30	A	319	CLA	C4D-ND	-2.98	1.33	1.37
30	b	722	CLA	CHC-C1C	2.97	1.42	1.35
30	b	720	CLA	C4D-ND	-2.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	702	CLA	C1D-ND	2.97	1.41	1.37
30	M	309	CLA	C4D-ND	-2.96	1.33	1.37
30	a	721	CLA	C4D-ND	-2.96	1.33	1.37
30	b	722	CLA	CMB-C2B	-2.96	1.45	1.51
30	a	712	CLA	C4D-ND	-2.96	1.33	1.37
31	N	308	KC1	C4A-C3A	-2.96	1.38	1.44
30	b	725	CLA	C4D-ND	-2.95	1.33	1.37
30	G	514	CLA	C4D-ND	-2.95	1.33	1.37
30	F	308	CLA	C4D-ND	-2.95	1.33	1.37
30	b	711	CLA	C4D-ND	-2.95	1.33	1.37
30	b	722	CLA	C4D-ND	-2.95	1.33	1.37
30	J	309	CLA	C4D-ND	-2.95	1.33	1.37
30	I	308	CLA	C4D-ND	-2.95	1.33	1.37
30	a	719	CLA	C4D-ND	-2.94	1.33	1.37
30	f	302	CLA	C4D-ND	-2.94	1.33	1.37
30	b	708	CLA	C4D-ND	-2.94	1.33	1.37
30	H	304	CLA	C4D-ND	-2.94	1.33	1.37
30	a	720	CLA	C4D-ND	-2.94	1.33	1.37
30	b	724	CLA	C4D-ND	-2.93	1.33	1.37
30	B	301	CLA	C4D-ND	-2.93	1.33	1.37
30	G	513	CLA	C4D-ND	-2.93	1.33	1.37
30	F	312	CLA	C1D-ND	2.93	1.41	1.37
30	f	303	CLA	C4D-ND	-2.93	1.33	1.37
28	J	304	DD6	C19-C20	2.93	1.56	1.52
30	L	314	CLA	C4D-ND	-2.93	1.33	1.37
30	N	305	CLA	C4D-ND	-2.93	1.33	1.37
30	a	711	CLA	C4D-ND	-2.93	1.33	1.37
30	K	308	CLA	C4D-ND	-2.93	1.33	1.37
30	K	309	CLA	C4D-ND	-2.93	1.33	1.37
30	B	309	CLA	C4D-ND	-2.93	1.33	1.37
30	O	311	CLA	C4D-ND	-2.93	1.33	1.37
30	a	716	CLA	C4D-ND	-2.93	1.33	1.37
30	K	307	CLA	CHC-C1C	2.93	1.42	1.35
30	b	728	CLA	C4D-ND	-2.92	1.33	1.37
30	F	312	CLA	CHC-C1C	2.92	1.42	1.35
30	b	727	CLA	C4D-ND	-2.92	1.33	1.37
30	b	707	CLA	C4D-ND	-2.92	1.33	1.37
30	D	313	CLA	C4D-ND	-2.92	1.33	1.37
30	O	309	CLA	C4D-ND	-2.92	1.33	1.37
30	K	315	CLA	C4D-ND	-2.92	1.33	1.37
30	A	317	CLA	C4D-ND	-2.92	1.33	1.37
30	l	305	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	731	CLA	C4D-ND	-2.92	1.33	1.37
28	J	304	DD6	O1-C20	-2.92	1.42	1.46
30	b	716	CLA	C4D-ND	-2.91	1.33	1.37
30	b	710	CLA	C4D-ND	-2.91	1.33	1.37
30	I	315	CLA	C4D-ND	-2.91	1.33	1.37
30	L	313	CLA	C4D-ND	-2.91	1.33	1.37
30	K	316	CLA	C4D-ND	-2.91	1.33	1.37
30	M	311	CLA	C4D-ND	-2.91	1.33	1.37
30	A	313	CLA	C4D-ND	-2.91	1.33	1.37
30	J	311	CLA	C4D-ND	-2.91	1.33	1.37
30	I	313	CLA	C4D-ND	-2.91	1.33	1.37
30	a	730	CLA	C4D-ND	-2.91	1.33	1.37
30	L	310	CLA	C4D-ND	-2.91	1.33	1.37
30	P	209	CLA	C4D-ND	-2.90	1.33	1.37
30	A	309	CLA	C4D-ND	-2.90	1.33	1.37
30	H	305	CLA	C4D-ND	-2.90	1.33	1.37
30	D	312	CLA	C4D-ND	-2.90	1.33	1.37
30	a	713	CLA	C4D-ND	-2.90	1.33	1.37
30	a	728	CLA	C4D-ND	-2.90	1.33	1.37
30	K	306	CLA	C4D-ND	-2.90	1.33	1.37
30	H	307	CLA	C4D-ND	-2.90	1.33	1.37
30	M	310	CLA	C4D-ND	-2.90	1.33	1.37
30	M	318	CLA	C4D-ND	-2.90	1.33	1.37
30	b	704	CLA	CHC-C1C	2.89	1.42	1.35
30	D	314	CLA	C4D-ND	-2.89	1.33	1.37
34	N	302	PID	C8-C9	-2.89	1.39	1.46
30	L	309	CLA	C4D-ND	-2.89	1.33	1.37
30	M	313	CLA	C4D-ND	-2.89	1.33	1.37
30	a	708	CLA	C4D-ND	-2.89	1.33	1.37
30	L	312	CLA	C4D-ND	-2.89	1.33	1.37
30	O	314	CLA	C4D-ND	-2.89	1.33	1.37
31	K	314	KC1	CBA-CGA	-2.89	1.41	1.48
30	I	316	CLA	C4D-ND	-2.89	1.33	1.37
30	b	706	CLA	C4D-ND	-2.89	1.33	1.37
30	a	701	CLA	C4D-ND	-2.88	1.33	1.37
34	G	506	PID	C8-C9	-2.88	1.39	1.46
30	M	317	CLA	C4D-ND	-2.88	1.33	1.37
30	a	722	CLA	C4D-ND	-2.88	1.33	1.37
30	J	316	CLA	C4D-ND	-2.88	1.33	1.37
30	L	316	CLA	C4D-ND	-2.88	1.33	1.37
30	a	723	CLA	C4D-ND	-2.88	1.33	1.37
30	b	719	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	303	CLA	C4D-ND	-2.88	1.33	1.37
34	O	302	PID	C20-C21	2.88	1.39	1.35
30	b	705	CLA	C4D-ND	-2.88	1.33	1.37
30	P	212	CLA	C4D-ND	-2.87	1.33	1.37
31	A	306	KC1	CBA-CGA	-2.87	1.41	1.48
30	P	214	CLA	C4D-ND	-2.87	1.33	1.37
30	G	517	CLA	C4D-ND	-2.87	1.33	1.37
30	a	707	CLA	C4D-ND	-2.87	1.33	1.37
30	a	718	CLA	C4D-ND	-2.87	1.33	1.37
30	l	312	CLA	C4D-ND	-2.87	1.33	1.37
30	A	310	CLA	C4D-ND	-2.87	1.33	1.37
30	K	311	CLA	C4D-ND	-2.87	1.33	1.37
30	A	311	CLA	C4D-ND	-2.87	1.33	1.37
30	H	309	CLA	C4D-ND	-2.86	1.33	1.37
30	K	310	CLA	C4D-ND	-2.86	1.33	1.37
30	H	312	CLA	C4D-ND	-2.86	1.33	1.37
30	l	308	CLA	C4D-ND	-2.86	1.33	1.37
30	L	311	CLA	C4D-ND	-2.86	1.33	1.37
30	F	312	CLA	CMB-C2B	-2.86	1.45	1.51
30	D	311	CLA	C4D-ND	-2.86	1.33	1.37
30	F	313	CLA	C4D-ND	-2.85	1.33	1.37
30	O	313	CLA	C4D-ND	-2.85	1.33	1.37
30	O	316	CLA	C4D-ND	-2.85	1.33	1.37
30	K	312	CLA	C4D-ND	-2.85	1.33	1.37
30	L	318	CLA	C4D-ND	-2.85	1.33	1.37
30	G	519	CLA	C4D-ND	-2.85	1.33	1.37
30	a	710	CLA	C4D-ND	-2.85	1.33	1.37
30	M	308	CLA	C4D-ND	-2.85	1.33	1.37
30	b	717	CLA	C4D-ND	-2.85	1.33	1.37
30	D	309	CLA	C4D-ND	-2.85	1.33	1.37
30	a	709	CLA	C4D-ND	-2.85	1.33	1.37
30	I	312	CLA	C4D-ND	-2.85	1.33	1.37
30	N	309	CLA	C4D-ND	-2.85	1.33	1.37
30	P	217	CLA	C4D-ND	-2.85	1.33	1.37
30	b	726	CLA	C4D-ND	-2.85	1.33	1.37
30	a	724	CLA	CMB-C2B	-2.84	1.45	1.51
30	B	308	CLA	C4D-ND	-2.84	1.33	1.37
30	a	702	CLA	CMB-C2B	-2.84	1.45	1.51
30	b	704	CLA	CMB-C2B	-2.84	1.45	1.51
30	a	727	CLA	C4D-ND	-2.84	1.33	1.37
30	D	308	CLA	C4D-ND	-2.84	1.33	1.37
30	G	509	CLA	C4D-ND	-2.84	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	316	CLA	C4D-ND	-2.84	1.33	1.37
30	l	311	CLA	C4D-ND	-2.84	1.33	1.37
30	a	715	CLA	C4D-ND	-2.84	1.33	1.37
30	b	704	CLA	C1D-ND	2.84	1.41	1.37
31	M	307	KC1	CBA-CGA	-2.84	1.41	1.48
30	L	308	CLA	C4D-ND	-2.83	1.33	1.37
31	L	307	KC1	CBA-CGA	-2.83	1.41	1.48
30	G	520	CLA	C4D-ND	-2.83	1.33	1.37
30	P	215	CLA	C4D-ND	-2.83	1.33	1.37
30	A	316	CLA	C4D-ND	-2.83	1.33	1.37
30	a	726	CLA	C4D-ND	-2.83	1.33	1.37
30	l	310	CLA	C1D-ND	2.83	1.42	1.37
30	b	721	CLA	C4D-ND	-2.83	1.33	1.37
30	B	312	CLA	C4D-ND	-2.83	1.33	1.37
30	G	512	CLA	C4D-ND	-2.83	1.33	1.37
30	h	202	CLA	C4D-ND	-2.83	1.33	1.37
30	N	304	CLA	C4D-ND	-2.83	1.33	1.37
30	J	312	CLA	C4D-ND	-2.82	1.33	1.37
28	I	303	DD6	O1-C20	-2.82	1.42	1.46
30	B	315	CLA	C4D-ND	-2.82	1.33	1.37
30	I	321	CLA	C4D-ND	-2.82	1.33	1.37
30	O	308	CLA	C4D-ND	-2.82	1.33	1.37
30	I	310	CLA	C4D-ND	-2.82	1.33	1.37
30	J	315	CLA	C4D-ND	-2.82	1.33	1.37
30	J	301	CLA	C4D-ND	-2.82	1.33	1.37
30	J	306	CLA	C4D-ND	-2.82	1.33	1.37
30	a	702	CLA	CHC-C1C	2.82	1.42	1.35
30	a	714	CLA	C4D-ND	-2.82	1.33	1.37
30	J	310	CLA	CMB-C2B	-2.82	1.45	1.51
29	O	306	UIX	O-C1	-2.81	1.42	1.46
30	a	717	CLA	C4D-ND	-2.81	1.33	1.37
30	J	314	CLA	C4D-ND	-2.81	1.33	1.37
31	N	308	KC1	C4B-NB	-2.81	1.34	1.37
30	J	307	CLA	C4D-ND	-2.81	1.33	1.37
29	P	207	UIX	O-C1	-2.81	1.42	1.46
30	G	511	CLA	C4D-ND	-2.81	1.33	1.37
30	f	301	CLA	C4D-ND	-2.81	1.33	1.37
31	J	313	KC1	C4B-NB	-2.81	1.34	1.37
30	B	317	CLA	C4D-ND	-2.81	1.33	1.37
30	b	709	CLA	C4D-ND	-2.80	1.33	1.37
30	b	715	CLA	C4D-ND	-2.80	1.33	1.37
30	F	307	CLA	C4D-ND	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	316	CLA	C4D-ND	-2.80	1.33	1.37
30	a	735	CLA	C4D-ND	-2.80	1.33	1.37
30	M	315	CLA	C4D-ND	-2.80	1.33	1.37
30	P	210	CLA	C4D-ND	-2.80	1.33	1.37
31	A	314	KC1	CBA-CGA	-2.80	1.42	1.48
30	b	701	CLA	C4D-ND	-2.80	1.33	1.37
31	J	313	KC1	CBA-CGA	-2.80	1.42	1.48
30	a	703	CLA	CHC-C1C	2.80	1.42	1.35
30	l	309	CLA	C4D-ND	-2.80	1.33	1.37
30	b	714	CLA	C4D-ND	-2.79	1.33	1.37
30	L	317	CLA	C4D-ND	-2.79	1.33	1.37
34	D	304	PID	C13-C12	2.79	1.44	1.36
30	B	316	CLA	C4D-ND	-2.79	1.33	1.37
30	j	106	CLA	C4D-ND	-2.79	1.33	1.37
30	b	712	CLA	C4D-ND	-2.79	1.33	1.37
31	B	314	KC1	CBA-CGA	-2.78	1.42	1.48
30	I	319	CLA	C4D-ND	-2.78	1.33	1.37
30	G	516	CLA	C4D-ND	-2.78	1.33	1.37
30	a	738	CLA	C4D-ND	-2.78	1.33	1.37
30	F	310	CLA	C4D-ND	-2.78	1.33	1.37
30	H	308	CLA	C4D-ND	-2.78	1.33	1.37
30	l	313	CLA	C4D-ND	-2.78	1.33	1.37
30	b	723	CLA	C4D-ND	-2.78	1.33	1.37
31	P	213	KC1	C4B-NB	-2.78	1.34	1.37
30	H	311	CLA	C4D-ND	-2.78	1.33	1.37
30	A	320	CLA	C4D-ND	-2.78	1.33	1.37
30	A	307	CLA	C4D-ND	-2.77	1.33	1.37
30	N	310	CLA	C4D-ND	-2.77	1.33	1.37
30	F	315	CLA	C4D-ND	-2.77	1.33	1.37
30	m	202	CLA	C4D-ND	-2.77	1.33	1.37
31	H	310	KC1	CBA-CGA	-2.77	1.42	1.48
30	J	310	CLA	C4D-ND	-2.77	1.33	1.37
30	b	710	CLA	CMB-C2B	-2.76	1.45	1.51
34	F	304	PID	C13-C12	2.76	1.44	1.36
30	l	304	CLA	C4D-ND	-2.76	1.33	1.37
34	P	203	PID	C20-C21	2.76	1.39	1.35
31	D	310	KC1	CBA-CGA	-2.76	1.42	1.48
31	P	216	KC1	CBA-CGA	-2.76	1.42	1.48
31	M	314	KC1	C4B-NB	-2.76	1.34	1.37
31	L	315	KC1	CBA-CGA	-2.76	1.42	1.48
30	I	311	CLA	C4D-ND	-2.76	1.33	1.37
31	M	307	KC1	C4B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	729	CLA	C4D-ND	-2.75	1.33	1.37
34	M	301	PID	C13-C12	2.75	1.44	1.36
34	P	206	PID	C13-C12	2.75	1.44	1.36
30	J	308	CLA	C4D-ND	-2.75	1.33	1.37
30	I	306	CLA	C4D-ND	-2.75	1.33	1.37
31	L	315	KC1	C4B-NB	-2.75	1.34	1.37
30	a	724	CLA	C4D-ND	-2.75	1.33	1.37
31	H	306	KC1	CBA-CGA	-2.75	1.42	1.48
30	A	315	CLA	C4D-ND	-2.75	1.33	1.37
30	b	718	CLA	C4D-ND	-2.75	1.33	1.37
30	F	311	CLA	C4D-ND	-2.75	1.33	1.37
31	K	314	KC1	C4B-NB	-2.74	1.34	1.37
30	j	104	CLA	C4D-ND	-2.74	1.33	1.37
30	M	312	CLA	CMB-C2B	-2.74	1.45	1.51
31	N	311	KC1	CBA-CGA	-2.74	1.42	1.48
31	M	314	KC1	CBA-CGA	-2.74	1.42	1.48
31	O	312	KC1	C4B-NB	-2.73	1.34	1.37
30	a	703	CLA	CMB-C2B	-2.73	1.46	1.51
31	F	314	KC1	CBA-CGA	-2.73	1.42	1.48
31	D	310	KC1	C4B-NB	-2.73	1.34	1.37
30	b	712	CLA	CMB-C2B	-2.73	1.46	1.51
31	G	515	KC1	CBA-CGA	-2.73	1.42	1.48
31	F	314	KC1	C4B-NB	-2.73	1.34	1.37
31	N	306	KC1	C4B-NB	-2.73	1.34	1.37
28	I	305	DD6	C36-C31	-2.73	1.31	1.34
30	b	703	CLA	C4D-ND	-2.73	1.33	1.37
31	N	306	KC1	CBA-CGA	-2.73	1.42	1.48
31	P	211	KC1	C4B-NB	-2.73	1.34	1.37
30	I	307	CLA	C4D-ND	-2.73	1.33	1.37
30	B	307	CLA	C4D-ND	-2.72	1.33	1.37
34	O	307	PID	C8-C9	-2.72	1.39	1.46
31	I	314	KC1	CBA-CGA	-2.72	1.42	1.48
31	G	515	KC1	C4B-NB	-2.72	1.34	1.37
31	F	309	KC1	CBA-CGA	-2.72	1.42	1.48
31	H	306	KC1	C4B-NB	-2.72	1.34	1.37
31	P	211	KC1	CBA-CGA	-2.72	1.42	1.48
34	F	302	PID	C13-C12	2.71	1.44	1.36
31	O	315	KC1	C4B-NB	-2.71	1.34	1.37
31	O	312	KC1	CBA-CGA	-2.71	1.42	1.48
31	B	314	KC1	C4B-NB	-2.71	1.34	1.37
31	O	310	KC1	CBA-CGA	-2.70	1.42	1.48
31	H	310	KC1	C4B-NB	-2.70	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	305	DD6	O1-C20	-2.70	1.42	1.46
31	D	315	KC1	CBA-CGA	-2.70	1.42	1.48
31	P	216	KC1	C4B-NB	-2.70	1.34	1.37
34	O	302	PID	C8-C9	-2.69	1.39	1.46
31	O	315	KC1	CBA-CGA	-2.69	1.42	1.48
31	L	307	KC1	C4B-NB	-2.69	1.34	1.37
34	P	203	PID	C8-C9	-2.69	1.39	1.46
34	P	202	PID	C13-C12	2.69	1.43	1.36
28	G	505	DD6	O1-C20	-2.69	1.42	1.46
34	O	304	PID	C13-C12	2.69	1.43	1.36
30	G	518	CLA	C4D-ND	-2.69	1.34	1.37
31	N	308	KC1	C1B-NB	-2.68	1.34	1.37
31	A	314	KC1	C4B-NB	-2.68	1.34	1.37
31	P	213	KC1	CBA-CGA	-2.68	1.42	1.48
34	D	307	PID	C13-C12	2.67	1.43	1.36
34	O	301	PID	C8-C9	-2.66	1.39	1.46
31	A	306	KC1	C4B-NB	-2.66	1.34	1.37
31	F	309	KC1	C4B-NB	-2.65	1.34	1.37
31	O	310	KC1	C4B-NB	-2.65	1.34	1.37
34	F	305	PID	C13-C12	2.65	1.43	1.36
34	H	302	PID	C8-C9	-2.65	1.39	1.46
34	P	208	PID	C13-C12	2.65	1.43	1.36
34	H	301	PID	C13-C12	2.64	1.43	1.36
31	I	314	KC1	C4B-NB	-2.64	1.34	1.37
34	F	306	PID	C13-C12	2.64	1.43	1.36
31	N	311	KC1	C4B-NB	-2.63	1.34	1.37
34	D	302	PID	C8-C9	-2.63	1.39	1.46
29	K	302	UIX	O-C1	-2.63	1.42	1.46
34	N	301	PID	C13-C12	2.63	1.43	1.36
34	O	304	PID	C8-C9	-2.62	1.39	1.46
28	I	305	DD6	C19-C20	2.61	1.55	1.52
34	j	105	PID	C13-C12	2.61	1.43	1.36
34	P	205	PID	C13-C12	2.61	1.43	1.36
30	b	718	CLA	CMB-C2B	-2.61	1.46	1.51
30	b	713	CLA	CMB-C2B	-2.60	1.46	1.51
34	G	506	PID	C20-C21	2.60	1.39	1.35
31	N	308	KC1	CBA-CGA	-2.60	1.42	1.48
30	a	703	CLA	C1D-ND	2.60	1.41	1.37
30	b	721	CLA	CMB-C2B	-2.59	1.46	1.51
34	F	306	PID	C8-C9	-2.59	1.39	1.46
34	O	305	PID	C8-C9	-2.59	1.39	1.46
30	l	313	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	518	CLA	CMB-C2B	-2.59	1.46	1.51
34	F	302	PID	C8-C9	-2.59	1.39	1.46
30	a	712	CLA	CMB-C2B	-2.59	1.46	1.51
30	b	719	CLA	CMB-C2B	-2.59	1.46	1.51
34	D	306	PID	C8-C9	-2.58	1.39	1.46
30	b	709	CLA	CMB-C2B	-2.58	1.46	1.51
34	P	205	PID	C8-C9	-2.58	1.39	1.46
30	b	701	CLA	CMB-C2B	-2.57	1.46	1.51
34	G	507	PID	C8-C9	-2.57	1.39	1.46
34	F	305	PID	C8-C9	-2.57	1.39	1.46
34	D	305	PID	C8-C9	-2.56	1.39	1.46
34	O	301	PID	C13-C12	2.56	1.43	1.36
34	P	206	PID	C8-C9	-2.56	1.39	1.46
30	b	717	CLA	CMB-C2B	-2.55	1.46	1.51
30	a	719	CLA	CMB-C2B	-2.54	1.46	1.51
34	H	301	PID	C8-C9	-2.54	1.40	1.46
30	l	312	CLA	CMB-C2B	-2.54	1.46	1.51
30	K	316	CLA	CMB-C2B	-2.53	1.46	1.51
30	J	308	CLA	CMB-C2B	-2.53	1.46	1.51
30	I	312	CLA	CMB-C2B	-2.53	1.46	1.51
30	P	215	CLA	CMB-C2B	-2.53	1.46	1.51
34	G	507	PID	C13-C12	2.52	1.43	1.36
34	j	105	PID	C8-C9	-2.52	1.40	1.46
34	D	306	PID	C13-C12	2.52	1.43	1.36
30	D	314	CLA	CMB-C2B	-2.51	1.46	1.51
30	a	703	CLA	CMD-C2D	-2.51	1.45	1.50
30	B	301	CLA	CMB-C2B	-2.51	1.46	1.51
30	a	709	CLA	CMB-C2B	-2.51	1.46	1.51
34	D	301	PID	C13-C12	2.51	1.43	1.36
32	L	301	DGD	O1G-C1A	2.51	1.45	1.33
30	I	311	CLA	CMB-C2B	-2.50	1.46	1.51
34	D	301	PID	C8-C9	-2.50	1.40	1.46
28	M	303	DD6	O1-C20	-2.50	1.42	1.46
29	h	201	UIX	O-C1	-2.50	1.42	1.46
29	G	503	UIX	O-C1	-2.49	1.42	1.46
34	P	202	PID	C8-C9	-2.49	1.40	1.46
30	L	312	CLA	CMB-C2B	-2.49	1.46	1.51
30	b	723	CLA	CMB-C2B	-2.48	1.46	1.51
30	a	717	CLA	CMB-C2B	-2.48	1.46	1.51
34	M	301	PID	C8-C9	-2.48	1.40	1.46
30	A	310	CLA	CMB-C2B	-2.48	1.46	1.51
34	H	302	PID	C13-C12	2.48	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	726	CLA	CMB-C2B	-2.48	1.46	1.51
30	K	311	CLA	CMB-C2B	-2.47	1.46	1.51
30	l	303	CLA	CMB-C2B	-2.47	1.46	1.51
34	P	208	PID	C8-C9	-2.47	1.40	1.46
28	G	504	DD6	C36-C31	-2.47	1.32	1.34
30	I	308	CLA	CMB-C2B	-2.47	1.46	1.51
30	b	706	CLA	CMB-C2B	-2.47	1.46	1.51
31	D	315	KC1	C4B-NB	-2.47	1.34	1.37
30	G	512	CLA	CMB-C2B	-2.47	1.46	1.51
34	D	305	PID	C13-C12	2.47	1.43	1.36
30	A	320	CLA	CMB-C2B	-2.46	1.46	1.51
30	H	309	CLA	CMB-C2B	-2.46	1.46	1.51
30	L	318	CLA	CMB-C2B	-2.46	1.46	1.51
30	B	316	CLA	CMB-C2B	-2.46	1.46	1.51
30	M	316	CLA	CMB-C2B	-2.46	1.46	1.51
30	a	701	CLA	CMB-C2B	-2.46	1.46	1.51
30	O	309	CLA	CMB-C2B	-2.45	1.46	1.51
30	L	317	CLA	CMB-C2B	-2.45	1.46	1.51
30	N	305	CLA	CMB-C2B	-2.45	1.46	1.51
30	a	702	CLA	CMD-C2D	-2.45	1.45	1.50
30	B	317	CLA	CMB-C2B	-2.45	1.46	1.51
30	M	311	CLA	CMB-C2B	-2.45	1.46	1.51
30	f	301	CLA	CMB-C2B	-2.44	1.46	1.51
30	J	316	CLA	CMB-C2B	-2.44	1.46	1.51
30	b	705	CLA	CMB-C2B	-2.44	1.46	1.51
30	L	308	CLA	CMB-C2B	-2.44	1.46	1.51
30	a	728	CLA	CMB-C2B	-2.44	1.46	1.51
30	b	704	CLA	C3B-C2B	-2.44	1.37	1.40
34	D	304	PID	C8-C9	-2.44	1.40	1.46
30	a	727	CLA	CMB-C2B	-2.44	1.46	1.51
30	I	315	CLA	CMB-C2B	-2.44	1.46	1.51
30	J	312	CLA	CMB-C2B	-2.44	1.46	1.51
30	K	307	CLA	CMB-C2B	-2.44	1.46	1.51
30	A	317	CLA	CMB-C2B	-2.44	1.46	1.51
30	a	726	CLA	CMB-C2B	-2.44	1.46	1.51
30	l	308	CLA	CMB-C2B	-2.44	1.46	1.51
30	L	316	CLA	CMB-C2B	-2.44	1.46	1.51
34	D	302	PID	C13-C12	2.43	1.43	1.36
30	L	313	CLA	CMB-C2B	-2.43	1.46	1.51
30	K	310	CLA	CMB-C2B	-2.43	1.46	1.51
30	a	715	CLA	CMB-C2B	-2.43	1.46	1.51
30	A	316	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	704	CLA	CMB-C2B	-2.43	1.46	1.51
30	B	307	CLA	CMB-C2B	-2.43	1.46	1.51
30	h	202	CLA	CMB-C2B	-2.43	1.46	1.51
30	a	708	CLA	CMB-C2B	-2.43	1.46	1.51
30	F	308	CLA	CMB-C2B	-2.43	1.46	1.51
30	N	304	CLA	CMB-C2B	-2.43	1.46	1.51
28	G	504	DD6	O1-C20	-2.43	1.42	1.46
31	G	515	KC1	CHD-C4C	2.43	1.41	1.35
30	l	310	CLA	CMB-C2B	-2.43	1.46	1.51
30	a	725	CLA	CMB-C2B	-2.43	1.46	1.51
30	K	306	CLA	CMB-C2B	-2.43	1.46	1.51
30	b	728	CLA	CMB-C2B	-2.43	1.46	1.51
34	N	301	PID	C8-C9	-2.42	1.40	1.46
30	B	311	CLA	CMB-C2B	-2.42	1.46	1.51
30	F	312	CLA	CMD-C2D	-2.42	1.45	1.50
30	a	720	CLA	CMB-C2B	-2.42	1.46	1.51
30	a	702	CLA	C3B-C2B	-2.42	1.37	1.40
30	G	509	CLA	CMB-C2B	-2.42	1.46	1.51
30	a	716	CLA	CMB-C2B	-2.42	1.46	1.51
30	b	724	CLA	CMB-C2B	-2.42	1.46	1.51
30	M	318	CLA	CMB-C2B	-2.42	1.46	1.51
30	B	312	CLA	CMB-C2B	-2.41	1.46	1.51
31	F	309	KC1	C1B-NB	-2.41	1.34	1.37
30	I	306	CLA	CMB-C2B	-2.41	1.46	1.51
30	a	738	CLA	CMB-C2B	-2.41	1.46	1.51
30	J	309	CLA	CMB-C2B	-2.41	1.46	1.51
31	N	306	KC1	CHD-C4C	2.41	1.41	1.35
30	l	310	CLA	C4D-ND	-2.41	1.33	1.37
31	M	307	KC1	CHD-C4C	2.41	1.41	1.35
30	F	307	CLA	CMB-C2B	-2.41	1.46	1.51
30	H	307	CLA	CMB-C2B	-2.41	1.46	1.51
31	H	310	KC1	CHD-C4C	2.41	1.41	1.35
30	a	731	CLA	CMB-C2B	-2.40	1.46	1.51
30	D	312	CLA	CMB-C2B	-2.40	1.46	1.51
30	B	313	CLA	CMB-C2B	-2.40	1.46	1.51
28	M	302	DD6	O1-C20	-2.40	1.42	1.46
31	A	306	KC1	CHD-C4C	2.40	1.41	1.35
31	J	313	KC1	CHD-C4C	2.40	1.41	1.35
34	N	302	PID	C20-C21	2.40	1.39	1.35
30	G	511	CLA	CMB-C2B	-2.40	1.46	1.51
30	a	730	CLA	CMB-C2B	-2.40	1.46	1.51
30	B	310	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	313	CLA	CMB-C2B	-2.40	1.46	1.51
31	P	211	KC1	CHD-C4C	2.40	1.41	1.35
30	I	309	CLA	CMB-C2B	-2.40	1.46	1.51
30	G	519	CLA	CMB-C2B	-2.40	1.46	1.51
30	H	311	CLA	CMB-C2B	-2.40	1.46	1.51
30	J	306	CLA	CMB-C2B	-2.40	1.46	1.51
30	b	708	CLA	CMB-C2B	-2.40	1.46	1.51
30	A	311	CLA	CMB-C2B	-2.40	1.46	1.51
30	N	310	CLA	CMB-C2B	-2.40	1.46	1.51
30	j	104	CLA	CMB-C2B	-2.40	1.46	1.51
30	F	311	CLA	CMB-C2B	-2.40	1.46	1.51
31	L	315	KC1	CHD-C4C	2.40	1.41	1.35
31	D	310	KC1	C1B-NB	-2.39	1.34	1.37
30	M	308	CLA	CMB-C2B	-2.39	1.46	1.51
30	G	514	CLA	CMB-C2B	-2.39	1.46	1.51
30	D	313	CLA	CMB-C2B	-2.39	1.46	1.51
30	O	314	CLA	CMB-C2B	-2.39	1.46	1.51
30	K	312	CLA	CMB-C2B	-2.39	1.46	1.51
31	P	216	KC1	CHD-C4C	2.39	1.41	1.35
30	f	303	CLA	CMB-C2B	-2.39	1.46	1.51
30	b	704	CLA	CMD-C2D	-2.39	1.45	1.50
31	M	314	KC1	CHD-C4C	2.39	1.41	1.35
30	a	723	CLA	CMB-C2B	-2.39	1.46	1.51
30	a	711	CLA	CMB-C2B	-2.39	1.46	1.51
28	K	301	DD6	O1-C20	-2.39	1.42	1.46
30	I	307	CLA	CMB-C2B	-2.39	1.46	1.51
30	B	315	CLA	CMB-C2B	-2.39	1.46	1.51
30	I	321	CLA	CMB-C2B	-2.39	1.46	1.51
30	H	304	CLA	CMB-C2B	-2.39	1.46	1.51
30	N	309	CLA	CMB-C2B	-2.39	1.46	1.51
30	f	302	CLA	CMB-C2B	-2.38	1.46	1.51
30	D	308	CLA	CMB-C2B	-2.38	1.46	1.51
30	J	311	CLA	CMB-C2B	-2.38	1.46	1.51
30	a	721	CLA	CMB-C2B	-2.38	1.46	1.51
30	I	310	CLA	CMB-C2B	-2.38	1.46	1.51
30	A	307	CLA	CMB-C2B	-2.38	1.46	1.51
30	A	319	CLA	CMB-C2B	-2.38	1.46	1.51
30	K	308	CLA	CMB-C2B	-2.38	1.46	1.51
30	P	209	CLA	CMB-C2B	-2.38	1.46	1.51
30	b	703	CLA	CMB-C2B	-2.38	1.46	1.51
30	G	516	CLA	CMB-C2B	-2.38	1.46	1.51
30	J	307	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	707	CLA	CMB-C2B	-2.38	1.46	1.51
34	O	307	PID	C13-C12	2.38	1.43	1.36
30	l	311	CLA	CMB-C2B	-2.38	1.46	1.51
31	O	315	KC1	CHD-C4C	2.38	1.41	1.35
30	F	313	CLA	CMB-C2B	-2.37	1.46	1.51
31	F	314	KC1	CHD-C4C	2.37	1.41	1.35
30	b	716	CLA	CMB-C2B	-2.37	1.46	1.51
31	D	315	KC1	C1B-NB	-2.37	1.34	1.37
30	H	312	CLA	CMB-C2B	-2.37	1.46	1.51
31	B	314	KC1	CHD-C4C	2.37	1.41	1.35
31	O	315	KC1	C1B-NB	-2.37	1.34	1.37
34	G	506	PID	C13-C12	2.37	1.43	1.36
30	G	510	CLA	CMB-C2B	-2.37	1.46	1.51
30	l	305	CLA	CMB-C2B	-2.37	1.46	1.51
30	a	713	CLA	CMB-C2B	-2.37	1.46	1.51
30	b	727	CLA	CMB-C2B	-2.37	1.46	1.51
30	A	315	CLA	CMB-C2B	-2.37	1.46	1.51
30	a	718	CLA	CMB-C2B	-2.37	1.46	1.51
30	H	308	CLA	CMB-C2B	-2.37	1.46	1.51
30	B	308	CLA	CMB-C2B	-2.37	1.46	1.51
31	H	306	KC1	CHD-C4C	2.37	1.41	1.35
30	L	309	CLA	CMB-C2B	-2.36	1.46	1.51
30	a	729	CLA	CMB-C2B	-2.36	1.46	1.51
30	G	520	CLA	CMB-C2B	-2.36	1.46	1.51
30	J	301	CLA	CMB-C2B	-2.36	1.46	1.51
30	P	217	CLA	CMB-C2B	-2.36	1.46	1.51
30	D	316	CLA	CMB-C2B	-2.36	1.46	1.51
31	N	308	KC1	CHD-C4C	2.36	1.41	1.35
30	l	304	CLA	CMB-C2B	-2.36	1.46	1.51
30	a	724	CLA	CMD-C2D	-2.36	1.45	1.50
30	O	311	CLA	CMB-C2B	-2.36	1.46	1.51
30	N	307	CLA	CMB-C2B	-2.36	1.46	1.51
34	O	302	PID	C13-C12	2.36	1.43	1.36
30	b	707	CLA	CMB-C2B	-2.36	1.46	1.51
30	b	711	CLA	CMB-C2B	-2.36	1.46	1.51
30	J	314	CLA	CMB-C2B	-2.36	1.46	1.51
30	M	317	CLA	CMB-C2B	-2.36	1.46	1.51
30	I	319	CLA	CMB-C2B	-2.35	1.46	1.51
31	A	314	KC1	CHD-C4C	2.35	1.41	1.35
30	P	214	CLA	CMB-C2B	-2.35	1.46	1.51
30	a	714	CLA	CMB-C2B	-2.35	1.46	1.51
30	O	316	CLA	CMB-C2B	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	314	CLA	CMB-C2B	-2.35	1.46	1.51
30	P	212	CLA	CMB-C2B	-2.35	1.46	1.51
34	D	307	PID	C8-C9	-2.35	1.40	1.46
31	P	213	KC1	CHD-C4C	2.35	1.41	1.35
30	l	309	CLA	CMB-C2B	-2.35	1.46	1.51
30	M	309	CLA	CMB-C2B	-2.35	1.46	1.51
30	b	725	CLA	CMB-C2B	-2.35	1.46	1.51
31	N	311	KC1	CHD-C4C	2.35	1.41	1.35
30	L	311	CLA	CMB-C2B	-2.35	1.46	1.51
30	a	705	CLA	CMB-C2B	-2.35	1.46	1.51
30	a	735	CLA	CMB-C2B	-2.35	1.46	1.51
31	D	310	KC1	CHD-C4C	2.35	1.41	1.35
30	b	715	CLA	CMB-C2B	-2.35	1.46	1.51
30	A	313	CLA	CMB-C2B	-2.35	1.46	1.51
34	O	305	PID	C13-C12	2.35	1.43	1.36
30	j	106	CLA	CMB-C2B	-2.35	1.46	1.51
30	A	312	CLA	CMB-C2B	-2.35	1.46	1.51
30	F	310	CLA	CMB-C2B	-2.35	1.46	1.51
31	O	310	KC1	CHD-C4C	2.35	1.41	1.35
30	P	210	CLA	CMB-C2B	-2.35	1.46	1.51
30	A	309	CLA	CMB-C2B	-2.34	1.46	1.51
31	L	307	KC1	C1B-NB	-2.34	1.34	1.37
30	M	310	CLA	CMB-C2B	-2.34	1.46	1.51
33	I	318	LMG	C4-C5	2.34	1.58	1.53
31	I	314	KC1	CHD-C4C	2.34	1.41	1.35
30	O	308	CLA	CMB-C2B	-2.34	1.46	1.51
30	b	714	CLA	CMB-C2B	-2.34	1.46	1.51
30	D	309	CLA	CMB-C2B	-2.34	1.46	1.51
30	J	315	CLA	CMB-C2B	-2.33	1.46	1.51
30	M	315	CLA	CMB-C2B	-2.33	1.46	1.51
31	P	211	KC1	C1B-NB	-2.33	1.34	1.37
30	F	312	CLA	C3B-C2B	-2.33	1.37	1.40
30	a	710	CLA	CMB-C2B	-2.33	1.46	1.51
30	O	313	CLA	CMB-C2B	-2.33	1.46	1.51
31	O	312	KC1	CHD-C4C	2.33	1.40	1.35
30	K	313	CLA	CMB-C2B	-2.33	1.46	1.51
30	G	513	CLA	CMB-C2B	-2.33	1.46	1.51
30	F	315	CLA	CMB-C2B	-2.33	1.46	1.51
30	I	313	CLA	CMB-C2B	-2.33	1.46	1.51
30	G	517	CLA	CMB-C2B	-2.33	1.46	1.51
30	b	720	CLA	CMB-C2B	-2.33	1.46	1.51
29	B	305	UIX	O-C1	-2.32	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	311	CLA	CMB-C2B	-2.32	1.46	1.51
28	I	302	DD6	O1-C20	-2.32	1.42	1.46
30	K	315	CLA	CMB-C2B	-2.32	1.46	1.51
28	L	304	DD6	O1-C20	-2.32	1.42	1.46
30	m	202	CLA	CMB-C2B	-2.32	1.46	1.51
30	b	704	CLA	CMC-C2C	-2.32	1.45	1.50
31	G	515	KC1	C1B-NB	-2.32	1.34	1.37
34	P	203	PID	C13-C12	2.32	1.42	1.36
28	B	302	DD6	O1-C20	-2.32	1.42	1.46
31	H	310	KC1	C1B-NB	-2.32	1.34	1.37
30	H	305	CLA	CMB-C2B	-2.32	1.46	1.51
30	A	308	CLA	CMB-C2B	-2.31	1.46	1.51
31	L	307	KC1	CHD-C4C	2.31	1.40	1.35
31	A	306	KC1	C1B-NB	-2.31	1.34	1.37
34	F	304	PID	C8-C9	-2.31	1.40	1.46
31	J	313	KC1	C1B-NB	-2.31	1.34	1.37
30	K	309	CLA	CMB-C2B	-2.30	1.46	1.51
30	L	310	CLA	CMB-C2B	-2.30	1.46	1.51
30	a	726	CLA	C3B-C2B	-2.30	1.37	1.40
31	O	310	KC1	C1B-NB	-2.30	1.35	1.37
30	B	309	CLA	CMB-C2B	-2.30	1.46	1.51
30	I	316	CLA	CMB-C2B	-2.29	1.46	1.51
31	K	314	KC1	CHD-C4C	2.29	1.40	1.35
28	A	302	DD6	C26-C27	-2.29	1.32	1.37
29	A	304	UIX	O-C1	-2.29	1.42	1.46
30	a	702	CLA	C3B-CAB	-2.28	1.43	1.47
31	F	309	KC1	CHD-C4C	2.28	1.40	1.35
31	I	314	KC1	C1B-NB	-2.28	1.35	1.37
28	K	304	DD6	O1-C20	-2.28	1.42	1.46
29	J	305	UIX	O-C1	-2.28	1.43	1.46
30	a	722	CLA	CMB-C2B	-2.28	1.46	1.51
30	a	706	CLA	CMB-C2B	-2.28	1.46	1.51
31	F	309	KC1	C4A-C3A	-2.28	1.40	1.44
29	I	304	UIX	O-C1	-2.27	1.43	1.46
31	A	314	KC1	C1B-NB	-2.27	1.35	1.37
31	P	213	KC1	C1B-NB	-2.27	1.35	1.37
31	D	315	KC1	CHD-C4C	2.27	1.40	1.35
31	A	306	KC1	C4A-C3A	-2.27	1.40	1.44
30	B	311	CLA	CMD-C2D	-2.26	1.46	1.50
30	b	704	CLA	C3B-CAB	-2.26	1.43	1.47
29	I	304	UIX	C15-C20	-2.26	1.50	1.54
28	B	304	DD6	O1-C20	-2.26	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	710	CLA	CMD-C2D	-2.26	1.46	1.50
31	M	314	KC1	C1B-NB	-2.26	1.35	1.37
31	K	314	KC1	C1B-NB	-2.25	1.35	1.37
28	G	508	DD6	O1-C20	-2.25	1.43	1.46
31	A	314	KC1	C4A-C3A	-2.25	1.40	1.44
31	F	314	KC1	C1B-NB	-2.25	1.35	1.37
31	G	515	KC1	C4A-C3A	-2.25	1.40	1.44
28	b	731	DD6	O1-C20	-2.25	1.43	1.46
30	a	702	CLA	CMC-C2C	-2.25	1.46	1.50
30	F	312	CLA	C3B-CAB	-2.25	1.43	1.47
31	B	314	KC1	C1B-NB	-2.25	1.35	1.37
31	N	311	KC1	C1B-NB	-2.24	1.35	1.37
33	K	317	LMG	O7-C8	-2.24	1.41	1.46
34	N	302	PID	C13-C12	2.24	1.42	1.36
30	a	726	CLA	C3B-CAB	-2.24	1.43	1.47
30	l	310	CLA	C1A-NA	2.24	1.40	1.35
31	M	307	KC1	C1B-NB	-2.24	1.35	1.37
28	I	303	DD6	C19-C20	2.24	1.55	1.52
31	O	312	KC1	C1B-NB	-2.24	1.35	1.37
30	b	721	CLA	CMD-C2D	-2.24	1.46	1.50
30	a	702	CLA	MG-ND	-2.23	2.01	2.05
31	D	310	KC1	C4A-C3A	-2.23	1.40	1.44
28	F	303	DD6	O1-C20	-2.23	1.43	1.46
31	L	315	KC1	C1B-NB	-2.22	1.35	1.37
28	K	303	DD6	O1-C20	-2.22	1.43	1.46
34	F	305	PID	C15-C14	2.22	1.38	1.35
30	a	703	CLA	CMC-C2C	-2.22	1.46	1.50
31	P	216	KC1	C1B-NB	-2.21	1.35	1.37
30	b	722	CLA	CMD-C2D	-2.20	1.46	1.50
30	l	310	CLA	C3D-C4D	2.20	1.48	1.43
28	H	303	DD6	O1-C20	-2.20	1.43	1.46
28	M	304	DD6	O1-C20	-2.20	1.43	1.46
31	H	306	KC1	C1B-NB	-2.19	1.35	1.37
28	M	306	DD6	O1-C20	-2.19	1.43	1.46
28	I	303	DD6	C21-C20	-2.19	1.48	1.51
31	N	306	KC1	C1B-NB	-2.19	1.35	1.37
31	J	313	KC1	C4A-C3A	-2.19	1.40	1.44
30	a	703	CLA	MG-ND	-2.19	2.01	2.05
37	i	201	BCR	C1-C6	-2.18	1.50	1.53
30	a	703	CLA	C3B-CAB	-2.18	1.43	1.47
31	M	307	KC1	C4A-C3A	-2.18	1.40	1.44
30	A	320	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	315	KC1	C4A-C3A	-2.18	1.40	1.44
30	F	312	CLA	CMC-C2C	-2.17	1.46	1.50
28	B	306	DD6	O1-C20	-2.16	1.43	1.46
28	O	303	DD6	O1-C20	-2.16	1.43	1.46
30	b	704	CLA	MG-ND	-2.16	2.01	2.05
30	J	308	CLA	CMD-C2D	-2.16	1.46	1.50
31	I	314	KC1	C4A-C3A	-2.15	1.40	1.44
31	O	310	KC1	C4A-C3A	-2.15	1.40	1.44
28	P	204	DD6	O1-C20	-2.15	1.43	1.46
31	P	213	KC1	C4A-C3A	-2.15	1.40	1.44
28	L	305	DD6	O1-C20	-2.15	1.43	1.46
30	P	212	CLA	CMD-C2D	-2.14	1.46	1.50
30	l	305	CLA	CMD-C2D	-2.14	1.46	1.50
35	A	318	SQD	O8-S	2.13	1.55	1.47
30	a	711	CLA	CMD-C2D	-2.13	1.46	1.50
31	K	314	KC1	C4A-C3A	-2.13	1.40	1.44
33	b	733	LMG	O7-C8	-2.13	1.41	1.46
33	D	317	LMG	O7-C8	-2.13	1.41	1.46
30	a	719	CLA	CMC-C2C	-2.13	1.46	1.50
28	M	305	DD6	O1-C20	-2.12	1.43	1.46
30	N	309	CLA	CMC-C2C	-2.12	1.46	1.50
31	P	216	KC1	C4A-C3A	-2.12	1.40	1.44
31	L	307	KC1	C4A-C3A	-2.12	1.40	1.44
31	L	315	KC1	C4A-C3A	-2.12	1.40	1.44
30	N	309	CLA	CMD-C2D	-2.12	1.46	1.50
31	F	314	KC1	C4A-C3A	-2.12	1.40	1.44
30	b	710	CLA	CMD-C2D	-2.12	1.46	1.50
30	b	703	CLA	CMD-C2D	-2.11	1.46	1.50
31	N	306	KC1	C4A-C3A	-2.11	1.40	1.44
28	L	306	DD6	O1-C20	-2.11	1.43	1.46
30	a	719	CLA	CMD-C2D	-2.11	1.46	1.50
31	B	314	KC1	C4A-C3A	-2.10	1.40	1.44
28	h	203	DD6	O1-C20	-2.10	1.43	1.46
30	l	310	CLA	CMD-C2D	-2.10	1.46	1.50
30	O	313	CLA	CMD-C2D	-2.10	1.46	1.50
28	K	305	DD6	O1-C20	-2.10	1.43	1.46
30	G	512	CLA	CMC-C2C	-2.09	1.46	1.50
30	M	316	CLA	CMD-C2D	-2.09	1.46	1.50
30	K	311	CLA	CMD-C2D	-2.09	1.46	1.50
30	D	313	CLA	CMD-C2D	-2.09	1.46	1.50
30	b	701	CLA	CMD-C2D	-2.09	1.46	1.50
30	j	106	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	727	CLA	CMD-C2D	-2.09	1.46	1.50
28	J	304	DD6	C36-C31	-2.09	1.32	1.34
30	P	214	CLA	CMD-C2D	-2.09	1.46	1.50
31	O	312	KC1	C4A-C3A	-2.09	1.40	1.44
30	K	315	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	703	CLA	C3B-C2B	-2.08	1.37	1.40
30	J	306	CLA	CMD-C2D	-2.08	1.46	1.50
30	a	723	CLA	CMD-C2D	-2.08	1.46	1.50
30	F	312	CLA	MG-ND	-2.08	2.01	2.05
28	M	303	DD6	C36-C31	-2.07	1.32	1.34
30	N	307	CLA	CMD-C2D	-2.07	1.46	1.50
31	M	314	KC1	C4A-C3A	-2.07	1.40	1.44
30	b	709	CLA	CMD-C2D	-2.07	1.46	1.50
30	F	313	CLA	CMD-C2D	-2.07	1.46	1.50
30	a	701	CLA	CMD-C2D	-2.07	1.46	1.50
30	P	217	CLA	CMD-C2D	-2.06	1.46	1.50
37	i	201	BCR	C30-C25	-2.06	1.50	1.53
28	I	305	DD6	C2-C1	-2.06	1.33	1.35
30	b	717	CLA	CMC-C2C	-2.06	1.46	1.50
30	G	511	CLA	CMD-C2D	-2.05	1.46	1.50
30	a	706	CLA	CMC-C2C	-2.05	1.46	1.50
30	a	715	CLA	CMD-C2D	-2.05	1.46	1.50
31	H	306	KC1	C4A-C3A	-2.05	1.40	1.44
30	F	308	CLA	CMC-C2C	-2.05	1.46	1.50
30	J	310	CLA	CMD-C2D	-2.05	1.46	1.50
30	D	314	CLA	C3B-C2B	-2.04	1.37	1.40
28	K	318	DD6	O1-C20	-2.04	1.43	1.46
30	P	217	CLA	CMC-C2C	-2.04	1.46	1.50
28	N	303	DD6	O1-C20	-2.04	1.43	1.46
30	H	308	CLA	CMD-C2D	-2.03	1.46	1.50
29	P	207	UIX	C15-C20	-2.03	1.51	1.54
30	A	319	CLA	CMD-C2D	-2.03	1.46	1.50
30	a	729	CLA	CMD-C2D	-2.03	1.46	1.50
30	L	318	CLA	CMC-C2C	-2.03	1.46	1.50
30	B	317	CLA	CMD-C2D	-2.03	1.46	1.50
30	H	311	CLA	CMD-C2D	-2.03	1.46	1.50
30	O	314	CLA	CMD-C2D	-2.03	1.46	1.50
30	K	310	CLA	CMD-C2D	-2.03	1.46	1.50
30	J	312	CLA	CMD-C2D	-2.03	1.46	1.50
30	L	317	CLA	CMD-C2D	-2.03	1.46	1.50
31	P	211	KC1	C4A-C3A	-2.03	1.40	1.44
30	b	713	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	730	CLA	CMC-C2C	-2.02	1.46	1.50
30	b	727	CLA	CMC-C2C	-2.02	1.46	1.50
30	I	319	CLA	CMD-C2D	-2.02	1.46	1.50
30	K	312	CLA	CMD-C2D	-2.02	1.46	1.50
30	b	724	CLA	CMD-C2D	-2.02	1.46	1.50
30	L	318	CLA	CMD-C2D	-2.02	1.46	1.50
30	I	312	CLA	CMD-C2D	-2.01	1.46	1.50
30	P	209	CLA	CMD-C2D	-2.01	1.46	1.50
30	K	312	CLA	CMC-C2C	-2.01	1.46	1.50
30	F	310	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	310	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	713	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	315	CLA	CMD-C2D	-2.01	1.46	1.50
30	G	520	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	731	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	316	CLA	CMC-C2C	-2.01	1.46	1.50
30	f	301	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	704	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	717	CLA	CMC-C2C	-2.01	1.46	1.50
30	D	316	CLA	CMC-C2C	-2.01	1.46	1.50
30	L	311	CLA	CMD-C2D	-2.01	1.46	1.50
30	F	307	CLA	CMD-C2D	-2.01	1.46	1.50
30	N	305	CLA	CMD-C2D	-2.01	1.46	1.50
30	J	307	CLA	CMD-C2D	-2.01	1.46	1.50
31	H	310	KC1	C4A-C3A	-2.01	1.40	1.44
28	I	301	DD6	O1-C20	-2.00	1.43	1.46
30	G	514	CLA	CMC-C2C	-2.00	1.46	1.50
30	B	315	CLA	CMD-C2D	-2.00	1.46	1.50
30	M	311	CLA	CMD-C2D	-2.00	1.46	1.50
30	a	722	CLA	CMC-C2C	-2.00	1.46	1.50
30	b	712	CLA	CMD-C2D	-2.00	1.46	1.50
30	b	728	CLA	CMC-C2C	-2.00	1.46	1.50

All (3152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	304	UIX	O-C1-C3	9.22	120.31	113.38
29	J	305	UIX	O-C1-C3	8.93	120.09	113.38
29	I	304	UIX	C6-C1-C	-8.91	107.33	122.26
29	B	305	UIX	O-C1-C3	8.34	119.65	113.38
37	m	201	BCR	C7-C8-C9	-8.14	113.94	126.23
29	O	306	UIX	C14-C13-C11	-7.64	116.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	503	UIX	O-C1-C3	7.60	119.09	113.38
30	l	304	CLA	C4A-NA-C1A	7.49	110.07	106.71
30	O	314	CLA	C4A-NA-C1A	7.39	110.03	106.71
29	h	201	UIX	O-C1-C3	7.27	118.84	113.38
30	P	215	CLA	C4A-NA-C1A	7.16	109.93	106.71
30	J	307	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	J	309	CLA	C4A-NA-C1A	7.08	109.89	106.71
29	G	503	UIX	C6-C1-C	-7.07	110.41	122.26
28	J	303	DD6	C3-C2-C1	-7.07	117.22	127.31
30	B	308	CLA	C4A-NA-C1A	7.05	109.88	106.71
30	P	210	CLA	C4A-NA-C1A	7.05	109.88	106.71
30	a	702	CLA	C4A-NA-C1A	7.04	109.87	106.71
30	a	715	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	L	311	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	N	310	CLA	C4A-NA-C1A	7.02	109.86	106.71
30	b	714	CLA	C4A-NA-C1A	7.01	109.86	106.71
30	G	512	CLA	C4A-NA-C1A	7.00	109.85	106.71
30	b	704	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	B	317	CLA	C4A-NA-C1A	6.99	109.85	106.71
30	L	309	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	M	317	CLA	C4A-NA-C1A	6.98	109.84	106.71
30	b	719	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	b	718	CLA	C4A-NA-C1A	6.97	109.84	106.71
30	L	318	CLA	C4A-NA-C1A	6.96	109.83	106.71
30	D	311	CLA	C4A-NA-C1A	6.94	109.83	106.71
30	J	312	CLA	C4A-NA-C1A	6.94	109.83	106.71
29	h	201	UIX	C6-C1-C	-6.94	110.64	122.26
30	a	730	CLA	C4A-NA-C1A	6.91	109.81	106.71
30	a	738	CLA	C4A-NA-C1A	6.91	109.81	106.71
30	A	310	CLA	C4A-NA-C1A	6.91	109.81	106.71
30	M	315	CLA	C4A-NA-C1A	6.90	109.81	106.71
30	h	202	CLA	C4A-NA-C1A	6.90	109.81	106.71
30	G	514	CLA	C4A-NA-C1A	6.88	109.80	106.71
30	b	728	CLA	C4A-NA-C1A	6.88	109.80	106.71
30	N	309	CLA	C4A-NA-C1A	6.88	109.80	106.71
30	M	310	CLA	C4A-NA-C1A	6.87	109.79	106.71
30	B	315	CLA	C4A-NA-C1A	6.83	109.78	106.71
30	A	308	CLA	C4A-NA-C1A	6.83	109.78	106.71
29	J	305	UIX	C6-C1-C	-6.83	110.82	122.26
30	P	212	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	l	303	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	K	312	CLA	C4A-NA-C1A	6.81	109.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	316	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	J	306	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	I	307	CLA	C4A-NA-C1A	6.80	109.77	106.71
30	b	720	CLA	C4A-NA-C1A	6.80	109.76	106.71
29	K	302	UIX	O-C1-C3	6.80	118.49	113.38
30	B	313	CLA	C4A-NA-C1A	6.80	109.76	106.71
30	I	306	CLA	C4A-NA-C1A	6.80	109.76	106.71
29	B	305	UIX	C6-C1-C	-6.79	110.89	122.26
30	A	307	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	a	731	CLA	C4A-NA-C1A	6.78	109.75	106.71
30	a	714	CLA	C4A-NA-C1A	6.77	109.75	106.71
30	F	315	CLA	C4A-NA-C1A	6.76	109.75	106.71
30	J	315	CLA	C4A-NA-C1A	6.76	109.74	106.71
30	b	701	CLA	C4A-NA-C1A	6.76	109.74	106.71
30	a	703	CLA	C4A-NA-C1A	6.75	109.74	106.71
30	F	313	CLA	C4A-NA-C1A	6.75	109.74	106.71
34	P	206	PID	C17-C16-C15	6.75	137.30	123.47
30	F	310	CLA	C4A-NA-C1A	6.75	109.74	106.71
30	P	217	CLA	C4A-NA-C1A	6.75	109.74	106.71
30	F	308	CLA	C4A-NA-C1A	6.74	109.74	106.71
30	A	320	CLA	C4A-NA-C1A	6.73	109.73	106.71
30	M	308	CLA	C4A-NA-C1A	6.73	109.73	106.71
30	a	720	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	b	716	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	I	319	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	b	705	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	K	307	CLA	C4A-NA-C1A	6.70	109.72	106.71
30	a	701	CLA	C4A-NA-C1A	6.70	109.72	106.71
30	K	316	CLA	C4A-NA-C1A	6.69	109.71	106.71
30	b	727	CLA	C4A-NA-C1A	6.69	109.71	106.71
30	a	718	CLA	C4A-NA-C1A	6.69	109.71	106.71
30	b	709	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	a	710	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	a	716	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	L	316	CLA	C4A-NA-C1A	6.68	109.71	106.71
30	I	311	CLA	C4A-NA-C1A	6.67	109.71	106.71
30	b	707	CLA	C4A-NA-C1A	6.67	109.70	106.71
29	P	207	UIX	C14-C13-C11	-6.67	117.80	127.31
30	O	309	CLA	C4A-NA-C1A	6.66	109.70	106.71
30	B	309	CLA	C4A-NA-C1A	6.65	109.70	106.71
30	G	518	CLA	C4A-NA-C1A	6.65	109.70	106.71
30	a	705	CLA	C4A-NA-C1A	6.65	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	304	CLA	C4A-NA-C1A	6.65	109.69	106.71
30	K	306	CLA	C4A-NA-C1A	6.63	109.69	106.71
37	b	702	BCR	C24-C23-C22	-6.63	116.22	126.23
37	b	730	BCR	C7-C8-C9	-6.63	116.22	126.23
30	I	310	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	G	519	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	O	316	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	D	309	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	M	303	DD6	C9-C10-C11	-6.61	117.87	127.31
30	I	313	CLA	C4A-NA-C1A	6.61	109.68	106.71
30	K	308	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	I	321	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	a	722	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	l	313	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	H	305	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	F	307	CLA	C4A-NA-C1A	6.59	109.67	106.71
30	H	312	CLA	C4A-NA-C1A	6.59	109.67	106.71
29	O	306	UIX	C7-C10-C11	-6.59	115.31	125.53
30	b	724	CLA	C4A-NA-C1A	6.58	109.67	106.71
30	a	727	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	b	712	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	a	725	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	D	316	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	G	517	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	a	711	CLA	C4A-NA-C1A	6.57	109.66	106.71
30	l	311	CLA	C4A-NA-C1A	6.56	109.66	106.71
30	G	510	CLA	C4A-NA-C1A	6.56	109.65	106.71
34	F	305	PID	C17-C16-C15	6.56	136.91	123.47
30	H	307	CLA	C4A-NA-C1A	6.56	109.65	106.71
30	f	301	CLA	C4A-NA-C1A	6.55	109.65	106.71
31	D	315	KC1	CHB-C1B-NB	6.55	130.47	124.45
30	a	708	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	B	312	CLA	C4A-NA-C1A	6.55	109.65	106.71
30	F	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
30	A	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
30	K	311	CLA	C4A-NA-C1A	6.54	109.64	106.71
30	L	314	CLA	C4A-NA-C1A	6.53	109.64	106.71
31	O	312	KC1	CHC-C4B-NB	6.53	130.45	124.45
30	L	312	CLA	C4A-NA-C1A	6.53	109.64	106.71
30	G	509	CLA	C4A-NA-C1A	6.52	109.64	106.71
30	b	726	CLA	C4A-NA-C1A	6.52	109.64	106.71
30	f	303	CLA	C4A-NA-C1A	6.51	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	308	CLA	C4A-NA-C1A	6.51	109.64	106.71
30	G	516	CLA	C4A-NA-C1A	6.51	109.63	106.71
30	a	728	CLA	C4A-NA-C1A	6.51	109.63	106.71
29	A	304	UIX	O-C1-C3	6.51	118.27	113.38
30	D	313	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	N	305	CLA	C4A-NA-C1A	6.50	109.63	106.71
31	H	310	KC1	CHB-C1B-NB	6.50	130.43	124.45
30	O	313	CLA	C4A-NA-C1A	6.49	109.63	106.71
30	l	308	CLA	C4A-NA-C1A	6.49	109.62	106.71
30	J	311	CLA	C4A-NA-C1A	6.49	109.62	106.71
30	j	106	CLA	C4A-NA-C1A	6.48	109.62	106.71
30	D	312	CLA	C4A-NA-C1A	6.48	109.62	106.71
30	I	315	CLA	C4A-NA-C1A	6.47	109.62	106.71
29	A	304	UIX	C6-C1-C	-6.47	111.41	122.26
31	P	216	KC1	CHB-C1B-NB	6.47	130.40	124.45
30	b	715	CLA	C4A-NA-C1A	6.47	109.61	106.71
30	b	723	CLA	C4A-NA-C1A	6.47	109.61	106.71
30	A	313	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	K	315	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	A	315	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	M	316	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	a	723	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	D	308	CLA	C4A-NA-C1A	6.45	109.61	106.71
30	b	708	CLA	C4A-NA-C1A	6.44	109.60	106.71
30	b	710	CLA	C4A-NA-C1A	6.44	109.60	106.71
31	D	310	KC1	CHC-C4B-NB	6.44	130.37	124.45
31	F	309	KC1	CHC-C4B-NB	6.44	130.37	124.45
30	f	302	CLA	C4A-NA-C1A	6.44	109.60	106.71
30	G	511	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	a	707	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	J	316	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	A	317	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	L	310	CLA	C4A-NA-C1A	6.42	109.59	106.71
30	A	312	CLA	C4A-NA-C1A	6.41	109.59	106.71
30	G	513	CLA	C4A-NA-C1A	6.41	109.59	106.71
30	a	712	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	b	725	CLA	C4A-NA-C1A	6.40	109.58	106.71
31	M	314	KC1	CHB-C1B-NB	6.40	130.34	124.45
30	O	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
31	H	306	KC1	CHB-C1B-NB	6.40	130.33	124.45
37	l	302	BCR	C24-C23-C22	-6.39	116.58	126.23
30	K	310	CLA	C4A-NA-C1A	6.39	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	314	KC1	CHB-C1B-NB	6.38	130.32	124.45
30	m	202	CLA	C4A-NA-C1A	6.38	109.58	106.71
34	P	205	PID	C17-C16-C15	6.38	136.55	123.47
28	F	301	DD6	C9-C10-C11	-6.38	118.20	127.31
30	b	722	CLA	C4A-NA-C1A	6.38	109.57	106.71
28	K	318	DD6	C9-C10-C11	-6.38	118.21	127.31
30	l	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	H	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	A	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	a	706	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	M	311	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	a	729	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	a	721	CLA	C4A-NA-C1A	6.36	109.57	106.71
30	K	313	CLA	C4A-NA-C1A	6.36	109.57	106.71
31	D	310	KC1	CHB-C1B-NB	6.36	130.30	124.45
30	K	309	CLA	C4A-NA-C1A	6.36	109.56	106.71
30	B	301	CLA	C4A-NA-C1A	6.36	109.56	106.71
30	J	301	CLA	C4A-NA-C1A	6.36	109.56	106.71
31	A	314	KC1	CHB-C1B-NB	6.36	130.30	124.45
30	P	214	CLA	C4A-NA-C1A	6.35	109.56	106.71
30	b	703	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	P	209	CLA	C4A-NA-C1A	6.34	109.56	106.71
30	A	319	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	B	316	CLA	C4A-NA-C1A	6.33	109.55	106.71
34	F	305	PID	C18-C19-C20	6.33	136.44	123.47
30	M	309	CLA	C4A-NA-C1A	6.33	109.55	106.71
30	I	316	CLA	C4A-NA-C1A	6.32	109.55	106.71
30	M	318	CLA	C4A-NA-C1A	6.32	109.55	106.71
31	L	315	KC1	CHB-C1B-NB	6.32	130.26	124.45
30	O	311	CLA	C4A-NA-C1A	6.31	109.54	106.71
30	b	721	CLA	C4A-NA-C1A	6.31	109.54	106.71
31	P	211	KC1	CHC-C4B-NB	6.30	130.25	124.45
30	b	713	CLA	C4A-NA-C1A	6.30	109.54	106.71
28	A	302	DD6	C9-C10-C11	-6.29	118.33	127.31
30	J	314	CLA	C4A-NA-C1A	6.29	109.53	106.71
31	I	314	KC1	CHB-C1B-NB	6.28	130.23	124.45
30	H	304	CLA	C4A-NA-C1A	6.28	109.53	106.71
31	O	310	KC1	CHB-C1B-NB	6.27	130.22	124.45
31	P	213	KC1	CHC-C4B-NB	6.27	130.22	124.45
28	M	302	DD6	C3-C2-C1	-6.27	118.36	127.31
29	P	207	UIX	C7-C10-C11	-6.27	115.81	125.53
30	b	717	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	711	CLA	C4A-NA-C1A	6.25	109.52	106.71
28	F	301	DD6	C4-C5-C6	-6.25	118.39	127.31
31	B	314	KC1	CHB-C1B-NB	6.25	130.20	124.45
30	B	307	CLA	C4A-NA-C1A	6.25	109.52	106.71
30	J	308	CLA	C4A-NA-C1A	6.25	109.52	106.71
31	N	311	KC1	CHC-C4B-NB	6.23	130.18	124.45
30	a	724	CLA	C4A-NA-C1A	6.23	109.51	106.71
30	L	317	CLA	C4A-NA-C1A	6.23	109.50	106.71
31	N	306	KC1	CHB-C1B-NB	6.22	130.17	124.45
31	H	306	KC1	CHC-C4B-NB	6.22	130.17	124.45
30	j	104	CLA	C4A-NA-C1A	6.21	109.50	106.71
31	K	314	KC1	CHC-C4B-NB	6.20	130.16	124.45
30	b	706	CLA	C4A-NA-C1A	6.20	109.49	106.71
31	L	307	KC1	CHC-C4B-NB	6.20	130.15	124.45
31	N	311	KC1	CHB-C1B-NB	6.19	130.15	124.45
30	H	311	CLA	C4A-NA-C1A	6.19	109.49	106.71
30	I	312	CLA	C4A-NA-C1A	6.18	109.48	106.71
30	l	305	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	a	709	CLA	C4A-NA-C1A	6.16	109.48	106.71
31	L	307	KC1	CHB-C1B-NB	6.16	130.12	124.45
30	B	311	CLA	C4A-NA-C1A	6.16	109.48	106.71
31	F	314	KC1	CHC-C4B-NB	6.16	130.12	124.45
29	P	207	UIX	O-C1-C3	6.15	118.00	113.38
30	L	308	CLA	C4A-NA-C1A	6.14	109.47	106.71
31	P	211	KC1	CHB-C1B-NB	6.14	130.10	124.45
31	I	314	KC1	CHC-C4B-NB	6.14	130.10	124.45
30	D	314	CLA	C4A-NA-C1A	6.14	109.47	106.71
31	F	309	KC1	CHB-C1B-NB	6.14	130.09	124.45
31	K	314	KC1	CHB-C1B-NB	6.14	130.09	124.45
30	G	520	CLA	C4A-NA-C1A	6.13	109.46	106.71
30	N	307	CLA	C4A-NA-C1A	6.12	109.46	106.71
31	O	315	KC1	CHB-C1B-NB	6.11	130.07	124.45
30	I	308	CLA	C4A-NA-C1A	6.11	109.45	106.71
34	H	301	PID	C17-C16-C15	6.10	135.98	123.47
31	N	306	KC1	CHC-C4B-NB	6.10	130.06	124.45
30	F	312	CLA	C4A-NA-C1A	6.09	109.45	106.71
31	J	313	KC1	CHB-C1B-NB	6.09	130.05	124.45
31	A	314	KC1	CHC-C4B-NB	6.09	130.05	124.45
29	K	302	UIX	C6-C1-C	-6.08	112.07	122.26
30	a	717	CLA	C4A-NA-C1A	6.08	109.44	106.71
30	M	313	CLA	C4A-NA-C1A	6.06	109.43	106.71
31	N	308	KC1	CHB-C1B-NB	6.04	130.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	H	310	KC1	CHC-C4B-NB	6.04	130.00	124.45
31	L	315	KC1	CHC-C4B-NB	6.04	130.00	124.45
30	I	309	CLA	C4A-NA-C1A	6.04	109.42	106.71
31	G	515	KC1	CHB-C1B-NB	6.03	129.99	124.45
31	M	314	KC1	CHC-C4B-NB	6.02	129.99	124.45
31	B	314	KC1	CHC-C4B-NB	6.01	129.98	124.45
30	M	312	CLA	C4A-NA-C1A	6.00	109.41	106.71
31	A	306	KC1	CHB-C1B-NB	5.98	129.95	124.45
30	l	312	CLA	C4A-NA-C1A	5.97	109.39	106.71
31	M	307	KC1	CHB-C1B-NB	5.96	129.93	124.45
31	A	306	KC1	CHC-C4B-NB	5.96	129.93	124.45
30	a	719	CLA	C4A-NA-C1A	5.95	109.38	106.71
31	P	216	KC1	CHC-C4B-NB	5.95	129.92	124.45
31	M	307	KC1	CHC-C4B-NB	5.95	129.92	124.45
29	K	302	UIX	C14-C13-C11	-5.95	118.82	127.31
37	m	201	BCR	C15-C14-C13	-5.93	118.85	127.31
28	A	302	DD6	C14-C13-C11	-5.91	116.36	125.53
31	O	312	KC1	CHB-C1B-NB	5.90	129.88	124.45
28	J	304	DD6	C9-C10-C11	-5.90	118.89	127.31
30	L	313	CLA	C4A-NA-C1A	5.89	109.35	106.71
29	P	207	UIX	C34-C30-C26	-5.88	118.91	127.31
37	a	736	BCR	C7-C8-C9	-5.88	117.35	126.23
31	O	310	KC1	CHC-C4B-NB	5.88	129.86	124.45
29	P	207	UIX	C6-C1-C	-5.86	112.43	122.26
29	O	306	UIX	C6-C1-C	-5.86	112.45	122.26
29	P	207	UIX	C37-C39-C40	-5.84	118.98	127.31
31	J	313	KC1	CHC-C4B-NB	5.83	129.81	124.45
30	a	735	CLA	C4A-NA-C1A	5.81	109.32	106.71
34	P	206	PID	CM4-C14-C15	-5.81	114.79	122.92
30	a	704	CLA	C4A-NA-C1A	5.80	109.31	106.71
30	a	726	CLA	C4A-NA-C1A	5.79	109.31	106.71
28	A	301	DD6	C21-C20-C19	5.79	120.80	114.28
37	j	102	BCR	C16-C17-C18	-5.79	119.04	127.31
34	M	301	PID	C17-C16-C15	5.79	135.34	123.47
28	P	204	DD6	C4-C5-C6	-5.79	119.05	127.31
34	F	304	PID	C17-C16-C15	5.78	135.32	123.47
31	N	308	KC1	O2D-CGD-CBD	5.78	121.54	111.27
29	O	306	UIX	C37-C39-C40	-5.76	119.09	127.31
29	J	305	UIX	C34-C30-C26	-5.76	119.09	127.31
31	O	315	KC1	CHC-C4B-NB	5.75	129.74	124.45
31	P	213	KC1	CHB-C1B-NB	5.74	129.73	124.45
28	M	306	DD6	C3-C2-C1	-5.74	119.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	504	DD6	O1-C20-C19	5.72	117.68	113.38
28	J	303	DD6	O1-C20-C19	5.72	117.68	113.38
28	J	302	DD6	C3-C2-C1	-5.71	119.16	127.31
28	I	305	DD6	C4-C5-C6	-5.71	119.17	127.31
28	G	504	DD6	C4-C5-C6	-5.71	119.17	127.31
37	b	702	BCR	C16-C17-C18	-5.70	119.18	127.31
30	J	310	CLA	C4A-NA-C1A	5.66	109.25	106.71
30	a	713	CLA	C4A-NA-C1A	5.65	109.25	106.71
29	K	302	UIX	C34-C30-C26	-5.65	119.25	127.31
29	O	306	UIX	O-C1-C3	5.65	117.62	113.38
28	I	305	DD6	C3-C2-C1	-5.64	119.26	127.31
34	F	302	PID	C18-C19-C20	5.64	135.02	123.47
31	N	308	KC1	CHC-C4B-NB	5.64	129.63	124.45
34	D	304	PID	C17-C16-C15	5.63	135.01	123.47
28	J	304	DD6	C3-C2-C1	-5.61	119.31	127.31
31	G	515	KC1	CHC-C4B-NB	5.59	129.59	124.45
28	G	505	DD6	C3-C2-C1	-5.58	119.35	127.31
30	B	310	CLA	C4A-NA-C1A	5.56	109.21	106.71
29	O	306	UIX	C34-C30-C26	-5.56	119.37	127.31
28	O	303	DD6	C4-C5-C6	-5.56	119.38	127.31
29	O	306	UIX	C36-C35-C32	-5.53	119.42	127.31
34	N	302	PID	C18-C19-C20	5.53	134.79	123.47
28	J	303	DD6	C4-C5-C6	-5.50	119.47	127.31
28	F	301	DD6	C21-C20-C19	5.49	120.45	114.28
37	a	736	BCR	C11-C10-C9	-5.47	119.50	127.31
28	A	303	DD6	C21-C20-C19	5.47	120.44	114.28
28	M	305	DD6	C3-C2-C1	-5.46	119.51	127.31
37	i	201	BCR	C24-C23-C22	-5.45	118.00	126.23
28	L	306	DD6	C9-C10-C11	-5.44	119.54	127.31
28	I	301	DD6	C21-C20-C19	5.44	120.40	114.28
28	B	303	DD6	C21-C20-C19	5.44	120.40	114.28
34	P	205	PID	CM4-C14-C15	-5.43	115.32	122.92
37	b	702	BCR	C20-C21-C22	-5.42	119.57	127.31
28	A	301	DD6	C9-C10-C11	-5.42	119.58	127.31
34	P	202	PID	C17-C16-C15	5.41	134.55	123.47
28	A	305	DD6	C21-C20-C19	5.40	120.35	114.28
28	G	502	DD6	C21-C20-C19	5.39	120.34	114.28
28	I	302	DD6	C9-C10-C11	-5.38	119.62	127.31
28	F	303	DD6	C4-C5-C6	-5.38	119.64	127.31
28	I	301	DD6	C9-C10-C11	-5.33	119.70	127.31
31	P	213	KC1	O2D-CGD-CBD	5.33	120.74	111.27
28	J	303	DD6	C9-C10-C11	-5.33	119.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	b	730	BCR	C15-C14-C13	-5.32	119.71	127.31
34	O	304	PID	CM4-C14-C15	-5.32	115.47	122.92
28	G	505	DD6	O1-C20-C21	5.32	121.43	115.06
28	A	301	DD6	O1-C20-C19	-5.31	109.39	113.38
37	b	730	BCR	C3-C4-C5	-5.30	104.61	114.08
34	M	301	PID	CM4-C14-C15	-5.30	115.50	122.92
28	I	301	DD6	C4-C5-C6	-5.23	119.84	127.31
34	D	304	PID	C18-C19-C20	5.23	134.19	123.47
34	P	202	PID	CM4-C14-C15	-5.22	115.61	122.92
28	J	302	DD6	C14-C13-C11	-5.22	117.43	125.53
37	f	304	BCR	C15-C14-C13	-5.22	119.87	127.31
28	J	302	DD6	C9-C10-C11	-5.21	119.87	127.31
28	L	302	DD6	C14-C13-C11	-5.21	117.45	125.53
28	K	304	DD6	C21-C20-C19	5.21	120.14	114.28
34	D	304	PID	CM4-C14-C15	-5.19	115.65	122.92
31	D	315	KC1	CHC-C4B-NB	5.18	129.21	124.45
37	l	307	BCR	C3-C4-C5	-5.18	104.83	114.08
28	A	302	DD6	C3-C2-C1	-5.16	119.94	127.31
28	G	508	DD6	C21-C20-C19	5.15	120.08	114.28
29	h	201	UIX	C37-C39-C40	-5.14	119.97	127.31
28	B	302	DD6	C3-C2-C1	-5.14	119.98	127.31
28	M	302	DD6	O1-C20-C19	5.12	117.23	113.38
34	H	301	PID	CM4-C14-C15	-5.11	115.77	122.92
28	N	303	DD6	C4-C5-C6	-5.09	120.04	127.31
31	L	307	KC1	O2D-CGD-CBD	5.08	120.29	111.27
34	O	305	PID	CM4-C14-C15	-5.08	115.81	122.92
28	P	204	DD6	C21-C20-C19	5.07	119.98	114.28
34	O	301	PID	CM4-C14-C15	-5.05	115.84	122.92
28	B	306	DD6	C3-C2-C1	-5.05	120.11	127.31
37	a	734	BCR	C15-C14-C13	-5.05	120.11	127.31
37	b	730	BCR	C11-C10-C9	-5.04	120.12	127.31
28	M	304	DD6	C21-C20-C19	5.04	119.95	114.28
28	F	301	DD6	O1-C20-C19	-5.03	109.60	113.38
29	B	305	UIX	O2-C27-C31	5.03	120.34	111.09
28	K	305	DD6	C3-C2-C1	-5.02	120.14	127.31
28	G	508	DD6	C3-C2-C1	-5.02	120.14	127.31
31	M	314	KC1	O2D-CGD-CBD	5.01	120.18	111.27
29	O	306	UIX	O-C1-C6	5.01	121.06	115.06
31	F	309	KC1	O2D-CGD-CBD	5.01	120.17	111.27
34	F	304	PID	CM4-C14-C15	-5.01	115.91	122.92
28	H	303	DD6	C21-C20-C19	5.00	119.91	114.28
28	G	502	DD6	C4-C5-C6	-5.00	120.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	301	DD6	C3-C2-C1	-5.00	120.17	127.31
28	K	301	DD6	C21-C20-C19	5.00	119.90	114.28
28	B	304	DD6	C21-C20-C19	4.99	119.89	114.28
34	O	301	PID	C17-C16-C15	4.99	133.69	123.47
31	A	306	KC1	O2D-CGD-CBD	4.98	120.11	111.27
28	G	504	DD6	C3-C2-C1	-4.98	120.21	127.31
28	G	508	DD6	C4-C5-C6	-4.98	120.21	127.31
37	f	304	BCR	C11-C10-C9	-4.97	120.22	127.31
28	B	306	DD6	C21-C20-C19	4.95	119.85	114.28
28	K	304	DD6	C3-C2-C1	-4.94	120.25	127.31
28	I	305	DD6	C15-C14-C13	-4.94	115.55	125.99
31	J	313	KC1	O2D-CGD-CBD	4.93	120.03	111.27
37	m	201	BCR	C11-C10-C9	-4.93	120.27	127.31
28	K	305	DD6	C21-C20-C19	4.92	119.82	114.28
28	L	306	DD6	C4-C5-C6	-4.92	120.29	127.31
28	N	303	DD6	C21-C20-C19	4.92	119.81	114.28
28	M	306	DD6	C4-C5-C6	-4.91	120.30	127.31
28	L	303	DD6	C21-C20-C19	4.91	119.80	114.28
29	I	304	UIX	O-C1-C6	4.90	120.93	115.06
28	h	203	DD6	C21-C20-C19	4.89	119.78	114.28
29	K	302	UIX	C16-C20-C15	4.88	124.54	119.70
28	L	303	DD6	C3-C2-C1	-4.88	120.34	127.31
34	F	302	PID	CM4-C14-C15	-4.88	116.08	122.92
28	L	305	DD6	C21-C20-C19	4.88	119.77	114.28
31	O	312	KC1	O2D-CGD-CBD	4.88	119.93	111.27
31	D	315	KC1	O2D-CGD-CBD	4.88	119.93	111.27
31	N	311	KC1	O2D-CGD-CBD	4.86	119.91	111.27
31	L	315	KC1	O2D-CGD-CBD	4.86	119.90	111.27
28	K	303	DD6	C21-C20-C19	4.86	119.74	114.28
28	O	303	DD6	C21-C20-C19	4.84	119.72	114.28
31	H	310	KC1	O2D-CGD-CBD	4.84	119.87	111.27
28	B	303	DD6	O1-C20-C19	-4.84	109.75	113.38
28	L	306	DD6	C21-C20-C19	4.84	119.72	114.28
34	N	301	PID	C17-C16-C15	4.82	133.35	123.47
28	F	303	DD6	C21-C20-C19	4.82	119.70	114.28
29	K	302	UIX	O-C1-C6	4.81	120.82	115.06
29	P	207	UIX	C36-C35-C32	-4.81	120.45	127.31
28	G	505	DD6	C4-C5-C6	-4.80	120.46	127.31
28	L	302	DD6	C21-C20-C19	4.80	119.68	114.28
29	h	201	UIX	O2-C27-C31	4.80	119.92	111.09
31	P	216	KC1	O2D-CGD-CBD	4.80	119.79	111.27
37	a	736	BCR	C16-C17-C18	-4.79	120.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	505	DD6	C9-C10-C11	-4.78	120.49	127.31
29	K	302	UIX	C17-C15-C20	4.78	113.86	109.21
28	M	302	DD6	C15-C14-C13	-4.77	115.91	125.99
28	I	301	DD6	C3-C2-C1	-4.76	120.52	127.31
31	F	314	KC1	O2D-CGD-CBD	4.75	119.71	111.27
29	A	304	UIX	O-C1-C6	4.75	120.75	115.06
28	M	305	DD6	C21-C20-C19	4.74	119.61	114.28
34	N	301	PID	CM4-C14-C15	-4.73	116.29	122.92
28	I	302	DD6	C21-C20-C19	4.72	119.59	114.28
37	l	306	BCR	C7-C8-C9	-4.72	119.10	126.23
37	i	201	BCR	C20-C21-C22	-4.72	120.58	127.31
37	l	306	BCR	C33-C5-C6	-4.71	119.24	124.53
28	M	304	DD6	C3-C2-C1	-4.71	120.59	127.31
31	H	306	KC1	O2D-CGD-CBD	4.71	119.63	111.27
31	A	314	KC1	O2D-CGD-CBD	4.70	119.63	111.27
28	K	318	DD6	C3-C2-C1	-4.70	120.60	127.31
28	M	306	DD6	C9-C10-C11	-4.70	120.60	127.31
31	N	308	KC1	O2D-CGD-O1D	-4.69	114.66	123.84
37	l	306	BCR	C16-C17-C18	-4.69	120.61	127.31
28	K	318	DD6	C4-C5-C6	-4.68	120.62	127.31
37	j	102	BCR	C15-C14-C13	-4.68	120.63	127.31
31	I	314	KC1	O2D-CGD-CBD	4.68	119.59	111.27
30	a	724	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
28	K	301	DD6	C4-C5-C6	-4.67	120.65	127.31
29	A	304	UIX	O2-C27-C31	4.66	119.67	111.09
34	D	301	PID	CM4-C14-C15	-4.64	116.42	122.92
28	D	303	DD6	C21-C20-C19	4.64	119.50	114.28
37	l	302	BCR	C28-C27-C26	-4.64	105.79	114.08
37	f	304	BCR	C16-C17-C18	-4.64	120.69	127.31
29	P	207	UIX	O-C1-C6	4.63	120.60	115.06
31	M	307	KC1	O2D-CGD-CBD	4.63	119.49	111.27
28	A	301	DD6	C3-C2-C1	-4.60	120.75	127.31
29	P	207	UIX	O2-C27-C31	4.59	119.54	111.09
28	L	305	DD6	C3-C2-C1	-4.59	120.76	127.31
28	M	303	DD6	C4-C5-C6	-4.59	120.76	127.31
28	N	303	DD6	C9-C10-C11	-4.59	120.77	127.31
28	b	731	DD6	C21-C20-C19	4.59	119.44	114.28
37	i	201	BCR	C15-C14-C13	-4.58	120.77	127.31
28	I	303	DD6	C9-C10-C11	-4.58	120.77	127.31
28	I	303	DD6	C21-C20-C19	4.57	119.42	114.28
31	G	515	KC1	O2D-CGD-CBD	4.57	119.39	111.27
28	B	302	DD6	C9-C10-C11	-4.57	120.79	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	O	306	UIX	O2-C27-C31	4.57	119.49	111.09
30	m	202	CLA	CMB-C2B-C1B	-4.57	121.45	128.46
34	F	306	PID	CM4-C14-C15	-4.55	116.54	122.92
31	O	310	KC1	O2D-CGD-CBD	4.55	119.34	111.27
31	K	314	KC1	O2D-CGD-CBD	4.54	119.34	111.27
31	B	314	KC1	O2D-CGD-CBD	4.54	119.34	111.27
34	G	506	PID	CM4-C14-C15	-4.54	116.57	122.92
34	F	304	PID	C6-C7-C8	4.54	135.59	125.99
28	I	302	DD6	C3-C2-C1	-4.53	120.85	127.31
37	a	736	BCR	C15-C14-C13	-4.52	120.86	127.31
28	F	303	DD6	O1-C20-C19	-4.52	109.99	113.38
28	L	304	DD6	C21-C20-C19	4.51	119.36	114.28
28	I	305	DD6	C20-C19-C18	-4.51	103.83	112.75
28	I	301	DD6	O1-C20-C19	-4.50	110.00	113.38
37	a	734	BCR	C16-C17-C18	-4.50	120.89	127.31
34	D	301	PID	C17-C16-C15	4.48	132.66	123.47
38	b	729	PQN	C11-C12-C13	-4.48	119.34	126.79
29	K	302	UIX	O2-C27-C31	4.48	119.33	111.09
37	l	302	BCR	C16-C17-C18	-4.47	120.93	127.31
28	b	731	DD6	C4-C5-C6	-4.47	120.94	127.31
28	J	302	DD6	C4-C5-C6	-4.47	120.94	127.31
28	M	303	DD6	C3-C2-C1	-4.46	120.95	127.31
29	G	503	UIX	O2-C27-C31	4.45	119.27	111.09
31	N	308	KC1	O1D-CGD-CBD	-4.44	115.41	124.48
37	l	307	BCR	C15-C14-C13	-4.43	120.98	127.31
28	N	303	DD6	C3-C2-C1	-4.42	121.00	127.31
28	J	303	DD6	C15-C14-C13	-4.42	116.65	125.99
28	A	305	DD6	C37-C36-C31	-4.42	118.35	124.35
28	G	502	DD6	C9-C10-C11	-4.41	121.01	127.31
31	N	306	KC1	O2D-CGD-CBD	4.41	119.10	111.27
28	M	303	DD6	C20-C19-C18	-4.40	104.04	112.75
28	M	306	DD6	C20-C19-C18	-4.40	104.04	112.75
29	h	201	UIX	C-C7-C10	-4.40	116.70	125.99
34	O	305	PID	C17-C16-C15	4.40	132.48	123.47
37	b	732	BCR	C33-C5-C6	-4.40	119.59	124.53
34	P	208	PID	CM4-C14-C15	-4.39	116.77	122.92
30	b	722	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
29	J	305	UIX	O2-C27-C31	4.39	119.16	111.09
34	D	307	PID	CM4-C14-C15	-4.39	116.78	122.92
29	K	302	UIX	C21-C15-C20	-4.39	106.55	110.47
28	I	305	DD6	C21-C20-C19	4.39	119.21	114.28
29	A	304	UIX	C6-C1-C3	4.38	119.21	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	j	102	BCR	C20-C21-C22	-4.38	121.06	127.31
28	B	304	DD6	C3-C2-C1	-4.38	121.06	127.31
31	O	315	KC1	O2D-CGD-CBD	4.37	119.04	111.27
29	I	304	UIX	O2-C27-C31	4.36	119.11	111.09
37	l	306	BCR	C38-C26-C25	-4.36	119.63	124.53
34	D	306	PID	CM4-C14-C15	-4.36	116.82	122.92
34	D	305	PID	C18-C19-C20	4.35	132.40	123.47
28	L	305	DD6	C9-C10-C11	-4.35	121.10	127.31
31	D	310	KC1	O2D-CGD-CBD	4.33	118.97	111.27
34	O	304	PID	C17-C16-C15	4.33	132.35	123.47
34	N	302	PID	CM4-C14-C15	-4.33	116.86	122.92
28	b	731	DD6	C15-C14-C13	-4.33	116.84	125.99
28	D	303	DD6	O1-C20-C19	4.33	116.64	113.38
28	F	303	DD6	C9-C10-C11	-4.32	121.14	127.31
28	h	203	DD6	C3-C2-C1	-4.32	121.14	127.31
28	H	303	DD6	C4-C5-C6	-4.31	121.16	127.31
37	b	732	BCR	C16-C17-C18	-4.30	121.17	127.31
28	J	303	DD6	O1-C20-C21	4.30	120.20	115.06
28	D	303	DD6	C10-C9-C8	-4.29	109.84	123.22
28	L	306	DD6	C3-C2-C1	-4.28	121.20	127.31
34	G	507	PID	CM4-C14-C15	-4.27	116.94	122.92
28	K	301	DD6	C15-C14-C13	-4.26	116.98	125.99
30	a	711	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
29	I	304	UIX	C7-C10-C11	-4.25	118.94	125.53
28	L	304	DD6	C3-C2-C1	-4.24	121.25	127.31
37	i	201	BCR	C16-C17-C18	-4.24	121.25	127.31
34	M	301	PID	C12-O4-C10	4.24	109.86	107.65
28	N	303	DD6	O1-C20-C19	-4.22	110.21	113.38
30	J	311	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
34	D	306	PID	C18-C19-C20	4.22	132.12	123.47
28	M	306	DD6	C25-C24-C1	-4.21	114.60	126.42
30	G	520	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
28	B	303	DD6	C4-C5-C6	-4.19	121.33	127.31
29	B	305	UIX	O-C1-C6	4.19	120.07	115.06
28	A	305	DD6	C4-C5-C6	-4.19	121.33	127.31
30	f	302	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
28	L	303	DD6	C37-C36-C31	-4.18	118.67	124.35
29	G	503	UIX	O-C1-C6	4.18	120.06	115.06
30	A	309	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
34	D	304	PID	C12-O4-C10	4.18	109.82	107.65
28	B	303	DD6	C37-C36-C31	-4.17	118.68	124.35
37	m	201	BCR	C38-C26-C25	-4.17	119.84	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	521	DGD	O2G-C1B-C2B	4.17	120.49	111.50
29	A	304	UIX	C16-C20-C15	4.17	123.83	119.70
30	L	310	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
28	B	304	DD6	C37-C36-C31	-4.16	118.69	124.35
28	O	303	DD6	C3-C2-C1	-4.16	121.37	127.31
28	O	303	DD6	C9-C10-C11	-4.16	121.38	127.31
28	H	303	DD6	C3-C2-C1	-4.15	121.38	127.31
31	P	211	KC1	O2D-CGD-CBD	4.15	118.65	111.27
34	O	307	PID	CM4-C14-C15	-4.15	117.11	122.92
28	K	304	DD6	C15-C14-C13	-4.15	117.22	125.99
28	B	302	DD6	C14-C13-C11	-4.15	119.09	125.53
30	K	313	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
29	h	201	UIX	O-C1-C6	4.14	120.02	115.06
28	L	303	DD6	C9-C10-C11	-4.14	121.41	127.31
34	D	306	PID	C17-C16-C15	4.13	131.94	123.47
32	j	103	DGD	O2G-C1B-C2B	4.13	120.40	111.50
28	I	303	DD6	C37-C36-C31	-4.13	118.74	124.35
30	G	513	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
30	A	312	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
28	M	302	DD6	O1-C20-C21	4.11	119.98	115.06
34	P	208	PID	C17-C16-C15	4.11	131.89	123.47
34	F	302	PID	C12-O4-C10	4.11	109.79	107.65
30	K	309	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
30	M	312	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
30	I	310	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
34	P	202	PID	C12-O4-C10	4.10	109.79	107.65
28	L	302	DD6	C3-C2-C1	-4.10	121.46	127.31
32	L	301	DGD	O2G-C1B-C2B	4.10	120.33	111.50
28	I	302	DD6	C7-C6-C8	4.10	124.53	118.08
30	J	310	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
28	L	305	DD6	C4-C5-C6	-4.09	121.47	127.31
28	P	204	DD6	C37-C36-C31	-4.08	118.80	124.35
34	D	301	PID	C18-C19-C20	4.08	131.84	123.47
30	G	510	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
34	P	203	PID	C18-C19-C20	4.07	131.82	123.47
28	M	303	DD6	O1-C20-C21	4.07	119.93	115.06
30	I	319	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
37	a	734	BCR	C11-C10-C9	-4.06	121.52	127.31
34	O	304	PID	C12-O4-C10	4.06	109.76	107.65
30	I	313	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
31	O	310	KC1	C3D-CAD-CBD	-4.06	102.26	107.61
28	J	303	DD6	C37-C36-C31	-4.05	118.84	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	318	DD6	C14-C13-C11	-4.05	119.25	125.53
30	P	214	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
30	a	703	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
34	F	304	PID	C12-O4-C10	4.04	109.75	107.65
28	J	302	DD6	C37-C36-C31	-4.04	118.86	124.35
30	J	308	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
30	a	722	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
30	M	315	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	L	302	DD6	C9-C10-C11	-4.03	121.56	127.31
30	b	717	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	A	301	DD6	C4-C5-C6	-4.03	121.56	127.31
37	a	734	BCR	C33-C5-C6	-4.02	120.01	124.53
28	O	303	DD6	C15-C14-C13	-4.02	117.49	125.99
28	K	318	DD6	O1-C20-C21	-4.01	110.25	115.06
32	y	201	DGD	O2G-C1B-C2B	4.01	120.15	111.50
29	J	305	UIX	C34-C37-C39	-4.01	115.26	123.47
37	b	732	BCR	C15-C14-C13	-4.01	121.59	127.31
30	O	313	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
29	h	201	UIX	C16-C20-C15	4.01	123.67	119.70
30	K	315	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
30	A	308	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
30	l	304	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
30	K	307	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
30	P	210	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
37	a	734	BCR	C28-C27-C26	-4.00	106.93	114.08
30	b	714	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
30	B	309	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
30	b	706	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
28	G	505	DD6	C37-C36-C31	-3.98	118.94	124.35
28	H	303	DD6	C15-C14-C13	-3.98	117.58	125.99
28	L	302	DD6	C4-C5-C6	-3.97	121.64	127.31
34	P	206	PID	C12-O4-C10	3.97	109.72	107.65
30	a	714	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
37	m	201	BCR	C3-C4-C5	-3.97	107.00	114.08
34	O	302	PID	CM4-C14-C15	-3.96	117.38	122.92
30	P	212	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
30	I	316	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
28	K	301	DD6	C37-C36-C31	-3.95	118.98	124.35
34	O	301	PID	C12-O4-C10	3.95	109.71	107.65
30	a	706	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
30	a	709	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
30	G	518	CLA	CMB-C2B-C1B	-3.95	122.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	201	UIX	C6-C1-C3	3.94	118.72	114.28
29	B	305	UIX	C37-C39-C40	-3.94	121.68	127.31
30	L	314	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
30	A	310	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
30	a	704	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
34	F	306	PID	C17-C16-C15	3.94	131.54	123.47
28	L	304	DD6	C37-C36-C31	-3.94	119.00	124.35
34	H	301	PID	C12-O4-C10	3.93	109.70	107.65
28	I	302	DD6	C12-C11-C13	3.93	124.27	118.08
37	l	306	BCR	C20-C21-C22	-3.93	121.70	127.31
28	I	303	DD6	O1-C20-C19	-3.92	110.44	113.38
37	i	201	BCR	C7-C8-C9	-3.92	120.31	126.23
28	B	304	DD6	C15-C14-C13	-3.92	117.71	125.99
30	D	309	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
29	A	304	UIX	C34-C30-C26	-3.91	121.73	127.31
28	B	304	DD6	C4-C5-C6	-3.91	121.73	127.31
30	m	202	CLA	CMB-C2B-C3B	3.90	131.98	124.68
37	m	201	BCR	C15-C16-C17	-3.90	115.48	123.47
28	A	305	DD6	O1-C20-C19	-3.90	110.45	113.38
31	H	310	KC1	C3D-CAD-CBD	-3.90	102.48	107.61
34	N	301	PID	C12-O4-C10	3.89	109.68	107.65
30	O	311	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
28	L	304	DD6	C4-C5-C6	-3.89	121.76	127.31
28	I	303	DD6	C4-C5-C6	-3.88	121.77	127.31
31	L	315	KC1	C3D-CAD-CBD	-3.88	102.49	107.61
28	M	304	DD6	C15-C14-C13	-3.88	117.78	125.99
30	H	305	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
28	P	204	DD6	C15-C14-C13	-3.88	117.78	125.99
30	b	725	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
31	J	313	KC1	C3D-CAD-CBD	-3.87	102.50	107.61
34	D	307	PID	C12-O4-C10	3.87	109.67	107.65
28	K	303	DD6	C15-C14-C13	-3.87	117.81	125.99
29	G	503	UIX	C-C7-C10	-3.87	117.81	125.99
34	D	302	PID	CM4-C14-C15	-3.87	117.51	122.92
30	a	713	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
32	I	317	DGD	O2G-C1B-C2B	3.86	119.83	111.50
37	j	102	BCR	C24-C23-C22	-3.85	120.41	126.23
37	f	304	BCR	C33-C5-C6	-3.85	120.20	124.53
32	G	501	DGD	O2G-C1B-C2B	3.85	119.81	111.50
30	F	315	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
31	F	314	KC1	C3D-CAD-CBD	-3.85	102.54	107.61
28	b	731	DD6	C9-C10-C11	-3.85	121.82	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	303	DD6	C37-C36-C31	-3.84	119.13	124.35
28	G	508	DD6	C9-C10-C11	-3.84	121.83	127.31
28	F	303	DD6	C15-C14-C13	-3.84	117.87	125.99
30	b	721	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
32	l	301	DGD	O2G-C1B-C2B	3.84	119.78	111.50
28	M	302	DD6	C21-C20-C15	-3.84	115.82	122.26
30	O	316	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
30	D	313	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
29	J	305	UIX	C14-C13-C11	-3.83	121.85	127.31
30	a	717	CLA	CMB-C2B-C1B	-3.82	122.58	128.46
30	N	307	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
37	b	730	BCR	C16-C17-C18	-3.82	121.85	127.31
30	a	723	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
37	l	302	BCR	C33-C5-C6	-3.82	120.24	124.53
30	P	215	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
28	M	302	DD6	C4-C5-C6	-3.81	121.87	127.31
37	f	304	BCR	C20-C21-C22	-3.81	121.87	127.31
34	G	506	PID	C17-C16-C15	3.81	131.28	123.47
30	l	312	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
34	F	302	PID	C17-C16-C15	3.81	131.27	123.47
34	P	203	PID	CM4-C14-C15	-3.80	117.59	122.92
28	F	303	DD6	C3-C2-C1	-3.80	121.88	127.31
34	j	105	PID	CM4-C14-C15	-3.80	117.60	122.92
29	G	503	UIX	C6-C1-C3	3.80	118.56	114.28
29	I	304	UIX	C14-C13-C11	-3.80	121.89	127.31
30	N	305	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
37	f	304	BCR	C28-C27-C26	-3.80	107.30	114.08
37	b	702	BCR	C16-C15-C14	-3.80	115.70	123.47
28	I	303	DD6	C3-C2-C1	-3.79	121.90	127.31
28	J	304	DD6	C24-C1-C2	3.79	124.76	118.94
28	M	302	DD6	C37-C36-C31	-3.79	119.20	124.35
34	F	306	PID	C12-O4-C10	3.79	109.62	107.65
28	A	302	DD6	C4-C5-C6	-3.78	121.91	127.31
30	a	705	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
28	I	302	DD6	C14-C13-C11	3.78	131.40	125.53
30	b	712	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
30	M	310	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
30	M	311	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
30	I	308	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
31	N	308	KC1	CBD-CHA-C1A	3.76	135.88	128.88
29	I	304	UIX	C37-C39-C40	-3.75	121.95	127.31
34	F	305	PID	C12-O4-C10	3.75	109.60	107.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	P	208	PID	C12-O4-C10	3.75	109.60	107.65
30	b	720	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
37	b	730	BCR	C4-C5-C6	-3.74	117.30	122.73
30	b	713	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
30	O	314	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
28	A	302	DD6	C21-C20-C19	3.73	118.48	114.28
34	D	301	PID	C12-O4-C10	3.73	109.59	107.65
30	b	707	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
30	F	312	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
34	D	302	PID	C18-C19-C20	3.73	131.10	123.47
30	G	519	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	b	716	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
37	f	304	BCR	C7-C8-C9	-3.72	120.61	126.23
30	K	310	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	K	304	DD6	O1-C20-C19	-3.71	110.60	113.38
30	a	735	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
28	J	304	DD6	C4-C5-C6	-3.71	122.02	127.31
29	O	306	UIX	C6-C1-C3	3.71	118.45	114.28
28	G	502	DD6	C3-C2-C1	-3.70	122.02	127.31
28	B	302	DD6	C21-C20-C19	3.70	118.45	114.28
30	H	312	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	J	314	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
28	L	306	DD6	C37-C36-C31	-3.70	119.33	124.35
28	I	302	DD6	C12-C11-C10	-3.69	117.75	122.92
30	M	313	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
30	L	313	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
28	G	505	DD6	C20-C19-C18	-3.69	105.45	112.75
30	b	708	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
30	b	715	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
30	l	305	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
34	O	305	PID	C18-C19-C20	3.69	131.03	123.47
28	M	306	DD6	C21-C20-C19	3.69	118.43	114.28
30	M	309	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
30	L	311	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
28	M	302	DD6	C-C1-C2	-3.68	117.77	122.92
30	I	309	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
34	D	305	PID	CM4-C14-C15	-3.68	117.77	122.92
31	P	211	KC1	C3D-CAD-CBD	-3.67	102.78	107.61
30	a	728	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
28	M	304	DD6	C37-C36-C31	-3.67	119.37	124.35
30	G	511	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
29	J	305	UIX	O-C1-C6	3.66	119.45	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	301	DD6	C15-C14-C13	-3.66	118.25	125.99
28	G	508	DD6	C15-C14-C13	-3.66	118.25	125.99
30	F	310	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
29	J	305	UIX	C14-C23-C26	-3.66	116.14	126.42
30	B	310	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
29	B	305	UIX	C34-C30-C26	-3.65	122.10	127.31
28	A	303	DD6	O1-C20-C19	-3.65	110.64	113.38
37	l	306	BCR	C11-C10-C9	-3.64	122.11	127.31
30	I	321	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
34	H	302	PID	C18-C19-C20	3.64	130.92	123.47
28	I	303	DD6	C14-C13-C11	-3.63	119.89	125.53
30	H	308	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
30	b	719	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
29	G	503	UIX	C34-C30-C26	-3.63	122.13	127.31
30	a	719	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
30	B	315	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
30	L	309	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
30	b	710	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
28	A	305	DD6	C3-C2-C1	-3.62	122.14	127.31
34	O	307	PID	C12-O4-C10	3.62	109.53	107.65
29	P	207	UIX	C6-C1-C3	3.62	118.35	114.28
34	O	302	PID	C18-C19-C20	3.61	130.87	123.47
31	M	314	KC1	C3D-CAD-CBD	-3.61	102.85	107.61
30	D	311	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
30	a	720	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
30	f	303	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
28	L	303	DD6	C4-C5-C6	-3.60	122.17	127.31
28	L	306	DD6	C14-C13-C11	-3.60	119.94	125.53
28	I	302	DD6	C37-C36-C31	-3.60	119.46	124.35
28	A	302	DD6	C37-C36-C31	-3.60	119.46	124.35
30	F	311	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
28	L	305	DD6	C37-C36-C31	-3.60	119.46	124.35
30	b	701	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
30	B	307	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
30	a	701	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
30	K	308	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
30	A	315	CLA	CMB-C2B-C1B	-3.58	122.95	128.46
30	B	313	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
34	D	306	PID	C12-O4-C10	3.58	109.51	107.65
30	a	712	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
28	K	318	DD6	C21-C20-C19	3.57	118.30	114.28
34	G	507	PID	C18-C19-C20	3.57	130.79	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	301	DD6	O1-C20-C21	-3.57	110.78	115.06
28	J	304	DD6	C21-C20-C19	3.56	118.29	114.28
28	M	305	DD6	C37-C36-C31	-3.56	119.51	124.35
28	G	502	DD6	C37-C36-C31	-3.56	119.51	124.35
30	I	312	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
31	M	307	KC1	O2D-CGD-O1D	-3.55	116.89	123.84
30	G	517	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
30	D	316	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
28	P	204	DD6	C9-C10-C11	-3.55	122.25	127.31
34	H	302	PID	CM4-C14-C15	-3.55	117.95	122.92
30	J	312	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
30	I	311	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
28	O	303	DD6	C37-C36-C31	-3.54	119.54	124.35
34	O	304	PID	C29-C24-C25	3.54	123.21	119.70
34	P	205	PID	C12-O4-C10	3.54	109.49	107.65
28	h	203	DD6	C15-C14-C13	-3.53	118.52	125.99
30	G	520	CLA	CMB-C2B-C3B	3.53	131.29	124.68
32	G	521	DGD	C4D-C3D-C2D	3.53	116.99	110.82
37	a	734	BCR	C7-C8-C9	-3.53	120.90	126.23
28	L	304	DD6	C15-C14-C13	-3.53	118.53	125.99
30	j	106	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
28	N	303	DD6	C15-C14-C13	-3.52	118.54	125.99
34	G	507	PID	C12-O4-C10	3.52	109.48	107.65
28	G	505	DD6	C14-C13-C11	-3.52	120.06	125.53
28	h	203	DD6	C4-C5-C6	-3.52	122.28	127.31
37	f	304	BCR	C24-C23-C22	-3.52	120.91	126.23
29	I	304	UIX	C6-C1-C3	3.52	118.24	114.28
30	a	711	CLA	CMB-C2B-C3B	3.52	131.26	124.68
30	A	309	CLA	CMB-C2B-C3B	3.52	131.26	124.68
30	a	722	CLA	CMB-C2B-C3B	3.52	131.26	124.68
28	A	303	DD6	C37-C36-C31	-3.52	119.57	124.35
30	K	313	CLA	CMB-C2B-C3B	3.52	131.26	124.68
28	B	303	DD6	C3-C2-C1	-3.52	122.29	127.31
28	K	318	DD6	C37-C36-C31	-3.51	119.57	124.35
30	H	307	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
34	F	305	PID	C16-C15-C14	3.51	132.32	127.31
28	B	302	DD6	O1-C20-C21	3.51	119.26	115.06
30	A	311	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
28	A	301	DD6	C37-C36-C31	-3.51	119.58	124.35
30	M	308	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
34	D	307	PID	C17-C16-C15	3.51	130.66	123.47
34	j	105	PID	C17-C16-C15	3.50	130.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	304	DD6	C9-C10-C11	-3.50	122.31	127.31
30	G	509	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
28	I	305	DD6	C37-C36-C31	-3.50	119.59	124.35
34	F	302	PID	CM5-C21-C20	-3.50	118.02	122.92
37	l	302	BCR	C15-C14-C13	-3.50	122.31	127.31
34	G	506	PID	C12-O4-C10	3.50	109.47	107.65
34	N	302	PID	CM5-C21-C20	-3.50	118.02	122.92
28	P	204	DD6	O1-C20-C19	-3.50	110.76	113.38
28	H	303	DD6	C37-C36-C31	-3.49	119.60	124.35
30	J	315	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
30	b	709	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
37	b	702	BCR	C11-C10-C9	-3.49	122.33	127.31
30	O	313	CLA	CMB-C2B-C3B	3.49	131.21	124.68
30	f	302	CLA	CMB-C2B-C3B	3.49	131.20	124.68
30	H	309	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
30	K	309	CLA	CMB-C2B-C3B	3.48	131.19	124.68
28	L	302	DD6	C37-C36-C31	-3.48	119.62	124.35
30	L	310	CLA	CMB-C2B-C3B	3.48	131.19	124.68
29	A	304	UIX	C18-O2-C27	-3.48	111.41	117.90
30	D	314	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
30	F	313	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
30	G	510	CLA	CMB-C2B-C3B	3.47	131.18	124.68
29	B	305	UIX	C14-C13-C11	-3.47	122.36	127.31
30	l	308	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
30	G	514	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
28	A	303	DD6	C3-C2-C1	-3.47	122.36	127.31
30	A	320	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
28	J	302	DD6	C21-C20-C19	3.47	118.18	114.28
30	G	513	CLA	CMB-C2B-C3B	3.47	131.17	124.68
34	D	305	PID	C12-O4-C10	3.47	109.46	107.65
30	P	217	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
30	M	316	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
30	A	312	CLA	CMB-C2B-C3B	3.46	131.16	124.68
30	P	214	CLA	CMB-C2B-C3B	3.46	131.15	124.68
31	M	307	KC1	O1D-CGD-CBD	-3.46	117.41	124.48
28	B	306	DD6	C4-C5-C6	-3.46	122.38	127.31
30	b	727	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
30	a	730	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
30	B	308	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
30	J	307	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
30	F	307	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
28	G	505	DD6	C24-C1-C2	3.44	124.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	724	CLA	CMB-C2B-C3B	3.44	131.12	124.68
30	b	705	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
30	a	731	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
30	A	313	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
30	I	316	CLA	CMB-C2B-C3B	3.44	131.11	124.68
30	A	317	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
30	I	306	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
30	l	311	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	J	311	CLA	CMB-C2B-C3B	3.42	131.08	124.68
37	b	702	BCR	C33-C5-C6	-3.42	120.69	124.53
29	A	304	UIX	C17-C15-C20	3.42	112.53	109.21
28	b	731	DD6	C37-C36-C31	-3.42	119.70	124.35
30	I	319	CLA	CMB-C2B-C3B	3.42	131.07	124.68
30	l	309	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
30	I	310	CLA	CMB-C2B-C3B	3.42	131.07	124.68
34	j	105	PID	C12-O4-C10	3.42	109.43	107.65
28	K	305	DD6	C37-C36-C31	-3.41	119.71	124.35
34	F	306	PID	C18-C19-C20	3.41	130.45	123.47
30	H	311	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
30	M	318	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
37	l	307	BCR	C7-C8-C9	-3.40	121.09	126.23
28	I	305	DD6	C9-C8-C6	-3.40	116.86	126.42
30	a	715	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
30	j	104	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
30	J	306	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
37	l	307	BCR	C38-C26-C25	-3.40	120.72	124.53
37	l	302	BCR	C20-C21-C22	-3.39	122.47	127.31
37	l	307	BCR	C11-C10-C9	-3.39	122.47	127.31
28	G	504	DD6	C21-C20-C19	3.39	118.10	114.28
28	M	304	DD6	C4-C5-C6	-3.39	122.47	127.31
28	I	301	DD6	C37-C36-C35	3.39	120.64	114.36
30	B	309	CLA	CMB-C2B-C3B	3.39	131.02	124.68
28	G	508	DD6	C37-C36-C31	-3.39	119.74	124.35
29	K	302	UIX	C18-O2-C27	-3.39	111.58	117.90
34	N	301	PID	C18-C19-C20	3.39	130.41	123.47
30	K	312	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
30	a	704	CLA	CMB-C2B-C3B	3.39	131.01	124.68
28	I	303	DD6	C24-C1-C2	3.38	124.13	118.94
28	B	306	DD6	C15-C14-C13	-3.38	118.84	125.99
30	K	307	CLA	CMB-C2B-C3B	3.38	131.01	124.68
30	G	512	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
30	I	313	CLA	CMB-C2B-C3B	3.38	131.00	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	J	309	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
30	M	317	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
30	b	718	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
30	a	703	CLA	CMB-C2B-C3B	3.37	130.98	124.68
30	A	308	CLA	CMB-C2B-C3B	3.37	130.98	124.68
30	G	516	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
37	j	102	BCR	C33-C5-C6	-3.36	120.75	124.53
28	J	303	DD6	C21-C20-C15	-3.36	116.62	122.26
30	l	310	CLA	C4D-CHA-C1A	-3.36	121.64	127.26
28	M	303	DD6	C37-C36-C31	-3.36	119.78	124.35
30	B	317	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
30	F	310	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
34	D	305	PID	CM5-C21-C20	-3.36	118.22	122.92
34	P	208	PID	C18-C19-C20	3.36	130.35	123.47
30	a	713	CLA	CMB-C2B-C3B	3.35	130.95	124.68
30	H	304	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
30	a	702	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
30	M	315	CLA	CMB-C2B-C3B	3.35	130.94	124.68
28	N	303	DD6	C37-C36-C31	-3.35	119.80	124.35
30	a	738	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
30	b	712	CLA	CAB-C3B-C4B	-3.35	123.32	128.46
38	a	732	PQN	C14-C13-C15	3.35	120.90	115.27
37	m	201	BCR	C11-C12-C13	-3.34	117.03	126.42
30	P	215	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
30	a	706	CLA	CMB-C2B-C3B	3.34	130.93	124.68
30	B	301	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
30	B	311	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
28	h	203	DD6	C37-C36-C31	-3.34	119.81	124.35
30	J	312	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
30	b	714	CLA	CMB-C2B-C3B	3.33	130.91	124.68
28	F	301	DD6	C14-C13-C11	-3.33	120.36	125.53
37	a	734	BCR	C20-C21-C22	-3.33	122.56	127.31
28	b	731	DD6	C3-C2-C1	-3.33	122.56	127.31
30	b	706	CLA	CMB-C2B-C3B	3.32	130.90	124.68
28	P	204	DD6	C3-C2-C1	-3.32	122.57	127.31
30	a	708	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
28	K	304	DD6	C37-C36-C31	-3.32	119.83	124.35
34	D	307	PID	C18-C19-C20	3.32	130.28	123.47
34	F	305	PID	CM4-C14-C15	-3.32	118.28	122.92
30	l	303	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
30	D	308	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
30	O	308	CLA	CMB-C2B-C1B	-3.31	123.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	209	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
30	D	312	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
34	D	302	PID	C12-O4-C10	3.31	109.37	107.65
30	L	317	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
28	K	303	DD6	C37-C36-C31	-3.30	119.86	124.35
30	L	314	CLA	CMB-C2B-C3B	3.30	130.86	124.68
30	a	718	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
30	N	304	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
30	K	315	CLA	CMB-C2B-C3B	3.30	130.86	124.68
30	a	727	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
30	a	710	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
30	O	309	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
30	l	304	CLA	CMB-C2B-C3B	3.30	130.85	124.68
37	l	307	BCR	C33-C5-C4	3.30	119.95	113.62
28	I	305	DD6	C3-C4-C5	-3.29	116.73	123.47
30	L	308	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
37	m	201	BCR	C4-C5-C6	-3.29	117.95	122.73
30	A	307	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
28	A	303	DD6	C15-C14-C13	-3.29	119.04	125.99
37	j	102	BCR	C3-C4-C5	-3.29	108.21	114.08
37	l	307	BCR	C4-C5-C6	-3.29	117.96	122.73
37	m	201	BCR	C20-C21-C22	-3.29	122.62	127.31
30	K	306	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
30	A	319	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
34	N	302	PID	C26-C25-C24	3.28	112.40	109.21
30	I	307	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
30	M	315	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
30	J	316	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
30	b	704	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
30	P	210	CLA	CMB-C2B-C3B	3.28	130.81	124.68
30	K	316	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
30	D	309	CLA	CMB-C2B-C3B	3.28	130.81	124.68
37	b	732	BCR	C21-C20-C19	-3.27	113.00	123.22
30	B	316	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
30	O	311	CLA	CMB-C2B-C3B	3.27	130.80	124.68
28	I	305	DD6	C37-C36-C35	3.27	120.41	114.36
28	G	505	DD6	C-C1-C2	-3.27	118.34	122.92
34	H	302	PID	C12-O4-C10	3.27	109.35	107.65
30	A	316	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
30	L	318	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
29	O	306	UIX	C14-C23-C26	-3.26	117.25	126.42
30	a	714	CLA	CMB-C2B-C3B	3.26	130.77	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	202	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
30	N	309	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
30	F	311	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
30	P	212	CLA	CMB-C2B-C3B	3.25	130.76	124.68
30	b	725	CLA	CMB-C2B-C3B	3.25	130.76	124.68
30	N	307	CLA	CMB-C2B-C3B	3.25	130.76	124.68
29	K	302	UIX	C34-C37-C39	-3.25	116.82	123.47
32	G	521	DGD	C1D-C2D-C3D	3.25	116.76	110.00
32	I	317	DGD	O1G-C1A-C2A	3.25	119.90	111.38
30	N	310	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
28	K	304	DD6	C4-C5-C6	-3.25	122.68	127.31
30	I	315	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
34	P	206	PID	C17-C18-C19	3.24	132.03	124.81
30	b	724	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
30	J	308	CLA	CMB-C2B-C3B	3.24	130.73	124.68
34	O	304	PID	C6-C7-C8	-3.24	119.15	125.99
29	B	305	UIX	C6-C1-C3	3.23	117.92	114.28
30	N	309	CLA	O2D-CGD-O1D	-3.23	117.51	123.84
30	I	319	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
28	L	305	DD6	C15-C14-C13	-3.23	119.16	125.99
30	a	716	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
28	G	505	DD6	O1-C20-C19	3.23	115.81	113.38
29	J	305	UIX	C6-C1-C3	3.23	117.91	114.28
34	G	507	PID	C17-C16-C15	3.23	130.09	123.47
34	D	301	PID	CM5-C21-C20	-3.23	118.40	122.92
30	a	709	CLA	CMB-C2B-C3B	3.23	130.71	124.68
30	J	301	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
34	P	203	PID	C12-O4-C10	3.22	109.33	107.65
30	A	310	CLA	CMB-C2B-C3B	3.22	130.71	124.68
30	b	720	CLA	CMB-C2B-C3B	3.22	130.71	124.68
30	b	722	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	H	303	DD6	C9-C10-C11	-3.22	122.71	127.31
30	D	313	CLA	CMB-C2B-C3B	3.22	130.70	124.68
37	l	302	BCR	C38-C26-C27	3.22	119.79	113.62
30	F	308	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
30	b	711	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
28	K	305	DD6	C15-C14-C13	-3.21	119.20	125.99
37	i	201	BCR	C11-C10-C9	-3.21	122.73	127.31
28	B	306	DD6	C37-C36-C31	-3.21	119.99	124.35
30	l	313	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
30	b	728	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
30	f	301	CLA	CMB-C2B-C1B	-3.20	123.54	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	731	DD6	C4-C3-C2	-3.20	116.92	123.47
28	B	302	DD6	C21-C20-C15	-3.20	116.90	122.26
30	H	305	CLA	CMB-C2B-C3B	3.20	130.66	124.68
30	L	316	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
30	a	735	CLA	CMB-C2B-C3B	3.20	130.66	124.68
28	G	502	DD6	C14-C13-C11	-3.20	120.57	125.53
30	K	311	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
30	a	726	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
30	B	312	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
30	a	705	CLA	CMB-C2B-C3B	3.20	130.66	124.68
37	i	201	BCR	C15-C16-C17	-3.20	116.93	123.47
30	b	723	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	D	303	DD6	C14-C13-C11	3.19	130.48	125.53
30	a	707	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	L	302	DD6	C33-C34-C35	-3.19	105.94	110.30
30	M	312	CLA	CMB-C2B-C3B	3.19	130.64	124.68
30	b	726	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
34	F	306	PID	CM5-C21-C20	-3.18	118.47	122.92
30	O	314	CLA	CMB-C2B-C3B	3.18	130.63	124.68
30	F	315	CLA	CMB-C2B-C3B	3.18	130.63	124.68
30	b	717	CLA	CMB-C2B-C3B	3.18	130.62	124.68
34	O	307	PID	C17-C16-C15	3.18	129.98	123.47
30	l	312	CLA	CMB-C2B-C3B	3.18	130.62	124.68
29	P	207	UIX	C14-C23-C26	-3.18	117.50	126.42
28	h	203	DD6	C9-C10-C11	-3.17	122.78	127.31
30	a	726	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
28	I	302	DD6	O1-C20-C19	-3.17	111.00	113.38
34	O	301	PID	C18-C19-C20	3.17	129.97	123.47
34	P	203	PID	CM5-C21-C20	-3.17	118.48	122.92
28	M	306	DD6	C25-C26-C27	-3.17	117.38	126.58
30	J	310	CLA	CMB-C2B-C3B	3.17	130.61	124.68
30	L	312	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
30	N	305	CLA	CMB-C2B-C3B	3.17	130.61	124.68
34	O	302	PID	C12-O4-C10	3.17	109.30	107.65
34	O	304	PID	C18-C19-C20	3.17	129.96	123.47
34	M	301	PID	C17-C18-C19	3.16	131.85	124.81
28	L	303	DD6	C21-C20-C15	-3.16	116.96	122.26
30	D	314	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
28	M	302	DD6	C21-C20-C19	3.16	117.83	114.28
30	b	723	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
30	O	316	CLA	CMB-C2B-C3B	3.16	130.58	124.68
30	a	721	CLA	CMB-C2B-C1B	-3.15	123.62	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	l	307	BCR	C16-C17-C18	-3.15	122.82	127.31
34	H	301	PID	C17-C18-C19	3.15	131.82	124.81
30	A	307	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
34	M	301	PID	C26-C25-C24	3.15	112.27	109.21
28	M	306	DD6	C37-C36-C35	3.15	120.19	114.36
37	l	302	BCR	C38-C26-C25	-3.15	120.99	124.53
30	P	215	CLA	CMB-C2B-C3B	3.15	130.56	124.68
34	P	208	PID	CM5-C21-C20	-3.14	118.52	122.92
30	a	717	CLA	CMB-C2B-C3B	3.14	130.56	124.68
34	P	206	PID	C16-C15-C14	-3.14	122.82	127.31
28	G	504	DD6	C32-C31-C36	-3.14	118.20	122.63
37	b	702	BCR	C28-C27-C26	-3.14	108.47	114.08
30	a	725	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
28	F	301	DD6	C9-C8-C6	-3.14	117.61	126.42
28	A	305	DD6	C37-C36-C35	3.13	120.16	114.36
30	b	716	CLA	CMB-C2B-C3B	3.13	130.54	124.68
30	H	307	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	J	305	UIX	C7-C10-C11	-3.13	120.67	125.53
30	G	516	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
30	I	311	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
30	L	313	CLA	CMB-C2B-C3B	3.13	130.53	124.68
30	a	723	CLA	CMB-C2B-C3B	3.13	130.53	124.68
28	J	304	DD6	C25-C24-C1	-3.13	117.63	126.42
28	F	301	DD6	C25-C26-C27	-3.12	117.51	126.58
30	M	313	CLA	CMB-C2B-C3B	3.12	130.52	124.68
28	M	306	DD6	C14-C13-C11	-3.12	120.69	125.53
31	O	315	KC1	C3D-CAD-CBD	-3.12	103.50	107.61
34	N	302	PID	C12-O4-C10	3.12	109.27	107.65
30	b	709	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
31	M	307	KC1	C3D-CAD-CBD	-3.12	103.50	107.61
34	P	205	PID	C17-C18-C19	3.12	131.74	124.81
30	l	310	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
30	J	314	CLA	CMB-C2B-C3B	3.11	130.50	124.68
30	G	519	CLA	CMB-C2B-C3B	3.11	130.50	124.68
30	M	310	CLA	CMB-C2B-C3B	3.11	130.50	124.68
28	M	305	DD6	C4-C5-C6	-3.11	122.87	127.31
30	F	315	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
28	K	301	DD6	C9-C10-C11	-3.11	122.88	127.31
30	b	707	CLA	CMB-C2B-C3B	3.10	130.49	124.68
28	M	305	DD6	C9-C10-C11	-3.10	122.88	127.31
28	K	303	DD6	C3-C2-C1	-3.10	122.88	127.31
30	a	704	CLA	C1B-CHB-C4A	-3.10	123.97	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	309	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
28	M	306	DD6	C24-C1-C2	3.10	123.70	118.94
37	i	201	BCR	C27-C26-C25	-3.10	118.23	122.73
31	N	311	KC1	C3D-CAD-CBD	-3.10	103.53	107.61
30	I	321	CLA	CMB-C2B-C3B	3.10	130.47	124.68
30	l	303	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
28	P	204	DD6	C37-C36-C35	3.09	120.08	114.36
34	D	304	PID	C17-C18-C19	3.09	131.69	124.81
28	D	303	DD6	C21-C20-C15	-3.09	117.08	122.26
30	I	308	CLA	CMB-C2B-C3B	3.09	130.46	124.68
34	P	202	PID	CM5-C21-C20	-3.09	118.59	122.92
30	I	306	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
34	F	304	PID	C17-C18-C19	3.09	131.68	124.81
28	L	303	DD6	C15-C14-C13	-3.09	119.47	125.99
30	H	312	CLA	CMB-C2B-C3B	3.09	130.45	124.68
37	m	201	BCR	C23-C24-C25	-3.08	118.55	127.20
30	G	517	CLA	CMB-C2B-C3B	3.08	130.44	124.68
30	I	309	CLA	CMB-C2B-C3B	3.08	130.44	124.68
31	O	312	KC1	CHC-C4B-C3B	-3.08	119.99	125.26
30	F	313	CLA	CHB-C4A-NA	3.08	128.76	124.51
30	a	738	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
28	K	305	DD6	C4-C5-C6	-3.07	122.92	127.31
28	I	305	DD6	C25-C24-C1	-3.07	117.78	126.42
30	F	310	CLA	CMB-C2B-C3B	3.07	130.43	124.68
34	O	301	PID	CM5-C21-C20	-3.07	118.62	122.92
28	b	731	DD6	C37-C36-C35	3.07	120.05	114.36
37	l	307	BCR	C20-C21-C22	-3.07	122.93	127.31
30	b	708	CLA	CMB-C2B-C3B	3.07	130.42	124.68
34	G	506	PID	CM5-C21-C20	-3.07	118.62	122.92
28	A	303	DD6	C4-C5-C6	-3.07	122.93	127.31
30	b	722	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
34	P	202	PID	C18-C19-C20	3.07	129.75	123.47
30	G	518	CLA	CMB-C2B-C3B	3.06	130.41	124.68
28	G	504	DD6	C37-C36-C35	3.06	120.03	114.36
30	L	311	CLA	CMB-C2B-C3B	3.06	130.41	124.68
30	H	308	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
34	G	507	PID	CM5-C21-C20	-3.06	118.63	122.92
30	b	715	CLA	CMB-C2B-C3B	3.06	130.41	124.68
30	M	309	CLA	CMB-C2B-C3B	3.06	130.40	124.68
29	K	302	UIX	C6-C1-C3	3.06	117.72	114.28
29	h	201	UIX	C37-C34-C30	-3.06	117.21	123.47
30	a	729	CLA	CMB-C2B-C1B	-3.05	123.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	303	DD6	C32-C33-C34	-3.05	106.75	113.64
29	B	305	UIX	C-C7-C10	-3.05	119.54	125.99
28	G	504	DD6	C21-C20-C15	-3.05	117.15	122.26
30	B	310	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
28	G	504	DD6	O1-C20-C21	3.05	118.71	115.06
30	K	315	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
28	G	508	DD6	O1-C20-C21	-3.05	111.40	115.06
30	L	317	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
30	K	310	CLA	CMB-C2B-C3B	3.05	130.38	124.68
28	I	305	DD6	O1-C20-C21	3.05	118.70	115.06
34	D	306	PID	CM5-C21-C20	-3.04	118.66	122.92
30	M	311	CLA	CMB-C2B-C3B	3.04	130.37	124.68
28	A	301	DD6	C14-C13-C11	-3.04	120.81	125.53
29	A	304	UIX	C37-C39-C40	-3.04	122.97	127.31
37	b	732	BCR	C8-C7-C6	-3.04	118.67	127.20
30	K	316	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
30	a	703	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
30	K	308	CLA	CMB-C2B-C3B	3.04	130.36	124.68
30	a	729	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
28	L	305	DD6	C33-C34-C35	-3.04	106.15	110.30
31	D	310	KC1	CHC-C4B-C3B	-3.03	120.07	125.26
30	J	308	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	L	309	CLA	CMB-C2B-C3B	3.03	130.35	124.68
34	N	301	PID	CM5-C21-C20	-3.03	118.68	122.92
30	F	312	CLA	CMB-C2B-C3B	3.03	130.34	124.68
37	a	734	BCR	C3-C4-C5	-3.03	108.67	114.08
37	b	730	BCR	C28-C27-C26	-3.03	108.67	114.08
30	O	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
30	b	721	CLA	CMB-C2B-C3B	3.03	130.34	124.68
37	i	201	BCR	C30-C25-C26	-3.02	118.35	122.61
30	I	310	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
30	l	305	CLA	CMB-C2B-C3B	3.02	130.33	124.68
30	l	310	CLA	C3D-C4D-ND	3.02	111.95	107.38
30	H	308	CLA	CMB-C2B-C3B	3.02	130.33	124.68
30	b	719	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
28	H	303	DD6	O1-C20-C19	-3.02	111.12	113.38
30	D	311	CLA	CMB-C2B-C3B	3.02	130.32	124.68
28	A	302	DD6	C21-C20-C15	-3.01	117.21	122.26
30	a	724	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
30	G	511	CLA	CMB-C2B-C3B	3.01	130.31	124.68
28	J	302	DD6	O1-C20-C21	-3.01	111.45	115.06
28	J	304	DD6	C14-C13-C11	-3.01	120.86	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	302	DD6	C37-C36-C31	-3.01	120.26	124.35
30	A	315	CLA	CMB-C2B-C3B	3.01	130.31	124.68
30	a	728	CLA	CMB-C2B-C3B	3.01	130.31	124.68
30	J	314	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
28	J	304	DD6	C37-C36-C31	-3.01	120.26	124.35
37	l	307	BCR	C24-C23-C22	-3.01	121.69	126.23
30	F	313	CLA	CMB-C2B-C3B	3.00	130.29	124.68
37	a	736	BCR	C20-C21-C22	-3.00	123.03	127.31
30	A	311	CLA	CMB-C2B-C3B	3.00	130.29	124.68
30	L	312	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
37	f	304	BCR	C38-C26-C25	-3.00	121.16	124.53
30	B	310	CLA	CMB-C2B-C3B	3.00	130.28	124.68
30	I	315	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
28	P	204	DD6	C4-C3-C2	-2.99	117.34	123.47
30	B	311	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
31	G	515	KC1	C3D-CAD-CBD	-2.99	103.67	107.61
34	D	304	PID	CM5-C21-C20	-2.99	118.73	122.92
34	O	304	PID	C26-C25-C24	2.99	112.12	109.21
28	L	304	DD6	O1-C20-C21	-2.99	111.47	115.06
28	M	305	DD6	C15-C14-C13	-2.99	119.67	125.99
31	F	309	KC1	CHC-C4B-C3B	-2.99	120.14	125.26
30	O	314	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
30	J	301	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
30	j	106	CLA	CMB-C2B-C3B	2.99	130.26	124.68
30	G	518	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
28	B	304	DD6	O1-C20-C21	-2.99	111.48	115.06
32	G	521	DGD	O6E-C5E-C4E	-2.98	104.28	109.69
29	B	305	UIX	C7-C10-C11	-2.98	120.90	125.53
31	P	213	KC1	CHC-C4B-C3B	-2.98	120.16	125.26
30	a	712	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
30	a	714	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
28	G	504	DD6	C24-C1-C2	2.98	123.51	118.94
37	b	702	BCR	C3-C4-C5	-2.98	108.76	114.08
34	j	105	PID	C6-C7-C8	-2.98	119.70	125.99
28	b	731	DD6	C32-C33-C34	-2.98	106.92	113.64
28	B	302	DD6	O1-C20-C19	2.98	115.62	113.38
30	a	723	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
28	M	306	DD6	C37-C36-C31	-2.98	120.31	124.35
30	B	315	CLA	CMB-C2B-C3B	2.97	130.24	124.68
34	O	302	PID	CM5-C21-C20	-2.97	118.76	122.92
30	K	306	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	J	307	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	O	305	PID	CM5-C21-C20	-2.97	118.76	122.92
34	F	305	PID	C29-C24-C25	2.97	122.64	119.70
34	H	302	PID	C17-C16-C15	2.97	129.56	123.47
30	B	313	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	a	720	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	H	309	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
28	L	304	DD6	C33-C34-C35	-2.96	106.25	110.30
28	B	306	DD6	C33-C34-C35	-2.96	106.26	110.30
30	a	725	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
30	f	303	CLA	CMB-C2B-C3B	2.95	130.21	124.68
30	b	705	CLA	CMB-C2B-C3B	2.95	130.20	124.68
30	J	310	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
30	H	307	CLA	CMB-C2B-C3B	2.95	130.19	124.68
34	D	302	PID	CM5-C21-C20	-2.95	118.79	122.92
30	J	307	CLA	CMB-C2B-C3B	2.95	130.19	124.68
37	b	702	BCR	C8-C7-C6	-2.95	118.93	127.20
32	G	501	DGD	O1G-C1A-C2A	2.95	121.15	111.91
31	N	308	KC1	CHB-C1B-C2B	-2.95	119.30	125.48
30	G	509	CLA	CMB-C2B-C3B	2.94	130.19	124.68
30	O	316	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	D	316	CLA	CMB-C2B-C3B	2.94	130.18	124.68
30	B	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
28	G	508	DD6	C4-C3-C2	-2.94	117.45	123.47
30	G	510	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	a	719	CLA	CMB-C2B-C3B	2.94	130.17	124.68
28	I	301	DD6	C37-C36-C31	-2.94	120.36	124.35
28	B	304	DD6	C33-C34-C35	-2.94	106.28	110.30
30	b	713	CLA	CMB-C2B-C3B	2.93	130.17	124.68
29	A	304	UIX	C35-C36-C38	-2.93	114.06	123.22
28	A	305	DD6	C9-C10-C11	-2.93	123.12	127.31
30	a	717	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
30	H	311	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	G	503	UIX	C36-C35-C32	-2.93	123.13	127.31
28	I	305	DD6	C24-C1-C2	2.93	123.43	118.94
28	L	302	DD6	O1-C20-C19	-2.93	111.18	113.38
28	O	303	DD6	C21-C20-C15	-2.92	117.36	122.26
28	I	302	DD6	O1-C20-C21	-2.92	111.55	115.06
37	b	730	BCR	C33-C5-C4	2.92	119.23	113.62
30	M	308	CLA	CMB-C2B-C3B	2.92	130.15	124.68
30	I	308	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
28	I	303	DD6	C12-C11-C10	-2.92	118.83	122.92
30	B	307	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	514	CLA	CMB-C2B-C3B	2.92	130.13	124.68
31	A	314	KC1	C3D-CAD-CBD	-2.92	103.77	107.61
28	M	303	DD6	C14-C13-C11	-2.92	121.00	125.53
31	L	307	KC1	CHC-C4B-C3B	-2.91	120.28	125.26
30	B	309	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	b	716	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	D	309	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	M	313	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	I	309	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
30	A	315	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
30	K	309	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
30	l	309	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	K	302	UIX	C35-C36-C38	-2.90	114.16	123.22
28	L	303	DD6	C33-C34-C35	-2.90	106.33	110.30
30	J	315	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
28	M	303	DD6	C12-C11-C10	-2.90	118.86	122.92
34	H	302	PID	CM5-C21-C20	-2.90	118.86	122.92
30	a	701	CLA	CMB-C2B-C3B	2.90	130.10	124.68
30	a	735	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
30	L	308	CLA	CBD-CHA-C1A	2.90	132.07	127.43
28	K	304	DD6	C3-C4-C5	-2.90	117.54	123.47
30	a	730	CLA	CMB-C2B-C3B	2.90	130.10	124.68
29	K	302	UIX	C7-C10-C11	-2.90	121.03	125.53
28	I	305	DD6	C-C1-C2	-2.90	118.86	122.92
31	D	315	KC1	C3D-CAD-CBD	-2.90	103.79	107.61
33	P	201	LMG	O6-C1-O1	-2.90	103.12	109.97
30	b	715	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
30	L	316	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
28	G	504	DD6	C37-C36-C31	-2.90	120.42	124.35
30	L	316	CLA	CAA-C2A-C3A	-2.89	109.34	116.10
29	O	306	UIX	C12-C11-C13	-2.89	118.87	122.92
37	l	302	BCR	C3-C4-C5	-2.89	108.92	114.08
30	F	313	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
28	K	305	DD6	C33-C34-C35	-2.89	106.35	110.30
30	A	308	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
28	G	504	DD6	C9-C10-C11	-2.89	123.19	127.31
30	a	705	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	b	707	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
28	K	301	DD6	C3-C2-C1	-2.88	123.19	127.31
31	N	308	KC1	C4B-CHC-C1C	-2.88	119.84	126.06
34	N	302	PID	C29-C24-C25	2.88	122.56	119.70
30	J	316	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	306	DD6	C9-C10-C11	-2.88	123.20	127.31
34	O	307	PID	CM5-C21-C20	-2.88	118.89	122.92
28	J	302	DD6	C25-C24-C1	-2.88	118.32	126.42
29	B	305	UIX	C18-O2-C27	-2.88	112.53	117.90
30	F	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	h	201	UIX	C34-C30-C26	-2.88	123.20	127.31
30	l	308	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	H	311	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	A	320	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
34	O	307	PID	C18-C19-C20	2.88	129.37	123.47
37	m	201	BCR	C33-C5-C4	2.88	119.14	113.62
37	b	732	BCR	C24-C23-C22	-2.88	121.89	126.23
30	b	718	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
30	b	727	CLA	CMB-C2B-C3B	2.87	130.06	124.68
37	l	302	BCR	C37-C22-C21	-2.87	118.90	122.92
37	a	734	BCR	C8-C7-C6	-2.87	119.13	127.20
30	b	710	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
37	b	732	BCR	C10-C11-C12	-2.87	114.26	123.22
30	J	315	CLA	CMB-C2B-C3B	2.87	130.05	124.68
30	b	724	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
28	F	301	DD6	C37-C36-C35	2.87	119.67	114.36
37	l	302	BCR	C16-C15-C14	-2.87	117.60	123.47
34	j	105	PID	CM5-C21-C20	-2.86	118.91	122.92
28	B	302	DD6	C20-C19-C18	-2.86	107.09	112.75
30	H	304	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
34	F	305	PID	C19-C20-C21	2.86	131.39	127.31
30	I	307	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	P	211	KC1	O1D-CGD-CBD	-2.86	118.63	124.48
30	B	301	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
30	l	309	CLA	CMB-C2B-C3B	2.85	130.02	124.68
30	A	317	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	a	722	CLA	C1B-CHB-C4A	-2.85	124.46	130.12
30	J	312	CLA	CMB-C2B-C3B	2.85	130.02	124.68
30	b	725	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
28	K	303	DD6	C4-C5-C6	-2.85	123.24	127.31
30	B	308	CLA	CMB-C2B-C3B	2.85	130.02	124.68
30	l	313	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	a	715	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	P	209	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	l	308	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	P	214	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
37	l	306	BCR	C28-C27-C26	-2.85	108.99	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	734	BCR	C33-C5-C4	2.85	119.09	113.62
30	K	308	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	M	308	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	a	726	CLA	CMB-C2B-C3B	2.85	130.01	124.68
37	l	302	BCR	C29-C30-C25	2.85	114.87	110.48
30	b	706	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	H	305	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
30	A	313	CLA	CMB-C2B-C3B	2.85	130.00	124.68
37	l	307	BCR	C15-C16-C17	-2.84	117.65	123.47
30	a	716	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	G	505	DD6	C21-C20-C19	2.84	117.48	114.28
29	G	503	UIX	C18-O2-C27	-2.84	112.60	117.90
30	b	701	CLA	CMB-C2B-C3B	2.84	130.00	124.68
30	a	728	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
30	L	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
30	a	726	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
30	F	307	CLA	CMB-C2B-C3B	2.84	130.00	124.68
30	I	312	CLA	CMB-C2B-C3B	2.84	129.99	124.68
30	M	317	CLA	CMB-C2B-C3B	2.84	129.99	124.68
31	K	314	KC1	CHC-C4B-C3B	-2.84	120.40	125.26
34	P	206	PID	CM5-C21-C20	-2.84	118.95	122.92
31	P	211	KC1	CHC-C4B-C3B	-2.84	120.40	125.26
30	b	711	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
30	P	217	CLA	CMB-C2B-C3B	2.84	129.99	124.68
30	L	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
30	P	210	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
30	a	715	CLA	CMB-C2B-C3B	2.84	129.98	124.68
30	M	317	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
28	J	304	DD6	C-C1-C2	-2.84	118.95	122.92
30	N	305	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
37	b	730	BCR	C21-C20-C19	-2.83	114.37	123.22
28	A	303	DD6	C33-C34-C35	-2.83	106.42	110.30
30	m	202	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	N	304	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	G	505	DD6	O1-C20-C15	-2.83	56.61	58.96
28	B	306	DD6	C25-C26-C27	-2.83	118.36	126.58
28	B	302	DD6	C24-C1-C2	2.83	123.29	118.94
30	b	717	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
31	P	216	KC1	CHB-C1B-C2B	-2.83	119.54	125.48
28	I	302	DD6	C7-C6-C5	-2.83	118.96	122.92
30	F	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	N	307	CLA	O2D-CGD-O1D	-2.83	118.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	311	CLA	CMB-C2B-C3B	2.83	129.97	124.68
31	H	306	KC1	CHC-C4B-C3B	-2.83	120.42	125.26
30	l	313	CLA	CHB-C4A-NA	2.83	128.42	124.51
30	I	321	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	K	311	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	a	718	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	f	303	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	b	712	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	K	313	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
30	D	314	CLA	CMB-C2B-C3B	2.83	129.96	124.68
30	a	710	CLA	CMB-C2B-C3B	2.82	129.96	124.68
30	a	722	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	l	304	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	K	310	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	L	303	DD6	O1-C20-C19	-2.82	111.26	113.38
31	A	314	KC1	CHB-C1B-C2B	-2.82	119.56	125.48
30	K	315	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
30	M	318	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	J	304	DD6	C12-C11-C10	-2.82	118.97	122.92
28	J	302	DD6	C37-C36-C35	2.82	119.58	114.36
30	G	509	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	D	303	DD6	C9-C10-C11	-2.82	123.29	127.31
33	b	734	LMG	O6-C1-O1	-2.82	103.30	109.97
30	O	308	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	M	316	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	K	304	DD6	C37-C36-C35	2.82	119.57	114.36
37	j	102	BCR	C28-C27-C26	-2.82	109.05	114.08
30	K	312	CLA	CMB-C2B-C3B	2.82	129.95	124.68
28	G	508	DD6	C14-C13-C11	-2.82	121.16	125.53
30	a	712	CLA	CMB-C2B-C3B	2.81	129.94	124.68
31	P	213	KC1	C3D-CAD-CBD	-2.81	103.90	107.61
30	O	313	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
30	P	217	CLA	CAA-C2A-C3A	-2.81	109.54	116.10
29	G	503	UIX	C14-C13-C11	-2.81	123.30	127.31
28	L	306	DD6	C37-C36-C35	2.81	119.56	114.36
31	N	311	KC1	CHC-C4B-C3B	-2.81	120.45	125.26
31	I	314	KC1	CHC-C4B-C3B	-2.81	120.45	125.26
30	A	319	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
30	l	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	I	304	UIX	C35-C36-C38	-2.81	114.45	123.22
30	P	217	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	b	719	CLA	CMB-C2B-C3B	2.81	129.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	313	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	I	321	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	j	104	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	A	313	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	a	708	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
30	I	316	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
37	b	702	BCR	C34-C9-C8	2.80	122.49	118.08
30	N	310	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	M	311	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
28	M	306	DD6	O1-C20-C21	2.80	118.41	115.06
28	G	504	DD6	C-C1-C2	-2.80	119.00	122.92
30	M	309	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	D	314	CLA	CHB-C4A-NA	2.80	128.38	124.51
28	M	303	DD6	C21-C20-C15	-2.80	117.57	122.26
37	j	102	BCR	C11-C10-C9	-2.80	123.31	127.31
30	B	315	CLA	CAA-C2A-C3A	-2.80	109.57	116.10
29	G	503	UIX	C34-C37-C39	-2.80	117.74	123.47
30	O	316	CLA	CAA-C2A-C3A	-2.80	109.57	116.10
37	b	730	BCR	C15-C16-C17	-2.80	117.74	123.47
29	A	304	UIX	C21-C15-C20	-2.80	107.97	110.47
30	M	312	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	a	709	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	N	307	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
34	D	302	PID	CM2-C5-C4	-2.79	104.13	108.98
31	N	306	KC1	CHC-C4B-C3B	-2.79	120.48	125.26
30	b	703	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	G	512	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	H	309	CLA	CMB-C2B-C3B	2.79	129.90	124.68
30	D	313	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
34	j	105	PID	C18-C19-C20	2.79	129.19	123.47
30	b	705	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
28	J	304	DD6	C32-C31-C36	-2.79	118.70	122.63
28	P	204	DD6	C33-C34-C35	-2.79	106.49	110.30
30	A	312	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	b	727	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
37	m	201	BCR	C28-C27-C26	-2.79	109.10	114.08
30	L	318	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
31	D	315	KC1	CHB-C1B-C2B	-2.78	119.64	125.48
30	K	307	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
37	b	702	BCR	C15-C14-C13	-2.78	123.34	127.31
30	b	712	CLA	CMB-C2B-C3B	2.78	130.14	124.69
30	J	306	CLA	CMB-C2B-C3B	2.78	129.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	304	UIX	C37-C34-C30	-2.78	117.77	123.47
30	J	309	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	I	312	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	P	216	KC1	C3D-CAD-CBD	-2.78	103.94	107.61
30	N	309	CLA	CMB-C2B-C3B	2.78	129.88	124.68
31	P	211	KC1	O2D-CGD-O1D	-2.78	118.40	123.84
32	G	521	DGD	C3E-C4E-C5E	2.78	115.20	110.24
30	b	720	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
30	a	701	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	O	306	UIX	C22-C15-C20	-2.78	107.98	110.47
30	B	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	A	316	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	B	317	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	a	735	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	O	306	UIX	C16-C20-C15	2.78	122.45	119.70
30	a	727	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
30	O	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
31	A	314	KC1	CHC-C4B-C3B	-2.78	120.51	125.26
37	a	734	BCR	C24-C23-C22	-2.77	122.04	126.23
37	m	201	BCR	C16-C17-C18	-2.77	123.35	127.31
29	B	305	UIX	C16-C20-C15	2.77	122.45	119.70
37	a	736	BCR	C3-C4-C5	-2.77	109.12	114.08
30	B	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	L	318	CLA	CHB-C4A-NA	2.77	128.35	124.51
37	j	102	BCR	C16-C15-C14	-2.77	117.80	123.47
30	P	214	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
28	F	301	DD6	C37-C36-C31	-2.77	120.58	124.35
30	l	312	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
28	M	304	DD6	C3-C4-C5	-2.77	117.80	123.47
28	M	305	DD6	C21-C20-C15	-2.77	117.62	122.26
37	m	201	BCR	C38-C26-C27	2.77	118.93	113.62
30	a	730	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
28	K	303	DD6	C10-C9-C8	-2.76	114.59	123.22
30	J	311	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	M	314	KC1	CHB-C1B-C2B	-2.76	119.68	125.48
31	N	306	KC1	C3D-CAD-CBD	-2.76	103.97	107.61
28	M	303	DD6	C25-C24-C1	-2.76	118.65	126.42
28	L	303	DD6	C37-C36-C35	2.76	119.47	114.36
28	I	301	DD6	C25-C26-C27	-2.76	118.56	126.58
28	F	301	DD6	C20-C19-C18	-2.76	107.28	112.75
30	M	318	CLA	CMB-C2B-C3B	2.76	129.84	124.68
28	B	303	DD6	C15-C14-C13	-2.76	120.15	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	l	311	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	A	306	KC1	C3D-CAD-CBD	-2.76	103.97	107.61
30	N	309	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
33	D	317	LMG	O6-C1-O1	-2.76	103.44	109.97
30	J	306	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
28	A	301	DD6	C20-C19-C18	-2.76	107.29	112.75
37	a	736	BCR	C38-C26-C25	-2.76	121.43	124.53
30	a	702	CLA	CMB-C2B-C3B	2.76	129.83	124.68
33	I	318	LMG	C1-C2-C3	-2.76	104.26	110.00
28	G	504	DD6	C15-C14-C13	-2.75	120.17	125.99
31	I	314	KC1	CHB-C1B-C2B	-2.75	119.70	125.48
30	O	309	CLA	CMB-C2B-C3B	2.75	129.83	124.68
29	P	207	UIX	C12-C11-C13	-2.75	119.06	122.92
34	H	301	PID	CM5-C21-C20	-2.75	119.06	122.92
28	I	305	DD6	C32-C31-C36	-2.75	118.75	122.63
30	G	516	CLA	CMB-C2B-C3B	2.75	129.83	124.68
37	j	102	BCR	C7-C8-C9	-2.75	122.08	126.23
31	B	314	KC1	CHC-C4B-C3B	-2.75	120.55	125.26
30	I	313	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	K	302	UIX	C14-C23-C26	-2.75	118.69	126.42
34	M	301	PID	C29-C24-C25	2.75	122.43	119.70
30	f	301	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	G	520	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
34	G	506	PID	C18-C19-C20	2.75	129.11	123.47
28	K	305	DD6	C14-C13-C11	-2.75	121.26	125.53
28	b	731	DD6	C14-C13-C11	-2.75	121.26	125.53
31	O	315	KC1	CHC-C4B-C3B	-2.75	120.56	125.26
28	G	505	DD6	C25-C24-C1	-2.75	118.70	126.42
28	D	303	DD6	C12-C11-C13	2.75	122.41	118.08
30	a	706	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	l	311	CLA	CMB-C2B-C3B	2.74	129.81	124.68
30	A	315	CLA	CAA-C2A-C3A	-2.74	109.69	116.10
30	b	726	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
30	A	311	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
30	H	304	CLA	CMB-C2B-C3B	2.74	129.81	124.68
30	a	708	CLA	CMB-C2B-C3B	2.74	129.81	124.68
30	J	310	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
30	a	711	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	l	310	CLA	CMB-C2B-C3B	2.74	129.80	124.68
30	b	728	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
30	j	106	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
33	I	320	LMG	O6-C1-O1	-2.74	103.49	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	317	CLA	CHB-C4A-NA	2.74	128.30	124.51
28	A	303	DD6	C9-C10-C11	-2.74	123.40	127.31
30	a	721	CLA	CMB-C2B-C3B	2.74	129.80	124.68
30	I	306	CLA	CMB-C2B-C3B	2.74	129.80	124.68
30	J	309	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
30	h	202	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
29	h	201	UIX	C13-C14-C23	-2.73	114.69	123.22
30	l	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
30	A	319	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	D	312	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
30	A	309	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
30	B	317	CLA	CMB-C2B-C3B	2.73	129.79	124.68
37	i	201	BCR	C10-C11-C12	-2.73	114.70	123.22
28	J	303	DD6	C-C1-C2	-2.73	119.10	122.92
30	A	317	CLA	CMB-C2B-C3B	2.73	129.78	124.68
28	B	302	DD6	C25-C24-C1	-2.73	118.75	126.42
30	l	304	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	F	310	CLA	CHB-C4A-NA	2.73	128.28	124.51
30	a	704	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
37	b	702	BCR	C20-C19-C18	-2.73	118.76	126.42
30	D	311	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
37	j	102	BCR	C8-C7-C6	-2.72	119.55	127.20
30	b	721	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
30	D	312	CLA	CMB-C2B-C3B	2.72	129.77	124.68
28	B	306	DD6	O1-C20-C19	-2.72	111.34	113.38
30	D	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
34	F	305	PID	C26-C25-C24	2.72	111.86	109.21
33	b	733	LMG	O6-C1-O1	-2.72	103.53	109.97
34	D	301	PID	CM2-C5-C4	-2.72	104.25	108.98
28	O	303	DD6	C4-C3-C2	-2.72	117.90	123.47
30	l	303	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
31	O	315	KC1	O1D-CGD-CBD	-2.72	118.92	124.48
30	b	704	CLA	CMB-C2B-C3B	2.72	129.76	124.68
30	B	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
28	O	303	DD6	C33-C34-C35	-2.72	106.58	110.30
31	B	314	KC1	CHB-C1B-C2B	-2.72	119.78	125.48
30	b	722	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
30	L	318	CLA	CMB-C2B-C3B	2.72	129.76	124.68
34	O	304	PID	CM5-C21-C20	-2.72	119.12	122.92
30	a	718	CLA	CMB-C2B-C3B	2.72	129.76	124.68
28	K	318	DD6	C33-C34-C35	-2.72	106.59	110.30
28	G	508	DD6	C33-C34-C35	2.71	114.02	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	b	702	BCR	C10-C11-C12	-2.71	114.75	123.22
31	D	310	KC1	CBD-CHA-C1A	2.71	133.94	128.88
37	a	734	BCR	C38-C26-C25	-2.71	121.48	124.53
30	N	304	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	M	303	DD6	C24-C1-C2	2.71	123.10	118.94
30	G	512	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	D	308	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	b	710	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	K	305	DD6	C21-C20-C15	-2.71	117.72	122.26
30	J	307	CLA	CHB-C4A-NA	2.71	128.26	124.51
37	b	732	BCR	C11-C10-C9	-2.71	123.45	127.31
30	L	311	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	J	312	CLA	CHB-C4A-NA	2.71	128.25	124.51
30	B	312	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	a	702	CLA	C1-C2-C3	-2.71	121.36	126.04
29	K	302	UIX	C37-C39-C40	-2.71	123.45	127.31
30	M	317	CLA	CHB-C4A-NA	2.71	128.25	124.51
28	G	504	DD6	C14-C13-C11	-2.70	121.33	125.53
30	b	708	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
34	D	307	PID	CM5-C21-C20	-2.70	119.14	122.92
31	L	315	KC1	CHB-C1B-C2B	-2.70	119.81	125.48
30	J	301	CLA	CMB-C2B-C3B	2.70	129.73	124.68
31	N	306	KC1	O1D-CGD-CBD	-2.70	118.96	124.48
28	I	302	DD6	C33-C34-C35	-2.70	106.61	110.30
31	D	310	KC1	CHB-C1B-C2B	-2.70	119.82	125.48
30	M	316	CLA	CMB-C2B-C3B	2.70	129.73	124.68
31	O	310	KC1	CHB-C1B-C2B	-2.70	119.82	125.48
30	P	215	CLA	CHB-C4A-NA	2.70	128.24	124.51
30	N	310	CLA	CMB-C2B-C3B	2.70	129.73	124.68
28	B	302	DD6	C8-C6-C5	-2.70	118.81	124.81
30	F	315	CLA	CAA-C2A-C3A	-2.70	109.81	116.10
30	f	302	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
37	a	736	BCR	C33-C5-C4	2.69	118.79	113.62
28	F	301	DD6	C25-C24-C1	-2.69	118.85	126.42
30	N	310	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	f	301	CLA	CMB-C2B-C3B	2.69	129.72	124.68
31	M	314	KC1	CHC-C4B-C3B	-2.69	120.65	125.26
30	I	321	CLA	CAC-C3C-C4C	2.69	128.30	124.81
37	a	736	BCR	C33-C5-C6	-2.69	121.50	124.53
30	a	731	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	b	723	CLA	CHB-C4A-NA	2.69	128.23	124.51
30	b	724	CLA	CMB-C2B-C3B	2.69	129.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	521	DGD	C6E-C5E-C4E	2.69	119.30	113.00
30	I	315	CLA	CMB-C2B-C3B	2.69	129.71	124.68
31	L	315	KC1	CHC-C4B-C3B	-2.69	120.66	125.26
31	F	314	KC1	CHB-C1B-C2B	-2.69	119.84	125.48
30	l	303	CLA	CMB-C2B-C3B	2.69	129.70	124.68
30	A	310	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
29	J	305	UIX	C29-C26-C30	-2.69	119.16	122.92
30	O	308	CLA	CMB-C2B-C3B	2.69	129.70	124.68
30	G	511	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
30	h	202	CLA	CMB-C2B-C3B	2.68	129.70	124.68
30	F	311	CLA	CMB-C2B-C3B	2.68	129.70	124.68
38	b	729	PQN	C2M-C2-C3	-2.68	120.02	124.40
29	I	304	UIX	C18-O2-C27	-2.68	112.90	117.90
30	a	725	CLA	CMB-C2B-C3B	2.68	129.69	124.68
30	B	310	CLA	C1-C2-C3	-2.68	121.41	126.04
31	A	306	KC1	CHC-C4B-C3B	-2.68	120.67	125.26
28	h	203	DD6	C37-C36-C35	2.68	119.32	114.36
37	b	730	BCR	C27-C26-C25	-2.68	118.84	122.73
33	K	317	LMG	O6-C1-O1	-2.68	103.63	109.97
28	F	303	DD6	C9-C8-C6	-2.68	118.89	126.42
30	a	716	CLA	CHB-C4A-NA	2.68	128.22	124.51
37	b	732	BCR	C16-C15-C14	-2.68	117.99	123.47
30	b	704	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
31	N	308	KC1	CHB-C4A-C3A	-2.68	120.80	124.98
30	j	104	CLA	CMB-C2B-C3B	2.68	129.68	124.68
30	a	721	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
33	B	318	LMG	O6-C1-O1	-2.68	103.64	109.97
37	l	306	BCR	C23-C24-C25	-2.67	119.69	127.20
30	J	316	CLA	CMB-C2B-C3B	2.67	129.68	124.68
31	O	315	KC1	CHB-C1B-C2B	-2.67	119.87	125.48
30	b	712	CLA	CAB-C3B-C2B	2.67	129.92	124.69
30	a	707	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
30	a	738	CLA	CMB-C2B-C3B	2.67	129.68	124.68
30	a	726	CLA	CHB-C4A-NA	2.67	128.21	124.51
30	F	308	CLA	CMB-C2B-C3B	2.67	129.68	124.68
28	M	305	DD6	C14-C13-C11	-2.67	121.38	125.53
30	M	310	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
30	a	710	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
37	j	102	BCR	C38-C26-C25	-2.67	121.53	124.53
30	K	312	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
30	l	313	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	b	709	CLA	O2A-CGA-O1A	-2.67	116.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	514	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	A	320	CLA	CMB-C2B-C3B	2.67	129.67	124.68
28	H	303	DD6	O1-C20-C21	-2.67	111.86	115.06
37	l	302	BCR	C8-C7-C6	-2.67	119.71	127.20
37	b	732	BCR	C7-C8-C9	-2.67	122.20	126.23
31	F	314	KC1	CHC-C4B-C3B	-2.67	120.70	125.26
30	L	308	CLA	CMB-C2B-C3B	2.67	129.67	124.68
31	H	310	KC1	CHC-C4B-C3B	-2.66	120.70	125.26
30	K	313	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
30	b	709	CLA	CMB-C2B-C3B	2.66	129.66	124.68
28	L	306	DD6	C15-C14-C13	-2.66	120.36	125.99
30	B	316	CLA	CMB-C2B-C3B	2.66	129.66	124.68
37	i	201	BCR	C1-C6-C5	-2.66	118.86	122.61
31	H	310	KC1	CHB-C1B-C2B	-2.66	119.90	125.48
30	N	307	CLA	CHD-C1D-ND	-2.66	122.01	124.45
31	B	314	KC1	O1D-CGD-CBD	-2.66	119.04	124.48
30	G	517	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	O	311	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	K	313	CLA	CHD-C1D-ND	-2.66	122.01	124.45
30	a	713	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
28	b	731	DD6	C26-C25-C24	-2.66	114.92	123.22
31	L	307	KC1	CHB-C1B-C2B	-2.66	119.91	125.48
30	a	719	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
28	M	302	DD6	C3-C4-C5	-2.66	118.03	123.47
31	H	306	KC1	CHB-C1B-C2B	-2.66	119.91	125.48
34	P	205	PID	CM5-C21-C20	-2.66	119.20	122.92
28	I	303	DD6	C20-C19-C18	-2.66	107.50	112.75
31	O	310	KC1	CHC-C4B-C3B	-2.65	120.72	125.26
37	i	201	BCR	C3-C4-C5	-2.65	109.34	114.08
37	l	302	BCR	C7-C8-C9	-2.65	122.22	126.23
28	D	303	DD6	C4-C5-C6	-2.65	123.52	127.31
30	L	311	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	I	303	DD6	C25-C24-C1	-2.65	118.96	126.42
37	l	302	BCR	C10-C11-C12	-2.65	114.94	123.22
30	L	317	CLA	CMB-C2B-C3B	2.65	129.64	124.68
31	O	312	KC1	CBD-CHA-C1A	2.65	133.82	128.88
28	B	302	DD6	C32-C33-C34	-2.65	107.66	113.64
28	M	304	DD6	C32-C33-C34	-2.65	107.66	113.64
30	a	731	CLA	CMB-C2B-C3B	2.65	129.64	124.68
31	F	309	KC1	CHB-C1B-C2B	-2.65	119.93	125.48
30	I	307	CLA	CMB-C2B-C3B	2.65	129.63	124.68
30	b	709	CLA	C1B-CHB-C4A	-2.65	124.88	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	303	DD6	C25-C24-C1	-2.65	118.98	126.42
31	K	314	KC1	CBD-CHA-C1A	2.65	133.81	128.88
30	a	701	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	b	707	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	B	312	CLA	CMB-C2B-C3B	2.64	129.62	124.68
30	M	313	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
30	a	716	CLA	CMB-C2B-C3B	2.64	129.62	124.68
30	a	703	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
30	G	510	CLA	CHB-C4A-NA	2.64	128.16	124.51
30	I	311	CLA	CMB-C2B-C3B	2.64	129.62	124.68
30	a	718	CLA	CHB-C4A-NA	2.64	128.16	124.51
34	P	205	PID	C16-C15-C14	-2.64	123.54	127.31
31	N	306	KC1	CHB-C1B-C2B	-2.64	119.94	125.48
30	a	727	CLA	CMB-C2B-C3B	2.64	129.62	124.68
28	L	302	DD6	C21-C20-C15	-2.64	117.84	122.26
30	G	519	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
30	b	712	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
37	j	102	BCR	C20-C19-C18	-2.64	119.01	126.42
30	a	721	CLA	CHB-C4A-NA	2.64	128.16	124.51
30	a	720	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
30	K	306	CLA	CMB-C2B-C3B	2.64	129.61	124.68
30	B	312	CLA	CHB-C4A-NA	2.64	128.16	124.51
31	K	314	KC1	CHB-C1B-C2B	-2.64	119.95	125.48
30	O	314	CLA	CHB-C4A-NA	2.63	128.16	124.51
28	J	304	DD6	C37-C36-C35	2.63	119.23	114.36
30	G	513	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	a	707	CLA	CMB-C2B-C3B	2.63	129.60	124.68
30	P	215	CLA	O2D-CGD-CBD	2.63	115.94	111.27
37	b	732	BCR	C20-C21-C22	-2.63	123.55	127.31
30	M	315	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	G	502	DD6	C33-C34-C35	-2.63	106.70	110.30
31	G	515	KC1	CHB-C1B-C2B	-2.63	119.96	125.48
30	b	703	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
30	G	514	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
30	J	312	CLA	O2D-CGD-CBD	2.63	115.94	111.27
30	m	202	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
30	b	713	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	O	312	KC1	O1D-CGD-CBD	-2.63	119.11	124.48
30	b	703	CLA	CMB-C2B-C1B	-2.63	124.43	128.46
30	D	308	CLA	CMB-C2B-C3B	2.63	129.59	124.68
31	O	312	KC1	O2D-CGD-O1D	-2.63	118.70	123.84
30	H	312	CLA	O2D-CGD-O1D	-2.63	118.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	316	CLA	CMB-C2B-C3B	2.63	129.59	124.68
29	K	302	UIX	C22-C15-C20	-2.62	108.12	110.47
30	A	312	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
30	N	305	CLA	CHB-C4A-NA	2.62	128.14	124.51
34	O	305	PID	C6-C7-C8	2.62	131.53	125.99
31	B	314	KC1	C3D-CAD-CBD	-2.62	104.15	107.61
30	A	317	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
30	G	519	CLA	CHB-C4A-NA	2.62	128.14	124.51
30	L	313	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
28	h	203	DD6	C21-C20-C15	-2.62	117.87	122.26
30	b	726	CLA	CMB-C2B-C3B	2.62	129.58	124.68
31	L	307	KC1	CBD-CHA-C1A	2.62	133.76	128.88
29	B	305	UIX	C37-C34-C30	-2.62	118.11	123.47
30	P	212	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
30	P	209	CLA	CMB-C2B-C3B	2.62	129.57	124.68
31	P	213	KC1	C4B-CHC-C1C	-2.62	120.42	126.06
29	h	201	UIX	C22-C15-C20	-2.61	108.13	110.47
30	b	701	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
31	H	306	KC1	C3D-CAD-CBD	-2.61	104.16	107.61
31	P	216	KC1	CHC-C4B-C3B	-2.61	120.79	125.26
30	a	705	CLA	CHB-C4A-NA	2.61	128.12	124.51
37	b	732	BCR	C23-C24-C25	-2.61	119.86	127.20
28	A	303	DD6	C21-C20-C15	-2.61	117.88	122.26
30	J	309	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	I	316	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	F	303	DD6	C41-C32-C31	-2.61	106.32	110.47
30	b	723	CLA	CMB-C2B-C3B	2.61	129.56	124.68
30	M	310	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	N	308	KC1	CHC-C4B-C3B	-2.61	120.79	125.26
31	L	307	KC1	C3D-CAD-CBD	-2.61	104.17	107.61
30	l	309	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
28	F	303	DD6	C37-C36-C31	-2.61	120.80	124.35
33	j	101	LMG	O6-C1-O1	-2.61	103.80	109.97
30	A	311	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	l	312	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
30	F	311	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	I	312	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
28	L	303	DD6	C14-C13-C11	-2.60	121.49	125.53
30	a	729	CLA	CMB-C2B-C3B	2.60	129.55	124.68
29	K	302	UIX	C3-C5-C4	-2.60	105.75	110.77
31	F	309	KC1	C3D-CAD-CBD	-2.60	104.18	107.61
28	L	305	DD6	C21-C20-C15	-2.60	117.90	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	304	DD6	O1-C20-C21	2.60	118.17	115.06
30	B	301	CLA	CMB-C2B-C3B	2.60	129.54	124.68
30	L	312	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	K	311	CLA	CMB-C2B-C3B	2.60	129.54	124.68
30	B	312	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
31	F	309	KC1	C4B-CHC-C1C	-2.60	120.45	126.06
30	I	306	CLA	CHB-C4A-NA	2.60	128.10	124.51
34	F	304	PID	CM5-C21-C20	-2.60	119.29	122.92
30	I	319	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	b	711	CLA	CMB-C2B-C3B	2.59	129.53	124.68
28	M	303	DD6	C9-C8-C6	-2.59	119.13	126.42
30	b	714	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	B	308	CLA	CHB-C4A-NA	2.59	128.10	124.51
38	b	729	PQN	C14-C13-C15	2.59	119.63	115.27
30	a	715	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	a	730	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	b	701	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	D	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	N	311	KC1	CHB-C1B-C2B	-2.59	120.05	125.48
30	M	312	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
30	I	316	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
30	K	312	CLA	CHB-C4A-NA	2.59	128.09	124.51
30	J	306	CLA	CHB-C4A-NA	2.59	128.09	124.51
30	A	316	CLA	CMB-C2B-C3B	2.59	129.52	124.68
37	b	732	BCR	C15-C16-C17	-2.58	118.18	123.47
30	b	708	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
31	J	313	KC1	C4B-CHC-C1C	-2.58	120.49	126.06
30	a	713	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
30	A	307	CLA	CMB-C2B-C3B	2.58	129.51	124.68
31	A	306	KC1	CHB-C1B-C2B	-2.58	120.07	125.48
31	G	515	KC1	CHC-C4B-C3B	-2.58	120.85	125.26
31	M	307	KC1	CHC-C4B-C3B	-2.58	120.85	125.26
30	b	716	CLA	CHB-C4A-NA	2.58	128.08	124.51
28	G	505	DD6	C21-C20-C15	-2.58	117.94	122.26
30	a	702	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
31	F	309	KC1	C2A-C3A-C4A	2.58	108.40	106.49
28	A	302	DD6	C3-C4-C5	-2.58	118.19	123.47
28	M	305	DD6	C3-C4-C5	-2.58	118.19	123.47
30	b	714	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
30	b	715	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
32	j	103	DGD	C2G-O2G-C1B	-2.57	111.45	117.79
30	L	308	CLA	C1-C2-C3	-2.57	122.59	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	303	DD6	C3-C4-C5	-2.57	118.21	123.47
30	b	706	CLA	CHD-C1D-ND	-2.57	122.09	124.45
28	I	305	DD6	C21-C20-C15	-2.57	117.95	122.26
31	J	313	KC1	CHC-C4B-C3B	-2.57	120.86	125.26
30	G	518	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	J	313	KC1	CHB-C1B-C2B	-2.57	120.09	125.48
28	M	306	DD6	C7-C6-C5	-2.57	119.33	122.92
30	A	310	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
30	h	202	CLA	CHB-C4A-NA	2.57	128.06	124.51
30	J	314	CLA	CAA-C2A-C3A	-2.57	110.11	116.10
30	H	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
31	F	309	KC1	CBD-CHA-C1A	2.57	133.67	128.88
31	I	314	KC1	CBD-CHA-C1A	2.57	133.67	128.88
30	H	305	CLA	C1-C2-C3	-2.57	121.61	126.04
31	D	310	KC1	C4B-CHC-C1C	-2.57	120.52	126.06
31	I	314	KC1	O1D-CGD-CBD	-2.56	119.24	124.48
34	P	208	PID	CM2-C5-C4	-2.56	104.53	108.98
30	D	313	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
30	G	510	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
30	M	315	CLA	CAA-C2A-C3A	-2.56	110.12	116.10
30	I	308	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
30	K	308	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
28	N	303	DD6	C14-C13-C11	-2.56	121.56	125.53
30	G	517	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	J	309	CLA	C1-C2-C3	-2.56	121.62	126.04
31	N	308	KC1	C3D-CAD-CBD	-2.56	104.24	107.61
28	M	306	DD6	C12-C11-C10	-2.56	119.34	122.92
30	L	312	CLA	CMB-C2B-C3B	2.56	129.46	124.68
28	J	302	DD6	C32-C33-C34	-2.56	107.87	113.64
31	P	211	KC1	CHB-C1B-C2B	-2.56	120.12	125.48
30	b	728	CLA	CMB-C2B-C3B	2.56	129.46	124.68
30	A	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
31	B	314	KC1	O2D-CGD-O1D	-2.55	118.84	123.84
30	K	306	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	a	706	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	J	301	CLA	CHB-C4A-NA	2.55	128.04	124.51
37	b	730	BCR	C38-C26-C27	2.55	118.52	113.62
30	I	310	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	I	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
37	a	734	BCR	C23-C24-C25	-2.55	120.03	127.20
30	b	720	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
30	A	310	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
28	F	301	DD6	O1-C20-C21	-2.55	112.00	115.06
28	F	303	DD6	C33-C34-C35	-2.55	106.82	110.30
30	B	309	CLA	CHB-C4A-NA	2.55	128.03	124.51
30	F	312	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
30	l	310	CLA	C1B-CHB-C4A	-2.54	125.28	128.57
32	L	301	DGD	C2G-O2G-C1B	-2.54	111.53	117.79
30	P	210	CLA	CHB-C4A-NA	2.54	128.03	124.51
29	G	503	UIX	C37-C39-C40	-2.54	123.68	127.31
30	F	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
32	G	521	DGD	O1G-C1A-C2A	2.54	119.88	111.91
31	L	315	KC1	O1D-CGD-CBD	-2.54	119.29	124.48
30	K	313	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	A	315	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	b	727	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	b	718	CLA	CMB-C2B-C3B	2.54	129.43	124.68
29	h	201	UIX	C18-O2-C27	-2.54	113.17	117.90
30	H	311	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	b	718	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	A	311	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
29	A	304	UIX	C22-C15-C20	-2.54	108.20	110.47
30	b	709	CLA	CHB-C4A-NA	2.53	128.02	124.51
28	M	304	DD6	C21-C20-C15	-2.53	118.01	122.26
30	G	516	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
30	f	301	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	l	309	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	L	316	CLA	CHB-C4A-NA	2.53	128.01	124.51
37	l	307	BCR	C2-C1-C6	2.53	114.38	110.48
30	l	313	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
30	b	717	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	H	306	KC1	O1D-CGD-CBD	-2.53	119.31	124.48
30	L	317	CLA	CHB-C4A-NA	2.53	128.01	124.51
30	b	712	CLA	CHB-C4A-NA	2.53	128.01	124.51
31	D	315	KC1	C2A-C3A-C4A	2.53	108.36	106.49
37	b	702	BCR	C27-C26-C25	-2.53	119.06	122.73
30	H	309	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	D	303	DD6	C4-C3-C2	-2.52	118.30	123.47
31	O	312	KC1	C1A-C2A-C3A	-2.52	105.11	107.11
28	K	305	DD6	C9-C10-C11	-2.52	123.71	127.31
30	N	304	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	A	316	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	a	711	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	308	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	O	311	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	M	305	DD6	C33-C34-C35	-2.52	106.85	110.30
30	A	317	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	M	308	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	B	306	DD6	C21-C20-C15	-2.52	118.04	122.26
28	L	304	DD6	C10-C9-C8	-2.52	115.35	123.22
30	B	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	M	303	DD6	C37-C36-C35	2.52	119.02	114.36
31	M	307	KC1	CHB-C1B-C2B	-2.52	120.20	125.48
29	P	207	UIX	C29-C26-C30	-2.52	119.40	122.92
30	P	212	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	A	302	DD6	C12-C11-C10	-2.52	119.40	122.92
30	G	509	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	a	731	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	a	738	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	b	704	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	F	303	DD6	C4-C3-C2	-2.52	118.32	123.47
30	J	315	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	K	316	CLA	CMB-C2B-C3B	2.52	129.38	124.68
31	O	310	KC1	O2D-CGD-O1D	-2.51	118.92	123.84
28	B	303	DD6	C9-C10-C11	-2.51	123.72	127.31
31	K	314	KC1	C3D-CAD-CBD	-2.51	104.30	107.61
29	B	305	UIX	C35-C36-C38	-2.51	115.38	123.22
30	K	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	b	705	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	a	720	CLA	CHB-C4A-NA	2.51	127.98	124.51
37	l	307	BCR	C28-C27-C26	-2.51	109.60	114.08
28	B	303	DD6	C20-C19-C18	-2.51	107.79	112.75
31	L	307	KC1	O2A-CGA-O1A	-2.51	117.46	122.67
30	I	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	J	316	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	M	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	I	316	CLA	CHD-C1D-ND	-2.51	122.15	124.45
30	M	313	CLA	CHD-C1D-ND	-2.51	122.15	124.45
30	A	309	CLA	CHB-C4A-NA	2.51	127.98	124.51
33	b	733	LMG	C1-C2-C3	-2.51	104.78	110.00
30	G	511	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	F	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	D	316	CLA	CAA-C2A-C3A	-2.50	110.26	116.10
28	K	305	DD6	C25-C26-C27	-2.50	119.31	126.58
30	b	719	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	708	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	K	311	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
31	I	314	KC1	C3D-CAD-CBD	-2.50	104.31	107.61
31	O	312	KC1	C4B-CHC-C1C	-2.50	120.67	126.06
30	b	704	CLA	CAC-C3C-C4C	2.50	128.05	124.81
32	I	317	DGD	C2G-O2G-C1B	-2.50	111.64	117.79
31	H	310	KC1	C4B-CHC-C1C	-2.50	120.67	126.06
30	b	728	CLA	CHB-C4A-NA	2.50	127.97	124.51
37	i	201	BCR	C33-C5-C4	2.50	118.41	113.62
30	O	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	A	307	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	A	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	a	714	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	D	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
37	m	201	BCR	C21-C20-C19	-2.49	115.44	123.22
30	K	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	a	726	CLA	CHD-C1D-ND	-2.49	122.16	124.45
28	K	303	DD6	C21-C20-C15	-2.49	118.08	122.26
30	O	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	G	516	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	J	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
37	l	302	BCR	C33-C5-C4	2.49	118.40	113.62
30	a	725	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
31	A	314	KC1	O1D-CGD-CBD	-2.49	119.39	124.48
31	M	307	KC1	C4B-CHC-C1C	-2.49	120.69	126.06
28	N	303	DD6	C37-C36-C35	2.49	118.97	114.36
29	O	306	UIX	C10-C11-C13	2.49	122.76	118.94
30	J	301	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
30	H	312	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	P	213	KC1	CBD-CHA-C1A	2.49	133.52	128.88
32	y	201	DGD	C2G-O2G-C1B	-2.49	111.67	117.79
30	a	723	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
30	D	312	CLA	CHB-C4A-NA	2.48	127.95	124.51
30	K	309	CLA	C1-C2-C3	-2.48	122.73	126.75
28	M	305	DD6	C25-C26-C27	-2.48	119.37	126.58
30	G	517	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
30	L	309	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
29	O	306	UIX	C36-C38-C40	-2.48	119.44	126.42
31	L	315	KC1	O2D-CGD-O1D	-2.48	118.98	123.84
28	M	306	DD6	C19-C18-C17	-2.48	105.98	110.77
30	M	316	CLA	CHB-C4A-NA	2.48	127.94	124.51
37	i	201	BCR	C4-C5-C6	-2.48	119.13	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	306	DD6	C21-C20-C15	-2.48	118.10	122.26
28	M	303	DD6	C13-C11-C10	2.48	122.75	118.94
28	J	304	DD6	C25-C26-C27	-2.48	119.38	126.58
30	b	708	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	A	305	DD6	C25-C26-C27	-2.48	119.38	126.58
30	j	104	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	a	709	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	B	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	B	304	DD6	C10-C9-C8	-2.48	115.49	123.22
30	a	704	CLA	CHD-C1D-ND	-2.48	122.18	124.45
30	f	303	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	J	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	N	303	DD6	C4-C3-C2	-2.47	118.41	123.47
30	I	321	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
30	b	715	CLA	CHB-C4A-NA	2.47	127.93	124.51
31	O	312	KC1	CHB-C1B-C2B	-2.47	120.29	125.48
30	L	313	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
31	O	315	KC1	O2D-CGD-O1D	-2.47	119.00	123.84
28	M	302	DD6	C9-C10-C11	-2.47	123.78	127.31
30	L	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	M	311	CLA	CHB-C4A-NA	2.47	127.93	124.51
34	O	302	PID	C17-C16-C15	2.47	128.54	123.47
29	P	207	UIX	C18-O2-C27	-2.47	113.29	117.90
37	i	201	BCR	C28-C27-C26	-2.47	109.66	114.08
30	a	727	CLA	CHB-C4A-NA	2.47	127.93	124.51
31	F	314	KC1	C4B-CHC-C1C	-2.47	120.73	126.06
31	O	310	KC1	O1D-CGD-CBD	-2.47	119.43	124.48
30	H	305	CLA	CHB-C4A-NA	2.47	127.92	124.51
30	D	316	CLA	CHB-C4A-NA	2.47	127.92	124.51
28	G	505	DD6	C32-C33-C34	-2.47	108.07	113.64
33	I	318	LMG	O7-C10-O9	-2.47	117.74	123.70
30	K	307	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
30	H	308	CLA	CHB-C4A-NA	2.47	127.92	124.51
29	B	305	UIX	O2-C27-O4	-2.46	118.07	122.96
28	K	318	DD6	C12-C11-C10	-2.46	119.47	122.92
30	J	314	CLA	CHB-C4A-NA	2.46	127.92	124.51
31	K	314	KC1	C4B-CHC-C1C	-2.46	120.74	126.06
29	I	304	UIX	O2-C27-O4	-2.46	118.07	122.96
28	L	305	DD6	C37-C36-C35	2.46	118.92	114.36
30	a	721	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
30	N	305	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
31	A	306	KC1	C4B-CHC-C1C	-2.46	120.75	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	305	PID	C18-C17-C16	2.46	130.29	124.81
30	a	711	CLA	CHD-C1D-ND	-2.46	122.19	124.45
30	a	712	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
29	O	306	UIX	C18-O2-C27	-2.46	113.31	117.90
28	G	504	DD6	O1-C20-C15	-2.46	56.92	58.96
30	L	309	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	G	510	CLA	CHD-C1D-ND	-2.46	122.19	124.45
30	a	728	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	I	308	CLA	CHD-C1D-ND	-2.46	122.20	124.45
30	F	311	CLA	O2D-CGD-CBD	2.46	115.63	111.27
28	F	301	DD6	C34-C35-C36	-2.46	106.96	111.85
28	B	303	DD6	C33-C34-C35	-2.46	106.94	110.30
28	I	302	DD6	C3-C4-C5	-2.46	118.44	123.47
37	i	201	BCR	C38-C26-C27	2.46	118.33	113.62
30	a	711	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
30	O	309	CLA	C1-C2-C3	-2.46	121.80	126.04
31	G	515	KC1	O1D-CGD-CBD	-2.45	119.46	124.48
37	a	734	BCR	C15-C16-C17	-2.45	118.45	123.47
29	J	305	UIX	C35-C36-C38	-2.45	115.56	123.22
28	J	302	DD6	C33-C34-C35	-2.45	106.94	110.30
30	b	724	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	a	712	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	G	515	KC1	C2A-C3A-C4A	2.45	108.31	106.49
30	G	513	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
37	a	736	BCR	C24-C23-C22	-2.45	122.53	126.23
31	G	515	KC1	C4B-CHC-C1C	-2.45	120.77	126.06
30	l	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
37	f	304	BCR	C11-C12-C13	-2.45	119.53	126.42
34	M	301	PID	C19-C20-C21	2.45	130.81	127.31
28	A	301	DD6	C33-C34-C35	-2.45	106.95	110.30
30	a	707	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	G	513	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	G	502	DD6	C37-C36-C35	2.45	118.89	114.36
30	I	307	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	K	310	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	H	306	KC1	C2A-C3A-C4A	2.45	108.30	106.49
31	O	310	KC1	C2A-C3A-C4A	2.45	108.30	106.49
28	O	303	DD6	C14-C13-C11	-2.45	121.73	125.53
28	L	306	DD6	C25-C26-C27	-2.45	119.48	126.58
28	K	301	DD6	C26-C25-C24	-2.45	115.58	123.22
31	I	314	KC1	C4B-CHC-C1C	-2.45	120.78	126.06
31	P	213	KC1	CHB-C1B-C2B	-2.45	120.35	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	304	DD6	C9-C10-C11	-2.45	123.82	127.31
30	b	703	CLA	C1-C2-C3	-2.45	121.81	126.04
34	P	203	PID	CM4-C14-C13	2.44	124.69	119.05
37	l	302	BCR	C27-C26-C25	-2.44	119.18	122.73
30	b	711	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	a	703	CLA	C1-C2-C3	-2.44	121.82	126.04
30	f	302	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
30	L	312	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
30	K	311	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	I	321	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
30	L	310	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	J	316	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
31	P	211	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
31	L	307	KC1	O2D-CGD-O1D	-2.44	119.07	123.84
30	A	319	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
30	B	311	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
30	L	313	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
30	a	706	CLA	CHD-C1D-ND	-2.44	122.22	124.45
30	b	705	CLA	C1-C2-C3	-2.44	121.83	126.04
30	L	317	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
31	N	311	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
29	P	207	UIX	C41-C40-C39	-2.44	119.51	122.92
30	b	726	CLA	CHB-C4A-NA	2.43	127.88	124.51
31	D	315	KC1	O1D-CGD-CBD	-2.43	119.50	124.48
30	D	314	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
28	h	203	DD6	C3-C4-C5	-2.43	118.49	123.47
30	F	308	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	K	316	CLA	CHB-C4A-NA	2.43	127.87	124.51
28	J	304	DD6	O1-C20-C19	-2.43	111.56	113.38
29	A	304	UIX	C34-C37-C39	-2.43	118.50	123.47
30	K	307	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	l	308	CLA	CAA-C2A-C3A	-2.43	110.43	116.10
30	A	320	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	I	315	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
28	G	502	DD6	O1-C20-C21	-2.43	112.15	115.06
28	I	301	DD6	C32-C31-C36	-2.43	119.21	122.63
28	G	508	DD6	C37-C36-C35	2.43	118.85	114.36
29	A	304	UIX	O2-C27-O4	-2.43	118.14	122.96
31	P	213	KC1	CAC-C3C-C4C	2.43	127.96	124.81
30	I	308	CLA	CHB-C4A-NA	2.43	127.87	124.51
31	O	312	KC1	C3D-CAD-CBD	-2.43	104.41	107.61
30	j	106	CLA	C1B-CHB-C4A	-2.43	125.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	314	KC1	C4B-CHC-C1C	-2.43	120.83	126.06
30	a	725	CLA	CHB-C4A-NA	2.43	127.87	124.51
28	N	303	DD6	C21-C20-C15	-2.42	118.20	122.26
28	A	302	DD6	C33-C34-C35	-2.42	106.99	110.30
28	N	303	DD6	C33-C34-C35	-2.42	106.99	110.30
30	a	707	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
30	l	308	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	N	309	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	L	318	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
30	a	710	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	K	308	CLA	CHD-C1D-ND	-2.42	122.23	124.45
30	a	703	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	f	301	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
30	O	316	CLA	CHB-C4A-NA	2.42	127.85	124.51
29	P	207	UIX	C22-C15-C20	-2.41	108.31	110.47
29	P	207	UIX	C16-C20-C15	2.41	122.09	119.70
31	H	306	KC1	CBD-CHA-C1A	2.41	133.38	128.88
32	G	521	DGD	C1D-O6D-C5D	-2.41	108.95	113.69
31	N	308	KC1	CGD-CBD-CAD	-2.41	102.92	110.73
31	F	314	KC1	O2D-CGD-O1D	-2.41	119.12	123.84
31	O	315	KC1	C4B-CHC-C1C	-2.41	120.85	126.06
37	b	730	BCR	C2-C1-C6	2.41	114.20	110.48
30	K	315	CLA	CHB-C4A-NA	2.41	127.85	124.51
31	L	307	KC1	C4B-CHC-C1C	-2.41	120.85	126.06
30	A	311	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	a	722	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	b	706	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
30	b	713	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	m	202	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	H	304	CLA	CHB-C4A-NA	2.41	127.84	124.51
31	L	315	KC1	C4B-CHC-C1C	-2.41	120.86	126.06
34	M	301	PID	CM5-C21-C20	-2.41	119.55	122.92
31	N	306	KC1	C4B-CHC-C1C	-2.41	120.87	126.06
30	G	512	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	a	705	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
30	M	312	CLA	CHB-C4A-NA	2.40	127.84	124.51
31	A	314	KC1	CBD-CHA-C1A	2.40	133.36	128.88
30	b	707	CLA	C1-C2-C3	-2.40	121.89	126.04
28	J	302	DD6	C12-C11-C10	-2.40	119.56	122.92
31	P	213	KC1	O1D-CGD-CBD	-2.40	119.57	124.48
31	M	307	KC1	O2A-CGA-O1A	-2.40	117.68	122.67
28	B	306	DD6	C37-C36-C35	2.40	118.80	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	I	315	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	J	312	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	K	304	DD6	C32-C33-C34	-2.40	108.22	113.64
30	K	310	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
30	b	709	CLA	O2D-CGD-CBD	2.40	115.53	111.27
30	a	724	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
37	b	732	BCR	C38-C26-C25	-2.40	121.83	124.53
28	L	306	DD6	C21-C20-C15	-2.40	118.24	122.26
31	I	314	KC1	O2D-CGD-O1D	-2.40	119.15	123.84
30	G	514	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
34	P	206	PID	C6-C7-C8	2.40	131.06	125.99
30	O	313	CLA	CHB-C4A-NA	2.39	127.82	124.51
32	j	103	DGD	O1G-C1A-C2A	2.39	119.42	111.91
28	B	302	DD6	C-C1-C2	-2.39	119.57	122.92
33	I	320	LMG	O1-C7-C8	-2.39	105.12	110.90
28	G	504	DD6	C25-C24-C1	-2.39	119.69	126.42
30	l	305	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	a	729	CLA	CHD-C1D-ND	-2.39	122.26	124.45
28	F	301	DD6	C7-C6-C5	-2.39	119.58	122.92
31	F	309	KC1	O1D-CGD-CBD	-2.39	119.60	124.48
30	A	308	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	O	314	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	I	311	CLA	CHB-C4A-NA	2.39	127.81	124.51
30	B	309	CLA	CHD-C1D-ND	-2.39	122.26	124.45
30	M	318	CLA	CHB-C4A-NA	2.39	127.81	124.51
30	O	309	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
30	J	311	CLA	CHD-C1D-ND	-2.39	122.26	124.45
34	N	302	PID	CM4-C14-C13	2.38	124.55	119.05
28	K	301	DD6	C4-C3-C2	-2.38	118.59	123.47
28	M	303	DD6	C7-C6-C5	-2.38	119.58	122.92
30	G	520	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	I	313	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
30	M	308	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
30	a	717	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	b	706	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	a	721	CLA	C1-C2-C3	-2.38	121.92	126.04
30	a	719	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
30	b	705	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
30	l	310	CLA	C4D-ND-C1D	-2.38	106.20	109.68
37	l	306	BCR	C35-C13-C12	2.38	121.83	118.08
30	D	314	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
28	L	305	DD6	O1-C20-C19	-2.38	111.59	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	723	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	b	720	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	A	312	CLA	CHB-C4A-NA	2.38	127.80	124.51
30	O	311	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
31	N	306	KC1	O2D-CGD-O1D	-2.38	119.19	123.84
31	G	515	KC1	CAC-C3C-C4C	2.38	127.89	124.81
28	P	204	DD6	C21-C20-C15	-2.38	118.28	122.26
30	f	302	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	h	201	UIX	C12-C11-C10	2.37	121.82	118.08
28	B	303	DD6	C3-C4-C5	-2.37	118.61	123.47
30	A	310	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
28	K	304	DD6	O1-C20-C21	-2.37	112.21	115.06
30	A	313	CLA	C1-C2-C3	-2.37	121.94	126.04
30	b	725	CLA	CHB-C4A-NA	2.37	127.79	124.51
30	P	217	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	P	216	KC1	C4B-CHC-C1C	-2.37	120.94	126.06
30	A	313	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
28	J	303	DD6	C20-C19-C18	-2.37	108.06	112.75
29	O	306	UIX	C33-C32-C35	-2.37	119.60	122.92
30	J	312	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	D	313	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	M	305	DD6	C37-C36-C35	2.37	118.75	114.36
30	L	312	CLA	CHD-C1D-ND	-2.37	122.28	124.45
30	a	717	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
29	h	201	UIX	O2-C27-O4	-2.37	118.26	122.96
28	B	306	DD6	C10-C9-C8	-2.37	115.83	123.22
30	b	707	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
30	K	312	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
30	H	309	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
30	M	309	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	B	309	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	H	307	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
28	A	305	DD6	C21-C20-C15	-2.36	118.30	122.26
30	b	703	CLA	CMB-C2B-C3B	2.36	129.10	124.68
30	J	307	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	A	304	UIX	C13-C14-C23	-2.36	115.84	123.22
28	I	303	DD6	C19-C18-C17	-2.36	106.21	110.77
30	N	310	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	I	313	CLA	CHD-C1D-ND	-2.36	122.28	124.45
31	O	310	KC1	C4B-CHC-C1C	-2.36	120.97	126.06
30	b	726	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
30	B	316	CLA	CHB-C4A-NA	2.36	127.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	l	312	CLA	CHD-C1D-ND	-2.36	122.29	124.45
30	G	509	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
30	l	308	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
30	I	310	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
29	P	207	UIX	C10-C11-C13	2.36	122.56	118.94
31	H	306	KC1	C4B-CHC-C1C	-2.36	120.97	126.06
30	a	715	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
28	B	306	DD6	C25-C24-C1	-2.36	119.80	126.42
30	a	701	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
30	b	709	CLA	C1-C2-C3	-2.35	121.97	126.04
30	b	719	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
37	f	304	BCR	C29-C30-C25	2.35	114.10	110.48
28	L	306	DD6	C33-C34-C35	-2.35	107.08	110.30
30	M	318	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	L	306	DD6	O1-C20-C21	-2.35	112.24	115.06
28	A	301	DD6	C37-C36-C35	2.35	118.71	114.36
30	j	106	CLA	CHB-C4A-NA	2.35	127.76	124.51
33	b	733	LMG	C38-C37-C36	-2.35	102.50	114.42
30	l	305	CLA	CHD-C1D-ND	-2.35	122.30	124.45
28	I	301	DD6	C14-C13-C11	-2.35	121.89	125.53
28	B	302	DD6	C8-C9-C10	-2.35	118.66	123.47
37	a	734	BCR	C29-C30-C25	2.35	114.10	110.48
30	I	309	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	h	203	DD6	C14-C13-C11	-2.35	121.89	125.53
30	b	710	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
30	P	212	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
37	b	702	BCR	C33-C5-C4	2.35	118.12	113.62
30	F	310	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
29	I	304	UIX	C41-C40-C38	2.35	121.77	118.08
30	a	705	CLA	CHD-C1D-ND	-2.34	122.30	124.45
30	J	308	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
37	m	201	BCR	C36-C18-C19	2.34	121.77	118.08
28	K	301	DD6	C37-C36-C35	2.34	118.70	114.36
30	a	710	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
31	B	314	KC1	C4B-CHC-C1C	-2.34	121.00	126.06
28	M	304	DD6	C10-C9-C8	-2.34	115.90	123.22
30	l	304	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	l	305	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	a	709	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	a	716	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
31	F	314	KC1	O1D-CGD-CBD	-2.34	119.69	124.48
28	A	305	DD6	C33-C34-C35	-2.34	107.10	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	312	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	J	309	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
31	N	311	KC1	O1D-CGD-CBD	-2.34	119.69	124.48
30	M	311	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	P	215	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
37	l	307	BCR	C21-C20-C19	-2.34	115.91	123.22
29	O	306	UIX	C41-C40-C39	-2.34	119.64	122.92
37	b	730	BCR	C36-C18-C19	2.34	121.76	118.08
30	B	301	CLA	CHD-C1D-ND	-2.34	122.30	124.45
30	A	317	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
31	M	307	KC1	C2A-C3A-C4A	2.34	108.22	106.49
33	D	317	LMG	O1-C7-C8	-2.34	105.26	110.90
30	B	310	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
31	L	315	KC1	C2A-C3A-C4A	2.34	108.22	106.49
37	j	102	BCR	C33-C5-C4	2.34	118.11	113.62
28	J	303	DD6	C37-C36-C35	2.34	118.68	114.36
30	M	316	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
28	F	303	DD6	C21-C20-C15	-2.34	118.35	122.26
31	D	315	KC1	CBD-CHA-C1A	2.33	133.24	128.88
30	b	704	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	b	719	CLA	CHD-C1D-ND	-2.33	122.31	124.45
30	L	313	CLA	CHB-C4A-NA	2.33	127.74	124.51
30	L	308	CLA	CHB-C4A-NA	2.33	127.74	124.51
37	a	736	BCR	C23-C24-C25	-2.33	120.65	127.20
29	A	304	UIX	C-C7-C10	-2.33	121.06	125.99
30	K	316	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	b	727	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	a	706	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	J	311	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
31	M	314	KC1	C4B-CHC-C1C	-2.33	121.03	126.06
30	a	724	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	K	316	CLA	CHD-C1D-ND	-2.33	122.31	124.45
30	l	312	CLA	CHB-C4A-NA	2.33	127.73	124.51
30	b	712	CLA	CHD-C1D-ND	-2.33	122.31	124.45
30	b	728	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
30	F	313	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
28	M	302	DD6	C37-C36-C35	2.33	118.66	114.36
30	D	311	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
30	M	317	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
30	b	703	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
29	P	207	UIX	O2-C27-O4	-2.32	118.35	122.96
28	M	304	DD6	O1-C20-C21	-2.32	112.27	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	j	102	BCR	C10-C11-C12	-2.32	115.97	123.22
30	H	305	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	M	303	DD6	C21-C20-C19	2.32	116.89	114.28
30	H	311	CLA	CAA-C2A-C3A	-2.32	110.68	116.10
38	a	732	PQN	C2M-C2-C3	-2.32	120.61	124.40
30	b	716	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
30	a	735	CLA	CHD-C1D-ND	-2.32	122.32	124.45
37	b	702	BCR	C35-C13-C12	2.32	121.73	118.08
30	D	308	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	N	303	DD6	C25-C26-C27	-2.32	119.85	126.58
30	b	725	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
30	J	311	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
30	D	309	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	I	312	CLA	CHB-C4A-NA	2.32	127.72	124.51
30	l	311	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	L	314	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
30	M	315	CLA	O2D-CGD-CBD	2.32	115.39	111.27
28	A	302	DD6	C25-C26-C27	-2.32	119.86	126.58
34	O	302	PID	CM4-C14-C13	2.32	124.39	119.05
30	j	104	CLA	C1-C2-C3	-2.32	122.04	126.04
30	l	303	CLA	CHD-C1D-ND	-2.32	122.33	124.45
37	f	304	BCR	C38-C26-C27	2.32	118.06	113.62
30	L	309	CLA	O2D-CGD-CBD	2.32	115.38	111.27
30	I	308	CLA	C1-C2-C3	-2.32	122.04	126.04
28	K	301	DD6	C10-C9-C8	-2.31	115.99	123.22
33	B	318	LMG	C38-C37-C36	-2.31	102.68	114.42
30	a	731	CLA	C1-C2-C3	-2.31	122.04	126.04
28	I	302	DD6	C4-C5-C6	-2.31	124.01	127.31
30	K	315	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
29	I	304	UIX	C34-C30-C26	-2.31	124.01	127.31
30	A	319	CLA	CHB-C4A-NA	2.31	127.71	124.51
30	I	316	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
30	I	306	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
28	B	302	DD6	C12-C11-C10	-2.31	119.69	122.92
28	A	301	DD6	O1-C20-C21	-2.31	112.29	115.06
30	J	306	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	a	708	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	B	316	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	b	723	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
30	a	709	CLA	CHD-C1D-ND	-2.31	122.33	124.45
30	A	320	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
30	b	713	CLA	C1B-CHB-C4A	-2.31	125.55	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	302	DD6	C10-C9-C8	-2.31	116.02	123.22
31	D	310	KC1	O1D-CGD-CBD	-2.31	119.77	124.48
30	a	728	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
28	A	301	DD6	C3-C4-C5	-2.31	118.75	123.47
30	a	702	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
30	J	314	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
30	H	311	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	I	316	CLA	C1-C2-C3	-2.30	122.06	126.04
28	B	304	DD6	C37-C36-C35	2.30	118.62	114.36
30	K	306	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
30	H	304	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
30	I	313	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
30	M	309	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	b	717	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	O	306	UIX	O2-C27-O4	-2.30	118.39	122.96
30	L	313	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	G	511	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
33	b	733	LMG	O1-C7-C8	-2.30	105.36	110.90
34	D	305	PID	CM4-C14-C13	2.30	124.35	119.05
30	a	730	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
33	B	318	LMG	O7-C10-O9	-2.30	118.15	123.70
30	G	510	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
30	N	305	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
30	a	710	CLA	C1-C2-C3	-2.30	122.07	126.04
30	a	729	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	P	209	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	b	707	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
30	G	519	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
34	D	302	PID	C17-C16-C15	2.29	128.17	123.47
28	b	731	DD6	C10-C9-C8	-2.29	116.06	123.22
30	A	309	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	M	309	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	O	308	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	K	313	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
28	A	302	DD6	C9-C8-C6	-2.29	119.98	126.42
30	L	310	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
29	A	304	UIX	C19-C18-C17	-2.29	105.88	109.88
28	B	303	DD6	C21-C20-C15	-2.29	118.42	122.26
31	H	306	KC1	O2D-CGD-O1D	-2.29	119.36	123.84
30	G	516	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	O	316	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	a	717	CLA	O2A-CGA-O1A	-2.29	117.81	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	503	UIX	C13-C14-C23	-2.29	116.07	123.22
29	A	304	UIX	C7-C10-C11	-2.29	121.98	125.53
30	a	724	CLA	C2D-C1D-ND	-2.29	108.42	110.10
30	b	706	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
31	K	314	KC1	C2A-C3A-C4A	2.29	108.18	106.49
30	F	310	CLA	O2D-CGD-CBD	2.29	115.33	111.27
28	K	318	DD6	C37-C36-C35	2.29	118.59	114.36
31	O	312	KC1	C2A-C3A-C4A	2.28	108.18	106.49
37	a	734	BCR	C38-C26-C27	2.28	118.00	113.62
34	D	302	PID	CM4-C14-C13	2.28	124.32	119.05
30	a	718	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
30	a	719	CLA	CHB-C4A-NA	2.28	127.67	124.51
28	G	505	DD6	C25-C26-C27	-2.28	119.95	126.58
28	B	302	DD6	C4-C3-C2	-2.28	118.80	123.47
30	b	722	CLA	C2D-C1D-ND	-2.28	108.42	110.10
30	f	303	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
30	b	718	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	F	301	DD6	C12-C11-C10	-2.28	119.73	122.92
30	L	308	CLA	CAC-C3C-C4C	2.28	127.77	124.81
30	b	715	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	G	505	DD6	C19-C18-C17	-2.28	106.37	110.77
30	b	728	CLA	CHD-C1D-ND	-2.28	122.36	124.45
28	L	306	DD6	C9-C8-C6	-2.28	120.01	126.42
30	F	312	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
30	b	711	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
30	F	312	CLA	CHB-C4A-NA	2.28	127.66	124.51
30	b	711	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	K	309	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	P	204	DD6	C9-C8-C6	-2.28	120.02	126.42
30	L	311	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
30	I	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	I	311	CLA	O2D-CGD-CBD	2.28	115.31	111.27
30	b	701	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
30	G	513	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	B	310	CLA	CHB-C4A-NA	2.28	127.66	124.51
30	F	307	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
28	A	305	DD6	C20-C19-C18	-2.27	108.25	112.75
37	b	732	BCR	C34-C9-C8	2.27	121.66	118.08
30	a	720	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
28	J	302	DD6	C25-C26-C27	-2.27	119.98	126.58
30	f	303	CLA	CHD-C1D-ND	-2.27	122.37	124.45
30	a	727	CLA	C1B-CHB-C4A	-2.27	125.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	520	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
30	b	721	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
30	L	309	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
30	L	317	CLA	CHD-C1D-ND	-2.27	122.37	124.45
37	l	306	BCR	C10-C11-C12	-2.27	116.14	123.22
28	N	303	DD6	C9-C8-C6	-2.27	120.05	126.42
30	B	313	CLA	CHD-C1D-ND	-2.27	122.37	124.45
30	J	309	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
30	B	311	CLA	CHB-C4A-NA	2.26	127.64	124.51
28	I	305	DD6	C28-C27-C29	2.26	121.32	116.84
30	H	307	CLA	CHD-C1D-ND	-2.26	122.37	124.45
30	I	315	CLA	O2D-CGD-CBD	2.26	115.29	111.27
28	O	303	DD6	C9-C8-C6	-2.26	120.06	126.42
28	B	304	DD6	C3-C4-C5	-2.26	118.84	123.47
34	P	206	PID	C15-C14-C13	2.26	123.19	117.00
30	a	730	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
37	l	302	BCR	C23-C22-C21	2.26	122.41	118.94
28	B	303	DD6	C37-C36-C35	2.26	118.54	114.36
30	b	710	CLA	CHB-C4A-NA	2.26	127.64	124.51
30	F	311	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
30	L	316	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
28	A	303	DD6	C20-C19-C18	-2.26	108.28	112.75
30	b	727	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
29	h	201	UIX	C35-C36-C38	-2.26	116.17	123.22
30	K	310	CLA	CHD-C1D-ND	-2.26	122.38	124.45
30	a	714	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
30	B	313	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
33	K	317	LMG	O1-C1-C2	-2.26	104.78	108.30
37	l	307	BCR	C8-C7-C6	-2.26	120.86	127.20
28	I	305	DD6	C9-C10-C11	-2.26	124.09	127.31
28	A	302	DD6	O1-C20-C21	-2.26	112.35	115.06
30	b	723	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
30	D	316	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
28	F	301	DD6	C4-C3-C2	-2.26	118.85	123.47
30	J	315	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
30	M	308	CLA	CHD-C1D-ND	-2.25	122.38	124.45
30	h	202	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
30	l	309	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
28	A	303	DD6	C4-C3-C2	-2.25	118.86	123.47
30	L	309	CLA	CHD-C1D-ND	-2.25	122.38	124.45
30	B	317	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
28	K	305	DD6	C37-C36-C35	2.25	118.53	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	714	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
37	a	734	BCR	C21-C20-C19	-2.25	116.19	123.22
30	l	313	CLA	CHD-C1D-ND	-2.25	122.39	124.45
30	F	310	CLA	CHD-C1D-ND	-2.25	122.39	124.45
34	N	302	PID	C6-C7-C8	-2.25	121.23	125.99
28	K	318	DD6	C9-C8-C6	-2.25	120.10	126.42
30	N	304	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
33	j	101	LMG	O3-C3-C2	-2.25	105.15	110.35
30	a	717	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	I	303	DD6	C37-C36-C35	2.25	118.52	114.36
31	D	315	KC1	CHC-C4B-C3B	-2.25	121.41	125.26
30	j	104	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
30	P	209	CLA	CHD-C1D-ND	-2.25	122.39	124.45
30	a	705	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
28	G	504	DD6	C25-C26-C27	-2.25	120.05	126.58
30	B	310	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
31	P	216	KC1	O1D-CGD-CBD	-2.25	119.89	124.48
37	l	302	BCR	C11-C10-C9	-2.25	124.10	127.31
29	h	201	UIX	C21-C15-C20	-2.25	108.46	110.47
30	K	306	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	B	302	DD6	C37-C36-C35	2.25	118.52	114.36
30	J	309	CLA	CHD-C1D-ND	-2.24	122.39	124.45
33	I	320	LMG	O7-C10-O9	-2.24	118.28	123.70
30	P	210	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
31	D	310	KC1	C3D-CAD-CBD	-2.24	104.65	107.61
30	I	312	CLA	CHD-C1D-ND	-2.24	122.39	124.45
28	B	303	DD6	C10-C9-C8	-2.24	116.22	123.22
37	b	730	BCR	C24-C23-C22	-2.24	122.84	126.23
28	K	318	DD6	C3-C4-C5	-2.24	118.88	123.47
28	h	203	DD6	C10-C9-C8	-2.24	116.22	123.22
30	a	713	CLA	CHB-C4A-NA	2.24	127.61	124.51
30	A	315	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
28	A	301	DD6	C12-C11-C10	-2.24	119.78	122.92
31	M	314	KC1	O1D-CGD-CBD	-2.24	119.90	124.48
30	b	716	CLA	C1-C2-C3	-2.24	123.13	126.75
30	a	718	CLA	CHD-C1D-ND	-2.24	122.39	124.45
28	B	306	DD6	O1-C20-C21	-2.24	112.37	115.06
30	H	308	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
30	B	310	CLA	CHD-C1D-ND	-2.24	122.40	124.45
37	a	736	BCR	C21-C20-C19	-2.24	116.23	123.22
37	b	730	BCR	C30-C25-C26	-2.24	119.46	122.61
37	b	732	BCR	C37-C22-C23	2.24	121.60	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	M	310	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
30	B	310	CLA	O2D-CGD-CBD	2.24	115.24	111.27
28	J	303	DD6	C9-C8-C6	-2.24	120.13	126.42
30	a	708	CLA	CHD-C1D-ND	-2.24	122.40	124.45
30	j	104	CLA	CHD-C1D-ND	-2.24	122.40	124.45
31	P	211	KC1	C2A-C3A-C4A	2.23	108.14	106.49
30	A	307	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
28	G	502	DD6	O1-C20-C19	-2.23	111.70	113.38
30	F	315	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
31	A	306	KC1	O1D-CGD-CBD	-2.23	119.92	124.48
30	I	307	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
30	a	725	CLA	CHD-C1D-ND	-2.23	122.40	124.45
30	M	308	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
31	J	313	KC1	O1D-CGD-CBD	-2.23	119.92	124.48
37	b	730	BCR	C20-C21-C22	-2.23	124.13	127.31
30	L	308	CLA	CHD-C1D-ND	-2.23	122.40	124.45
29	K	302	UIX	O2-C27-O4	-2.23	118.53	122.96
30	G	512	CLA	CHD-C1D-ND	-2.23	122.41	124.45
30	D	308	CLA	CHD-C1D-ND	-2.23	122.41	124.45
28	G	505	DD6	C12-C11-C10	-2.23	119.80	122.92
30	B	307	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	A	312	CLA	CHD-C1D-ND	-2.23	122.41	124.45
30	a	707	CLA	CHD-C1D-ND	-2.23	122.41	124.45
30	M	315	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	P	209	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	K	309	CLA	CHD-C1D-ND	-2.22	122.41	124.45
30	O	311	CLA	CHD-C1D-ND	-2.22	122.41	124.45
30	I	310	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	G	503	UIX	C12-C11-C10	2.22	121.57	118.08
33	K	317	LMG	O1-C7-C8	-2.22	105.54	110.90
30	b	701	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
31	D	315	KC1	CAB-C3B-C4B	2.22	130.25	124.90
30	B	308	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
37	f	304	BCR	C8-C7-C6	-2.22	120.97	127.20
30	B	315	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	G	502	DD6	C25-C24-C1	-2.22	120.19	126.42
28	L	306	DD6	C12-C11-C10	-2.22	119.82	122.92
30	L	314	CLA	CHD-C1D-ND	-2.22	122.42	124.45
28	K	301	DD6	C33-C34-C35	-2.22	107.27	110.30
30	a	713	CLA	CHD-C1D-ND	-2.22	122.42	124.45
28	b	731	DD6	C21-C20-C15	-2.21	118.55	122.26
30	b	716	CLA	CHD-C1D-ND	-2.21	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	311	KC1	O2D-CGD-O1D	-2.21	119.51	123.84
30	G	518	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
33	b	734	LMG	O3-C3-C2	-2.21	105.23	110.35
29	K	302	UIX	C12-C11-C13	-2.21	119.82	122.92
30	J	314	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	M	304	DD6	C28-C27-C29	2.21	121.22	116.84
37	b	730	BCR	C37-C22-C23	2.21	121.56	118.08
37	b	732	BCR	C35-C13-C12	2.21	121.56	118.08
28	A	302	DD6	O1-C20-C19	2.21	115.04	113.38
30	D	309	CLA	CHD-C1D-ND	-2.21	122.42	124.45
31	M	314	KC1	C2A-C3A-C4A	2.21	108.13	106.49
30	a	731	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
29	O	306	UIX	C3-C5-C4	-2.21	106.50	110.77
30	b	722	CLA	CHB-C4A-NA	2.21	127.57	124.51
30	a	735	CLA	C1-C2-C3	-2.21	122.22	126.04
30	b	728	CLA	C1-C2-C3	-2.21	122.22	126.04
30	l	310	CLA	C4B-CHC-C1C	-2.21	126.17	128.81
31	L	315	KC1	CAC-C3C-C4C	2.21	127.68	124.81
28	L	302	DD6	C32-C33-C34	-2.21	108.66	113.64
28	G	502	DD6	C20-C19-C18	-2.21	108.38	112.75
28	I	303	DD6	C33-C34-C35	-2.21	107.28	110.30
29	O	306	UIX	C1-C3-C5	-2.21	108.38	112.75
30	a	728	CLA	CHD-C1D-ND	-2.21	122.43	124.45
30	b	724	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
30	B	301	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
30	H	309	CLA	CHD-C1D-ND	-2.20	122.43	124.45
30	L	318	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	O	306	UIX	C29-C26-C30	-2.20	119.83	122.92
33	P	201	LMG	O7-C10-O9	-2.20	118.38	123.70
34	O	305	PID	C1-C2-C3	-2.20	108.39	112.75
37	a	736	BCR	C34-C9-C10	-2.20	119.84	122.92
29	G	503	UIX	O2-C27-O4	-2.20	118.59	122.96
31	A	306	KC1	CBD-CHA-C1A	2.20	132.99	128.88
31	B	314	KC1	CBD-CHA-C1A	2.20	132.99	128.88
30	a	703	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	I	319	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
28	A	305	DD6	C15-C14-C13	-2.20	121.34	125.99
30	K	311	CLA	CHD-C1D-ND	-2.20	122.43	124.45
28	A	302	DD6	C25-C24-C1	-2.20	120.23	126.42
30	D	311	CLA	CHD-C1D-ND	-2.20	122.43	124.45
30	M	312	CLA	CHD-C1D-ND	-2.20	122.43	124.45
30	a	738	CLA	C1B-CHB-C4A	-2.20	125.76	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	316	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
30	A	313	CLA	CHD-C1D-ND	-2.20	122.43	124.45
30	H	309	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
30	A	319	CLA	CHD-C1D-ND	-2.20	122.44	124.45
28	L	302	DD6	C28-C27-C29	2.20	121.19	116.84
28	K	304	DD6	C21-C20-C15	-2.20	118.58	122.26
32	y	201	DGD	O1G-C1A-C2A	2.20	118.80	111.91
28	L	302	DD6	C37-C36-C35	2.20	118.42	114.36
37	l	307	BCR	C33-C5-C6	-2.19	122.06	124.53
28	M	302	DD6	C24-C1-C2	2.19	122.31	118.94
30	b	715	CLA	CHD-C1D-ND	-2.19	122.44	124.45
30	a	726	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
28	M	306	DD6	C32-C31-C36	-2.19	119.54	122.63
30	G	519	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	J	305	UIX	C18-O2-C27	-2.19	113.81	117.90
30	a	728	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
33	I	320	LMG	O3-C3-C2	-2.19	105.28	110.35
31	F	309	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
30	M	318	CLA	CHD-C1D-ND	-2.19	122.44	124.45
30	G	518	CLA	O2D-CGD-CBD	2.19	115.16	111.27
30	G	512	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
30	I	306	CLA	CHD-C1D-ND	-2.19	122.44	124.45
34	j	105	PID	O4-C12-C13	2.19	127.56	122.89
30	a	720	CLA	CHD-C1D-ND	-2.19	122.44	124.45
30	P	214	CLA	CHB-C4A-NA	2.19	127.53	124.51
34	F	305	PID	CM5-C21-C20	-2.19	119.86	122.92
30	b	713	CLA	CHD-C1D-ND	-2.19	122.45	124.45
28	h	203	DD6	C33-C34-C35	-2.18	107.31	110.30
37	b	732	BCR	C33-C5-C4	2.18	117.81	113.62
30	D	314	CLA	O2D-CGD-CBD	2.18	115.15	111.27
28	K	304	DD6	C25-C24-C1	-2.18	120.28	126.42
28	G	505	DD6	C37-C36-C35	2.18	118.40	114.36
30	P	217	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
28	M	302	DD6	C33-C34-C35	-2.18	107.31	110.30
30	a	721	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	b	703	CLA	CHB-C4A-NA	2.18	127.53	124.51
31	D	310	KC1	O2D-CGD-O1D	-2.18	119.57	123.84
30	O	309	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	A	309	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	a	719	CLA	CHD-C1D-ND	-2.18	122.45	124.45
28	J	303	DD6	C12-C11-C10	-2.18	119.87	122.92
28	M	305	DD6	C10-C9-C8	-2.18	116.41	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	P	211	KC1	O2A-CGA-O1A	-2.18	118.14	122.67
30	I	321	CLA	C1-C2-C3	-2.18	122.27	126.04
30	G	517	CLA	CHD-C1D-ND	-2.18	122.45	124.45
37	l	306	BCR	C21-C20-C19	-2.18	116.41	123.22
28	K	304	DD6	C14-C13-C11	-2.18	122.15	125.53
30	f	301	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
30	a	705	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
30	G	514	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
30	a	712	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	a	713	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
30	a	722	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
30	f	302	CLA	CHD-C1D-ND	-2.18	122.45	124.45
34	P	202	PID	CM3-C5-C4	-2.18	105.20	108.98
30	a	713	CLA	C1-C2-C3	-2.18	122.28	126.04
30	B	307	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	F	308	CLA	CHD-C1D-ND	-2.18	122.45	124.45
31	A	314	KC1	O2A-CGA-O1A	-2.18	118.15	122.67
30	A	317	CLA	CMA-C3A-C2A	-2.18	111.02	116.10
30	L	314	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
37	l	302	BCR	C34-C9-C8	2.18	121.50	118.08
28	G	504	DD6	C4-C3-C2	-2.18	119.02	123.47
30	L	310	CLA	CHD-C1D-ND	-2.18	122.45	124.45
31	P	213	KC1	O2D-CGD-O1D	-2.17	119.59	123.84
28	O	303	DD6	C25-C26-C27	-2.17	120.27	126.58
34	H	301	PID	C16-C15-C14	-2.17	124.21	127.31
28	J	303	DD6	C21-C20-C19	2.17	116.72	114.28
28	M	303	DD6	C32-C33-C34	-2.17	108.74	113.64
30	G	511	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	I	308	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
28	K	301	DD6	C-C1-C24	2.17	121.50	118.08
30	A	310	CLA	CHD-C1D-ND	-2.17	122.46	124.45
30	a	722	CLA	CHD-C1D-ND	-2.17	122.46	124.45
37	a	736	BCR	C16-C15-C14	-2.17	119.03	123.47
28	I	301	DD6	C9-C8-C6	-2.17	120.33	126.42
30	a	738	CLA	O2D-CGD-CBD	2.17	115.12	111.27
28	I	301	DD6	C34-C35-C36	-2.17	107.54	111.85
28	N	303	DD6	C25-C24-C1	-2.17	120.33	126.42
28	B	302	DD6	C28-C27-C29	2.17	121.13	116.84
30	a	725	CLA	C1-C2-C3	-2.17	122.30	126.04
30	a	728	CLA	C1-C2-C3	-2.17	122.30	126.04
31	J	313	KC1	C2A-C3A-C4A	2.16	108.09	106.49
37	b	732	BCR	C36-C18-C19	2.16	121.49	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	207	UIX	C3-C5-C4	-2.16	106.59	110.77
30	M	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	K	303	DD6	C3-C4-C5	-2.16	119.04	123.47
30	b	701	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	b	725	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	I	301	DD6	C21-C20-C15	-2.16	118.64	122.26
33	I	318	LMG	O3-C3-C2	-2.16	105.35	110.35
28	M	306	DD6	O1-C20-C15	-2.16	57.17	58.96
37	b	730	BCR	C23-C24-C25	-2.16	121.13	127.20
30	b	717	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	l	313	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	B	309	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
28	I	301	DD6	C25-C24-C1	-2.16	120.35	126.42
30	D	312	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
31	P	216	KC1	CBD-CHA-C1A	2.16	132.91	128.88
30	b	718	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	a	717	CLA	C1-C2-C3	-2.16	122.31	126.04
30	G	520	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	L	306	DD6	C4-C3-C2	-2.16	119.05	123.47
28	O	303	DD6	O1-C20-C19	-2.16	111.76	113.38
37	l	306	BCR	C33-C5-C4	2.16	117.76	113.62
30	a	710	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
30	a	702	CLA	CHB-C4A-NA	2.16	127.49	124.51
31	H	310	KC1	O2D-CGD-O1D	-2.16	119.62	123.84
33	j	101	LMG	O7-C10-O9	-2.16	118.49	123.70
30	G	514	CLA	CHD-C1D-ND	-2.16	122.47	124.45
30	H	311	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	J	302	DD6	C21-C20-C15	-2.16	118.65	122.26
31	N	311	KC1	C2A-C3A-C4A	2.16	108.08	106.49
30	a	726	CLA	O2D-CGD-CBD	2.16	115.10	111.27
30	I	311	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
30	H	305	CLA	CHD-C1D-ND	-2.15	122.47	124.45
31	D	310	KC1	C2A-C3A-C4A	2.15	108.08	106.49
30	a	724	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
31	O	315	KC1	C2A-C3A-C4A	2.15	108.08	106.49
30	P	210	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
30	a	712	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
30	O	309	CLA	CHD-C1D-ND	-2.15	122.48	124.45
30	J	301	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
28	M	303	DD6	C19-C18-C17	-2.15	106.62	110.77
37	f	304	BCR	C35-C13-C14	-2.15	119.91	122.92
28	G	502	DD6	C4-C3-C2	-2.15	119.07	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	314	KC1	C1A-C2A-C3A	-2.15	105.41	107.11
30	a	701	CLA	CHD-C1D-ND	-2.15	122.48	124.45
30	M	315	CLA	CHD-C1D-ND	-2.15	122.48	124.45
37	b	730	BCR	C11-C12-C13	-2.15	120.39	126.42
31	I	314	KC1	O2A-CGA-O1A	-2.15	118.21	122.67
31	N	306	KC1	C2A-C3A-C4A	2.14	108.08	106.49
30	b	710	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
30	b	727	CLA	CHD-C1D-ND	-2.14	122.48	124.45
28	F	303	DD6	C25-C26-C27	-2.14	120.36	126.58
28	J	303	DD6	C28-C27-C29	2.14	121.08	116.84
34	F	302	PID	C17-C18-C19	2.14	129.57	124.81
28	I	301	DD6	C20-C19-C18	-2.14	108.51	112.75
28	A	303	DD6	C26-C25-C24	-2.14	116.54	123.22
33	j	101	LMG	O2-C2-C1	-2.14	104.85	110.05
33	B	318	LMG	O1-C7-C8	-2.14	105.74	110.90
28	J	304	DD6	C15-C14-C13	-2.14	121.47	125.99
28	G	508	DD6	C21-C20-C15	-2.14	118.68	122.26
33	D	317	LMG	O3-C3-C2	-2.14	105.41	110.35
33	K	317	LMG	O3-C3-C2	-2.14	105.41	110.35
30	l	309	CLA	CHD-C1D-ND	-2.14	122.49	124.45
30	b	725	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
33	B	318	LMG	O2-C2-C1	-2.13	104.86	110.05
30	b	705	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	A	314	KC1	O2D-CGD-O1D	-2.13	119.67	123.84
28	G	504	DD6	C7-C6-C5	-2.13	119.94	122.92
34	F	304	PID	C19-C20-C21	2.13	130.35	127.31
37	f	304	BCR	C23-C24-C25	-2.13	121.21	127.20
28	B	306	DD6	C3-C4-C5	-2.13	119.11	123.47
28	D	303	DD6	C-C1-C24	2.13	121.43	118.08
30	h	202	CLA	CHD-C1D-ND	-2.13	122.50	124.45
30	b	726	CLA	CHD-C1D-ND	-2.13	122.50	124.45
28	B	303	DD6	C26-C25-C24	-2.13	116.57	123.22
33	P	201	LMG	C6-C5-C4	-2.13	108.01	113.00
30	H	312	CLA	CHD-C1D-ND	-2.13	122.50	124.45
28	G	502	DD6	C7-C6-C5	-2.13	119.94	122.92
31	N	306	KC1	CBD-CHA-C1A	2.13	132.85	128.88
30	B	301	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
30	G	513	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
28	L	305	DD6	C25-C26-C27	-2.13	120.40	126.58
34	G	506	PID	CM4-C14-C13	2.13	123.96	119.05
30	J	312	CLA	CHD-C1D-ND	-2.13	122.50	124.45
28	J	302	DD6	C-C1-C2	-2.13	119.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	304	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
30	F	307	CLA	CHD-C1D-ND	-2.13	122.50	124.45
33	P	201	LMG	O3-C3-C2	-2.13	105.44	110.35
28	K	303	DD6	C41-C32-C31	-2.12	107.09	110.47
30	b	708	CLA	C1-C2-C3	-2.12	122.37	126.04
30	l	310	CLA	CHC-C1C-NC	-2.12	125.88	128.83
30	a	703	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
30	G	512	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
30	l	303	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
30	j	106	CLA	C1-C2-C3	-2.12	122.37	126.04
33	I	320	LMG	O2-C2-C1	-2.12	104.89	110.05
30	K	316	CLA	O2D-CGD-CBD	2.12	115.04	111.27
34	O	305	PID	O4-C12-C11	-2.12	106.07	107.36
34	O	305	PID	C15-C14-C13	2.12	122.81	117.00
30	N	307	CLA	CHB-C4A-NA	2.12	127.44	124.51
37	f	304	BCR	C3-C4-C5	-2.12	110.29	114.08
29	B	305	UIX	C22-C15-C20	-2.12	108.58	110.47
31	G	515	KC1	O2D-CGD-O1D	-2.12	119.69	123.84
28	G	505	DD6	C7-C6-C5	-2.12	119.95	122.92
30	I	306	CLA	O2D-CGD-CBD	2.12	115.03	111.27
31	O	310	KC1	O2A-CGA-O1A	-2.12	118.27	122.67
30	F	313	CLA	C2A-C1A-CHA	2.12	127.56	123.86
37	a	736	BCR	C4-C5-C6	-2.12	119.66	122.73
33	I	320	LMG	O1-C1-C2	-2.12	105.00	108.30
34	P	206	PID	C28-C27-C26	2.12	113.57	109.88
28	H	303	DD6	C33-C34-C35	-2.11	107.41	110.30
33	K	317	LMG	O2-C2-C1	-2.11	104.91	110.05
34	G	507	PID	C28-C27-C26	2.11	113.56	109.88
30	G	509	CLA	CHD-C1D-ND	-2.11	122.51	124.45
30	B	312	CLA	CHD-C1D-ND	-2.11	122.51	124.45
30	B	316	CLA	CHD-C1D-ND	-2.11	122.51	124.45
31	K	314	KC1	O1D-CGD-CBD	-2.11	120.16	124.48
30	b	724	CLA	CHD-C1D-ND	-2.11	122.51	124.45
28	K	304	DD6	C28-C27-C29	2.11	121.02	116.84
30	G	514	CLA	C1-C2-C3	-2.11	122.39	126.04
28	I	301	DD6	C3-C4-C5	-2.11	119.15	123.47
30	I	311	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
30	I	312	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
28	K	305	DD6	C3-C4-C5	-2.11	119.16	123.47
30	a	727	CLA	CHD-C1D-ND	-2.11	122.52	124.45
31	H	310	KC1	O1D-CGD-CBD	-2.11	120.17	124.48
28	A	301	DD6	C9-C8-C6	-2.11	120.50	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	716	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
28	M	305	DD6	C25-C24-C1	-2.11	120.50	126.42
29	K	302	UIX	C19-C18-C17	-2.10	106.20	109.88
33	D	317	LMG	O1-C1-C2	-2.10	105.02	108.30
30	b	704	CLA	C2D-C1D-ND	-2.10	108.55	110.10
37	i	201	BCR	C20-C19-C18	-2.10	120.51	126.42
34	G	507	PID	CM4-C14-C13	2.10	123.90	119.05
32	I	317	DGD	O6D-C5D-C6D	2.10	110.91	106.67
33	B	318	LMG	O3-C3-C2	-2.10	105.49	110.35
30	b	720	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
28	I	303	DD6	O1-C20-C15	-2.10	57.22	58.96
28	B	306	DD6	C14-C13-C11	-2.10	122.27	125.53
29	K	302	UIX	C41-C40-C38	2.10	121.39	118.08
30	b	723	CLA	C1-C2-C3	-2.10	123.36	126.75
28	L	303	DD6	C25-C24-C1	-2.10	120.52	126.42
30	K	306	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
30	l	311	CLA	CHD-C1D-ND	-2.10	122.53	124.45
30	H	305	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	D	303	DD6	C7-C6-C8	2.10	121.38	118.08
33	D	317	LMG	O2-C2-C1	-2.10	104.95	110.05
28	A	305	DD6	C25-C24-C1	-2.10	120.53	126.42
30	h	202	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
28	B	303	DD6	C40-C32-C31	-2.09	107.14	110.47
28	h	203	DD6	C34-C35-C36	-2.09	107.69	111.85
30	b	707	CLA	CHD-C1D-ND	-2.09	122.53	124.45
30	b	722	CLA	CHD-C1D-ND	-2.09	122.53	124.45
28	A	303	DD6	C37-C36-C35	2.09	118.23	114.36
28	P	204	DD6	C7-C6-C5	-2.09	119.99	122.92
37	l	306	BCR	C15-C16-C17	-2.09	119.19	123.47
28	b	731	DD6	C-C1-C24	2.09	121.37	118.08
28	I	302	DD6	C9-C8-C6	2.09	132.29	126.42
31	P	216	KC1	C2A-C3A-C4A	2.09	108.04	106.49
33	K	317	LMG	C1-C2-C3	-2.09	105.65	110.00
28	O	303	DD6	C37-C36-C35	2.09	118.22	114.36
30	b	710	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	M	307	KC1	C1A-C2A-C3A	-2.09	105.46	107.11
31	I	314	KC1	C2A-C3A-C4A	2.09	108.03	106.49
37	a	734	BCR	C16-C15-C14	-2.09	119.20	123.47
34	H	302	PID	C6-C7-C8	-2.09	121.58	125.99
30	F	311	CLA	CHD-C1D-ND	-2.09	122.54	124.45
30	N	304	CLA	CHD-C1D-ND	-2.09	122.54	124.45
30	a	731	CLA	O2A-CGA-O1A	-2.09	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	310	CLA	C2A-C1A-CHA	2.09	127.51	123.86
28	N	303	DD6	O1-C20-C21	-2.09	112.56	115.06
37	l	302	BCR	C35-C13-C12	2.09	121.36	118.08
30	a	729	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
30	B	301	CLA	CHB-C4A-NA	2.08	127.39	124.51
31	L	307	KC1	C2A-C3A-C4A	2.08	108.03	106.49
37	l	307	BCR	C10-C11-C12	-2.08	116.71	123.22
28	B	306	DD6	C34-C35-C36	-2.08	107.70	111.85
30	N	304	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
28	G	508	DD6	C28-C27-C29	2.08	120.96	116.84
28	B	303	DD6	C28-C27-C29	2.08	120.96	116.84
34	N	301	PID	C15-C14-C13	2.08	122.70	117.00
30	L	308	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
30	M	309	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
28	K	305	DD6	C25-C24-C1	-2.08	120.57	126.42
30	m	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
37	b	702	BCR	C34-C9-C10	-2.08	120.01	122.92
30	b	723	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	A	313	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
37	i	201	BCR	C35-C13-C12	2.08	121.35	118.08
30	l	308	CLA	CHD-C1D-ND	-2.08	122.55	124.45
38	a	732	PQN	C12-C11-C3	-2.08	106.44	112.05
30	a	729	CLA	C1-C2-C3	-2.08	122.45	126.04
33	b	734	LMG	O2-C2-C1	-2.08	105.00	110.05
30	B	311	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
30	P	215	CLA	CED-O2D-CGD	2.08	120.63	115.94
33	b	733	LMG	O7-C10-O9	-2.08	118.69	123.70
30	L	317	CLA	O2D-CGD-CBD	2.08	114.96	111.27
30	O	308	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
28	M	303	DD6	C25-C26-C27	-2.07	120.56	126.58
30	K	312	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
31	L	307	KC1	O1D-CGD-CBD	-2.07	120.24	124.48
30	a	715	CLA	CHD-C1D-ND	-2.07	122.55	124.45
37	a	736	BCR	C15-C16-C17	-2.07	119.23	123.47
30	a	731	CLA	CHD-C1D-ND	-2.07	122.55	124.45
28	I	302	DD6	C37-C36-C35	2.07	118.19	114.36
30	L	311	CLA	CHD-C1D-ND	-2.07	122.55	124.45
30	L	314	CLA	C1-C2-C3	-2.07	122.47	126.04
30	D	316	CLA	CHD-C1D-ND	-2.07	122.55	124.45
37	a	736	BCR	C11-C12-C13	-2.07	120.61	126.42
30	b	708	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
30	J	308	CLA	O2D-CGD-CBD	2.06	114.94	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	j	102	BCR	C38-C26-C27	2.06	117.58	113.62
30	K	310	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
30	M	312	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
30	O	311	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
31	A	306	KC1	O2D-CGD-O1D	-2.06	119.81	123.84
30	b	720	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	P	212	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	A	302	DD6	C37-C36-C35	2.06	118.17	114.36
28	I	303	DD6	C25-C26-C27	-2.06	120.60	126.58
31	P	213	KC1	C2A-C3A-C4A	2.06	108.02	106.49
30	a	720	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	J	305	UIX	C3-C5-C4	-2.06	106.79	110.77
28	M	304	DD6	C37-C36-C35	2.06	118.17	114.36
37	l	307	BCR	C23-C24-C25	-2.06	121.42	127.20
30	I	319	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
38	a	732	PQN	C11-C12-C13	-2.06	123.36	126.79
33	b	733	LMG	O3-C3-C2	-2.06	105.59	110.35
28	L	304	DD6	C40-C32-C31	-2.06	107.20	110.47
30	B	308	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	a	711	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
29	J	305	UIX	O2-C27-O4	-2.06	118.88	122.96
28	A	305	DD6	C10-C9-C8	-2.06	116.80	123.22
30	D	308	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
31	G	515	KC1	CBD-CHA-C1A	2.06	132.71	128.88
30	b	723	CLA	O2D-CGD-CBD	2.05	114.92	111.27
32	G	501	DGD	C2G-O2G-C1B	-2.05	112.73	117.79
30	B	307	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
29	h	201	UIX	C36-C35-C32	-2.05	124.38	127.31
30	b	721	CLA	CHB-C4A-NA	2.05	127.35	124.51
31	D	315	KC1	C4B-CHC-C1C	-2.05	121.63	126.06
30	f	301	CLA	CHD-C1D-ND	-2.05	122.57	124.45
28	L	304	DD6	C12-C11-C13	2.05	121.31	118.08
28	L	302	DD6	C25-C26-C27	-2.05	120.62	126.58
30	I	308	CLA	O2D-CGD-CBD	2.05	114.91	111.27
37	a	736	BCR	C37-C22-C23	2.05	121.31	118.08
30	a	716	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	j	106	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
34	D	305	PID	C17-C16-C15	2.05	127.67	123.47
30	A	317	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	K	315	CLA	CMA-C3A-C2A	-2.05	111.32	116.10
30	A	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	G	520	CLA	O2A-CGA-O1A	-2.05	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	j	105	PID	CM4-C14-C13	2.05	123.77	119.05
37	l	307	BCR	C36-C18-C19	2.05	121.30	118.08
30	I	315	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	P	204	DD6	C25-C26-C27	-2.05	120.64	126.58
30	a	730	CLA	C1-C2-C3	-2.05	122.50	126.04
30	a	724	CLA	O2D-CGD-CBD	2.05	114.91	111.27
30	L	311	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
37	i	201	BCR	C34-C9-C8	2.05	121.30	118.08
30	P	210	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	M	317	CLA	O2D-CGD-CBD	2.05	114.91	111.27
28	I	302	DD6	C15-C14-C13	2.05	130.32	125.99
31	A	314	KC1	C2A-C3A-C4A	2.05	108.00	106.49
30	b	722	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
30	b	712	CLA	O2A-C1-C2	2.05	114.01	108.64
31	A	306	KC1	C2A-C3A-C4A	2.04	108.00	106.49
30	a	708	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
28	b	731	DD6	C12-C11-C13	2.04	121.30	118.08
37	a	734	BCR	C37-C22-C23	2.04	121.30	118.08
30	J	301	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	D	315	KC1	O2D-CGD-O1D	-2.04	119.85	123.84
30	j	104	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
28	H	303	DD6	C21-C20-C15	-2.04	118.84	122.26
31	L	307	KC1	CAA-CBA-CGA	-2.04	116.77	127.26
30	O	308	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	G	509	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
30	B	317	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
30	M	310	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	L	308	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	b	717	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	O	314	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	b	708	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	I	301	DD6	C4-C3-C2	-2.04	119.30	123.47
30	I	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	G	518	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	b	726	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	l	301	DGD	O1G-C1A-C2A	2.04	118.30	111.91
28	F	301	DD6	C-C1-C2	-2.04	120.07	122.92
28	B	306	DD6	C7-C6-C8	2.03	121.28	118.08
30	a	725	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
34	j	105	PID	O1-C1-C2	-2.03	111.86	113.38
28	F	303	DD6	C7-C6-C5	-2.03	120.08	122.92
30	F	315	CLA	O2D-CGD-CBD	2.03	114.88	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	316	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
30	a	714	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
28	K	303	DD6	C25-C26-C27	-2.03	120.69	126.58
29	G	503	UIX	C3-C5-C4	-2.03	106.85	110.77
28	M	304	DD6	C-C1-C2	-2.03	120.08	122.92
30	L	316	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	J	303	DD6	C3-C4-C5	-2.03	119.32	123.47
30	D	313	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
30	A	308	CLA	CHD-C1D-ND	-2.03	122.59	124.45
30	A	309	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
28	G	502	DD6	C9-C8-C6	-2.03	120.72	126.42
28	B	303	DD6	C12-C11-C13	2.03	121.27	118.08
29	K	302	UIX	C29-C26-C30	-2.03	120.08	122.92
34	P	202	PID	C17-C18-C19	2.03	129.32	124.81
37	i	201	BCR	C16-C15-C14	-2.03	119.33	123.47
34	N	302	PID	O4-C12-C13	2.02	127.21	122.89
28	D	303	DD6	C32-C33-C34	-2.02	109.07	113.64
31	L	307	KC1	C1A-C2A-C3A	-2.02	105.51	107.11
30	a	723	CLA	CHD-C1D-ND	-2.02	122.59	124.45
28	B	306	DD6	C4-C3-C2	-2.02	119.33	123.47
28	M	302	DD6	C28-C27-C29	2.02	120.85	116.84
28	H	303	DD6	C3-C4-C5	-2.02	119.33	123.47
30	J	316	CLA	CHD-C1D-ND	-2.02	122.59	124.45
30	a	710	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
31	N	311	KC1	CBD-CHA-C1A	2.02	132.65	128.88
28	G	505	DD6	C33-C34-C35	-2.02	107.54	110.30
30	I	309	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
30	a	707	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
30	N	310	CLA	C3A-C2A-C1A	2.02	104.37	101.34
37	b	732	BCR	C28-C29-C30	-2.02	107.38	114.60
30	b	704	CLA	O1D-CGD-CBD	2.02	128.62	124.48
28	L	305	DD6	O1-C20-C21	-2.02	112.64	115.06
28	I	301	DD6	C12-C11-C10	-2.02	120.09	122.92
28	L	304	DD6	C25-C26-C27	-2.02	120.72	126.58
30	A	308	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
30	P	209	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	J	305	UIX	C37-C39-C40	-2.02	124.43	127.31
28	B	302	DD6	C4-C5-C6	-2.02	120.32	124.81
30	K	315	CLA	CHD-C1D-ND	-2.02	122.60	124.45
30	D	314	CLA	CHD-C1D-ND	-2.02	122.60	124.45
31	B	314	KC1	C2A-C3A-C4A	2.02	107.98	106.49
37	f	304	BCR	C33-C5-C4	2.02	117.49	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	b	729	PQN	C2M-C2-C1	2.02	119.61	116.27
28	I	303	DD6	C-C1-C2	-2.02	120.10	122.92
28	I	301	DD6	C28-C27-C29	2.02	120.83	116.84
31	M	314	KC1	O2A-CGA-O1A	-2.02	118.48	122.67
28	B	304	DD6	C21-C20-C15	-2.02	118.88	122.26
28	L	304	DD6	C3-C4-C5	-2.02	119.34	123.47
30	B	312	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
28	J	304	DD6	C20-C19-C18	-2.02	108.76	112.75
30	B	308	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
30	b	712	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	O	314	CLA	C2A-C1A-CHA	2.01	127.38	123.86
30	K	308	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	l	303	CLA	O2D-CGD-CBD	2.01	114.84	111.27
31	N	308	KC1	O2A-CGA-O1A	-2.01	118.49	122.67
30	I	311	CLA	CHD-C1D-ND	-2.01	122.61	124.45
28	L	302	DD6	O1-C20-C21	-2.01	112.65	115.06
30	H	307	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
30	L	317	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
34	D	304	PID	CM2-C5-C4	-2.01	105.49	108.98
30	b	711	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	J	305	UIX	C-C7-C10	-2.01	121.75	125.99
29	A	304	UIX	C37-C34-C30	-2.01	119.36	123.47
30	l	311	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	F	314	KC1	C1A-C2A-C3A	-2.01	105.52	107.11
28	H	303	DD6	C14-C13-C11	-2.01	122.42	125.53
31	F	309	KC1	CMD-C2D-C1D	-2.01	125.38	128.46
34	j	105	PID	C17-C18-C19	2.01	129.27	124.81
30	a	723	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
30	K	306	CLA	O2D-CGD-CBD	2.00	114.83	111.27
30	a	721	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	M	314	KC1	O2D-CGD-O1D	-2.00	119.92	123.84
29	h	201	UIX	C3-C5-C4	-2.00	106.91	110.77
28	J	304	DD6	C19-C18-C17	-2.00	106.91	110.77
30	J	310	CLA	C2D-C1D-ND	-2.00	108.63	110.10
28	G	502	DD6	C12-C11-C10	-2.00	120.12	122.92
28	L	303	DD6	C34-C35-C36	-2.00	107.87	111.85
30	b	714	CLA	CHD-C1D-ND	-2.00	122.62	124.45
30	J	315	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (198) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
30	I	306	CLA	ND
30	I	307	CLA	ND
30	I	308	CLA	ND
30	I	309	CLA	ND
30	I	310	CLA	ND
30	I	311	CLA	ND
30	I	312	CLA	ND
30	I	313	CLA	ND
30	I	315	CLA	ND
30	I	316	CLA	ND
30	I	319	CLA	ND
30	I	321	CLA	ND
30	K	306	CLA	ND
30	K	307	CLA	ND
30	K	308	CLA	ND
30	K	309	CLA	ND
30	K	310	CLA	ND
30	K	311	CLA	ND
30	K	312	CLA	ND
30	K	313	CLA	ND
30	K	315	CLA	ND
30	K	316	CLA	ND
30	G	509	CLA	ND
30	G	510	CLA	ND
30	G	511	CLA	ND
30	G	512	CLA	ND
30	G	513	CLA	ND
30	G	514	CLA	ND
30	G	516	CLA	ND
30	G	517	CLA	ND
30	G	518	CLA	ND
30	G	519	CLA	ND
30	G	520	CLA	ND
30	A	307	CLA	ND
30	A	308	CLA	ND
30	A	309	CLA	ND
30	A	310	CLA	ND
30	A	311	CLA	ND
30	A	312	CLA	ND
30	A	313	CLA	ND
30	A	315	CLA	ND

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Mol	Chain	Res	Type	Atom
30	A	316	CLA	ND
30	A	317	CLA	ND
30	A	319	CLA	ND
30	A	320	CLA	ND
30	f	301	CLA	ND
30	f	302	CLA	ND
30	f	303	CLA	ND
30	h	202	CLA	ND
30	j	104	CLA	ND
30	j	106	CLA	ND
30	l	303	CLA	ND
30	l	304	CLA	ND
30	l	305	CLA	ND
30	l	308	CLA	ND
30	l	309	CLA	ND
30	l	311	CLA	ND
30	l	312	CLA	ND
30	l	313	CLA	ND
30	m	202	CLA	ND
30	a	701	CLA	ND
30	a	702	CLA	ND
30	a	703	CLA	ND
30	a	704	CLA	ND
30	a	705	CLA	ND
30	a	706	CLA	ND
30	a	707	CLA	ND
30	a	708	CLA	ND
30	a	709	CLA	ND
30	a	710	CLA	ND
30	a	711	CLA	ND
30	a	712	CLA	ND
30	a	713	CLA	ND
30	a	714	CLA	ND
30	a	715	CLA	ND
30	a	716	CLA	ND
30	a	717	CLA	ND
30	a	718	CLA	ND
30	a	719	CLA	ND
30	a	720	CLA	ND
30	a	721	CLA	ND
30	a	722	CLA	ND
30	a	723	CLA	ND

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Mol	Chain	Res	Type	Atom
30	a	724	CLA	ND
30	a	725	CLA	ND
30	a	726	CLA	ND
30	a	727	CLA	ND
30	a	728	CLA	ND
30	a	729	CLA	ND
30	a	730	CLA	ND
30	a	731	CLA	ND
30	a	735	CLA	ND
30	a	738	CLA	ND
30	b	701	CLA	ND
30	b	703	CLA	ND
30	b	704	CLA	ND
30	b	705	CLA	ND
30	b	706	CLA	ND
30	b	707	CLA	ND
30	b	708	CLA	ND
30	b	709	CLA	ND
30	b	710	CLA	ND
30	b	711	CLA	ND
30	b	712	CLA	ND
30	b	713	CLA	ND
30	b	714	CLA	ND
30	b	715	CLA	ND
30	b	716	CLA	ND
30	b	717	CLA	ND
30	b	718	CLA	ND
30	b	719	CLA	ND
30	b	720	CLA	ND
30	b	721	CLA	ND
30	b	722	CLA	ND
30	b	723	CLA	ND
30	b	724	CLA	ND
30	b	725	CLA	ND
30	b	726	CLA	ND
30	b	727	CLA	ND
30	b	728	CLA	ND
30	B	301	CLA	ND
30	B	307	CLA	ND
30	B	308	CLA	ND
30	B	309	CLA	ND
30	B	310	CLA	ND

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Mol	Chain	Res	Type	Atom
30	B	311	CLA	ND
30	B	312	CLA	ND
30	B	313	CLA	ND
30	B	315	CLA	ND
30	B	316	CLA	ND
30	B	317	CLA	ND
30	D	308	CLA	ND
30	D	309	CLA	ND
30	D	311	CLA	ND
30	D	312	CLA	ND
30	D	313	CLA	ND
30	D	314	CLA	ND
30	D	316	CLA	ND
30	F	307	CLA	ND
30	F	308	CLA	ND
30	F	310	CLA	ND
30	F	311	CLA	ND
30	F	312	CLA	ND
30	F	313	CLA	ND
30	F	315	CLA	ND
30	H	304	CLA	ND
30	H	305	CLA	ND
30	H	307	CLA	ND
30	H	308	CLA	ND
30	H	309	CLA	ND
30	H	312	CLA	ND
30	J	301	CLA	ND
30	J	306	CLA	ND
30	J	307	CLA	ND
30	J	308	CLA	ND
30	J	309	CLA	ND
30	J	310	CLA	ND
30	J	311	CLA	ND
30	J	312	CLA	ND
30	J	314	CLA	ND
30	J	315	CLA	ND
30	L	308	CLA	ND
30	L	309	CLA	ND
30	L	310	CLA	ND
30	L	311	CLA	ND
30	L	312	CLA	ND
30	L	313	CLA	ND

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Mol	Chain	Res	Type	Atom
30	L	314	CLA	ND
30	L	316	CLA	ND
30	L	317	CLA	ND
30	L	318	CLA	ND
30	M	308	CLA	ND
30	M	309	CLA	ND
30	M	310	CLA	ND
30	M	311	CLA	ND
30	M	312	CLA	ND
30	M	313	CLA	ND
30	M	315	CLA	ND
30	M	316	CLA	ND
30	M	317	CLA	ND
30	M	318	CLA	ND
30	N	304	CLA	ND
30	N	305	CLA	ND
30	N	307	CLA	ND
30	N	309	CLA	ND
30	N	310	CLA	ND
30	O	308	CLA	ND
30	O	309	CLA	ND
30	O	311	CLA	ND
30	O	313	CLA	ND
30	O	314	CLA	ND
30	O	316	CLA	ND
30	P	209	CLA	ND
30	P	210	CLA	ND
30	P	212	CLA	ND
30	P	214	CLA	ND
30	P	215	CLA	ND
30	P	217	CLA	ND

All (2300) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	I	302	DD6	C27-C29-C30-C31
28	K	301	DD6	C12-C11-C13-C14
28	G	502	DD6	C-C1-C24-C25
28	G	502	DD6	C2-C1-C24-C25
28	G	504	DD6	C10-C11-C13-C14
28	G	504	DD6	C12-C11-C13-C14
28	G	504	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
28	G	505	DD6	C5-C6-C8-C9
28	G	505	DD6	C7-C6-C8-C9
28	A	301	DD6	C13-C14-C15-C16
28	A	303	DD6	C27-C29-C30-C31
28	A	305	DD6	C13-C14-C15-O1
28	B	303	DD6	C13-C14-C15-O1
28	B	306	DD6	C13-C14-C15-O1
28	D	303	DD6	C13-C14-C15-O1
28	D	303	DD6	C27-C29-C30-C31
28	F	301	DD6	C10-C11-C13-C14
28	F	301	DD6	C12-C11-C13-C14
28	J	302	DD6	C10-C11-C13-C14
28	J	302	DD6	C12-C11-C13-C14
28	J	302	DD6	C27-C29-C30-C31
28	J	303	DD6	C10-C11-C13-C14
28	J	303	DD6	C12-C11-C13-C14
28	J	304	DD6	C10-C11-C13-C14
28	L	302	DD6	C13-C14-C15-O1
28	L	305	DD6	C13-C14-C15-O1
28	M	305	DD6	C13-C14-C15-O1
28	M	306	DD6	C10-C11-C13-C14
28	M	306	DD6	C12-C11-C13-C14
29	I	304	UIX	C2-C-C7-C10
29	I	304	UIX	C31-C27-O2-C18
29	K	302	UIX	O4-C27-O2-C18
29	K	302	UIX	C31-C27-O2-C18
29	G	503	UIX	C31-C27-O2-C18
29	h	201	UIX	O4-C27-O2-C18
29	J	305	UIX	O-C-C7-C10
29	J	305	UIX	C14-C23-C26-C29
29	J	305	UIX	C14-C23-C26-C30
29	P	207	UIX	C36-C38-C40-C39
30	I	307	CLA	CBA-CGA-O2A-C1
30	I	307	CLA	O1A-CGA-O2A-C1
30	I	310	CLA	CHA-CBD-CGD-O1D
30	I	310	CLA	CHA-CBD-CGD-O2D
30	I	310	CLA	CAD-CBD-CGD-O1D
30	I	311	CLA	C1A-C2A-CAA-CBA
30	I	311	CLA	C3A-C2A-CAA-CBA
30	I	311	CLA	CHA-CBD-CGD-O1D
30	I	311	CLA	CHA-CBD-CGD-O2D
30	I	312	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	I	312	CLA	C4-C3-C5-C6
30	I	313	CLA	CBD-CGD-O2D-CED
30	I	313	CLA	C2-C3-C5-C6
30	I	313	CLA	C4-C3-C5-C6
30	I	316	CLA	C1A-C2A-CAA-CBA
30	I	316	CLA	C3A-C2A-CAA-CBA
30	I	319	CLA	CHA-CBD-CGD-O1D
30	I	319	CLA	CHA-CBD-CGD-O2D
30	K	306	CLA	CHA-CBD-CGD-O1D
30	K	306	CLA	CHA-CBD-CGD-O2D
30	K	308	CLA	CBD-CGD-O2D-CED
30	K	308	CLA	C2-C3-C5-C6
30	K	308	CLA	C4-C3-C5-C6
30	K	310	CLA	CHA-CBD-CGD-O1D
30	K	311	CLA	C1A-C2A-CAA-CBA
30	K	311	CLA	C3A-C2A-CAA-CBA
30	K	311	CLA	C3-C5-C6-C7
30	K	313	CLA	C2-C3-C5-C6
30	K	313	CLA	C4-C3-C5-C6
30	K	315	CLA	CBD-CGD-O2D-CED
30	G	509	CLA	C2-C3-C5-C6
30	G	509	CLA	C4-C3-C5-C6
30	G	514	CLA	C2-C3-C5-C6
30	G	514	CLA	C4-C3-C5-C6
30	G	516	CLA	CAD-CBD-CGD-O1D
30	G	516	CLA	CAD-CBD-CGD-O2D
30	G	516	CLA	CBD-CGD-O2D-CED
30	G	517	CLA	CBA-CGA-O2A-C1
30	G	518	CLA	C1A-C2A-CAA-CBA
30	G	518	CLA	C3A-C2A-CAA-CBA
30	G	519	CLA	C1A-C2A-CAA-CBA
30	G	519	CLA	C3A-C2A-CAA-CBA
30	G	520	CLA	C1A-C2A-CAA-CBA
30	G	520	CLA	C3A-C2A-CAA-CBA
30	A	307	CLA	CHA-CBD-CGD-O1D
30	A	307	CLA	CHA-CBD-CGD-O2D
30	A	311	CLA	CBA-CGA-O2A-C1
30	A	315	CLA	CAD-CBD-CGD-O1D
30	A	315	CLA	CAD-CBD-CGD-O2D
30	A	319	CLA	CHA-CBD-CGD-O1D
30	A	319	CLA	CHA-CBD-CGD-O2D
30	A	319	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	A	320	CLA	CBA-CGA-O2A-C1
30	f	301	CLA	C1A-C2A-CAA-CBA
30	f	301	CLA	C3A-C2A-CAA-CBA
30	f	301	CLA	CBD-CGD-O2D-CED
30	f	302	CLA	CBA-CGA-O2A-C1
30	f	303	CLA	C1A-C2A-CAA-CBA
30	f	303	CLA	C3A-C2A-CAA-CBA
30	f	303	CLA	CHA-CBD-CGD-O1D
30	j	106	CLA	C1A-C2A-CAA-CBA
30	j	106	CLA	C3A-C2A-CAA-CBA
30	j	106	CLA	C2-C3-C5-C6
30	j	106	CLA	C4-C3-C5-C6
30	l	309	CLA	CHA-CBD-CGD-O1D
30	l	309	CLA	CHA-CBD-CGD-O2D
30	l	309	CLA	CAD-CBD-CGD-O1D
30	l	310	CLA	CBA-CGA-O2A-C1
30	l	310	CLA	CHA-CBD-CGD-O1D
30	l	310	CLA	CHA-CBD-CGD-O2D
30	l	310	CLA	CBD-CGD-O2D-CED
30	l	311	CLA	C1A-C2A-CAA-CBA
30	l	312	CLA	C3A-C2A-CAA-CBA
30	l	312	CLA	CBD-CGD-O2D-CED
30	l	313	CLA	CHA-CBD-CGD-O1D
30	l	313	CLA	CHA-CBD-CGD-O2D
30	a	702	CLA	CHA-CBD-CGD-O1D
30	a	702	CLA	CBD-CGD-O2D-CED
30	a	703	CLA	CHA-CBD-CGD-O1D
30	a	705	CLA	C1A-C2A-CAA-CBA
30	a	705	CLA	C3A-C2A-CAA-CBA
30	a	706	CLA	CHA-CBD-CGD-O1D
30	a	706	CLA	CHA-CBD-CGD-O2D
30	a	706	CLA	CAD-CBD-CGD-O1D
30	a	706	CLA	C2-C3-C5-C6
30	a	706	CLA	C4-C3-C5-C6
30	a	707	CLA	C3A-C2A-CAA-CBA
30	a	707	CLA	CBD-CGD-O2D-CED
30	a	709	CLA	C1A-C2A-CAA-CBA
30	a	709	CLA	C3A-C2A-CAA-CBA
30	a	711	CLA	C2A-CAA-CBA-CGA
30	a	712	CLA	CHA-CBD-CGD-O1D
30	a	712	CLA	CHA-CBD-CGD-O2D
30	a	713	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	713	CLA	C4-C3-C5-C6
30	a	715	CLA	CBD-CGD-O2D-CED
30	a	716	CLA	C1A-C2A-CAA-CBA
30	a	716	CLA	C3A-C2A-CAA-CBA
30	a	717	CLA	C3A-C2A-CAA-CBA
30	a	717	CLA	C6-C7-C8-C9
30	a	718	CLA	C1A-C2A-CAA-CBA
30	a	718	CLA	CHA-CBD-CGD-O1D
30	a	718	CLA	CHA-CBD-CGD-O2D
30	a	720	CLA	C3A-C2A-CAA-CBA
30	a	721	CLA	C2A-CAA-CBA-CGA
30	a	721	CLA	CHA-CBD-CGD-O1D
30	a	721	CLA	CHA-CBD-CGD-O2D
30	a	721	CLA	CBD-CGD-O2D-CED
30	a	722	CLA	CHA-CBD-CGD-O1D
30	a	722	CLA	CBD-CGD-O2D-CED
30	a	723	CLA	CHA-CBD-CGD-O1D
30	a	723	CLA	CHA-CBD-CGD-O2D
30	a	724	CLA	C4-C3-C5-C6
30	a	726	CLA	CHA-CBD-CGD-O1D
30	a	726	CLA	CHA-CBD-CGD-O2D
30	a	727	CLA	CBA-CGA-O2A-C1
30	a	727	CLA	O1A-CGA-O2A-C1
30	a	728	CLA	C2-C3-C5-C6
30	a	728	CLA	C4-C3-C5-C6
30	a	731	CLA	C1A-C2A-CAA-CBA
30	a	731	CLA	C3A-C2A-CAA-CBA
30	a	731	CLA	CBD-CGD-O2D-CED
30	a	735	CLA	CHA-CBD-CGD-O1D
30	a	735	CLA	CHA-CBD-CGD-O2D
30	a	735	CLA	CAD-CBD-CGD-O1D
30	a	735	CLA	C4-C3-C5-C6
30	a	738	CLA	CHA-CBD-CGD-O1D
30	a	738	CLA	CHA-CBD-CGD-O2D
30	b	701	CLA	CHA-CBD-CGD-O1D
30	b	701	CLA	CHA-CBD-CGD-O2D
30	b	701	CLA	CBD-CGD-O2D-CED
30	b	701	CLA	C2-C3-C5-C6
30	b	701	CLA	C4-C3-C5-C6
30	b	703	CLA	CHA-CBD-CGD-O1D
30	b	703	CLA	CHA-CBD-CGD-O2D
30	b	703	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	b	704	CLA	C1A-C2A-CAA-CBA
30	b	704	CLA	C3A-C2A-CAA-CBA
30	b	704	CLA	CBD-CGD-O2D-CED
30	b	704	CLA	C14-C13-C15-C16
30	b	709	CLA	CHA-CBD-CGD-O1D
30	b	709	CLA	CHA-CBD-CGD-O2D
30	b	710	CLA	C1A-C2A-CAA-CBA
30	b	710	CLA	C3A-C2A-CAA-CBA
30	b	711	CLA	CHA-CBD-CGD-O1D
30	b	711	CLA	CHA-CBD-CGD-O2D
30	b	711	CLA	CAD-CBD-CGD-O1D
30	b	711	CLA	CBD-CGD-O2D-CED
30	b	714	CLA	C2A-CAA-CBA-CGA
30	b	715	CLA	C1A-C2A-CAA-CBA
30	b	715	CLA	C3A-C2A-CAA-CBA
30	b	715	CLA	C2-C3-C5-C6
30	b	715	CLA	C4-C3-C5-C6
30	b	717	CLA	C1A-C2A-CAA-CBA
30	b	717	CLA	C3A-C2A-CAA-CBA
30	b	717	CLA	C14-C13-C15-C16
30	b	719	CLA	CHA-CBD-CGD-O1D
30	b	719	CLA	CHA-CBD-CGD-O2D
30	b	719	CLA	CAD-CBD-CGD-O1D
30	b	720	CLA	CBD-CGD-O2D-CED
30	b	723	CLA	C3A-C2A-CAA-CBA
30	b	723	CLA	CHA-CBD-CGD-O2D
30	b	724	CLA	C1A-C2A-CAA-CBA
30	b	725	CLA	C2-C3-C5-C6
30	b	725	CLA	C4-C3-C5-C6
30	B	308	CLA	C1A-C2A-CAA-CBA
30	B	309	CLA	CHA-CBD-CGD-O1D
30	B	309	CLA	CHA-CBD-CGD-O2D
30	B	311	CLA	CBD-CGD-O2D-CED
30	B	311	CLA	C14-C13-C15-C16
30	B	315	CLA	CHA-CBD-CGD-O1D
30	B	315	CLA	CHA-CBD-CGD-O2D
30	B	315	CLA	CAD-CBD-CGD-O1D
30	B	315	CLA	CAD-CBD-CGD-O2D
30	B	315	CLA	CBD-CGD-O2D-CED
30	B	317	CLA	C1A-C2A-CAA-CBA
30	D	309	CLA	CBA-CGA-O2A-C1
30	D	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	D	314	CLA	CBA-CGA-O2A-C1
30	D	314	CLA	CBD-CGD-O2D-CED
30	F	310	CLA	C1A-C2A-CAA-CBA
30	F	313	CLA	CBD-CGD-O2D-CED
30	F	315	CLA	CHA-CBD-CGD-O2D
30	H	304	CLA	CHA-CBD-CGD-O1D
30	H	304	CLA	CHA-CBD-CGD-O2D
30	H	307	CLA	CBD-CGD-O2D-CED
30	H	308	CLA	CBA-CGA-O2A-C1
30	H	309	CLA	C3A-C2A-CAA-CBA
30	H	309	CLA	CBD-CGD-O2D-CED
30	H	311	CLA	CAD-CBD-CGD-O1D
30	H	311	CLA	CAD-CBD-CGD-O2D
30	H	311	CLA	CBD-CGD-O2D-CED
30	H	312	CLA	C1A-C2A-CAA-CBA
30	H	312	CLA	C3A-C2A-CAA-CBA
30	H	312	CLA	CHA-CBD-CGD-O1D
30	H	312	CLA	CBD-CGD-O2D-CED
30	J	307	CLA	C1A-C2A-CAA-CBA
30	J	307	CLA	C3A-C2A-CAA-CBA
30	J	307	CLA	C2-C3-C5-C6
30	J	307	CLA	C4-C3-C5-C6
30	J	308	CLA	C2A-CAA-CBA-CGA
30	J	311	CLA	C1A-C2A-CAA-CBA
30	J	311	CLA	C3A-C2A-CAA-CBA
30	J	314	CLA	CHA-CBD-CGD-O1D
30	J	314	CLA	CHA-CBD-CGD-O2D
30	L	308	CLA	C1A-C2A-CAA-CBA
30	L	308	CLA	C3A-C2A-CAA-CBA
30	L	312	CLA	C3A-C2A-CAA-CBA
30	L	312	CLA	CBD-CGD-O2D-CED
30	L	313	CLA	C3A-C2A-CAA-CBA
30	L	317	CLA	C3-C5-C6-C7
30	L	318	CLA	CBD-CGD-O2D-CED
30	M	313	CLA	CHA-CBD-CGD-O1D
30	M	313	CLA	CHA-CBD-CGD-O2D
30	M	317	CLA	CBD-CGD-O2D-CED
30	M	317	CLA	O1D-CGD-O2D-CED
30	M	318	CLA	C1A-C2A-CAA-CBA
30	M	318	CLA	C3A-C2A-CAA-CBA
30	M	318	CLA	C2A-CAA-CBA-CGA
30	M	318	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	M	318	CLA	CAD-CBD-CGD-O2D
30	N	305	CLA	CHA-CBD-CGD-O1D
30	N	305	CLA	CHA-CBD-CGD-O2D
30	N	309	CLA	C1A-C2A-CAA-CBA
30	N	310	CLA	C1A-C2A-CAA-CBA
30	N	310	CLA	CBD-CGD-O2D-CED
30	O	314	CLA	CBD-CGD-O2D-CED
30	O	316	CLA	CAD-CBD-CGD-O1D
30	O	316	CLA	CAD-CBD-CGD-O2D
30	P	214	CLA	CBD-CGD-O2D-CED
30	P	215	CLA	CBD-CGD-O2D-CED
31	I	314	KC1	C2B-C3B-CAB-CBB
31	I	314	KC1	C4B-C3B-CAB-CBB
31	I	314	KC1	C2A-CAA-CBA-CGA
31	I	314	KC1	CHA-CBD-CGD-O2D
31	K	314	KC1	C1A-C2A-CAA-CBA
31	K	314	KC1	C2B-C3B-CAB-CBB
31	K	314	KC1	C4B-C3B-CAB-CBB
31	K	314	KC1	CAA-CBA-CGA-O1A
31	G	515	KC1	C4B-C3B-CAB-CBB
31	A	306	KC1	C1A-C2A-CAA-CBA
31	A	306	KC1	C2B-C3B-CAB-CBB
31	A	306	KC1	C4B-C3B-CAB-CBB
31	A	306	KC1	CHA-CBD-CGD-O2D
31	A	314	KC1	C2B-C3B-CAB-CBB
31	A	314	KC1	C4B-C3B-CAB-CBB
31	A	314	KC1	C2A-CAA-CBA-CGA
31	A	314	KC1	CHA-CBD-CGD-O1D
31	B	314	KC1	C2B-C3B-CAB-CBB
31	B	314	KC1	C4B-C3B-CAB-CBB
31	B	314	KC1	CBD-CGD-O2D-CED
31	D	310	KC1	C1A-C2A-CAA-CBA
31	D	310	KC1	C3A-C2A-CAA-CBA
31	D	310	KC1	C2B-C3B-CAB-CBB
31	D	310	KC1	C4B-C3B-CAB-CBB
31	D	310	KC1	C2A-CAA-CBA-CGA
31	D	310	KC1	CAA-CBA-CGA-O2A
31	D	310	KC1	CHA-CBD-CGD-O2D
31	F	309	KC1	C2B-C3B-CAB-CBB
31	F	309	KC1	C4B-C3B-CAB-CBB
31	F	309	KC1	CHA-CBD-CGD-O1D
31	F	309	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	F	314	KC1	C2B-C3B-CAB-CBB
31	F	314	KC1	C4B-C3B-CAB-CBB
31	F	314	KC1	CHA-CBD-CGD-O2D
31	H	306	KC1	C1A-C2A-CAA-CBA
31	H	306	KC1	C3A-C2A-CAA-CBA
31	H	306	KC1	C2B-C3B-CAB-CBB
31	H	306	KC1	C4B-C3B-CAB-CBB
31	H	310	KC1	C3A-C2A-CAA-CBA
31	H	310	KC1	C2B-C3B-CAB-CBB
31	H	310	KC1	C4B-C3B-CAB-CBB
31	H	310	KC1	CBD-CGD-O2D-CED
31	J	313	KC1	C1A-C2A-CAA-CBA
31	J	313	KC1	C2B-C3B-CAB-CBB
31	J	313	KC1	C4B-C3B-CAB-CBB
31	L	307	KC1	CHA-CBD-CGD-O1D
31	L	307	KC1	CHA-CBD-CGD-O2D
31	L	315	KC1	C1A-C2A-CAA-CBA
31	L	315	KC1	C2B-C3B-CAB-CBB
31	L	315	KC1	C4B-C3B-CAB-CBB
31	L	315	KC1	C2A-CAA-CBA-CGA
31	L	315	KC1	CBD-CGD-O2D-CED
31	M	307	KC1	C2B-C3B-CAB-CBB
31	M	307	KC1	C4B-C3B-CAB-CBB
31	M	314	KC1	C3A-C2A-CAA-CBA
31	M	314	KC1	C2B-C3B-CAB-CBB
31	M	314	KC1	C4B-C3B-CAB-CBB
31	M	314	KC1	CBD-CGD-O2D-CED
31	N	306	KC1	C1A-C2A-CAA-CBA
31	N	306	KC1	C3A-C2A-CAA-CBA
31	N	306	KC1	C2B-C3B-CAB-CBB
31	N	306	KC1	C4B-C3B-CAB-CBB
31	N	308	KC1	C2B-C3B-CAB-CBB
31	N	308	KC1	C2A-CAA-CBA-CGA
31	N	311	KC1	C1A-C2A-CAA-CBA
31	N	311	KC1	C3A-C2A-CAA-CBA
31	N	311	KC1	C2B-C3B-CAB-CBB
31	N	311	KC1	C4B-C3B-CAB-CBB
31	N	311	KC1	CBD-CGD-O2D-CED
31	O	310	KC1	C1A-C2A-CAA-CBA
31	O	310	KC1	C3A-C2A-CAA-CBA
31	O	310	KC1	C4B-C3B-CAB-CBB
31	O	310	KC1	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	O	312	KC1	C2B-C3B-CAB-CBB
31	O	312	KC1	C4B-C3B-CAB-CBB
31	O	312	KC1	C2A-CAA-CBA-CGA
31	O	312	KC1	CHA-CBD-CGD-O1D
31	O	315	KC1	C1A-C2A-CAA-CBA
31	O	315	KC1	CBD-CGD-O2D-CED
31	P	211	KC1	C1A-C2A-CAA-CBA
31	P	211	KC1	C2B-C3B-CAB-CBB
31	P	211	KC1	C4B-C3B-CAB-CBB
31	P	211	KC1	C2A-CAA-CBA-CGA
31	P	211	KC1	CHA-CBD-CGD-O2D
31	P	213	KC1	C2B-C3B-CAB-CBB
31	P	213	KC1	C4B-C3B-CAB-CBB
31	P	213	KC1	C2A-CAA-CBA-CGA
31	P	216	KC1	C1A-C2A-CAA-CBA
31	P	216	KC1	C3A-C2A-CAA-CBA
31	P	216	KC1	C2B-C3B-CAB-CBB
31	P	216	KC1	CBD-CGD-O2D-CED
32	G	521	DGD	C2E-C1E-O5D-C6D
32	G	521	DGD	O6E-C1E-O5D-C6D
32	j	103	DGD	C2B-C1B-O2G-C2G
33	I	318	LMG	O6-C1-O1-C7
33	K	317	LMG	O7-C8-C9-O8
33	K	317	LMG	C11-C10-O7-C8
33	j	101	LMG	O9-C10-O7-C8
33	j	101	LMG	C11-C10-O7-C8
33	b	734	LMG	C2-C1-O1-C7
33	b	734	LMG	O6-C1-O1-C7
33	b	734	LMG	O1-C7-C8-O7
33	b	734	LMG	C11-C10-O7-C8
33	B	318	LMG	O10-C28-O8-C9
33	P	201	LMG	C2-C1-O1-C7
33	P	201	LMG	O6-C1-O1-C7
33	P	201	LMG	C11-C10-O7-C8
34	G	506	PID	O1-C6-C7-C8
34	j	105	PID	C20-C21-C22-C23
34	j	105	PID	CM5-C21-C22-C23
34	D	301	PID	O1-C6-C7-C8
34	D	301	PID	O4-C12-C13-C14
34	D	302	PID	C26-C27-O6-C30
34	D	306	PID	O1-C6-C7-C8
34	D	307	PID	O1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	F	304	PID	O7-C30-O6-C27
34	F	305	PID	O7-C30-O6-C27
34	H	301	PID	O1-C6-C7-C8
34	N	301	PID	O4-C12-C13-C14
34	N	301	PID	C12-C13-C14-CM4
34	N	301	PID	O7-C30-O6-C27
34	N	302	PID	O7-C30-O6-C27
34	O	301	PID	O1-C6-C7-C8
34	O	301	PID	O7-C30-O6-C27
34	O	305	PID	C1-C6-C7-C8
34	O	305	PID	C19-C20-C21-C22
34	O	305	PID	C19-C20-C21-CM5
34	O	305	PID	C31-C30-O6-C27
34	O	305	PID	O7-C30-O6-C27
34	O	307	PID	O1-C6-C7-C8
34	P	202	PID	O1-C6-C7-C8
34	P	203	PID	O7-C30-O6-C27
34	P	205	PID	O4-C12-C13-C14
34	P	205	PID	C26-C27-O6-C30
34	P	208	PID	O7-C30-O6-C27
35	A	318	SQD	C46-C45-O47-C7
35	A	318	SQD	C8-C7-O47-C45
37	i	201	BCR	C5-C6-C7-C8
37	i	201	BCR	C7-C8-C9-C10
37	i	201	BCR	C7-C8-C9-C34
37	i	201	BCR	C21-C22-C23-C24
37	i	201	BCR	C37-C22-C23-C24
37	i	201	BCR	C23-C24-C25-C26
37	i	201	BCR	C23-C24-C25-C30
37	j	102	BCR	C7-C8-C9-C10
37	j	102	BCR	C7-C8-C9-C34
37	m	201	BCR	C7-C8-C9-C10
37	m	201	BCR	C7-C8-C9-C34
37	a	734	BCR	C7-C8-C9-C10
37	a	734	BCR	C7-C8-C9-C34
37	a	736	BCR	C7-C8-C9-C10
37	a	736	BCR	C7-C8-C9-C34
37	b	730	BCR	C21-C22-C23-C24
37	b	730	BCR	C37-C22-C23-C24
38	a	732	PQN	C12-C13-C15-C16
38	a	732	PQN	C14-C13-C15-C16
29	h	201	UIX	C31-C27-O2-C18

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Mol	Chain	Res	Type	Atoms
29	O	306	UIX	C31-C27-O2-C18
29	P	207	UIX	C31-C27-O2-C18
34	j	105	PID	O7-C30-O6-C27
34	F	304	PID	C31-C30-O6-C27
34	F	305	PID	C31-C30-O6-C27
34	H	302	PID	C31-C30-O6-C27
34	N	301	PID	C31-C30-O6-C27
34	N	302	PID	C31-C30-O6-C27
34	O	304	PID	O7-C30-O6-C27
34	P	203	PID	C31-C30-O6-C27
34	P	208	PID	C31-C30-O6-C27
30	a	722	CLA	O1D-CGD-O2D-CED
30	a	731	CLA	O1D-CGD-O2D-CED
30	H	309	CLA	O1D-CGD-O2D-CED
30	H	311	CLA	O1D-CGD-O2D-CED
31	I	314	KC1	O1D-CGD-O2D-CED
31	H	310	KC1	O1D-CGD-O2D-CED
31	L	315	KC1	O1D-CGD-O2D-CED
31	M	314	KC1	O1D-CGD-O2D-CED
31	N	311	KC1	O1D-CGD-O2D-CED
31	O	315	KC1	O1D-CGD-O2D-CED
31	P	216	KC1	O1D-CGD-O2D-CED
29	G	503	UIX	O4-C27-O2-C18
29	J	305	UIX	C31-C27-O2-C18
34	j	105	PID	C31-C30-O6-C27
34	O	301	PID	C31-C30-O6-C27
34	O	304	PID	C31-C30-O6-C27
30	K	312	CLA	O1D-CGD-O2D-CED
30	a	712	CLA	O1D-CGD-O2D-CED
30	a	715	CLA	O1D-CGD-O2D-CED
30	B	311	CLA	O1D-CGD-O2D-CED
30	F	312	CLA	O1D-CGD-O2D-CED
30	L	312	CLA	O1D-CGD-O2D-CED
30	N	310	CLA	O1D-CGD-O2D-CED
31	B	314	KC1	O1D-CGD-O2D-CED
30	I	309	CLA	CBD-CGD-O2D-CED
30	I	316	CLA	CBD-CGD-O2D-CED
30	K	312	CLA	CBD-CGD-O2D-CED
30	A	313	CLA	CBD-CGD-O2D-CED
30	A	319	CLA	CBD-CGD-O2D-CED
30	j	106	CLA	CBD-CGD-O2D-CED
30	a	704	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	712	CLA	CBD-CGD-O2D-CED
30	a	714	CLA	CBD-CGD-O2D-CED
30	a	730	CLA	CBD-CGD-O2D-CED
30	B	317	CLA	CBD-CGD-O2D-CED
30	D	313	CLA	CBD-CGD-O2D-CED
30	F	310	CLA	CBD-CGD-O2D-CED
30	F	312	CLA	CBD-CGD-O2D-CED
30	L	316	CLA	CBD-CGD-O2D-CED
30	M	315	CLA	CBD-CGD-O2D-CED
30	M	316	CLA	CBD-CGD-O2D-CED
30	M	318	CLA	CBD-CGD-O2D-CED
30	N	307	CLA	CBD-CGD-O2D-CED
30	O	313	CLA	CBD-CGD-O2D-CED
30	O	316	CLA	CBD-CGD-O2D-CED
30	P	212	CLA	CBD-CGD-O2D-CED
30	P	217	CLA	CBD-CGD-O2D-CED
31	I	314	KC1	CBD-CGD-O2D-CED
31	P	211	KC1	CBD-CGD-O2D-CED
30	b	701	CLA	O1A-CGA-O2A-C1
30	H	304	CLA	O1A-CGA-O2A-C1
30	J	307	CLA	O1A-CGA-O2A-C1
30	J	311	CLA	O1A-CGA-O2A-C1
30	N	310	CLA	O1A-CGA-O2A-C1
30	O	308	CLA	O1A-CGA-O2A-C1
30	O	314	CLA	O1A-CGA-O2A-C1
30	A	311	CLA	O1A-CGA-O2A-C1
30	A	320	CLA	O1A-CGA-O2A-C1
30	D	312	CLA	O1A-CGA-O2A-C1
30	D	314	CLA	O1A-CGA-O2A-C1
30	H	308	CLA	O1A-CGA-O2A-C1
34	H	302	PID	O7-C30-O6-C27
30	I	309	CLA	O1D-CGD-O2D-CED
30	D	313	CLA	O1D-CGD-O2D-CED
30	D	314	CLA	O1D-CGD-O2D-CED
30	H	312	CLA	O1D-CGD-O2D-CED
30	M	318	CLA	O1D-CGD-O2D-CED
30	N	307	CLA	O1D-CGD-O2D-CED
30	O	316	CLA	O1D-CGD-O2D-CED
30	P	215	CLA	O1D-CGD-O2D-CED
30	G	518	CLA	CBA-CGA-O2A-C1
30	F	307	CLA	CBA-CGA-O2A-C1
30	F	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	J	310	CLA	CBA-CGA-O2A-C1
29	J	305	UIX	C19-C18-O2-C27
30	I	313	CLA	O1D-CGD-O2D-CED
30	I	316	CLA	O1D-CGD-O2D-CED
30	K	308	CLA	O1D-CGD-O2D-CED
30	f	301	CLA	O1D-CGD-O2D-CED
30	a	702	CLA	O1D-CGD-O2D-CED
30	a	707	CLA	O1D-CGD-O2D-CED
30	b	701	CLA	O1D-CGD-O2D-CED
30	b	711	CLA	O1D-CGD-O2D-CED
30	B	315	CLA	O1D-CGD-O2D-CED
30	F	313	CLA	O1D-CGD-O2D-CED
30	O	314	CLA	O1D-CGD-O2D-CED
30	P	214	CLA	O1D-CGD-O2D-CED
30	b	701	CLA	CBA-CGA-O2A-C1
30	H	304	CLA	CBA-CGA-O2A-C1
30	J	307	CLA	CBA-CGA-O2A-C1
30	J	311	CLA	CBA-CGA-O2A-C1
30	O	308	CLA	CBA-CGA-O2A-C1
30	O	314	CLA	CBA-CGA-O2A-C1
32	G	521	DGD	C2A-C1A-O1G-C1G
33	K	317	LMG	C29-C28-O8-C9
33	j	101	LMG	C29-C28-O8-C9
30	I	319	CLA	CBD-CGD-O2D-CED
30	I	321	CLA	CBD-CGD-O2D-CED
30	A	315	CLA	CBD-CGD-O2D-CED
30	l	308	CLA	CBD-CGD-O2D-CED
30	m	202	CLA	CBD-CGD-O2D-CED
30	a	711	CLA	CBD-CGD-O2D-CED
30	a	725	CLA	CBD-CGD-O2D-CED
30	a	726	CLA	CBD-CGD-O2D-CED
30	b	707	CLA	CBD-CGD-O2D-CED
30	b	713	CLA	CBD-CGD-O2D-CED
30	H	304	CLA	CBD-CGD-O2D-CED
30	H	308	CLA	CBD-CGD-O2D-CED
30	J	306	CLA	CBD-CGD-O2D-CED
30	J	307	CLA	CBD-CGD-O2D-CED
30	J	308	CLA	CBD-CGD-O2D-CED
30	J	315	CLA	CBD-CGD-O2D-CED
30	L	313	CLA	CBD-CGD-O2D-CED
30	M	308	CLA	CBD-CGD-O2D-CED
30	M	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	M	310	CLA	CBD-CGD-O2D-CED
30	P	209	CLA	CBD-CGD-O2D-CED
29	O	306	UIX	O4-C27-O2-C18
34	P	202	PID	C31-C30-O6-C27
34	P	202	PID	O7-C30-O6-C27
30	I	308	CLA	O1A-CGA-O2A-C1
30	I	315	CLA	O1A-CGA-O2A-C1
30	K	308	CLA	O1A-CGA-O2A-C1
30	G	513	CLA	O1A-CGA-O2A-C1
30	a	706	CLA	O1A-CGA-O2A-C1
30	a	721	CLA	O1A-CGA-O2A-C1
30	b	707	CLA	O1A-CGA-O2A-C1
30	b	717	CLA	O1A-CGA-O2A-C1
30	B	311	CLA	O1A-CGA-O2A-C1
30	H	309	CLA	O1A-CGA-O2A-C1
30	L	313	CLA	O1A-CGA-O2A-C1
32	G	521	DGD	O1A-C1A-O1G-C1G
33	I	318	LMG	O10-C28-O8-C9
33	K	317	LMG	O10-C28-O8-C9
33	j	101	LMG	O10-C28-O8-C9
33	b	733	LMG	O10-C28-O8-C9
30	G	517	CLA	O1A-CGA-O2A-C1
30	f	302	CLA	O1A-CGA-O2A-C1
30	F	311	CLA	O1A-CGA-O2A-C1
30	K	315	CLA	O1D-CGD-O2D-CED
30	l	312	CLA	O1D-CGD-O2D-CED
30	b	703	CLA	O1D-CGD-O2D-CED
30	H	307	CLA	O1D-CGD-O2D-CED
31	B	314	KC1	CAA-CBA-CGA-O1A
29	P	207	UIX	O4-C27-O2-C18
30	b	720	CLA	O1D-CGD-O2D-CED
30	L	318	CLA	O1D-CGD-O2D-CED
29	I	304	UIX	O4-C27-O2-C18
34	G	506	PID	C31-C30-O6-C27
30	A	312	CLA	CBD-CGD-O2D-CED
30	b	715	CLA	CBD-CGD-O2D-CED
30	J	311	CLA	CBD-CGD-O2D-CED
30	M	311	CLA	CBD-CGD-O2D-CED
31	O	312	KC1	CBD-CGD-O2D-CED
30	G	516	CLA	O1D-CGD-O2D-CED
30	l	310	CLA	O1D-CGD-O2D-CED
30	a	713	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	a	721	CLA	O1D-CGD-O2D-CED
30	b	704	CLA	O1D-CGD-O2D-CED
30	F	310	CLA	O1D-CGD-O2D-CED
30	M	315	CLA	O1D-CGD-O2D-CED
32	j	103	DGD	O1B-C1B-O2G-C2G
33	I	318	LMG	O9-C10-O7-C8
33	I	320	LMG	O9-C10-O7-C8
33	K	317	LMG	O9-C10-O7-C8
33	b	734	LMG	O9-C10-O7-C8
33	B	318	LMG	O9-C10-O7-C8
35	A	318	SQD	O49-C7-O47-C45
30	F	313	CLA	CBA-CGA-O2A-C1
30	a	718	CLA	O1A-CGA-O2A-C1
30	F	310	CLA	O1A-CGA-O2A-C1
30	I	311	CLA	C3-C5-C6-C7
30	I	312	CLA	C3-C5-C6-C7
30	I	316	CLA	C3-C5-C6-C7
30	K	313	CLA	C3-C5-C6-C7
30	G	514	CLA	C3-C5-C6-C7
30	G	519	CLA	C3-C5-C6-C7
30	j	104	CLA	C3-C5-C6-C7
30	l	305	CLA	C3-C5-C6-C7
30	a	702	CLA	C3-C5-C6-C7
30	a	705	CLA	C3-C5-C6-C7
30	a	706	CLA	C3-C5-C6-C7
30	b	701	CLA	C3-C5-C6-C7
30	b	707	CLA	C3-C5-C6-C7
30	b	717	CLA	C3-C5-C6-C7
30	B	310	CLA	C3-C5-C6-C7
30	J	307	CLA	C3-C5-C6-C7
30	L	309	CLA	C3-C5-C6-C7
30	I	315	CLA	CBA-CGA-O2A-C1
30	K	308	CLA	CBA-CGA-O2A-C1
30	G	513	CLA	CBA-CGA-O2A-C1
30	a	706	CLA	CBA-CGA-O2A-C1
30	a	728	CLA	CBA-CGA-O2A-C1
30	b	720	CLA	CBA-CGA-O2A-C1
30	B	310	CLA	CBA-CGA-O2A-C1
30	H	309	CLA	CBA-CGA-O2A-C1
30	L	314	CLA	CBA-CGA-O2A-C1
30	L	317	CLA	CBA-CGA-O2A-C1
30	N	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	b	733	LMG	C29-C28-O8-C9
34	G	506	PID	O7-C30-O6-C27
33	I	318	LMG	C11-C10-O7-C8
33	I	320	LMG	C11-C10-O7-C8
33	B	318	LMG	C11-C10-O7-C8
30	O	313	CLA	O1D-CGD-O2D-CED
30	G	512	CLA	CBD-CGD-O2D-CED
30	L	314	CLA	CBD-CGD-O2D-CED
31	M	307	KC1	CBD-CGD-O2D-CED
34	D	305	PID	C31-C30-O6-C27
34	D	305	PID	O7-C30-O6-C27
30	N	304	CLA	O1A-CGA-O2A-C1
30	P	215	CLA	O1A-CGA-O2A-C1
30	D	309	CLA	O1A-CGA-O2A-C1
30	F	313	CLA	O1A-CGA-O2A-C1
31	F	309	KC1	CAA-CBA-CGA-O2A
30	a	718	CLA	CBA-CGA-O2A-C1
30	F	310	CLA	CBA-CGA-O2A-C1
30	M	316	CLA	C3-C5-C6-C7
30	I	308	CLA	C4-C3-C5-C6
30	A	313	CLA	C4-C3-C5-C6
30	l	305	CLA	C4-C3-C5-C6
30	l	311	CLA	C4-C3-C5-C6
30	a	731	CLA	C4-C3-C5-C6
30	L	309	CLA	C4-C3-C5-C6
30	L	317	CLA	C4-C3-C5-C6
30	M	308	CLA	C4-C3-C5-C6
30	M	316	CLA	C4-C3-C5-C6
30	a	713	CLA	C2-C3-C5-C6
30	a	724	CLA	C2-C3-C5-C6
30	a	731	CLA	C2-C3-C5-C6
30	a	735	CLA	C2-C3-C5-C6
30	M	308	CLA	C2-C3-C5-C6
30	a	723	CLA	CBD-CGD-O2D-CED
30	B	312	CLA	CBD-CGD-O2D-CED
30	K	308	CLA	C2A-CAA-CBA-CGA
30	G	513	CLA	C2A-CAA-CBA-CGA
30	G	520	CLA	C2A-CAA-CBA-CGA
30	A	319	CLA	C2A-CAA-CBA-CGA
30	a	709	CLA	C2A-CAA-CBA-CGA
30	a	719	CLA	C2A-CAA-CBA-CGA
30	N	305	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	O	314	CLA	C2A-CAA-CBA-CGA
30	G	518	CLA	O1A-CGA-O2A-C1
30	J	310	CLA	O1A-CGA-O2A-C1
30	A	308	CLA	C3-C5-C6-C7
30	A	312	CLA	C3-C5-C6-C7
30	h	202	CLA	C3-C5-C6-C7
30	I	308	CLA	CBA-CGA-O2A-C1
30	G	514	CLA	CBA-CGA-O2A-C1
30	a	721	CLA	CBA-CGA-O2A-C1
30	b	707	CLA	CBA-CGA-O2A-C1
30	b	717	CLA	CBA-CGA-O2A-C1
30	B	311	CLA	CBA-CGA-O2A-C1
30	L	313	CLA	CBA-CGA-O2A-C1
30	N	304	CLA	CBA-CGA-O2A-C1
30	P	215	CLA	CBA-CGA-O2A-C1
33	I	318	LMG	C29-C28-O8-C9
33	B	318	LMG	C29-C28-O8-C9
29	J	305	UIX	O4-C27-O2-C18
30	j	106	CLA	O1D-CGD-O2D-CED
30	B	317	CLA	O1D-CGD-O2D-CED
30	A	313	CLA	O1D-CGD-O2D-CED
30	A	319	CLA	O1D-CGD-O2D-CED
30	a	714	CLA	O1D-CGD-O2D-CED
30	a	730	CLA	O1D-CGD-O2D-CED
30	P	212	CLA	O1D-CGD-O2D-CED
33	B	318	LMG	C4-C5-C6-O5
30	G	514	CLA	O1A-CGA-O2A-C1
30	l	313	CLA	O1A-CGA-O2A-C1
30	a	728	CLA	O1A-CGA-O2A-C1
30	b	720	CLA	O1A-CGA-O2A-C1
30	L	317	CLA	O1A-CGA-O2A-C1
30	l	310	CLA	O1A-CGA-O2A-C1
30	F	307	CLA	O1A-CGA-O2A-C1
30	M	316	CLA	O1D-CGD-O2D-CED
28	I	301	DD6	C24-C25-C26-C27
28	G	502	DD6	C24-C25-C26-C27
28	M	302	DD6	C1-C2-C3-C4
34	F	305	PID	C14-C15-C16-C17
34	F	305	PID	C18-C19-C20-C21
34	O	305	PID	C14-C15-C16-C17
34	P	206	PID	C31-C30-O6-C27
31	P	213	KC1	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
31	P	213	KC1	CAA-CBA-CGA-O2A
30	I	306	CLA	CBD-CGD-O2D-CED
30	I	311	CLA	CBD-CGD-O2D-CED
30	A	308	CLA	CBD-CGD-O2D-CED
30	A	320	CLA	CBD-CGD-O2D-CED
30	f	303	CLA	CBD-CGD-O2D-CED
30	l	313	CLA	CBD-CGD-O2D-CED
30	a	705	CLA	CBD-CGD-O2D-CED
30	a	709	CLA	CBD-CGD-O2D-CED
30	b	712	CLA	CBD-CGD-O2D-CED
30	b	727	CLA	CBD-CGD-O2D-CED
30	J	301	CLA	CBD-CGD-O2D-CED
30	J	314	CLA	CBD-CGD-O2D-CED
30	L	317	CLA	CBD-CGD-O2D-CED
31	D	310	KC1	CBD-CGD-O2D-CED
30	G	511	CLA	C3-C5-C6-C7
30	A	309	CLA	C3-C5-C6-C7
30	J	301	CLA	CBA-CGA-O2A-C1
29	B	305	UIX	C31-C27-O2-C18
34	F	302	PID	C31-C30-O6-C27
34	H	301	PID	C31-C30-O6-C27
34	O	302	PID	C31-C30-O6-C27
30	B	310	CLA	O1A-CGA-O2A-C1
30	L	314	CLA	O1A-CGA-O2A-C1
30	a	704	CLA	O1D-CGD-O2D-CED
30	L	316	CLA	O1D-CGD-O2D-CED
30	P	217	CLA	O1D-CGD-O2D-CED
29	B	305	UIX	O4-C27-O2-C18
34	F	302	PID	O7-C30-O6-C27
34	H	301	PID	O7-C30-O6-C27
34	O	302	PID	O7-C30-O6-C27
34	P	206	PID	O7-C30-O6-C27
30	K	316	CLA	CBA-CGA-O2A-C1
30	H	312	CLA	CBA-CGA-O2A-C1
30	G	519	CLA	CBD-CGD-O2D-CED
30	a	710	CLA	CBD-CGD-O2D-CED
30	B	316	CLA	CBD-CGD-O2D-CED
30	J	309	CLA	CBD-CGD-O2D-CED
31	N	306	KC1	CBD-CGD-O2D-CED
33	K	317	LMG	O6-C5-C6-O5
30	b	703	CLA	C3-C5-C6-C7
30	l	313	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	P	201	LMG	O6-C5-C6-O5
31	D	315	KC1	CAA-CBA-CGA-O2A
31	F	309	KC1	CAA-CBA-CGA-O1A
31	J	313	KC1	CAA-CBA-CGA-O2A
31	O	310	KC1	CAA-CBA-CGA-O2A
30	b	704	CLA	C2C-C3C-CAC-CBC
30	J	301	CLA	O1A-CGA-O2A-C1
30	G	510	CLA	C4-C3-C5-C6
30	b	703	CLA	C4-C3-C5-C6
30	P	210	CLA	C4-C3-C5-C6
30	G	510	CLA	C2-C3-C5-C6
30	b	703	CLA	C2-C3-C5-C6
30	P	210	CLA	C2-C3-C5-C6
30	a	735	CLA	CBD-CGD-O2D-CED
30	a	722	CLA	C2A-CAA-CBA-CGA
30	b	727	CLA	C2A-CAA-CBA-CGA
33	B	318	LMG	O6-C5-C6-O5
32	G	501	DGD	O6E-C1E-O5D-C6D
33	D	317	LMG	O6-C1-O1-C7
30	a	708	CLA	CBA-CGA-O2A-C1
30	a	709	CLA	CBA-CGA-O2A-C1
30	b	723	CLA	CBA-CGA-O2A-C1
30	B	309	CLA	CBA-CGA-O2A-C1
30	M	308	CLA	CBA-CGA-O2A-C1
30	G	514	CLA	CBD-CGD-O2D-CED
31	B	314	KC1	CAA-CBA-CGA-O2A
31	P	216	KC1	CAA-CBA-CGA-O2A
30	b	707	CLA	O1D-CGD-O2D-CED
30	H	308	CLA	O1D-CGD-O2D-CED
30	J	308	CLA	O1D-CGD-O2D-CED
30	M	309	CLA	O1D-CGD-O2D-CED
30	O	308	CLA	CBD-CGD-O2D-CED
30	a	708	CLA	O1A-CGA-O2A-C1
30	b	723	CLA	O1A-CGA-O2A-C1
30	M	308	CLA	O1A-CGA-O2A-C1
30	b	728	CLA	C3-C5-C6-C7
30	M	308	CLA	C3-C5-C6-C7
30	I	319	CLA	O1D-CGD-O2D-CED
30	b	713	CLA	O1D-CGD-O2D-CED
30	J	307	CLA	O1D-CGD-O2D-CED
30	I	321	CLA	CBA-CGA-O2A-C1
30	G	519	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	A	313	CLA	CBA-CGA-O2A-C1
30	l	311	CLA	CBA-CGA-O2A-C1
30	a	707	CLA	CBA-CGA-O2A-C1
30	a	712	CLA	CBA-CGA-O2A-C1
30	M	312	CLA	CBA-CGA-O2A-C1
30	B	313	CLA	CBD-CGD-O2D-CED
30	F	315	CLA	CBD-CGD-O2D-CED
30	O	311	CLA	CBD-CGD-O2D-CED
30	K	316	CLA	O1A-CGA-O2A-C1
30	H	312	CLA	O1A-CGA-O2A-C1
30	a	721	CLA	C10-C11-C12-C13
30	b	717	CLA	C5-C6-C7-C8
31	K	314	KC1	CAA-CBA-CGA-O2A
31	A	314	KC1	CAA-CBA-CGA-O2A
31	N	308	KC1	CAA-CBA-CGA-O2A
31	O	315	KC1	CAA-CBA-CGA-O1A
30	a	730	CLA	C5-C6-C7-C8
30	b	719	CLA	CBA-CGA-O2A-C1
30	M	317	CLA	CBA-CGA-O2A-C1
32	y	201	DGD	C1B-C2B-C3B-C4B
35	A	318	SQD	C2-C1-O6-C44
32	y	201	DGD	O2G-C2G-C3G-O3G
30	I	308	CLA	C2-C3-C5-C6
30	A	313	CLA	C2-C3-C5-C6
30	L	309	CLA	C2-C3-C5-C6
30	M	316	CLA	C2-C3-C5-C6
30	I	312	CLA	C14-C13-C15-C16
30	l	303	CLA	C11-C12-C13-C14
30	l	304	CLA	C11-C10-C8-C9
30	l	305	CLA	C11-C12-C13-C14
30	a	707	CLA	C11-C10-C8-C9
30	a	720	CLA	C11-C12-C13-C14
30	a	721	CLA	C14-C13-C15-C16
30	a	722	CLA	C6-C7-C8-C9
30	a	724	CLA	C6-C7-C8-C9
30	a	731	CLA	C11-C12-C13-C14
30	b	704	CLA	C6-C7-C8-C9
30	b	708	CLA	C6-C7-C8-C9
30	B	311	CLA	C6-C7-C8-C9
30	A	315	CLA	O1D-CGD-O2D-CED
30	J	306	CLA	O1D-CGD-O2D-CED
30	J	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	L	313	CLA	O1D-CGD-O2D-CED
30	J	310	CLA	CBD-CGD-O2D-CED
30	b	713	CLA	C10-C11-C12-C13
30	B	313	CLA	C10-C11-C12-C13
30	f	303	CLA	C2A-CAA-CBA-CGA
30	a	717	CLA	C2A-CAA-CBA-CGA
30	B	309	CLA	C2A-CAA-CBA-CGA
30	F	311	CLA	C2A-CAA-CBA-CGA
30	J	315	CLA	C2A-CAA-CBA-CGA
28	I	305	DD6	C7-C6-C8-C9
28	K	305	DD6	C12-C11-C13-C14
28	G	502	DD6	C12-C11-C13-C14
28	b	731	DD6	C12-C11-C13-C14
28	D	303	DD6	C12-C11-C13-C14
28	L	302	DD6	C12-C11-C13-C14
29	P	207	UIX	C36-C38-C40-C41
37	l	306	BCR	C37-C22-C23-C24
37	b	702	BCR	C37-C22-C23-C24
37	b	730	BCR	C7-C8-C9-C34
28	K	301	DD6	C10-C11-C13-C14
28	B	302	DD6	C10-C11-C13-C14
28	D	303	DD6	C10-C11-C13-C14
28	L	302	DD6	C10-C11-C13-C14
37	l	306	BCR	C21-C22-C23-C24
37	b	702	BCR	C21-C22-C23-C24
37	b	730	BCR	C7-C8-C9-C10
33	I	318	LMG	C28-C29-C30-C31
30	G	519	CLA	O1A-CGA-O2A-C1
30	A	313	CLA	O1A-CGA-O2A-C1
30	a	707	CLA	O1A-CGA-O2A-C1
30	M	312	CLA	O1A-CGA-O2A-C1
30	I	312	CLA	C13-C15-C16-C17
30	I	313	CLA	C5-C6-C7-C8
30	j	106	CLA	C5-C6-C7-C8
30	B	313	CLA	C8-C10-C11-C12
30	J	307	CLA	C8-C10-C11-C12
30	l	308	CLA	O1D-CGD-O2D-CED
30	a	725	CLA	O1D-CGD-O2D-CED
30	M	308	CLA	O1D-CGD-O2D-CED
31	L	307	KC1	CAA-CBA-CGA-O2A
31	M	307	KC1	CAA-CBA-CGA-O2A
31	P	211	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	P	216	KC1	CAA-CBA-CGA-O1A
30	H	304	CLA	O1D-CGD-O2D-CED
30	l	303	CLA	C8-C10-C11-C12
30	a	706	CLA	C5-C6-C7-C8
30	a	713	CLA	C10-C11-C12-C13
30	b	713	CLA	C8-C10-C11-C12
30	J	309	CLA	C5-C6-C7-C8
33	I	318	LMG	C10-C11-C12-C13
30	a	711	CLA	O1D-CGD-O2D-CED
30	a	726	CLA	O1D-CGD-O2D-CED
30	P	209	CLA	O1D-CGD-O2D-CED
33	P	201	LMG	C4-C5-C6-O5
31	F	314	KC1	CBD-CGD-O2D-CED
34	O	305	PID	C17-C18-C19-C20
30	I	309	CLA	C5-C6-C7-C8
30	m	202	CLA	C5-C6-C7-C8
30	a	723	CLA	C13-C15-C16-C17
30	a	724	CLA	C15-C16-C17-C18
30	a	726	CLA	C15-C16-C17-C18
30	b	722	CLA	C15-C16-C17-C18
30	B	310	CLA	C5-C6-C7-C8
30	J	307	CLA	C13-C15-C16-C17
30	I	321	CLA	C2C-C3C-CAC-CBC
30	l	311	CLA	O1A-CGA-O2A-C1
33	j	101	LMG	C28-C29-C30-C31
31	O	310	KC1	CBD-CGD-O2D-CED
30	I	312	CLA	C15-C16-C17-C18
30	a	707	CLA	C5-C6-C7-C8
30	b	707	CLA	C10-C11-C12-C13
30	P	210	CLA	C15-C16-C17-C18
30	I	321	CLA	O1D-CGD-O2D-CED
30	m	202	CLA	O1D-CGD-O2D-CED
30	M	310	CLA	O1D-CGD-O2D-CED
31	D	310	KC1	CAA-CBA-CGA-O1A
31	N	308	KC1	CAA-CBA-CGA-O1A
30	H	305	CLA	C15-C16-C17-C18
30	A	309	CLA	CBD-CGD-O2D-CED
30	a	706	CLA	CBD-CGD-O2D-CED
30	K	312	CLA	O2A-C1-C2-C3
30	a	735	CLA	C13-C15-C16-C17
30	b	705	CLA	C10-C11-C12-C13
30	b	722	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	B	309	CLA	C13-C15-C16-C17
30	b	715	CLA	O1D-CGD-O2D-CED
30	M	311	CLA	O1D-CGD-O2D-CED
30	a	731	CLA	C11-C12-C13-C15
30	b	708	CLA	C6-C7-C8-C10
30	b	717	CLA	C6-C7-C8-C10
30	b	717	CLA	C12-C13-C15-C16
30	b	724	CLA	C11-C12-C13-C15
28	I	305	DD6	C11-C10-C9-C8
28	M	302	DD6	C24-C25-C26-C27
28	M	306	DD6	C24-C25-C26-C27
29	P	207	UIX	C32-C35-C36-C38
34	O	305	PID	C18-C19-C20-C21
30	I	308	CLA	C2A-CAA-CBA-CGA
30	b	719	CLA	C2A-CAA-CBA-CGA
30	b	724	CLA	C2A-CAA-CBA-CGA
30	H	312	CLA	C2A-CAA-CBA-CGA
30	L	312	CLA	C2A-CAA-CBA-CGA
30	M	310	CLA	C2A-CAA-CBA-CGA
30	P	215	CLA	C2A-CAA-CBA-CGA
30	A	312	CLA	O1D-CGD-O2D-CED
30	J	311	CLA	O1D-CGD-O2D-CED
30	I	312	CLA	C10-C11-C12-C13
30	G	510	CLA	C5-C6-C7-C8
30	l	305	CLA	C5-C6-C7-C8
30	l	313	CLA	C5-C6-C7-C8
30	a	709	CLA	C5-C6-C7-C8
30	b	705	CLA	C13-C15-C16-C17
30	I	321	CLA	O1A-CGA-O2A-C1
30	a	712	CLA	O1A-CGA-O2A-C1
32	y	201	DGD	O6D-C1D-O3G-C3G
33	j	101	LMG	O6-C1-O1-C7
35	A	318	SQD	O5-C1-O6-C44
30	I	311	CLA	C5-C6-C7-C8
30	l	311	CLA	C8-C10-C11-C12
30	a	723	CLA	C15-C16-C17-C18
30	b	707	CLA	C15-C16-C17-C18
30	B	311	CLA	C13-C15-C16-C17
30	K	313	CLA	CBA-CGA-O2A-C1
30	a	709	CLA	O1A-CGA-O2A-C1
30	B	309	CLA	O1A-CGA-O2A-C1
30	I	308	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	h	202	CLA	C5-C6-C7-C8
30	l	311	CLA	C5-C6-C7-C8
30	a	705	CLA	C5-C6-C7-C8
30	a	723	CLA	C5-C6-C7-C8
30	B	311	CLA	C10-C11-C12-C13
30	L	314	CLA	O1D-CGD-O2D-CED
32	G	521	DGD	C4A-C5A-C6A-C7A
30	I	312	CLA	C5-C6-C7-C8
30	I	316	CLA	C5-C6-C7-C8
30	A	313	CLA	C3-C5-C6-C7
30	a	716	CLA	CBD-CGD-O2D-CED
30	B	309	CLA	C15-C16-C17-C18
38	b	729	PQN	C20-C21-C22-C23
30	G	512	CLA	O1D-CGD-O2D-CED
32	G	501	DGD	O6D-C5D-C6D-O5D
30	a	723	CLA	O1D-CGD-O2D-CED
33	j	101	LMG	O6-C5-C6-O5
32	G	521	DGD	O1B-C1B-O2G-C2G
30	L	317	CLA	C2-C3-C5-C6
30	I	319	CLA	C2A-CAA-CBA-CGA
30	B	317	CLA	C2A-CAA-CBA-CGA
30	D	312	CLA	C2A-CAA-CBA-CGA
30	J	316	CLA	C2A-CAA-CBA-CGA
30	L	308	CLA	C2A-CAA-CBA-CGA
30	M	311	CLA	C2A-CAA-CBA-CGA
30	m	202	CLA	C11-C12-C13-C15
30	b	720	CLA	C3-C5-C6-C7
30	L	313	CLA	C3-C5-C6-C7
30	L	314	CLA	C3-C5-C6-C7
34	F	305	PID	C16-C17-C18-C19
31	I	314	KC1	CAA-CBA-CGA-O2A
30	I	306	CLA	CBA-CGA-O2A-C1
30	b	716	CLA	CBA-CGA-O2A-C1
30	B	313	CLA	CBA-CGA-O2A-C1
30	L	309	CLA	CBA-CGA-O2A-C1
30	G	513	CLA	C5-C6-C7-C8
32	G	521	DGD	C1A-C2A-C3A-C4A
30	a	707	CLA	C8-C10-C11-C12
29	J	305	UIX	C11-C13-C14-C23
30	D	309	CLA	CBD-CGD-O2D-CED
31	N	308	KC1	CBD-CGD-O2D-CED
32	G	521	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
34	D	307	PID	C19-C20-C21-CM5
34	F	305	PID	C19-C20-C21-CM5
30	I	313	CLA	C3-C5-C6-C7
30	b	709	CLA	C3-C5-C6-C7
33	I	318	LMG	C29-C30-C31-C32
30	B	312	CLA	O1D-CGD-O2D-CED
31	K	314	KC1	C2A-CAA-CBA-CGA
31	B	314	KC1	C2A-CAA-CBA-CGA
31	F	314	KC1	C2A-CAA-CBA-CGA
31	J	313	KC1	C2A-CAA-CBA-CGA
30	G	512	CLA	C11-C12-C13-C14
30	B	311	CLA	C16-C17-C18-C20
32	l	301	DGD	C2B-C3B-C4B-C5B
33	D	317	LMG	C32-C33-C34-C35
33	B	318	LMG	C7-C8-O7-C10
33	P	201	LMG	O9-C10-O7-C8
31	M	307	KC1	CAA-CBA-CGA-O1A
31	O	312	KC1	CAA-CBA-CGA-O2A
33	K	317	LMG	C32-C33-C34-C35
33	D	317	LMG	C15-C16-C17-C18
33	K	317	LMG	C4-C5-C6-O5
30	I	311	CLA	O1D-CGD-O2D-CED
32	G	521	DGD	C2D-C1D-O3G-C3G
33	I	318	LMG	C2-C1-O1-C7
33	j	101	LMG	C2-C1-O1-C7
34	D	306	PID	C19-C20-C21-C22
34	D	307	PID	C19-C20-C21-C22
34	F	305	PID	C19-C20-C21-C22
30	b	704	CLA	C4C-C3C-CAC-CBC
33	b	733	LMG	C33-C34-C35-C36
30	I	316	CLA	C6-C7-C8-C9
30	h	202	CLA	C6-C7-C8-C9
30	j	104	CLA	C6-C7-C8-C10
30	b	708	CLA	C16-C17-C18-C20
30	b	715	CLA	C11-C12-C13-C15
30	b	717	CLA	C16-C17-C18-C20
33	K	317	LMG	C34-C35-C36-C37
33	B	318	LMG	C31-C32-C33-C34
30	l	305	CLA	C2-C3-C5-C6
30	l	311	CLA	C2-C3-C5-C6
30	a	702	CLA	C11-C12-C13-C14
30	a	723	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	b	701	CLA	C11-C12-C13-C14
30	b	717	CLA	C6-C7-C8-C9
30	b	717	CLA	C11-C12-C13-C14
30	b	727	CLA	C14-C13-C15-C16
32	I	317	DGD	C1B-C2B-C3B-C4B
33	K	317	LMG	C31-C32-C33-C34
31	P	211	KC1	CAA-CBA-CGA-O1A
30	f	302	CLA	C2A-CAA-CBA-CGA
30	j	106	CLA	C2A-CAA-CBA-CGA
30	b	701	CLA	C2A-CAA-CBA-CGA
30	B	308	CLA	C2A-CAA-CBA-CGA
30	N	310	CLA	C2A-CAA-CBA-CGA
28	K	318	DD6	C12-C11-C13-C14
28	A	301	DD6	C12-C11-C13-C14
28	B	302	DD6	C12-C11-C13-C14
28	J	304	DD6	C12-C11-C13-C14
28	M	303	DD6	C12-C11-C13-C14
29	J	305	UIX	C7-C10-C11-C12
33	b	733	LMG	C36-C37-C38-C39
28	K	318	DD6	C10-C11-C13-C14
28	A	301	DD6	C10-C11-C13-C14
28	M	303	DD6	C10-C11-C13-C14
29	J	305	UIX	C7-C10-C11-C13
38	a	732	PQN	C13-C15-C16-C17
30	j	104	CLA	C5-C6-C7-C8
30	a	702	CLA	C8-C10-C11-C12
33	b	733	LMG	C32-C33-C34-C35
30	a	709	CLA	O1D-CGD-O2D-CED
30	G	512	CLA	C11-C12-C13-C15
30	l	311	CLA	C16-C17-C18-C20
30	B	301	CLA	C11-C12-C13-C14
30	B	311	CLA	C16-C17-C18-C19
30	J	307	CLA	C16-C17-C18-C19
30	J	307	CLA	C16-C17-C18-C20
30	L	313	CLA	C6-C7-C8-C10
38	a	732	PQN	C26-C27-C28-C29
38	a	732	PQN	C26-C27-C28-C30
32	G	521	DGD	O6D-C1D-O3G-C3G
30	A	312	CLA	C5-C6-C7-C8
30	a	735	CLA	C15-C16-C17-C18
38	a	732	PQN	C18-C20-C21-C22
30	J	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	L	317	CLA	O1D-CGD-O2D-CED
33	D	317	LMG	C30-C31-C32-C33
30	b	717	CLA	CBD-CGD-O2D-CED
30	a	705	CLA	O1D-CGD-O2D-CED
30	L	308	CLA	C2C-C3C-CAC-CBC
33	B	318	LMG	C32-C33-C34-C35
31	A	314	KC1	CAA-CBA-CGA-O1A
31	D	315	KC1	CAA-CBA-CGA-O1A
31	L	307	KC1	CAA-CBA-CGA-O1A
31	N	306	KC1	CAA-CBA-CGA-O2A
30	L	309	CLA	O1A-CGA-O2A-C1
30	J	314	CLA	O1D-CGD-O2D-CED
30	I	309	CLA	C3-C5-C6-C7
32	G	521	DGD	O6D-C5D-C6D-O5D
30	A	320	CLA	O1D-CGD-O2D-CED
30	b	712	CLA	O1D-CGD-O2D-CED
30	b	727	CLA	O1D-CGD-O2D-CED
30	f	302	CLA	C3A-C2A-CAA-CBA
30	a	718	CLA	C3A-C2A-CAA-CBA
30	a	719	CLA	C3A-C2A-CAA-CBA
30	a	725	CLA	C3A-C2A-CAA-CBA
30	a	727	CLA	C3A-C2A-CAA-CBA
30	a	735	CLA	C3A-C2A-CAA-CBA
30	B	308	CLA	C3A-C2A-CAA-CBA
30	D	314	CLA	C3A-C2A-CAA-CBA
30	F	310	CLA	C3A-C2A-CAA-CBA
30	J	308	CLA	C3A-C2A-CAA-CBA
30	L	317	CLA	C3A-C2A-CAA-CBA
30	N	310	CLA	C3A-C2A-CAA-CBA
30	O	314	CLA	C3A-C2A-CAA-CBA
30	P	215	CLA	C3A-C2A-CAA-CBA
33	D	317	LMG	C33-C34-C35-C36
30	G	519	CLA	O1D-CGD-O2D-CED
30	A	308	CLA	O1D-CGD-O2D-CED
30	K	313	CLA	O1A-CGA-O2A-C1
30	h	202	CLA	C6-C7-C8-C10
30	j	104	CLA	C6-C7-C8-C9
30	l	311	CLA	C16-C17-C18-C19
30	b	717	CLA	C16-C17-C18-C19
30	B	301	CLA	C11-C12-C13-C15
30	L	313	CLA	C6-C7-C8-C9
33	b	733	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	I	310	CLA	O2A-C1-C2-C3
30	I	306	CLA	O1D-CGD-O2D-CED
30	f	303	CLA	O1D-CGD-O2D-CED
30	l	313	CLA	O1D-CGD-O2D-CED
30	B	301	CLA	CBD-CGD-O2D-CED
33	I	318	LMG	C14-C15-C16-C17
33	j	101	LMG	C33-C34-C35-C36
34	D	307	PID	C17-C18-C19-C20
34	O	305	PID	C15-C16-C17-C18
33	K	317	LMG	C28-C29-C30-C31
33	D	317	LMG	C10-C11-C12-C13
33	K	317	LMG	C30-C31-C32-C33
30	B	301	CLA	CBA-CGA-O2A-C1
30	a	707	CLA	C2-C3-C5-C6
30	B	311	CLA	C2-C3-C5-C6
31	J	313	KC1	CAA-CBA-CGA-O1A
32	G	501	DGD	C4D-C5D-C6D-O5D
33	I	318	LMG	C30-C31-C32-C33
33	B	318	LMG	C33-C34-C35-C36
30	J	309	CLA	O1D-CGD-O2D-CED
30	a	728	CLA	C6-C7-C8-C9
30	M	317	CLA	O1A-CGA-O2A-C1
30	a	704	CLA	C15-C16-C17-C18
30	b	724	CLA	C3-C5-C6-C7
30	b	725	CLA	C3-C5-C6-C7
32	G	521	DGD	C4D-C5D-C6D-O5D
30	I	313	CLA	CBA-CGA-O2A-C1
30	I	306	CLA	O1A-CGA-O2A-C1
30	b	716	CLA	O1A-CGA-O2A-C1
30	B	313	CLA	O1A-CGA-O2A-C1
30	l	303	CLA	C10-C11-C12-C13
33	K	317	LMG	C12-C13-C14-C15
30	K	311	CLA	C2-C1-O2A-CGA
39	a	733	LHG	C26-C27-C28-C29
30	b	715	CLA	C11-C12-C13-C14
30	b	719	CLA	O1A-CGA-O2A-C1
30	J	312	CLA	C3-C5-C6-C7
37	i	201	BCR	C1-C6-C7-C8
37	b	730	BCR	C1-C6-C7-C8
37	b	730	BCR	C5-C6-C7-C8
33	D	317	LMG	O6-C5-C6-O5
30	b	703	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	l	311	CLA	C10-C11-C12-C13
30	a	712	CLA	C10-C11-C12-C13
30	b	712	CLA	C5-C6-C7-C8
33	D	317	LMG	C13-C14-C15-C16
30	a	707	CLA	C4-C3-C5-C6
30	b	722	CLA	C4-C3-C5-C6
30	a	710	CLA	O1D-CGD-O2D-CED
30	G	513	CLA	C12-C13-C15-C16
30	l	313	CLA	C12-C13-C15-C16
30	a	702	CLA	C11-C12-C13-C15
30	a	707	CLA	C11-C10-C8-C7
30	a	721	CLA	C12-C13-C15-C16
30	a	722	CLA	C6-C7-C8-C10
30	b	701	CLA	C11-C12-C13-C15
30	b	704	CLA	C11-C10-C8-C7
30	b	707	CLA	C11-C10-C8-C7
30	b	709	CLA	C2-C3-C5-C6
30	b	717	CLA	C11-C12-C13-C15
30	b	724	CLA	C12-C13-C15-C16
30	B	311	CLA	C11-C10-C8-C7
30	K	308	CLA	C3-C5-C6-C7
30	a	729	CLA	C3-C5-C6-C7
30	I	313	CLA	O1A-CGA-O2A-C1
30	B	301	CLA	O1A-CGA-O2A-C1
30	b	704	CLA	C13-C15-C16-C17
38	a	732	PQN	C15-C16-C17-C18
30	I	316	CLA	C6-C7-C8-C10
30	b	708	CLA	C16-C17-C18-C19
30	B	316	CLA	O1D-CGD-O2D-CED
30	K	311	CLA	CBA-CGA-O2A-C1
30	G	510	CLA	CBA-CGA-O2A-C1
30	h	202	CLA	CBA-CGA-O2A-C1
30	a	705	CLA	CBA-CGA-O2A-C1
30	a	735	CLA	CBA-CGA-O2A-C1
32	l	301	DGD	C2A-C1A-O1G-C1G
30	I	316	CLA	C2A-CAA-CBA-CGA
30	G	510	CLA	C2A-CAA-CBA-CGA
30	G	514	CLA	C2A-CAA-CBA-CGA
30	m	202	CLA	C2A-CAA-CBA-CGA
30	b	708	CLA	C2A-CAA-CBA-CGA
30	b	718	CLA	C2A-CAA-CBA-CGA
30	b	723	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	D	309	CLA	C2A-CAA-CBA-CGA
30	J	312	CLA	C2A-CAA-CBA-CGA
30	B	311	CLA	C5-C6-C7-C8
30	b	722	CLA	CBD-CGD-O2D-CED
31	G	515	KC1	C2C-C3C-CAC-CBC
31	G	515	KC1	C2B-C3B-CAB-CBB
31	L	307	KC1	C2B-C3B-CAB-CBB
31	O	310	KC1	C2B-C3B-CAB-CBB
31	M	314	KC1	CAA-CBA-CGA-O2A
33	D	317	LMG	C14-C15-C16-C17
30	f	301	CLA	CBA-CGA-O2A-C1
30	I	313	CLA	C6-C7-C8-C10
33	I	320	LMG	O6-C1-O1-C7
33	b	733	LMG	C15-C16-C17-C18
32	G	501	DGD	C2B-C1B-O2G-C2G
39	a	733	LHG	C8-C7-O7-C5
33	I	320	LMG	C16-C17-C18-C19
31	L	307	KC1	C4B-C3B-CAB-CBB
31	N	308	KC1	C4B-C3B-CAB-CBB
31	P	216	KC1	C4B-C3B-CAB-CBB
30	l	304	CLA	C8-C10-C11-C12
30	b	701	CLA	C10-C11-C12-C13
30	b	711	CLA	C5-C6-C7-C8
38	b	729	PQN	C23-C25-C26-C27
33	D	317	LMG	C18-C19-C20-C21
30	M	310	CLA	O2A-C1-C2-C3
31	O	310	KC1	CAA-CBA-CGA-O1A
30	A	310	CLA	C16-C17-C18-C20
33	b	733	LMG	C14-C15-C16-C17
32	L	301	DGD	O6E-C5E-C6E-O5E
30	b	709	CLA	C4-C3-C5-C6
28	K	301	DD6	C27-C29-C30-C31
28	K	305	DD6	C27-C29-C30-C31
28	K	318	DD6	C27-C29-C30-C31
28	G	502	DD6	C27-C29-C30-C31
28	G	508	DD6	C27-C29-C30-C31
28	h	203	DD6	C27-C29-C30-C31
28	B	303	DD6	C27-C29-C30-C31
28	F	303	DD6	C27-C29-C30-C31
28	L	306	DD6	C27-C29-C30-C31
30	G	510	CLA	C11-C12-C13-C14
30	G	513	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	l	313	CLA	C14-C13-C15-C16
30	b	704	CLA	C11-C10-C8-C9
30	b	724	CLA	C11-C12-C13-C14
30	b	724	CLA	C14-C13-C15-C16
30	B	311	CLA	C11-C10-C8-C9
30	B	313	CLA	C11-C10-C8-C9
30	I	310	CLA	CBD-CGD-O2D-CED
30	I	307	CLA	C2A-CAA-CBA-CGA
30	I	313	CLA	C2A-CAA-CBA-CGA
30	I	315	CLA	C2A-CAA-CBA-CGA
30	A	310	CLA	C2A-CAA-CBA-CGA
30	A	311	CLA	C2A-CAA-CBA-CGA
30	H	307	CLA	C2A-CAA-CBA-CGA
30	J	301	CLA	C2A-CAA-CBA-CGA
30	M	316	CLA	C2A-CAA-CBA-CGA
28	I	301	DD6	C12-C11-C13-C14
37	j	102	BCR	C36-C18-C19-C20
30	a	731	CLA	C8-C10-C11-C12
28	I	301	DD6	C10-C11-C13-C14
28	I	305	DD6	C5-C6-C8-C9
30	a	705	CLA	O1A-CGA-O2A-C1
30	b	703	CLA	O1A-CGA-O2A-C1
30	I	315	CLA	C1A-C2A-CAA-CBA
30	A	319	CLA	C1A-C2A-CAA-CBA
30	f	302	CLA	C1A-C2A-CAA-CBA
30	l	312	CLA	C1A-C2A-CAA-CBA
30	a	707	CLA	C1A-C2A-CAA-CBA
30	a	711	CLA	C1A-C2A-CAA-CBA
30	a	712	CLA	C1A-C2A-CAA-CBA
30	a	715	CLA	C1A-C2A-CAA-CBA
30	a	717	CLA	C1A-C2A-CAA-CBA
30	a	719	CLA	C1A-C2A-CAA-CBA
30	a	720	CLA	C1A-C2A-CAA-CBA
30	a	725	CLA	C1A-C2A-CAA-CBA
30	a	727	CLA	C1A-C2A-CAA-CBA
30	a	735	CLA	C1A-C2A-CAA-CBA
30	b	706	CLA	C1A-C2A-CAA-CBA
30	b	720	CLA	C1A-C2A-CAA-CBA
30	b	721	CLA	C1A-C2A-CAA-CBA
30	b	723	CLA	C1A-C2A-CAA-CBA
30	D	314	CLA	C1A-C2A-CAA-CBA
30	F	308	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	H	309	CLA	C1A-C2A-CAA-CBA
30	J	301	CLA	C1A-C2A-CAA-CBA
30	J	308	CLA	C1A-C2A-CAA-CBA
30	L	312	CLA	C1A-C2A-CAA-CBA
30	L	313	CLA	C1A-C2A-CAA-CBA
30	L	317	CLA	C1A-C2A-CAA-CBA
30	M	313	CLA	C1A-C2A-CAA-CBA
30	N	305	CLA	C1A-C2A-CAA-CBA
30	O	314	CLA	C1A-C2A-CAA-CBA
30	P	215	CLA	C1A-C2A-CAA-CBA
30	I	313	CLA	C6-C7-C8-C9
30	m	202	CLA	C11-C12-C13-C14
30	a	728	CLA	C6-C7-C8-C10
30	a	735	CLA	C16-C17-C18-C20
32	G	501	DGD	O1B-C1B-O2G-C2G
31	A	306	KC1	CAA-CBA-CGA-O2A
33	K	317	LMG	C29-C30-C31-C32
30	G	514	CLA	O1D-CGD-O2D-CED
30	G	512	CLA	C5-C6-C7-C8
30	a	731	CLA	C15-C16-C17-C18
30	b	701	CLA	C5-C6-C7-C8
30	b	707	CLA	C5-C6-C7-C8
30	a	735	CLA	O1D-CGD-O2D-CED
30	a	721	CLA	C8-C10-C11-C12
30	b	704	CLA	C10-C11-C12-C13
30	b	717	CLA	C13-C15-C16-C17
30	O	308	CLA	O1D-CGD-O2D-CED
32	l	301	DGD	C3B-C4B-C5B-C6B
30	A	310	CLA	C8-C10-C11-C12
30	b	712	CLA	C6-C7-C8-C10
29	J	305	UIX	C17-C18-O2-C27
30	l	304	CLA	C3-C5-C6-C7
32	I	317	DGD	O6E-C5E-C6E-O5E
30	B	311	CLA	C4-C3-C5-C6
30	K	311	CLA	O1A-CGA-O2A-C1
30	G	510	CLA	O1A-CGA-O2A-C1
30	h	202	CLA	O1A-CGA-O2A-C1
30	l	303	CLA	C16-C17-C18-C20
30	O	311	CLA	O1D-CGD-O2D-CED
32	G	501	DGD	C1G-C2G-C3G-O3G
33	K	317	LMG	C7-C8-C9-O8
33	b	734	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	B	318	LMG	C7-C8-C9-O8
30	D	311	CLA	CBA-CGA-O2A-C1
31	O	315	KC1	CAA-CBA-CGA-O2A
30	a	729	CLA	C5-C6-C7-C8
33	I	318	LMG	C15-C16-C17-C18
33	I	320	LMG	C32-C33-C34-C35
32	l	301	DGD	O1A-C1A-O1G-C1G
33	b	734	LMG	O6-C5-C6-O5
32	G	521	DGD	C1B-C2B-C3B-C4B
30	f	301	CLA	O1A-CGA-O2A-C1
30	a	735	CLA	O1A-CGA-O2A-C1
30	a	735	CLA	C3-C5-C6-C7
30	f	303	CLA	CBA-CGA-O2A-C1
30	b	712	CLA	C6-C7-C8-C9
30	l	311	CLA	C13-C15-C16-C17
30	F	315	CLA	O1D-CGD-O2D-CED
30	b	706	CLA	O2A-C1-C2-C3
30	J	306	CLA	CBA-CGA-O2A-C1
34	D	306	PID	C19-C20-C21-CM5
34	O	305	PID	CM4-C14-C15-C16
30	a	721	CLA	C16-C17-C18-C19
30	b	705	CLA	CBA-CGA-O2A-C1
30	L	308	CLA	CBA-CGA-O2A-C1
30	l	303	CLA	CBD-CGD-O2D-CED
30	P	210	CLA	CBD-CGD-O2D-CED
30	K	308	CLA	C6-C7-C8-C9
30	B	313	CLA	O1D-CGD-O2D-CED
30	a	723	CLA	C2A-CAA-CBA-CGA
30	K	310	CLA	C5-C6-C7-C8
30	b	704	CLA	C15-C16-C17-C18
30	J	310	CLA	O1D-CGD-O2D-CED
30	A	311	CLA	CBD-CGD-O2D-CED
30	A	312	CLA	CBA-CGA-O2A-C1
30	b	704	CLA	CBA-CGA-O2A-C1
33	b	734	LMG	C29-C28-O8-C9
30	L	318	CLA	CAA-CBA-CGA-O2A
30	A	309	CLA	O1D-CGD-O2D-CED
30	b	711	CLA	C6-C7-C8-C9
33	I	320	LMG	C17-C18-C19-C20
30	l	313	CLA	C15-C16-C17-C18
30	a	713	CLA	C8-C10-C11-C12
30	a	731	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	O	305	PID	C13-C14-C15-C16
32	G	521	DGD	O2G-C2G-C3G-O3G
30	A	310	CLA	C16-C17-C18-C19
30	l	303	CLA	C16-C17-C18-C19
33	b	733	LMG	C38-C39-C40-C41
30	I	312	CLA	C12-C13-C15-C16
30	G	510	CLA	C11-C12-C13-C15
30	G	519	CLA	C6-C7-C8-C10
30	G	519	CLA	C11-C10-C8-C7
30	A	310	CLA	C11-C12-C13-C15
30	l	313	CLA	C6-C7-C8-C10
30	a	702	CLA	C12-C13-C15-C16
30	a	709	CLA	C12-C13-C15-C16
30	a	717	CLA	C11-C10-C8-C7
30	b	703	CLA	C11-C10-C8-C7
30	b	709	CLA	C11-C10-C8-C7
30	B	301	CLA	C11-C10-C8-C7
30	B	309	CLA	C6-C7-C8-C10
30	B	309	CLA	C11-C12-C13-C15
30	B	311	CLA	C11-C12-C13-C15
30	B	311	CLA	C12-C13-C15-C16
30	B	313	CLA	C11-C10-C8-C7
30	J	307	CLA	C11-C10-C8-C7
30	J	309	CLA	C6-C7-C8-C10
30	N	305	CLA	C11-C12-C13-C15
30	P	210	CLA	C11-C12-C13-C15
30	b	714	CLA	CAA-CBA-CGA-O2A
30	P	210	CLA	C3-C5-C6-C7
30	I	312	CLA	C11-C12-C13-C14
30	G	510	CLA	C6-C7-C8-C9
30	G	512	CLA	C11-C10-C8-C9
30	A	310	CLA	C11-C12-C13-C14
30	A	310	CLA	C14-C13-C15-C16
30	l	313	CLA	C6-C7-C8-C9
30	a	707	CLA	C11-C12-C13-C14
30	a	709	CLA	C14-C13-C15-C16
30	a	717	CLA	C11-C10-C8-C9
30	a	724	CLA	C14-C13-C15-C16
30	b	703	CLA	C11-C10-C8-C9
30	b	705	CLA	C14-C13-C15-C16
30	b	709	CLA	C11-C10-C8-C9
30	B	309	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	B	309	CLA	C11-C12-C13-C14
30	N	305	CLA	C11-C12-C13-C14
30	P	210	CLA	C11-C12-C13-C14
38	a	732	PQN	C21-C22-C23-C24
37	l	306	BCR	C13-C14-C15-C16
30	I	312	CLA	CBA-CGA-O2A-C1
30	I	310	CLA	C2A-CAA-CBA-CGA
30	L	308	CLA	O1A-CGA-O2A-C1
28	G	505	DD6	C12-C11-C13-C14
28	L	305	DD6	C12-C11-C13-C14
30	a	721	CLA	C16-C17-C18-C20
28	I	303	DD6	C10-C11-C13-C14
28	G	504	DD6	C5-C6-C8-C9
28	G	505	DD6	C10-C11-C13-C14
30	b	711	CLA	C3-C5-C6-C7
30	a	723	CLA	C10-C11-C12-C13
33	b	733	LMG	C28-C29-C30-C31
30	a	724	CLA	C5-C6-C7-C8
30	B	309	CLA	C4-C3-C5-C6
30	a	716	CLA	O1D-CGD-O2D-CED
30	D	309	CLA	O1D-CGD-O2D-CED
31	G	515	KC1	CAA-CBA-CGA-O2A
31	O	312	KC1	CAA-CBA-CGA-O1A
30	I	311	CLA	C6-C7-C8-C10
30	f	301	CLA	C6-C7-C8-C10
30	a	720	CLA	C10-C11-C12-C13
30	K	306	CLA	CBA-CGA-O2A-C1
30	a	724	CLA	CBA-CGA-O2A-C1
30	a	726	CLA	CBA-CGA-O2A-C1
30	b	712	CLA	CBA-CGA-O2A-C1
30	P	209	CLA	CBA-CGA-O2A-C1
33	j	101	LMG	C31-C32-C33-C34
39	a	733	LHG	C2-C3-O3-P
30	I	310	CLA	C3A-C2A-CAA-CBA
30	b	706	CLA	C3A-C2A-CAA-CBA
30	b	724	CLA	C3A-C2A-CAA-CBA
30	B	317	CLA	C3A-C2A-CAA-CBA
33	I	318	LMG	C12-C13-C14-C15
29	P	207	UIX	C11-C13-C14-C23
30	a	735	CLA	C16-C17-C18-C19
30	b	728	CLA	CBA-CGA-O2A-C1
30	a	721	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	P	211	KC1	O1D-CGD-O2D-CED
32	y	201	DGD	C1G-C2G-C3G-O3G
33	I	318	LMG	O1-C7-C8-C9
33	I	318	LMG	C7-C8-C9-O8
33	D	317	LMG	C7-C8-C9-O8
33	I	318	LMG	C32-C33-C34-C35
30	a	726	CLA	C3-C5-C6-C7
30	a	706	CLA	O1D-CGD-O2D-CED
30	b	704	CLA	O1A-CGA-O2A-C1
30	H	305	CLA	C4-C3-C5-C6
33	I	320	LMG	C31-C32-C33-C34
30	A	312	CLA	O1A-CGA-O2A-C1
30	b	705	CLA	O1A-CGA-O2A-C1
31	D	315	KC1	C3A-C2A-CAA-CBA
31	F	309	KC1	C3A-C2A-CAA-CBA
31	L	315	KC1	C3A-C2A-CAA-CBA
30	B	310	CLA	C6-C7-C8-C9
30	b	708	CLA	C5-C6-C7-C8
30	B	316	CLA	CBA-CGA-O2A-C1
30	b	717	CLA	O1D-CGD-O2D-CED
33	b	734	LMG	C11-C12-C13-C14
30	I	312	CLA	O1A-CGA-O2A-C1
32	G	521	DGD	O1G-C1G-C2G-O2G
32	j	103	DGD	O1G-C1G-C2G-O2G
32	l	301	DGD	O2G-C2G-C3G-O3G
33	I	318	LMG	O1-C7-C8-O7
33	I	318	LMG	O7-C8-C9-O8
33	j	101	LMG	O7-C8-C9-O8
33	b	734	LMG	O7-C8-C9-O8
30	b	719	CLA	CBD-CGD-O2D-CED
30	l	313	CLA	C2C-C3C-CAC-CBC
30	b	711	CLA	C6-C7-C8-C10
30	a	704	CLA	C5-C6-C7-C8
30	I	307	CLA	CBD-CGD-O2D-CED
30	f	301	CLA	C2-C1-O2A-CGA
30	a	703	CLA	C2-C1-O2A-CGA
30	b	725	CLA	C2-C1-O2A-CGA
30	B	301	CLA	O1D-CGD-O2D-CED
30	G	510	CLA	C14-C13-C15-C16
30	G	519	CLA	C6-C7-C8-C9
30	m	202	CLA	C6-C7-C8-C9
30	b	704	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	b	727	CLA	C11-C12-C13-C14
30	a	724	CLA	C13-C15-C16-C17
31	M	314	KC1	C1A-C2A-CAA-CBA
33	I	318	LMG	C31-C32-C33-C34
30	l	310	CLA	C2A-CAA-CBA-CGA
30	b	712	CLA	C2A-CAA-CBA-CGA
30	I	311	CLA	C6-C7-C8-C9
37	j	102	BCR	C23-C24-C25-C30
37	l	306	BCR	C1-C6-C7-C8
37	l	306	BCR	C5-C6-C7-C8
37	l	306	BCR	C23-C24-C25-C26
37	l	306	BCR	C23-C24-C25-C30
28	I	303	DD6	C12-C11-C13-C14
28	A	302	DD6	C7-C6-C8-C9
28	K	305	DD6	C10-C11-C13-C14
28	b	731	DD6	C10-C11-C13-C14
28	L	305	DD6	C10-C11-C13-C14
37	j	102	BCR	C17-C18-C19-C20
37	m	201	BCR	C11-C12-C13-C14
34	D	306	PID	C15-C16-C17-C18
30	M	312	CLA	O2A-C1-C2-C3
30	f	301	CLA	C6-C7-C8-C9
30	I	321	CLA	C4C-C3C-CAC-CBC
30	b	722	CLA	O1D-CGD-O2D-CED
31	L	315	KC1	C2C-C3C-CAC-CBC
30	G	510	CLA	C6-C7-C8-C10
30	G	512	CLA	C11-C10-C8-C7
30	A	310	CLA	C11-C10-C8-C7
30	A	310	CLA	C12-C13-C15-C16
30	l	305	CLA	C11-C12-C13-C15
30	l	313	CLA	C11-C12-C13-C15
30	m	202	CLA	C6-C7-C8-C10
30	a	709	CLA	C11-C10-C8-C7
30	a	713	CLA	C11-C10-C8-C7
30	a	717	CLA	C6-C7-C8-C10
30	a	725	CLA	C11-C10-C8-C7
30	b	704	CLA	C6-C7-C8-C10
30	b	704	CLA	C12-C13-C15-C16
30	b	705	CLA	C11-C12-C13-C15
30	b	707	CLA	C6-C7-C8-C10
30	b	727	CLA	C12-C13-C15-C16
30	b	728	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	B	309	CLA	C12-C13-C15-C16
30	H	305	CLA	C11-C12-C13-C15
30	a	702	CLA	C15-C16-C17-C18
28	I	305	DD6	C1-C2-C3-C4
28	I	305	DD6	C3-C4-C5-C6
30	G	519	CLA	C10-C11-C12-C13
30	K	310	CLA	C2A-CAA-CBA-CGA
34	D	306	PID	CM4-C14-C15-C16
30	a	713	CLA	C3-C5-C6-C7
30	a	722	CLA	C5-C6-C7-C8
30	J	308	CLA	CAA-CBA-CGA-O2A
29	O	306	UIX	C25-C28-C32-C33
30	I	310	CLA	CAD-CBD-CGD-O2D
30	I	315	CLA	CAD-CBD-CGD-O2D
30	K	311	CLA	CAD-CBD-CGD-O2D
30	K	315	CLA	CAD-CBD-CGD-O2D
30	G	513	CLA	CAD-CBD-CGD-O2D
30	G	517	CLA	CAD-CBD-CGD-O2D
30	G	519	CLA	CAD-CBD-CGD-O2D
30	f	302	CLA	CAD-CBD-CGD-O2D
30	l	305	CLA	CAD-CBD-CGD-O2D
30	l	309	CLA	CAD-CBD-CGD-O2D
30	a	705	CLA	CAD-CBD-CGD-O2D
30	a	708	CLA	CAD-CBD-CGD-O2D
30	a	735	CLA	CAD-CBD-CGD-O2D
30	b	708	CLA	CAD-CBD-CGD-O2D
30	b	714	CLA	CAD-CBD-CGD-O2D
30	b	715	CLA	CAD-CBD-CGD-O2D
30	b	719	CLA	CAD-CBD-CGD-O2D
30	B	316	CLA	CAD-CBD-CGD-O2D
30	D	311	CLA	CAD-CBD-CGD-O2D
30	D	312	CLA	CAD-CBD-CGD-O2D
30	D	313	CLA	CAD-CBD-CGD-O2D
30	J	315	CLA	CAD-CBD-CGD-O2D
30	L	318	CLA	CAD-CBD-CGD-O2D
30	O	309	CLA	CAD-CBD-CGD-O2D
30	O	311	CLA	CAD-CBD-CGD-O2D
30	O	313	CLA	CAD-CBD-CGD-O2D
30	P	214	CLA	CAD-CBD-CGD-O2D
31	N	308	KC1	CAD-CBD-CGD-O2D
32	G	521	DGD	C1G-C2G-O2G-C1B
33	I	320	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	a	717	CLA	CBA-CGA-O2A-C1
30	a	720	CLA	CBA-CGA-O2A-C1
30	b	722	CLA	C2-C3-C5-C6
32	G	521	DGD	O1G-C1G-C2G-C3G
32	j	103	DGD	O1G-C1G-C2G-C3G
32	l	301	DGD	C1G-C2G-C3G-O3G
33	b	734	LMG	C7-C8-C9-O8
39	a	733	LHG	C24-C25-C26-C27
33	I	318	LMG	C11-C12-C13-C14
30	a	704	CLA	C2A-CAA-CBA-CGA
30	b	705	CLA	C2A-CAA-CBA-CGA
30	L	309	CLA	C2A-CAA-CBA-CGA
30	b	712	CLA	O1A-CGA-O2A-C1
39	a	733	LHG	O9-C7-O7-C5
30	I	306	CLA	CHA-CBD-CGD-O1D
30	I	306	CLA	CHA-CBD-CGD-O2D
30	K	310	CLA	CHA-CBD-CGD-O2D
30	G	512	CLA	CHA-CBD-CGD-O1D
30	G	512	CLA	CHA-CBD-CGD-O2D
30	A	315	CLA	CHA-CBD-CGD-O1D
30	A	320	CLA	CHA-CBD-CGD-O1D
30	f	303	CLA	CHA-CBD-CGD-O2D
30	l	304	CLA	CHA-CBD-CGD-O1D
30	l	304	CLA	CHA-CBD-CGD-O2D
30	a	714	CLA	CHA-CBD-CGD-O1D
30	a	714	CLA	CHA-CBD-CGD-O2D
30	a	722	CLA	CHA-CBD-CGD-O2D
30	a	724	CLA	CHA-CBD-CGD-O1D
30	a	724	CLA	CHA-CBD-CGD-O2D
30	a	727	CLA	CHA-CBD-CGD-O1D
30	a	727	CLA	CHA-CBD-CGD-O2D
30	a	729	CLA	CHA-CBD-CGD-O1D
30	a	729	CLA	CHA-CBD-CGD-O2D
30	b	705	CLA	CHA-CBD-CGD-O1D
30	b	723	CLA	CHA-CBD-CGD-O1D
30	F	310	CLA	CHA-CBD-CGD-O1D
30	F	310	CLA	CHA-CBD-CGD-O2D
30	F	315	CLA	CHA-CBD-CGD-O1D
30	H	312	CLA	CHA-CBD-CGD-O2D
30	J	301	CLA	CHA-CBD-CGD-O1D
30	J	301	CLA	CHA-CBD-CGD-O2D
30	J	312	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	J	312	CLA	CHA-CBD-CGD-O2D
30	L	316	CLA	CHA-CBD-CGD-O1D
30	L	316	CLA	CHA-CBD-CGD-O2D
30	N	307	CLA	CHA-CBD-CGD-O1D
30	P	210	CLA	CHA-CBD-CGD-O1D
30	P	212	CLA	CHA-CBD-CGD-O1D
30	P	212	CLA	CHA-CBD-CGD-O2D
30	P	217	CLA	CHA-CBD-CGD-O1D
30	P	217	CLA	CHA-CBD-CGD-O2D
31	I	314	KC1	CHA-CBD-CGD-O1D
31	K	314	KC1	CHA-CBD-CGD-O1D
31	K	314	KC1	CHA-CBD-CGD-O2D
31	A	306	KC1	CHA-CBD-CGD-O1D
31	D	310	KC1	CHA-CBD-CGD-O1D
31	N	308	KC1	CHA-CBD-CGD-O1D
31	O	312	KC1	CHA-CBD-CGD-O2D
34	N	301	PID	C12-C13-C14-C15
34	O	305	PID	C12-C13-C14-C15
34	D	306	PID	C13-C14-C15-C16
32	G	501	DGD	O2G-C2G-C3G-O3G
33	B	318	LMG	O7-C8-C9-O8
30	K	306	CLA	O1A-CGA-O2A-C1
30	a	724	CLA	O1A-CGA-O2A-C1
30	b	728	CLA	O1A-CGA-O2A-C1
30	P	209	CLA	O1A-CGA-O2A-C1
30	B	310	CLA	C6-C7-C8-C10
33	b	733	LMG	C35-C36-C37-C38
33	P	201	LMG	C28-C29-C30-C31
30	a	721	CLA	C13-C15-C16-C17
30	a	726	CLA	O1A-CGA-O2A-C1
28	K	304	DD6	C27-C29-C30-C31
28	b	731	DD6	C27-C29-C30-C31
28	B	302	DD6	C27-C29-C30-C31
28	B	306	DD6	C27-C29-C30-C31
28	H	303	DD6	C27-C29-C30-C31
28	L	302	DD6	C27-C29-C30-C31
28	M	306	DD6	C27-C29-C30-C31
30	a	725	CLA	C5-C6-C7-C8
30	G	513	CLA	C6-C7-C8-C9
30	l	304	CLA	C6-C7-C8-C9
30	l	311	CLA	C14-C13-C15-C16
30	a	709	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	a	713	CLA	C11-C10-C8-C9
30	a	725	CLA	C11-C10-C8-C9
30	b	715	CLA	C6-C7-C8-C9
30	b	728	CLA	C6-C7-C8-C9
30	J	301	CLA	C11-C10-C8-C9
30	I	310	CLA	O1D-CGD-O2D-CED
31	P	213	KC1	C2C-C3C-CAC-CBC
30	N	305	CLA	C3-C5-C6-C7
30	A	319	CLA	CAA-CBA-CGA-O2A
30	b	703	CLA	CAA-CBA-CGA-O2A
30	a	709	CLA	C8-C10-C11-C12
28	L	306	DD6	C12-C11-C13-C14
29	K	302	UIX	C7-C10-C11-C12
37	m	201	BCR	C11-C12-C13-C35
30	b	720	CLA	C5-C6-C7-C8
28	G	502	DD6	C10-C11-C13-C14
28	L	306	DD6	C10-C11-C13-C14
29	K	302	UIX	C7-C10-C11-C13
30	a	703	CLA	C3-C5-C6-C7
30	A	311	CLA	O1D-CGD-O2D-CED
30	a	724	CLA	C1A-C2A-CAA-CBA
30	H	305	CLA	C1A-C2A-CAA-CBA
33	D	317	LMG	C28-C29-C30-C31
30	b	709	CLA	C11-C12-C13-C14
30	b	707	CLA	C2-C1-O2A-CGA
30	l	303	CLA	O1D-CGD-O2D-CED
30	P	210	CLA	O1D-CGD-O2D-CED
30	K	311	CLA	C4-C3-C5-C6
38	b	729	PQN	C14-C13-C15-C16
30	K	313	CLA	C6-C7-C8-C10
31	M	314	KC1	C2C-C3C-CAC-CBC
39	a	733	LHG	C24-C23-O8-C6
30	F	312	CLA	C2C-C3C-CAC-CBC
30	A	313	CLA	C6-C7-C8-C9
30	N	305	CLA	C16-C17-C18-C20
33	b	733	LMG	C31-C32-C33-C34
29	O	306	UIX	C25-C28-C32-C35
30	K	310	CLA	CAD-CBD-CGD-O1D
30	G	512	CLA	CAD-CBD-CGD-O1D
30	a	708	CLA	C2-C3-C5-C6
30	a	718	CLA	CAD-CBD-CGD-O1D
30	a	721	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	a	729	CLA	CAD-CBD-CGD-O1D
30	F	311	CLA	CAD-CBD-CGD-O1D
30	H	312	CLA	CAD-CBD-CGD-O1D
30	J	307	CLA	CAD-CBD-CGD-O1D
30	O	311	CLA	C2-C3-C5-C6
30	P	212	CLA	C2-C3-C5-C6
30	P	217	CLA	CAD-CBD-CGD-O1D
30	l	312	CLA	CBA-CGA-O2A-C1
30	J	301	CLA	C8-C10-C11-C12
30	a	717	CLA	O1A-CGA-O2A-C1
30	a	720	CLA	O1A-CGA-O2A-C1
30	b	725	CLA	CBA-CGA-O2A-C1
30	b	704	CLA	C16-C17-C18-C20
30	b	707	CLA	C4-C3-C5-C6
30	A	310	CLA	C6-C7-C8-C10
30	l	303	CLA	C11-C12-C13-C15
30	a	706	CLA	C3A-C2A-CAA-CBA
30	a	722	CLA	C11-C10-C8-C7
30	a	724	CLA	C6-C7-C8-C10
30	b	708	CLA	C11-C10-C8-C7
30	B	301	CLA	C6-C7-C8-C10
30	B	311	CLA	C6-C7-C8-C10
30	J	301	CLA	C11-C10-C8-C7
30	N	305	CLA	C12-C13-C15-C16
30	O	313	CLA	C2A-CAA-CBA-CGA
30	a	703	CLA	C6-C7-C8-C9
34	O	305	PID	C16-C17-C18-C19
30	A	316	CLA	CAA-CBA-CGA-O2A
30	M	317	CLA	CAA-CBA-CGA-O2A
32	G	521	DGD	C1G-C2G-C3G-O3G
34	D	306	PID	O4-C12-C13-C14
34	H	301	PID	O4-C12-C13-C14
34	O	301	PID	O4-C12-C13-C14
34	O	307	PID	O4-C12-C13-C14
33	D	317	LMG	O7-C8-C9-O8
30	a	702	CLA	CAA-CBA-CGA-O2A
30	l	303	CLA	C15-C16-C17-C18
30	b	724	CLA	C5-C6-C7-C8
30	b	712	CLA	C3-C5-C6-C7
30	b	719	CLA	O1D-CGD-O2D-CED
30	B	309	CLA	C10-C11-C12-C13
30	A	310	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	l	311	CLA	C11-C12-C13-C14
30	l	313	CLA	C11-C12-C13-C14
30	a	723	CLA	C14-C13-C15-C16
30	a	726	CLA	C14-C13-C15-C16
30	b	705	CLA	C11-C12-C13-C14
30	b	707	CLA	C6-C7-C8-C9
30	B	309	CLA	C14-C13-C15-C16
30	H	305	CLA	C11-C12-C13-C14
30	J	309	CLA	C6-C7-C8-C9
33	b	733	LMG	C34-C35-C36-C37
28	I	302	DD6	C6-C8-C9-C10
28	D	303	DD6	C11-C10-C9-C8
33	P	201	LMG	C10-C11-C12-C13
30	l	313	CLA	C13-C15-C16-C17
30	b	725	CLA	O1A-CGA-O2A-C1
39	a	733	LHG	C23-C24-C25-C26
30	f	303	CLA	CAA-CBA-CGA-O2A
30	K	311	CLA	C2-C3-C5-C6
31	F	309	KC1	C2A-CAA-CBA-CGA
30	A	313	CLA	C6-C7-C8-C10
30	a	726	CLA	C13-C15-C16-C17
30	P	210	CLA	C10-C11-C12-C13
30	G	520	CLA	C1-C2-C3-C4
33	I	318	LMG	C9-C8-O7-C10
30	G	512	CLA	C2A-CAA-CBA-CGA
30	P	212	CLA	C2A-CAA-CBA-CGA
30	M	310	CLA	CBA-CGA-O2A-C1
30	I	308	CLA	C2-C1-O2A-CGA
30	j	106	CLA	C2-C1-O2A-CGA
30	L	313	CLA	C2-C1-O2A-CGA
30	M	308	CLA	C2-C1-O2A-CGA
30	M	309	CLA	C2-C1-O2A-CGA
31	M	314	KC1	C4C-C3C-CAC-CBC
34	D	306	PID	C17-C18-C19-C20
30	D	311	CLA	O1A-CGA-O2A-C1
33	B	318	LMG	C34-C35-C36-C37
30	b	710	CLA	O1A-CGA-O2A-C1
30	M	310	CLA	O1A-CGA-O2A-C1
30	M	316	CLA	O1A-CGA-O2A-C1
30	G	513	CLA	C8-C10-C11-C12
30	b	710	CLA	CBA-CGA-O2A-C1
30	M	316	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	D	317	LMG	C29-C28-O8-C9
32	y	201	DGD	C9B-CAB-CBB-CCB
33	B	318	LMG	C36-C37-C38-C39
30	f	303	CLA	O1A-CGA-O2A-C1
37	j	102	BCR	C23-C24-C25-C26
38	b	729	PQN	C12-C13-C15-C16
30	L	308	CLA	C4C-C3C-CAC-CBC
30	l	304	CLA	C11-C12-C13-C14
33	b	733	LMG	C11-C10-O7-C8
30	J	307	CLA	C10-C11-C12-C13
30	L	318	CLA	C2A-CAA-CBA-CGA
33	I	320	LMG	C2-C1-O1-C7
34	D	304	PID	C19-C20-C21-C22
39	a	733	LHG	C3-O3-P-O6
39	a	733	LHG	C4-O6-P-O3
33	b	733	LMG	C29-C30-C31-C32
30	N	305	CLA	C16-C17-C18-C19
30	I	307	CLA	O1D-CGD-O2D-CED
30	G	510	CLA	C12-C13-C15-C16
30	G	513	CLA	C6-C7-C8-C10
30	l	304	CLA	C11-C10-C8-C7
30	a	707	CLA	C11-C12-C13-C15
30	a	724	CLA	C12-C13-C15-C16
30	B	309	CLA	C11-C10-C8-C7
30	a	722	CLA	C11-C10-C8-C9
30	B	301	CLA	C6-C7-C8-C9
33	b	733	LMG	C30-C31-C32-C33
39	a	733	LHG	C32-C33-C34-C35
30	l	305	CLA	C10-C11-C12-C13
30	B	309	CLA	C2-C3-C5-C6
30	J	306	CLA	O1A-CGA-O2A-C1
30	G	518	CLA	C2A-CAA-CBA-CGA
30	L	311	CLA	C2A-CAA-CBA-CGA
29	P	207	UIX	C34-C37-C39-C40
33	b	734	LMG	C14-C15-C16-C17
30	a	717	CLA	C4-C3-C5-C6
30	b	728	CLA	C5-C6-C7-C8
39	a	733	LHG	O2-C2-C3-O3
34	O	305	PID	C28-C27-O6-C30
30	K	313	CLA	C6-C7-C8-C9
30	b	707	CLA	C16-C17-C18-C20
30	a	728	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	D	311	CLA	C2A-CAA-CBA-CGA
30	b	716	CLA	C3A-C2A-CAA-CBA
30	b	719	CLA	C3A-C2A-CAA-CBA
30	B	307	CLA	C3A-C2A-CAA-CBA
30	F	313	CLA	C3A-C2A-CAA-CBA
30	D	308	CLA	CBA-CGA-O2A-C1
39	a	733	LHG	C29-C30-C31-C32
32	G	501	DGD	C3A-C4A-C5A-C6A
30	l	303	CLA	C14-C13-C15-C16
30	a	721	CLA	C11-C12-C13-C14
30	b	724	CLA	C11-C10-C8-C9
30	b	727	CLA	C6-C7-C8-C9
30	N	305	CLA	C14-C13-C15-C16
30	I	315	CLA	C4C-C3C-CAC-CBC
30	O	314	CLA	C2-C1-O2A-CGA
28	I	302	DD6	C9-C10-C11-C12
32	G	501	DGD	O1G-C1G-C2G-C3G
34	D	304	PID	C19-C20-C21-CM5
37	f	304	BCR	C35-C13-C14-C15
37	l	302	BCR	C20-C21-C22-C37
30	l	304	CLA	C11-C12-C13-C15
30	b	727	CLA	C16-C17-C18-C20
29	G	503	UIX	C36-C38-C40-C41
30	B	316	CLA	O1A-CGA-O2A-C1
33	I	320	LMG	C7-C8-O7-C10
39	a	733	LHG	C4-C5-O7-C7
39	a	733	LHG	C6-C5-O7-C7
30	I	308	CLA	C1A-C2A-CAA-CBA
30	I	310	CLA	C1A-C2A-CAA-CBA
30	a	706	CLA	C1A-C2A-CAA-CBA
30	b	716	CLA	C1A-C2A-CAA-CBA
30	B	313	CLA	C1A-C2A-CAA-CBA
30	H	305	CLA	C16-C17-C18-C20
30	a	735	CLA	C12-C13-C15-C16
30	b	713	CLA	C11-C10-C8-C7
30	a	723	CLA	C3-C5-C6-C7
30	L	318	CLA	CAA-CBA-CGA-O1A
28	F	303	DD6	C11-C10-C9-C8
30	D	308	CLA	O1A-CGA-O2A-C1
30	A	308	CLA	C2A-CAA-CBA-CGA
30	b	725	CLA	C2A-CAA-CBA-CGA
30	L	314	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	b	715	CLA	CBA-CGA-O2A-C1
32	j	103	DGD	C2A-C3A-C4A-C5A
31	P	211	KC1	C3A-C2A-CAA-CBA
34	O	305	PID	C26-C27-O6-C30
31	G	515	KC1	C4C-C3C-CAC-CBC
28	I	302	DD6	C9-C10-C11-C13
37	f	304	BCR	C12-C13-C14-C15
37	l	302	BCR	C20-C21-C22-C23
30	I	308	CLA	C10-C11-C12-C13
28	G	504	DD6	C24-C25-C26-C27
28	M	302	DD6	C3-C4-C5-C6
34	O	307	PID	C28-C27-O6-C30
30	I	321	CLA	C2-C1-O2A-CGA
30	G	514	CLA	C2-C1-O2A-CGA
30	A	309	CLA	C2-C1-O2A-CGA
30	I	312	CLA	C6-C7-C8-C9
30	b	707	CLA	C11-C10-C8-C9
30	b	725	CLA	C6-C7-C8-C9
30	J	307	CLA	C14-C13-C15-C16
30	B	316	CLA	C2C-C3C-CAC-CBC
30	O	311	CLA	C4-C3-C5-C6
30	P	212	CLA	C4-C3-C5-C6
31	G	515	KC1	C1A-C2A-CAA-CBA
31	A	314	KC1	C1A-C2A-CAA-CBA
31	F	314	KC1	C1A-C2A-CAA-CBA
31	H	310	KC1	C1A-C2A-CAA-CBA
31	M	307	KC1	C1A-C2A-CAA-CBA
30	l	305	CLA	CAA-CBA-CGA-O2A
30	a	710	CLA	C2A-CAA-CBA-CGA
30	b	720	CLA	C2A-CAA-CBA-CGA
30	J	309	CLA	C2A-CAA-CBA-CGA
30	P	210	CLA	C2A-CAA-CBA-CGA
30	I	316	CLA	O1A-CGA-O2A-C1
30	b	715	CLA	O1A-CGA-O2A-C1
39	a	733	LHG	O10-C23-O8-C6
37	f	304	BCR	C23-C24-C25-C30
37	a	734	BCR	C23-C24-C25-C30
37	b	730	BCR	C23-C24-C25-C30
37	b	732	BCR	C1-C6-C7-C8
30	a	728	CLA	C5-C6-C7-C8
30	A	316	CLA	O1A-CGA-O2A-C1
28	P	204	DD6	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
30	a	725	CLA	CBA-CGA-O2A-C1
28	A	302	DD6	C5-C6-C8-C9
30	A	310	CLA	C13-C15-C16-C17
30	B	309	CLA	C5-C6-C7-C8
30	a	729	CLA	CAA-CBA-CGA-O2A
30	b	714	CLA	CAA-CBA-CGA-O1A
33	b	733	LMG	C8-C7-O1-C1
35	A	318	SQD	C45-C44-O6-C1
30	a	727	CLA	O1D-CGD-O2D-CED
30	a	725	CLA	O1A-CGA-O2A-C1
30	b	707	CLA	C16-C17-C18-C19
30	G	517	CLA	C2A-CAA-CBA-CGA
30	a	710	CLA	C6-C7-C8-C10
33	j	101	LMG	C4-C5-C6-O5
33	b	733	LMG	C17-C18-C19-C20
30	L	311	CLA	C4-C3-C5-C6
30	l	311	CLA	C11-C12-C13-C15
30	a	704	CLA	C11-C10-C8-C7
30	a	709	CLA	C6-C7-C8-C10
30	b	725	CLA	C6-C7-C8-C10
30	H	305	CLA	C2-C3-C5-C6
28	K	301	DD6	C24-C25-C26-C27
29	J	305	UIX	C26-C30-C34-C37
30	B	308	CLA	CAA-CBA-CGA-O2A
30	G	509	CLA	O1A-CGA-O2A-C1
30	l	312	CLA	O1A-CGA-O2A-C1
30	b	722	CLA	C2A-CAA-CBA-CGA
30	G	509	CLA	CBA-CGA-O2A-C1
30	A	316	CLA	CBA-CGA-O2A-C1
33	D	317	LMG	C16-C17-C18-C19
34	D	304	PID	CM4-C14-C15-C16
30	b	713	CLA	CAA-CBA-CGA-O2A
30	b	720	CLA	C4-C3-C5-C6
30	L	313	CLA	C4-C3-C5-C6
30	l	303	CLA	C13-C15-C16-C17
31	N	311	KC1	C2A-CAA-CBA-CGA
30	J	312	CLA	CBD-CGD-O2D-CED
33	K	317	LMG	C18-C19-C20-C21
30	m	202	CLA	CAA-CBA-CGA-O2A
30	B	310	CLA	CAA-CBA-CGA-O2A
30	a	729	CLA	C11-C10-C8-C7
30	A	310	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	a	723	CLA	C11-C10-C8-C9
30	a	729	CLA	C6-C7-C8-C9
30	a	735	CLA	C14-C13-C15-C16
30	b	708	CLA	C11-C10-C8-C9
30	B	309	CLA	C11-C10-C8-C9
30	B	311	CLA	C11-C12-C13-C14
30	J	307	CLA	C11-C10-C8-C9
30	l	311	CLA	C3A-C2A-CAA-CBA
30	H	307	CLA	C3A-C2A-CAA-CBA
30	L	318	CLA	C3A-C2A-CAA-CBA
30	M	311	CLA	C3A-C2A-CAA-CBA
33	D	317	LMG	C20-C21-C22-C23
30	b	724	CLA	CAA-CBA-CGA-O2A
30	L	317	CLA	CAA-CBA-CGA-O2A
30	a	715	CLA	CAA-CBA-CGA-O2A
29	P	207	UIX	C25-C28-C32-C33
30	I	312	CLA	CAD-CBD-CGD-O2D
30	I	313	CLA	CAD-CBD-CGD-O2D
30	I	316	CLA	CAD-CBD-CGD-O2D
30	K	312	CLA	CAD-CBD-CGD-O2D
30	G	510	CLA	CAD-CBD-CGD-O2D
30	G	518	CLA	CAD-CBD-CGD-O2D
30	G	520	CLA	CAD-CBD-CGD-O2D
30	A	309	CLA	CAD-CBD-CGD-O2D
30	j	106	CLA	CAD-CBD-CGD-O2D
30	l	303	CLA	CAD-CBD-CGD-O2D
30	l	311	CLA	CAD-CBD-CGD-O2D
30	a	706	CLA	CAD-CBD-CGD-O2D
30	a	713	CLA	CAD-CBD-CGD-O2D
30	b	722	CLA	CAD-CBD-CGD-O2D
30	b	724	CLA	CAD-CBD-CGD-O2D
30	b	725	CLA	CAD-CBD-CGD-O2D
30	b	726	CLA	CAD-CBD-CGD-O2D
30	B	301	CLA	CAD-CBD-CGD-O2D
30	B	311	CLA	CAD-CBD-CGD-O2D
30	F	312	CLA	CAD-CBD-CGD-O2D
30	H	309	CLA	CAD-CBD-CGD-O2D
30	J	311	CLA	CAD-CBD-CGD-O2D
30	M	311	CLA	CAD-CBD-CGD-O2D
30	M	312	CLA	CAD-CBD-CGD-O2D
30	M	316	CLA	CAD-CBD-CGD-O2D
30	N	309	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	N	310	CLA	CAD-CBD-CGD-O2D
30	O	314	CLA	CAD-CBD-CGD-O2D
31	G	515	KC1	CAD-CBD-CGD-O2D
33	I	320	LMG	C9-C8-O7-C10
30	a	703	CLA	C6-C7-C8-C10
33	j	101	LMG	C10-C11-C12-C13
30	l	310	CLA	CAA-CBA-CGA-O2A
30	a	723	CLA	CAA-CBA-CGA-O2A
30	I	315	CLA	C2C-C3C-CAC-CBC
30	I	308	CLA	CAA-CBA-CGA-O2A
30	I	316	CLA	CAA-CBA-CGA-O2A
30	A	310	CLA	CAA-CBA-CGA-O2A
33	I	320	LMG	O8-C28-C29-C30
29	G	503	UIX	C36-C38-C40-C39
28	K	301	DD6	C13-C14-C15-O1
28	K	305	DD6	C13-C14-C15-O1
28	K	318	DD6	C13-C14-C15-O1
28	A	302	DD6	C13-C14-C15-O1
28	M	306	DD6	C13-C14-C15-O1
29	I	304	UIX	O-C-C7-C10
33	j	101	LMG	O1-C7-C8-C9
34	F	305	PID	O1-C6-C7-C8
34	M	301	PID	O1-C6-C7-C8
34	N	301	PID	O1-C6-C7-C8
34	O	305	PID	O1-C6-C7-C8
30	G	511	CLA	CAA-CBA-CGA-O2A
30	a	706	CLA	CAA-CBA-CGA-O2A
30	a	717	CLA	CAA-CBA-CGA-O2A
30	H	305	CLA	C16-C17-C18-C19
30	B	307	CLA	O2A-C1-C2-C3
30	I	309	CLA	O2A-C1-C2-C3
30	G	510	CLA	O2A-C1-C2-C3
30	l	304	CLA	O2A-C1-C2-C3
30	l	313	CLA	O2A-C1-C2-C3
30	a	723	CLA	O2A-C1-C2-C3
30	b	716	CLA	O2A-C1-C2-C3
30	b	717	CLA	O2A-C1-C2-C3
30	B	309	CLA	O2A-C1-C2-C3
30	B	311	CLA	O2A-C1-C2-C3
30	J	307	CLA	O2A-C1-C2-C3
30	L	309	CLA	O2A-C1-C2-C3
30	L	310	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	b	708	CLA	CAA-CBA-CGA-O2A
30	b	711	CLA	CAA-CBA-CGA-O2A
30	a	711	CLA	CAA-CBA-CGA-O2A
30	a	715	CLA	CAA-CBA-CGA-O1A
30	I	308	CLA	C11-C12-C13-C15
30	a	731	CLA	C16-C17-C18-C19
30	I	321	CLA	CHA-CBD-CGD-O2D
30	K	308	CLA	CHA-CBD-CGD-O1D
30	K	308	CLA	CHA-CBD-CGD-O2D
30	A	315	CLA	CHA-CBD-CGD-O2D
30	A	320	CLA	CHA-CBD-CGD-O2D
30	j	104	CLA	CHA-CBD-CGD-O1D
30	l	303	CLA	CHA-CBD-CGD-O1D
30	l	312	CLA	CHA-CBD-CGD-O1D
30	l	312	CLA	CHA-CBD-CGD-O2D
30	a	702	CLA	CHA-CBD-CGD-O2D
30	a	703	CLA	CHA-CBD-CGD-O2D
30	a	707	CLA	CHA-CBD-CGD-O1D
30	a	707	CLA	CHA-CBD-CGD-O2D
30	a	709	CLA	CHA-CBD-CGD-O1D
30	a	709	CLA	CHA-CBD-CGD-O2D
30	a	719	CLA	CHA-CBD-CGD-O2D
30	b	705	CLA	CHA-CBD-CGD-O2D
30	b	710	CLA	CHA-CBD-CGD-O1D
30	b	710	CLA	CHA-CBD-CGD-O2D
30	b	714	CLA	CHA-CBD-CGD-O2D
30	b	721	CLA	CHA-CBD-CGD-O1D
30	b	721	CLA	CHA-CBD-CGD-O2D
30	b	727	CLA	CHA-CBD-CGD-O1D
30	b	727	CLA	CHA-CBD-CGD-O2D
30	B	313	CLA	CHA-CBD-CGD-O1D
30	B	313	CLA	CHA-CBD-CGD-O2D
30	D	308	CLA	CHA-CBD-CGD-O1D
30	D	308	CLA	CHA-CBD-CGD-O2D
30	F	307	CLA	CHA-CBD-CGD-O1D
30	F	307	CLA	CHA-CBD-CGD-O2D
30	H	311	CLA	CHA-CBD-CGD-O1D
30	H	311	CLA	CHA-CBD-CGD-O2D
30	J	308	CLA	CHA-CBD-CGD-O1D
30	J	308	CLA	CHA-CBD-CGD-O2D
30	J	309	CLA	CHA-CBD-CGD-O1D
30	J	309	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	L	309	CLA	CHA-CBD-CGD-O1D
30	L	309	CLA	CHA-CBD-CGD-O2D
30	L	311	CLA	CHA-CBD-CGD-O1D
30	M	310	CLA	CHA-CBD-CGD-O1D
30	M	315	CLA	CHA-CBD-CGD-O1D
30	M	315	CLA	CHA-CBD-CGD-O2D
30	M	318	CLA	CHA-CBD-CGD-O1D
30	M	318	CLA	CHA-CBD-CGD-O2D
30	N	307	CLA	CHA-CBD-CGD-O2D
30	P	210	CLA	CHA-CBD-CGD-O2D
31	G	515	KC1	CHA-CBD-CGD-O1D
31	F	314	KC1	CHA-CBD-CGD-O1D
31	M	307	KC1	CHA-CBD-CGD-O2D
31	P	211	KC1	CHA-CBD-CGD-O1D
31	P	213	KC1	CHA-CBD-CGD-O1D
31	P	213	KC1	CHA-CBD-CGD-O2D
30	l	305	CLA	C15-C16-C17-C18
30	D	309	CLA	CAA-CBA-CGA-O2A
30	J	310	CLA	CAA-CBA-CGA-O2A
30	M	316	CLA	CAA-CBA-CGA-O2A
32	l	301	DGD	C3A-C4A-C5A-C6A
33	K	317	LMG	C19-C20-C21-C22
30	a	711	CLA	CAA-CBA-CGA-O1A
30	G	514	CLA	CAA-CBA-CGA-O2A
30	l	305	CLA	O1A-CGA-O2A-C1
30	B	308	CLA	CAA-CBA-CGA-O1A
33	D	317	LMG	C36-C37-C38-C39
30	L	309	CLA	C5-C6-C7-C8
30	I	309	CLA	O1A-CGA-O2A-C1
30	J	312	CLA	O1D-CGD-O2D-CED
30	M	317	CLA	C2A-CAA-CBA-CGA
30	I	319	CLA	CAA-CBA-CGA-O2A
30	l	305	CLA	CBA-CGA-O2A-C1
30	a	706	CLA	C10-C11-C12-C13
30	K	309	CLA	CAA-CBA-CGA-O2A
30	b	707	CLA	C2-C3-C5-C6
32	j	103	DGD	O6D-C5D-C6D-O5D
30	b	725	CLA	C16-C17-C18-C20
30	a	724	CLA	C11-C10-C8-C9
30	a	725	CLA	C6-C7-C8-C9
30	B	301	CLA	C11-C10-C8-C9
30	G	520	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	j	103	DGD	C1A-C2A-C3A-C4A
30	I	309	CLA	CBA-CGA-O2A-C1
30	A	310	CLA	CAA-CBA-CGA-O1A
30	A	313	CLA	C2A-CAA-CBA-CGA
30	a	735	CLA	C2A-CAA-CBA-CGA
30	a	717	CLA	CAA-CBA-CGA-O1A
30	I	316	CLA	CBA-CGA-O2A-C1
30	B	316	CLA	C4C-C3C-CAC-CBC
37	m	201	BCR	C37-C22-C23-C24
30	m	202	CLA	CAA-CBA-CGA-O1A
30	a	706	CLA	CAA-CBA-CGA-O1A
30	b	724	CLA	CAA-CBA-CGA-O1A
30	P	212	CLA	CAA-CBA-CGA-O2A
30	B	310	CLA	CAA-CBA-CGA-O1A
37	l	302	BCR	C17-C18-C19-C20
30	I	307	CLA	C1A-C2A-CAA-CBA
30	b	713	CLA	C1A-C2A-CAA-CBA
30	b	719	CLA	C1A-C2A-CAA-CBA
30	b	728	CLA	C1A-C2A-CAA-CBA
30	B	307	CLA	C1A-C2A-CAA-CBA
30	B	309	CLA	C1A-C2A-CAA-CBA
30	H	307	CLA	C1A-C2A-CAA-CBA
30	L	318	CLA	C1A-C2A-CAA-CBA
30	M	311	CLA	C1A-C2A-CAA-CBA
30	P	210	CLA	C1A-C2A-CAA-CBA
30	G	511	CLA	C6-C7-C8-C10
30	I	308	CLA	CAA-CBA-CGA-O1A
30	I	316	CLA	CAA-CBA-CGA-O1A
30	b	713	CLA	CAA-CBA-CGA-O1A
34	D	302	PID	C28-C27-O6-C30
31	F	314	KC1	CAA-CBA-CGA-O2A
32	G	501	DGD	C2A-C3A-C4A-C5A
30	L	310	CLA	C2-C1-O2A-CGA
30	J	310	CLA	CAA-CBA-CGA-O1A
30	J	312	CLA	CAA-CBA-CGA-O2A
30	I	321	CLA	C2A-CAA-CBA-CGA
30	l	305	CLA	C2A-CAA-CBA-CGA
30	J	307	CLA	C2A-CAA-CBA-CGA
30	M	313	CLA	C2A-CAA-CBA-CGA
30	a	727	CLA	CBD-CGD-O2D-CED
30	D	312	CLA	CBD-CGD-O2D-CED
30	b	724	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	M	316	CLA	CAA-CBA-CGA-O1A
30	O	309	CLA	C13-C15-C16-C17
30	K	308	CLA	CAA-CBA-CGA-O2A
30	l	313	CLA	C3-C5-C6-C7
30	a	730	CLA	C3-C5-C6-C7
32	y	201	DGD	C2A-C3A-C4A-C5A
30	a	723	CLA	CAA-CBA-CGA-O1A
39	a	733	LHG	C3-O3-P-O5
39	a	733	LHG	C4-O6-P-O5
30	B	309	CLA	C16-C17-C18-C19
30	G	514	CLA	CAA-CBA-CGA-O1A
30	l	310	CLA	CAA-CBA-CGA-O1A
30	b	708	CLA	CAA-CBA-CGA-O1A
30	D	309	CLA	CAA-CBA-CGA-O1A
30	L	317	CLA	CAA-CBA-CGA-O1A
30	a	718	CLA	CAA-CBA-CGA-O2A
30	L	311	CLA	CAA-CBA-CGA-O2A
34	O	304	PID	CM4-C14-C15-C16
37	a	734	BCR	C23-C24-C25-C26
37	a	736	BCR	C5-C6-C7-C8
37	b	730	BCR	C23-C24-C25-C26
37	b	732	BCR	C5-C6-C7-C8
30	b	705	CLA	C5-C6-C7-C8
28	I	302	DD6	C11-C13-C14-C15
28	D	303	DD6	C11-C13-C14-C15
34	F	304	PID	C6-C7-C8-C9
33	B	318	LMG	O9-C10-C11-C12
30	a	729	CLA	CBD-CGD-O2D-CED
30	K	310	CLA	CAA-CBA-CGA-O2A
30	G	519	CLA	C11-C12-C13-C14
30	I	319	CLA	CAA-CBA-CGA-O1A
32	I	317	DGD	O6D-C5D-C6D-O5D
30	l	303	CLA	C2A-CAA-CBA-CGA
30	G	511	CLA	CAA-CBA-CGA-O1A
30	b	711	CLA	CAA-CBA-CGA-O1A
33	I	320	LMG	O9-C10-C11-C12
30	M	309	CLA	CAA-CBA-CGA-O2A
30	b	713	CLA	C13-C15-C16-C17
30	D	312	CLA	O1D-CGD-O2D-CED
30	b	701	CLA	C8-C10-C11-C12
30	I	319	CLA	CAD-CBD-CGD-O1D
30	b	705	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	b	713	CLA	CAD-CBD-CGD-O1D
30	b	721	CLA	CAD-CBD-CGD-O1D
30	F	307	CLA	CAD-CBD-CGD-O1D
30	H	307	CLA	CAD-CBD-CGD-O1D
30	J	316	CLA	CAD-CBD-CGD-O1D
30	L	309	CLA	CAD-CBD-CGD-O1D
30	N	304	CLA	CAD-CBD-CGD-O1D
30	N	307	CLA	CAD-CBD-CGD-O1D
30	N	307	CLA	C2-C3-C5-C6
30	O	308	CLA	CAD-CBD-CGD-O1D
30	j	106	CLA	O1A-CGA-O2A-C1
30	J	312	CLA	CAA-CBA-CGA-O1A
33	I	320	LMG	O10-C28-C29-C30
39	a	733	LHG	C31-C32-C33-C34
30	a	726	CLA	C5-C6-C7-C8
30	a	702	CLA	C14-C13-C15-C16
30	a	709	CLA	C6-C7-C8-C9
30	b	713	CLA	C14-C13-C15-C16
30	J	308	CLA	CAA-CBA-CGA-O1A
30	j	106	CLA	CBA-CGA-O2A-C1
30	G	512	CLA	CAA-CBA-CGA-O2A
30	A	309	CLA	CAA-CBA-CGA-O2A
30	l	311	CLA	C2A-CAA-CBA-CGA
30	a	703	CLA	C2A-CAA-CBA-CGA
30	M	309	CLA	C2A-CAA-CBA-CGA
30	h	202	CLA	CAA-CBA-CGA-O2A
30	a	703	CLA	CAA-CBA-CGA-O2A
30	b	705	CLA	CAA-CBA-CGA-O2A
30	b	706	CLA	CAA-CBA-CGA-O2A
30	b	716	CLA	CAA-CBA-CGA-O2A
30	b	725	CLA	CAA-CBA-CGA-O2A
30	P	210	CLA	CAA-CBA-CGA-O2A
33	b	733	LMG	C10-C11-C12-C13
32	y	201	DGD	C2B-C3B-C4B-C5B
30	l	313	CLA	C4-C3-C5-C6
30	l	304	CLA	C6-C7-C8-C10
30	a	717	CLA	C2-C3-C5-C6
30	a	721	CLA	C11-C12-C13-C15
30	a	725	CLA	C6-C7-C8-C10
30	J	307	CLA	C12-C13-C15-C16
30	N	309	CLA	C3A-C2A-CAA-CBA
30	K	308	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	P	212	CLA	CAA-CBA-CGA-O1A
30	I	306	CLA	O2A-C1-C2-C3
37	l	302	BCR	C21-C22-C23-C24
30	K	309	CLA	CAA-CBA-CGA-O1A
30	a	703	CLA	CAA-CBA-CGA-O1A
30	J	311	CLA	C2-C1-O2A-CGA
30	I	309	CLA	CAA-CBA-CGA-O2A
30	j	104	CLA	CAA-CBA-CGA-O2A
30	b	715	CLA	CAA-CBA-CGA-O2A
32	L	301	DGD	O2G-C1B-C2B-C3B
30	b	715	CLA	C8-C10-C11-C12
30	N	310	CLA	C2-C1-O2A-CGA
30	G	512	CLA	CAA-CBA-CGA-O1A
30	a	731	CLA	CAA-CBA-CGA-O2A
30	b	721	CLA	CAA-CBA-CGA-O2A
30	H	307	CLA	CAA-CBA-CGA-O2A
30	N	307	CLA	CAA-CBA-CGA-O2A
33	K	317	LMG	C16-C17-C18-C19
30	A	309	CLA	CAA-CBA-CGA-O1A
30	b	705	CLA	CAA-CBA-CGA-O1A
30	b	716	CLA	CAA-CBA-CGA-O1A
30	b	725	CLA	CAA-CBA-CGA-O1A
30	M	315	CLA	C2C-C3C-CAC-CBC
30	G	518	CLA	CAA-CBA-CGA-O2A
30	A	308	CLA	CAA-CBA-CGA-O2A

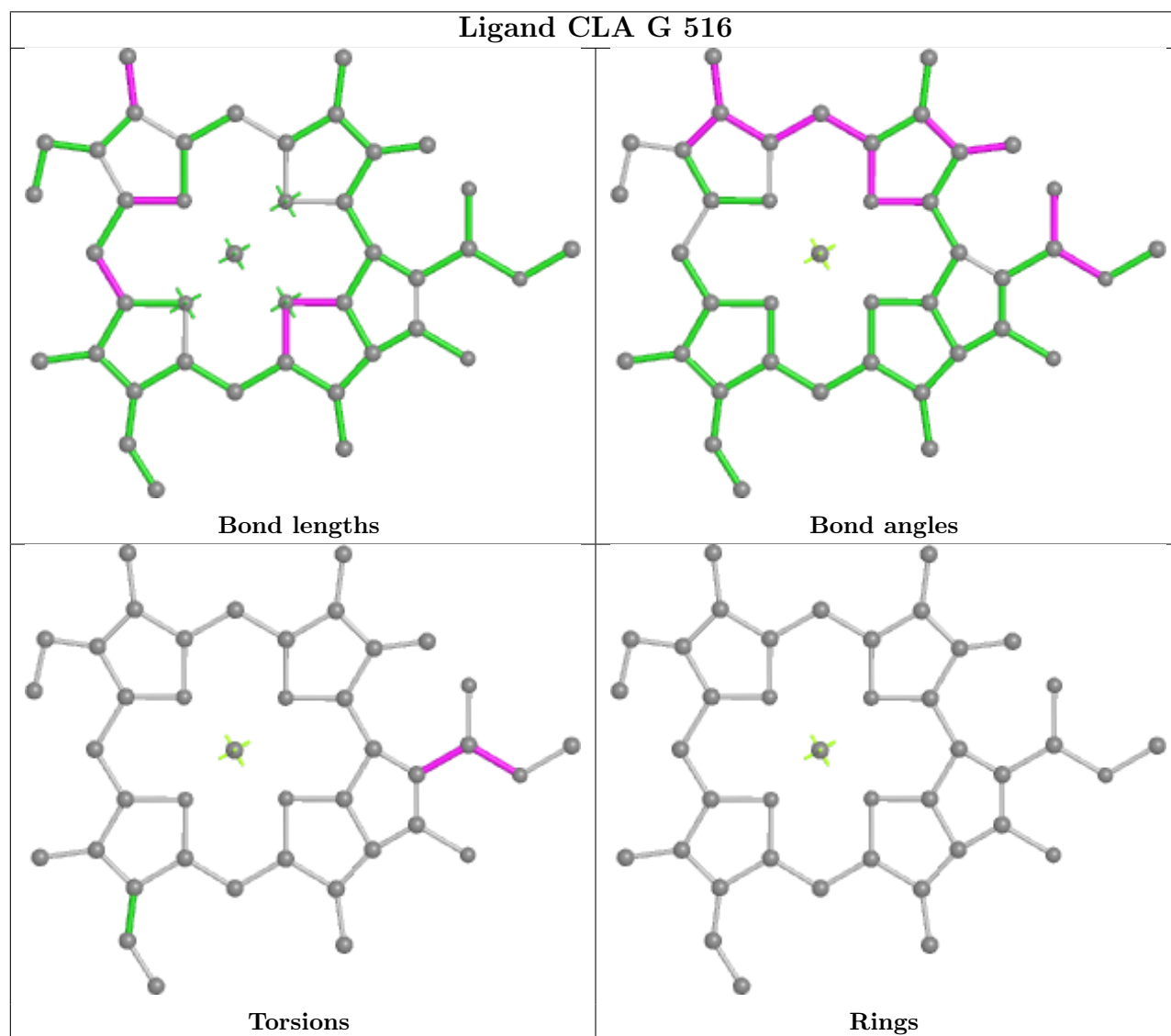
All (1) ring outliers are listed below:

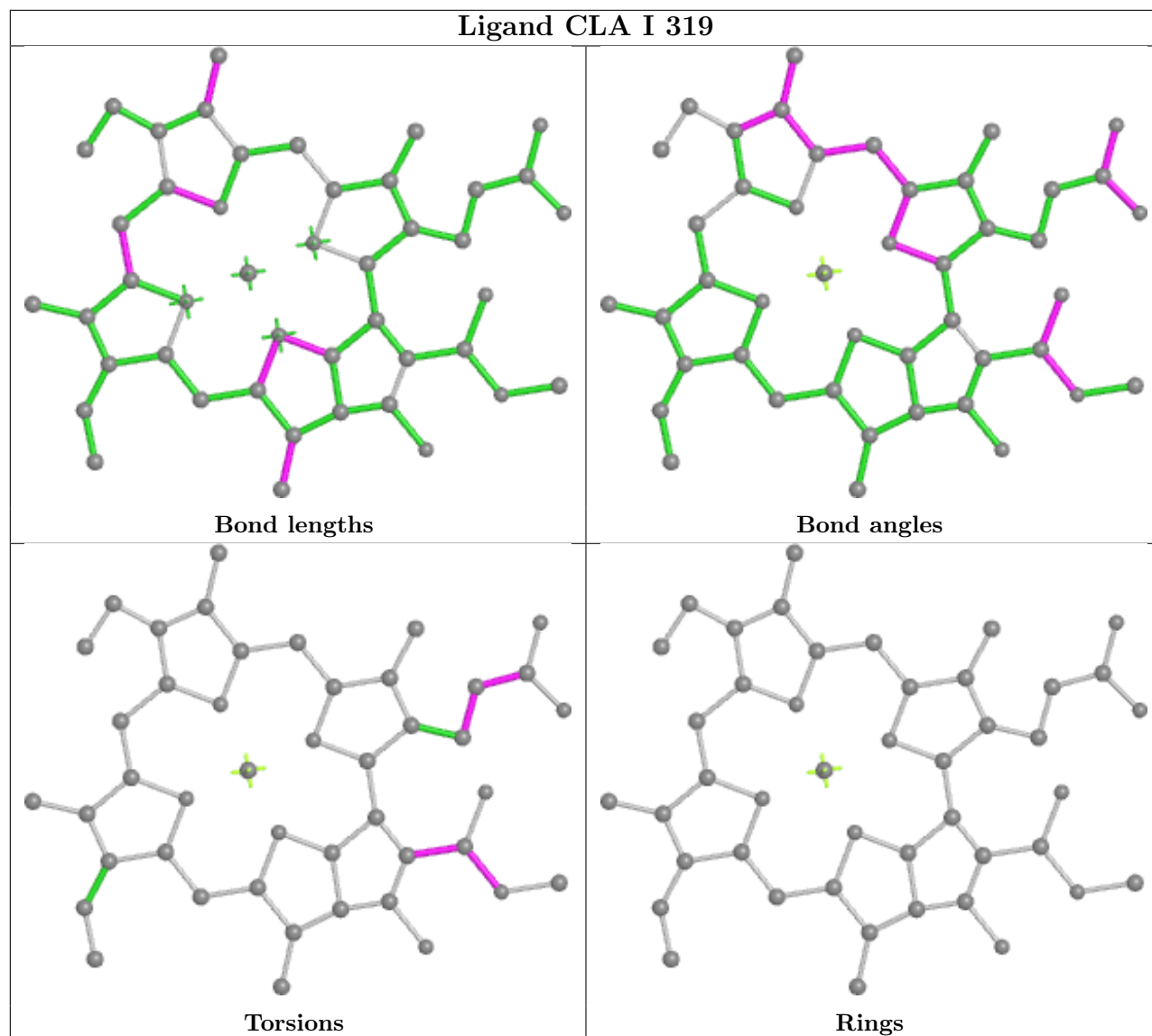
Mol	Chain	Res	Type	Atoms
34	G	507	PID	C24-C25-C26-C27-C28-C29

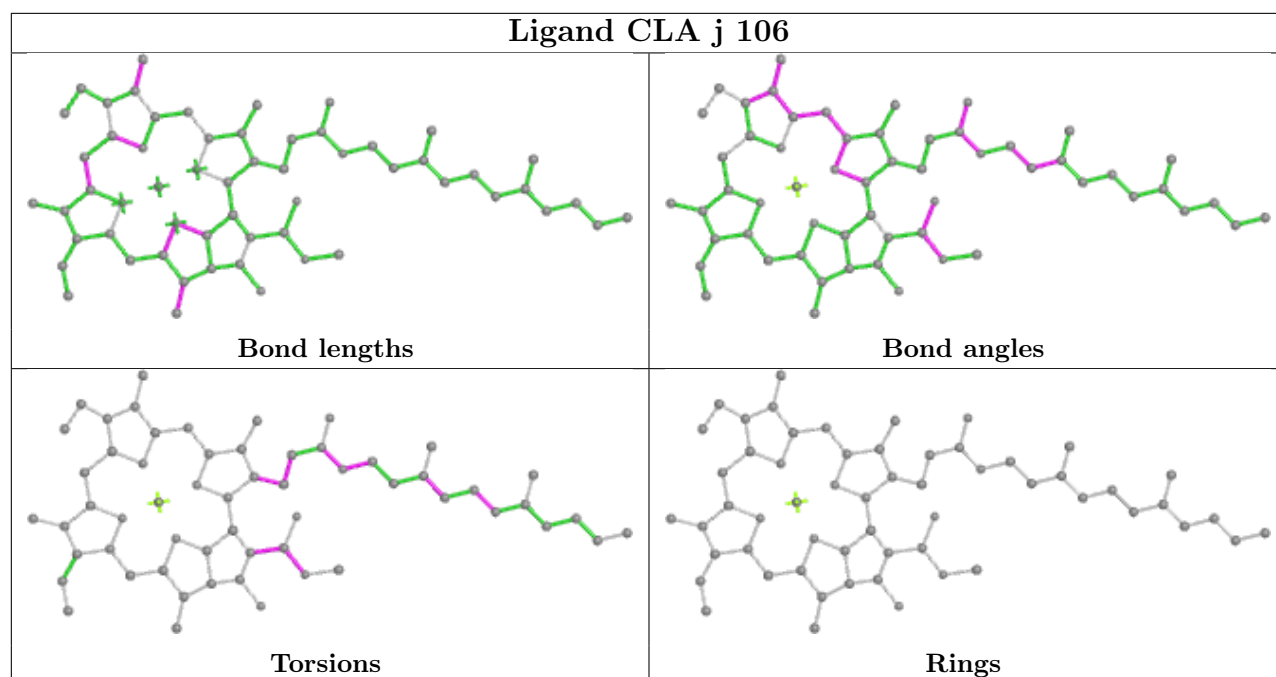
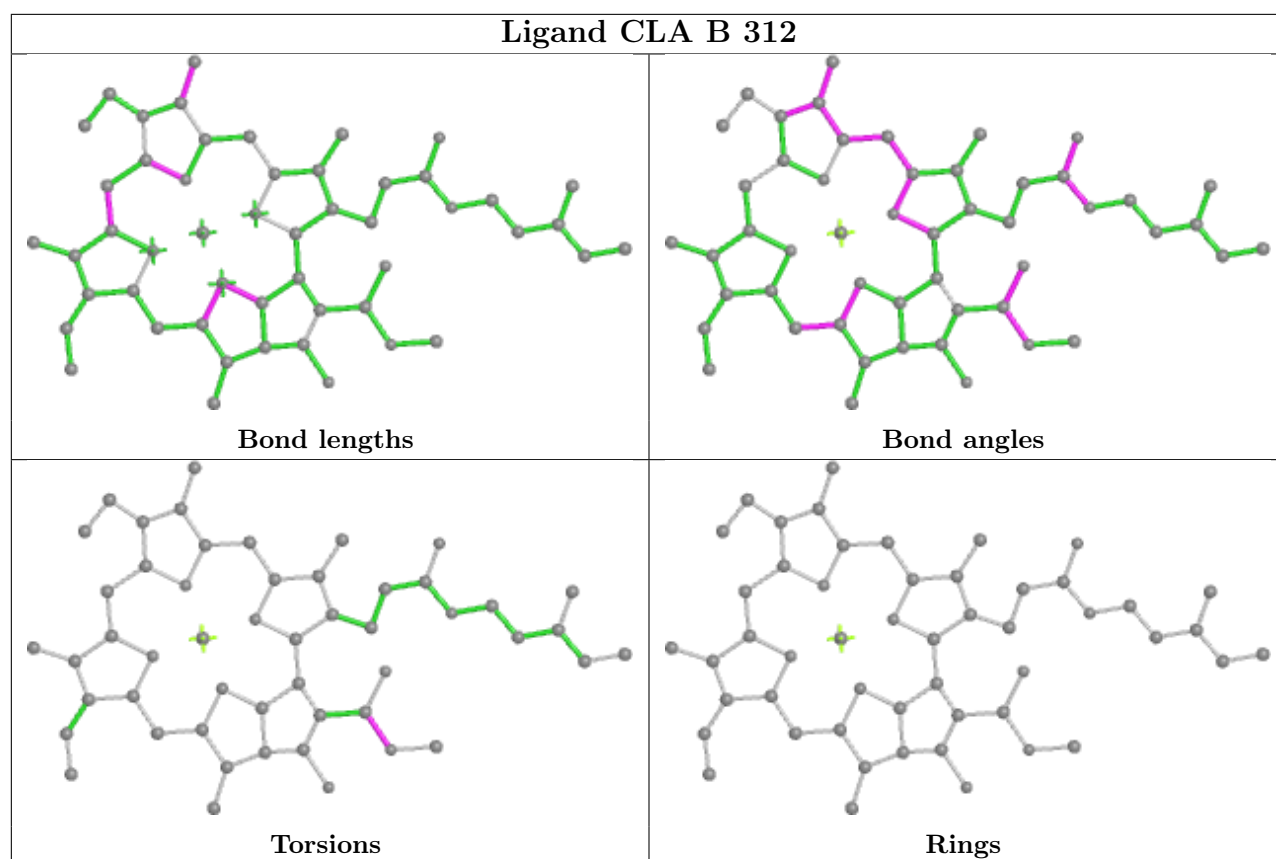
No monomer is involved in short contacts.

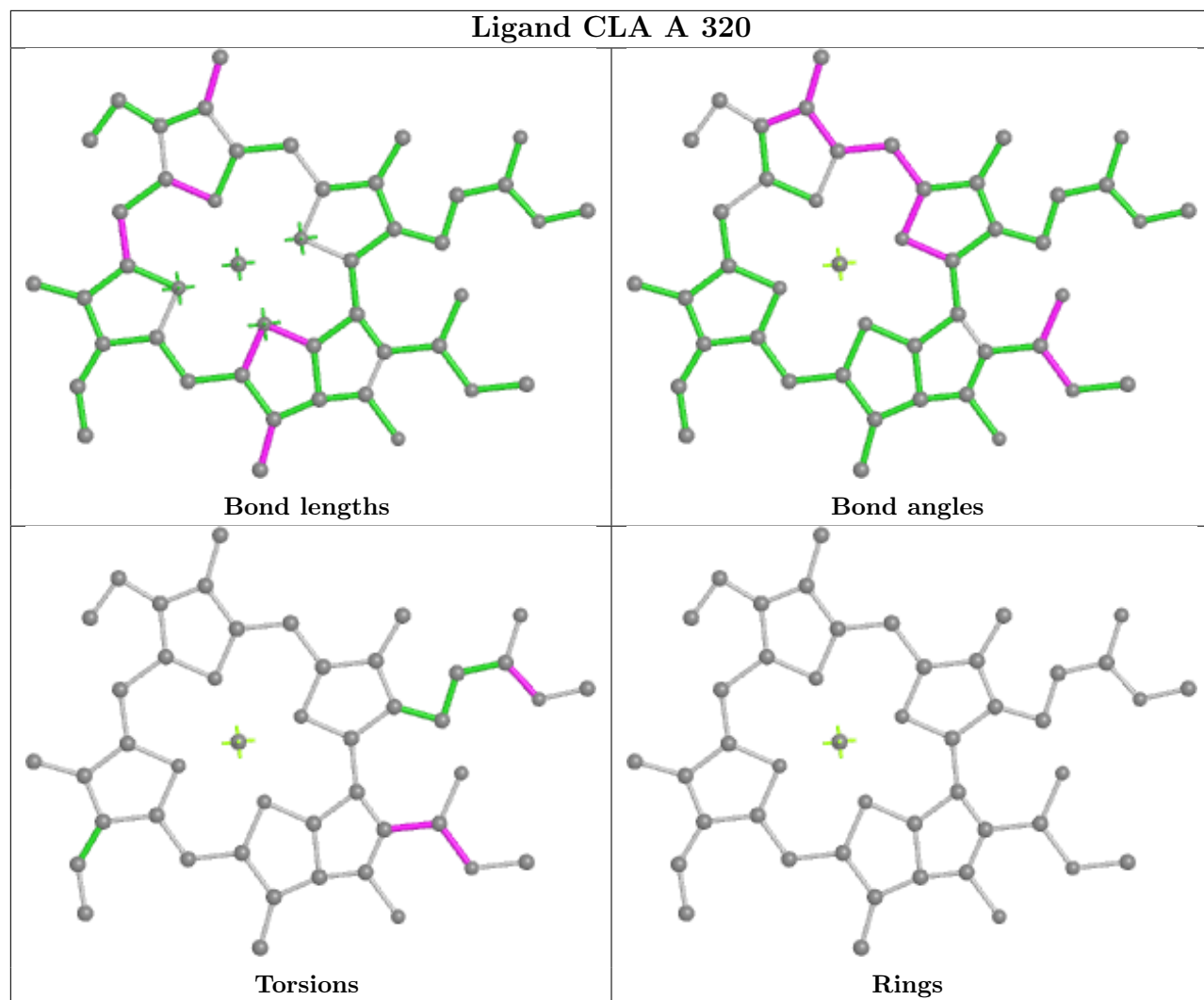
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

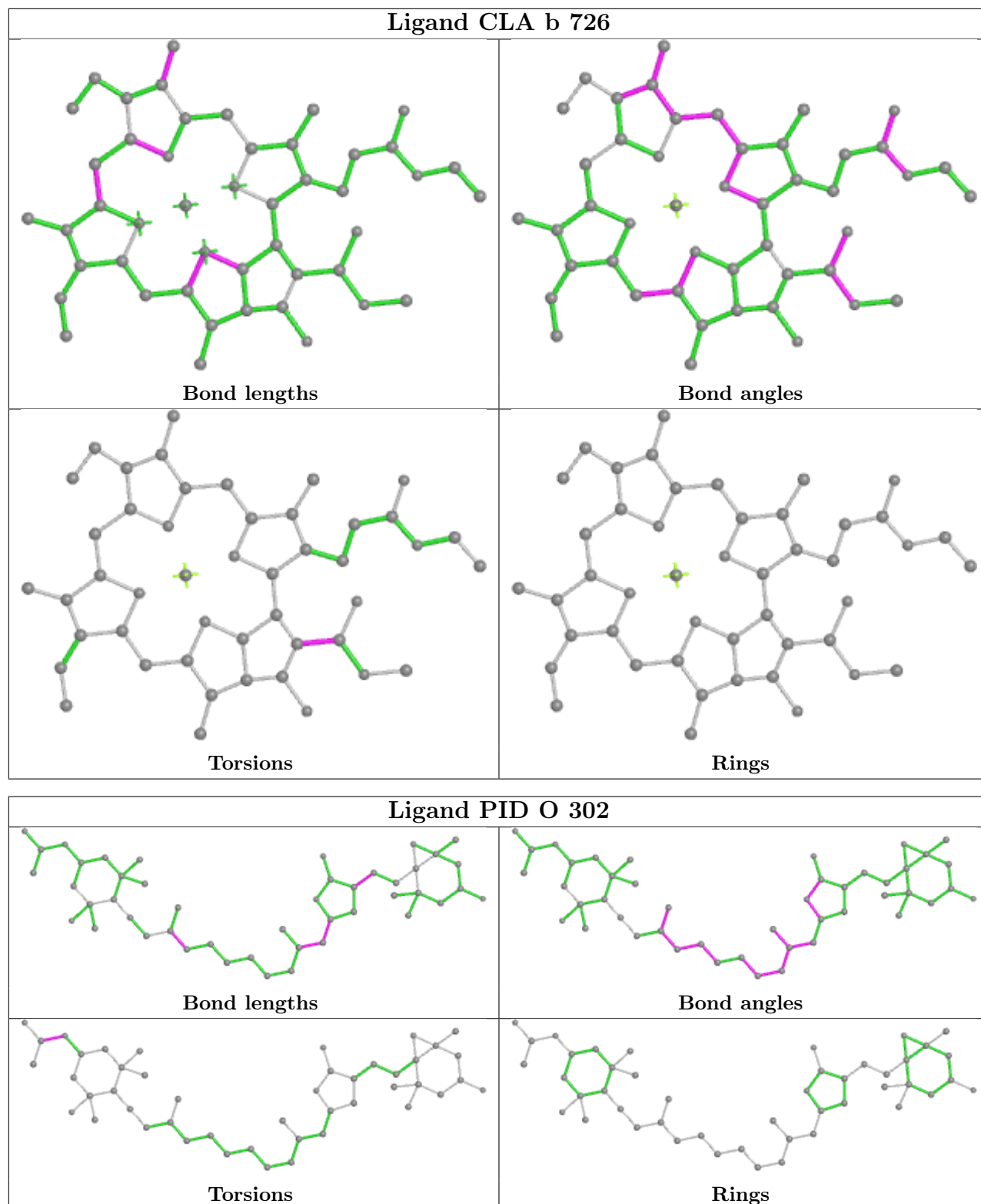
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

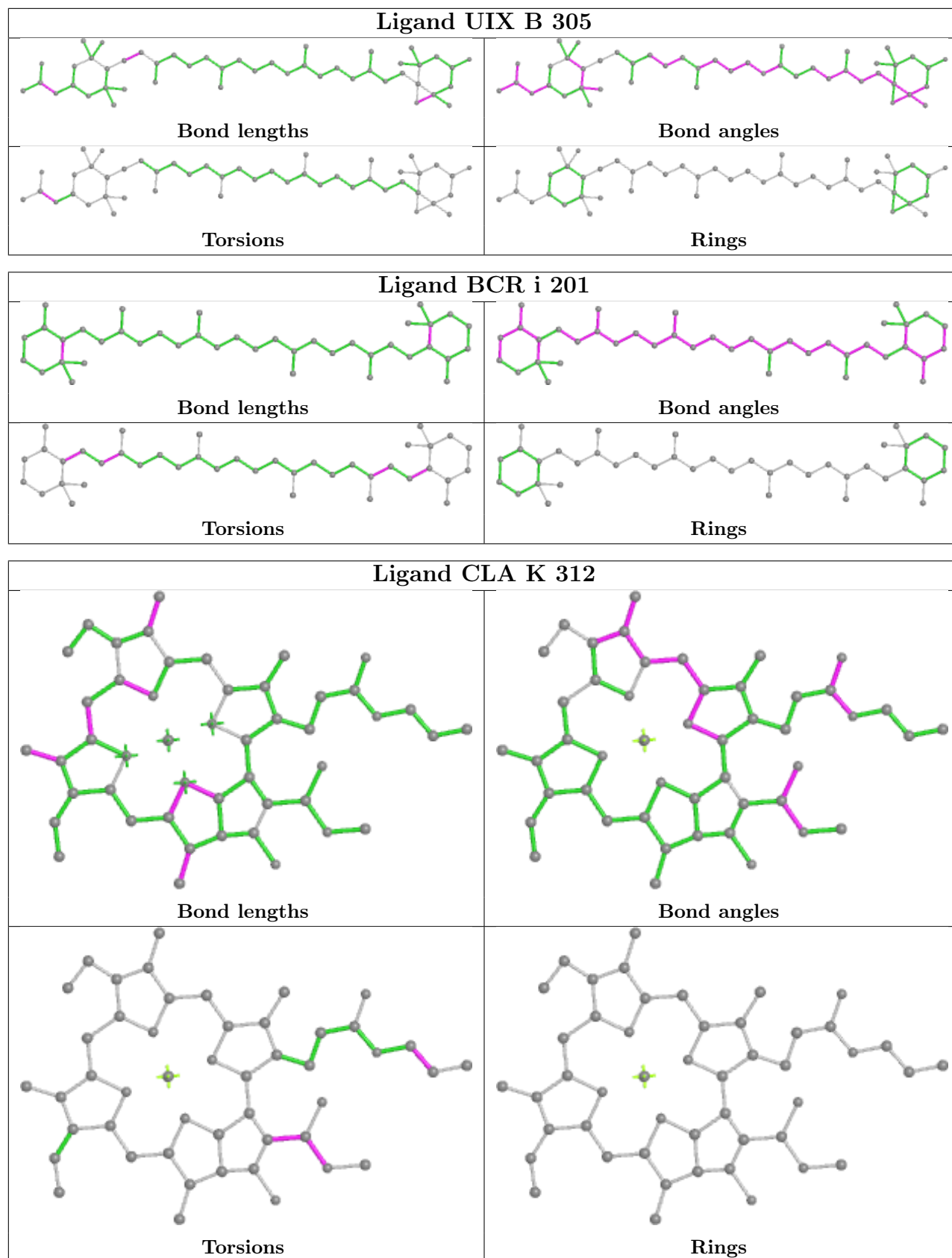


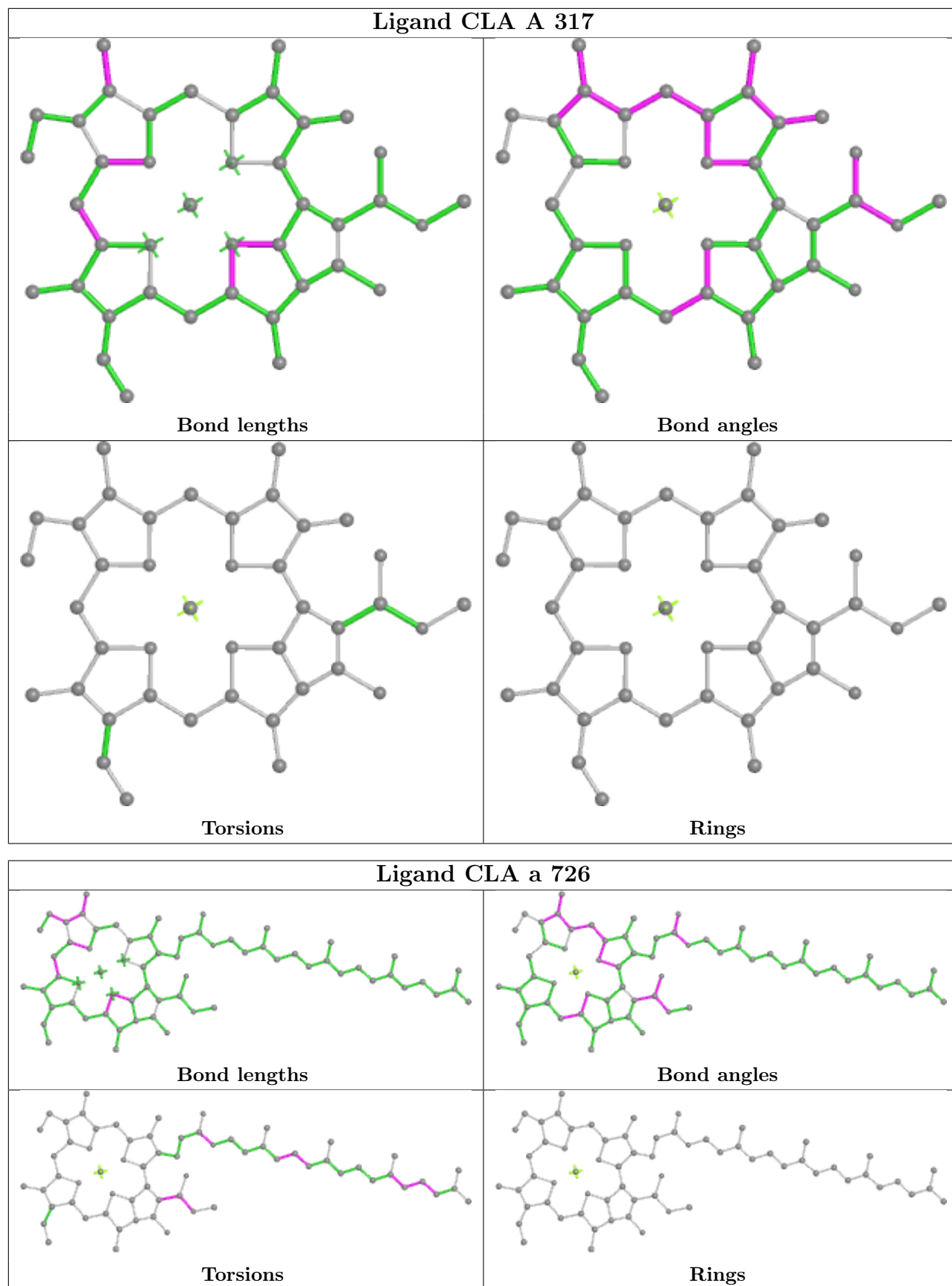


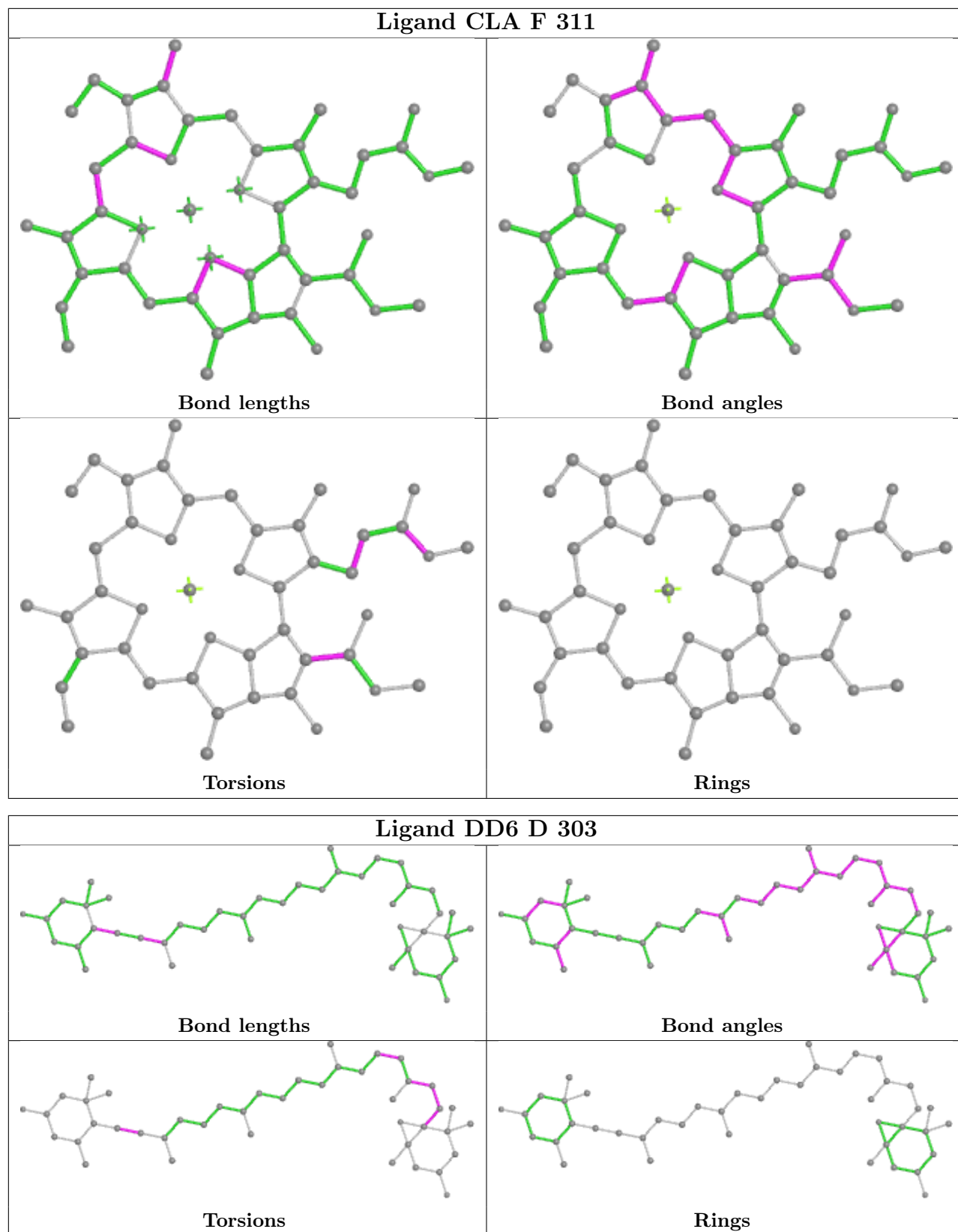


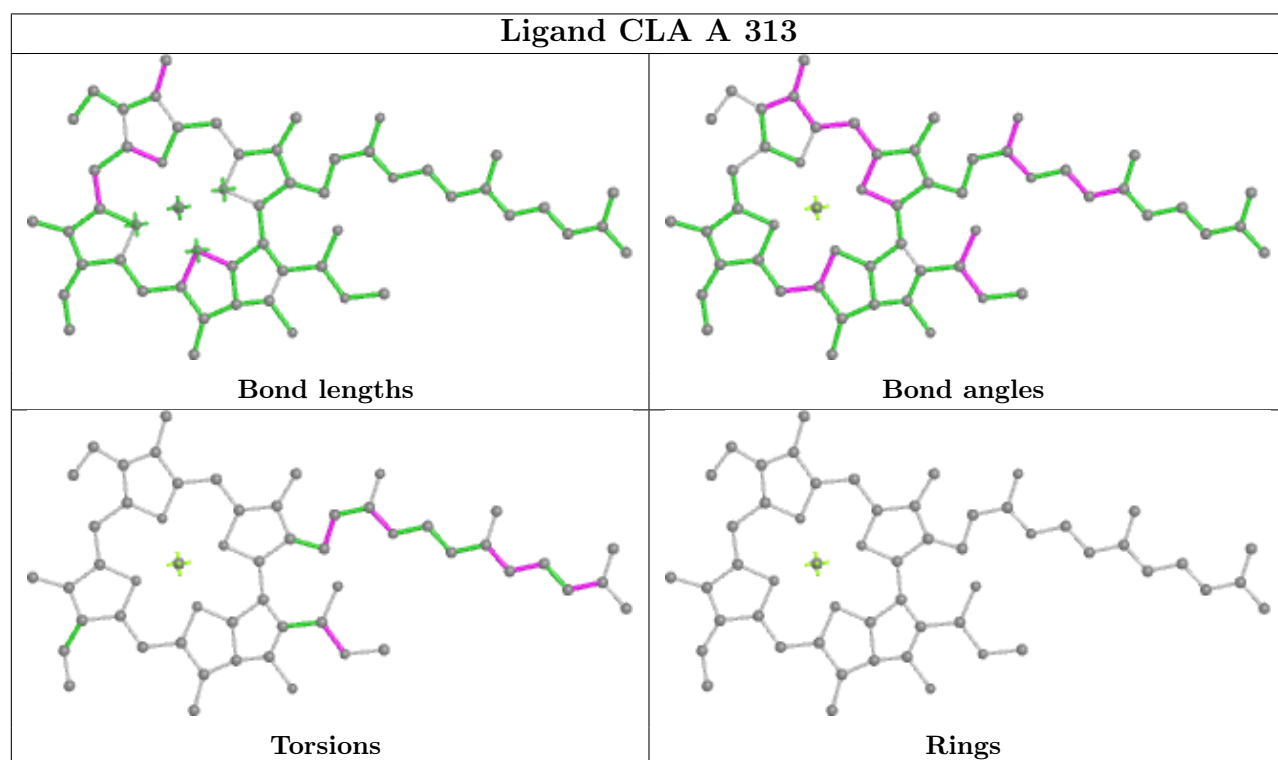
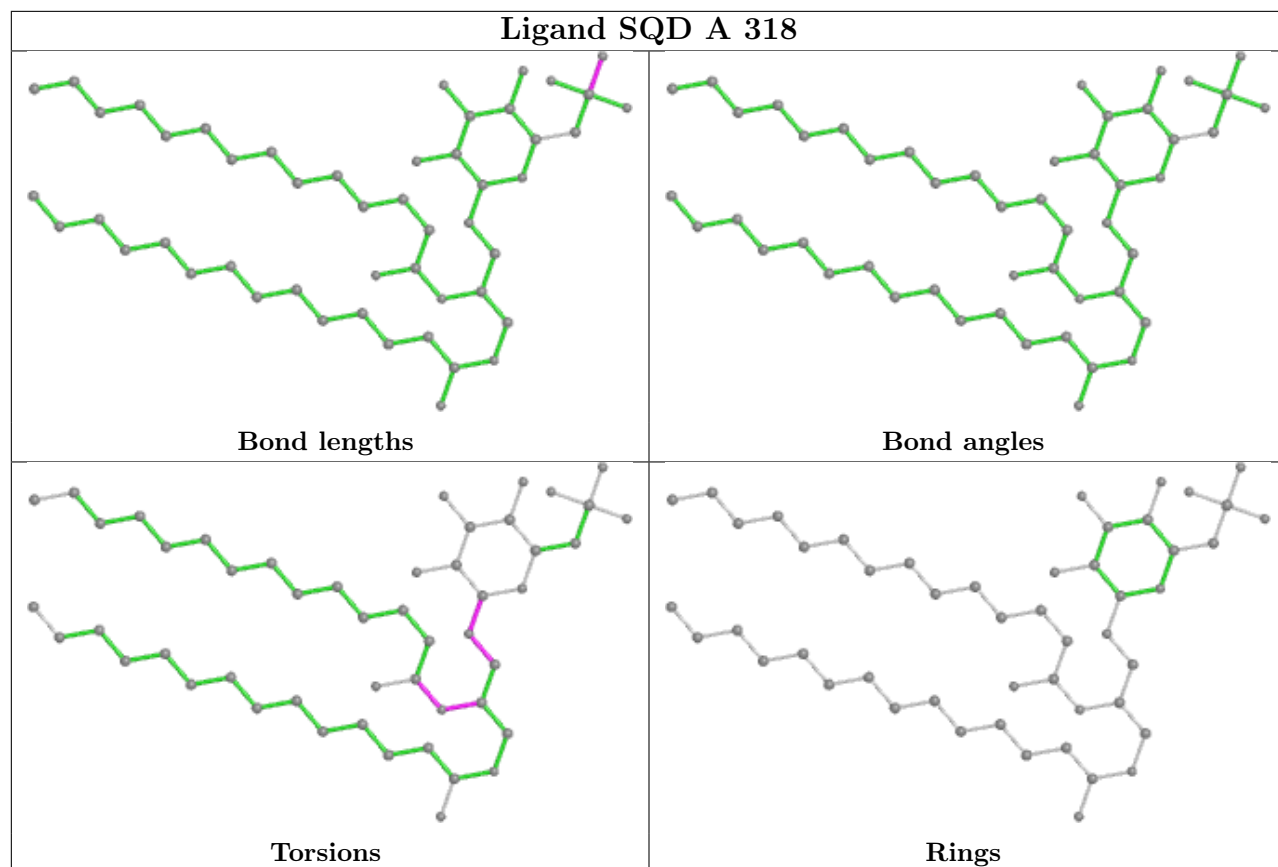


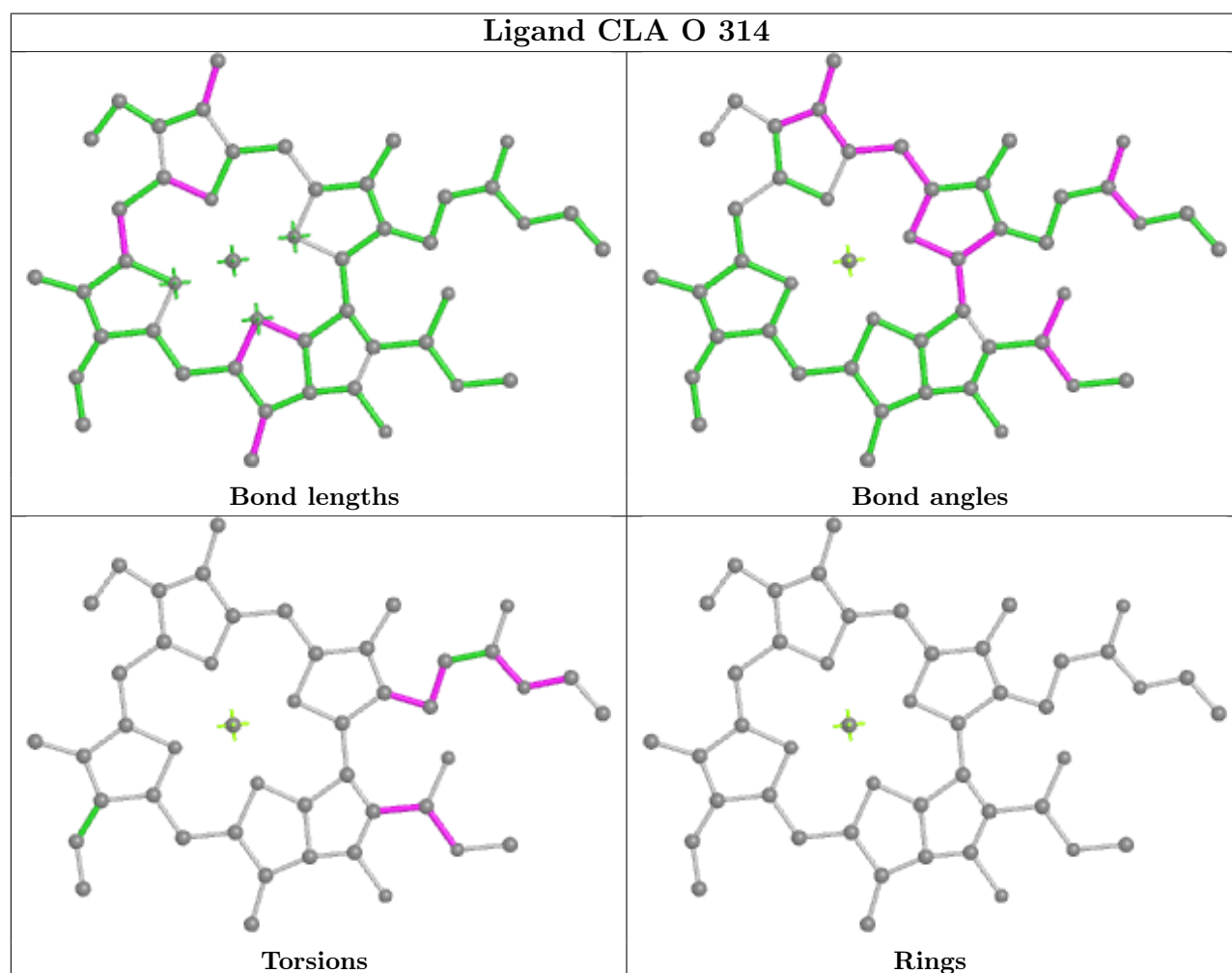
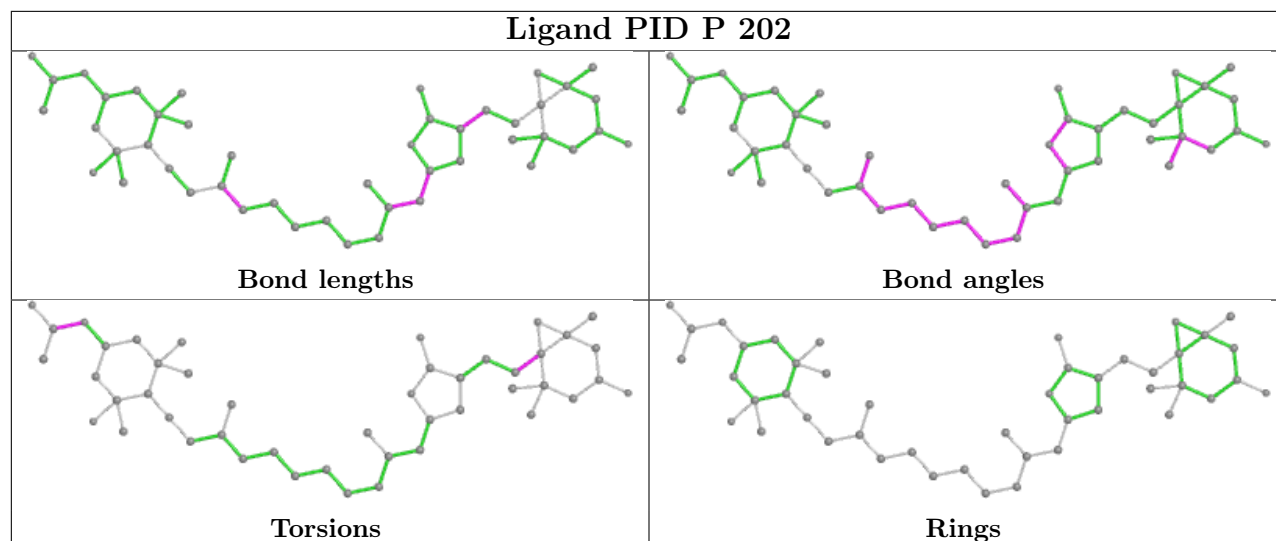


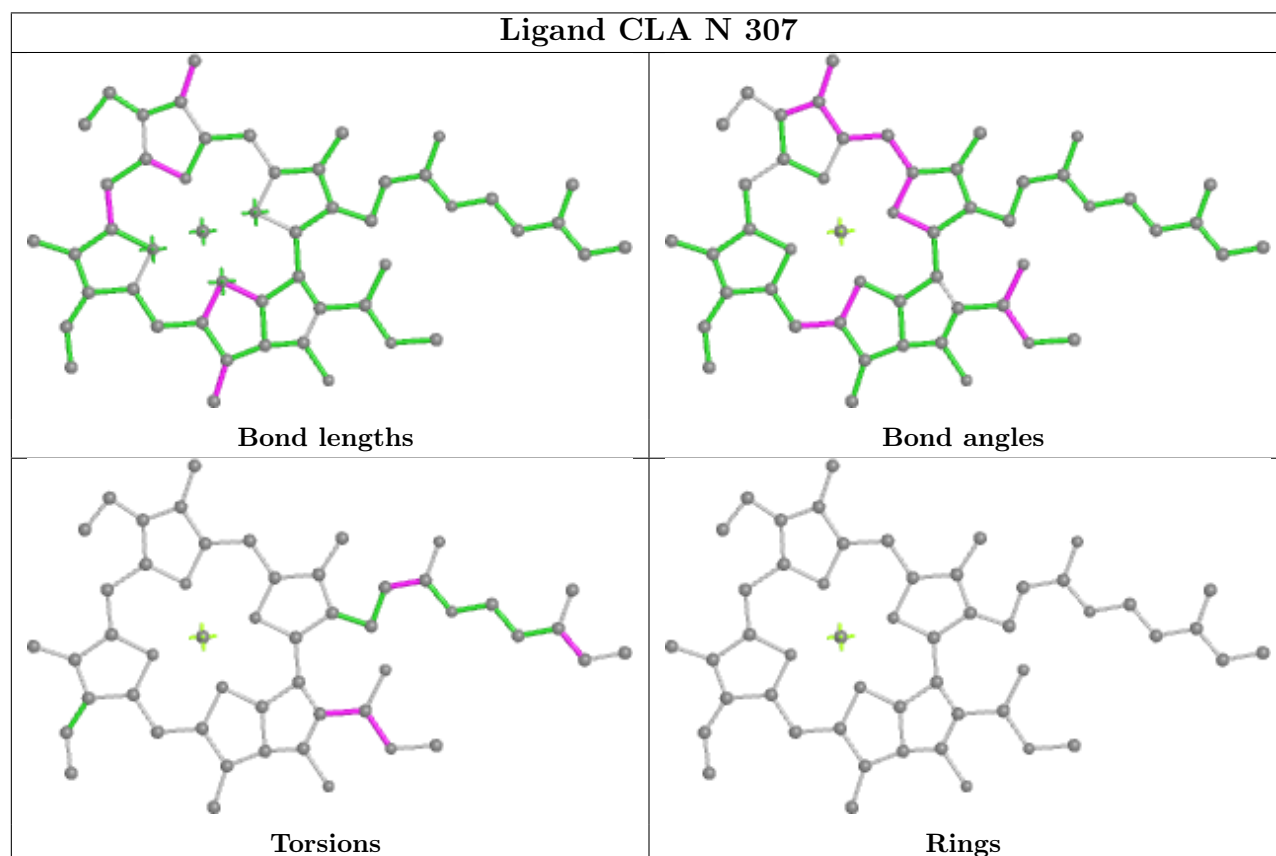
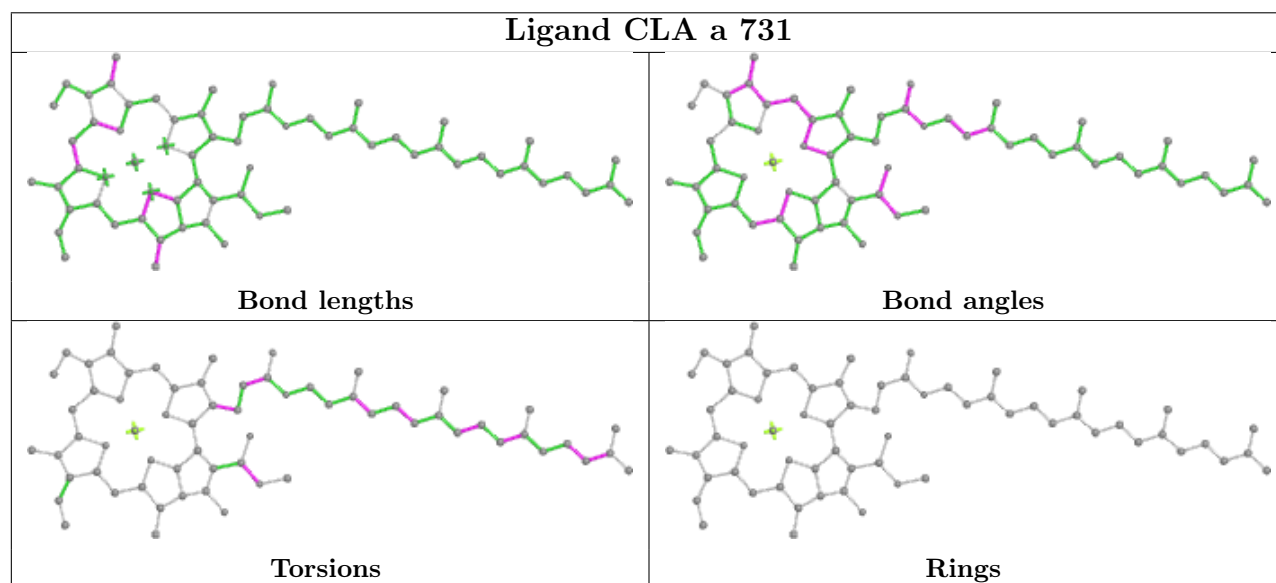
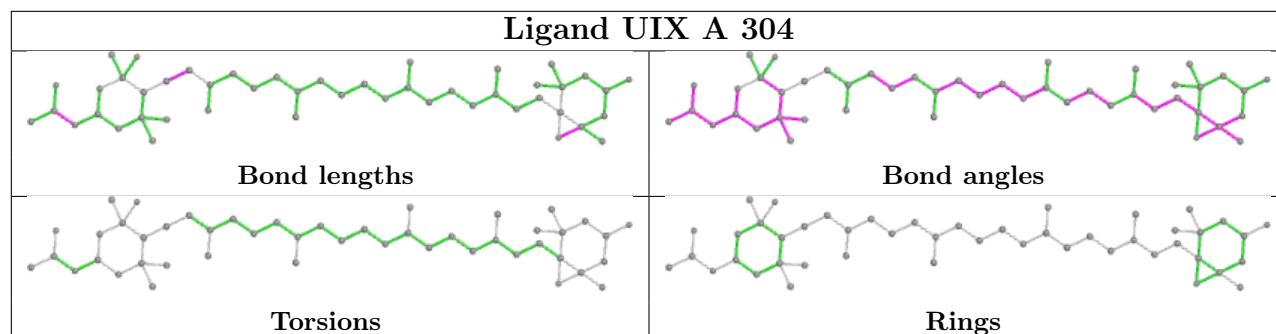


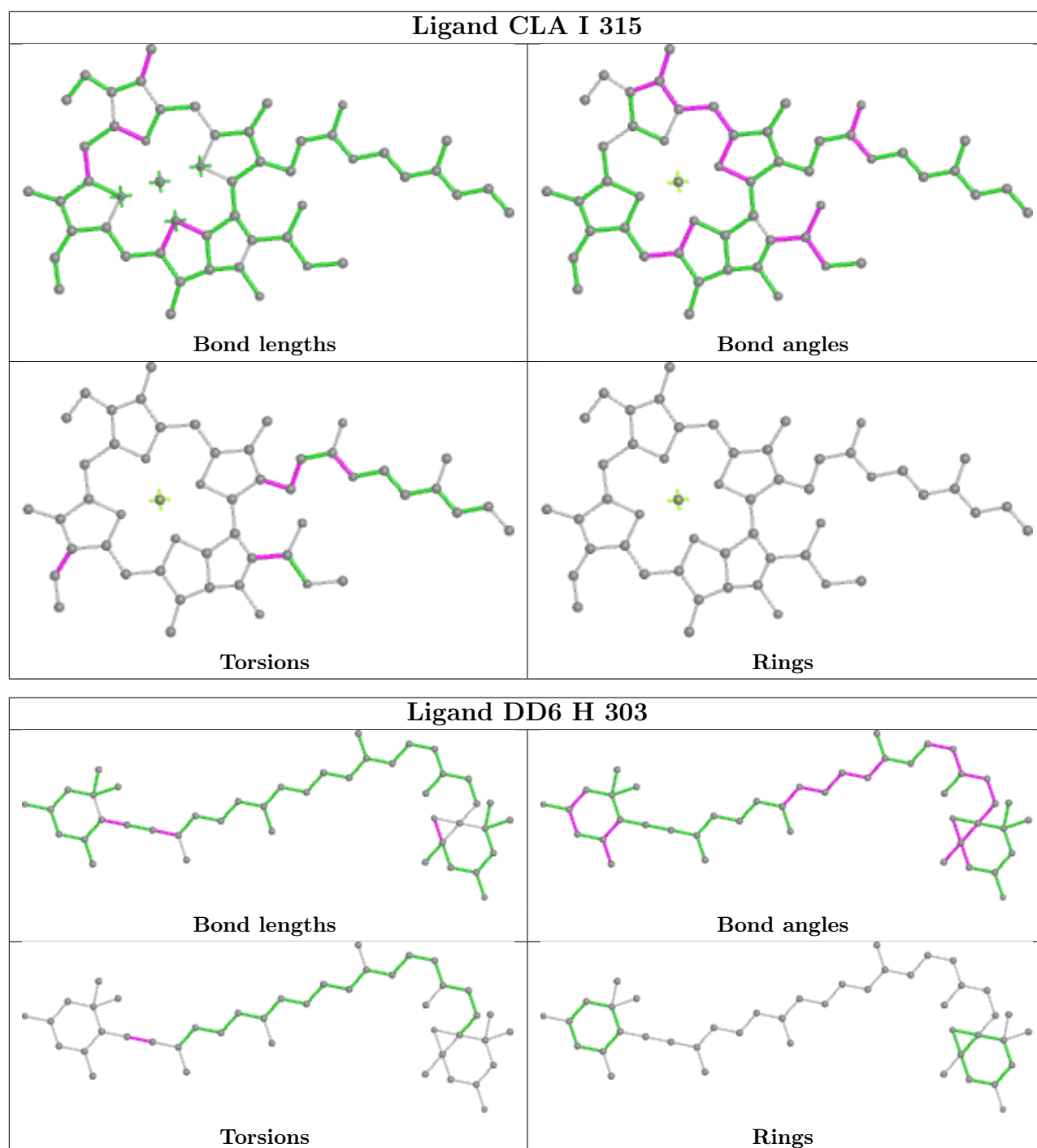


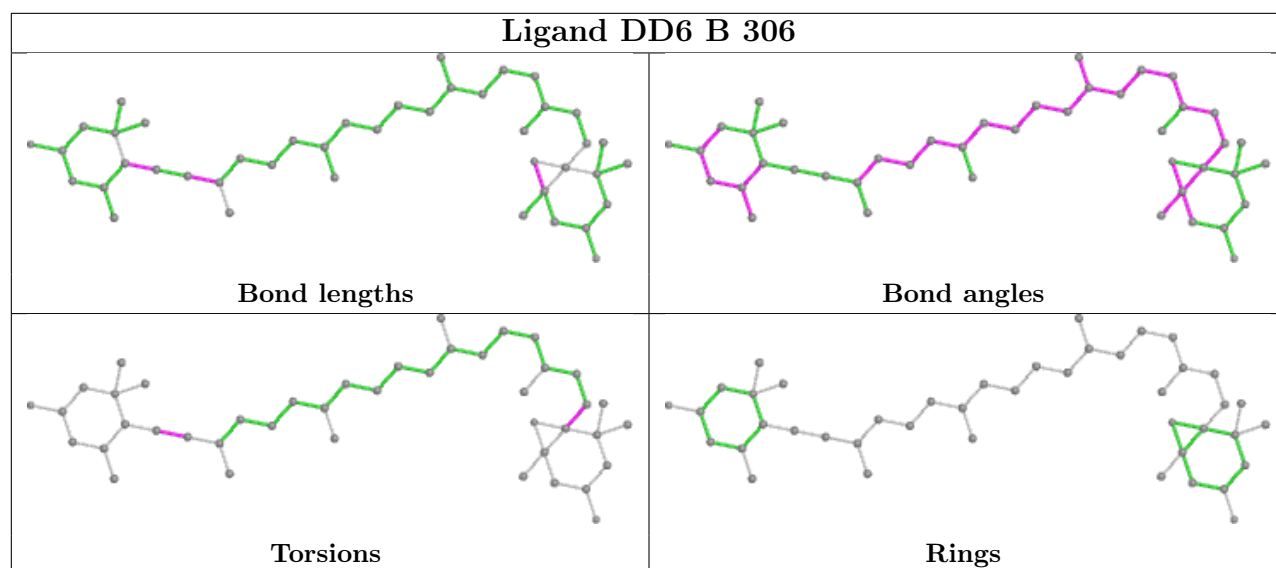
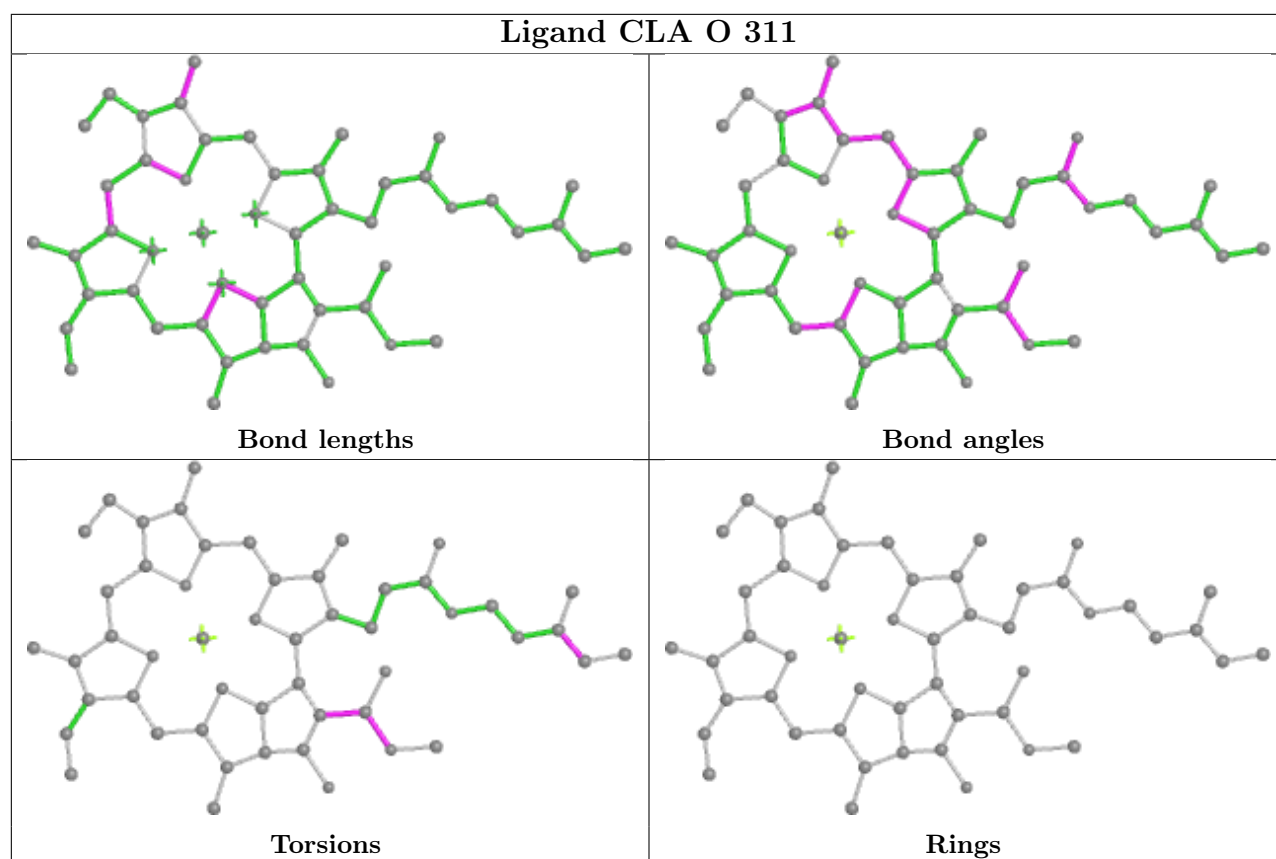


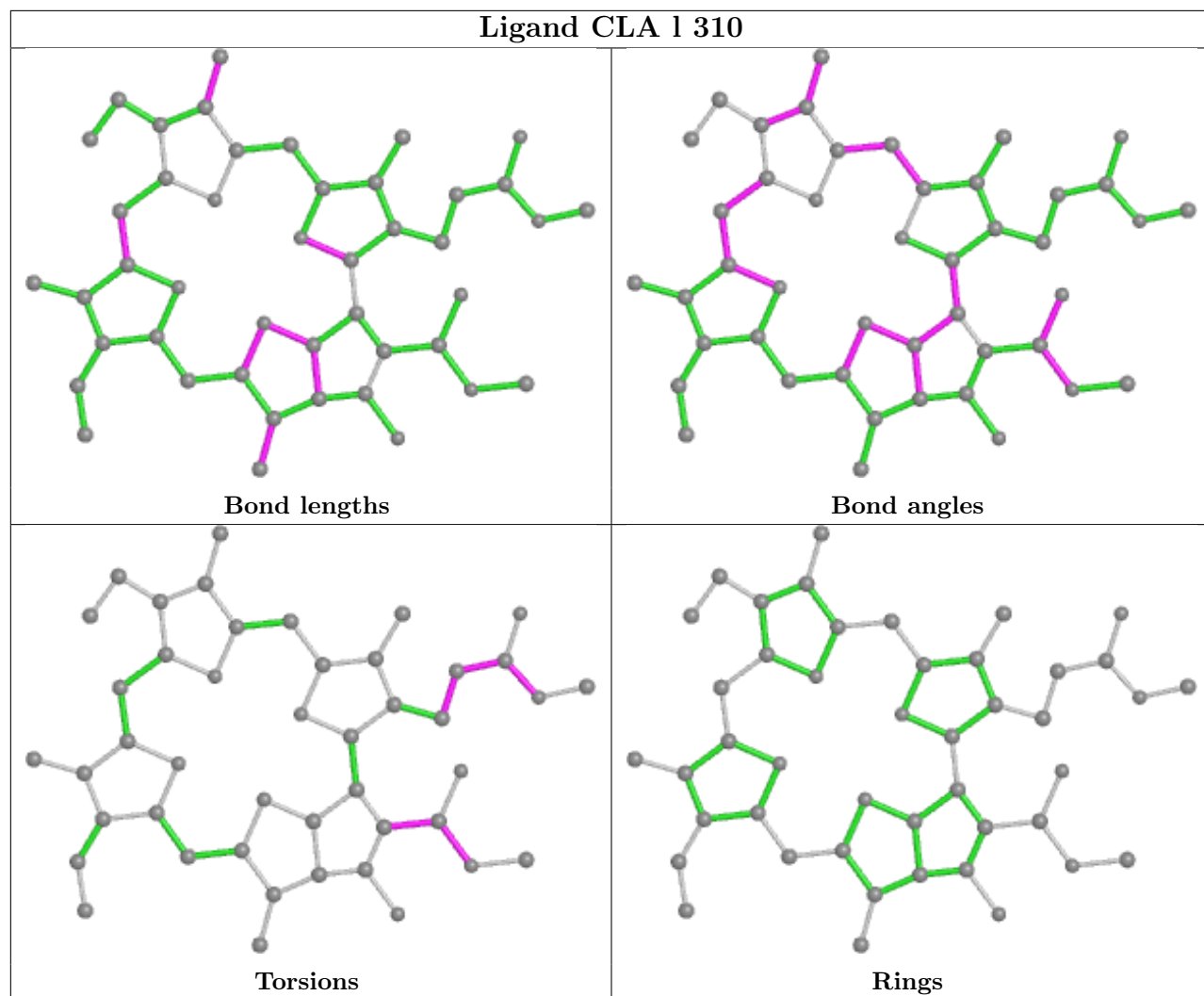


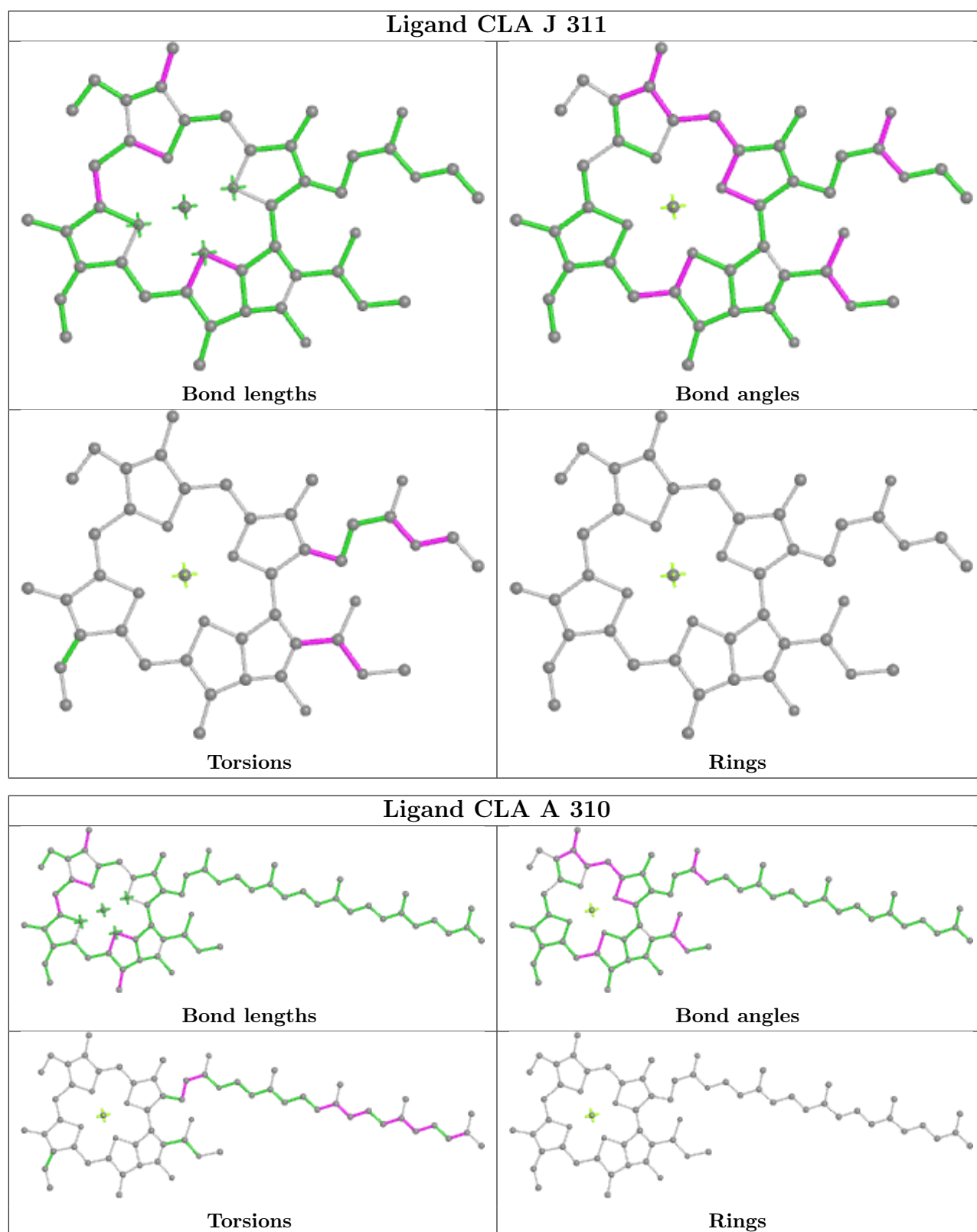


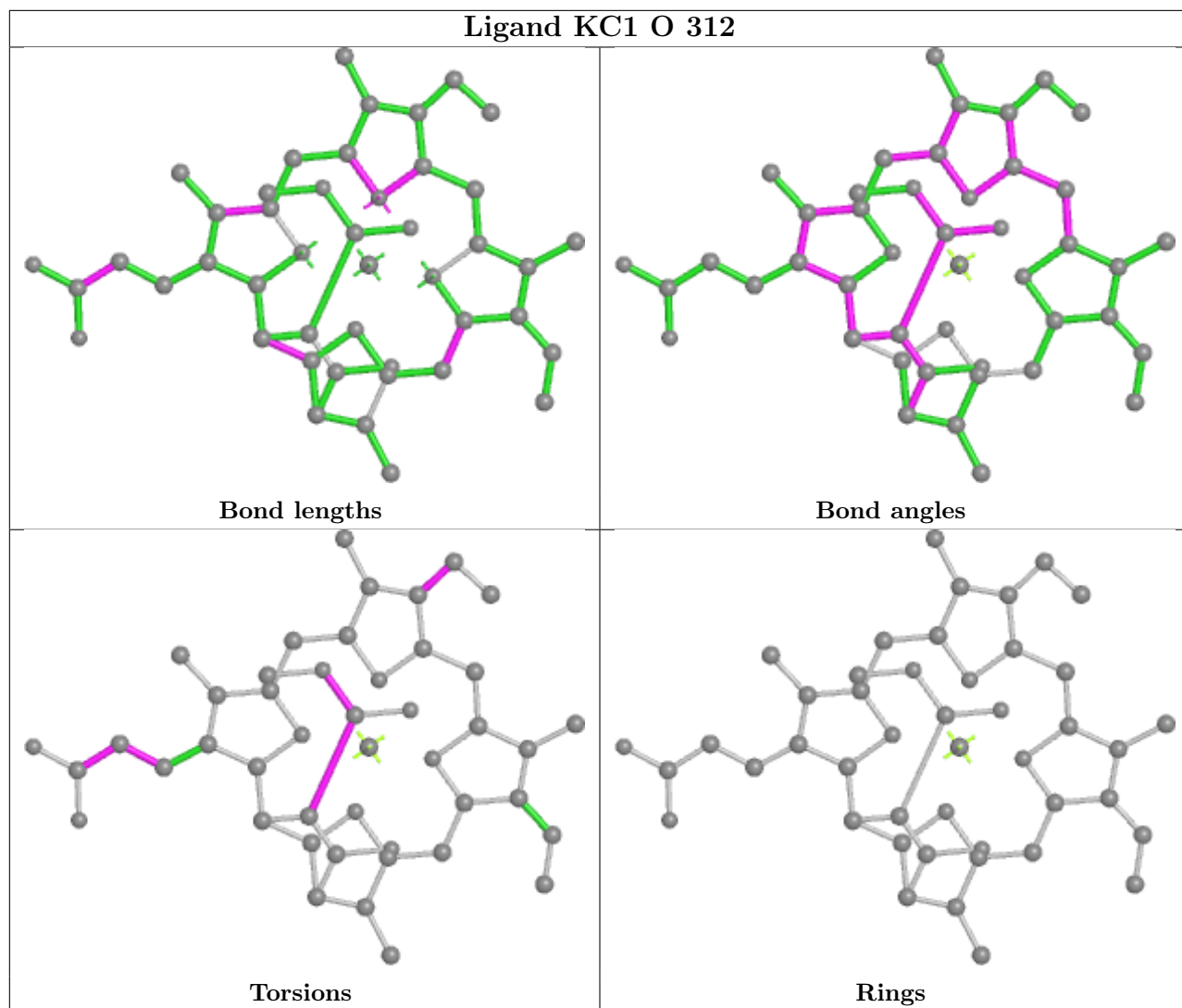


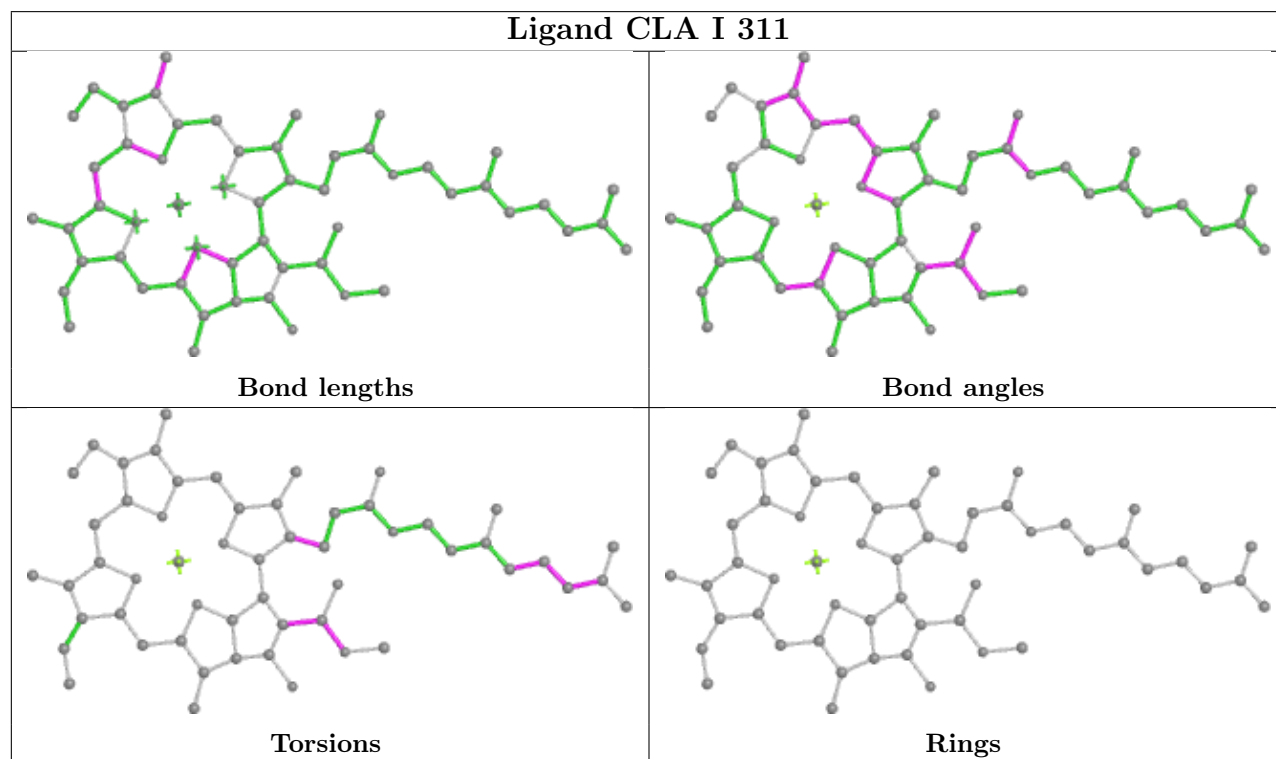
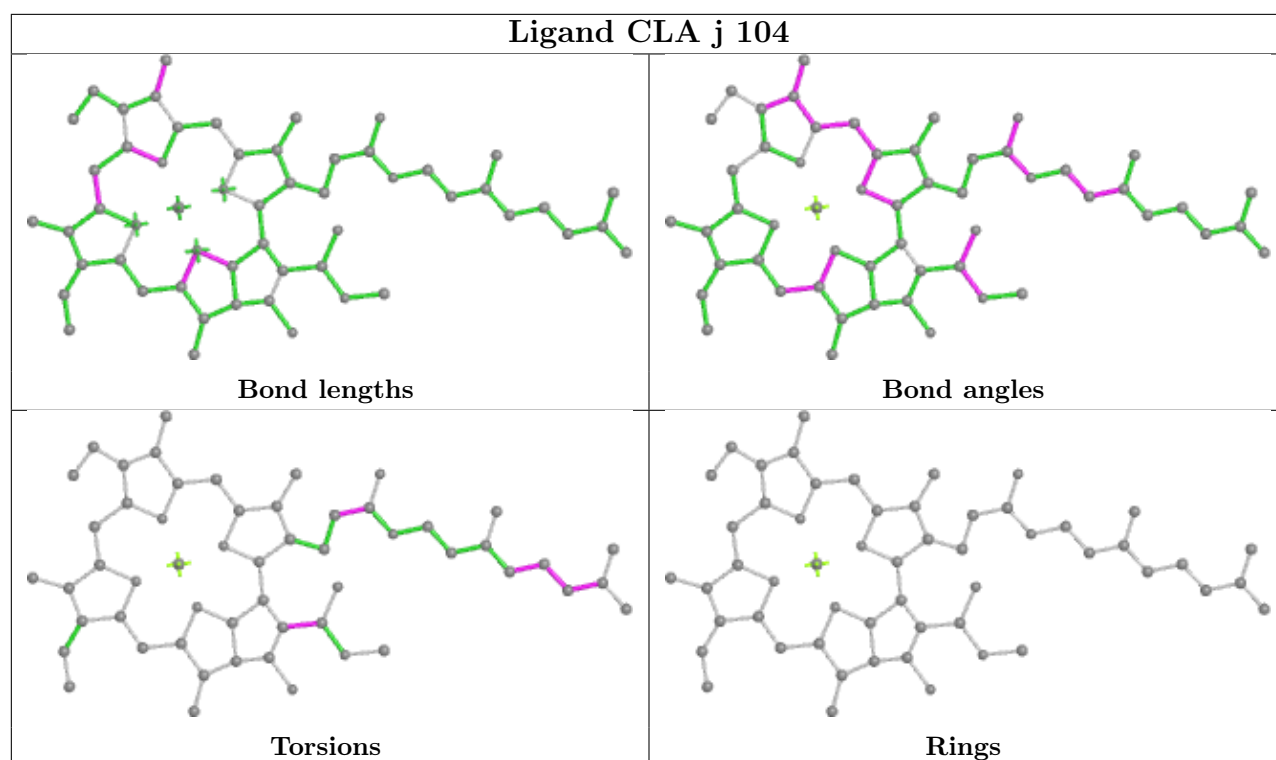


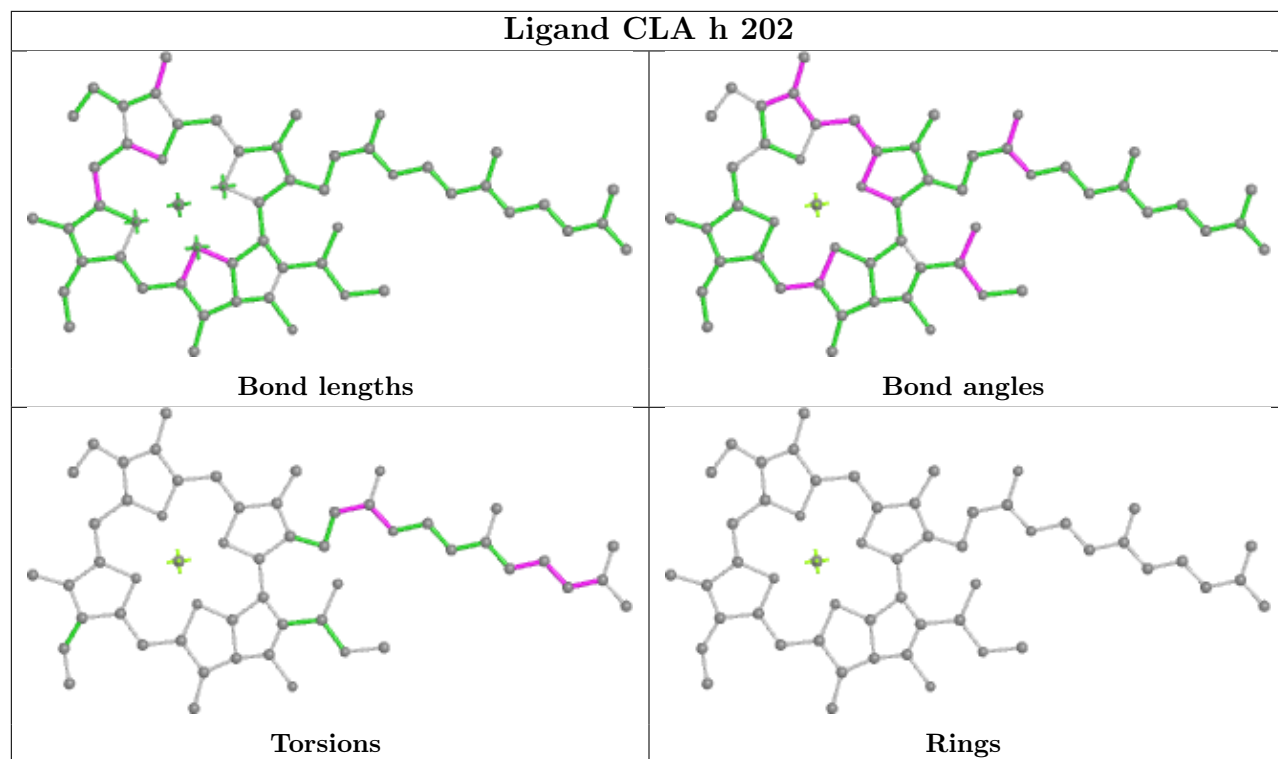


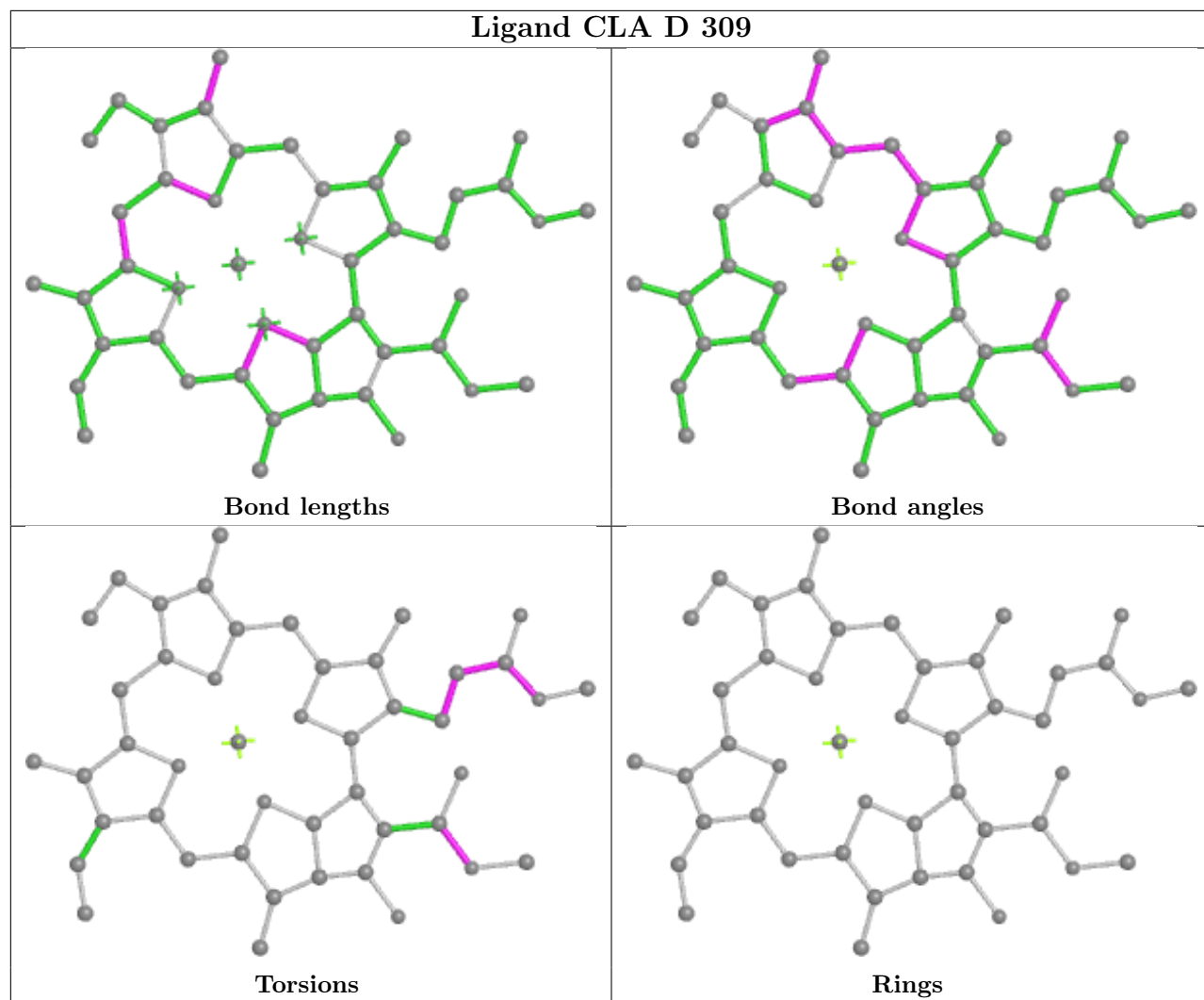


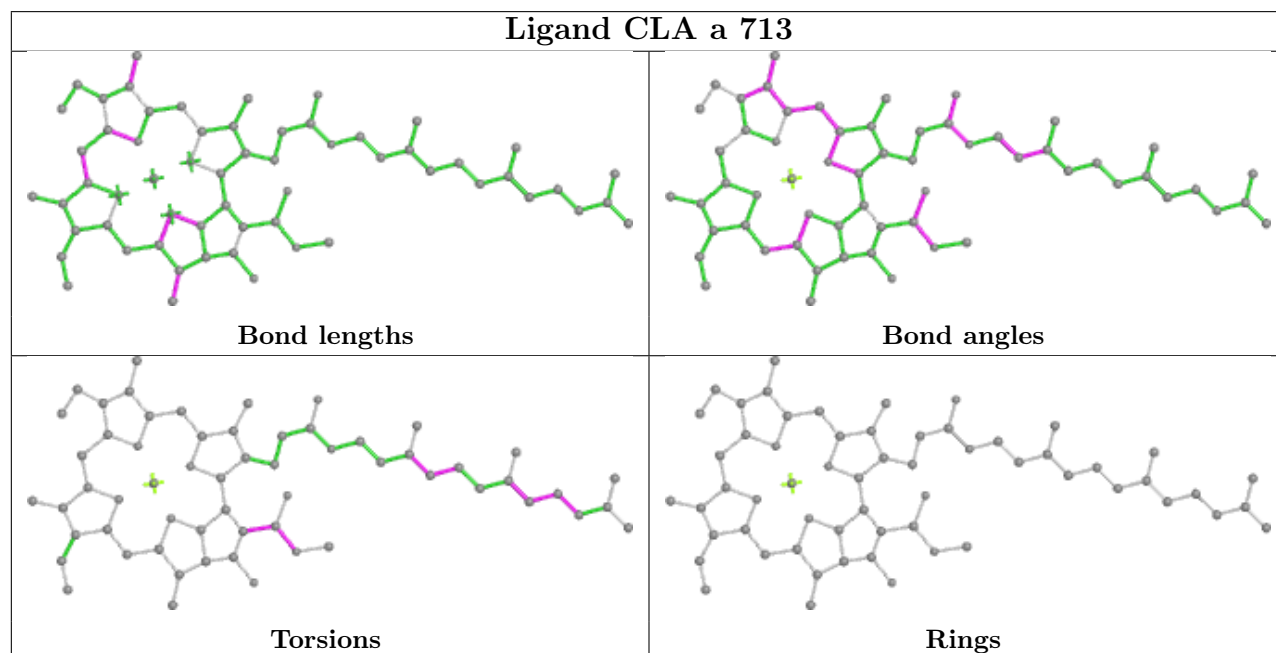
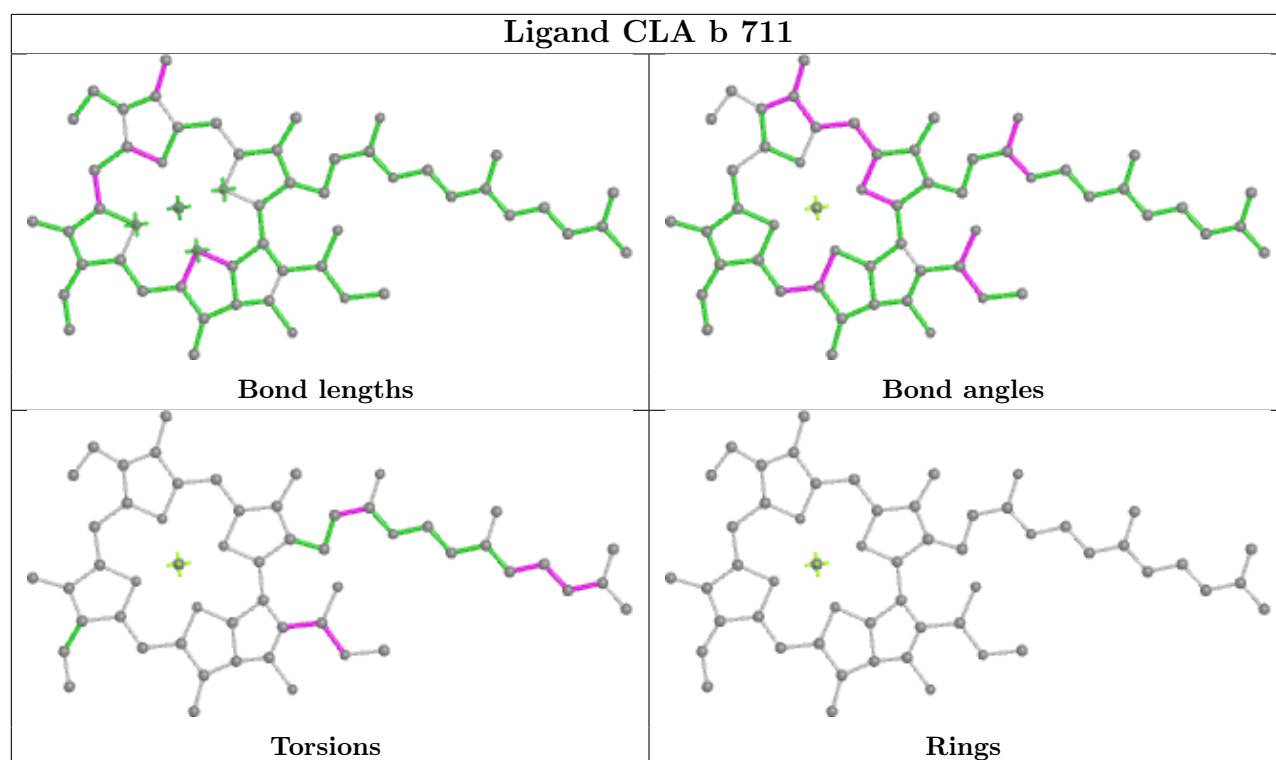


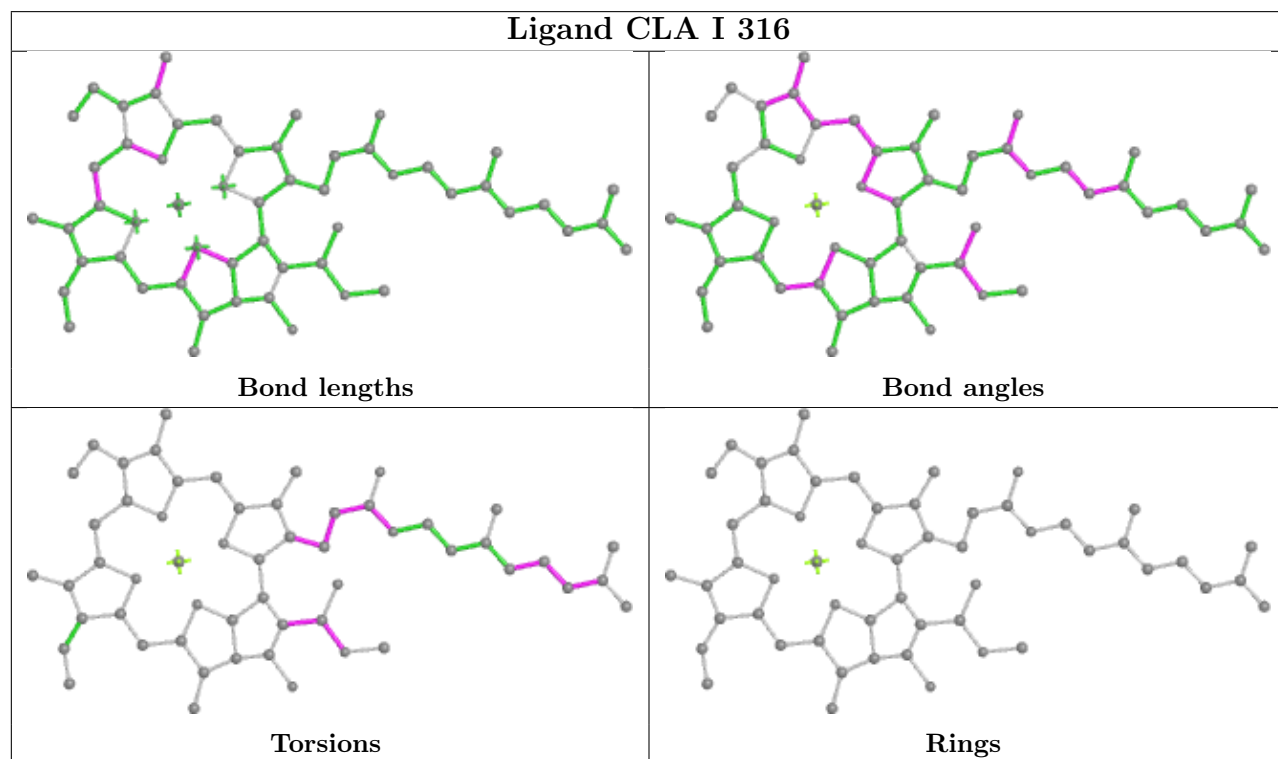
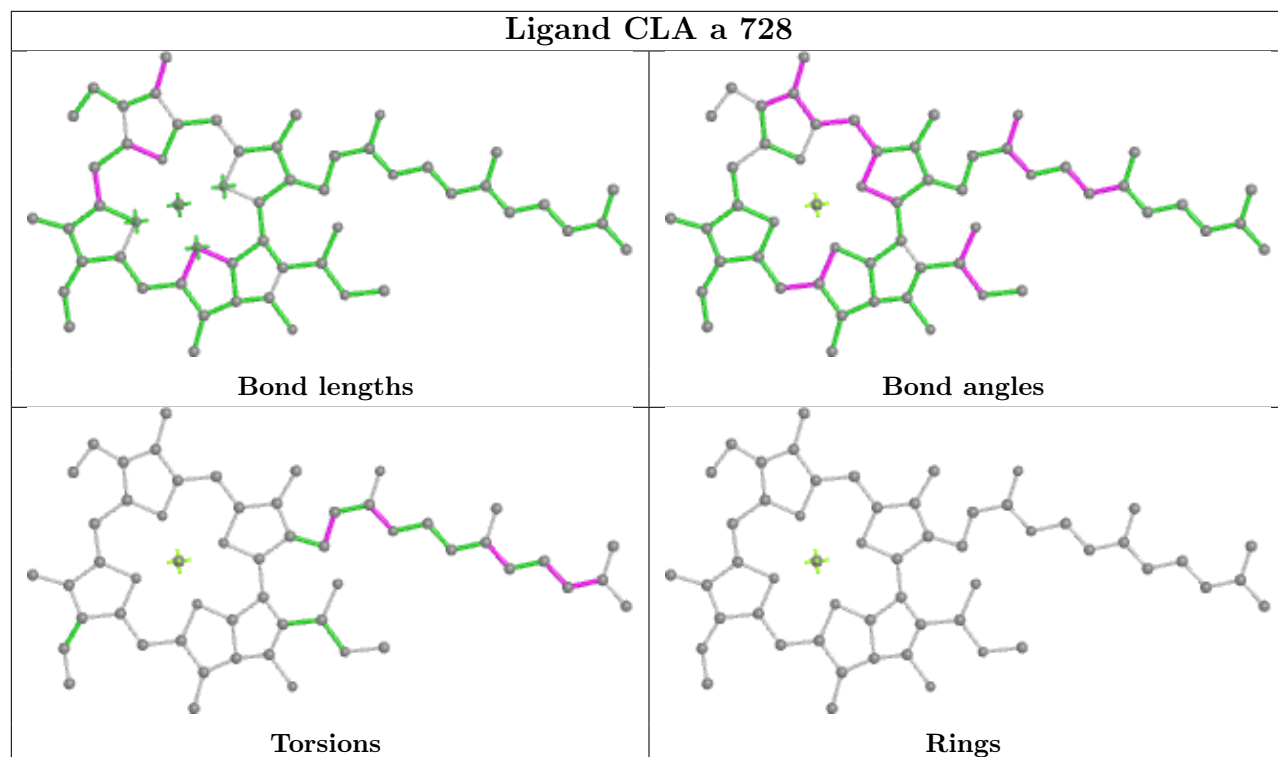


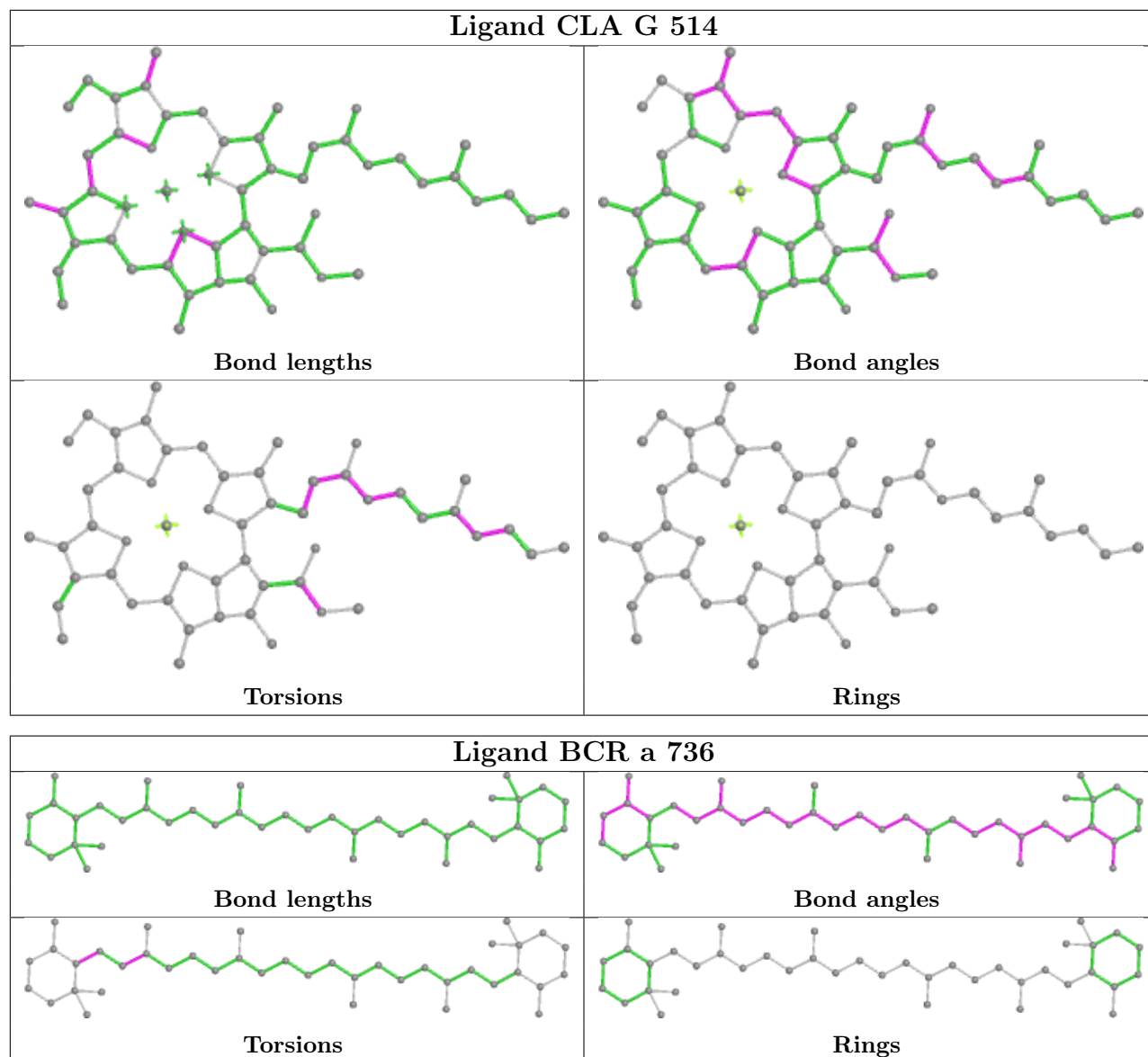


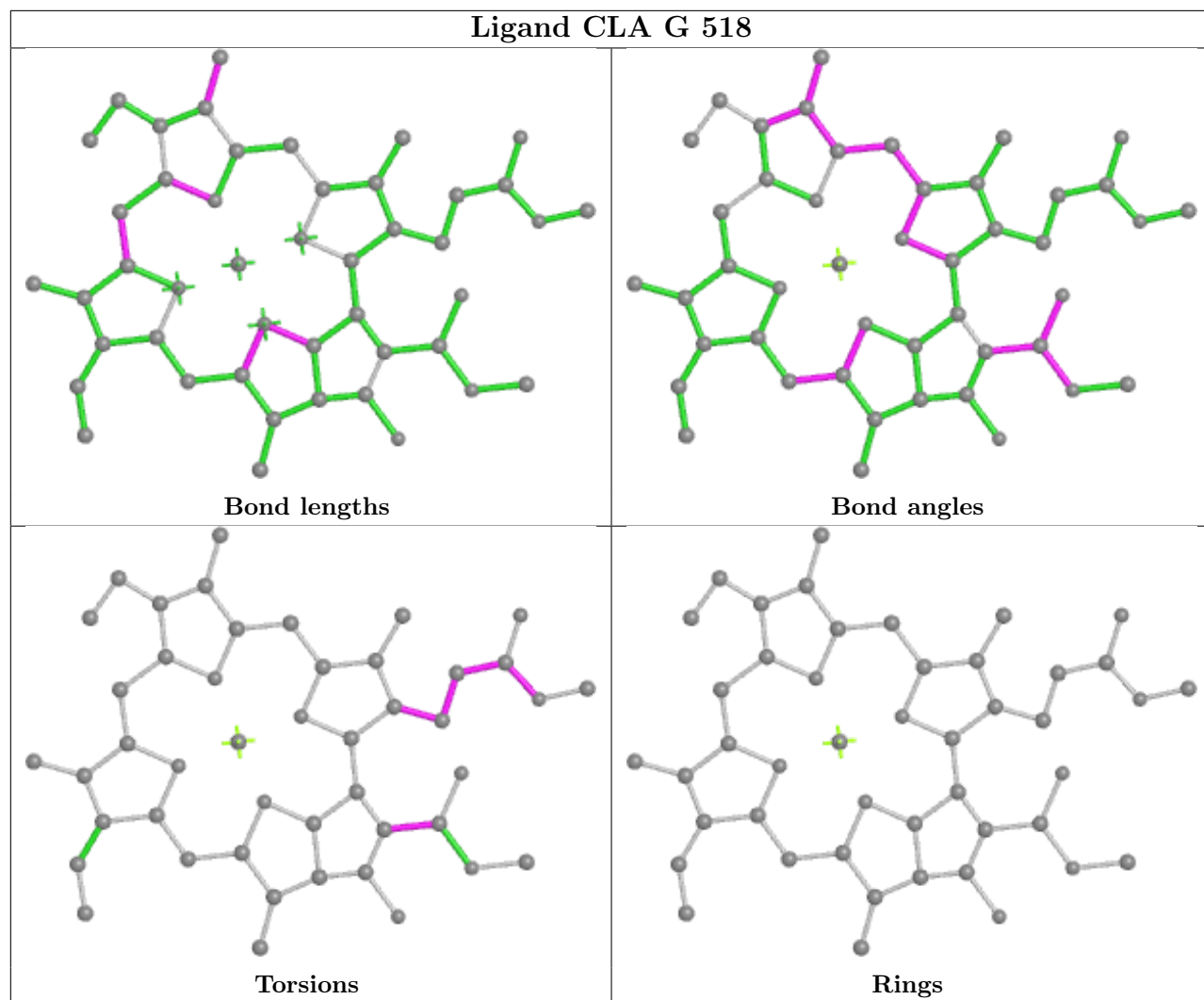


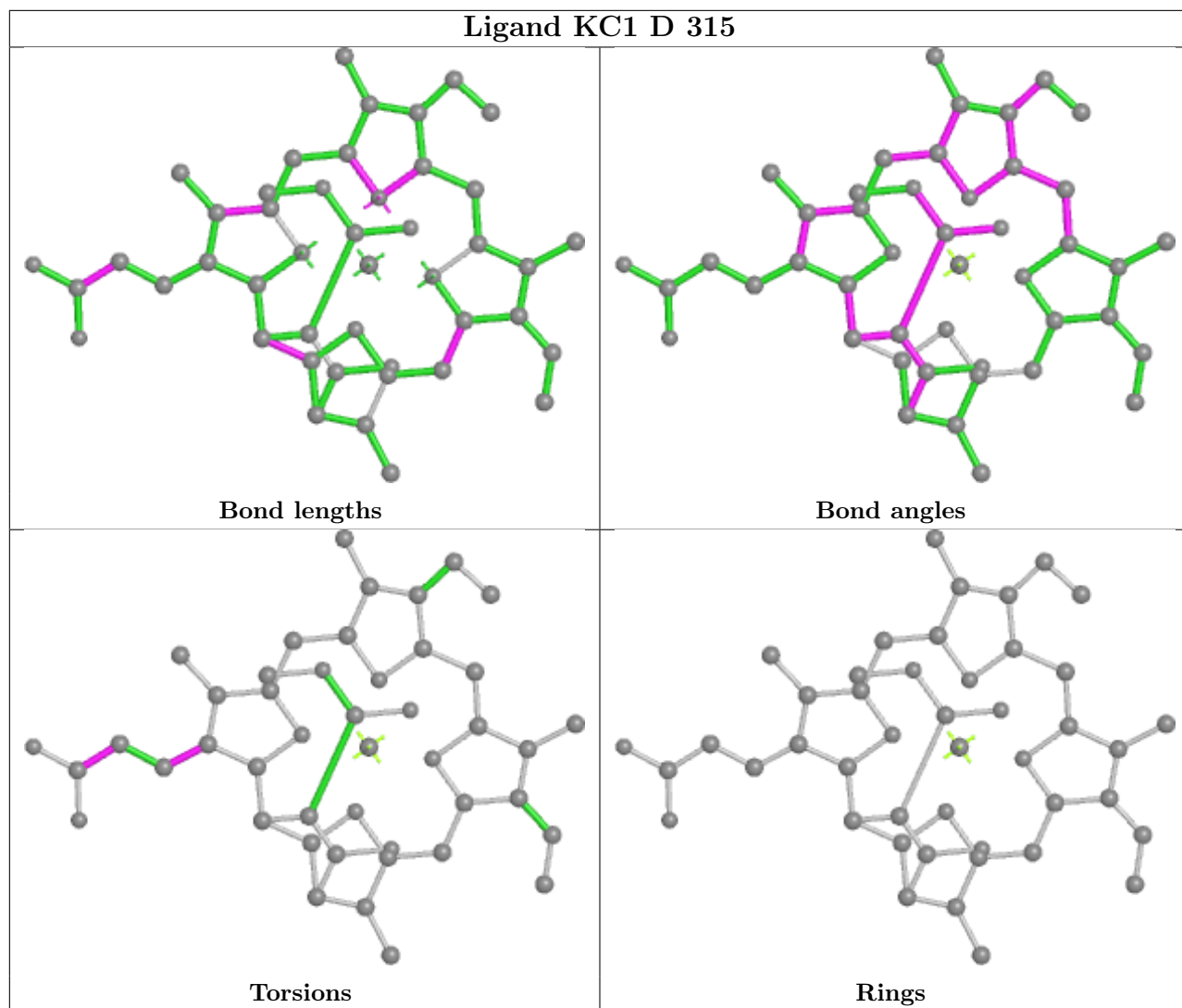


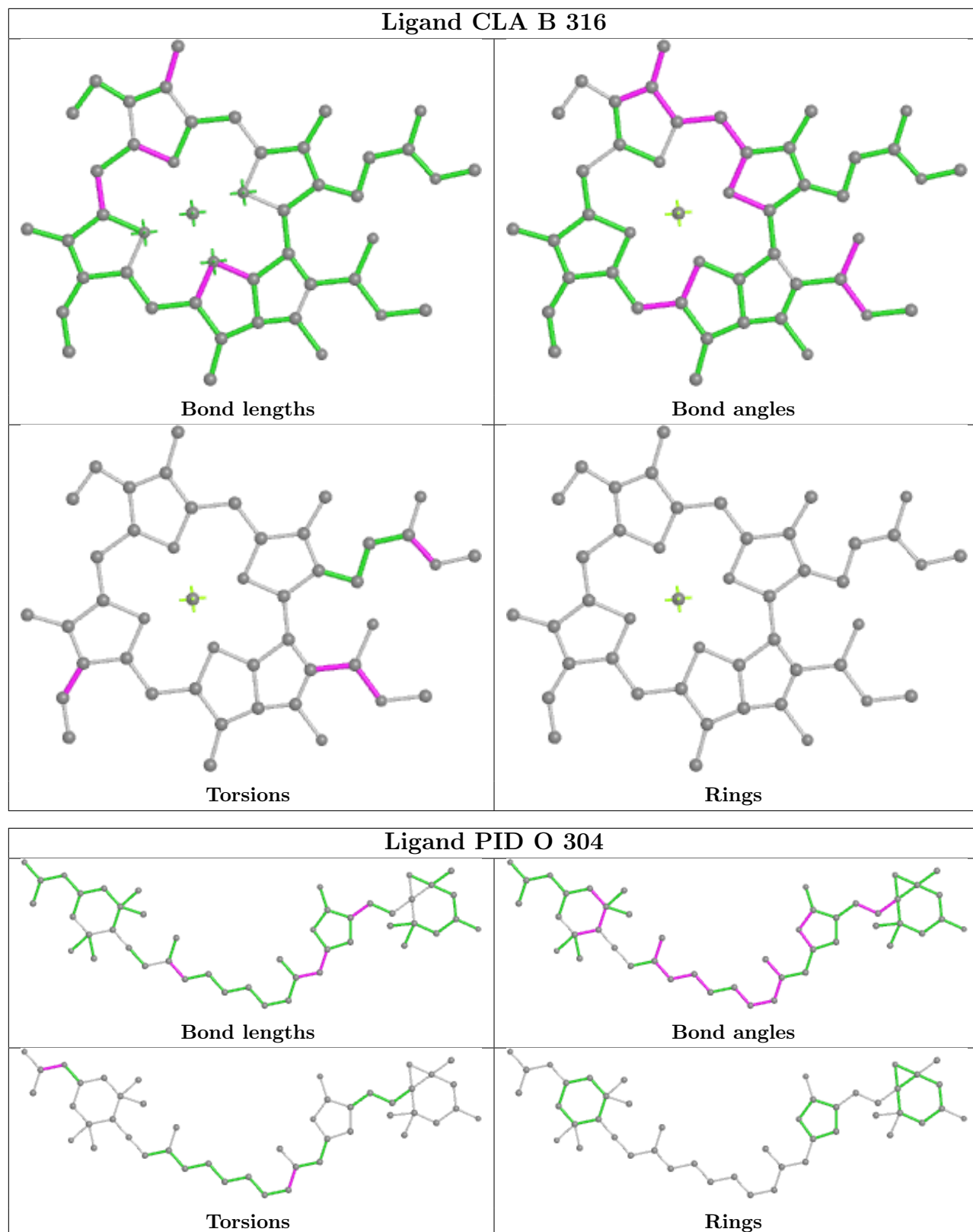


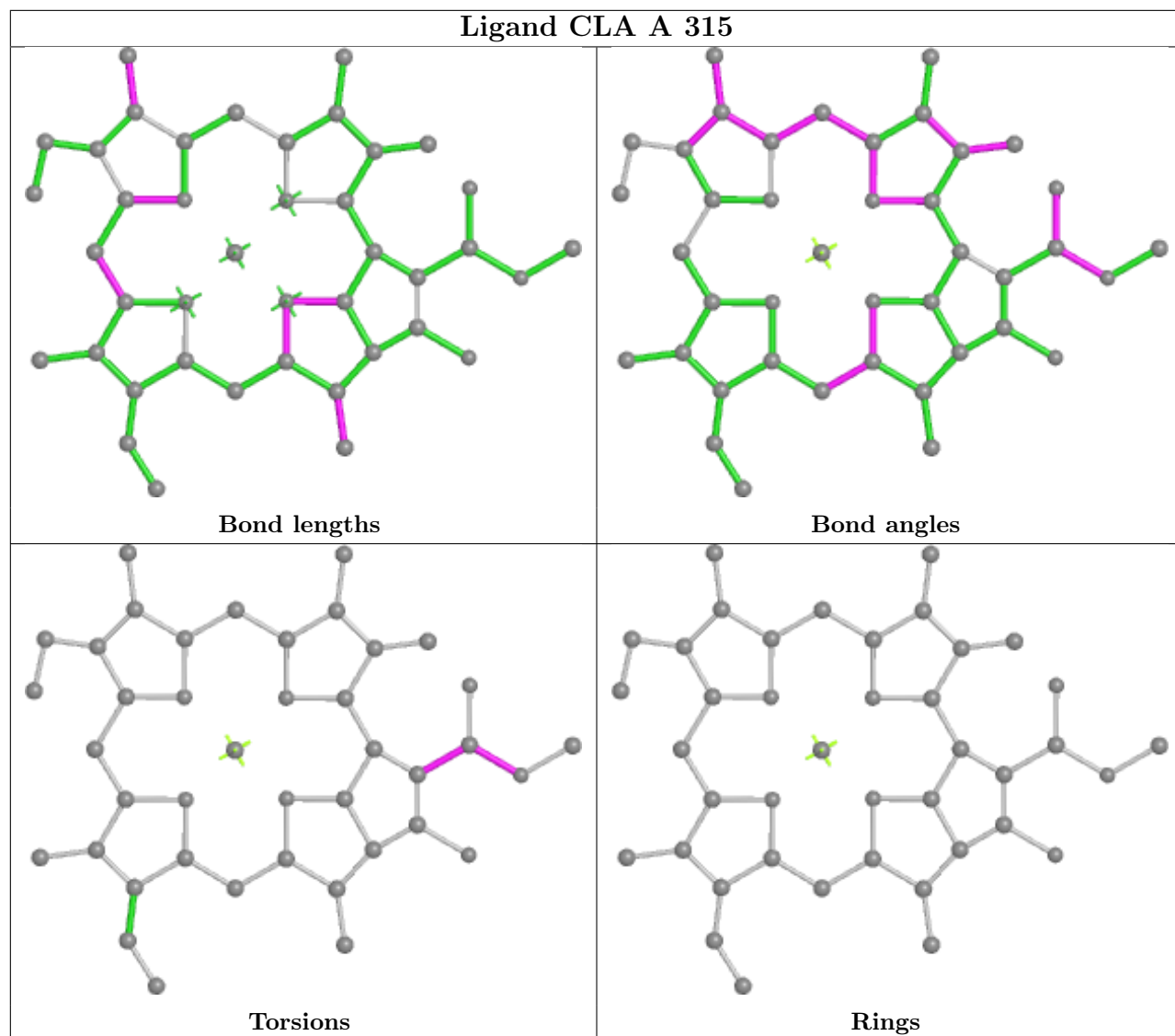


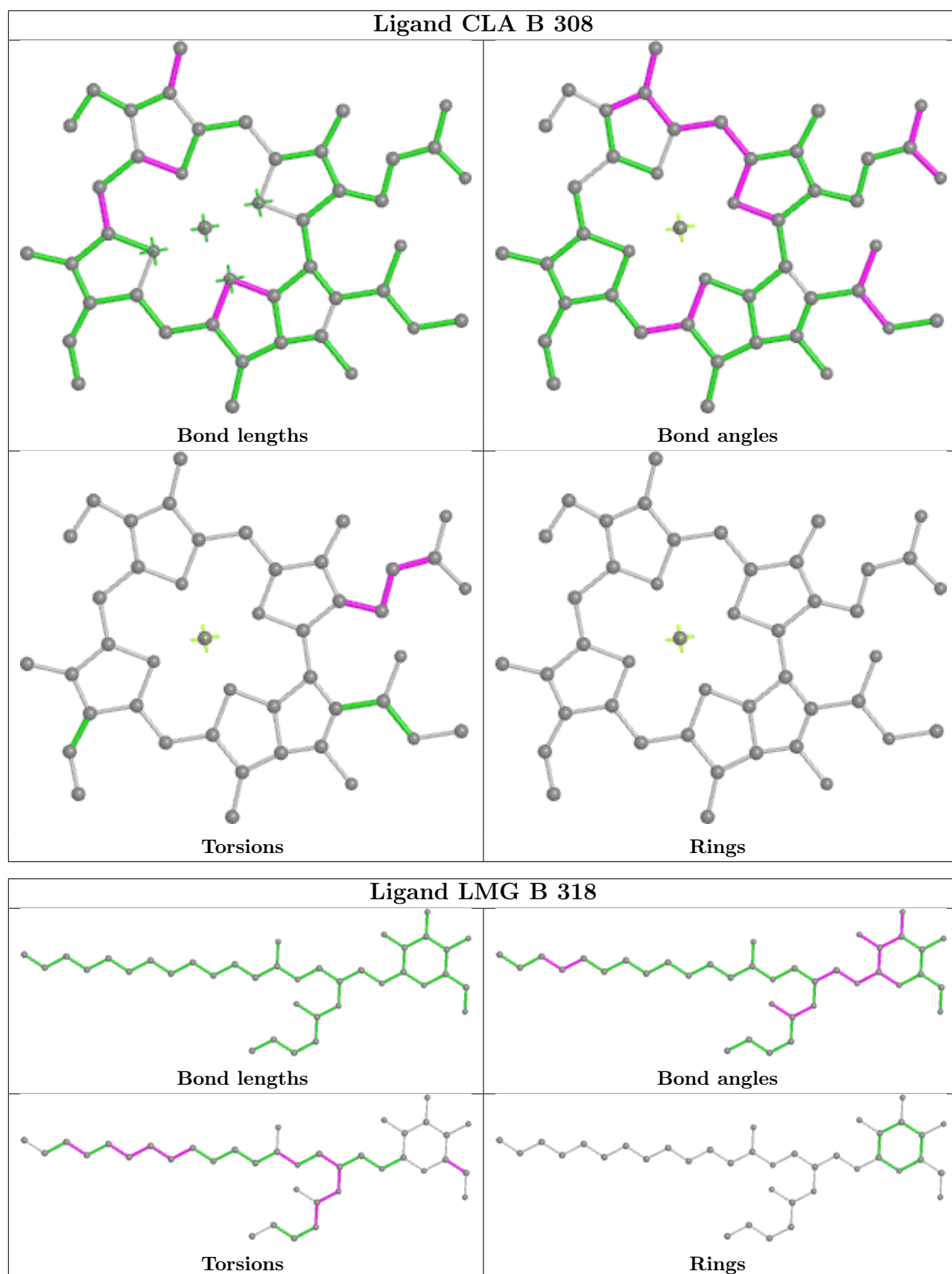


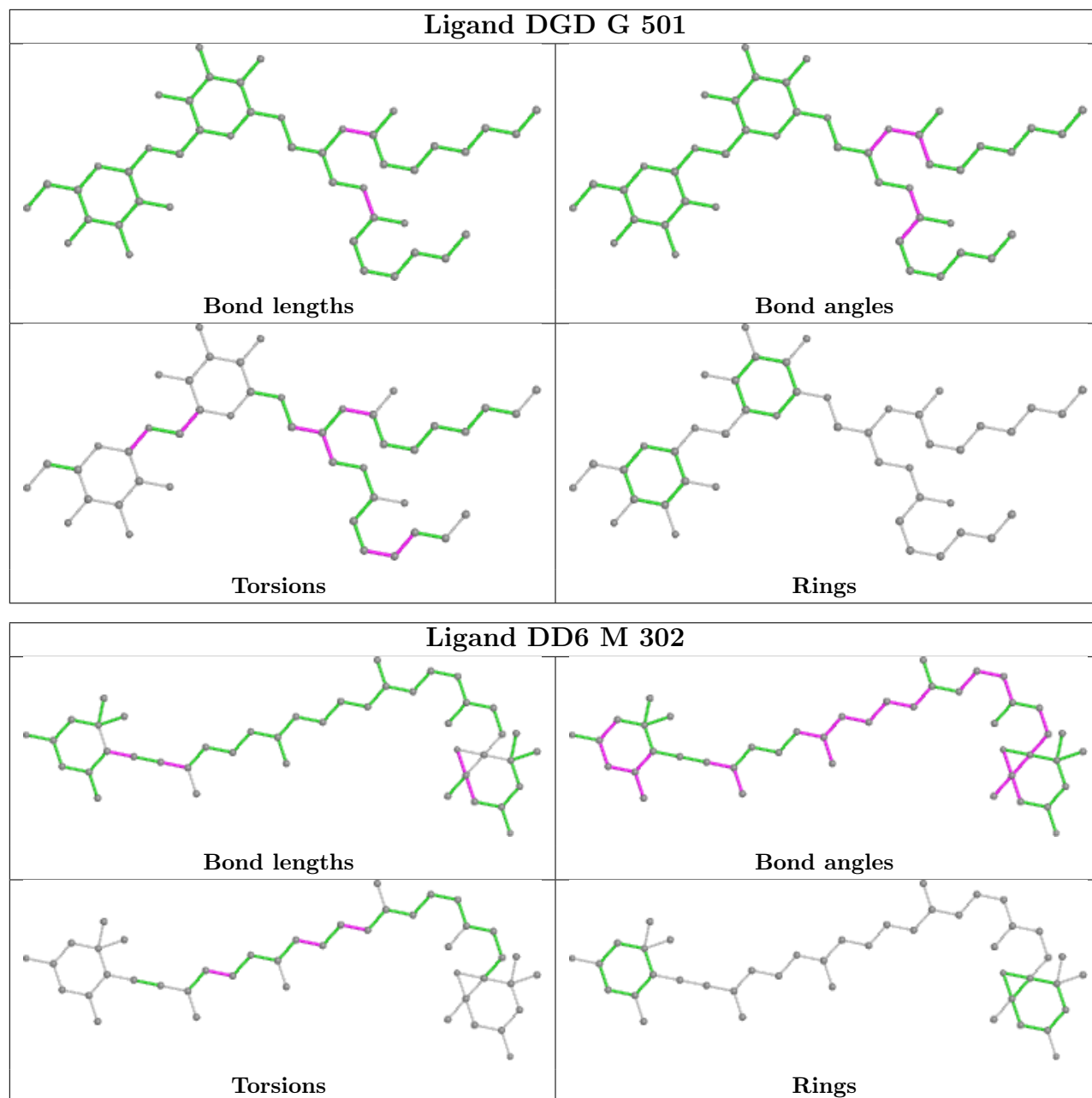


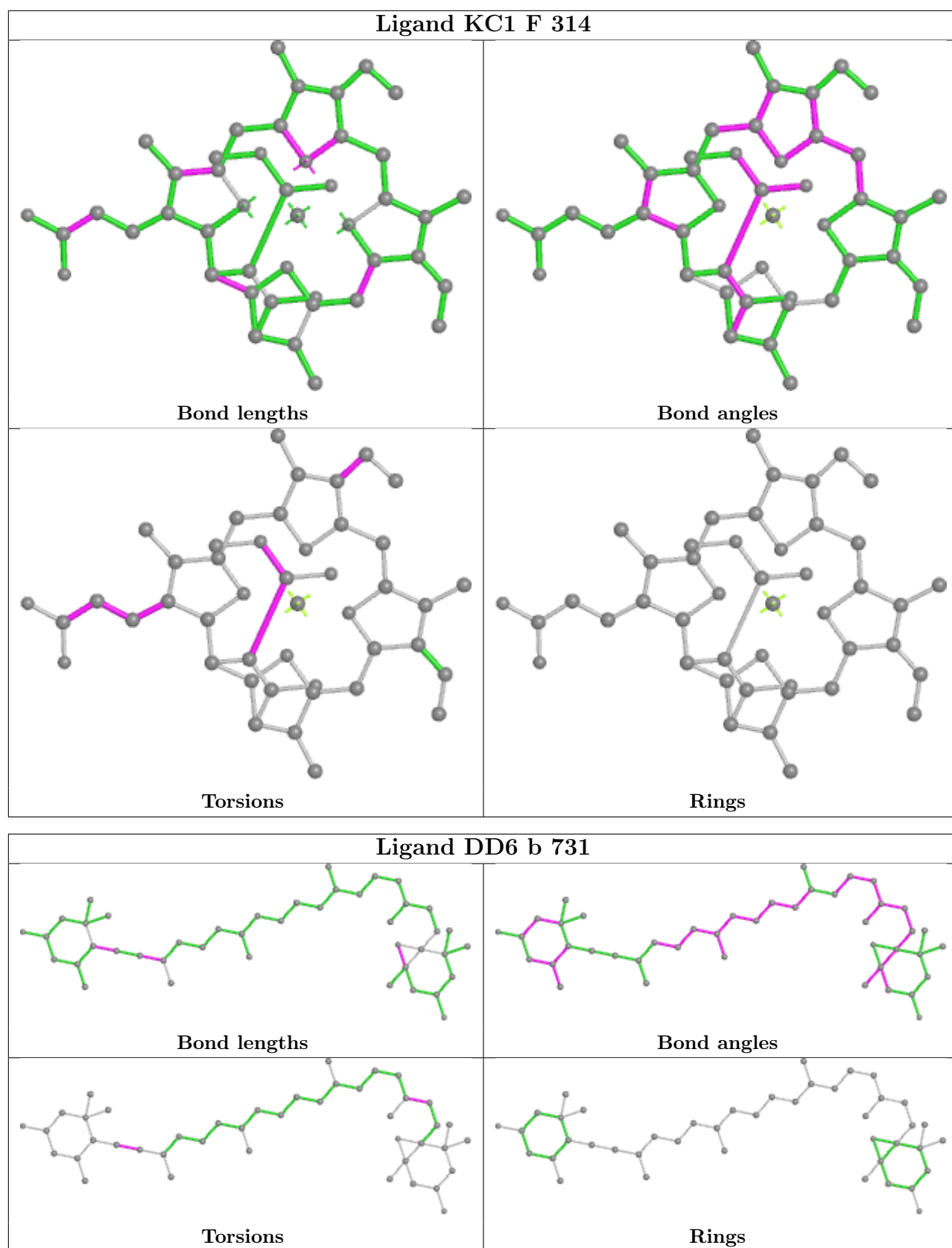


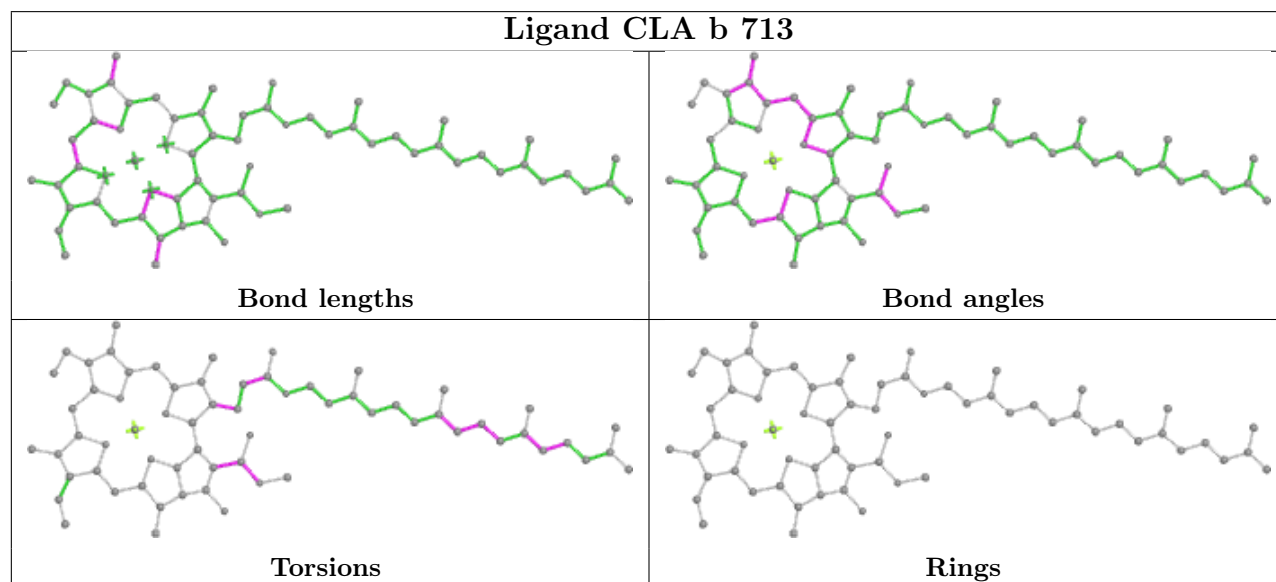
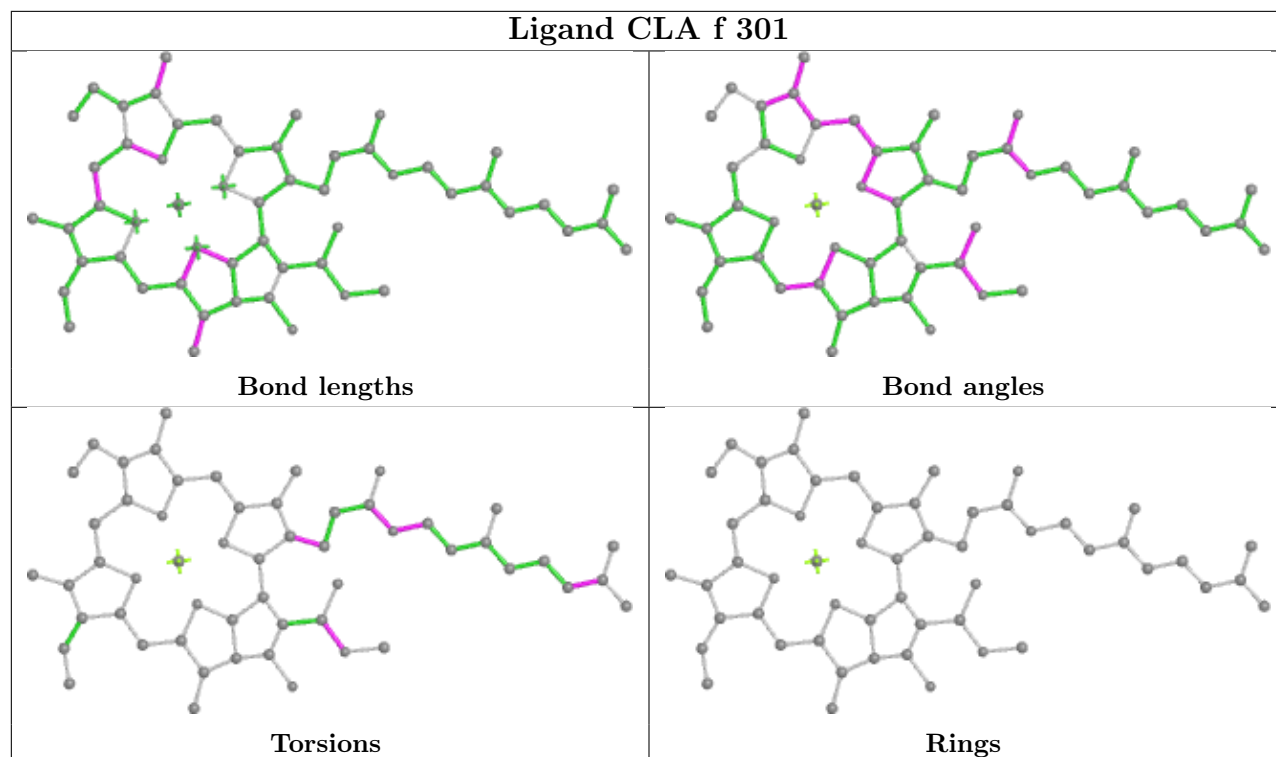


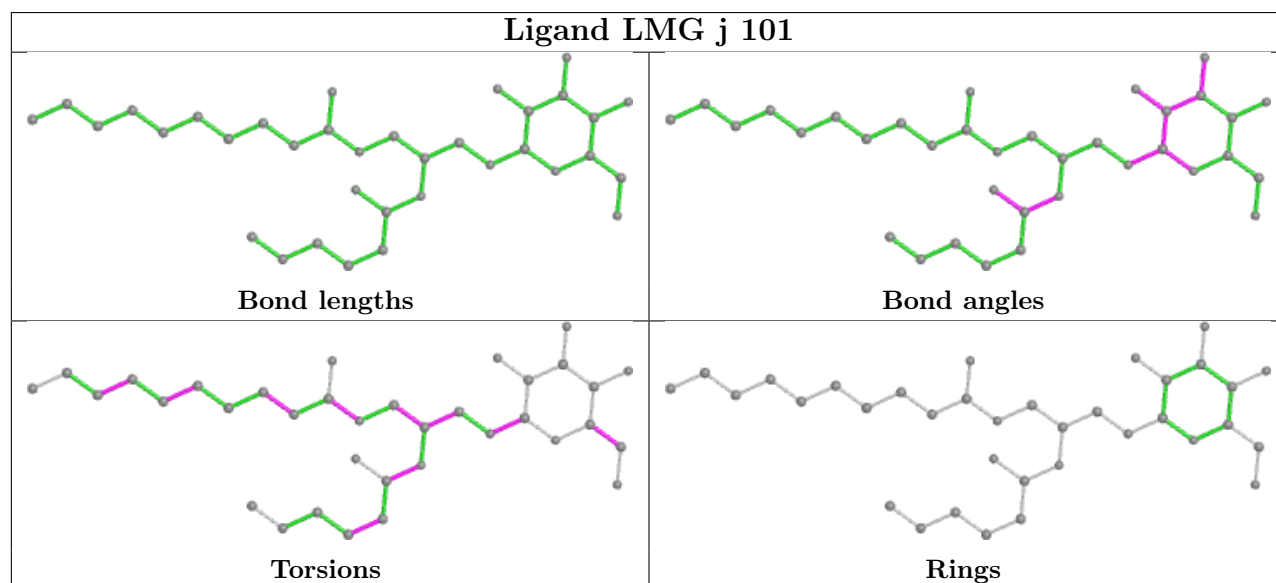
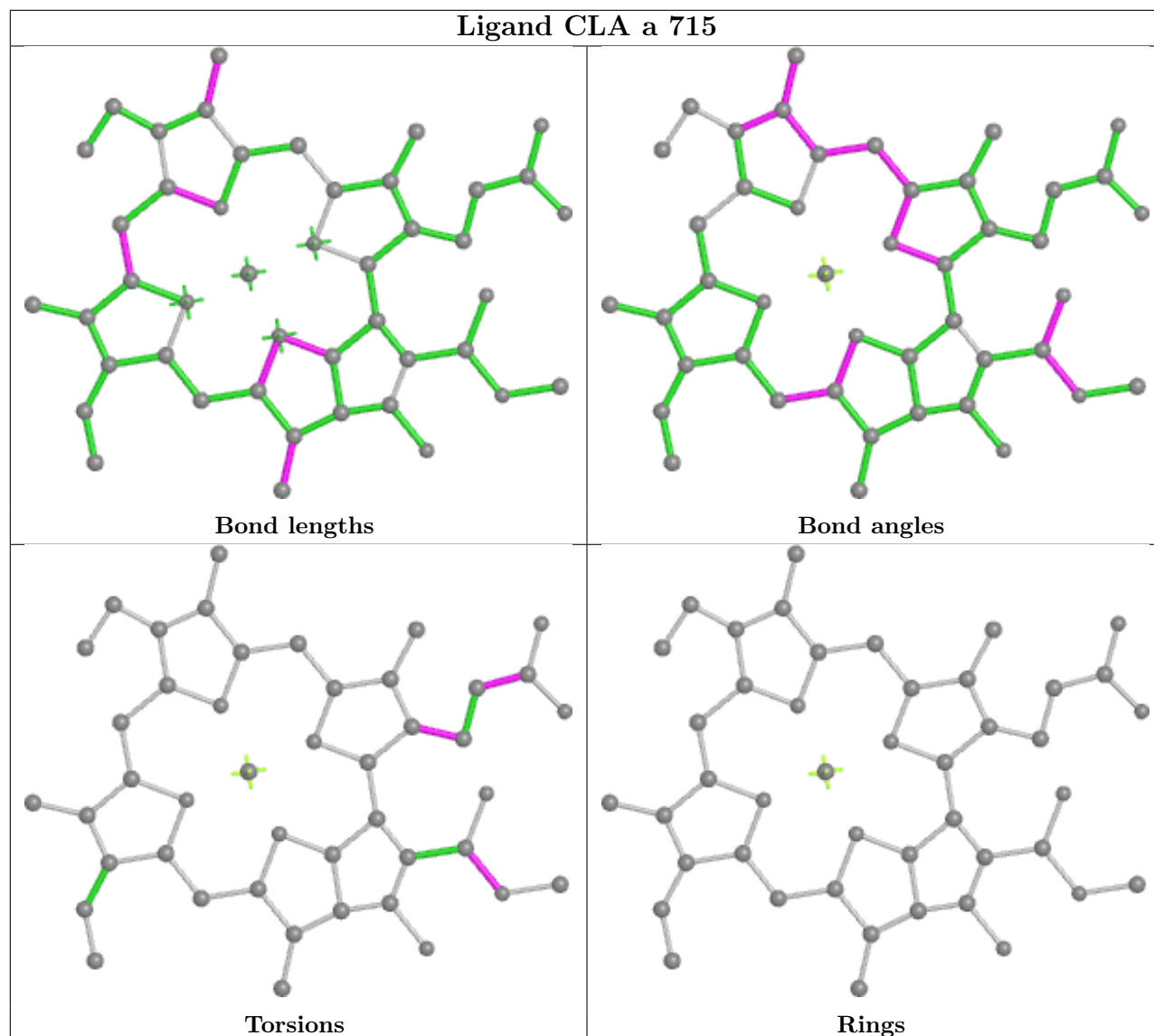


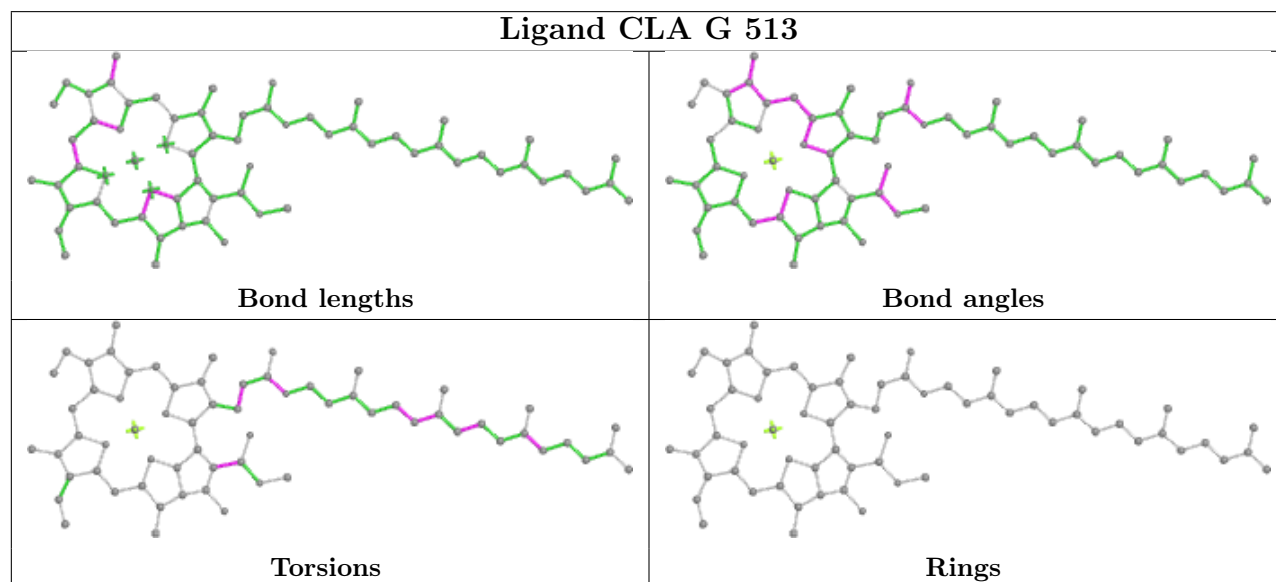
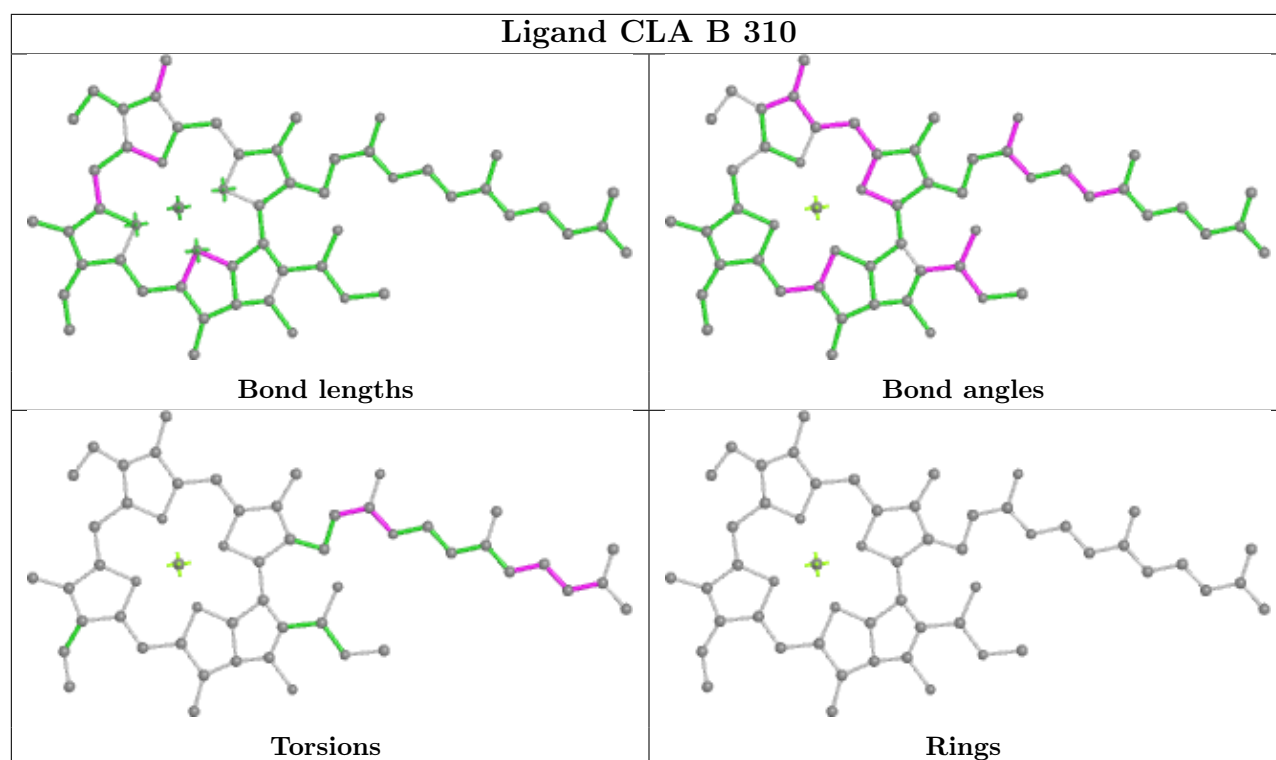


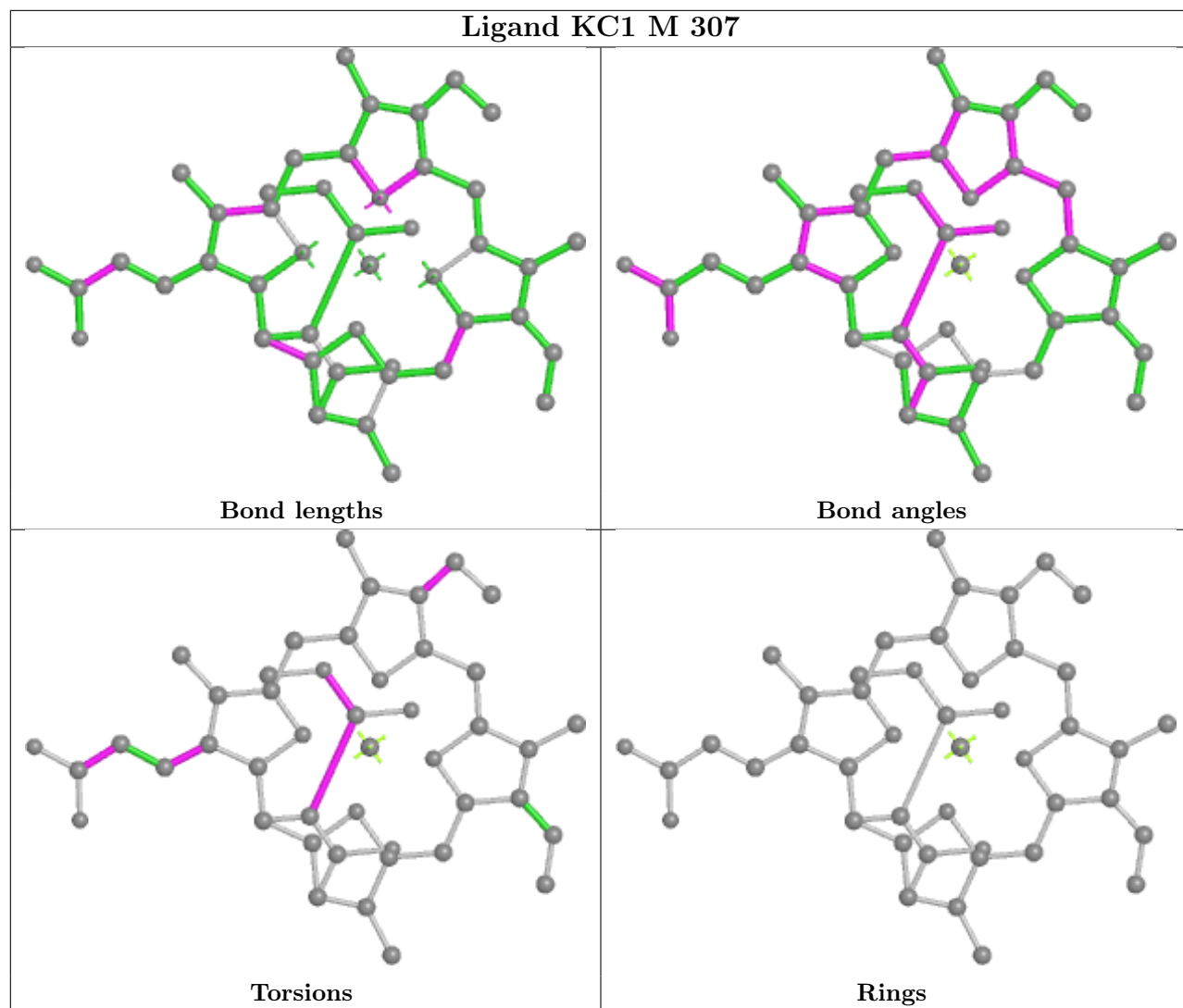


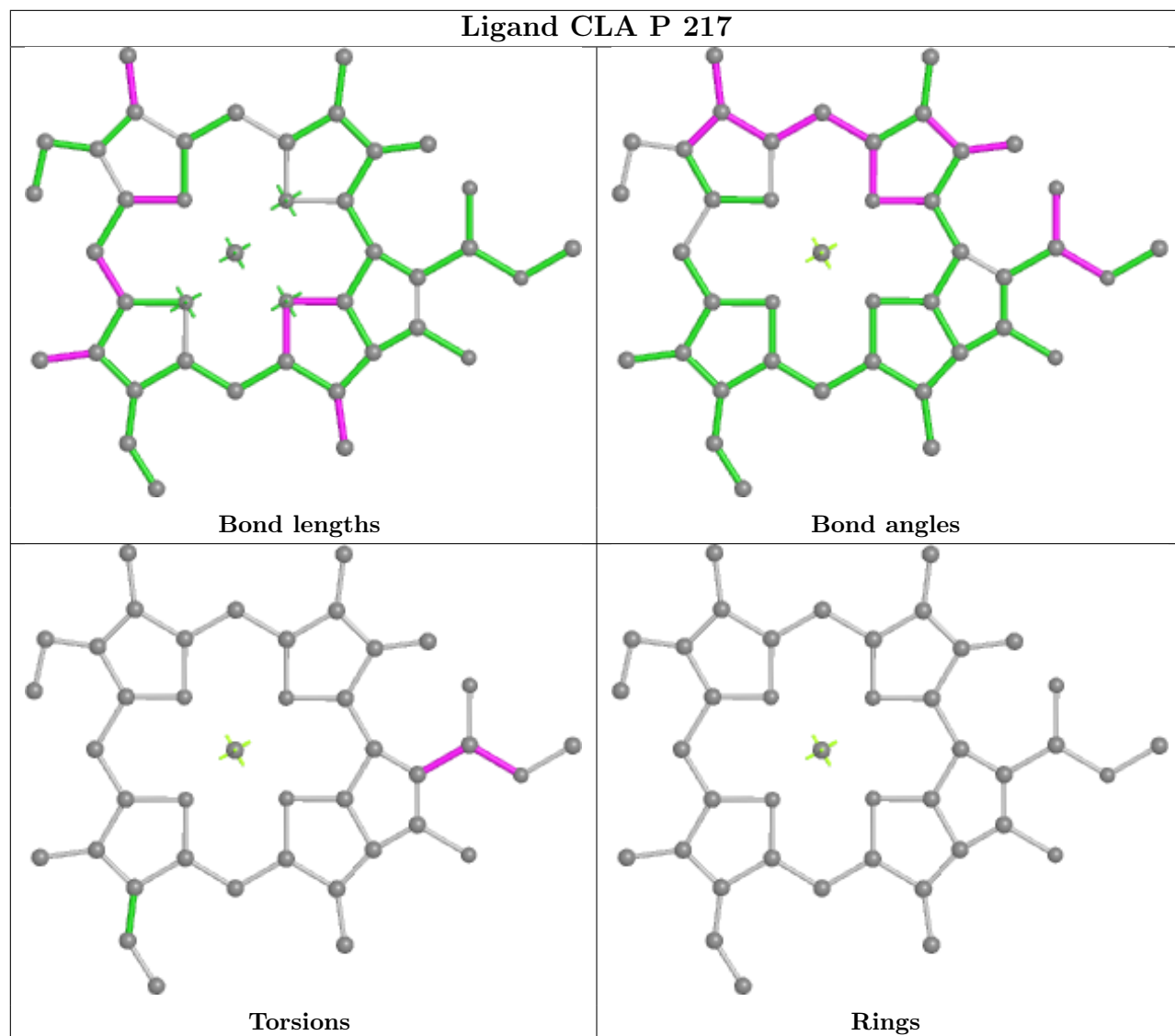


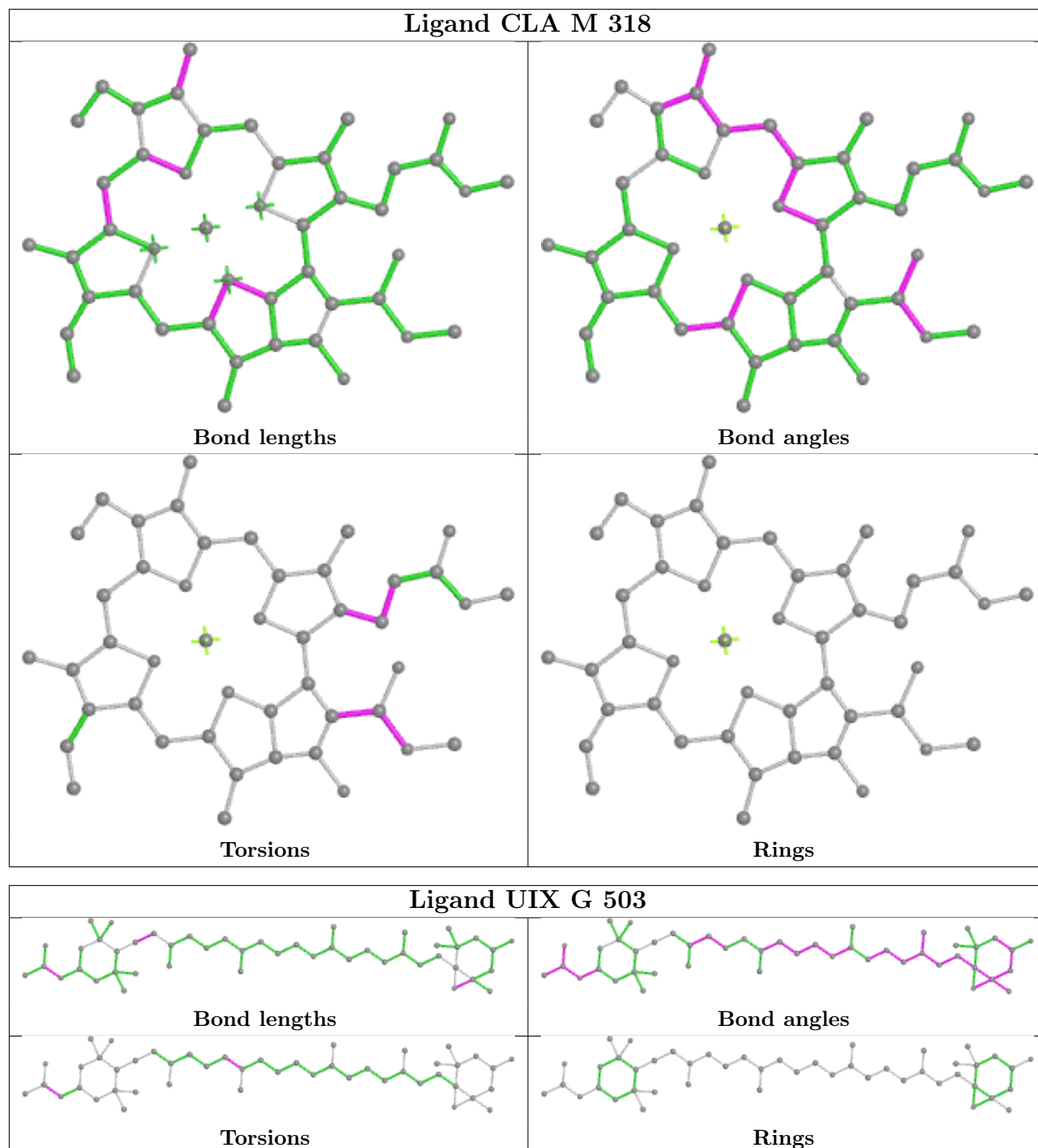


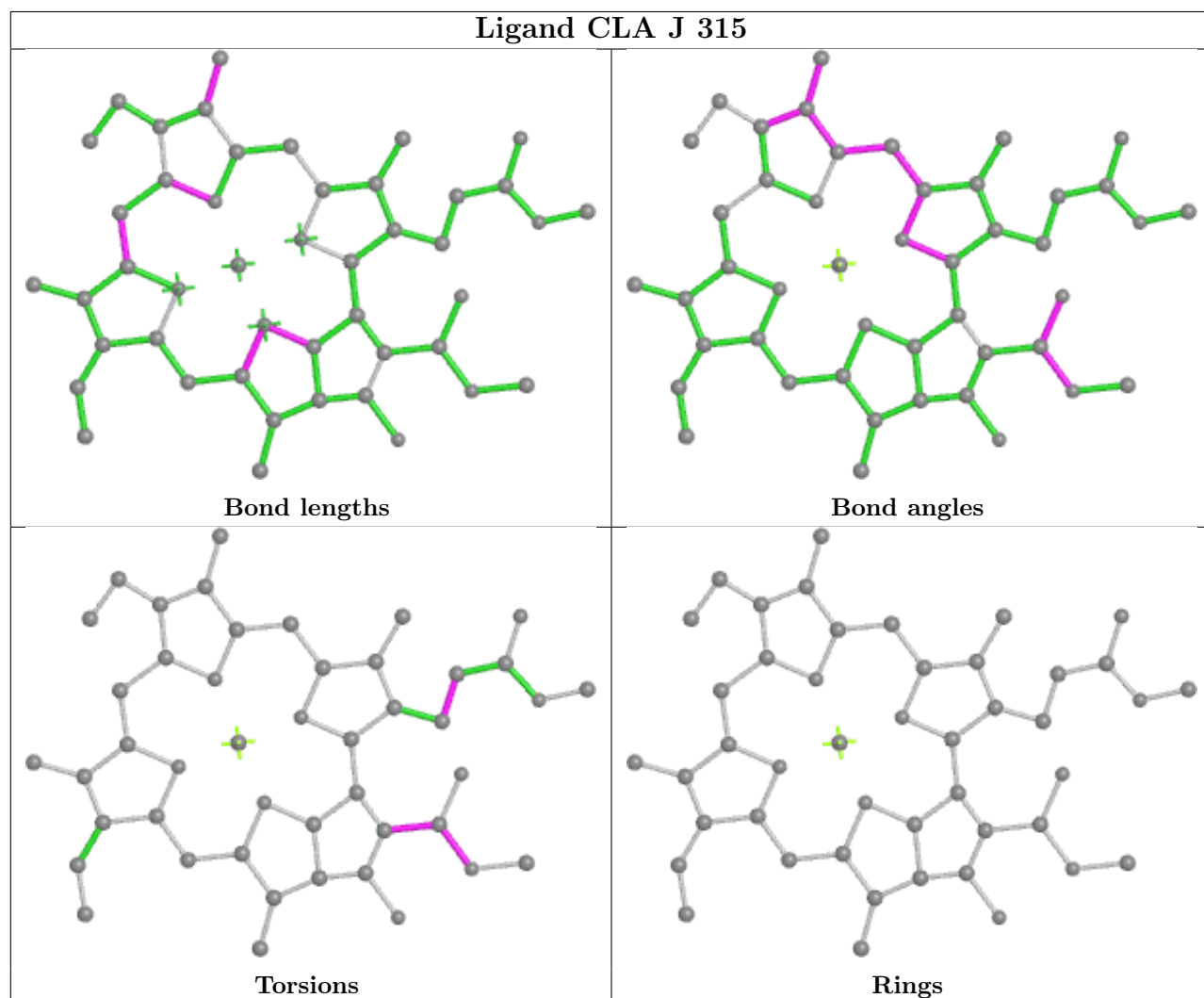
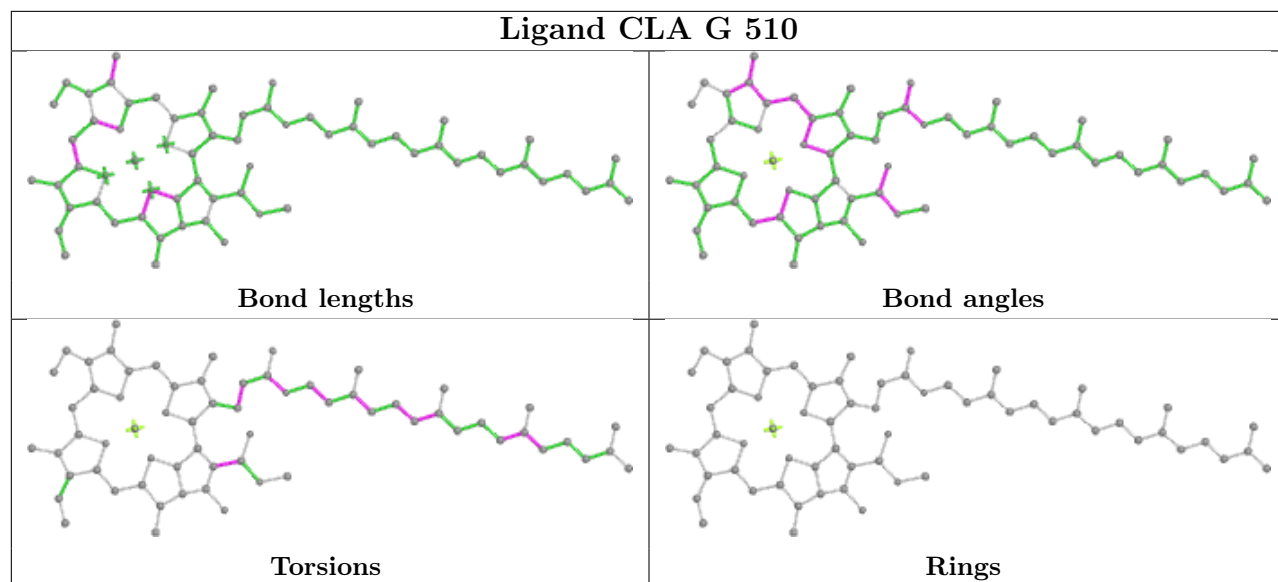


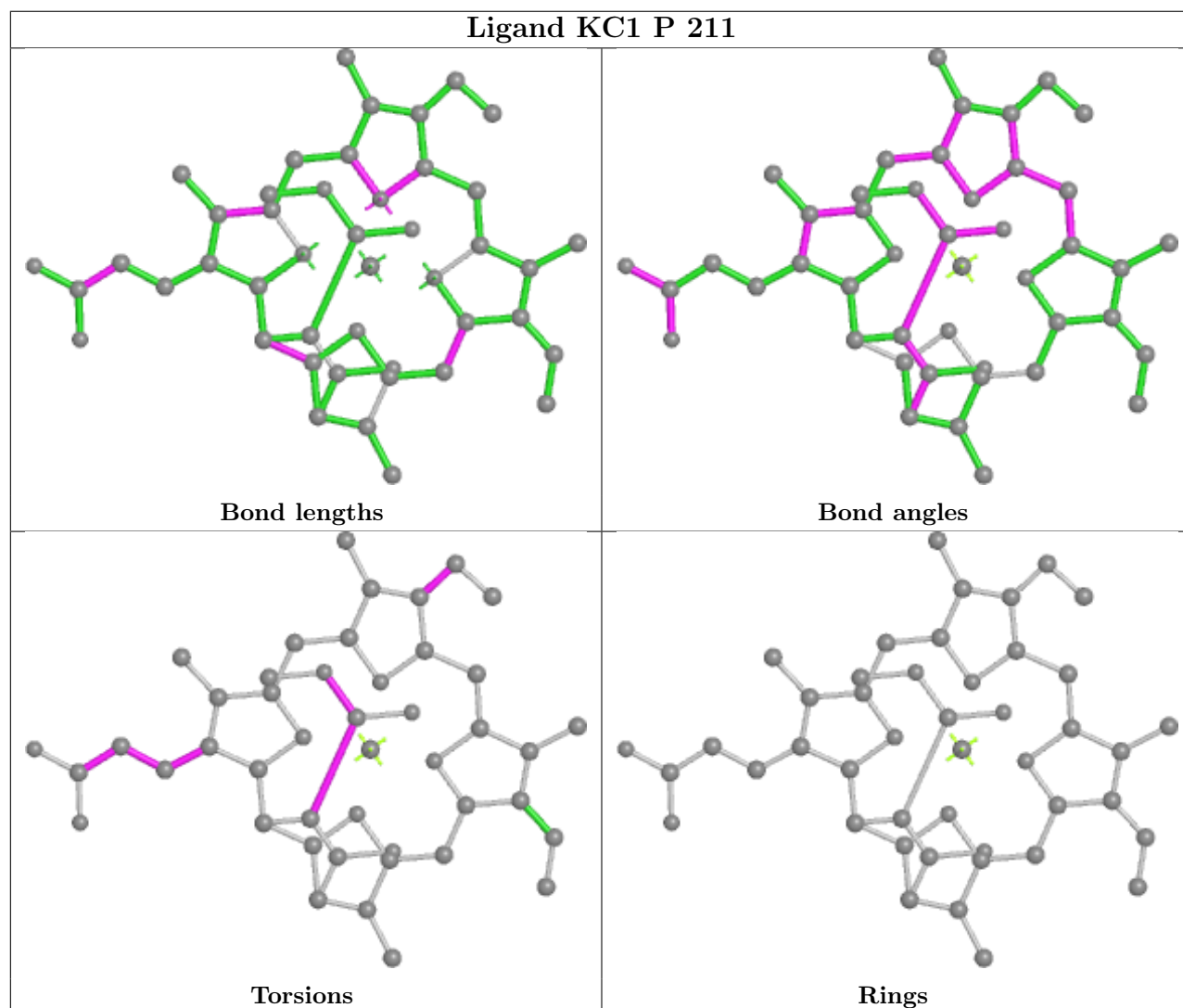
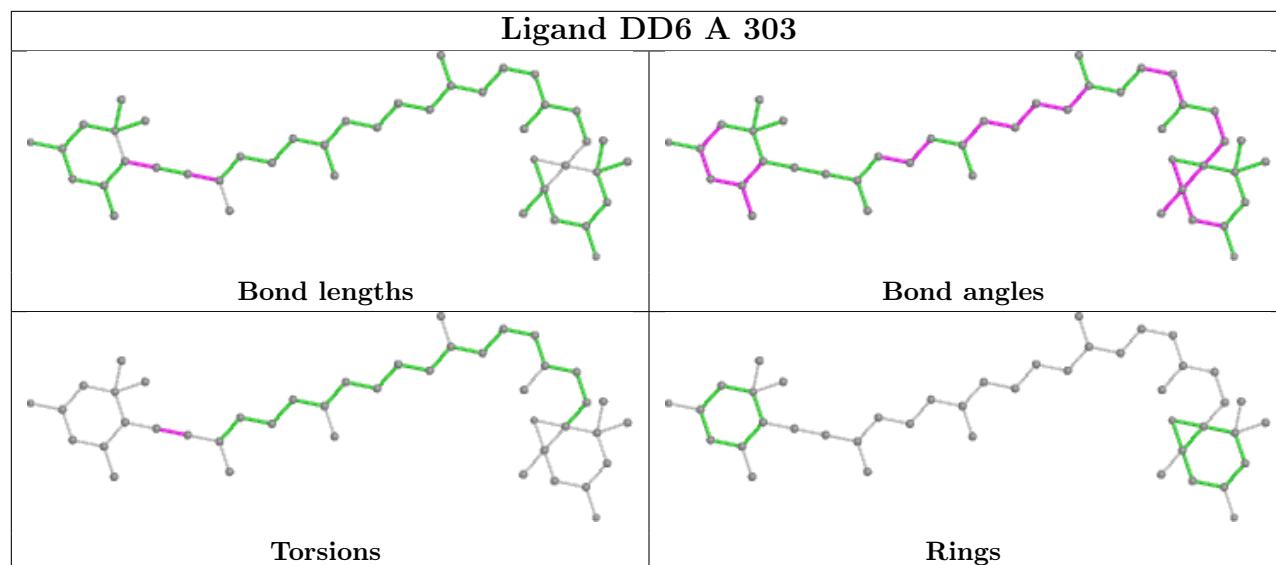


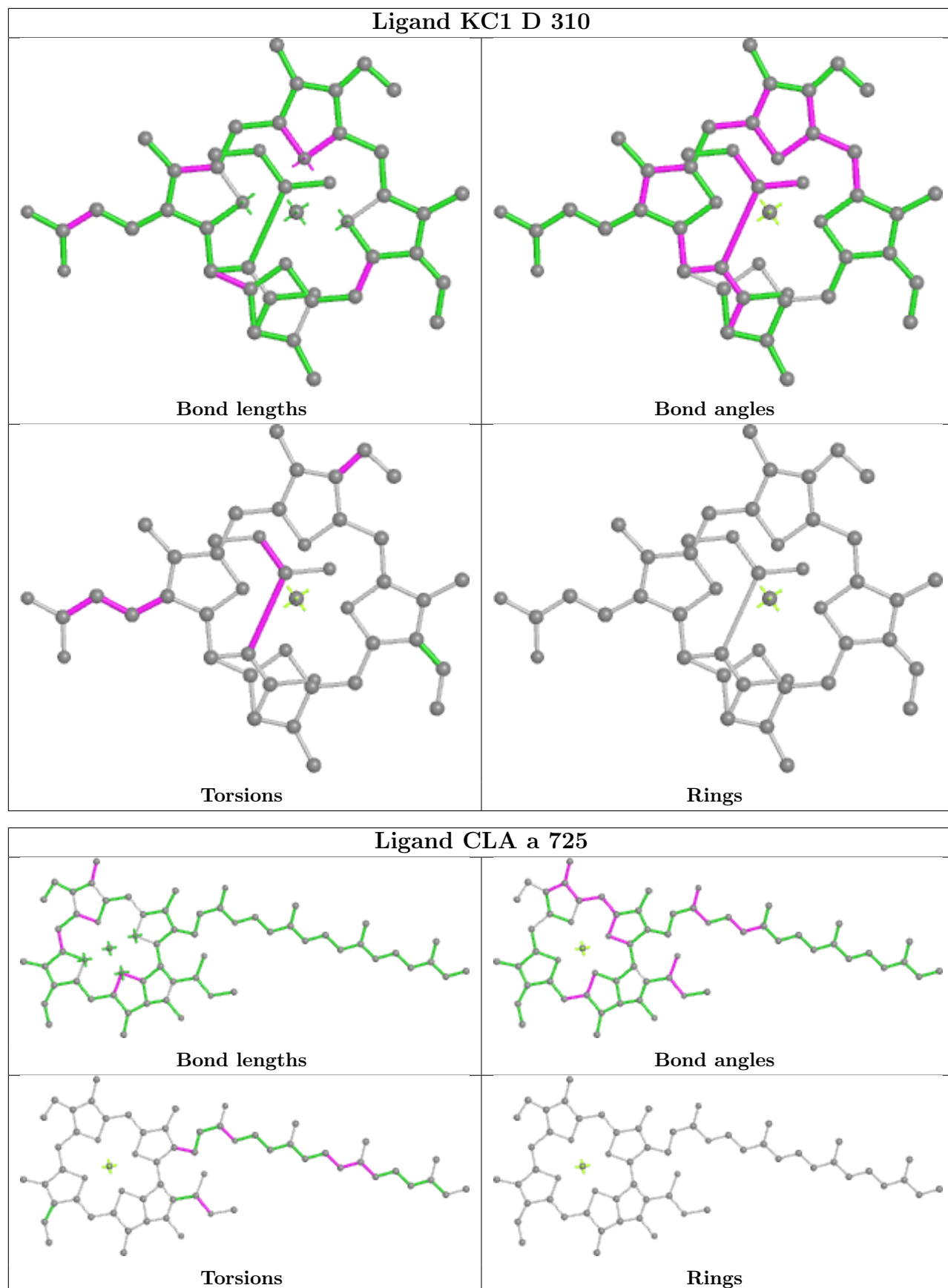


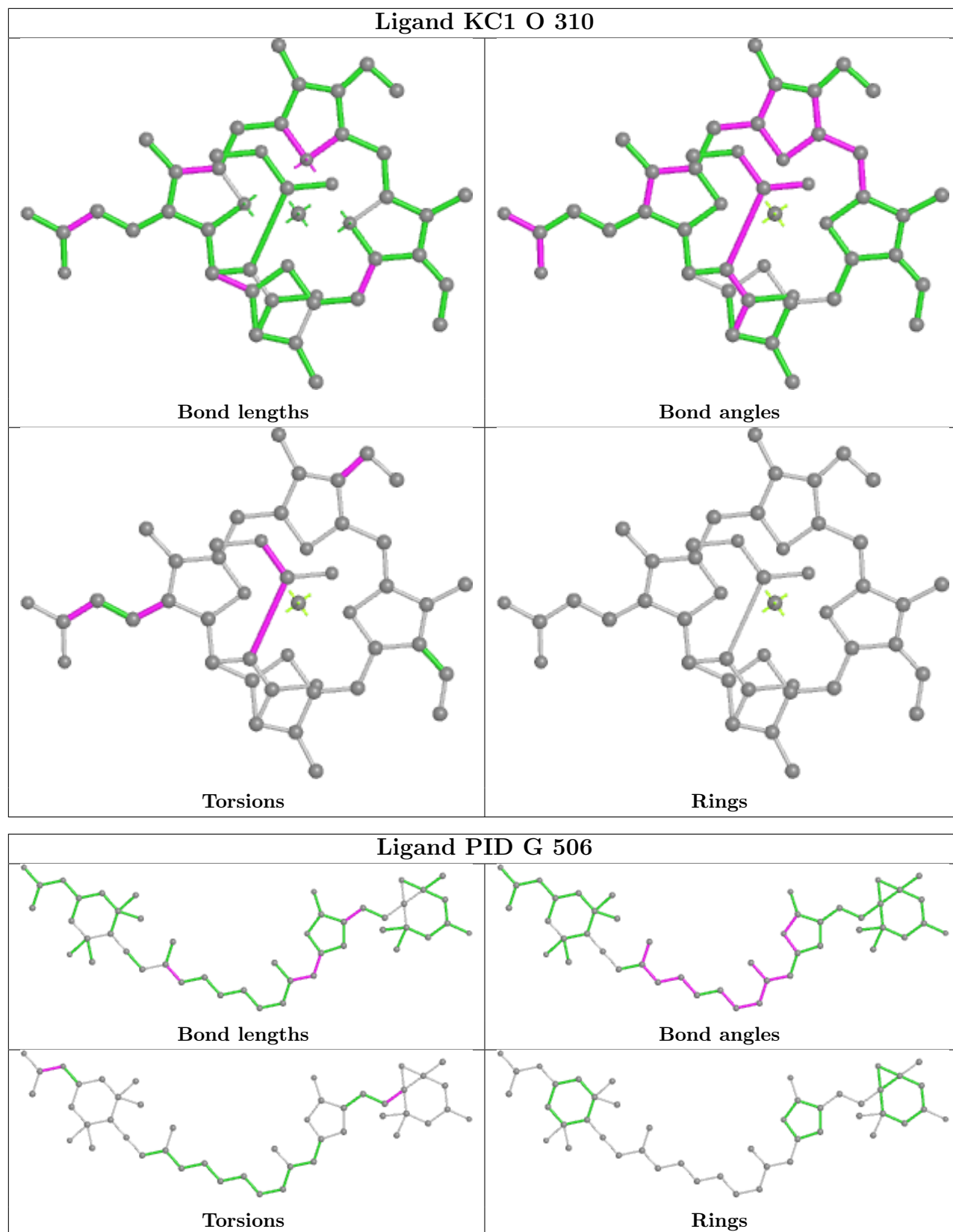


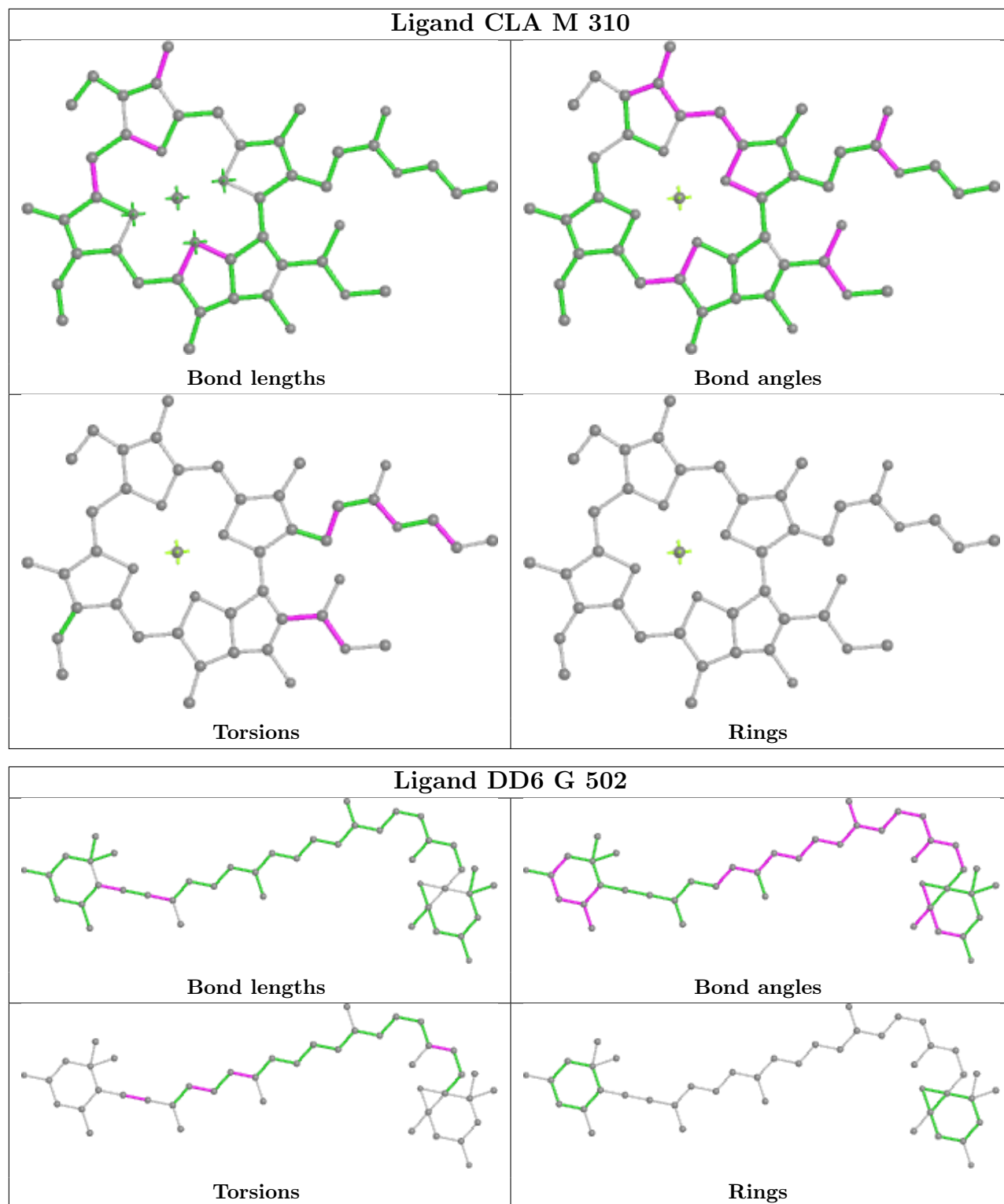


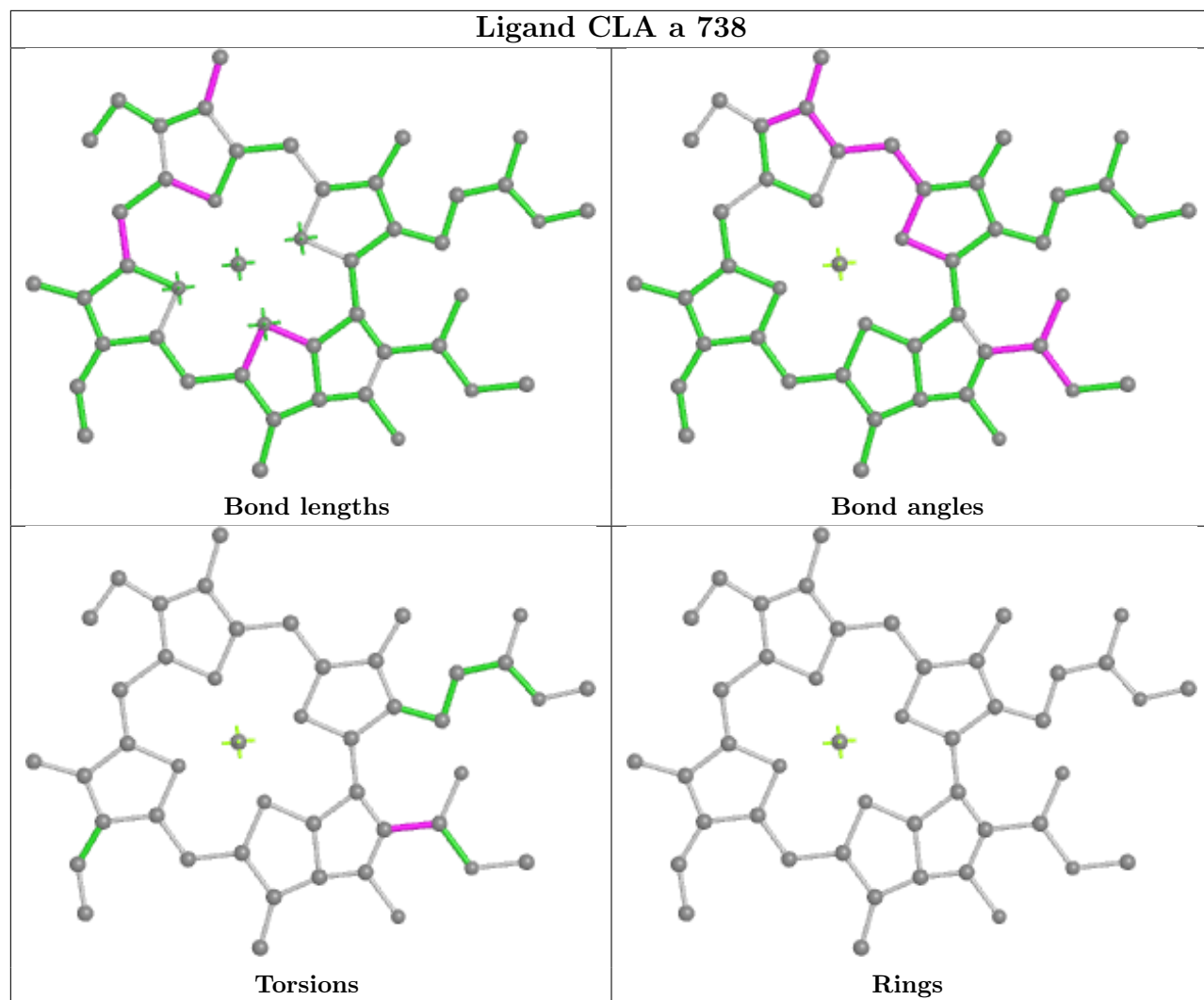


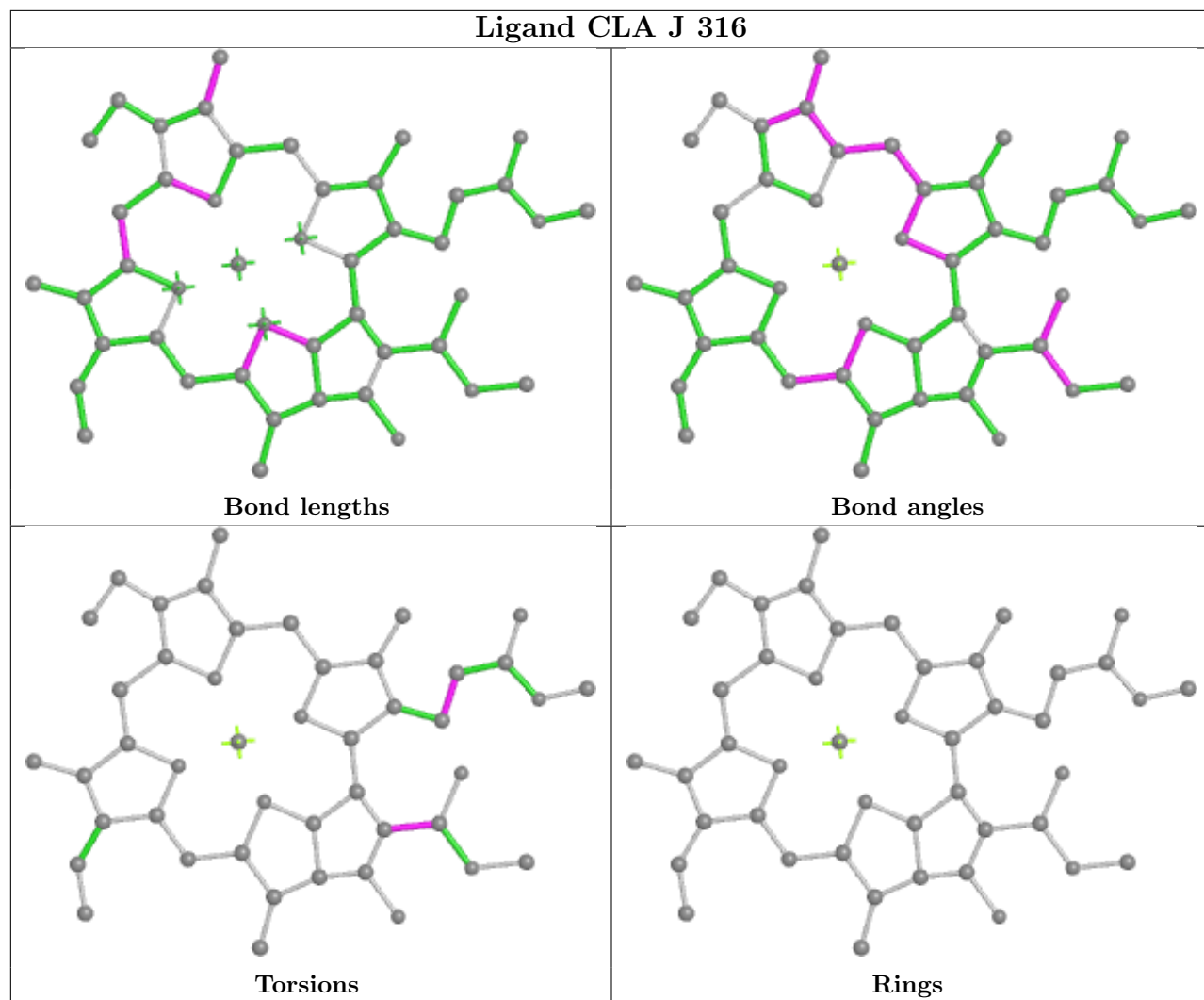


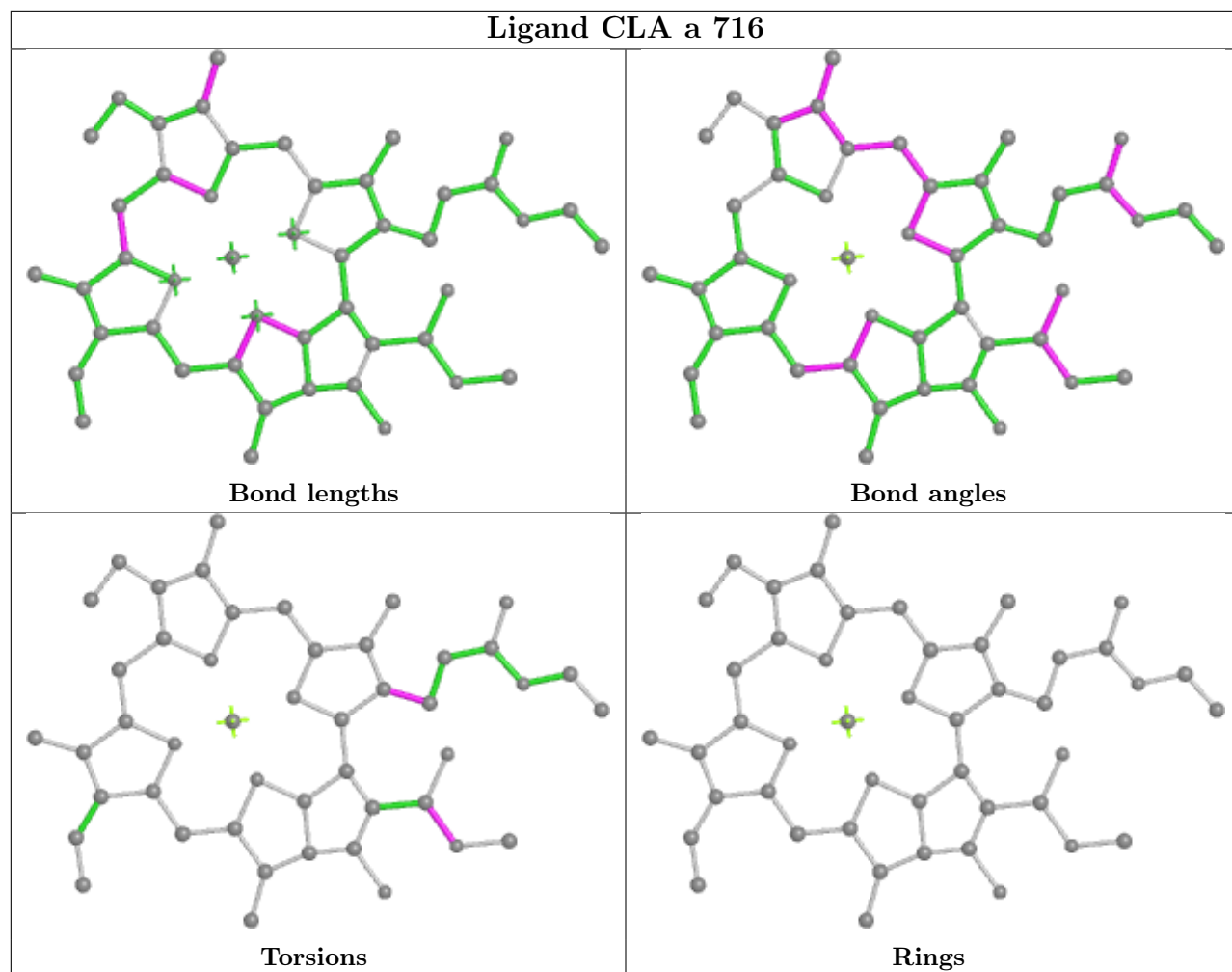


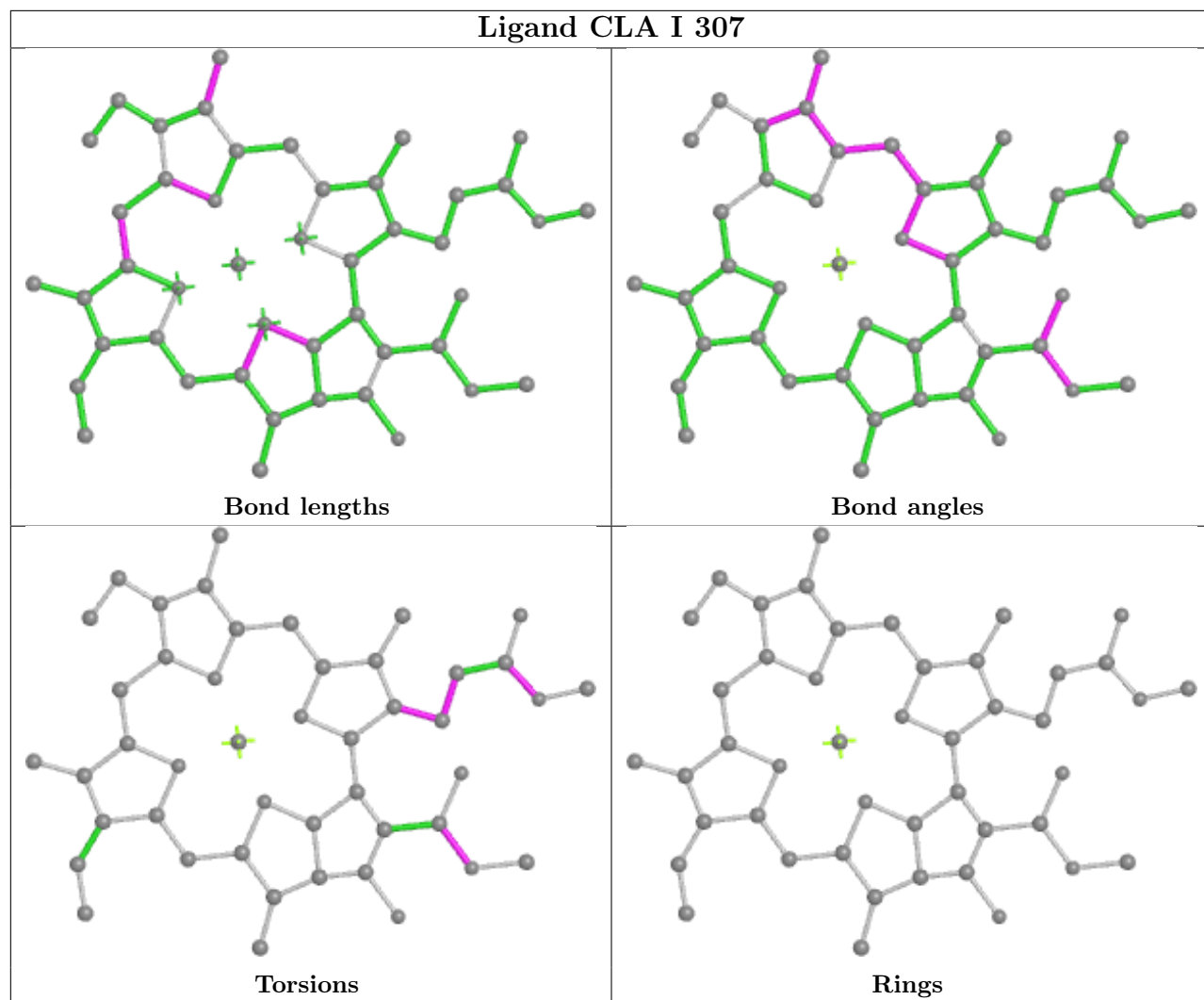


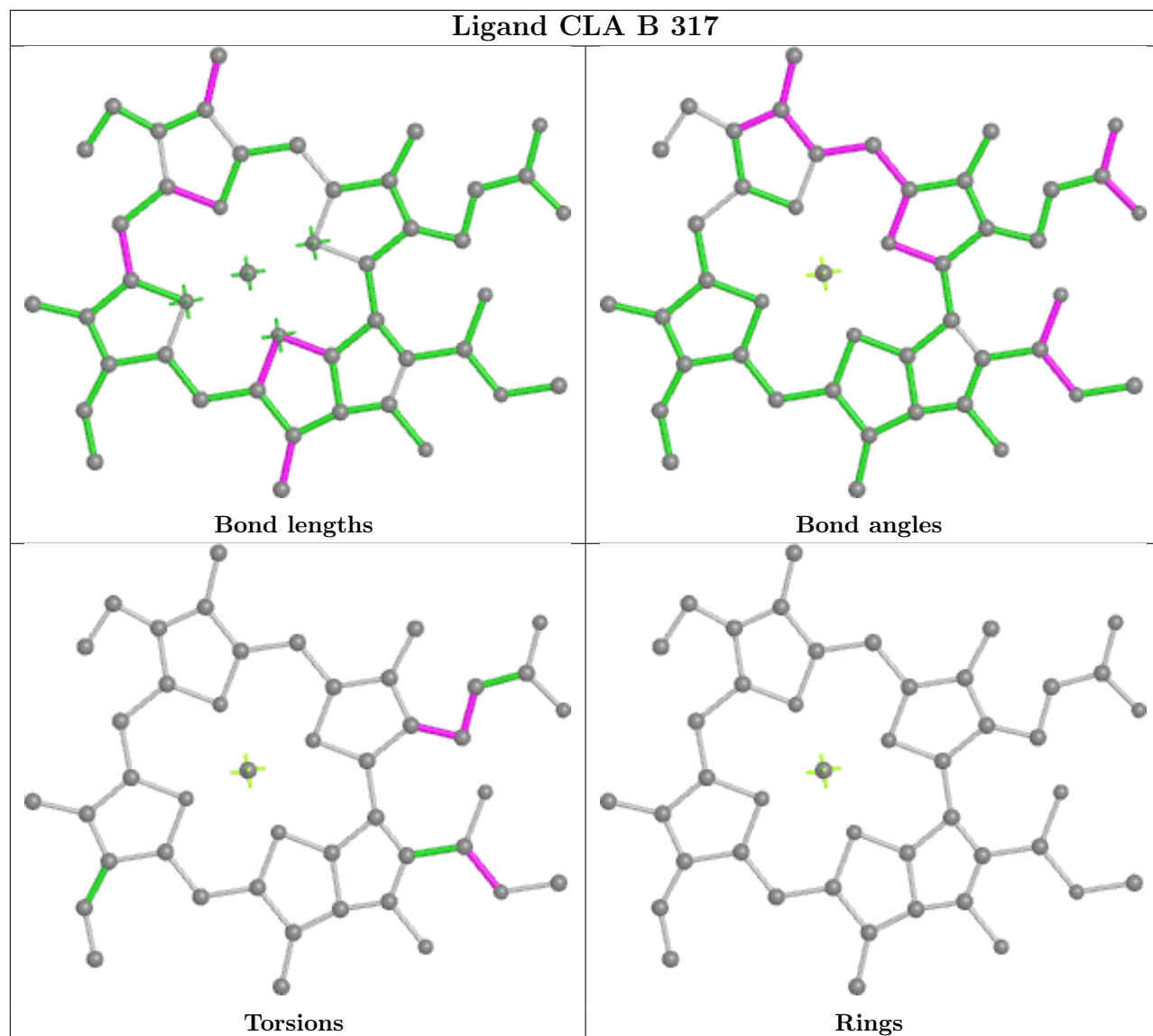


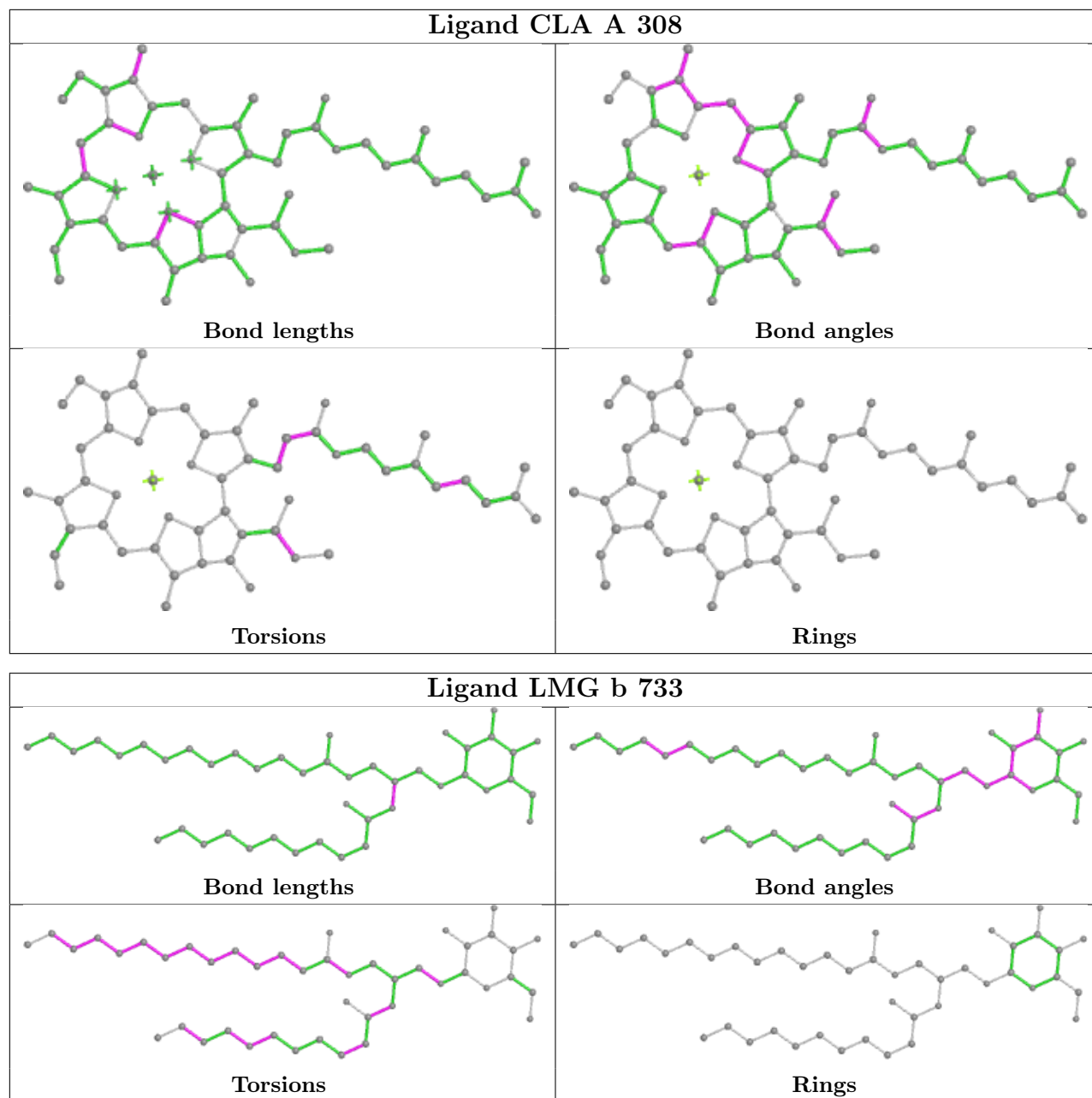


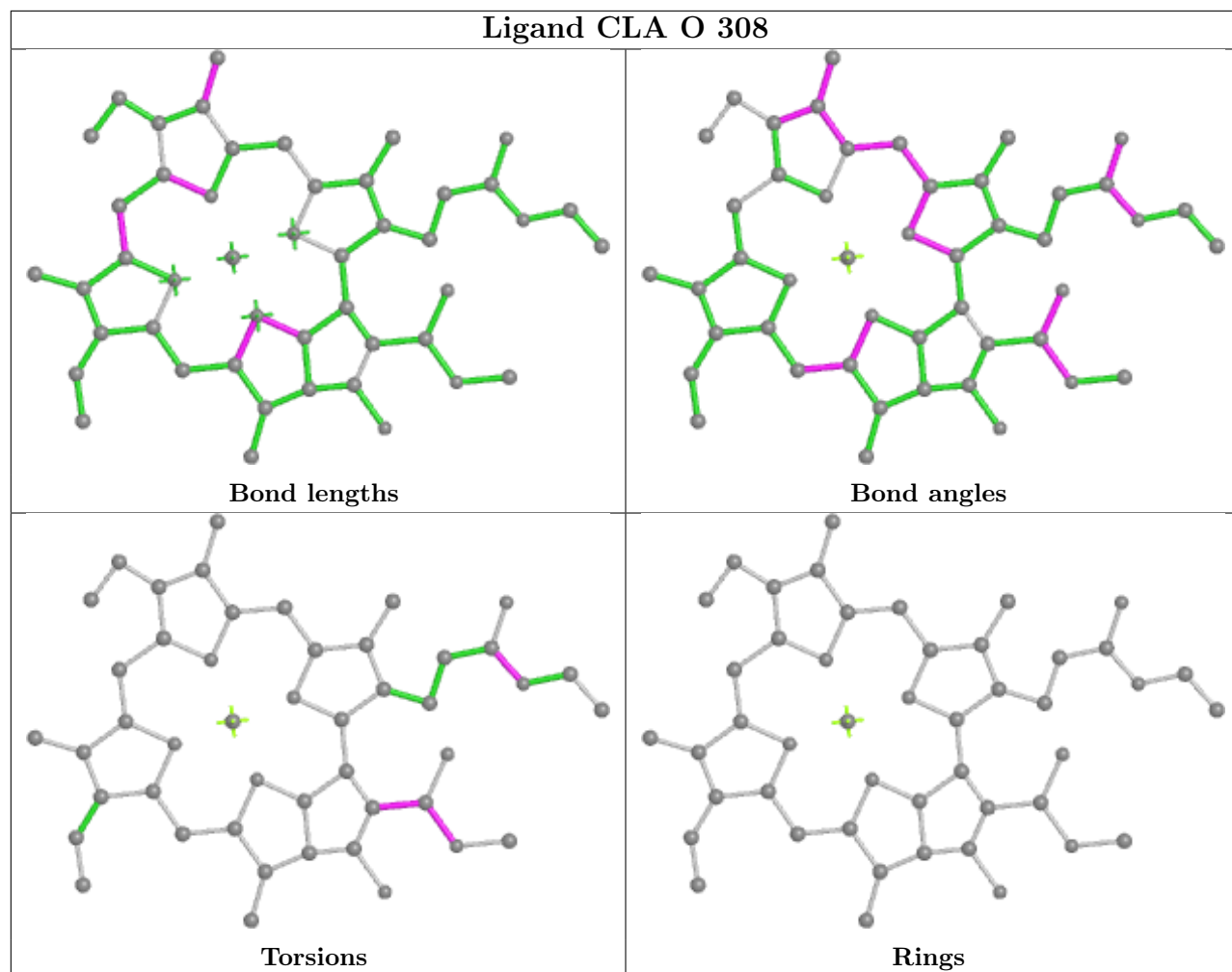


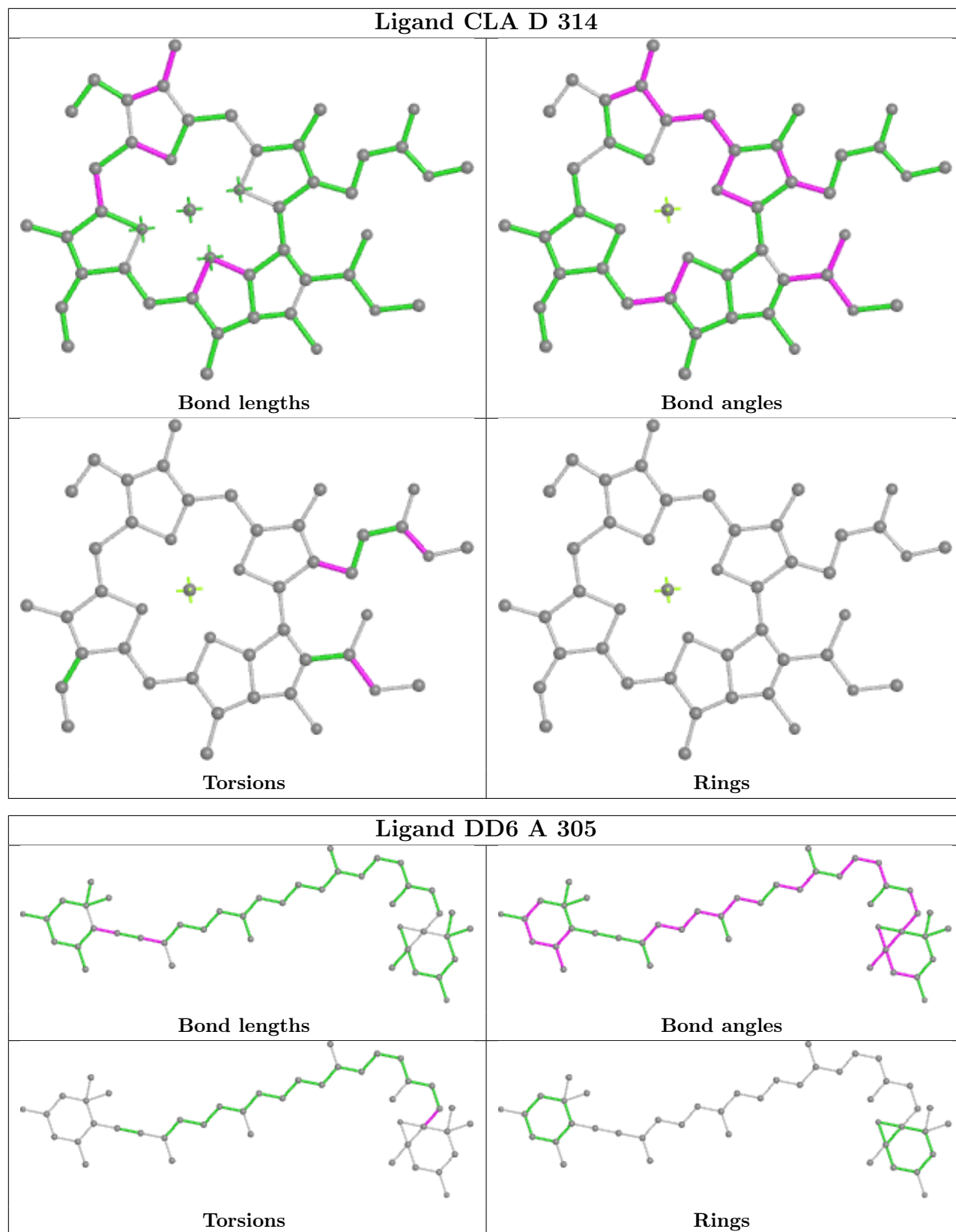


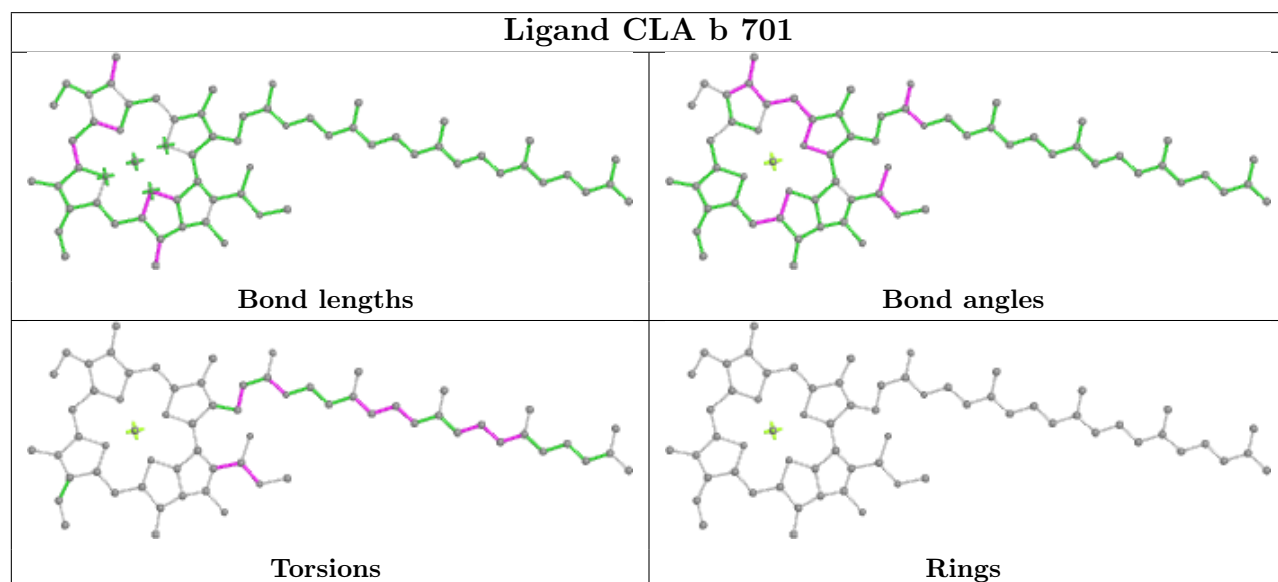
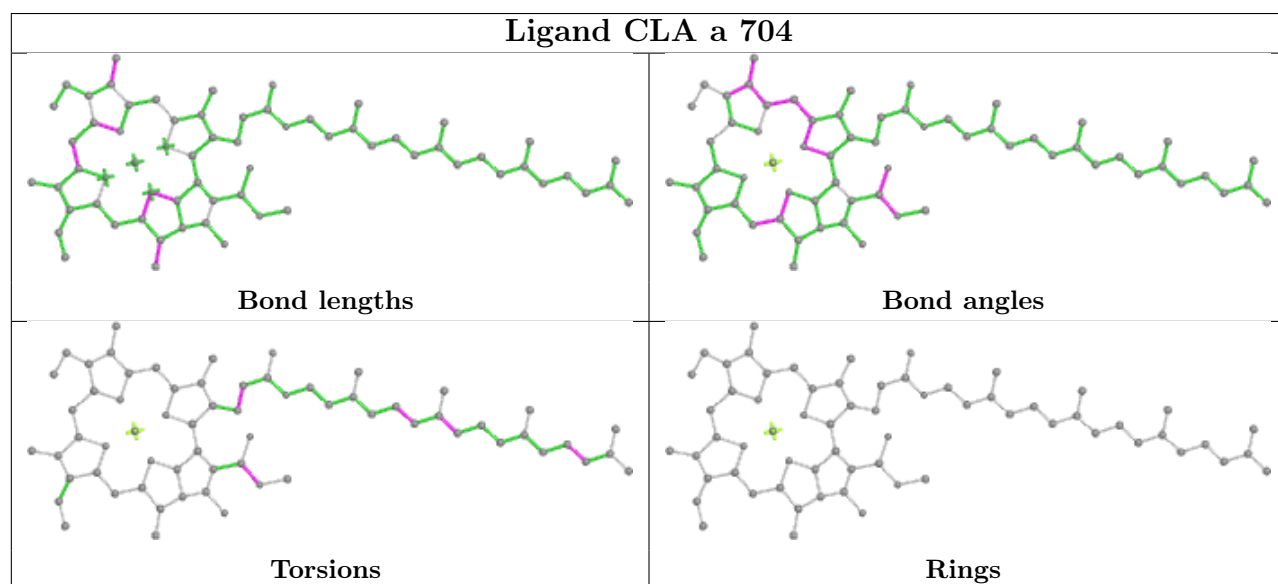
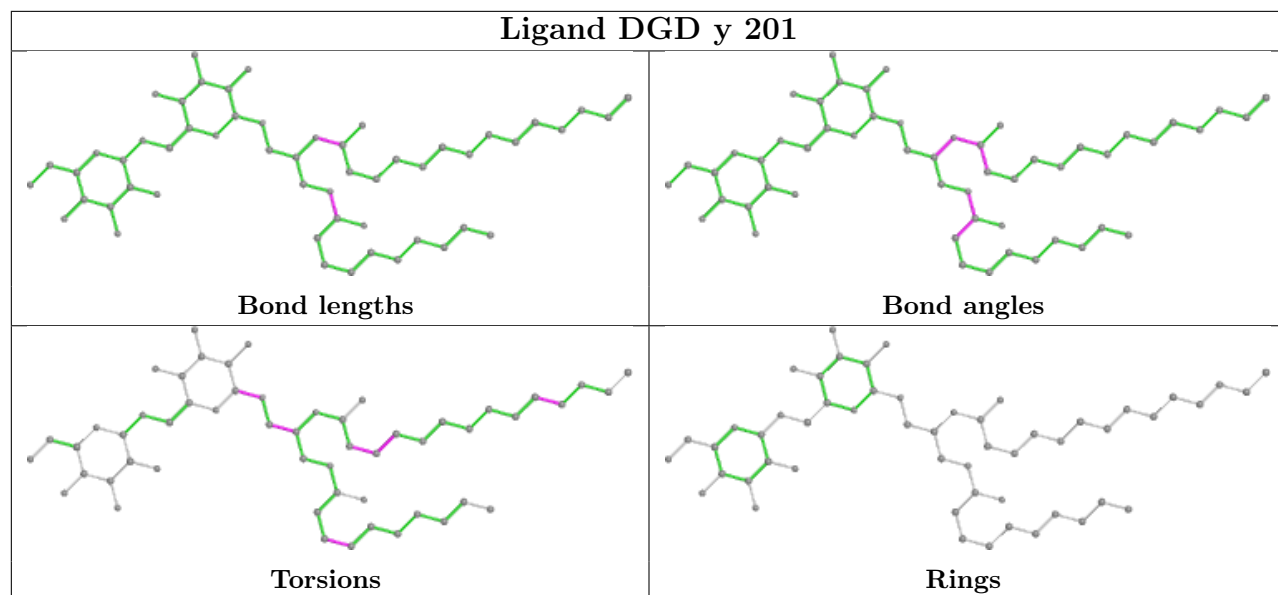


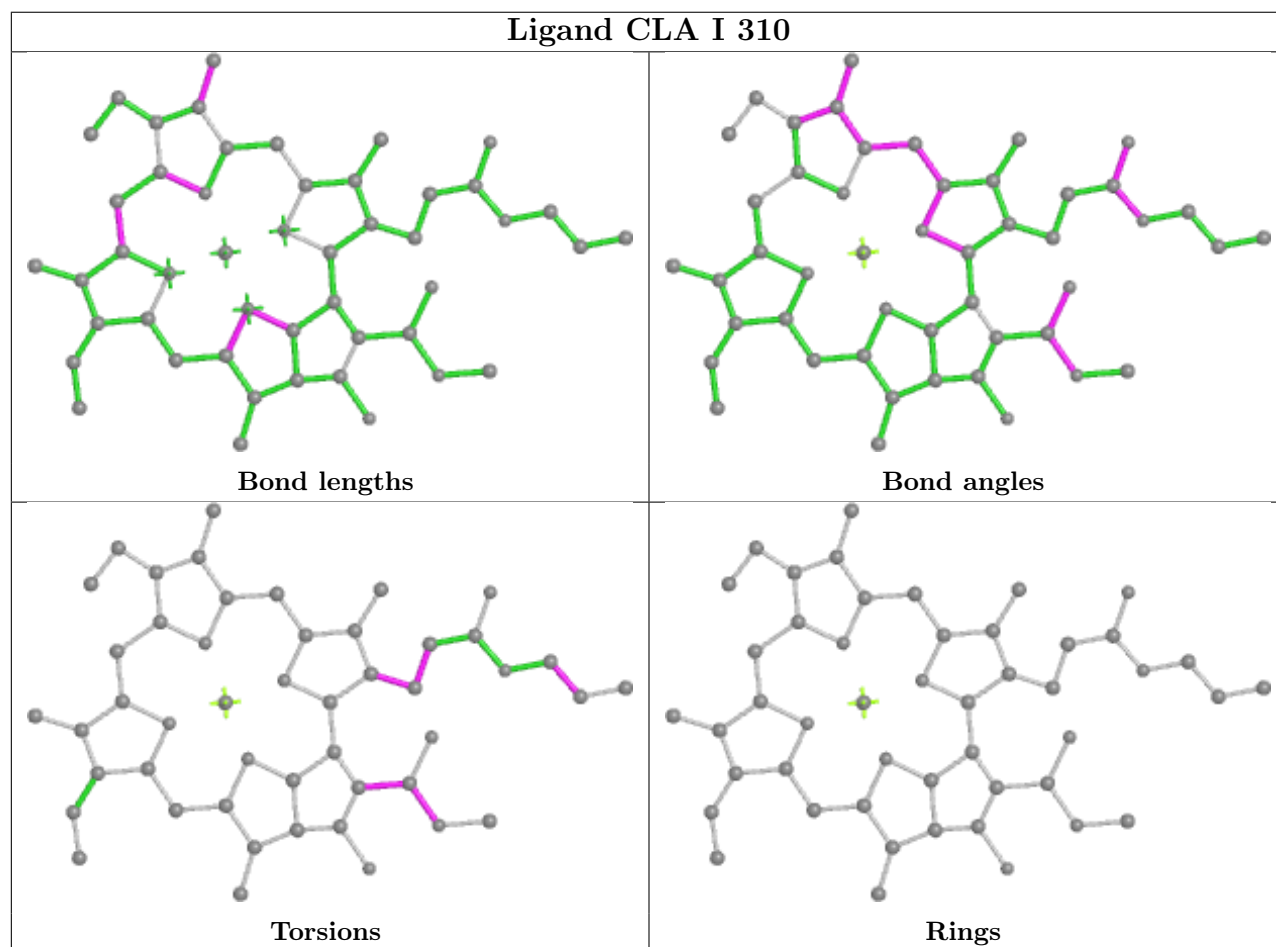
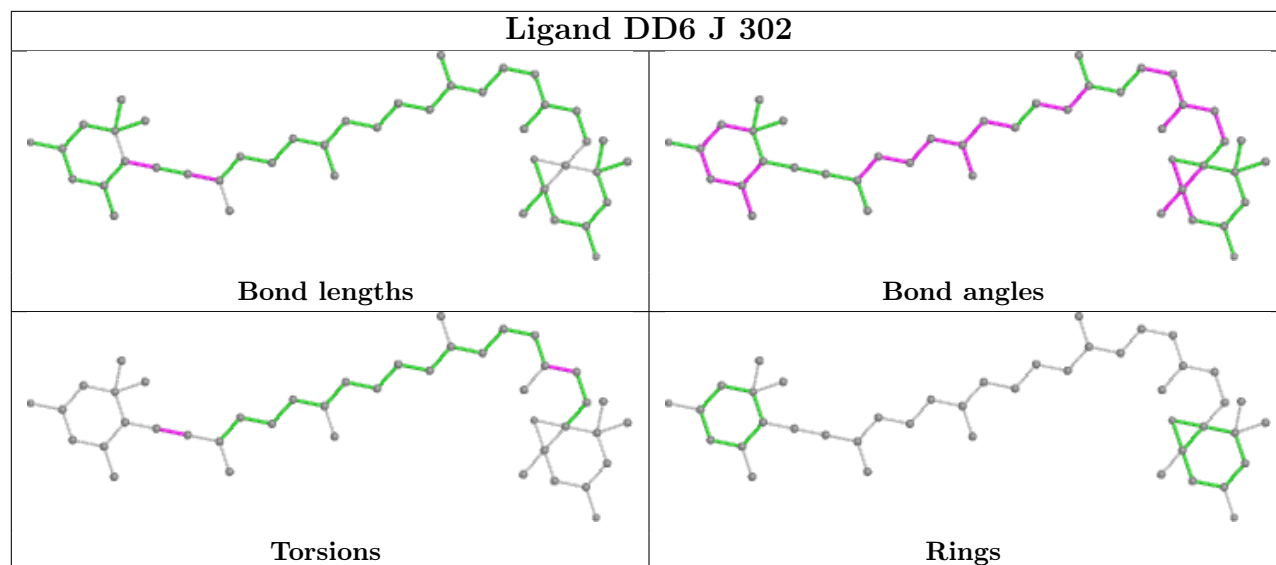


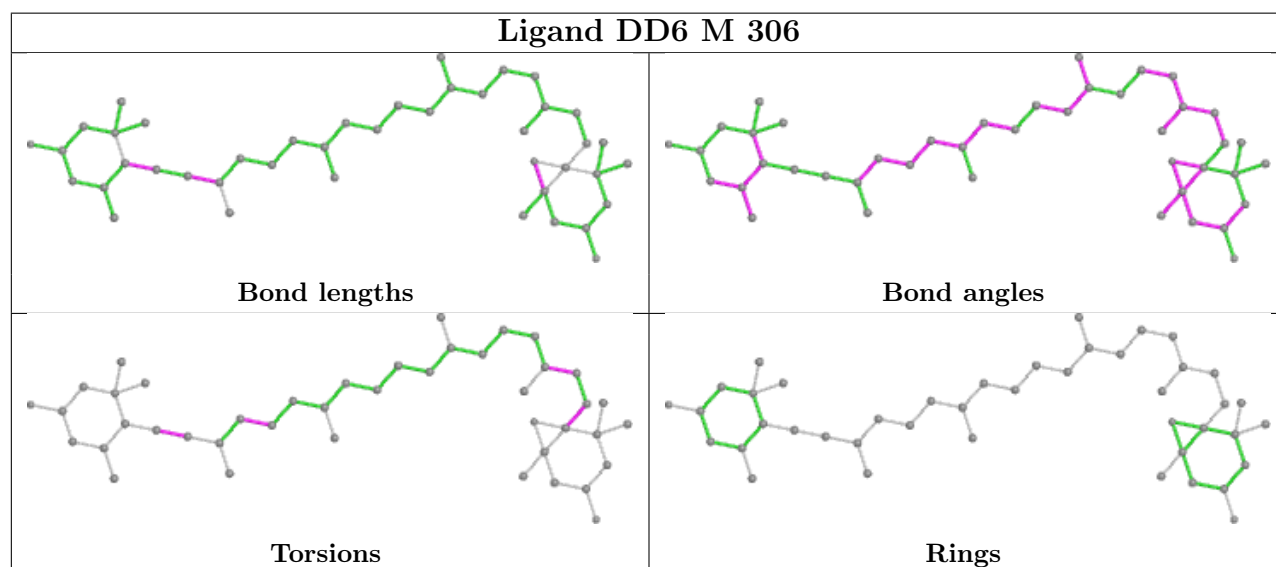
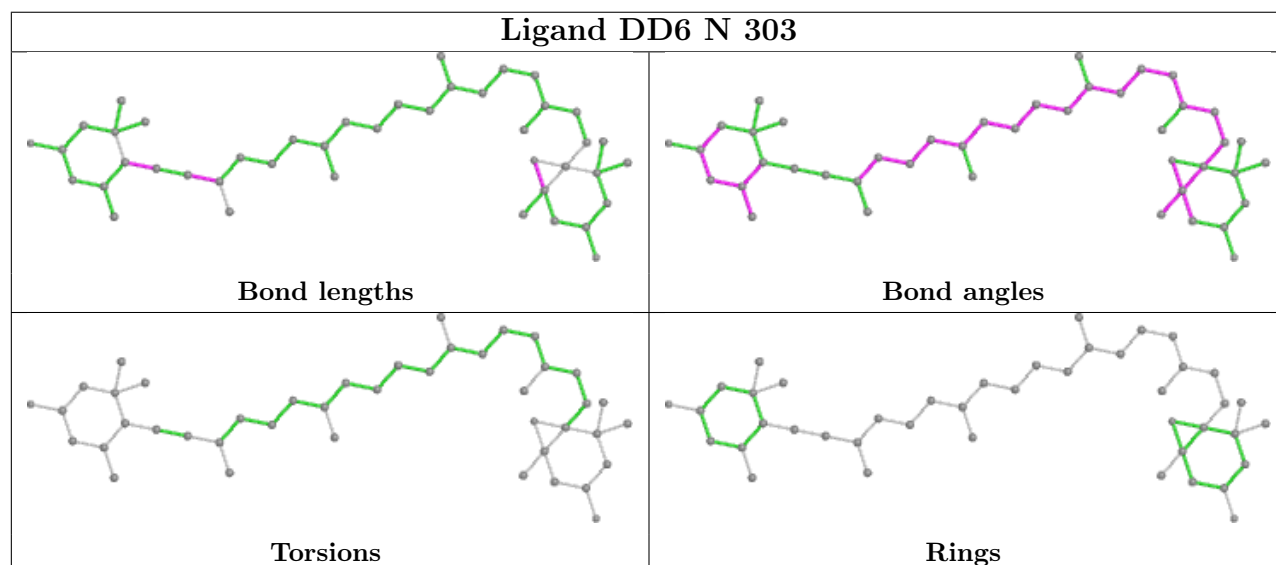
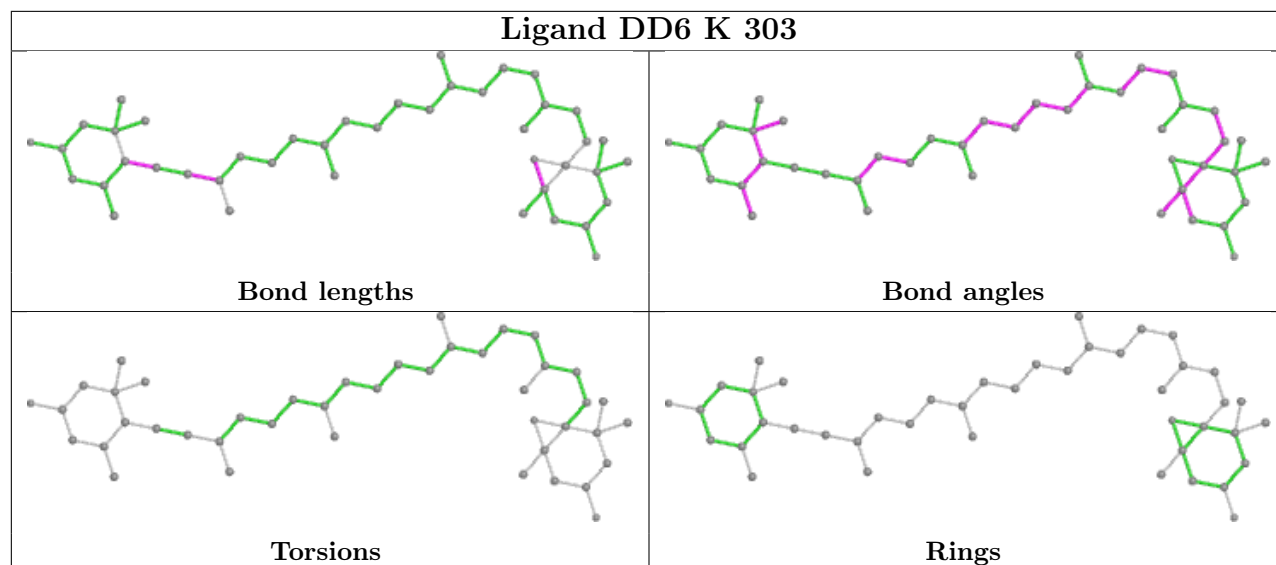


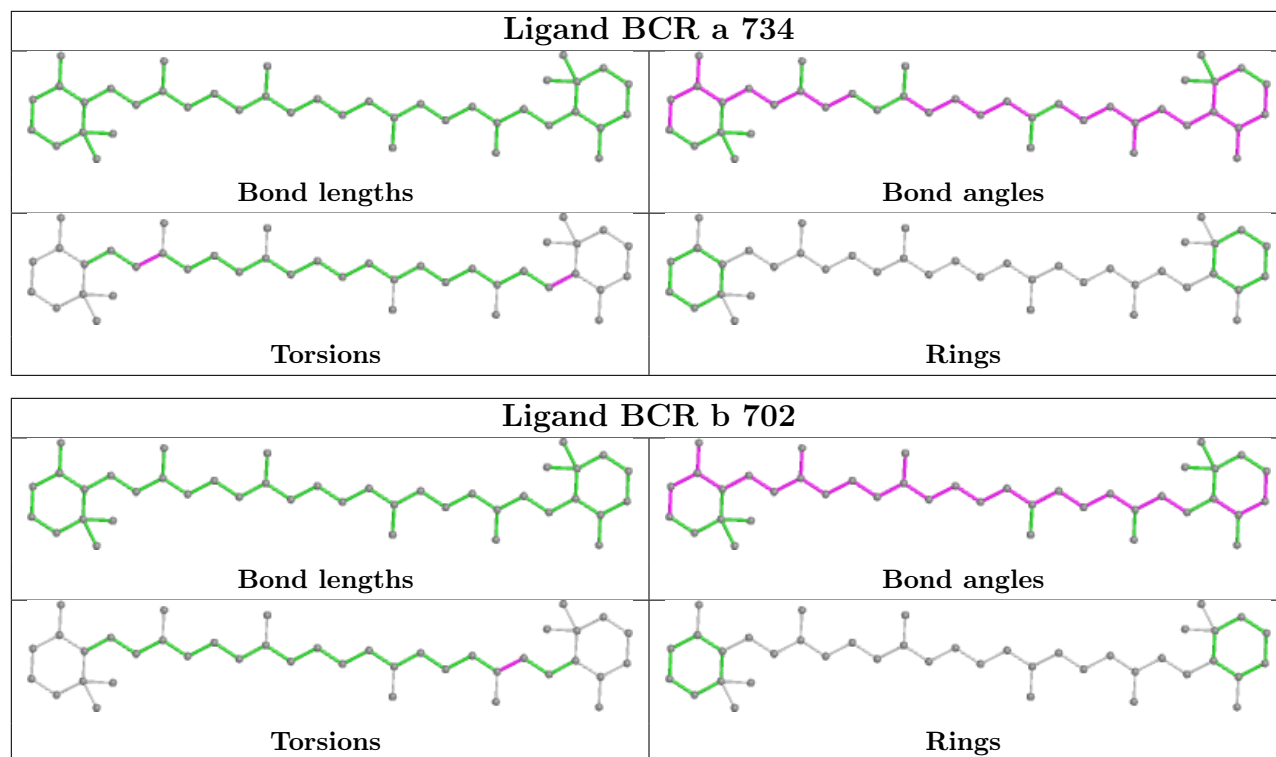


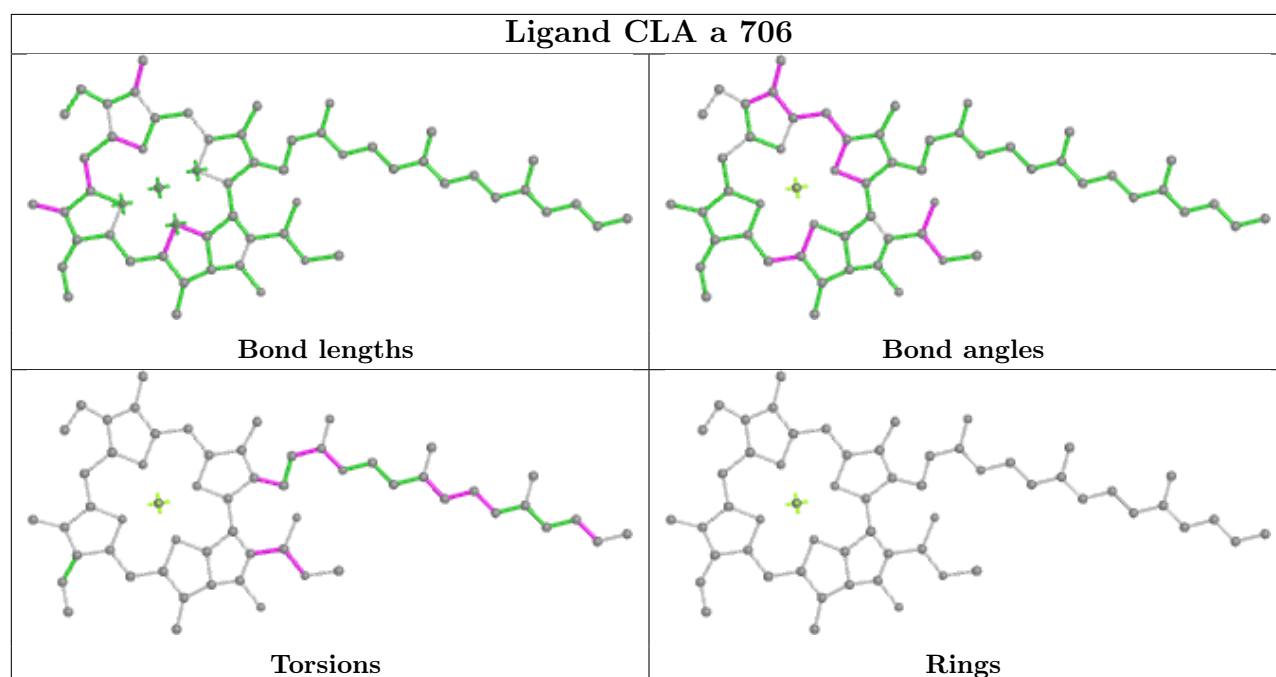
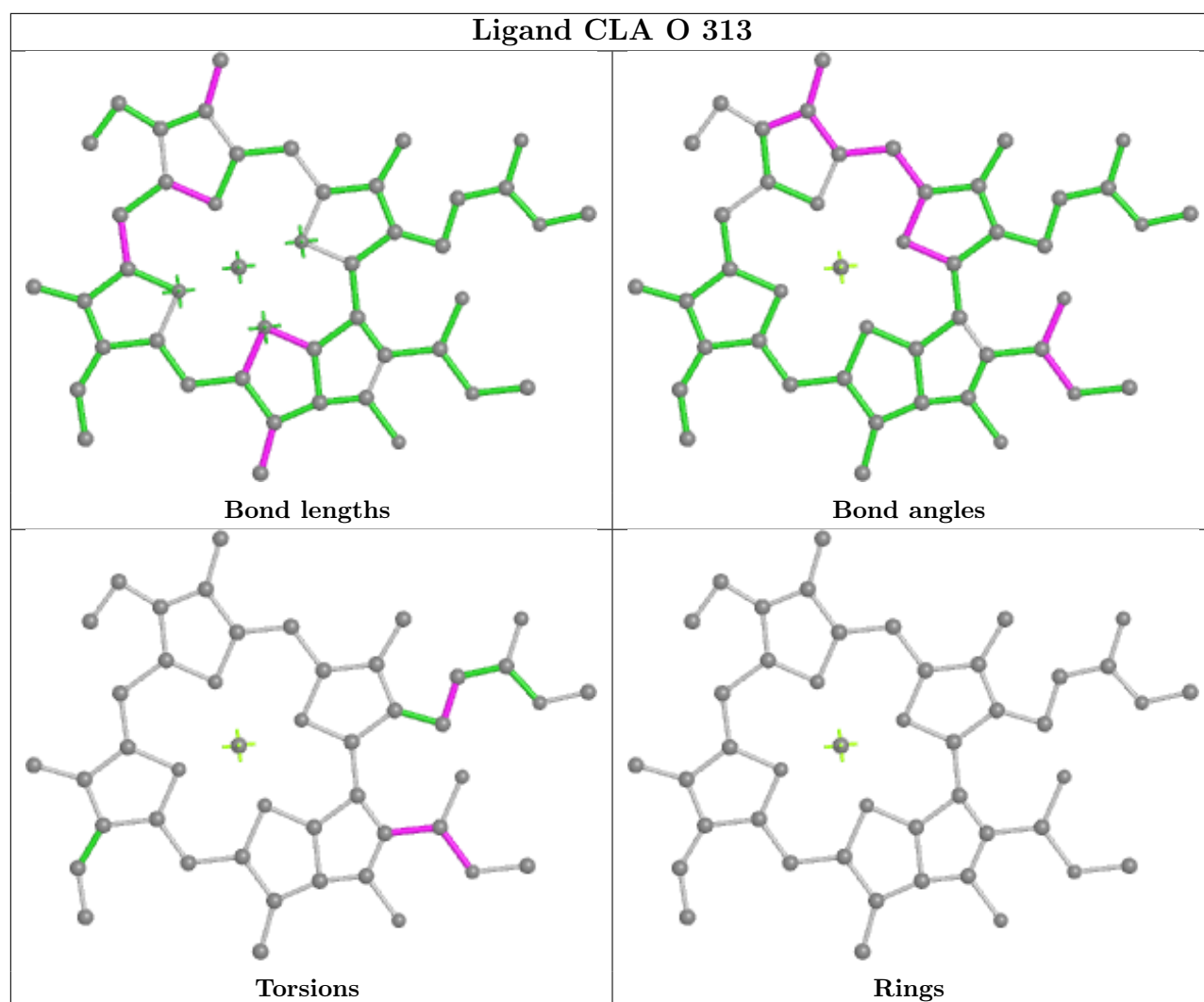


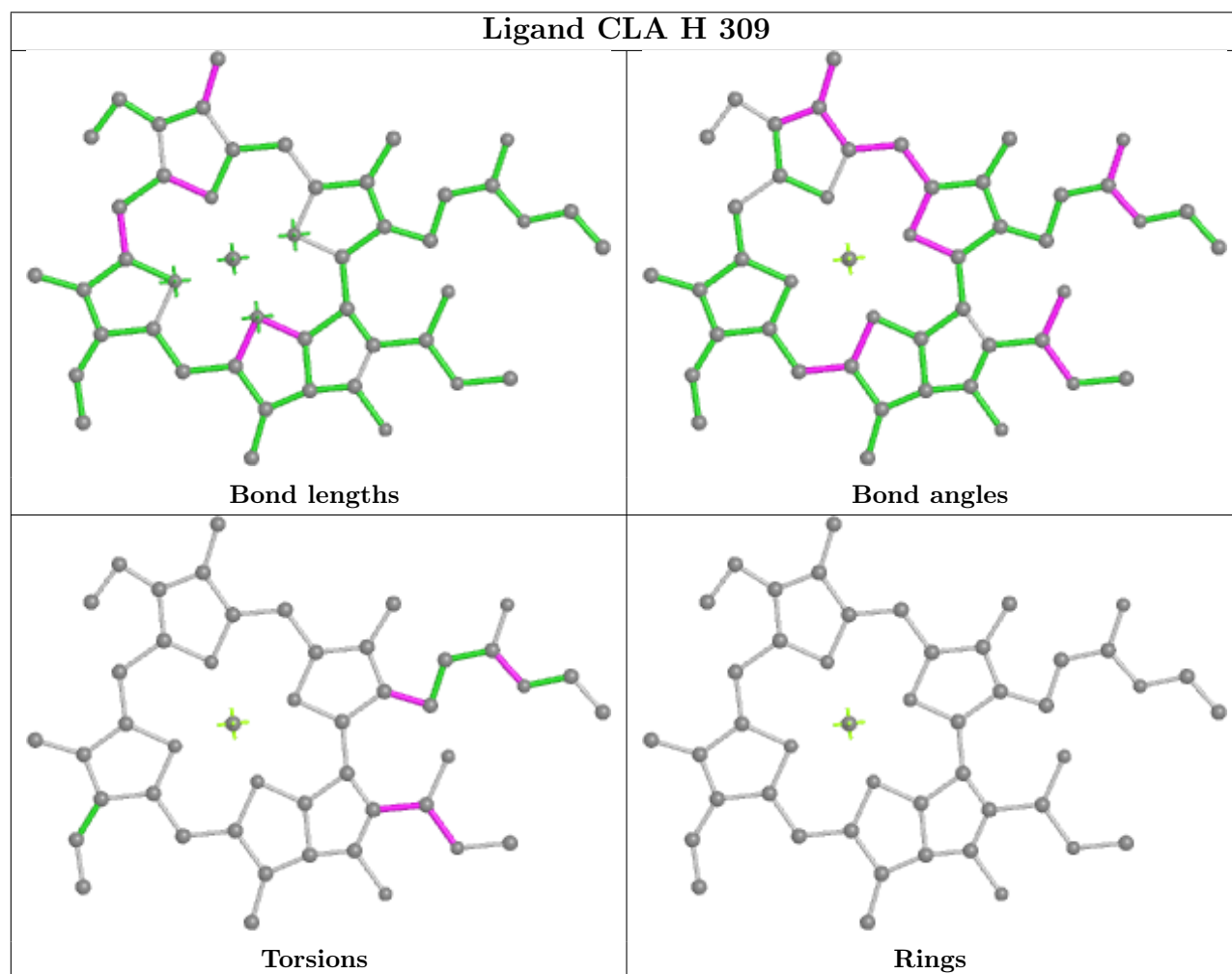
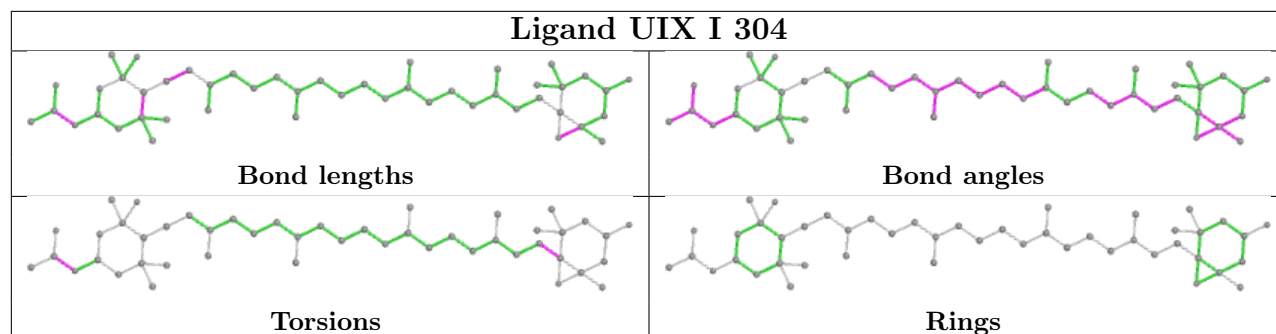


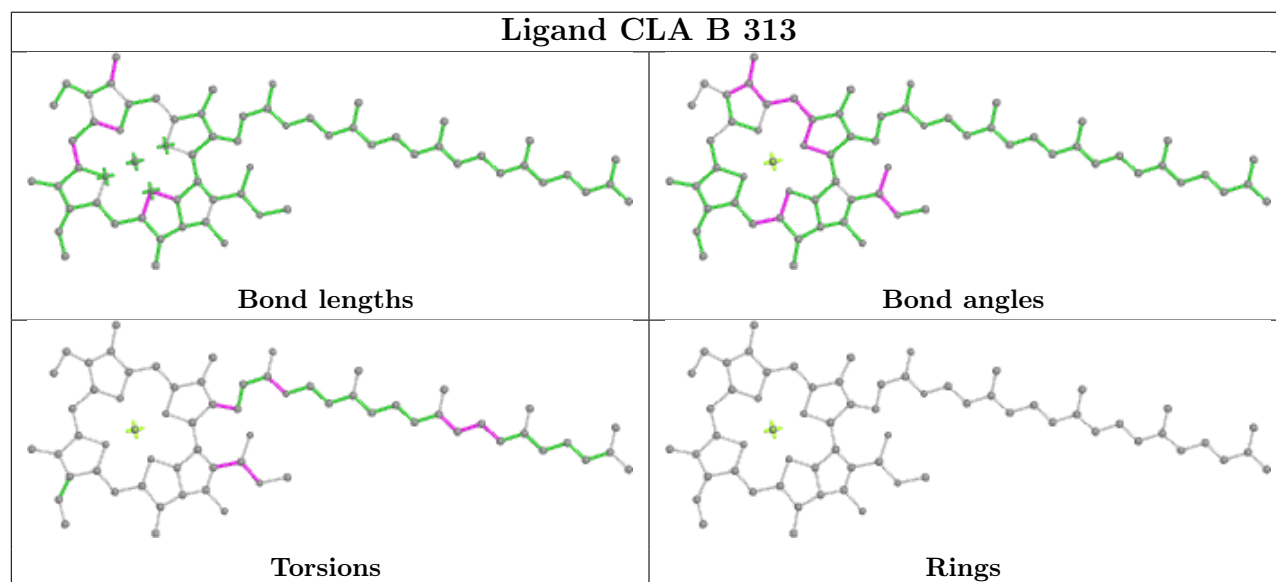
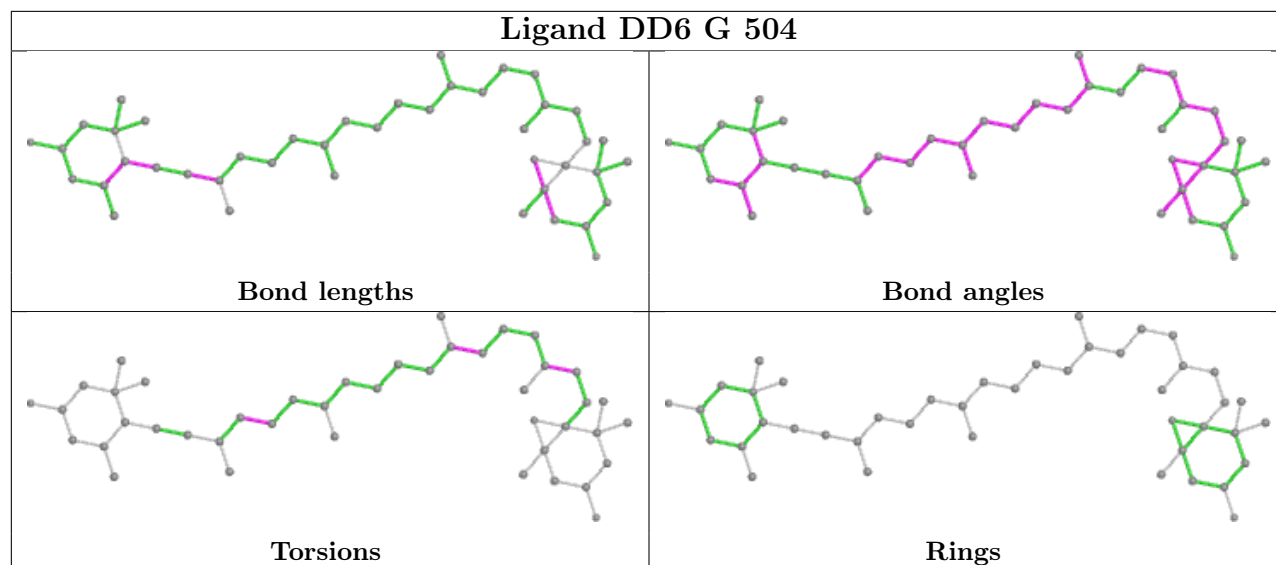


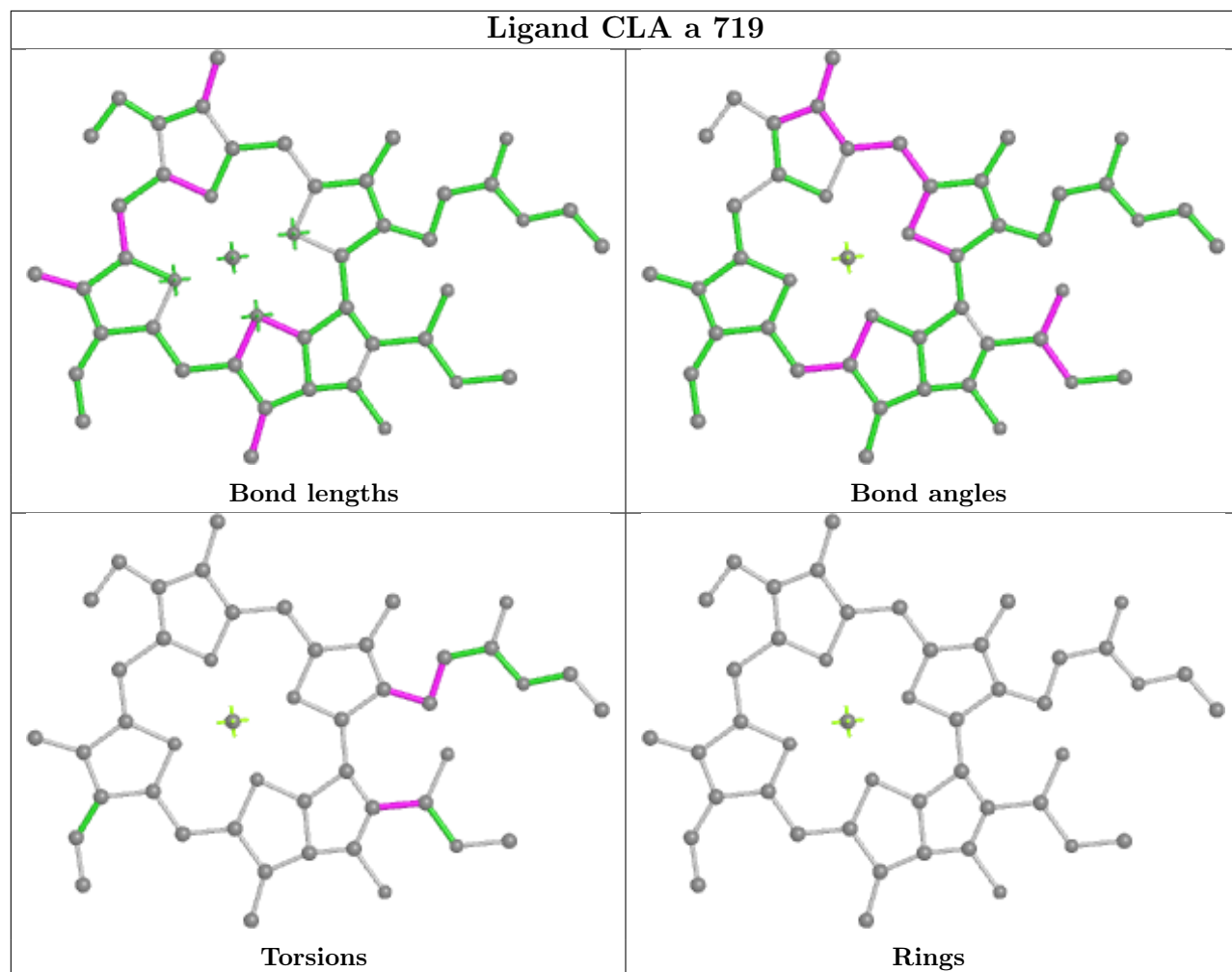


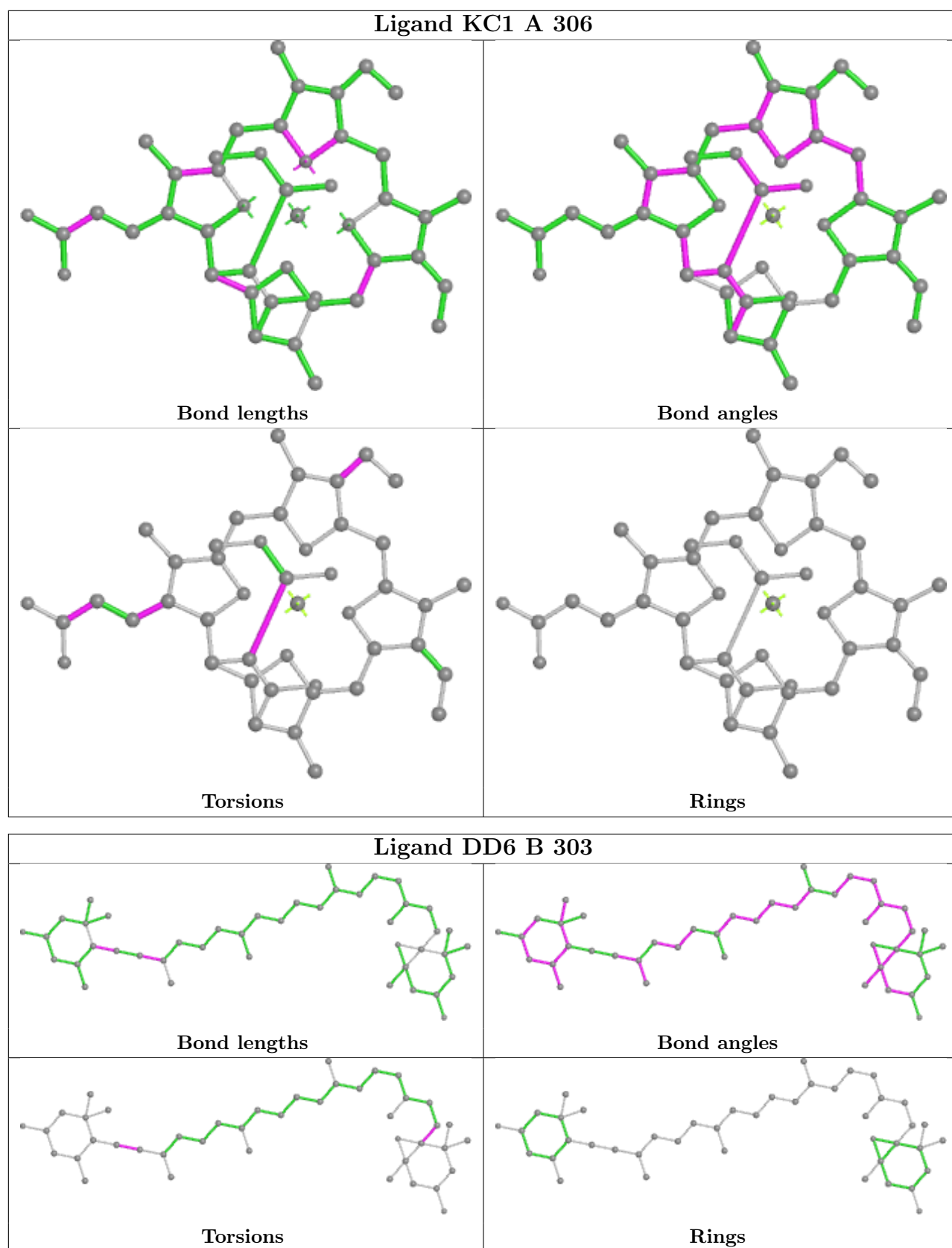


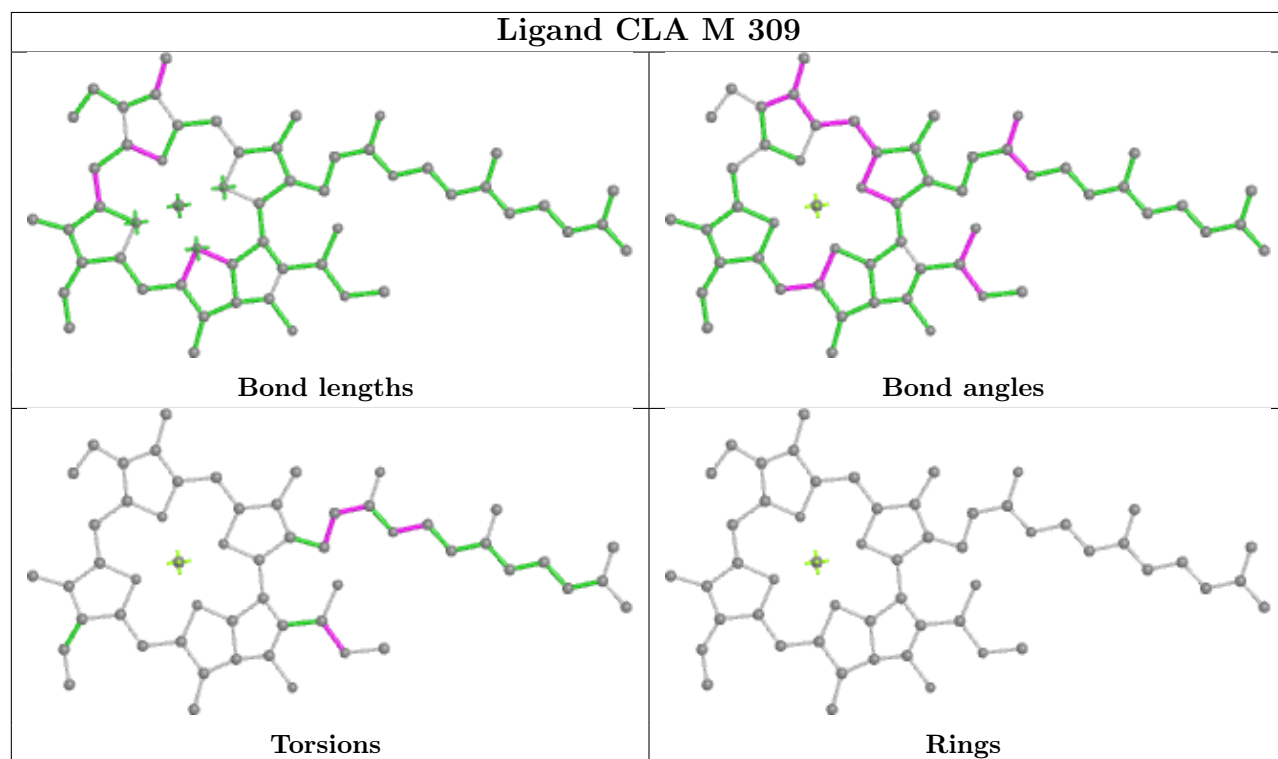
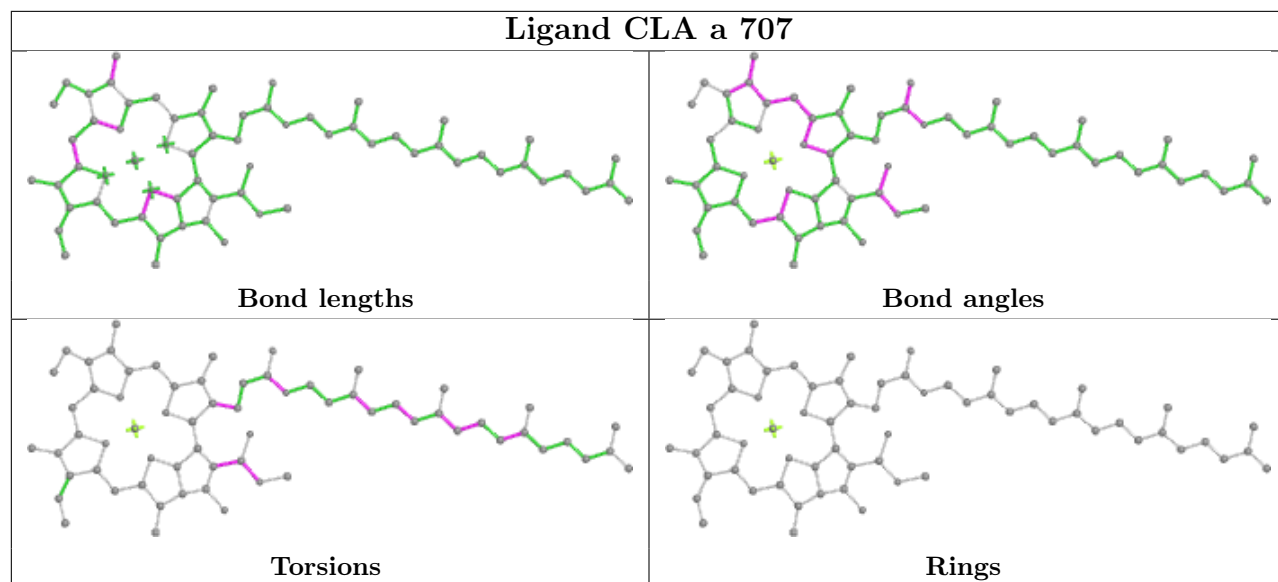


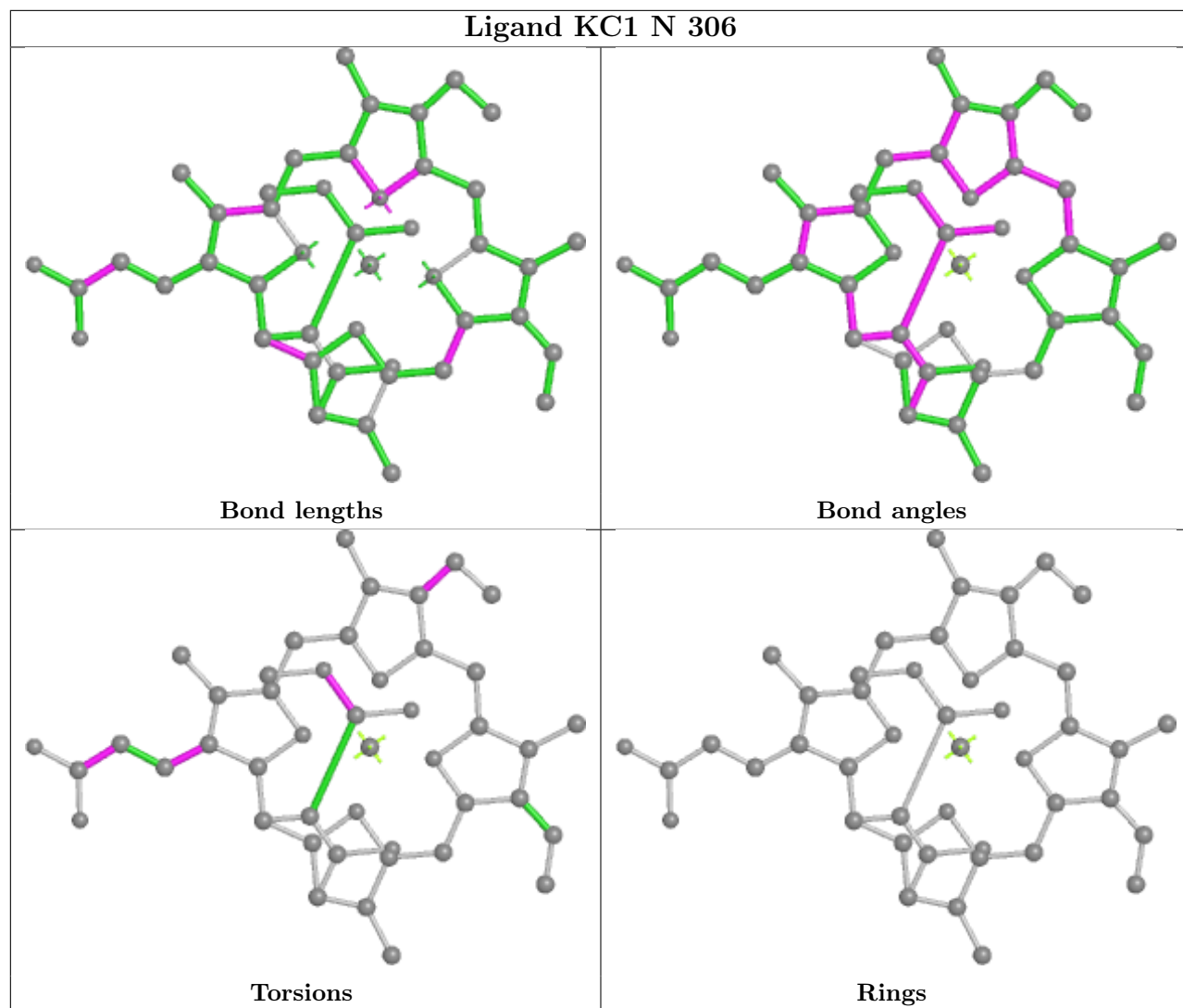


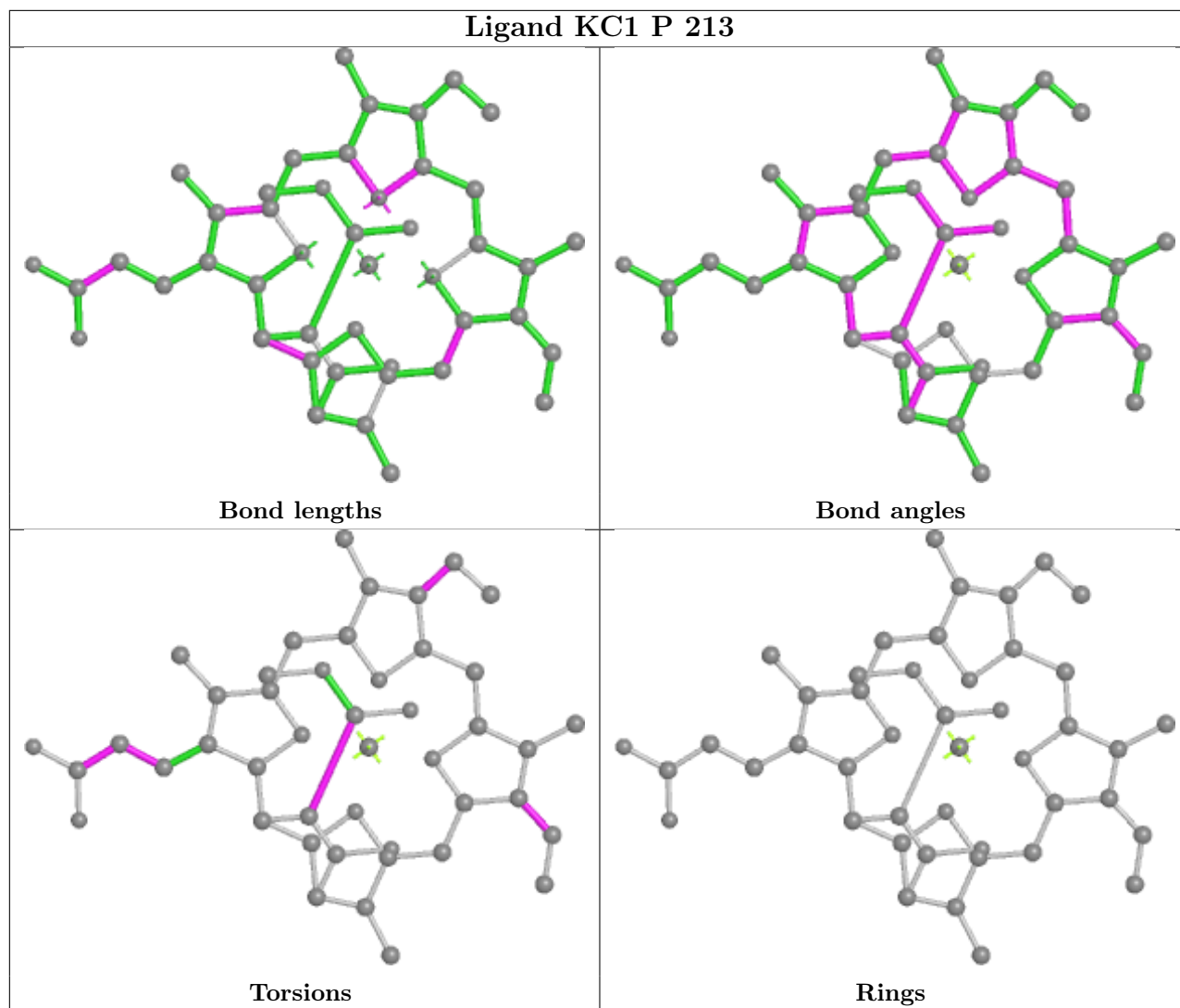


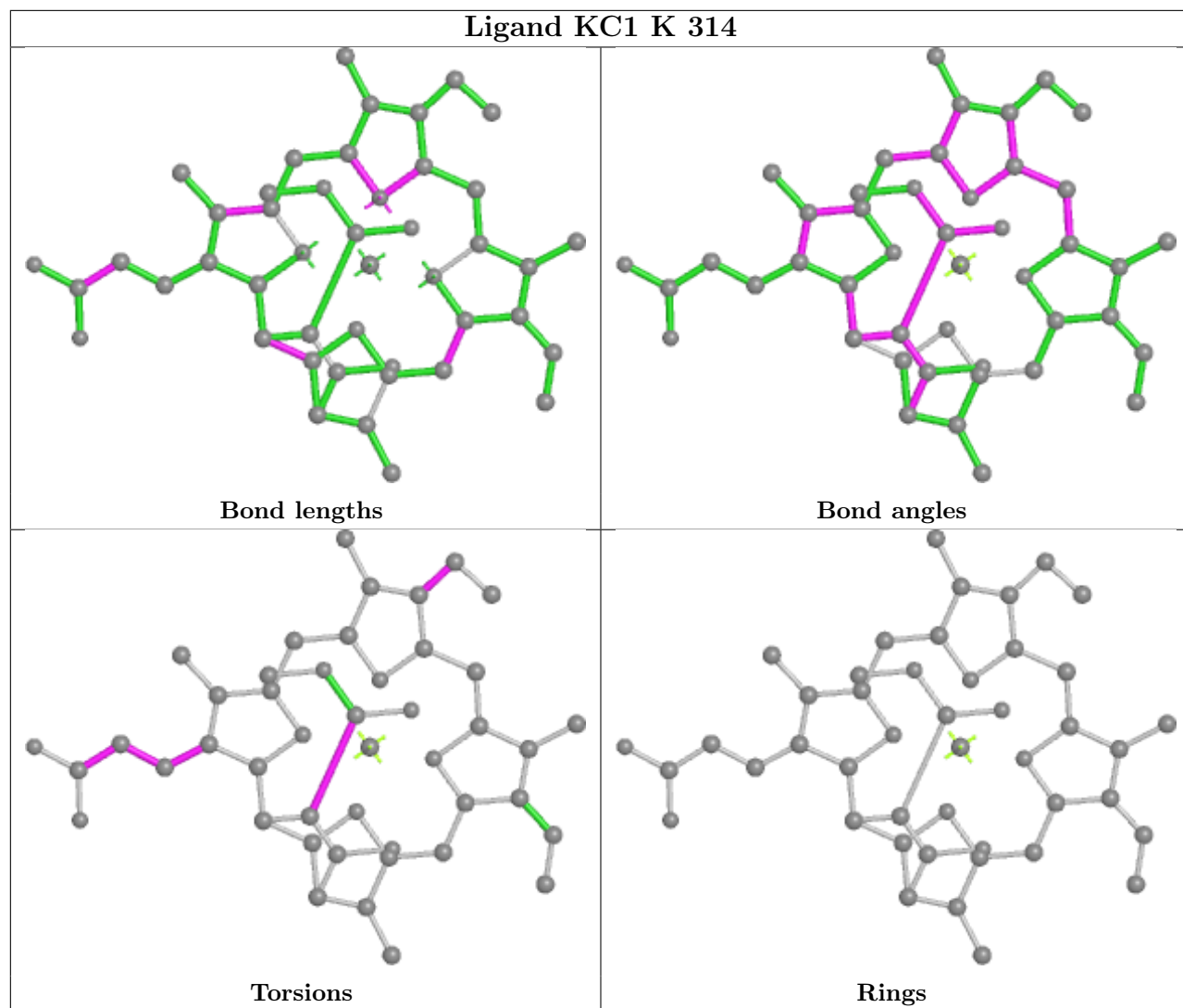


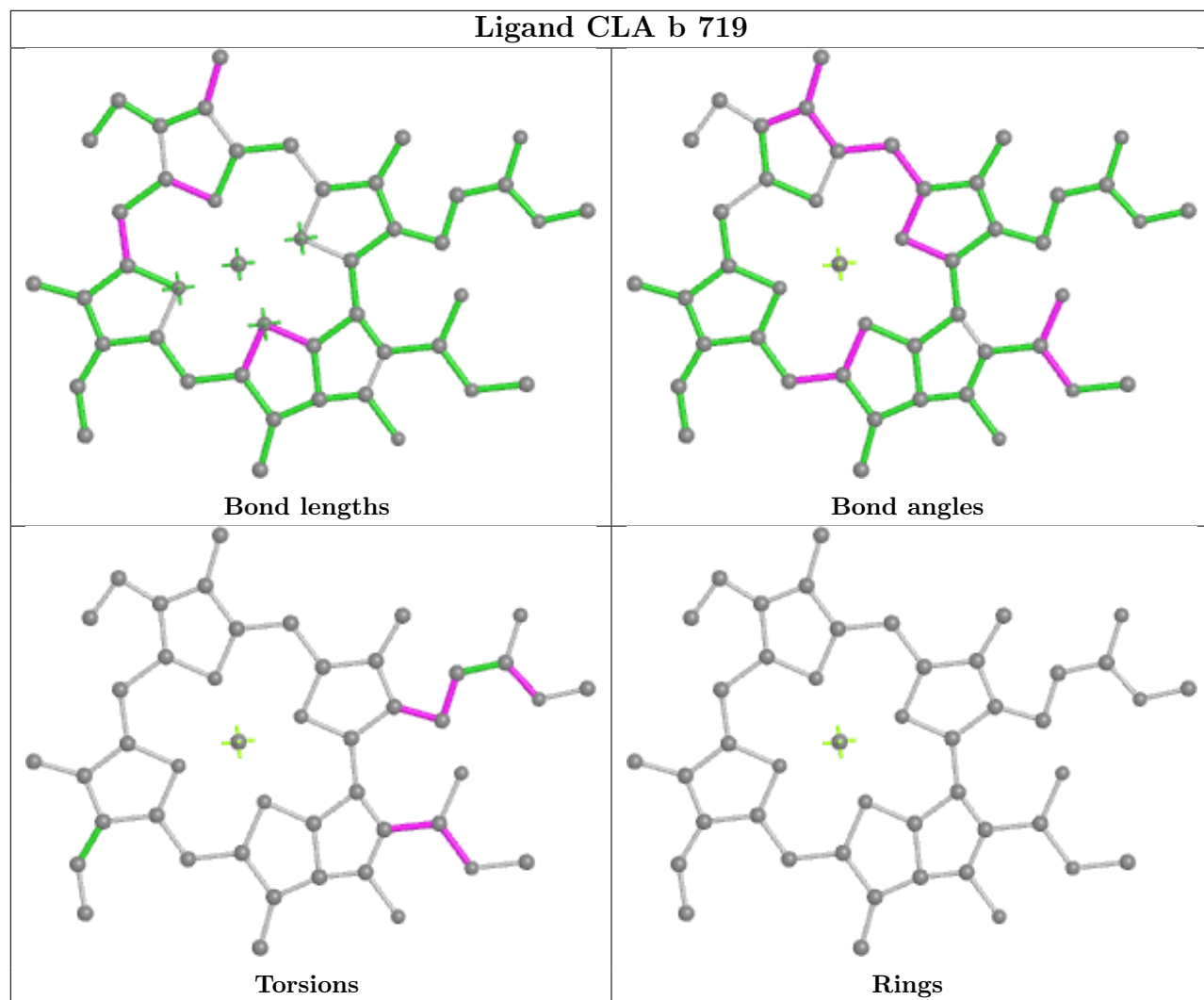


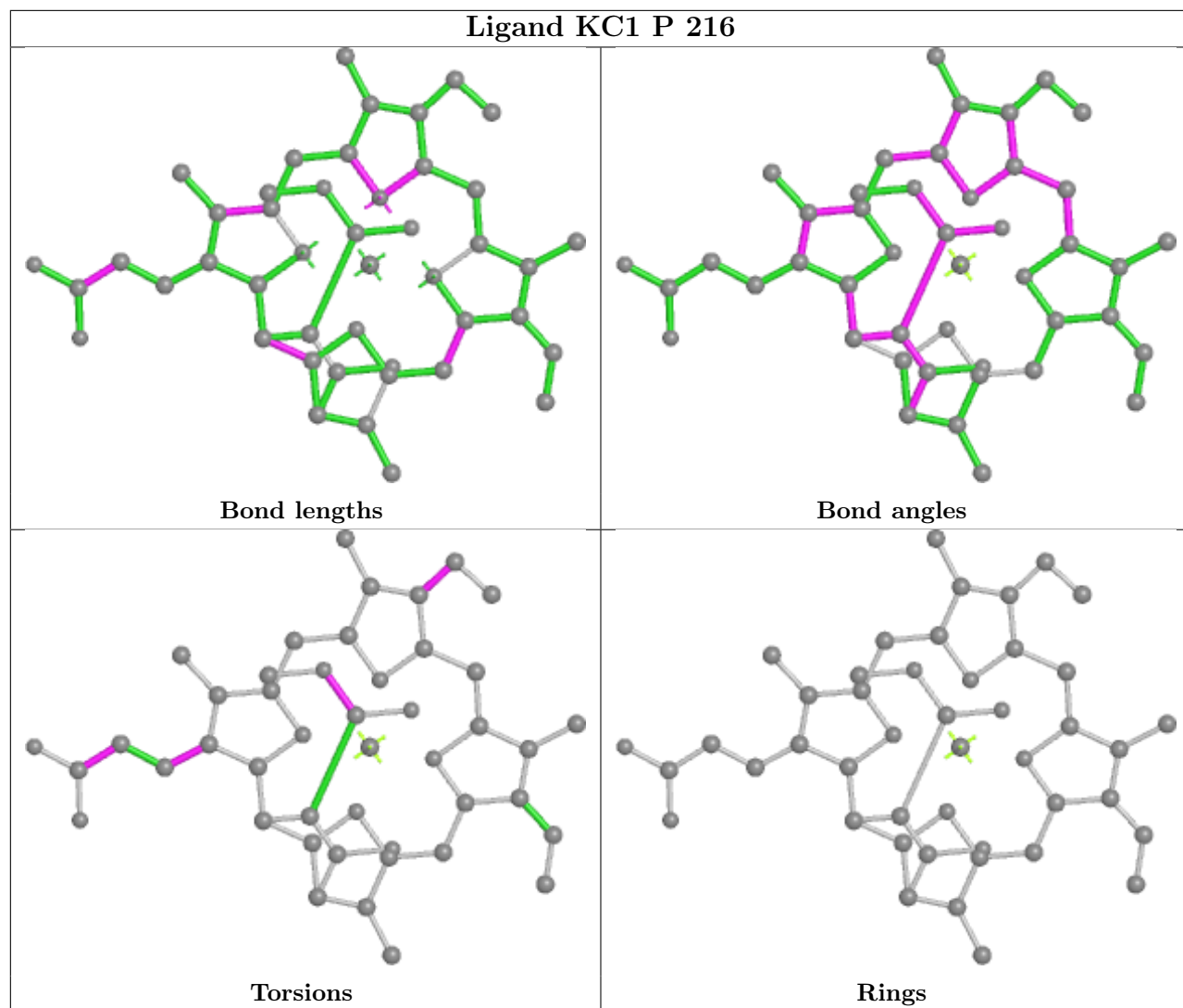


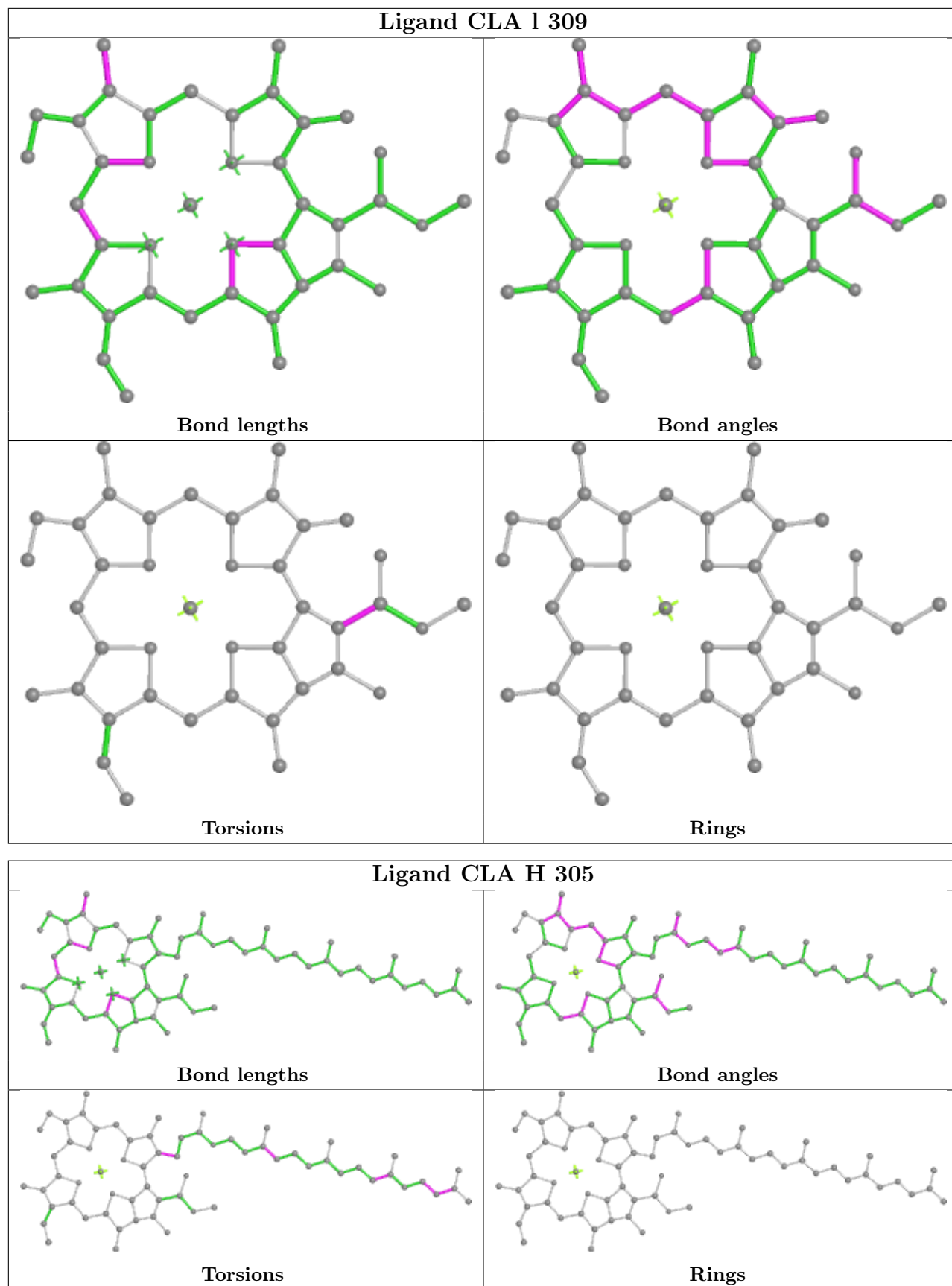


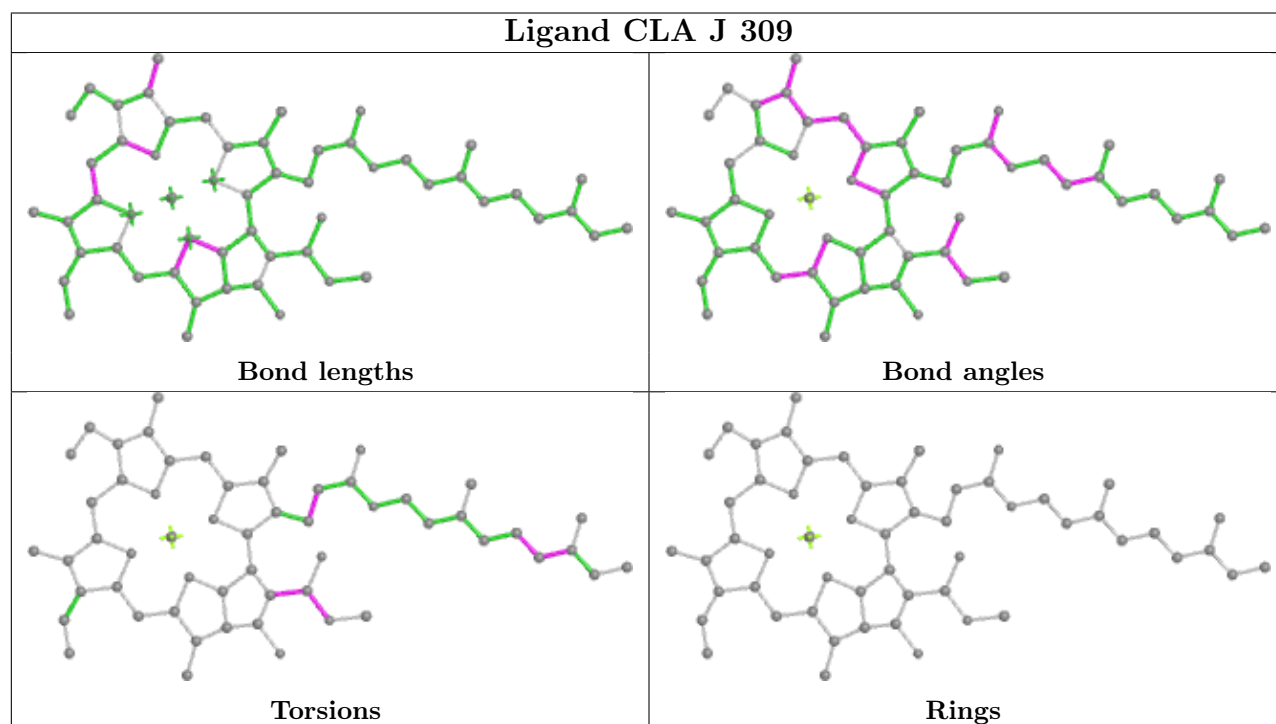
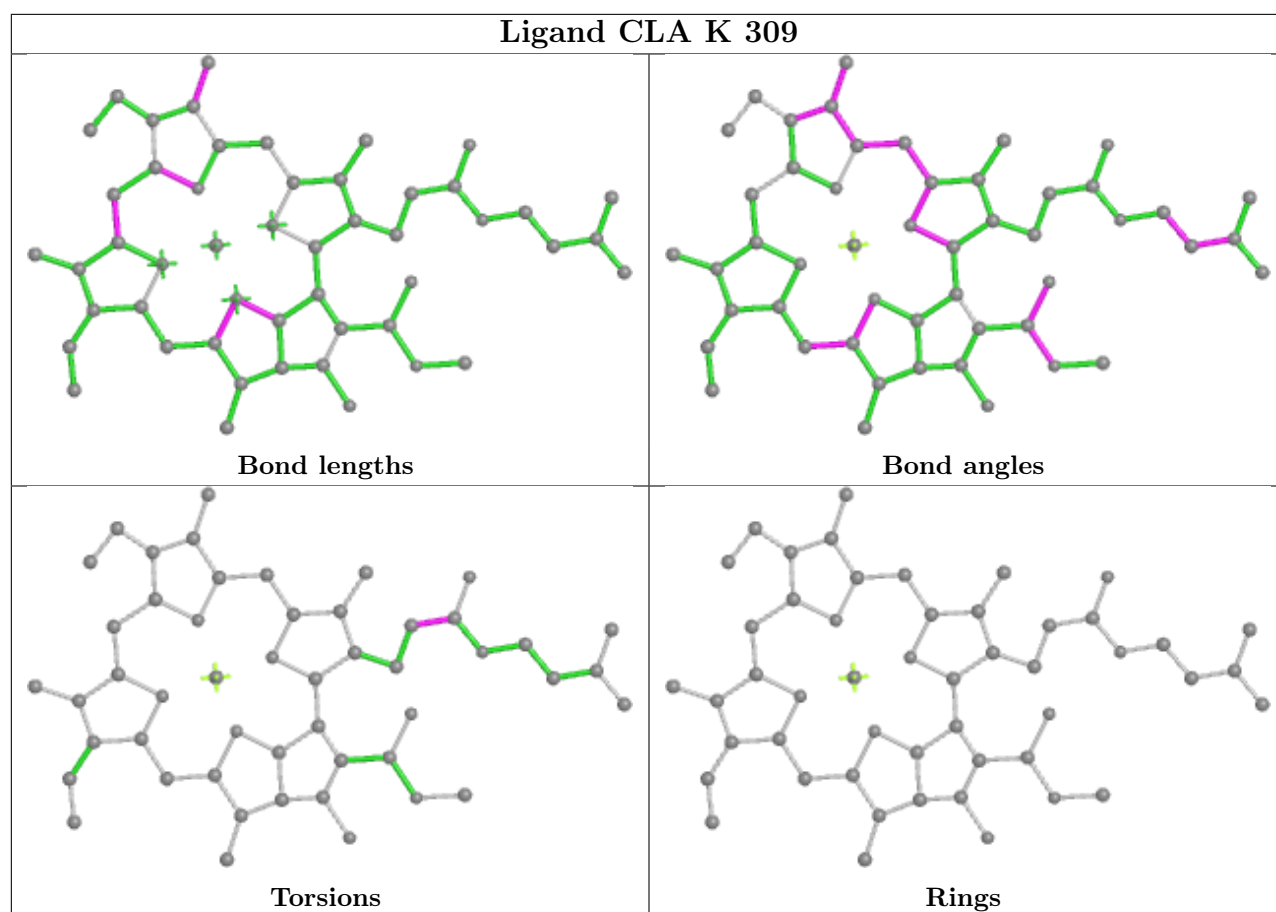


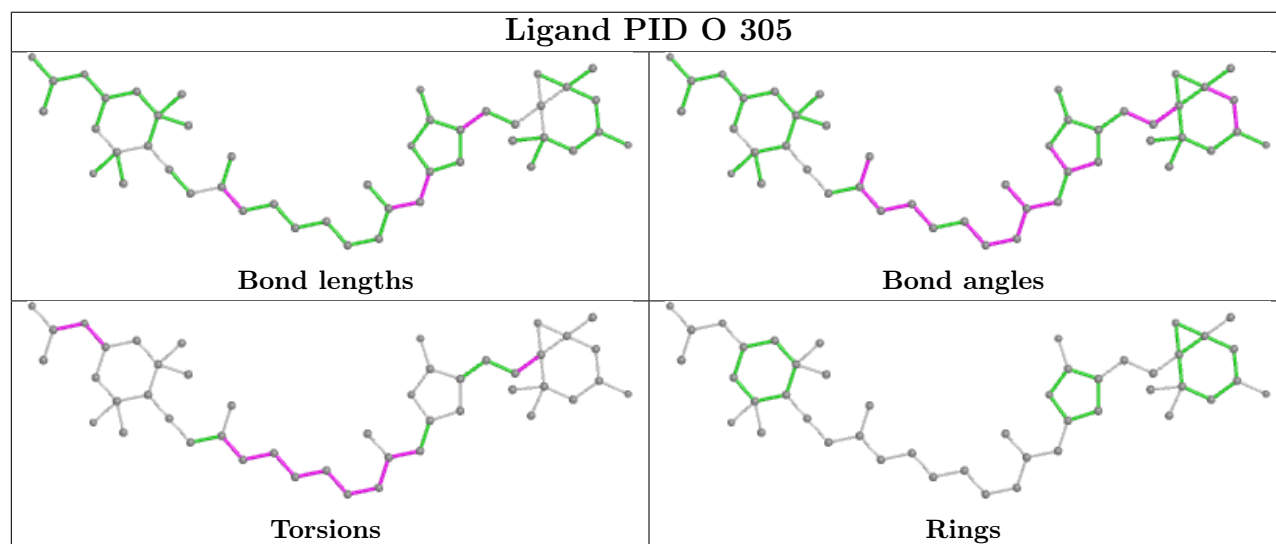
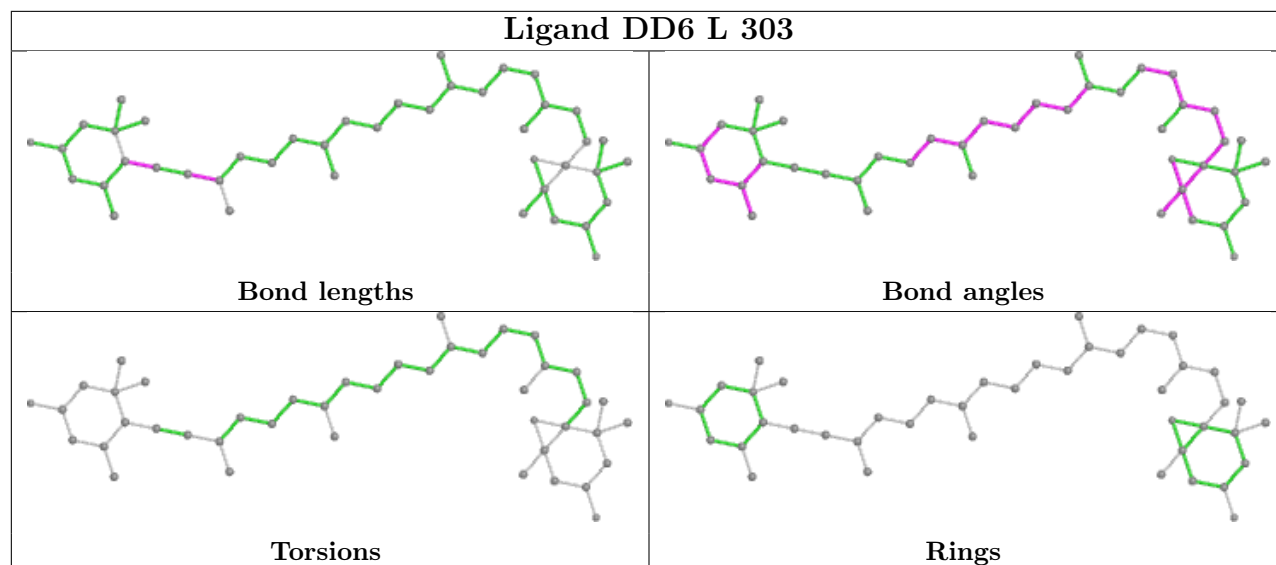


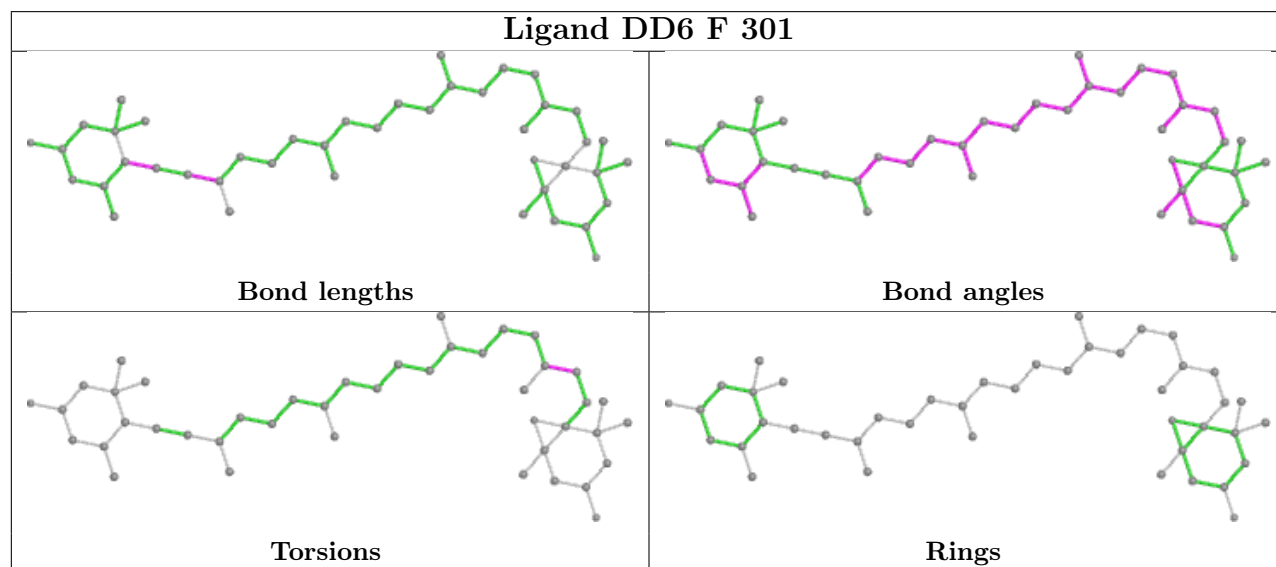
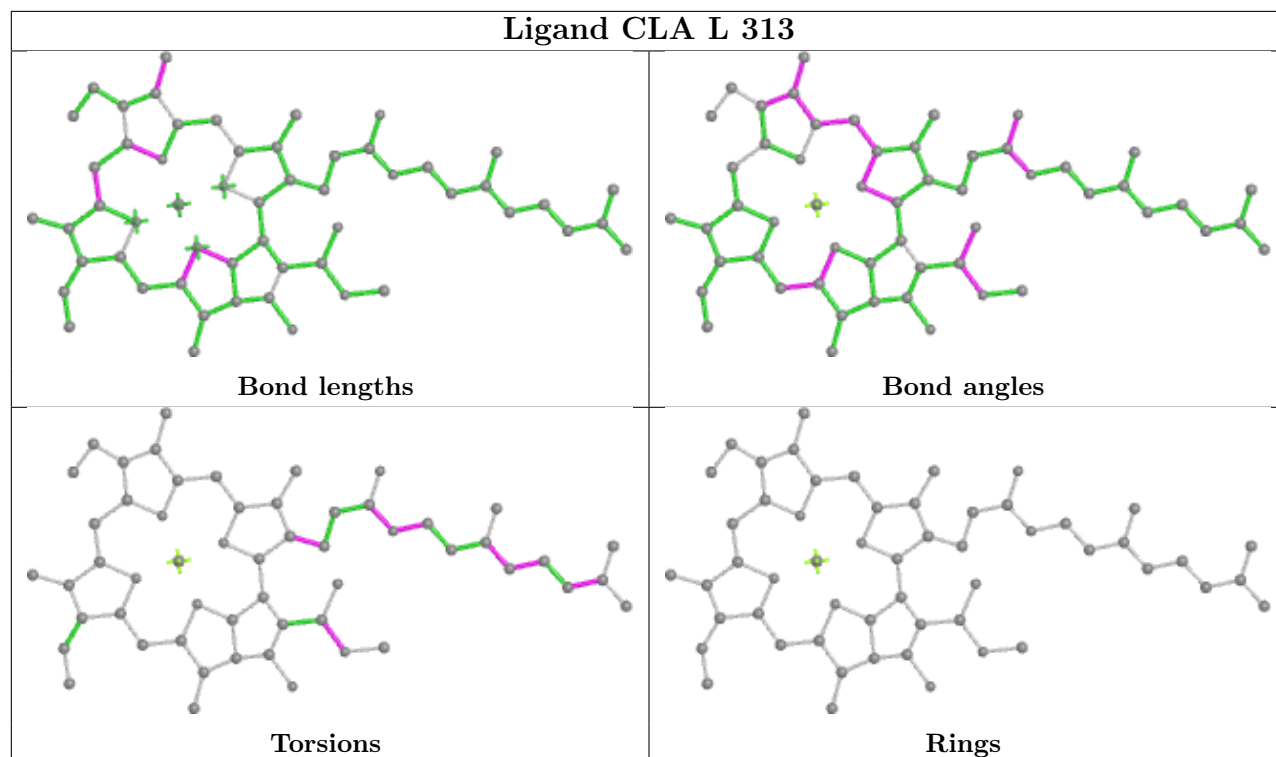


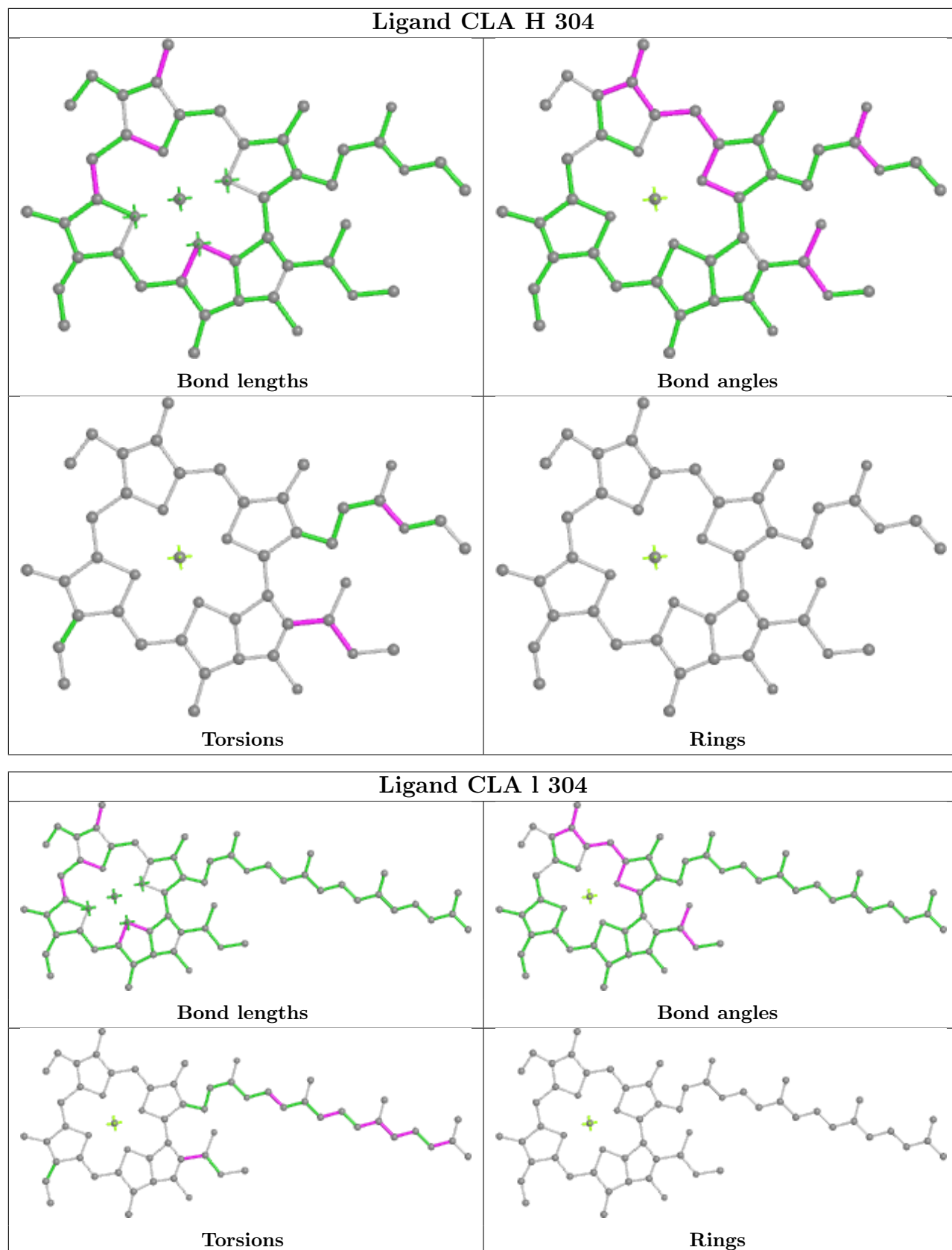


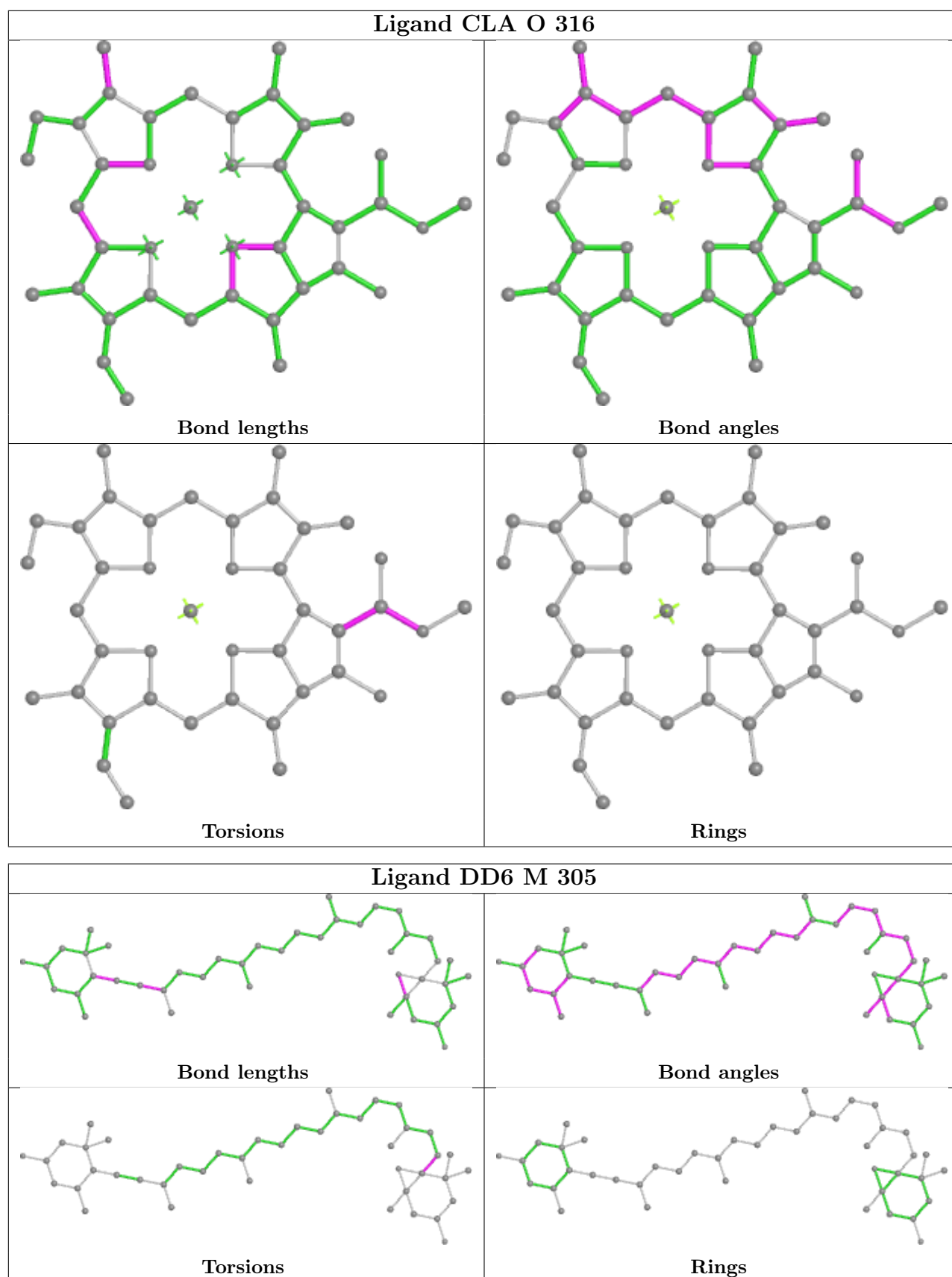


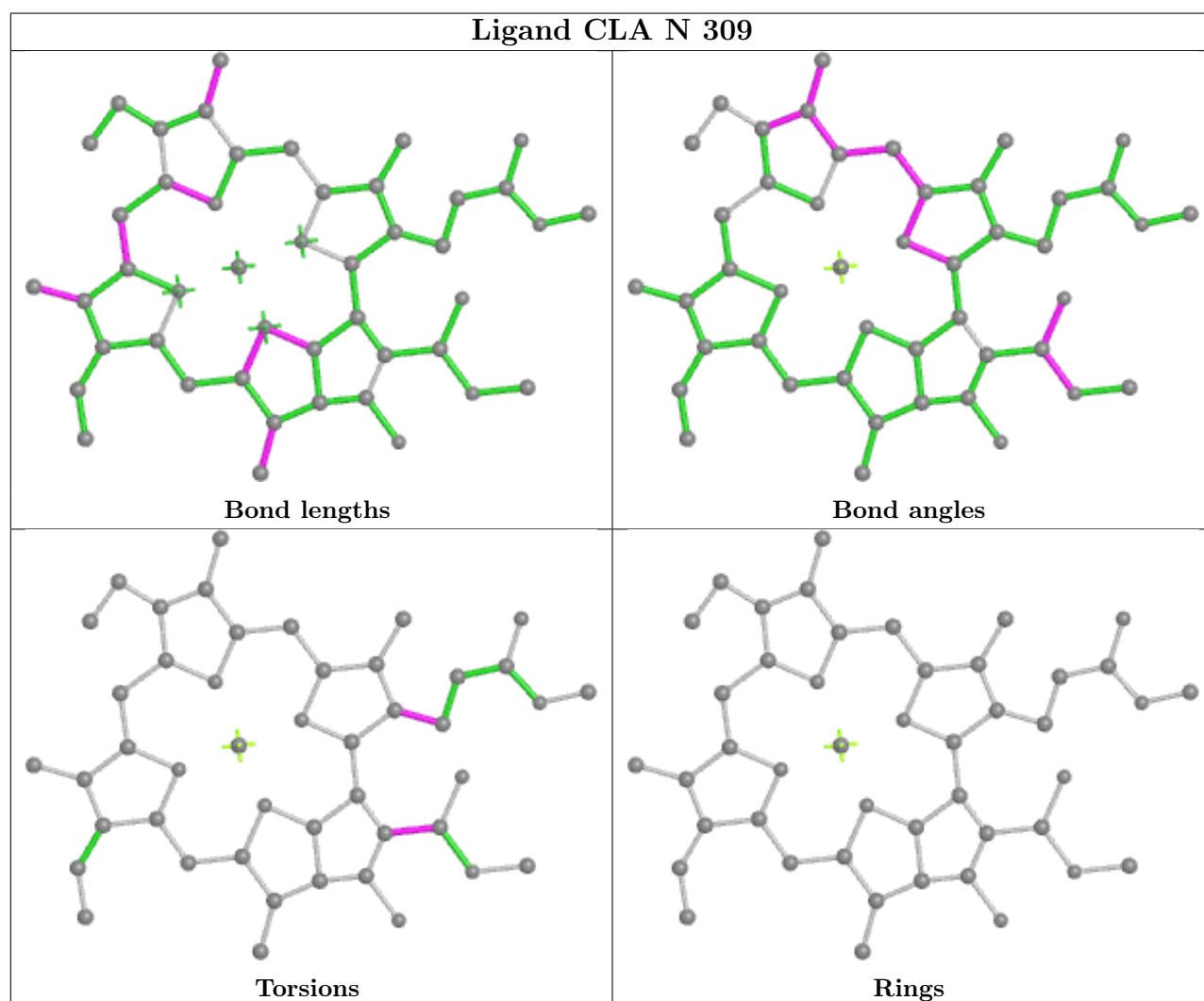
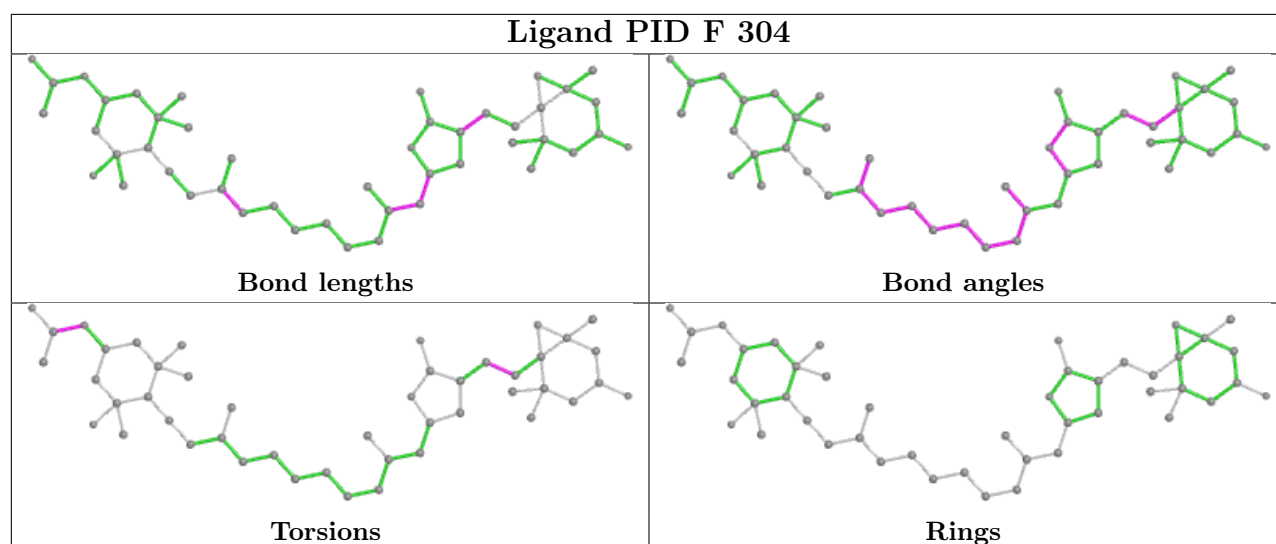


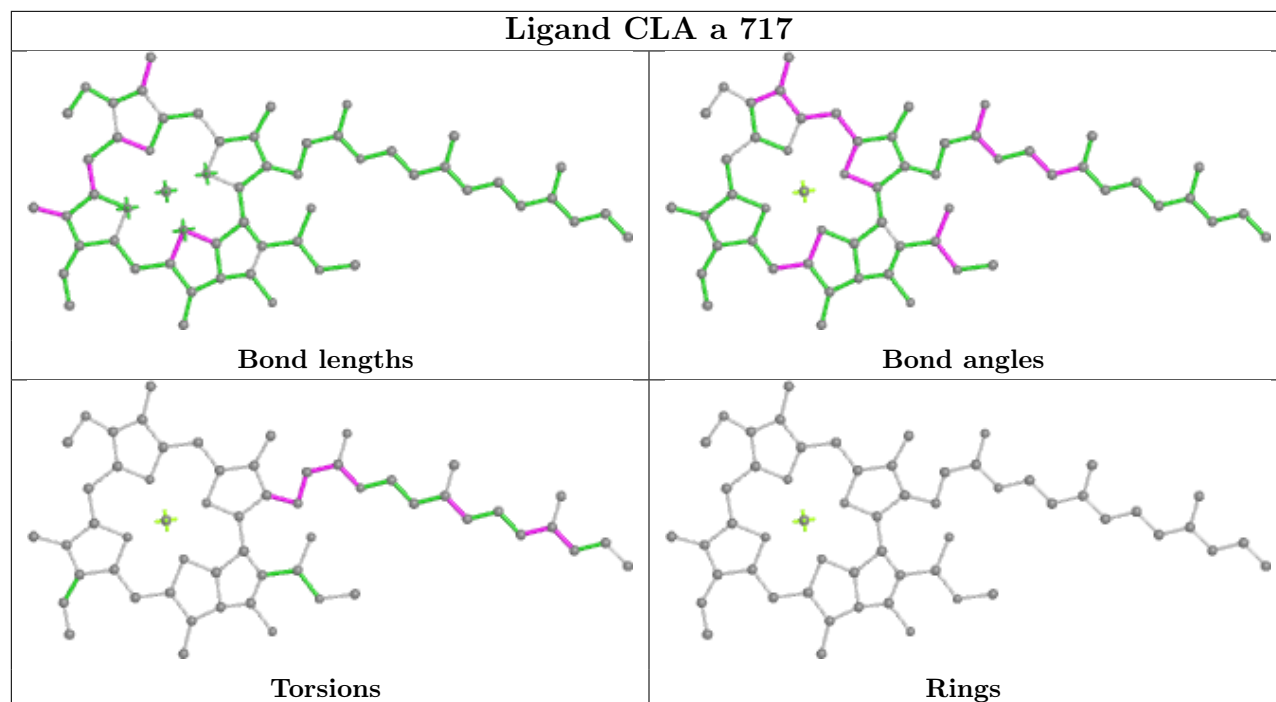


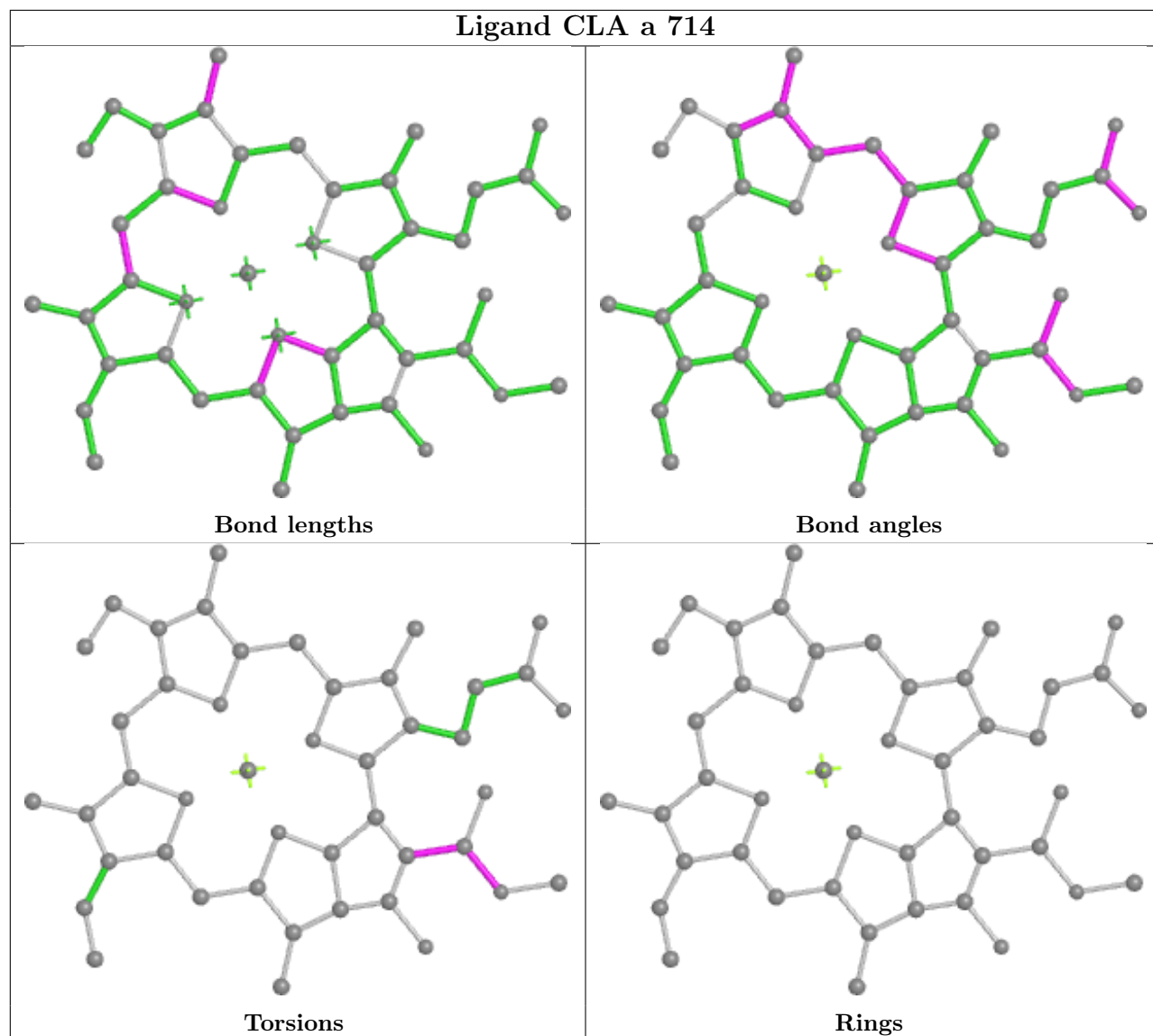


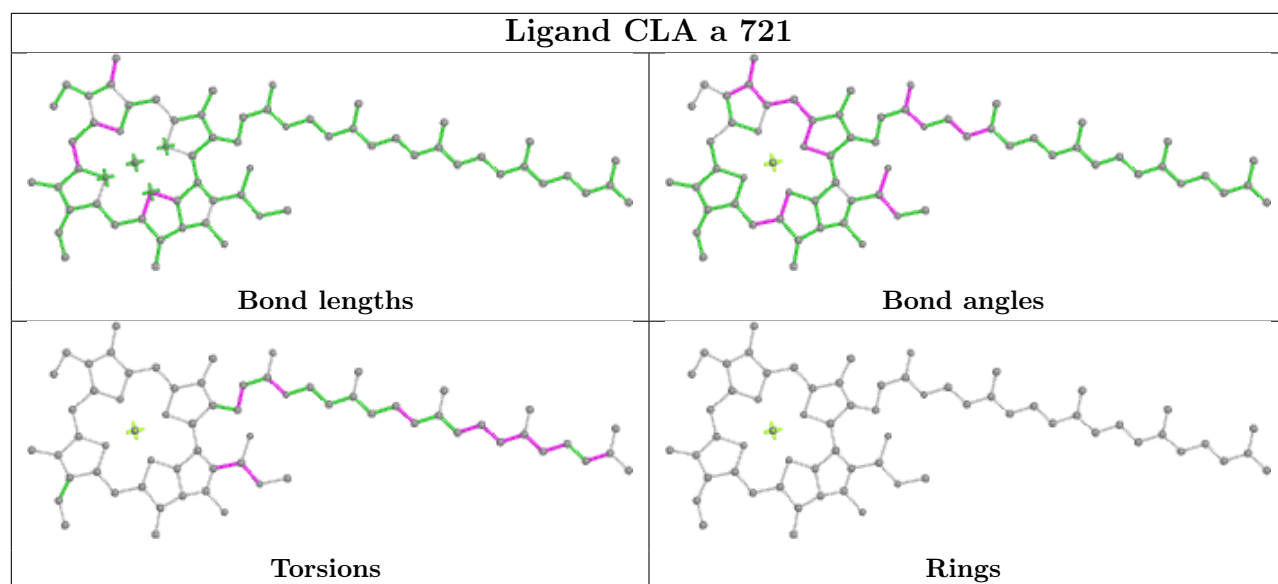
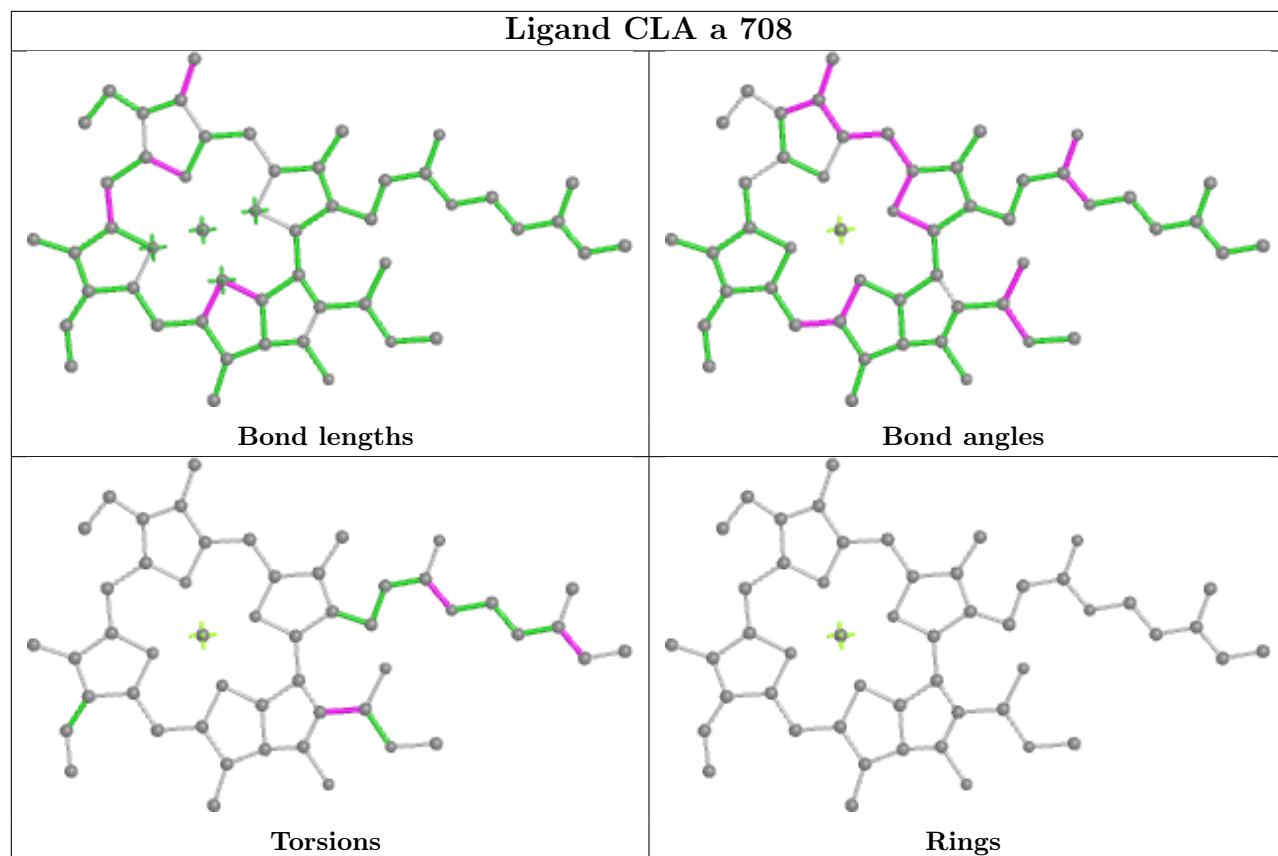


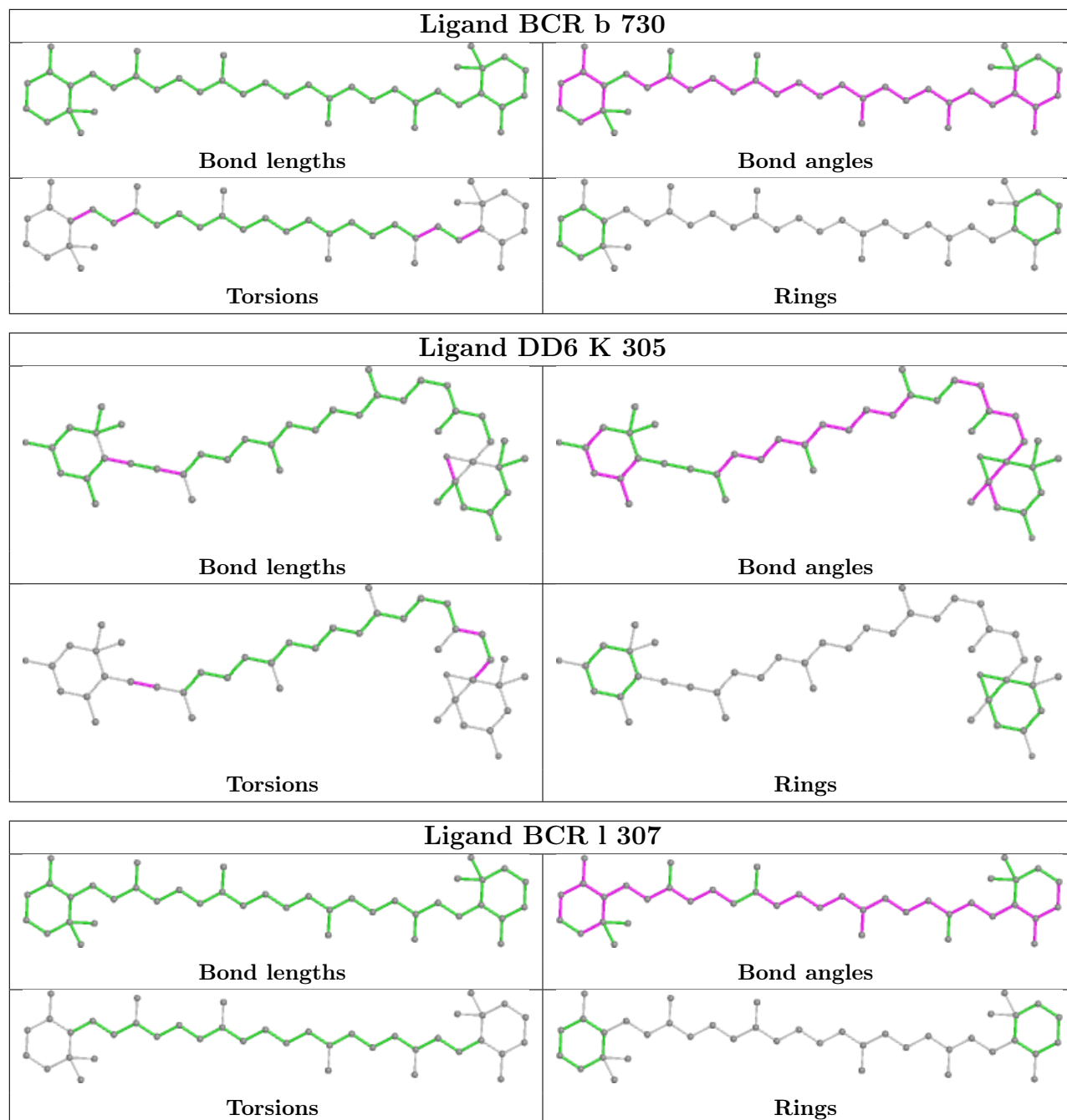


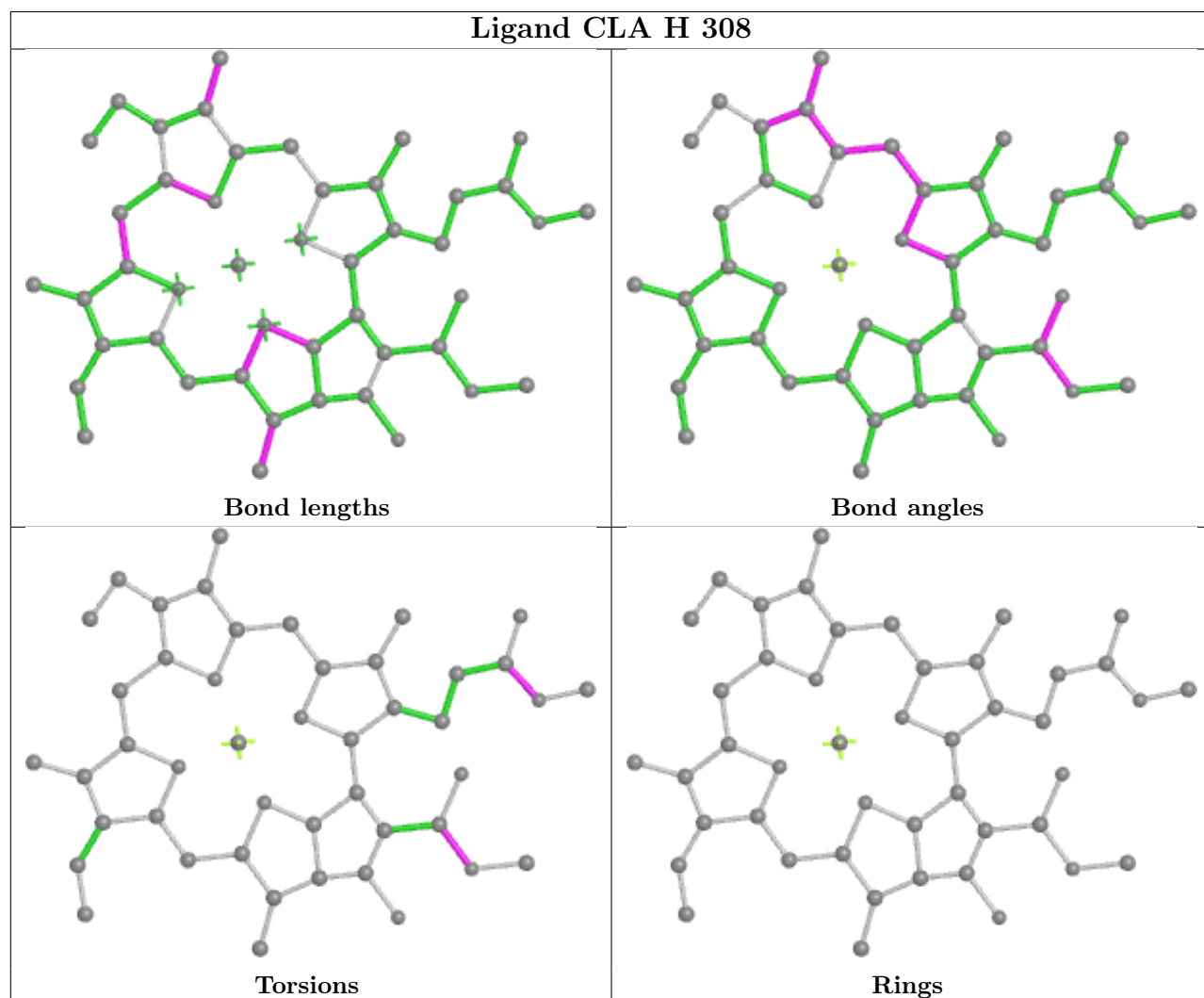
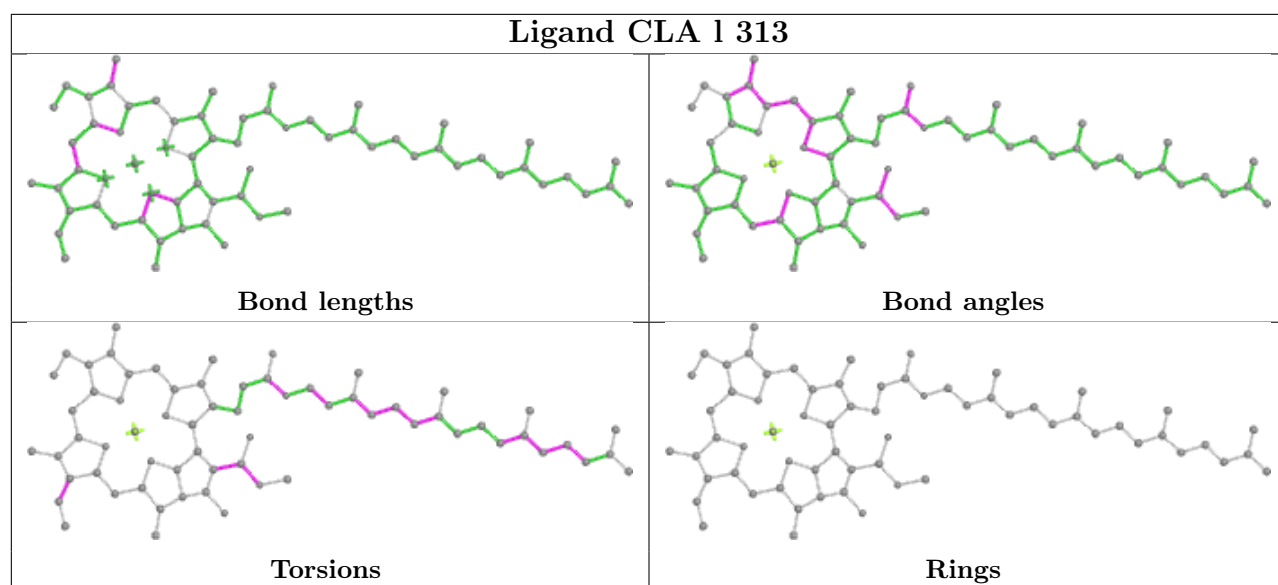


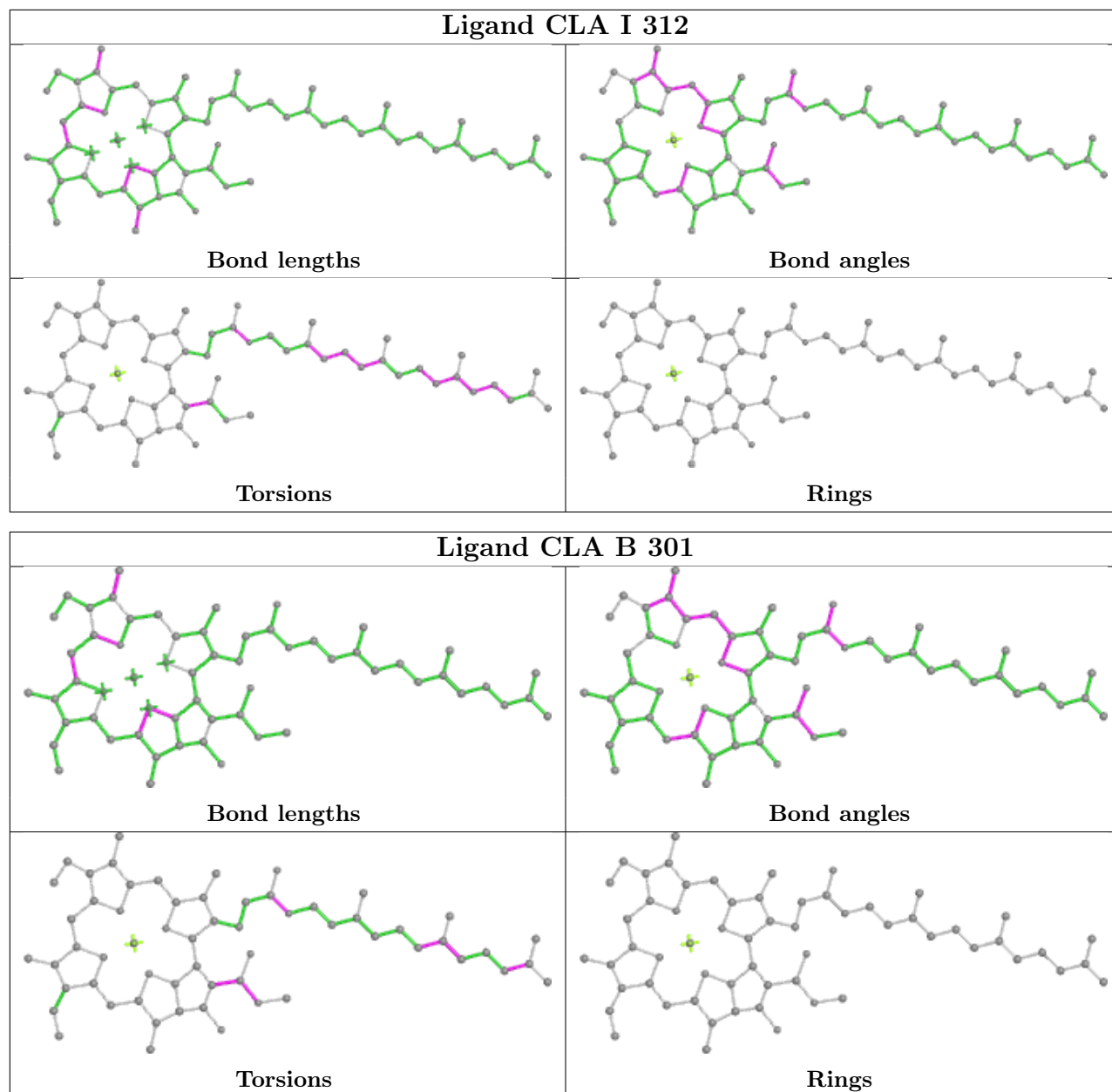


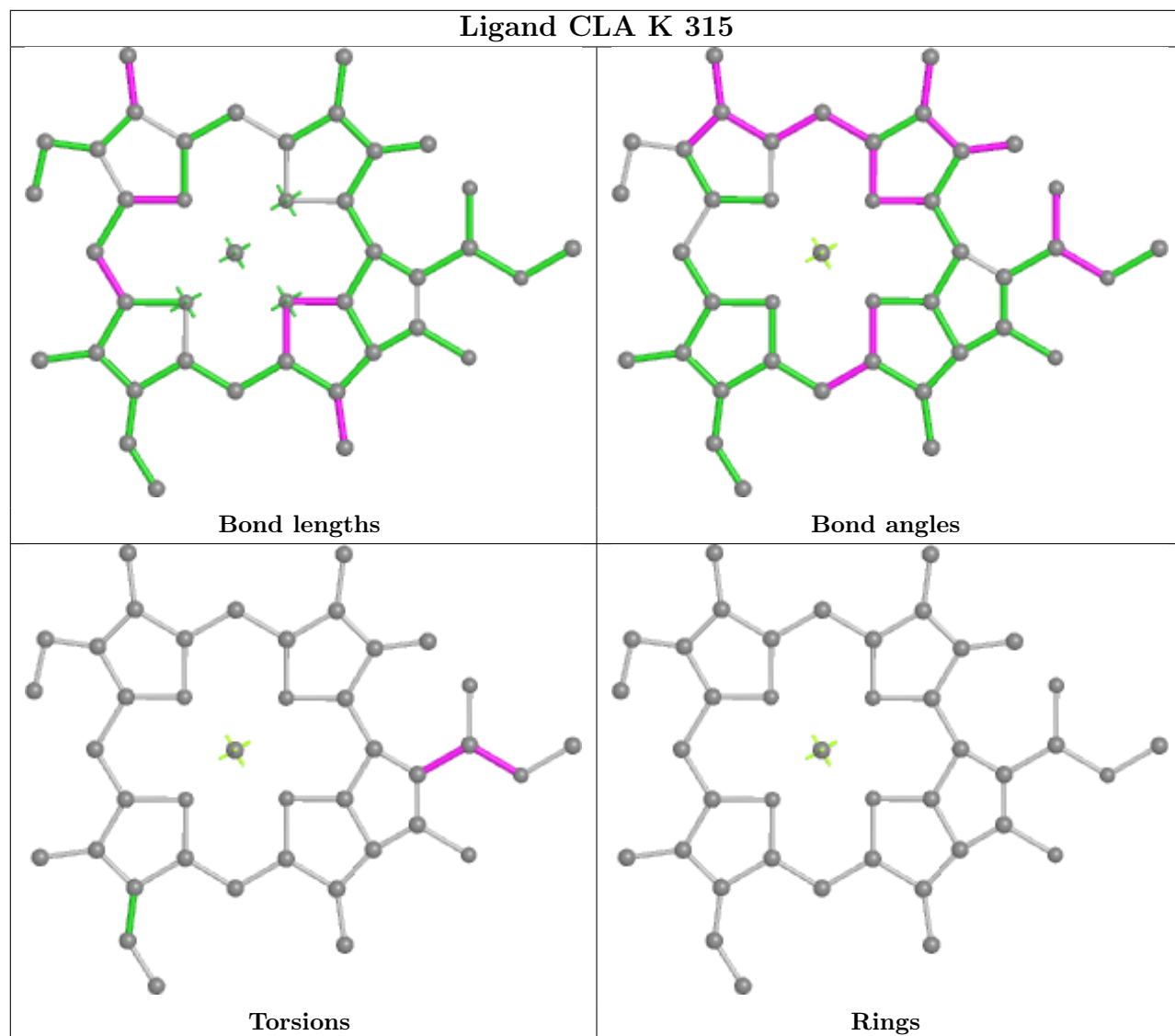


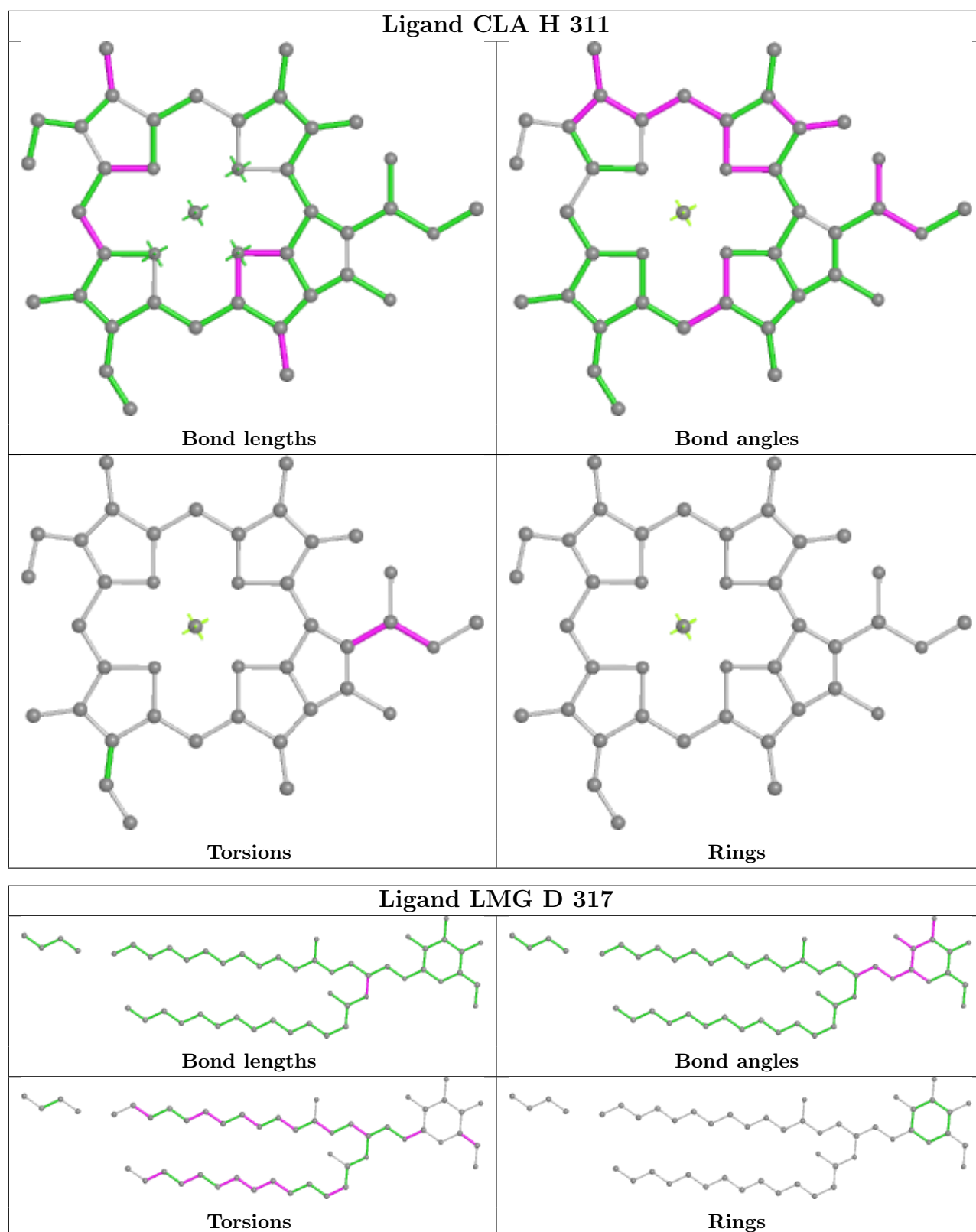


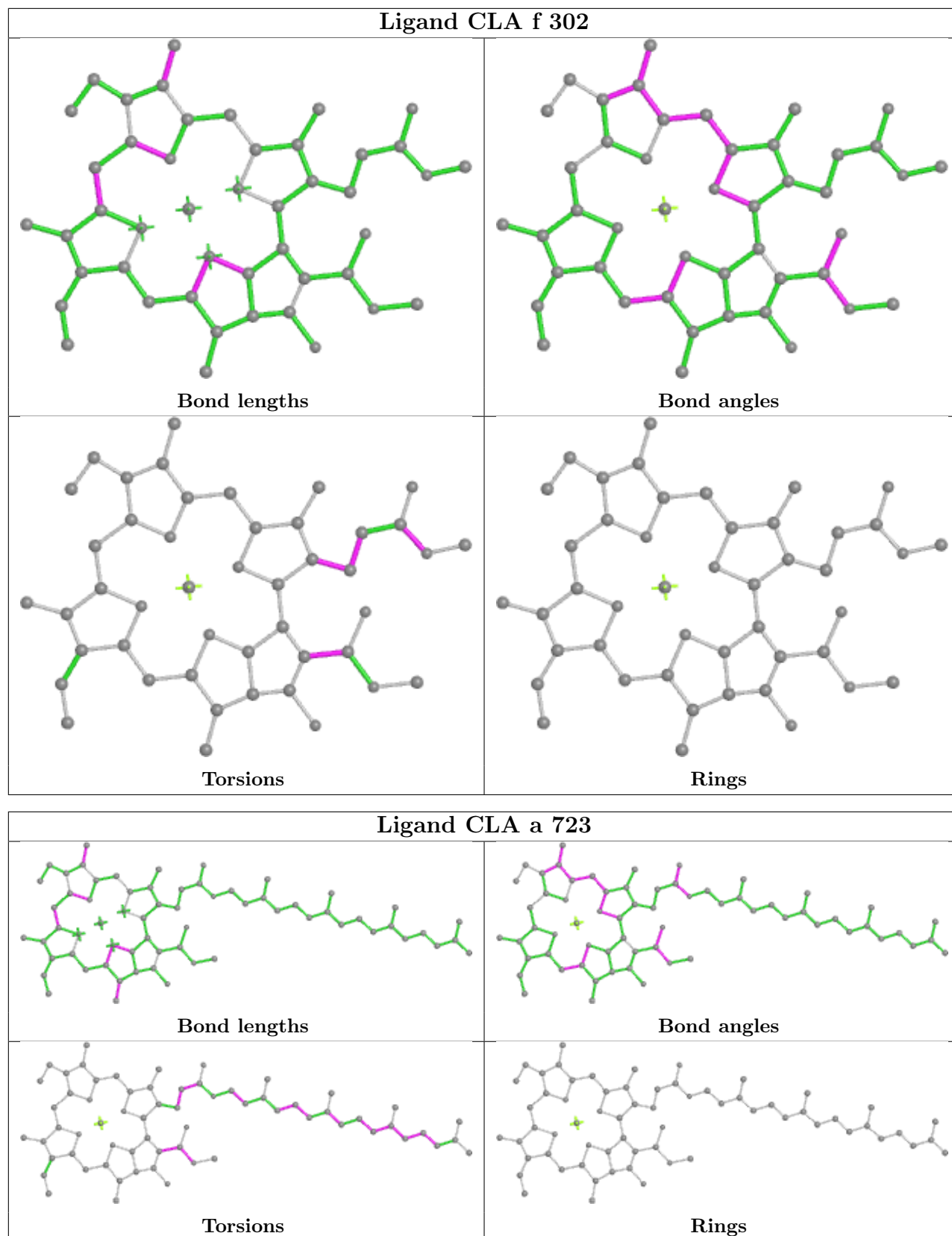


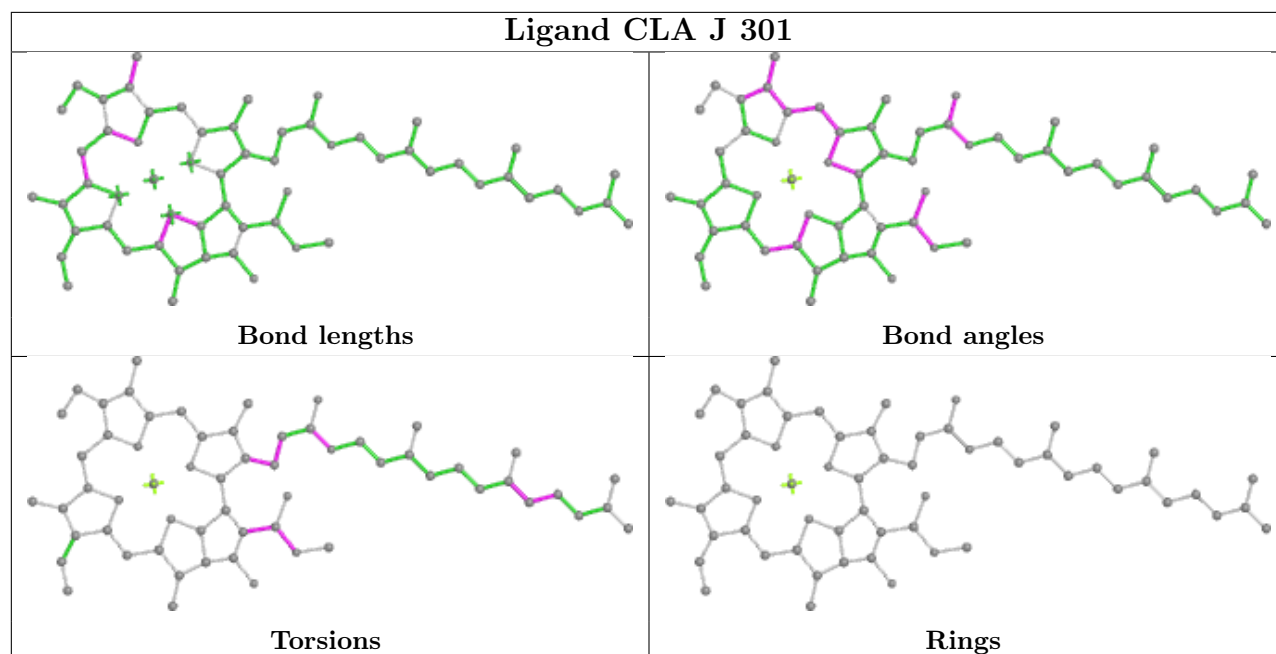
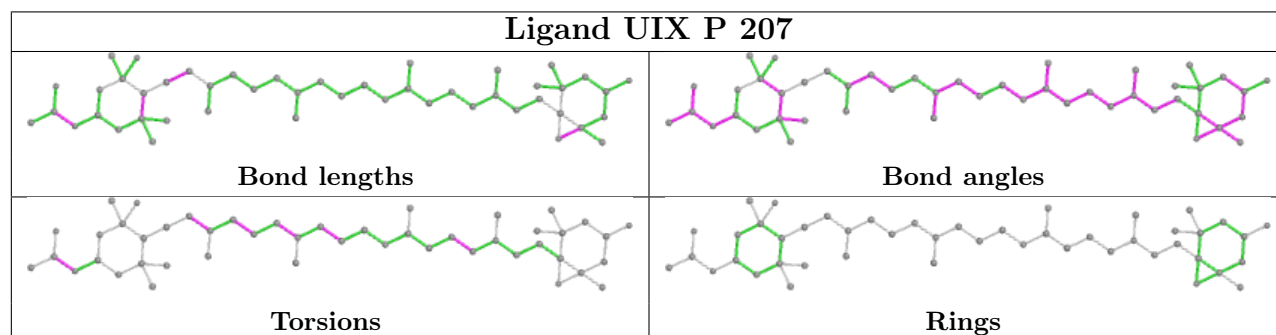
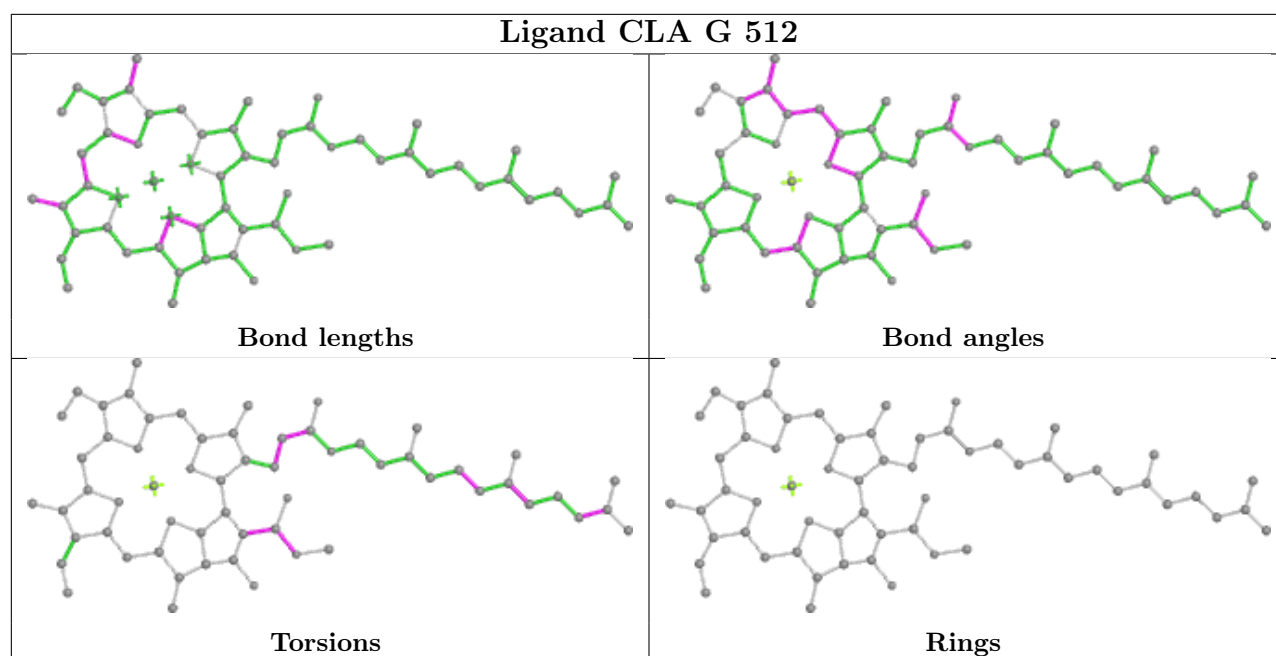


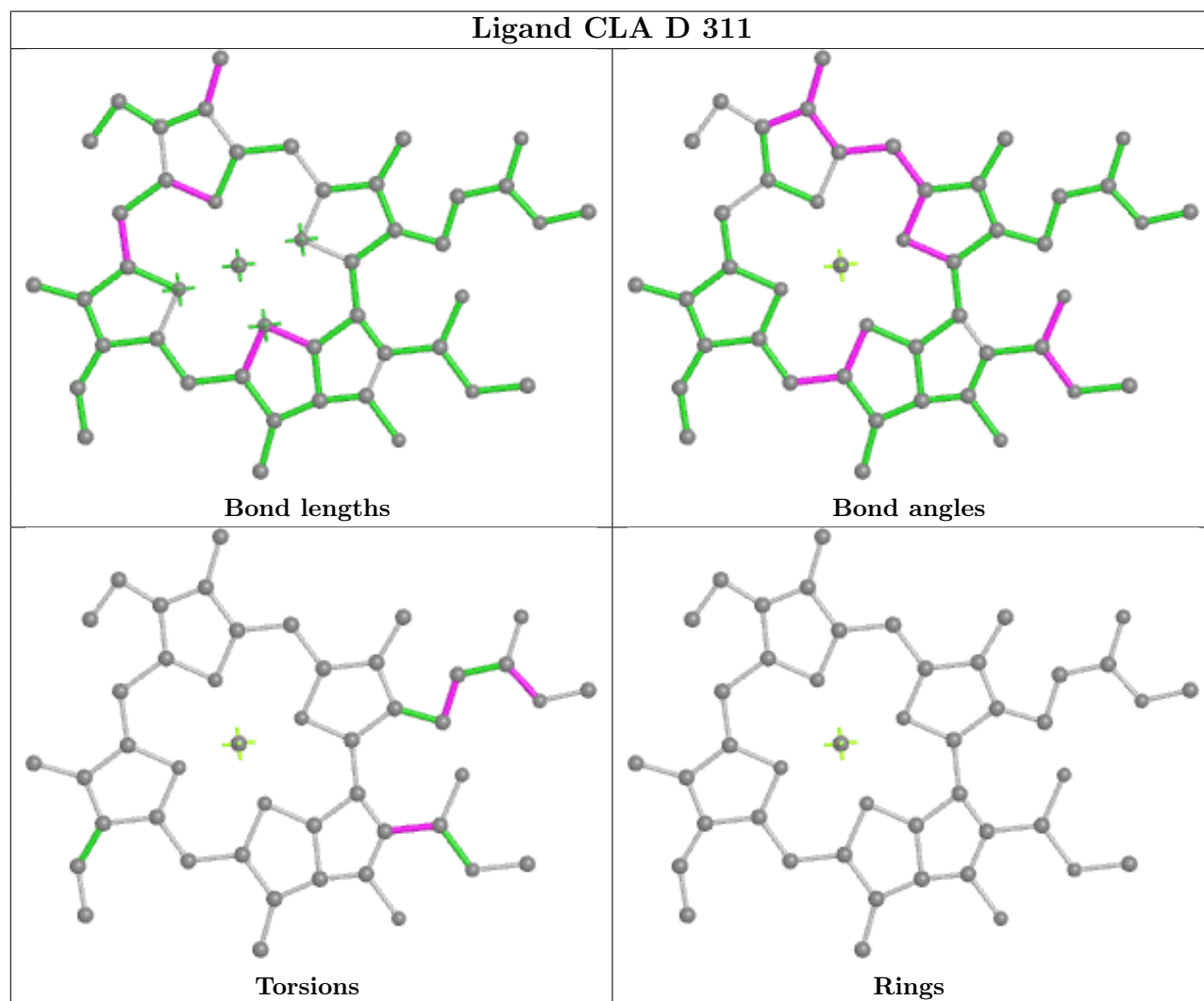
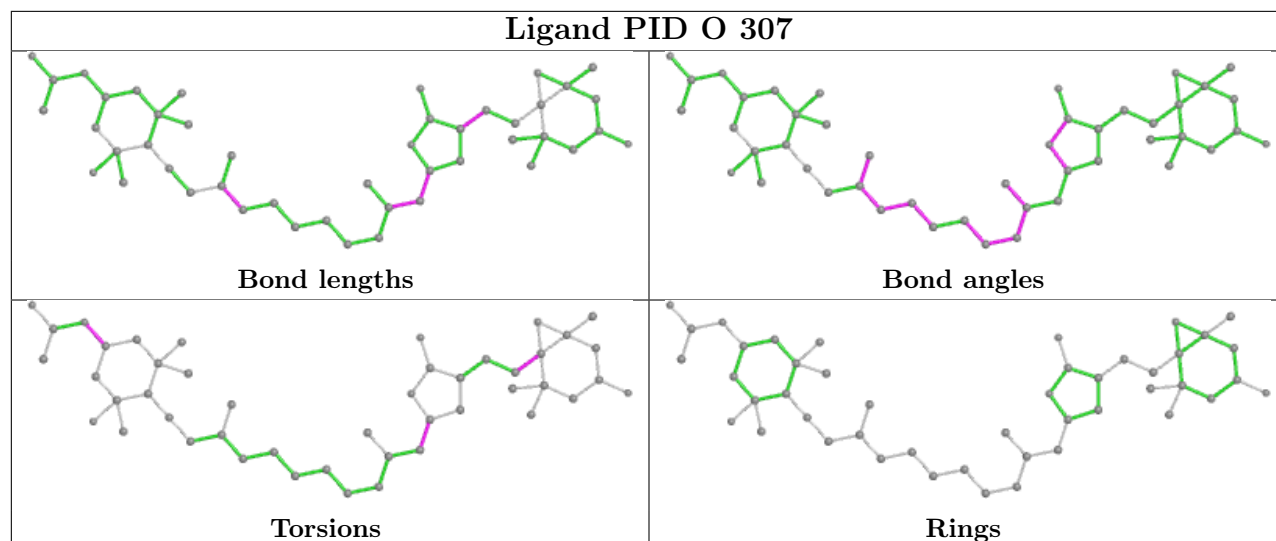


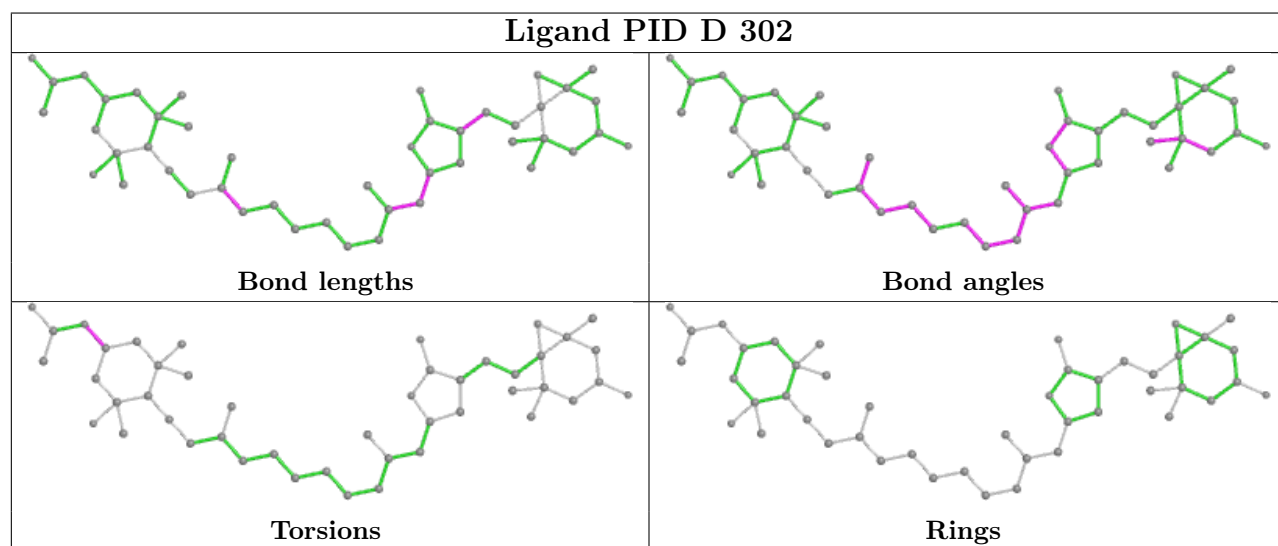
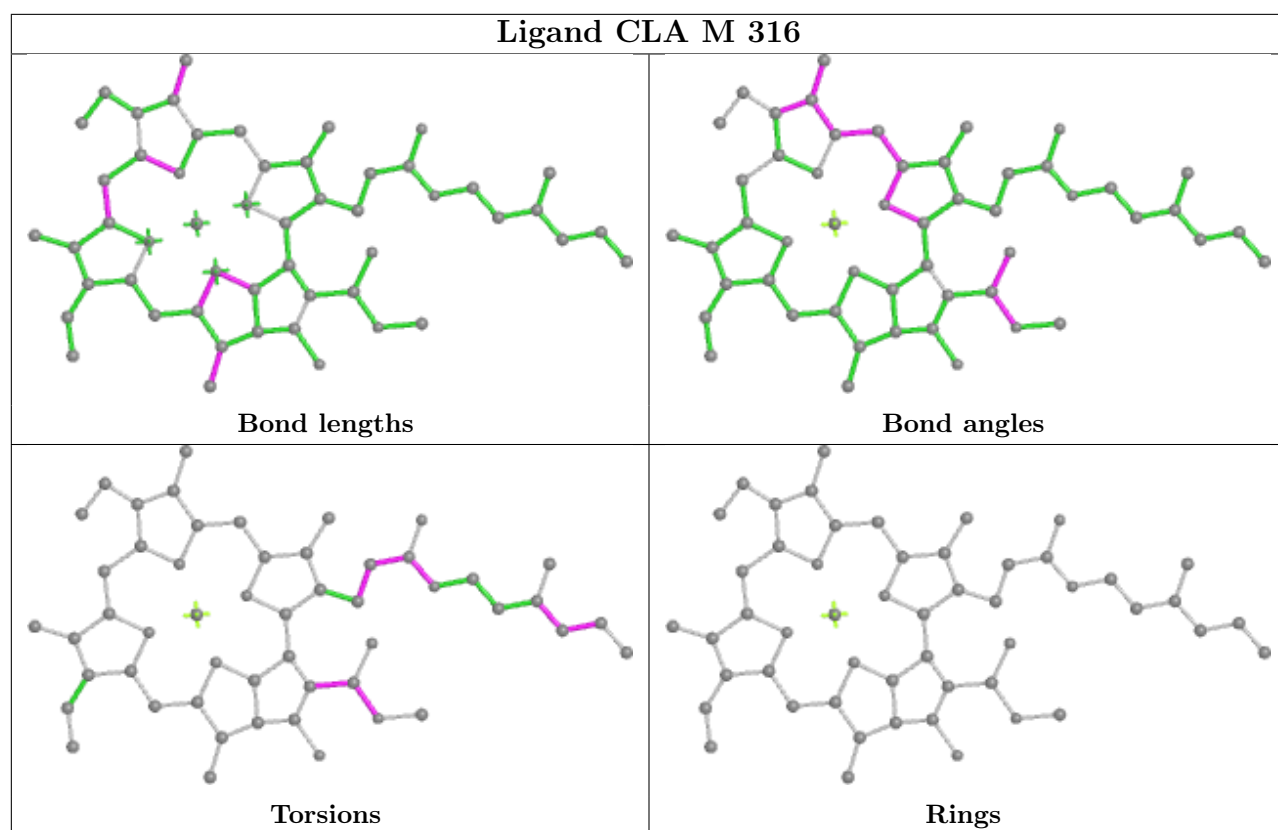


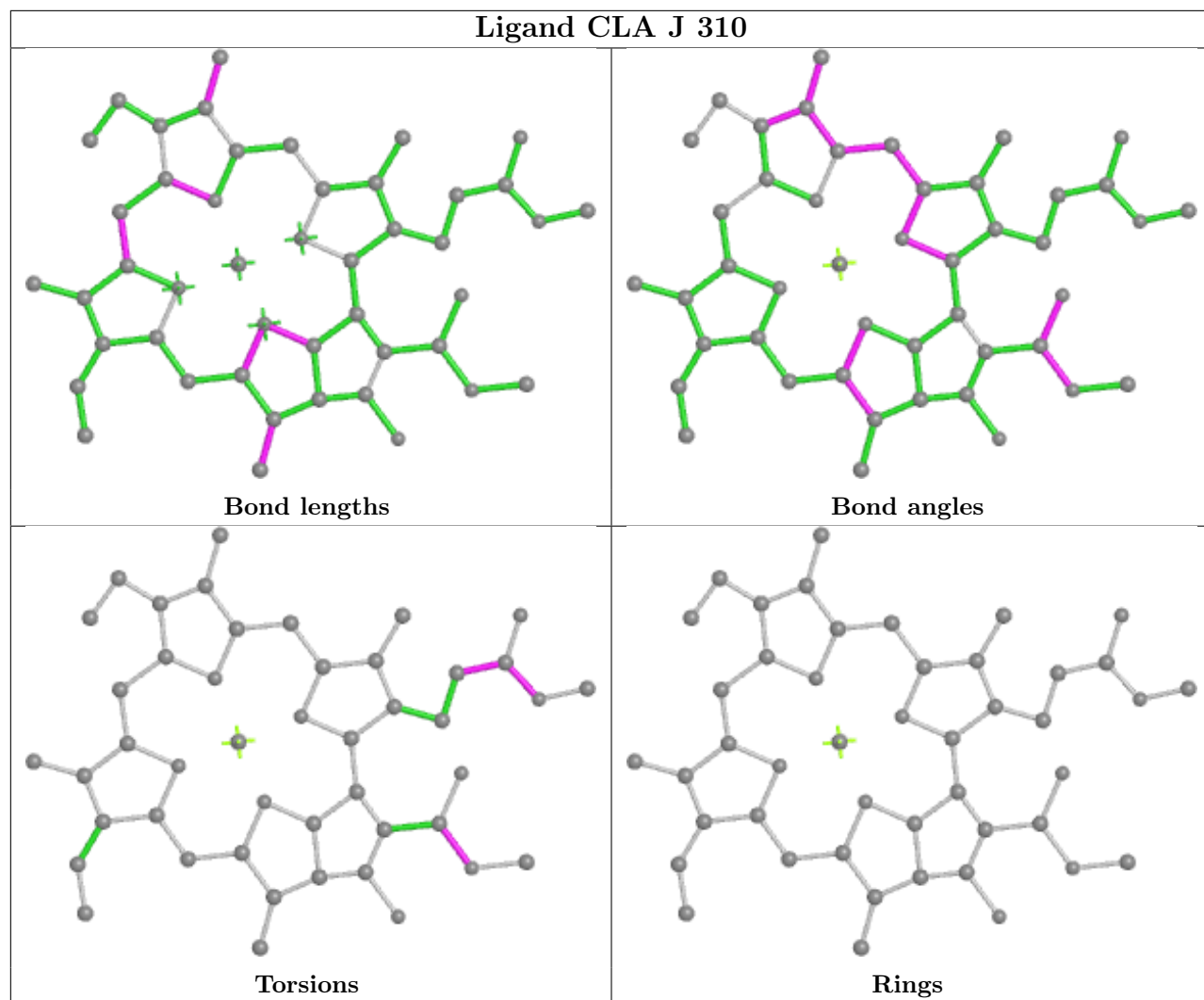


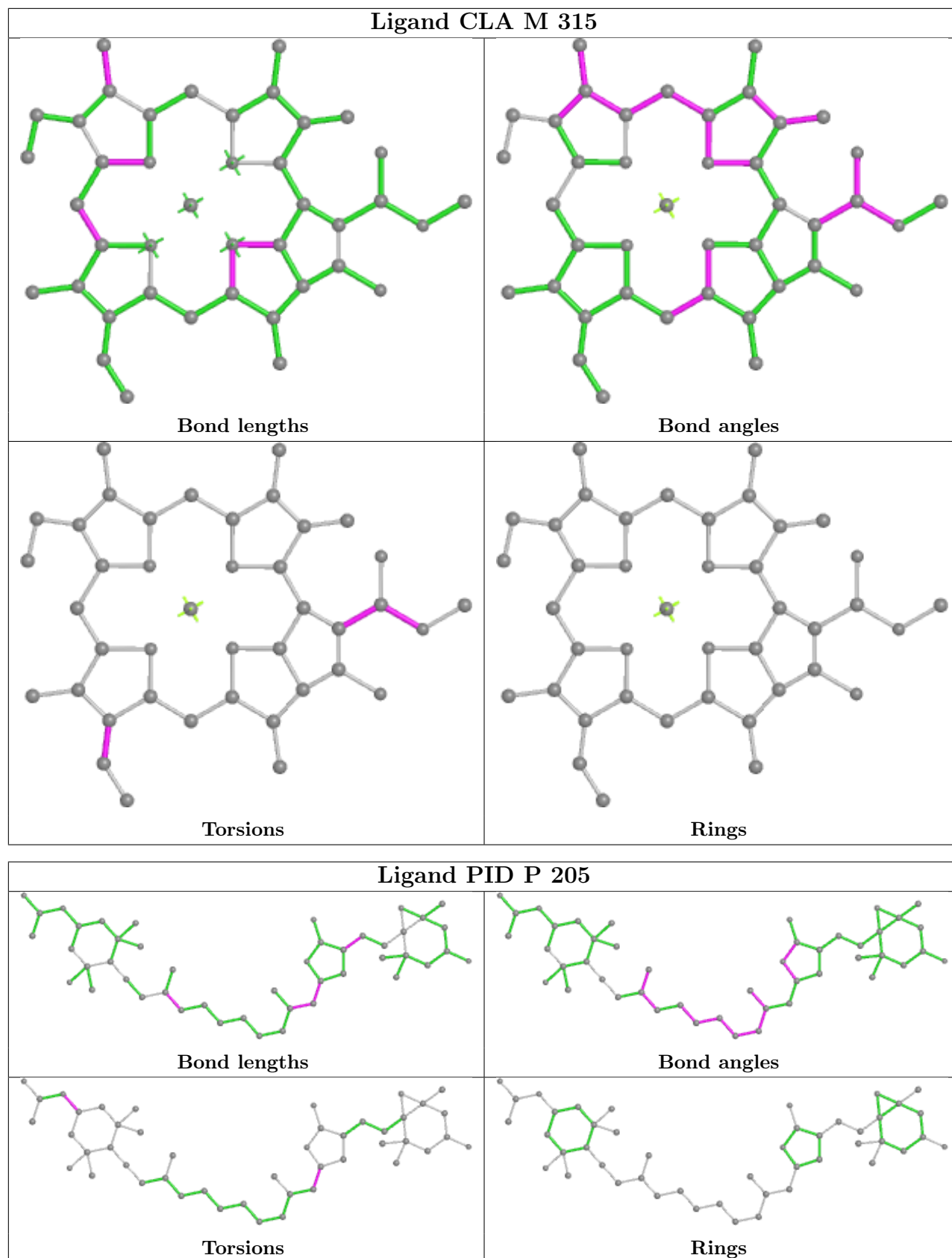


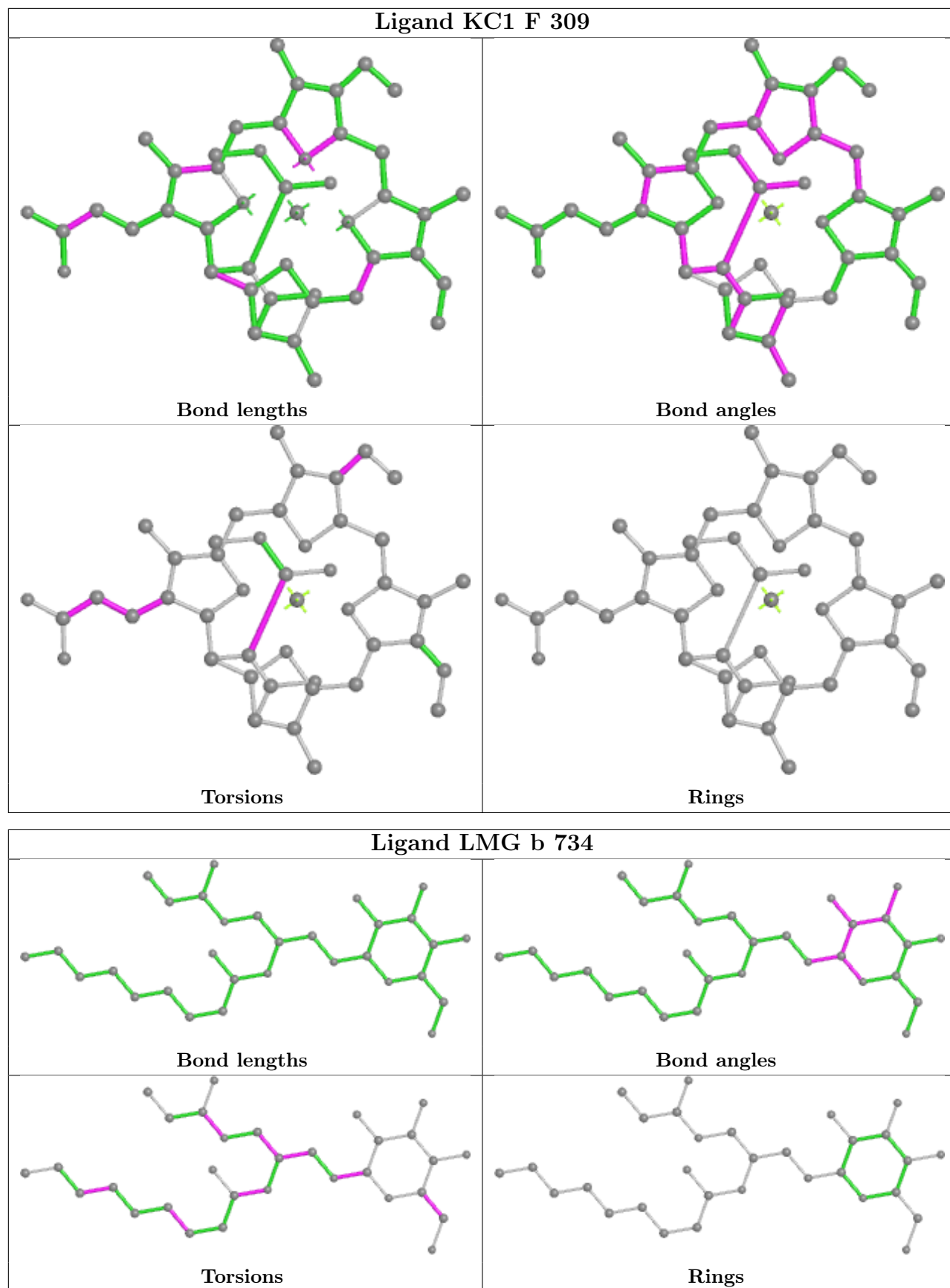


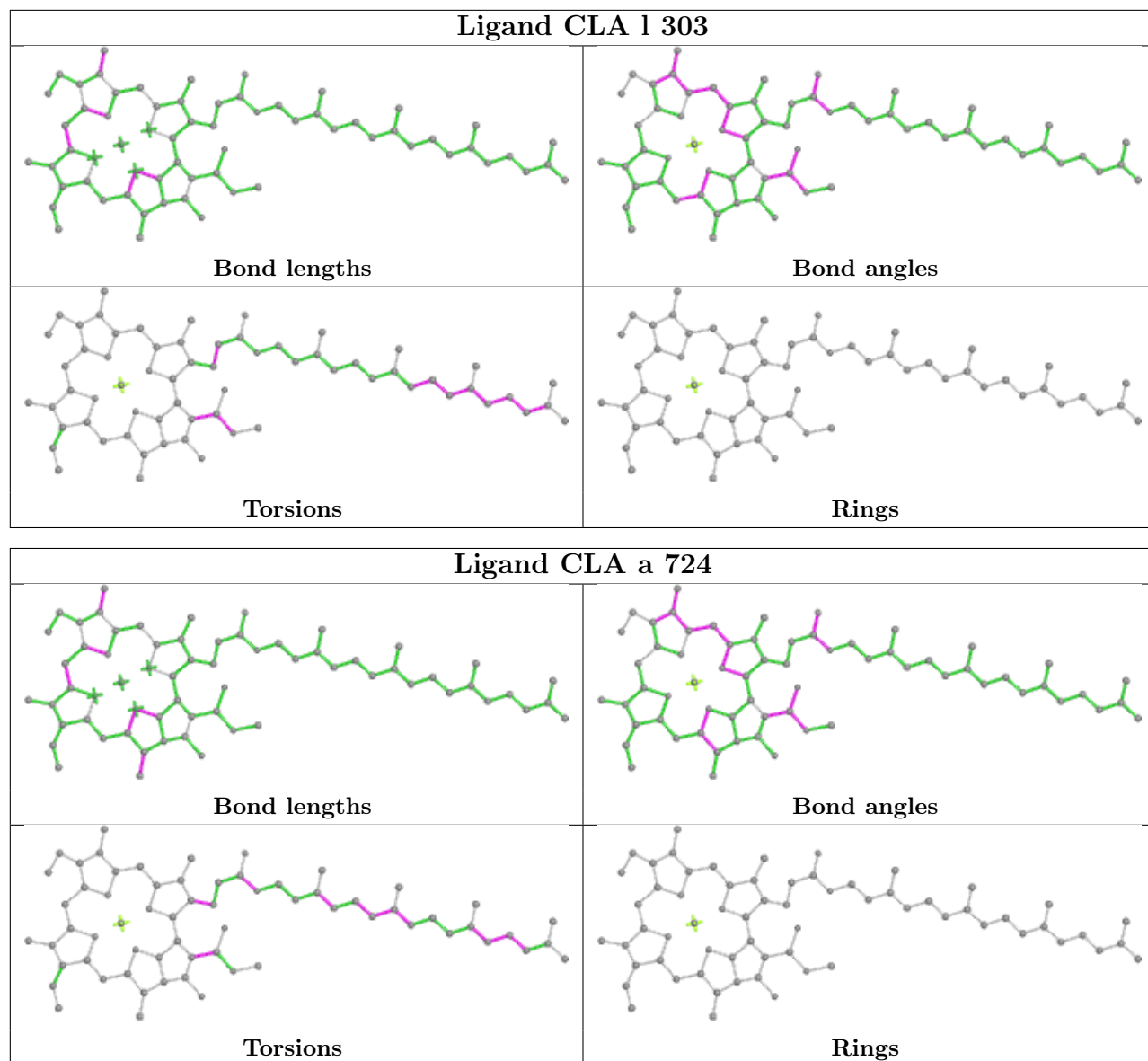


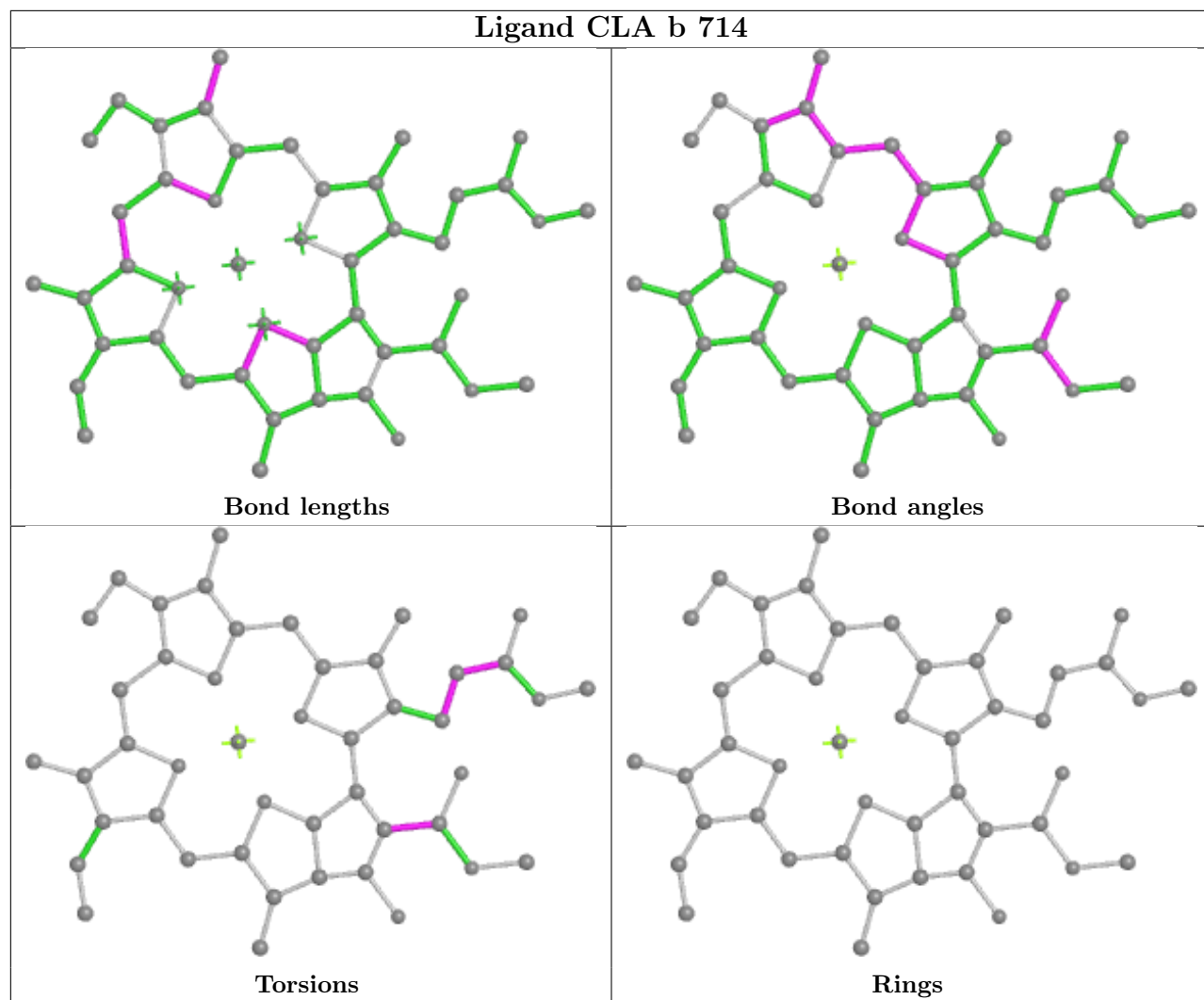


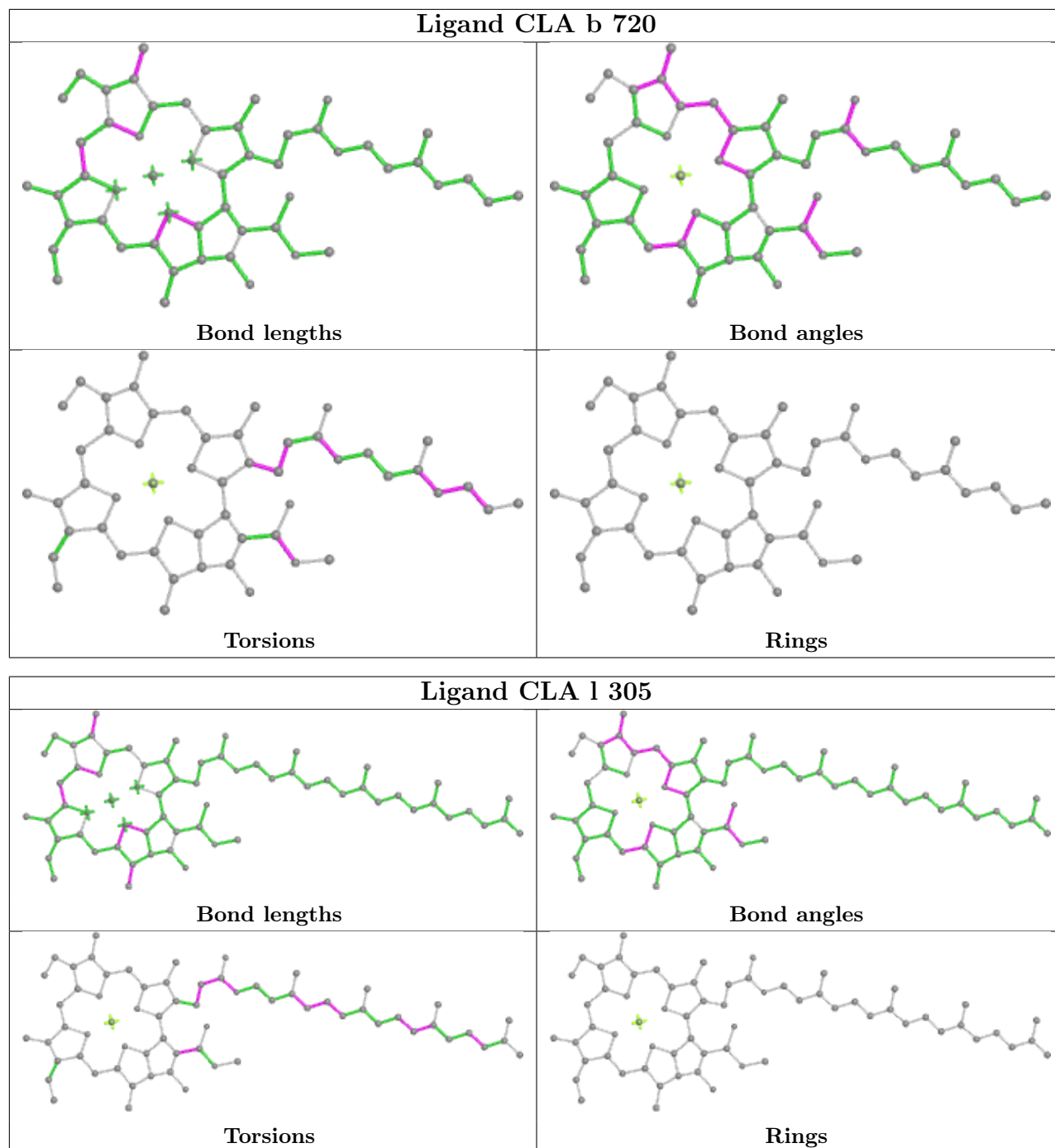


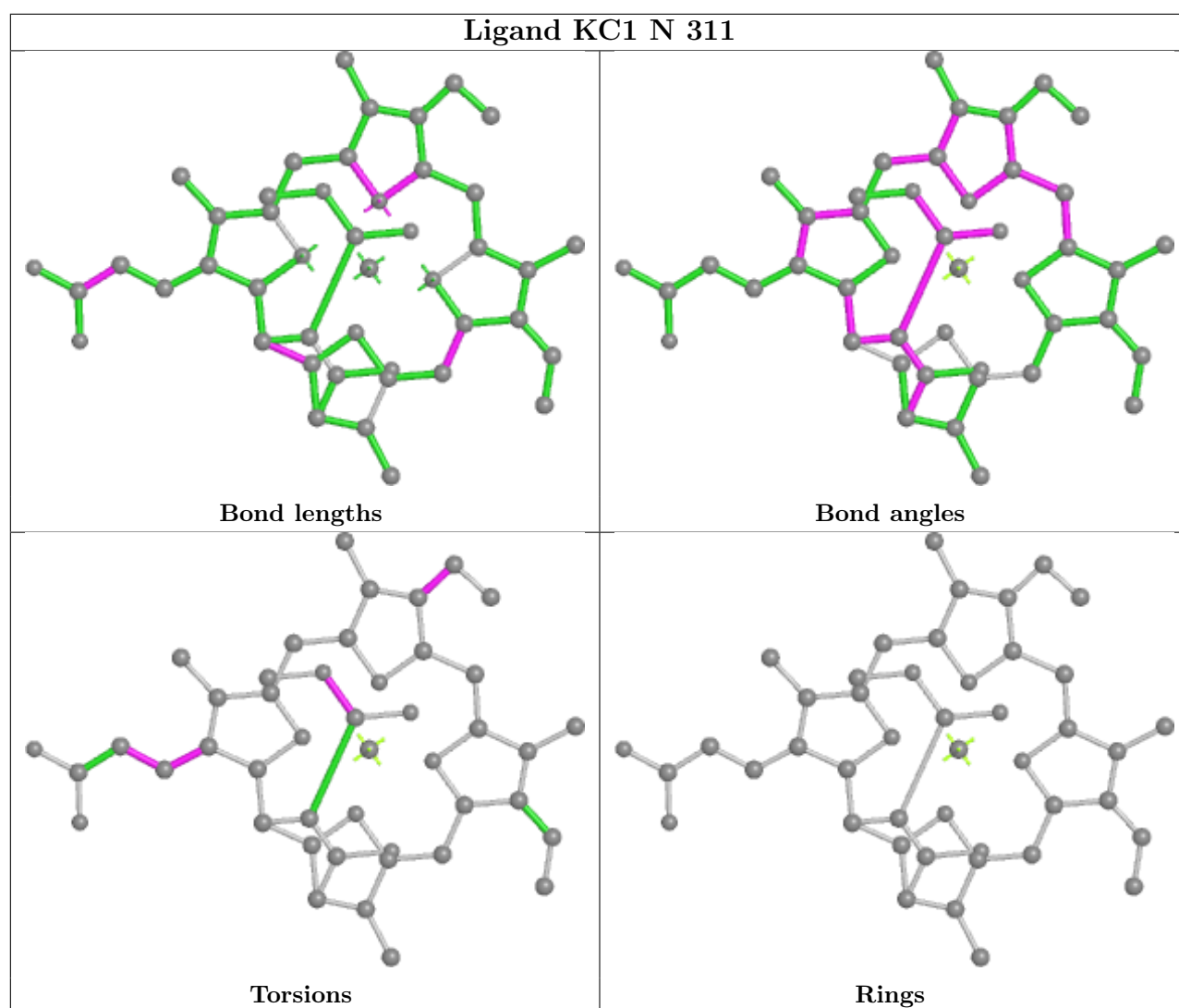
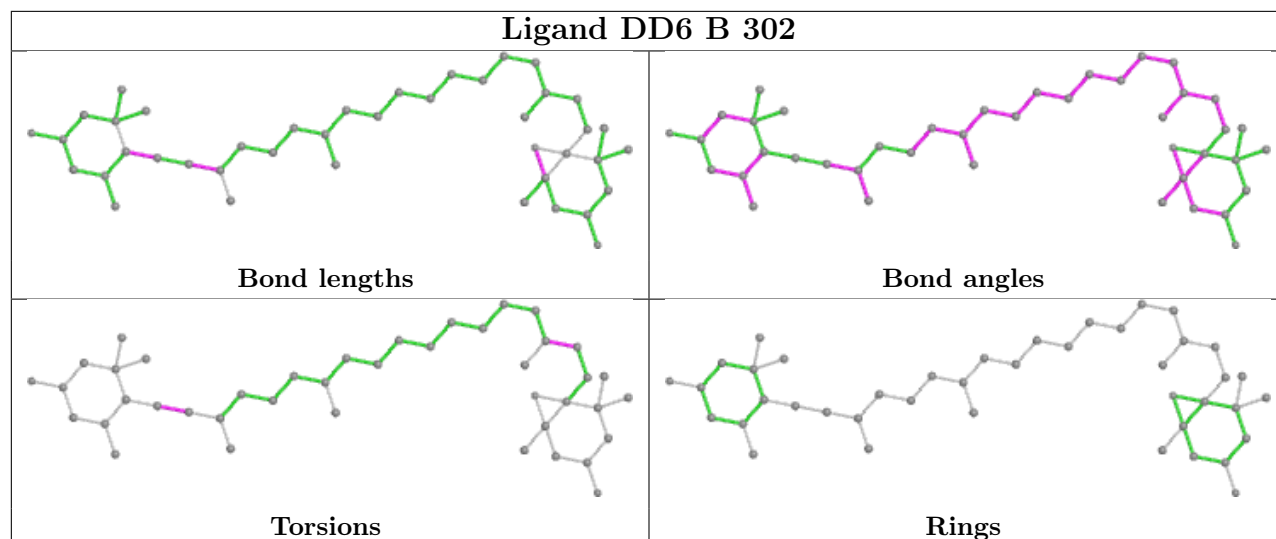


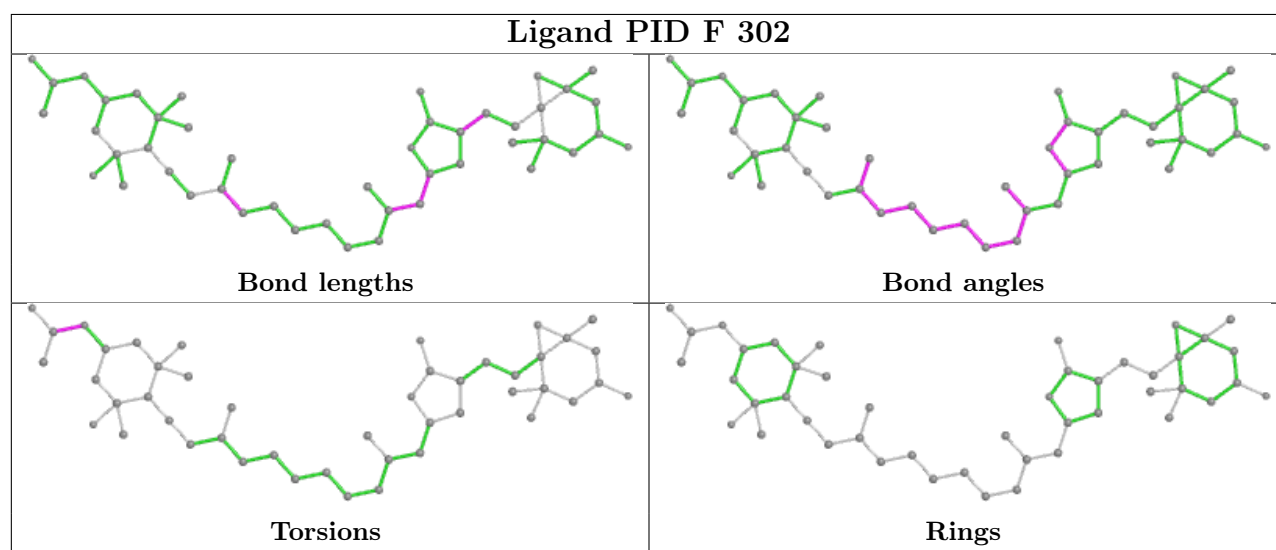
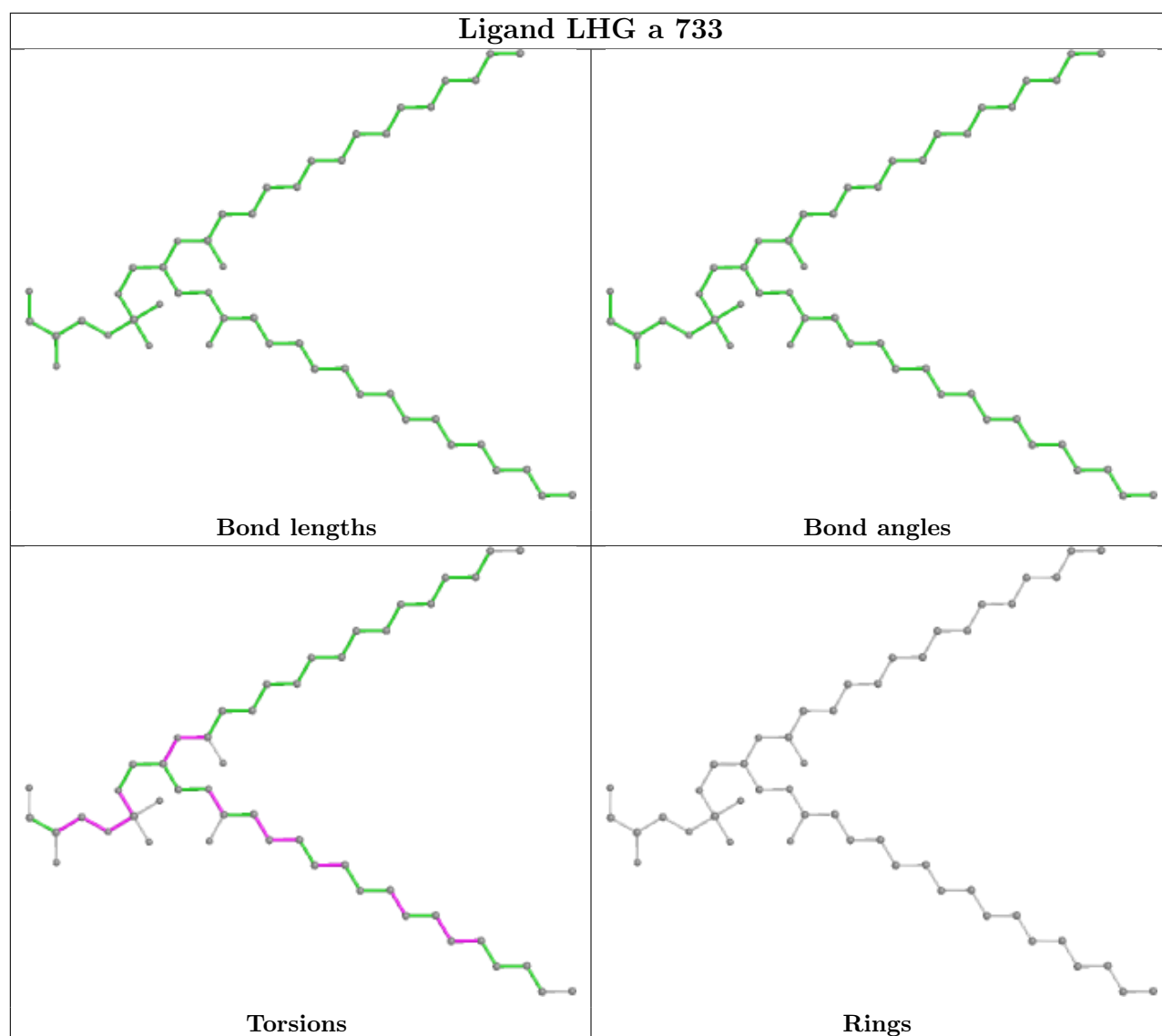


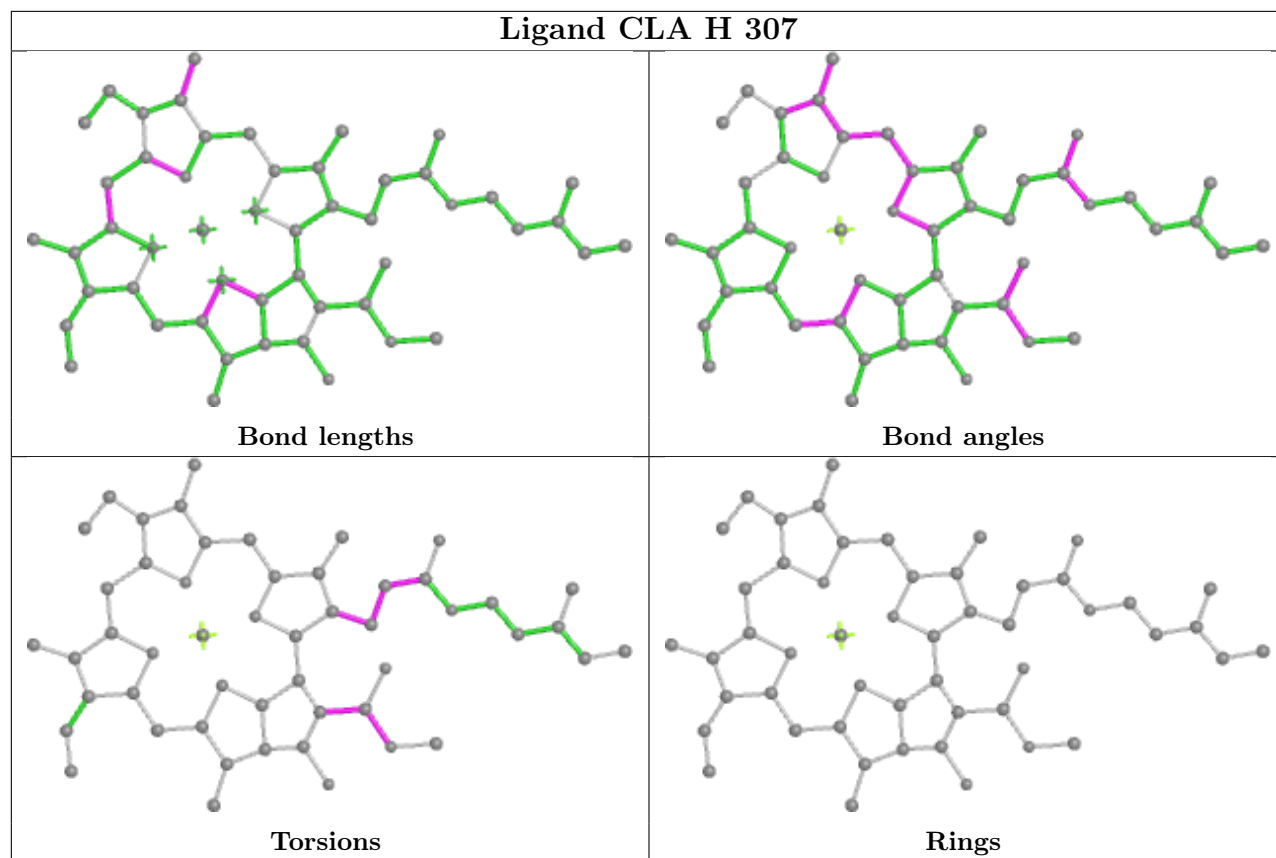


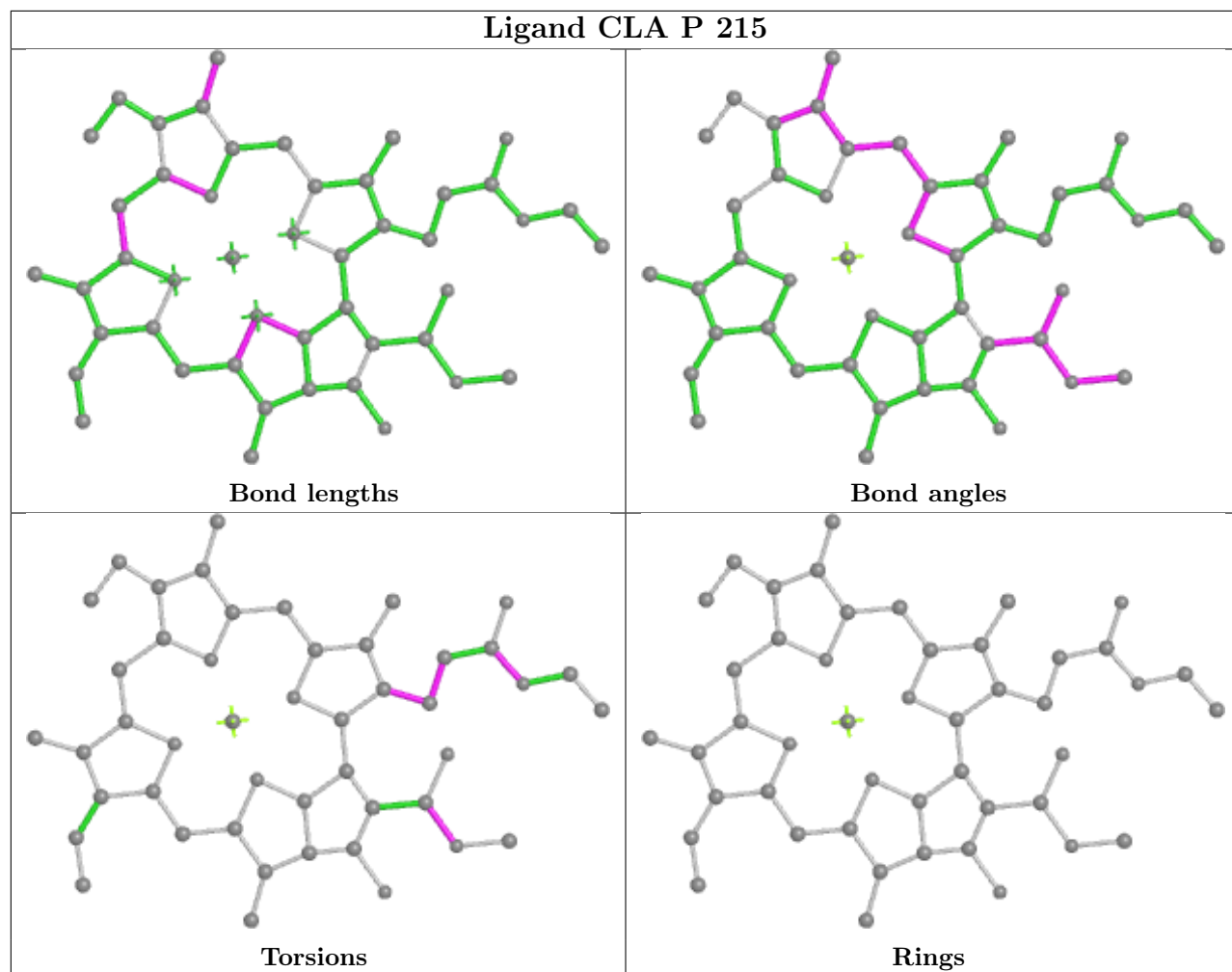


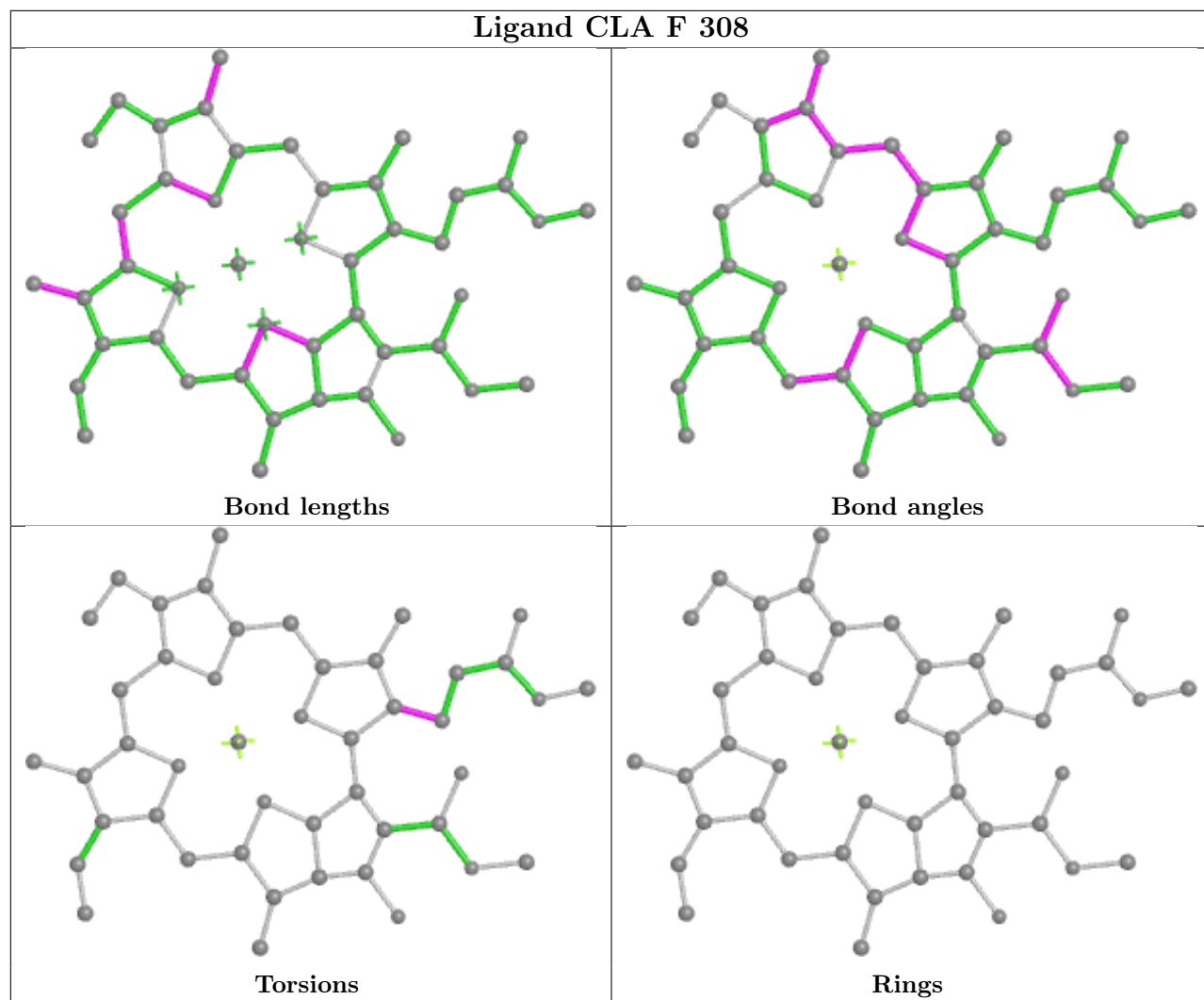


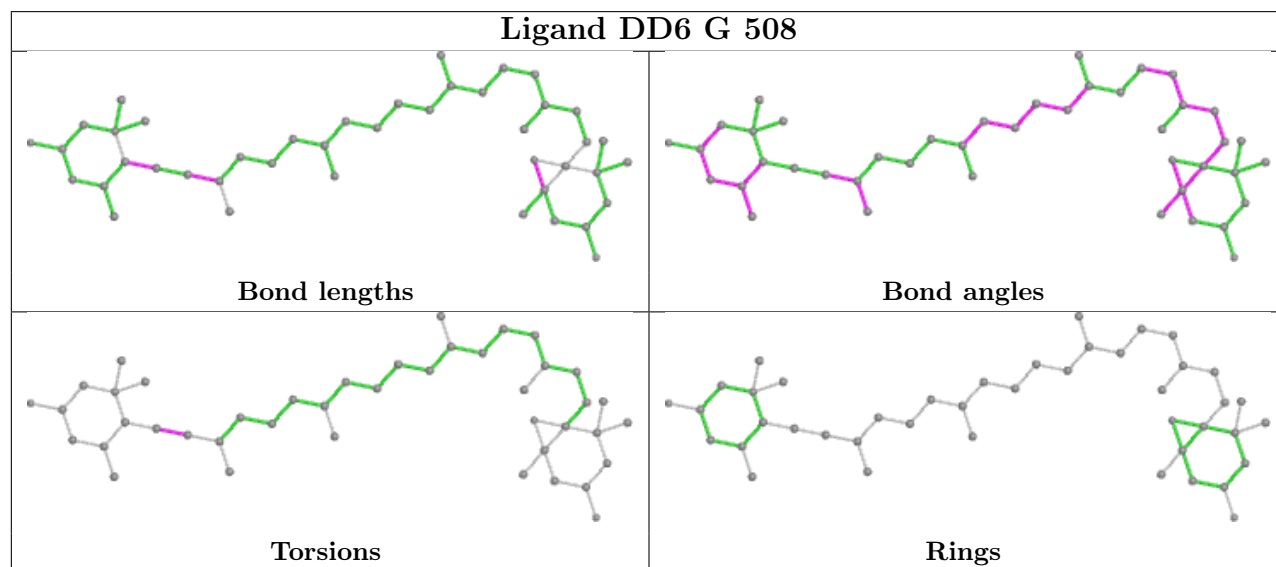
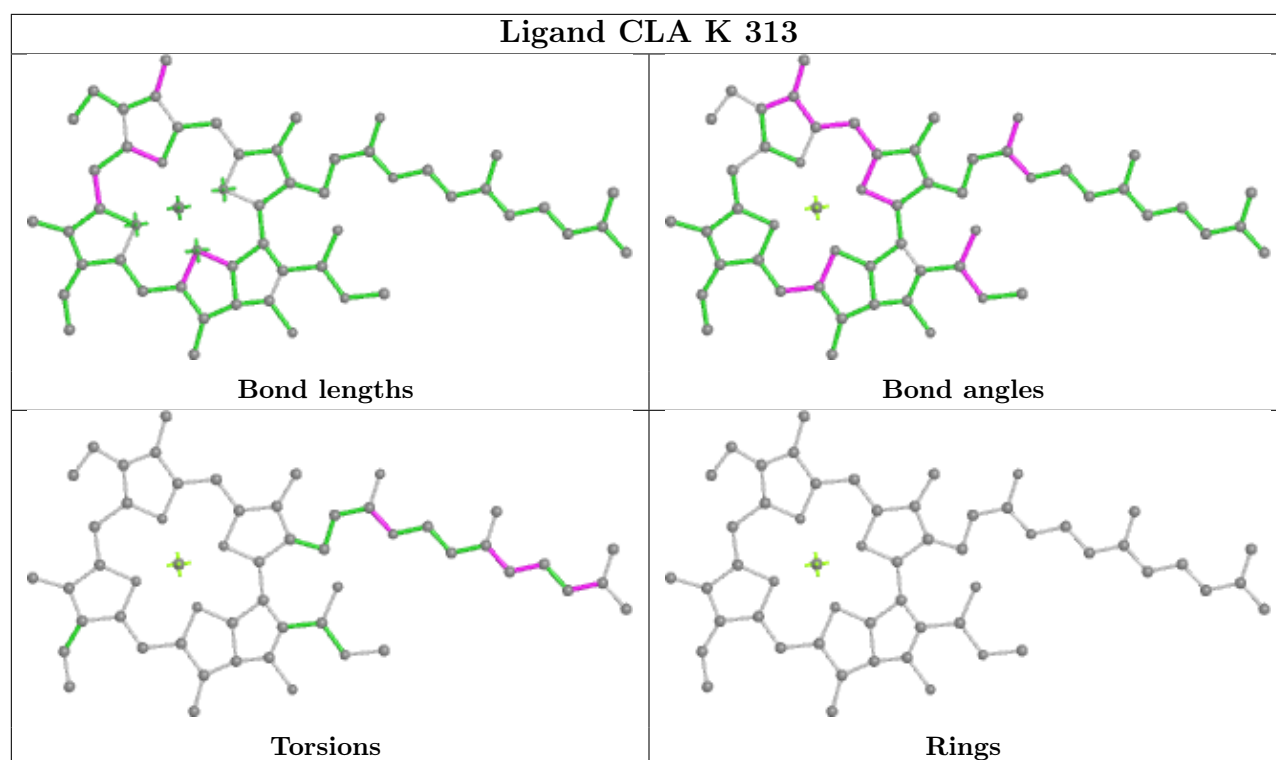


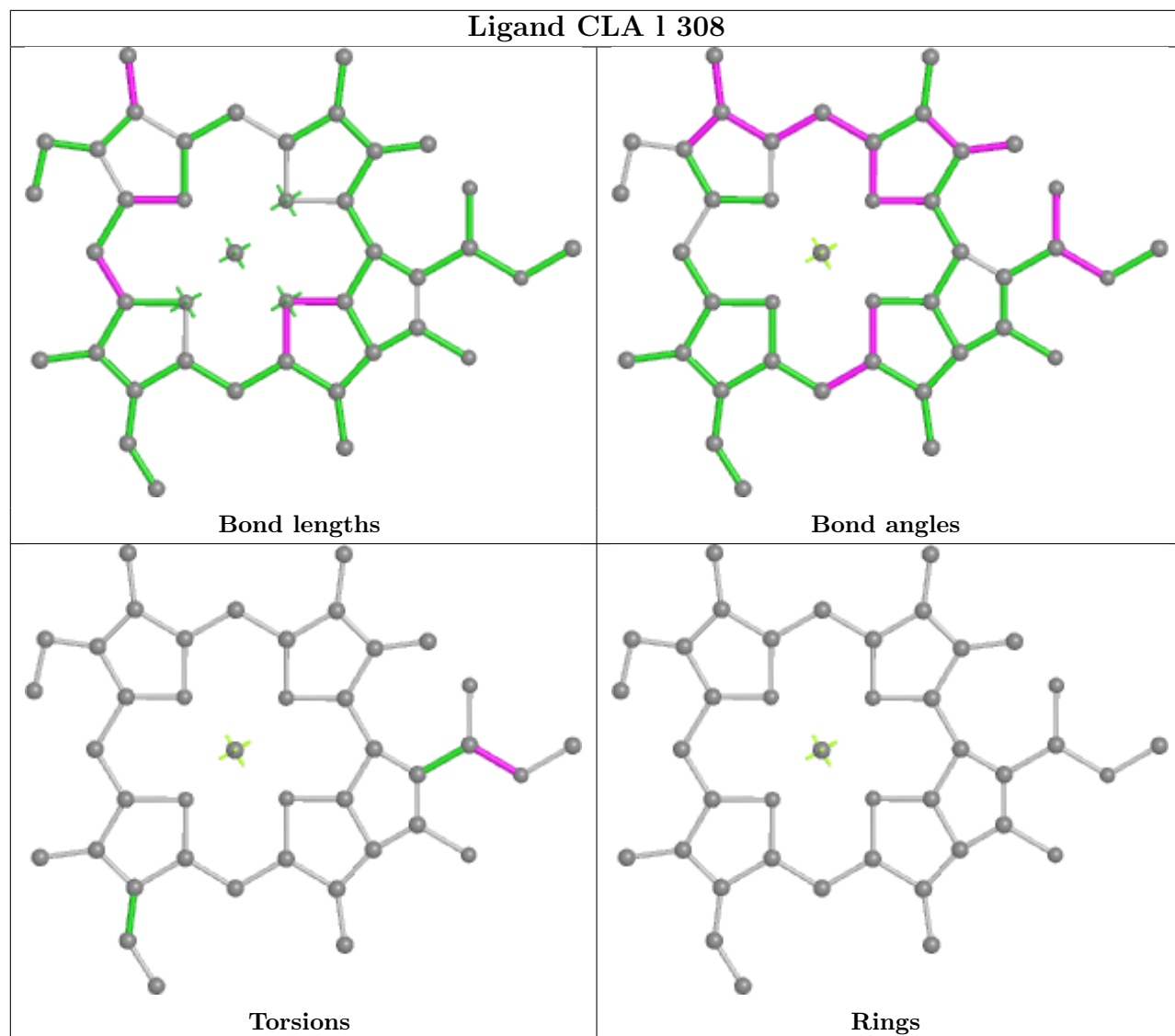


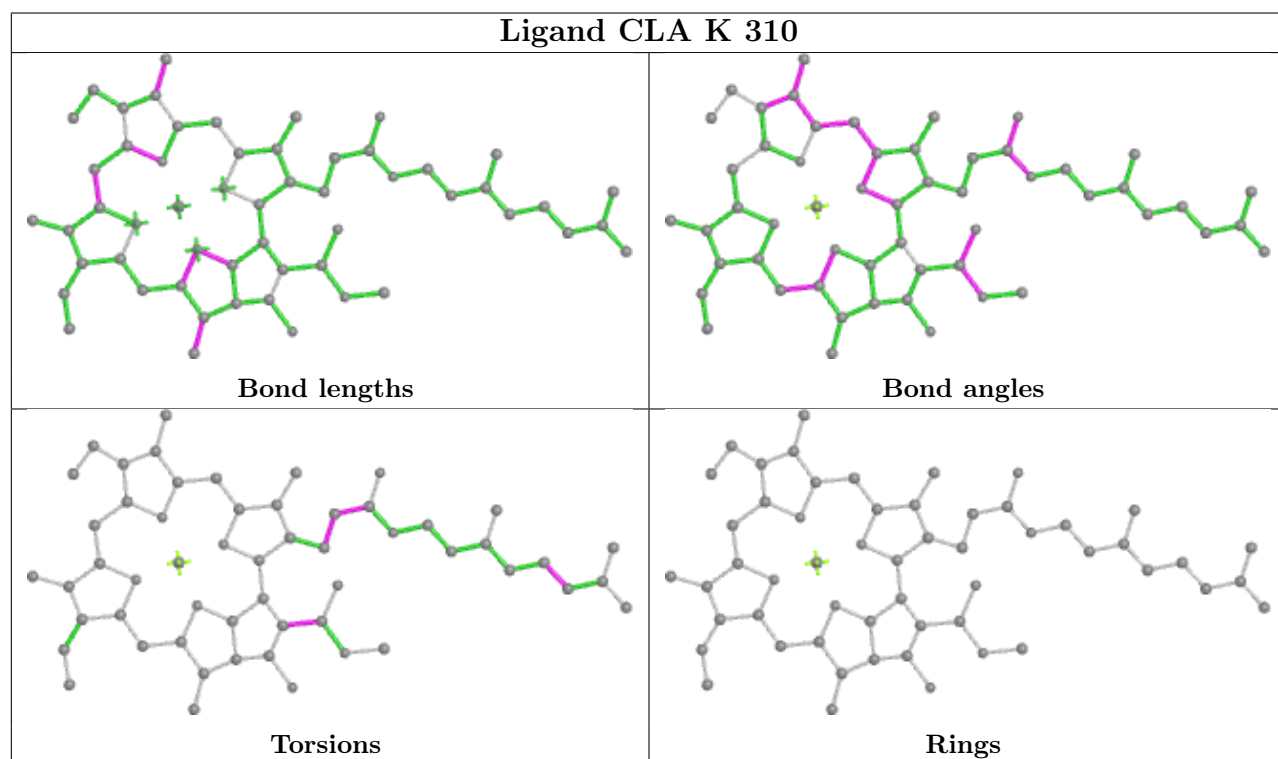
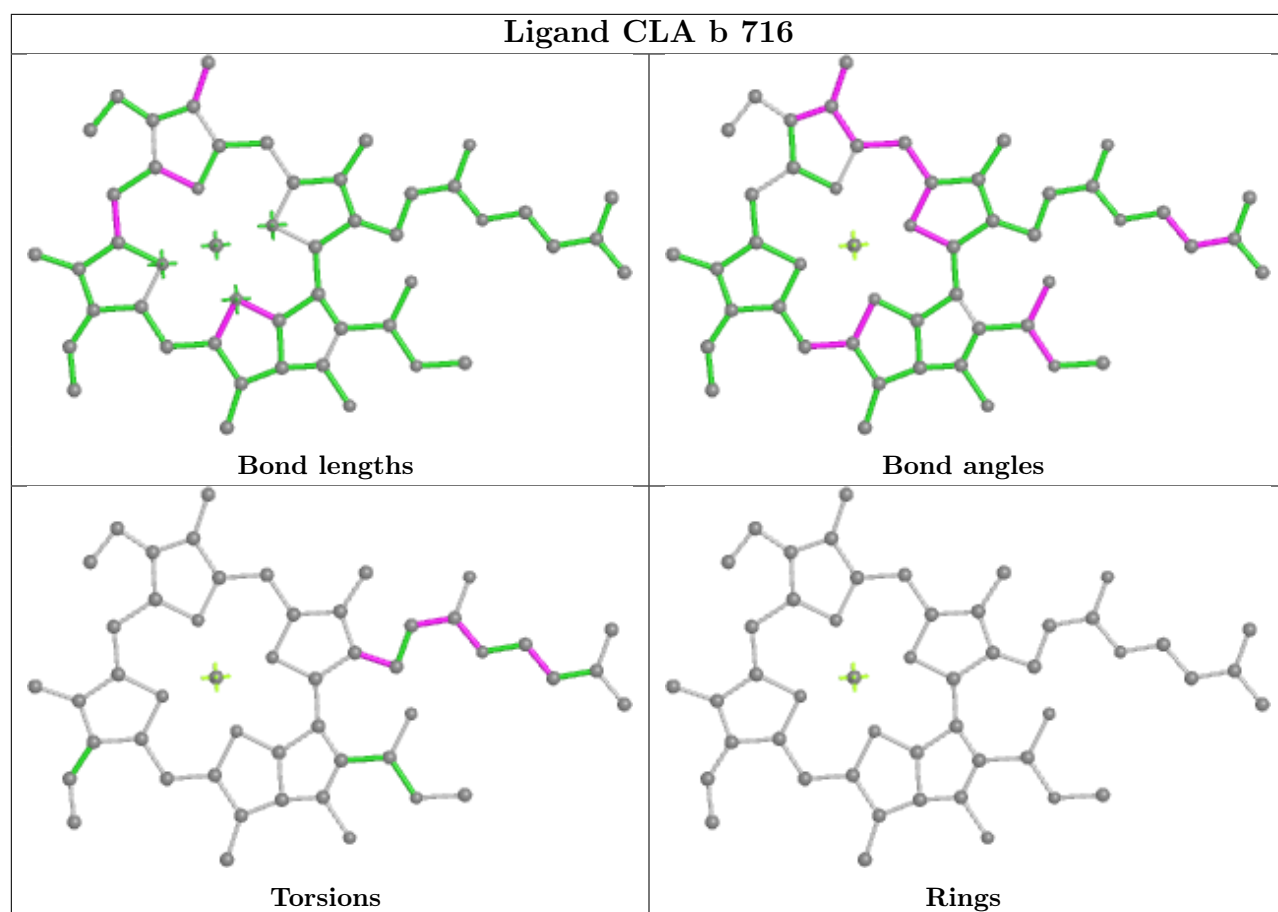


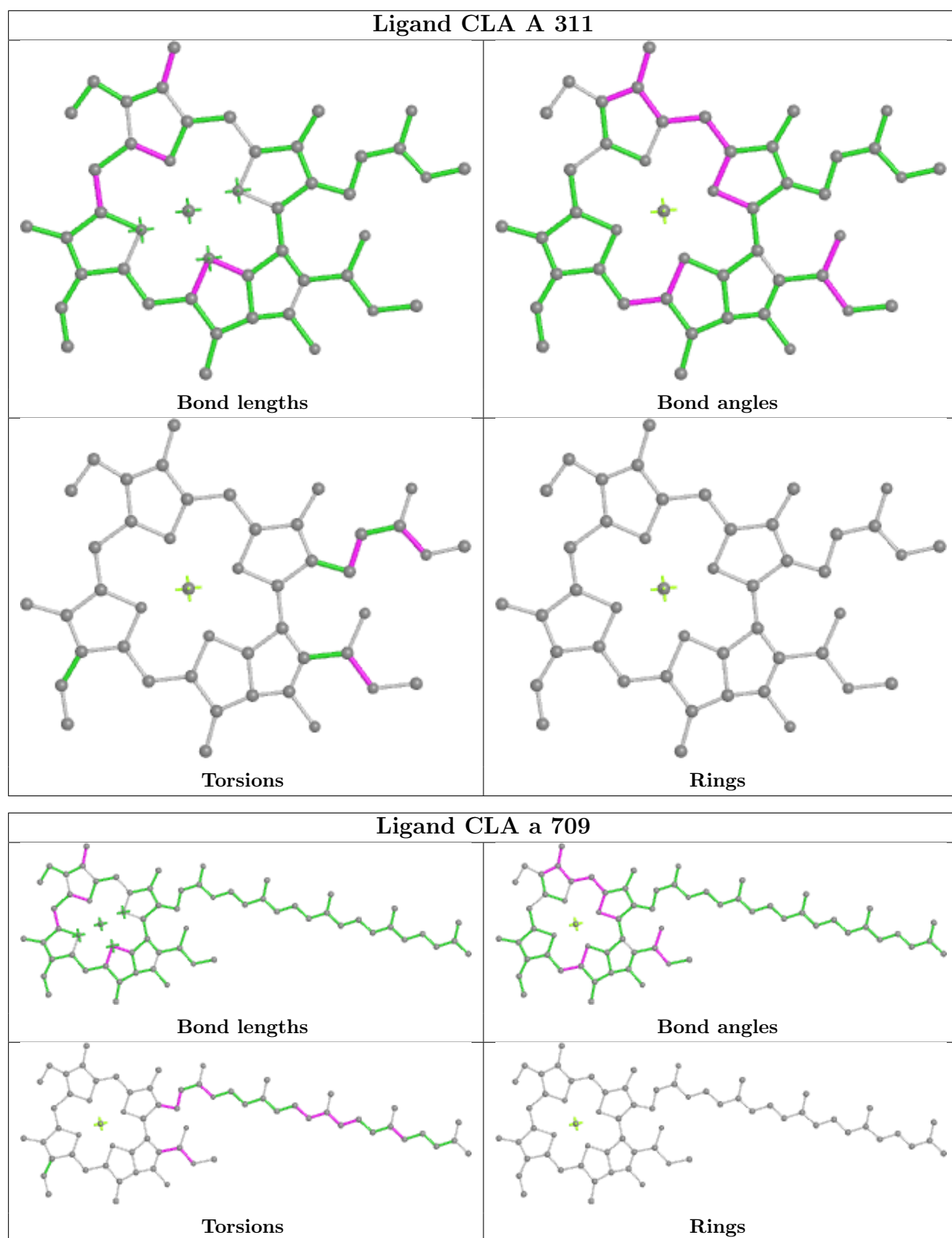


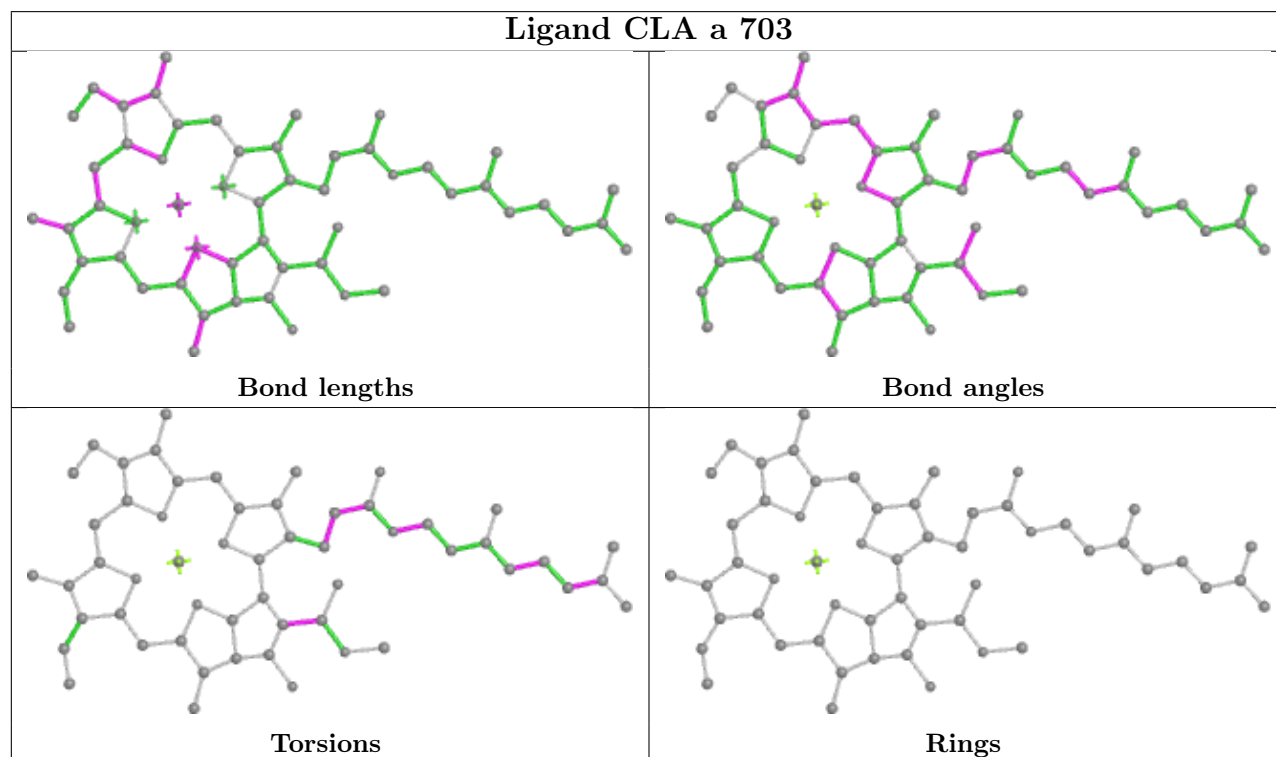
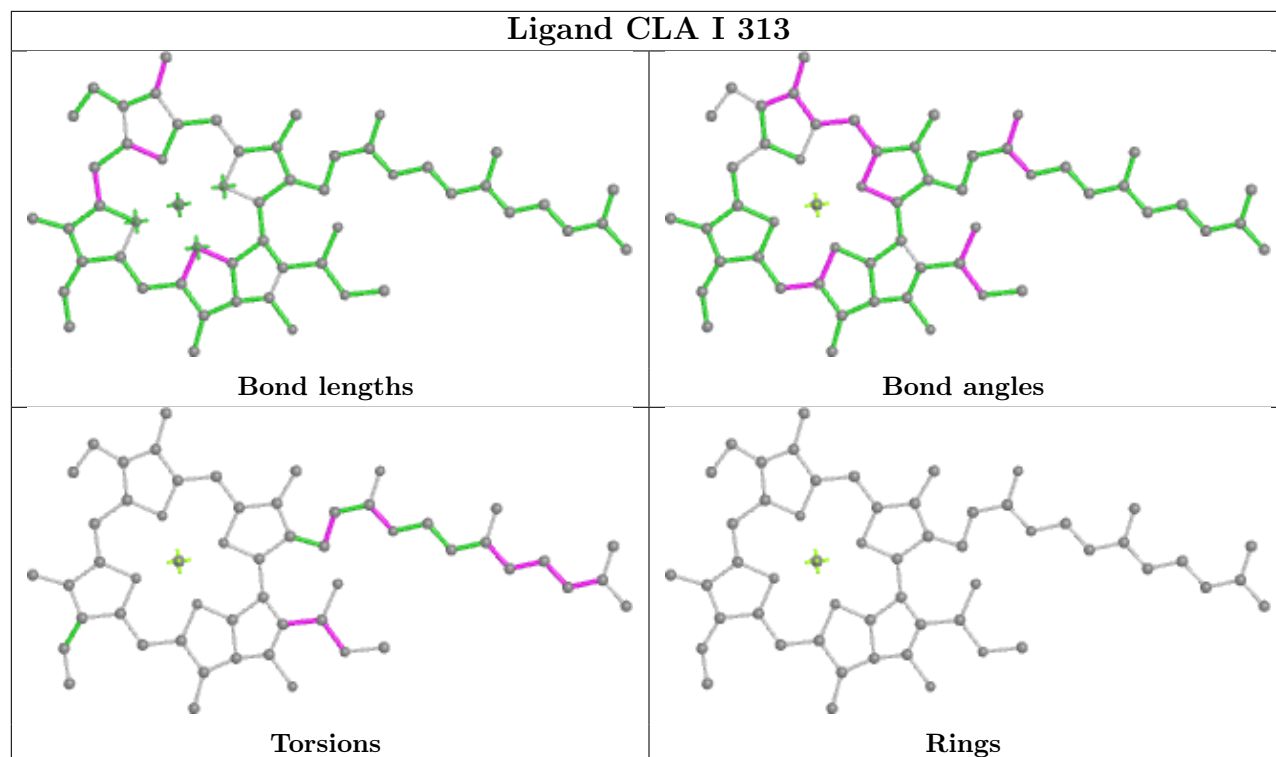


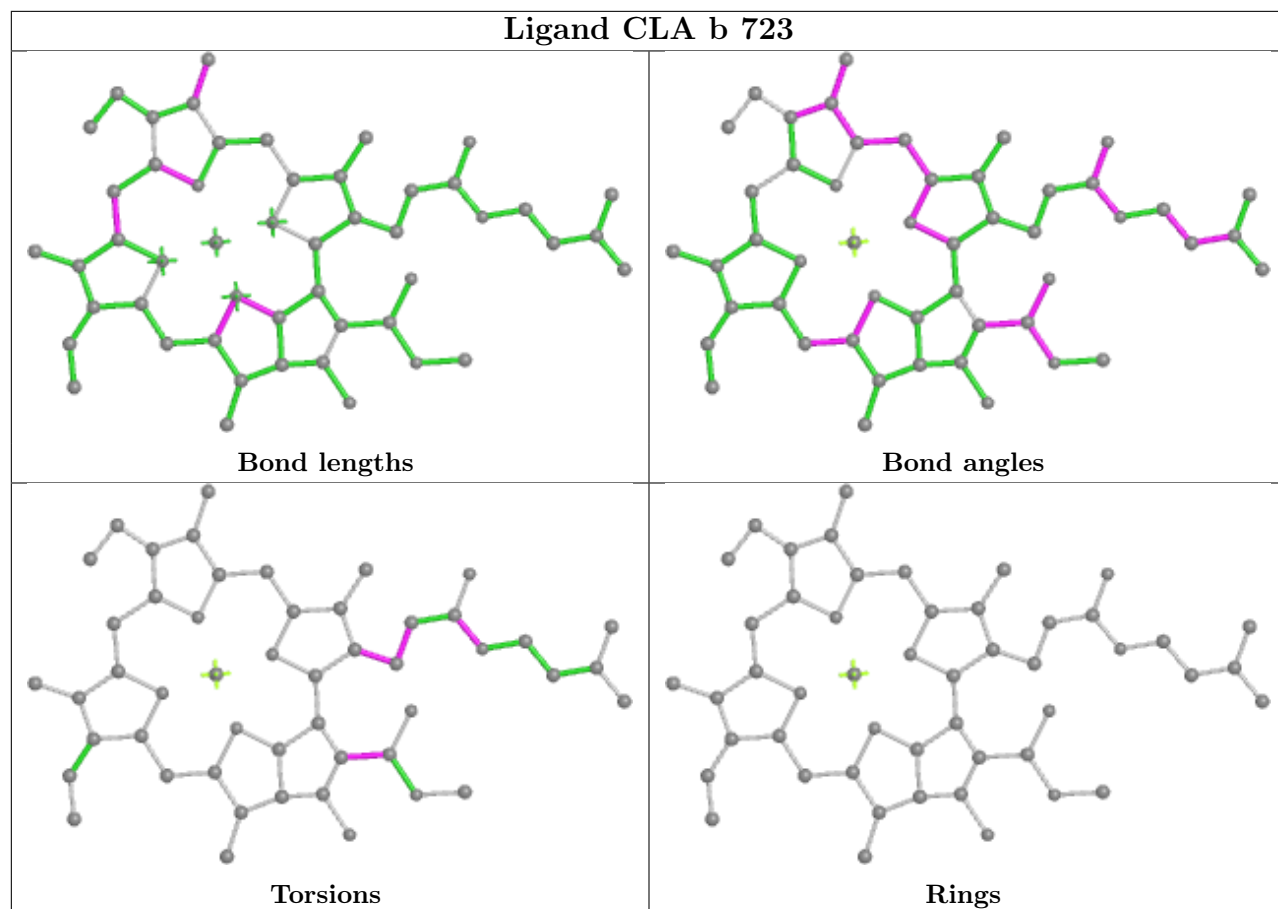


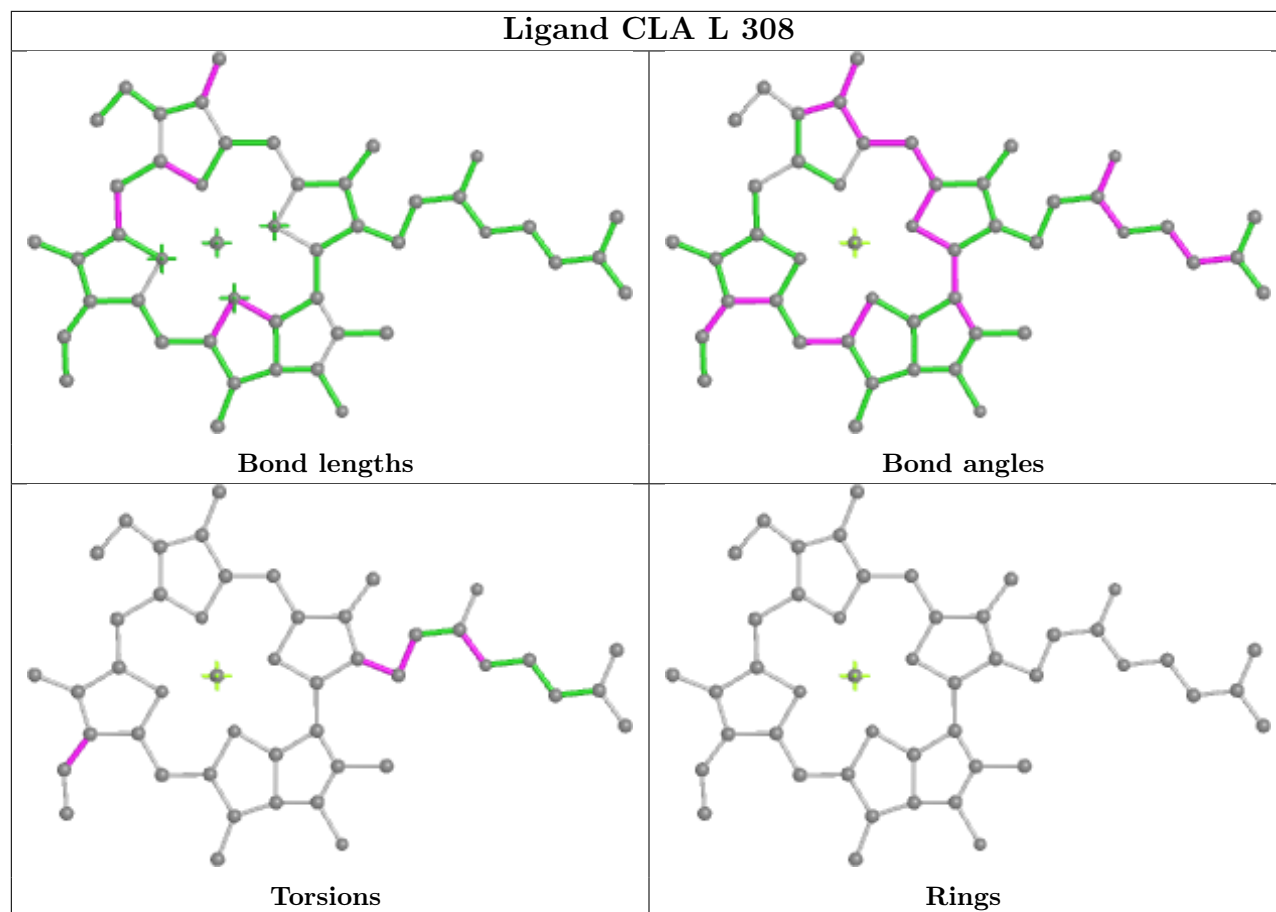


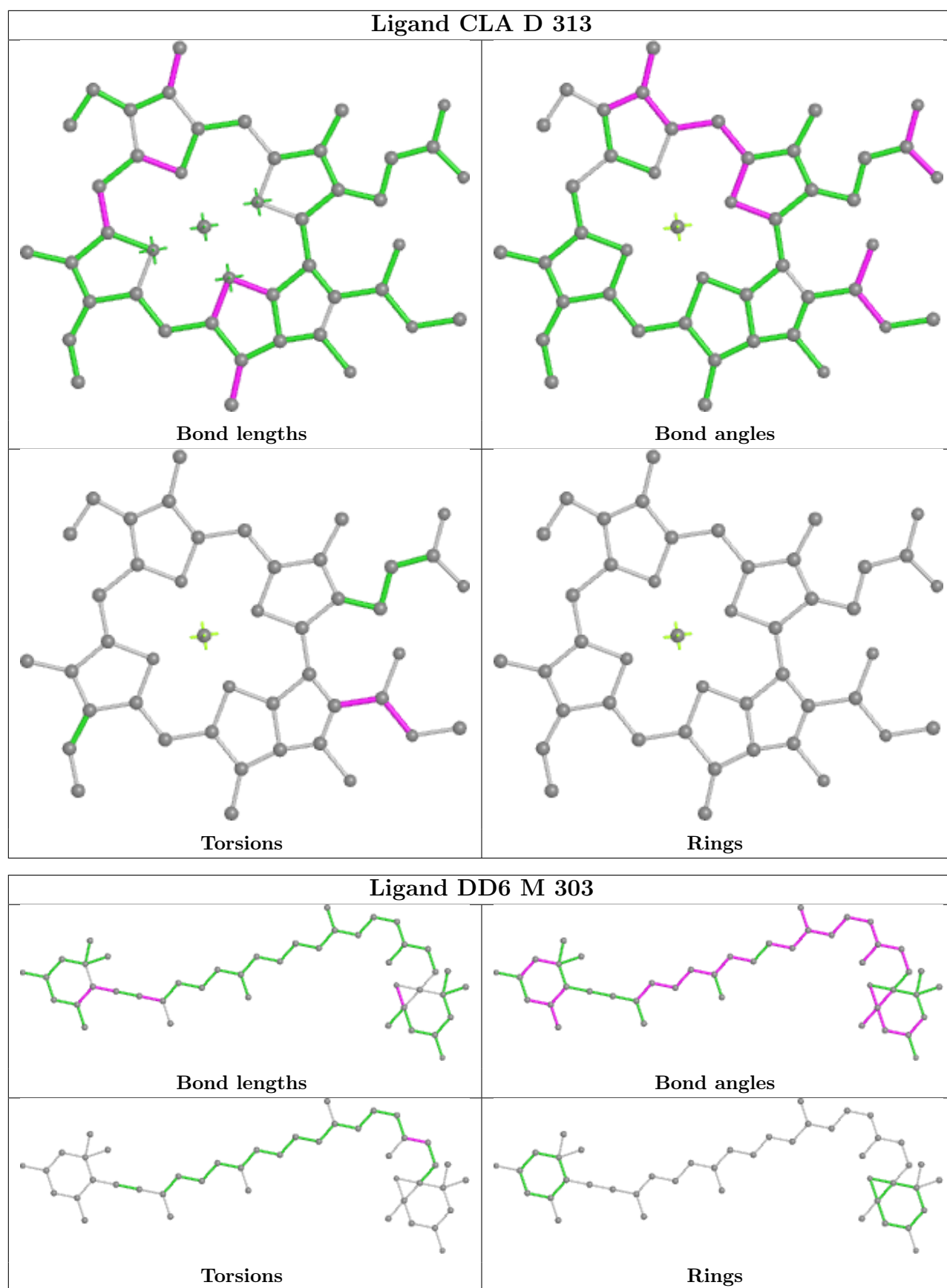


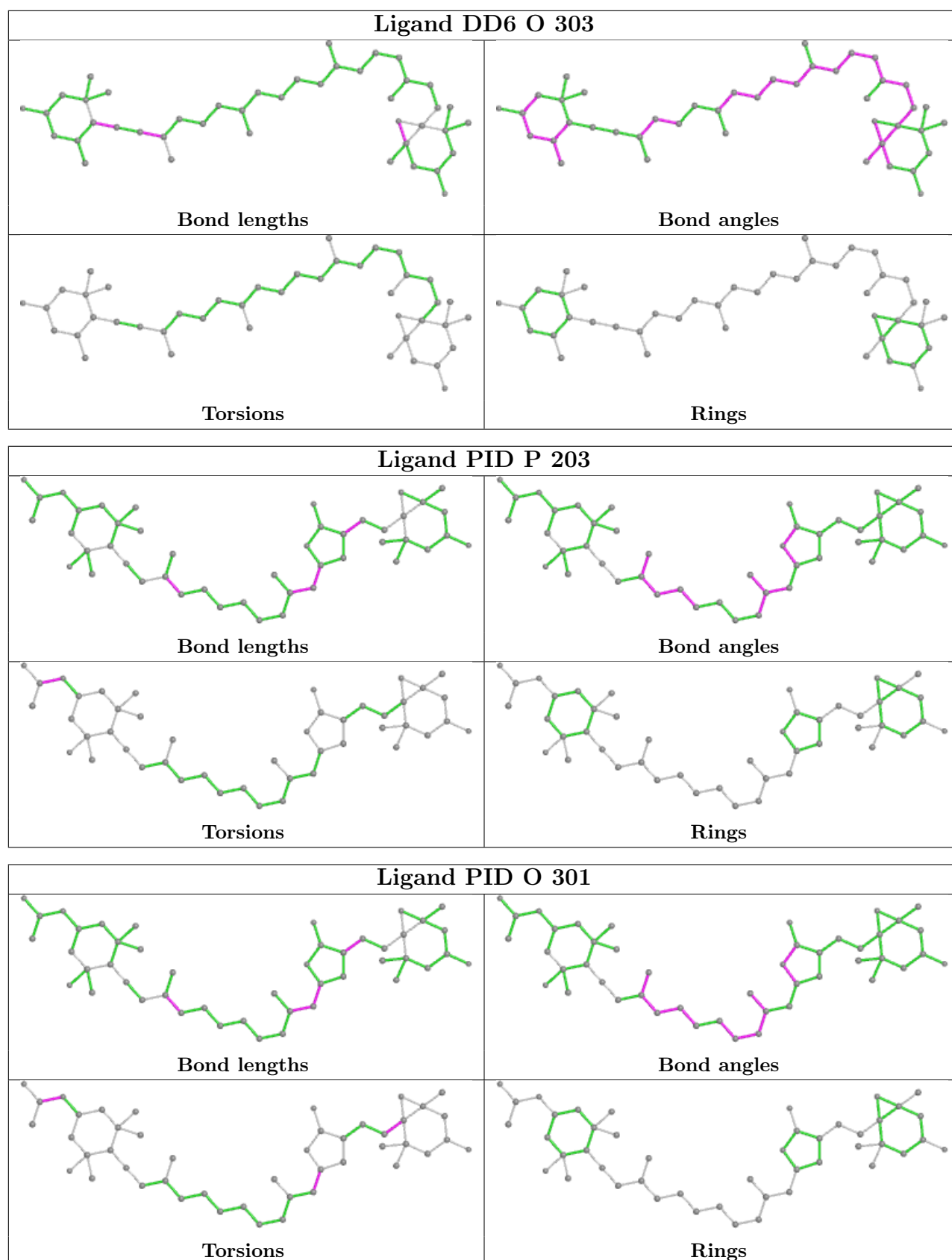


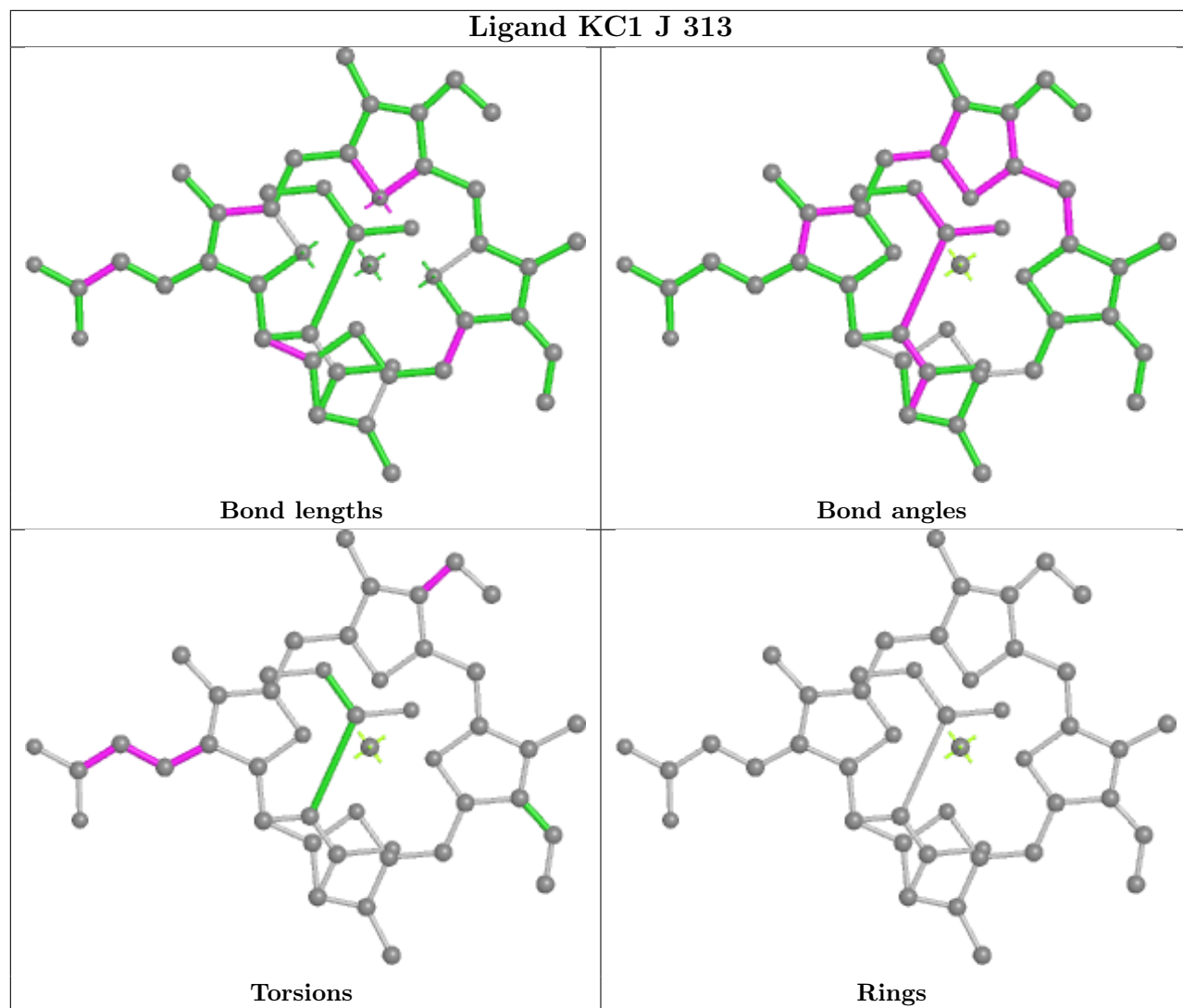


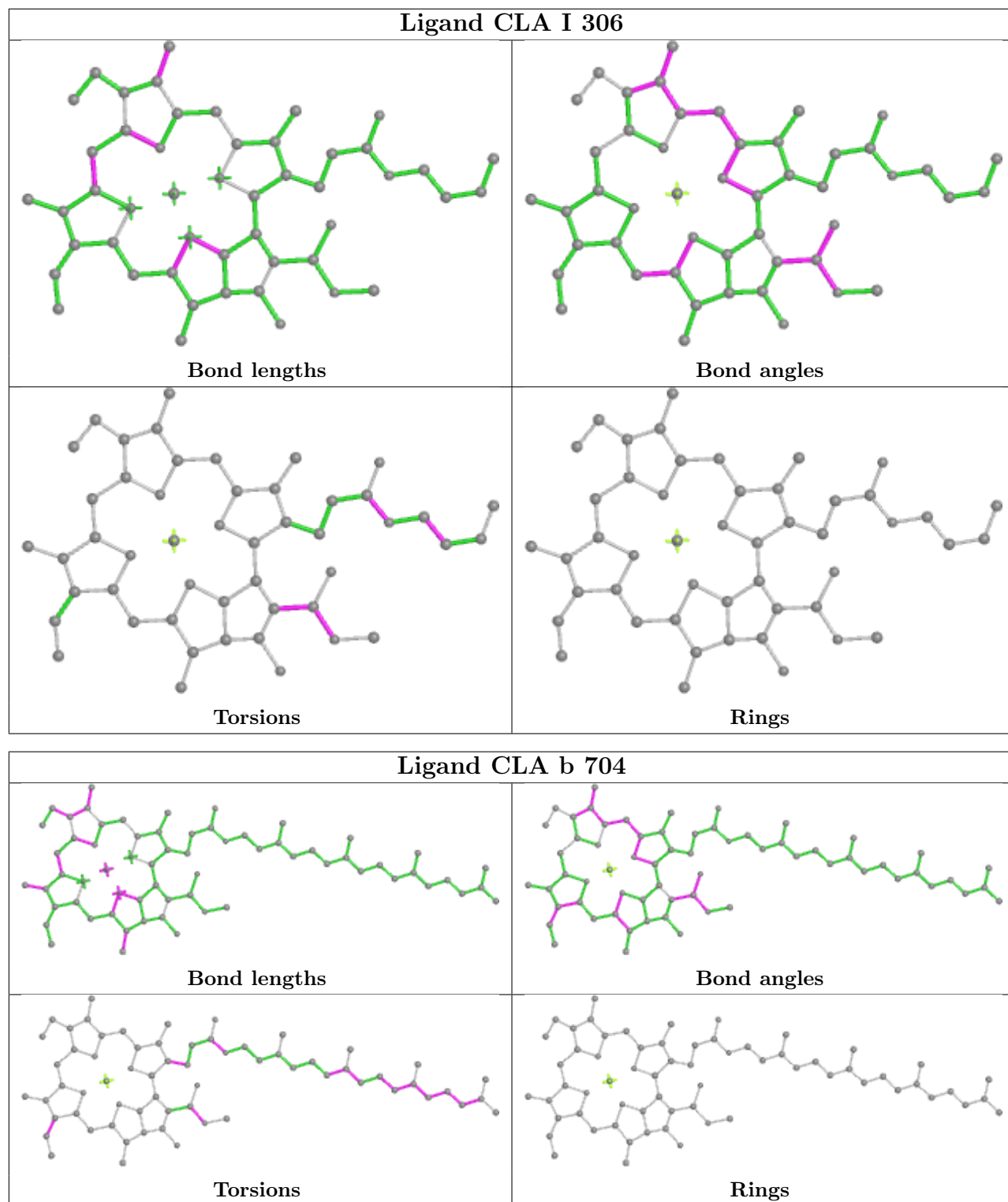


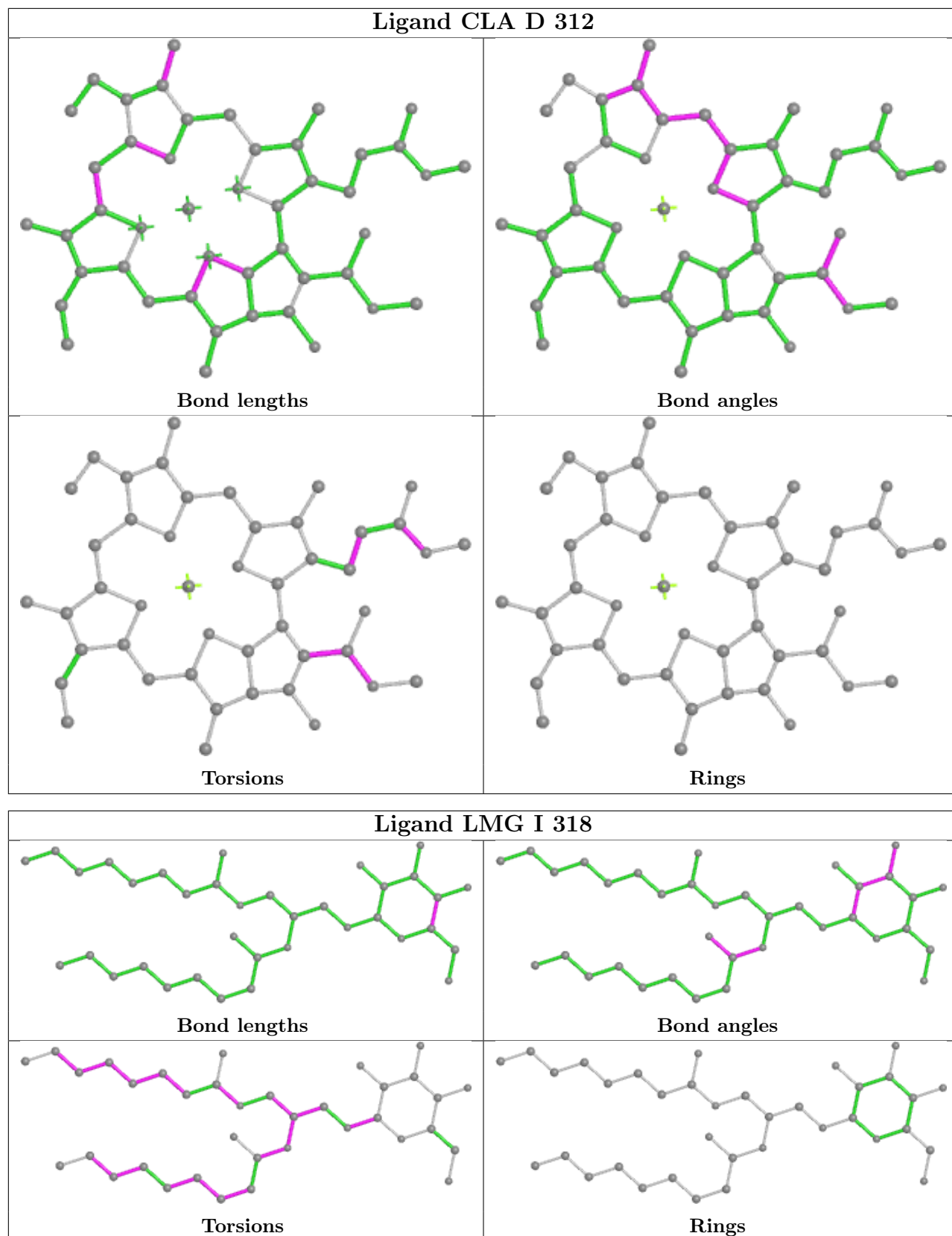


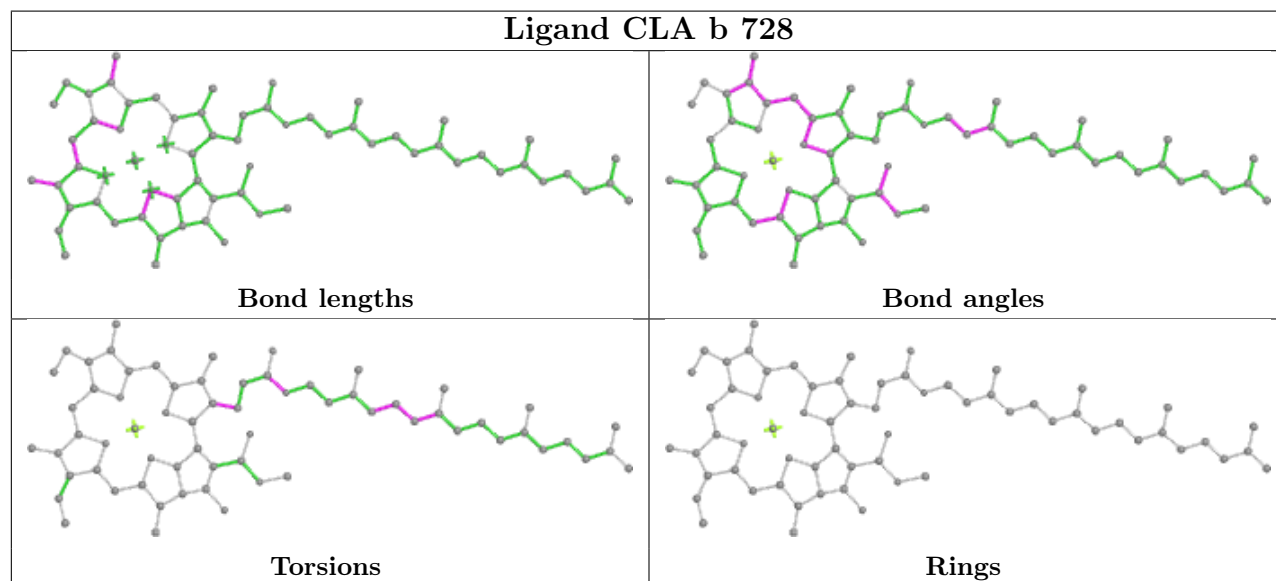
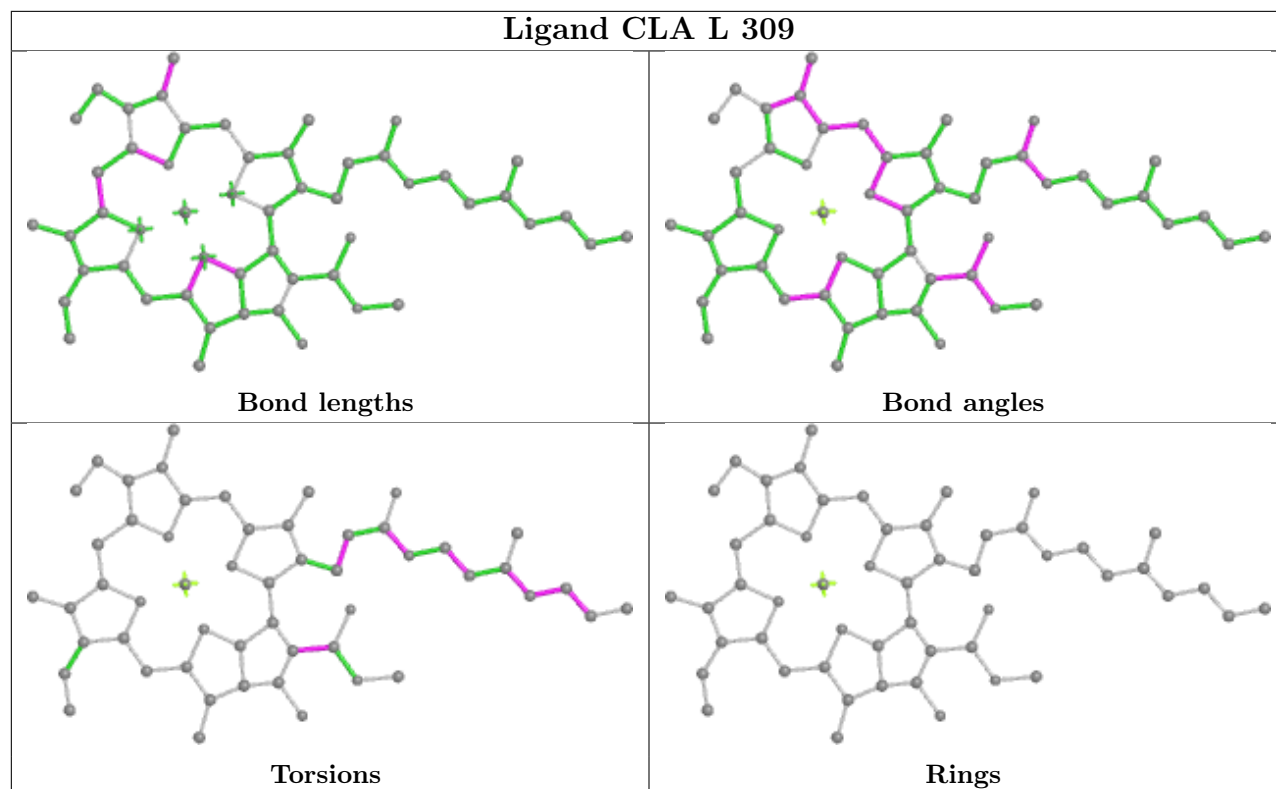


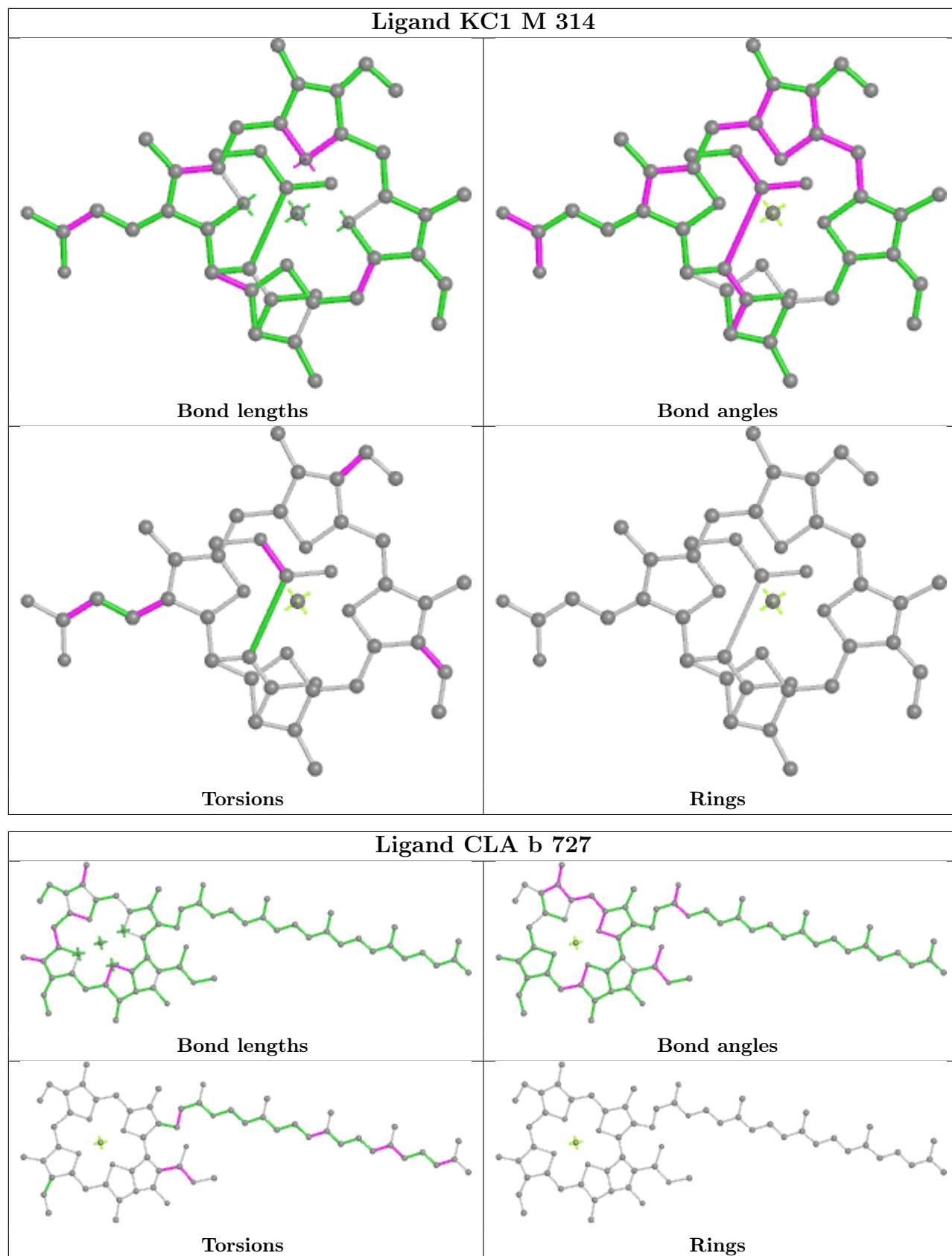


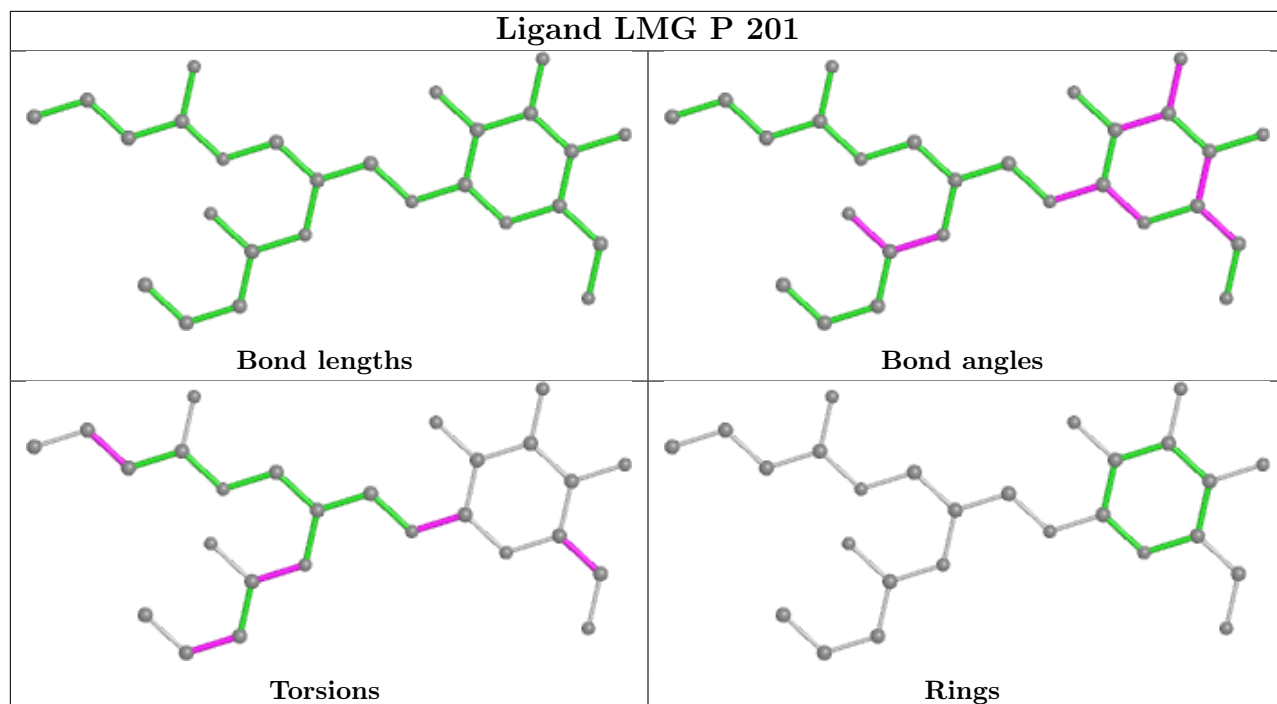


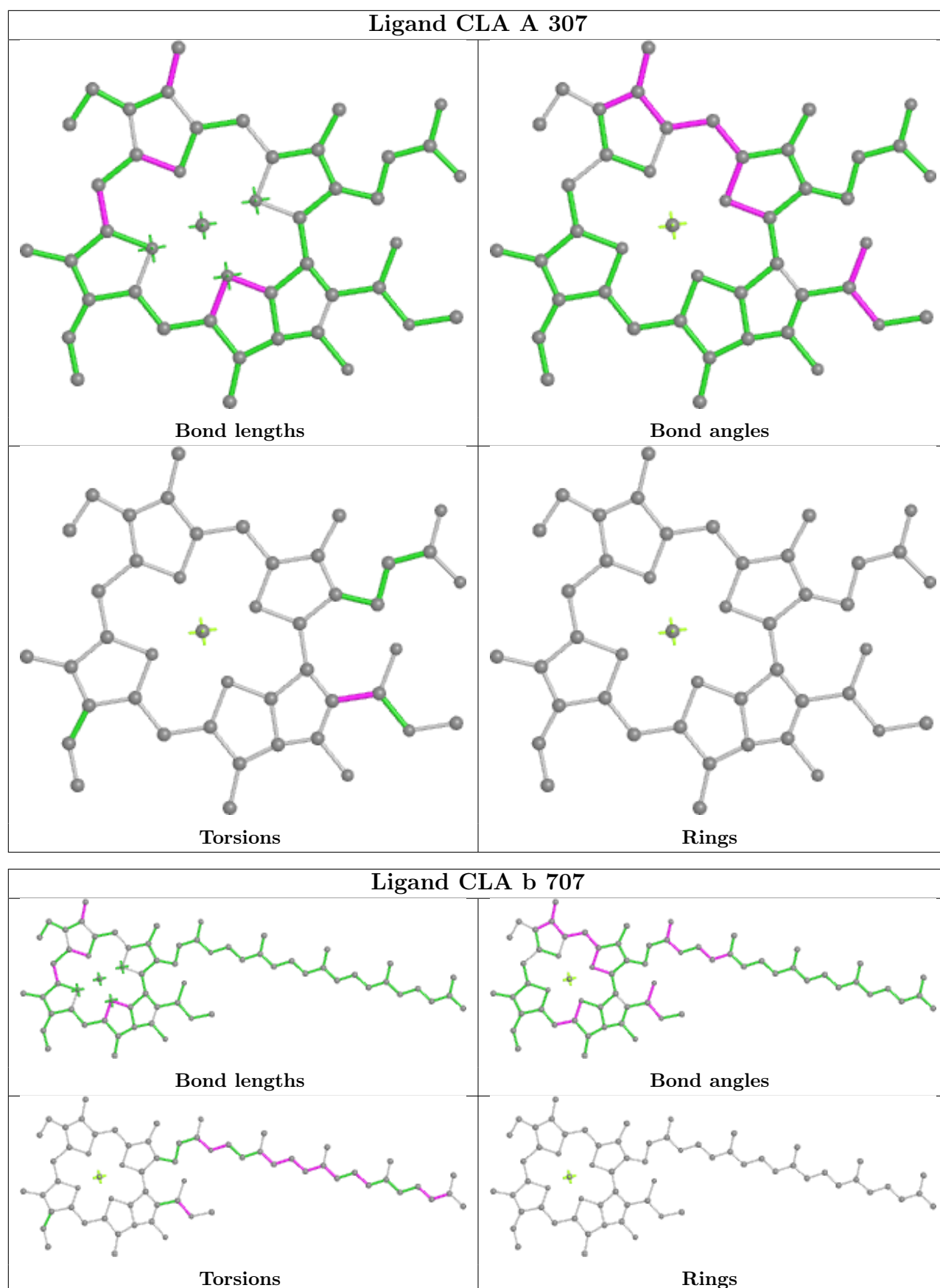


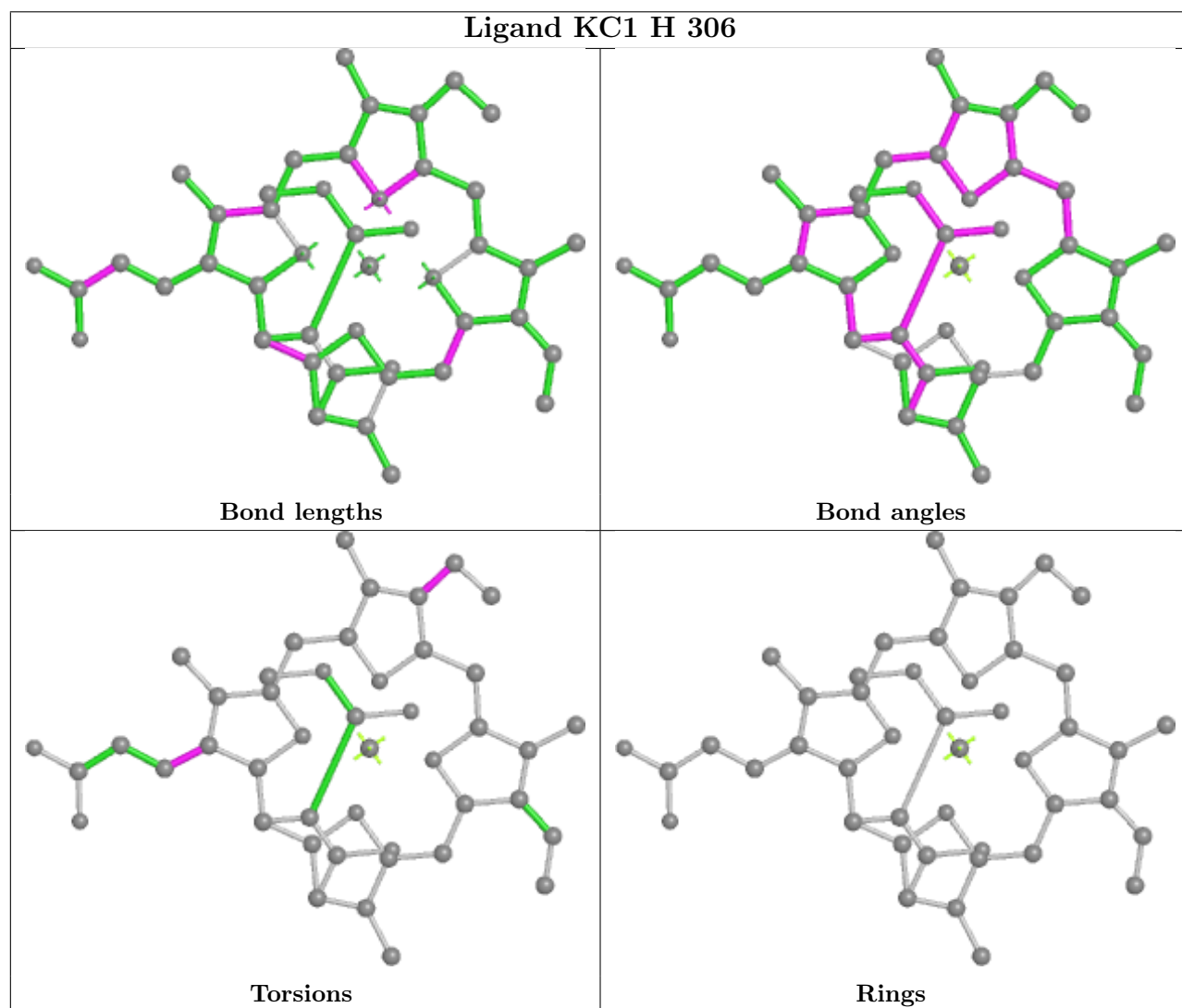
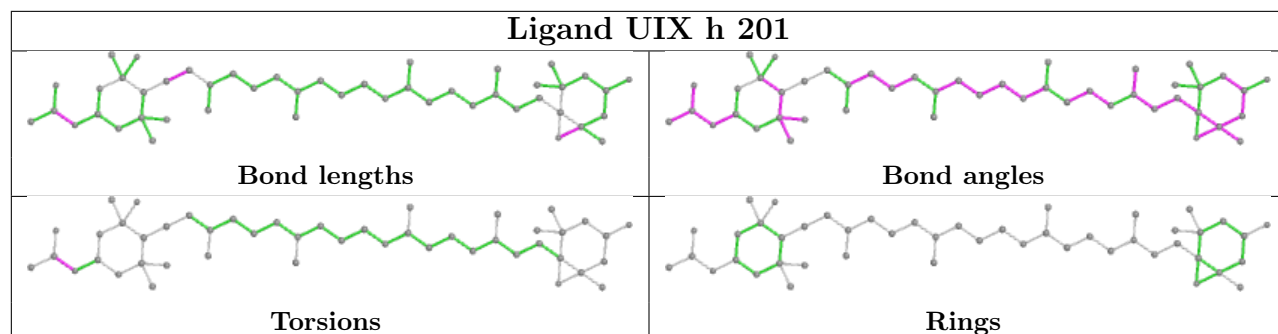


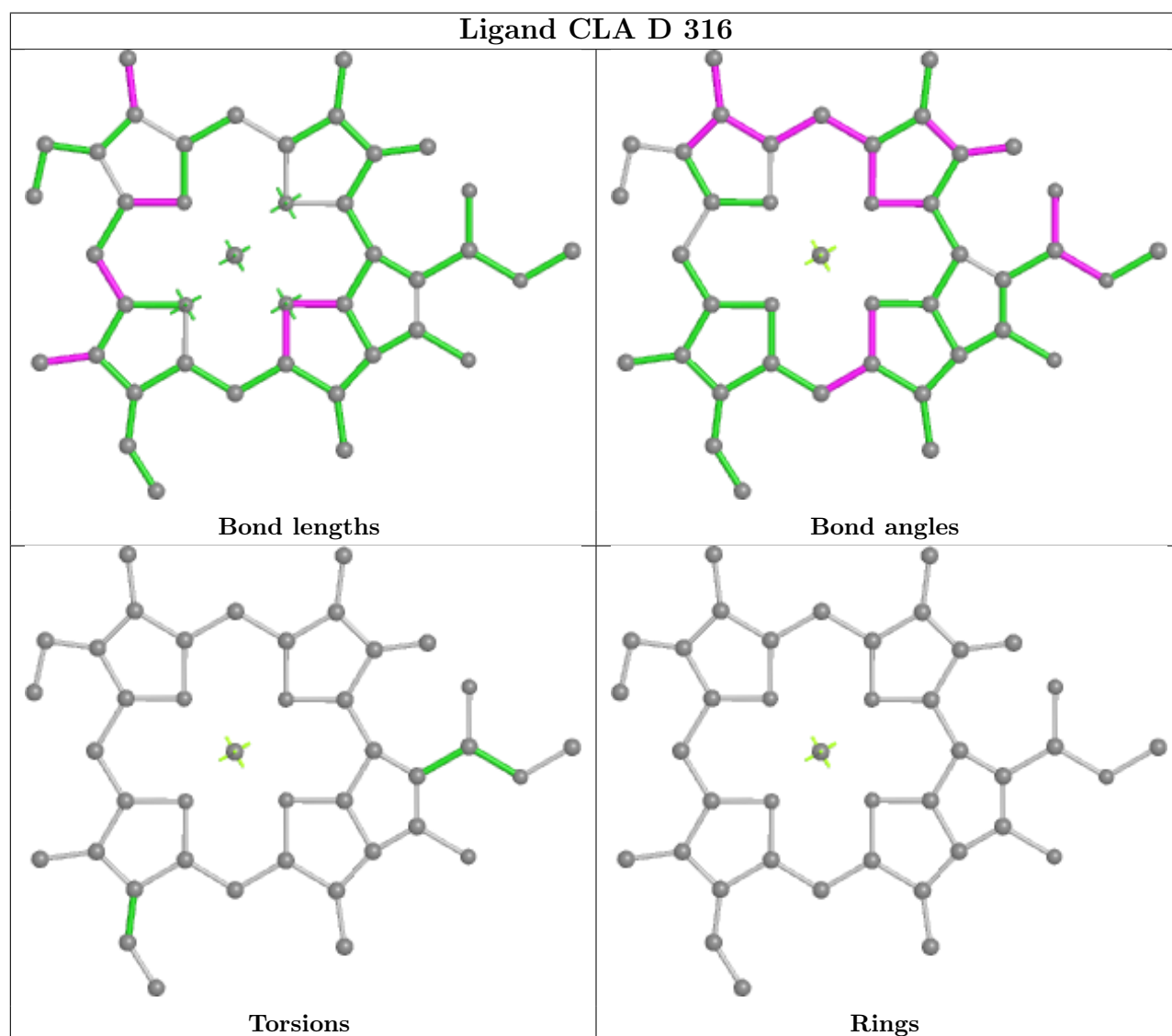
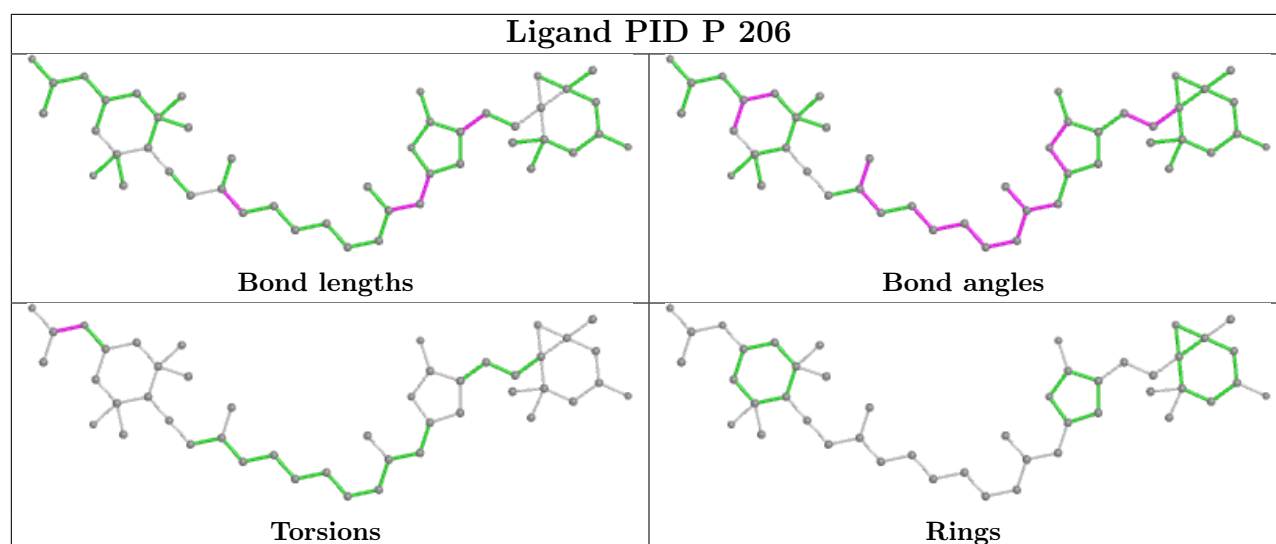


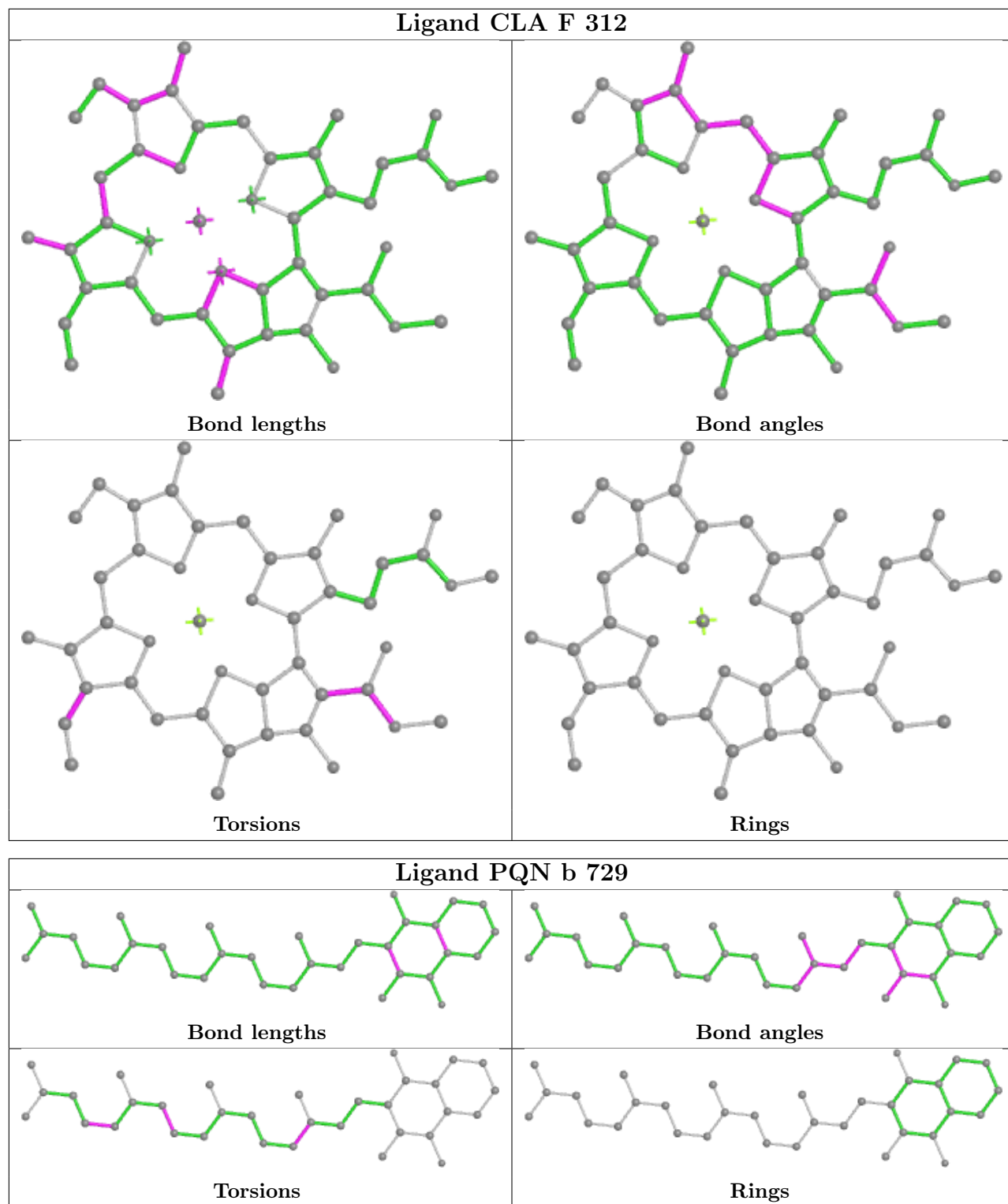


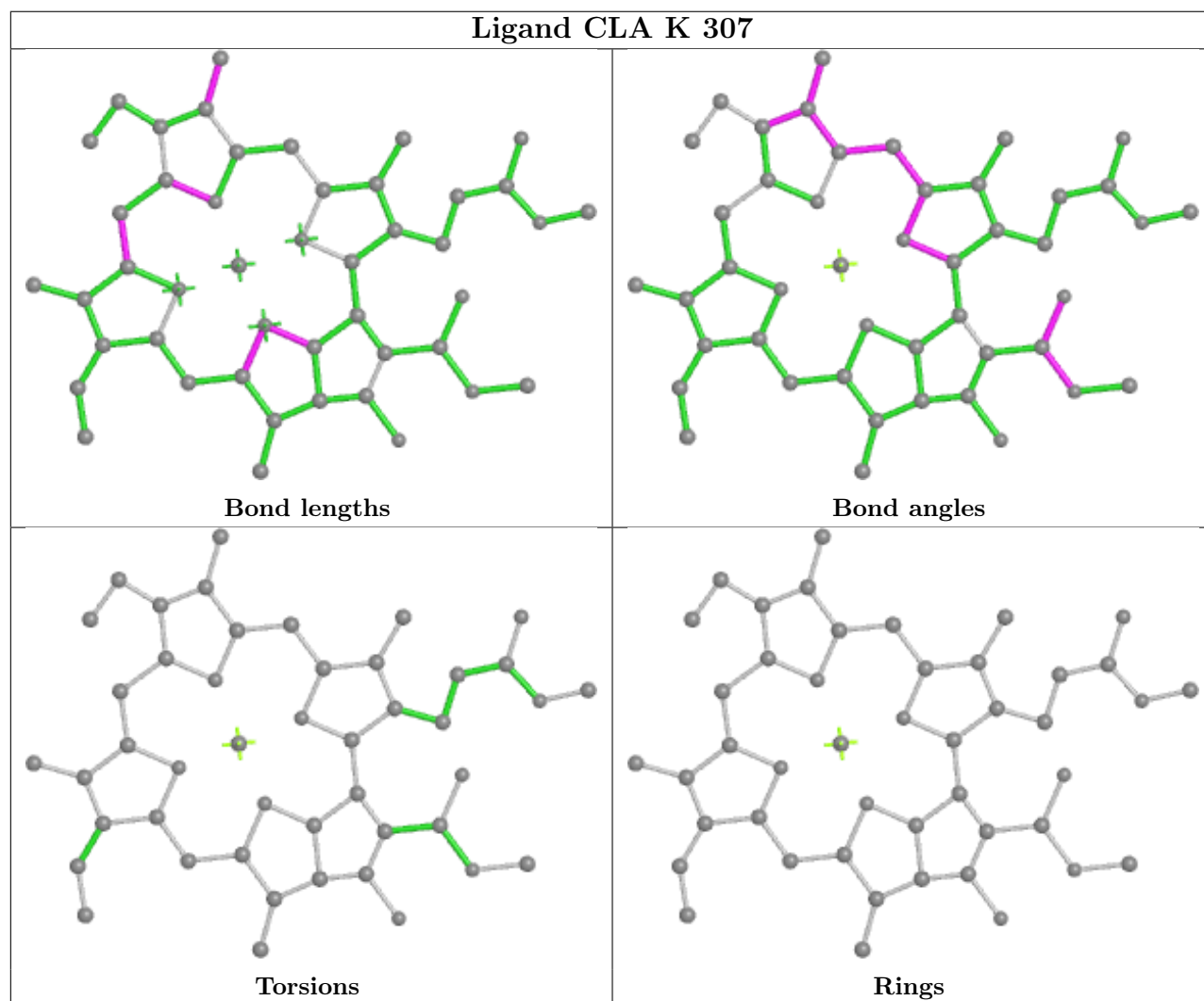
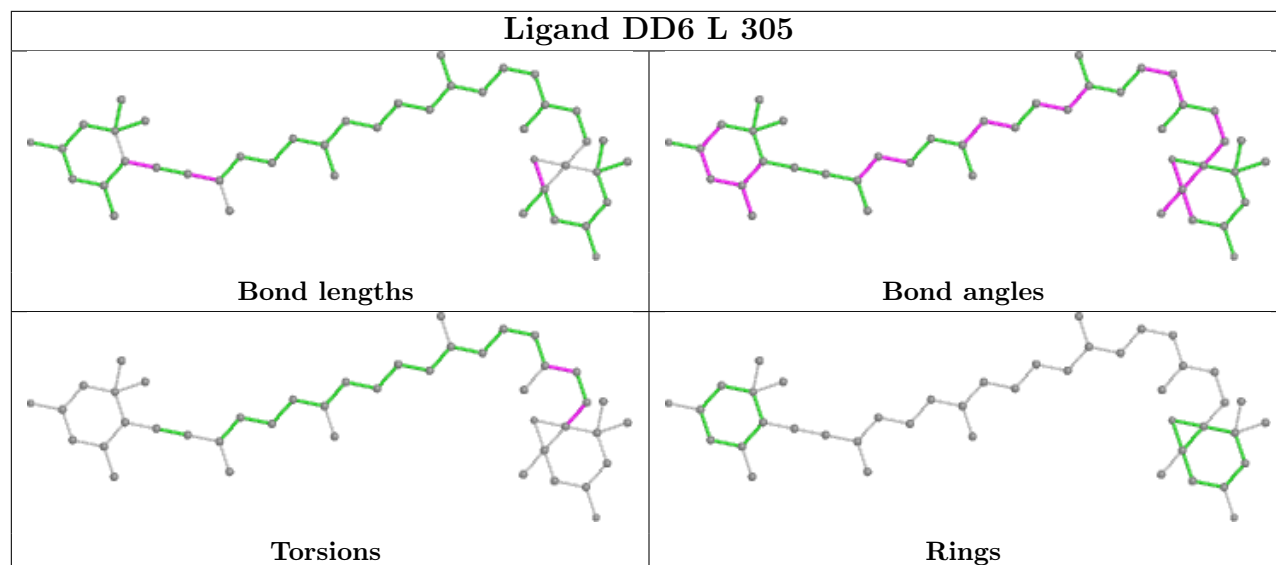


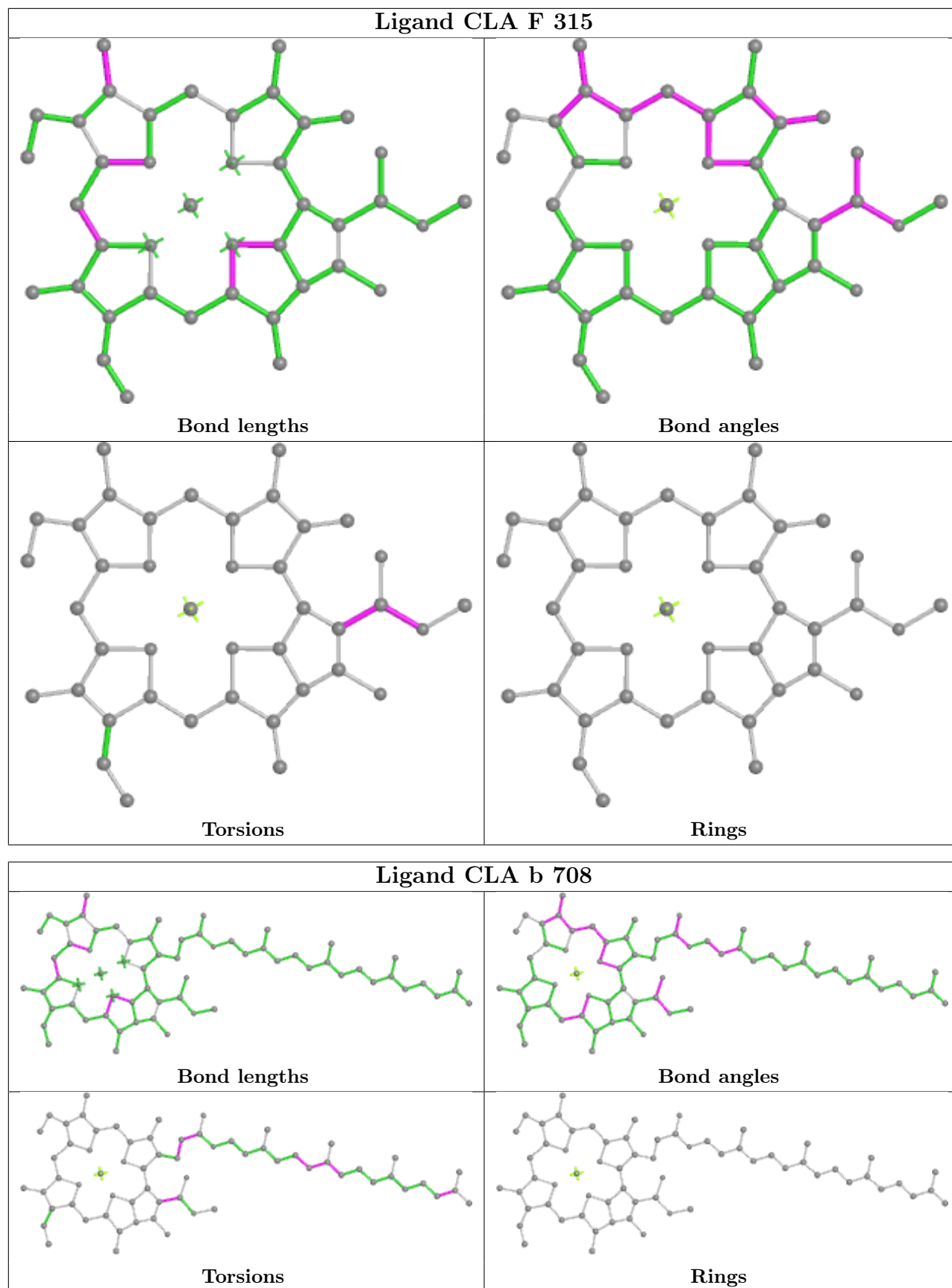


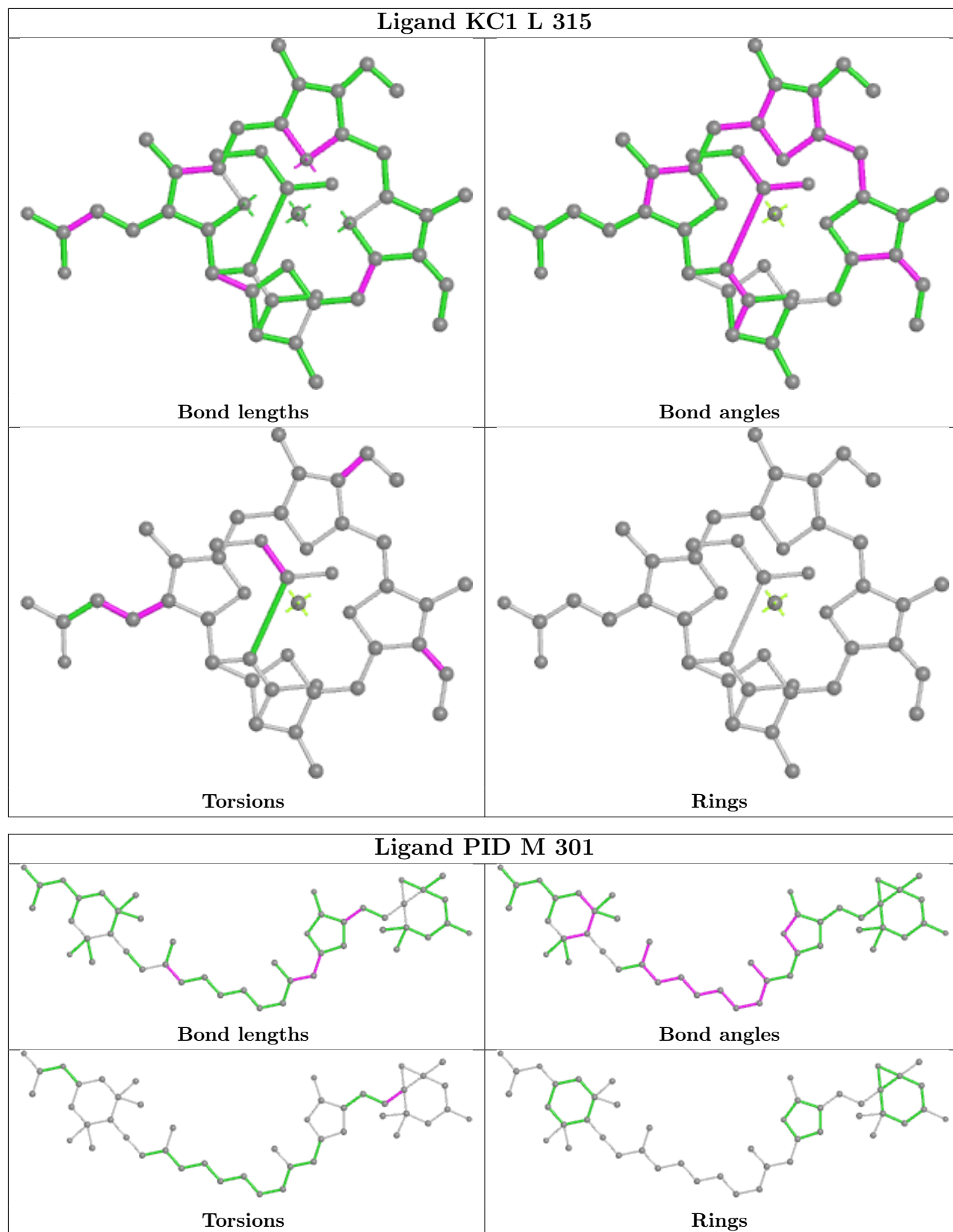


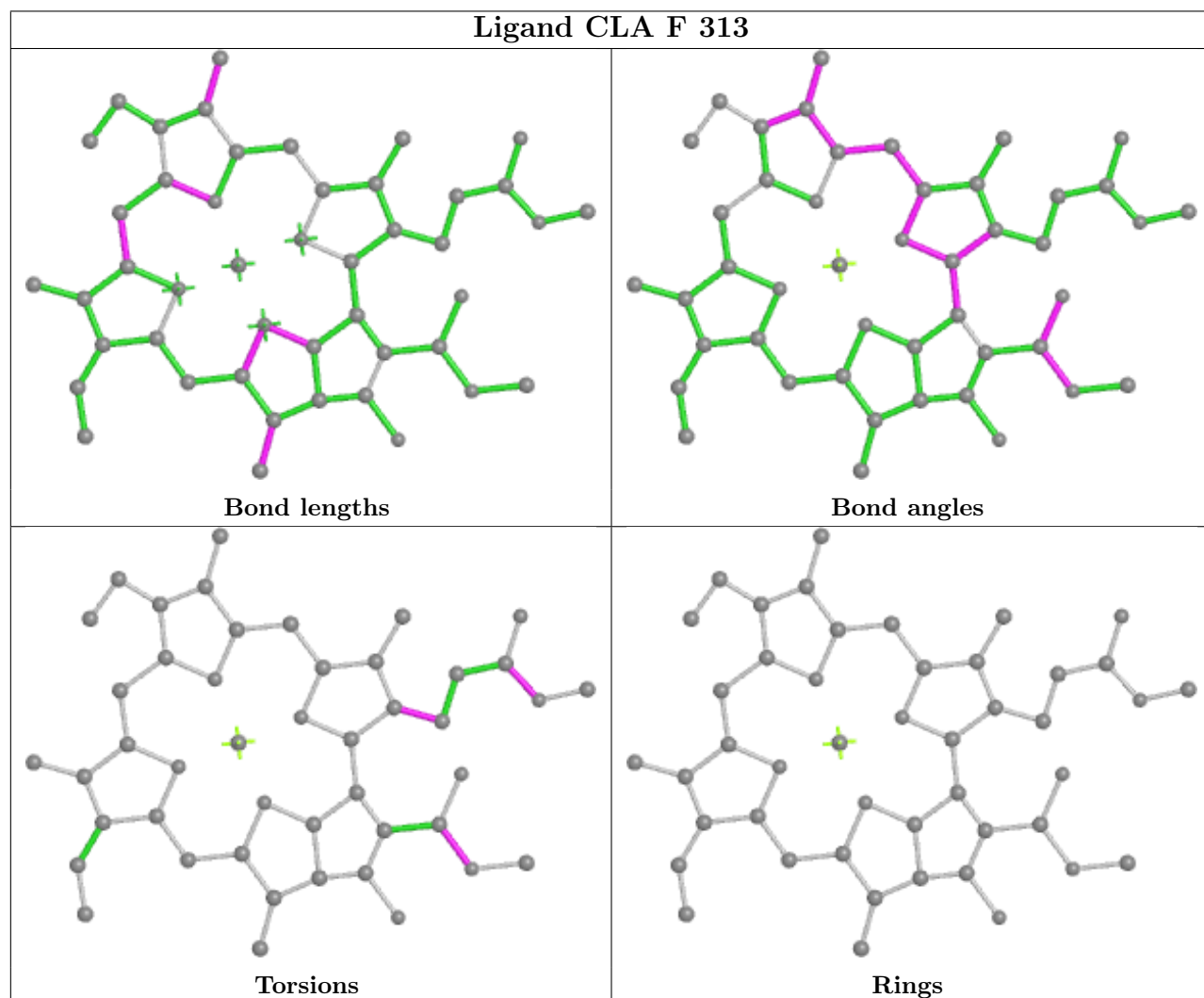
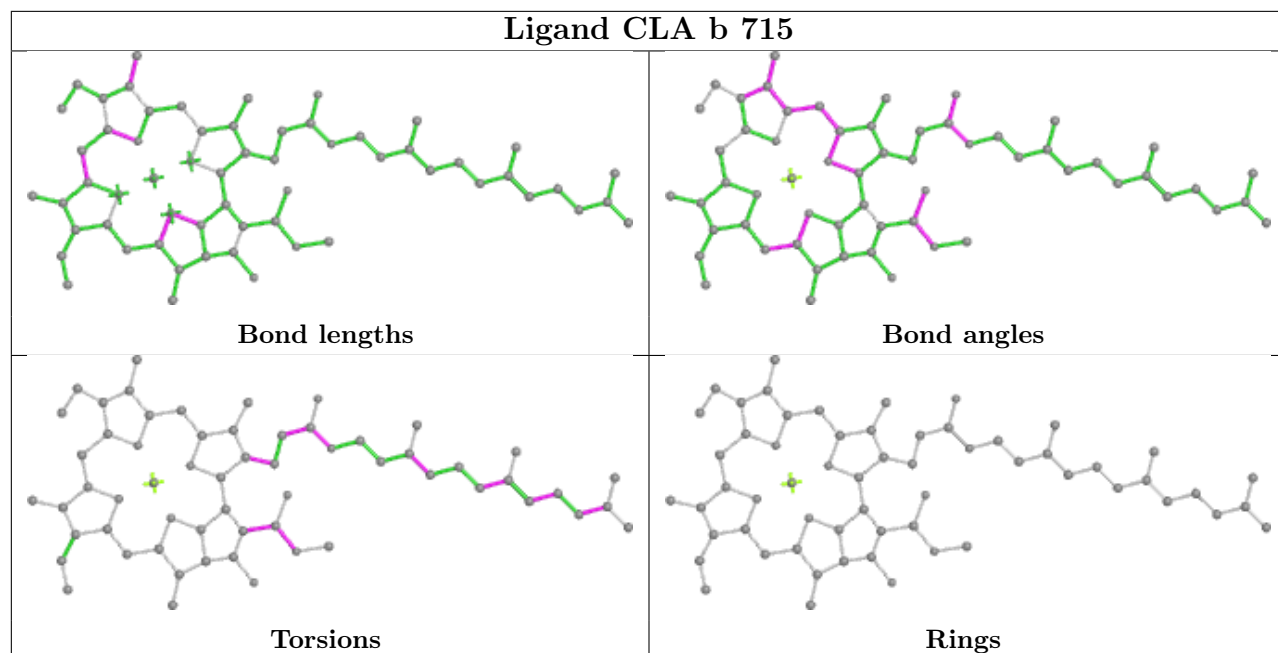


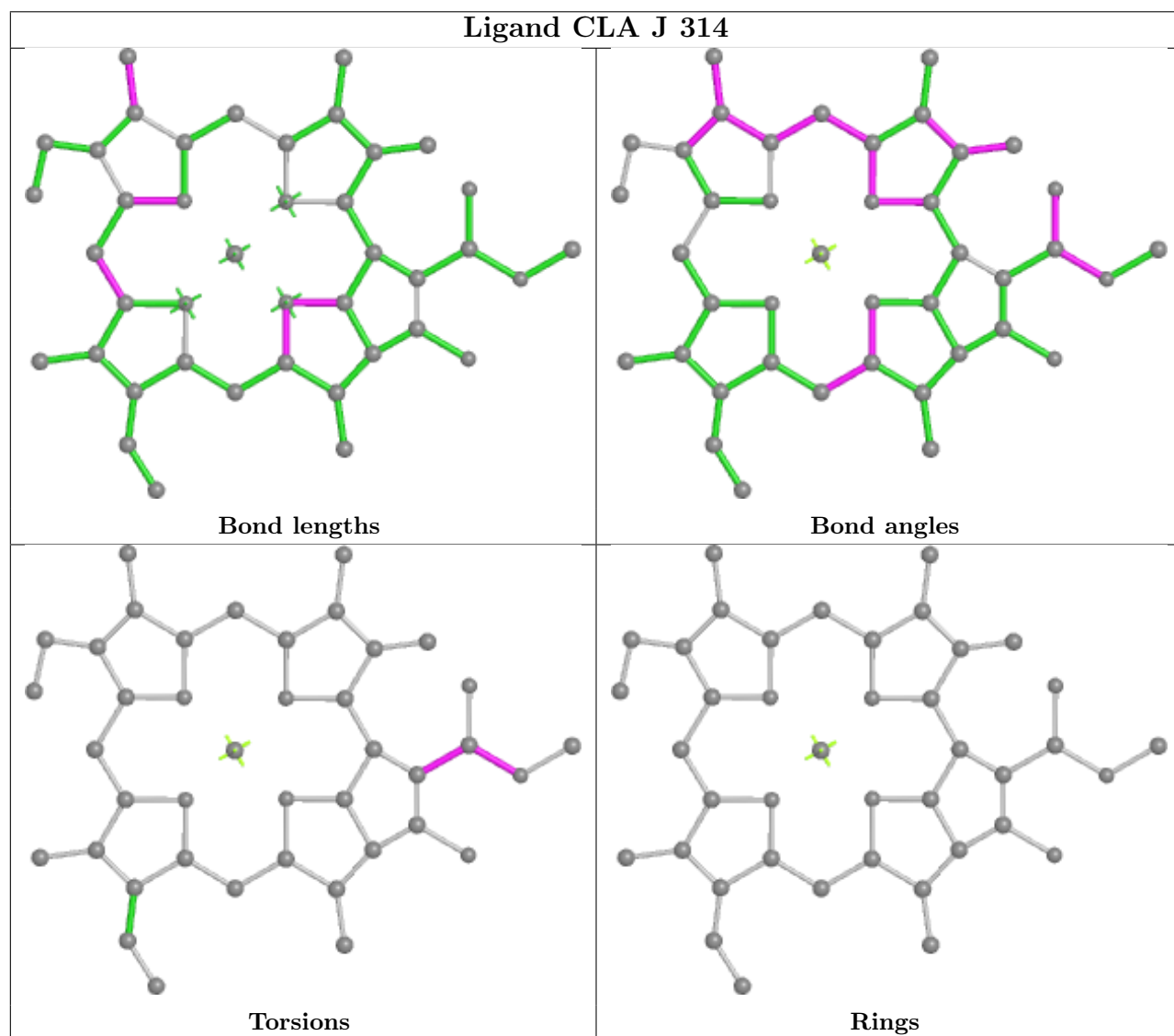
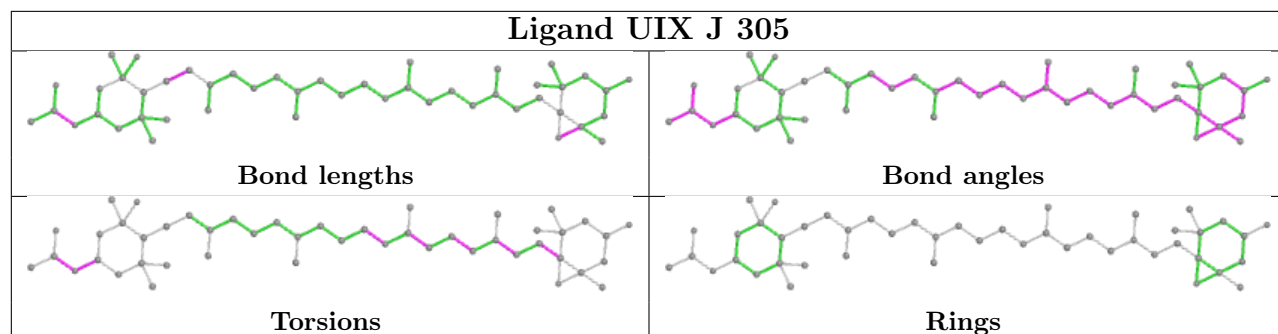


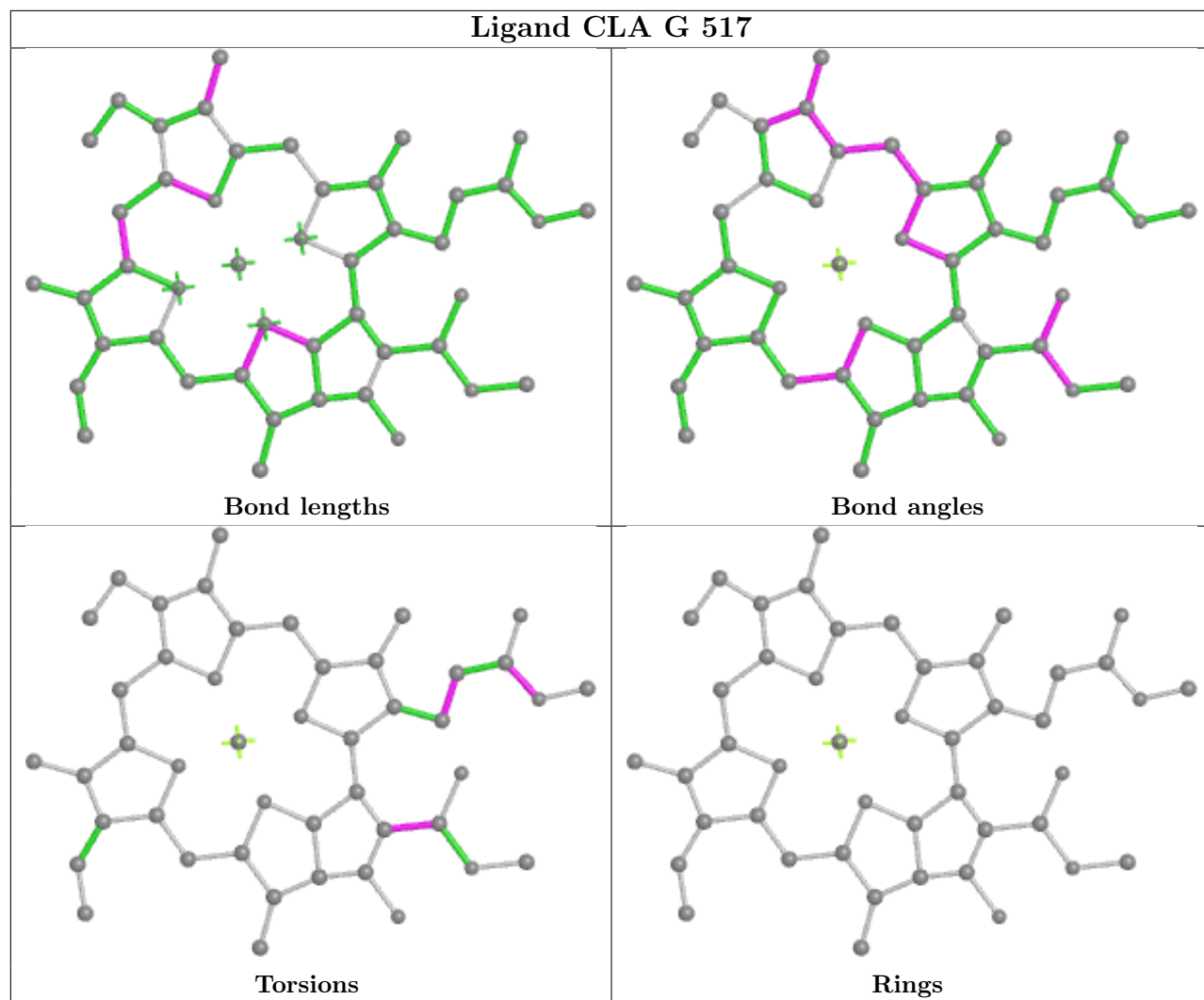


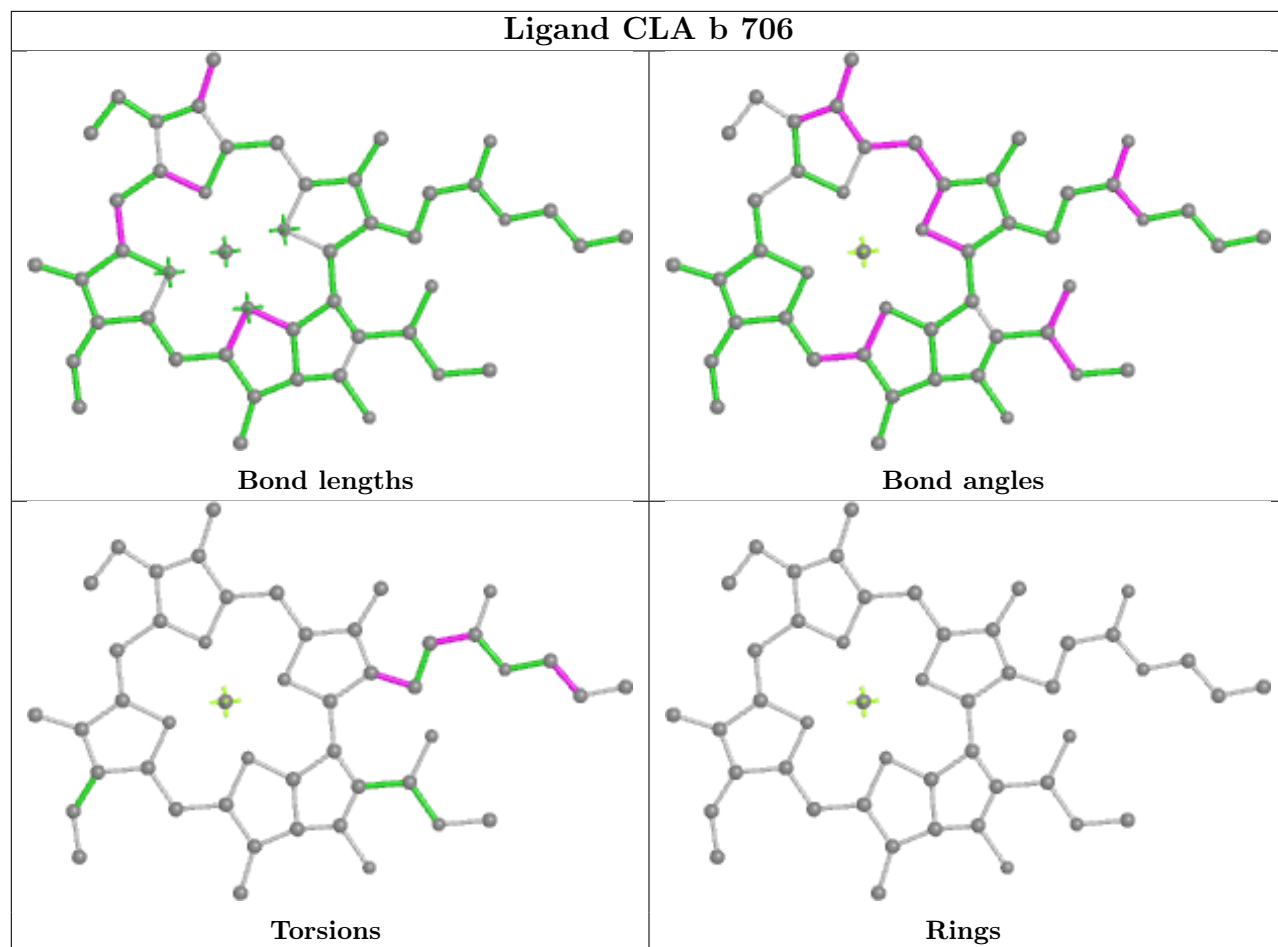


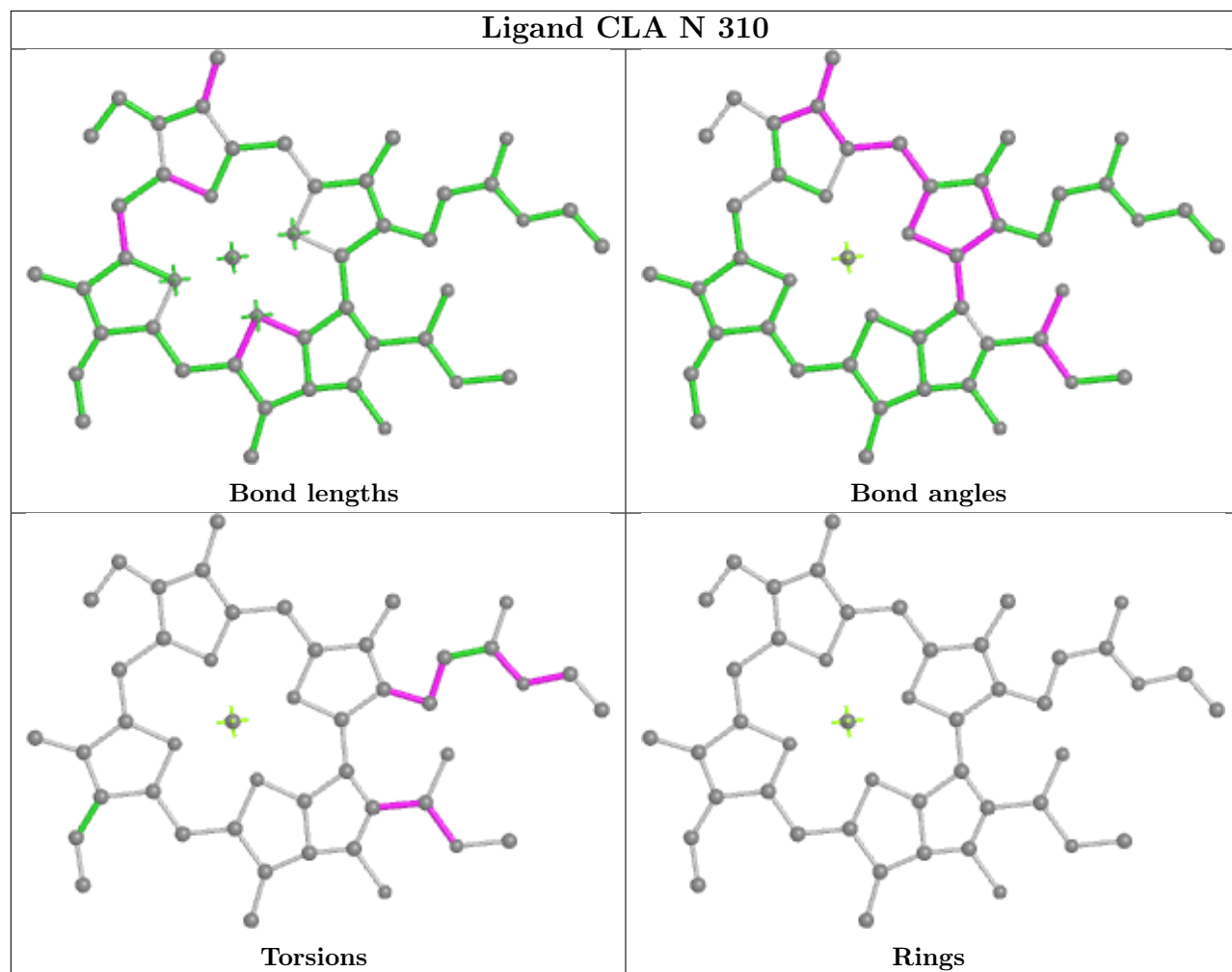


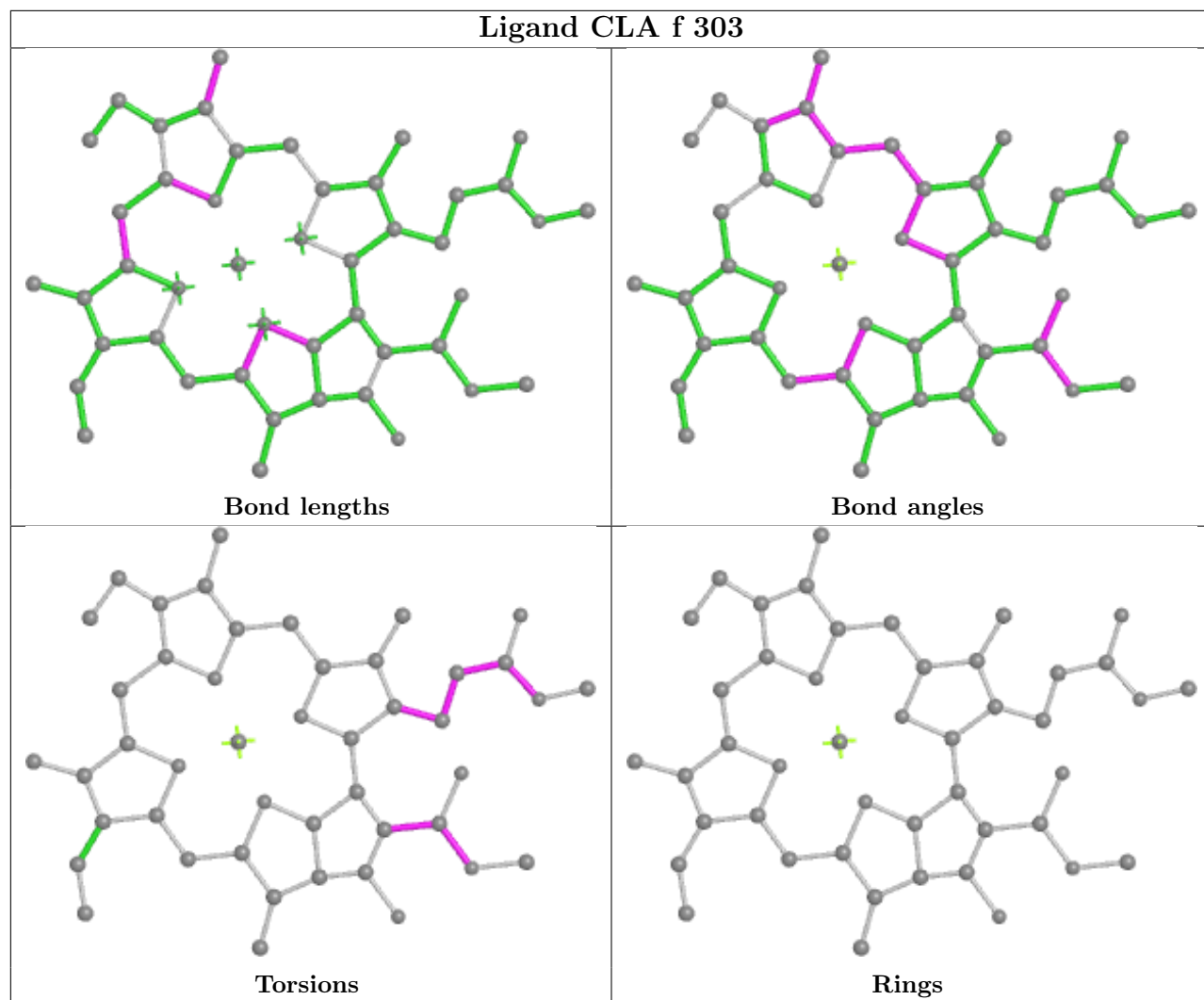


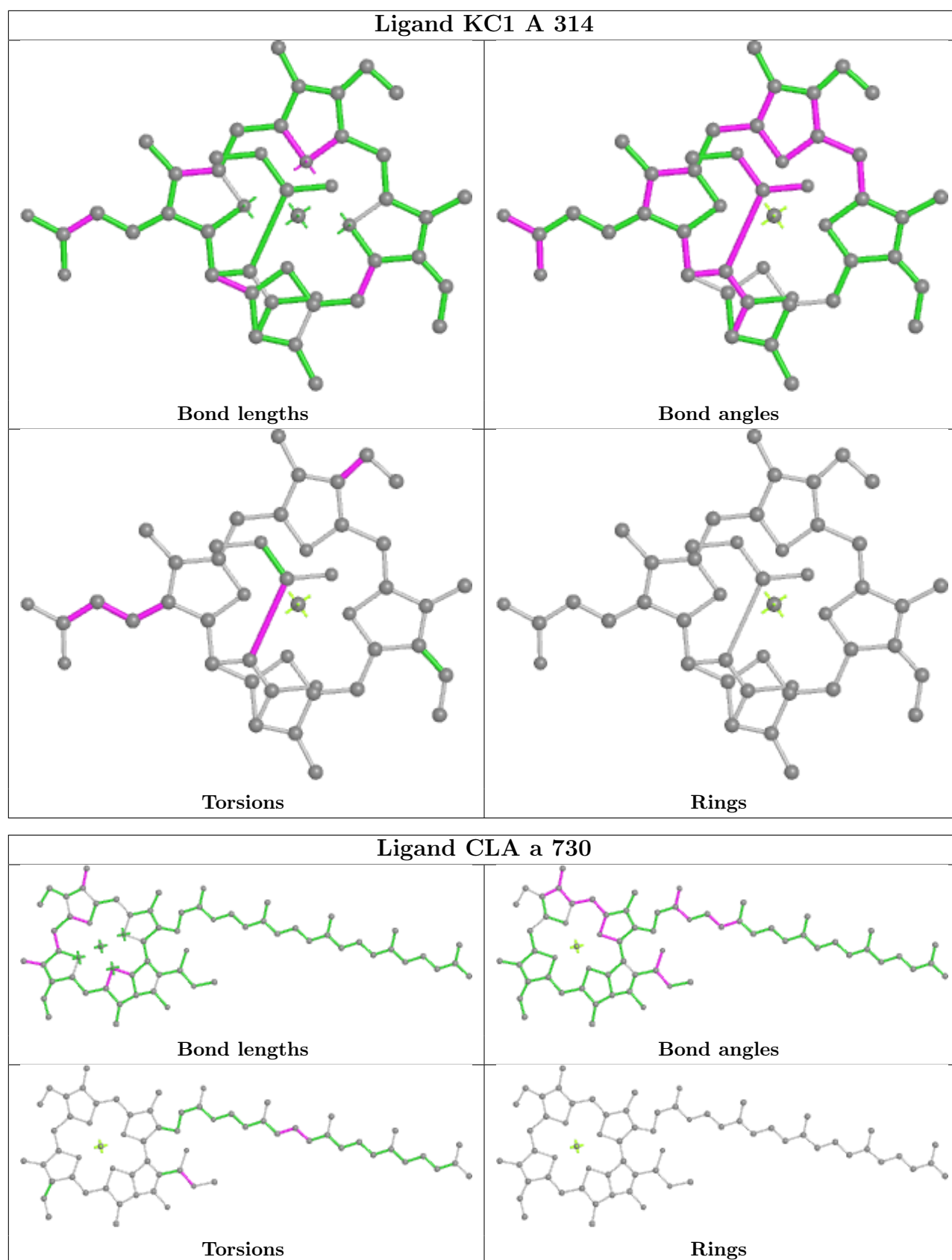


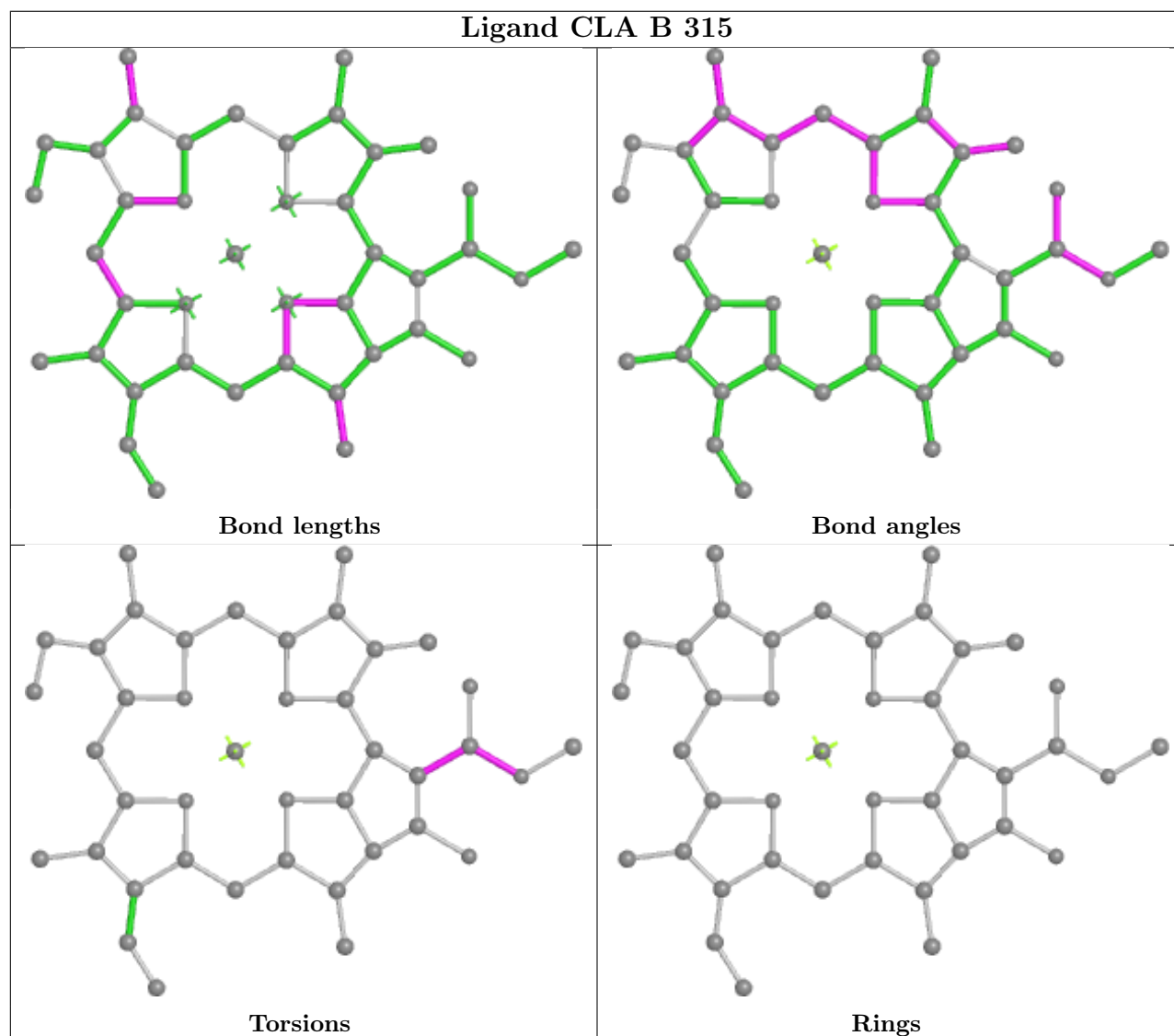
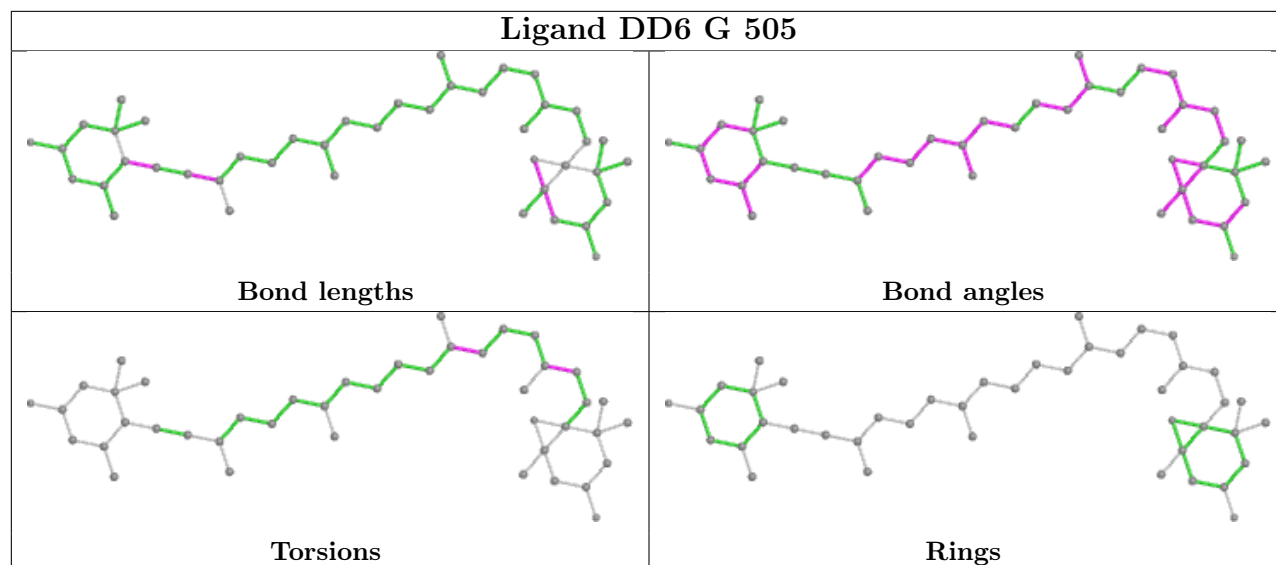


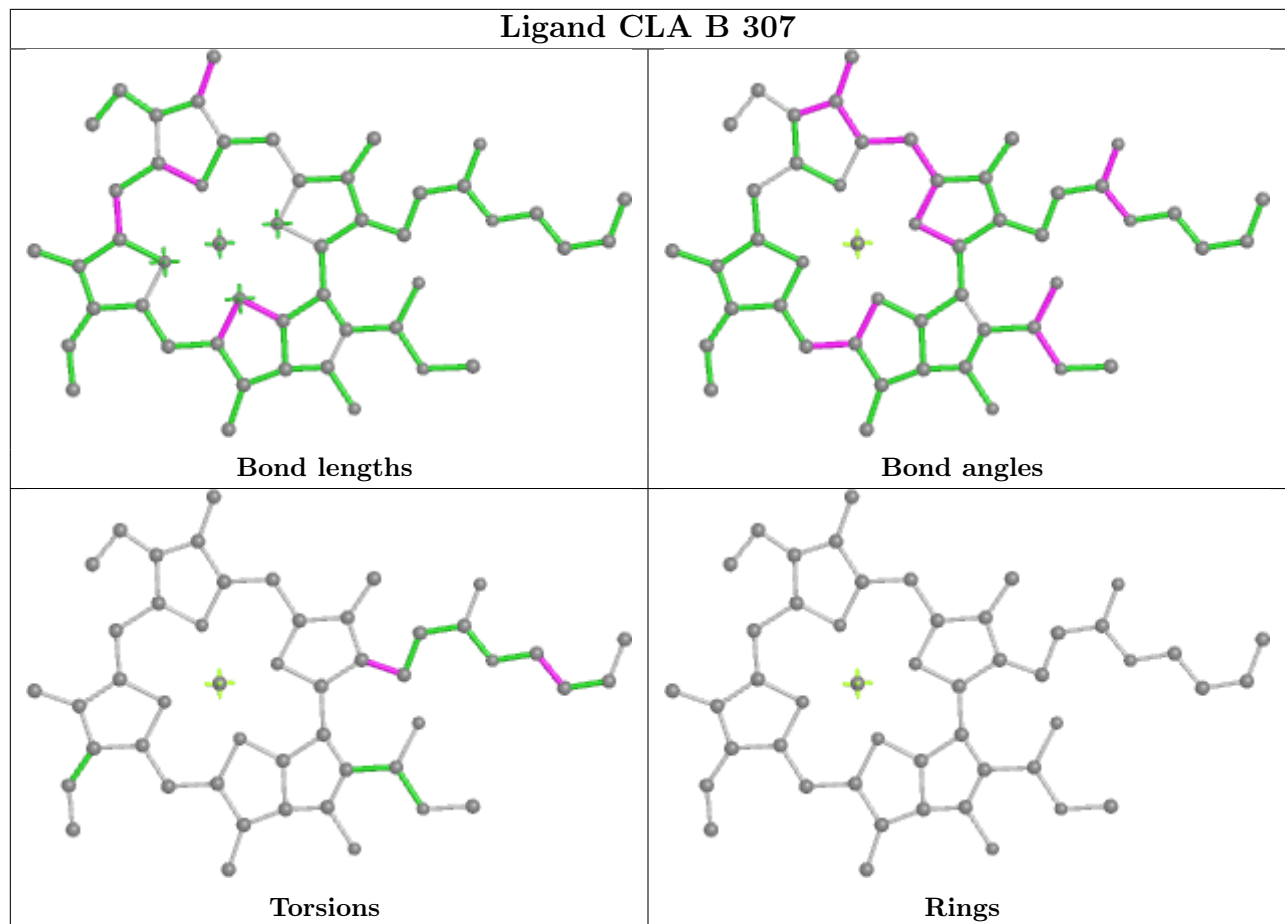


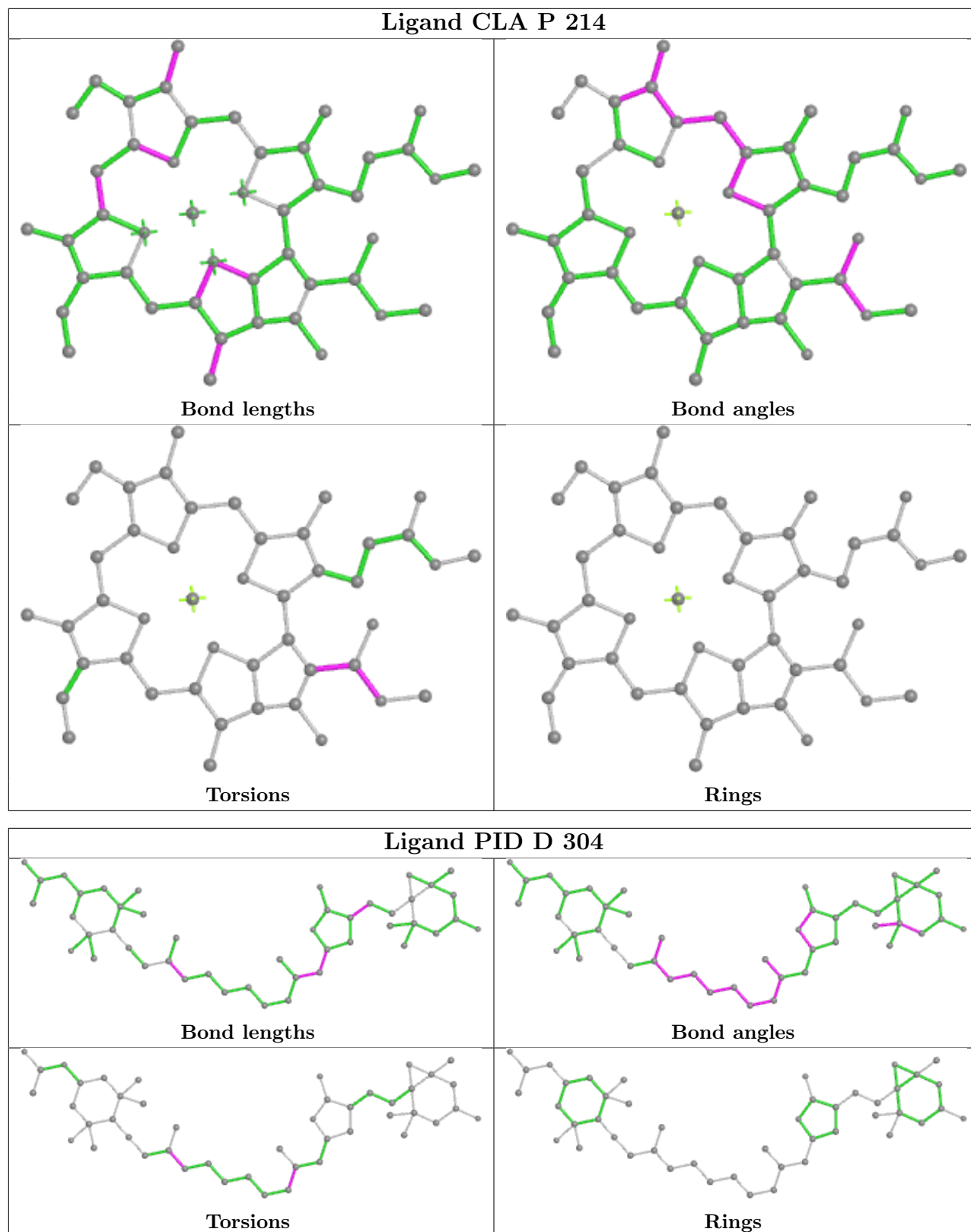


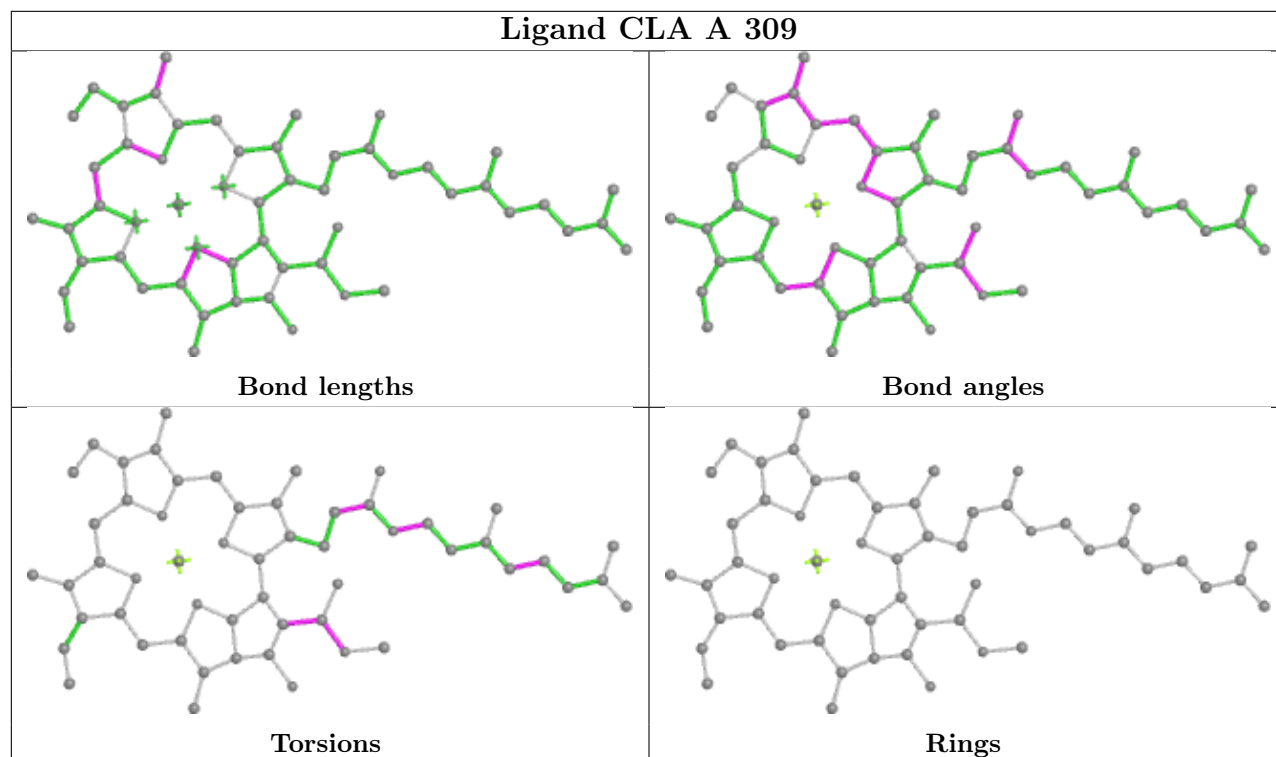
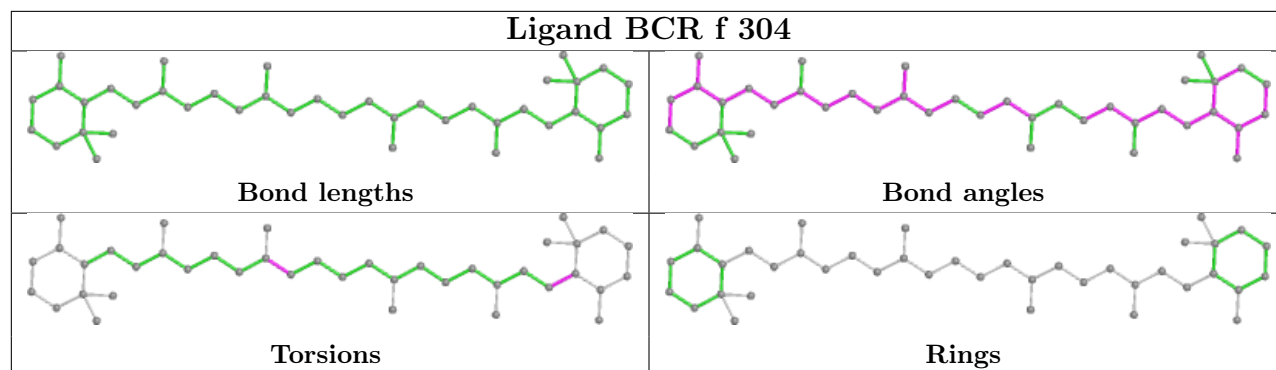


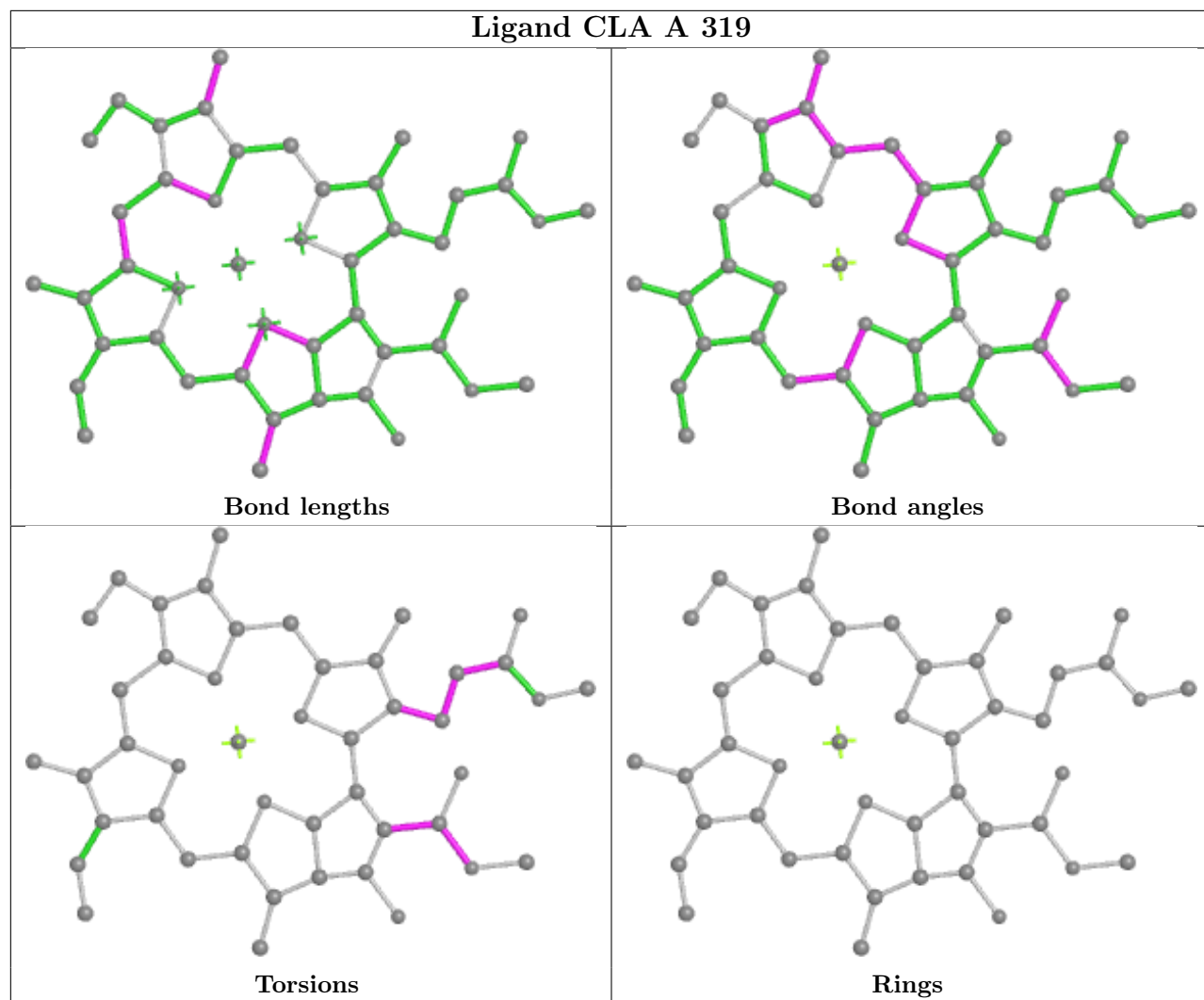


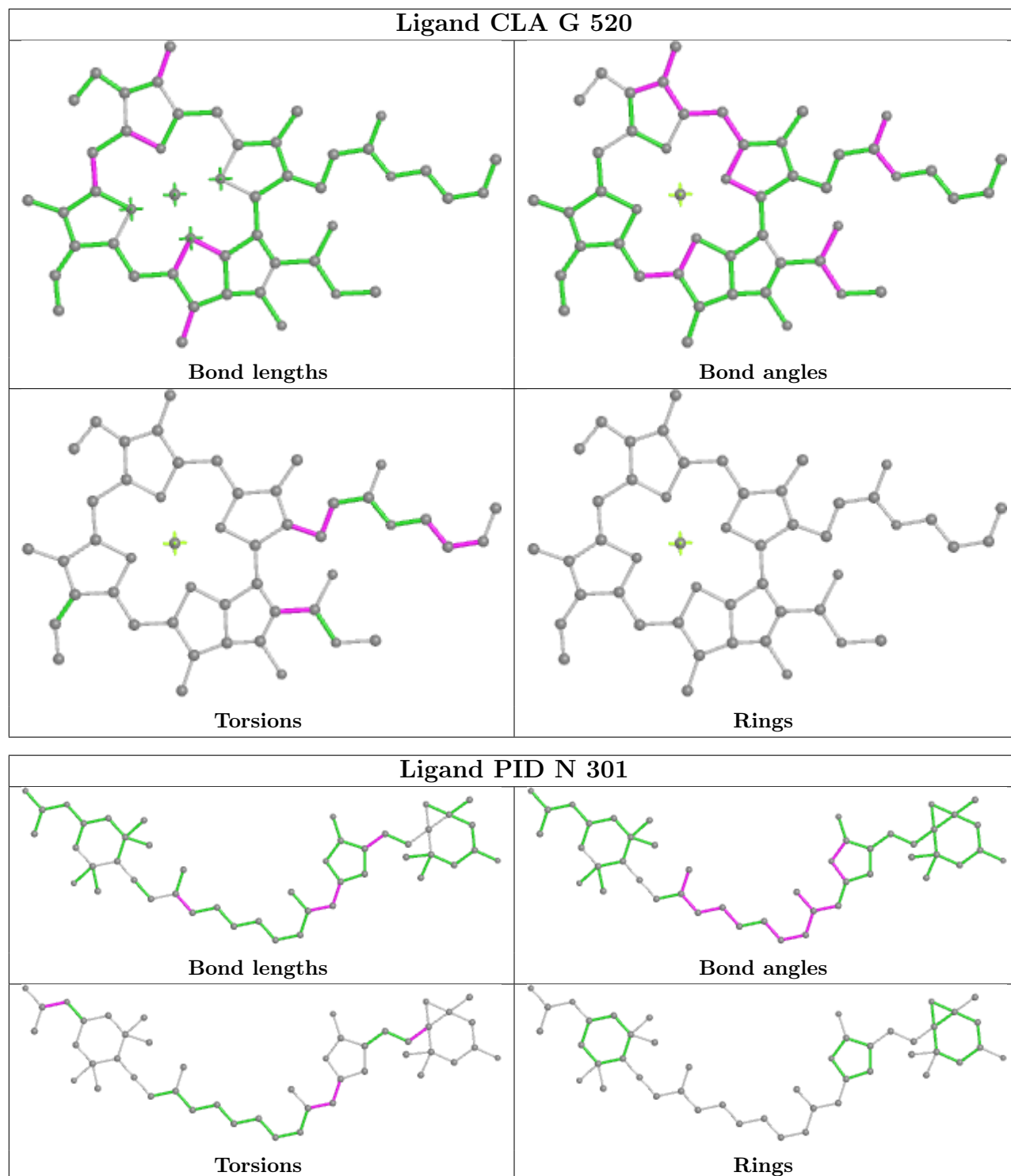


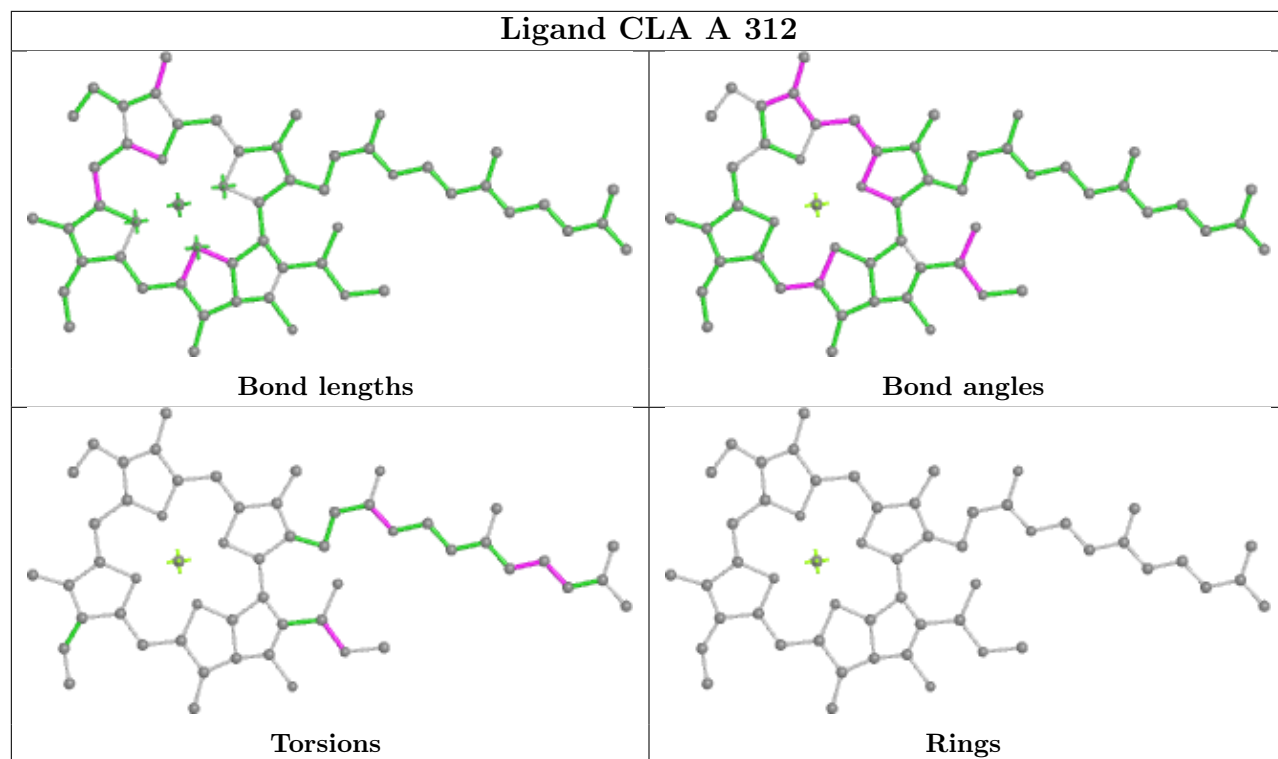


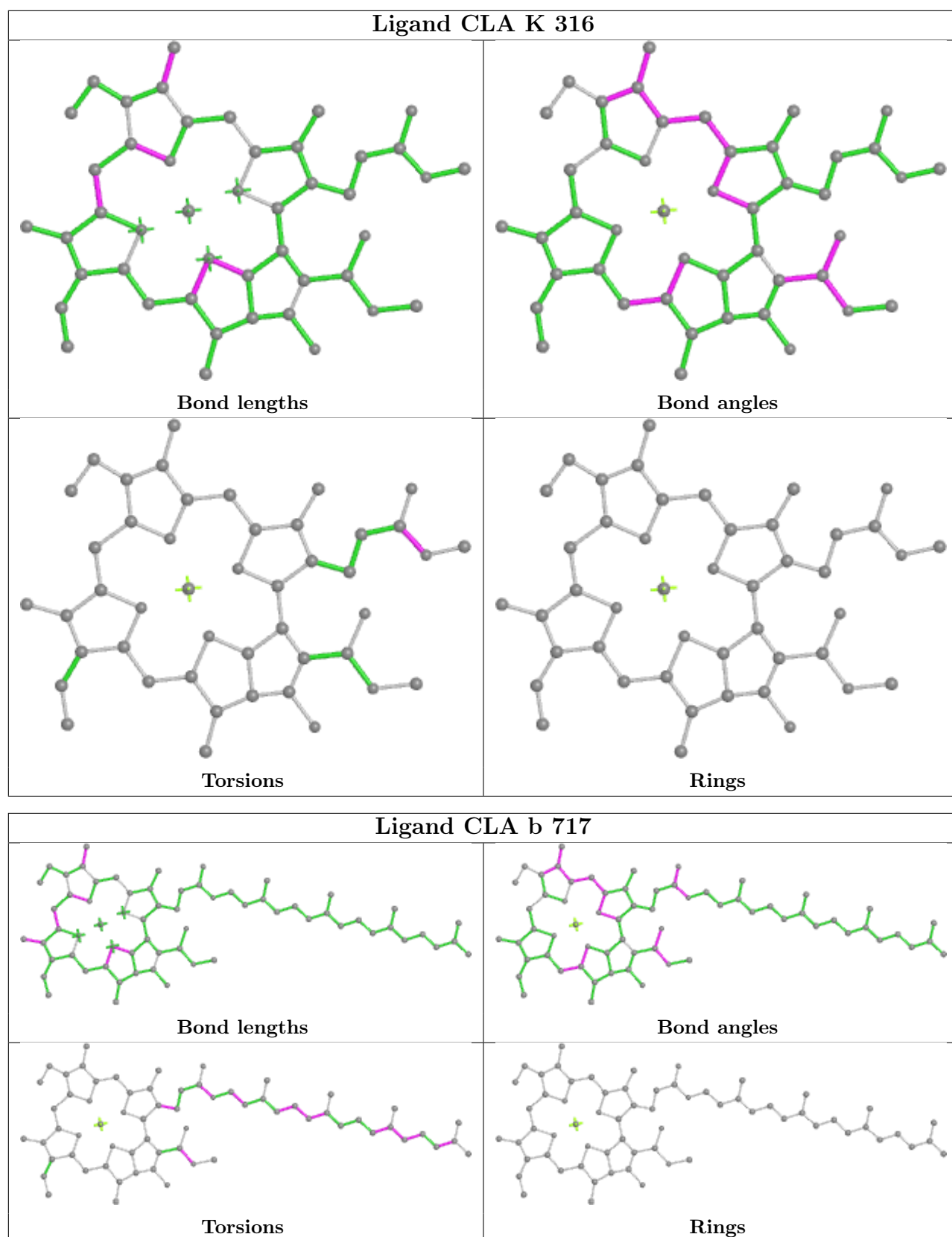


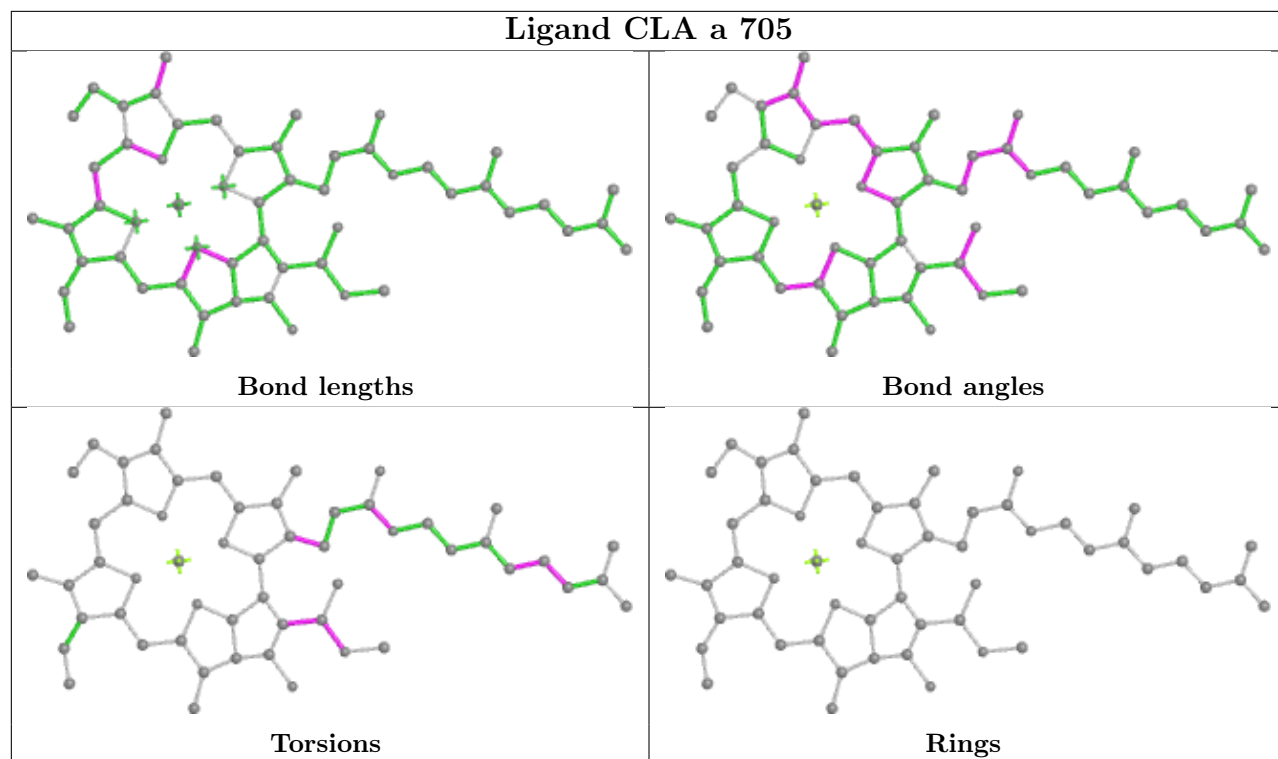


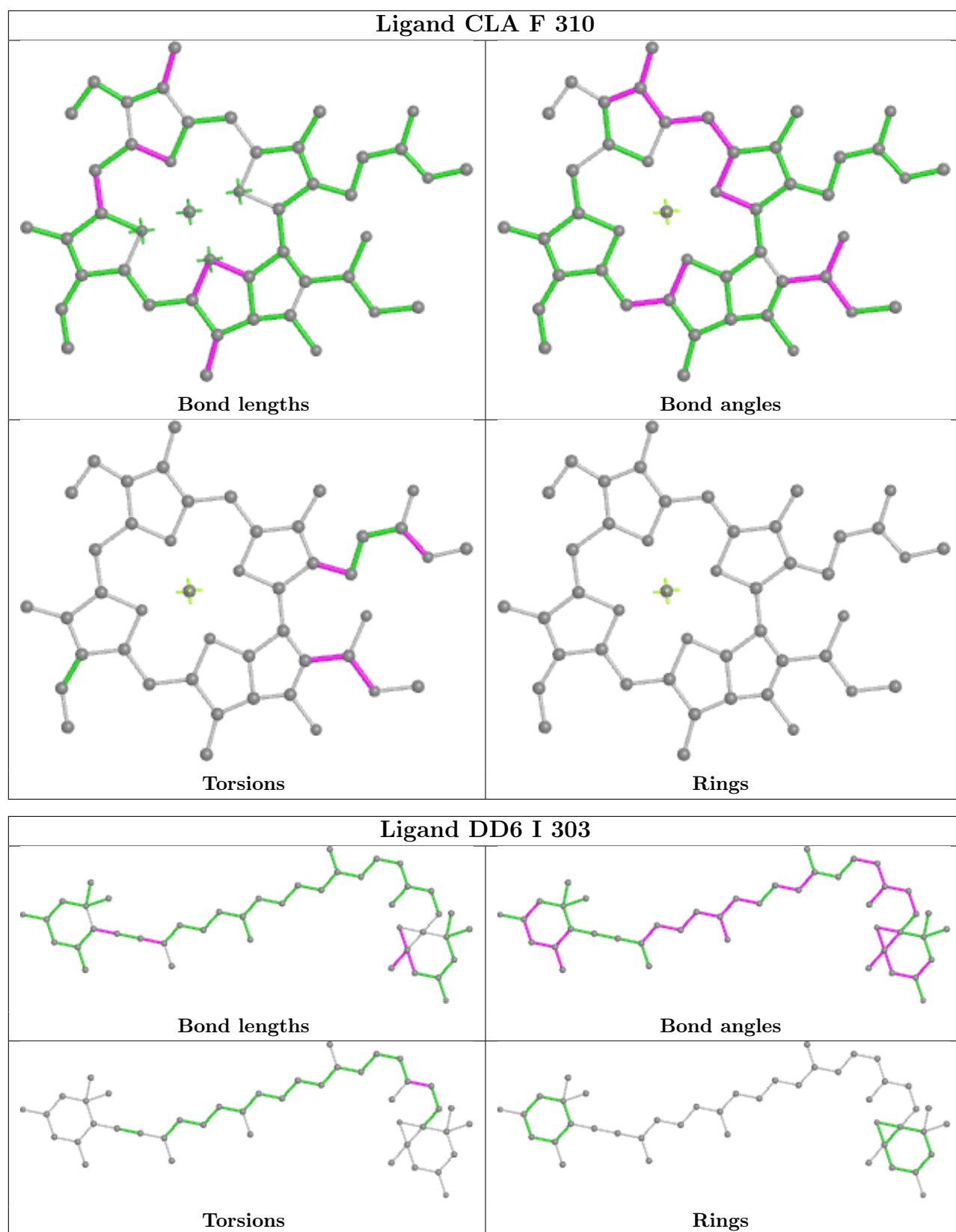


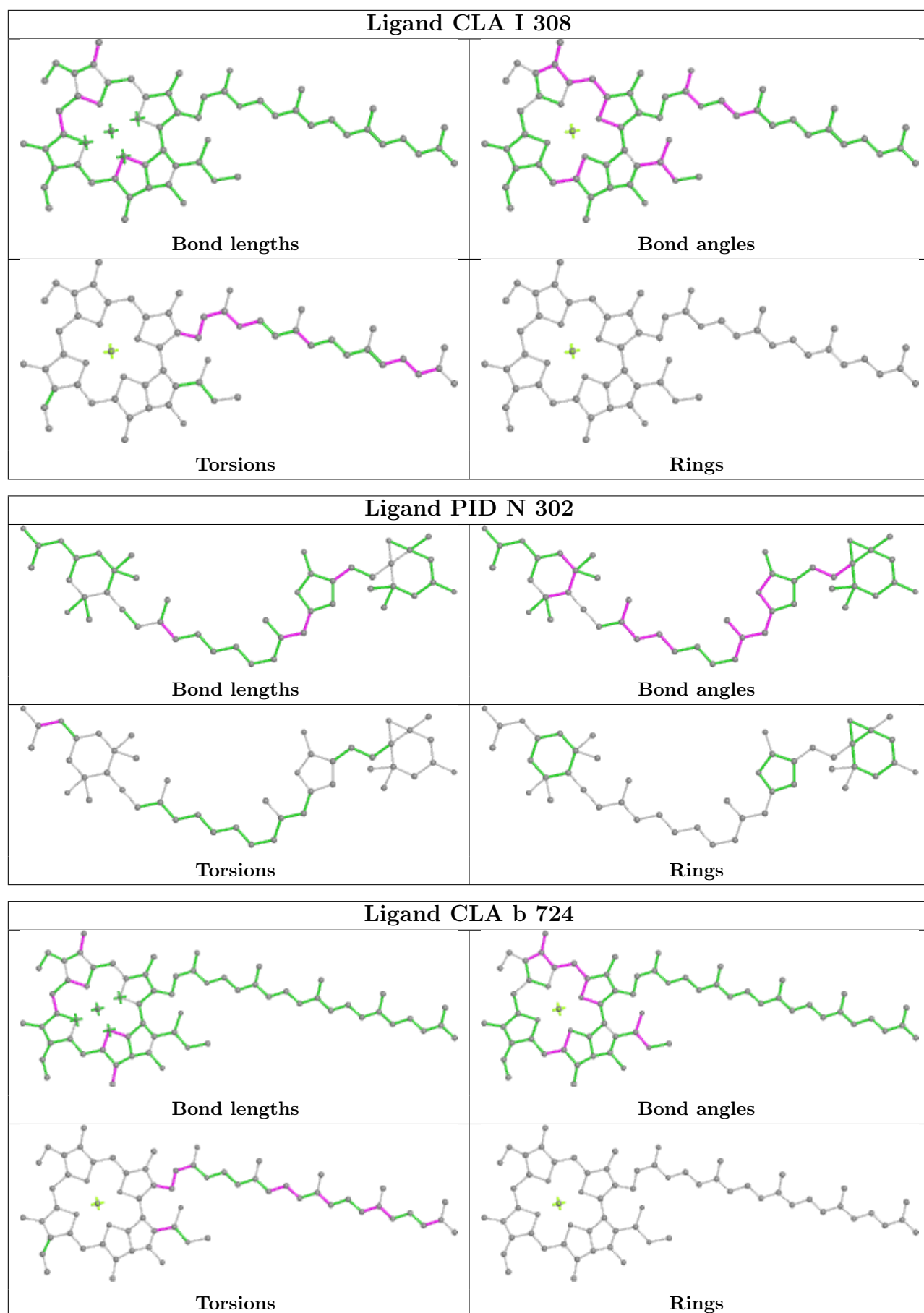


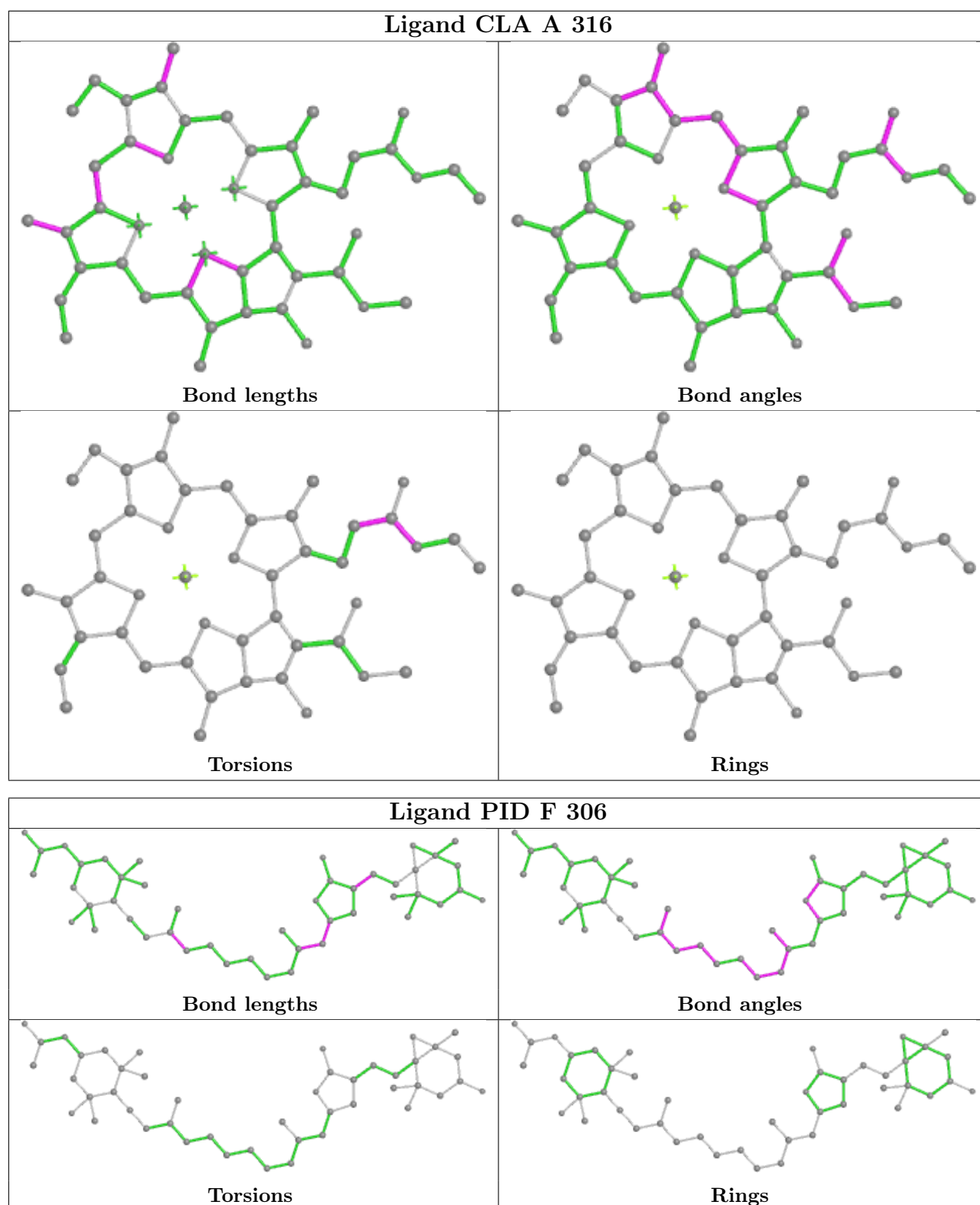


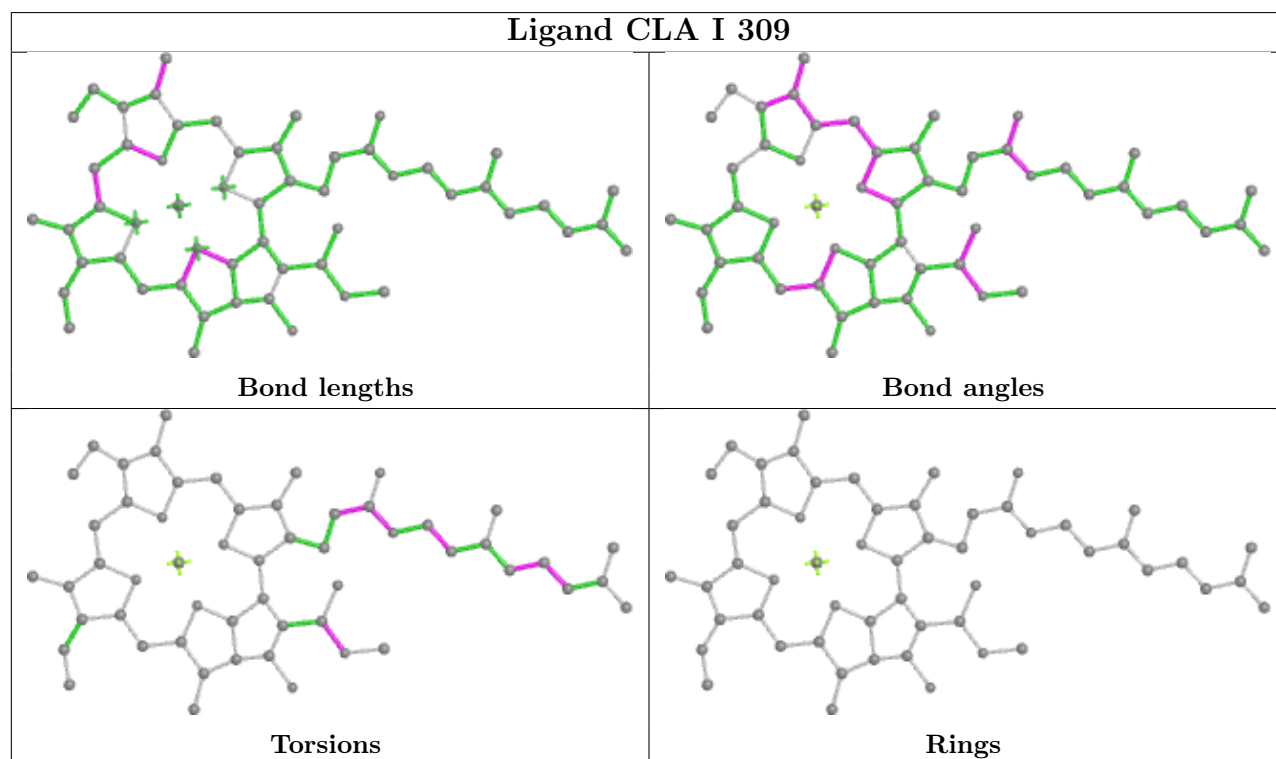
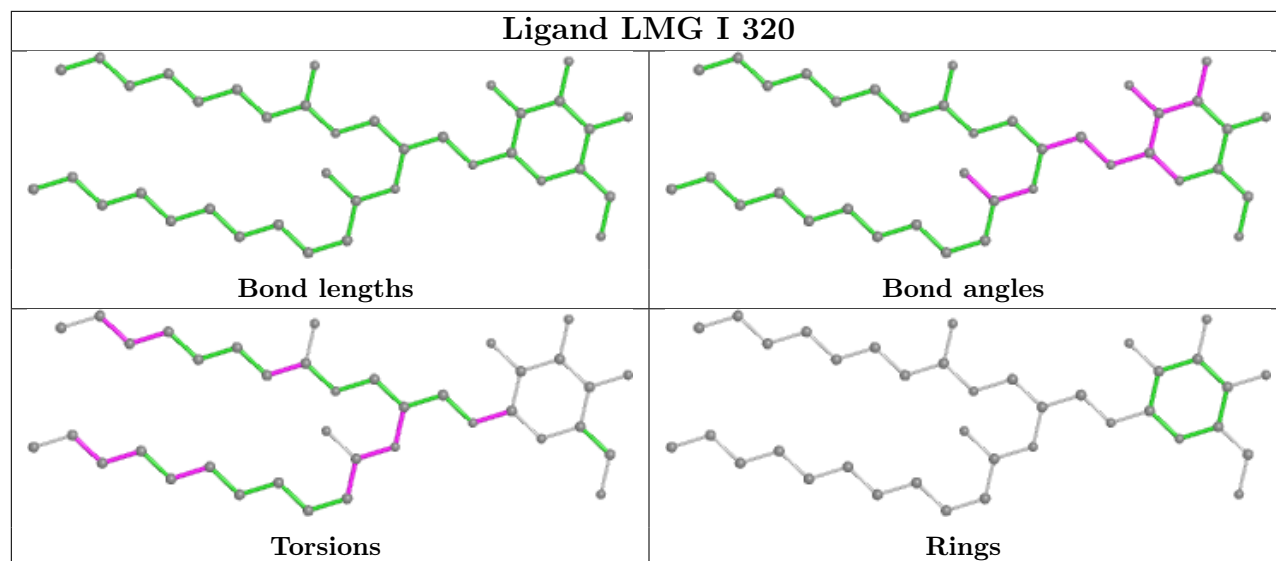


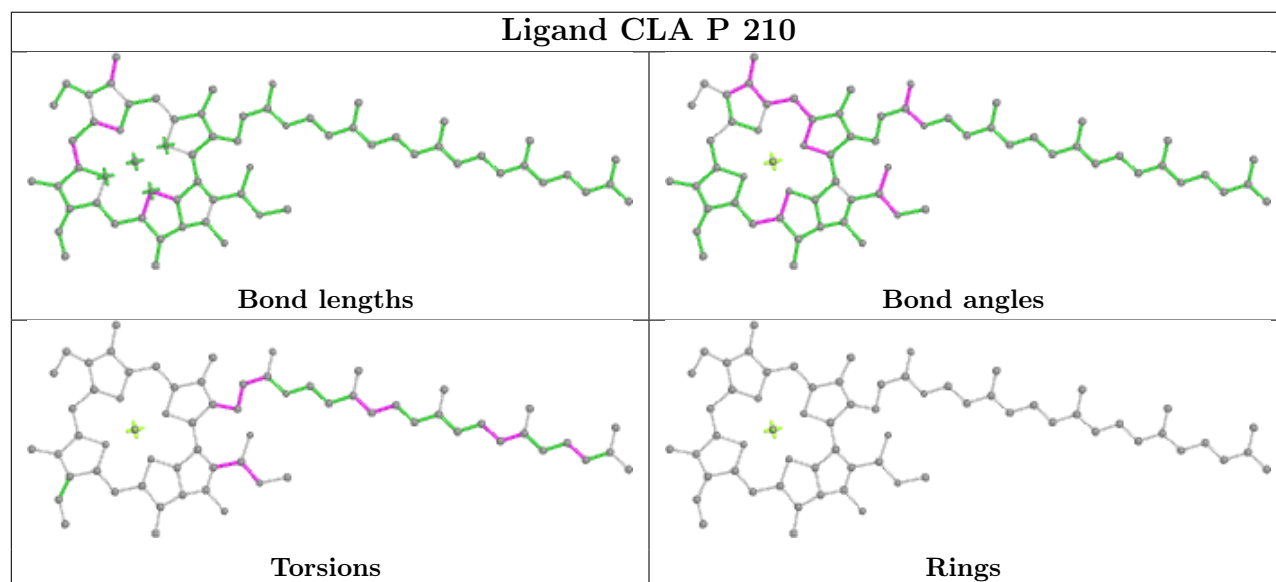
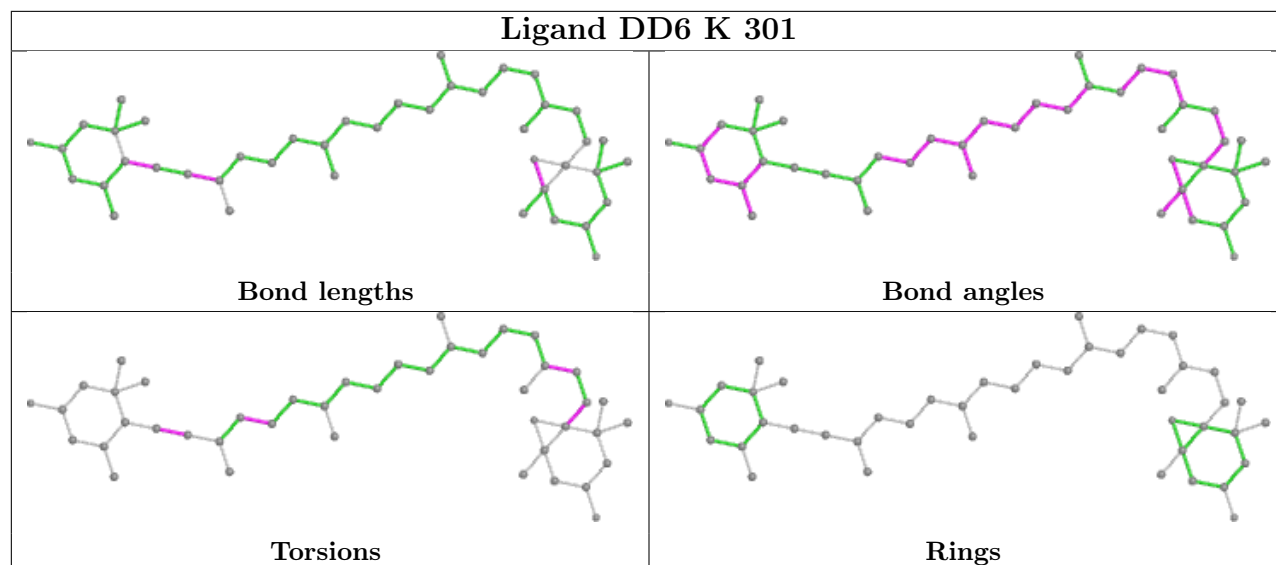


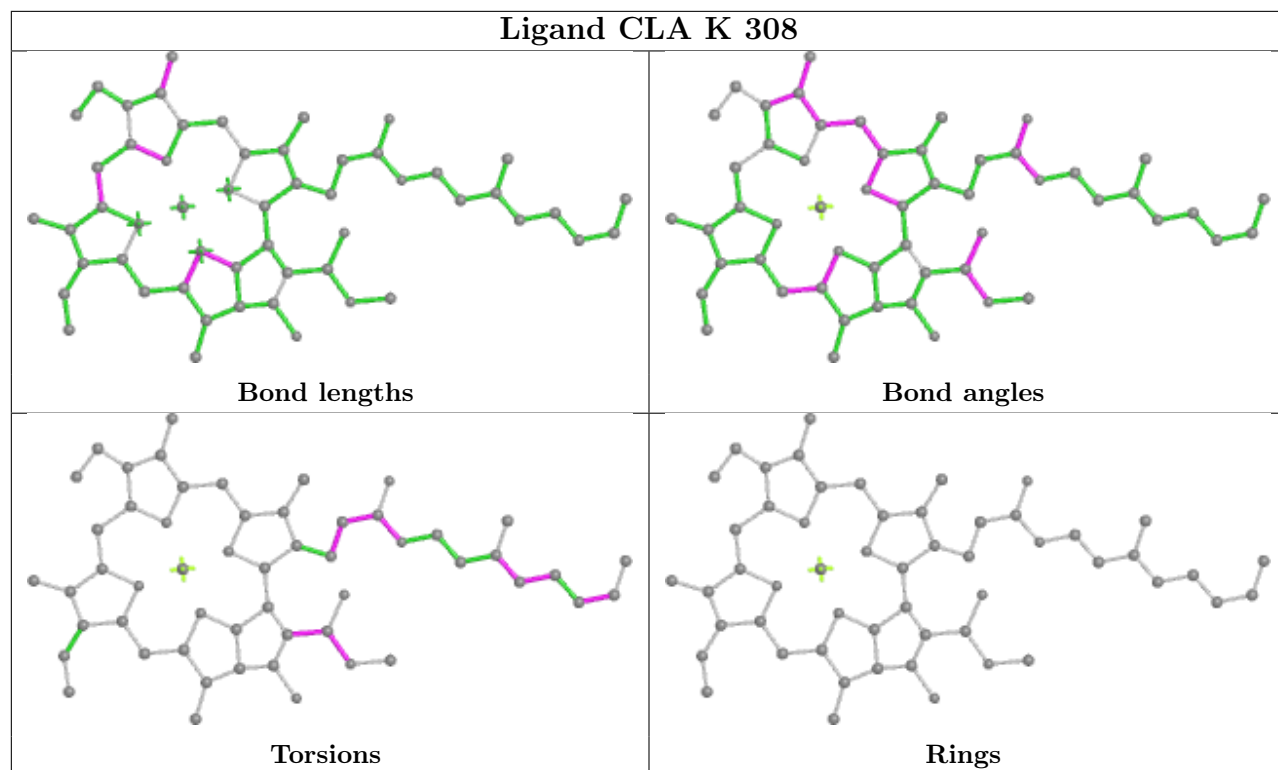


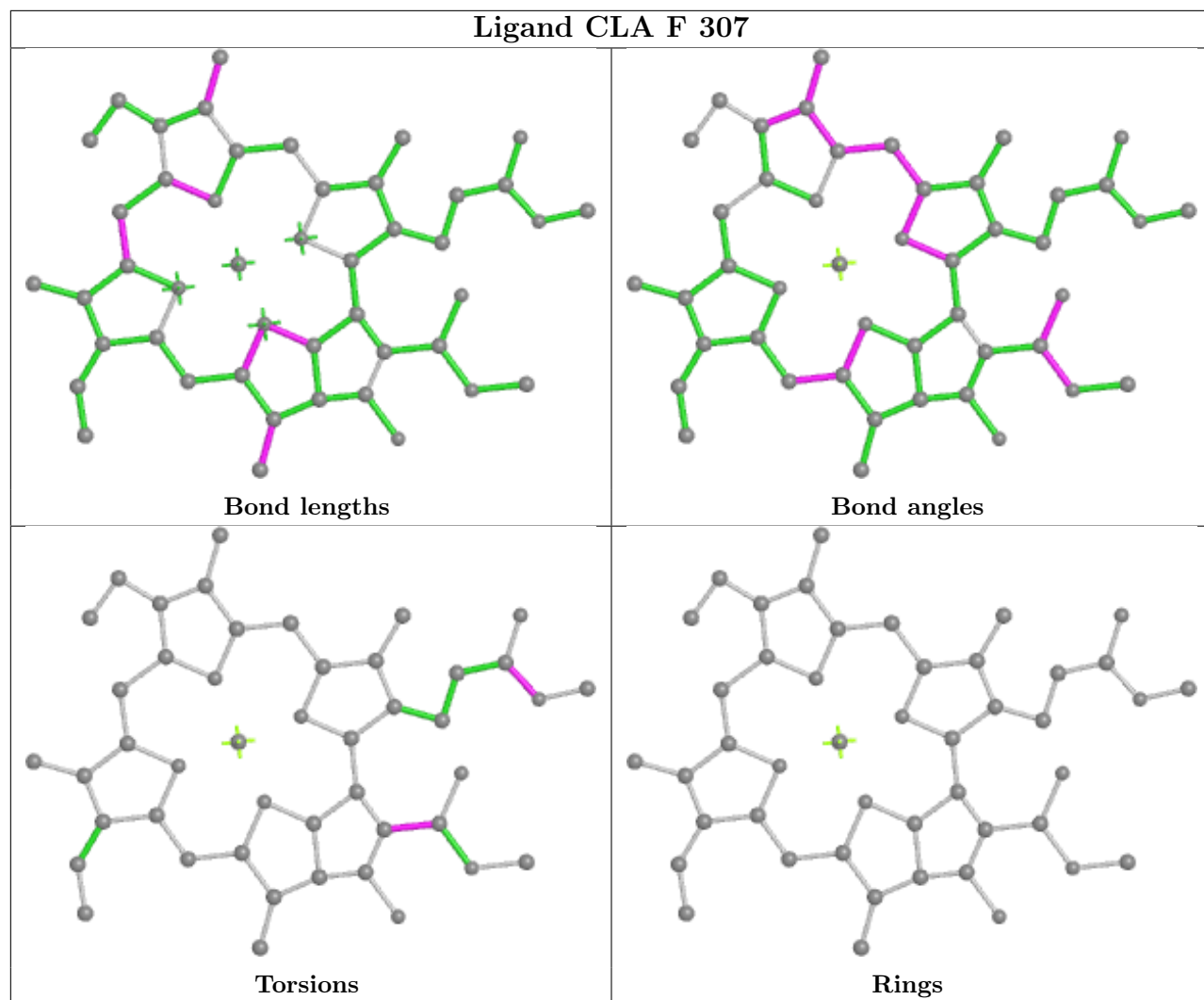


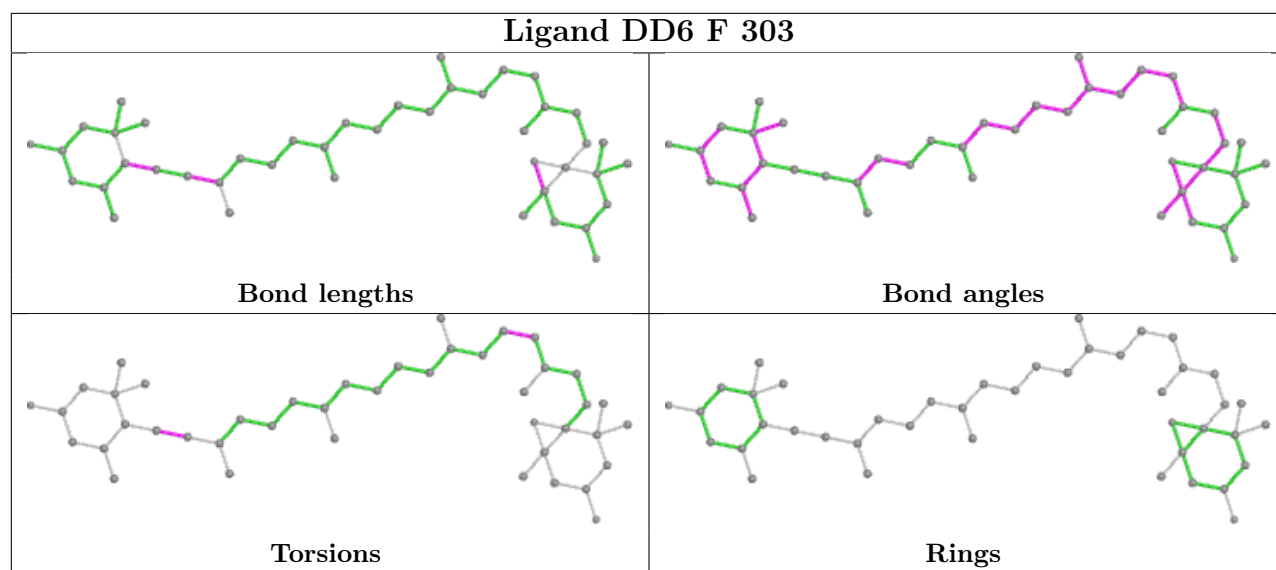
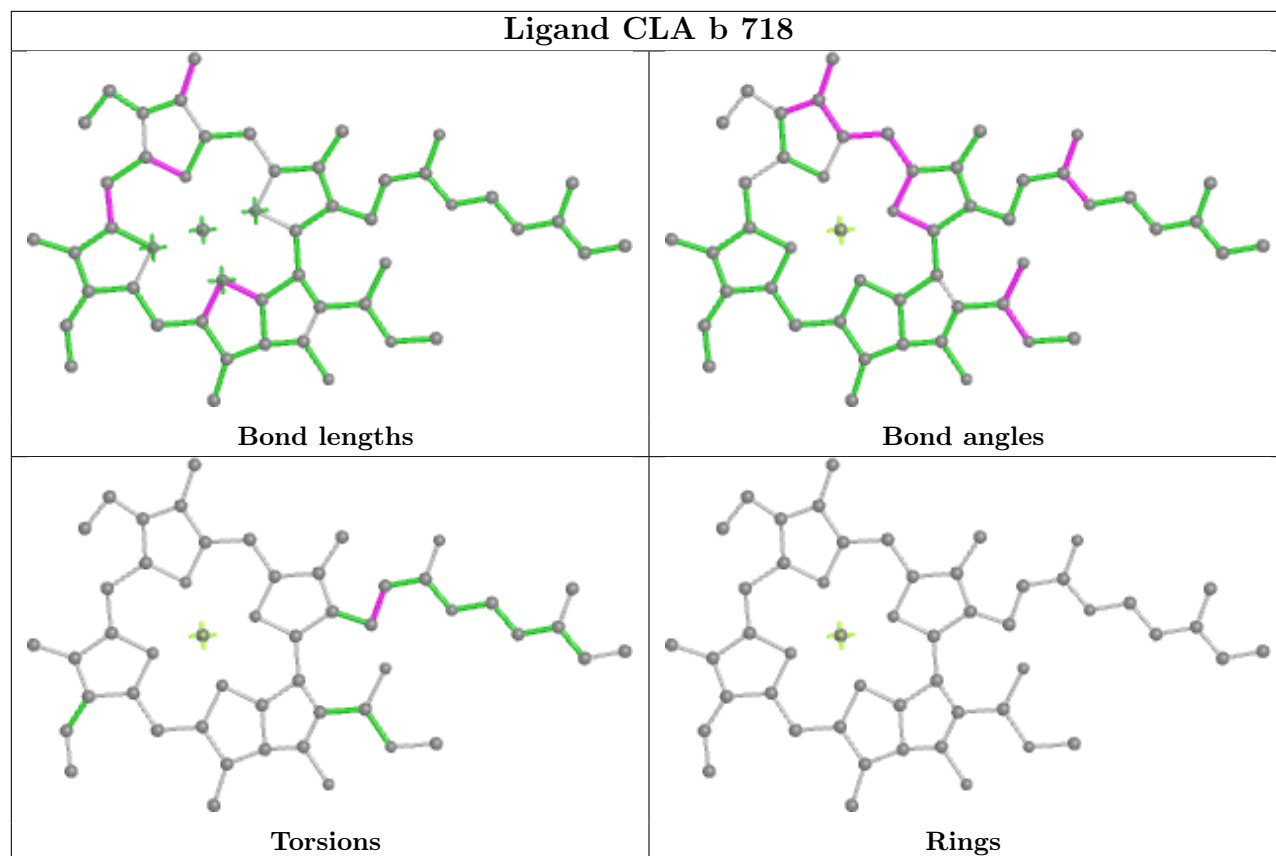


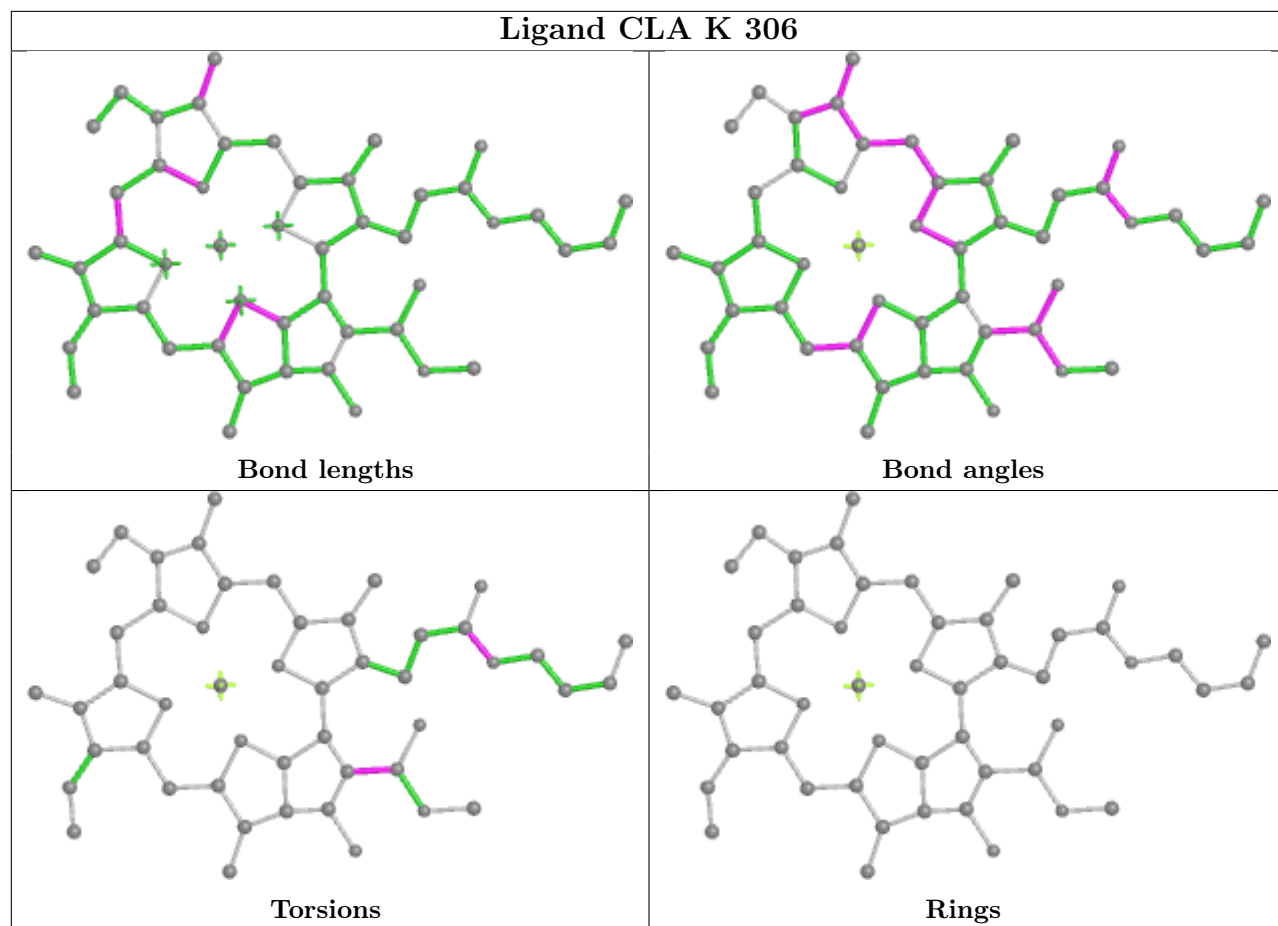


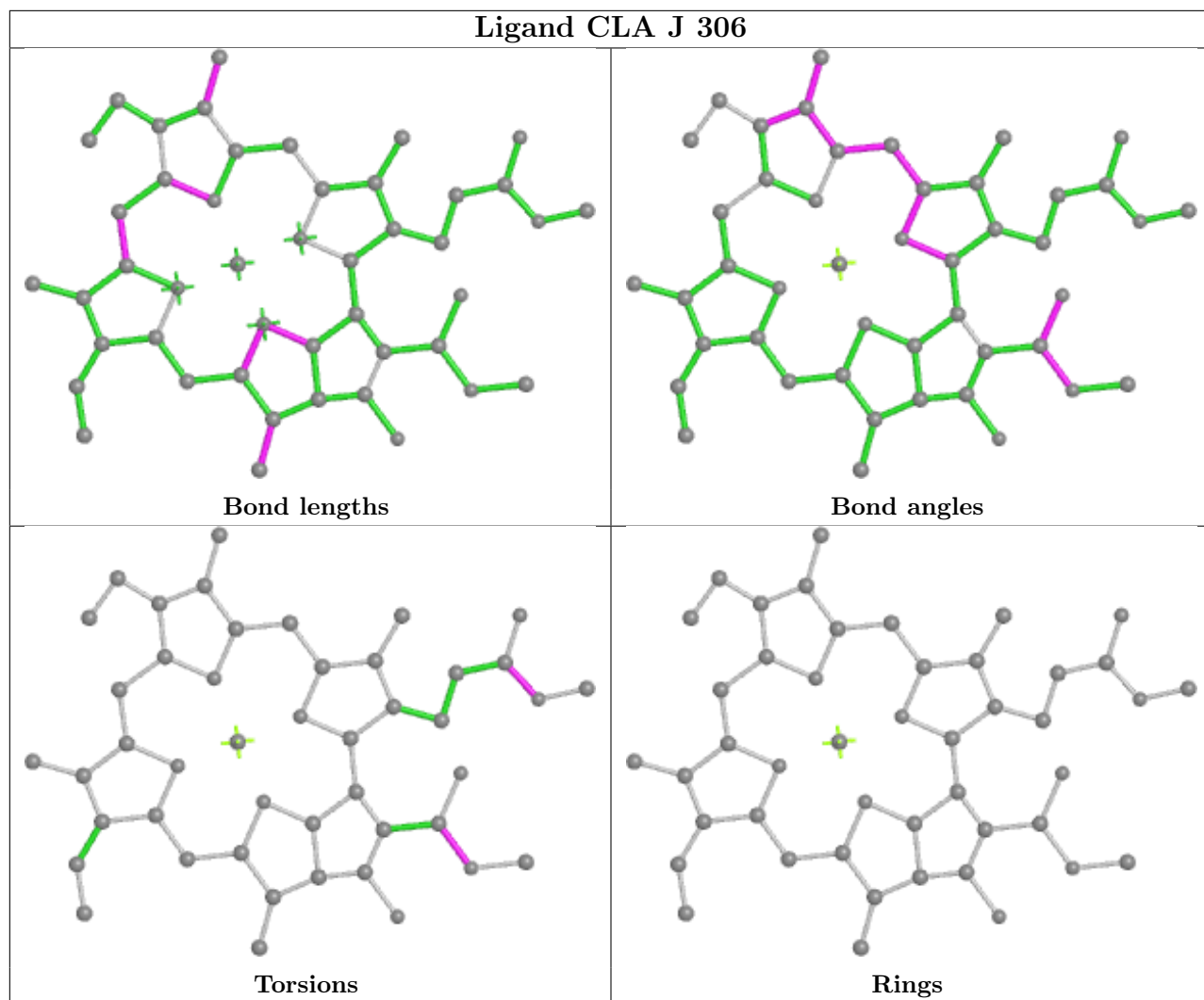


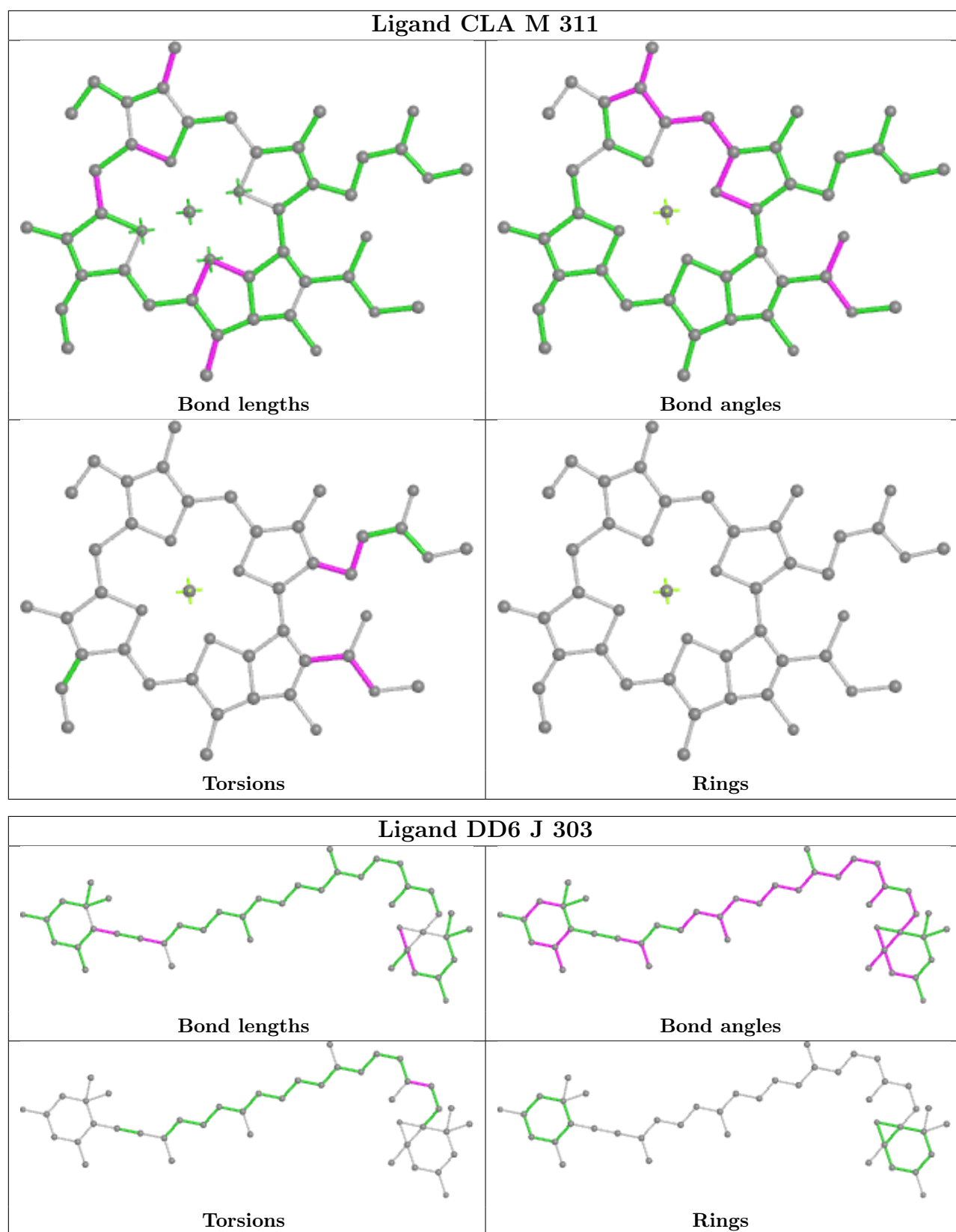


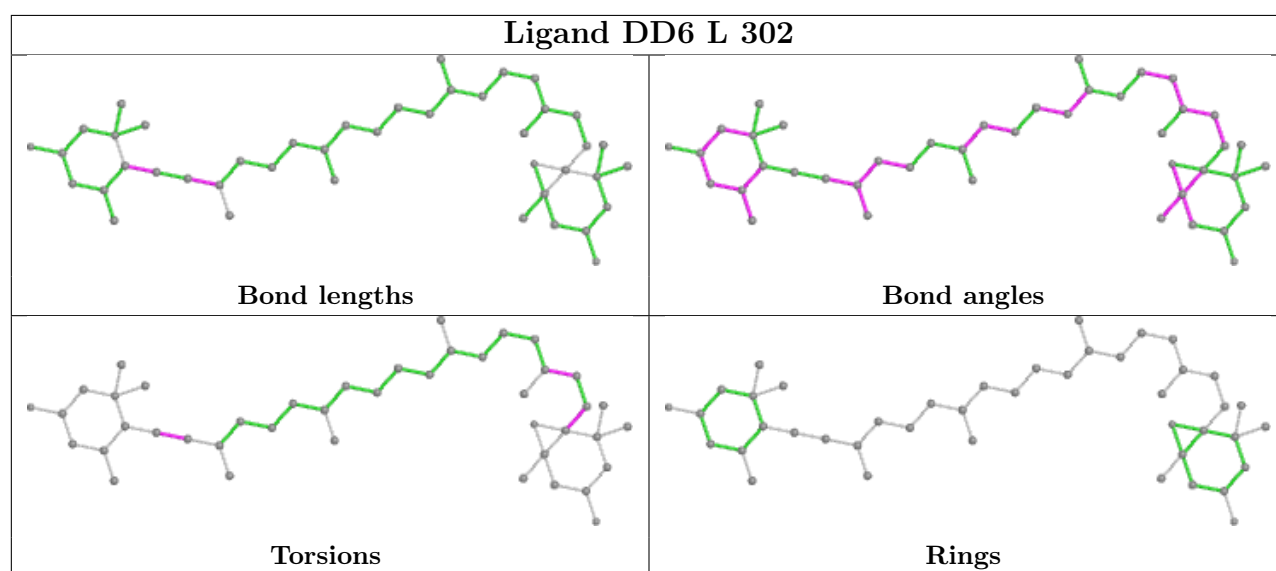
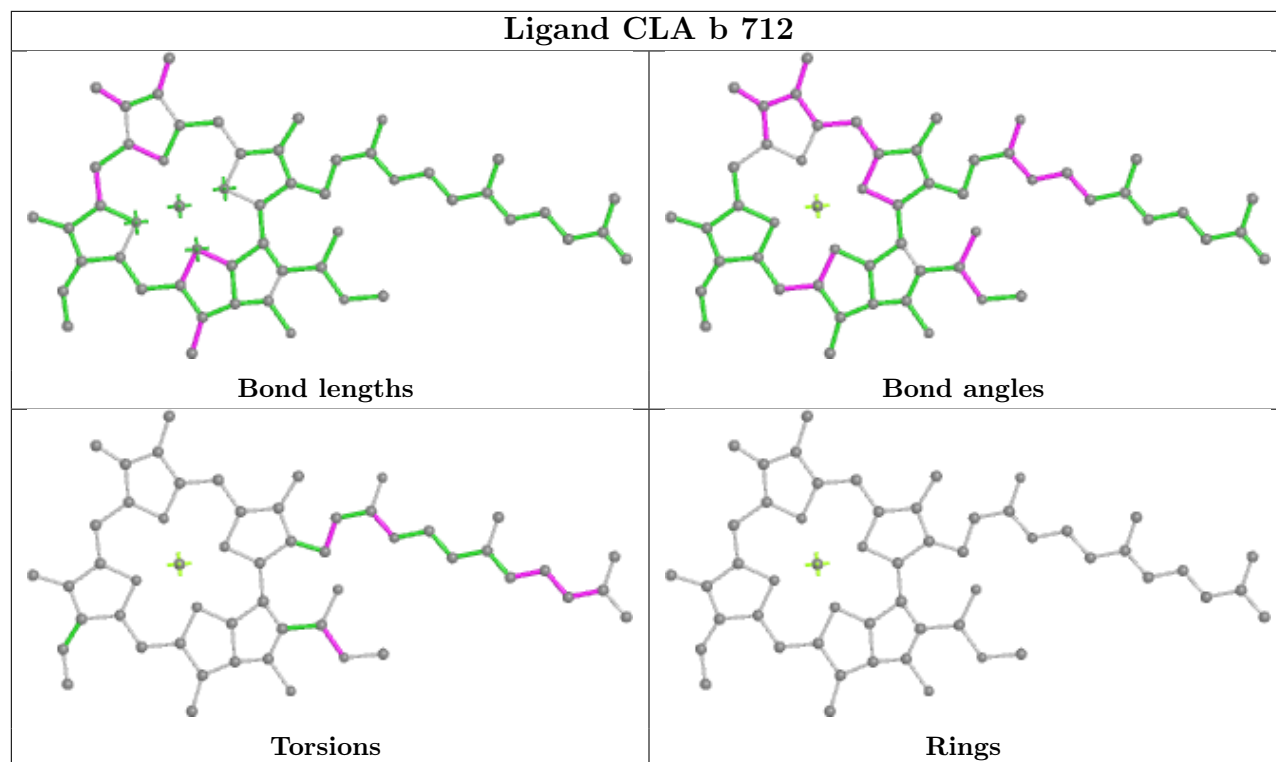


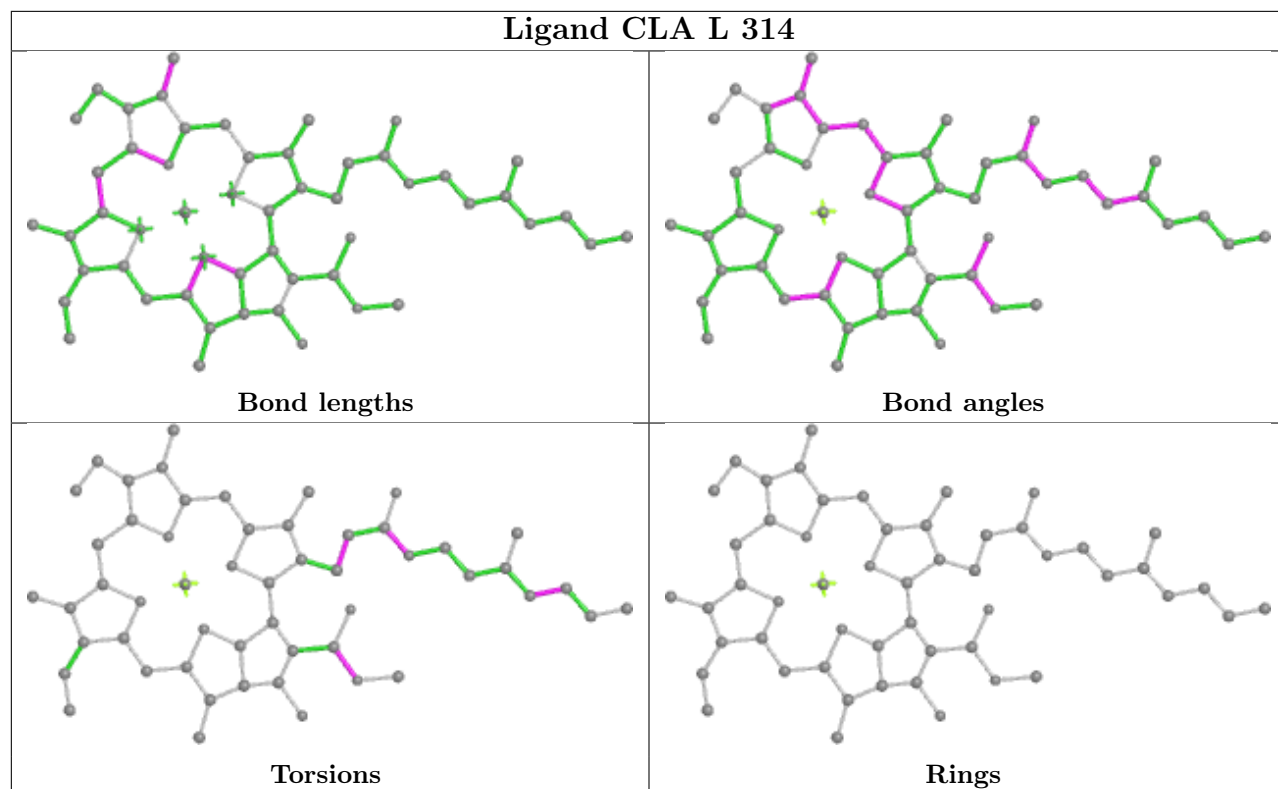


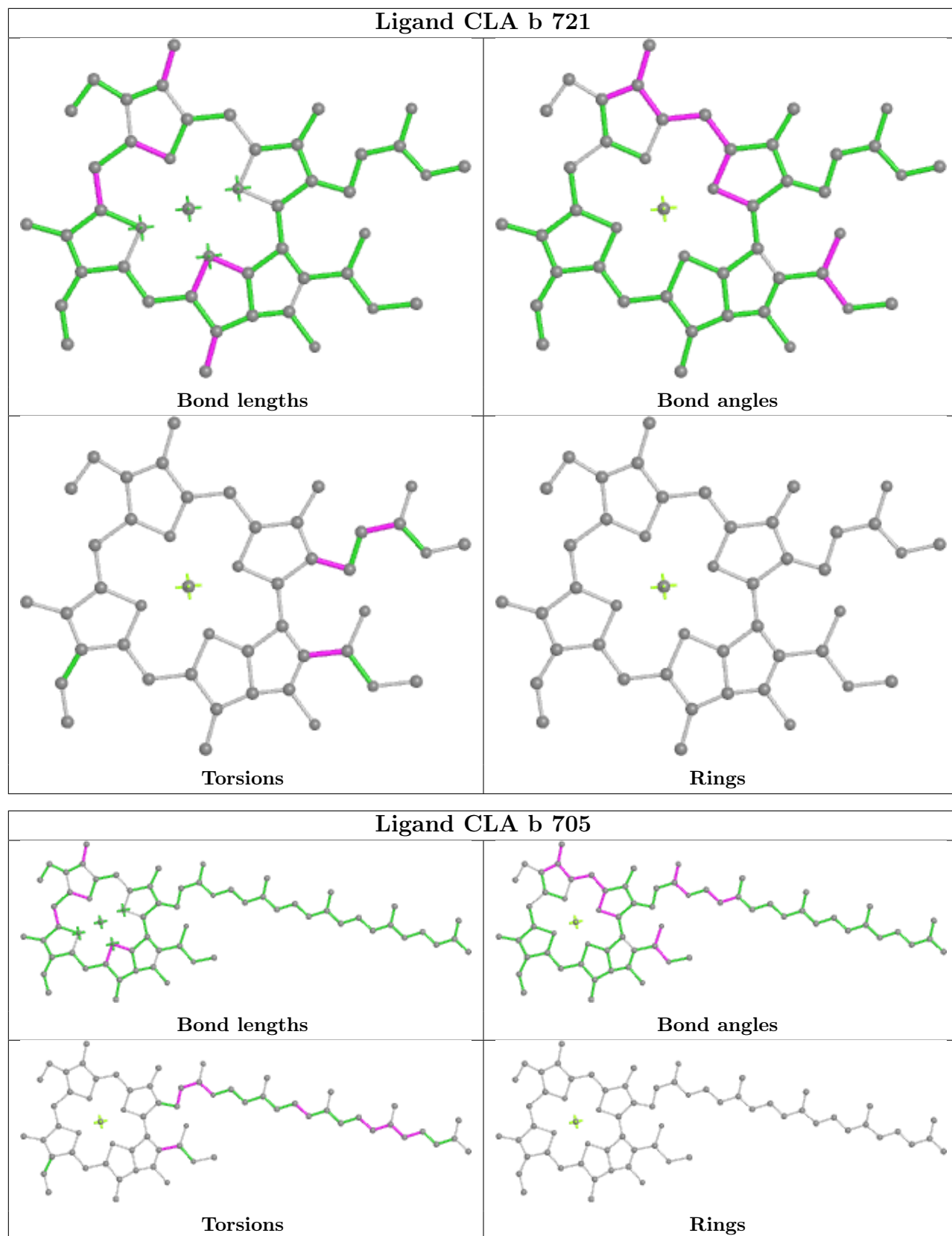


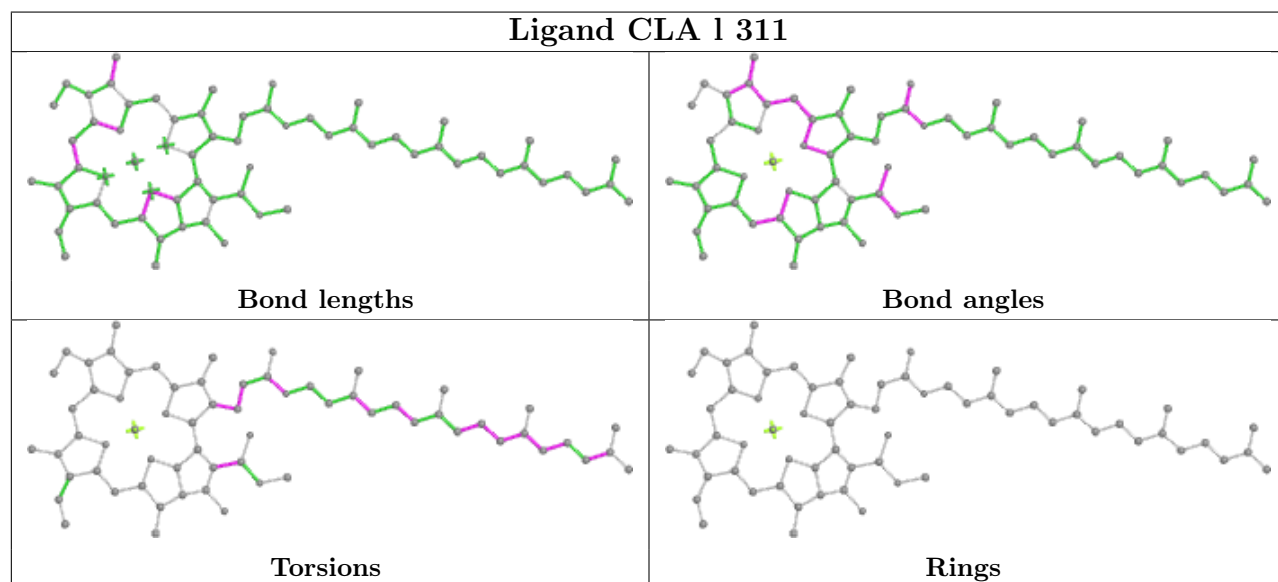
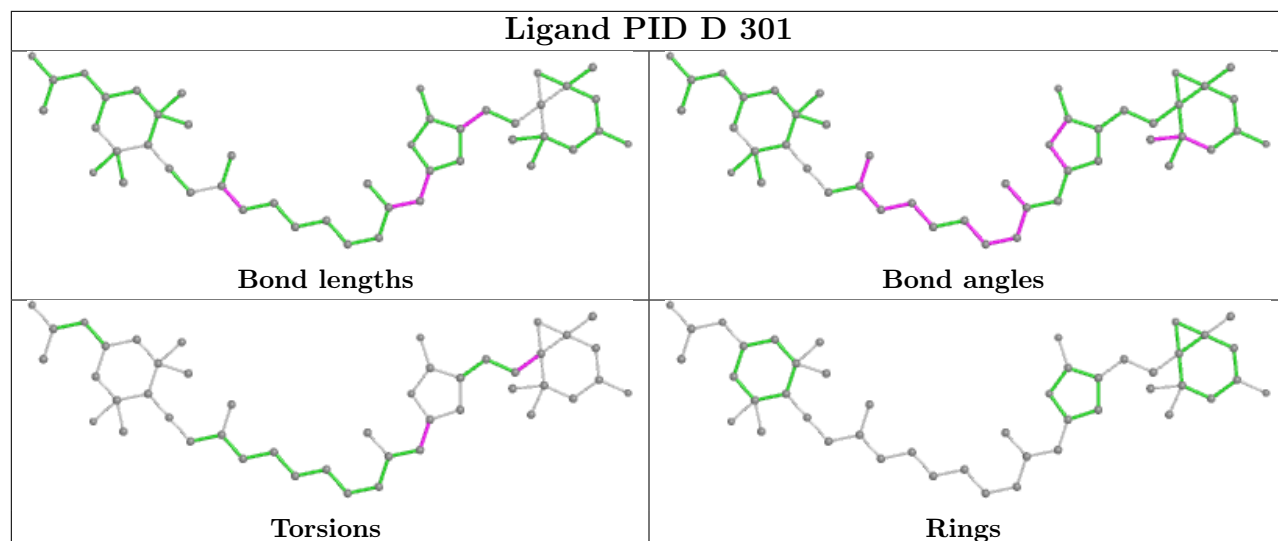


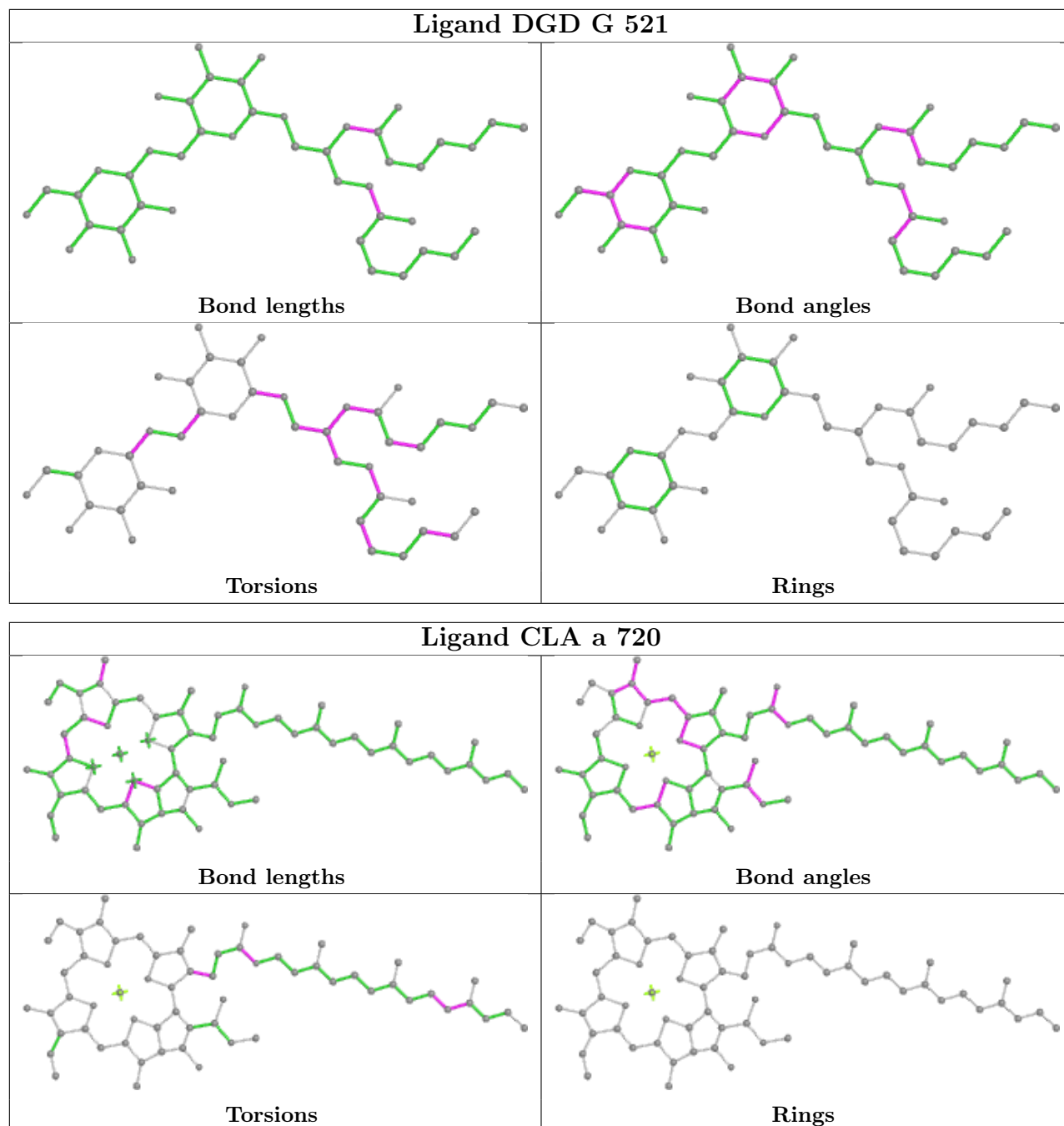


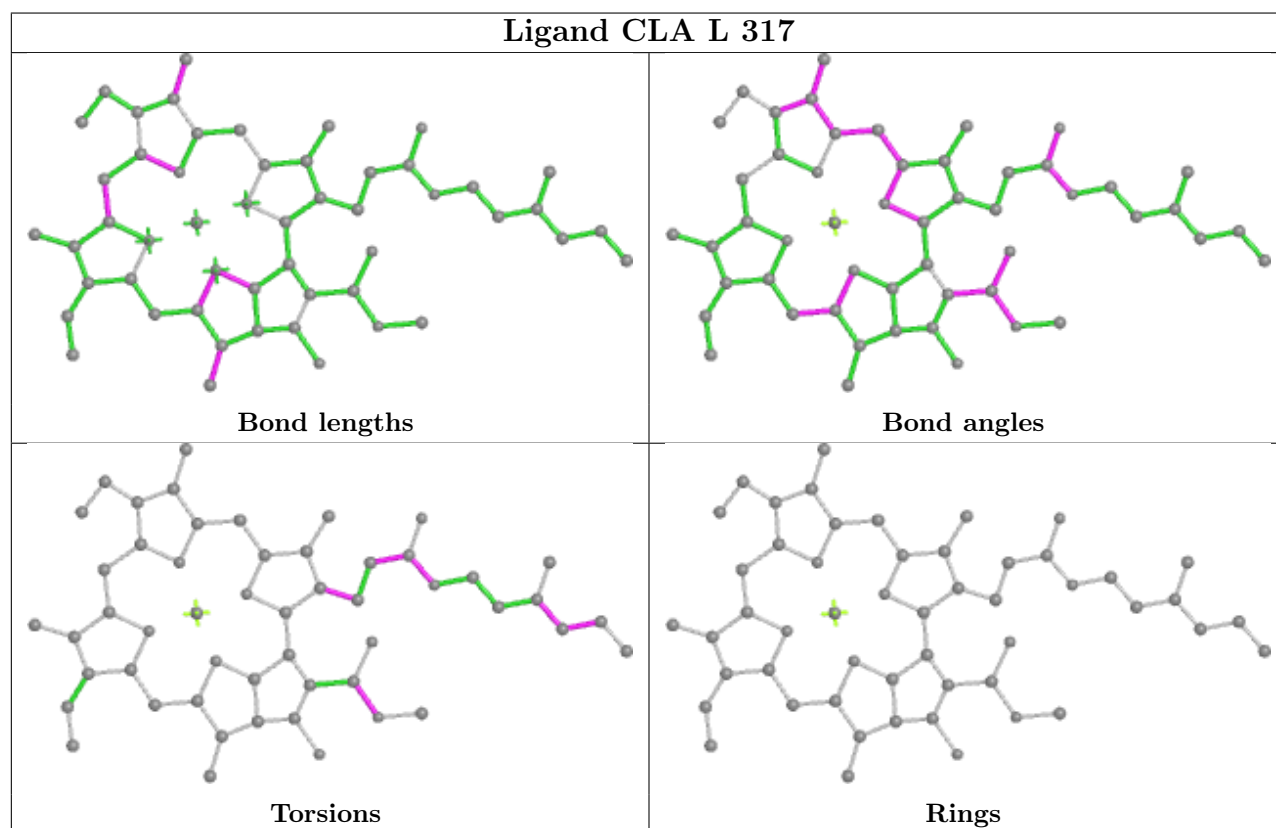
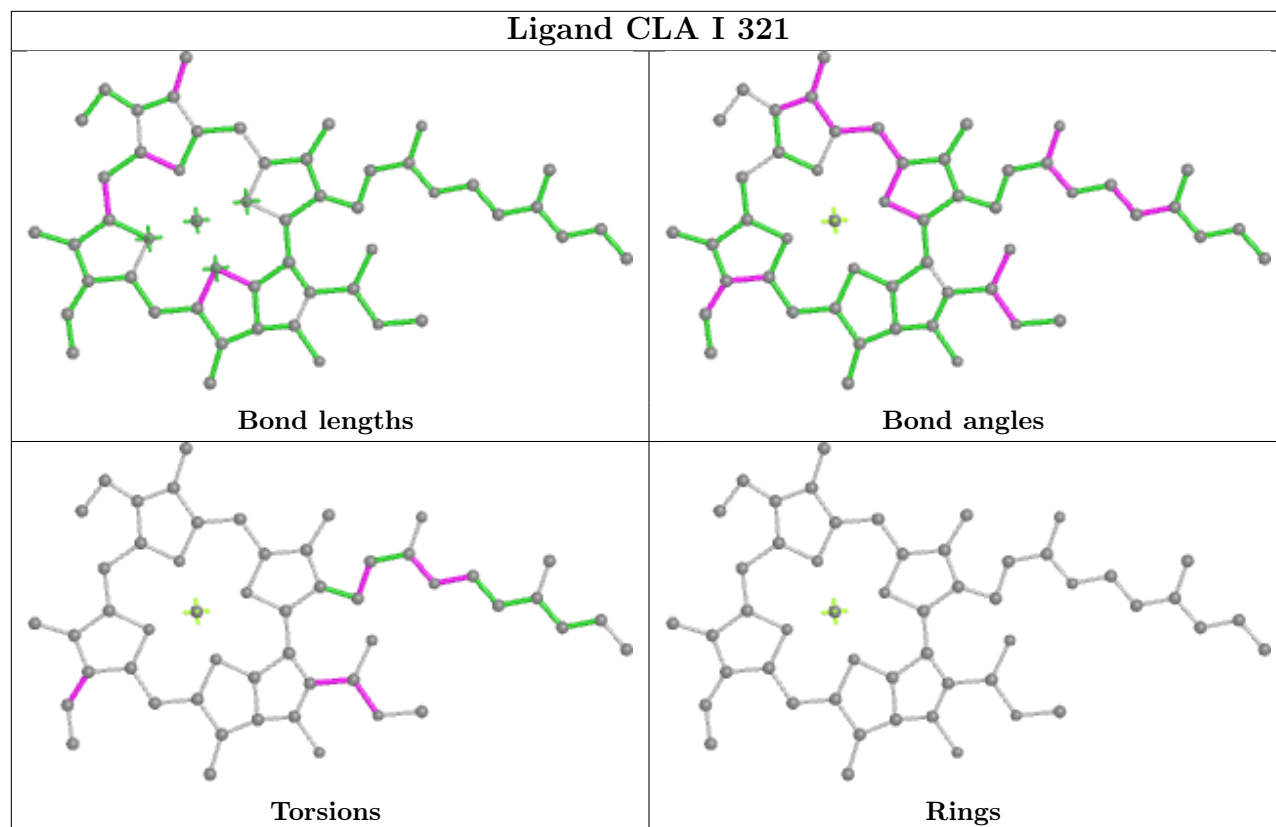


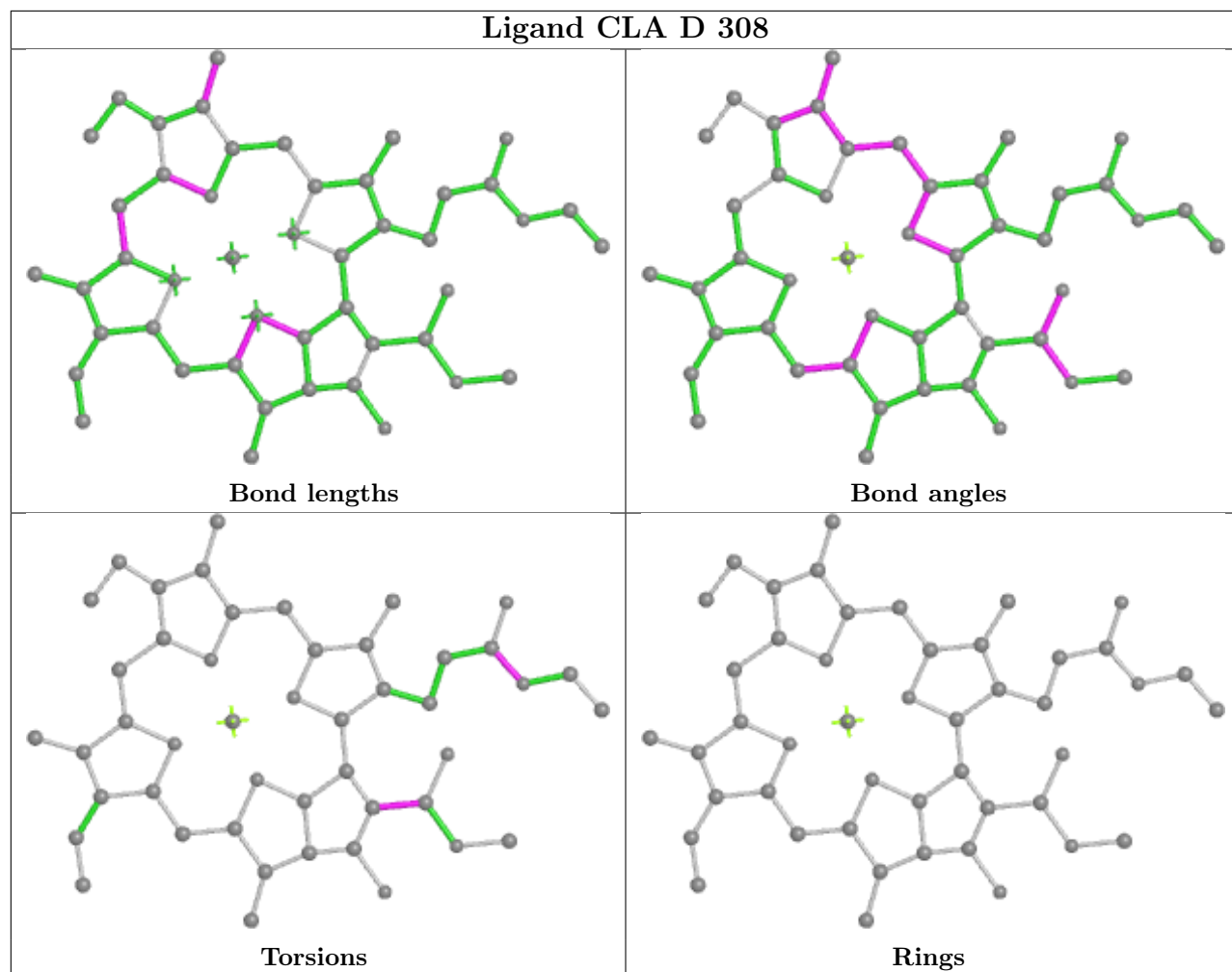


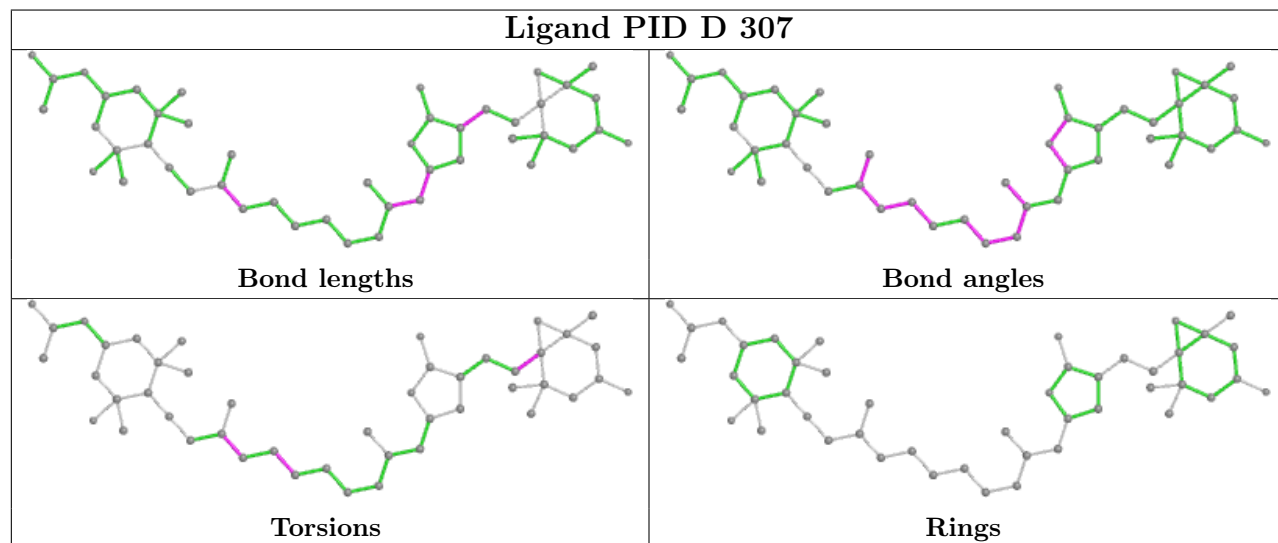
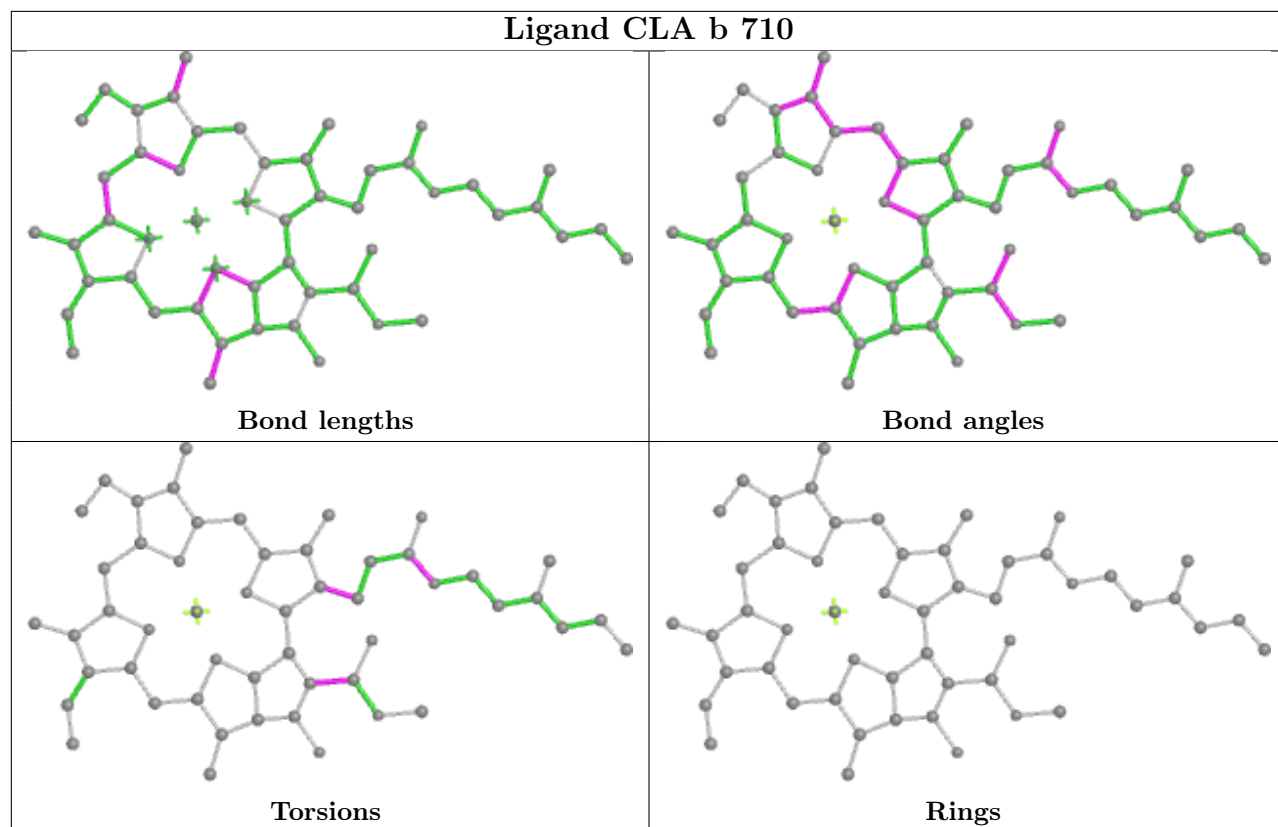


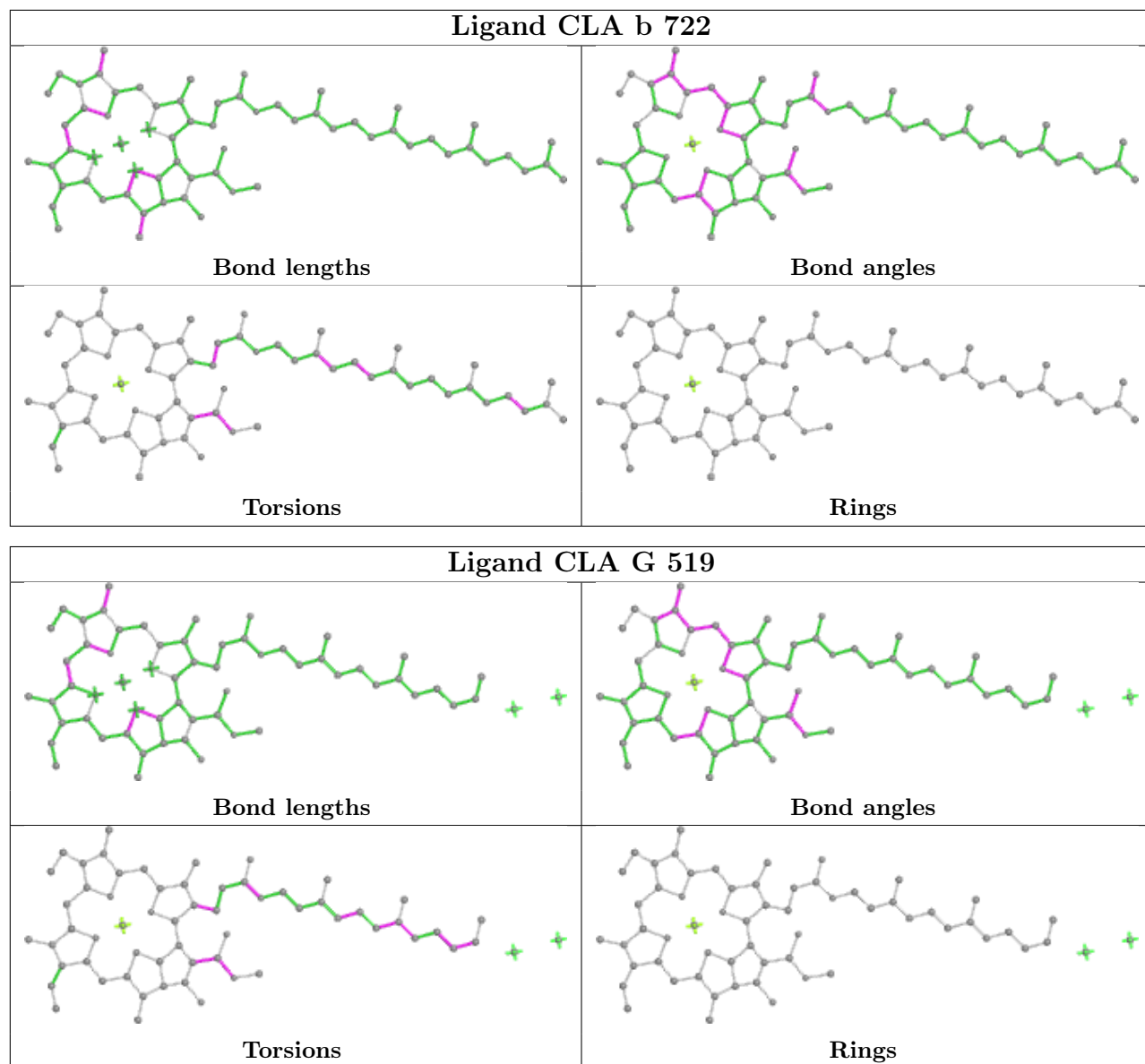


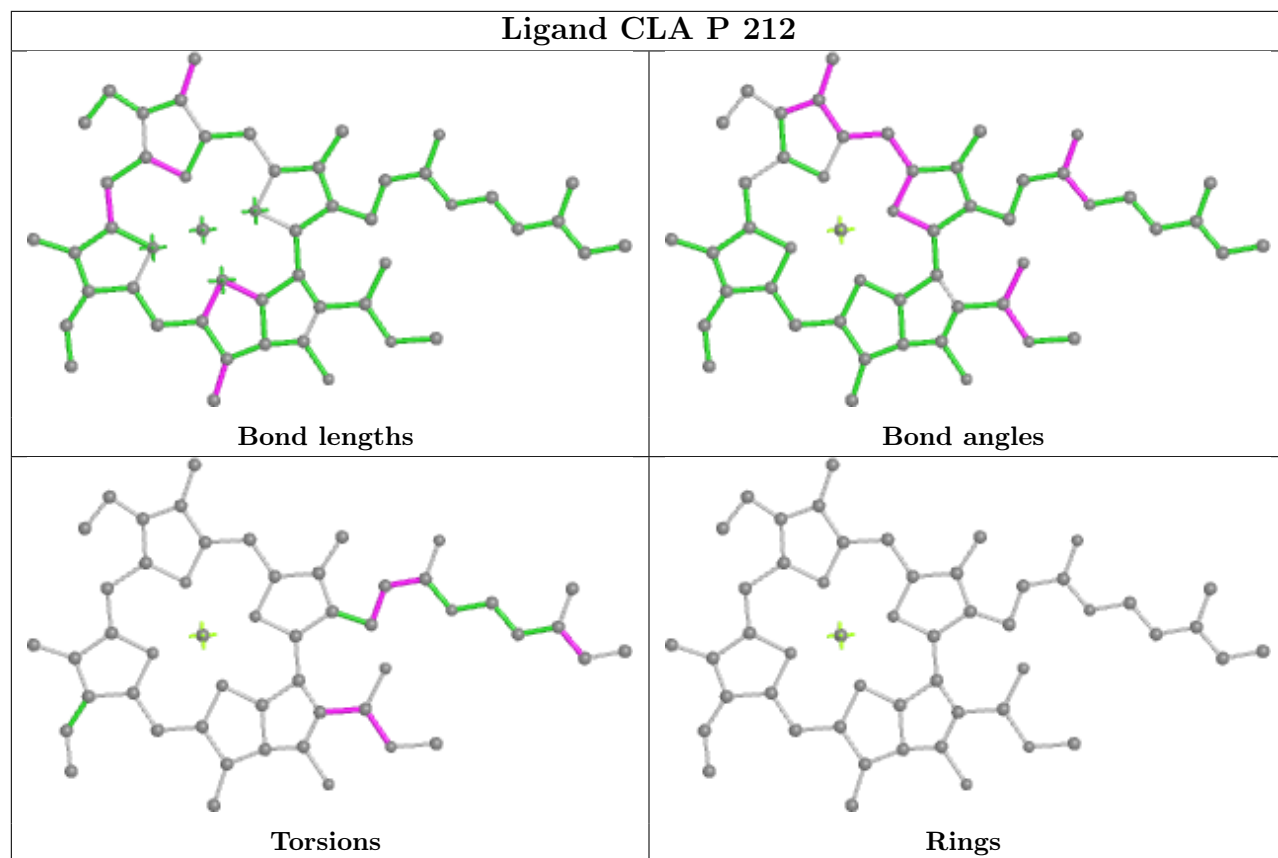


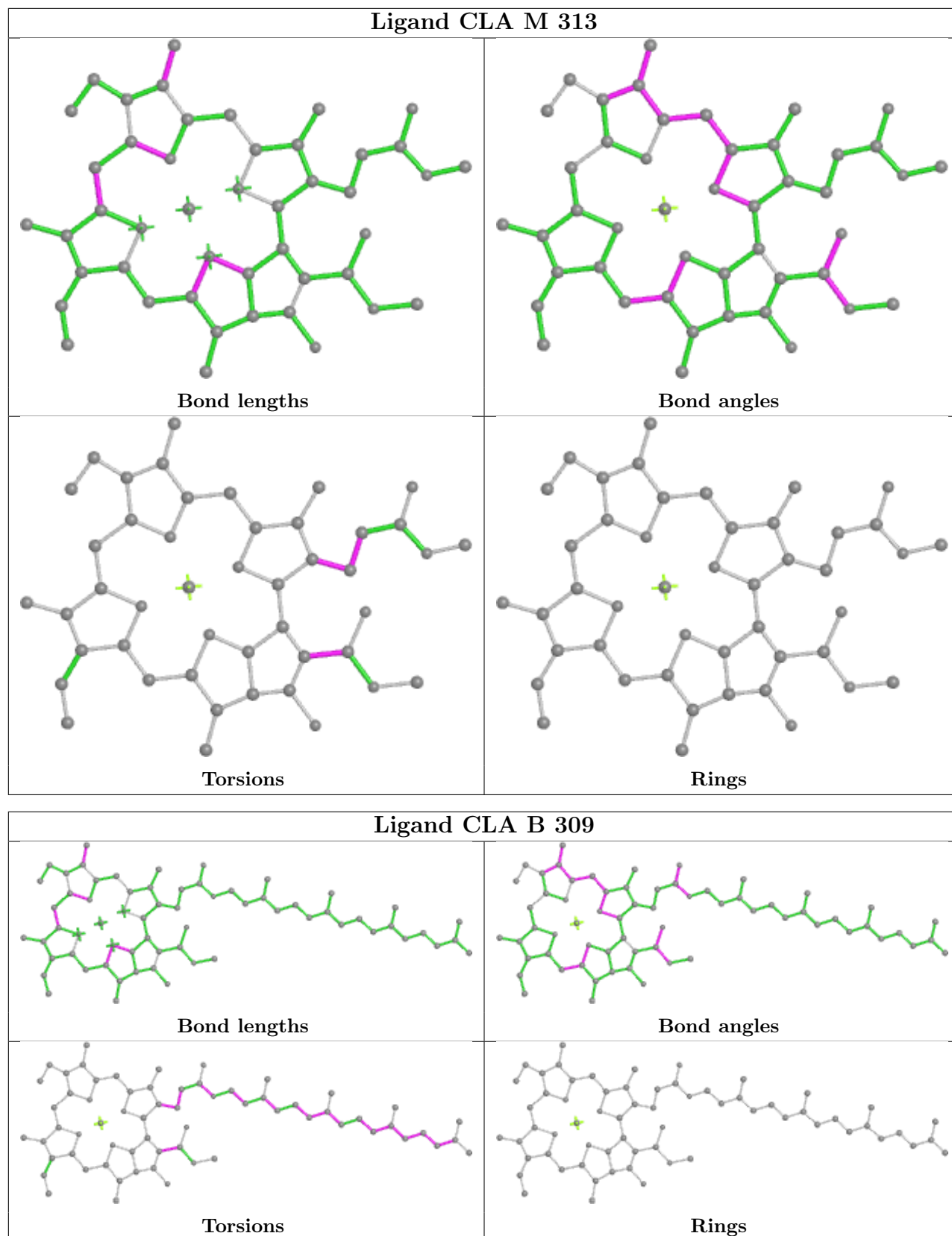


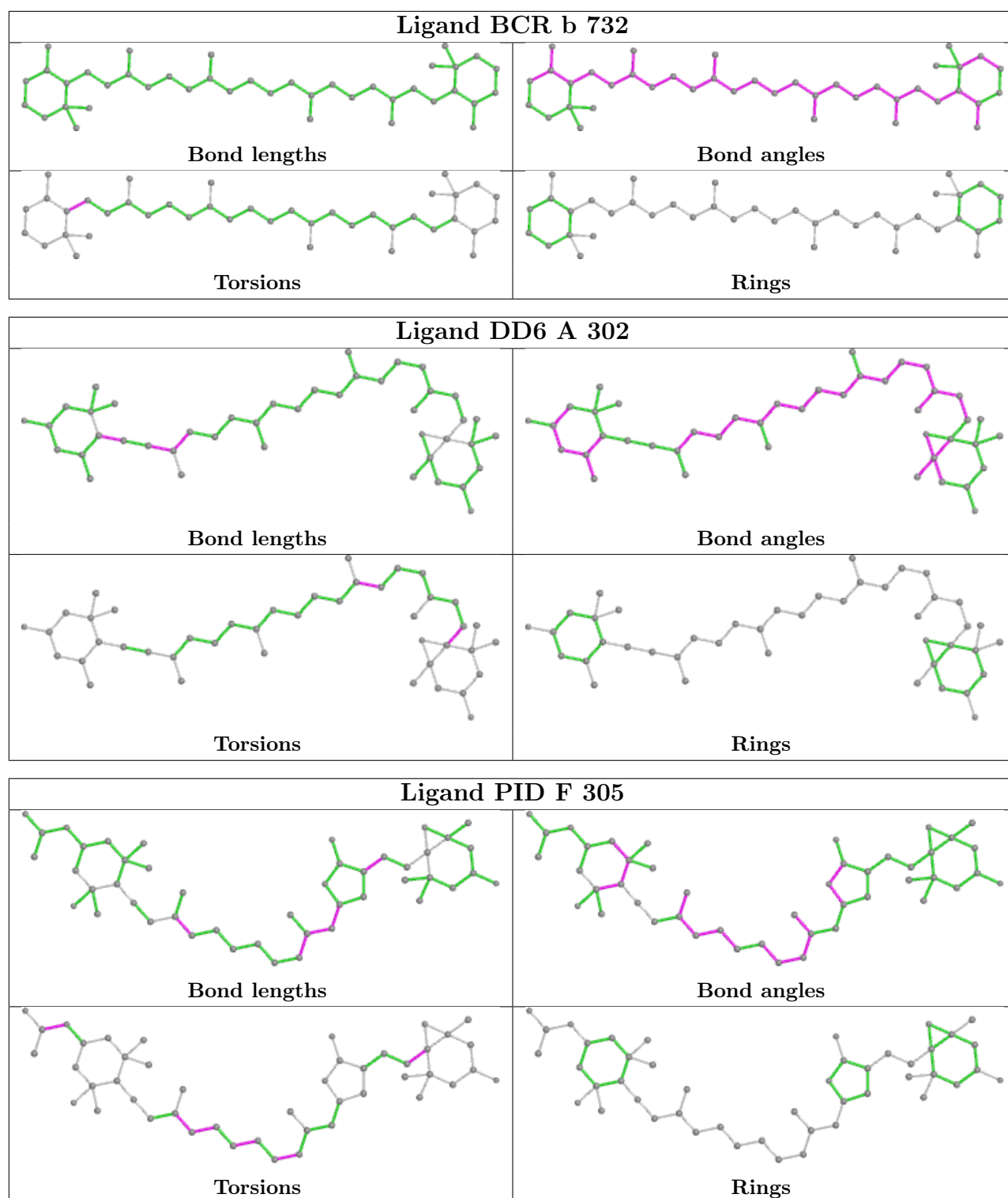


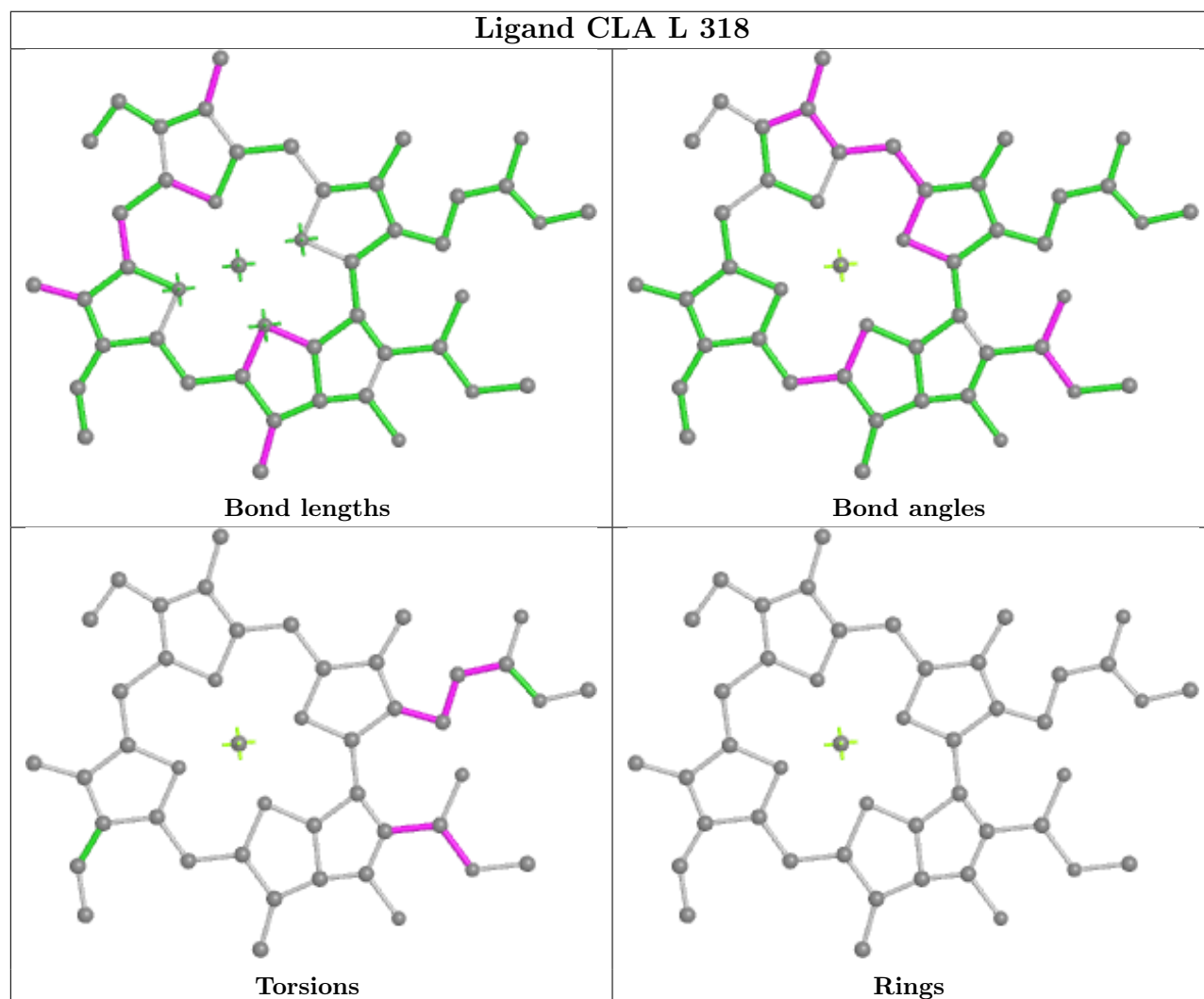
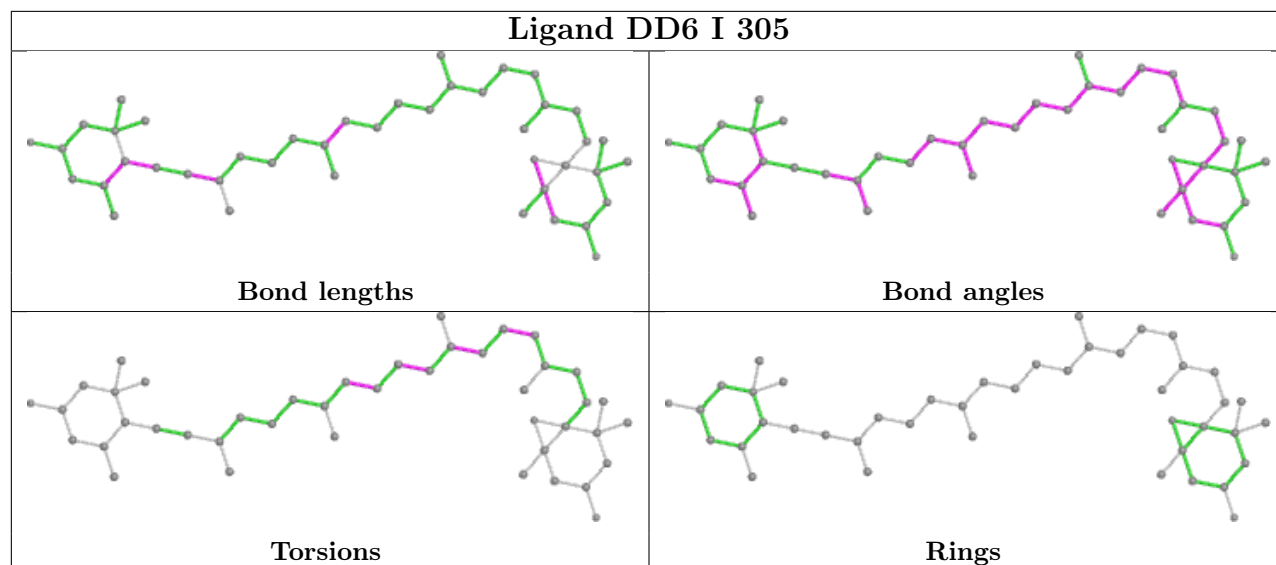


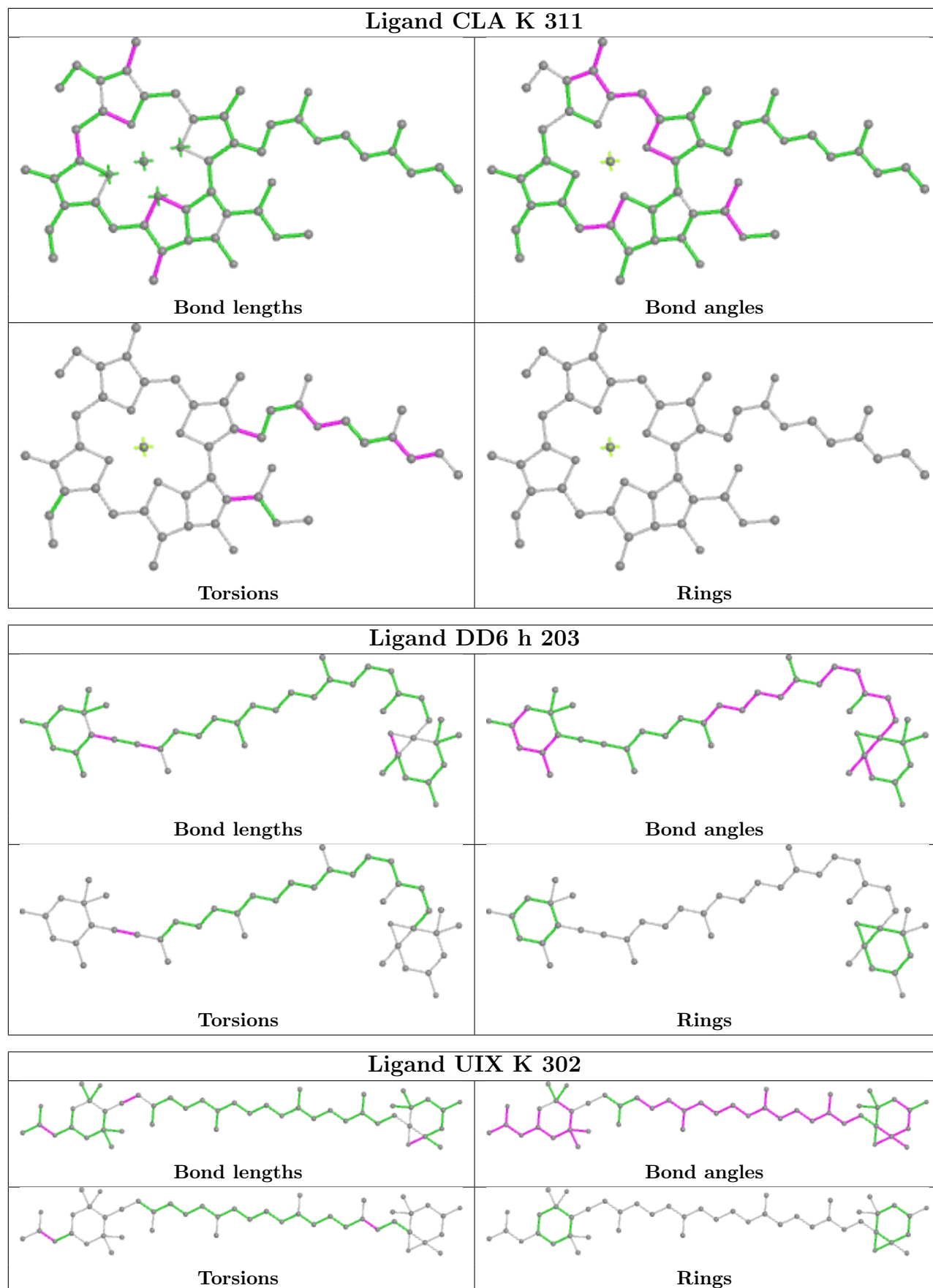


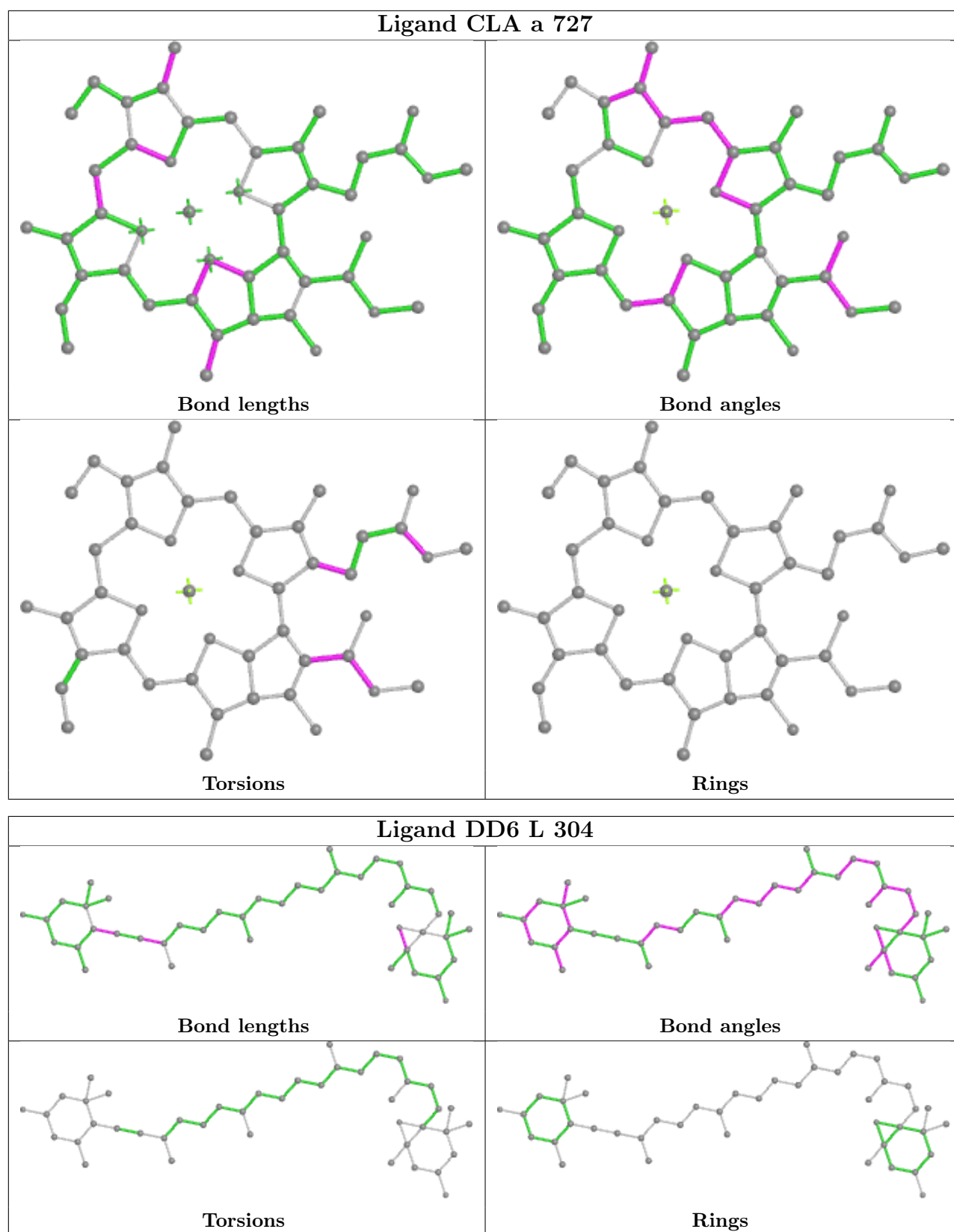


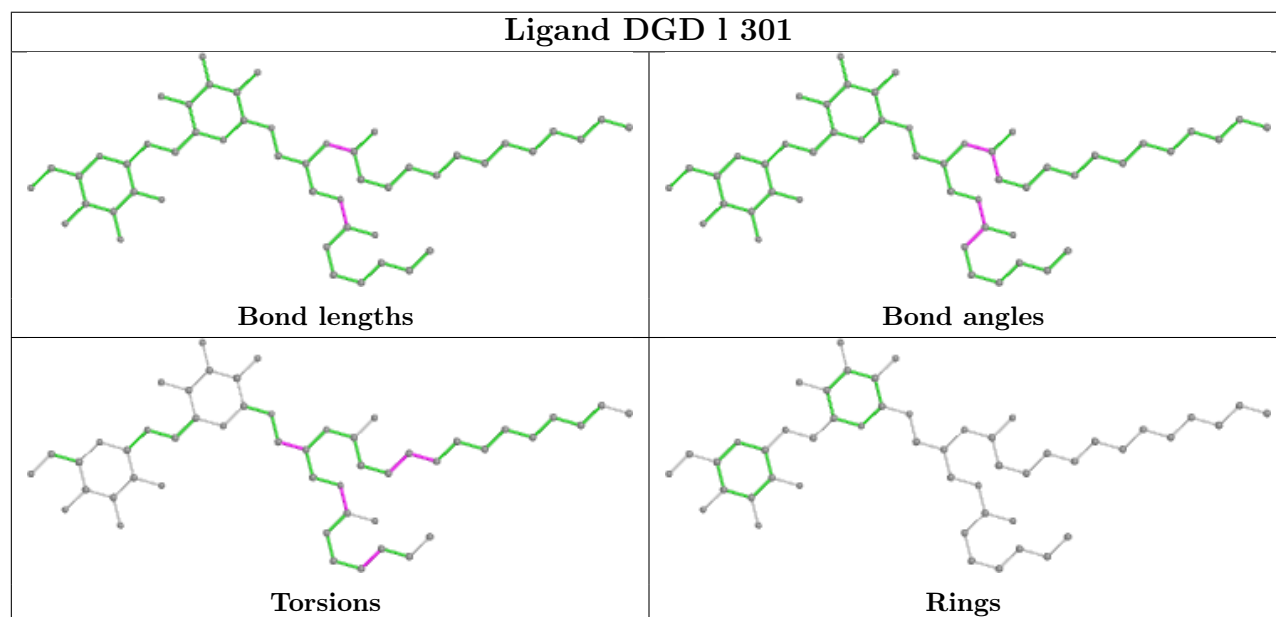
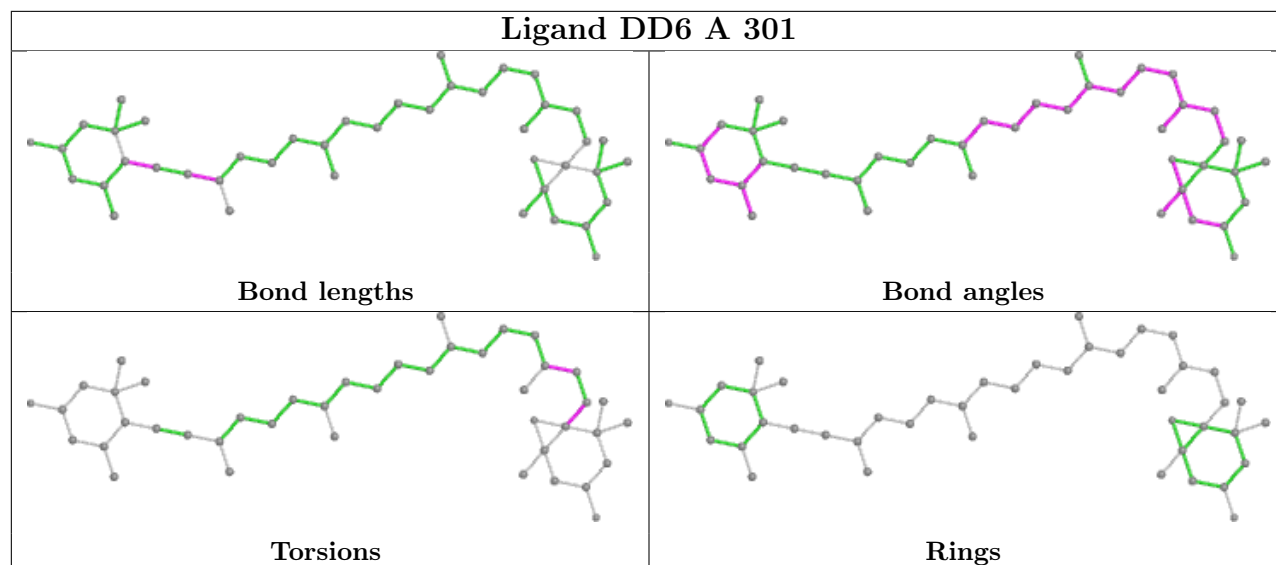


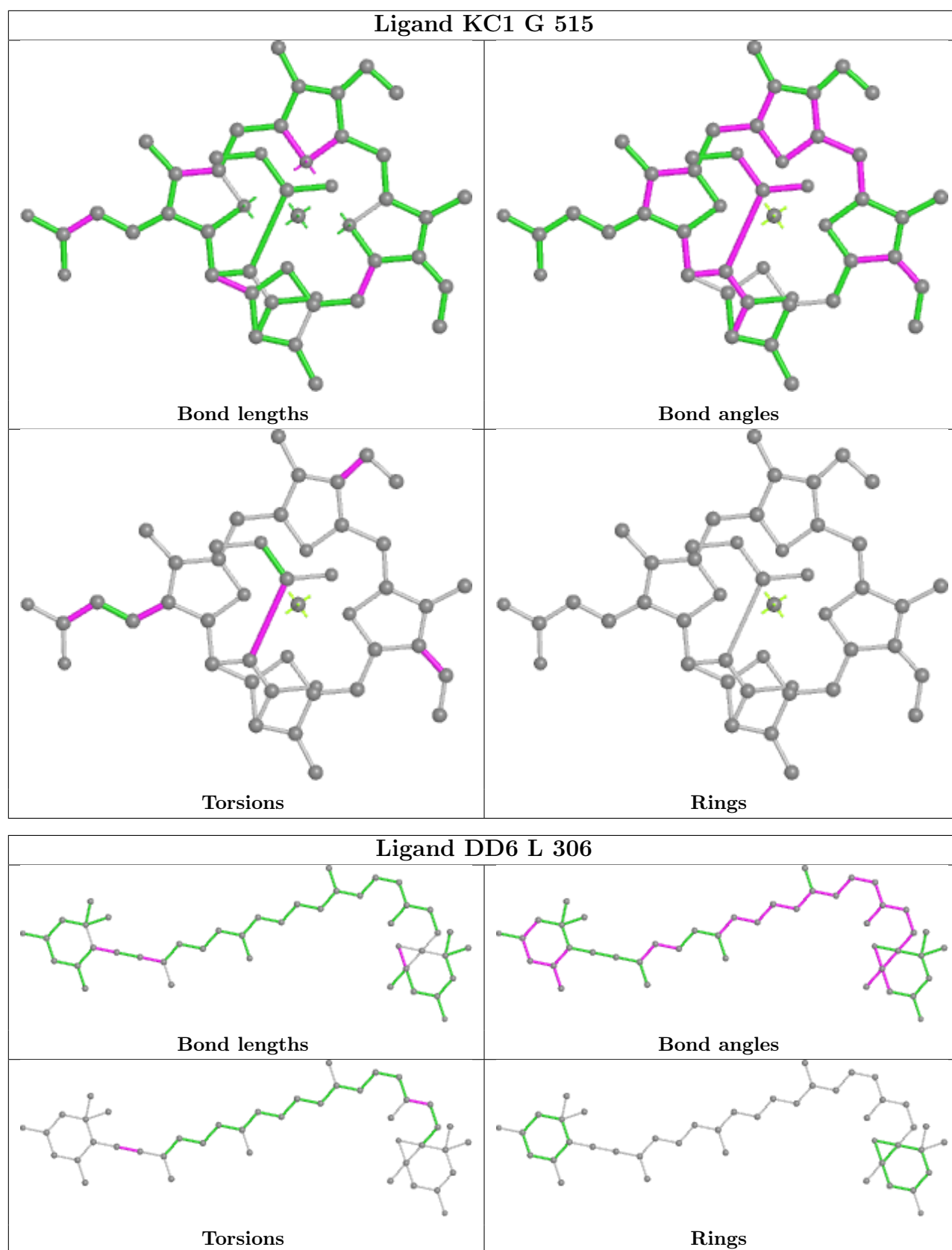


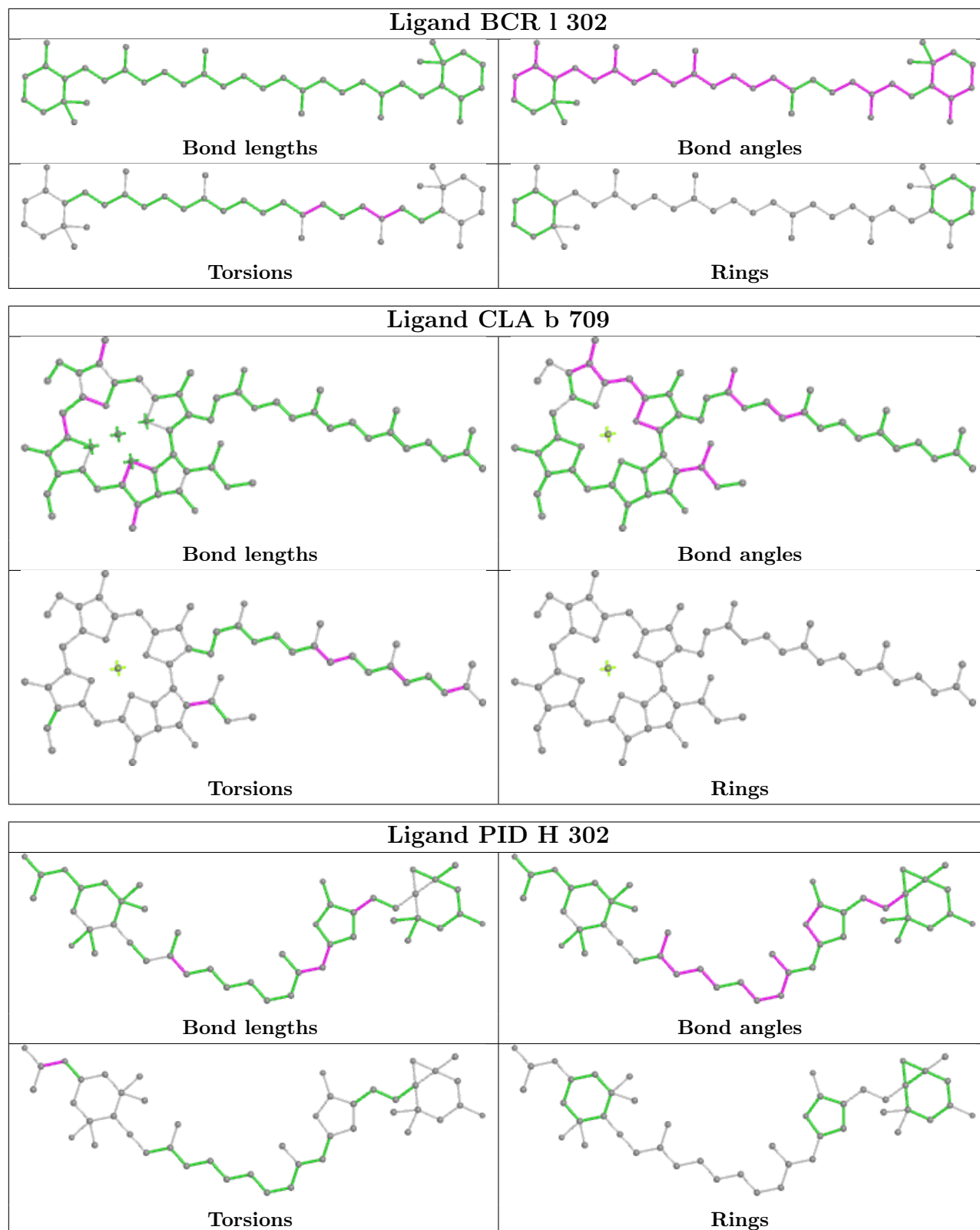


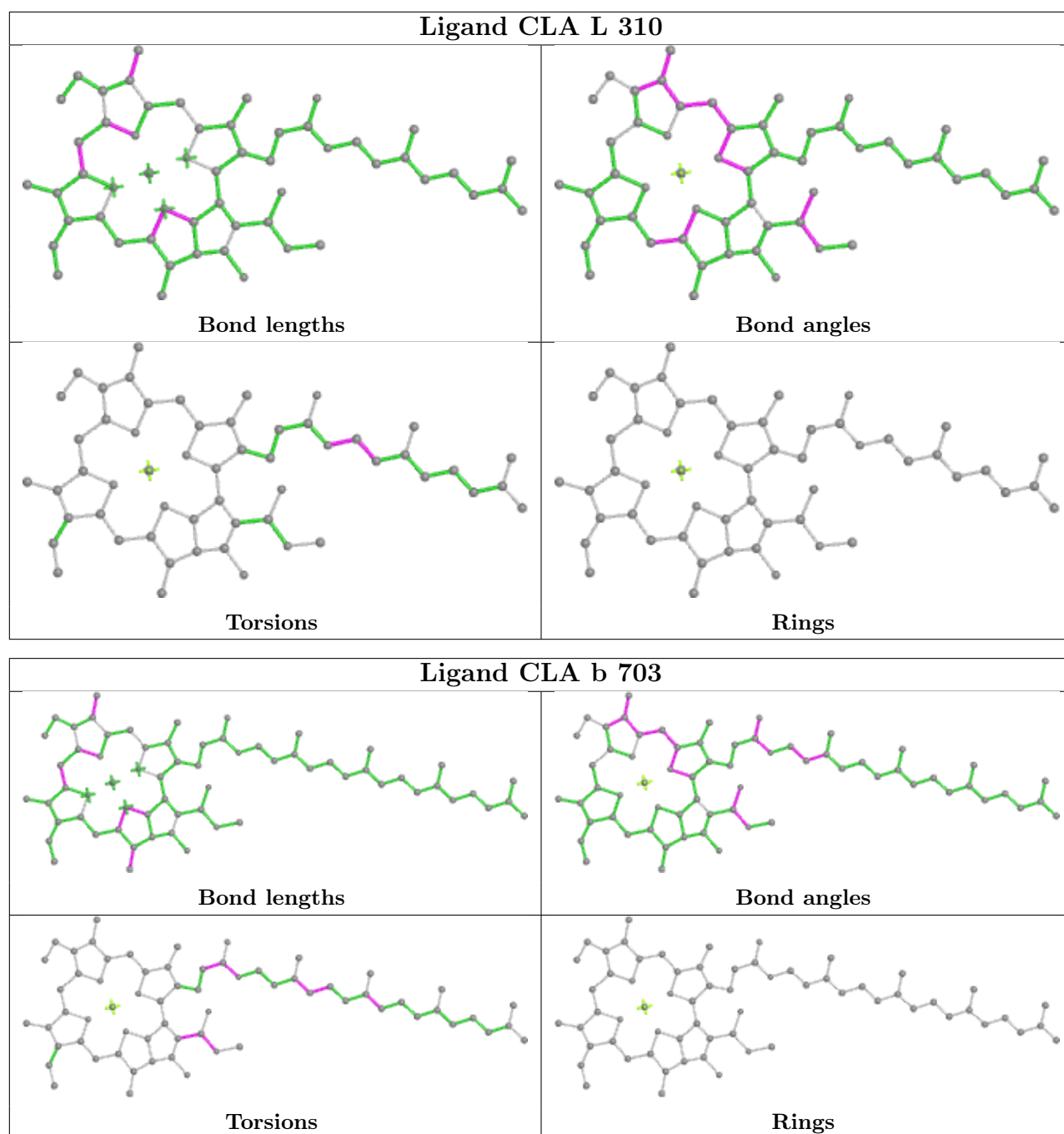


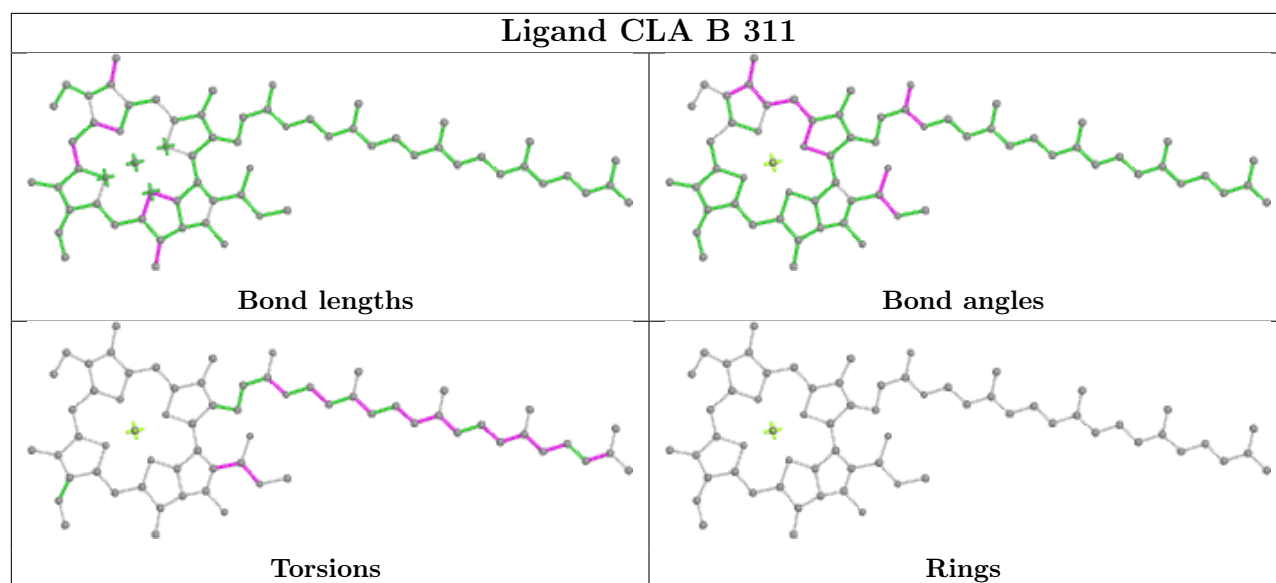
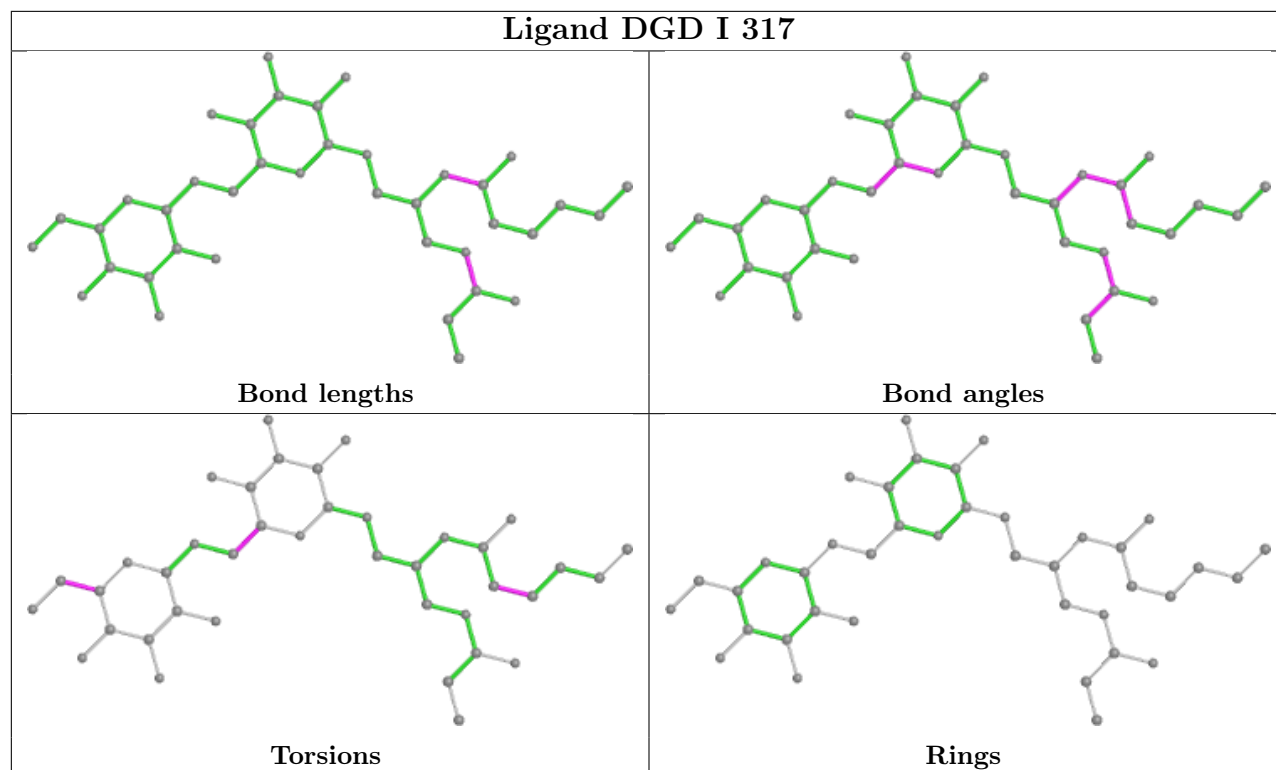


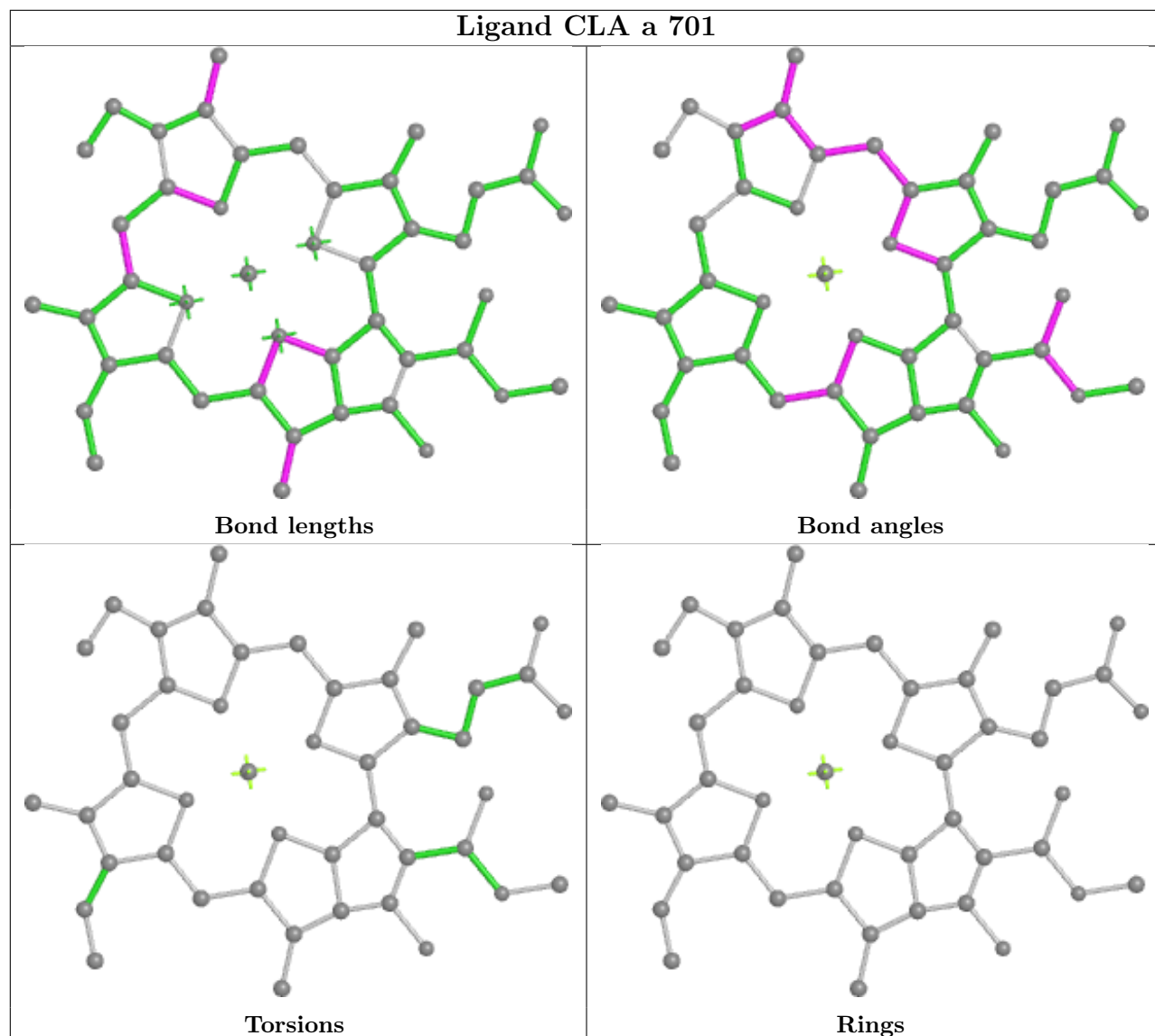


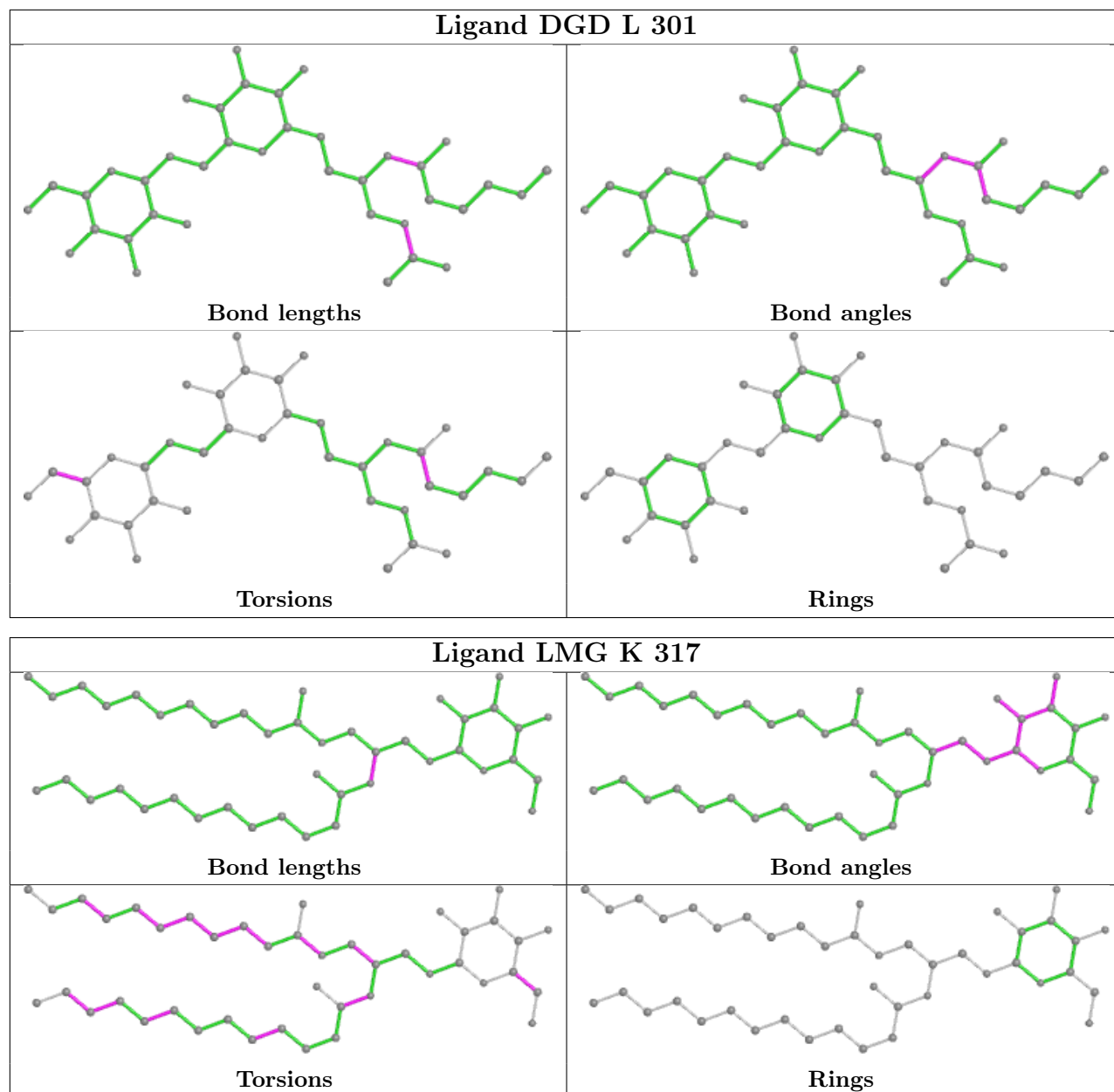


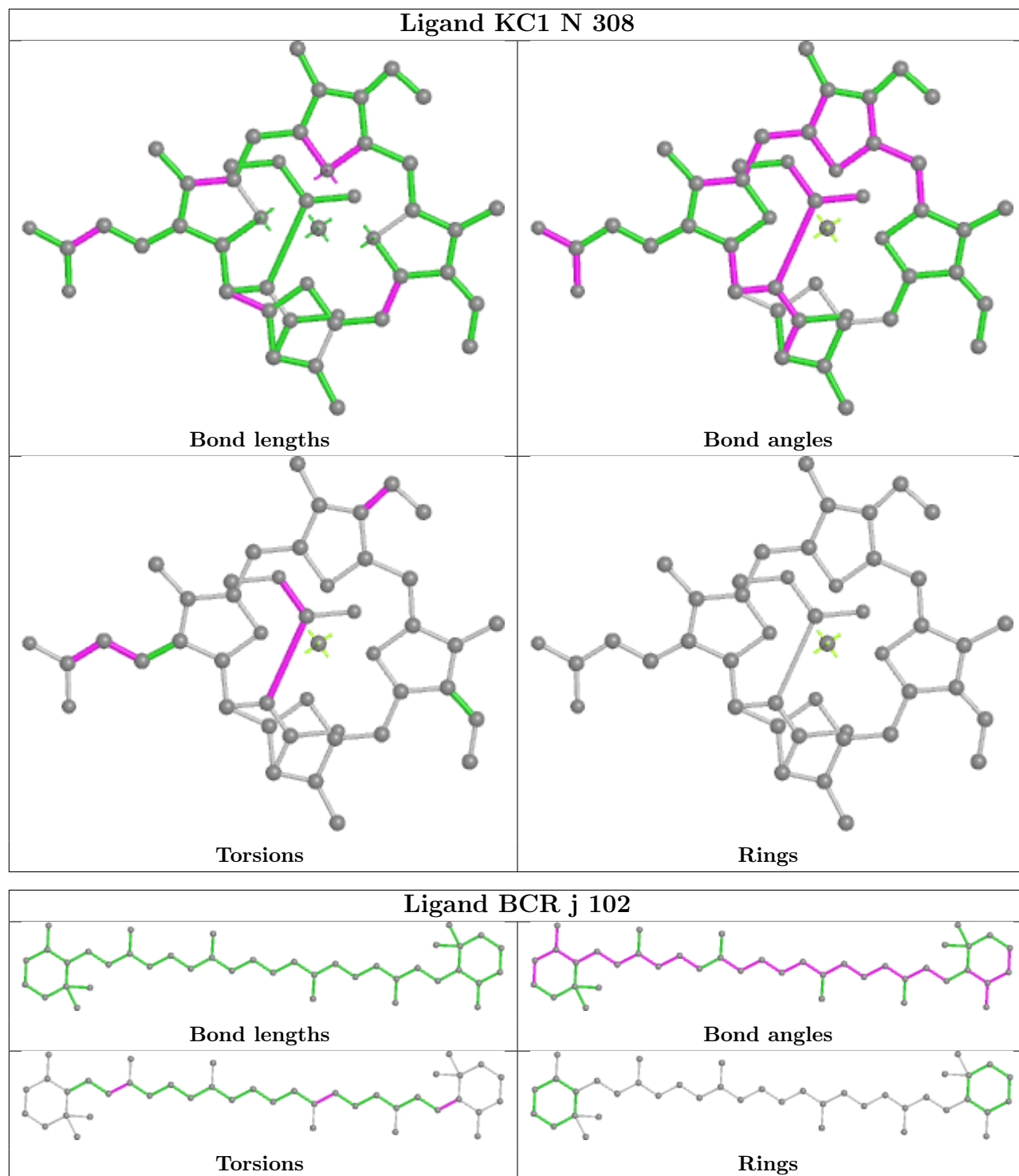


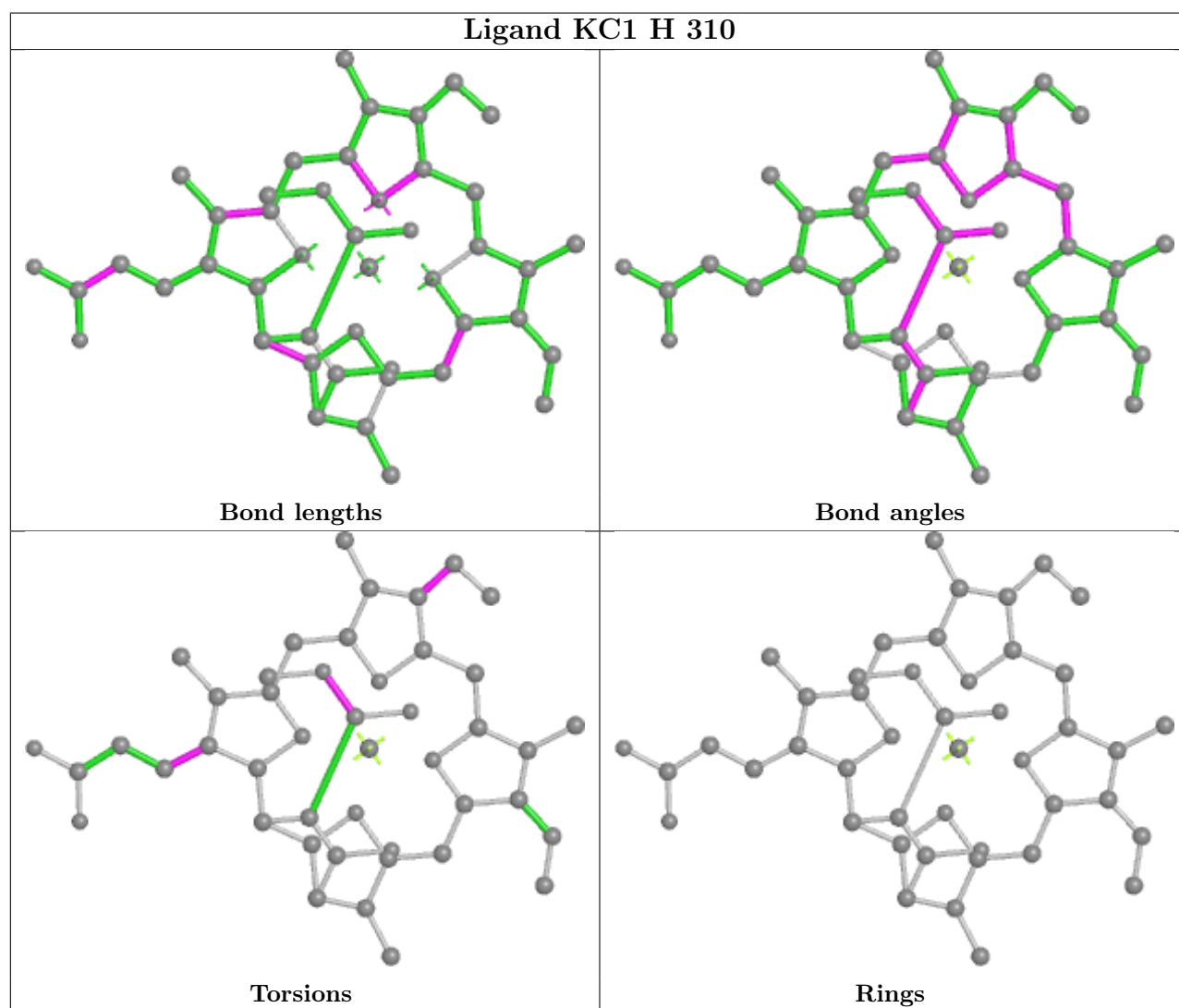
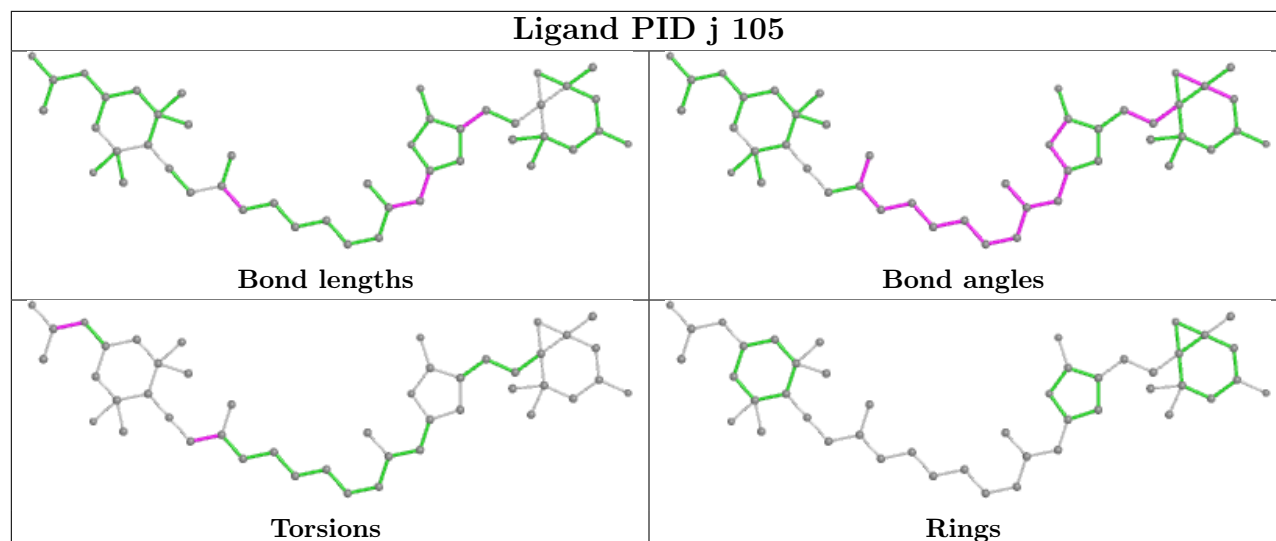


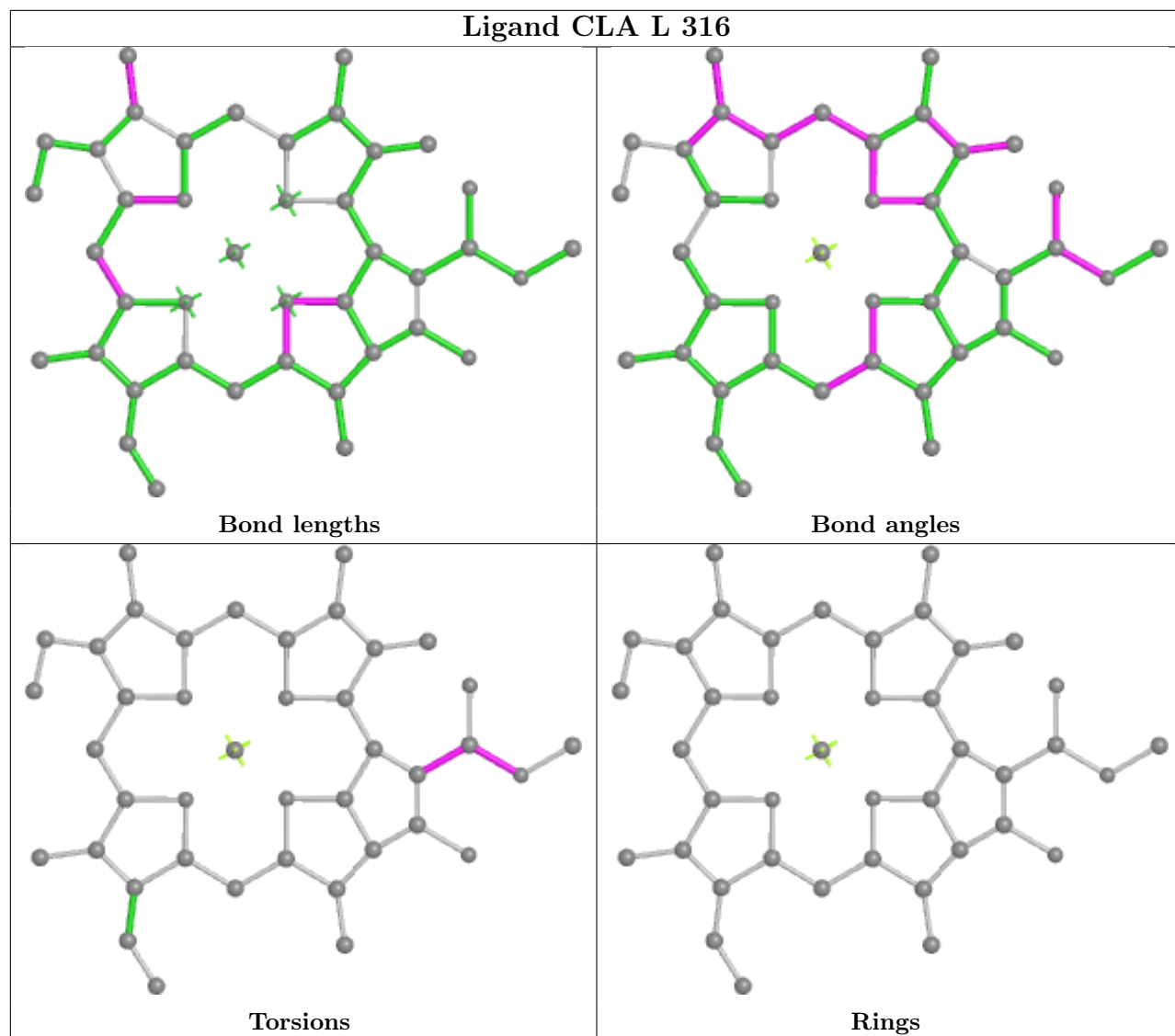


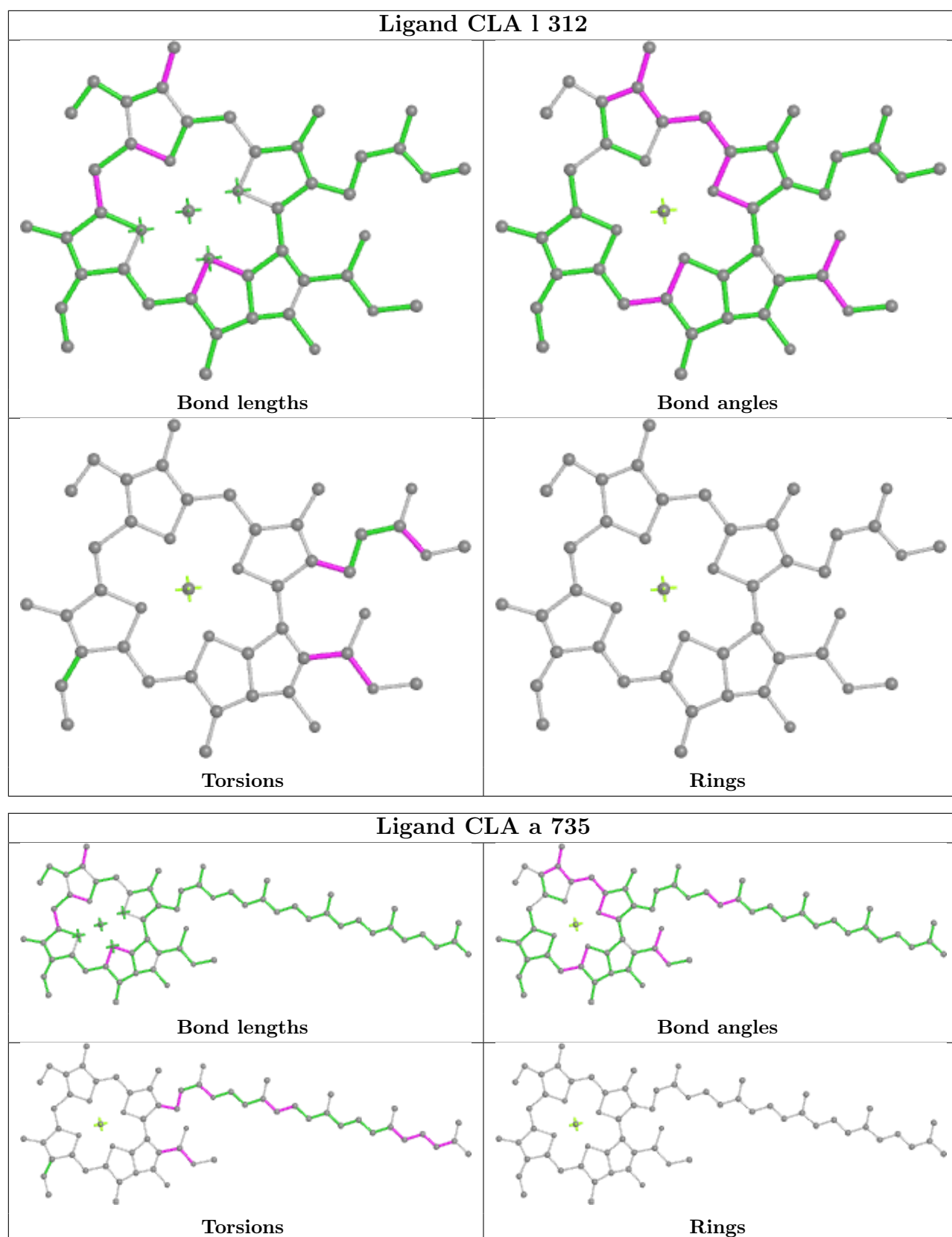


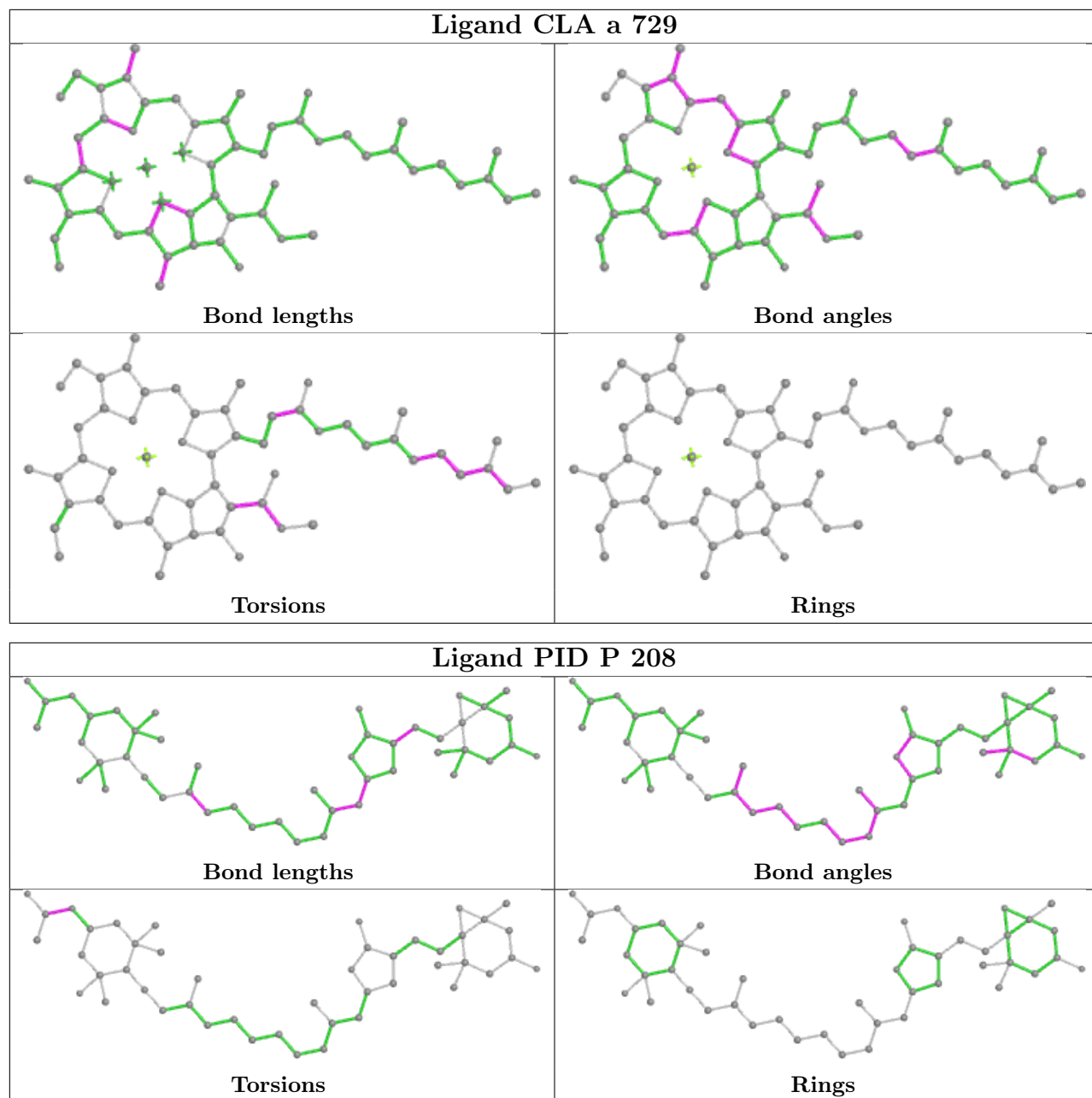


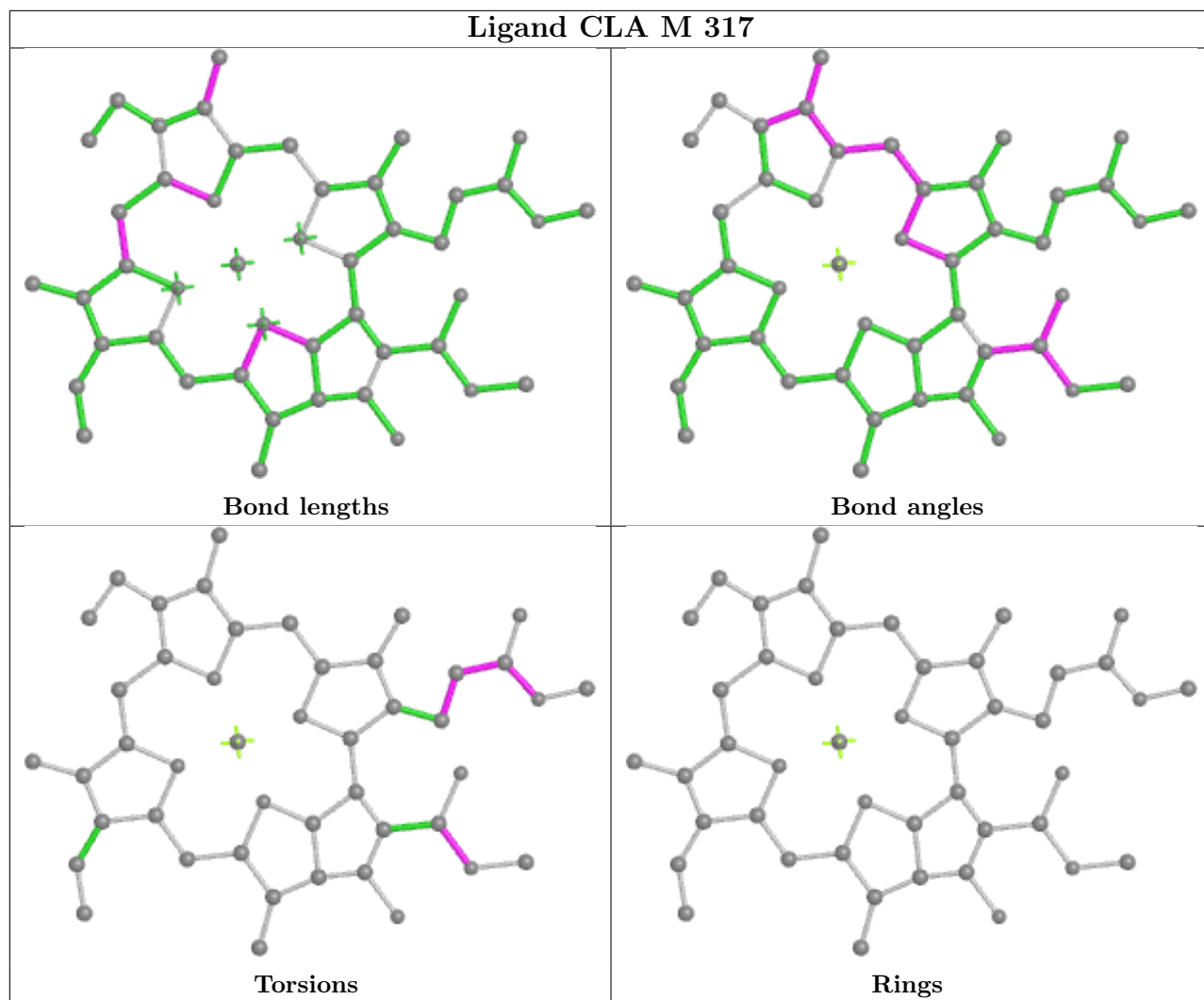


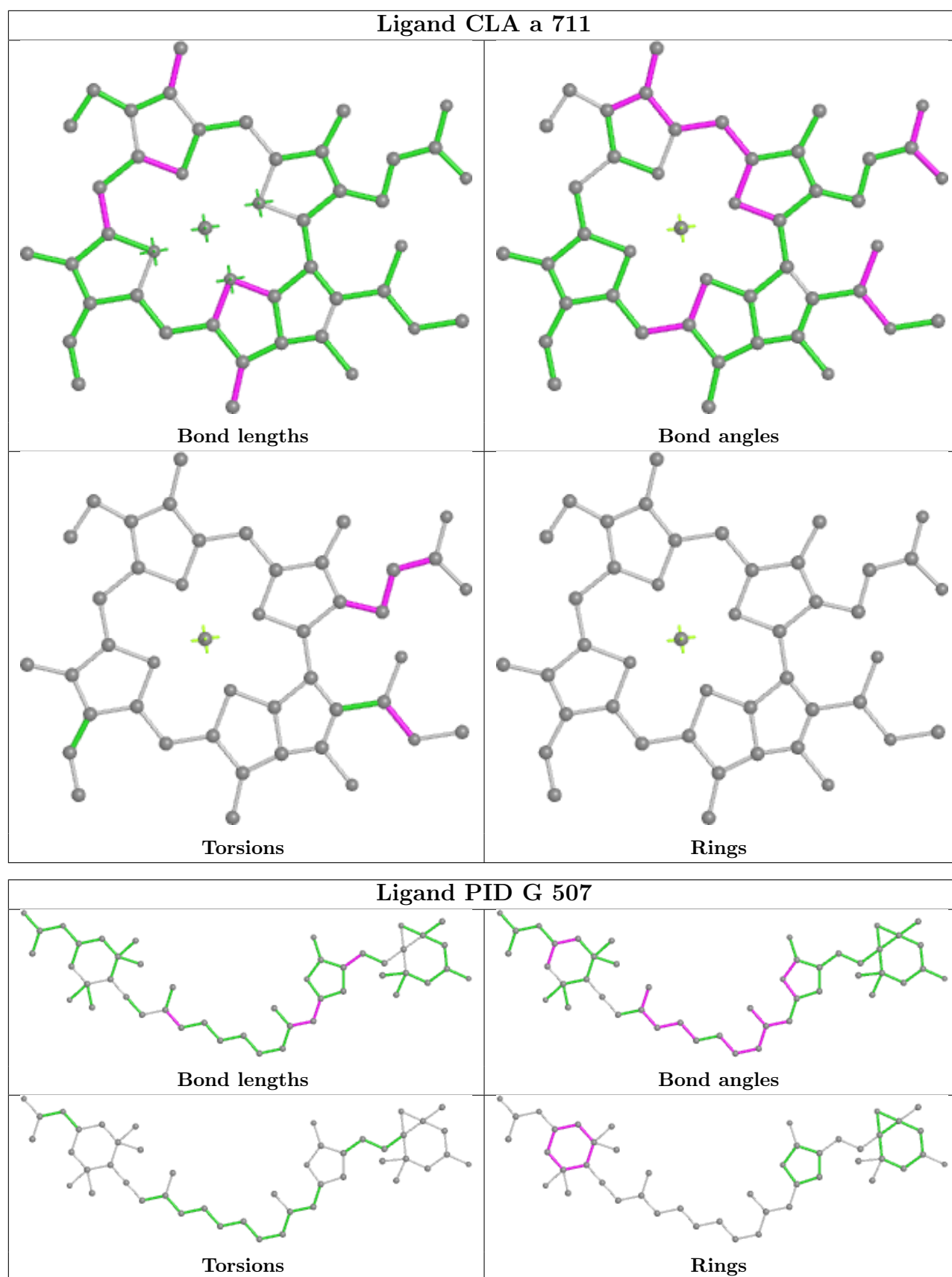


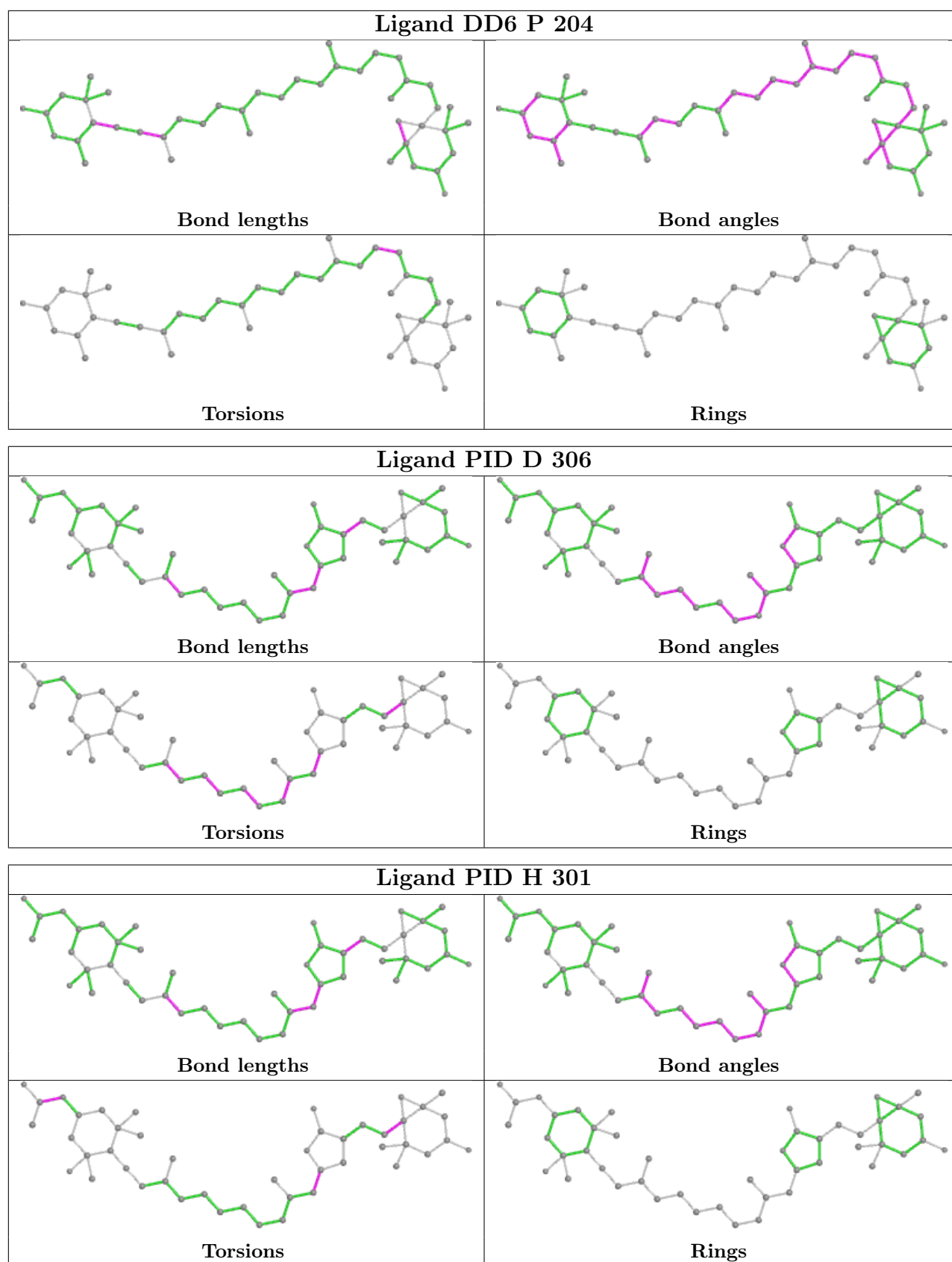


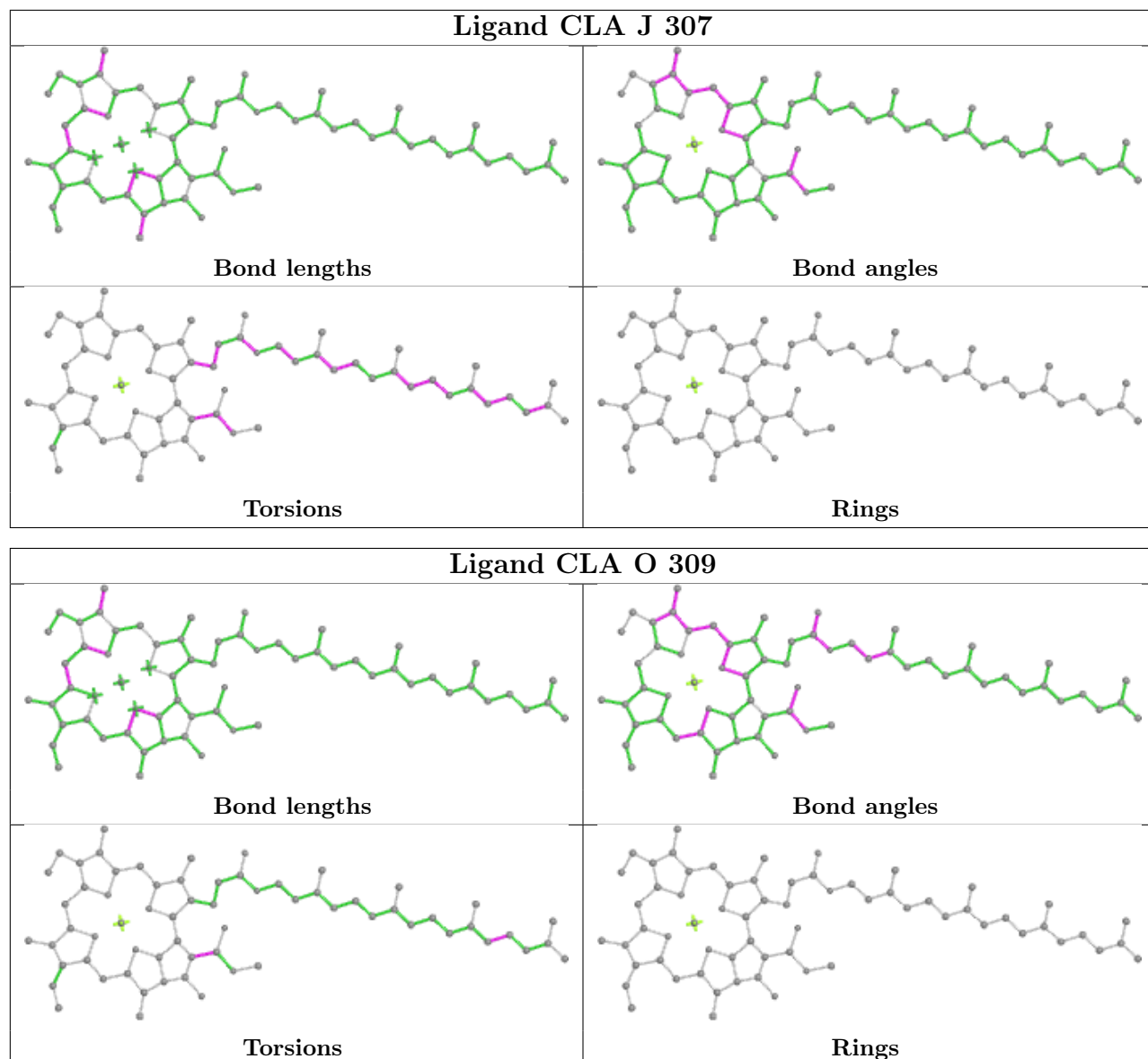


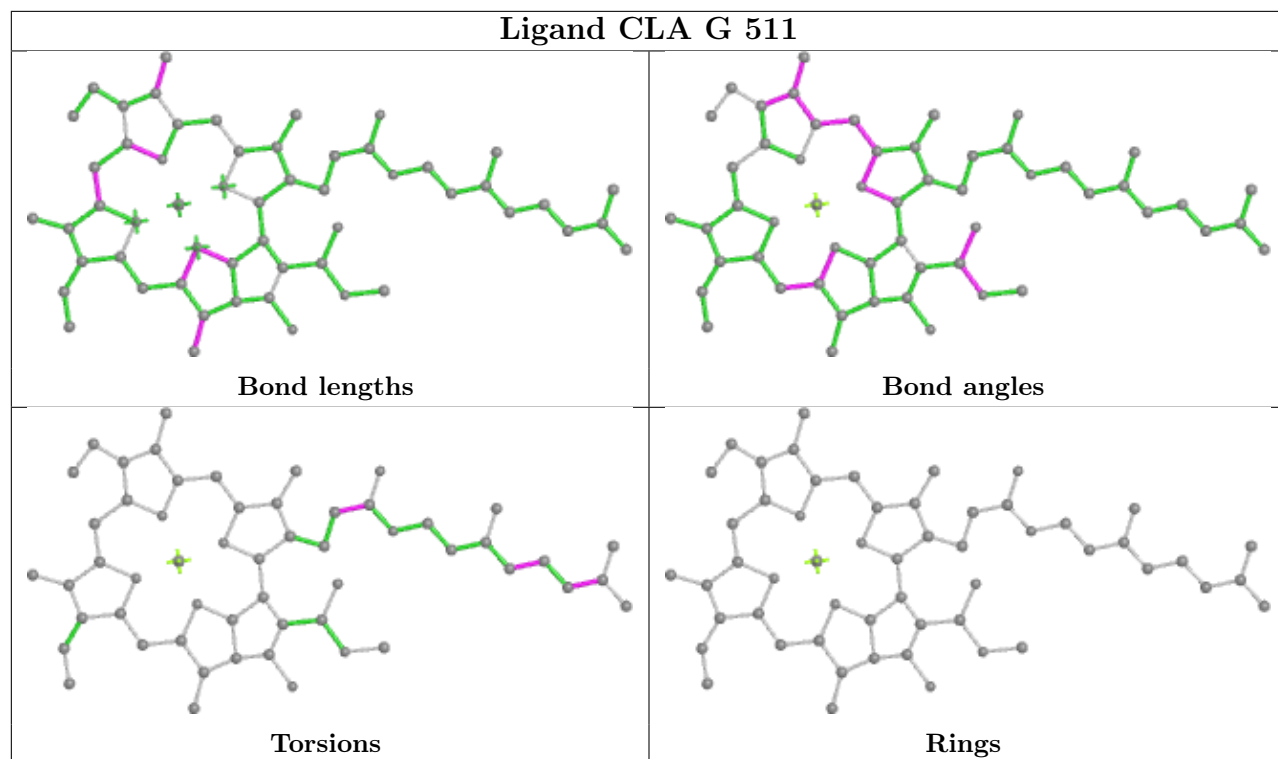


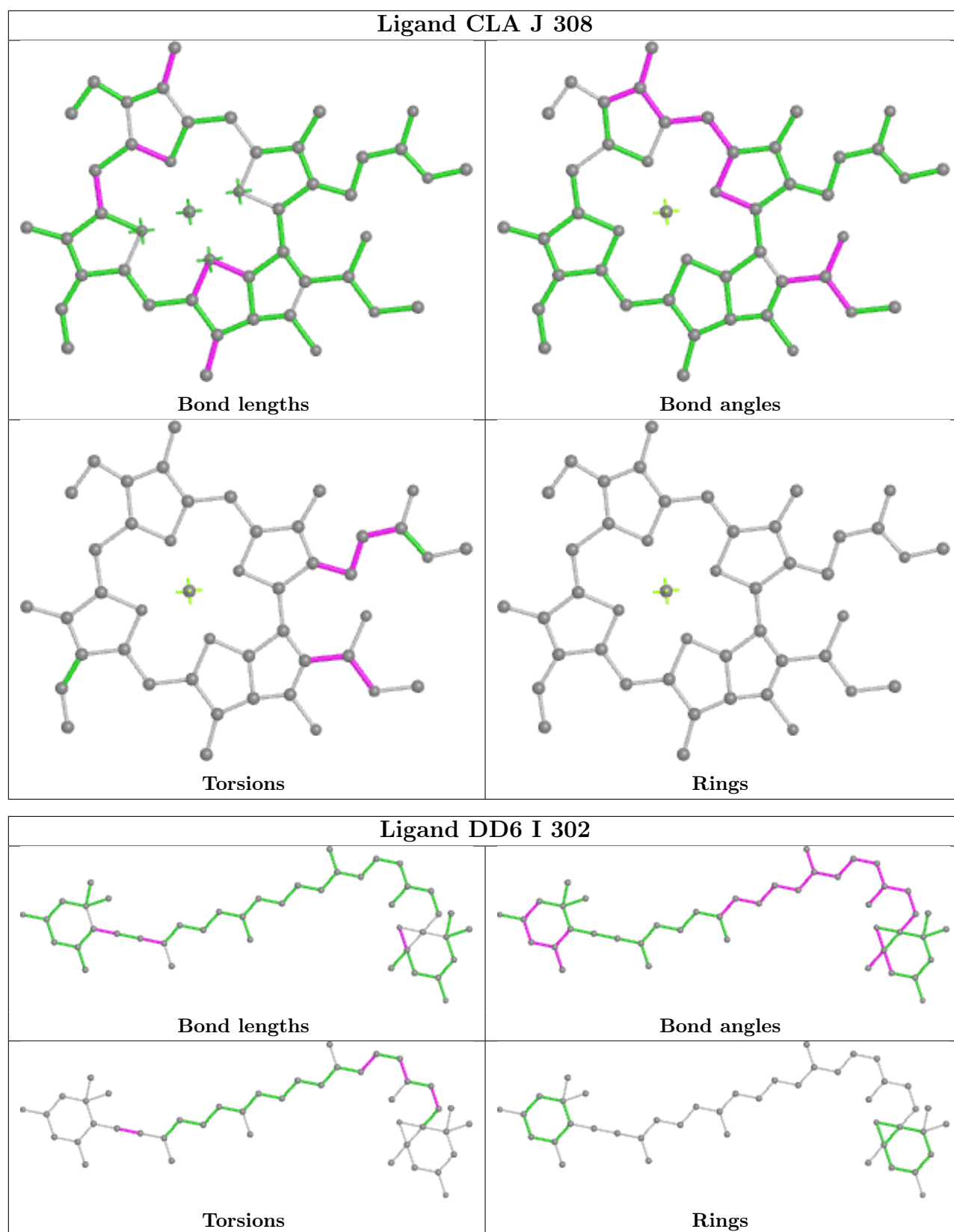


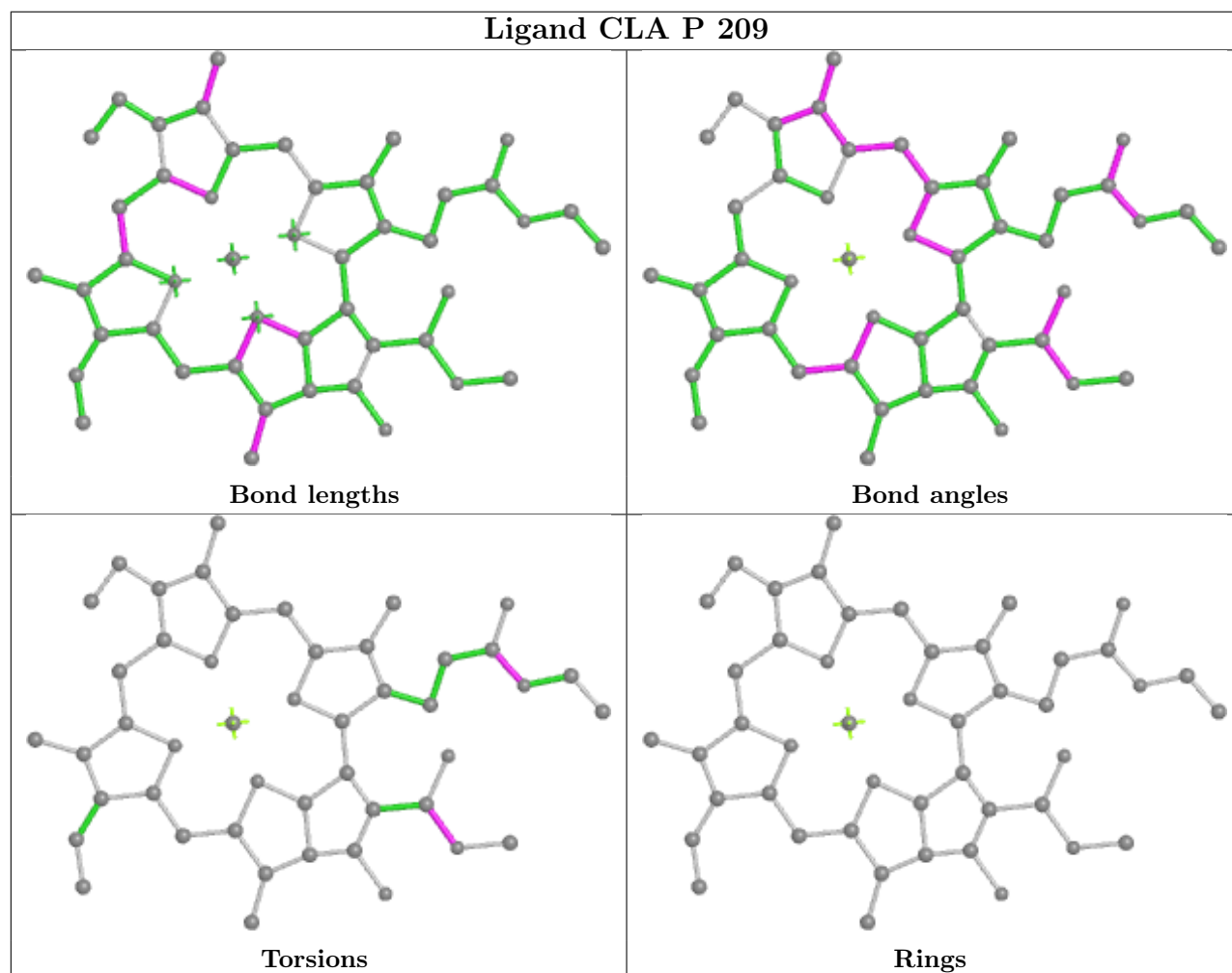
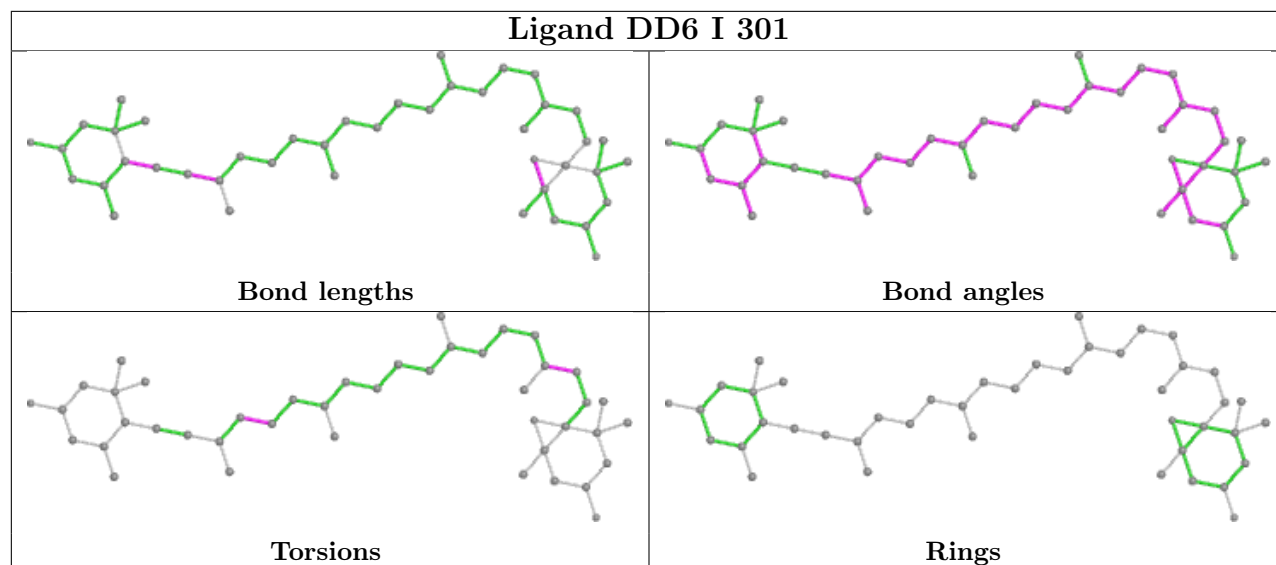


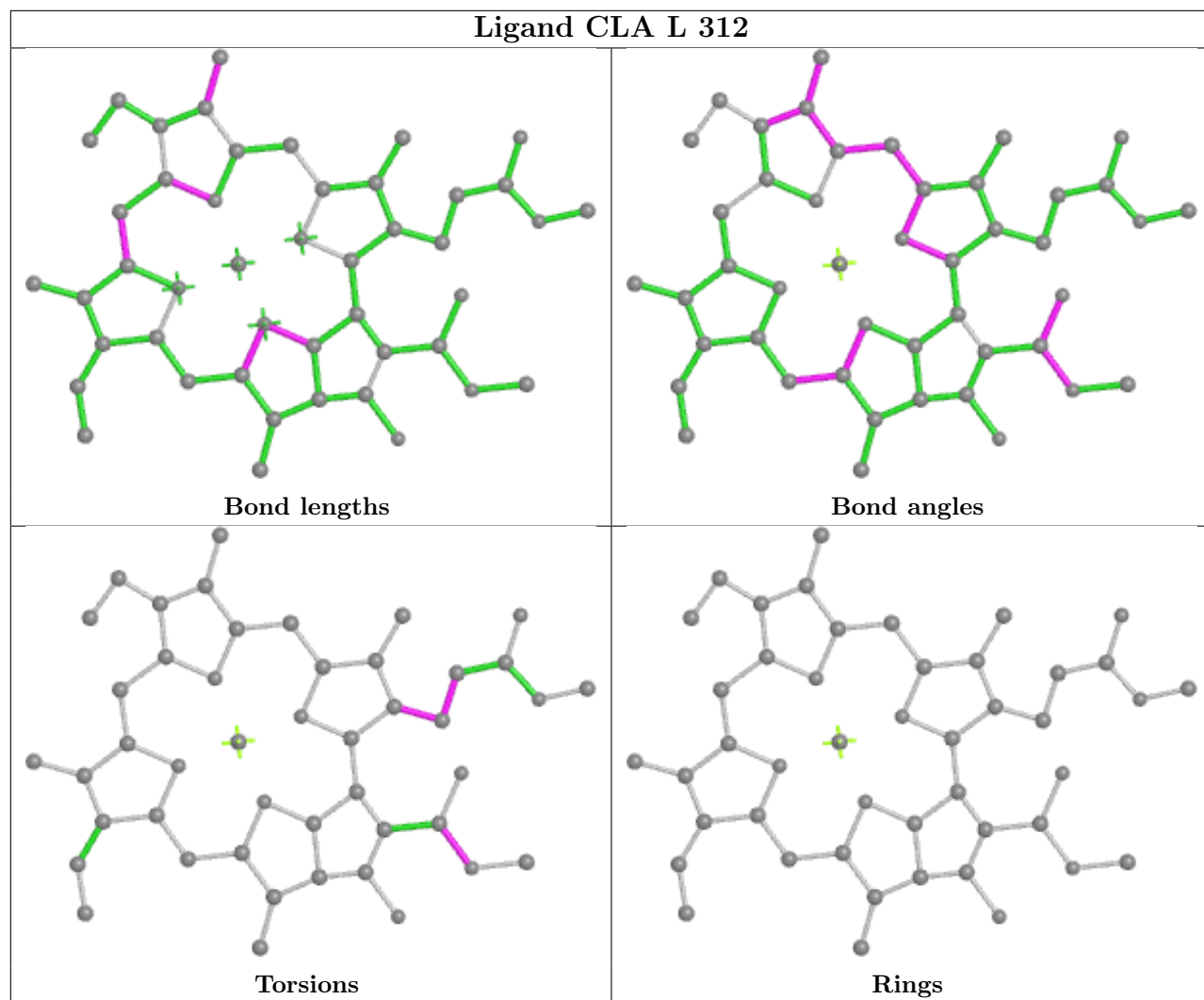


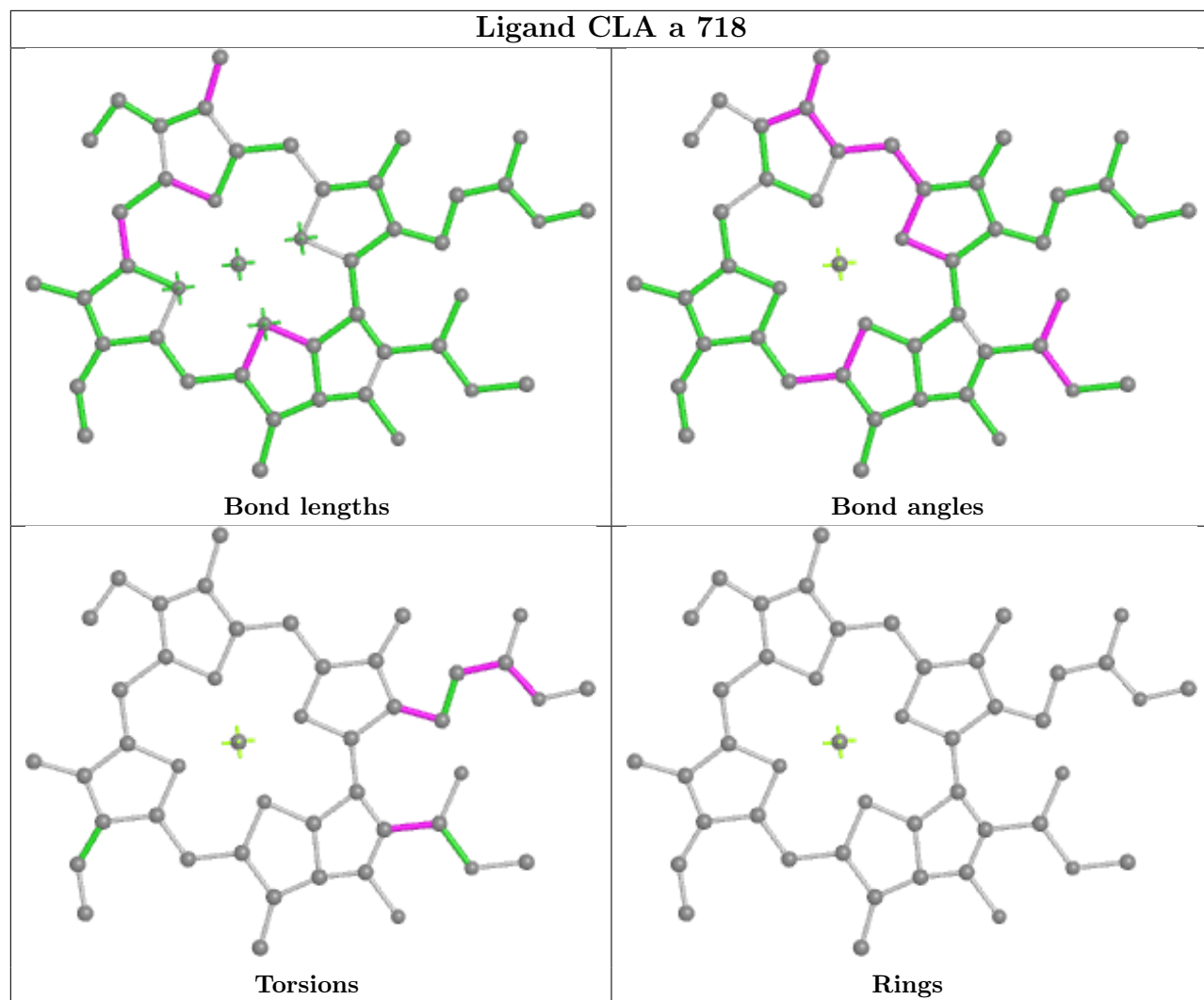


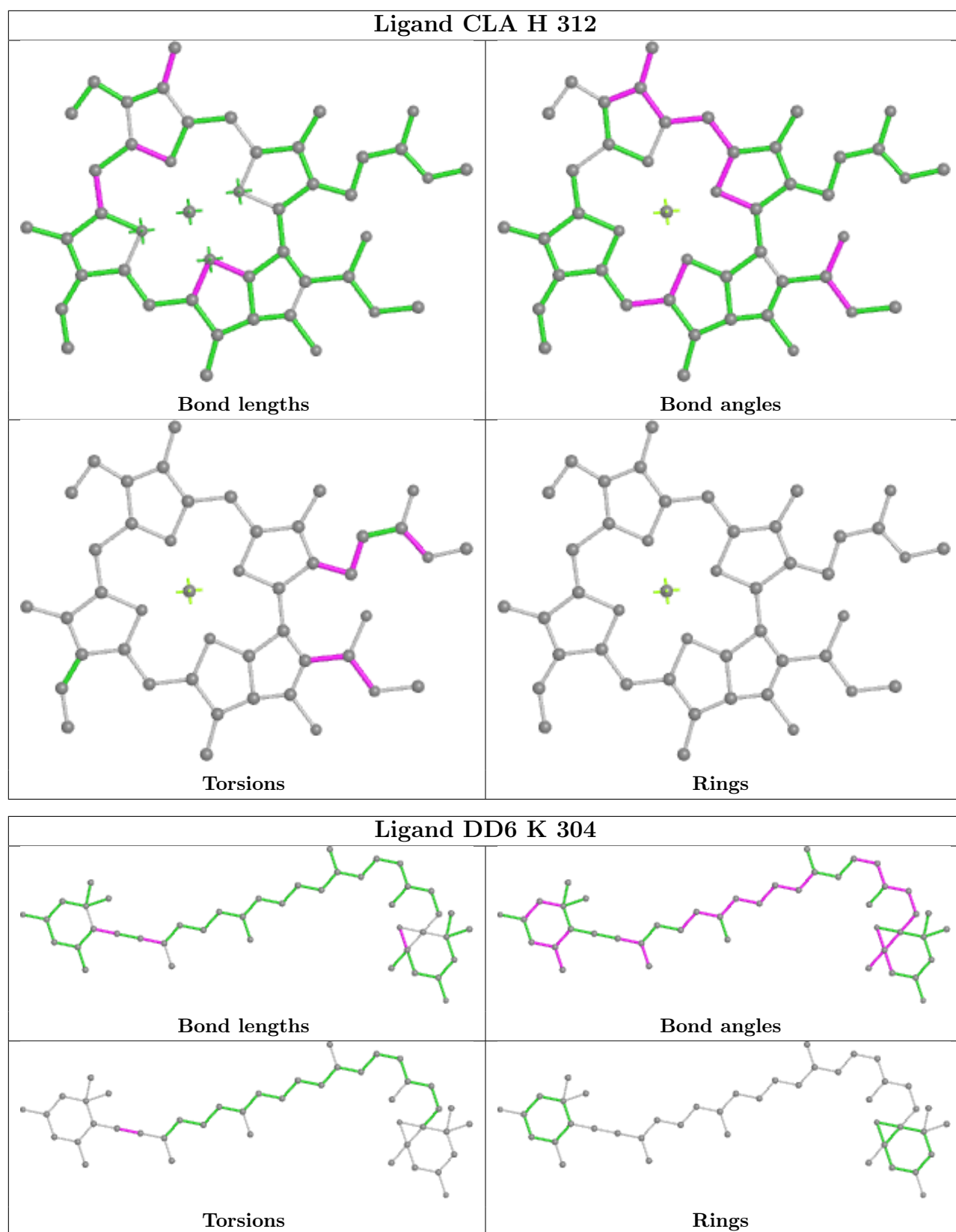


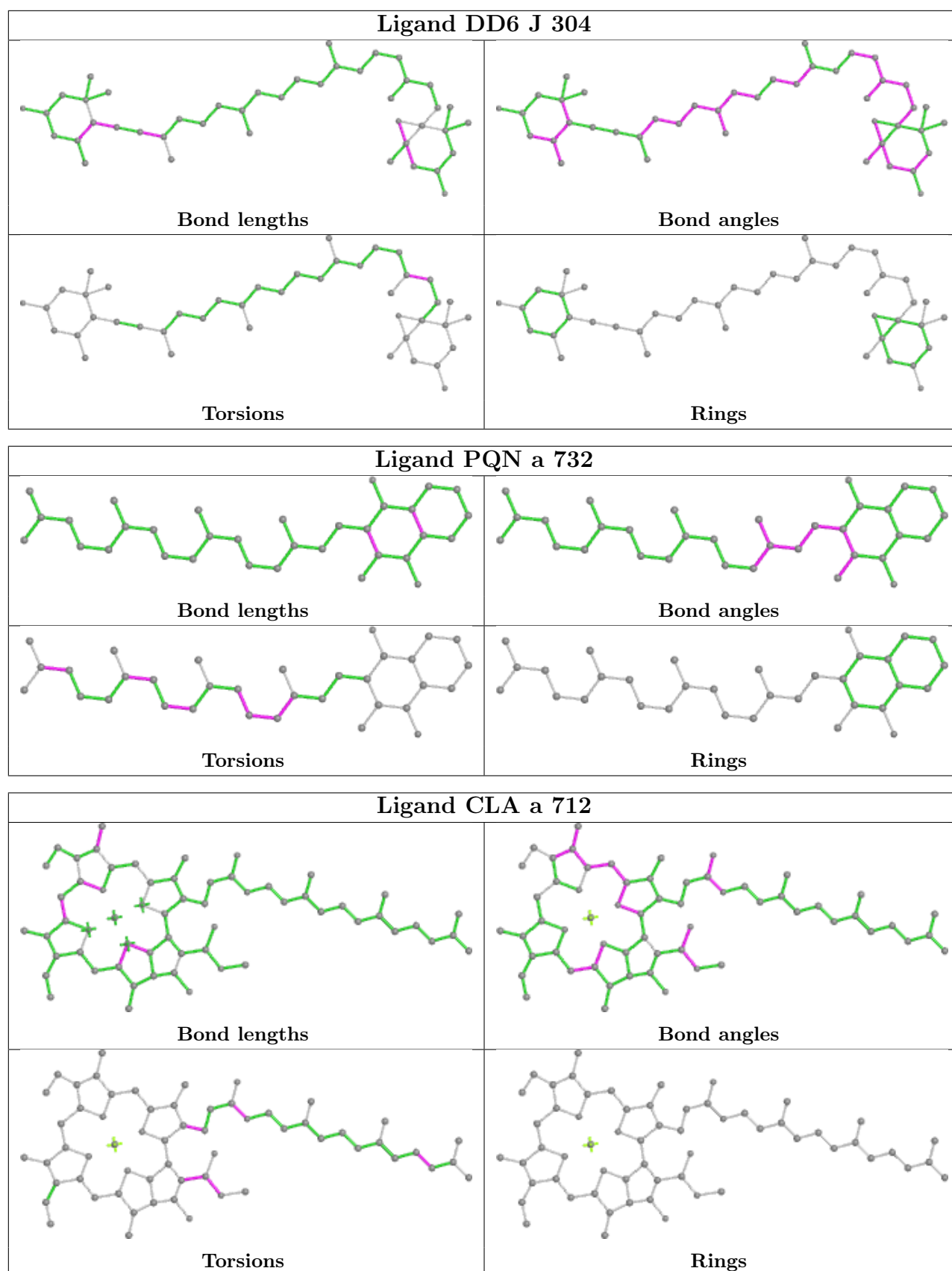


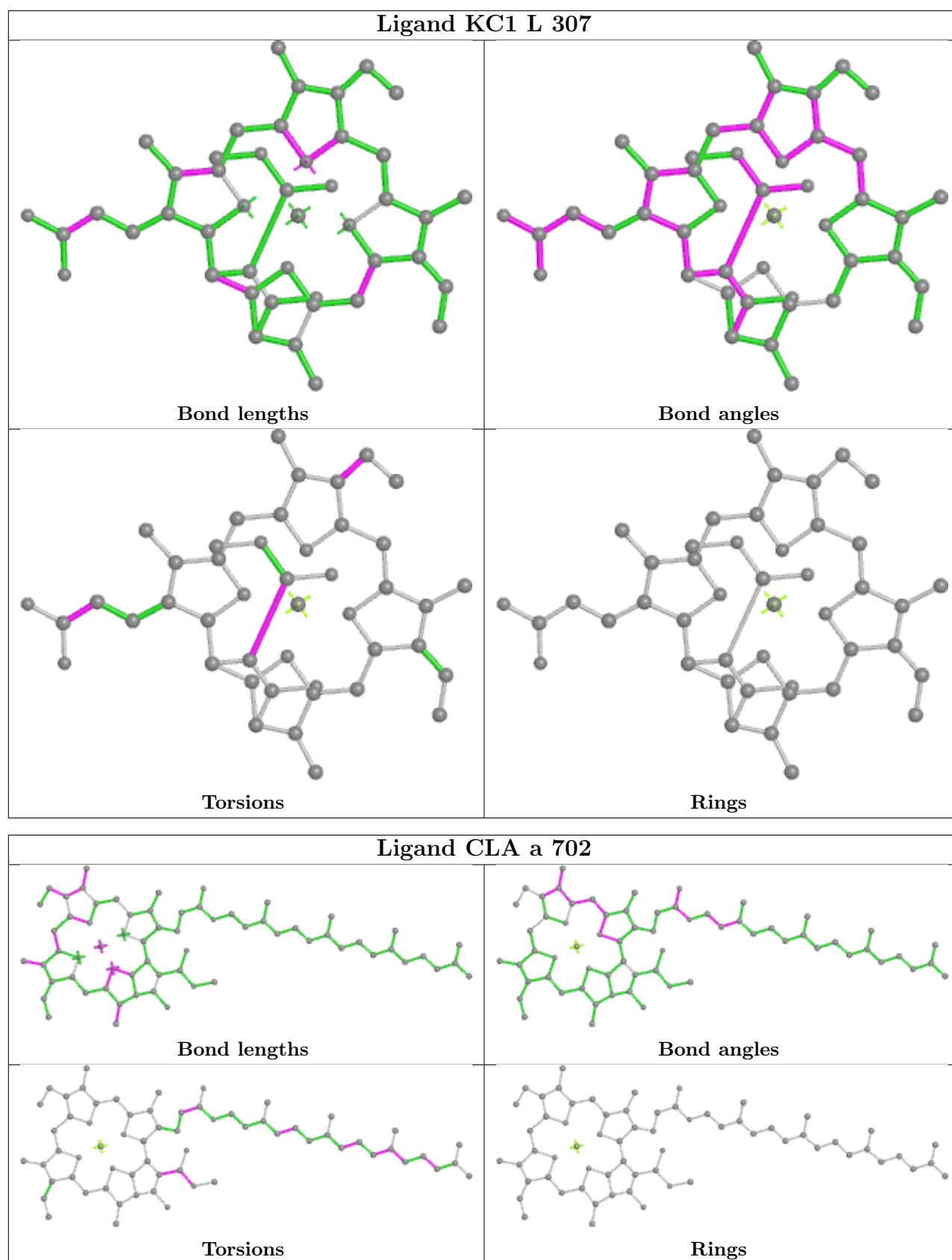


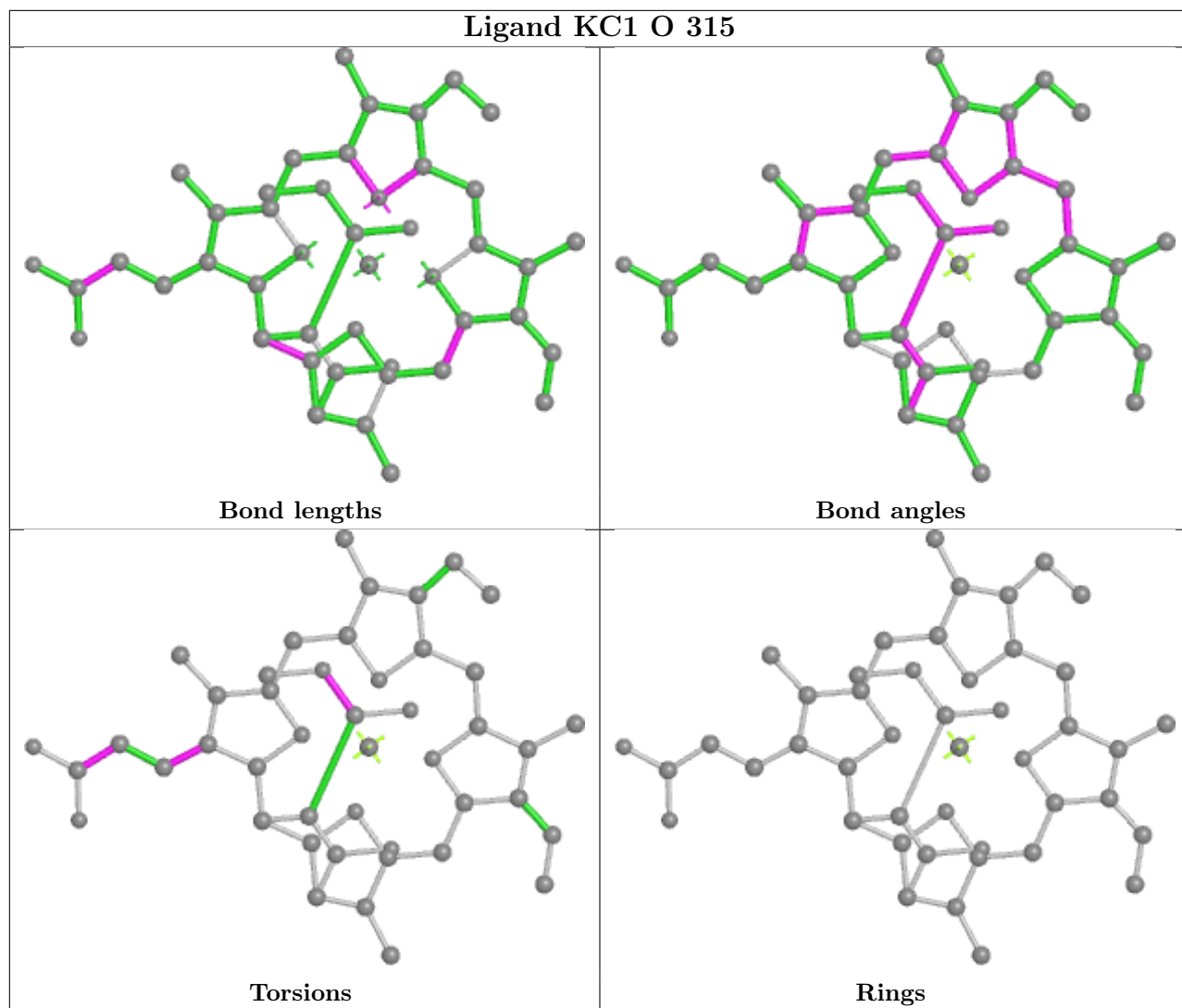


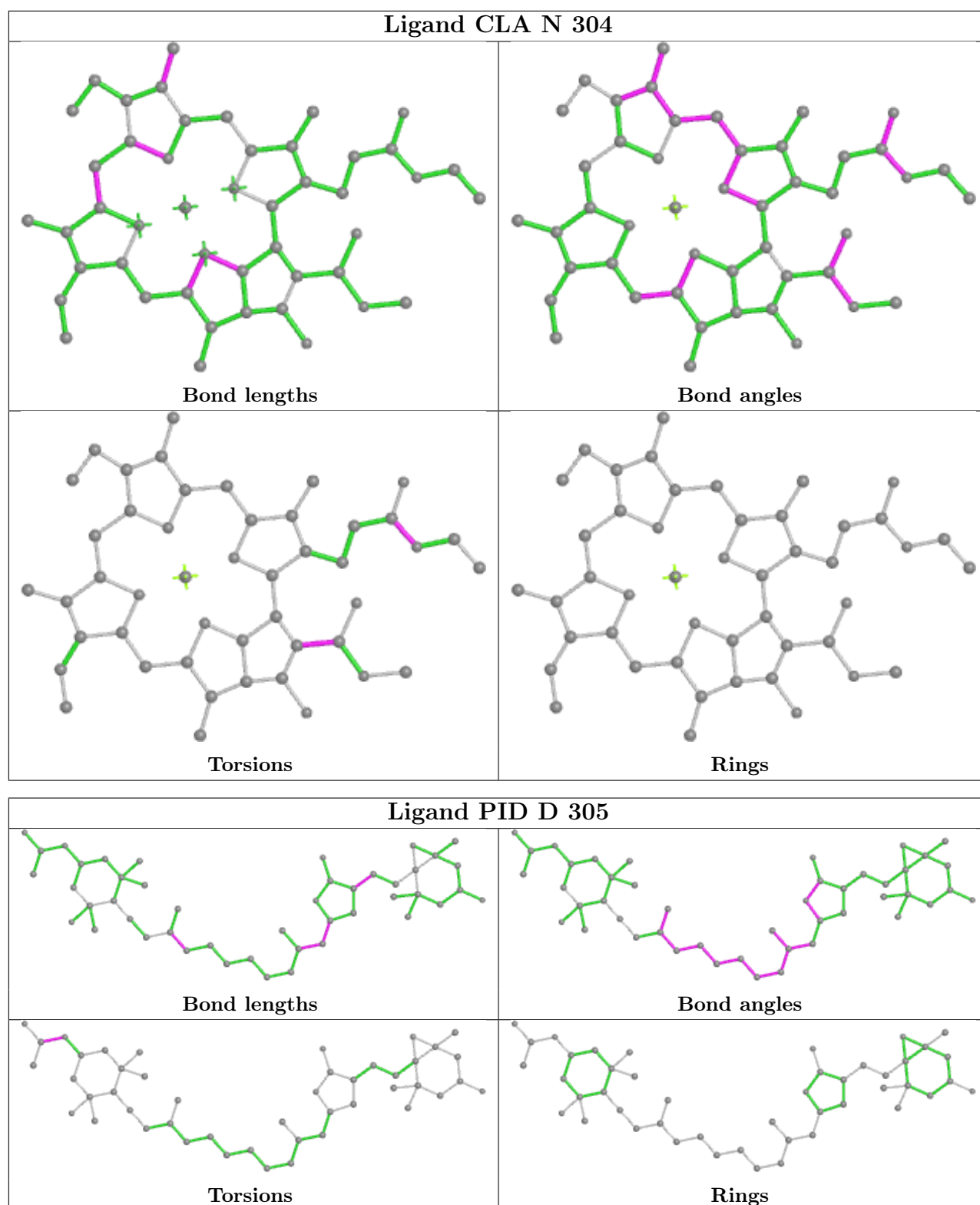


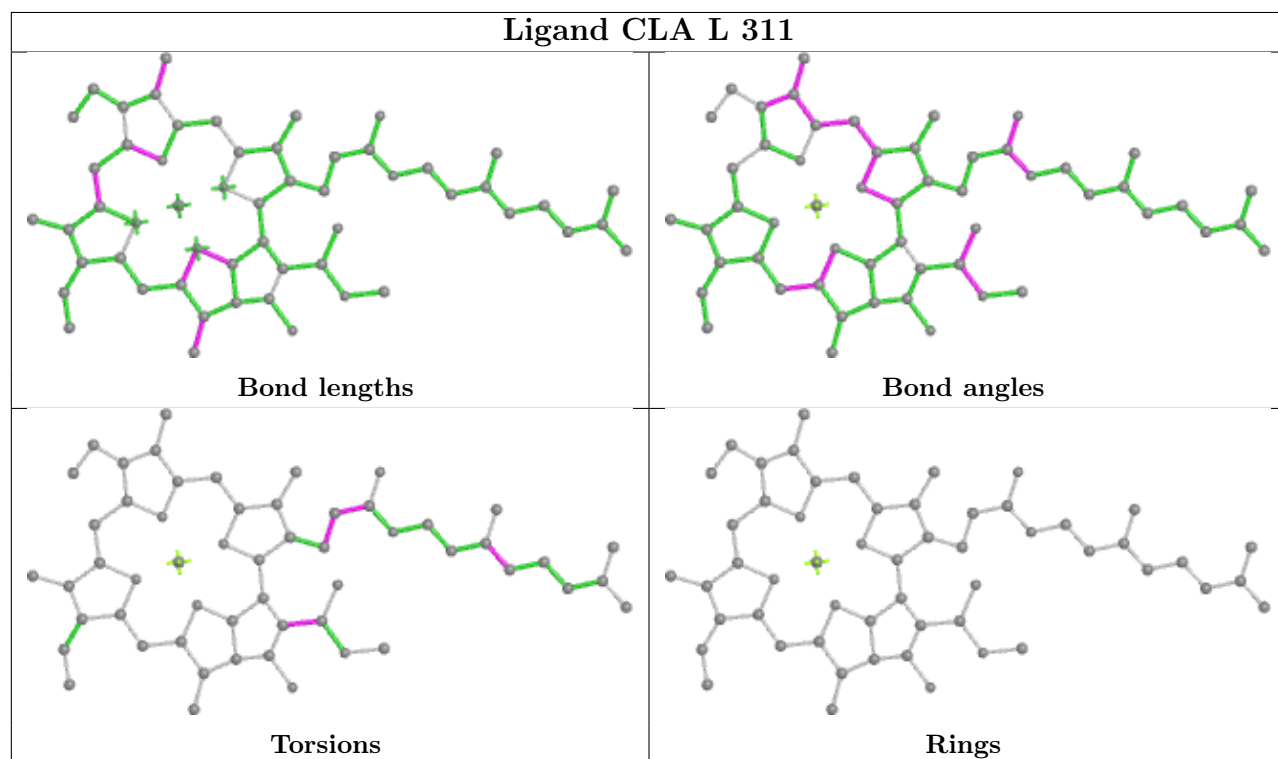
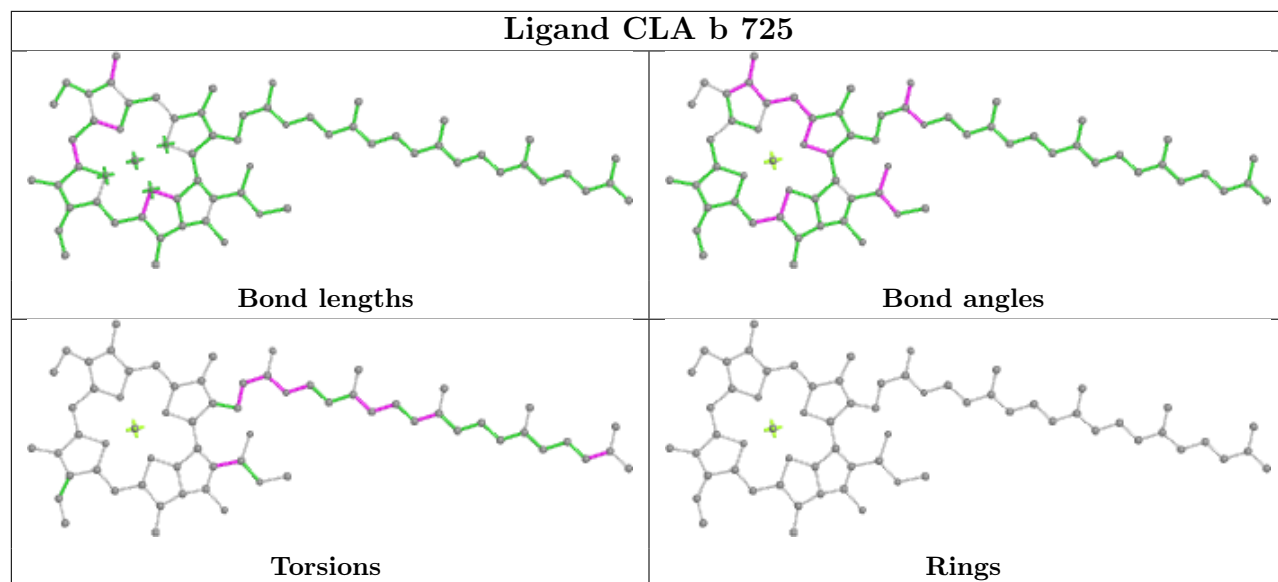


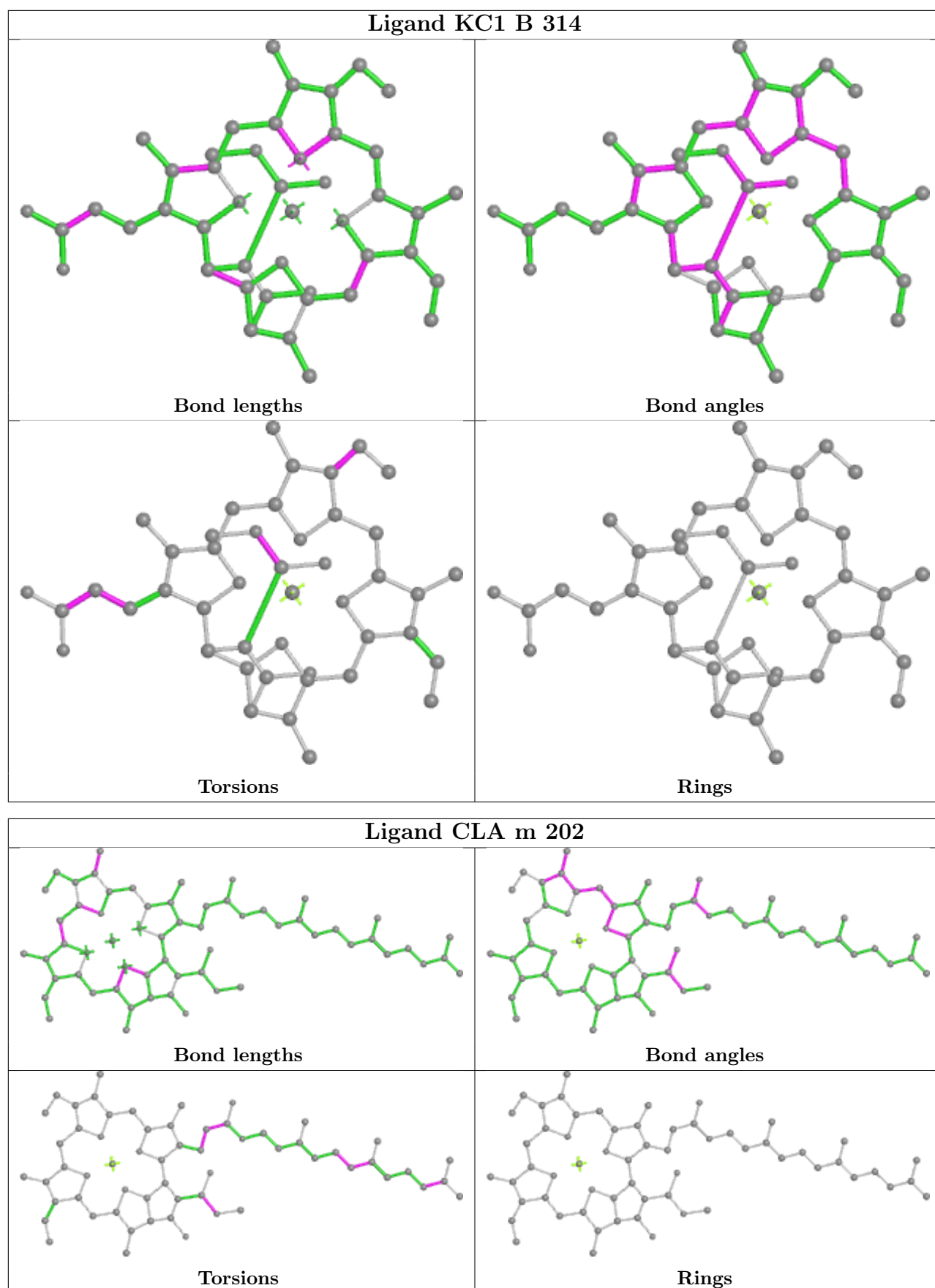


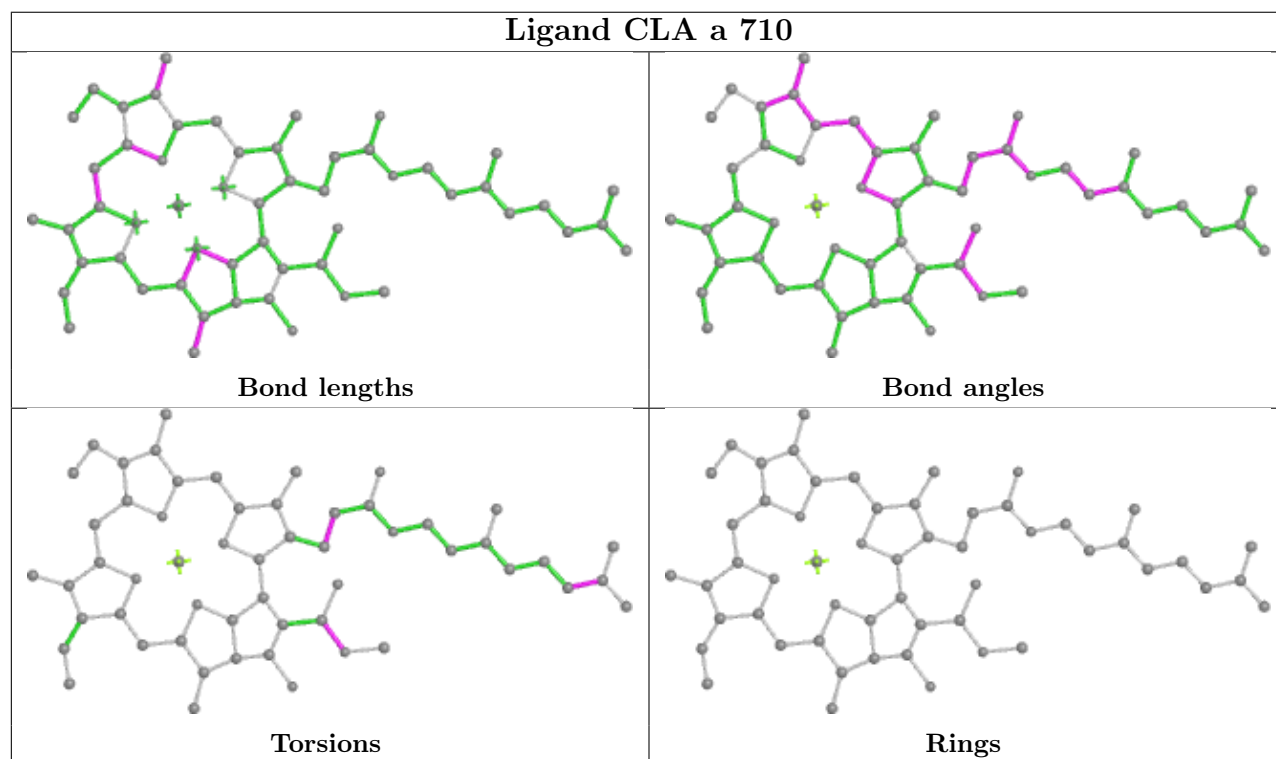
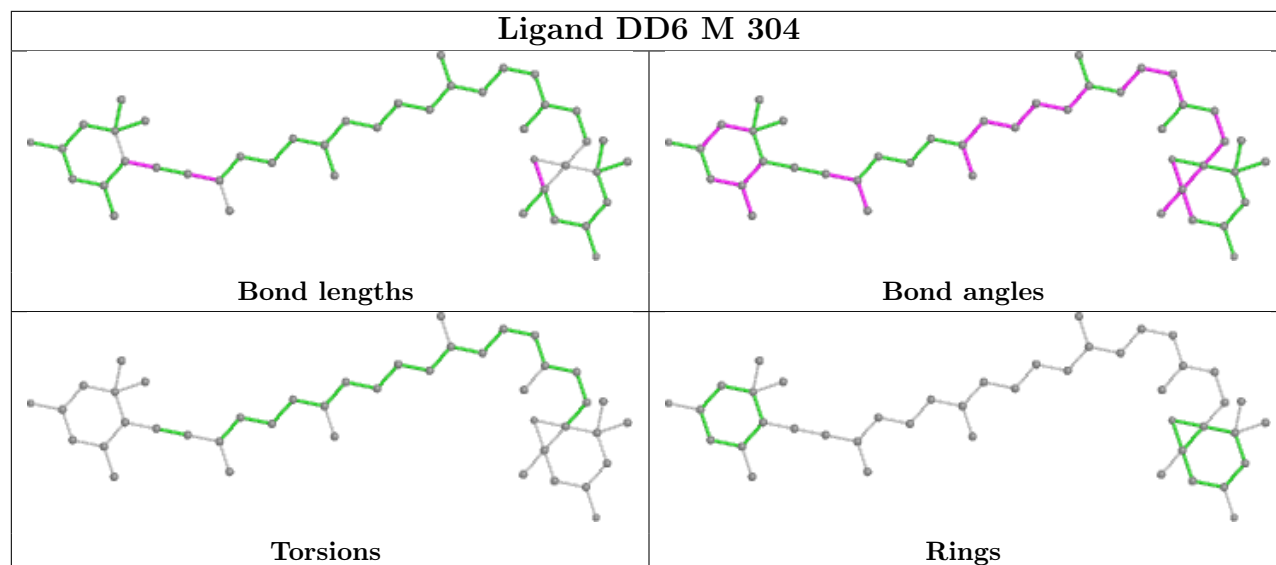


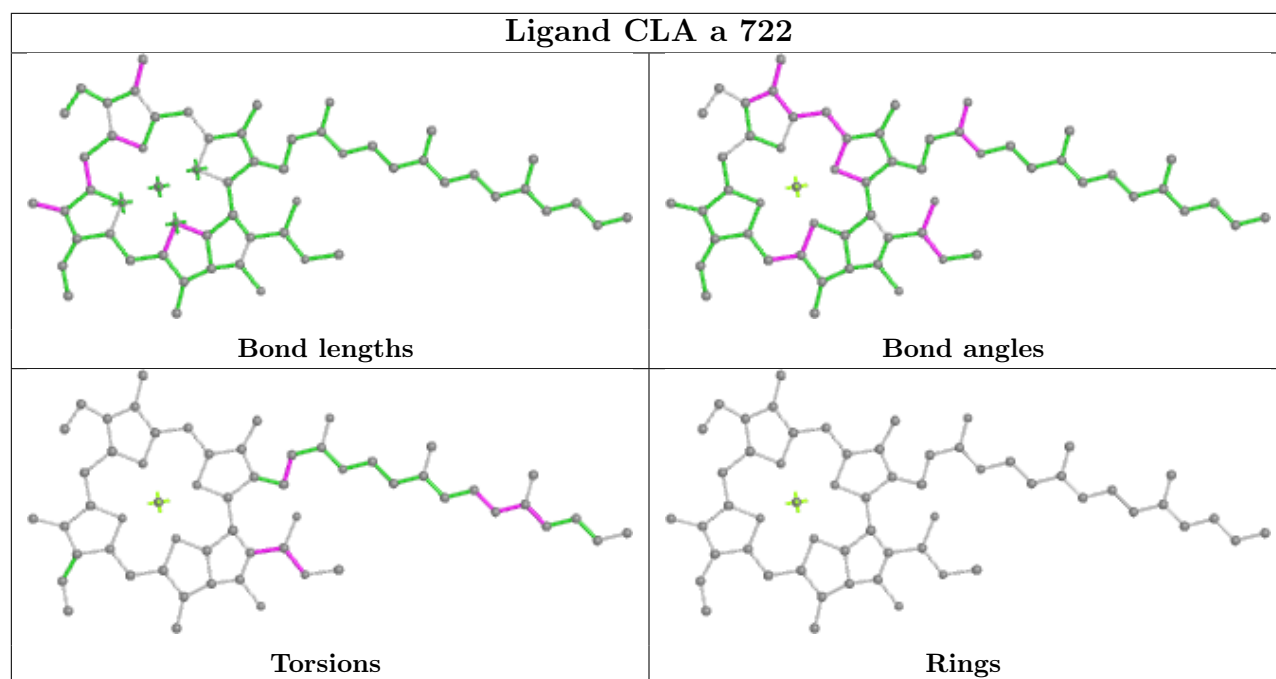
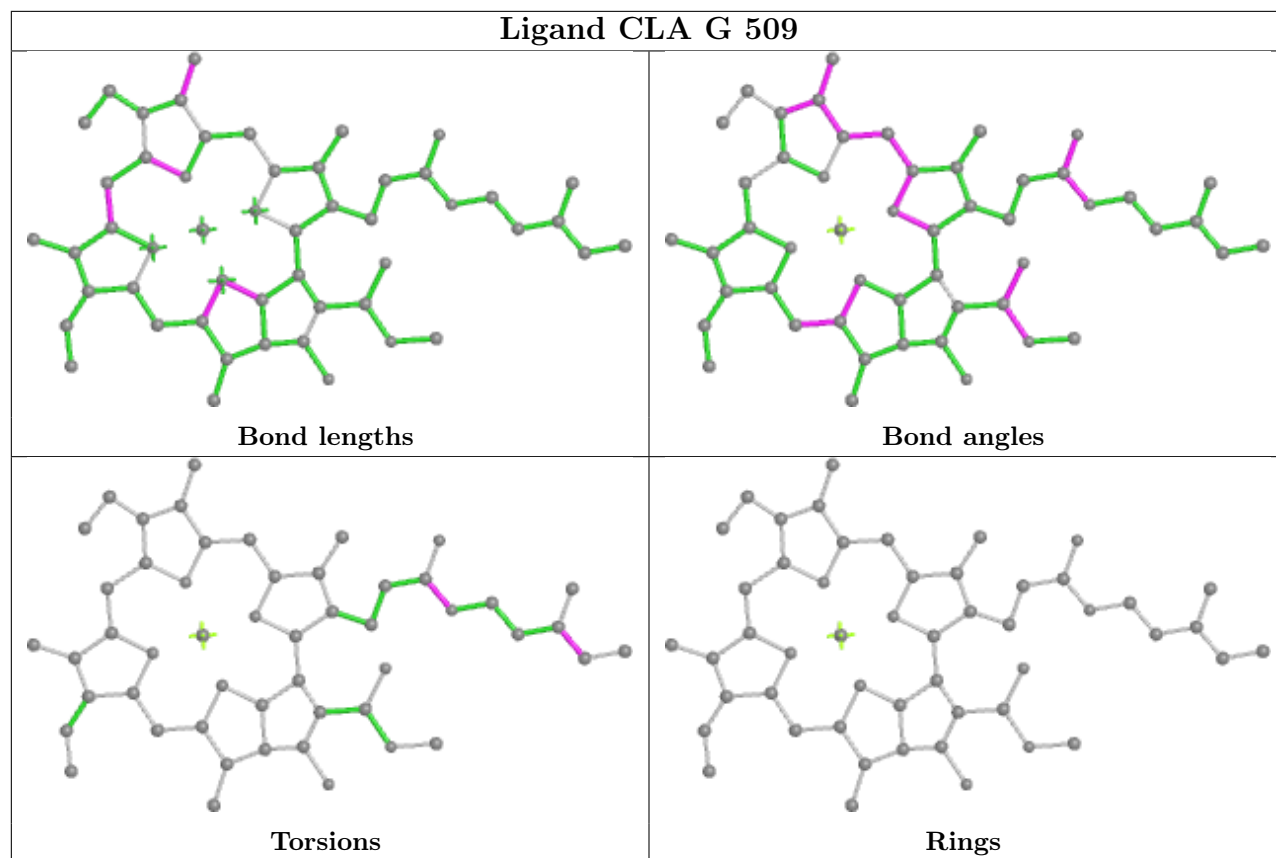


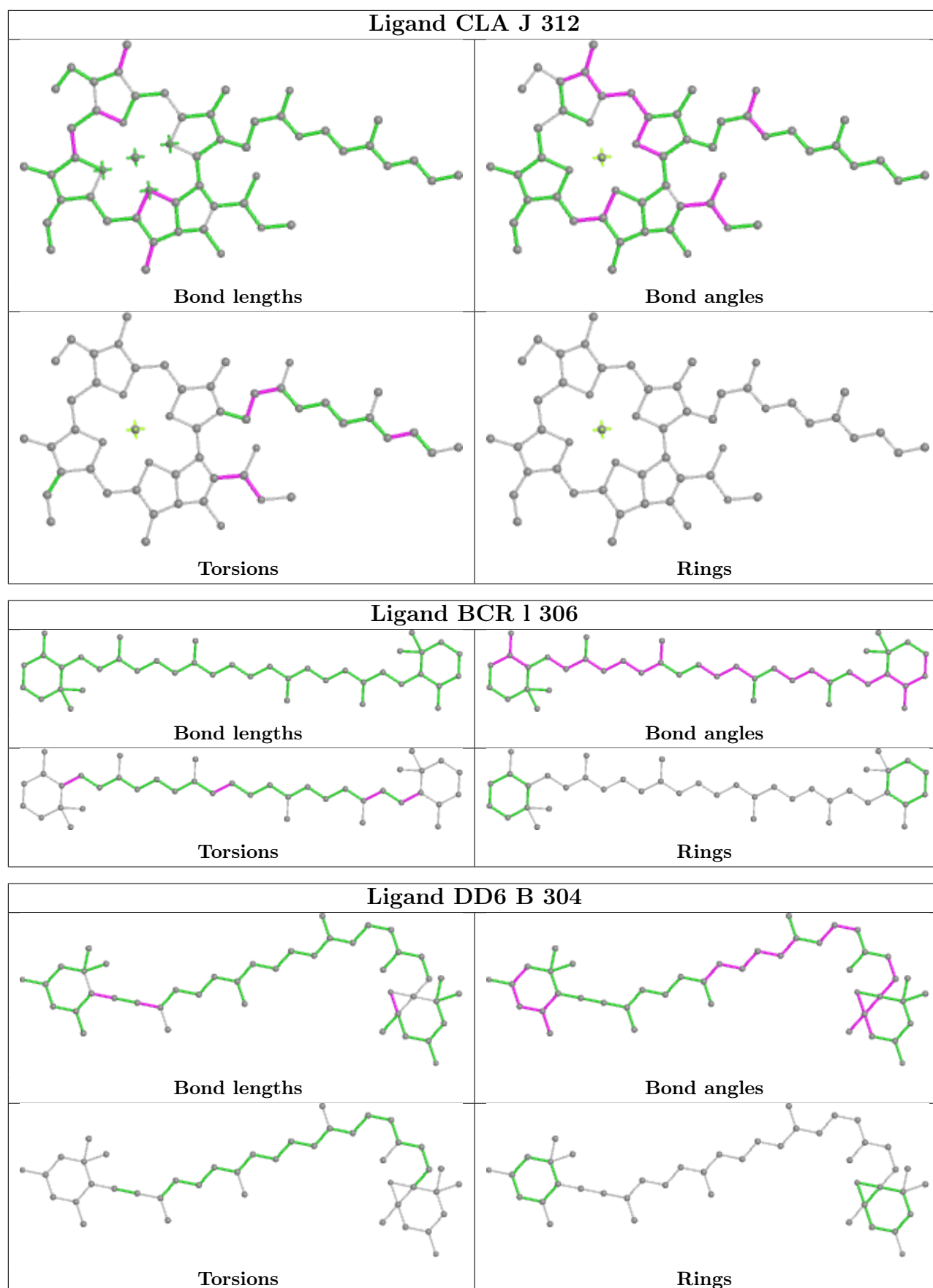


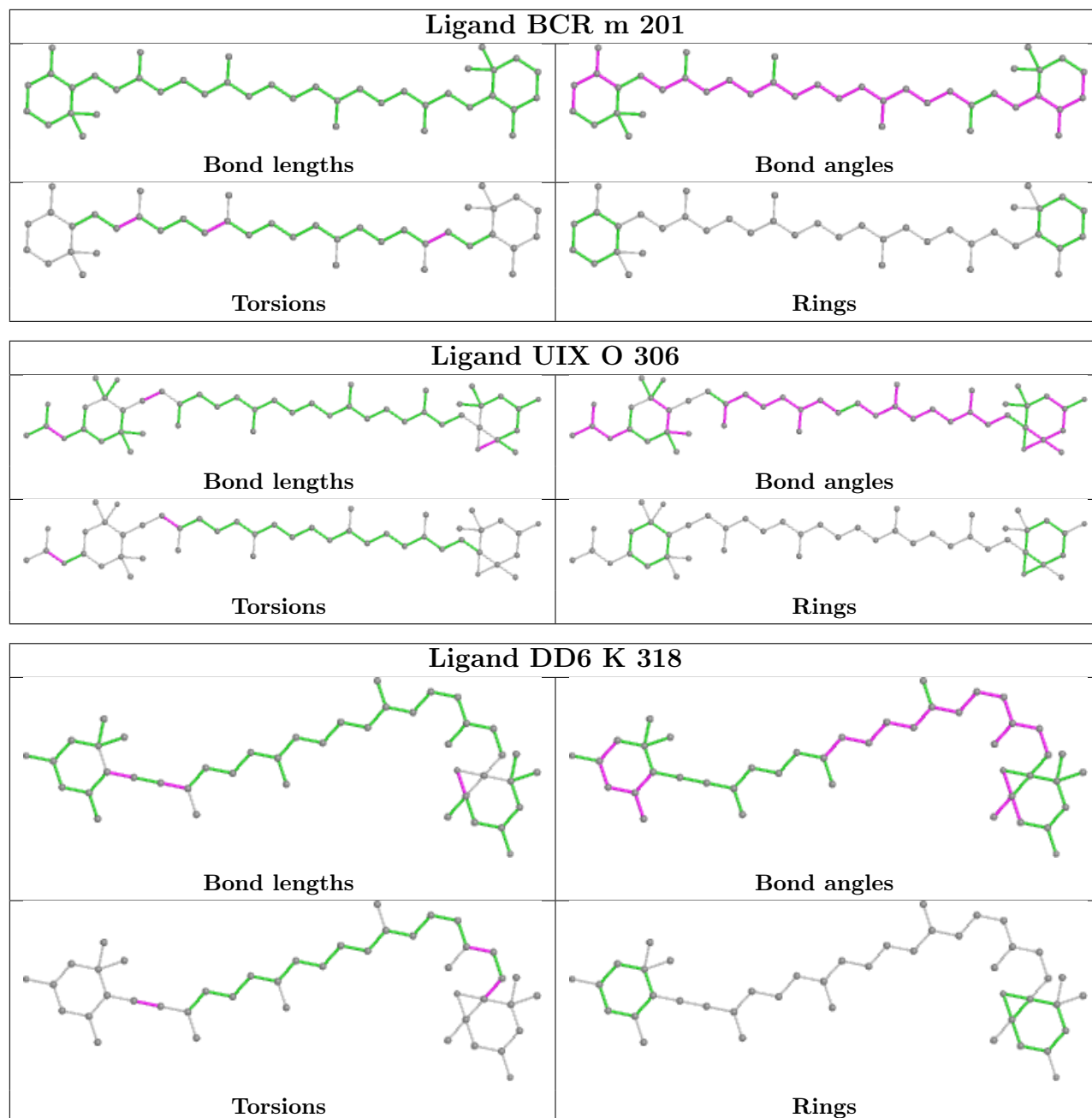


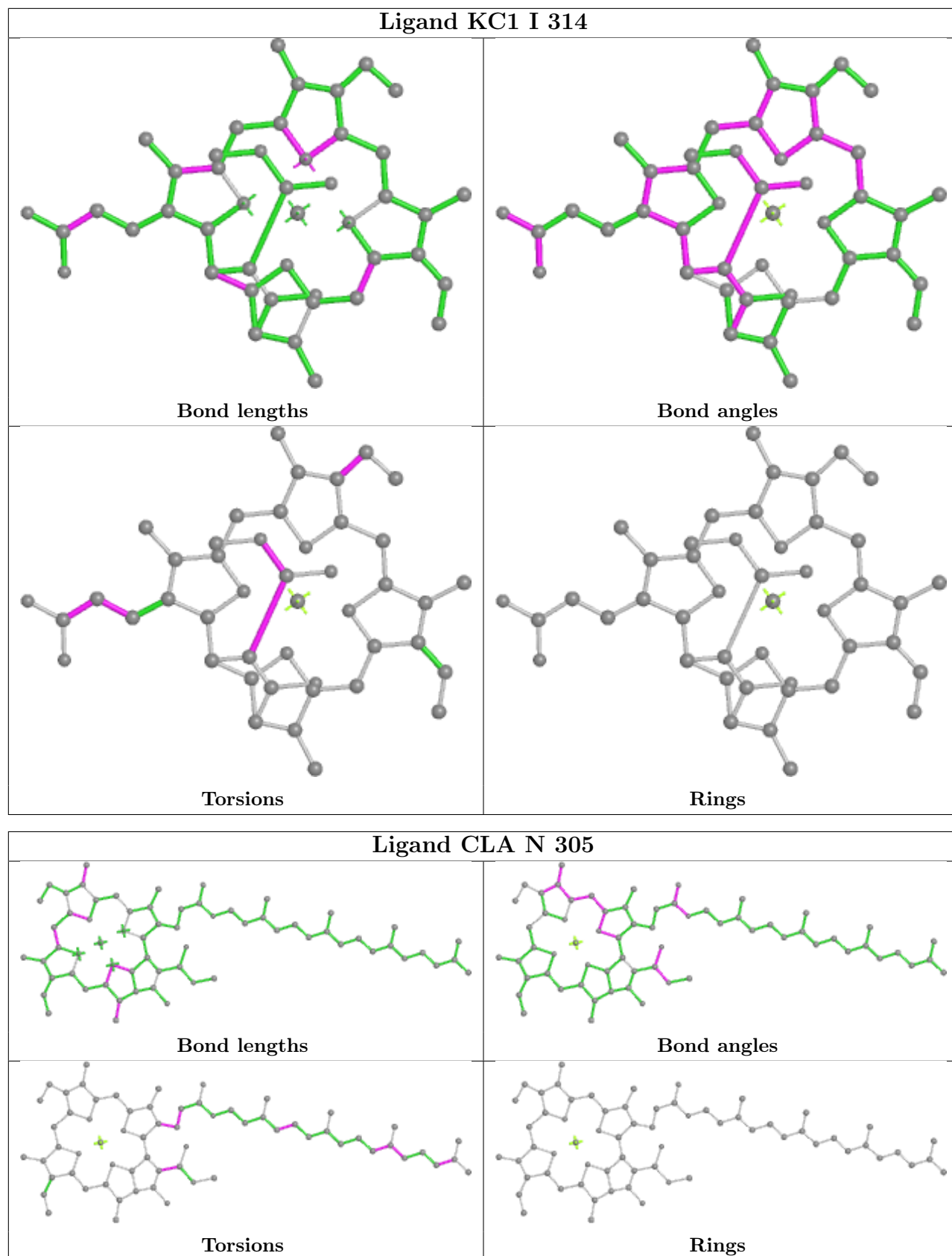


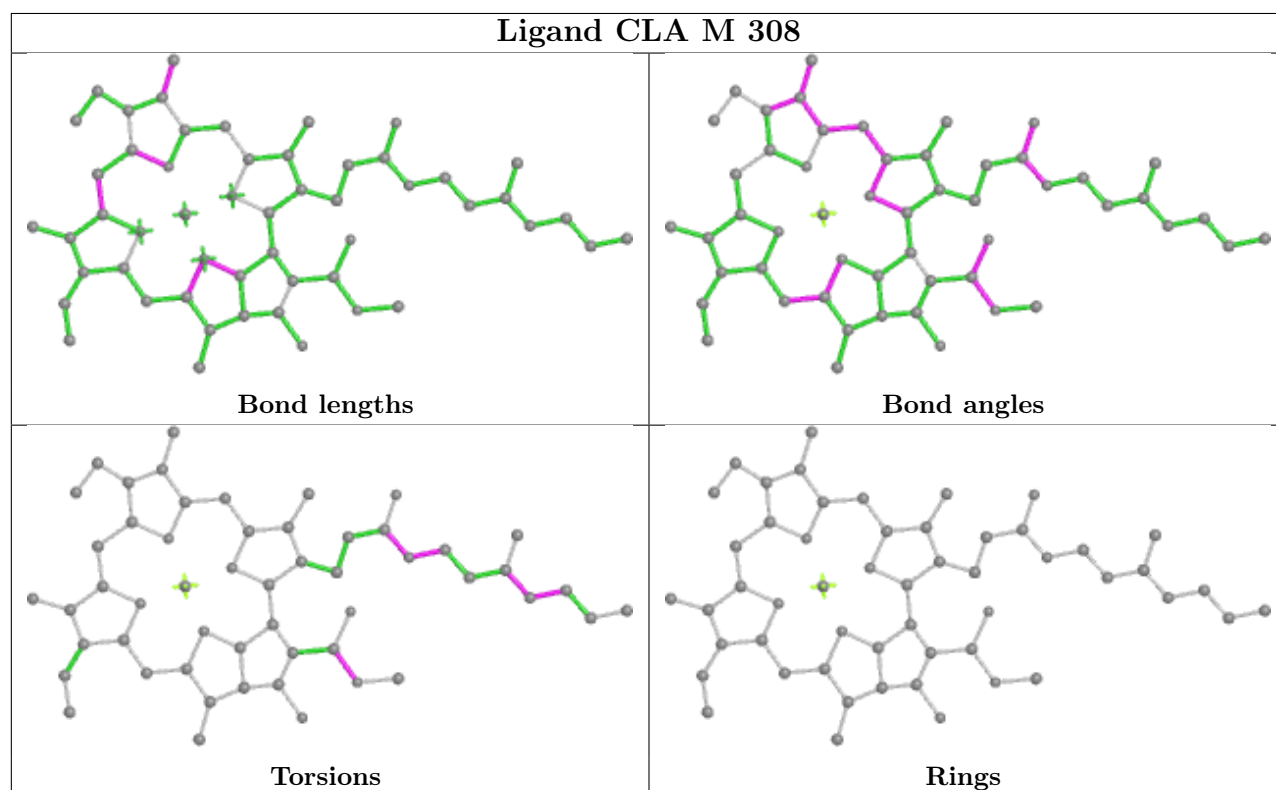
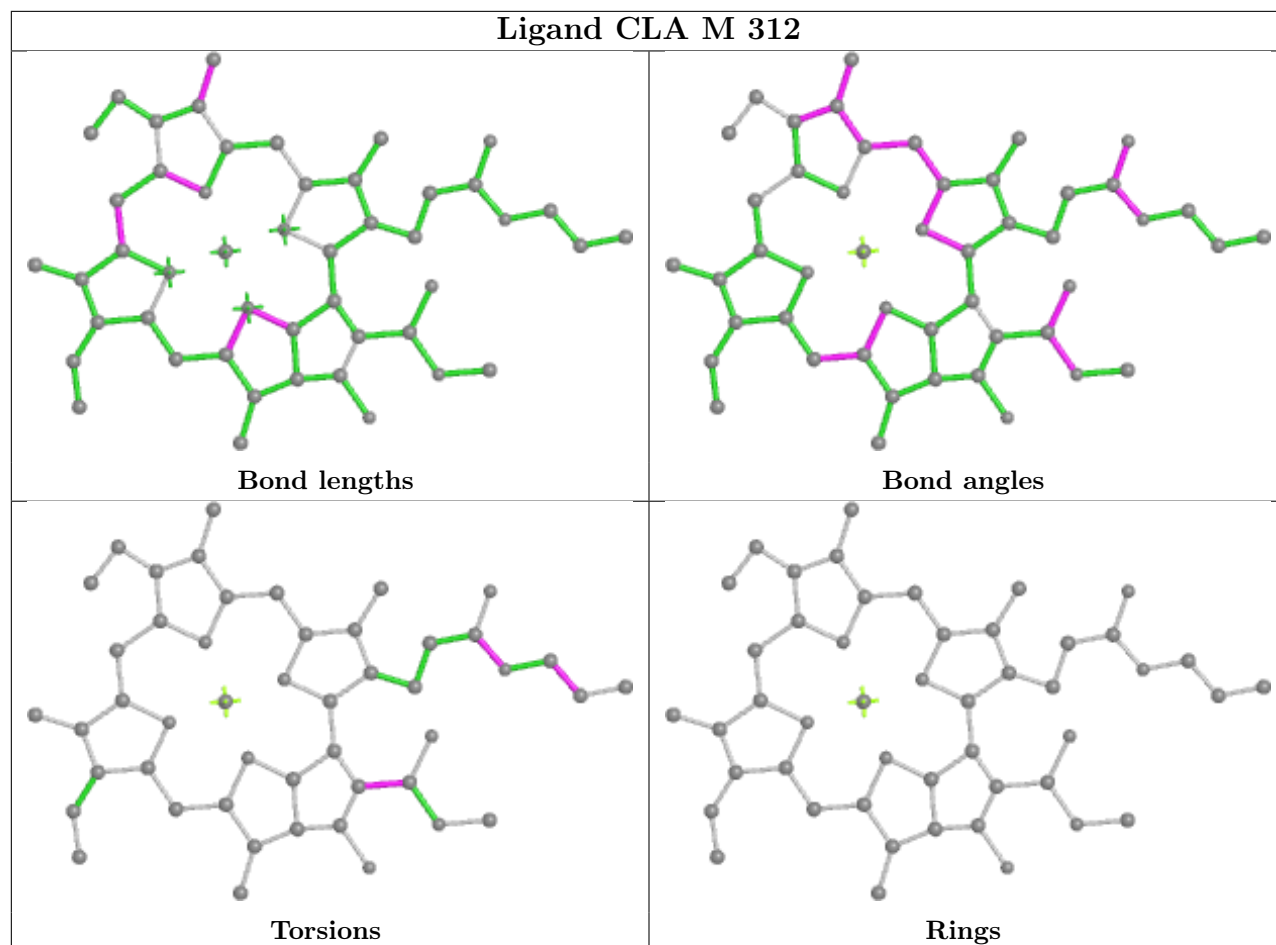


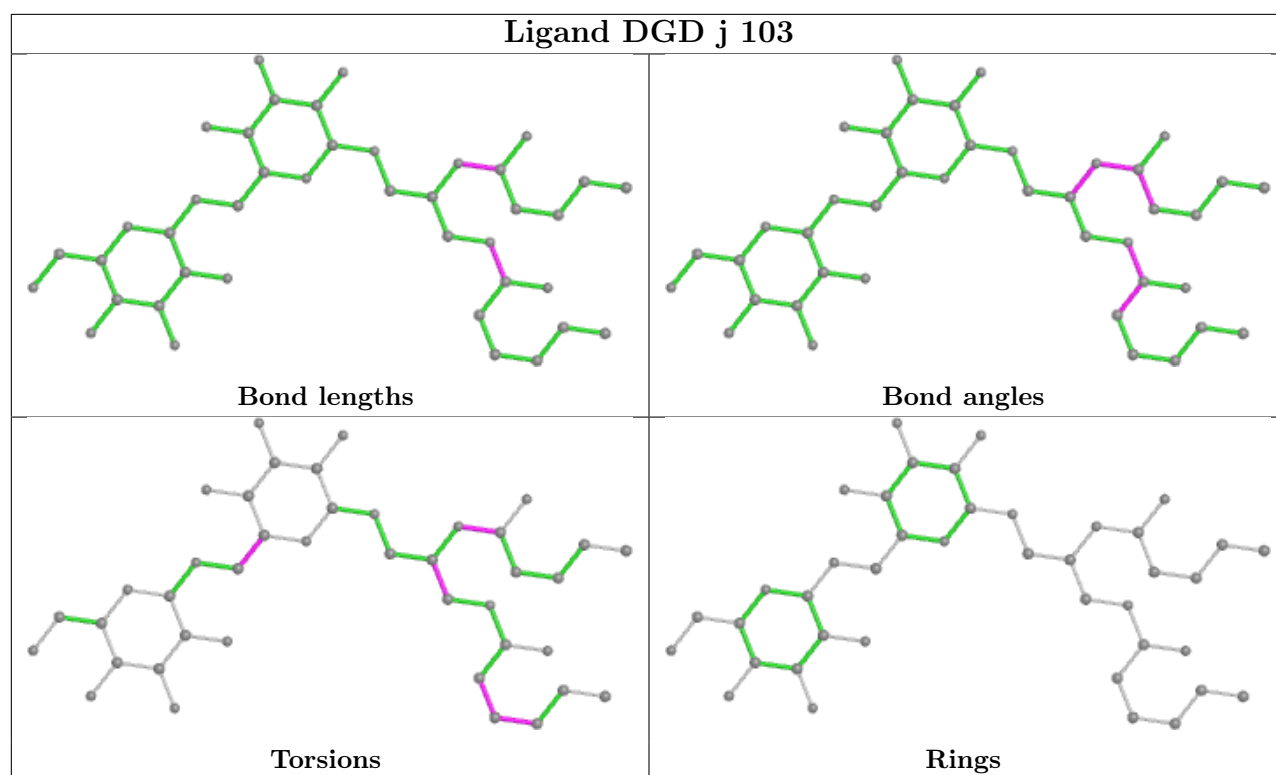












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

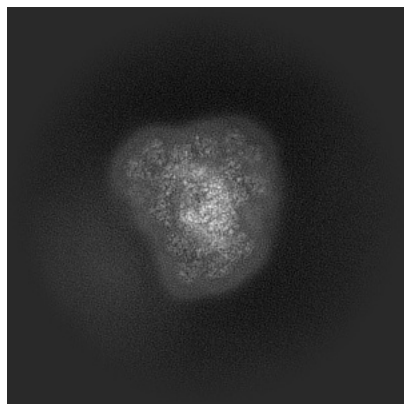
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36742. These allow visual inspection of the internal detail of the map and identification of artifacts.

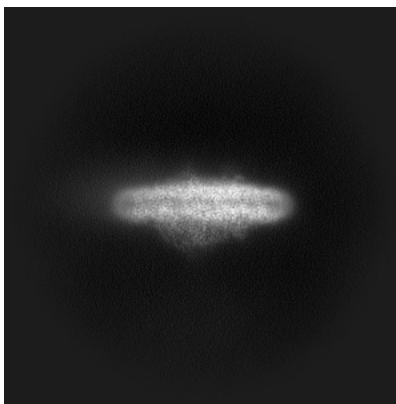
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

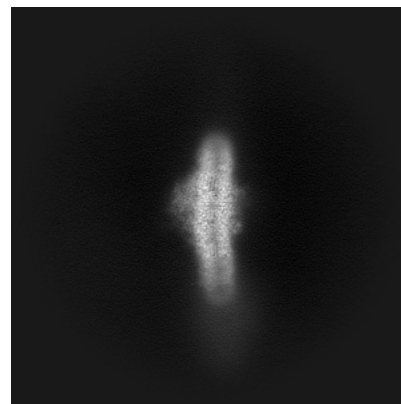
6.1.1 Primary map



X

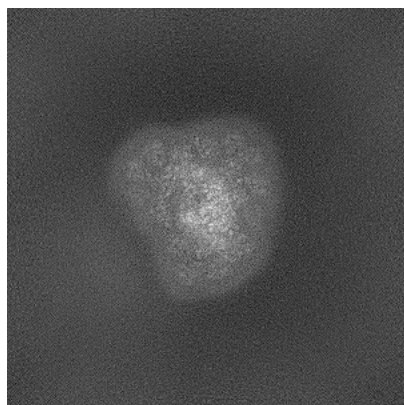


Y

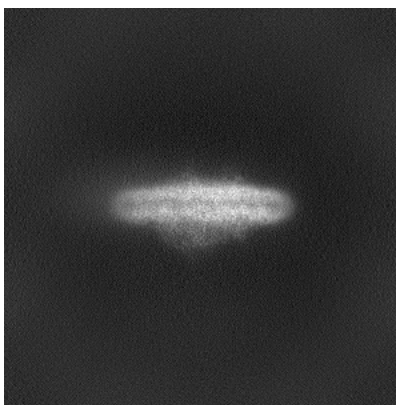


Z

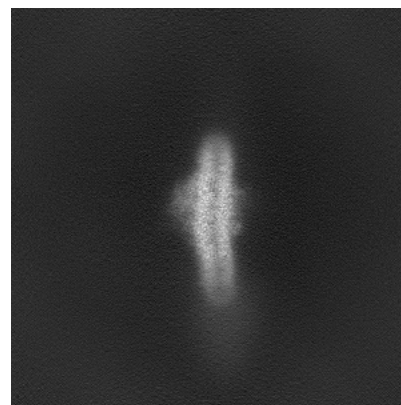
6.1.2 Raw map



X



Y

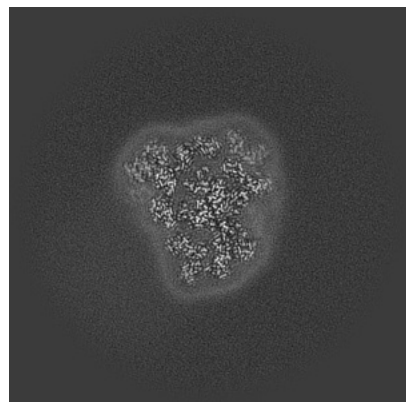


Z

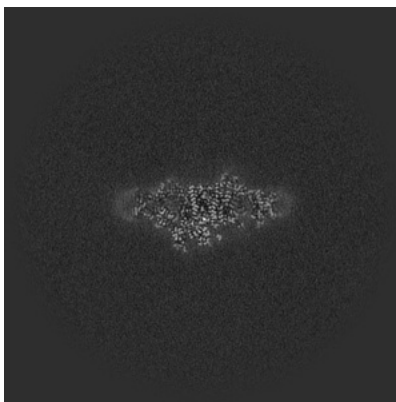
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

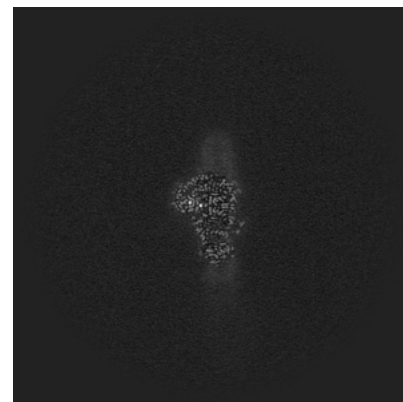
6.2.1 Primary map



X Index: 256

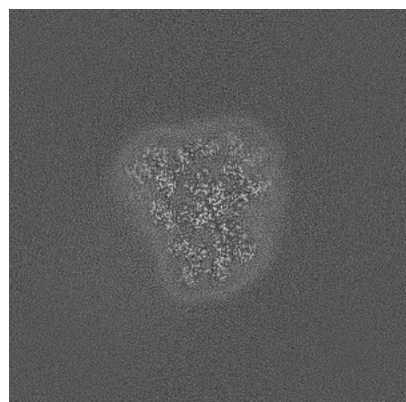


Y Index: 256

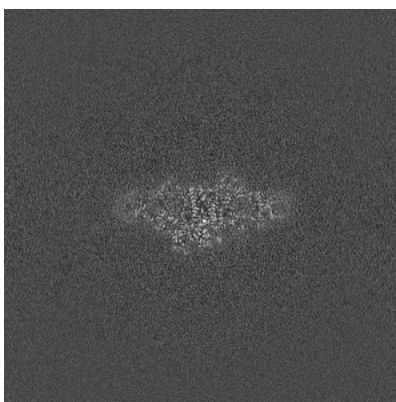


Z Index: 256

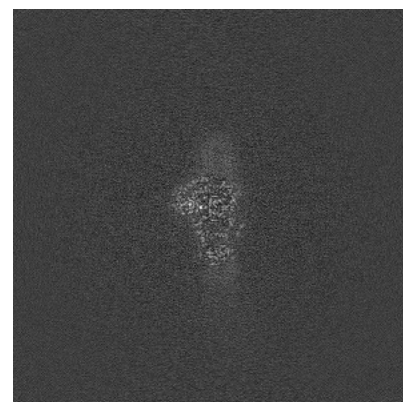
6.2.2 Raw map



X Index: 256



Y Index: 256

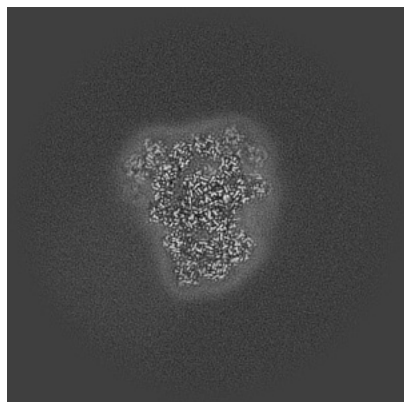


Z Index: 256

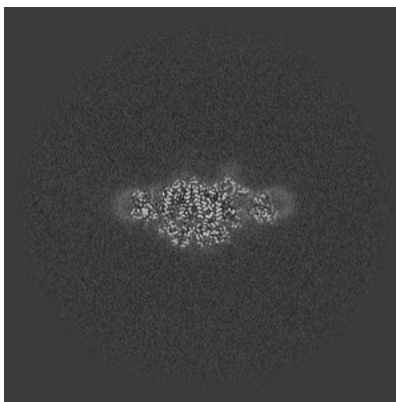
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

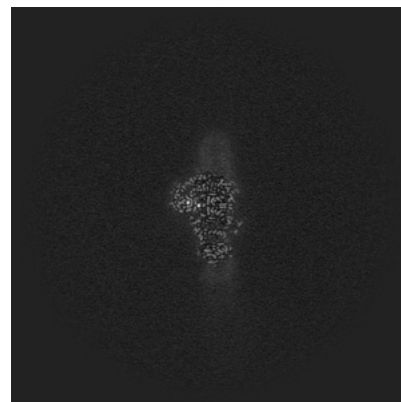
6.3.1 Primary map



X Index: 250

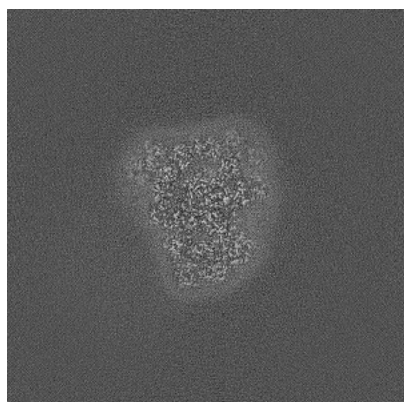


Y Index: 264

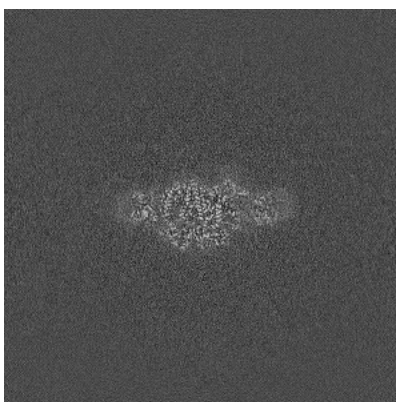


Z Index: 256

6.3.2 Raw map



X Index: 250



Y Index: 264

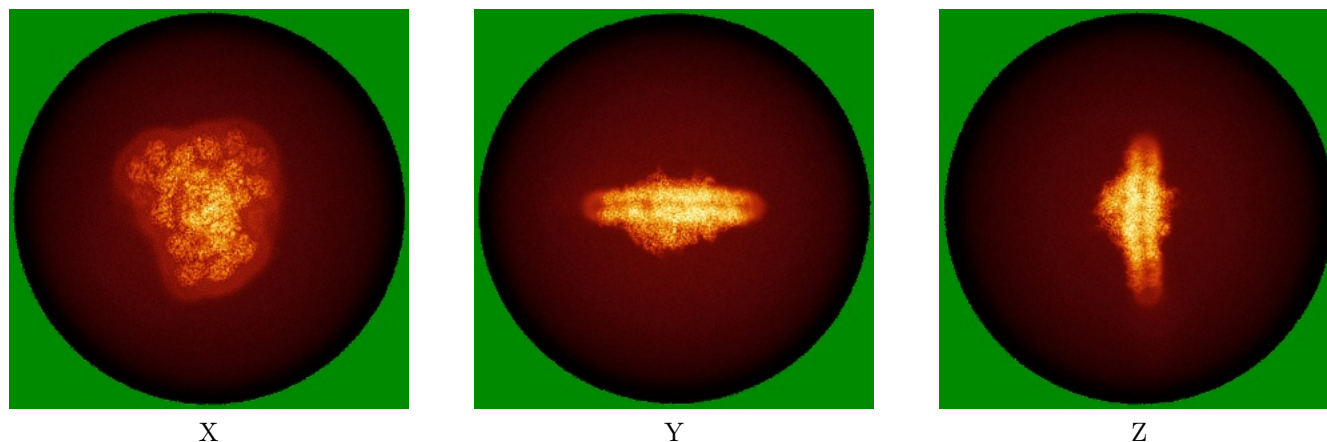


Z Index: 256

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

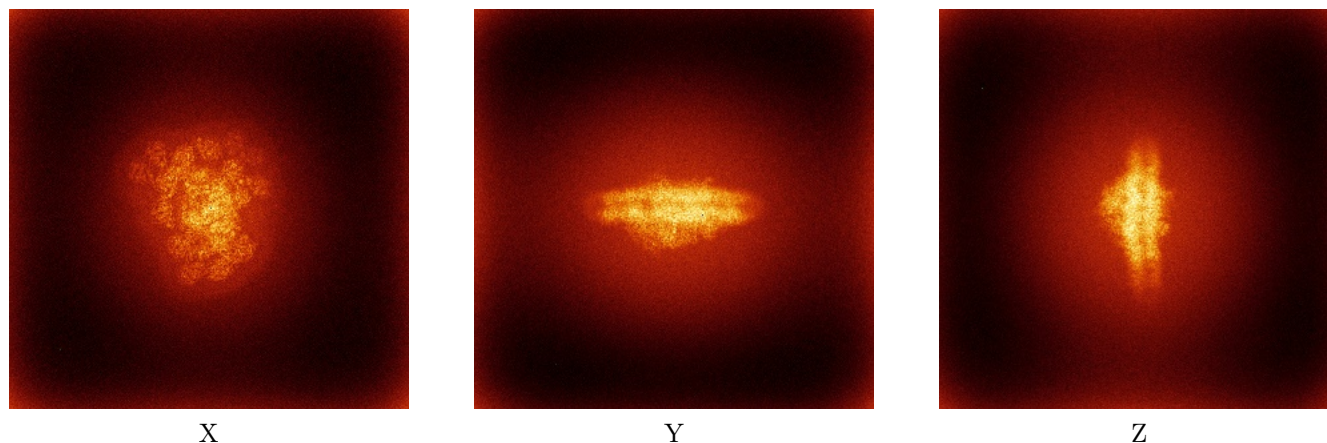


X

Y

Z

6.4.2 Raw map



X

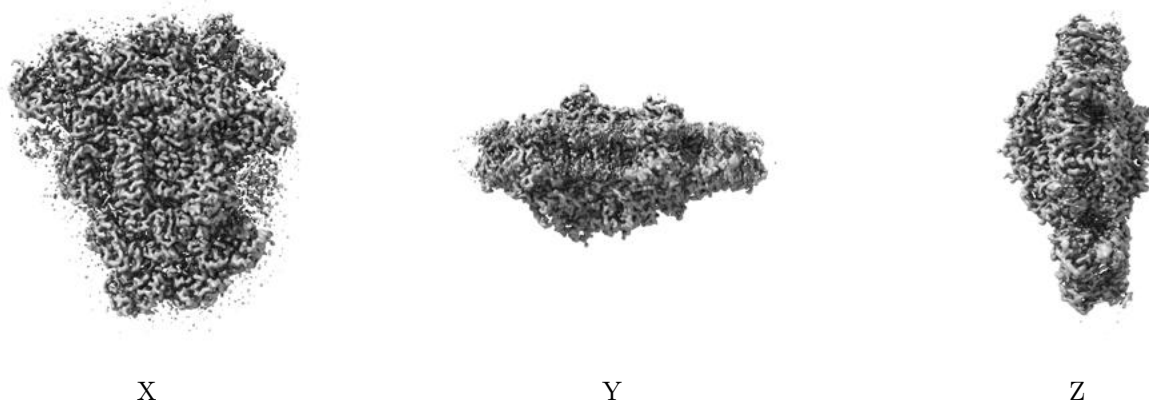
Y

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.

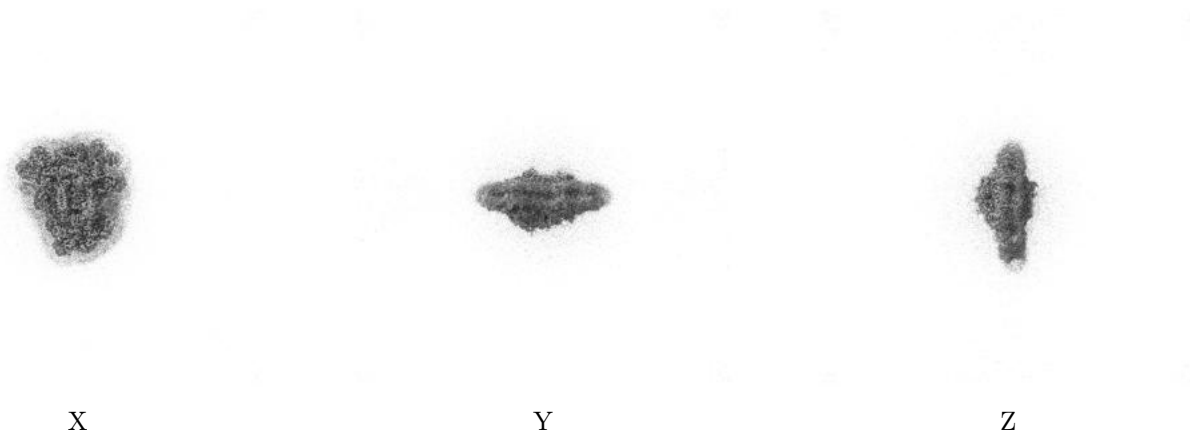
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

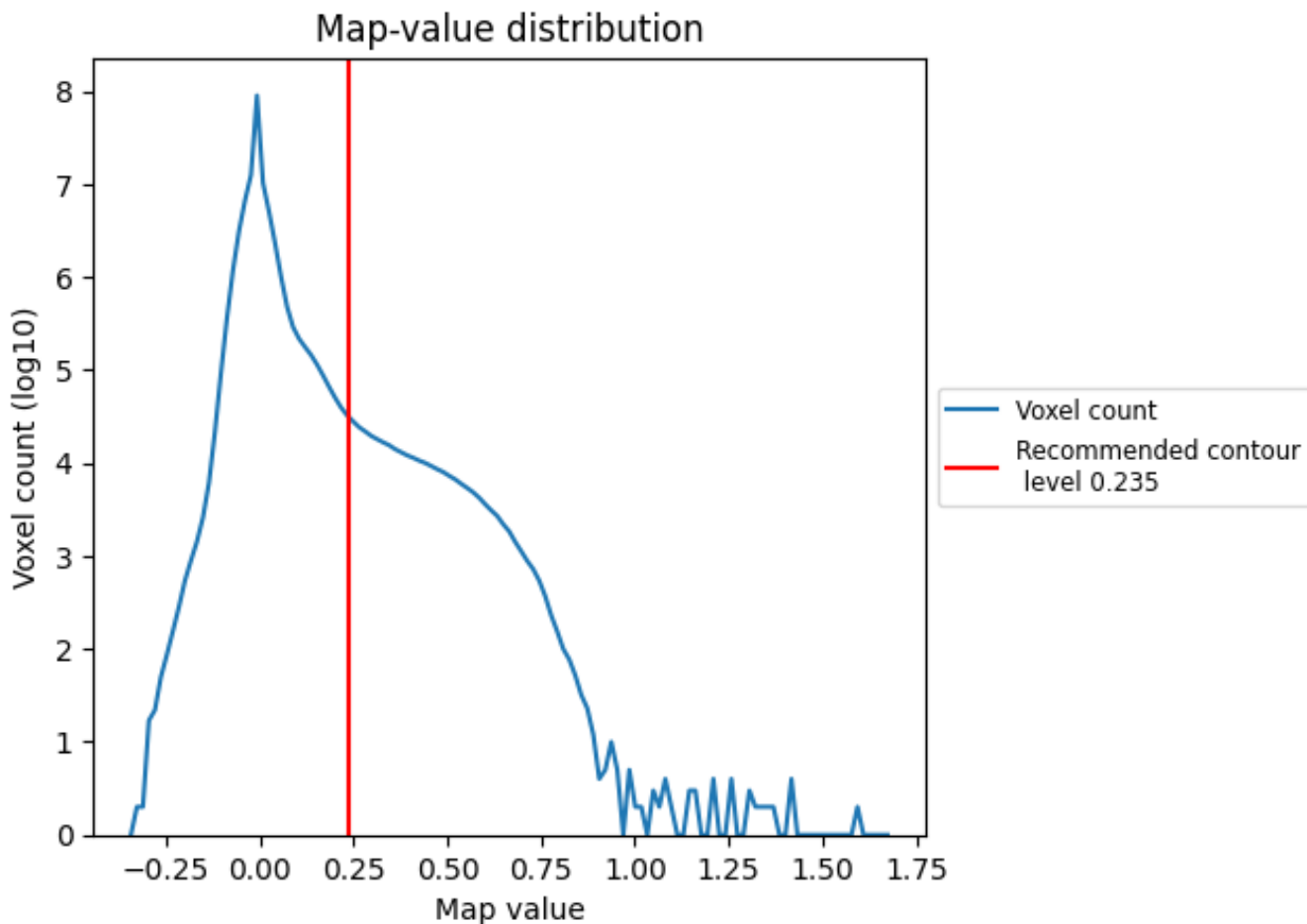
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

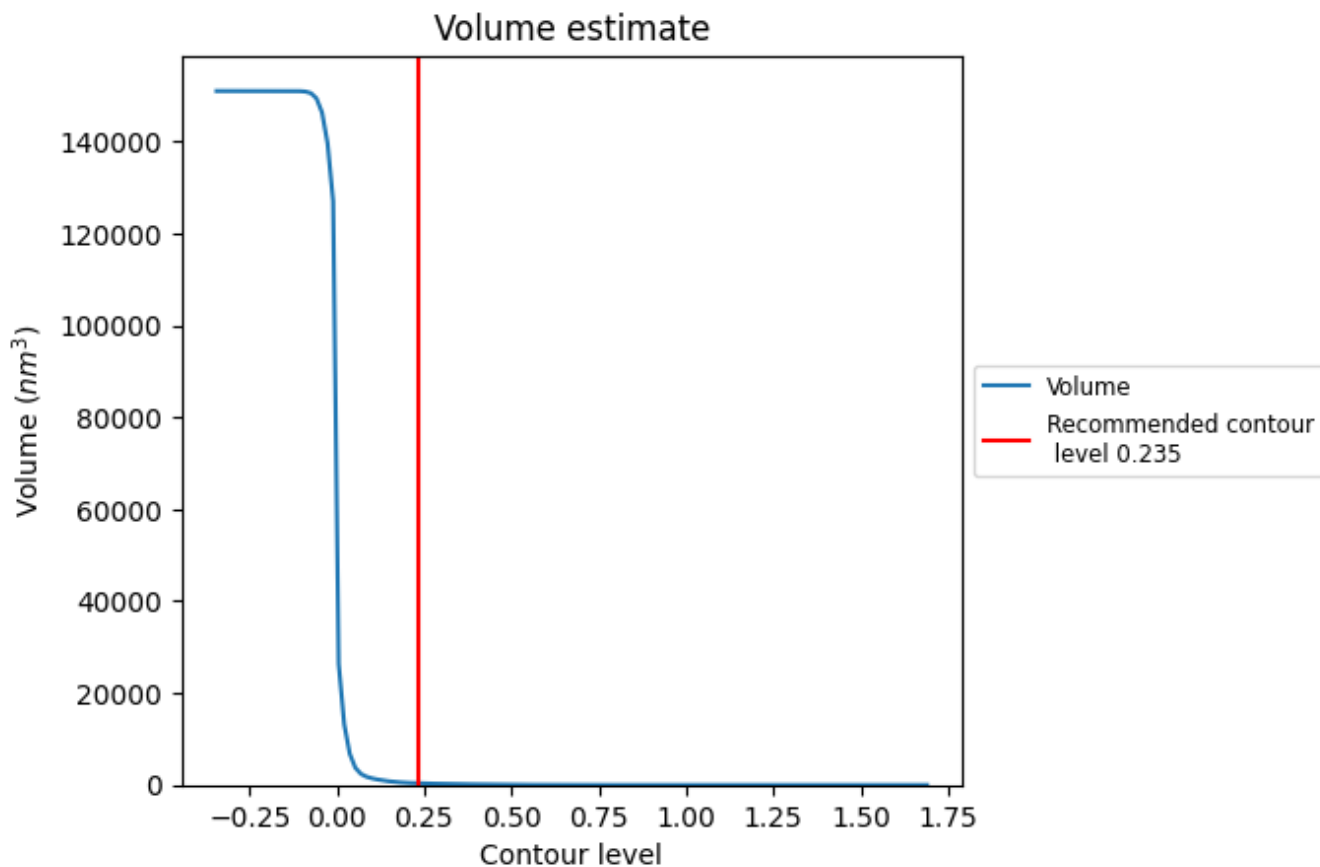
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

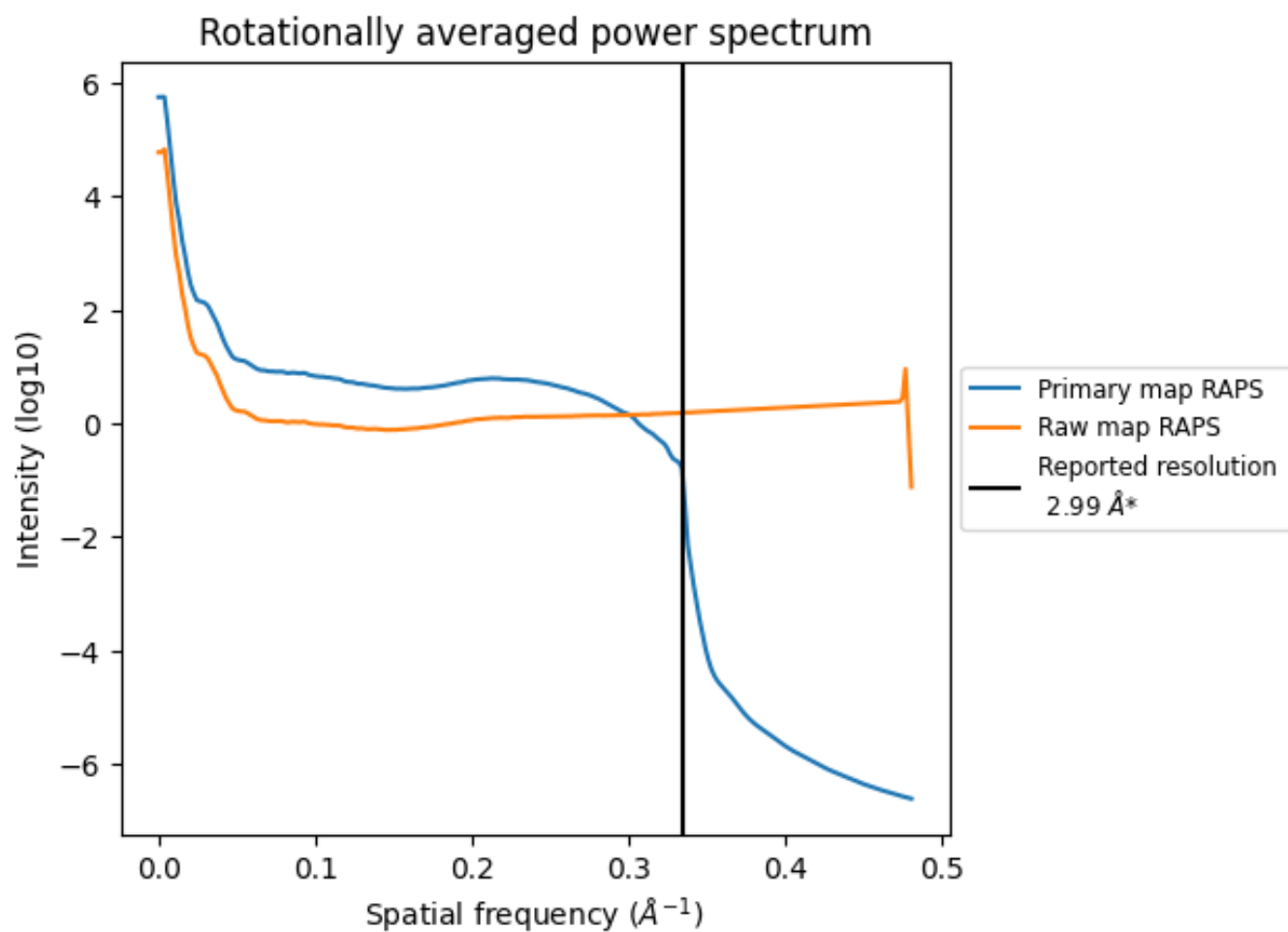
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 kDa.

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

7.3 Rotationally averaged power spectrum i

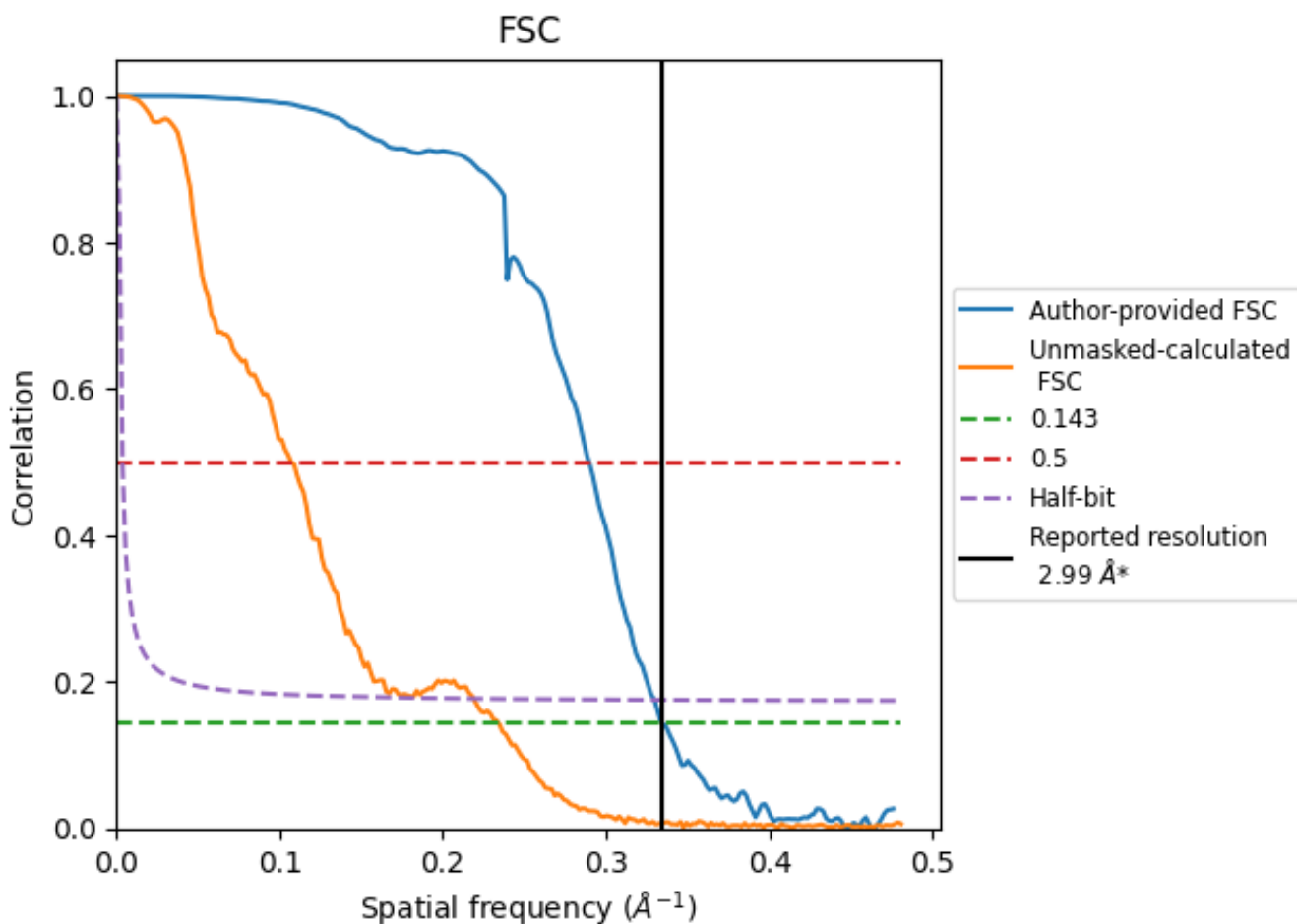


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

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 0.334 \AA^{-1}

8.2 Resolution estimates [i](#)

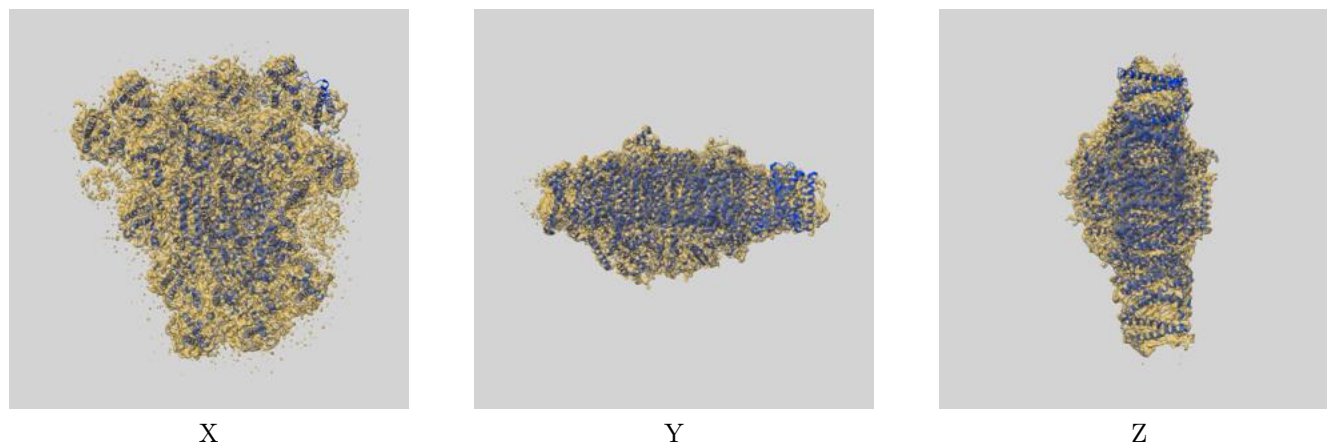
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.45	3.03
Unmasked-calculated*	4.27	9.35	4.57

*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 4.27 differs from the reported value 2.99 by more than 10 %

9 Map-model fit [i](#)

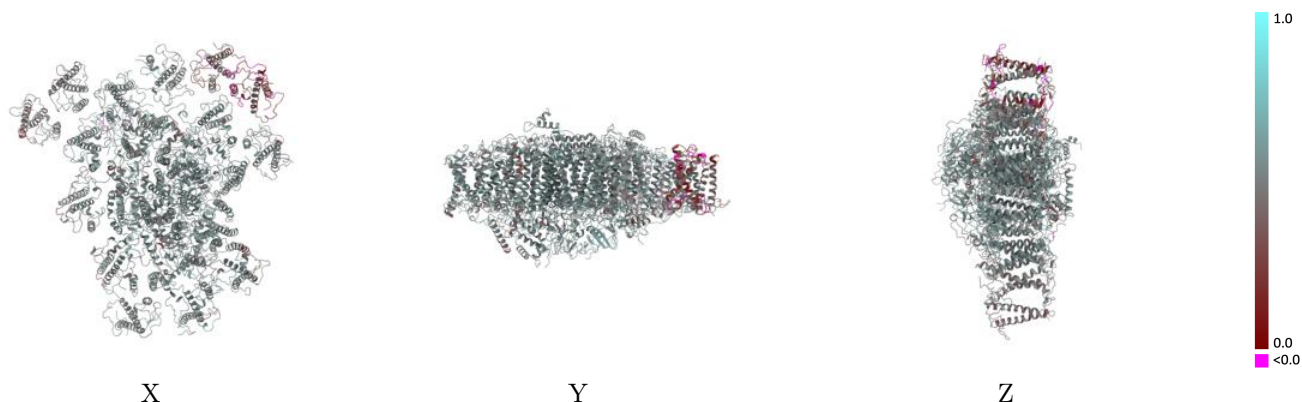
This section contains information regarding the fit between EMDB map EMD-36742 and PDB model 8JZE. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



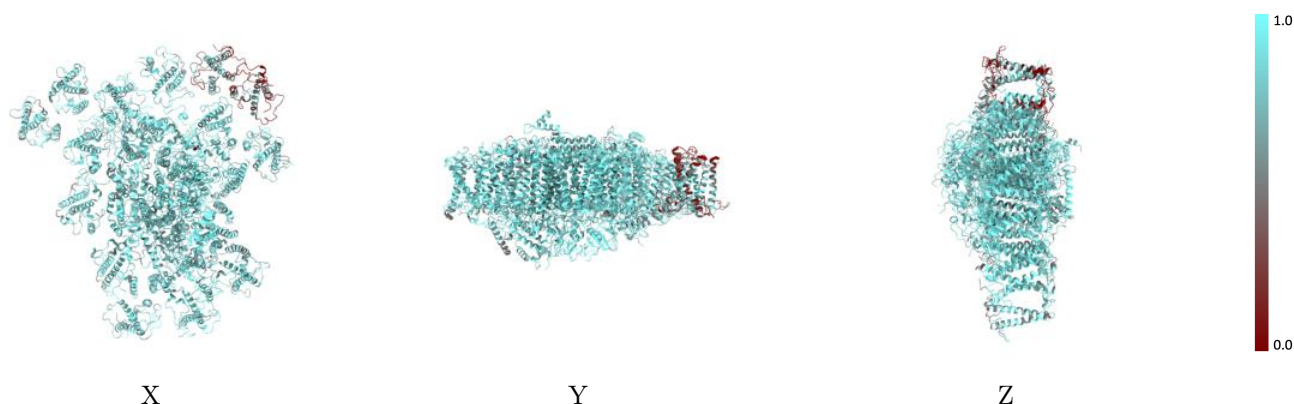
The images above show the 3D surface view of the map at the recommended contour level 0.235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



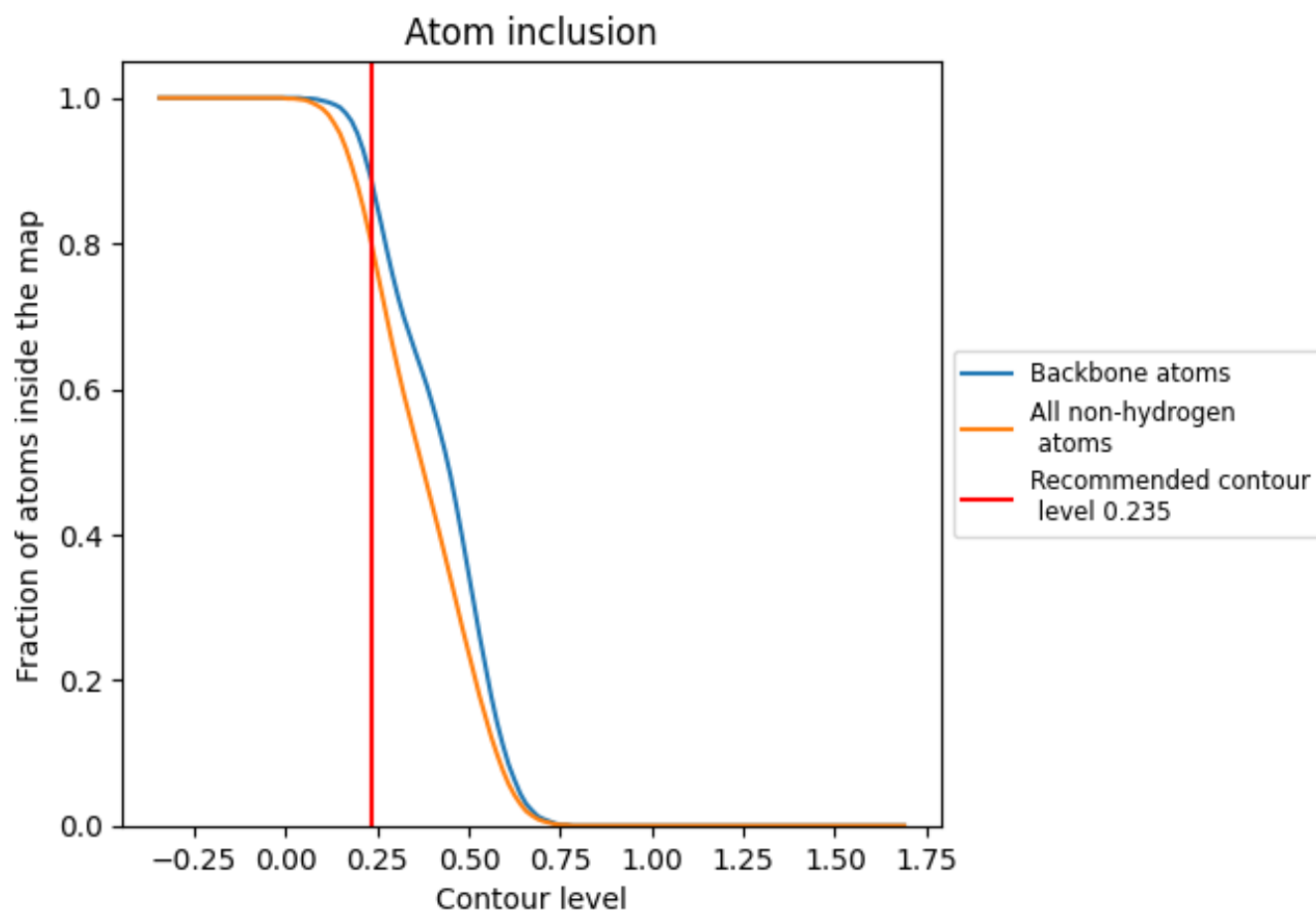
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.235).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5180
A	 0.8360	 0.5390
B	 0.7940	 0.5260
D	 0.7490	 0.5080
F	 0.7320	 0.4980
G	 0.8000	 0.5170
H	 0.3060	 0.2340
I	 0.7850	 0.5140
J	 0.8410	 0.5330
K	 0.8600	 0.5510
L	 0.8440	 0.5460
M	 0.7800	 0.5200
N	 0.4940	 0.3650
O	 0.6780	 0.4560
P	 0.7250	 0.4850
a	 0.8560	 0.5470
b	 0.8710	 0.5530
c	 0.9280	 0.5570
d	 0.8550	 0.5450
e	 0.8990	 0.5640
f	 0.8330	 0.5420
h	 0.8660	 0.5480
i	 0.8360	 0.5320
j	 0.7800	 0.5310
l	 0.8610	 0.5490
m	 0.8270	 0.5380
y	 0.8670	 0.5260
z	 0.9150	 0.5230

