



Full wwPDB EM Validation Report ⓘ

Feb 18, 2024 – 07:23 PM JST

PDB ID : 8JZF
EMDB ID : EMD-36743
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, X.Y.; Li, Z.H.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.70 Å (reported)

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

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

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:

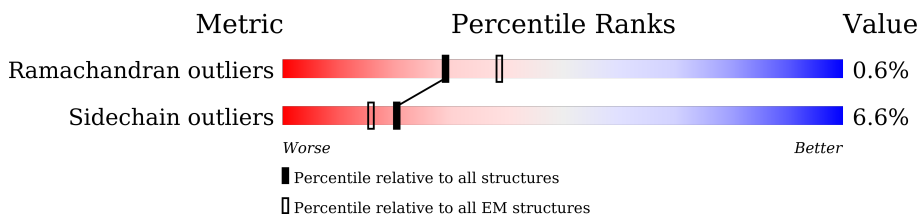
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

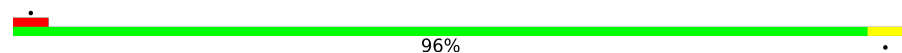
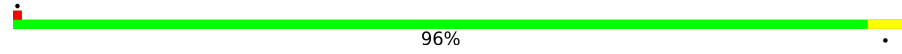
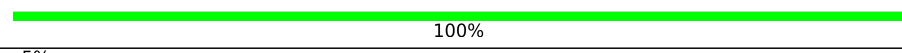
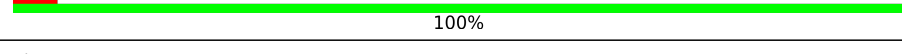
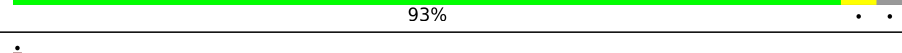
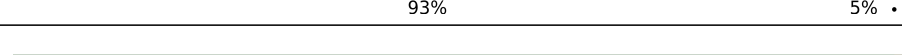
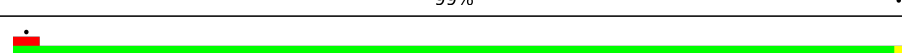
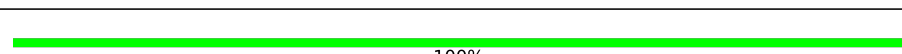

The reported resolution of this entry is 2.70 Å.

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



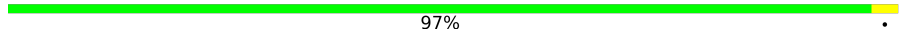
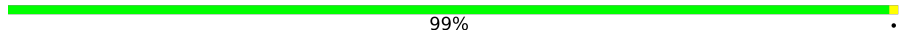
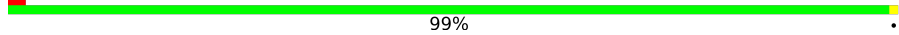
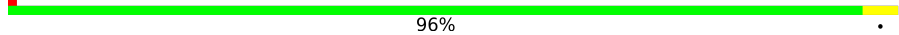
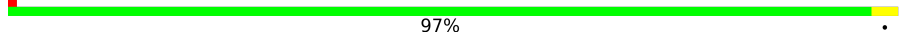
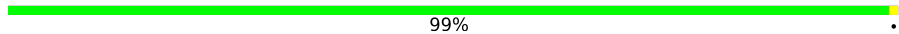
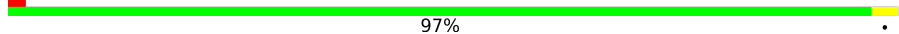
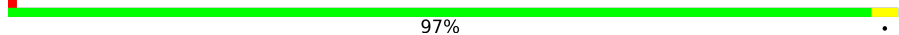



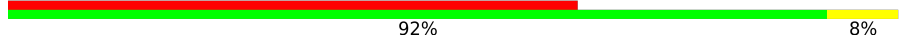




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 96%
2	K	177	 96%
3	z	78	 100%
4	y	131	 100%
5	G	224	 93%
6	A	189	 93% 5%
7	c	86	 99%
8	d	218	 99%
9	e	73	 100%

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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	 87% 9%
21	H	160	 64% 92% 8%
22	J	220	 92% 8%
23	L	185	 86% 14%
24	M	173	 86% 12%
25	N	160	 38% 74% 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
28	CLA	A	307	X	-	-	-
28	CLA	A	308	X	-	-	-
28	CLA	A	309	X	-	-	-
28	CLA	A	310	X	-	-	-
28	CLA	A	311	X	-	-	-
28	CLA	A	312	X	-	-	-
28	CLA	A	313	X	-	-	-
28	CLA	A	315	X	-	-	-
28	CLA	A	316	X	-	-	-
28	CLA	A	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	319	X	-	-	-
28	CLA	A	320	X	-	-	-
28	CLA	B	301	X	-	-	-
28	CLA	B	307	X	-	-	-
28	CLA	B	308	X	-	-	-
28	CLA	B	309	X	-	-	-
28	CLA	B	310	X	-	-	-
28	CLA	B	311	X	-	-	-
28	CLA	B	312	X	-	-	-
28	CLA	B	313	X	-	-	-
28	CLA	B	315	X	-	-	-
28	CLA	B	316	X	-	-	-
28	CLA	B	317	X	-	-	-
28	CLA	D	308	X	-	-	-
28	CLA	D	309	X	-	-	-
28	CLA	D	311	X	-	-	-
28	CLA	D	312	X	-	-	-
28	CLA	D	313	X	-	-	-
28	CLA	D	314	X	-	-	-
28	CLA	D	316	X	-	-	-
28	CLA	F	307	X	-	-	-
28	CLA	F	308	X	-	-	-
28	CLA	F	310	X	-	-	-
28	CLA	F	311	X	-	-	-
28	CLA	F	312	X	-	-	-
28	CLA	F	313	X	-	-	-
28	CLA	F	315	X	-	-	-
28	CLA	G	509	X	-	-	-
28	CLA	G	510	X	-	-	-
28	CLA	G	511	X	-	-	-
28	CLA	G	512	X	-	-	-
28	CLA	G	513	X	-	-	-
28	CLA	G	514	X	-	-	-
28	CLA	G	516	X	-	-	-
28	CLA	G	517	X	-	-	-
28	CLA	G	518	X	-	-	-
28	CLA	G	519	X	-	-	-
28	CLA	G	520	X	-	-	-
28	CLA	H	304	X	-	-	-
28	CLA	H	305	X	-	-	-
28	CLA	H	307	X	-	-	-
28	CLA	H	308	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	L	317	X	-	-	-
28	CLA	L	318	X	-	-	-
28	CLA	M	308	X	-	-	-
28	CLA	M	309	X	-	-	-
28	CLA	M	310	X	-	-	-
28	CLA	M	311	X	-	-	-
28	CLA	M	312	X	-	-	-
28	CLA	M	313	X	-	-	-
28	CLA	M	315	X	-	-	-
28	CLA	M	316	X	-	-	-
28	CLA	M	317	X	-	-	-
28	CLA	M	318	X	-	-	-
28	CLA	N	304	X	-	-	-
28	CLA	N	305	X	-	-	-
28	CLA	N	307	X	-	-	-
28	CLA	N	309	X	-	-	-
28	CLA	N	310	X	-	-	-
28	CLA	a	701	X	-	-	-
28	CLA	a	702	X	-	-	-
28	CLA	a	703	X	-	-	-
28	CLA	a	704	X	-	-	-
28	CLA	a	705	X	-	-	-
28	CLA	a	706	X	-	-	-
28	CLA	a	707	X	-	-	-
28	CLA	a	708	X	-	-	-
28	CLA	a	709	X	-	-	-
28	CLA	a	710	X	-	-	-
28	CLA	a	711	X	-	-	-
28	CLA	a	712	X	-	-	-
28	CLA	a	713	X	-	-	-
28	CLA	a	714	X	-	-	-
28	CLA	a	715	X	-	-	-
28	CLA	a	716	X	-	-	-
28	CLA	a	717	X	-	-	-
28	CLA	a	718	X	-	-	-
28	CLA	a	719	X	-	-	-
28	CLA	a	720	X	-	-	-
28	CLA	a	721	X	-	-	-
28	CLA	a	722	X	-	-	-
28	CLA	a	723	X	-	-	-
28	CLA	a	724	X	-	-	-
28	CLA	a	725	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	a	726	X	-	-	-
28	CLA	a	727	X	-	-	-
28	CLA	a	728	X	-	-	-
28	CLA	a	729	X	-	-	-
28	CLA	a	730	X	-	-	-
28	CLA	a	731	X	-	-	-
28	CLA	a	735	X	-	-	-
28	CLA	a	738	X	-	-	-
28	CLA	b	701	X	-	-	-
28	CLA	b	703	X	-	-	-
28	CLA	b	704	X	-	-	-
28	CLA	b	705	X	-	-	-
28	CLA	b	706	X	-	-	-
28	CLA	b	707	X	-	-	-
28	CLA	b	708	X	-	-	-
28	CLA	b	709	X	-	-	-
28	CLA	b	710	X	-	-	-
28	CLA	b	711	X	-	-	-
28	CLA	b	712	X	-	-	-
28	CLA	b	713	X	-	-	-
28	CLA	b	714	X	-	-	-
28	CLA	b	715	X	-	-	-
28	CLA	b	716	X	-	-	-
28	CLA	b	717	X	-	-	-
28	CLA	b	718	X	-	-	-
28	CLA	b	719	X	-	-	-
28	CLA	b	720	X	-	-	-
28	CLA	b	721	X	-	-	-
28	CLA	b	722	X	-	-	-
28	CLA	b	723	X	-	-	-
28	CLA	b	724	X	-	-	-
28	CLA	b	725	X	-	-	-
28	CLA	b	726	X	-	-	-
28	CLA	b	727	X	-	-	-
28	CLA	b	728	X	-	-	-
28	CLA	f	301	X	-	-	-
28	CLA	f	302	X	-	-	-
28	CLA	f	303	X	-	-	-
28	CLA	h	202	X	-	-	-
28	CLA	j	104	X	-	-	-
28	CLA	j	106	X	-	-	-
28	CLA	l	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	1	304	X	-	-	-
28	CLA	1	305	X	-	-	-
28	CLA	1	308	X	-	-	-
28	CLA	1	309	X	-	-	-
28	CLA	1	311	X	-	-	-
28	CLA	1	312	X	-	-	-
28	CLA	1	313	X	-	-	-
28	CLA	m	202	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 52237 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

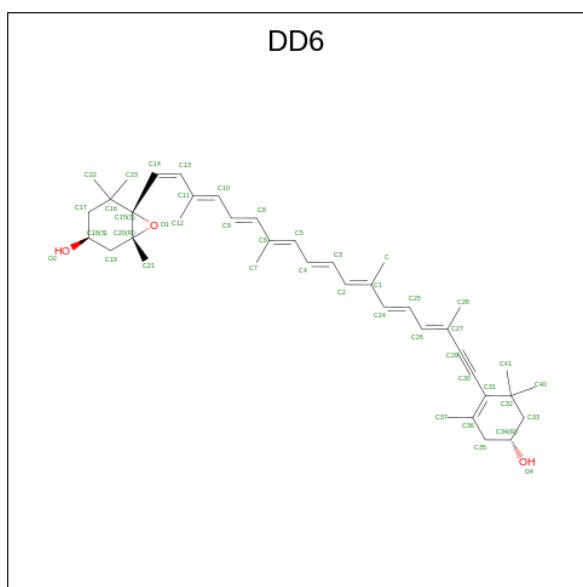
- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

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 (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
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	

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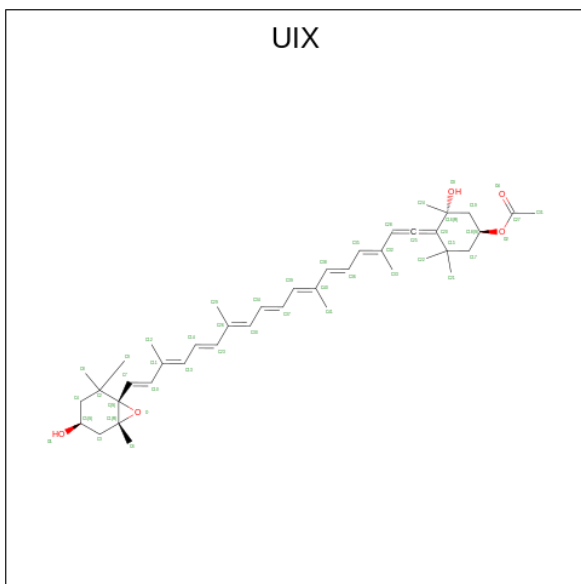
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	A	1	43	40	3	0
26	A	1	43	40	3	0
26	A	1	43	40	3	0
26	h	1	43	40	3	0
26	b	1	43	40	3	0
26	B	1	42	39	3	0
26	B	1	43	40	3	0
26	B	1	43	40	3	0
26	B	1	43	40	3	0
26	B	1	43	40	3	0
26	D	1	43	40	3	0
26	F	1	43	40	3	0
26	F	1	43	40	3	0
26	H	1	43	40	3	0
26	J	1	43	40	3	0
26	J	1	43	40	3	0
26	J	1	43	40	3	0
26	L	1	43	40	3	0
26	L	1	43	40	3	0
26	L	1	43	40	3	0
26	L	1	43	40	3	0
26	L	1	43	40	3	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	M	1	43	40	3	0
26	M	1	43	40	3	0
26	M	1	43	40	3	0
26	M	1	43	40	3	0
26	M	1	43	40	3	0
26	N	1	43	40	3	0

- Molecule 27 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-nonaenylidene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



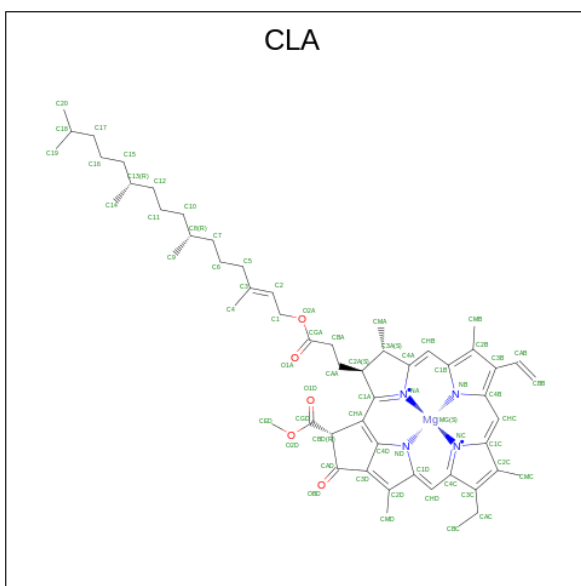
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	I	1	47	42	5	0
27	K	1	47	42	5	0
27	G	1	47	42	5	0

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Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			47	42	5	
27	h	1	Total	C	O	0
			47	42	5	
27	B	1	Total	C	O	0
			47	42	5	
27	J	1	Total	C	O	0
			47	42	5	

- Molecule 28 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	
28	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	G	1	41	33	1	4	3	0
28	G	1	46	36	1	4	5	0
28	G	1	46	36	1	4	5	0
28	G	1	61	51	1	4	5	0
28	G	1	49	39	1	4	5	0
28	A	1	45	35	1	4	5	0
28	A	1	55	45	1	4	5	0
28	A	1	55	45	1	4	5	0
28	A	1	65	55	1	4	5	0
28	A	1	46	36	1	4	5	0
28	A	1	55	45	1	4	5	0
28	A	1	55	45	1	4	5	0
28	A	1	41	33	1	4	3	0
28	A	1	47	37	1	4	5	0
28	A	1	41	33	1	4	3	0
28	A	1	46	36	1	4	5	0
28	A	1	46	36	1	4	5	0
28	f	1	55	45	1	4	5	0
28	f	1	46	36	1	4	5	0
28	f	1	46	36	1	4	5	0
28	h	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	j	1	55	45	1	4	5	0
28	j	1	58	48	1	4	5	0
28	l	1	65	55	1	4	5	0
28	l	1	60	50	1	4	5	0
28	l	1	65	55	1	4	5	0
28	l	1	41	33	1	4	3	0
28	l	1	41	33	1	4	3	0
28	l	1	45	36	4	5		0
28	l	1	65	55	1	4	5	0
28	l	1	46	36	1	4	5	0
28	l	1	65	55	1	4	5	0
28	m	1	60	50	1	4	5	0
28	a	1	45	35	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	55	45	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	55	45	1	4	5	0
28	a	1	58	48	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	51	41	1	4	5	0
28	a	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	a	1	55	45	1	4	5	0
28	a	1	45	35	1	4	5	0
28	a	1	60	50	1	4	5	0
28	a	1	60	50	1	4	5	0
28	a	1	45	35	1	4	5	0
28	a	1	45	35	1	4	5	0
28	a	1	47	37	1	4	5	0
28	a	1	57	47	1	4	5	0
28	a	1	46	36	1	4	5	0
28	a	1	47	37	1	4	5	0
28	a	1	62	52	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	58	48	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	61	51	1	4	5	0
28	a	1	65	55	1	4	5	0
28	a	1	46	36	1	4	5	0
28	a	1	55	45	1	4	5	0
28	a	1	56	46	1	4	5	0
28	a	1	65	55	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	b	1	53	43	1	4	5	0
28	b	1	46	36	1	4	5	0
28	b	1	65	55	1	4	5	0
28	b	1	50	40	1	4	5	0
28	b	1	65	55	1	4	5	0
28	b	1	65	55	1	4	5	0
28	b	1	47	37	1	4	5	0
28	b	1	65	55	1	4	5	0
28	b	1	65	55	1	4	5	0
28	B	1	60	50	1	4	5	0
28	B	1	49	39	1	4	5	0
28	B	1	45	35	1	4	5	0
28	B	1	65	55	1	4	5	0
28	B	1	55	45	1	4	5	0
28	B	1	65	55	1	4	5	0
28	B	1	51	41	1	4	5	0
28	B	1	65	55	1	4	5	0
28	B	1	41	33	1	4	3	0
28	B	1	46	36	1	4	5	0
28	B	1	45	35	1	4	5	0
28	D	1	47	37	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	D	1	46	36	1	4	5	0
28	D	1	46	36	1	4	5	0
28	D	1	46	36	1	4	5	0
28	D	1	45	35	1	4	5	0
28	D	1	46	36	1	4	5	0
28	D	1	41	33	1	4	3	0
28	F	1	46	36	1	4	5	0
28	F	1	46	36	1	4	5	0
28	F	1	46	36	1	4	5	0
28	F	1	46	36	1	4	5	0
28	F	1	46	36	1	4	5	0
28	F	1	46	36	1	4	5	0
28	F	1	41	33	1	4	3	0
28	H	1	47	37	1	4	5	0
28	H	1	65	55	1	4	5	0
28	H	1	51	41	1	4	5	0
28	H	1	46	36	1	4	5	0
28	H	1	47	37	1	4	5	0
28	H	1	41	33	1	4	3	0
28	H	1	46	36	1	4	5	0
28	J	1	60	50	1	4	5	0

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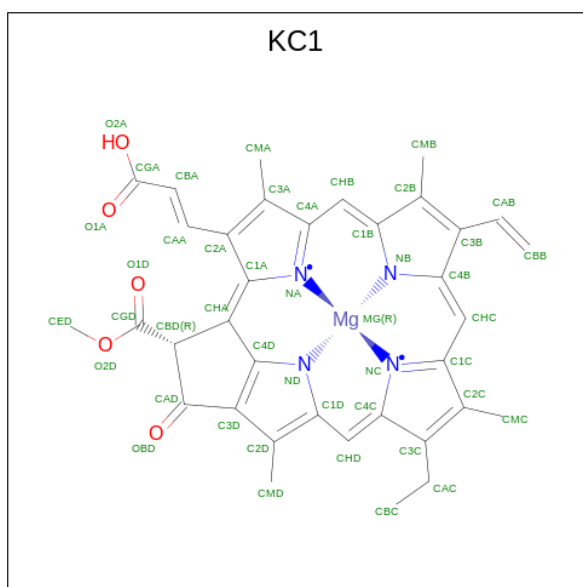
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	J	1	46	36	1	4	5	0
28	J	1	65	55	1	4	5	0
28	J	1	46	36	1	4	5	0
28	J	1	56	46	1	4	5	0
28	J	1	46	36	1	4	5	0
28	J	1	47	37	1	4	5	0
28	J	1	53	43	1	4	5	0
28	J	1	41	33	1	4	3	0
28	J	1	46	36	1	4	5	0
28	J	1	46	36	1	4	5	0
28	L	1	47	39	1	4	3	0
28	L	1	53	43	1	4	5	0
28	L	1	55	45	1	4	5	0
28	L	1	55	45	1	4	5	0
28	L	1	46	36	1	4	5	0
28	L	1	55	45	1	4	5	0
28	L	1	53	43	1	4	5	0
28	L	1	41	33	1	4	3	0
28	L	1	52	42	1	4	5	0
28	L	1	46	36	1	4	5	0
28	M	1	53	43	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
28	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 29 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



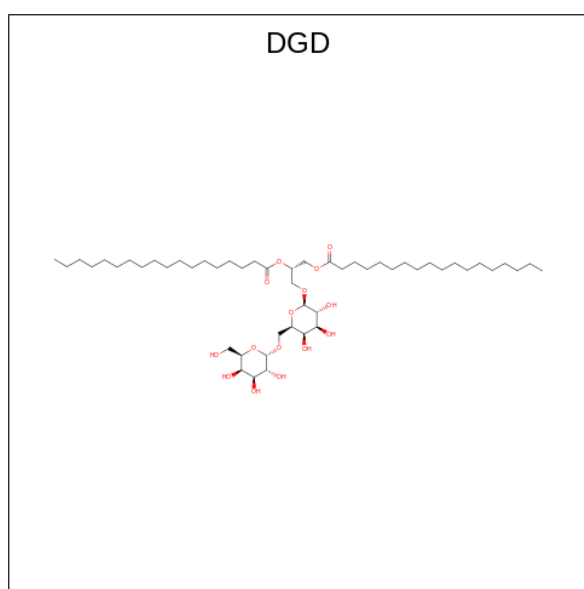
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
29	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



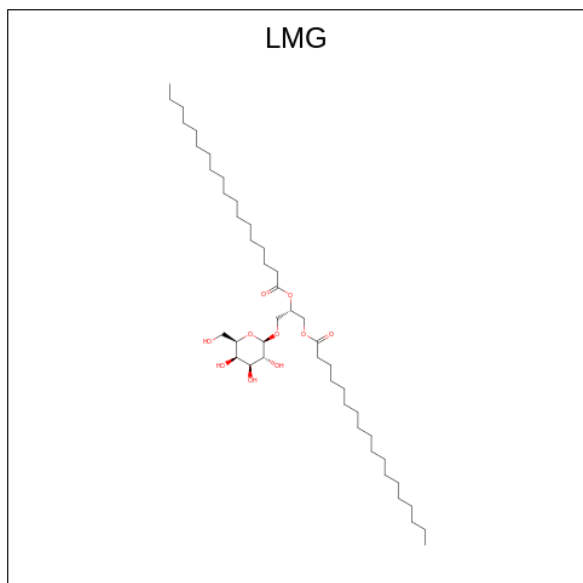
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	I	1	Total 39	C 24	O 15	0
30	y	1	Total 54	C 39	O 15	0
30	G	1	Total 45	C 30	O 15	0
30	G	1	Total 44	C 29	O 15	0
30	j	1	Total 41	C 26	O 15	0

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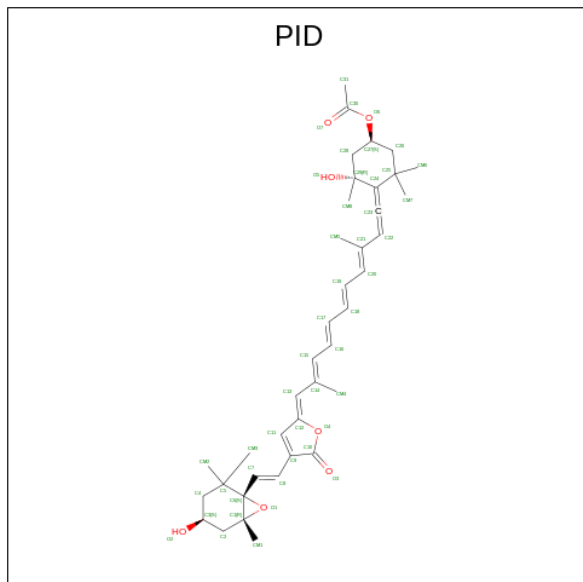
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	l	1	50	35	15	0
30	L	1	38	23	15	0

- Molecule 31 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
			Total	C	O	
31	I	1	36	26	10	0
31	I	1	38	28	10	0
31	K	1	27	17	10	0
31	K	1	43	33	10	0
31	j	1	35	25	10	0
31	b	1	44	34	10	0
31	b	1	31	21	10	0
31	B	1	37	27	10	0
31	D	1	49	39	10	0

- Molecule 32 is PERIDININ (three-letter code: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



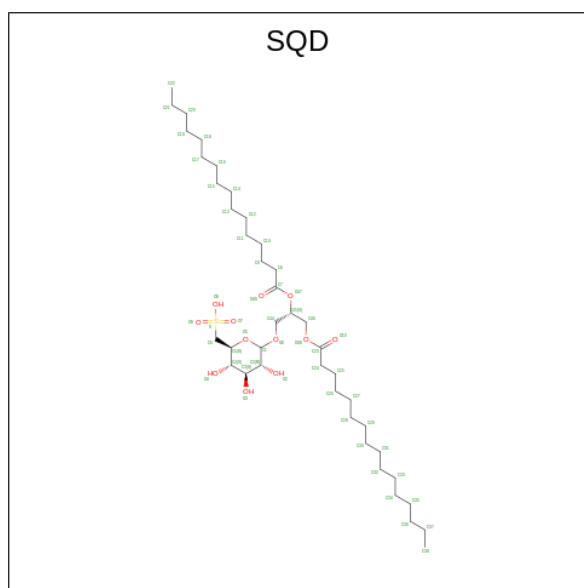
Mol	Chain	Residues	Atoms			AltConf
32	G	1	Total	C	O	0
			46	39	7	
32	G	1	Total	C	O	0
			46	39	7	
32	j	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0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

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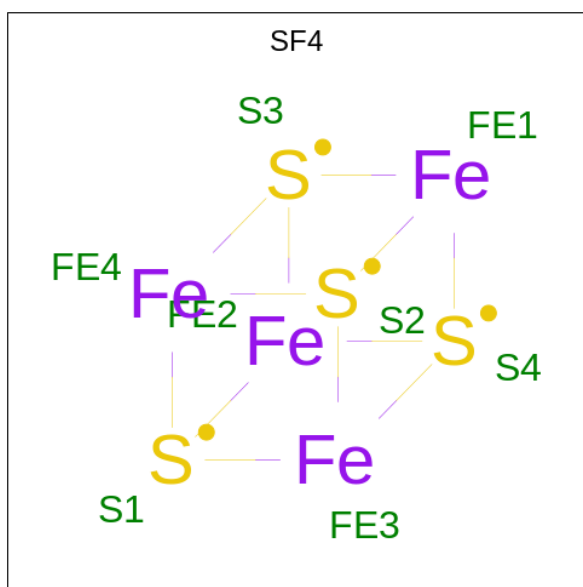
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	F	1	46	39	7	0
32	H	1	46	39	7	0
32	H	1	46	39	7	0
32	M	1	46	39	7	0
32	N	1	46	39	7	0
32	N	1	46	39	7	0

- Molecule 33 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).



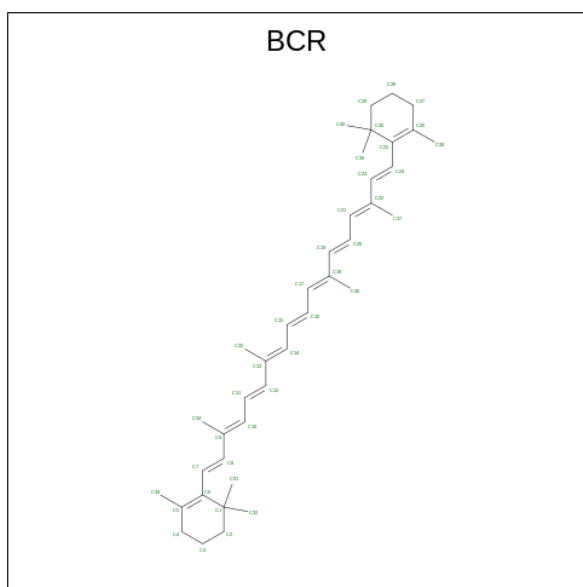
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
33	A	1	50	37	12	1	0

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 35 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



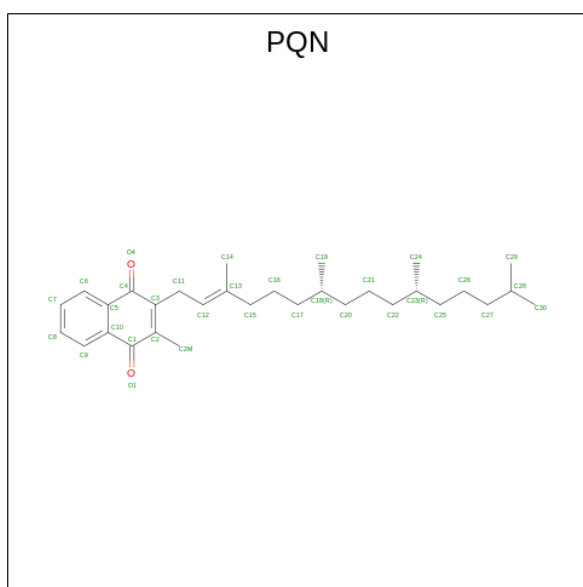
Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total	C	0
			40	40	

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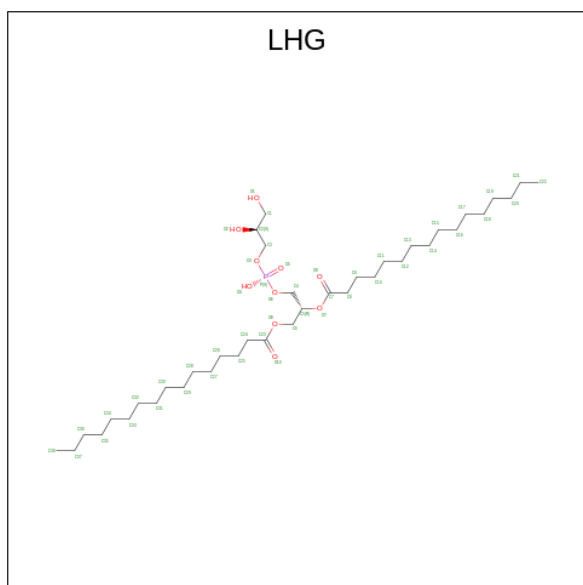
Mol	Chain	Residues	Atoms	AltConf
35	i	1	Total C 40 40	0
35	j	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	m	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0

- Molecule 36 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 37 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).

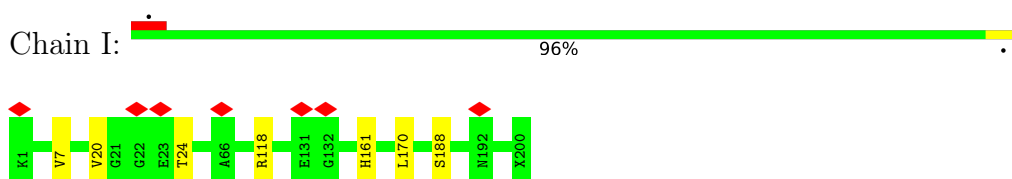


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
37	a	1	48	37	10	1	0

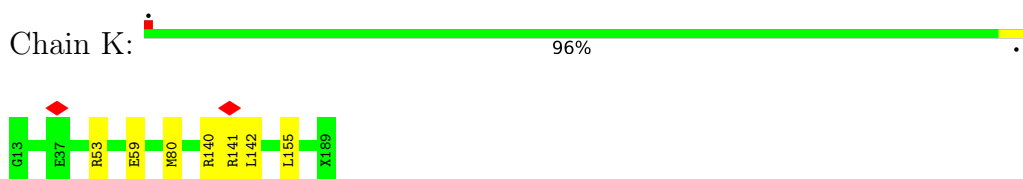
3 Residue-property plots [i](#)

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

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



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

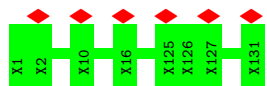


- Molecule 3: Photosystem I unk

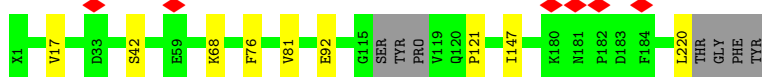


There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I unk

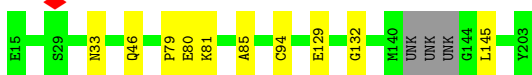


- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



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

Chain A:  93% 5%



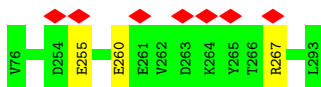
- Molecule 7: Photosystem I PsaC

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%



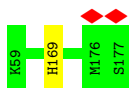
- Molecule 11: Photosystem I PsaR

Chain h:  99%



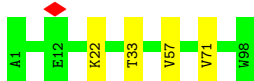
- Molecule 12: Photosystem I PsaI

Chain i:  99%



- Molecule 13: Photosystem I PsaJ

Chain j:  96%



- Molecule 14: Photosystem I PsaL

Chain l:  97%



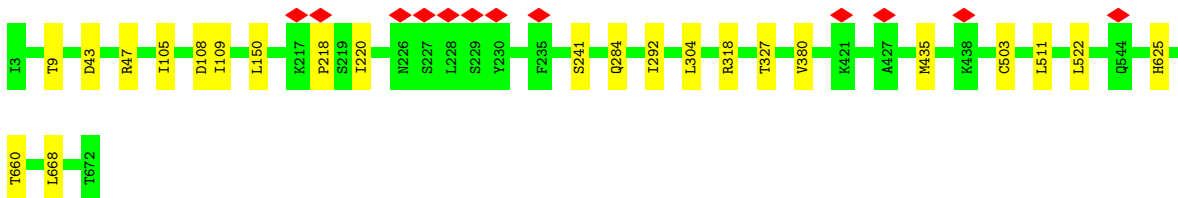
- Molecule 15: Photosystem I PsaM

Chain m:  99%



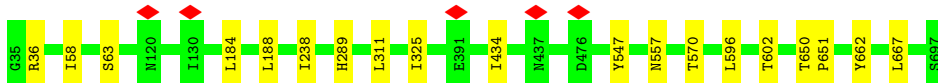
- Molecule 16: Photosystem I PsaA

Chain a:  97%



- Molecule 17: Photosystem I PsaB

Chain b:  97%




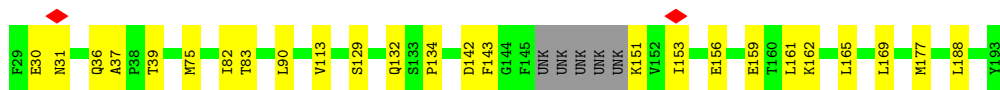
- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

Chain B:  91%

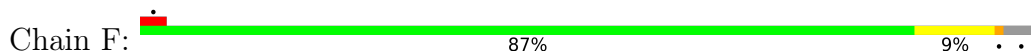


- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

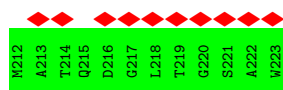
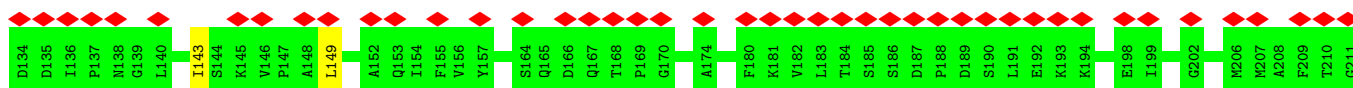
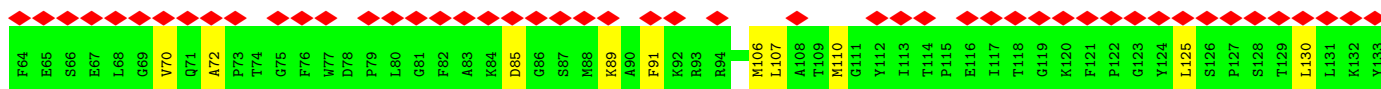
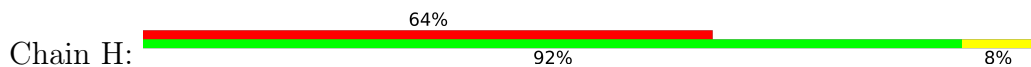
Chain D:  82%



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



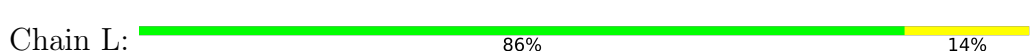
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



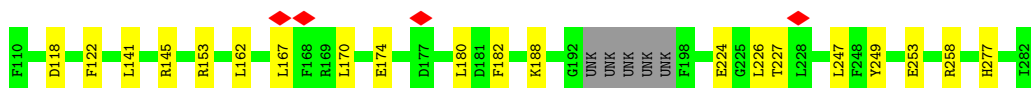
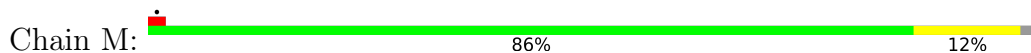
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



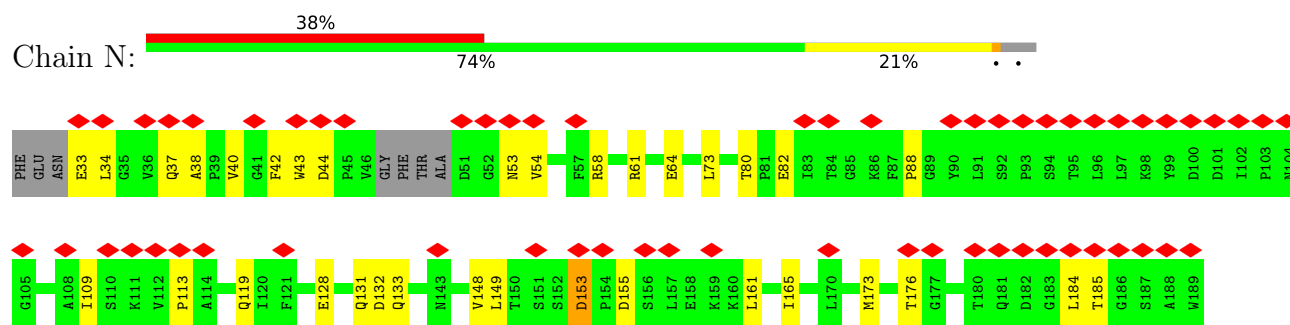
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216895	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	1.628	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: DGD, SF4, PID, DD6, CLA, PQN, UIX, KC1, SQD, LHG, LMG, BCR

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	0.27	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	0.31	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	0.30	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	0.44	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
All	All	0.28	0/36403	0.47	0/49437

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%)	164 (86%)	27 (14%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	176 (86%)	26 (13%)	2 (1%)	15	37
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	5	14
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	54
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	60
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	34	60
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	47	73
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	8	21
19	D	156/165 (94%)	130 (83%)	23 (15%)	3 (2%)	8	20
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	13	32
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	12	30
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	25	50
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	3	6
All	All	4587/4792 (96%)	4182 (91%)	376 (8%)	29 (1%)	29	50

All (29) 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
5	G	76	PHE
21	H	125	LEU
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
19	D	37	ALA
6	A	132	GLY
18	B	165	VAL
25	N	38	ALA

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%)	132 (95%)	7 (5%)	24	51
2	K	133/138 (96%)	126 (95%)	7 (5%)	22	48
5	G	147/171 (86%)	140 (95%)	7 (5%)	25	53
6	A	122/129 (95%)	116 (95%)	6 (5%)	25	52
7	c	76/76 (100%)	75 (99%)	1 (1%)	69	87
8	d	182/184 (99%)	179 (98%)	3 (2%)	62	85
9	e	63/63 (100%)	63 (100%)	0	100	100
10	f	148/148 (100%)	144 (97%)	4 (3%)	44	74
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	55
14	l	199/201 (99%)	192 (96%)	7 (4%)	36	65
15	m	60/63 (95%)	59 (98%)	1 (2%)	60	84
16	a	540/592 (91%)	520 (96%)	20 (4%)	34	63
17	b	557/581 (96%)	539 (97%)	18 (3%)	39	68
18	B	142/146 (97%)	128 (90%)	14 (10%)	8	18
19	D	116/123 (94%)	94 (81%)	22 (19%)	1	4
20	F	126/140 (90%)	111 (88%)	15 (12%)	5	12
21	H	123/123 (100%)	113 (92%)	10 (8%)	11	27
22	J	124/136 (91%)	108 (87%)	16 (13%)	4	10
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	4
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	4
25	N	80/124 (64%)	51 (64%)	29 (36%)	0	0
All	All	3623/3870 (94%)	3385 (93%)	238 (7%)	20	38

All (238) 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

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Mol	Chain	Res	Type
1	I	118	ARG
1	I	161	HIS
1	I	170	LEU
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	53	LYS
20	F	88	LEU
20	F	103	MET
20	F	107	LYS
20	F	111	THR

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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

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](#)

310 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
28	CLA	H	305	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
31	LMG	K	318	-	43,43,55	0.81	1 (2%)	51,51,63	1.31	6 (11%)
28	CLA	a	702	-	65,73,73	1.47	10 (15%)	76,113,113	1.42	7 (9%)
31	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
28	CLA	M	310	-	48,56,73	1.73	6 (12%)	55,92,113	1.56	8 (14%)
28	CLA	b	712	-	54,62,73	1.69	7 (12%)	67,100,113	1.54	11 (16%)
28	CLA	B	317	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
28	CLA	b	717	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
32	PID	G	507	-	41,49,49	1.34	4 (9%)	49,76,76	1.40	7 (14%)
35	BCR	j	102	-	41,41,41	0.70	0	56,56,56	2.01	16 (28%)
28	CLA	a	730	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	9 (11%)
29	KC1	F	309	20	48,53,53	1.50	7 (14%)	55,89,89	1.92	12 (21%)
28	CLA	N	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.58	6 (11%)
28	CLA	l	313	14	65,73,73	1.51	5 (7%)	76,113,113	1.40	8 (10%)
28	CLA	H	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.52	8 (14%)
28	CLA	l	310	-	44,50,73	1.88	7 (15%)	48,76,113	1.38	8 (16%)
27	UIX	G	503	-	41,49,49	1.23	3 (7%)	52,74,74	2.34	17 (32%)
28	CLA	l	305	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	L	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.95	12 (23%)
28	CLA	a	703	-	55,63,73	1.56	10 (18%)	64,101,113	1.60	9 (14%)
27	UIX	J	305	-	41,49,49	1.25	3 (7%)	52,74,74	2.47	17 (32%)
28	CLA	b	725	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
26	DD6	K	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	13 (25%)
28	CLA	b	723	-	50,58,73	1.70	5 (10%)	58,95,113	1.51	10 (17%)
27	UIX	I	304	-	41,49,49	1.32	4 (9%)	52,74,74	2.59	14 (26%)
28	CLA	J	312	-	53,61,73	1.64	5 (9%)	61,98,113	1.56	9 (14%)
28	CLA	b	703	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	8 (10%)
28	CLA	A	316	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
35	BCR	a	736	-	41,41,41	0.74	0	56,56,56	2.03	18 (32%)
28	CLA	B	307	18	49,57,73	1.74	5 (10%)	55,93,113	1.52	8 (14%)
28	CLA	a	708	-	51,59,73	1.70	5 (9%)	59,96,113	1.50	8 (13%)
28	CLA	a	713	-	60,68,73	1.55	5 (8%)	70,107,113	1.40	9 (12%)
28	CLA	L	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.55	7 (13%)
28	CLA	a	715	-	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
28	CLA	a	701	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
36	PQN	a	732	-	34,34,34	1.57	2 (5%)	42,45,45	1.10	4 (9%)
26	DD6	M	302	-	39,45,45	2.17	4 (10%)	52,67,67	2.24	16 (30%)
29	KC1	D	315	19	48,53,53	1.49	7 (14%)	55,89,89	1.85	13 (23%)
28	CLA	J	306	-	46,54,73	1.77	6 (13%)	53,90,113	1.58	6 (11%)
28	CLA	I	316	-	55,63,73	1.60	5 (9%)	64,101,113	1.52	9 (14%)
28	CLA	l	303	14	65,73,73	1.52	5 (7%)	76,113,113	1.38	9 (11%)
28	CLA	G	513	5	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
28	CLA	b	708	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
32	PID	F	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.66	6 (12%)
32	PID	N	301	-	41,49,49	1.35	4 (9%)	49,76,76	1.51	6 (12%)
32	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.68	9 (18%)
28	CLA	B	312	-	51,59,73	1.68	5 (9%)	59,96,113	1.50	8 (13%)
26	DD6	I	301	-	39,45,45	2.05	2 (5%)	52,67,67	2.20	20 (38%)
28	CLA	F	308	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	7 (13%)
28	CLA	a	718	-	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
28	CLA	D	313	19	45,53,73	1.77	6 (13%)	52,89,113	1.60	7 (13%)
28	CLA	b	707	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	9 (11%)
28	CLA	b	714	-	46,54,73	1.75	5 (10%)	53,90,113	1.60	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	G	512	-	60,68,73	1.55	6 (10%)	70,107,113	1.44	8 (11%)
28	CLA	B	308	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	8 (15%)
28	CLA	L	314	-	53,61,73	1.63	5 (9%)	61,98,113	1.52	9 (14%)
35	BCR	b	730	-	41,41,41	0.75	0	56,56,56	2.25	20 (35%)
28	CLA	A	312	-	55,63,73	1.62	6 (10%)	64,101,113	1.48	7 (10%)
28	CLA	J	316	-	46,54,73	1.78	6 (13%)	53,90,113	1.53	7 (13%)
29	KC1	N	308	-	48,53,53	1.52	7 (14%)	55,89,89	2.12	13 (23%)
28	CLA	A	313	-	55,63,73	1.60	5 (9%)	64,101,113	1.45	9 (14%)
28	CLA	G	510	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	8 (10%)
26	DD6	K	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.69	11 (21%)
28	CLA	j	104	-	55,63,73	1.65	5 (9%)	64,101,113	1.42	9 (14%)
28	CLA	I	319	28	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
26	DD6	B	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	11 (21%)
29	KC1	H	310	-	48,53,53	1.49	7 (14%)	55,89,89	1.86	9 (16%)
30	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	3 (5%)
32	PID	G	506	-	41,49,49	1.34	4 (9%)	49,76,76	1.39	6 (12%)
28	CLA	K	311	-	52,60,73	1.68	6 (11%)	60,97,113	1.49	7 (11%)
28	CLA	L	317	-	52,60,73	1.69	6 (11%)	60,97,113	1.51	9 (15%)
32	PID	j	105	-	41,49,49	1.41	4 (9%)	49,76,76	1.49	10 (20%)
28	CLA	f	303	10	46,54,73	1.75	5 (10%)	53,90,113	1.56	7 (13%)
26	DD6	F	303	-	39,45,45	2.03	3 (7%)	52,67,67	2.01	14 (26%)
26	DD6	L	304	-	39,45,45	2.01	3 (7%)	52,67,67	1.82	11 (21%)
28	CLA	J	301	-	60,68,73	1.55	5 (8%)	70,107,113	1.40	8 (11%)
28	CLA	b	718	-	51,59,73	1.72	5 (9%)	59,96,113	1.53	7 (11%)
30	DGD	l	301	-	51,51,67	0.96	2 (3%)	65,65,81	0.89	2 (3%)
28	CLA	A	308	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
28	CLA	J	315	-	46,54,73	1.76	5 (10%)	53,90,113	1.56	7 (13%)
28	CLA	H	307	-	51,59,73	1.68	5 (9%)	59,96,113	1.52	8 (13%)
28	CLA	b	720	-	53,61,73	1.63	5 (9%)	61,98,113	1.49	8 (13%)
28	CLA	M	318	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	7 (13%)
35	BCR	b	732	-	41,41,41	0.80	0	56,56,56	1.88	20 (35%)
28	CLA	A	309	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
28	CLA	A	320	-	46,54,73	1.79	6 (13%)	53,90,113	1.54	6 (11%)
28	CLA	A	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	8 (10%)
37	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	316	-	46,54,73	1.76	5 (10%)	53,90,113	1.50	7 (13%)
28	CLA	l	308	-	41,49,73	1.86	5 (12%)	47,84,113	1.63	8 (17%)
31	LMG	K	317	-	27,27,55	1.00	0	35,35,63	1.19	4 (11%)
32	PID	F	305	-	41,49,49	1.39	5 (12%)	49,76,76	1.87	9 (18%)
29	KC1	N	306	-	48,53,53	1.49	7 (14%)	55,89,89	1.84	11 (20%)
30	DGD	y	201	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
28	CLA	b	704	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	9 (11%)
28	CLA	K	316	-	46,54,73	1.78	6 (13%)	53,90,113	1.57	8 (15%)
35	BCR	m	201	-	41,41,41	0.70	0	56,56,56	2.33	17 (30%)
26	DD6	G	505	-	39,45,45	2.26	4 (10%)	52,67,67	2.31	21 (40%)
32	PID	D	302	-	41,49,49	1.35	4 (9%)	49,76,76	1.44	7 (14%)
28	CLA	m	202	-	60,68,73	1.55	5 (8%)	70,107,113	1.49	7 (10%)
26	DD6	K	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.90	13 (25%)
28	CLA	J	314	-	41,49,73	1.85	5 (12%)	47,84,113	1.68	8 (17%)
28	CLA	a	719	-	47,55,73	1.76	7 (14%)	54,91,113	1.51	8 (14%)
26	DD6	B	303	-	39,45,45	2.00	2 (5%)	52,67,67	2.00	17 (32%)
28	CLA	b	705	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
29	KC1	B	314	18	48,53,53	1.51	7 (14%)	55,89,89	1.84	11 (20%)
28	CLA	j	106	-	58,66,73	1.58	6 (10%)	67,104,113	1.46	8 (11%)
28	CLA	a	738	22	46,54,73	1.77	5 (10%)	53,90,113	1.58	7 (13%)
28	CLA	f	301	-	55,63,73	1.62	5 (9%)	64,101,113	1.44	8 (12%)
28	CLA	b	716	-	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
28	CLA	J	308	-	46,54,73	1.76	6 (13%)	53,90,113	1.57	7 (13%)
28	CLA	B	311	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	7 (9%)
29	KC1	K	314	2	48,53,53	1.51	7 (14%)	55,89,89	1.84	10 (18%)
29	KC1	L	315	-	48,53,53	1.51	7 (14%)	55,89,89	1.90	11 (20%)
28	CLA	l	312	-	46,54,73	1.76	5 (10%)	53,90,113	1.53	7 (13%)
28	CLA	b	726	-	47,55,73	1.76	5 (10%)	54,91,113	1.51	8 (14%)
26	DD6	A	303	-	39,45,45	1.94	2 (5%)	52,67,67	1.88	13 (25%)
28	CLA	l	309	-	41,49,73	1.86	5 (12%)	47,84,113	1.65	8 (17%)
28	CLA	F	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.58	8 (15%)
26	DD6	J	304	-	39,45,45	2.20	5 (12%)	52,67,67	2.12	18 (34%)
28	CLA	A	319	-	46,54,73	1.77	6 (13%)	53,90,113	1.50	7 (13%)
31	LMG	b	734	-	31,31,55	0.99	0	39,39,63	1.18	3 (7%)
28	CLA	b	722	-	65,73,73	1.51	6 (9%)	76,113,113	1.45	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PID	H	301	-	41,49,49	1.33	4 (9%)	49,76,76	1.65	6 (12%)
32	PID	M	301	-	41,49,49	1.33	4 (9%)	49,76,76	1.74	8 (16%)
35	BCR	f	304	-	41,41,41	0.72	0	56,56,56	2.07	17 (30%)
28	CLA	a	711	-	45,53,73	1.77	6 (13%)	52,89,113	1.66	8 (15%)
32	PID	F	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.76	7 (14%)
33	SQD	A	318	-	49,50,54	0.40	1 (2%)	58,61,65	0.58	0
28	CLA	L	308	29	46,55,73	1.76	5 (10%)	55,91,113	1.53	10 (18%)
35	BCR	l	302	-	41,41,41	0.72	0	56,56,56	2.19	21 (37%)
29	KC1	J	313	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
28	CLA	a	707	-	65,73,73	1.52	6 (9%)	76,113,113	1.33	8 (10%)
28	CLA	M	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.77	9 (19%)
28	CLA	A	317	-	41,49,73	1.86	5 (12%)	47,84,113	1.65	9 (19%)
28	CLA	I	310	-	48,56,73	1.71	5 (10%)	55,92,113	1.60	7 (12%)
26	DD6	b	731	28	39,45,45	2.11	3 (7%)	52,67,67	1.96	16 (30%)
28	CLA	G	509	5	51,59,73	1.68	5 (9%)	59,96,113	1.51	8 (13%)
30	DGD	I	317	-	40,40,67	1.09	2 (5%)	54,54,81	1.02	4 (7%)
28	CLA	A	315	-	41,49,73	1.85	6 (14%)	47,84,113	1.65	8 (17%)
28	CLA	l	311	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
29	KC1	F	314	20	48,53,53	1.49	7 (14%)	55,89,89	1.88	10 (18%)
34	SF4	a	737	17,16	0,12,12	-	-	-	-	-
28	CLA	a	731	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	9 (11%)
32	PID	D	306	-	41,49,49	1.34	4 (9%)	49,76,76	1.43	5 (10%)
28	CLA	I	315	-	52,60,73	1.68	5 (9%)	60,97,113	1.50	8 (13%)
26	DD6	G	504	-	39,45,45	2.24	5 (12%)	52,67,67	2.19	19 (36%)
28	CLA	N	304	-	47,55,73	1.76	5 (10%)	54,91,113	1.54	8 (14%)
26	DD6	A	302	-	39,45,45	2.02	3 (7%)	52,67,67	2.13	16 (30%)
32	PID	D	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.41	5 (10%)
26	DD6	J	303	-	39,45,45	2.31	4 (10%)	52,67,67	2.44	18 (34%)
28	CLA	J	310	-	46,54,73	1.81	6 (13%)	53,90,113	1.56	6 (11%)
28	CLA	G	519	-	59,67,73	1.57	5 (8%)	68,105,113	1.45	7 (10%)
28	CLA	I	308	-	60,68,73	1.57	5 (8%)	70,107,113	1.42	10 (14%)
28	CLA	M	308	29	53,61,73	1.66	5 (9%)	61,98,113	1.52	8 (13%)
28	CLA	D	314	-	46,54,73	1.79	6 (13%)	53,90,113	1.59	9 (16%)
28	CLA	a	717	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	9 (13%)
28	CLA	K	315	-	41,49,73	1.85	6 (14%)	47,84,113	1.70	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	J	311	22	47,55,73	1.73	5 (10%)	54,91,113	1.60	8 (14%)
28	CLA	H	308	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	6 (11%)
28	CLA	G	514	-	53,61,73	1.64	6 (11%)	61,98,113	1.51	9 (14%)
28	CLA	b	713	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
26	DD6	M	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.19	19 (36%)
28	CLA	H	309	-	47,55,73	1.73	5 (10%)	54,91,113	1.55	8 (14%)
29	KC1	M	314	24	48,53,53	1.51	7 (14%)	55,89,89	1.87	11 (20%)
26	DD6	F	301	-	39,45,45	1.99	2 (5%)	52,67,67	2.34	17 (32%)
28	CLA	a	729	-	56,64,73	1.59	6 (10%)	65,102,113	1.42	8 (12%)
28	CLA	I	307	-	46,54,73	1.76	5 (10%)	53,90,113	1.53	6 (11%)
26	DD6	G	508	-	39,45,45	2.04	3 (7%)	52,67,67	2.02	13 (25%)
28	CLA	a	720	-	62,70,73	1.52	5 (8%)	72,109,113	1.42	8 (11%)
29	KC1	H	306	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
30	DGD	L	301	-	39,39,67	0.95	2 (5%)	53,53,81	0.98	2 (3%)
28	CLA	a	725	-	61,69,73	1.55	5 (8%)	71,108,113	1.40	9 (12%)
26	DD6	I	302	-	39,45,45	2.04	3 (7%)	52,67,67	2.16	18 (34%)
28	CLA	A	307	29	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
26	DD6	L	306	-	39,45,45	2.01	3 (7%)	52,67,67	2.03	15 (28%)
28	CLA	F	307	-	46,54,73	1.77	6 (13%)	53,90,113	1.60	7 (13%)
30	DGD	j	103	-	42,42,67	1.05	2 (4%)	56,56,81	1.00	3 (5%)
28	CLA	M	317	-	46,54,73	1.75	6 (13%)	53,90,113	1.58	7 (13%)
28	CLA	b	711	-	55,63,73	1.63	5 (9%)	64,101,113	1.43	8 (12%)
28	CLA	H	312	-	46,54,73	1.78	6 (13%)	53,90,113	1.56	7 (13%)
28	CLA	I	313	-	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
26	DD6	M	304	-	39,45,45	2.05	3 (7%)	52,67,67	1.90	14 (26%)
28	CLA	G	511	-	55,63,73	1.63	6 (10%)	64,101,113	1.47	7 (10%)
28	CLA	M	312	-	48,56,73	1.74	5 (10%)	55,92,113	1.56	8 (14%)
29	KC1	M	307	28	48,53,53	1.51	7 (14%)	55,89,89	1.88	12 (21%)
34	SF4	c	201	7	0,12,12	-	-	-	-	-
28	CLA	D	309	-	46,54,73	1.74	5 (10%)	53,90,113	1.59	7 (13%)
35	BCR	l	306	-	41,41,41	0.72	0	56,56,56	1.92	13 (23%)
28	CLA	H	311	-	41,49,73	1.88	6 (14%)	47,84,113	1.63	8 (17%)
28	CLA	L	318	-	46,54,73	1.75	7 (15%)	53,90,113	1.57	7 (13%)
26	DD6	B	302	-	38,44,45	2.18	3 (7%)	50,65,67	2.12	20 (40%)
29	KC1	L	307	28	48,53,53	1.52	7 (14%)	55,89,89	1.89	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	L	310	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
28	CLA	b	719	-	46,54,73	1.79	6 (13%)	53,90,113	1.61	7 (13%)
28	CLA	f	302	-	46,54,73	1.76	5 (10%)	53,90,113	1.58	7 (13%)
28	CLA	a	716	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	8 (14%)
28	CLA	B	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.45	10 (15%)
28	CLA	B	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.70	7 (14%)
28	CLA	F	313	-	46,54,73	1.76	6 (13%)	53,90,113	1.65	7 (13%)
31	LMG	j	101	-	35,35,55	0.88	0	43,43,63	1.22	4 (9%)
28	CLA	G	516	5	41,49,73	1.87	5 (12%)	47,84,113	1.65	7 (14%)
28	CLA	K	310	-	55,63,73	1.62	5 (9%)	64,101,113	1.46	8 (12%)
28	CLA	a	735	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
29	KC1	G	515	5	48,53,53	1.49	7 (14%)	55,89,89	1.81	12 (21%)
28	CLA	I	309	-	55,63,73	1.64	5 (9%)	64,101,113	1.45	8 (12%)
31	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.33	6 (13%)
28	CLA	F	310	-	46,54,73	1.76	5 (10%)	53,90,113	1.63	8 (15%)
35	BCR	i	201	-	41,41,41	0.83	2 (4%)	56,56,56	2.12	20 (35%)
28	CLA	K	308	2	54,62,73	1.63	5 (9%)	62,99,113	1.48	8 (12%)
34	SF4	c	202	7	0,12,12	-	-	-	-	-
29	KC1	N	311	25	48,53,53	1.49	7 (14%)	55,89,89	1.85	11 (20%)
28	CLA	h	202	-	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)
26	DD6	N	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.09	16 (30%)
28	CLA	M	316	-	52,60,73	1.68	6 (11%)	60,97,113	1.48	6 (10%)
28	CLA	M	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.54	6 (11%)
28	CLA	K	306	2	49,57,73	1.73	5 (10%)	55,93,113	1.55	9 (16%)
26	DD6	L	303	-	39,45,45	1.98	2 (5%)	52,67,67	1.99	14 (26%)
28	CLA	K	312	-	48,56,73	1.72	7 (14%)	55,92,113	1.53	7 (12%)
28	CLA	D	308	-	47,55,73	1.76	5 (10%)	54,91,113	1.51	7 (12%)
35	BCR	b	702	-	41,41,41	0.73	0	56,56,56	2.17	17 (30%)
32	PID	D	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.78	7 (14%)
28	CLA	a	724	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
31	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
28	CLA	b	710	-	52,60,73	1.69	6 (11%)	60,97,113	1.50	8 (13%)
28	CLA	L	311	-	55,63,73	1.62	5 (9%)	64,101,113	1.48	8 (12%)
30	DGD	G	521	-	45,45,67	1.02	2 (4%)	59,59,81	1.46	8 (13%)
26	DD6	D	303	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	K	307	-	46,54,73	1.71	5 (10%)	53,90,113	1.60	6 (11%)
27	UIX	A	304	-	41,49,49	1.23	3 (7%)	52,74,74	2.44	20 (38%)
28	CLA	a	714	-	45,53,73	1.80	6 (13%)	52,89,113	1.62	7 (13%)
28	CLA	G	518	-	46,54,73	1.79	5 (10%)	53,90,113	1.60	8 (15%)
28	CLA	b	709	-	60,68,73	1.57	6 (10%)	70,107,113	1.43	9 (12%)
28	CLA	a	722	-	58,66,73	1.58	5 (8%)	67,104,113	1.48	8 (11%)
28	CLA	a	705	28	55,63,73	1.62	5 (9%)	64,101,113	1.53	9 (14%)
28	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.71	8 (17%)
35	BCR	l	307	-	41,41,41	0.72	0	56,56,56	2.01	19 (33%)
28	CLA	B	313	18	65,73,73	1.47	5 (7%)	76,113,113	1.39	7 (9%)
28	CLA	a	723	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	8 (10%)
28	CLA	b	724	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
28	CLA	a	710	16	55,63,73	1.64	6 (10%)	64,101,113	1.46	9 (14%)
28	CLA	J	307	-	65,73,73	1.48	5 (7%)	76,113,113	1.43	6 (7%)
26	DD6	I	303	-	39,45,45	2.23	5 (12%)	52,67,67	2.03	16 (30%)
28	CLA	N	305	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
28	CLA	K	313	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	8 (12%)
26	DD6	A	301	-	39,45,45	2.00	3 (7%)	52,67,67	2.12	14 (26%)
28	CLA	a	704	-	65,73,73	1.51	6 (9%)	76,113,113	1.35	6 (7%)
28	CLA	b	727	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	8 (10%)
31	LMG	b	733	-	44,44,55	0.82	1 (2%)	52,52,63	1.30	6 (11%)
28	CLA	b	715	-	60,68,73	1.55	5 (8%)	70,107,113	1.43	8 (11%)
28	CLA	a	726	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	9 (11%)
28	CLA	D	312	19	46,54,73	1.77	5 (10%)	53,90,113	1.51	6 (11%)
28	CLA	b	721	26	46,54,73	1.77	6 (13%)	53,90,113	1.50	6 (11%)
27	UIX	B	305	-	41,49,49	1.24	3 (7%)	52,74,74	2.45	16 (30%)
26	DD6	L	302	-	39,45,45	1.94	3 (7%)	52,67,67	2.00	13 (25%)
28	CLA	J	309	-	56,64,73	1.59	5 (8%)	65,102,113	1.51	9 (13%)
28	CLA	A	311	6	46,54,73	1.77	5 (10%)	53,90,113	1.56	7 (13%)
26	DD6	H	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.90	11 (21%)
28	CLA	l	304	-	60,68,73	1.54	5 (8%)	70,107,113	1.49	6 (8%)
26	DD6	M	305	-	39,45,45	2.01	3 (7%)	52,67,67	1.89	14 (26%)
28	CLA	a	727	-	46,54,73	1.78	6 (13%)	53,90,113	1.50	7 (13%)
36	PQN	b	729	-	34,34,34	1.55	2 (5%)	42,45,45	1.23	4 (9%)
31	LMG	I	318	-	36,36,55	0.91	1 (2%)	44,44,63	1.24	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	A	305	29	39,45,45	1.99	2 (5%)	52,67,67	1.96	14 (26%)
27	UIX	K	302	-	41,49,49	1.27	3 (7%)	52,74,74	2.71	23 (44%)
28	CLA	K	309	-	50,58,73	1.66	5 (10%)	58,95,113	1.57	8 (13%)
28	CLA	B	309	18	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
26	DD6	K	319	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
28	CLA	N	310	-	47,55,73	1.76	5 (10%)	54,91,113	1.66	8 (14%)
28	CLA	B	301	-	60,68,73	1.56	5 (8%)	70,107,113	1.38	8 (11%)
32	PID	D	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.51	6 (12%)
35	BCR	a	734	-	41,41,41	0.71	0	56,56,56	2.07	19 (33%)
26	DD6	B	306	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	19 (36%)
28	CLA	G	520	-	49,57,73	1.69	5 (10%)	55,93,113	1.54	8 (14%)
29	KC1	A	314	6	48,53,53	1.52	7 (14%)	55,89,89	1.87	12 (21%)
28	CLA	a	706	16	58,66,73	1.57	6 (10%)	67,104,113	1.47	7 (10%)
27	UIX	h	201	-	41,49,49	1.28	3 (7%)	52,74,74	2.48	19 (36%)
28	CLA	I	306	1	49,57,73	1.71	5 (10%)	55,93,113	1.58	8 (14%)
29	KC1	I	314	1	48,53,53	1.50	7 (14%)	55,89,89	1.87	13 (23%)
26	DD6	I	305	-	39,45,45	2.28	6 (15%)	52,67,67	2.28	17 (32%)
29	KC1	A	306	28,26	48,53,53	1.49	7 (14%)	55,89,89	1.81	10 (18%)
28	CLA	L	309	-	53,61,73	1.66	5 (9%)	61,98,113	1.52	9 (14%)
28	CLA	b	728	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	8 (10%)
28	CLA	D	316	-	41,49,73	1.86	6 (14%)	47,84,113	1.65	8 (17%)
29	KC1	D	310	-	48,53,53	1.50	7 (14%)	55,89,89	1.88	11 (20%)
28	CLA	D	311	-	46,54,73	1.75	5 (10%)	53,90,113	1.57	7 (13%)
26	DD6	h	203	-	39,45,45	2.03	3 (7%)	52,67,67	1.87	13 (25%)
28	CLA	I	312	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
28	CLA	M	313	-	46,54,73	1.78	6 (13%)	53,90,113	1.55	7 (13%)
28	CLA	F	312	-	46,54,73	1.70	10 (21%)	53,90,113	1.51	6 (11%)
28	CLA	G	517	-	46,54,73	1.76	5 (10%)	53,90,113	1.57	7 (13%)
28	CLA	M	309	24	55,63,73	1.62	5 (9%)	64,101,113	1.44	8 (12%)
28	CLA	a	728	-	55,63,73	1.60	5 (9%)	64,101,113	1.48	9 (14%)
32	PID	F	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.49	5 (10%)
28	CLA	L	313	-	55,63,73	1.62	5 (9%)	64,101,113	1.45	8 (12%)
26	DD6	M	306	-	39,45,45	2.17	3 (7%)	52,67,67	2.24	19 (36%)
26	DD6	J	302	-	39,45,45	2.02	2 (5%)	52,67,67	2.11	15 (28%)
32	PID	D	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.47	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	a	721	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	9 (11%)
26	DD6	G	502	-	39,45,45	1.99	2 (5%)	52,67,67	1.94	15 (28%)
26	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	15 (28%)
28	CLA	I	321	28	52,60,73	1.67	5 (9%)	60,97,113	1.60	9 (15%)
28	CLA	I	311	1	55,63,73	1.65	5 (9%)	64,101,113	1.46	9 (14%)
32	PID	H	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.37	6 (12%)
28	CLA	b	706	-	48,56,73	1.74	5 (10%)	55,92,113	1.58	8 (14%)
28	CLA	a	709	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
28	CLA	L	316	-	41,49,73	1.85	5 (12%)	47,84,113	1.64	7 (14%)
28	CLA	b	701	-	65,73,73	1.50	6 (9%)	76,113,113	1.40	8 (10%)
28	CLA	a	712	28	60,68,73	1.55	5 (8%)	70,107,113	1.41	8 (11%)
28	CLA	N	307	-	51,59,73	1.73	6 (11%)	59,96,113	1.52	7 (11%)

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
28	CLA	H	305	-	1/1/15/20	8/37/115/115	-
31	LMG	K	318	-	-	18/38/58/70	0/1/1/1
28	CLA	a	702	-	1/1/15/20	12/37/115/115	-
31	LMG	D	317	-	-	17/41/61/70	0/1/1/1
28	CLA	M	310	-	1/1/11/20	7/17/95/115	-
28	CLA	b	712	-	1/1/13/20	9/25/101/115	-
28	CLA	B	317	-	1/1/11/20	5/13/91/115	-
28	CLA	b	717	-	1/1/15/20	18/37/115/115	-
32	PID	G	507	-	-	0/24/93/93	1/4/4/4
35	BCR	j	102	-	-	6/29/63/63	0/2/2/2
28	CLA	a	730	-	1/1/15/20	4/37/115/115	-
29	KC1	F	309	20	-	8/15/71/71	-
28	CLA	N	309	25	1/1/11/20	3/15/93/115	-
28	CLA	l	313	14	1/1/15/20	19/37/115/115	-
28	CLA	H	304	-	1/1/11/20	6/16/94/115	-
28	CLA	l	310	-	-	9/26/65/115	0/5/5/9
27	UIX	G	503	-	-	4/31/87/87	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	l	305	-	1/1/15/20	13/37/115/115	-
26	DD6	L	305	-	-	3/26/80/80	0/3/3/3
28	CLA	a	703	-	1/1/13/20	9/25/103/115	-
27	UIX	J	305	-	-	11/31/87/87	0/3/3/3
28	CLA	b	725	-	1/1/15/20	13/37/115/115	-
26	DD6	K	305	-	-	4/26/80/80	0/3/3/3
28	CLA	b	723	-	1/1/12/20	7/19/97/115	-
27	UIX	I	304	-	-	4/31/87/87	0/3/3/3
28	CLA	J	312	-	1/1/12/20	8/23/101/115	-
28	CLA	b	703	-	1/1/15/20	12/37/115/115	-
28	CLA	A	316	-	1/1/11/20	3/16/94/115	-
35	BCR	a	736	-	-	3/29/63/63	0/2/2/2
28	CLA	B	307	18	1/1/11/20	3/18/96/115	-
28	CLA	a	708	-	1/1/12/20	4/21/99/115	-
28	CLA	a	713	-	1/1/14/20	10/31/109/115	-
28	CLA	L	312	-	1/1/11/20	5/15/93/115	-
28	CLA	a	715	-	1/1/11/20	5/13/91/115	-
28	CLA	a	701	-	1/1/11/20	0/13/91/115	-
36	PQN	a	732	-	-	8/23/43/43	0/2/2/2
26	DD6	M	302	-	-	3/26/80/80	0/3/3/3
29	KC1	D	315	19	-	3/15/71/71	-
28	CLA	J	306	-	1/1/11/20	4/15/93/115	-
28	CLA	I	316	-	1/1/13/20	14/25/103/115	-
28	CLA	l	303	14	1/1/15/20	14/37/115/115	-
28	CLA	G	513	5	1/1/15/20	10/37/115/115	-
28	CLA	b	708	-	1/1/15/20	11/37/115/115	-
32	PID	F	302	-	-	2/24/93/93	0/4/4/4
32	PID	N	301	-	-	6/24/93/93	0/4/4/4
32	PID	N	302	-	-	2/24/93/93	0/4/4/4
28	CLA	B	312	-	1/1/12/20	2/21/99/115	-
26	DD6	I	301	-	-	3/26/80/80	0/3/3/3
28	CLA	F	308	-	1/1/11/20	1/15/93/115	-
28	CLA	a	718	-	1/1/11/20	8/15/93/115	-
28	CLA	D	313	19	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	707	-	1/1/15/20	17/37/115/115	-
28	CLA	b	714	-	1/1/11/20	5/15/93/115	-
28	CLA	G	512	-	1/1/14/20	13/31/109/115	-
28	CLA	B	308	-	1/1/11/20	5/13/91/115	-
28	CLA	L	314	-	1/1/12/20	6/23/101/115	-
35	BCR	b	730	-	-	8/29/63/63	0/2/2/2
28	CLA	A	312	-	1/1/13/20	6/25/103/115	-
28	CLA	J	316	-	-	2/15/93/115	-
29	KC1	N	308	-	-	8/15/71/71	-
28	CLA	A	313	-	1/1/13/20	10/25/103/115	-
28	CLA	G	510	-	1/1/15/20	14/37/115/115	-
26	DD6	K	303	-	-	0/26/80/80	0/3/3/3
28	CLA	j	104	-	1/1/13/20	6/25/103/115	-
28	CLA	I	319	28	1/1/11/20	8/13/91/115	-
26	DD6	B	304	-	-	0/26/80/80	0/3/3/3
29	KC1	H	310	-	-	6/15/71/71	-
30	DGD	G	501	-	-	10/34/74/95	0/2/2/2
32	PID	G	506	-	-	3/24/93/93	0/4/4/4
28	CLA	K	311	-	1/1/12/20	9/22/100/115	-
28	CLA	L	317	-	1/1/12/20	11/22/100/115	-
32	PID	j	105	-	-	4/24/93/93	0/4/4/4
28	CLA	f	303	10	1/1/11/20	10/15/93/115	-
26	DD6	F	303	-	-	2/26/80/80	0/3/3/3
26	DD6	L	304	-	-	0/26/80/80	0/3/3/3
28	CLA	J	301	-	1/1/14/20	11/31/109/115	-
28	CLA	b	718	-	1/1/12/20	1/21/99/115	-
30	DGD	l	301	-	-	7/39/79/95	0/2/2/2
28	CLA	A	308	-	1/1/13/20	4/25/103/115	-
28	CLA	J	315	-	1/1/11/20	4/15/93/115	-
28	CLA	H	307	-	1/1/12/20	7/21/99/115	-
28	CLA	b	720	-	1/1/12/20	9/23/101/115	-
28	CLA	M	318	-	1/1/11/20	9/15/93/115	-
35	BCR	b	732	-	-	2/29/63/63	0/2/2/2
28	CLA	A	309	-	1/1/13/20	7/25/103/115	-
28	CLA	A	320	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	310	-	1/1/15/20	15/37/115/115	-
37	LHG	a	733	-	-	18/52/52/53	-
28	CLA	B	316	-	1/1/11/20	7/15/93/115	-
28	CLA	l	308	-	1/1/10/20	2/8/86/115	-
31	LMG	K	317	-	-	8/22/42/70	0/1/1/1
32	PID	F	305	-	-	8/24/93/93	0/4/4/4
29	KC1	N	306	-	-	6/15/71/71	-
30	DGD	y	201	-	-	7/43/83/95	0/2/2/2
28	CLA	b	704	-	1/1/15/20	19/37/115/115	-
28	CLA	K	316	-	1/1/11/20	2/15/93/115	-
35	BCR	m	201	-	-	5/29/63/63	0/2/2/2
26	DD6	G	505	-	-	4/26/80/80	0/3/3/3
32	PID	D	302	-	-	2/24/93/93	0/4/4/4
28	CLA	m	202	-	1/1/14/20	10/31/109/115	-
26	DD6	K	301	-	-	5/26/80/80	0/3/3/3
28	CLA	J	314	-	1/1/10/20	4/8/86/115	-
28	CLA	a	719	-	1/1/11/20	4/16/94/115	-
26	DD6	B	303	-	-	2/26/80/80	0/3/3/3
28	CLA	b	705	-	1/1/15/20	14/37/115/115	-
29	KC1	B	314	18	-	7/15/71/71	-
28	CLA	j	106	-	1/1/13/20	12/29/107/115	-
28	CLA	a	738	22	1/1/11/20	2/15/93/115	-
28	CLA	f	301	-	1/1/13/20	9/25/103/115	-
28	CLA	b	716	-	1/1/12/20	7/19/97/115	-
28	CLA	J	308	-	1/1/11/20	9/15/93/115	-
28	CLA	B	311	-	1/1/15/20	21/37/115/115	-
29	KC1	K	314	2	-	8/15/71/71	-
29	KC1	L	315	-	-	8/15/71/71	-
28	CLA	l	312	-	1/1/11/20	8/15/93/115	-
28	CLA	b	726	-	1/1/11/20	1/16/94/115	-
26	DD6	A	303	-	-	1/26/80/80	0/3/3/3
28	CLA	l	309	-	1/1/10/20	4/8/86/115	-
28	CLA	F	311	-	1/1/11/20	4/15/93/115	-
26	DD6	J	304	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	319	-	1/1/11/20	8/15/93/115	-
31	LMG	b	734	-	-	12/26/46/70	0/1/1/1
28	CLA	b	722	-	1/1/15/20	8/37/115/115	-
32	PID	H	301	-	-	4/24/93/93	0/4/4/4
32	PID	M	301	-	-	1/24/93/93	0/4/4/4
35	BCR	f	304	-	-	3/29/63/63	0/2/2/2
28	CLA	a	711	-	1/1/11/20	6/13/91/115	-
32	PID	F	304	-	-	3/24/93/93	0/4/4/4
33	SQD	A	318	-	-	6/45/65/69	0/1/1/1
28	CLA	L	308	29	1/1/11/20	7/13/91/115	-
35	BCR	l	302	-	-	4/29/63/63	0/2/2/2
29	KC1	J	313	-	-	6/15/71/71	-
28	CLA	a	707	-	1/1/15/20	16/37/115/115	-
28	CLA	M	315	-	1/1/10/20	5/8/86/115	-
28	CLA	A	317	-	1/1/10/20	0/8/86/115	-
28	CLA	I	310	-	1/1/11/20	10/17/95/115	-
26	DD6	b	731	28	-	3/26/80/80	0/3/3/3
28	CLA	G	509	5	1/1/12/20	4/21/99/115	-
30	DGD	I	317	-	-	3/28/68/95	0/2/2/2
28	CLA	A	315	-	1/1/10/20	6/8/86/115	-
28	CLA	l	311	-	1/1/15/20	17/37/115/115	-
29	KC1	F	314	20	-	8/15/71/71	-
34	SF4	a	737	17,16	-	-	0/6/5/5
28	CLA	a	731	-	1/1/15/20	13/37/115/115	-
32	PID	D	306	-	-	8/24/93/93	0/4/4/4
28	CLA	I	315	-	1/1/12/20	7/22/100/115	-
26	DD6	G	504	-	-	5/26/80/80	0/3/3/3
28	CLA	N	304	-	1/1/11/20	3/16/94/115	-
26	DD6	A	302	-	-	3/26/80/80	0/3/3/3
32	PID	D	307	-	-	4/24/93/93	0/4/4/4
26	DD6	J	303	-	-	2/26/80/80	0/3/3/3
28	CLA	J	310	-	1/1/11/20	6/15/93/115	-
28	CLA	G	519	-	1/1/13/20	13/30/108/115	-
28	CLA	I	308	-	1/1/14/20	12/31/109/115	-
28	CLA	M	308	29	1/1/12/20	8/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	D	314	-	1/1/11/20	6/15/93/115	-
28	CLA	a	717	-	1/1/13/20	13/28/106/115	-
28	CLA	K	315	-	1/1/10/20	3/8/86/115	-
28	CLA	J	311	22	1/1/11/20	8/16/94/115	-
28	CLA	H	308	-	1/1/11/20	4/15/93/115	-
28	CLA	G	514	-	1/1/12/20	11/23/101/115	-
28	CLA	b	713	-	1/1/15/20	11/37/115/115	-
26	DD6	M	303	-	-	2/26/80/80	0/3/3/3
28	CLA	H	309	-	1/1/11/20	7/16/94/115	-
29	KC1	M	314	24	-	9/15/71/71	-
26	DD6	F	301	-	-	2/26/80/80	0/3/3/3
28	CLA	a	729	-	1/1/13/20	9/27/105/115	-
28	CLA	I	307	-	1/1/11/20	6/15/93/115	-
26	DD6	G	508	-	-	1/26/80/80	0/3/3/3
28	CLA	a	720	-	1/1/14/20	6/34/112/115	-
29	KC1	H	306	-	-	4/15/71/71	-
30	DGD	L	301	-	-	2/26/66/95	0/2/2/2
28	CLA	a	725	-	1/1/14/20	11/33/111/115	-
26	DD6	I	302	-	-	5/26/80/80	0/3/3/3
28	CLA	A	307	29	1/1/11/20	2/13/91/115	-
26	DD6	L	306	-	-	3/26/80/80	0/3/3/3
28	CLA	F	307	-	1/1/11/20	5/15/93/115	-
30	DGD	j	103	-	-	7/30/70/95	0/2/2/2
28	CLA	M	317	-	1/1/11/20	6/15/93/115	-
28	CLA	b	711	-	1/1/13/20	11/25/103/115	-
28	CLA	H	312	-	1/1/11/20	10/15/93/115	-
28	CLA	I	313	-	1/1/13/20	12/25/103/115	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
28	CLA	G	511	-	1/1/13/20	4/25/103/115	-
28	CLA	M	312	-	1/1/11/20	4/17/95/115	-
29	KC1	M	307	28	-	7/15/71/71	-
34	SF4	c	201	7	-	-	0/6/5/5
28	CLA	D	309	-	1/1/11/20	7/15/93/115	-
35	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	CLA	L	318	-	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	H	311	-	-	6/8/86/115	-
26	DD6	B	302	-	-	3/24/78/80	0/3/3/3
29	KC1	L	307	28	-	6/15/71/71	-
28	CLA	L	310	-	1/1/13/20	2/25/103/115	-
28	CLA	b	719	-	1/1/11/20	11/15/93/115	-
28	CLA	f	302	-	1/1/11/20	6/15/93/115	-
28	CLA	a	716	-	1/1/11/20	4/16/94/115	-
28	CLA	B	310	-	1/1/13/20	8/25/103/115	-
28	CLA	B	315	-	1/1/10/20	6/8/86/115	-
28	CLA	F	313	-	1/1/11/20	5/15/93/115	-
31	LMG	j	101	-	-	14/30/50/70	0/1/1/1
28	CLA	G	516	5	1/1/10/20	4/8/86/115	-
28	CLA	K	310	-	1/1/13/20	6/25/103/115	-
28	CLA	a	735	-	1/1/15/20	20/37/115/115	-
29	KC1	G	515	5	-	8/15/71/71	-
28	CLA	I	309	-	1/1/13/20	8/25/103/115	-
31	LMG	B	318	-	-	15/32/52/70	0/1/1/1
28	CLA	F	310	-	1/1/11/20	8/15/93/115	-
35	BCR	i	201	-	-	8/29/63/63	0/2/2/2
28	CLA	K	308	2	1/1/12/20	13/24/102/115	-
34	SF4	c	202	7	-	-	0/6/5/5
29	KC1	N	311	25	-	7/15/71/71	-
28	CLA	h	202	-	1/1/13/20	7/25/103/115	-
26	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	CLA	M	316	-	1/1/12/20	11/22/100/115	-
28	CLA	M	311	-	1/1/11/20	6/15/93/115	-
28	CLA	K	306	2	1/1/11/20	4/18/96/115	-
28	CLA	K	312	-	1/1/11/20	4/17/95/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
28	CLA	D	308	-	1/1/11/20	4/16/94/115	-
35	BCR	b	702	-	-	2/29/63/63	0/2/2/2
32	PID	D	304	-	-	3/24/93/93	0/4/4/4
28	CLA	a	724	-	1/1/15/20	15/37/115/115	-
31	LMG	I	320	-	-	14/33/53/70	0/1/1/1
28	CLA	b	710	-	1/1/12/20	6/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	L	311	-	1/1/13/20	4/25/103/115	-
30	DGD	G	521	-	-	18/33/73/95	0/2/2/2
26	DD6	D	303	-	-	6/26/80/80	0/3/3/3
28	CLA	K	307	-	1/1/11/20	0/15/93/115	-
28	CLA	a	714	-	1/1/11/20	4/13/91/115	-
27	UIX	A	304	-	-	0/31/87/87	0/3/3/3
28	CLA	G	518	-	1/1/11/20	7/15/93/115	-
28	CLA	b	709	-	1/1/14/20	8/31/109/115	-
28	CLA	a	722	-	1/1/13/20	10/29/107/115	-
28	CLA	a	705	28	1/1/13/20	9/25/103/115	-
28	CLA	F	315	-	1/1/10/20	4/8/86/115	-
35	BCR	l	307	-	-	0/29/63/63	0/2/2/2
28	CLA	B	313	18	1/1/15/20	11/37/115/115	-
28	CLA	a	723	-	1/1/15/20	16/37/115/115	-
28	CLA	b	724	-	1/1/15/20	14/37/115/115	-
28	CLA	a	710	16	1/1/13/20	4/25/103/115	-
28	CLA	J	307	-	1/1/15/20	21/37/115/115	-
26	DD6	I	303	-	-	2/26/80/80	0/3/3/3
28	CLA	N	305	-	1/1/15/20	11/37/115/115	-
28	CLA	K	313	-	1/1/13/20	7/25/103/115	-
26	DD6	A	301	-	-	3/26/80/80	0/3/3/3
28	CLA	a	704	-	1/1/15/20	6/37/115/115	-
28	CLA	b	727	-	1/1/15/20	10/37/115/115	-
31	LMG	b	733	-	-	18/39/59/70	0/1/1/1
28	CLA	b	715	-	1/1/14/20	14/31/109/115	-
28	CLA	a	726	-	1/1/15/20	11/37/115/115	-
28	CLA	D	312	19	1/1/11/20	6/15/93/115	-
28	CLA	b	721	26	1/1/11/20	5/15/93/115	-
27	UIX	B	305	-	-	2/31/87/87	0/3/3/3
26	DD6	L	302	-	-	4/26/80/80	0/3/3/3
28	CLA	J	309	-	1/1/13/20	8/27/105/115	-
28	CLA	A	311	6	1/1/11/20	5/15/93/115	-
26	DD6	H	303	-	-	1/26/80/80	0/3/3/3
28	CLA	l	304	-	1/1/14/20	11/31/109/115	-
26	DD6	M	305	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	a	727	-	1/1/11/20	8/15/93/115	-
36	PQN	b	729	-	-	4/23/43/43	0/2/2/2
31	LMG	I	318	-	-	21/31/51/70	0/1/1/1
26	DD6	A	305	29	-	1/26/80/80	0/3/3/3
27	UIX	K	302	-	-	4/31/87/87	0/3/3/3
28	CLA	K	309	-	1/1/12/20	2/19/97/115	-
28	CLA	B	309	18	1/1/15/20	22/37/115/115	-
26	DD6	K	319	-	-	4/26/80/80	0/3/3/3
28	CLA	N	310	-	1/1/11/20	9/16/94/115	-
28	CLA	B	301	-	1/1/14/20	11/31/109/115	-
32	PID	D	301	-	-	2/24/93/93	0/4/4/4
35	BCR	a	734	-	-	4/29/63/63	0/2/2/2
26	DD6	B	306	-	-	2/26/80/80	0/3/3/3
28	CLA	G	520	-	1/1/11/20	6/18/96/115	-
29	KC1	A	314	6	-	7/15/71/71	-
28	CLA	a	706	16	1/1/13/20	17/29/107/115	-
27	UIX	h	201	-	-	2/31/87/87	0/3/3/3
28	CLA	I	306	1	1/1/11/20	7/18/96/115	-
29	KC1	I	314	1	-	8/15/71/71	-
26	DD6	I	305	-	-	5/26/80/80	0/3/3/3
29	KC1	A	306	28,26	-	6/15/71/71	-
28	CLA	L	309	-	1/1/12/20	11/23/101/115	-
28	CLA	b	728	-	1/1/15/20	7/37/115/115	-
28	CLA	D	316	-	1/1/10/20	0/8/86/115	-
29	KC1	D	310	-	-	10/15/71/71	-
28	CLA	D	311	-	1/1/11/20	4/15/93/115	-
26	DD6	h	203	-	-	1/26/80/80	0/3/3/3
28	CLA	I	312	-	1/1/15/20	14/37/115/115	-
28	CLA	M	313	-	1/1/11/20	4/15/93/115	-
28	CLA	F	312	-	1/1/11/20	4/15/93/115	-
28	CLA	G	517	-	1/1/11/20	4/15/93/115	-
28	CLA	M	309	24	1/1/13/20	5/25/103/115	-
28	CLA	a	728	-	1/1/13/20	8/25/103/115	-
32	PID	F	306	-	-	0/24/93/93	0/4/4/4
28	CLA	L	313	-	1/1/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DD6	M	306	-	-	5/26/80/80	0/3/3/3
26	DD6	J	302	-	-	3/26/80/80	0/3/3/3
32	PID	D	305	-	-	2/24/93/93	0/4/4/4
28	CLA	a	721	-	1/1/15/20	18/37/115/115	-
26	DD6	G	502	-	-	6/26/80/80	0/3/3/3
26	DD6	K	304	-	-	1/26/80/80	0/3/3/3
28	CLA	I	321	28	1/1/12/20	9/22/100/115	-
28	CLA	I	311	1	1/1/13/20	10/25/103/115	-
32	PID	H	302	-	-	2/24/93/93	0/4/4/4
28	CLA	b	706	-	1/1/11/20	4/17/95/115	-
28	CLA	a	709	-	1/1/15/20	17/37/115/115	-
28	CLA	L	316	-	1/1/10/20	4/8/86/115	-
28	CLA	b	701	-	1/1/15/20	15/37/115/115	-
28	CLA	a	712	28	1/1/14/20	8/31/109/115	-
28	CLA	N	307	-	1/1/12/20	7/21/99/115	-

All (1436) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	310	CLA	CHC-C1C	9.32	1.42	1.35
26	I	305	DD6	C29-C27	-9.13	1.25	1.42
26	M	303	DD6	C29-C27	-9.08	1.25	1.42
26	J	303	DD6	C29-C27	-9.06	1.25	1.42
26	b	731	DD6	C29-C27	-9.02	1.25	1.42
26	M	306	DD6	C29-C27	-9.01	1.25	1.42
26	G	505	DD6	C29-C27	-8.98	1.25	1.42
26	I	303	DD6	C29-C27	-8.95	1.25	1.42
26	G	504	DD6	C29-C27	-8.87	1.25	1.42
26	M	304	DD6	C29-C27	-8.86	1.25	1.42
26	I	301	DD6	C29-C27	-8.81	1.25	1.42
26	B	302	DD6	C29-C27	-8.80	1.25	1.42
26	F	303	DD6	C29-C27	-8.80	1.25	1.42
26	G	508	DD6	C29-C27	-8.77	1.25	1.42
26	B	306	DD6	C29-C27	-8.74	1.25	1.42
26	N	303	DD6	C29-C27	-8.71	1.25	1.42
26	K	319	DD6	C29-C27	-8.70	1.25	1.42
26	I	302	DD6	C29-C27	-8.70	1.25	1.42
26	J	302	DD6	C29-C27	-8.70	1.25	1.42
26	h	203	DD6	C29-C27	-8.69	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	304	DD6	C29-C27	-8.69	1.25	1.42
26	M	302	DD6	C29-C27	-8.68	1.25	1.42
26	B	303	DD6	C29-C27	-8.68	1.25	1.42
26	M	305	DD6	C29-C27	-8.67	1.25	1.42
26	L	306	DD6	C29-C27	-8.62	1.26	1.42
26	K	304	DD6	C29-C27	-8.62	1.26	1.42
26	L	303	DD6	C29-C27	-8.61	1.26	1.42
26	K	305	DD6	C29-C27	-8.59	1.26	1.42
26	A	301	DD6	C29-C27	-8.59	1.26	1.42
26	A	305	DD6	C29-C27	-8.58	1.26	1.42
26	K	301	DD6	C29-C27	-8.58	1.26	1.42
26	B	304	DD6	C29-C27	-8.58	1.26	1.42
26	G	502	DD6	C29-C27	-8.56	1.26	1.42
26	L	304	DD6	C29-C27	-8.54	1.26	1.42
26	F	301	DD6	C29-C27	-8.53	1.26	1.42
26	D	303	DD6	C29-C27	-8.52	1.26	1.42
26	A	302	DD6	C29-C27	-8.50	1.26	1.42
26	L	305	DD6	C29-C27	-8.48	1.26	1.42
26	H	303	DD6	C29-C27	-8.48	1.26	1.42
26	A	303	DD6	C29-C27	-8.33	1.26	1.42
26	L	302	DD6	C29-C27	-8.31	1.26	1.42
26	K	303	DD6	C29-C27	-8.31	1.26	1.42
26	I	305	DD6	C30-C31	-8.31	1.25	1.42
26	J	303	DD6	C30-C31	-8.30	1.25	1.42
26	M	306	DD6	C30-C31	-8.29	1.25	1.42
26	G	505	DD6	C30-C31	-8.27	1.25	1.42
26	M	303	DD6	C30-C31	-8.23	1.25	1.42
26	b	731	DD6	C30-C31	-8.12	1.25	1.42
26	G	504	DD6	C30-C31	-8.09	1.25	1.42
26	I	303	DD6	C30-C31	-8.08	1.25	1.42
26	B	302	DD6	C30-C31	-8.06	1.25	1.42
26	J	304	DD6	C30-C31	-8.04	1.25	1.42
26	M	302	DD6	C30-C31	-8.01	1.25	1.42
26	h	203	DD6	C30-C31	-7.90	1.25	1.42
28	I	311	CLA	C4B-NB	7.90	1.42	1.35
28	A	320	CLA	C4B-NB	7.89	1.42	1.35
26	N	303	DD6	C30-C31	-7.86	1.25	1.42
26	I	301	DD6	C30-C31	-7.86	1.25	1.42
26	M	304	DD6	C30-C31	-7.85	1.26	1.42
26	B	306	DD6	C30-C31	-7.85	1.26	1.42
28	B	307	CLA	C4B-NB	7.83	1.42	1.35
28	b	718	CLA	C4B-NB	7.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	508	DD6	C30-C31	-7.82	1.26	1.42
28	b	709	CLA	C4B-NB	7.81	1.42	1.35
26	A	302	DD6	C30-C31	-7.80	1.26	1.42
26	G	502	DD6	C30-C31	-7.78	1.26	1.42
26	K	304	DD6	C30-C31	-7.78	1.26	1.42
26	K	303	DD6	C30-C31	-7.77	1.26	1.42
26	A	301	DD6	C30-C31	-7.77	1.26	1.42
26	I	302	DD6	C30-C31	-7.77	1.26	1.42
26	B	303	DD6	C30-C31	-7.76	1.26	1.42
26	M	305	DD6	C30-C31	-7.76	1.26	1.42
28	N	307	CLA	C4B-NB	7.76	1.42	1.35
28	G	518	CLA	C4B-NB	7.76	1.42	1.35
28	J	310	CLA	C4B-NB	7.75	1.42	1.35
26	F	303	DD6	C30-C31	-7.75	1.26	1.42
26	L	305	DD6	C30-C31	-7.74	1.26	1.42
26	F	301	DD6	C30-C31	-7.74	1.26	1.42
26	K	319	DD6	C30-C31	-7.73	1.26	1.42
28	b	719	CLA	C4B-NB	7.72	1.42	1.35
28	l	303	CLA	C4B-NB	7.71	1.42	1.35
26	L	306	DD6	C30-C31	-7.71	1.26	1.42
28	A	307	CLA	C4B-NB	7.70	1.42	1.35
28	a	707	CLA	C4B-NB	7.70	1.42	1.35
26	A	305	DD6	C30-C31	-7.70	1.26	1.42
28	j	104	CLA	C4B-NB	7.69	1.42	1.35
28	a	727	CLA	C4B-NB	7.69	1.42	1.35
28	a	735	CLA	C4B-NB	7.69	1.42	1.35
28	M	313	CLA	C4B-NB	7.68	1.42	1.35
28	a	731	CLA	C4B-NB	7.67	1.42	1.35
26	B	304	DD6	C30-C31	-7.67	1.26	1.42
26	K	305	DD6	C30-C31	-7.67	1.26	1.42
28	D	308	CLA	C4B-NB	7.66	1.42	1.35
28	a	724	CLA	C4B-NB	7.66	1.42	1.35
28	M	316	CLA	C4B-NB	7.65	1.42	1.35
28	b	728	CLA	C4B-NB	7.65	1.42	1.35
28	b	706	CLA	C4B-NB	7.64	1.42	1.35
28	b	723	CLA	C4B-NB	7.63	1.42	1.35
28	H	308	CLA	C4B-NB	7.63	1.42	1.35
26	D	303	DD6	C30-C31	-7.63	1.26	1.42
28	G	516	CLA	C4B-NB	7.63	1.42	1.35
28	b	721	CLA	C4B-NB	7.63	1.42	1.35
28	N	304	CLA	C4B-NB	7.62	1.42	1.35
28	L	317	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	316	CLA	C4B-NB	7.61	1.42	1.35
26	L	303	DD6	C30-C31	-7.61	1.26	1.42
28	H	311	CLA	C4B-NB	7.61	1.42	1.35
28	M	311	CLA	C4B-NB	7.60	1.42	1.35
28	I	321	CLA	C4B-NB	7.60	1.42	1.35
28	J	306	CLA	C4B-NB	7.60	1.42	1.35
28	L	309	CLA	C4B-NB	7.60	1.42	1.35
28	b	712	CLA	C4B-NB	7.60	1.42	1.35
28	l	309	CLA	C4B-NB	7.59	1.42	1.35
28	I	307	CLA	C4B-NB	7.59	1.42	1.35
26	L	304	DD6	C30-C31	-7.59	1.26	1.42
28	A	316	CLA	C4B-NB	7.59	1.42	1.35
28	a	738	CLA	C4B-NB	7.59	1.42	1.35
28	B	317	CLA	C4B-NB	7.59	1.42	1.35
28	I	309	CLA	C4B-NB	7.59	1.42	1.35
28	l	308	CLA	C4B-NB	7.59	1.42	1.35
26	H	303	DD6	C30-C31	-7.58	1.26	1.42
28	b	701	CLA	C4B-NB	7.58	1.42	1.35
26	J	302	DD6	C30-C31	-7.58	1.26	1.42
28	a	710	CLA	C4B-NB	7.58	1.42	1.35
28	a	714	CLA	C4B-NB	7.58	1.42	1.35
28	F	311	CLA	C4B-NB	7.57	1.42	1.35
28	K	306	CLA	C4B-NB	7.57	1.42	1.35
28	M	318	CLA	C4B-NB	7.57	1.42	1.35
28	H	304	CLA	C4B-NB	7.57	1.42	1.35
28	H	312	CLA	C4B-NB	7.57	1.42	1.35
26	K	301	DD6	C30-C31	-7.57	1.26	1.42
28	I	308	CLA	C4B-NB	7.57	1.42	1.35
28	a	716	CLA	C4B-NB	7.56	1.42	1.35
28	B	308	CLA	C4B-NB	7.56	1.42	1.35
28	J	316	CLA	C4B-NB	7.56	1.42	1.35
26	A	303	DD6	C30-C31	-7.56	1.26	1.42
28	G	511	CLA	C4B-NB	7.56	1.41	1.35
28	B	301	CLA	C4B-NB	7.56	1.41	1.35
28	I	313	CLA	C4B-NB	7.55	1.41	1.35
28	L	311	CLA	C4B-NB	7.55	1.41	1.35
28	A	317	CLA	C4B-NB	7.55	1.41	1.35
28	A	319	CLA	C4B-NB	7.55	1.41	1.35
28	a	718	CLA	C4B-NB	7.55	1.41	1.35
28	G	519	CLA	C4B-NB	7.55	1.41	1.35
28	b	722	CLA	C4B-NB	7.55	1.41	1.35
28	b	711	CLA	C4B-NB	7.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	719	CLA	C4B-NB	7.54	1.41	1.35
28	L	316	CLA	C4B-NB	7.54	1.41	1.35
28	L	308	CLA	C4B-NB	7.54	1.41	1.35
28	l	311	CLA	C4B-NB	7.54	1.41	1.35
28	l	304	CLA	C4B-NB	7.54	1.41	1.35
28	b	726	CLA	C4B-NB	7.54	1.41	1.35
28	b	707	CLA	C4B-NB	7.54	1.41	1.35
28	b	727	CLA	C4B-NB	7.53	1.41	1.35
28	a	704	CLA	C4B-NB	7.53	1.41	1.35
28	F	310	CLA	C4B-NB	7.53	1.41	1.35
28	b	710	CLA	C4B-NB	7.53	1.41	1.35
28	J	314	CLA	C4B-NB	7.53	1.41	1.35
28	B	315	CLA	C4B-NB	7.53	1.41	1.35
28	F	307	CLA	C4B-NB	7.53	1.41	1.35
28	M	310	CLA	C4B-NB	7.53	1.41	1.35
28	m	202	CLA	C4B-NB	7.53	1.41	1.35
28	a	722	CLA	C4B-NB	7.53	1.41	1.35
28	b	716	CLA	C4B-NB	7.53	1.41	1.35
28	D	311	CLA	C4B-NB	7.53	1.41	1.35
28	D	312	CLA	C4B-NB	7.52	1.41	1.35
28	A	311	CLA	C4B-NB	7.52	1.41	1.35
28	D	316	CLA	C4B-NB	7.52	1.41	1.35
28	K	315	CLA	C4B-NB	7.52	1.41	1.35
28	a	709	CLA	C4B-NB	7.51	1.41	1.35
28	I	306	CLA	C4B-NB	7.51	1.41	1.35
28	M	308	CLA	C4B-NB	7.51	1.41	1.35
28	I	315	CLA	C4B-NB	7.51	1.41	1.35
28	l	305	CLA	C4B-NB	7.51	1.41	1.35
28	l	313	CLA	C4B-NB	7.51	1.41	1.35
28	J	315	CLA	C4B-NB	7.51	1.41	1.35
28	J	312	CLA	C4B-NB	7.51	1.41	1.35
28	L	310	CLA	C4B-NB	7.51	1.41	1.35
36	a	732	PQN	C3-C2	7.51	1.48	1.35
28	K	311	CLA	C4B-NB	7.51	1.41	1.35
28	A	308	CLA	C4B-NB	7.50	1.41	1.35
26	L	302	DD6	C30-C31	-7.50	1.26	1.42
28	b	714	CLA	C4B-NB	7.50	1.41	1.35
28	L	312	CLA	C4B-NB	7.50	1.41	1.35
28	H	305	CLA	C4B-NB	7.50	1.41	1.35
28	l	312	CLA	C4B-NB	7.50	1.41	1.35
28	J	308	CLA	C4B-NB	7.49	1.41	1.35
28	a	708	CLA	C4B-NB	7.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	717	CLA	C4B-NB	7.49	1.41	1.35
28	a	713	CLA	C4B-NB	7.48	1.41	1.35
28	M	315	CLA	C4B-NB	7.48	1.41	1.35
28	B	316	CLA	C4B-NB	7.48	1.41	1.35
28	j	106	CLA	C4B-NB	7.48	1.41	1.35
28	N	310	CLA	C4B-NB	7.48	1.41	1.35
28	D	314	CLA	C4B-NB	7.48	1.41	1.35
28	a	712	CLA	C4B-NB	7.47	1.41	1.35
28	I	316	CLA	C4B-NB	7.46	1.41	1.35
28	f	301	CLA	C4B-NB	7.46	1.41	1.35
28	H	307	CLA	C4B-NB	7.46	1.41	1.35
28	b	703	CLA	C4B-NB	7.46	1.41	1.35
28	B	311	CLA	C4B-NB	7.46	1.41	1.35
28	b	715	CLA	C4B-NB	7.46	1.41	1.35
28	I	319	CLA	C4B-NB	7.45	1.41	1.35
28	F	315	CLA	C4B-NB	7.45	1.41	1.35
28	K	310	CLA	C4B-NB	7.45	1.41	1.35
28	K	308	CLA	C4B-NB	7.45	1.41	1.35
28	A	315	CLA	C4B-NB	7.45	1.41	1.35
28	A	312	CLA	C4B-NB	7.44	1.41	1.35
28	b	713	CLA	C4B-NB	7.44	1.41	1.35
28	H	309	CLA	C4B-NB	7.44	1.41	1.35
28	B	310	CLA	C4B-NB	7.44	1.41	1.35
28	a	706	CLA	C4B-NB	7.43	1.41	1.35
28	J	307	CLA	C4B-NB	7.43	1.41	1.35
28	a	701	CLA	C4B-NB	7.43	1.41	1.35
28	h	202	CLA	C4B-NB	7.43	1.41	1.35
28	f	302	CLA	C4B-NB	7.43	1.41	1.35
28	b	717	CLA	C4B-NB	7.43	1.41	1.35
28	a	705	CLA	C4B-NB	7.42	1.41	1.35
28	G	517	CLA	C4B-NB	7.42	1.41	1.35
28	K	313	CLA	C4B-NB	7.42	1.41	1.35
28	b	724	CLA	C4B-NB	7.42	1.41	1.35
28	B	309	CLA	C4B-NB	7.42	1.41	1.35
28	D	309	CLA	C4B-NB	7.42	1.41	1.35
28	G	512	CLA	C4B-NB	7.41	1.41	1.35
28	G	520	CLA	C4B-NB	7.41	1.41	1.35
28	I	310	CLA	C4B-NB	7.40	1.41	1.35
28	M	317	CLA	C4B-NB	7.39	1.41	1.35
28	a	725	CLA	C4B-NB	7.39	1.41	1.35
28	A	309	CLA	C4B-NB	7.38	1.41	1.35
28	M	309	CLA	C4B-NB	7.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	509	CLA	C4B-NB	7.38	1.41	1.35
28	J	311	CLA	C4B-NB	7.37	1.41	1.35
28	a	711	CLA	C4B-NB	7.37	1.41	1.35
28	b	720	CLA	C4B-NB	7.37	1.41	1.35
28	B	312	CLA	C4B-NB	7.37	1.41	1.35
28	a	729	CLA	C4B-NB	7.36	1.41	1.35
28	A	310	CLA	C4B-NB	7.36	1.41	1.35
28	f	303	CLA	C4B-NB	7.36	1.41	1.35
28	J	301	CLA	C4B-NB	7.36	1.41	1.35
28	a	723	CLA	C4B-NB	7.35	1.41	1.35
28	L	314	CLA	C4B-NB	7.35	1.41	1.35
28	I	312	CLA	C4B-NB	7.35	1.41	1.35
28	a	715	CLA	C4B-NB	7.35	1.41	1.35
36	b	729	PQN	C3-C2	7.34	1.48	1.35
28	F	308	CLA	C4B-NB	7.33	1.41	1.35
28	L	313	CLA	C4B-NB	7.33	1.41	1.35
28	L	318	CLA	C4B-NB	7.33	1.41	1.35
28	K	312	CLA	C4B-NB	7.33	1.41	1.35
28	M	312	CLA	C4B-NB	7.33	1.41	1.35
28	a	720	CLA	C4B-NB	7.33	1.41	1.35
28	b	725	CLA	C4B-NB	7.32	1.41	1.35
28	J	309	CLA	C4B-NB	7.32	1.41	1.35
28	F	313	CLA	C4B-NB	7.32	1.41	1.35
28	G	510	CLA	C4B-NB	7.32	1.41	1.35
28	B	313	CLA	C4B-NB	7.32	1.41	1.35
28	G	514	CLA	C4B-NB	7.31	1.41	1.35
28	b	708	CLA	C4B-NB	7.31	1.41	1.35
28	a	726	CLA	C4B-NB	7.31	1.41	1.35
28	N	305	CLA	C4B-NB	7.30	1.41	1.35
28	a	730	CLA	C4B-NB	7.29	1.41	1.35
28	a	728	CLA	C4B-NB	7.29	1.41	1.35
28	K	309	CLA	C4B-NB	7.29	1.41	1.35
28	a	721	CLA	C4B-NB	7.26	1.41	1.35
28	b	705	CLA	C4B-NB	7.25	1.41	1.35
28	A	313	CLA	C4B-NB	7.20	1.41	1.35
28	D	313	CLA	C4B-NB	7.20	1.41	1.35
28	N	309	CLA	C4B-NB	7.19	1.41	1.35
28	G	513	CLA	C4B-NB	7.17	1.41	1.35
28	K	307	CLA	C4B-NB	6.99	1.41	1.35
29	H	306	KC1	C4D-CHA	-6.92	1.36	1.45
29	L	307	KC1	C4D-CHA	-6.77	1.36	1.45
29	A	314	KC1	C4D-CHA	-6.74	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	314	KC1	C4D-CHA	-6.73	1.36	1.45
29	M	314	KC1	C4D-CHA	-6.70	1.36	1.45
29	I	314	KC1	C4D-CHA	-6.65	1.36	1.45
29	K	314	KC1	C4D-CHA	-6.64	1.36	1.45
29	L	315	KC1	C4D-CHA	-6.63	1.36	1.45
29	D	315	KC1	C4D-CHA	-6.58	1.36	1.45
29	J	313	KC1	C4D-CHA	-6.58	1.36	1.45
29	N	311	KC1	C4D-CHA	-6.57	1.36	1.45
29	M	307	KC1	C4D-CHA	-6.53	1.36	1.45
29	N	306	KC1	C4D-CHA	-6.53	1.36	1.45
29	F	309	KC1	C4D-CHA	-6.51	1.36	1.45
29	D	310	KC1	C4D-CHA	-6.46	1.37	1.45
28	F	312	CLA	C4B-NB	6.44	1.41	1.35
29	A	306	KC1	C4D-CHA	-6.43	1.37	1.45
29	H	310	KC1	C4D-CHA	-6.43	1.37	1.45
29	G	515	KC1	C4D-CHA	-6.40	1.37	1.45
29	F	314	KC1	C4D-CHA	-6.39	1.37	1.45
28	b	704	CLA	C4B-NB	6.15	1.40	1.35
28	a	703	CLA	C4B-NB	6.15	1.40	1.35
28	a	702	CLA	C4B-NB	6.07	1.40	1.35
32	N	302	PID	C13-C14	-5.97	1.34	1.45
32	H	302	PID	C13-C14	-5.77	1.34	1.45
29	N	308	KC1	C4D-CHA	-5.76	1.37	1.45
32	G	506	PID	C13-C14	-5.73	1.34	1.45
32	D	302	PID	C13-C14	-5.57	1.34	1.45
32	D	305	PID	C13-C14	-5.56	1.34	1.45
32	D	301	PID	C13-C14	-5.49	1.34	1.45
32	j	105	PID	C13-C14	-5.48	1.35	1.45
32	G	507	PID	C13-C14	-5.48	1.35	1.45
32	D	306	PID	C13-C14	-5.48	1.35	1.45
32	N	301	PID	C13-C14	-5.44	1.35	1.45
32	F	306	PID	C13-C14	-5.35	1.35	1.45
32	H	301	PID	C13-C14	-5.32	1.35	1.45
32	F	304	PID	C13-C14	-5.25	1.35	1.45
32	F	302	PID	C13-C14	-5.25	1.35	1.45
32	F	305	PID	C13-C14	-5.23	1.35	1.45
32	D	307	PID	C13-C14	-5.19	1.35	1.45
32	D	304	PID	C13-C14	-5.12	1.35	1.45
32	M	301	PID	C13-C14	-5.07	1.35	1.45
27	B	305	UIX	O2-C27	4.88	1.46	1.35
36	b	729	PQN	C10-C5	4.83	1.48	1.40
27	J	305	UIX	O2-C27	4.81	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	h	201	UIX	O2-C27	4.81	1.46	1.35
36	a	732	PQN	C10-C5	4.77	1.48	1.40
27	G	503	UIX	O2-C27	4.77	1.46	1.35
29	M	307	KC1	MG-NB	-4.75	1.96	2.05
27	K	302	UIX	O2-C27	4.72	1.45	1.35
29	H	310	KC1	MG-NB	-4.69	1.96	2.05
27	A	304	UIX	O2-C27	4.69	1.45	1.35
29	F	314	KC1	MG-NB	-4.68	1.96	2.05
29	N	311	KC1	MG-NB	-4.65	1.96	2.05
29	F	309	KC1	MG-NB	-4.64	1.96	2.05
29	D	310	KC1	MG-NB	-4.63	1.96	2.05
29	M	314	KC1	MG-NB	-4.63	1.96	2.05
29	N	306	KC1	MG-NB	-4.61	1.96	2.05
29	H	306	KC1	MG-NB	-4.61	1.96	2.05
29	N	308	KC1	MG-NB	-4.60	1.96	2.05
29	I	314	KC1	MG-NB	-4.59	1.96	2.05
29	A	314	KC1	MG-NB	-4.58	1.96	2.05
29	J	313	KC1	MG-NB	-4.57	1.96	2.05
29	L	315	KC1	MG-NB	-4.57	1.96	2.05
29	K	314	KC1	MG-NB	-4.56	1.96	2.05
29	L	307	KC1	MG-NB	-4.54	1.96	2.05
29	B	314	KC1	MG-NB	-4.53	1.96	2.05
29	A	306	KC1	MG-NB	-4.53	1.96	2.05
29	G	515	KC1	MG-NB	-4.50	1.96	2.05
29	D	315	KC1	MG-NB	-4.46	1.97	2.05
30	I	317	DGD	O1G-C1A	4.25	1.45	1.33
27	I	304	UIX	O2-C27	4.24	1.44	1.35
30	G	501	DGD	O1G-C1A	4.23	1.45	1.33
30	j	103	DGD	O1G-C1A	4.23	1.45	1.33
30	l	301	DGD	O1G-C1A	4.23	1.45	1.33
26	J	303	DD6	C19-C20	4.20	1.58	1.52
30	y	201	DGD	O1G-C1A	4.20	1.45	1.33
30	G	521	DGD	O2G-C1B	4.17	1.46	1.34
30	G	501	DGD	O2G-C1B	4.15	1.46	1.34
30	l	301	DGD	O2G-C1B	4.12	1.45	1.34
30	j	103	DGD	O2G-C1B	4.11	1.45	1.34
28	a	702	CLA	C4D-ND	-4.09	1.32	1.37
28	b	718	CLA	C1D-ND	4.07	1.42	1.37
28	M	318	CLA	C1D-ND	4.05	1.42	1.37
28	J	316	CLA	C1D-ND	4.05	1.42	1.37
30	y	201	DGD	O2G-C1B	4.04	1.45	1.34
28	H	304	CLA	C1D-ND	4.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	301	DGD	O2G-C1B	4.03	1.45	1.34
28	H	311	CLA	C1D-ND	4.03	1.42	1.37
28	L	317	CLA	C1D-ND	4.03	1.42	1.37
30	I	317	DGD	O2G-C1B	4.01	1.45	1.34
28	K	306	CLA	C1D-ND	4.01	1.42	1.37
28	A	307	CLA	C1D-ND	4.00	1.42	1.37
28	N	307	CLA	C1D-ND	4.00	1.42	1.37
28	N	310	CLA	C1D-ND	4.00	1.42	1.37
28	a	703	CLA	C4D-ND	-3.99	1.32	1.37
28	G	518	CLA	C1D-ND	3.99	1.42	1.37
30	G	521	DGD	O1G-C1A	3.99	1.45	1.33
28	b	704	CLA	C4D-ND	-3.98	1.32	1.37
28	a	738	CLA	C1D-ND	3.98	1.42	1.37
28	F	313	CLA	C1D-ND	3.97	1.42	1.37
28	H	312	CLA	C1D-ND	3.97	1.42	1.37
28	H	308	CLA	C1D-ND	3.97	1.42	1.37
28	L	313	CLA	C1D-ND	3.97	1.42	1.37
28	G	509	CLA	C1D-ND	3.96	1.42	1.37
28	J	311	CLA	C1D-ND	3.96	1.42	1.37
28	M	308	CLA	C1D-ND	3.96	1.42	1.37
28	G	512	CLA	C1D-ND	3.96	1.42	1.37
28	B	307	CLA	C1D-ND	3.96	1.42	1.37
28	j	104	CLA	C1D-ND	3.95	1.42	1.37
28	F	315	CLA	C1D-ND	3.95	1.42	1.37
28	b	705	CLA	C1D-ND	3.94	1.42	1.37
28	K	312	CLA	C1D-ND	3.94	1.42	1.37
28	J	308	CLA	C1D-ND	3.94	1.42	1.37
28	J	314	CLA	C1D-ND	3.94	1.42	1.37
28	b	726	CLA	C1D-ND	3.94	1.42	1.37
28	l	309	CLA	C1D-ND	3.93	1.42	1.37
28	b	708	CLA	C1D-ND	3.93	1.42	1.37
28	h	202	CLA	C1D-ND	3.93	1.42	1.37
28	b	717	CLA	C1D-ND	3.93	1.42	1.37
28	G	516	CLA	C1D-ND	3.93	1.42	1.37
28	K	307	CLA	C1D-ND	3.92	1.42	1.37
28	a	726	CLA	C1D-ND	3.92	1.42	1.37
28	K	316	CLA	C1D-ND	3.92	1.42	1.37
28	A	315	CLA	C1D-ND	3.92	1.42	1.37
32	j	105	PID	C20-C21	3.92	1.41	1.35
28	a	714	CLA	C1D-ND	3.92	1.42	1.37
28	B	316	CLA	C1D-ND	3.91	1.42	1.37
28	L	318	CLA	C1D-ND	3.91	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	717	CLA	C1D-ND	3.91	1.42	1.37
28	D	314	CLA	C1D-ND	3.91	1.42	1.37
28	a	728	CLA	C1D-ND	3.91	1.42	1.37
28	N	305	CLA	C1D-ND	3.91	1.42	1.37
28	l	303	CLA	C1D-ND	3.91	1.42	1.37
28	I	311	CLA	C1D-ND	3.91	1.42	1.37
28	l	305	CLA	C1D-ND	3.91	1.42	1.37
28	A	312	CLA	C1D-ND	3.91	1.42	1.37
28	b	707	CLA	C1D-ND	3.90	1.42	1.37
28	b	711	CLA	C1D-ND	3.90	1.42	1.37
28	a	707	CLA	C1D-ND	3.90	1.42	1.37
28	A	311	CLA	C1D-ND	3.90	1.42	1.37
28	M	315	CLA	C1D-ND	3.90	1.42	1.37
28	K	311	CLA	C1D-ND	3.90	1.42	1.37
28	b	719	CLA	C1D-ND	3.90	1.42	1.37
28	D	316	CLA	C1D-ND	3.90	1.42	1.37
28	M	309	CLA	C1D-ND	3.90	1.42	1.37
28	B	301	CLA	C1D-ND	3.90	1.42	1.37
28	G	511	CLA	C1D-ND	3.89	1.42	1.37
28	A	316	CLA	C1D-ND	3.89	1.42	1.37
28	b	714	CLA	C1D-ND	3.88	1.42	1.37
28	J	310	CLA	C1D-ND	3.88	1.42	1.37
28	N	304	CLA	C1D-ND	3.88	1.42	1.37
28	b	715	CLA	C1D-ND	3.88	1.42	1.37
28	H	305	CLA	C1D-ND	3.88	1.42	1.37
28	a	708	CLA	C1D-ND	3.88	1.42	1.37
28	K	310	CLA	C1D-ND	3.88	1.42	1.37
28	m	202	CLA	C1D-ND	3.88	1.42	1.37
28	a	705	CLA	C1D-ND	3.88	1.42	1.37
28	D	313	CLA	C1D-ND	3.87	1.42	1.37
28	I	315	CLA	C1D-ND	3.87	1.42	1.37
28	F	311	CLA	C1D-ND	3.87	1.42	1.37
28	D	311	CLA	C1D-ND	3.87	1.42	1.37
28	a	722	CLA	C1D-ND	3.87	1.42	1.37
28	F	310	CLA	C1D-ND	3.87	1.42	1.37
28	I	306	CLA	C1D-ND	3.87	1.42	1.37
28	G	517	CLA	C1D-ND	3.87	1.42	1.37
28	a	723	CLA	C1D-ND	3.87	1.42	1.37
28	A	309	CLA	C1D-ND	3.86	1.42	1.37
28	I	308	CLA	C1D-ND	3.86	1.42	1.37
28	l	311	CLA	C1D-ND	3.86	1.42	1.37
28	B	312	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	301	CLA	C1D-ND	3.86	1.42	1.37
28	I	307	CLA	C1D-ND	3.86	1.42	1.37
28	F	307	CLA	C1D-ND	3.86	1.42	1.37
28	G	513	CLA	C1D-ND	3.86	1.42	1.37
28	a	721	CLA	C1D-ND	3.86	1.42	1.37
28	f	302	CLA	C1D-ND	3.86	1.42	1.37
28	f	301	CLA	C1D-ND	3.86	1.42	1.37
28	D	309	CLA	C1D-ND	3.86	1.42	1.37
28	M	312	CLA	C1D-ND	3.85	1.42	1.37
28	a	718	CLA	C1D-ND	3.85	1.42	1.37
28	L	316	CLA	C1D-ND	3.85	1.42	1.37
28	l	308	CLA	C1D-ND	3.84	1.42	1.37
28	B	308	CLA	C1D-ND	3.84	1.42	1.37
28	A	313	CLA	C1D-ND	3.84	1.42	1.37
28	K	315	CLA	C1D-ND	3.84	1.42	1.37
28	a	715	CLA	C1D-ND	3.84	1.42	1.37
26	G	505	DD6	C19-C20	3.84	1.57	1.52
28	L	308	CLA	C1D-ND	3.84	1.42	1.37
28	M	317	CLA	C1D-ND	3.84	1.42	1.37
28	a	720	CLA	C1D-ND	3.84	1.42	1.37
28	b	724	CLA	C1D-ND	3.84	1.42	1.37
28	B	317	CLA	C1D-ND	3.84	1.42	1.37
28	a	731	CLA	C1D-ND	3.84	1.42	1.37
28	a	704	CLA	C1D-ND	3.84	1.42	1.37
28	J	315	CLA	C1D-ND	3.84	1.42	1.37
28	j	106	CLA	C1D-ND	3.83	1.42	1.37
28	a	709	CLA	C1D-ND	3.83	1.42	1.37
28	a	706	CLA	C1D-ND	3.83	1.42	1.37
28	b	716	CLA	C1D-ND	3.83	1.42	1.37
28	D	312	CLA	C1D-ND	3.83	1.42	1.37
28	M	310	CLA	C1D-ND	3.83	1.42	1.37
28	L	312	CLA	C1D-ND	3.83	1.42	1.37
28	a	729	CLA	C1D-ND	3.83	1.42	1.37
28	H	307	CLA	C1D-ND	3.82	1.42	1.37
28	M	311	CLA	C1D-ND	3.82	1.42	1.37
32	F	305	PID	C20-C21	3.82	1.40	1.35
28	f	303	CLA	C1D-ND	3.82	1.42	1.37
27	h	201	UIX	C25-C28	-3.82	1.25	1.32
28	I	312	CLA	C1D-ND	3.82	1.42	1.37
28	A	319	CLA	C1D-ND	3.82	1.42	1.37
28	l	313	CLA	C1D-ND	3.82	1.42	1.37
28	I	310	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	314	CLA	C1D-ND	3.82	1.42	1.37
28	G	510	CLA	C1D-ND	3.82	1.42	1.37
28	B	310	CLA	C1D-ND	3.81	1.42	1.37
28	B	313	CLA	C1D-ND	3.81	1.42	1.37
28	D	308	CLA	C1D-ND	3.81	1.42	1.37
28	L	311	CLA	C1D-ND	3.81	1.42	1.37
28	M	313	CLA	C1D-ND	3.81	1.42	1.37
28	a	716	CLA	C1D-ND	3.81	1.42	1.37
28	A	317	CLA	C1D-ND	3.81	1.42	1.37
28	a	725	CLA	C1D-ND	3.81	1.42	1.37
28	J	306	CLA	C1D-ND	3.81	1.42	1.37
28	b	706	CLA	C1D-ND	3.81	1.42	1.37
28	B	309	CLA	C1D-ND	3.81	1.42	1.37
28	L	310	CLA	C1D-ND	3.80	1.42	1.37
28	b	701	CLA	C1D-ND	3.80	1.42	1.37
28	L	309	CLA	C1D-ND	3.80	1.42	1.37
28	a	711	CLA	C1D-ND	3.79	1.42	1.37
28	N	309	CLA	C1D-ND	3.79	1.42	1.37
28	J	309	CLA	C1D-ND	3.79	1.42	1.37
28	b	720	CLA	C1D-ND	3.79	1.42	1.37
28	b	722	CLA	C1D-ND	3.78	1.42	1.37
28	K	308	CLA	C1D-ND	3.78	1.42	1.37
28	H	309	CLA	C1D-ND	3.78	1.42	1.37
28	I	316	CLA	C1D-ND	3.78	1.42	1.37
28	b	727	CLA	C1D-ND	3.78	1.42	1.37
28	b	725	CLA	C1D-ND	3.78	1.42	1.37
27	I	304	UIX	C25-C28	-3.78	1.25	1.32
28	b	710	CLA	C1D-ND	3.77	1.42	1.37
28	F	308	CLA	C1D-ND	3.77	1.42	1.37
28	a	701	CLA	C1D-ND	3.77	1.42	1.37
28	b	728	CLA	C1D-ND	3.76	1.42	1.37
28	A	310	CLA	C1D-ND	3.75	1.42	1.37
28	I	309	CLA	C1D-ND	3.75	1.42	1.37
28	J	312	CLA	C1D-ND	3.74	1.42	1.37
28	G	519	CLA	C1D-ND	3.74	1.42	1.37
28	A	308	CLA	C1D-ND	3.74	1.42	1.37
28	M	316	CLA	C1D-ND	3.73	1.42	1.37
28	a	727	CLA	C1D-ND	3.73	1.42	1.37
28	a	730	CLA	C1D-ND	3.73	1.42	1.37
28	a	735	CLA	C1D-ND	3.73	1.42	1.37
28	I	319	CLA	C1D-ND	3.73	1.42	1.37
28	b	713	CLA	C1D-ND	3.73	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	307	CLA	C1D-ND	3.73	1.42	1.37
28	G	520	CLA	C1D-ND	3.72	1.42	1.37
28	b	723	CLA	C1D-ND	3.72	1.42	1.37
27	K	302	UIX	C25-C28	-3.72	1.25	1.32
28	I	313	CLA	C1D-ND	3.72	1.42	1.37
28	b	712	CLA	C1D-ND	3.71	1.42	1.37
28	K	309	CLA	C1D-ND	3.71	1.42	1.37
28	l	312	CLA	C1D-ND	3.71	1.42	1.37
28	G	514	CLA	C1D-ND	3.71	1.42	1.37
28	l	304	CLA	C1D-ND	3.70	1.42	1.37
28	a	719	CLA	C1D-ND	3.70	1.42	1.37
28	b	703	CLA	C1D-ND	3.70	1.42	1.37
28	a	710	CLA	C1D-ND	3.69	1.42	1.37
28	b	709	CLA	C1D-ND	3.69	1.42	1.37
28	K	313	CLA	C1D-ND	3.69	1.42	1.37
28	B	315	CLA	C1D-ND	3.69	1.42	1.37
28	A	320	CLA	C1D-ND	3.68	1.42	1.37
28	I	321	CLA	C1D-ND	3.68	1.42	1.37
27	A	304	UIX	C25-C28	-3.67	1.25	1.32
28	a	712	CLA	C1D-ND	3.67	1.42	1.37
32	D	307	PID	C20-C21	3.65	1.40	1.35
28	a	713	CLA	C1D-ND	3.63	1.42	1.37
26	G	504	DD6	C19-C20	3.62	1.57	1.52
28	B	311	CLA	C1D-ND	3.61	1.42	1.37
28	a	724	CLA	C1D-ND	3.61	1.42	1.37
28	b	721	CLA	C1D-ND	3.60	1.42	1.37
27	B	305	UIX	C25-C28	-3.57	1.26	1.32
28	F	312	CLA	C4D-ND	-3.53	1.32	1.37
28	b	712	CLA	CAB-C3B	-3.50	1.44	1.51
32	M	301	PID	C20-C21	3.43	1.40	1.35
32	D	304	PID	C20-C21	3.42	1.40	1.35
32	N	301	PID	C20-C21	3.41	1.40	1.35
28	a	726	CLA	CHC-C1C	3.37	1.43	1.35
28	a	735	CLA	CHC-C1C	3.35	1.43	1.35
27	G	503	UIX	C25-C28	-3.35	1.26	1.32
32	F	304	PID	C20-C21	3.34	1.40	1.35
28	M	313	CLA	CHC-C1C	3.34	1.43	1.35
27	J	305	UIX	C25-C28	-3.33	1.26	1.32
32	F	302	PID	C20-C21	3.31	1.40	1.35
28	I	308	CLA	CHC-C1C	3.31	1.43	1.35
28	I	309	CLA	CHC-C1C	3.31	1.43	1.35
28	I	316	CLA	CHC-C1C	3.30	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	705	CLA	CHC-C1C	3.30	1.43	1.35
28	K	309	CLA	CHC-C1C	3.29	1.43	1.35
28	A	319	CLA	CHC-C1C	3.27	1.43	1.35
28	A	311	CLA	CHC-C1C	3.26	1.43	1.35
28	b	725	CLA	CHC-C1C	3.26	1.43	1.35
28	b	715	CLA	CHC-C1C	3.26	1.43	1.35
32	D	301	PID	C20-C21	3.26	1.40	1.35
28	L	310	CLA	CHC-C1C	3.26	1.43	1.35
28	a	711	CLA	CHC-C1C	3.26	1.43	1.35
28	D	316	CLA	CHC-C1C	3.26	1.43	1.35
28	a	709	CLA	CHC-C1C	3.25	1.43	1.35
28	F	310	CLA	CHC-C1C	3.25	1.43	1.35
28	a	701	CLA	CHC-C1C	3.25	1.43	1.35
28	L	313	CLA	CHC-C1C	3.25	1.43	1.35
28	K	308	CLA	CHC-C1C	3.25	1.43	1.35
32	H	302	PID	C20-C21	3.25	1.40	1.35
28	b	724	CLA	CHC-C1C	3.25	1.43	1.35
28	L	316	CLA	CHC-C1C	3.25	1.43	1.35
28	A	313	CLA	CHC-C1C	3.25	1.43	1.35
28	D	314	CLA	CHC-C1C	3.24	1.43	1.35
28	J	312	CLA	CHC-C1C	3.24	1.43	1.35
28	b	714	CLA	CHC-C1C	3.24	1.43	1.35
28	j	104	CLA	CHC-C1C	3.24	1.43	1.35
28	A	309	CLA	CHC-C1C	3.24	1.43	1.35
28	J	301	CLA	CHC-C1C	3.24	1.43	1.35
32	H	301	PID	C20-C21	3.23	1.40	1.35
28	J	311	CLA	CHC-C1C	3.23	1.43	1.35
28	N	309	CLA	CHC-C1C	3.23	1.43	1.35
28	b	706	CLA	CHC-C1C	3.23	1.43	1.35
28	l	312	CLA	CHC-C1C	3.23	1.43	1.35
32	F	306	PID	C20-C21	3.23	1.40	1.35
28	K	310	CLA	CHC-C1C	3.23	1.43	1.35
28	b	703	CLA	CHC-C1C	3.23	1.43	1.35
28	l	309	CLA	CHC-C1C	3.23	1.43	1.35
28	L	314	CLA	CHC-C1C	3.23	1.43	1.35
28	I	313	CLA	CHC-C1C	3.23	1.43	1.35
28	f	303	CLA	CHC-C1C	3.23	1.43	1.35
28	b	707	CLA	CHC-C1C	3.23	1.43	1.35
28	H	305	CLA	CHC-C1C	3.22	1.43	1.35
28	M	310	CLA	CHC-C1C	3.22	1.43	1.35
28	I	321	CLA	CHC-C1C	3.22	1.43	1.35
28	b	727	CLA	CHC-C1C	3.22	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	K	313	CLA	CHC-C1C	3.22	1.43	1.35
28	l	308	CLA	CHC-C1C	3.22	1.43	1.35
28	D	311	CLA	CHC-C1C	3.22	1.43	1.35
28	B	317	CLA	CHC-C1C	3.22	1.43	1.35
28	a	717	CLA	CHC-C1C	3.22	1.43	1.35
28	M	318	CLA	CHC-C1C	3.22	1.43	1.35
28	a	704	CLA	CHC-C1C	3.21	1.43	1.35
28	L	308	CLA	CHC-C1C	3.21	1.43	1.35
28	M	309	CLA	CHC-C1C	3.21	1.43	1.35
28	M	311	CLA	CHC-C1C	3.21	1.43	1.35
28	B	312	CLA	CHC-C1C	3.21	1.43	1.35
28	J	314	CLA	CHC-C1C	3.21	1.43	1.35
28	b	716	CLA	CHC-C1C	3.21	1.43	1.35
28	G	510	CLA	CHC-C1C	3.21	1.43	1.35
28	A	312	CLA	CHC-C1C	3.21	1.43	1.35
28	I	319	CLA	CHC-C1C	3.20	1.43	1.35
28	l	313	CLA	CHC-C1C	3.20	1.43	1.35
28	a	714	CLA	CHC-C1C	3.20	1.43	1.35
28	L	311	CLA	CHC-C1C	3.20	1.43	1.35
28	G	513	CLA	CHC-C1C	3.20	1.43	1.35
28	a	707	CLA	CHC-C1C	3.20	1.43	1.35
32	D	306	PID	C20-C21	3.20	1.40	1.35
28	L	309	CLA	CHC-C1C	3.20	1.43	1.35
28	b	726	CLA	CHC-C1C	3.20	1.43	1.35
28	G	520	CLA	CHC-C1C	3.20	1.43	1.35
28	j	106	CLA	CHC-C1C	3.20	1.43	1.35
28	H	308	CLA	CHC-C1C	3.20	1.43	1.35
28	a	708	CLA	CHC-C1C	3.20	1.43	1.35
28	J	315	CLA	CHC-C1C	3.20	1.43	1.35
28	A	315	CLA	CHC-C1C	3.20	1.43	1.35
28	F	315	CLA	CHC-C1C	3.20	1.43	1.35
28	a	725	CLA	CHC-C1C	3.19	1.43	1.35
28	a	729	CLA	CHC-C1C	3.19	1.43	1.35
28	f	301	CLA	CHC-C1C	3.19	1.43	1.35
28	H	307	CLA	CHC-C1C	3.19	1.43	1.35
28	I	312	CLA	CHC-C1C	3.19	1.43	1.35
28	a	722	CLA	CHC-C1C	3.19	1.43	1.35
28	a	727	CLA	CHC-C1C	3.19	1.43	1.35
28	L	312	CLA	CHC-C1C	3.19	1.43	1.35
28	B	309	CLA	CHC-C1C	3.19	1.43	1.35
28	G	519	CLA	CHC-C1C	3.19	1.43	1.35
28	K	315	CLA	CHC-C1C	3.19	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	719	CLA	CHC-C1C	3.19	1.43	1.35
28	a	706	CLA	CHC-C1C	3.19	1.43	1.35
28	D	309	CLA	CHC-C1C	3.19	1.43	1.35
28	A	317	CLA	CHC-C1C	3.19	1.43	1.35
28	b	705	CLA	CHC-C1C	3.19	1.43	1.35
28	l	305	CLA	CHC-C1C	3.19	1.43	1.35
28	M	316	CLA	CHC-C1C	3.19	1.43	1.35
28	a	710	CLA	CHC-C1C	3.19	1.43	1.35
28	f	302	CLA	CHC-C1C	3.18	1.43	1.35
28	l	311	CLA	CHC-C1C	3.18	1.43	1.35
28	D	312	CLA	CHC-C1C	3.18	1.43	1.35
28	a	716	CLA	CHC-C1C	3.18	1.43	1.35
28	K	312	CLA	CHC-C1C	3.18	1.43	1.35
28	a	723	CLA	CHC-C1C	3.18	1.43	1.35
28	H	312	CLA	CHC-C1C	3.18	1.43	1.35
28	M	315	CLA	CHC-C1C	3.18	1.43	1.35
28	B	308	CLA	CHC-C1C	3.18	1.43	1.35
28	b	709	CLA	CHC-C1C	3.18	1.43	1.35
28	l	304	CLA	CHC-C1C	3.18	1.43	1.35
28	A	308	CLA	CHC-C1C	3.17	1.43	1.35
28	b	723	CLA	CHC-C1C	3.17	1.43	1.35
28	a	718	CLA	CHC-C1C	3.17	1.43	1.35
28	b	713	CLA	CHC-C1C	3.17	1.43	1.35
28	a	712	CLA	CHC-C1C	3.17	1.43	1.35
28	L	318	CLA	CHC-C1C	3.17	1.43	1.35
28	b	720	CLA	CHC-C1C	3.17	1.43	1.35
28	M	317	CLA	CHC-C1C	3.17	1.43	1.35
28	B	315	CLA	CHC-C1C	3.17	1.43	1.35
28	H	311	CLA	CHC-C1C	3.17	1.43	1.35
28	G	514	CLA	CHC-C1C	3.17	1.43	1.35
28	D	308	CLA	CHC-C1C	3.17	1.43	1.35
32	D	305	PID	C20-C21	3.16	1.40	1.35
28	J	308	CLA	CHC-C1C	3.16	1.43	1.35
28	h	202	CLA	CHC-C1C	3.16	1.43	1.35
28	b	701	CLA	CHC-C1C	3.16	1.43	1.35
28	A	310	CLA	CHC-C1C	3.16	1.43	1.35
28	B	311	CLA	CHC-C1C	3.16	1.43	1.35
28	B	310	CLA	CHC-C1C	3.16	1.43	1.35
28	a	730	CLA	CHC-C1C	3.16	1.43	1.35
28	N	307	CLA	CHC-C1C	3.16	1.43	1.35
28	G	516	CLA	CHC-C1C	3.16	1.43	1.35
28	m	202	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M	302	DD6	C19-C20	3.16	1.56	1.52
28	F	311	CLA	CHC-C1C	3.16	1.43	1.35
32	D	302	PID	C20-C21	3.15	1.40	1.35
28	a	721	CLA	CHC-C1C	3.15	1.43	1.35
28	G	517	CLA	CHC-C1C	3.15	1.43	1.35
28	G	511	CLA	CHC-C1C	3.15	1.43	1.35
28	l	303	CLA	CHC-C1C	3.15	1.43	1.35
28	b	712	CLA	CHC-C1C	3.15	1.43	1.35
28	I	315	CLA	CHC-C1C	3.15	1.43	1.35
28	K	311	CLA	CHC-C1C	3.15	1.43	1.35
28	a	713	CLA	CHC-C1C	3.15	1.43	1.35
28	a	720	CLA	CHC-C1C	3.15	1.43	1.35
28	B	307	CLA	CHC-C1C	3.15	1.43	1.35
32	G	507	PID	C20-C21	3.15	1.40	1.35
28	G	518	CLA	CHC-C1C	3.15	1.43	1.35
28	b	728	CLA	CHC-C1C	3.14	1.43	1.35
28	I	310	CLA	CHC-C1C	3.14	1.43	1.35
28	M	308	CLA	CHC-C1C	3.14	1.43	1.35
28	b	711	CLA	CHC-C1C	3.14	1.43	1.35
28	a	738	CLA	CHC-C1C	3.14	1.43	1.35
28	N	304	CLA	CHC-C1C	3.14	1.43	1.35
28	A	320	CLA	CHC-C1C	3.14	1.43	1.35
28	a	715	CLA	CHC-C1C	3.14	1.43	1.35
28	H	309	CLA	CHC-C1C	3.14	1.43	1.35
28	G	509	CLA	CHC-C1C	3.14	1.43	1.35
28	a	731	CLA	CHC-C1C	3.13	1.43	1.35
28	J	316	CLA	CHC-C1C	3.13	1.43	1.35
28	b	710	CLA	CHC-C1C	3.13	1.43	1.35
28	B	313	CLA	CHC-C1C	3.13	1.43	1.35
28	a	728	CLA	CHC-C1C	3.13	1.43	1.35
28	H	304	CLA	CHC-C1C	3.13	1.43	1.35
28	I	307	CLA	CHC-C1C	3.13	1.43	1.35
28	K	306	CLA	CHC-C1C	3.13	1.43	1.35
28	b	719	CLA	CHC-C1C	3.12	1.43	1.35
28	B	301	CLA	CHC-C1C	3.12	1.43	1.35
28	J	307	CLA	CHC-C1C	3.12	1.43	1.35
28	b	721	CLA	CHC-C1C	3.12	1.43	1.35
28	B	316	CLA	CHC-C1C	3.12	1.43	1.35
28	I	311	CLA	CHC-C1C	3.11	1.43	1.35
28	N	305	CLA	CHC-C1C	3.11	1.42	1.35
28	A	307	CLA	CHC-C1C	3.11	1.42	1.35
28	J	306	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	M	312	CLA	CHC-C1C	3.11	1.42	1.35
28	N	307	CLA	C4D-ND	-3.10	1.33	1.37
28	a	725	CLA	C4D-ND	-3.10	1.33	1.37
28	b	708	CLA	CHC-C1C	3.09	1.42	1.35
28	I	306	CLA	CHC-C1C	3.09	1.42	1.35
28	b	717	CLA	CHC-C1C	3.09	1.42	1.35
28	J	309	CLA	CHC-C1C	3.07	1.42	1.35
28	F	308	CLA	CHC-C1C	3.07	1.42	1.35
28	G	512	CLA	CHC-C1C	3.07	1.42	1.35
28	D	313	CLA	CHC-C1C	3.06	1.42	1.35
28	a	724	CLA	CHC-C1C	3.06	1.42	1.35
28	K	316	CLA	CHC-C1C	3.05	1.42	1.35
28	F	307	CLA	CHC-C1C	3.05	1.42	1.35
28	K	313	CLA	C4D-ND	-3.04	1.33	1.37
28	G	510	CLA	C4D-ND	-3.04	1.33	1.37
28	F	313	CLA	CHC-C1C	3.04	1.42	1.35
28	L	317	CLA	CHC-C1C	3.04	1.42	1.35
28	a	706	CLA	C4D-ND	-3.04	1.33	1.37
28	A	316	CLA	CHC-C1C	3.03	1.42	1.35
28	b	718	CLA	CHC-C1C	3.03	1.42	1.35
28	B	310	CLA	C4D-ND	-3.03	1.33	1.37
28	a	705	CLA	C4D-ND	-3.03	1.33	1.37
26	J	303	DD6	O1-C20	-3.03	1.41	1.46
28	b	713	CLA	C4D-ND	-3.02	1.33	1.37
28	N	310	CLA	CHC-C1C	3.02	1.42	1.35
28	K	307	CLA	C4D-ND	-3.01	1.33	1.37
28	J	310	CLA	CHC-C1C	3.00	1.42	1.35
28	b	725	CLA	C4D-ND	-3.00	1.33	1.37
28	A	319	CLA	C4D-ND	-2.99	1.33	1.37
28	M	312	CLA	C4D-ND	-2.99	1.33	1.37
28	M	309	CLA	C4D-ND	-2.99	1.33	1.37
28	B	313	CLA	C4D-ND	-2.99	1.33	1.37
28	A	308	CLA	C4D-ND	-2.98	1.33	1.37
28	b	722	CLA	CMB-C2B	-2.98	1.45	1.51
28	F	312	CLA	C1D-ND	2.98	1.41	1.37
29	N	308	KC1	C4A-C3A	-2.97	1.38	1.44
28	b	711	CLA	C4D-ND	-2.97	1.33	1.37
26	J	304	DD6	O1-C20	-2.97	1.42	1.46
28	G	514	CLA	C4D-ND	-2.97	1.33	1.37
28	a	704	CLA	C4D-ND	-2.97	1.33	1.37
28	K	315	CLA	C4D-ND	-2.96	1.33	1.37
28	B	311	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	308	CLA	C4D-ND	-2.96	1.33	1.37
28	b	722	CLA	CHC-C1C	2.96	1.42	1.35
28	I	313	CLA	C4D-ND	-2.96	1.33	1.37
28	b	708	CLA	C4D-ND	-2.96	1.33	1.37
28	a	712	CLA	C4D-ND	-2.96	1.33	1.37
28	I	308	CLA	C4D-ND	-2.96	1.33	1.37
28	l	305	CLA	C4D-ND	-2.95	1.33	1.37
28	a	702	CLA	C1D-ND	2.95	1.41	1.37
28	a	719	CLA	C4D-ND	-2.95	1.33	1.37
28	I	309	CLA	C4D-ND	-2.95	1.33	1.37
28	B	301	CLA	C4D-ND	-2.95	1.33	1.37
28	b	724	CLA	C4D-ND	-2.95	1.33	1.37
28	b	722	CLA	C4D-ND	-2.95	1.33	1.37
28	f	302	CLA	C4D-ND	-2.94	1.33	1.37
28	B	309	CLA	C4D-ND	-2.94	1.33	1.37
28	L	312	CLA	C4D-ND	-2.94	1.33	1.37
28	a	720	CLA	C4D-ND	-2.94	1.33	1.37
28	H	307	CLA	C4D-ND	-2.93	1.33	1.37
28	J	309	CLA	C4D-ND	-2.93	1.33	1.37
28	a	708	CLA	C4D-ND	-2.93	1.33	1.37
28	M	317	CLA	C4D-ND	-2.93	1.33	1.37
28	b	720	CLA	C4D-ND	-2.93	1.33	1.37
28	K	306	CLA	C4D-ND	-2.93	1.33	1.37
26	J	304	DD6	C19-C20	2.92	1.56	1.52
28	K	309	CLA	C4D-ND	-2.92	1.33	1.37
28	N	305	CLA	C4D-ND	-2.92	1.33	1.37
28	f	303	CLA	C4D-ND	-2.92	1.33	1.37
28	D	312	CLA	C4D-ND	-2.92	1.33	1.37
28	b	710	CLA	C4D-ND	-2.92	1.33	1.37
28	H	304	CLA	C4D-ND	-2.92	1.33	1.37
28	b	727	CLA	C4D-ND	-2.92	1.33	1.37
32	N	302	PID	C8-C9	-2.92	1.39	1.46
28	a	711	CLA	C4D-ND	-2.91	1.33	1.37
28	b	704	CLA	CHC-C1C	2.91	1.42	1.35
28	L	313	CLA	C4D-ND	-2.91	1.33	1.37
28	K	307	CLA	CHC-C1C	2.91	1.42	1.35
28	M	310	CLA	C4D-ND	-2.91	1.33	1.37
28	A	312	CLA	C4D-ND	-2.91	1.33	1.37
28	b	716	CLA	C4D-ND	-2.90	1.33	1.37
28	L	314	CLA	C4D-ND	-2.90	1.33	1.37
28	a	721	CLA	C4D-ND	-2.90	1.33	1.37
28	I	315	CLA	C4D-ND	-2.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	313	CLA	C4D-ND	-2.90	1.33	1.37
28	a	718	CLA	C4D-ND	-2.90	1.33	1.37
28	J	316	CLA	C4D-ND	-2.90	1.33	1.37
28	F	312	CLA	CHC-C1C	2.89	1.42	1.35
28	K	316	CLA	C4D-ND	-2.89	1.33	1.37
28	L	309	CLA	C4D-ND	-2.89	1.33	1.37
28	a	731	CLA	C4D-ND	-2.89	1.33	1.37
28	b	728	CLA	C4D-ND	-2.89	1.33	1.37
28	A	317	CLA	C4D-ND	-2.89	1.33	1.37
28	H	312	CLA	C4D-ND	-2.89	1.33	1.37
28	a	709	CLA	C4D-ND	-2.89	1.33	1.37
28	M	318	CLA	C4D-ND	-2.89	1.33	1.37
28	l	303	CLA	C4D-ND	-2.89	1.33	1.37
28	b	717	CLA	C4D-ND	-2.89	1.33	1.37
28	G	513	CLA	C4D-ND	-2.89	1.33	1.37
28	A	313	CLA	C4D-ND	-2.89	1.33	1.37
28	M	313	CLA	C4D-ND	-2.89	1.33	1.37
28	a	728	CLA	C4D-ND	-2.89	1.33	1.37
28	b	719	CLA	C4D-ND	-2.89	1.33	1.37
28	D	314	CLA	C4D-ND	-2.89	1.33	1.37
28	I	316	CLA	C4D-ND	-2.89	1.33	1.37
28	a	723	CLA	C4D-ND	-2.89	1.33	1.37
28	A	311	CLA	C4D-ND	-2.88	1.33	1.37
28	a	701	CLA	C4D-ND	-2.88	1.33	1.37
29	A	306	KC1	CBA-CGA	-2.88	1.41	1.48
28	D	311	CLA	C4D-ND	-2.88	1.33	1.37
28	K	310	CLA	C4D-ND	-2.88	1.33	1.37
28	a	707	CLA	C4D-ND	-2.88	1.33	1.37
28	L	310	CLA	C4D-ND	-2.88	1.33	1.37
28	K	308	CLA	C4D-ND	-2.88	1.33	1.37
28	b	707	CLA	C4D-ND	-2.88	1.33	1.37
32	G	506	PID	C8-C9	-2.87	1.39	1.46
28	b	706	CLA	C4D-ND	-2.87	1.33	1.37
28	M	311	CLA	C4D-ND	-2.87	1.33	1.37
28	H	305	CLA	C4D-ND	-2.87	1.33	1.37
29	K	314	KC1	CBA-CGA	-2.87	1.41	1.48
28	A	309	CLA	C4D-ND	-2.87	1.33	1.37
28	J	315	CLA	C4D-ND	-2.87	1.33	1.37
28	F	312	CLA	CMB-C2B	-2.87	1.45	1.51
28	G	509	CLA	C4D-ND	-2.86	1.33	1.37
28	a	713	CLA	C4D-ND	-2.86	1.33	1.37
28	a	702	CLA	CMB-C2B	-2.86	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	714	CLA	C4D-ND	-2.86	1.33	1.37
28	a	716	CLA	C4D-ND	-2.86	1.33	1.37
28	L	308	CLA	C4D-ND	-2.86	1.33	1.37
28	G	511	CLA	C4D-ND	-2.86	1.33	1.37
28	M	308	CLA	C4D-ND	-2.86	1.33	1.37
28	a	730	CLA	C4D-ND	-2.86	1.33	1.37
28	b	715	CLA	C4D-ND	-2.86	1.33	1.37
28	b	705	CLA	C4D-ND	-2.86	1.33	1.37
28	B	315	CLA	C4D-ND	-2.86	1.33	1.37
28	a	722	CLA	C4D-ND	-2.86	1.33	1.37
28	K	311	CLA	C4D-ND	-2.85	1.33	1.37
28	G	520	CLA	C4D-ND	-2.85	1.33	1.37
29	N	308	KC1	C4B-NB	-2.85	1.34	1.37
28	F	313	CLA	C4D-ND	-2.85	1.33	1.37
28	J	306	CLA	C4D-ND	-2.85	1.33	1.37
28	N	309	CLA	C4D-ND	-2.85	1.33	1.37
28	A	310	CLA	C4D-ND	-2.85	1.33	1.37
28	l	311	CLA	C4D-ND	-2.85	1.33	1.37
29	M	307	KC1	CBA-CGA	-2.85	1.41	1.48
28	l	308	CLA	C4D-ND	-2.85	1.33	1.37
28	D	309	CLA	C4D-ND	-2.85	1.33	1.37
29	J	313	KC1	C4B-NB	-2.84	1.34	1.37
28	K	312	CLA	C4D-ND	-2.84	1.33	1.37
28	l	309	CLA	C4D-ND	-2.84	1.33	1.37
28	D	316	CLA	C4D-ND	-2.84	1.33	1.37
29	L	307	KC1	CBA-CGA	-2.84	1.41	1.48
28	L	318	CLA	C4D-ND	-2.83	1.33	1.37
28	I	310	CLA	C4D-ND	-2.83	1.33	1.37
28	G	517	CLA	C4D-ND	-2.83	1.33	1.37
28	h	202	CLA	C4D-ND	-2.83	1.33	1.37
28	H	309	CLA	C4D-ND	-2.83	1.33	1.37
28	a	710	CLA	C4D-ND	-2.83	1.33	1.37
28	M	316	CLA	C4D-ND	-2.83	1.33	1.37
28	a	724	CLA	CMB-C2B	-2.83	1.45	1.51
28	a	727	CLA	C4D-ND	-2.83	1.33	1.37
28	b	723	CLA	C4D-ND	-2.83	1.33	1.37
28	B	308	CLA	C4D-ND	-2.83	1.33	1.37
28	G	512	CLA	C4D-ND	-2.83	1.33	1.37
28	J	310	CLA	CMB-C2B	-2.83	1.45	1.51
28	J	311	CLA	C4D-ND	-2.82	1.33	1.37
28	N	304	CLA	C4D-ND	-2.82	1.33	1.37
28	l	310	CLA	C1D-ND	2.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	311	CLA	C4D-ND	-2.82	1.33	1.37
28	b	704	CLA	C1D-ND	2.82	1.41	1.37
28	I	312	CLA	C4D-ND	-2.82	1.33	1.37
28	I	321	CLA	C4D-ND	-2.82	1.33	1.37
28	G	519	CLA	C4D-ND	-2.82	1.33	1.37
28	f	301	CLA	C4D-ND	-2.82	1.33	1.37
28	a	735	CLA	C4D-ND	-2.82	1.33	1.37
28	F	307	CLA	C4D-ND	-2.81	1.33	1.37
28	H	308	CLA	C4D-ND	-2.81	1.33	1.37
28	L	316	CLA	C4D-ND	-2.81	1.33	1.37
28	a	702	CLA	CHC-C1C	2.81	1.42	1.35
28	A	316	CLA	C4D-ND	-2.81	1.33	1.37
28	j	106	CLA	C4D-ND	-2.81	1.33	1.37
28	D	308	CLA	C4D-ND	-2.81	1.33	1.37
28	b	726	CLA	C4D-ND	-2.81	1.33	1.37
28	l	312	CLA	C4D-ND	-2.81	1.33	1.37
28	J	301	CLA	C4D-ND	-2.81	1.33	1.37
28	b	714	CLA	C4D-ND	-2.81	1.33	1.37
28	a	717	CLA	C4D-ND	-2.80	1.33	1.37
28	B	312	CLA	C4D-ND	-2.80	1.33	1.37
28	b	712	CLA	C4D-ND	-2.80	1.33	1.37
28	b	709	CLA	C4D-ND	-2.80	1.33	1.37
28	J	312	CLA	C4D-ND	-2.80	1.33	1.37
29	J	313	KC1	CBA-CGA	-2.80	1.42	1.48
28	a	703	CLA	CHC-C1C	2.80	1.42	1.35
26	I	303	DD6	O1-C20	-2.80	1.42	1.46
28	B	317	CLA	C4D-ND	-2.80	1.33	1.37
29	L	315	KC1	CBA-CGA	-2.80	1.42	1.48
28	G	516	CLA	C4D-ND	-2.80	1.33	1.37
28	A	315	CLA	C4D-ND	-2.79	1.33	1.37
28	I	306	CLA	C4D-ND	-2.79	1.33	1.37
28	F	315	CLA	C4D-ND	-2.79	1.33	1.37
28	H	311	CLA	C4D-ND	-2.79	1.33	1.37
28	B	316	CLA	C4D-ND	-2.79	1.33	1.37
28	J	307	CLA	C4D-ND	-2.79	1.33	1.37
28	j	104	CLA	C4D-ND	-2.79	1.33	1.37
28	b	704	CLA	CMB-C2B	-2.79	1.45	1.51
28	J	314	CLA	C4D-ND	-2.78	1.33	1.37
28	F	310	CLA	C4D-ND	-2.78	1.33	1.37
28	a	738	CLA	C4D-ND	-2.78	1.33	1.37
28	a	724	CLA	C4D-ND	-2.78	1.33	1.37
29	B	314	KC1	CBA-CGA	-2.78	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	311	CLA	C4D-ND	-2.78	1.33	1.37
28	b	721	CLA	C4D-ND	-2.78	1.33	1.37
28	a	726	CLA	C4D-ND	-2.78	1.33	1.37
28	L	317	CLA	C4D-ND	-2.78	1.33	1.37
32	D	304	PID	C13-C12	2.78	1.44	1.36
28	N	310	CLA	C4D-ND	-2.77	1.33	1.37
29	M	314	KC1	C4B-NB	-2.77	1.34	1.37
32	F	304	PID	C13-C12	2.77	1.44	1.36
29	A	314	KC1	CBA-CGA	-2.77	1.42	1.48
28	l	304	CLA	C4D-ND	-2.77	1.33	1.37
28	a	715	CLA	C4D-ND	-2.77	1.33	1.37
28	b	710	CLA	CMB-C2B	-2.76	1.45	1.51
29	H	310	KC1	CBA-CGA	-2.76	1.42	1.48
28	A	320	CLA	C4D-ND	-2.76	1.33	1.37
28	b	718	CLA	C4D-ND	-2.76	1.33	1.37
29	B	314	KC1	C4B-NB	-2.76	1.34	1.37
28	I	311	CLA	C4D-ND	-2.76	1.33	1.37
28	I	319	CLA	C4D-ND	-2.76	1.33	1.37
28	b	701	CLA	C4D-ND	-2.76	1.33	1.37
28	B	307	CLA	C4D-ND	-2.76	1.33	1.37
28	A	307	CLA	C4D-ND	-2.76	1.33	1.37
28	l	313	CLA	C4D-ND	-2.76	1.33	1.37
29	F	314	KC1	C4B-NB	-2.76	1.34	1.37
28	M	315	CLA	C4D-ND	-2.75	1.33	1.37
29	K	314	KC1	C4B-NB	-2.75	1.34	1.37
29	D	310	KC1	CBA-CGA	-2.75	1.42	1.48
29	M	307	KC1	C4B-NB	-2.75	1.34	1.37
29	H	306	KC1	CBA-CGA	-2.74	1.42	1.48
29	N	311	KC1	CBA-CGA	-2.74	1.42	1.48
28	m	202	CLA	C4D-ND	-2.74	1.33	1.37
28	J	308	CLA	C4D-ND	-2.73	1.33	1.37
32	M	301	PID	C13-C12	2.73	1.44	1.36
29	F	309	KC1	CBA-CGA	-2.73	1.42	1.48
28	b	712	CLA	CMB-C2B	-2.73	1.46	1.51
29	G	515	KC1	CBA-CGA	-2.73	1.42	1.48
28	J	310	CLA	C4D-ND	-2.73	1.33	1.37
29	D	310	KC1	C4B-NB	-2.73	1.34	1.37
29	F	314	KC1	CBA-CGA	-2.73	1.42	1.48
28	I	307	CLA	C4D-ND	-2.73	1.33	1.37
29	M	314	KC1	CBA-CGA	-2.73	1.42	1.48
28	M	312	CLA	CMB-C2B	-2.72	1.46	1.51
29	H	306	KC1	C4B-NB	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	L	315	KC1	C4B-NB	-2.72	1.34	1.37
28	a	703	CLA	CMB-C2B	-2.72	1.46	1.51
26	G	505	DD6	O1-C20	-2.72	1.42	1.46
28	a	729	CLA	C4D-ND	-2.71	1.34	1.37
29	N	306	KC1	CBA-CGA	-2.71	1.42	1.48
32	F	302	PID	C13-C12	2.71	1.44	1.36
29	I	314	KC1	CBA-CGA	-2.71	1.42	1.48
29	G	515	KC1	C4B-NB	-2.70	1.34	1.37
26	I	305	DD6	O1-C20	-2.69	1.42	1.46
26	I	305	DD6	C36-C31	-2.69	1.31	1.34
29	N	308	KC1	C1B-NB	-2.69	1.34	1.37
32	D	307	PID	C13-C12	2.68	1.43	1.36
28	G	518	CLA	C4D-ND	-2.68	1.34	1.37
29	L	307	KC1	C4B-NB	-2.68	1.34	1.37
32	F	305	PID	C13-C12	2.67	1.43	1.36
28	b	703	CLA	C4D-ND	-2.67	1.34	1.37
29	H	310	KC1	C4B-NB	-2.66	1.34	1.37
27	K	302	UIX	O-C1	-2.66	1.42	1.46
29	D	315	KC1	CBA-CGA	-2.66	1.42	1.48
32	H	302	PID	C8-C9	-2.66	1.39	1.46
29	N	306	KC1	C4B-NB	-2.66	1.34	1.37
29	A	314	KC1	C4B-NB	-2.65	1.34	1.37
28	a	703	CLA	C1D-ND	2.64	1.41	1.37
29	A	306	KC1	C4B-NB	-2.64	1.34	1.37
32	N	301	PID	C13-C12	2.63	1.43	1.36
29	N	311	KC1	C4B-NB	-2.63	1.34	1.37
28	b	721	CLA	CMB-C2B	-2.63	1.46	1.51
32	H	301	PID	C13-C12	2.63	1.43	1.36
28	l	313	CLA	CMB-C2B	-2.62	1.46	1.51
32	F	306	PID	C13-C12	2.62	1.43	1.36
32	D	302	PID	C8-C9	-2.62	1.39	1.46
32	j	105	PID	C13-C12	2.62	1.43	1.36
26	I	305	DD6	C19-C20	2.62	1.55	1.52
29	F	309	KC1	C4B-NB	-2.61	1.34	1.37
29	I	314	KC1	C4B-NB	-2.61	1.34	1.37
32	G	506	PID	C20-C21	2.61	1.39	1.35
28	b	718	CLA	CMB-C2B	-2.61	1.46	1.51
32	F	306	PID	C8-C9	-2.60	1.39	1.46
28	b	713	CLA	CMB-C2B	-2.59	1.46	1.51
28	b	717	CLA	CMB-C2B	-2.58	1.46	1.51
28	a	712	CLA	CMB-C2B	-2.58	1.46	1.51
28	b	719	CLA	CMB-C2B	-2.58	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	308	KC1	CBA-CGA	-2.57	1.42	1.48
32	D	306	PID	C8-C9	-2.57	1.39	1.46
32	F	302	PID	C8-C9	-2.57	1.39	1.46
32	D	305	PID	C8-C9	-2.56	1.39	1.46
32	G	507	PID	C8-C9	-2.56	1.39	1.46
28	b	709	CLA	CMB-C2B	-2.56	1.46	1.51
32	F	305	PID	C8-C9	-2.56	1.39	1.46
28	I	312	CLA	CMB-C2B	-2.56	1.46	1.51
32	G	507	PID	C13-C12	2.55	1.43	1.36
28	b	701	CLA	CMB-C2B	-2.55	1.46	1.51
28	G	518	CLA	CMB-C2B	-2.55	1.46	1.51
28	a	709	CLA	CMB-C2B	-2.54	1.46	1.51
28	a	719	CLA	CMB-C2B	-2.54	1.46	1.51
26	M	303	DD6	O1-C20	-2.53	1.42	1.46
28	a	703	CLA	CMD-C2D	-2.53	1.45	1.50
32	H	301	PID	C8-C9	-2.53	1.40	1.46
28	K	316	CLA	CMB-C2B	-2.53	1.46	1.51
28	J	308	CLA	CMB-C2B	-2.52	1.46	1.51
32	D	306	PID	C13-C12	2.52	1.43	1.36
28	I	311	CLA	CMB-C2B	-2.52	1.46	1.51
32	D	301	PID	C13-C12	2.52	1.43	1.36
28	l	312	CLA	CMB-C2B	-2.51	1.46	1.51
28	A	310	CLA	CMB-C2B	-2.51	1.46	1.51
28	K	311	CLA	CMB-C2B	-2.51	1.46	1.51
28	l	303	CLA	CMB-C2B	-2.50	1.46	1.51
30	L	301	DGD	O1G-C1A	2.50	1.45	1.33
28	b	704	CLA	C3B-C2B	-2.50	1.36	1.40
28	B	301	CLA	CMB-C2B	-2.49	1.46	1.51
28	b	706	CLA	CMB-C2B	-2.49	1.46	1.51
32	j	105	PID	C8-C9	-2.49	1.40	1.46
28	D	314	CLA	CMB-C2B	-2.49	1.46	1.51
28	b	723	CLA	CMB-C2B	-2.49	1.46	1.51
28	B	316	CLA	CMB-C2B	-2.48	1.46	1.51
28	a	717	CLA	CMB-C2B	-2.48	1.46	1.51
32	H	302	PID	C13-C12	2.48	1.43	1.36
28	N	305	CLA	CMB-C2B	-2.48	1.46	1.51
32	M	301	PID	C8-C9	-2.48	1.40	1.46
28	G	512	CLA	CMB-C2B	-2.48	1.46	1.51
28	M	311	CLA	CMB-C2B	-2.48	1.46	1.51
28	I	308	CLA	CMB-C2B	-2.47	1.46	1.51
28	A	320	CLA	CMB-C2B	-2.47	1.46	1.51
32	D	305	PID	C13-C12	2.47	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	312	CLA	CMB-C2B	-2.47	1.46	1.51
26	G	504	DD6	C36-C31	-2.47	1.32	1.34
28	B	317	CLA	CMB-C2B	-2.47	1.46	1.51
28	b	726	CLA	CMB-C2B	-2.46	1.46	1.51
32	D	301	PID	C8-C9	-2.46	1.40	1.46
26	G	504	DD6	O1-C20	-2.46	1.42	1.46
28	K	310	CLA	CMB-C2B	-2.46	1.46	1.51
28	a	715	CLA	CMB-C2B	-2.46	1.46	1.51
28	L	318	CLA	CMB-C2B	-2.46	1.46	1.51
27	h	201	UIX	O-C1	-2.46	1.42	1.46
29	D	315	KC1	C4B-NB	-2.46	1.34	1.37
27	G	503	UIX	O-C1	-2.46	1.42	1.46
28	H	309	CLA	CMB-C2B	-2.46	1.46	1.51
28	J	316	CLA	CMB-C2B	-2.46	1.46	1.51
28	L	316	CLA	CMB-C2B	-2.45	1.46	1.51
28	B	312	CLA	CMB-C2B	-2.45	1.46	1.51
28	G	519	CLA	CMB-C2B	-2.45	1.46	1.51
28	A	317	CLA	CMB-C2B	-2.45	1.46	1.51
28	b	728	CLA	CMB-C2B	-2.45	1.46	1.51
28	L	308	CLA	CMB-C2B	-2.45	1.46	1.51
28	N	310	CLA	CMB-C2B	-2.45	1.46	1.51
28	M	316	CLA	CMB-C2B	-2.44	1.46	1.51
28	N	304	CLA	CMB-C2B	-2.44	1.46	1.51
28	f	301	CLA	CMB-C2B	-2.44	1.46	1.51
32	D	302	PID	C13-C12	2.44	1.43	1.36
28	a	725	CLA	CMB-C2B	-2.44	1.46	1.51
28	a	701	CLA	CMB-C2B	-2.44	1.46	1.51
28	K	306	CLA	CMB-C2B	-2.44	1.46	1.51
28	G	514	CLA	CMB-C2B	-2.44	1.46	1.51
28	A	316	CLA	CMB-C2B	-2.44	1.46	1.51
28	M	318	CLA	CMB-C2B	-2.44	1.46	1.51
28	I	306	CLA	CMB-C2B	-2.43	1.46	1.51
28	B	307	CLA	CMB-C2B	-2.43	1.46	1.51
28	F	307	CLA	CMB-C2B	-2.43	1.46	1.51
28	F	308	CLA	CMB-C2B	-2.43	1.46	1.51
29	G	515	KC1	CHD-C4C	2.43	1.41	1.35
28	a	708	CLA	CMB-C2B	-2.43	1.46	1.51
28	a	702	CLA	CMD-C2D	-2.43	1.45	1.50
28	I	315	CLA	CMB-C2B	-2.43	1.46	1.51
28	L	317	CLA	CMB-C2B	-2.43	1.46	1.51
32	D	304	PID	C8-C9	-2.43	1.40	1.46
28	a	716	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	308	CLA	CMB-C2B	-2.43	1.46	1.51
29	M	307	KC1	CHD-C4C	2.42	1.41	1.35
28	b	705	CLA	CMB-C2B	-2.42	1.46	1.51
28	H	311	CLA	CMB-C2B	-2.42	1.46	1.51
28	F	311	CLA	CMB-C2B	-2.42	1.46	1.51
28	A	311	CLA	CMB-C2B	-2.42	1.46	1.51
28	b	724	CLA	CMB-C2B	-2.42	1.46	1.51
28	a	726	CLA	CMB-C2B	-2.42	1.46	1.51
28	F	312	CLA	CMD-C2D	-2.42	1.45	1.50
28	G	511	CLA	CMB-C2B	-2.42	1.46	1.51
28	l	310	CLA	CMB-C2B	-2.42	1.46	1.51
28	J	312	CLA	CMB-C2B	-2.42	1.46	1.51
26	M	302	DD6	O1-C20	-2.41	1.42	1.46
28	K	307	CLA	CMB-C2B	-2.41	1.46	1.51
29	F	309	KC1	C1B-NB	-2.41	1.34	1.37
28	a	728	CLA	CMB-C2B	-2.41	1.46	1.51
29	D	315	KC1	C1B-NB	-2.41	1.34	1.37
28	a	727	CLA	CMB-C2B	-2.41	1.46	1.51
28	h	202	CLA	CMB-C2B	-2.41	1.46	1.51
28	H	307	CLA	CMB-C2B	-2.41	1.46	1.51
28	K	312	CLA	CMB-C2B	-2.41	1.46	1.51
32	N	301	PID	C8-C9	-2.41	1.40	1.46
29	N	306	KC1	CHD-C4C	2.41	1.41	1.35
32	N	302	PID	C20-C21	2.41	1.39	1.35
28	a	723	CLA	CMB-C2B	-2.41	1.46	1.51
29	H	310	KC1	CHD-C4C	2.41	1.41	1.35
28	M	308	CLA	CMB-C2B	-2.41	1.46	1.51
29	L	315	KC1	CHD-C4C	2.41	1.41	1.35
28	D	312	CLA	CMB-C2B	-2.41	1.46	1.51
28	L	313	CLA	CMB-C2B	-2.41	1.46	1.51
28	a	720	CLA	CMB-C2B	-2.40	1.46	1.51
26	K	301	DD6	O1-C20	-2.40	1.42	1.46
28	G	510	CLA	CMB-C2B	-2.40	1.46	1.51
28	a	704	CLA	CMB-C2B	-2.40	1.46	1.51
28	j	104	CLA	CMB-C2B	-2.40	1.46	1.51
28	B	311	CLA	CMB-C2B	-2.40	1.46	1.51
28	b	708	CLA	CMB-C2B	-2.40	1.46	1.51
28	J	309	CLA	CMB-C2B	-2.40	1.46	1.51
28	D	308	CLA	CMB-C2B	-2.40	1.46	1.51
28	a	702	CLA	C3B-C2B	-2.40	1.37	1.40
28	a	721	CLA	CMB-C2B	-2.40	1.46	1.51
29	J	313	KC1	CHD-C4C	2.40	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	311	CLA	CMB-C2B	-2.40	1.46	1.51
28	G	509	CLA	CMB-C2B	-2.40	1.46	1.51
28	B	313	CLA	CMB-C2B	-2.39	1.46	1.51
28	f	302	CLA	CMB-C2B	-2.39	1.46	1.51
28	l	310	CLA	C4D-ND	-2.39	1.33	1.37
28	l	305	CLA	CMB-C2B	-2.39	1.46	1.51
28	B	310	CLA	CMB-C2B	-2.39	1.46	1.51
28	a	711	CLA	CMB-C2B	-2.39	1.46	1.51
28	a	731	CLA	CMB-C2B	-2.39	1.46	1.51
29	N	308	KC1	CHD-C4C	2.39	1.41	1.35
26	I	302	DD6	O1-C20	-2.39	1.42	1.46
28	f	303	CLA	CMB-C2B	-2.39	1.46	1.51
28	a	730	CLA	CMB-C2B	-2.39	1.46	1.51
29	B	314	KC1	CHD-C4C	2.39	1.41	1.35
28	A	319	CLA	CMB-C2B	-2.39	1.46	1.51
28	a	738	CLA	CMB-C2B	-2.39	1.46	1.51
28	N	309	CLA	CMB-C2B	-2.38	1.46	1.51
28	J	306	CLA	CMB-C2B	-2.38	1.46	1.51
28	b	703	CLA	CMB-C2B	-2.38	1.46	1.51
28	a	714	CLA	CMB-C2B	-2.38	1.46	1.51
28	I	309	CLA	CMB-C2B	-2.38	1.46	1.51
28	I	321	CLA	CMB-C2B	-2.38	1.46	1.51
28	A	315	CLA	CMB-C2B	-2.38	1.46	1.51
29	A	306	KC1	CHD-C4C	2.38	1.41	1.35
28	b	711	CLA	CMB-C2B	-2.38	1.46	1.51
28	B	315	CLA	CMB-C2B	-2.38	1.46	1.51
28	M	313	CLA	CMB-C2B	-2.38	1.46	1.51
28	a	707	CLA	CMB-C2B	-2.38	1.46	1.51
28	b	704	CLA	CMD-C2D	-2.38	1.45	1.50
28	l	311	CLA	CMB-C2B	-2.38	1.46	1.51
28	D	313	CLA	CMB-C2B	-2.38	1.46	1.51
28	K	308	CLA	CMB-C2B	-2.38	1.46	1.51
26	L	304	DD6	O1-C20	-2.37	1.42	1.46
28	H	304	CLA	CMB-C2B	-2.37	1.46	1.51
29	F	314	KC1	CHD-C4C	2.37	1.41	1.35
28	H	312	CLA	CMB-C2B	-2.37	1.46	1.51
28	L	311	CLA	CMB-C2B	-2.37	1.46	1.51
29	H	306	KC1	CHD-C4C	2.37	1.41	1.35
28	I	319	CLA	CMB-C2B	-2.37	1.46	1.51
29	A	314	KC1	CHD-C4C	2.37	1.41	1.35
29	M	314	KC1	CHD-C4C	2.37	1.41	1.35
28	G	520	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	301	CLA	CMB-C2B	-2.37	1.46	1.51
29	D	310	KC1	C1B-NB	-2.37	1.34	1.37
28	L	309	CLA	CMB-C2B	-2.37	1.46	1.51
28	J	307	CLA	CMB-C2B	-2.37	1.46	1.51
28	N	307	CLA	CMB-C2B	-2.37	1.46	1.51
28	a	735	CLA	CMB-C2B	-2.36	1.46	1.51
28	b	716	CLA	CMB-C2B	-2.36	1.46	1.51
28	b	727	CLA	CMB-C2B	-2.36	1.46	1.51
28	A	307	CLA	CMB-C2B	-2.36	1.46	1.51
28	a	724	CLA	CMD-C2D	-2.36	1.45	1.50
31	I	318	LMG	C4-C5	2.36	1.58	1.53
28	H	308	CLA	CMB-C2B	-2.36	1.46	1.51
29	N	311	KC1	CHD-C4C	2.36	1.41	1.35
29	L	307	KC1	C1B-NB	-2.36	1.34	1.37
29	D	310	KC1	CHD-C4C	2.36	1.41	1.35
26	B	302	DD6	O1-C20	-2.36	1.42	1.46
32	G	506	PID	C13-C12	2.36	1.43	1.36
28	A	312	CLA	CMB-C2B	-2.36	1.46	1.51
28	F	313	CLA	CMB-C2B	-2.35	1.46	1.51
28	D	316	CLA	CMB-C2B	-2.35	1.46	1.51
28	F	315	CLA	CMB-C2B	-2.35	1.46	1.51
28	b	707	CLA	CMB-C2B	-2.35	1.46	1.51
28	I	310	CLA	CMB-C2B	-2.35	1.46	1.51
28	G	513	CLA	CMB-C2B	-2.35	1.46	1.51
28	I	307	CLA	CMB-C2B	-2.35	1.46	1.51
28	a	713	CLA	CMB-C2B	-2.35	1.46	1.51
28	M	309	CLA	CMB-C2B	-2.35	1.46	1.51
28	a	718	CLA	CMB-C2B	-2.35	1.46	1.51
28	B	308	CLA	CMB-C2B	-2.35	1.46	1.51
28	G	516	CLA	CMB-C2B	-2.35	1.46	1.51
29	I	314	KC1	CHD-C4C	2.35	1.41	1.35
28	b	715	CLA	CMB-C2B	-2.35	1.46	1.51
28	M	315	CLA	CMB-C2B	-2.35	1.46	1.51
28	A	313	CLA	CMB-C2B	-2.34	1.46	1.51
28	L	314	CLA	CMB-C2B	-2.34	1.46	1.51
28	F	312	CLA	C3B-C2B	-2.34	1.37	1.40
28	l	309	CLA	CMB-C2B	-2.34	1.46	1.51
28	M	310	CLA	CMB-C2B	-2.34	1.46	1.51
28	l	304	CLA	CMB-C2B	-2.34	1.46	1.51
28	F	310	CLA	CMB-C2B	-2.34	1.46	1.51
28	M	317	CLA	CMB-C2B	-2.34	1.46	1.51
28	a	729	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	309	CLA	CMB-C2B	-2.34	1.46	1.51
28	j	106	CLA	CMB-C2B	-2.34	1.46	1.51
28	a	705	CLA	CMB-C2B	-2.34	1.46	1.51
28	b	725	CLA	CMB-C2B	-2.34	1.46	1.51
29	A	306	KC1	C1B-NB	-2.34	1.34	1.37
28	b	714	CLA	CMB-C2B	-2.33	1.46	1.51
29	L	307	KC1	CHD-C4C	2.33	1.40	1.35
28	K	313	CLA	CMB-C2B	-2.33	1.46	1.51
28	G	517	CLA	CMB-C2B	-2.33	1.46	1.51
29	G	515	KC1	C1B-NB	-2.32	1.34	1.37
28	D	311	CLA	CMB-C2B	-2.32	1.46	1.51
28	J	314	CLA	CMB-C2B	-2.32	1.46	1.51
32	D	307	PID	C8-C9	-2.32	1.40	1.46
28	K	315	CLA	CMB-C2B	-2.32	1.46	1.51
28	a	710	CLA	CMB-C2B	-2.32	1.46	1.51
28	J	315	CLA	CMB-C2B	-2.32	1.46	1.51
28	I	313	CLA	CMB-C2B	-2.31	1.46	1.51
28	b	720	CLA	CMB-C2B	-2.31	1.46	1.51
32	F	304	PID	C8-C9	-2.31	1.40	1.46
28	D	309	CLA	CMB-C2B	-2.31	1.46	1.51
28	m	202	CLA	CMB-C2B	-2.31	1.46	1.51
28	H	305	CLA	CMB-C2B	-2.31	1.46	1.51
29	F	309	KC1	CHD-C4C	2.31	1.40	1.35
28	a	722	CLA	CMB-C2B	-2.30	1.46	1.51
28	B	309	CLA	CMB-C2B	-2.30	1.46	1.51
27	A	304	UIX	O-C1	-2.30	1.42	1.46
27	I	304	UIX	C15-C20	-2.30	1.50	1.54
28	a	710	CLA	CMD-C2D	-2.30	1.45	1.50
28	B	311	CLA	CMD-C2D	-2.30	1.45	1.50
26	A	302	DD6	C26-C27	-2.30	1.32	1.37
28	a	726	CLA	C3B-C2B	-2.29	1.37	1.40
27	J	305	UIX	O-C1	-2.29	1.42	1.46
29	I	314	KC1	C1B-NB	-2.29	1.35	1.37
28	a	702	CLA	C3B-CAB	-2.28	1.43	1.47
28	a	706	CLA	CMB-C2B	-2.28	1.46	1.51
28	L	310	CLA	CMB-C2B	-2.28	1.46	1.51
29	G	515	KC1	C4A-C3A	-2.28	1.40	1.44
28	K	309	CLA	CMB-C2B	-2.28	1.46	1.51
27	B	305	UIX	O-C1	-2.28	1.43	1.46
28	b	704	CLA	CMC-C2C	-2.27	1.46	1.50
29	J	313	KC1	C1B-NB	-2.27	1.35	1.37
28	A	308	CLA	CMB-C2B	-2.27	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	702	CLA	CMC-C2C	-2.27	1.46	1.50
29	A	314	KC1	C1B-NB	-2.27	1.35	1.37
29	K	314	KC1	CHD-C4C	2.26	1.40	1.35
29	A	314	KC1	C4A-C3A	-2.26	1.40	1.44
29	H	310	KC1	C1B-NB	-2.26	1.35	1.37
29	F	314	KC1	C1B-NB	-2.26	1.35	1.37
26	I	303	DD6	C19-C20	2.26	1.55	1.52
28	b	721	CLA	CMD-C2D	-2.26	1.46	1.50
31	K	318	LMG	O7-C8	-2.25	1.41	1.46
29	D	315	KC1	CHD-C4C	2.25	1.40	1.35
29	A	306	KC1	C4A-C3A	-2.25	1.40	1.44
28	I	316	CLA	CMB-C2B	-2.25	1.47	1.51
29	K	314	KC1	C1B-NB	-2.25	1.35	1.37
29	F	309	KC1	C4A-C3A	-2.25	1.40	1.44
26	K	304	DD6	O1-C20	-2.24	1.43	1.46
26	B	304	DD6	O1-C20	-2.24	1.43	1.46
26	G	508	DD6	O1-C20	-2.24	1.43	1.46
29	M	314	KC1	C1B-NB	-2.24	1.35	1.37
29	D	310	KC1	C4A-C3A	-2.24	1.40	1.44
28	a	726	CLA	C3B-CAB	-2.23	1.43	1.47
28	F	312	CLA	C3B-CAB	-2.23	1.43	1.47
28	l	310	CLA	C1A-NA	2.23	1.40	1.35
29	J	313	KC1	C4A-C3A	-2.23	1.40	1.44
26	b	731	DD6	O1-C20	-2.23	1.43	1.46
28	b	704	CLA	C3B-CAB	-2.23	1.43	1.47
28	l	310	CLA	C3D-C4D	2.22	1.48	1.43
32	F	305	PID	C15-C14	2.22	1.38	1.35
32	N	302	PID	C13-C12	2.22	1.42	1.36
27	I	304	UIX	O-C1	-2.22	1.43	1.46
29	N	306	KC1	C1B-NB	-2.21	1.35	1.37
29	L	315	KC1	C1B-NB	-2.21	1.35	1.37
26	F	303	DD6	O1-C20	-2.21	1.43	1.46
26	M	304	DD6	O1-C20	-2.20	1.43	1.46
29	M	307	KC1	C1B-NB	-2.20	1.35	1.37
28	a	703	CLA	CMC-C2C	-2.20	1.46	1.50
28	b	722	CLA	CMD-C2D	-2.20	1.46	1.50
29	B	314	KC1	C1B-NB	-2.20	1.35	1.37
26	I	303	DD6	C21-C20	-2.20	1.48	1.51
28	a	702	CLA	MG-ND	-2.19	2.01	2.05
29	N	311	KC1	C1B-NB	-2.19	1.35	1.37
26	K	303	DD6	O1-C20	-2.18	1.43	1.46
28	F	312	CLA	CMC-C2C	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	703	CLA	C3B-CAB	-2.18	1.43	1.47
26	B	306	DD6	O1-C20	-2.18	1.43	1.46
29	D	315	KC1	C4A-C3A	-2.18	1.40	1.44
28	a	703	CLA	MG-ND	-2.18	2.01	2.05
29	H	306	KC1	C1B-NB	-2.18	1.35	1.37
28	b	704	CLA	MG-ND	-2.17	2.01	2.05
29	M	307	KC1	C4A-C3A	-2.17	1.40	1.44
29	L	315	KC1	C4A-C3A	-2.16	1.40	1.44
26	H	303	DD6	O1-C20	-2.16	1.43	1.46
28	J	308	CLA	CMD-C2D	-2.16	1.46	1.50
28	A	320	CLA	CMD-C2D	-2.16	1.46	1.50
26	M	305	DD6	O1-C20	-2.15	1.43	1.46
29	K	314	KC1	C4A-C3A	-2.15	1.40	1.44
31	b	733	LMG	O7-C8	-2.15	1.41	1.46
28	N	309	CLA	CMD-C2D	-2.15	1.46	1.50
26	M	306	DD6	O1-C20	-2.14	1.43	1.46
28	N	309	CLA	CMC-C2C	-2.14	1.46	1.50
33	A	318	SQD	O8-S	2.14	1.55	1.47
35	i	201	BCR	C1-C6	-2.14	1.50	1.53
28	l	305	CLA	CMD-C2D	-2.13	1.46	1.50
28	b	710	CLA	CMD-C2D	-2.13	1.46	1.50
29	I	314	KC1	C4A-C3A	-2.12	1.40	1.44
28	D	313	CLA	CMD-C2D	-2.12	1.46	1.50
28	M	316	CLA	CMD-C2D	-2.12	1.46	1.50
26	I	305	DD6	C2-C1	-2.12	1.33	1.35
28	a	711	CLA	CMD-C2D	-2.12	1.46	1.50
26	M	303	DD6	C36-C31	-2.11	1.32	1.34
29	N	306	KC1	C4A-C3A	-2.11	1.40	1.44
29	L	307	KC1	C4A-C3A	-2.11	1.40	1.44
28	G	512	CLA	CMC-C2C	-2.11	1.46	1.50
26	h	203	DD6	O1-C20	-2.11	1.43	1.46
28	a	719	CLA	CMD-C2D	-2.11	1.46	1.50
28	K	311	CLA	CMD-C2D	-2.11	1.46	1.50
28	l	310	CLA	CMD-C2D	-2.11	1.46	1.50
26	L	305	DD6	O1-C20	-2.10	1.43	1.46
28	a	719	CLA	CMC-C2C	-2.10	1.46	1.50
31	D	317	LMG	O7-C8	-2.10	1.41	1.46
28	b	709	CLA	CMD-C2D	-2.10	1.46	1.50
29	F	314	KC1	C4A-C3A	-2.10	1.40	1.44
26	J	304	DD6	C36-C31	-2.10	1.32	1.34
28	b	703	CLA	CMD-C2D	-2.10	1.46	1.50
28	D	314	CLA	C3B-C2B	-2.09	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	723	CLA	CMD-C2D	-2.09	1.46	1.50
28	F	312	CLA	MG-ND	-2.09	2.01	2.05
29	B	314	KC1	C4A-C3A	-2.09	1.40	1.44
28	K	315	CLA	CMD-C2D	-2.09	1.46	1.50
26	K	305	DD6	O1-C20	-2.08	1.43	1.46
28	j	106	CLA	CMD-C2D	-2.08	1.46	1.50
28	b	717	CLA	CMC-C2C	-2.08	1.46	1.50
28	a	727	CLA	CMD-C2D	-2.08	1.46	1.50
26	L	306	DD6	O1-C20	-2.08	1.43	1.46
28	b	701	CLA	CMD-C2D	-2.08	1.46	1.50
28	J	306	CLA	CMD-C2D	-2.08	1.46	1.50
28	a	706	CLA	CMC-C2C	-2.08	1.46	1.50
29	M	314	KC1	C4A-C3A	-2.08	1.40	1.44
26	K	319	DD6	O1-C20	-2.07	1.43	1.46
28	a	701	CLA	CMD-C2D	-2.07	1.46	1.50
28	G	511	CLA	CMD-C2D	-2.07	1.46	1.50
28	a	715	CLA	CMD-C2D	-2.06	1.46	1.50
35	i	201	BCR	C30-C25	-2.06	1.50	1.53
28	N	307	CLA	CMD-C2D	-2.06	1.46	1.50
28	a	703	CLA	C3B-C2B	-2.06	1.37	1.40
28	F	313	CLA	CMD-C2D	-2.06	1.46	1.50
28	A	315	CLA	CMD-C2D	-2.06	1.46	1.50
29	H	306	KC1	C4A-C3A	-2.05	1.40	1.44
28	H	308	CLA	CMD-C2D	-2.05	1.46	1.50
29	H	310	KC1	C4A-C3A	-2.05	1.40	1.44
28	A	319	CLA	CMD-C2D	-2.04	1.46	1.50
28	A	310	CLA	CMD-C2D	-2.04	1.46	1.50
26	N	303	DD6	O1-C20	-2.04	1.43	1.46
28	a	729	CLA	CMD-C2D	-2.04	1.46	1.50
28	b	713	CLA	CMD-C2D	-2.04	1.46	1.50
28	J	310	CLA	CMD-C2D	-2.03	1.46	1.50
28	F	308	CLA	CMC-C2C	-2.03	1.46	1.50
28	H	311	CLA	CMD-C2D	-2.03	1.46	1.50
28	D	316	CLA	CMC-C2C	-2.03	1.46	1.50
28	a	704	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	301	DD6	O1-C20	-2.03	1.43	1.46
28	K	312	CLA	CMD-C2D	-2.03	1.46	1.50
28	K	313	CLA	CMC-C2C	-2.03	1.46	1.50
28	a	707	CLA	CMD-C2D	-2.02	1.46	1.50
28	H	312	CLA	CMD-C2D	-2.02	1.46	1.50
28	B	317	CLA	CMD-C2D	-2.02	1.46	1.50
28	M	317	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	712	CLA	CMD-C2D	-2.02	1.46	1.50
28	I	313	CLA	CMD-C2D	-2.02	1.46	1.50
28	K	312	CLA	CMC-C2C	-2.02	1.46	1.50
28	F	307	CLA	CMD-C2D	-2.02	1.46	1.50
28	a	730	CLA	CMC-C2C	-2.02	1.46	1.50
28	L	317	CLA	CMD-C2D	-2.01	1.46	1.50
28	G	513	CLA	CMD-C2D	-2.01	1.46	1.50
28	A	316	CLA	CMC-C2C	-2.01	1.46	1.50
26	M	303	DD6	C21-C20	2.01	1.55	1.51
28	M	310	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	731	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	717	CLA	CMC-C2C	-2.01	1.46	1.50
28	K	316	CLA	CMD-C2D	-2.01	1.46	1.50
28	b	727	CLA	CMC-C2C	-2.01	1.46	1.50
28	b	724	CLA	CMD-C2D	-2.01	1.46	1.50
28	b	705	CLA	CMD-C2D	-2.01	1.46	1.50
28	a	714	CLA	CMD-C2D	-2.01	1.46	1.50
28	I	312	CLA	CMD-C2D	-2.00	1.46	1.50
26	L	302	DD6	O1-C20	-2.00	1.43	1.46
28	J	316	CLA	CMD-C2D	-2.00	1.46	1.50
28	G	514	CLA	CMC-C2C	-2.00	1.46	1.50
28	b	719	CLA	CMD-C2D	-2.00	1.46	1.50
28	b	725	CLA	CMC-C2C	-2.00	1.46	1.50
28	l	311	CLA	CMD-C2D	-2.00	1.46	1.50
28	L	318	CLA	CMC-C2C	-2.00	1.46	1.50
28	A	312	CLA	CMD-C2D	-2.00	1.46	1.50
29	N	311	KC1	C4A-C3A	-2.00	1.40	1.44
28	I	319	CLA	CMD-C2D	-2.00	1.46	1.50
28	L	318	CLA	CMD-C2D	-2.00	1.46	1.50
28	M	313	CLA	CMD-C2D	-2.00	1.46	1.50

All (2862) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	304	UIX	O-C1-C3	9.16	120.27	113.38
27	J	305	UIX	O-C1-C3	8.93	120.09	113.38
27	I	304	UIX	C6-C1-C	-8.90	107.34	122.26
27	B	305	UIX	O-C1-C3	8.31	119.63	113.38
35	m	201	BCR	C7-C8-C9	-8.11	113.98	126.23
27	G	503	UIX	O-C1-C3	7.60	119.09	113.38
28	l	304	CLA	C4A-NA-C1A	7.52	110.09	106.71
27	h	201	UIX	O-C1-C3	7.30	118.86	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	307	CLA	C4A-NA-C1A	7.18	109.94	106.71
26	J	303	DD6	C3-C2-C1	-7.10	117.18	127.31
28	N	310	CLA	C4A-NA-C1A	7.09	109.89	106.71
27	G	503	UIX	C6-C1-C	-7.08	110.40	122.26
28	B	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
28	a	702	CLA	C4A-NA-C1A	7.06	109.88	106.71
28	G	512	CLA	C4A-NA-C1A	7.03	109.87	106.71
28	J	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	L	309	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	a	738	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	b	714	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	A	310	CLA	C4A-NA-C1A	7.01	109.86	106.71
28	M	317	CLA	C4A-NA-C1A	7.00	109.85	106.71
28	b	704	CLA	C4A-NA-C1A	6.99	109.85	106.71
28	L	311	CLA	C4A-NA-C1A	6.98	109.84	106.71
28	a	730	CLA	C4A-NA-C1A	6.97	109.84	106.71
28	a	715	CLA	C4A-NA-C1A	6.97	109.84	106.71
28	b	719	CLA	C4A-NA-C1A	6.96	109.83	106.71
28	J	312	CLA	C4A-NA-C1A	6.95	109.83	106.71
28	M	315	CLA	C4A-NA-C1A	6.94	109.83	106.71
27	h	201	UIX	C6-C1-C	-6.94	110.63	122.26
28	b	728	CLA	C4A-NA-C1A	6.94	109.83	106.71
28	B	317	CLA	C4A-NA-C1A	6.93	109.82	106.71
28	b	718	CLA	C4A-NA-C1A	6.91	109.81	106.71
28	L	318	CLA	C4A-NA-C1A	6.91	109.81	106.71
28	D	311	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	J	306	CLA	C4A-NA-C1A	6.87	109.80	106.71
28	K	312	CLA	C4A-NA-C1A	6.86	109.79	106.71
28	a	703	CLA	C4A-NA-C1A	6.86	109.79	106.71
28	l	303	CLA	C4A-NA-C1A	6.85	109.79	106.71
28	B	313	CLA	C4A-NA-C1A	6.85	109.79	106.71
28	N	309	CLA	C4A-NA-C1A	6.85	109.79	106.71
27	J	305	UIX	C6-C1-C	-6.85	110.78	122.26
28	h	202	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	B	315	CLA	C4A-NA-C1A	6.84	109.78	106.71
28	M	310	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	F	310	CLA	C4A-NA-C1A	6.82	109.77	106.71
28	a	714	CLA	C4A-NA-C1A	6.80	109.76	106.71
28	I	306	CLA	C4A-NA-C1A	6.80	109.76	106.71
28	A	308	CLA	C4A-NA-C1A	6.80	109.76	106.71
28	J	315	CLA	C4A-NA-C1A	6.80	109.76	106.71
28	A	307	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	514	CLA	C4A-NA-C1A	6.79	109.76	106.71
27	K	302	UIX	O-C1-C3	6.79	118.48	113.38
28	b	720	CLA	C4A-NA-C1A	6.79	109.76	106.71
28	a	720	CLA	C4A-NA-C1A	6.78	109.76	106.71
28	I	307	CLA	C4A-NA-C1A	6.78	109.75	106.71
27	B	305	UIX	C6-C1-C	-6.78	110.89	122.26
28	a	705	CLA	C4A-NA-C1A	6.77	109.75	106.71
28	F	313	CLA	C4A-NA-C1A	6.77	109.75	106.71
28	A	316	CLA	C4A-NA-C1A	6.76	109.75	106.71
28	A	320	CLA	C4A-NA-C1A	6.76	109.74	106.71
28	b	705	CLA	C4A-NA-C1A	6.74	109.74	106.71
28	b	707	CLA	C4A-NA-C1A	6.74	109.74	106.71
28	a	701	CLA	C4A-NA-C1A	6.74	109.73	106.71
28	b	701	CLA	C4A-NA-C1A	6.74	109.73	106.71
28	a	731	CLA	C4A-NA-C1A	6.72	109.73	106.71
28	b	709	CLA	C4A-NA-C1A	6.72	109.73	106.71
28	I	319	CLA	C4A-NA-C1A	6.72	109.72	106.71
28	F	308	CLA	C4A-NA-C1A	6.72	109.72	106.71
28	F	315	CLA	C4A-NA-C1A	6.70	109.72	106.71
28	K	316	CLA	C4A-NA-C1A	6.70	109.72	106.71
28	b	727	CLA	C4A-NA-C1A	6.69	109.72	106.71
28	G	517	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	a	718	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	I	311	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	G	519	CLA	C4A-NA-C1A	6.67	109.71	106.71
28	N	304	CLA	C4A-NA-C1A	6.67	109.70	106.71
28	b	716	CLA	C4A-NA-C1A	6.67	109.70	106.71
28	B	312	CLA	C4A-NA-C1A	6.67	109.70	106.71
28	B	309	CLA	C4A-NA-C1A	6.66	109.70	106.71
28	a	716	CLA	C4A-NA-C1A	6.65	109.70	106.71
28	M	308	CLA	C4A-NA-C1A	6.65	109.70	106.71
28	K	307	CLA	C4A-NA-C1A	6.65	109.70	106.71
28	G	518	CLA	C4A-NA-C1A	6.65	109.70	106.71
35	b	702	BCR	C24-C23-C22	-6.64	116.19	126.23
28	a	711	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	H	308	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	a	722	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	D	313	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	L	312	CLA	C4A-NA-C1A	6.64	109.69	106.71
28	F	307	CLA	C4A-NA-C1A	6.63	109.69	106.71
28	N	305	CLA	C4A-NA-C1A	6.63	109.69	106.71
35	b	730	BCR	C7-C8-C9	-6.63	116.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	306	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	D	312	CLA	C4A-NA-C1A	6.62	109.68	106.71
26	M	303	DD6	C9-C10-C11	-6.62	117.87	127.31
28	a	725	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	L	316	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	A	311	CLA	C4A-NA-C1A	6.61	109.68	106.71
28	f	303	CLA	C4A-NA-C1A	6.60	109.67	106.71
28	l	313	CLA	C4A-NA-C1A	6.58	109.67	106.71
28	D	309	CLA	C4A-NA-C1A	6.58	109.67	106.71
28	D	316	CLA	C4A-NA-C1A	6.58	109.67	106.71
28	H	312	CLA	C4A-NA-C1A	6.58	109.66	106.71
28	H	305	CLA	C4A-NA-C1A	6.58	109.66	106.71
28	a	710	CLA	C4A-NA-C1A	6.57	109.66	106.71
28	a	728	CLA	C4A-NA-C1A	6.57	109.66	106.71
28	l	311	CLA	C4A-NA-C1A	6.57	109.66	106.71
28	K	308	CLA	C4A-NA-C1A	6.56	109.66	106.71
28	b	724	CLA	C4A-NA-C1A	6.56	109.66	106.71
32	F	305	PID	C17-C16-C15	6.56	136.91	123.47
29	D	315	KC1	CHB-C1B-NB	6.54	130.47	124.45
28	I	310	CLA	C4A-NA-C1A	6.54	109.65	106.71
28	K	311	CLA	C4A-NA-C1A	6.54	109.65	106.71
28	A	317	CLA	C4A-NA-C1A	6.54	109.65	106.71
28	G	510	CLA	C4A-NA-C1A	6.53	109.64	106.71
28	G	516	CLA	C4A-NA-C1A	6.53	109.64	106.71
28	J	311	CLA	C4A-NA-C1A	6.52	109.64	106.71
27	A	304	UIX	O-C1-C3	6.52	118.28	113.38
28	D	308	CLA	C4A-NA-C1A	6.52	109.64	106.71
28	L	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
28	G	509	CLA	C4A-NA-C1A	6.50	109.63	106.71
28	A	312	CLA	C4A-NA-C1A	6.50	109.63	106.71
28	b	726	CLA	C4A-NA-C1A	6.50	109.63	106.71
28	I	315	CLA	C4A-NA-C1A	6.50	109.63	106.71
28	j	106	CLA	C4A-NA-C1A	6.49	109.62	106.71
28	b	712	CLA	C4A-NA-C1A	6.49	109.62	106.71
28	a	708	CLA	C4A-NA-C1A	6.49	109.62	106.71
28	F	311	CLA	C4A-NA-C1A	6.49	109.62	106.71
28	H	307	CLA	C4A-NA-C1A	6.48	109.62	106.71
29	D	310	KC1	CHC-C4B-NB	6.48	130.41	124.45
28	a	707	CLA	C4A-NA-C1A	6.48	109.62	106.71
28	J	316	CLA	C4A-NA-C1A	6.48	109.62	106.71
28	f	301	CLA	C4A-NA-C1A	6.47	109.62	106.71
28	I	321	CLA	C4A-NA-C1A	6.47	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	723	CLA	C4A-NA-C1A	6.47	109.61	106.71
28	M	316	CLA	C4A-NA-C1A	6.47	109.61	106.71
28	l	308	CLA	C4A-NA-C1A	6.47	109.61	106.71
28	I	313	CLA	C4A-NA-C1A	6.46	109.61	106.71
28	b	710	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	A	304	UIX	C6-C1-C	-6.46	111.43	122.26
28	b	715	CLA	C4A-NA-C1A	6.46	109.61	106.71
29	H	310	KC1	CHB-C1B-NB	6.46	130.39	124.45
28	a	706	CLA	C4A-NA-C1A	6.44	109.60	106.71
28	K	315	CLA	C4A-NA-C1A	6.44	109.60	106.71
28	l	309	CLA	C4A-NA-C1A	6.44	109.60	106.71
28	G	511	CLA	C4A-NA-C1A	6.43	109.60	106.71
28	A	313	CLA	C4A-NA-C1A	6.43	109.59	106.71
28	b	723	CLA	C4A-NA-C1A	6.42	109.59	106.71
29	F	309	KC1	CHC-C4B-NB	6.42	130.35	124.45
28	A	319	CLA	C4A-NA-C1A	6.41	109.59	106.71
28	G	513	CLA	C4A-NA-C1A	6.41	109.59	106.71
28	a	727	CLA	C4A-NA-C1A	6.41	109.59	106.71
28	J	301	CLA	C4A-NA-C1A	6.40	109.58	106.71
28	A	315	CLA	C4A-NA-C1A	6.40	109.58	106.71
28	B	301	CLA	C4A-NA-C1A	6.40	109.58	106.71
28	K	310	CLA	C4A-NA-C1A	6.40	109.58	106.71
28	b	708	CLA	C4A-NA-C1A	6.39	109.58	106.71
26	F	301	DD6	C9-C10-C11	-6.39	118.19	127.31
29	F	314	KC1	CHB-C1B-NB	6.39	130.33	124.45
28	a	729	CLA	C4A-NA-C1A	6.39	109.58	106.71
28	b	722	CLA	C4A-NA-C1A	6.38	109.58	106.71
29	H	306	KC1	CHB-C1B-NB	6.38	130.32	124.45
29	M	314	KC1	CHB-C1B-NB	6.38	130.31	124.45
28	f	302	CLA	C4A-NA-C1A	6.37	109.57	106.71
29	D	310	KC1	CHB-C1B-NB	6.37	130.31	124.45
28	H	309	CLA	C4A-NA-C1A	6.37	109.57	106.71
28	b	717	CLA	C4A-NA-C1A	6.36	109.57	106.71
28	b	703	CLA	C4A-NA-C1A	6.36	109.56	106.71
28	A	309	CLA	C4A-NA-C1A	6.35	109.56	106.71
35	l	302	BCR	C24-C23-C22	-6.35	116.64	126.23
26	K	319	DD6	C9-C10-C11	-6.35	118.25	127.31
28	I	316	CLA	C4A-NA-C1A	6.35	109.56	106.71
28	b	725	CLA	C4A-NA-C1A	6.34	109.56	106.71
28	L	310	CLA	C4A-NA-C1A	6.34	109.56	106.71
28	J	314	CLA	C4A-NA-C1A	6.33	109.55	106.71
32	F	305	PID	C18-C19-C20	6.32	136.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	m	202	CLA	C4A-NA-C1A	6.32	109.55	106.71
28	M	311	CLA	C4A-NA-C1A	6.31	109.55	106.71
28	a	712	CLA	C4A-NA-C1A	6.31	109.54	106.71
28	K	309	CLA	C4A-NA-C1A	6.31	109.54	106.71
28	b	713	CLA	C4A-NA-C1A	6.31	109.54	106.71
28	M	318	CLA	C4A-NA-C1A	6.31	109.54	106.71
29	A	314	KC1	CHB-C1B-NB	6.31	130.25	124.45
28	B	316	CLA	C4A-NA-C1A	6.30	109.54	106.71
29	L	315	KC1	CHB-C1B-NB	6.30	130.24	124.45
28	b	721	CLA	C4A-NA-C1A	6.29	109.53	106.71
28	a	721	CLA	C4A-NA-C1A	6.29	109.53	106.71
28	H	304	CLA	C4A-NA-C1A	6.29	109.53	106.71
29	B	314	KC1	CHB-C1B-NB	6.28	130.23	124.45
26	M	302	DD6	C3-C2-C1	-6.28	118.35	127.31
28	l	305	CLA	C4A-NA-C1A	6.27	109.53	106.71
26	A	302	DD6	C9-C10-C11	-6.27	118.36	127.31
28	K	313	CLA	C4A-NA-C1A	6.27	109.52	106.71
28	b	706	CLA	C4A-NA-C1A	6.27	109.52	106.71
28	b	711	CLA	C4A-NA-C1A	6.26	109.52	106.71
29	I	314	KC1	CHB-C1B-NB	6.25	130.20	124.45
29	N	311	KC1	CHC-C4B-NB	6.24	130.19	124.45
28	L	317	CLA	C4A-NA-C1A	6.23	109.51	106.71
28	B	307	CLA	C4A-NA-C1A	6.23	109.51	106.71
29	H	306	KC1	CHC-C4B-NB	6.23	130.18	124.45
29	N	306	KC1	CHB-C1B-NB	6.22	130.17	124.45
26	F	301	DD6	C4-C5-C6	-6.22	118.43	127.31
29	L	307	KC1	CHC-C4B-NB	6.22	130.17	124.45
28	M	309	CLA	C4A-NA-C1A	6.21	109.50	106.71
28	I	312	CLA	C4A-NA-C1A	6.21	109.50	106.71
29	K	314	KC1	CHC-C4B-NB	6.20	130.16	124.45
28	J	308	CLA	C4A-NA-C1A	6.20	109.49	106.71
28	a	724	CLA	C4A-NA-C1A	6.20	109.49	106.71
28	H	311	CLA	C4A-NA-C1A	6.19	109.49	106.71
28	D	314	CLA	C4A-NA-C1A	6.19	109.49	106.71
28	I	308	CLA	C4A-NA-C1A	6.18	109.48	106.71
28	j	104	CLA	C4A-NA-C1A	6.18	109.48	106.71
28	G	520	CLA	C4A-NA-C1A	6.17	109.48	106.71
29	F	314	KC1	CHC-C4B-NB	6.17	130.12	124.45
29	N	311	KC1	CHB-C1B-NB	6.17	130.12	124.45
29	K	314	KC1	CHB-C1B-NB	6.15	130.10	124.45
29	F	309	KC1	CHB-C1B-NB	6.15	130.10	124.45
28	N	307	CLA	C4A-NA-C1A	6.15	109.47	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	308	CLA	C4A-NA-C1A	6.14	109.47	106.71
29	J	313	KC1	CHB-C1B-NB	6.14	130.09	124.45
28	B	311	CLA	C4A-NA-C1A	6.13	109.46	106.71
29	L	307	KC1	CHB-C1B-NB	6.12	130.08	124.45
28	M	313	CLA	C4A-NA-C1A	6.12	109.46	106.71
28	a	709	CLA	C4A-NA-C1A	6.11	109.45	106.71
29	N	306	KC1	CHC-C4B-NB	6.11	130.07	124.45
29	I	314	KC1	CHC-C4B-NB	6.11	130.07	124.45
32	H	301	PID	C17-C16-C15	6.10	135.98	123.47
29	N	308	KC1	CHB-C1B-NB	6.10	130.06	124.45
28	l	312	CLA	C4A-NA-C1A	6.09	109.44	106.71
27	K	302	UIX	C6-C1-C	-6.08	112.07	122.26
28	F	312	CLA	C4A-NA-C1A	6.06	109.43	106.71
29	M	314	KC1	CHC-C4B-NB	6.05	130.02	124.45
29	A	314	KC1	CHC-C4B-NB	6.05	130.01	124.45
28	M	312	CLA	C4A-NA-C1A	6.04	109.42	106.71
28	a	717	CLA	C4A-NA-C1A	6.03	109.42	106.71
28	L	313	CLA	C4A-NA-C1A	6.03	109.42	106.71
28	a	719	CLA	C4A-NA-C1A	6.03	109.42	106.71
29	G	515	KC1	CHB-C1B-NB	6.02	129.99	124.45
29	B	314	KC1	CHC-C4B-NB	6.02	129.99	124.45
29	L	315	KC1	CHC-C4B-NB	6.02	129.99	124.45
29	A	306	KC1	CHB-C1B-NB	6.02	129.98	124.45
28	I	309	CLA	C4A-NA-C1A	6.02	109.41	106.71
29	H	310	KC1	CHC-C4B-NB	5.99	129.96	124.45
29	M	307	KC1	CHC-C4B-NB	5.98	129.95	124.45
29	A	306	KC1	CHC-C4B-NB	5.96	129.94	124.45
27	K	302	UIX	C14-C13-C11	-5.96	118.80	127.31
35	m	201	BCR	C15-C14-C13	-5.93	118.85	127.31
26	A	302	DD6	C14-C13-C11	-5.92	116.34	125.53
29	M	307	KC1	CHB-C1B-NB	5.92	129.89	124.45
26	J	304	DD6	C9-C10-C11	-5.91	118.87	127.31
29	J	313	KC1	CHC-C4B-NB	5.89	129.86	124.45
35	a	736	BCR	C7-C8-C9	-5.86	117.38	126.23
28	a	704	CLA	C4A-NA-C1A	5.82	109.32	106.71
32	M	301	PID	C17-C16-C15	5.80	135.35	123.47
26	A	301	DD6	C21-C20-C19	5.79	120.79	114.28
29	N	308	KC1	O2D-CGD-CBD	5.78	121.54	111.27
28	a	735	CLA	C4A-NA-C1A	5.78	109.30	106.71
32	F	304	PID	C17-C16-C15	5.78	135.30	123.47
27	J	305	UIX	C34-C30-C26	-5.76	119.08	127.31
35	j	102	BCR	C16-C17-C18	-5.75	119.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	306	DD6	C3-C2-C1	-5.75	119.11	127.31
26	G	504	DD6	O1-C20-C19	5.75	117.70	113.38
26	J	302	DD6	C3-C2-C1	-5.72	119.14	127.31
26	I	305	DD6	C4-C5-C6	-5.71	119.16	127.31
28	a	726	CLA	C4A-NA-C1A	5.71	109.27	106.71
28	J	310	CLA	C4A-NA-C1A	5.70	109.27	106.71
35	b	702	BCR	C16-C17-C18	-5.70	119.18	127.31
26	J	303	DD6	O1-C20-C19	5.70	117.66	113.38
26	G	504	DD6	C4-C5-C6	-5.70	119.18	127.31
32	F	302	PID	C18-C19-C20	5.66	135.06	123.47
26	I	305	DD6	C3-C2-C1	-5.64	119.25	127.31
32	D	304	PID	C17-C16-C15	5.63	135.01	123.47
27	K	302	UIX	C34-C30-C26	-5.63	119.28	127.31
29	N	308	KC1	CHC-C4B-NB	5.61	129.61	124.45
26	J	304	DD6	C3-C2-C1	-5.59	119.33	127.31
26	G	505	DD6	C3-C2-C1	-5.56	119.37	127.31
28	B	310	CLA	C4A-NA-C1A	5.56	109.20	106.71
29	G	515	KC1	CHC-C4B-NB	5.55	129.56	124.45
28	a	713	CLA	C4A-NA-C1A	5.55	109.20	106.71
32	N	302	PID	C18-C19-C20	5.53	134.81	123.47
26	A	303	DD6	C21-C20-C19	5.51	120.48	114.28
26	J	303	DD6	C4-C5-C6	-5.48	119.48	127.31
26	F	301	DD6	C21-C20-C19	5.48	120.44	114.28
35	i	201	BCR	C24-C23-C22	-5.47	117.98	126.23
35	a	736	BCR	C11-C10-C9	-5.45	119.54	127.31
26	M	305	DD6	C3-C2-C1	-5.44	119.55	127.31
26	I	301	DD6	C21-C20-C19	5.44	120.40	114.28
35	b	702	BCR	C20-C21-C22	-5.44	119.55	127.31
26	A	301	DD6	C9-C10-C11	-5.42	119.57	127.31
26	L	306	DD6	C9-C10-C11	-5.42	119.58	127.31
26	G	502	DD6	C21-C20-C19	5.41	120.37	114.28
26	B	303	DD6	C21-C20-C19	5.41	120.36	114.28
26	A	305	DD6	C21-C20-C19	5.39	120.35	114.28
26	G	505	DD6	O1-C20-C21	5.37	121.48	115.06
26	F	303	DD6	C4-C5-C6	-5.36	119.66	127.31
26	I	302	DD6	C9-C10-C11	-5.35	119.68	127.31
26	I	301	DD6	C9-C10-C11	-5.35	119.68	127.31
26	J	303	DD6	C9-C10-C11	-5.33	119.70	127.31
35	b	730	BCR	C15-C14-C13	-5.31	119.73	127.31
35	b	730	BCR	C3-C4-C5	-5.30	104.62	114.08
32	M	301	PID	CM4-C14-C15	-5.29	115.51	122.92
26	A	301	DD6	O1-C20-C19	-5.25	109.44	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	301	DD6	C4-C5-C6	-5.24	119.83	127.31
26	K	304	DD6	C21-C20-C19	5.24	120.17	114.28
26	J	302	DD6	C14-C13-C11	-5.23	117.41	125.53
26	J	302	DD6	C9-C10-C11	-5.23	119.84	127.31
32	D	304	PID	C18-C19-C20	5.22	134.17	123.47
26	L	302	DD6	C14-C13-C11	-5.21	117.45	125.53
35	f	304	BCR	C15-C14-C13	-5.20	119.89	127.31
35	l	307	BCR	C3-C4-C5	-5.19	104.80	114.08
32	D	304	PID	CM4-C14-C15	-5.19	115.65	122.92
29	D	315	KC1	CHC-C4B-NB	5.18	129.22	124.45
26	G	508	DD6	C21-C20-C19	5.17	120.10	114.28
26	A	302	DD6	C3-C2-C1	-5.17	119.94	127.31
27	h	201	UIX	C37-C39-C40	-5.14	119.97	127.31
26	B	302	DD6	C3-C2-C1	-5.13	119.98	127.31
26	M	302	DD6	O1-C20-C19	5.13	117.23	113.38
29	L	307	KC1	O2D-CGD-CBD	5.09	120.32	111.27
26	N	303	DD6	C4-C5-C6	-5.08	120.06	127.31
35	b	730	BCR	C11-C10-C9	-5.08	120.07	127.31
32	H	301	PID	CM4-C14-C15	-5.07	115.82	122.92
26	K	305	DD6	C3-C2-C1	-5.06	120.09	127.31
27	B	305	UIX	O2-C27-C31	5.06	120.40	111.09
26	B	306	DD6	C3-C2-C1	-5.06	120.09	127.31
35	a	734	BCR	C15-C14-C13	-5.05	120.10	127.31
26	M	304	DD6	C21-C20-C19	5.05	119.96	114.28
26	F	301	DD6	C3-C2-C1	-5.05	120.11	127.31
26	F	301	DD6	O1-C20-C19	-5.04	109.60	113.38
26	H	303	DD6	C21-C20-C19	5.04	119.95	114.28
29	F	309	KC1	O2D-CGD-CBD	5.01	120.17	111.27
26	G	502	DD6	C4-C5-C6	-5.00	120.17	127.31
26	G	508	DD6	C3-C2-C1	-5.00	120.17	127.31
26	B	304	DD6	C21-C20-C19	5.00	119.90	114.28
29	M	314	KC1	O2D-CGD-CBD	5.00	120.14	111.27
29	A	306	KC1	O2D-CGD-CBD	4.99	120.13	111.27
32	F	304	PID	CM4-C14-C15	-4.98	115.95	122.92
26	K	301	DD6	C21-C20-C19	4.97	119.87	114.28
26	G	508	DD6	C4-C5-C6	-4.96	120.23	127.31
26	G	504	DD6	C3-C2-C1	-4.96	120.23	127.31
35	f	304	BCR	C11-C10-C9	-4.95	120.24	127.31
35	m	201	BCR	C11-C10-C9	-4.95	120.25	127.31
26	K	304	DD6	C3-C2-C1	-4.95	120.25	127.31
26	B	306	DD6	C21-C20-C19	4.94	119.84	114.28
26	I	305	DD6	C15-C14-C13	-4.94	115.56	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	303	DD6	C21-C20-C19	4.93	119.83	114.28
26	L	306	DD6	C4-C5-C6	-4.93	120.27	127.31
26	K	305	DD6	C21-C20-C19	4.93	119.83	114.28
29	J	313	KC1	O2D-CGD-CBD	4.92	120.01	111.27
26	M	306	DD6	C4-C5-C6	-4.92	120.29	127.31
26	L	303	DD6	C21-C20-C19	4.91	119.81	114.28
27	I	304	UIX	O-C1-C6	4.91	120.94	115.06
32	F	302	PID	CM4-C14-C15	-4.90	116.05	122.92
27	K	302	UIX	C16-C20-C15	4.88	124.54	119.70
26	h	203	DD6	C21-C20-C19	4.87	119.76	114.28
26	L	305	DD6	C21-C20-C19	4.87	119.75	114.28
29	L	315	KC1	O2D-CGD-CBD	4.87	119.92	111.27
29	D	315	KC1	O2D-CGD-CBD	4.87	119.91	111.27
29	H	310	KC1	O2D-CGD-CBD	4.86	119.91	111.27
26	K	303	DD6	C21-C20-C19	4.86	119.75	114.28
26	L	303	DD6	C3-C2-C1	-4.86	120.37	127.31
29	N	311	KC1	O2D-CGD-CBD	4.85	119.89	111.27
26	B	303	DD6	O1-C20-C19	-4.84	109.75	113.38
32	N	301	PID	C17-C16-C15	4.83	133.38	123.47
27	h	201	UIX	O2-C27-C31	4.83	119.97	111.09
26	L	306	DD6	C21-C20-C19	4.82	119.70	114.28
27	K	302	UIX	O-C1-C6	4.82	120.83	115.06
26	L	302	DD6	C21-C20-C19	4.80	119.68	114.28
26	G	505	DD6	C9-C10-C11	-4.79	120.47	127.31
27	K	302	UIX	C17-C15-C20	4.79	113.87	109.21
26	F	303	DD6	C21-C20-C19	4.79	119.66	114.28
35	a	736	BCR	C16-C17-C18	-4.78	120.49	127.31
26	M	302	DD6	C15-C14-C13	-4.78	115.89	125.99
26	G	505	DD6	C4-C5-C6	-4.75	120.53	127.31
27	A	304	UIX	O-C1-C6	4.75	120.75	115.06
32	N	301	PID	CM4-C14-C15	-4.75	116.28	122.92
26	I	301	DD6	C3-C2-C1	-4.75	120.54	127.31
35	l	306	BCR	C7-C8-C9	-4.74	119.07	126.23
29	F	314	KC1	O2D-CGD-CBD	4.73	119.68	111.27
26	M	305	DD6	C21-C20-C19	4.73	119.60	114.28
26	K	319	DD6	C4-C5-C6	-4.72	120.57	127.31
35	i	201	BCR	C20-C21-C22	-4.72	120.57	127.31
35	l	306	BCR	C33-C5-C6	-4.71	119.24	124.53
26	K	319	DD6	C3-C2-C1	-4.71	120.59	127.31
29	H	306	KC1	O2D-CGD-CBD	4.71	119.64	111.27
26	I	302	DD6	C21-C20-C19	4.71	119.57	114.28
26	M	304	DD6	C3-C2-C1	-4.71	120.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	306	DD6	C9-C10-C11	-4.70	120.60	127.31
28	a	724	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
29	A	314	KC1	O2D-CGD-CBD	4.70	119.62	111.27
29	N	308	KC1	O2D-CGD-O1D	-4.69	114.67	123.84
27	A	304	UIX	O2-C27-C31	4.68	119.69	111.09
35	l	306	BCR	C16-C17-C18	-4.68	120.64	127.31
26	K	301	DD6	C4-C5-C6	-4.67	120.64	127.31
29	I	314	KC1	O2D-CGD-CBD	4.67	119.56	111.27
35	j	102	BCR	C15-C14-C13	-4.66	120.66	127.31
26	D	303	DD6	C21-C20-C19	4.64	119.50	114.28
35	l	302	BCR	C28-C27-C26	-4.64	105.79	114.08
32	D	301	PID	CM4-C14-C15	-4.64	116.42	122.92
29	M	307	KC1	O2D-CGD-CBD	4.63	119.50	111.27
35	f	304	BCR	C16-C17-C18	-4.63	120.71	127.31
26	L	305	DD6	C3-C2-C1	-4.62	120.72	127.31
26	M	303	DD6	C4-C5-C6	-4.60	120.75	127.31
35	i	201	BCR	C15-C14-C13	-4.59	120.76	127.31
26	I	303	DD6	C9-C10-C11	-4.59	120.76	127.31
26	b	731	DD6	C21-C20-C19	4.58	119.44	114.28
26	I	303	DD6	C21-C20-C19	4.58	119.43	114.28
28	m	202	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
26	A	301	DD6	C3-C2-C1	-4.58	120.78	127.31
26	B	302	DD6	C9-C10-C11	-4.56	120.80	127.31
29	G	515	KC1	O2D-CGD-CBD	4.56	119.37	111.27
29	B	314	KC1	O2D-CGD-CBD	4.56	119.37	111.27
26	N	303	DD6	C9-C10-C11	-4.55	120.81	127.31
32	G	506	PID	CM4-C14-C15	-4.54	116.56	122.92
32	F	306	PID	CM4-C14-C15	-4.53	116.58	122.92
29	K	314	KC1	O2D-CGD-CBD	4.53	119.32	111.27
35	a	736	BCR	C15-C14-C13	-4.52	120.86	127.31
32	F	304	PID	C6-C7-C8	4.52	135.54	125.99
26	I	305	DD6	C20-C19-C18	-4.51	103.83	112.75
26	F	303	DD6	O1-C20-C19	-4.50	110.00	113.38
26	L	304	DD6	C21-C20-C19	4.50	119.34	114.28
26	I	302	DD6	C3-C2-C1	-4.49	120.91	127.31
35	a	734	BCR	C16-C17-C18	-4.49	120.91	127.31
26	I	301	DD6	O1-C20-C19	-4.48	110.01	113.38
35	l	302	BCR	C16-C17-C18	-4.48	120.92	127.31
26	M	303	DD6	C3-C2-C1	-4.47	120.92	127.31
32	D	301	PID	C17-C16-C15	4.47	132.64	123.47
27	K	302	UIX	O2-C27-C31	4.47	119.32	111.09
26	b	731	DD6	C4-C5-C6	-4.47	120.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	729	PQN	C11-C12-C13	-4.46	119.36	126.79
26	J	302	DD6	C4-C5-C6	-4.46	120.95	127.31
27	G	503	UIX	O2-C27-C31	4.45	119.28	111.09
35	l	307	BCR	C15-C14-C13	-4.43	120.98	127.31
35	b	732	BCR	C33-C5-C6	-4.43	119.55	124.53
26	G	502	DD6	C9-C10-C11	-4.43	120.99	127.31
29	N	308	KC1	O1D-CGD-CBD	-4.43	115.43	124.48
26	N	303	DD6	C3-C2-C1	-4.42	121.00	127.31
26	M	303	DD6	C20-C19-C18	-4.42	104.00	112.75
26	J	303	DD6	C15-C14-C13	-4.42	116.64	125.99
29	N	306	KC1	O2D-CGD-CBD	4.42	119.12	111.27
27	h	201	UIX	C-C7-C10	-4.42	116.65	125.99
26	A	305	DD6	C37-C36-C31	-4.41	118.36	124.35
35	j	102	BCR	C20-C21-C22	-4.40	121.03	127.31
27	K	302	UIX	C21-C15-C20	-4.40	106.53	110.47
27	J	305	UIX	O2-C27-C31	4.40	119.18	111.09
26	M	306	DD6	C20-C19-C18	-4.40	104.05	112.75
26	B	304	DD6	C3-C2-C1	-4.39	121.04	127.31
27	I	304	UIX	O2-C27-C31	4.39	119.16	111.09
28	b	722	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
32	D	307	PID	CM4-C14-C15	-4.38	116.79	122.92
27	A	304	UIX	C6-C1-C3	4.37	119.20	114.28
26	L	305	DD6	C9-C10-C11	-4.37	121.07	127.31
26	I	305	DD6	C21-C20-C19	4.37	119.19	114.28
32	D	305	PID	C18-C19-C20	4.37	132.42	123.47
35	l	306	BCR	C38-C26-C25	-4.37	119.63	124.53
26	h	203	DD6	C3-C2-C1	-4.34	121.12	127.31
26	b	731	DD6	C15-C14-C13	-4.33	116.83	125.99
26	F	303	DD6	C9-C10-C11	-4.33	121.13	127.31
32	D	306	PID	CM4-C14-C15	-4.33	116.86	122.92
29	D	310	KC1	O2D-CGD-CBD	4.33	118.96	111.27
32	N	302	PID	CM4-C14-C15	-4.32	116.87	122.92
26	D	303	DD6	O1-C20-C19	4.32	116.62	113.38
26	J	303	DD6	O1-C20-C21	4.30	120.21	115.06
26	L	306	DD6	C3-C2-C1	-4.29	121.18	127.31
26	D	303	DD6	C10-C9-C8	-4.29	109.82	123.22
26	H	303	DD6	C4-C5-C6	-4.28	121.21	127.31
26	K	301	DD6	C15-C14-C13	-4.28	116.95	125.99
32	G	507	PID	CM4-C14-C15	-4.26	116.95	122.92
26	N	303	DD6	O1-C20-C19	-4.26	110.18	113.38
28	a	711	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
35	b	732	BCR	C16-C17-C18	-4.25	121.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	201	BCR	C16-C17-C18	-4.25	121.25	127.31
26	L	304	DD6	C3-C2-C1	-4.24	121.25	127.31
27	I	304	UIX	C7-C10-C11	-4.24	118.95	125.53
26	M	306	DD6	C25-C24-C1	-4.22	114.57	126.42
28	J	311	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
32	D	306	PID	C18-C19-C20	4.21	132.09	123.47
26	B	303	DD6	C37-C36-C31	-4.20	118.64	124.35
32	D	304	PID	C12-O4-C10	4.20	109.84	107.65
27	B	305	UIX	O-C1-C6	4.20	120.09	115.06
32	M	301	PID	C12-O4-C10	4.20	109.83	107.65
28	L	310	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
26	L	303	DD6	C37-C36-C31	-4.19	118.65	124.35
28	G	520	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	B	303	DD6	C4-C5-C6	-4.18	121.35	127.31
28	f	302	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
26	B	304	DD6	C37-C36-C31	-4.17	118.68	124.35
30	G	521	DGD	O2G-C1B-C2B	4.17	120.48	111.50
26	H	303	DD6	C3-C2-C1	-4.17	121.36	127.31
27	G	503	UIX	O-C1-C6	4.16	120.05	115.06
28	K	313	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
26	K	304	DD6	C15-C14-C13	-4.16	117.20	125.99
26	I	303	DD6	C37-C36-C31	-4.16	118.70	124.35
28	A	309	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
26	A	305	DD6	C4-C5-C6	-4.15	121.38	127.31
35	m	201	BCR	C38-C26-C25	-4.15	119.86	124.53
26	B	302	DD6	C14-C13-C11	-4.14	119.10	125.53
27	A	304	UIX	C16-C20-C15	4.14	123.80	119.70
32	D	306	PID	C17-C16-C15	4.13	131.94	123.47
28	G	513	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
27	h	201	UIX	O-C1-C6	4.13	120.00	115.06
26	M	302	DD6	O1-C20-C21	4.12	119.99	115.06
30	j	103	DGD	O2G-C1B-C2B	4.12	120.37	111.50
26	I	302	DD6	C7-C6-C8	4.11	124.56	118.08
26	L	303	DD6	C9-C10-C11	-4.11	121.44	127.31
28	M	312	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
26	L	305	DD6	C4-C5-C6	-4.11	121.44	127.31
28	I	310	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
28	A	312	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
26	L	302	DD6	C3-C2-C1	-4.11	121.45	127.31
28	K	309	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
32	F	302	PID	C12-O4-C10	4.09	109.78	107.65
30	L	301	DGD	O2G-C1B-C2B	4.08	120.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	734	BCR	C11-C10-C9	-4.07	121.50	127.31
26	J	303	DD6	C37-C36-C31	-4.07	118.81	124.35
28	J	310	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
26	K	319	DD6	C14-C13-C11	-4.07	119.22	125.53
28	I	319	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
32	D	301	PID	C18-C19-C20	4.06	131.79	123.47
28	G	510	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
28	I	313	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	J	302	DD6	C37-C36-C31	-4.04	118.86	124.35
28	M	315	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
27	J	305	UIX	C34-C37-C39	-4.03	115.22	123.47
28	l	304	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	a	703	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
28	b	714	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
28	K	307	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
28	J	308	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
30	y	201	DGD	O2G-C1B-C2B	4.02	120.17	111.50
35	a	734	BCR	C33-C5-C6	-4.02	120.01	124.53
26	A	301	DD6	C4-C5-C6	-4.02	121.58	127.31
35	b	732	BCR	C15-C14-C13	-4.02	121.58	127.31
28	b	717	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
26	M	303	DD6	O1-C20-C21	4.02	119.87	115.06
28	A	308	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
28	K	315	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
28	a	722	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
26	L	302	DD6	C9-C10-C11	-3.99	121.61	127.31
26	K	319	DD6	O1-C20-C21	-3.99	110.27	115.06
35	a	734	BCR	C28-C27-C26	-3.99	106.95	114.08
32	H	301	PID	C12-O4-C10	3.99	109.72	107.65
26	H	303	DD6	C15-C14-C13	-3.98	117.58	125.99
28	b	706	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
28	B	309	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
27	h	201	UIX	C16-C20-C15	3.97	123.64	119.70
35	l	306	BCR	C20-C21-C22	-3.97	121.64	127.31
26	I	302	DD6	C12-C11-C13	3.97	124.33	118.08
28	G	518	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
28	L	314	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
26	G	505	DD6	C37-C36-C31	-3.96	118.97	124.35
28	a	704	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
26	L	302	DD6	C4-C5-C6	-3.95	121.67	127.31
26	I	303	DD6	O1-C20-C19	-3.95	110.41	113.38
32	F	304	PID	C12-O4-C10	3.95	109.71	107.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	m	201	BCR	C3-C4-C5	-3.95	107.03	114.08
26	K	301	DD6	C37-C36-C31	-3.94	118.99	124.35
28	a	714	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
27	B	305	UIX	C37-C39-C40	-3.94	121.68	127.31
28	I	316	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
28	a	709	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
27	h	201	UIX	C6-C1-C3	3.94	118.71	114.28
28	A	310	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
32	F	306	PID	C17-C16-C15	3.93	131.53	123.47
28	a	706	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
26	B	304	DD6	C15-C14-C13	-3.92	117.70	125.99
26	B	304	DD6	C4-C5-C6	-3.92	121.72	127.31
32	N	301	PID	C12-O4-C10	3.92	109.69	107.65
28	D	309	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
28	m	202	CLA	CMB-C2B-C3B	3.92	132.00	124.68
35	i	201	BCR	C7-C8-C9	-3.91	120.32	126.23
29	H	310	KC1	C3D-CAD-CBD	-3.91	102.46	107.61
26	L	304	DD6	C37-C36-C31	-3.91	119.04	124.35
28	H	305	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	I	303	DD6	C4-C5-C6	-3.90	121.75	127.31
27	A	304	UIX	C34-C30-C26	-3.90	121.75	127.31
35	m	201	BCR	C15-C16-C17	-3.89	115.50	123.47
29	J	313	KC1	C3D-CAD-CBD	-3.89	102.48	107.61
30	G	501	DGD	O2G-C1B-C2B	3.87	119.85	111.50
29	L	315	KC1	C3D-CAD-CBD	-3.87	102.50	107.61
30	I	317	DGD	O2G-C1B-C2B	3.87	119.85	111.50
26	K	303	DD6	C15-C14-C13	-3.87	117.81	125.99
26	L	304	DD6	C4-C5-C6	-3.87	121.79	127.31
28	a	713	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
26	b	731	DD6	C9-C10-C11	-3.86	121.80	127.31
32	D	302	PID	CM4-C14-C15	-3.86	117.51	122.92
26	M	304	DD6	C15-C14-C13	-3.86	117.83	125.99
35	f	304	BCR	C33-C5-C6	-3.86	120.19	124.53
26	D	303	DD6	C37-C36-C31	-3.86	119.11	124.35
26	G	508	DD6	C9-C10-C11	-3.86	121.81	127.31
26	F	303	DD6	C15-C14-C13	-3.85	117.86	125.99
29	F	314	KC1	C3D-CAD-CBD	-3.84	102.54	107.61
28	b	725	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
26	A	305	DD6	O1-C20-C19	-3.84	110.49	113.38
35	b	730	BCR	C16-C17-C18	-3.84	121.82	127.31
32	D	307	PID	C12-O4-C10	3.84	109.65	107.65
28	N	307	CLA	CMB-C2B-C1B	-3.84	122.56	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	102	BCR	C24-C23-C22	-3.84	120.43	126.23
27	G	503	UIX	C-C7-C10	-3.84	117.87	125.99
26	M	302	DD6	C21-C20-C15	-3.84	115.82	122.26
28	a	717	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
30	l	301	DGD	O2G-C1B-C2B	3.83	119.76	111.50
32	j	105	PID	CM4-C14-C15	-3.83	117.56	122.92
26	F	303	DD6	C3-C2-C1	-3.83	121.84	127.31
28	l	312	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
28	F	315	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
35	l	302	BCR	C33-C5-C6	-3.82	120.24	124.53
32	G	506	PID	C17-C16-C15	3.82	131.29	123.47
32	F	302	PID	C17-C16-C15	3.82	131.29	123.47
35	f	304	BCR	C20-C21-C22	-3.81	121.87	127.31
27	J	305	UIX	C14-C13-C11	-3.81	121.87	127.31
26	I	303	DD6	C3-C2-C1	-3.81	121.88	127.31
28	b	721	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
27	G	503	UIX	C6-C1-C3	3.81	118.56	114.28
26	J	304	DD6	C24-C1-C2	3.81	124.78	118.94
26	M	302	DD6	C4-C5-C6	-3.80	121.88	127.31
28	a	723	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
28	D	313	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
32	F	306	PID	C12-O4-C10	3.79	109.62	107.65
26	M	302	DD6	C37-C36-C31	-3.79	119.20	124.35
28	N	305	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
35	b	702	BCR	C16-C15-C14	-3.79	115.71	123.47
28	M	310	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
35	f	304	BCR	C28-C27-C26	-3.79	107.31	114.08
28	a	705	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
28	b	712	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
27	I	304	UIX	C37-C39-C40	-3.77	121.93	127.31
29	N	308	KC1	CBD-CHA-C1A	3.77	135.90	128.88
28	M	311	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
28	I	308	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
26	I	302	DD6	C14-C13-C11	3.76	131.36	125.53
27	I	304	UIX	C14-C13-C11	-3.76	121.95	127.31
32	D	301	PID	C12-O4-C10	3.75	109.60	107.65
28	b	713	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
26	A	302	DD6	C4-C5-C6	-3.74	121.98	127.31
26	K	304	DD6	O1-C20-C19	-3.74	110.58	113.38
35	f	304	BCR	C7-C8-C9	-3.73	120.59	126.23
35	b	730	BCR	C4-C5-C6	-3.73	117.31	122.73
28	J	314	CLA	CMB-C2B-C1B	-3.73	122.73	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	302	DD6	C21-C20-C19	3.73	118.47	114.28
28	a	735	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
32	D	302	PID	C18-C19-C20	3.72	131.10	123.47
28	b	720	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	F	312	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	b	707	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
26	M	306	DD6	C21-C20-C19	3.71	118.45	114.28
28	b	716	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
28	I	309	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
28	b	715	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
28	L	313	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
28	G	519	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
26	L	306	DD6	C37-C36-C31	-3.70	119.32	124.35
26	G	502	DD6	C3-C2-C1	-3.70	122.03	127.31
28	M	313	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
28	K	310	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
26	J	304	DD6	C4-C5-C6	-3.69	122.04	127.31
26	I	302	DD6	C12-C11-C10	-3.69	117.76	122.92
28	H	312	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
26	G	505	DD6	C20-C19-C18	-3.68	105.46	112.75
26	B	302	DD6	C21-C20-C19	3.68	118.42	114.28
28	l	305	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
28	b	708	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
28	B	310	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	I	301	DD6	C15-C14-C13	-3.67	118.22	125.99
28	M	309	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
28	L	311	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
26	M	302	DD6	C-C1-C2	-3.67	117.79	122.92
28	F	310	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
32	F	305	PID	C12-O4-C10	3.66	109.56	107.65
26	M	304	DD6	C37-C36-C31	-3.66	119.38	124.35
26	A	303	DD6	O1-C20-C19	-3.66	110.64	113.38
28	a	728	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
28	B	315	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
32	D	305	PID	CM4-C14-C15	-3.65	117.81	122.92
27	B	305	UIX	C34-C30-C26	-3.65	122.10	127.31
27	J	305	UIX	C14-C23-C26	-3.65	116.17	126.42
27	J	305	UIX	O-C1-C6	3.65	119.43	115.06
28	G	511	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
35	l	306	BCR	C11-C10-C9	-3.65	122.11	127.31
26	G	508	DD6	C15-C14-C13	-3.64	118.29	125.99
28	I	321	CLA	CMB-C2B-C1B	-3.64	122.87	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	719	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
27	G	503	UIX	C34-C30-C26	-3.64	122.12	127.31
28	H	308	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
28	a	701	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
32	H	302	PID	C18-C19-C20	3.62	130.90	123.47
28	b	701	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
26	I	303	DD6	C14-C13-C11	-3.62	119.92	125.53
28	D	311	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
26	L	305	DD6	C37-C36-C31	-3.62	119.43	124.35
28	b	710	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
26	A	305	DD6	C3-C2-C1	-3.61	122.16	127.31
29	M	314	KC1	C3D-CAD-CBD	-3.61	102.85	107.61
28	a	719	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
26	I	302	DD6	C37-C36-C31	-3.61	119.45	124.35
28	a	720	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
28	L	309	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
28	G	517	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
28	A	315	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
28	f	303	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
28	F	311	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
26	L	303	DD6	C4-C5-C6	-3.58	122.20	127.31
28	B	313	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
26	A	302	DD6	C37-C36-C31	-3.58	119.49	124.35
28	B	307	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
32	H	302	PID	CM4-C14-C15	-3.58	117.92	122.92
26	L	306	DD6	C14-C13-C11	-3.57	119.99	125.53
28	K	308	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
28	a	712	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
28	D	316	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
32	D	306	PID	C12-O4-C10	3.57	109.51	107.65
26	M	305	DD6	C37-C36-C31	-3.57	119.50	124.35
26	K	319	DD6	C21-C20-C19	3.56	118.29	114.28
29	M	307	KC1	O2D-CGD-O1D	-3.56	116.88	123.84
26	K	301	DD6	O1-C20-C21	-3.56	110.79	115.06
27	I	304	UIX	C6-C1-C3	3.55	118.28	114.28
26	G	502	DD6	C37-C36-C31	-3.55	119.52	124.35
28	J	312	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
32	G	507	PID	C18-C19-C20	3.55	130.74	123.47
28	I	312	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
26	h	203	DD6	C15-C14-C13	-3.55	118.49	125.99
32	G	507	PID	C12-O4-C10	3.55	109.50	107.65
30	G	521	DGD	C4D-C3D-C2D	3.54	117.01	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	j	106	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	J	304	DD6	C21-C20-C19	3.54	118.26	114.28
28	a	711	CLA	CMB-C2B-C3B	3.53	131.29	124.68
32	F	305	PID	C16-C15-C14	3.53	132.35	127.31
28	I	311	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
32	F	302	PID	CM5-C21-C20	-3.53	117.98	122.92
28	G	520	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	L	304	DD6	C15-C14-C13	-3.52	118.54	125.99
26	h	203	DD6	C4-C5-C6	-3.52	122.28	127.31
28	K	313	CLA	CMB-C2B-C3B	3.52	131.27	124.68
26	K	319	DD6	C37-C36-C31	-3.52	119.57	124.35
28	a	722	CLA	CMB-C2B-C3B	3.52	131.26	124.68
32	D	305	PID	C12-O4-C10	3.52	109.48	107.65
26	N	303	DD6	C15-C14-C13	-3.51	118.57	125.99
28	F	313	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
26	K	304	DD6	C9-C10-C11	-3.51	122.30	127.31
28	H	307	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
28	M	308	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
32	N	302	PID	CM5-C21-C20	-3.51	118.01	122.92
35	b	702	BCR	C11-C10-C9	-3.51	122.30	127.31
26	B	302	DD6	O1-C20-C21	3.51	119.26	115.06
28	D	314	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
28	L	310	CLA	CMB-C2B-C3B	3.50	131.24	124.68
28	A	311	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
35	f	304	BCR	C24-C23-C22	-3.50	120.94	126.23
26	A	303	DD6	C37-C36-C31	-3.50	119.59	124.35
32	j	105	PID	C17-C16-C15	3.50	130.65	123.47
28	A	309	CLA	CMB-C2B-C3B	3.50	131.23	124.68
28	H	309	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
32	G	506	PID	C12-O4-C10	3.50	109.47	107.65
26	H	303	DD6	C37-C36-C31	-3.50	119.60	124.35
26	J	302	DD6	C21-C20-C19	3.50	118.21	114.28
26	B	303	DD6	C3-C2-C1	-3.50	122.32	127.31
32	D	307	PID	C17-C16-C15	3.49	130.63	123.47
26	G	505	DD6	C14-C13-C11	-3.49	120.11	125.53
35	a	734	BCR	C7-C8-C9	-3.49	120.96	126.23
28	b	709	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	I	305	DD6	C37-C36-C31	-3.49	119.61	124.35
28	J	315	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
28	G	509	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
28	M	316	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
35	l	302	BCR	C15-C14-C13	-3.48	122.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	730	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
28	l	308	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
27	A	304	UIX	C18-O2-C27	-3.47	111.42	117.90
28	f	302	CLA	CMB-C2B-C3B	3.47	131.18	124.68
28	G	513	CLA	CMB-C2B-C3B	3.47	131.17	124.68
26	A	301	DD6	C37-C36-C31	-3.47	119.64	124.35
28	K	309	CLA	CMB-C2B-C3B	3.46	131.16	124.68
26	A	303	DD6	C3-C2-C1	-3.46	122.37	127.31
27	A	304	UIX	C17-C15-C20	3.46	112.58	109.21
29	M	307	KC1	O1D-CGD-CBD	-3.46	117.40	124.48
28	A	320	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
28	G	514	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
28	G	510	CLA	CMB-C2B-C3B	3.46	131.15	124.68
28	a	731	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
26	B	306	DD6	C4-C5-C6	-3.46	122.38	127.31
26	G	505	DD6	C24-C1-C2	3.45	124.24	118.94
28	A	313	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
28	A	312	CLA	CMB-C2B-C3B	3.45	131.14	124.68
28	b	727	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
26	L	302	DD6	C37-C36-C31	-3.45	119.66	124.35
27	B	305	UIX	C14-C13-C11	-3.44	122.39	127.31
28	a	724	CLA	CMB-C2B-C3B	3.44	131.11	124.68
28	B	308	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
28	I	306	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
28	J	307	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
28	F	307	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
28	I	316	CLA	CMB-C2B-C3B	3.42	131.07	124.68
28	l	309	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
28	A	317	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
28	b	705	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	K	305	DD6	C37-C36-C31	-3.42	119.71	124.35
35	l	307	BCR	C11-C10-C9	-3.41	122.44	127.31
35	l	307	BCR	C7-C8-C9	-3.41	121.08	126.23
28	I	319	CLA	CMB-C2B-C3B	3.41	131.05	124.68
28	I	310	CLA	CMB-C2B-C3B	3.41	131.05	124.68
26	M	304	DD6	C4-C5-C6	-3.41	122.45	127.31
26	I	301	DD6	C37-C36-C35	3.41	120.66	114.36
28	H	311	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
35	l	302	BCR	C20-C21-C22	-3.40	122.45	127.31
28	J	311	CLA	CMB-C2B-C3B	3.40	131.04	124.68
35	b	702	BCR	C33-C5-C6	-3.40	120.71	124.53
32	F	306	PID	C18-C19-C20	3.40	130.44	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	j	105	PID	C12-O4-C10	3.40	109.42	107.65
28	l	311	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
26	I	305	DD6	C9-C8-C6	-3.40	116.88	126.42
28	J	306	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	G	504	DD6	C21-C20-C19	3.39	118.10	114.28
26	b	731	DD6	C37-C36-C31	-3.39	119.74	124.35
28	G	516	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
28	M	318	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	G	508	DD6	C37-C36-C31	-3.39	119.74	124.35
28	K	307	CLA	CMB-C2B-C3B	3.39	131.02	124.68
28	a	704	CLA	CMB-C2B-C3B	3.39	131.02	124.68
28	a	715	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	B	306	DD6	C15-C14-C13	-3.39	118.83	125.99
28	B	309	CLA	CMB-C2B-C3B	3.39	131.01	124.68
32	N	301	PID	C18-C19-C20	3.38	130.40	123.47
28	K	312	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
36	a	732	PQN	C14-C13-C15	3.37	120.95	115.27
28	b	718	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
27	K	302	UIX	C18-O2-C27	-3.37	111.61	117.90
28	l	310	CLA	C4D-CHA-C1A	-3.37	121.63	127.26
28	M	315	CLA	CMB-C2B-C3B	3.37	130.99	124.68
28	J	309	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
28	G	512	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
26	M	303	DD6	C37-C36-C31	-3.37	119.77	124.35
28	j	104	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
28	I	313	CLA	CMB-C2B-C3B	3.37	130.97	124.68
26	I	303	DD6	C24-C1-C2	3.36	124.10	118.94
28	B	317	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
28	M	317	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
28	A	308	CLA	CMB-C2B-C3B	3.36	130.96	124.68
35	m	201	BCR	C11-C12-C13	-3.35	116.99	126.42
35	l	307	BCR	C38-C26-C25	-3.35	120.76	124.53
28	B	301	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
28	a	703	CLA	CMB-C2B-C3B	3.35	130.95	124.68
32	D	305	PID	CM5-C21-C20	-3.35	118.23	122.92
28	b	712	CLA	CAB-C3B-C4B	-3.35	123.31	128.46
28	a	702	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
28	H	304	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
28	J	312	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
26	b	731	DD6	C3-C2-C1	-3.34	122.55	127.31
32	F	305	PID	CM4-C14-C15	-3.34	118.25	122.92
26	h	203	DD6	C37-C36-C31	-3.34	119.81	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	J	303	DD6	C21-C20-C15	-3.34	116.67	122.26
28	a	708	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
32	N	302	PID	C26-C25-C24	3.33	112.45	109.21
28	a	713	CLA	CMB-C2B-C3B	3.33	130.91	124.68
28	b	714	CLA	CMB-C2B-C3B	3.33	130.91	124.68
35	a	734	BCR	C20-C21-C22	-3.33	122.56	127.31
28	K	306	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
28	F	310	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
35	j	102	BCR	C33-C5-C6	-3.33	120.79	124.53
28	a	738	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
32	D	307	PID	C18-C19-C20	3.33	130.29	123.47
26	F	301	DD6	C14-C13-C11	-3.33	120.37	125.53
28	l	304	CLA	CMB-C2B-C3B	3.32	130.90	124.68
28	a	706	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	N	303	DD6	C37-C36-C31	-3.32	119.84	124.35
28	b	706	CLA	CMB-C2B-C3B	3.32	130.89	124.68
28	a	718	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
26	K	304	DD6	C37-C36-C31	-3.32	119.84	124.35
28	L	308	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
28	l	303	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
28	a	710	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
28	B	311	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
28	D	308	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
28	L	314	CLA	CMB-C2B-C3B	3.31	130.86	124.68
35	l	307	BCR	C4-C5-C6	-3.31	117.93	122.73
26	K	303	DD6	C37-C36-C31	-3.30	119.86	124.35
28	K	315	CLA	CMB-C2B-C3B	3.30	130.86	124.68
28	D	312	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
28	M	315	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
35	m	201	BCR	C20-C21-C22	-3.30	122.61	127.31
28	I	307	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
28	a	727	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
28	L	317	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
35	m	201	BCR	C4-C5-C6	-3.29	117.95	122.73
26	A	303	DD6	C15-C14-C13	-3.29	119.03	125.99
28	A	307	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
32	H	302	PID	C12-O4-C10	3.29	109.36	107.65
35	l	307	BCR	C33-C5-C4	3.29	119.93	113.62
28	b	704	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
28	J	316	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
26	I	305	DD6	C3-C4-C5	-3.29	116.74	123.47
35	j	102	BCR	C3-C4-C5	-3.28	108.22	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	318	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
26	G	505	DD6	C-C1-C2	-3.28	118.33	122.92
28	K	316	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
26	I	305	DD6	C37-C36-C35	3.27	120.42	114.36
35	b	732	BCR	C21-C20-C19	-3.27	113.01	123.22
28	B	316	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
28	N	304	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
27	J	305	UIX	C6-C1-C3	3.26	117.95	114.28
28	N	307	CLA	CMB-C2B-C3B	3.26	130.78	124.68
28	A	319	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
32	D	302	PID	C12-O4-C10	3.26	109.35	107.65
28	D	309	CLA	CMB-C2B-C3B	3.26	130.77	124.68
28	a	714	CLA	CMB-C2B-C3B	3.25	130.77	124.68
28	A	316	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
27	K	302	UIX	C34-C37-C39	-3.25	116.81	123.47
28	h	202	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
30	I	317	DGD	O1G-C1A-C2A	3.25	119.89	111.38
30	G	521	DGD	C1D-C2D-C3D	3.25	116.76	110.00
27	B	305	UIX	C6-C1-C3	3.24	117.93	114.28
26	H	303	DD6	C9-C10-C11	-3.24	122.68	127.31
28	a	716	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
28	I	315	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
26	K	304	DD6	C4-C5-C6	-3.24	122.69	127.31
32	G	507	PID	C17-C16-C15	3.24	130.10	123.47
28	F	308	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
28	N	309	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
26	L	305	DD6	C15-C14-C13	-3.24	119.15	125.99
28	b	711	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
28	I	319	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
28	N	310	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
28	b	728	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
28	b	722	CLA	CMB-C2B-C3B	3.23	130.71	124.68
28	b	725	CLA	CMB-C2B-C3B	3.22	130.71	124.68
28	l	313	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
26	G	502	DD6	C14-C13-C11	-3.22	120.53	125.53
28	A	310	CLA	CMB-C2B-C3B	3.22	130.71	124.68
28	a	709	CLA	CMB-C2B-C3B	3.22	130.71	124.68
32	D	301	PID	CM5-C21-C20	-3.22	118.41	122.92
28	b	724	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
28	J	301	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
28	J	308	CLA	CMB-C2B-C3B	3.22	130.69	124.68
28	F	311	CLA	CMB-C2B-C1B	-3.22	123.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	BCR	C38-C26-C27	3.21	119.79	113.62
26	b	731	DD6	C4-C3-C2	-3.21	116.89	123.47
28	N	309	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
28	a	735	CLA	CMB-C2B-C3B	3.21	130.69	124.68
28	H	305	CLA	CMB-C2B-C3B	3.21	130.69	124.68
35	i	201	BCR	C15-C16-C17	-3.21	116.89	123.47
28	a	726	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
28	b	726	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
26	B	302	DD6	C21-C20-C15	-3.20	116.89	122.26
26	K	305	DD6	C15-C14-C13	-3.20	119.23	125.99
28	L	316	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
35	l	307	BCR	C16-C17-C18	-3.20	122.75	127.31
26	G	505	DD6	O1-C20-C19	3.20	115.78	113.38
26	L	302	DD6	C33-C34-C35	-3.19	105.93	110.30
28	a	705	CLA	CMB-C2B-C3B	3.19	130.65	124.68
35	i	201	BCR	C11-C10-C9	-3.19	122.75	127.31
32	F	306	PID	CM5-C21-C20	-3.19	118.45	122.92
26	B	306	DD6	C37-C36-C31	-3.19	120.01	124.35
28	b	723	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	f	301	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	b	720	CLA	CMB-C2B-C3B	3.18	130.64	124.68
28	D	313	CLA	CMB-C2B-C3B	3.18	130.64	124.68
26	D	303	DD6	C14-C13-C11	3.18	130.47	125.53
28	a	726	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
28	K	311	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
28	a	707	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
26	I	302	DD6	O1-C20-C19	-3.18	110.99	113.38
28	F	315	CLA	CMB-C2B-C3B	3.18	130.62	124.68
28	b	717	CLA	CMB-C2B-C3B	3.18	130.62	124.68
26	M	306	DD6	C25-C26-C27	-3.18	117.36	126.58
28	B	312	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
28	L	312	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
26	L	303	DD6	C21-C20-C15	-3.17	116.95	122.26
28	l	312	CLA	CMB-C2B-C3B	3.17	130.61	124.68
26	M	302	DD6	C21-C20-C19	3.17	117.85	114.28
28	M	312	CLA	CMB-C2B-C3B	3.17	130.60	124.68
32	M	301	PID	C17-C18-C19	3.16	131.85	124.81
26	h	203	DD6	C9-C10-C11	-3.16	122.80	127.31
35	l	302	BCR	C38-C26-C25	-3.16	120.98	124.53
28	J	310	CLA	CMB-C2B-C3B	3.15	130.58	124.68
28	A	307	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
28	N	305	CLA	CMB-C2B-C3B	3.15	130.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	723	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
28	a	721	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
27	J	305	UIX	C7-C10-C11	-3.15	120.64	125.53
28	D	314	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
28	G	516	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
32	H	301	PID	C17-C18-C19	3.15	131.81	124.81
35	b	702	BCR	C28-C27-C26	-3.14	108.46	114.08
28	a	717	CLA	CMB-C2B-C3B	3.14	130.56	124.68
26	G	504	DD6	C32-C31-C36	-3.14	118.20	122.63
28	M	310	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	M	306	DD6	C37-C36-C35	3.14	120.17	114.36
28	l	310	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
26	M	305	DD6	C9-C10-C11	-3.13	122.84	127.31
28	M	313	CLA	CMB-C2B-C3B	3.13	130.54	124.68
28	L	313	CLA	CMB-C2B-C3B	3.13	130.53	124.68
26	F	301	DD6	C25-C26-C27	-3.13	117.50	126.58
26	A	305	DD6	C37-C36-C35	3.13	120.15	114.36
28	a	725	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
28	I	311	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
28	b	716	CLA	CMB-C2B-C3B	3.12	130.52	124.68
26	F	301	DD6	C9-C8-C6	-3.12	117.64	126.42
26	M	305	DD6	C4-C5-C6	-3.12	122.85	127.31
28	J	314	CLA	CMB-C2B-C3B	3.12	130.52	124.68
26	M	306	DD6	C14-C13-C11	-3.12	120.69	125.53
28	L	309	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
26	J	304	DD6	C25-C24-C1	-3.12	117.66	126.42
28	a	723	CLA	CMB-C2B-C3B	3.11	130.50	124.68
32	M	301	PID	C26-C25-C24	3.11	112.23	109.21
28	b	709	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
28	H	307	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
28	I	306	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
28	I	308	CLA	CMB-C2B-C3B	3.10	130.48	124.68
29	M	307	KC1	C3D-CAD-CBD	-3.10	103.52	107.61
28	G	519	CLA	CMB-C2B-C3B	3.10	130.48	124.68
35	i	201	BCR	C27-C26-C25	-3.10	118.23	122.73
28	F	315	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
32	G	506	PID	CM5-C21-C20	-3.10	118.58	122.92
28	G	517	CLA	CMB-C2B-C3B	3.10	130.47	124.68
28	b	707	CLA	CMB-C2B-C3B	3.10	130.47	124.68
29	N	311	KC1	C3D-CAD-CBD	-3.09	103.53	107.61
28	l	303	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
32	F	304	PID	C17-C18-C19	3.09	131.69	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	306	DD6	C24-C1-C2	3.09	123.69	118.94
28	a	704	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
28	I	321	CLA	CMB-C2B-C3B	3.09	130.46	124.68
28	I	309	CLA	CMB-C2B-C3B	3.09	130.45	124.68
26	L	303	DD6	C15-C14-C13	-3.09	119.47	125.99
28	B	310	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
35	m	201	BCR	C23-C24-C25	-3.09	118.53	127.20
28	F	313	CLA	CHB-C4A-NA	3.09	128.78	124.51
26	D	303	DD6	C21-C20-C15	-3.09	117.09	122.26
26	K	303	DD6	C3-C2-C1	-3.09	122.91	127.31
26	K	305	DD6	C4-C5-C6	-3.09	122.91	127.31
32	N	302	PID	C12-O4-C10	3.08	109.25	107.65
28	a	738	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
35	l	307	BCR	C20-C21-C22	-3.08	122.92	127.31
32	D	304	PID	C17-C18-C19	3.08	131.66	124.81
26	G	504	DD6	C37-C36-C35	3.07	120.05	114.36
28	a	729	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
28	H	308	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
28	H	312	CLA	CMB-C2B-C3B	3.07	130.42	124.68
26	I	305	DD6	C25-C24-C1	-3.07	117.80	126.42
26	K	301	DD6	C9-C10-C11	-3.07	122.93	127.31
28	b	715	CLA	CMB-C2B-C3B	3.07	130.41	124.68
28	K	316	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
28	M	309	CLA	CMB-C2B-C3B	3.06	130.41	124.68
28	L	311	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	b	731	DD6	C37-C36-C35	3.06	120.02	114.36
27	A	304	UIX	C37-C39-C40	-3.06	122.94	127.31
28	G	518	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	A	303	DD6	C4-C5-C6	-3.06	122.95	127.31
28	F	310	CLA	CMB-C2B-C3B	3.05	130.39	124.68
28	b	722	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
32	D	306	PID	CM5-C21-C20	-3.05	118.64	122.92
28	b	708	CLA	CMB-C2B-C3B	3.05	130.39	124.68
28	L	317	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
26	I	305	DD6	O1-C20-C21	3.05	118.71	115.06
26	J	303	DD6	C32-C33-C34	-3.05	106.75	113.64
28	K	315	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
27	K	302	UIX	C6-C1-C3	3.05	117.71	114.28
32	G	507	PID	CM5-C21-C20	-3.04	118.66	122.92
26	B	302	DD6	O1-C20-C19	3.04	115.67	113.38
26	G	504	DD6	C21-C20-C15	-3.04	117.16	122.26
28	K	310	CLA	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	729	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
28	a	703	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
27	h	201	UIX	C37-C34-C30	-3.04	117.25	123.47
27	B	305	UIX	C-C7-C10	-3.04	119.57	125.99
28	H	308	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	G	504	DD6	O1-C20-C21	3.04	118.69	115.06
28	J	308	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
28	M	311	CLA	CMB-C2B-C3B	3.03	130.36	124.68
35	a	734	BCR	C3-C4-C5	-3.03	108.66	114.08
28	a	724	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	D	310	KC1	CHC-C4B-C3B	-3.03	120.07	125.26
28	b	719	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
32	N	301	PID	CM5-C21-C20	-3.03	118.68	122.92
26	J	304	DD6	C37-C36-C31	-3.03	120.23	124.35
28	b	721	CLA	CMB-C2B-C3B	3.03	130.35	124.68
28	F	312	CLA	CMB-C2B-C3B	3.03	130.35	124.68
35	i	201	BCR	C30-C25-C26	-3.03	118.35	122.61
35	b	732	BCR	C8-C7-C6	-3.03	118.70	127.20
35	b	730	BCR	C28-C27-C26	-3.03	108.67	114.08
35	f	304	BCR	C38-C26-C25	-3.03	121.13	124.53
28	B	310	CLA	CMB-C2B-C3B	3.03	130.34	124.68
26	G	508	DD6	O1-C20-C21	-3.02	111.43	115.06
28	L	309	CLA	CMB-C2B-C3B	3.02	130.34	124.68
28	D	311	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	L	304	DD6	O1-C20-C21	-3.02	111.44	115.06
26	H	303	DD6	O1-C20-C19	-3.02	111.11	113.38
28	l	305	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	L	305	DD6	C33-C34-C35	-3.02	106.17	110.30
26	B	304	DD6	O1-C20-C21	-3.02	111.44	115.06
28	F	313	CLA	CMB-C2B-C3B	3.02	130.32	124.68
28	A	315	CLA	CMB-C2B-C3B	3.01	130.32	124.68
26	A	301	DD6	C14-C13-C11	-3.01	120.86	125.53
26	B	302	DD6	C37-C36-C31	-3.01	120.26	124.35
28	K	308	CLA	CMB-C2B-C3B	3.01	130.31	124.68
28	I	310	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
35	a	736	BCR	C20-C21-C22	-3.01	123.02	127.31
35	l	307	BCR	C24-C23-C22	-3.01	121.69	126.23
26	A	302	DD6	C21-C20-C15	-3.01	117.22	122.26
28	J	314	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
28	a	728	CLA	CMB-C2B-C3B	3.00	130.29	124.68
28	J	301	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	M	305	DD6	C15-C14-C13	-3.00	119.65	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	518	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
28	A	311	CLA	CMB-C2B-C3B	3.00	130.29	124.68
28	I	315	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
28	l	310	CLA	C3D-C4D-ND	3.00	111.91	107.38
26	J	302	DD6	O1-C20-C21	-3.00	111.47	115.06
32	F	305	PID	C29-C24-C25	2.99	122.67	119.70
28	L	312	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
28	G	511	CLA	CMB-C2B-C3B	2.99	130.28	124.68
28	j	106	CLA	CMB-C2B-C3B	2.99	130.28	124.68
29	G	515	KC1	C3D-CAD-CBD	-2.99	103.67	107.61
32	j	105	PID	C6-C7-C8	-2.99	119.67	125.99
26	I	301	DD6	C37-C36-C31	-2.99	120.29	124.35
28	B	311	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
26	G	504	DD6	C24-C1-C2	2.98	123.52	118.94
29	F	309	KC1	CHC-C4B-C3B	-2.98	120.16	125.26
28	B	315	CLA	CMB-C2B-C3B	2.98	130.25	124.68
26	b	731	DD6	C32-C33-C34	-2.98	106.91	113.64
35	b	702	BCR	C3-C4-C5	-2.98	108.75	114.08
26	J	304	DD6	C14-C13-C11	-2.98	120.91	125.53
28	a	714	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
32	D	304	PID	CM5-C21-C20	-2.98	118.75	122.92
30	G	521	DGD	O6E-C5E-C4E	-2.97	104.30	109.69
28	J	310	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
28	J	307	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
32	H	302	PID	C17-C16-C15	2.97	129.55	123.47
28	a	712	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
27	B	305	UIX	C7-C10-C11	-2.96	120.93	125.53
28	K	306	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
28	H	309	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	M	306	DD6	C37-C36-C31	-2.96	120.32	124.35
27	G	503	UIX	C36-C35-C32	-2.96	123.09	127.31
32	D	302	PID	CM5-C21-C20	-2.96	118.78	122.92
29	N	308	KC1	CHB-C1B-C2B	-2.96	119.28	125.48
28	a	723	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
28	B	315	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	A	305	DD6	C9-C10-C11	-2.96	123.09	127.31
35	b	702	BCR	C8-C7-C6	-2.95	118.90	127.20
30	G	501	DGD	O1G-C1A-C2A	2.95	121.18	111.91
26	B	306	DD6	C33-C34-C35	-2.95	106.26	110.30
28	a	720	CLA	CMB-C2B-C3B	2.95	130.20	124.68
28	a	725	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
26	L	302	DD6	O1-C20-C19	-2.95	111.17	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	314	KC1	C3D-CAD-CBD	-2.95	103.73	107.61
28	B	313	CLA	CMB-C2B-C3B	2.95	130.19	124.68
28	D	316	CLA	CMB-C2B-C3B	2.94	130.19	124.68
28	f	303	CLA	CMB-C2B-C3B	2.94	130.19	124.68
28	G	510	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	L	304	DD6	C33-C34-C35	-2.94	106.28	110.30
26	I	305	DD6	C24-C1-C2	2.94	123.45	118.94
28	H	307	CLA	CMB-C2B-C3B	2.94	130.18	124.68
27	A	304	UIX	C35-C36-C38	-2.94	114.04	123.22
26	G	508	DD6	C4-C3-C2	-2.94	117.45	123.47
28	a	719	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	B	304	DD6	C33-C34-C35	-2.94	106.28	110.30
28	D	309	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	L	303	DD6	C33-C34-C35	-2.93	106.30	110.30
28	G	514	CLA	CMB-C2B-C3B	2.93	130.15	124.68
28	b	713	CLA	CMB-C2B-C3B	2.92	130.15	124.68
28	I	308	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
28	F	313	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
28	a	717	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	K	305	DD6	C33-C34-C35	-2.92	106.31	110.30
35	b	730	BCR	C33-C5-C4	2.92	119.22	113.62
28	a	730	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	I	303	DD6	C12-C11-C10	-2.92	118.84	122.92
28	J	307	CLA	CMB-C2B-C3B	2.92	130.14	124.68
28	M	308	CLA	CMB-C2B-C3B	2.92	130.14	124.68
28	H	311	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
28	L	308	CLA	CBD-CHA-C1A	2.92	132.10	127.43
35	l	302	BCR	C3-C4-C5	-2.92	108.87	114.08
28	J	315	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
28	G	509	CLA	CMB-C2B-C3B	2.91	130.13	124.68
29	L	307	KC1	CHC-C4B-C3B	-2.91	120.28	125.26
28	K	309	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
27	K	302	UIX	C35-C36-C38	-2.91	114.14	123.22
26	M	303	DD6	C14-C13-C11	-2.91	121.02	125.53
28	b	705	CLA	CMB-C2B-C3B	2.91	130.12	124.68
28	I	309	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
28	a	701	CLA	CMB-C2B-C3B	2.91	130.12	124.68
28	A	315	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
28	b	707	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
28	B	307	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
28	M	313	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
28	A	320	CLA	O2D-CGD-O1D	-2.90	118.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	715	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
28	l	309	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
28	B	309	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
27	K	302	UIX	C7-C10-C11	-2.89	121.04	125.53
26	I	305	DD6	C-C1-C2	-2.89	118.87	122.92
28	L	316	CLA	CAA-C2A-C3A	-2.89	109.35	116.10
31	K	317	LMG	O6-C1-O1	-2.89	103.13	109.97
26	K	304	DD6	C3-C4-C5	-2.89	117.56	123.47
28	L	316	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
28	b	718	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
28	F	307	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	I	302	DD6	O1-C20-C21	-2.88	111.60	115.06
28	b	716	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
28	J	316	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	G	504	DD6	C9-C10-C11	-2.88	123.20	127.31
28	l	308	CLA	CMB-C2B-C3B	2.88	130.07	124.68
35	b	732	BCR	C10-C11-C12	-2.88	114.23	123.22
27	B	305	UIX	C18-O2-C27	-2.88	112.53	117.90
28	a	735	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
28	a	715	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
35	l	302	BCR	C37-C22-C21	-2.88	118.89	122.92
26	G	504	DD6	C37-C36-C31	-2.88	120.44	124.35
35	b	732	BCR	C24-C23-C22	-2.88	121.89	126.23
26	B	306	DD6	C9-C10-C11	-2.87	123.21	127.31
35	l	302	BCR	C29-C30-C25	2.87	114.91	110.48
26	J	304	DD6	C-C1-C2	-2.87	118.90	122.92
28	b	724	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
35	m	201	BCR	C33-C5-C4	2.87	119.14	113.62
28	H	311	CLA	CMB-C2B-C3B	2.87	130.05	124.68
32	F	305	PID	C19-C20-C21	2.87	131.41	127.31
28	H	304	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	b	701	CLA	CMB-C2B-C3B	2.87	130.05	124.68
26	K	301	DD6	C3-C2-C1	-2.87	123.21	127.31
32	H	302	PID	CM5-C21-C20	-2.87	118.90	122.92
28	B	301	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
26	B	302	DD6	C20-C19-C18	-2.87	107.07	112.75
26	J	302	DD6	C25-C24-C1	-2.87	118.36	126.42
35	l	302	BCR	C16-C15-C14	-2.87	117.60	123.47
26	M	303	DD6	C12-C11-C10	-2.87	118.91	122.92
28	a	722	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
28	b	710	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	D	315	KC1	C3D-CAD-CBD	-2.87	103.83	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	705	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	j	105	PID	CM5-C21-C20	-2.87	118.91	122.92
28	A	317	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
28	J	315	CLA	CMB-C2B-C3B	2.86	130.04	124.68
28	N	304	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
28	A	313	CLA	CMB-C2B-C3B	2.86	130.03	124.68
28	A	308	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
35	a	734	BCR	C8-C7-C6	-2.86	119.17	127.20
29	N	308	KC1	C4B-CHC-C1C	-2.86	119.89	126.06
35	l	307	BCR	C15-C16-C17	-2.86	117.62	123.47
27	h	201	UIX	C34-C30-C26	-2.86	123.23	127.31
32	N	302	PID	C29-C24-C25	2.86	122.53	119.70
28	b	727	CLA	CMB-C2B-C3B	2.86	130.02	124.68
26	F	301	DD6	C37-C36-C35	2.85	119.64	114.36
35	a	734	BCR	C33-C5-C4	2.85	119.10	113.62
26	J	302	DD6	C37-C36-C35	2.85	119.64	114.36
28	K	308	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
27	G	503	UIX	C18-O2-C27	-2.85	112.58	117.90
28	I	307	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
28	b	725	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
28	H	305	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
28	a	726	CLA	CMB-C2B-C3B	2.85	130.00	124.68
26	B	306	DD6	C25-C26-C27	-2.85	118.32	126.58
28	L	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	B	308	CLA	CMB-C2B-C3B	2.84	130.00	124.68
35	l	306	BCR	C28-C27-C26	-2.84	109.00	114.08
28	a	728	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	l	308	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	a	718	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	N	305	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	b	717	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	K	314	KC1	CHC-C4B-C3B	-2.84	120.40	125.26
28	N	310	CLA	CHB-C4A-NA	2.84	128.44	124.51
28	M	317	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	G	505	DD6	C21-C20-C19	2.84	117.47	114.28
28	J	312	CLA	CMB-C2B-C3B	2.84	129.99	124.68
28	l	309	CLA	CMB-C2B-C3B	2.84	129.98	124.68
35	b	730	BCR	C21-C20-C19	-2.84	114.37	123.22
28	l	304	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
28	L	314	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
28	I	312	CLA	CMB-C2B-C3B	2.83	129.98	124.68
28	l	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	715	CLA	CMB-C2B-C3B	2.83	129.98	124.68
28	I	321	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	B	313	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	a	726	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
28	m	202	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	D	314	CLA	CMB-C2B-C3B	2.83	129.98	124.68
29	N	311	KC1	CHC-C4B-C3B	-2.83	120.41	125.26
26	G	505	DD6	O1-C20-C15	-2.83	56.62	58.96
28	D	314	CLA	CHB-C4A-NA	2.83	128.43	124.51
28	K	310	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	K	303	DD6	C4-C5-C6	-2.83	123.27	127.31
28	b	719	CLA	CMB-C2B-C3B	2.83	129.97	124.68
28	N	307	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	f	303	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	J	304	DD6	C12-C11-C10	-2.83	118.96	122.92
28	b	706	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	b	711	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	F	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	M	317	CLA	CMB-C2B-C3B	2.83	129.97	124.68
28	a	722	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
27	G	503	UIX	C14-C13-C11	-2.83	123.28	127.31
28	a	716	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	j	104	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	M	308	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	K	312	CLA	CMB-C2B-C3B	2.82	129.96	124.68
28	F	307	CLA	CMB-C2B-C3B	2.82	129.96	124.68
28	a	710	CLA	CMB-C2B-C3B	2.82	129.96	124.68
26	B	302	DD6	C24-C1-C2	2.82	123.27	118.94
28	b	712	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	A	319	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	H	306	KC1	CHC-C4B-C3B	-2.82	120.44	125.26
26	I	302	DD6	C7-C6-C5	-2.82	118.98	122.92
31	b	734	LMG	O6-C1-O1	-2.82	103.30	109.97
26	A	303	DD6	C33-C34-C35	-2.82	106.45	110.30
28	M	309	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
29	A	314	KC1	CHB-C1B-C2B	-2.82	119.58	125.48
28	G	509	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	L	303	DD6	O1-C20-C19	-2.81	111.27	113.38
35	j	102	BCR	C28-C27-C26	-2.81	109.05	114.08
28	l	313	CLA	CHB-C4A-NA	2.81	128.40	124.51
28	b	712	CLA	CMB-C2B-C3B	2.81	130.19	124.69
32	j	105	PID	C18-C19-C20	2.81	129.24	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	318	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	a	712	CLA	CMB-C2B-C3B	2.81	129.94	124.68
28	K	315	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	M	316	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	D	303	DD6	C9-C10-C11	-2.81	123.30	127.31
26	G	508	DD6	C14-C13-C11	-2.81	121.17	125.53
26	L	306	DD6	C37-C36-C35	2.81	119.56	114.36
28	K	311	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	K	304	DD6	C37-C36-C35	2.81	119.56	114.36
27	G	503	UIX	C34-C37-C39	-2.81	117.72	123.47
27	I	304	UIX	C35-C36-C38	-2.81	114.46	123.22
28	K	313	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
28	B	315	CLA	CAA-C2A-C3A	-2.81	109.55	116.10
28	a	701	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	J	304	DD6	C32-C31-C36	-2.80	118.67	122.63
28	A	313	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	I	314	KC1	CHC-C4B-C3B	-2.80	120.46	125.26
26	G	504	DD6	C-C1-C2	-2.80	119.00	122.92
28	I	316	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
26	M	306	DD6	O1-C20-C21	2.80	118.41	115.06
28	M	312	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	M	303	DD6	C21-C20-C15	-2.80	117.57	122.26
28	I	321	CLA	CHB-C4A-NA	2.80	128.38	124.51
28	K	307	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	b	702	BCR	C34-C9-C8	2.80	122.48	118.08
28	M	311	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
28	l	305	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
27	A	304	UIX	C21-C15-C20	-2.80	107.97	110.47
28	B	311	CLA	CMB-C2B-C3B	2.79	129.91	124.68
28	A	312	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
28	a	735	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
28	H	309	CLA	CMB-C2B-C3B	2.79	129.91	124.68
28	a	708	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
35	m	201	BCR	C28-C27-C26	-2.79	109.09	114.08
30	G	521	DGD	C3E-C4E-C5E	2.79	115.22	110.24
28	J	309	CLA	CMB-C2B-C3B	2.79	129.90	124.68
28	I	312	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
28	B	317	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
28	N	307	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
28	b	720	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
28	G	512	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
35	b	730	BCR	C15-C16-C17	-2.79	117.77	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	318	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
29	A	306	KC1	C3D-CAD-CBD	-2.78	103.94	107.61
29	N	306	KC1	CHC-C4B-C3B	-2.78	120.50	125.26
35	j	102	BCR	C11-C10-C9	-2.78	123.34	127.31
28	B	308	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	A	316	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	b	705	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	D	313	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	b	703	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
32	D	302	PID	CM2-C5-C4	-2.78	104.15	108.98
28	J	311	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	M	303	DD6	C25-C24-C1	-2.78	118.61	126.42
26	M	305	DD6	C21-C20-C15	-2.78	117.60	122.26
28	J	306	CLA	CMB-C2B-C3B	2.78	129.88	124.68
29	D	315	KC1	CHB-C1B-C2B	-2.78	119.65	125.48
28	a	709	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	N	306	KC1	C3D-CAD-CBD	-2.78	103.95	107.61
28	B	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
28	M	318	CLA	CMB-C2B-C3B	2.78	129.88	124.68
32	M	301	PID	C29-C24-C25	2.78	122.45	119.70
35	m	201	BCR	C16-C17-C18	-2.77	123.35	127.31
26	B	303	DD6	C15-C14-C13	-2.77	120.13	125.99
29	B	314	KC1	CHC-C4B-C3B	-2.77	120.52	125.26
28	f	301	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
27	I	304	UIX	C37-C34-C30	-2.77	117.80	123.47
28	N	309	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
28	b	727	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	M	304	DD6	C3-C4-C5	-2.77	117.81	123.47
35	b	702	BCR	C15-C14-C13	-2.77	123.36	127.31
28	a	706	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	I	313	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	a	730	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
27	B	305	UIX	C16-C20-C15	2.76	122.44	119.70
28	b	726	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
32	H	301	PID	CM5-C21-C20	-2.76	119.05	122.92
35	j	102	BCR	C16-C15-C14	-2.76	117.81	123.47
31	D	317	LMG	O6-C1-O1	-2.76	103.43	109.97
26	A	301	DD6	C20-C19-C18	-2.76	107.28	112.75
26	K	303	DD6	C10-C9-C8	-2.76	114.60	123.22
35	m	201	BCR	C38-C26-C27	2.76	118.92	113.62
26	I	301	DD6	C25-C26-C27	-2.76	118.57	126.58
32	G	506	PID	C18-C19-C20	2.76	129.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	309	CLA	CMB-C2B-C3B	2.76	129.84	124.68
28	J	306	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	A	303	DD6	C9-C10-C11	-2.76	123.37	127.31
28	B	317	CLA	CMB-C2B-C3B	2.76	129.84	124.68
26	b	731	DD6	C14-C13-C11	-2.76	121.25	125.53
28	a	727	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	F	301	DD6	C20-C19-C18	-2.76	107.30	112.75
26	L	303	DD6	C37-C36-C35	2.76	119.46	114.36
26	F	301	DD6	C37-C36-C31	-2.76	120.60	124.35
29	A	314	KC1	CHC-C4B-C3B	-2.76	120.54	125.26
29	M	314	KC1	CHB-C1B-C2B	-2.75	119.70	125.48
28	G	516	CLA	CMB-C2B-C3B	2.75	129.83	124.68
35	a	736	BCR	C3-C4-C5	-2.75	109.16	114.08
28	l	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
35	j	102	BCR	C7-C8-C9	-2.75	122.08	126.23
31	I	320	LMG	O6-C1-O1	-2.75	103.46	109.97
26	G	504	DD6	C15-C14-C13	-2.75	120.18	125.99
28	G	520	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	G	505	DD6	C25-C24-C1	-2.75	118.69	126.42
35	a	736	BCR	C38-C26-C25	-2.75	121.44	124.53
26	D	303	DD6	C12-C11-C13	2.75	122.41	118.08
28	H	304	CLA	CMB-C2B-C3B	2.75	129.82	124.68
28	D	312	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
27	K	302	UIX	C14-C23-C26	-2.75	118.70	126.42
31	I	318	LMG	C1-C2-C3	-2.75	104.28	110.00
28	b	728	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	K	305	DD6	C14-C13-C11	-2.74	121.27	125.53
28	A	315	CLA	CAA-C2A-C3A	-2.74	109.69	116.10
27	h	201	UIX	C13-C14-C23	-2.74	114.65	123.22
28	I	306	CLA	CMB-C2B-C3B	2.74	129.81	124.68
28	a	708	CLA	CMB-C2B-C3B	2.74	129.81	124.68
28	a	702	CLA	CMB-C2B-C3B	2.74	129.81	124.68
28	B	317	CLA	CHB-C4A-NA	2.74	128.30	124.51
28	F	310	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	I	305	DD6	C32-C31-C36	-2.74	118.77	122.63
28	l	312	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	I	314	KC1	CHB-C1B-C2B	-2.74	119.74	125.48
28	a	721	CLA	CMB-C2B-C3B	2.74	129.80	124.68
28	l	311	CLA	CMB-C2B-C3B	2.74	129.80	124.68
35	b	702	BCR	C20-C19-C18	-2.73	118.73	126.42
28	D	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
35	j	102	BCR	C8-C7-C6	-2.73	119.53	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	l	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
35	i	201	BCR	C10-C11-C12	-2.73	114.69	123.22
28	j	106	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
28	L	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
28	L	318	CLA	CHB-C4A-NA	2.73	128.29	124.51
32	D	301	PID	CM2-C5-C4	-2.73	104.24	108.98
31	b	733	LMG	O6-C1-O1	-2.73	103.51	109.97
26	B	302	DD6	C25-C24-C1	-2.73	118.75	126.42
35	b	702	BCR	C10-C11-C12	-2.73	114.70	123.22
35	a	734	BCR	C24-C23-C22	-2.73	122.11	126.23
28	b	721	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
28	B	312	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
28	l	310	CLA	CMB-C2B-C3B	2.73	129.78	124.68
28	J	309	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
28	J	310	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
28	A	311	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
28	h	202	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
35	a	736	BCR	C33-C5-C4	2.72	118.85	113.62
35	a	736	BCR	C33-C5-C6	-2.72	121.47	124.53
28	L	318	CLA	CMB-C2B-C3B	2.72	129.77	124.68
28	I	321	CLA	CAC-C3C-C4C	2.72	128.34	124.81
28	J	312	CLA	CHB-C4A-NA	2.72	128.28	124.51
28	D	316	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
28	l	303	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
29	D	310	KC1	CBD-CHA-C1A	2.72	133.95	128.88
28	a	718	CLA	CMB-C2B-C3B	2.72	129.76	124.68
28	a	711	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
28	b	722	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
28	l	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
28	J	307	CLA	CHB-C4A-NA	2.72	128.27	124.51
28	D	312	CLA	CMB-C2B-C3B	2.72	129.76	124.68
28	a	704	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
29	B	314	KC1	CHB-C1B-C2B	-2.71	119.79	125.48
35	b	732	BCR	C11-C10-C9	-2.71	123.44	127.31
29	N	306	KC1	O1D-CGD-CBD	-2.71	118.94	124.48
28	A	319	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	J	301	CLA	CMB-C2B-C3B	2.71	129.75	124.68
27	K	302	UIX	C37-C39-C40	-2.71	123.44	127.31
28	D	308	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	F	305	PID	C26-C25-C24	2.71	111.84	109.21
28	M	316	CLA	CMB-C2B-C3B	2.71	129.75	124.68
28	N	310	CLA	CMB-C2B-C3B	2.71	129.75	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	704	CLA	CMB-C2B-C3B	2.71	129.75	124.68
29	M	314	KC1	CHC-C4B-C3B	-2.71	120.62	125.26
28	a	702	CLA	C1-C2-C3	-2.71	121.36	126.04
28	A	309	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	J	303	DD6	C-C1-C2	-2.71	119.13	122.92
28	M	317	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	D	310	KC1	CHB-C1B-C2B	-2.71	119.80	125.48
26	F	301	DD6	C25-C24-C1	-2.71	118.81	126.42
28	F	315	CLA	CAA-C2A-C3A	-2.71	109.78	116.10
28	l	303	CLA	CMB-C2B-C3B	2.71	129.74	124.68
28	B	316	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
29	L	315	KC1	CHB-C1B-C2B	-2.70	119.81	125.48
26	B	302	DD6	C8-C6-C5	-2.70	118.79	124.81
28	f	302	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
28	N	304	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	K	305	DD6	C21-C20-C15	-2.70	117.73	122.26
26	B	306	DD6	O1-C20-C19	-2.70	111.35	113.38
28	G	512	CLA	CMB-C2B-C3B	2.70	129.73	124.68
28	A	317	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	I	302	DD6	C33-C34-C35	-2.70	106.61	110.30
26	G	508	DD6	C33-C34-C35	2.70	114.00	110.30
28	l	313	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	G	504	DD6	C14-C13-C11	-2.70	121.34	125.53
28	b	708	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
32	D	307	PID	CM5-C21-C20	-2.70	119.15	122.92
28	L	308	CLA	CMB-C2B-C3B	2.69	129.72	124.68
28	b	710	CLA	CMB-C2B-C3B	2.69	129.72	124.68
26	M	305	DD6	C14-C13-C11	-2.69	121.35	125.53
27	J	305	UIX	C29-C26-C30	-2.69	119.16	122.92
30	G	521	DGD	C6E-C5E-C4E	2.69	119.30	113.00
26	M	303	DD6	C24-C1-C2	2.69	123.07	118.94
26	K	319	DD6	C33-C34-C35	-2.69	106.62	110.30
28	a	710	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
28	a	731	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
28	A	310	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
31	K	318	LMG	O6-C1-O1	-2.69	103.61	109.97
28	I	315	CLA	CMB-C2B-C3B	2.68	129.70	124.68
29	F	314	KC1	CHB-C1B-C2B	-2.68	119.85	125.48
26	h	203	DD6	C37-C36-C35	2.68	119.33	114.36
28	b	707	CLA	CHB-C4A-NA	2.68	128.22	124.51
28	J	316	CLA	CMB-C2B-C3B	2.68	129.70	124.68
28	B	310	CLA	C1-C2-C3	-2.68	121.41	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	729	PQN	C2M-C2-C3	-2.68	120.03	124.40
28	K	313	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
35	b	732	BCR	C16-C15-C14	-2.68	117.98	123.47
28	a	721	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
28	B	316	CLA	CMB-C2B-C3B	2.68	129.69	124.68
27	I	304	UIX	C18-O2-C27	-2.68	112.90	117.90
28	b	724	CLA	CMB-C2B-C3B	2.68	129.69	124.68
28	G	511	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
35	i	201	BCR	C1-C6-C5	-2.68	118.84	122.61
28	b	709	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
35	l	306	BCR	C23-C24-C25	-2.68	119.69	127.20
31	B	318	LMG	O6-C1-O1	-2.68	103.64	109.97
29	F	314	KC1	CHC-C4B-C3B	-2.68	120.68	125.26
28	b	723	CLA	CHB-C4A-NA	2.67	128.21	124.51
28	N	310	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
28	F	308	CLA	CMB-C2B-C3B	2.67	129.68	124.68
28	M	310	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
28	b	704	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
28	h	202	CLA	CMB-C2B-C3B	2.67	129.68	124.68
28	F	311	CLA	CMB-C2B-C3B	2.67	129.68	124.68
35	a	734	BCR	C38-C26-C25	-2.67	121.53	124.53
28	N	307	CLA	CHD-C1D-ND	-2.67	122.00	124.45
35	j	102	BCR	C38-C26-C25	-2.67	121.53	124.53
29	L	315	KC1	CHC-C4B-C3B	-2.67	120.69	125.26
28	f	301	CLA	CMB-C2B-C3B	2.67	129.67	124.68
28	G	517	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
28	G	514	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	F	303	DD6	C9-C8-C6	-2.67	118.92	126.42
35	b	730	BCR	C27-C26-C25	-2.67	118.86	122.73
29	N	308	KC1	CHB-C4A-C3A	-2.67	120.81	124.98
35	b	732	BCR	C7-C8-C9	-2.67	122.21	126.23
28	a	716	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	M	304	DD6	C32-C33-C34	-2.66	107.63	113.64
26	H	303	DD6	O1-C20-C21	-2.66	111.87	115.06
26	M	302	DD6	C3-C4-C5	-2.66	118.03	123.47
28	j	104	CLA	CMB-C2B-C3B	2.66	129.65	124.68
26	D	303	DD6	C4-C5-C6	-2.66	123.52	127.31
29	A	306	KC1	CHC-C4B-C3B	-2.66	120.71	125.26
28	a	719	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	B	302	DD6	C32-C33-C34	-2.66	107.64	113.64
28	a	738	CLA	CMB-C2B-C3B	2.66	129.65	124.68
28	a	703	CLA	C1B-CHB-C4A	-2.66	124.86	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	303	DD6	C25-C24-C1	-2.66	118.95	126.42
29	F	309	KC1	CHB-C1B-C2B	-2.66	119.91	125.48
28	a	716	CLA	CMB-C2B-C3B	2.66	129.65	124.68
28	a	725	CLA	CMB-C2B-C3B	2.65	129.65	124.68
26	I	303	DD6	C20-C19-C18	-2.65	107.50	112.75
28	b	712	CLA	CAB-C3B-C2B	2.65	129.88	124.69
28	G	519	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
28	A	320	CLA	CMB-C2B-C3B	2.65	129.64	124.68
28	b	713	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
28	b	709	CLA	CMB-C2B-C3B	2.65	129.64	124.68
28	N	305	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	K	306	CLA	CMB-C2B-C3B	2.65	129.63	124.68
28	b	712	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
28	L	317	CLA	CMB-C2B-C3B	2.65	129.63	124.68
35	j	102	BCR	C20-C19-C18	-2.65	118.97	126.42
26	L	306	DD6	C15-C14-C13	-2.65	120.39	125.99
35	l	302	BCR	C8-C7-C6	-2.65	119.77	127.20
28	a	707	CLA	CMB-C2B-C3B	2.65	129.63	124.68
26	b	731	DD6	C26-C25-C24	-2.65	114.96	123.22
29	K	314	KC1	CHB-C1B-C2B	-2.65	119.93	125.48
29	H	310	KC1	CHB-C1B-C2B	-2.65	119.93	125.48
35	l	302	BCR	C7-C8-C9	-2.65	122.24	126.23
28	a	701	CLA	CHB-C4A-NA	2.65	128.17	124.51
28	B	312	CLA	CHB-C4A-NA	2.65	128.17	124.51
28	M	315	CLA	CHB-C4A-NA	2.65	128.17	124.51
28	M	313	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
29	H	306	KC1	CHB-C1B-C2B	-2.64	119.93	125.48
35	b	732	BCR	C20-C21-C22	-2.64	123.54	127.31
29	N	306	KC1	CHB-C1B-C2B	-2.64	119.93	125.48
28	B	312	CLA	CMB-C2B-C3B	2.64	129.62	124.68
28	a	718	CLA	CHB-C4A-NA	2.64	128.17	124.51
29	L	307	KC1	CHB-C1B-C2B	-2.64	119.94	125.48
28	K	313	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	H	310	KC1	CHC-C4B-C3B	-2.64	120.74	125.26
28	G	514	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	h	201	UIX	C22-C15-C20	-2.64	108.11	110.47
28	b	709	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
26	J	304	DD6	C37-C36-C35	2.64	119.25	114.36
29	B	314	KC1	O1D-CGD-CBD	-2.64	119.08	124.48
28	I	307	CLA	CMB-C2B-C3B	2.64	129.62	124.68
28	a	731	CLA	CMB-C2B-C3B	2.64	129.62	124.68
28	a	707	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	l	302	BCR	C10-C11-C12	-2.64	114.98	123.22
28	G	513	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	J	303	DD6	C25-C24-C1	-2.64	119.00	126.42
28	a	726	CLA	CHB-C4A-NA	2.64	128.16	124.51
28	J	312	CLA	O2D-CGD-CBD	2.64	115.95	111.27
28	a	720	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
28	I	311	CLA	CMB-C2B-C3B	2.63	129.61	124.68
29	L	307	KC1	C3D-CAD-CBD	-2.63	104.14	107.61
28	G	519	CLA	CHB-C4A-NA	2.63	128.15	124.51
35	i	201	BCR	C3-C4-C5	-2.63	109.38	114.08
29	K	314	KC1	CBD-CHA-C1A	2.63	133.78	128.88
28	m	202	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
29	G	515	KC1	CHB-C1B-C2B	-2.63	119.97	125.48
28	a	705	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	K	312	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
28	a	713	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	L	302	DD6	C21-C20-C15	-2.63	117.86	122.26
26	G	502	DD6	C33-C34-C35	-2.63	106.71	110.30
28	b	711	CLA	CMB-C2B-C3B	2.63	129.59	124.68
28	L	316	CLA	CMB-C2B-C3B	2.62	129.59	124.68
28	b	703	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
35	b	732	BCR	C23-C24-C25	-2.62	119.84	127.20
28	a	727	CLA	CMB-C2B-C3B	2.62	129.58	124.68
28	G	510	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	a	729	CLA	CMB-C2B-C3B	2.62	129.58	124.68
28	A	312	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
27	K	302	UIX	C22-C15-C20	-2.62	108.13	110.47
28	L	311	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	I	316	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	b	726	CLA	CMB-C2B-C3B	2.62	129.58	124.68
28	L	313	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
28	a	721	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	a	730	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	A	303	DD6	C21-C20-C15	-2.62	117.88	122.26
28	b	703	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
28	b	701	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	J	306	CLA	CHB-C4A-NA	2.62	128.13	124.51
28	D	308	CLA	CMB-C2B-C3B	2.62	129.57	124.68
27	B	305	UIX	C37-C34-C30	-2.61	118.12	123.47
28	I	312	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
29	F	309	KC1	C3D-CAD-CBD	-2.61	104.16	107.61
28	b	723	CLA	CMB-C2B-C3B	2.61	129.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	307	KC1	CBD-CHA-C1A	2.61	133.75	128.88
28	l	309	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
28	K	312	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	l	312	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
28	A	311	CLA	CHB-C4A-NA	2.61	128.12	124.51
36	b	729	PQN	C14-C13-C15	2.61	119.66	115.27
26	L	303	DD6	C14-C13-C11	-2.61	121.48	125.53
27	K	302	UIX	C3-C5-C4	-2.61	105.73	110.77
29	B	314	KC1	C3D-CAD-CBD	-2.61	104.17	107.61
31	j	101	LMG	O6-C1-O1	-2.61	103.80	109.97
28	A	310	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	b	701	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
28	H	312	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	J	304	DD6	O1-C20-C21	2.61	118.18	115.06
26	F	303	DD6	C37-C36-C31	-2.60	120.81	124.35
29	F	309	KC1	C2A-C3A-C4A	2.60	108.42	106.49
28	G	517	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	B	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	M	307	KC1	CHC-C4B-C3B	-2.60	120.81	125.26
28	B	312	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
28	A	317	CLA	CAA-C2A-C3A	-2.60	110.03	116.10
29	H	306	KC1	C3D-CAD-CBD	-2.60	104.18	107.61
28	L	312	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	N	308	KC1	CHC-C4B-C3B	-2.60	120.81	125.26
28	A	316	CLA	CMB-C2B-C3B	2.60	129.54	124.68
28	K	311	CLA	CMB-C2B-C3B	2.60	129.54	124.68
29	F	309	KC1	C4B-CHC-C1C	-2.60	120.46	126.06
26	F	303	DD6	C41-C32-C31	-2.60	106.34	110.47
26	M	303	DD6	C9-C8-C6	-2.60	119.13	126.42
28	M	310	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	h	203	DD6	C21-C20-C15	-2.59	117.91	122.26
28	B	301	CLA	CMB-C2B-C3B	2.59	129.53	124.68
28	J	309	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	L	305	DD6	C21-C20-C15	-2.59	117.92	122.26
29	J	313	KC1	C4B-CHC-C1C	-2.59	120.47	126.06
28	I	316	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
32	F	304	PID	CM5-C21-C20	-2.59	119.30	122.92
28	b	708	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
29	J	313	KC1	CHC-C4B-C3B	-2.59	120.83	125.26
28	H	305	CLA	C1-C2-C3	-2.59	121.57	126.04
28	J	309	CLA	C1-C2-C3	-2.59	121.57	126.04
29	D	310	KC1	C4B-CHC-C1C	-2.58	120.48	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	301	CLA	CHB-C4A-NA	2.58	128.09	124.51
28	a	702	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
29	I	314	KC1	O1D-CGD-CBD	-2.58	119.20	124.48
28	D	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	B	314	KC1	O2D-CGD-O1D	-2.58	118.79	123.84
28	M	315	CLA	CAA-C2A-C3A	-2.58	110.08	116.10
26	G	505	DD6	C21-C20-C15	-2.58	117.94	122.26
28	F	311	CLA	CHB-C4A-NA	2.58	128.08	124.51
29	A	306	KC1	CHB-C1B-C2B	-2.58	120.07	125.48
28	L	308	CLA	C1-C2-C3	-2.58	122.58	126.75
28	I	306	CLA	CHB-C4A-NA	2.58	128.07	124.51
29	D	315	KC1	C2A-C3A-C4A	2.58	108.40	106.49
29	G	515	KC1	CHC-C4B-C3B	-2.58	120.85	125.26
26	M	305	DD6	C3-C4-C5	-2.58	118.20	123.47
28	A	310	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
28	b	728	CLA	CMB-C2B-C3B	2.57	129.49	124.68
28	M	312	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
28	b	715	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
30	j	103	DGD	C2G-O2G-C1B	-2.57	111.46	117.79
28	a	706	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	M	306	DD6	C12-C11-C10	-2.57	119.32	122.92
28	D	313	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	L	303	DD6	C3-C4-C5	-2.57	118.21	123.47
28	b	714	CLA	CHB-C4A-NA	2.57	128.06	124.51
28	b	714	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
28	l	310	CLA	C1B-CHB-C4A	-2.57	125.25	128.57
29	J	313	KC1	CHB-C1B-C2B	-2.57	120.09	125.48
28	A	307	CLA	CMB-C2B-C3B	2.57	129.48	124.68
28	b	720	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	I	305	DD6	C21-C20-C15	-2.56	117.96	122.26
26	J	302	DD6	C32-C33-C34	-2.56	107.85	113.64
26	N	303	DD6	C14-C13-C11	-2.56	121.55	125.53
27	h	201	UIX	C18-O2-C27	-2.56	113.12	117.90
27	G	503	UIX	C37-C39-C40	-2.56	123.65	127.31
28	G	510	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
29	N	311	KC1	CHB-C1B-C2B	-2.56	120.11	125.48
35	b	732	BCR	C15-C16-C17	-2.56	118.23	123.47
28	I	308	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
28	G	518	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	M	306	DD6	C7-C6-C5	-2.56	119.34	122.92
28	I	319	CLA	CHB-C4A-NA	2.56	128.05	124.51
28	a	711	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	309	KC1	CBD-CHA-C1A	2.56	133.65	128.88
28	J	314	CLA	CAA-C2A-C3A	-2.56	110.13	116.10
30	L	301	DGD	C2G-O2G-C1B	-2.56	111.50	117.79
28	a	713	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
28	K	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
29	I	314	KC1	CBD-CHA-C1A	2.55	133.64	128.88
28	L	317	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	K	305	DD6	C9-C10-C11	-2.55	123.67	127.31
26	A	302	DD6	C3-C4-C5	-2.55	118.25	123.47
28	I	310	CLA	CHB-C4A-NA	2.55	128.04	124.51
29	L	315	KC1	O1D-CGD-CBD	-2.55	119.27	124.48
28	a	715	CLA	CHB-C4A-NA	2.55	128.03	124.51
28	b	727	CLA	CHB-C4A-NA	2.55	128.03	124.51
28	B	309	CLA	CHB-C4A-NA	2.55	128.03	124.51
28	B	313	CLA	CHB-C4A-NA	2.55	128.03	124.51
28	H	307	CLA	CHB-C4A-NA	2.55	128.03	124.51
28	H	311	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
26	F	303	DD6	C33-C34-C35	-2.55	106.82	110.30
28	A	313	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	M	304	DD6	C21-C20-C15	-2.54	118.00	122.26
29	N	308	KC1	C3D-CAD-CBD	-2.54	104.26	107.61
28	b	706	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	F	301	DD6	O1-C20-C21	-2.54	112.01	115.06
35	b	730	BCR	C38-C26-C27	2.54	118.50	113.62
28	L	312	CLA	CMB-C2B-C3B	2.54	129.43	124.68
28	b	716	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	b	718	CLA	CMB-C2B-C3B	2.54	129.43	124.68
28	K	313	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	b	709	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	K	306	CLA	CHB-C4A-NA	2.54	128.03	124.51
28	h	202	CLA	CHB-C4A-NA	2.54	128.03	124.51
35	a	734	BCR	C23-C24-C25	-2.54	120.07	127.20
26	A	302	DD6	C12-C11-C10	-2.54	119.37	122.92
28	l	309	CLA	CHB-C4A-NA	2.54	128.02	124.51
30	G	521	DGD	O1G-C1A-C2A	2.53	119.86	111.91
28	G	516	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
28	A	317	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	L	304	DD6	C10-C9-C8	-2.53	115.32	123.22
28	A	311	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
28	M	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
28	F	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
28	J	316	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	305	UIX	C35-C36-C38	-2.53	115.33	123.22
28	b	704	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	D	303	DD6	C4-C3-C2	-2.53	118.30	123.47
26	B	306	DD6	C21-C20-C15	-2.53	118.03	122.26
28	a	738	CLA	CHB-C4A-NA	2.53	128.00	124.51
35	l	307	BCR	C2-C1-C6	2.52	114.37	110.48
28	B	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	I	316	CLA	CHD-C1D-ND	-2.52	122.13	124.45
28	l	313	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
27	A	304	UIX	C22-C15-C20	-2.52	108.21	110.47
26	M	305	DD6	C33-C34-C35	-2.52	106.85	110.30
28	b	705	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	N	304	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	D	316	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
35	i	201	BCR	C33-C5-C4	2.52	118.45	113.62
29	H	306	KC1	O1D-CGD-CBD	-2.52	119.33	124.48
28	J	315	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	b	728	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	F	315	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	a	720	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	a	731	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	A	315	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	F	303	DD6	C4-C3-C2	-2.52	118.32	123.47
28	K	316	CLA	CMB-C2B-C3B	2.51	129.38	124.68
28	I	309	CLA	CHB-C4A-NA	2.51	127.99	124.51
28	a	726	CLA	CHD-C1D-ND	-2.51	122.14	124.45
28	b	704	CLA	CAC-C3C-C4C	2.51	128.07	124.81
29	K	314	KC1	C3D-CAD-CBD	-2.51	104.30	107.61
28	b	718	CLA	CHB-C4A-NA	2.51	127.99	124.51
31	b	733	LMG	C1-C2-C3	-2.51	104.76	110.00
29	M	307	KC1	CHB-C1B-C2B	-2.51	120.21	125.48
28	I	313	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	G	517	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
28	J	314	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	b	717	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
28	G	511	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	K	305	DD6	C25-C26-C27	-2.51	119.29	126.58
28	J	301	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
28	b	712	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	L	316	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	B	303	DD6	C20-C19-C18	-2.51	107.79	112.75
29	M	307	KC1	C4B-CHC-C1C	-2.50	120.66	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	516	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	D	312	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	K	309	CLA	C1-C2-C3	-2.50	122.70	126.75
28	K	311	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
35	b	702	BCR	C27-C26-C25	-2.50	119.10	122.73
26	M	303	DD6	C37-C36-C35	2.50	118.99	114.36
28	f	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	L	307	KC1	O2A-CGA-O1A	-2.50	117.47	122.67
28	a	714	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	F	308	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	H	309	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	A	314	KC1	O1D-CGD-CBD	-2.50	119.37	124.48
28	F	307	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	B	303	DD6	C9-C10-C11	-2.50	123.75	127.31
28	b	719	CLA	CHB-C4A-NA	2.50	127.97	124.51
28	L	309	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
35	m	201	BCR	C21-C20-C19	-2.50	115.43	123.22
28	A	309	CLA	CHB-C4A-NA	2.50	127.96	124.51
28	A	316	CLA	CHB-C4A-NA	2.50	127.96	124.51
35	i	201	BCR	C4-C5-C6	-2.50	119.11	122.73
28	M	313	CLA	CHD-C1D-ND	-2.49	122.16	124.45
28	A	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	K	303	DD6	C21-C20-C15	-2.49	118.08	122.26
28	M	308	CLA	CHB-C4A-NA	2.49	127.96	124.51
29	H	306	KC1	C2A-C3A-C4A	2.49	108.33	106.49
28	a	704	CLA	CHD-C1D-ND	-2.49	122.17	124.45
29	I	314	KC1	C3D-CAD-CBD	-2.49	104.33	107.61
28	f	301	CLA	CHB-C4A-NA	2.49	127.95	124.51
28	G	509	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	I	304	UIX	O2-C27-O4	-2.49	118.02	122.96
28	a	709	CLA	CHB-C4A-NA	2.49	127.95	124.51
28	K	309	CLA	CHB-C4A-NA	2.49	127.95	124.51
35	l	307	BCR	C28-C27-C26	-2.49	109.64	114.08
28	J	311	CLA	CHB-C4A-NA	2.48	127.95	124.51
29	H	310	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
28	H	308	CLA	CHB-C4A-NA	2.48	127.95	124.51
26	M	302	DD6	C9-C10-C11	-2.48	123.77	127.31
29	L	315	KC1	O2D-CGD-O1D	-2.48	118.98	123.84
29	F	314	KC1	C4B-CHC-C1C	-2.48	120.70	126.06
31	I	318	LMG	O7-C10-O9	-2.48	117.70	123.70
30	I	317	DGD	C2G-O2G-C1B	-2.48	111.68	117.79
28	A	307	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	725	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
28	M	316	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	G	515	KC1	C2A-C3A-C4A	2.48	108.33	106.49
26	K	319	DD6	C12-C11-C10	-2.48	119.45	122.92
28	a	706	CLA	CHD-C1D-ND	-2.48	122.18	124.45
28	G	513	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	L	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	D	316	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	J	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	M	306	DD6	C21-C20-C15	-2.48	118.11	122.26
28	a	723	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
26	M	306	DD6	C19-C18-C17	-2.48	105.99	110.77
26	N	303	DD6	C4-C3-C2	-2.48	118.40	123.47
26	J	302	DD6	C33-C34-C35	-2.47	106.92	110.30
28	L	313	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	J	304	DD6	C25-C26-C27	-2.47	119.40	126.58
28	D	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	L	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
30	y	201	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
26	F	301	DD6	C34-C35-C36	-2.47	106.93	111.85
26	B	304	DD6	C10-C9-C8	-2.47	115.50	123.22
27	B	305	UIX	O2-C27-O4	-2.47	118.05	122.96
28	I	321	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
28	H	312	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	M	305	DD6	C25-C26-C27	-2.47	119.41	126.58
28	b	724	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	N	303	DD6	C37-C36-C35	2.47	118.93	114.36
28	a	728	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	b	715	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	B	307	CLA	CHB-C4A-NA	2.47	127.93	124.51
35	l	302	BCR	C33-C5-C4	2.47	118.36	113.62
28	I	308	CLA	CHD-C1D-ND	-2.47	122.19	124.45
28	K	308	CLA	CHD-C1D-ND	-2.47	122.19	124.45
28	a	711	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
28	j	104	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	A	305	DD6	C25-C26-C27	-2.47	119.42	126.58
28	a	712	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
28	K	308	CLA	CHB-C4A-NA	2.46	127.92	124.51
28	K	307	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
29	K	314	KC1	C4B-CHC-C1C	-2.46	120.75	126.06
28	M	311	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	G	505	DD6	C32-C33-C34	-2.46	108.08	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	708	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	I	301	DD6	C32-C31-C36	-2.46	119.16	122.63
28	A	319	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
28	G	510	CLA	CHD-C1D-ND	-2.46	122.19	124.45
35	i	201	BCR	C28-C27-C26	-2.46	109.69	114.08
28	b	708	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	G	502	DD6	C37-C36-C35	2.46	118.91	114.36
35	a	734	BCR	C15-C16-C17	-2.46	118.44	123.47
29	L	307	KC1	O2D-CGD-O1D	-2.46	119.04	123.84
26	M	303	DD6	C13-C11-C10	2.45	122.71	118.94
28	j	106	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
27	J	305	UIX	C35-C36-C38	-2.45	115.56	123.22
28	F	311	CLA	O2D-CGD-CBD	2.45	115.62	111.27
35	i	201	BCR	C38-C26-C27	2.45	118.33	113.62
32	M	301	PID	C19-C20-C21	2.45	130.81	127.31
26	L	305	DD6	C37-C36-C35	2.45	118.90	114.36
28	f	302	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
26	K	301	DD6	C26-C25-C24	-2.45	115.57	123.22
26	G	504	DD6	O1-C20-C15	-2.45	56.93	58.96
26	I	302	DD6	C3-C4-C5	-2.45	118.46	123.47
28	N	305	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
28	H	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	G	515	KC1	O1D-CGD-CBD	-2.45	119.47	124.48
28	G	513	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
28	l	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
28	a	707	CLA	CHB-C4A-NA	2.45	127.90	124.51
28	b	713	CLA	CHB-C4A-NA	2.45	127.89	124.51
28	J	316	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
28	K	311	CLA	CHB-C4A-NA	2.45	127.89	124.51
26	M	304	DD6	C9-C10-C11	-2.44	123.82	127.31
28	L	317	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
26	N	303	DD6	C33-C34-C35	-2.44	106.96	110.30
27	A	304	UIX	C34-C37-C39	-2.44	118.47	123.47
28	a	721	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
28	L	312	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	D	305	PID	C18-C17-C16	2.44	130.24	124.81
35	f	304	BCR	C11-C12-C13	-2.44	119.56	126.42
26	G	508	DD6	C37-C36-C35	2.44	118.88	114.36
28	b	711	CLA	CHB-C4A-NA	2.44	127.89	124.51
28	I	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
28	b	703	CLA	C1-C2-C3	-2.44	121.82	126.04
26	L	306	DD6	C25-C26-C27	-2.44	119.50	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	725	CLA	CHB-C4A-NA	2.44	127.88	124.51
28	I	321	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
35	a	736	BCR	C24-C23-C22	-2.44	122.55	126.23
28	D	314	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
35	l	302	BCR	C27-C26-C25	-2.44	119.19	122.73
28	I	307	CLA	CHB-C4A-NA	2.44	127.88	124.51
28	a	729	CLA	CHD-C1D-ND	-2.44	122.22	124.45
29	I	314	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
29	A	306	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
27	A	304	UIX	O2-C27-O4	-2.44	118.12	122.96
28	B	311	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
28	a	703	CLA	CHB-C4A-NA	2.43	127.88	124.51
28	L	313	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
26	B	303	DD6	C33-C34-C35	-2.43	106.97	110.30
29	N	311	KC1	C4B-CHC-C1C	-2.43	120.81	126.06
28	a	712	CLA	CHB-C4A-NA	2.43	127.88	124.51
28	L	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	A	301	DD6	C33-C34-C35	-2.43	106.97	110.30
28	a	703	CLA	C1-C2-C3	-2.43	121.83	126.04
29	M	307	KC1	O2A-CGA-O1A	-2.43	117.62	122.67
28	K	310	CLA	CHB-C4A-NA	2.43	127.88	124.51
28	J	311	CLA	CHD-C1D-ND	-2.43	122.22	124.45
28	N	309	CLA	CHB-C4A-NA	2.43	127.87	124.51
28	G	512	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	G	515	KC1	C4B-CHC-C1C	-2.43	120.82	126.06
28	l	308	CLA	CAA-C2A-C3A	-2.43	110.43	116.10
28	K	316	CLA	CHB-C4A-NA	2.43	127.87	124.51
28	b	705	CLA	C1-C2-C3	-2.42	121.85	126.04
26	J	304	DD6	O1-C20-C19	-2.42	111.56	113.38
26	A	302	DD6	C33-C34-C35	-2.42	106.99	110.30
26	N	303	DD6	C21-C20-C15	-2.42	118.20	122.26
28	l	308	CLA	CHB-C4A-NA	2.42	127.86	124.51
28	F	308	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
28	D	313	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	h	203	DD6	C3-C4-C5	-2.42	118.52	123.47
28	a	711	CLA	CHD-C1D-ND	-2.42	122.23	124.45
28	K	307	CLA	CHB-C4A-NA	2.42	127.86	124.51
35	l	306	BCR	C35-C13-C12	2.42	121.89	118.08
28	b	706	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
28	A	320	CLA	CHB-C4A-NA	2.42	127.85	124.51
28	a	724	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
29	L	307	KC1	C4B-CHC-C1C	-2.42	120.84	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	707	CLA	C1-C2-C3	-2.42	121.86	126.04
28	l	312	CLA	CHD-C1D-ND	-2.41	122.24	124.45
28	b	720	CLA	CHB-C4A-NA	2.41	127.85	124.51
28	M	312	CLA	CHB-C4A-NA	2.41	127.85	124.51
28	a	727	CLA	CHB-C4A-NA	2.41	127.84	124.51
28	a	719	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
28	A	311	CLA	CHD-C1D-ND	-2.41	122.24	124.45
26	B	306	DD6	C37-C36-C35	2.41	118.82	114.36
28	a	722	CLA	CHB-C4A-NA	2.41	127.84	124.51
28	a	707	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	N	306	KC1	C4B-CHC-C1C	-2.41	120.86	126.06
26	G	502	DD6	O1-C20-C21	-2.41	112.17	115.06
29	N	308	KC1	CGD-CBD-CAD	-2.41	102.94	110.73
28	I	315	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
28	b	726	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	G	521	DGD	C1D-O6D-C5D	-2.41	108.97	113.69
29	D	315	KC1	O1D-CGD-CBD	-2.41	119.56	124.48
29	A	314	KC1	CBD-CHA-C1A	2.40	133.37	128.88
29	A	314	KC1	C4B-CHC-C1C	-2.40	120.87	126.06
28	b	706	CLA	CHB-C4A-NA	2.40	127.84	124.51
28	A	310	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	G	514	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
30	j	103	DGD	O1G-C1A-C2A	2.40	119.45	111.91
28	m	202	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	B	302	DD6	C-C1-C2	-2.40	119.56	122.92
26	F	301	DD6	C7-C6-C5	-2.40	119.56	122.92
28	b	705	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	a	710	CLA	CHB-C4A-NA	2.40	127.83	124.51
28	M	318	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	L	315	KC1	C2A-C3A-C4A	2.40	108.27	106.49
28	l	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
35	b	732	BCR	C38-C26-C25	-2.40	121.83	124.53
29	H	306	KC1	CBD-CHA-C1A	2.40	133.35	128.88
28	a	723	CLA	CHB-C4A-NA	2.40	127.83	124.51
32	M	301	PID	CM5-C21-C20	-2.40	119.56	122.92
29	G	515	KC1	CAC-C3C-C4C	2.40	127.92	124.81
26	L	305	DD6	O1-C20-C19	-2.39	111.58	113.38
28	f	301	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
28	a	705	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
29	L	315	KC1	C4B-CHC-C1C	-2.39	120.89	126.06
35	b	730	BCR	C2-C1-C6	2.39	114.17	110.48
26	G	504	DD6	C25-C24-C1	-2.39	119.69	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	312	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
29	F	309	KC1	O1D-CGD-CBD	-2.39	119.59	124.48
28	K	315	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	J	302	DD6	C12-C11-C10	-2.39	119.57	122.92
28	A	313	CLA	C1-C2-C3	-2.39	121.91	126.04
28	H	304	CLA	CHB-C4A-NA	2.39	127.82	124.51
28	A	308	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
26	M	305	DD6	C37-C36-C35	2.39	118.78	114.36
28	b	709	CLA	O2D-CGD-CBD	2.39	115.51	111.27
28	L	318	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
26	K	304	DD6	C32-C33-C34	-2.39	108.25	113.64
28	K	310	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
31	I	320	LMG	O1-C7-C8	-2.39	105.14	110.90
28	D	314	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
27	h	201	UIX	C12-C11-C10	2.38	121.83	118.08
29	F	314	KC1	O2D-CGD-O1D	-2.38	119.18	123.84
28	A	312	CLA	CHB-C4A-NA	2.38	127.81	124.51
28	b	707	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
26	L	306	DD6	C21-C20-C15	-2.38	118.27	122.26
27	h	201	UIX	O2-C27-O4	-2.38	118.23	122.96
28	B	309	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
28	N	310	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
28	K	312	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
28	f	302	CLA	CHB-C4A-NA	2.38	127.80	124.51
28	I	311	CLA	CHB-C4A-NA	2.38	127.80	124.51
28	M	308	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
28	J	312	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
28	J	307	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
28	j	106	CLA	CHB-C4A-NA	2.37	127.80	124.51
28	K	316	CLA	CHD-C1D-ND	-2.37	122.27	124.45
26	K	301	DD6	C4-C3-C2	-2.37	118.61	123.47
29	I	314	KC1	O2D-CGD-O1D	-2.37	119.20	123.84
28	b	719	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
28	a	717	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	J	303	DD6	C20-C19-C18	-2.37	108.06	112.75
28	M	318	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	I	304	UIX	C41-C40-C38	2.37	121.81	118.08
29	N	306	KC1	O2D-CGD-O1D	-2.37	119.20	123.84
28	L	312	CLA	CHD-C1D-ND	-2.37	122.28	124.45
28	I	313	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
28	l	308	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
28	I	315	CLA	CHB-C4A-NA	2.37	127.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	304	DD6	O1-C20-C21	-2.37	112.22	115.06
28	l	310	CLA	C4D-ND-C1D	-2.37	106.22	109.68
28	l	312	CLA	CHB-C4A-NA	2.37	127.78	124.51
32	N	302	PID	CM4-C14-C13	2.37	124.51	119.05
28	b	719	CLA	CHD-C1D-ND	-2.36	122.28	124.45
26	M	303	DD6	C7-C6-C5	-2.36	119.61	122.92
26	B	306	DD6	C25-C24-C1	-2.36	119.78	126.42
26	h	203	DD6	C14-C13-C11	-2.36	121.87	125.53
28	b	725	CLA	CHB-C4A-NA	2.36	127.78	124.51
35	m	201	BCR	C36-C18-C19	2.36	121.80	118.08
26	J	303	DD6	C37-C36-C35	2.36	118.73	114.36
28	G	520	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	B	303	DD6	C3-C4-C5	-2.36	118.64	123.47
28	b	703	CLA	CMB-C2B-C3B	2.36	129.09	124.68
28	a	701	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	F	314	KC1	O1D-CGD-CBD	-2.36	119.66	124.48
28	a	717	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
26	I	303	DD6	C19-C18-C17	-2.36	106.22	110.77
26	B	306	DD6	C10-C9-C8	-2.36	115.86	123.22
26	A	305	DD6	C21-C20-C15	-2.36	118.31	122.26
27	A	304	UIX	C13-C14-C23	-2.36	115.86	123.22
28	G	509	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
28	H	307	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
29	B	314	KC1	C4B-CHC-C1C	-2.35	120.98	126.06
35	b	702	BCR	C33-C5-C4	2.35	118.14	113.62
28	H	309	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
28	A	317	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	a	706	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	J	308	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	a	721	CLA	C1-C2-C3	-2.35	121.97	126.04
28	L	313	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	a	705	CLA	CHD-C1D-ND	-2.35	122.29	124.45
28	B	309	CLA	CHD-C1D-ND	-2.35	122.29	124.45
28	A	313	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	a	710	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
28	I	309	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
31	b	733	LMG	C38-C37-C36	-2.35	102.50	114.42
28	b	728	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
26	I	301	DD6	C14-C13-C11	-2.35	121.89	125.53
29	H	306	KC1	C4B-CHC-C1C	-2.35	120.99	126.06
29	N	311	KC1	O1D-CGD-CBD	-2.35	119.68	124.48
28	a	715	CLA	C1B-CHB-C4A	-2.35	125.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	725	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	b	704	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
26	L	306	DD6	O1-C20-C21	-2.35	112.25	115.06
28	A	319	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	K	301	DD6	C37-C36-C35	2.35	118.70	114.36
29	M	314	KC1	C4B-CHC-C1C	-2.35	121.00	126.06
28	I	310	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	l	305	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
35	l	307	BCR	C21-C20-C19	-2.34	115.90	123.22
28	L	309	CLA	O2D-CGD-CBD	2.34	115.43	111.27
26	I	302	DD6	C4-C5-C6	-2.34	123.97	127.31
26	M	302	DD6	C37-C36-C35	2.34	118.70	114.36
28	F	310	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
28	M	317	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
35	b	730	BCR	C36-C18-C19	2.34	121.77	118.08
28	J	309	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
28	M	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
26	M	304	DD6	C10-C9-C8	-2.34	115.91	123.22
28	a	709	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
35	f	304	BCR	C29-C30-C25	2.34	114.08	110.48
26	B	302	DD6	C8-C9-C10	-2.34	118.69	123.47
28	I	313	CLA	CHD-C1D-ND	-2.34	122.31	124.45
28	b	709	CLA	C1-C2-C3	-2.34	122.00	126.04
28	B	301	CLA	CHD-C1D-ND	-2.34	122.31	124.45
28	D	308	CLA	CHB-C4A-NA	2.34	127.74	124.51
28	K	316	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
28	b	726	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
28	M	316	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
28	a	724	CLA	CHB-C4A-NA	2.33	127.74	124.51
28	B	316	CLA	CHB-C4A-NA	2.33	127.74	124.51
31	D	317	LMG	O1-C7-C8	-2.33	105.27	110.90
28	b	727	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
35	a	734	BCR	C29-C30-C25	2.33	114.07	110.48
28	a	731	CLA	C1-C2-C3	-2.33	122.01	126.04
28	b	722	CLA	C2D-C1D-ND	-2.33	108.39	110.10
35	j	102	BCR	C33-C5-C4	2.33	118.09	113.62
28	b	712	CLA	CHD-C1D-ND	-2.33	122.31	124.45
28	H	312	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
28	L	314	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
28	I	312	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	A	301	DD6	C37-C36-C35	2.33	118.67	114.36
26	F	303	DD6	C21-C20-C15	-2.33	118.36	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	713	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
28	J	314	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
28	j	104	CLA	C1-C2-C3	-2.33	122.02	126.04
28	l	303	CLA	CHD-C1D-ND	-2.33	122.32	124.45
35	f	304	BCR	C38-C26-C27	2.33	118.08	113.62
29	D	315	KC1	CBD-CHA-C1A	2.33	133.22	128.88
28	a	716	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
28	I	316	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
28	b	710	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
28	I	308	CLA	C1-C2-C3	-2.32	122.02	126.04
26	A	301	DD6	C3-C4-C5	-2.32	118.71	123.47
28	L	308	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	J	311	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	l	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	J	306	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	J	311	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
26	N	303	DD6	C25-C26-C27	-2.32	119.84	126.58
28	B	316	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	M	311	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	M	315	CLA	O2D-CGD-CBD	2.32	115.39	111.27
28	a	702	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
28	b	716	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
31	B	318	LMG	O7-C10-O9	-2.32	118.10	123.70
28	K	315	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	l	311	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	F	313	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
28	b	723	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
26	B	302	DD6	C12-C11-C10	-2.32	119.68	122.92
35	j	102	BCR	C10-C11-C12	-2.32	115.99	123.22
28	a	730	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	B	304	DD6	C37-C36-C35	2.32	118.64	114.36
28	H	311	CLA	CHB-C4A-NA	2.32	127.71	124.51
26	L	306	DD6	C33-C34-C35	-2.32	107.14	110.30
35	a	736	BCR	C23-C24-C25	-2.31	120.70	127.20
29	M	307	KC1	C2A-C3A-C4A	2.31	108.20	106.49
28	D	311	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
27	A	304	UIX	C-C7-C10	-2.31	121.10	125.99
26	A	302	DD6	C25-C26-C27	-2.31	119.86	126.58
28	b	711	CLA	CHD-C1D-ND	-2.31	122.33	124.45
28	a	719	CLA	CHB-C4A-NA	2.31	127.71	124.51
28	a	729	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	A	305	DD6	C33-C34-C35	-2.31	107.14	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	305	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	K	301	DD6	C10-C9-C8	-2.31	116.00	123.22
28	B	310	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
28	b	703	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
32	D	302	PID	C17-C16-C15	2.31	128.21	123.47
31	B	318	LMG	C38-C37-C36	-2.31	102.70	114.42
26	M	304	DD6	O1-C20-C21	-2.31	112.29	115.06
28	N	305	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
28	I	306	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
28	H	311	CLA	CAA-C2A-C3A	-2.31	110.71	116.10
28	a	710	CLA	C1-C2-C3	-2.31	122.05	126.04
28	b	728	CLA	CHD-C1D-ND	-2.31	122.33	124.45
28	G	511	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
28	G	519	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	G	505	DD6	C25-C26-C27	-2.30	119.89	126.58
26	A	301	DD6	O1-C20-C21	-2.30	112.30	115.06
27	G	503	UIX	C13-C14-C23	-2.30	116.03	123.22
28	a	735	CLA	CHD-C1D-ND	-2.30	122.34	124.45
28	b	707	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	M	303	DD6	C21-C20-C19	2.30	116.87	114.28
28	G	510	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
29	H	306	KC1	O2D-CGD-O1D	-2.30	119.34	123.84
26	M	302	DD6	C10-C9-C8	-2.30	116.05	123.22
36	a	732	PQN	C2M-C2-C3	-2.30	120.65	124.40
26	G	505	DD6	C19-C18-C17	-2.30	106.34	110.77
28	A	320	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
28	f	303	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
28	H	304	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
32	D	305	PID	CM4-C14-C13	2.30	124.34	119.05
28	l	305	CLA	CHD-C1D-ND	-2.29	122.34	124.45
28	l	313	CLA	CHD-C1D-ND	-2.29	122.34	124.45
28	b	711	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
28	D	309	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
26	b	731	DD6	C10-C9-C8	-2.29	116.06	123.22
26	K	319	DD6	C37-C36-C35	2.29	118.61	114.36
31	b	733	LMG	O1-C7-C8	-2.29	105.36	110.90
28	I	309	CLA	CHD-C1D-ND	-2.29	122.35	124.45
28	b	717	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	B	303	DD6	C21-C20-C15	-2.29	118.42	122.26
28	A	309	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	I	304	UIX	C34-C30-C26	-2.29	124.04	127.31
28	L	314	CLA	CHD-C1D-ND	-2.29	122.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	310	KC1	O1D-CGD-CBD	-2.29	119.80	124.48
28	K	313	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
26	A	302	DD6	C9-C8-C6	-2.29	119.98	126.42
28	L	309	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
28	I	316	CLA	C1-C2-C3	-2.29	122.08	126.04
28	b	706	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
28	G	516	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
35	a	734	BCR	C38-C26-C27	2.29	118.01	113.62
29	K	314	KC1	C2A-C3A-C4A	2.29	108.18	106.49
28	b	701	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
28	K	306	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
28	a	708	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
28	a	718	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
26	L	306	DD6	C9-C8-C6	-2.28	120.00	126.42
35	b	702	BCR	C35-C13-C12	2.28	121.68	118.08
29	D	310	KC1	C3D-CAD-CBD	-2.28	104.60	107.61
28	L	313	CLA	CHD-C1D-ND	-2.28	122.36	124.45
28	M	309	CLA	CHD-C1D-ND	-2.28	122.36	124.45
28	a	728	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
28	L	310	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	a	717	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
26	I	303	DD6	C37-C36-C35	2.28	118.58	114.36
28	b	716	CLA	C1-C2-C3	-2.28	123.06	126.75
35	l	306	BCR	C10-C11-C12	-2.28	116.10	123.22
28	a	730	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
28	A	312	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	K	305	DD6	C37-C36-C35	2.28	118.57	114.36
28	F	312	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
28	b	721	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
28	M	309	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
28	K	306	CLA	CHD-C1D-ND	-2.28	122.36	124.45
35	a	734	BCR	C21-C20-C19	-2.27	116.12	123.22
28	b	715	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
35	l	302	BCR	C23-C22-C21	2.27	122.43	118.94
26	A	305	DD6	C20-C19-C18	-2.27	108.25	112.75
27	A	304	UIX	C19-C18-C17	-2.27	105.91	109.88
26	F	301	DD6	C4-C3-C2	-2.27	118.82	123.47
28	b	718	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	J	302	DD6	C25-C26-C27	-2.27	119.98	126.58
28	B	317	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	B	304	DD6	C3-C4-C5	-2.27	118.82	123.47
32	D	302	PID	CM4-C14-C13	2.27	124.29	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M	314	KC1	C2A-C3A-C4A	2.27	108.17	106.49
28	a	720	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
28	B	313	CLA	CHD-C1D-ND	-2.27	122.37	124.45
28	H	307	CLA	CHD-C1D-ND	-2.27	122.37	124.45
28	B	311	CLA	CHB-C4A-NA	2.27	127.65	124.51
28	F	312	CLA	CHB-C4A-NA	2.27	127.65	124.51
28	L	311	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
28	I	312	CLA	CHD-C1D-ND	-2.27	122.37	124.45
28	I	313	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
28	a	714	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
28	J	309	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
28	I	315	CLA	O2D-CGD-CBD	2.27	115.29	111.27
28	f	303	CLA	CHD-C1D-ND	-2.27	122.37	124.45
27	A	304	UIX	C7-C10-C11	-2.27	122.02	125.53
35	b	730	BCR	C30-C25-C26	-2.27	119.42	122.61
26	I	305	DD6	C28-C27-C29	2.26	121.32	116.84
28	L	308	CLA	CAC-C3C-C4C	2.26	127.75	124.81
35	b	732	BCR	C34-C9-C8	2.26	121.64	118.08
28	a	717	CLA	CHD-C1D-ND	-2.26	122.38	124.45
28	a	724	CLA	C2D-C1D-ND	-2.26	108.44	110.10
27	h	201	UIX	C35-C36-C38	-2.26	116.16	123.22
28	D	316	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
26	N	303	DD6	C9-C8-C6	-2.26	120.06	126.42
26	G	502	DD6	O1-C20-C19	-2.26	111.68	113.38
28	G	520	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
26	K	319	DD6	C3-C4-C5	-2.26	118.84	123.47
26	B	302	DD6	C4-C3-C2	-2.26	118.84	123.47
26	A	303	DD6	C4-C3-C2	-2.26	118.85	123.47
28	I	311	CLA	O2D-CGD-CBD	2.26	115.28	111.27
35	b	730	BCR	C24-C23-C22	-2.26	122.82	126.23
28	L	308	CLA	CHD-C1D-ND	-2.26	122.38	124.45
28	b	727	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
28	J	314	CLA	CHD-C1D-ND	-2.26	122.38	124.45
28	B	310	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
28	G	513	CLA	CHD-C1D-ND	-2.26	122.38	124.45
28	J	315	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
28	a	705	CLA	CAA-CBA-CGA	-2.25	106.66	113.25
28	a	718	CLA	CHD-C1D-ND	-2.25	122.38	124.45
32	N	302	PID	C6-C7-C8	-2.25	121.23	125.99
26	F	301	DD6	C12-C11-C10	-2.25	119.77	122.92
35	l	307	BCR	C8-C7-C6	-2.25	120.87	127.20
26	A	302	DD6	O1-C20-C21	-2.25	112.36	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	304	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
28	F	311	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
28	K	311	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	a	713	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	B	310	CLA	CHB-C4A-NA	2.25	127.62	124.51
28	j	104	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
35	l	302	BCR	C11-C10-C9	-2.25	124.10	127.31
28	K	309	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
28	F	307	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
28	F	310	CLA	O2D-CGD-CBD	2.25	115.27	111.27
28	F	310	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	B	313	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
28	a	709	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	K	319	DD6	C9-C8-C6	-2.25	120.11	126.42
28	B	310	CLA	O2D-CGD-CBD	2.25	115.26	111.27
26	G	504	DD6	C25-C26-C27	-2.25	120.06	126.58
28	l	309	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
28	A	307	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
26	I	305	DD6	C9-C10-C11	-2.24	124.11	127.31
28	h	202	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
28	a	727	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
28	b	723	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
26	B	303	DD6	C10-C9-C8	-2.24	116.22	123.22
28	b	710	CLA	CHB-C4A-NA	2.24	127.61	124.51
31	I	320	LMG	O7-C10-O9	-2.24	118.29	123.70
31	K	318	LMG	O1-C7-C8	-2.24	105.49	110.90
28	M	310	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
28	M	315	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
35	b	732	BCR	C37-C22-C23	2.24	121.61	118.08
28	B	308	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
28	L	316	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
26	A	303	DD6	C20-C19-C18	-2.24	108.32	112.75
35	a	736	BCR	C21-C20-C19	-2.24	116.23	123.22
31	j	101	LMG	O3-C3-C2	-2.24	105.18	110.35
28	b	714	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	h	201	UIX	C21-C15-C20	-2.24	108.47	110.47
26	A	301	DD6	C12-C11-C10	-2.24	119.79	122.92
26	B	303	DD6	C37-C36-C35	2.24	118.50	114.36
28	L	317	CLA	CHD-C1D-ND	-2.24	122.40	124.45
28	F	315	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
31	K	318	LMG	O1-C1-C2	-2.23	104.82	108.30
35	b	732	BCR	C35-C13-C12	2.23	121.59	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	203	DD6	C10-C9-C8	-2.23	116.25	123.22
27	K	302	UIX	O2-C27-O4	-2.23	118.53	122.96
28	a	708	CLA	CHD-C1D-ND	-2.23	122.40	124.45
29	A	306	KC1	O1D-CGD-CBD	-2.23	119.92	124.48
28	A	313	CLA	CHD-C1D-ND	-2.23	122.41	124.45
28	A	315	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
28	H	308	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	J	303	DD6	C9-C8-C6	-2.23	120.16	126.42
26	B	306	DD6	O1-C20-C21	-2.23	112.39	115.06
29	J	313	KC1	O1D-CGD-CBD	-2.23	119.93	124.48
27	G	503	UIX	O2-C27-O4	-2.23	118.54	122.96
26	G	502	DD6	C25-C24-C1	-2.23	120.16	126.42
35	b	730	BCR	C37-C22-C23	2.23	121.58	118.08
26	B	302	DD6	C37-C36-C35	2.23	118.48	114.36
29	M	314	KC1	O1D-CGD-CBD	-2.23	119.93	124.48
28	G	512	CLA	CHD-C1D-ND	-2.23	122.41	124.45
28	b	701	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
35	f	304	BCR	C8-C7-C6	-2.22	120.96	127.20
28	M	308	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
26	b	731	DD6	C21-C20-C15	-2.22	118.53	122.26
28	L	309	CLA	CHD-C1D-ND	-2.22	122.41	124.45
28	L	318	CLA	CHD-C1D-ND	-2.22	122.41	124.45
35	b	730	BCR	C20-C21-C22	-2.22	124.14	127.31
28	H	305	CLA	CHD-C1D-ND	-2.22	122.41	124.45
28	B	301	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	D	315	KC1	CHC-C4B-C3B	-2.22	121.46	125.26
28	M	312	CLA	CHD-C1D-ND	-2.22	122.41	124.45
28	b	724	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
26	L	306	DD6	C12-C11-C10	-2.22	119.81	122.92
26	A	302	DD6	C25-C24-C1	-2.22	120.18	126.42
28	I	307	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	B	307	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
28	b	728	CLA	C1-C2-C3	-2.22	122.21	126.04
29	B	314	KC1	CBD-CHA-C1A	2.22	133.01	128.88
28	l	310	CLA	C4B-CHC-C1C	-2.22	126.16	128.81
28	B	315	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
28	a	725	CLA	CHD-C1D-ND	-2.21	122.42	124.45
35	a	736	BCR	C34-C9-C10	-2.21	119.82	122.92
28	a	735	CLA	C1-C2-C3	-2.21	122.22	126.04
26	M	304	DD6	C28-C27-C29	2.21	121.22	116.84
28	a	721	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	K	309	CLA	CHD-C1D-ND	-2.21	122.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	303	DD6	C33-C34-C35	-2.21	107.28	110.30
28	I	310	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
31	b	734	LMG	O3-C3-C2	-2.21	105.24	110.35
28	a	707	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	J	309	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	K	304	DD6	C14-C13-C11	-2.21	122.10	125.53
28	a	728	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	A	305	DD6	C15-C14-C13	-2.21	121.32	125.99
28	a	722	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	G	502	DD6	C20-C19-C18	-2.21	108.38	112.75
28	a	728	CLA	CHD-C1D-ND	-2.21	122.43	124.45
28	M	308	CLA	CHD-C1D-ND	-2.21	122.43	124.45
26	G	505	DD6	C12-C11-C10	-2.21	119.83	122.92
27	K	302	UIX	C12-C11-C13	-2.21	119.83	122.92
28	F	308	CLA	CHD-C1D-ND	-2.21	122.43	124.45
28	a	738	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
28	B	310	CLA	CHD-C1D-ND	-2.20	122.43	124.45
29	N	311	KC1	O2D-CGD-O1D	-2.20	119.53	123.84
28	G	512	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
28	a	731	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
26	M	306	DD6	C32-C31-C36	-2.20	119.52	122.63
28	G	518	CLA	O2D-CGD-CBD	2.20	115.18	111.27
27	J	305	UIX	C18-O2-C27	-2.20	113.79	117.90
28	A	319	CLA	CHD-C1D-ND	-2.20	122.43	124.45
28	G	518	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
26	L	302	DD6	C32-C33-C34	-2.20	108.67	113.64
28	K	310	CLA	CHD-C1D-ND	-2.20	122.43	124.45
27	G	503	UIX	C12-C11-C10	2.20	121.54	118.08
28	a	713	CLA	CHB-C4A-NA	2.20	127.55	124.51
29	D	315	KC1	CAB-C3B-C4B	2.20	130.21	124.90
28	D	308	CLA	CHD-C1D-ND	-2.20	122.43	124.45
28	H	309	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
28	j	104	CLA	CHD-C1D-ND	-2.20	122.44	124.45
29	L	315	KC1	CAC-C3C-C4C	2.20	127.66	124.81
35	l	306	BCR	C21-C20-C19	-2.20	116.36	123.22
28	D	309	CLA	CHD-C1D-ND	-2.20	122.44	124.45
26	K	304	DD6	C21-C20-C15	-2.20	118.58	122.26
28	a	726	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
28	a	703	CLA	C2D-C1D-ND	-2.19	108.49	110.10
26	M	305	DD6	C10-C9-C8	-2.19	116.37	123.22
28	a	722	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	h	203	DD6	C33-C34-C35	-2.19	107.30	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	320	LMG	O3-C3-C2	-2.19	105.28	110.35
28	b	716	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	H	309	CLA	CHD-C1D-ND	-2.19	122.44	124.45
30	y	201	DGD	O1G-C1A-C2A	2.19	118.78	111.91
32	j	105	PID	O4-C12-C13	2.19	127.56	122.89
26	A	302	DD6	O1-C20-C19	2.19	115.03	113.38
29	A	306	KC1	CBD-CHA-C1A	2.19	132.96	128.88
26	L	302	DD6	C37-C36-C35	2.19	118.41	114.36
28	G	511	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	M	302	DD6	C24-C1-C2	2.19	122.30	118.94
26	K	301	DD6	C-C1-C24	2.19	121.52	118.08
31	K	317	LMG	O7-C10-O9	-2.19	118.42	123.70
26	K	301	DD6	C33-C34-C35	-2.19	107.31	110.30
28	G	517	CLA	CHD-C1D-ND	-2.19	122.45	124.45
26	J	303	DD6	C12-C11-C10	-2.18	119.86	122.92
28	a	713	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
28	b	722	CLA	CHB-C4A-NA	2.18	127.53	124.51
28	M	318	CLA	CHD-C1D-ND	-2.18	122.45	124.45
28	a	705	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
35	a	736	BCR	C16-C15-C14	-2.18	119.00	123.47
28	L	314	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
35	b	730	BCR	C23-C24-C25	-2.18	121.07	127.20
35	l	302	BCR	C34-C9-C8	2.18	121.52	118.08
32	H	301	PID	C16-C15-C14	-2.18	124.20	127.31
28	f	302	CLA	CHD-C1D-ND	-2.18	122.45	124.45
32	F	305	PID	CM5-C21-C20	-2.18	119.87	122.92
29	D	310	KC1	O2D-CGD-O1D	-2.18	119.57	123.84
29	F	309	KC1	O2D-CGD-O1D	-2.18	119.57	123.84
29	J	313	KC1	C2A-C3A-C4A	2.18	108.10	106.49
28	G	519	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	M	306	DD6	O1-C20-C15	-2.18	57.15	58.96
26	K	304	DD6	C25-C24-C1	-2.18	120.29	126.42
29	H	310	KC1	O2D-CGD-O1D	-2.18	119.58	123.84
28	f	301	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
28	b	713	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	M	302	DD6	C33-C34-C35	-2.18	107.32	110.30
26	N	303	DD6	C25-C24-C1	-2.18	120.30	126.42
28	a	738	CLA	O2D-CGD-CBD	2.18	115.14	111.27
28	G	514	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
28	I	319	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
35	b	732	BCR	C33-C5-C4	2.18	117.80	113.62
28	A	316	CLA	C1B-CHB-C4A	-2.17	125.81	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	302	DD6	C28-C27-C29	2.17	121.14	116.84
28	a	725	CLA	C1-C2-C3	-2.17	122.29	126.04
28	a	728	CLA	C1-C2-C3	-2.17	122.29	126.04
28	l	309	CLA	CHD-C1D-ND	-2.17	122.46	124.45
28	b	715	CLA	CHD-C1D-ND	-2.17	122.46	124.45
28	D	311	CLA	CHD-C1D-ND	-2.17	122.46	124.45
28	l	313	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
28	D	314	CLA	O2D-CGD-CBD	2.17	115.12	111.27
26	I	301	DD6	C25-C24-C1	-2.17	120.33	126.42
26	I	301	DD6	C9-C8-C6	-2.17	120.33	126.42
28	B	309	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	J	302	DD6	C21-C20-C15	-2.17	118.63	122.26
28	A	309	CLA	CHD-C1D-ND	-2.17	122.46	124.45
29	A	314	KC1	O2A-CGA-O1A	-2.17	118.17	122.67
28	a	724	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
26	L	306	DD6	C4-C3-C2	-2.17	119.04	123.47
28	I	321	CLA	C1-C2-C3	-2.16	122.30	126.04
28	a	702	CLA	CHB-C4A-NA	2.16	127.50	124.51
29	D	310	KC1	C2A-C3A-C4A	2.16	108.09	106.49
26	I	301	DD6	C34-C35-C36	-2.16	107.55	111.85
26	G	504	DD6	C4-C3-C2	-2.16	119.04	123.47
28	I	308	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	I	301	DD6	C21-C20-C15	-2.16	118.64	122.26
26	K	303	DD6	C3-C4-C5	-2.16	119.05	123.47
28	b	725	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	I	306	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	B	312	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	M	315	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	a	710	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
26	J	303	DD6	C21-C20-C19	2.16	116.71	114.28
28	J	301	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
28	L	310	CLA	CHD-C1D-ND	-2.16	122.47	124.45
35	f	304	BCR	C35-C13-C14	-2.16	119.90	122.92
28	a	713	CLA	C1-C2-C3	-2.16	122.31	126.04
28	A	317	CLA	CMA-C3A-C2A	-2.16	111.06	116.10
26	G	505	DD6	C7-C6-C5	-2.16	119.90	122.92
28	a	712	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	b	726	CLA	CHD-C1D-ND	-2.15	122.47	124.45
26	D	303	DD6	C-C1-C24	2.15	121.47	118.08
26	G	505	DD6	C37-C36-C35	2.15	118.34	114.36
28	M	310	CLA	CHD-C1D-ND	-2.15	122.47	124.45
35	l	307	BCR	C33-C5-C6	-2.15	122.11	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	318	LMG	O3-C3-C2	-2.15	105.37	110.35
26	G	502	DD6	C7-C6-C5	-2.15	119.91	122.92
29	N	306	KC1	C2A-C3A-C4A	2.15	108.08	106.49
28	H	311	CLA	CHD-C1D-ND	-2.15	122.48	124.45
28	b	703	CLA	CHB-C4A-NA	2.15	127.49	124.51
28	J	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	M	303	DD6	C19-C18-C17	-2.15	106.62	110.77
26	B	302	DD6	C28-C27-C29	2.15	121.10	116.84
35	b	732	BCR	C36-C18-C19	2.15	121.47	118.08
28	B	307	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	G	502	DD6	C4-C3-C2	-2.15	119.07	123.47
28	I	311	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
28	F	307	CLA	CHD-C1D-ND	-2.15	122.48	124.45
31	j	101	LMG	O7-C10-O9	-2.15	118.51	123.70
28	a	720	CLA	CHD-C1D-ND	-2.15	122.48	124.45
28	H	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	F	303	DD6	C25-C26-C27	-2.15	120.34	126.58
26	B	306	DD6	C3-C4-C5	-2.15	119.08	123.47
28	G	514	CLA	C1-C2-C3	-2.15	122.33	126.04
28	G	514	CLA	CHD-C1D-ND	-2.15	122.48	124.45
28	A	310	CLA	CHD-C1D-ND	-2.15	122.48	124.45
35	l	306	BCR	C33-C5-C4	2.15	117.74	113.62
28	D	312	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
31	B	318	LMG	O1-C7-C8	-2.15	105.72	110.90
29	I	314	KC1	C1A-C2A-C3A	-2.14	105.41	107.11
31	D	317	LMG	O3-C3-C2	-2.14	105.39	110.35
28	b	718	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	M	303	DD6	C32-C33-C34	-2.14	108.80	113.64
35	b	730	BCR	C11-C12-C13	-2.14	120.39	126.42
28	b	725	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	I	301	DD6	C20-C19-C18	-2.14	108.51	112.75
28	a	726	CLA	O2D-CGD-CBD	2.14	115.07	111.27
31	K	318	LMG	O3-C3-C2	-2.14	105.40	110.35
31	j	101	LMG	O2-C2-C1	-2.14	104.85	110.05
32	G	507	PID	C28-C27-C26	2.14	113.61	109.88
28	F	313	CLA	C2A-C1A-CHA	2.14	127.60	123.86
29	N	306	KC1	CBD-CHA-C1A	2.14	132.87	128.88
28	a	701	CLA	CHD-C1D-ND	-2.14	122.49	124.45
28	a	719	CLA	CHD-C1D-ND	-2.14	122.49	124.45
28	b	717	CLA	CHD-C1D-ND	-2.14	122.49	124.45
28	a	717	CLA	C1-C2-C3	-2.14	122.34	126.04
28	K	316	CLA	O2D-CGD-CBD	2.14	115.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	303	DD6	C26-C25-C24	-2.14	116.55	123.22
28	b	710	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	G	504	DD6	C7-C6-C5	-2.14	119.93	122.92
28	a	712	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
28	b	704	CLA	C2D-C1D-ND	-2.13	108.53	110.10
28	H	304	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	B	303	DD6	C26-C25-C24	-2.13	116.56	123.22
28	B	301	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
26	J	303	DD6	C28-C27-C29	2.13	121.06	116.84
35	a	736	BCR	C4-C5-C6	-2.13	119.64	122.73
26	B	306	DD6	C14-C13-C11	-2.13	122.22	125.53
28	l	303	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
28	I	306	CLA	O2D-CGD-CBD	2.13	115.05	111.27
31	K	317	LMG	C6-C5-C4	-2.13	108.02	113.00
29	N	311	KC1	C2A-C3A-C4A	2.13	108.07	106.49
28	b	705	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
28	b	708	CLA	C1-C2-C3	-2.13	122.36	126.04
31	K	318	LMG	O2-C2-C1	-2.13	104.88	110.05
26	J	302	DD6	C-C1-C2	-2.13	119.94	122.92
26	J	304	DD6	C15-C14-C13	-2.13	121.49	125.99
32	G	506	PID	CM4-C14-C13	2.13	123.96	119.05
29	L	307	KC1	C2A-C3A-C4A	2.13	108.06	106.49
29	I	314	KC1	O2A-CGA-O1A	-2.13	118.25	122.67
28	N	307	CLA	CHB-C4A-NA	2.12	127.45	124.51
26	K	303	DD6	C41-C32-C31	-2.12	107.09	110.47
35	f	304	BCR	C23-C24-C25	-2.12	121.24	127.20
28	b	722	CLA	CHD-C1D-ND	-2.12	122.50	124.45
32	F	302	PID	C17-C18-C19	2.12	129.53	124.81
31	K	317	LMG	O3-C3-C2	-2.12	105.44	110.35
28	b	701	CLA	CHD-C1D-ND	-2.12	122.50	124.45
31	B	318	LMG	O2-C2-C1	-2.12	104.89	110.05
32	F	304	PID	C19-C20-C21	2.12	130.34	127.31
28	j	106	CLA	C1-C2-C3	-2.12	122.37	126.04
31	D	317	LMG	O2-C2-C1	-2.12	104.89	110.05
28	l	311	CLA	CHD-C1D-ND	-2.12	122.50	124.45
28	a	716	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
35	f	304	BCR	C3-C4-C5	-2.12	110.29	114.08
26	L	305	DD6	C25-C26-C27	-2.12	120.43	126.58
26	I	301	DD6	C3-C4-C5	-2.12	119.13	123.47
29	G	515	KC1	O2D-CGD-O1D	-2.12	119.70	123.84
28	G	512	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
28	G	520	CLA	CHD-C1D-ND	-2.12	122.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	727	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	B	305	UIX	C22-C15-C20	-2.12	108.58	110.47
28	b	720	CLA	CHD-C1D-ND	-2.12	122.51	124.45
28	G	513	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
26	G	508	DD6	C21-C20-C15	-2.12	118.71	122.26
28	b	723	CLA	C1-C2-C3	-2.12	123.33	126.75
28	G	509	CLA	CHD-C1D-ND	-2.12	122.51	124.45
28	b	707	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	H	303	DD6	C33-C34-C35	-2.11	107.41	110.30
31	I	320	LMG	O2-C2-C1	-2.11	104.91	110.05
29	A	314	KC1	O2D-CGD-O1D	-2.11	119.71	123.84
35	i	201	BCR	C20-C19-C18	-2.11	120.48	126.42
28	L	311	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	M	305	DD6	C25-C24-C1	-2.11	120.49	126.42
26	K	304	DD6	C28-C27-C29	2.11	121.02	116.84
28	a	703	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
31	B	318	LMG	O3-C3-C2	-2.11	105.47	110.35
31	I	320	LMG	O1-C1-C2	-2.11	105.01	108.30
26	K	305	DD6	C3-C4-C5	-2.11	119.16	123.47
31	D	317	LMG	O1-C1-C2	-2.11	105.01	108.30
27	K	302	UIX	C19-C18-C17	-2.11	106.20	109.88
26	L	303	DD6	C25-C24-C1	-2.11	120.50	126.42
28	b	724	CLA	CHD-C1D-ND	-2.11	122.52	124.45
32	G	507	PID	CM4-C14-C13	2.11	123.91	119.05
28	H	305	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
29	H	310	KC1	O1D-CGD-CBD	-2.10	120.18	124.48
26	A	305	DD6	C25-C24-C1	-2.10	120.51	126.42
28	l	310	CLA	CHC-C1C-NC	-2.10	125.91	128.83
29	K	314	KC1	O1D-CGD-CBD	-2.10	120.18	124.48
28	B	308	CLA	CHD-C1D-ND	-2.10	122.52	124.45
28	K	306	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
28	b	720	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	h	202	CLA	CHD-C1D-ND	-2.10	122.53	124.45
28	B	316	CLA	CHD-C1D-ND	-2.10	122.53	124.45
26	B	303	DD6	C40-C32-C31	-2.10	107.13	110.47
28	I	312	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	B	301	CLA	CHB-C4A-NA	2.10	127.41	124.51
26	K	305	DD6	C25-C24-C1	-2.09	120.53	126.42
26	A	301	DD6	C9-C8-C6	-2.09	120.53	126.42
26	I	303	DD6	O1-C20-C15	-2.09	57.23	58.96
35	l	302	BCR	C35-C13-C12	2.09	121.37	118.08
28	I	311	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	734	BCR	C16-C15-C14	-2.09	119.20	123.47
32	N	301	PID	C15-C14-C13	2.09	122.72	117.00
32	H	302	PID	C6-C7-C8	-2.09	121.58	125.99
35	l	307	BCR	C10-C11-C12	-2.09	116.70	123.22
31	b	734	LMG	O2-C2-C1	-2.09	104.98	110.05
28	D	316	CLA	CHD-C1D-ND	-2.09	122.54	124.45
28	M	309	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	A	303	DD6	C37-C36-C35	2.09	118.22	114.36
26	h	203	DD6	C34-C35-C36	-2.08	107.70	111.85
28	N	310	CLA	C2A-C1A-CHA	2.08	127.50	123.86
28	a	729	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
30	I	317	DGD	O6D-C5D-C6D	2.08	110.87	106.67
27	K	302	UIX	C41-C40-C38	2.08	121.36	118.08
31	K	318	LMG	C1-C2-C3	-2.08	105.66	110.00
28	L	314	CLA	C1-C2-C3	-2.08	122.44	126.04
26	N	303	DD6	O1-C20-C21	-2.08	112.56	115.06
28	a	715	CLA	CHD-C1D-ND	-2.08	122.54	124.45
35	a	736	BCR	C15-C16-C17	-2.08	119.21	123.47
26	b	731	DD6	C-C1-C24	2.08	121.36	118.08
28	B	311	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	I	302	DD6	C37-C36-C35	2.08	118.21	114.36
28	N	304	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
28	m	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	I	302	DD6	C9-C8-C6	2.08	132.26	126.42
28	A	313	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
28	a	731	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
35	b	702	BCR	C34-C9-C10	-2.08	120.01	122.92
31	b	733	LMG	O7-C10-O9	-2.08	118.68	123.70
28	L	308	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
26	G	508	DD6	C28-C27-C29	2.08	120.95	116.84
29	B	314	KC1	C2A-C3A-C4A	2.08	108.03	106.49
26	M	303	DD6	C25-C26-C27	-2.07	120.56	126.58
35	l	307	BCR	C23-C24-C25	-2.07	121.38	127.20
31	b	733	LMG	O3-C3-C2	-2.07	105.55	110.35
28	a	727	CLA	CHD-C1D-ND	-2.07	122.55	124.45
28	h	202	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
29	A	306	KC1	O2D-CGD-O1D	-2.07	119.78	123.84
28	K	312	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
35	l	306	BCR	C15-C16-C17	-2.07	119.23	123.47
35	a	736	BCR	C11-C12-C13	-2.07	120.60	126.42
28	A	317	CLA	CHD-C1D-ND	-2.07	122.55	124.45
35	j	102	BCR	C38-C26-C27	2.07	117.59	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	732	PQN	C12-C11-C3	-2.07	106.47	112.05
35	i	201	BCR	C35-C13-C12	2.07	121.34	118.08
29	L	307	KC1	O1D-CGD-CBD	-2.07	120.25	124.48
28	a	731	CLA	CHD-C1D-ND	-2.07	122.55	124.45
26	L	302	DD6	C25-C26-C27	-2.07	120.58	126.58
26	I	303	DD6	C25-C26-C27	-2.07	120.58	126.58
28	L	317	CLA	O2D-CGD-CBD	2.07	114.94	111.27
26	D	303	DD6	C7-C6-C8	2.07	121.33	118.08
28	b	721	CLA	CHB-C4A-NA	2.07	127.37	124.51
28	a	729	CLA	C1-C2-C3	-2.07	122.47	126.04
26	B	306	DD6	C34-C35-C36	-2.07	107.74	111.85
26	A	305	DD6	C10-C9-C8	-2.07	116.77	123.22
26	B	303	DD6	C28-C27-C29	2.06	120.93	116.84
28	a	711	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
29	D	315	KC1	O2D-CGD-O1D	-2.06	119.80	123.84
28	j	106	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	b	712	CLA	O2A-C1-C2	2.06	114.05	108.64
26	A	302	DD6	C37-C36-C35	2.06	118.17	114.36
28	b	726	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	I	319	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
28	J	316	CLA	CHD-C1D-ND	-2.06	122.56	124.45
27	J	305	UIX	C3-C5-C4	-2.06	106.79	110.77
28	b	708	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
32	j	105	PID	CM4-C14-C13	2.06	123.80	119.05
28	b	710	CLA	CHD-C1D-ND	-2.06	122.56	124.45
27	h	201	UIX	C36-C35-C32	-2.06	124.37	127.31
28	a	724	CLA	O2D-CGD-CBD	2.06	114.92	111.27
28	K	310	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	L	304	DD6	C40-C32-C31	-2.06	107.20	110.47
29	I	314	KC1	C2A-C3A-C4A	2.06	108.01	106.49
26	L	304	DD6	C12-C11-C13	2.06	121.32	118.08
28	a	708	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	L	307	KC1	C1A-C2A-C3A	-2.06	105.48	107.11
29	M	307	KC1	C1A-C2A-C3A	-2.06	105.48	107.11
27	J	305	UIX	O2-C27-O4	-2.06	118.88	122.96
28	b	723	CLA	O2D-CGD-CBD	2.05	114.92	111.27
28	F	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	G	515	KC1	CBD-CHA-C1A	2.05	132.71	128.88
28	M	312	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
35	a	736	BCR	C37-C22-C23	2.05	121.31	118.08
28	G	520	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	b	731	DD6	C12-C11-C13	2.05	121.31	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	j	105	PID	O1-C1-C2	-2.05	111.84	113.38
27	J	305	UIX	C37-C39-C40	-2.05	124.38	127.31
26	L	305	DD6	O1-C20-C21	-2.05	112.60	115.06
28	D	308	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
30	G	501	DGD	C2G-O2G-C1B	-2.05	112.75	117.79
29	D	315	KC1	C4B-CHC-C1C	-2.05	121.64	126.06
28	A	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
28	J	308	CLA	O2D-CGD-CBD	2.05	114.91	111.27
28	I	315	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	a	720	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	B	306	DD6	C4-C3-C2	-2.05	119.28	123.47
26	B	306	DD6	C7-C6-C8	2.05	121.30	118.08
28	M	317	CLA	O2D-CGD-CBD	2.05	114.91	111.27
28	l	308	CLA	CHD-C1D-ND	-2.05	122.57	124.45
28	K	315	CLA	CMA-C3A-C2A	-2.05	111.32	116.10
28	b	717	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
28	L	311	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
28	I	311	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	M	304	DD6	C37-C36-C35	2.04	118.14	114.36
26	H	303	DD6	C21-C20-C15	-2.04	118.84	122.26
30	l	301	DGD	O1G-C1A-C2A	2.04	118.32	111.91
35	l	307	BCR	C36-C18-C19	2.04	121.30	118.08
26	I	301	DD6	C4-C3-C2	-2.04	119.29	123.47
28	f	301	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	a	710	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	i	201	BCR	C16-C15-C14	-2.04	119.29	123.47
26	K	303	DD6	O1-C20-C19	-2.04	111.85	113.38
36	a	732	PQN	C11-C12-C13	-2.04	123.39	126.79
28	J	301	CLA	CHD-C1D-ND	-2.04	122.58	124.45
29	N	311	KC1	CBD-CHA-C1A	2.04	132.69	128.88
28	B	307	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	L	307	KC1	CAA-CBA-CGA	-2.04	116.78	127.26
28	H	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
35	i	201	BCR	C34-C9-C8	2.04	121.29	118.08
27	K	302	UIX	C29-C26-C30	-2.04	120.07	122.92
28	a	716	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	M	302	DD6	C28-C27-C29	2.04	120.87	116.84
26	J	303	DD6	C3-C4-C5	-2.04	119.30	123.47
26	I	302	DD6	C15-C14-C13	2.04	130.30	125.99
28	N	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	a	714	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
28	I	308	CLA	O2D-CGD-CBD	2.03	114.88	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	308	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
28	A	309	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
26	G	505	DD6	C33-C34-C35	-2.03	107.52	110.30
28	j	104	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
28	b	722	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
35	a	734	BCR	C37-C22-C23	2.03	121.28	118.08
28	G	518	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	B	317	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
26	K	303	DD6	C25-C26-C27	-2.03	120.69	126.58
26	G	502	DD6	C9-C8-C6	-2.03	120.71	126.42
35	m	201	BCR	C24-C23-C22	-2.03	123.17	126.23
28	B	312	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	L	304	DD6	C25-C26-C27	-2.03	120.69	126.58
28	a	730	CLA	C1-C2-C3	-2.03	122.53	126.04
28	b	714	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	b	723	CLA	CHD-C1D-ND	-2.03	122.59	124.45
28	D	314	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	D	305	PID	C17-C16-C15	2.03	127.63	123.47
28	G	509	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
28	a	725	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	F	303	DD6	C7-C6-C5	-2.02	120.09	122.92
35	b	732	BCR	C28-C29-C30	-2.02	107.37	114.60
28	a	707	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	H	307	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	A	308	CLA	CHD-C1D-ND	-2.02	122.60	124.45
28	A	316	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
32	N	302	PID	O4-C12-C13	2.02	127.20	122.89
26	M	304	DD6	C-C1-C2	-2.02	120.09	122.92
28	M	310	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
27	A	304	UIX	C37-C34-C30	-2.02	119.34	123.47
28	I	309	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	J	315	CLA	CHD-C1D-ND	-2.02	122.60	124.45
28	b	712	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	J	304	DD6	C20-C19-C18	-2.02	108.75	112.75
26	M	306	DD6	C3-C4-C5	-2.02	119.34	123.47
26	B	304	DD6	C21-C20-C15	-2.02	118.88	122.26
28	F	315	CLA	O2D-CGD-CBD	2.02	114.85	111.27
26	H	303	DD6	C3-C4-C5	-2.02	119.34	123.47
35	f	304	BCR	C33-C5-C4	2.02	117.49	113.62
26	I	301	DD6	C12-C11-C10	-2.02	120.10	122.92
28	a	723	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
32	D	304	PID	CM2-C5-C4	-2.01	105.48	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	303	DD6	C12-C11-C13	2.01	121.25	118.08
28	b	704	CLA	O1D-CGD-CBD	2.01	128.60	124.48
27	J	305	UIX	C-C7-C10	-2.01	121.74	125.99
26	D	303	DD6	C32-C33-C34	-2.01	109.10	113.64
27	G	503	UIX	C3-C5-C4	-2.01	106.89	110.77
28	A	308	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
26	I	302	DD6	C-C1-C2	-2.01	120.10	122.92
26	I	301	DD6	C28-C27-C29	2.01	120.83	116.84
28	D	313	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
28	J	310	CLA	C2D-C1D-ND	-2.01	108.62	110.10
28	a	719	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
28	a	721	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	L	303	DD6	C34-C35-C36	-2.01	107.85	111.85
28	L	317	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
36	b	729	PQN	C2M-C2-C1	2.01	119.60	116.27
28	l	311	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	A	314	KC1	C2A-C3A-C4A	2.01	107.98	106.49
29	M	314	KC1	O2A-CGA-O1A	-2.01	118.50	122.67
26	B	302	DD6	C4-C5-C6	-2.01	120.34	124.81
28	l	303	CLA	O2D-CGD-CBD	2.01	114.84	111.27
28	N	305	CLA	CHD-C1D-ND	-2.01	122.61	124.45
28	K	315	CLA	CHD-C1D-ND	-2.01	122.61	124.45
28	N	310	CLA	C3A-C2A-C1A	2.01	104.34	101.34
28	K	306	CLA	O2D-CGD-CBD	2.00	114.83	111.27
28	b	713	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	F	309	KC1	O2A-CGA-O1A	-2.00	118.51	122.67
28	B	308	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
29	N	308	KC1	O2A-CGA-O1A	-2.00	118.51	122.67
32	j	105	PID	C17-C18-C19	2.00	129.27	124.81
29	D	315	KC1	C1A-C2A-C3A	-2.00	105.53	107.11
28	b	711	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	b	731	DD6	C3-C4-C5	-2.00	119.37	123.47
28	a	723	CLA	CHD-C1D-ND	-2.00	122.61	124.45
27	G	503	UIX	C41-C40-C38	2.00	121.23	118.08
29	F	314	KC1	C2A-C3A-C4A	2.00	107.97	106.49
29	M	314	KC1	O2D-CGD-O1D	-2.00	119.92	123.84
27	h	201	UIX	C3-C5-C4	-2.00	106.91	110.77
28	K	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	J	304	DD6	C19-C18-C17	-2.00	106.91	110.77
28	a	730	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (186) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	I	306	CLA	ND
28	I	307	CLA	ND
28	I	308	CLA	ND
28	I	309	CLA	ND
28	I	310	CLA	ND
28	I	311	CLA	ND
28	I	312	CLA	ND
28	I	313	CLA	ND
28	I	315	CLA	ND
28	I	316	CLA	ND
28	I	319	CLA	ND
28	I	321	CLA	ND
28	K	306	CLA	ND
28	K	307	CLA	ND
28	K	308	CLA	ND
28	K	309	CLA	ND
28	K	310	CLA	ND
28	K	311	CLA	ND
28	K	312	CLA	ND
28	K	313	CLA	ND
28	K	315	CLA	ND
28	K	316	CLA	ND
28	G	509	CLA	ND
28	G	510	CLA	ND
28	G	511	CLA	ND
28	G	512	CLA	ND
28	G	513	CLA	ND
28	G	514	CLA	ND
28	G	516	CLA	ND
28	G	517	CLA	ND
28	G	518	CLA	ND
28	G	519	CLA	ND
28	G	520	CLA	ND
28	A	307	CLA	ND
28	A	308	CLA	ND
28	A	309	CLA	ND
28	A	310	CLA	ND
28	A	311	CLA	ND
28	A	312	CLA	ND
28	A	313	CLA	ND
28	A	315	CLA	ND
28	A	316	CLA	ND
28	A	317	CLA	ND

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Mol	Chain	Res	Type	Atom
28	A	319	CLA	ND
28	A	320	CLA	ND
28	f	301	CLA	ND
28	f	302	CLA	ND
28	f	303	CLA	ND
28	h	202	CLA	ND
28	j	104	CLA	ND
28	j	106	CLA	ND
28	l	303	CLA	ND
28	l	304	CLA	ND
28	l	305	CLA	ND
28	l	308	CLA	ND
28	l	309	CLA	ND
28	l	311	CLA	ND
28	l	312	CLA	ND
28	l	313	CLA	ND
28	m	202	CLA	ND
28	a	701	CLA	ND
28	a	702	CLA	ND
28	a	703	CLA	ND
28	a	704	CLA	ND
28	a	705	CLA	ND
28	a	706	CLA	ND
28	a	707	CLA	ND
28	a	708	CLA	ND
28	a	709	CLA	ND
28	a	710	CLA	ND
28	a	711	CLA	ND
28	a	712	CLA	ND
28	a	713	CLA	ND
28	a	714	CLA	ND
28	a	715	CLA	ND
28	a	716	CLA	ND
28	a	717	CLA	ND
28	a	718	CLA	ND
28	a	719	CLA	ND
28	a	720	CLA	ND
28	a	721	CLA	ND
28	a	722	CLA	ND
28	a	723	CLA	ND
28	a	724	CLA	ND
28	a	725	CLA	ND

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Mol	Chain	Res	Type	Atom
28	a	726	CLA	ND
28	a	727	CLA	ND
28	a	728	CLA	ND
28	a	729	CLA	ND
28	a	730	CLA	ND
28	a	731	CLA	ND
28	a	735	CLA	ND
28	a	738	CLA	ND
28	b	701	CLA	ND
28	b	703	CLA	ND
28	b	704	CLA	ND
28	b	705	CLA	ND
28	b	706	CLA	ND
28	b	707	CLA	ND
28	b	708	CLA	ND
28	b	709	CLA	ND
28	b	710	CLA	ND
28	b	711	CLA	ND
28	b	712	CLA	ND
28	b	713	CLA	ND
28	b	714	CLA	ND
28	b	715	CLA	ND
28	b	716	CLA	ND
28	b	717	CLA	ND
28	b	718	CLA	ND
28	b	719	CLA	ND
28	b	720	CLA	ND
28	b	721	CLA	ND
28	b	722	CLA	ND
28	b	723	CLA	ND
28	b	724	CLA	ND
28	b	725	CLA	ND
28	b	726	CLA	ND
28	b	727	CLA	ND
28	b	728	CLA	ND
28	B	301	CLA	ND
28	B	307	CLA	ND
28	B	308	CLA	ND
28	B	309	CLA	ND
28	B	310	CLA	ND
28	B	311	CLA	ND
28	B	312	CLA	ND

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

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Mol	Chain	Res	Type	Atom
28	L	317	CLA	ND
28	L	318	CLA	ND
28	M	308	CLA	ND
28	M	309	CLA	ND
28	M	310	CLA	ND
28	M	311	CLA	ND
28	M	312	CLA	ND
28	M	313	CLA	ND
28	M	315	CLA	ND
28	M	316	CLA	ND
28	M	317	CLA	ND
28	M	318	CLA	ND
28	N	304	CLA	ND
28	N	305	CLA	ND
28	N	307	CLA	ND
28	N	309	CLA	ND
28	N	310	CLA	ND

All (2127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	K	301	DD6	C12-C11-C13-C14
26	G	502	DD6	C-C1-C24-C25
26	G	502	DD6	C2-C1-C24-C25
26	G	504	DD6	C10-C11-C13-C14
26	G	504	DD6	C12-C11-C13-C14
26	G	504	DD6	C7-C6-C8-C9
26	G	505	DD6	C5-C6-C8-C9
26	G	505	DD6	C7-C6-C8-C9
26	A	301	DD6	C13-C14-C15-C16
26	A	303	DD6	C27-C29-C30-C31
26	A	305	DD6	C13-C14-C15-O1
26	B	303	DD6	C13-C14-C15-O1
26	B	306	DD6	C13-C14-C15-O1
26	D	303	DD6	C13-C14-C15-O1
26	D	303	DD6	C27-C29-C30-C31
26	F	301	DD6	C10-C11-C13-C14
26	F	301	DD6	C12-C11-C13-C14
26	J	302	DD6	C10-C11-C13-C14
26	J	302	DD6	C12-C11-C13-C14
26	J	303	DD6	C10-C11-C13-C14
26	J	303	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	J	304	DD6	C10-C11-C13-C14
26	L	302	DD6	C13-C14-C15-O1
26	L	305	DD6	C13-C14-C15-O1
26	M	305	DD6	C13-C14-C15-O1
26	M	306	DD6	C10-C11-C13-C14
26	M	306	DD6	C12-C11-C13-C14
27	I	304	UIX	C2-C-C7-C10
27	I	304	UIX	C31-C27-O2-C18
27	K	302	UIX	O4-C27-O2-C18
27	K	302	UIX	C31-C27-O2-C18
27	G	503	UIX	C31-C27-O2-C18
27	h	201	UIX	O4-C27-O2-C18
27	J	305	UIX	O-C-C7-C10
27	J	305	UIX	C14-C23-C26-C29
27	J	305	UIX	C14-C23-C26-C30
28	I	307	CLA	CBA-CGA-O2A-C1
28	I	307	CLA	O1A-CGA-O2A-C1
28	I	310	CLA	CHA-CBD-CGD-O1D
28	I	310	CLA	CHA-CBD-CGD-O2D
28	I	310	CLA	CAD-CBD-CGD-O1D
28	I	311	CLA	C1A-C2A-CAA-CBA
28	I	311	CLA	C3A-C2A-CAA-CBA
28	I	311	CLA	CHA-CBD-CGD-O1D
28	I	311	CLA	CHA-CBD-CGD-O2D
28	I	312	CLA	C2-C3-C5-C6
28	I	312	CLA	C4-C3-C5-C6
28	I	313	CLA	CBD-CGD-O2D-CED
28	I	313	CLA	C2-C3-C5-C6
28	I	313	CLA	C4-C3-C5-C6
28	I	316	CLA	C1A-C2A-CAA-CBA
28	I	316	CLA	C3A-C2A-CAA-CBA
28	I	319	CLA	CHA-CBD-CGD-O1D
28	I	319	CLA	CHA-CBD-CGD-O2D
28	K	306	CLA	CHA-CBD-CGD-O1D
28	K	306	CLA	CHA-CBD-CGD-O2D
28	K	308	CLA	CBD-CGD-O2D-CED
28	K	308	CLA	C2-C3-C5-C6
28	K	308	CLA	C4-C3-C5-C6
28	K	310	CLA	CHA-CBD-CGD-O1D
28	K	311	CLA	C1A-C2A-CAA-CBA
28	K	311	CLA	C3A-C2A-CAA-CBA
28	K	311	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	K	313	CLA	C2-C3-C5-C6
28	K	313	CLA	C4-C3-C5-C6
28	K	315	CLA	CBD-CGD-O2D-CED
28	G	509	CLA	C2-C3-C5-C6
28	G	509	CLA	C4-C3-C5-C6
28	G	514	CLA	C2-C3-C5-C6
28	G	514	CLA	C4-C3-C5-C6
28	G	516	CLA	CAD-CBD-CGD-O1D
28	G	516	CLA	CAD-CBD-CGD-O2D
28	G	516	CLA	CBD-CGD-O2D-CED
28	G	517	CLA	CBA-CGA-O2A-C1
28	G	518	CLA	C1A-C2A-CAA-CBA
28	G	518	CLA	C3A-C2A-CAA-CBA
28	G	519	CLA	C1A-C2A-CAA-CBA
28	G	519	CLA	C3A-C2A-CAA-CBA
28	G	520	CLA	C1A-C2A-CAA-CBA
28	G	520	CLA	C3A-C2A-CAA-CBA
28	A	307	CLA	CHA-CBD-CGD-O1D
28	A	307	CLA	CHA-CBD-CGD-O2D
28	A	311	CLA	CBA-CGA-O2A-C1
28	A	315	CLA	CAD-CBD-CGD-O1D
28	A	315	CLA	CAD-CBD-CGD-O2D
28	A	319	CLA	CHA-CBD-CGD-O1D
28	A	319	CLA	CHA-CBD-CGD-O2D
28	A	319	CLA	CAD-CBD-CGD-O1D
28	A	320	CLA	CBA-CGA-O2A-C1
28	f	301	CLA	C1A-C2A-CAA-CBA
28	f	301	CLA	C3A-C2A-CAA-CBA
28	f	301	CLA	CBD-CGD-O2D-CED
28	f	302	CLA	CBA-CGA-O2A-C1
28	f	303	CLA	C1A-C2A-CAA-CBA
28	f	303	CLA	C3A-C2A-CAA-CBA
28	f	303	CLA	CHA-CBD-CGD-O1D
28	j	106	CLA	C1A-C2A-CAA-CBA
28	j	106	CLA	C3A-C2A-CAA-CBA
28	j	106	CLA	C2-C3-C5-C6
28	j	106	CLA	C4-C3-C5-C6
28	l	309	CLA	CHA-CBD-CGD-O1D
28	l	309	CLA	CHA-CBD-CGD-O2D
28	l	309	CLA	CAD-CBD-CGD-O1D
28	l	310	CLA	CBA-CGA-O2A-C1
28	l	310	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	l	310	CLA	CHA-CBD-CGD-O2D
28	l	310	CLA	CBD-CGD-O2D-CED
28	l	311	CLA	C1A-C2A-CAA-CBA
28	l	312	CLA	C3A-C2A-CAA-CBA
28	l	312	CLA	CBD-CGD-O2D-CED
28	l	313	CLA	CHA-CBD-CGD-O1D
28	l	313	CLA	CHA-CBD-CGD-O2D
28	a	702	CLA	CHA-CBD-CGD-O1D
28	a	702	CLA	CBD-CGD-O2D-CED
28	a	703	CLA	CHA-CBD-CGD-O1D
28	a	705	CLA	C1A-C2A-CAA-CBA
28	a	705	CLA	C3A-C2A-CAA-CBA
28	a	706	CLA	CHA-CBD-CGD-O1D
28	a	706	CLA	CHA-CBD-CGD-O2D
28	a	706	CLA	CAD-CBD-CGD-O1D
28	a	706	CLA	C2-C3-C5-C6
28	a	706	CLA	C4-C3-C5-C6
28	a	707	CLA	C3A-C2A-CAA-CBA
28	a	707	CLA	CBD-CGD-O2D-CED
28	a	709	CLA	C1A-C2A-CAA-CBA
28	a	709	CLA	C3A-C2A-CAA-CBA
28	a	711	CLA	C2A-CAA-CBA-CGA
28	a	712	CLA	CHA-CBD-CGD-O1D
28	a	712	CLA	CHA-CBD-CGD-O2D
28	a	713	CLA	CBD-CGD-O2D-CED
28	a	713	CLA	C4-C3-C5-C6
28	a	715	CLA	CBD-CGD-O2D-CED
28	a	716	CLA	C1A-C2A-CAA-CBA
28	a	716	CLA	C3A-C2A-CAA-CBA
28	a	717	CLA	C3A-C2A-CAA-CBA
28	a	717	CLA	C6-C7-C8-C9
28	a	718	CLA	C1A-C2A-CAA-CBA
28	a	718	CLA	CHA-CBD-CGD-O1D
28	a	718	CLA	CHA-CBD-CGD-O2D
28	a	720	CLA	C3A-C2A-CAA-CBA
28	a	721	CLA	C2A-CAA-CBA-CGA
28	a	721	CLA	CHA-CBD-CGD-O1D
28	a	721	CLA	CHA-CBD-CGD-O2D
28	a	721	CLA	CBD-CGD-O2D-CED
28	a	722	CLA	CHA-CBD-CGD-O1D
28	a	722	CLA	CBD-CGD-O2D-CED
28	a	723	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	a	723	CLA	CHA-CBD-CGD-O2D
28	a	724	CLA	C4-C3-C5-C6
28	a	726	CLA	CHA-CBD-CGD-O1D
28	a	726	CLA	CHA-CBD-CGD-O2D
28	a	727	CLA	CBA-CGA-O2A-C1
28	a	727	CLA	O1A-CGA-O2A-C1
28	a	728	CLA	C2-C3-C5-C6
28	a	728	CLA	C4-C3-C5-C6
28	a	731	CLA	C1A-C2A-CAA-CBA
28	a	731	CLA	C3A-C2A-CAA-CBA
28	a	731	CLA	CBD-CGD-O2D-CED
28	a	735	CLA	CHA-CBD-CGD-O1D
28	a	735	CLA	CHA-CBD-CGD-O2D
28	a	735	CLA	CAD-CBD-CGD-O1D
28	a	735	CLA	C4-C3-C5-C6
28	a	738	CLA	CHA-CBD-CGD-O1D
28	a	738	CLA	CHA-CBD-CGD-O2D
28	b	701	CLA	CHA-CBD-CGD-O1D
28	b	701	CLA	CHA-CBD-CGD-O2D
28	b	701	CLA	CBD-CGD-O2D-CED
28	b	701	CLA	C2-C3-C5-C6
28	b	701	CLA	C4-C3-C5-C6
28	b	703	CLA	CHA-CBD-CGD-O1D
28	b	703	CLA	CHA-CBD-CGD-O2D
28	b	703	CLA	CBD-CGD-O2D-CED
28	b	704	CLA	C1A-C2A-CAA-CBA
28	b	704	CLA	C3A-C2A-CAA-CBA
28	b	704	CLA	CBD-CGD-O2D-CED
28	b	704	CLA	C14-C13-C15-C16
28	b	709	CLA	CHA-CBD-CGD-O1D
28	b	709	CLA	CHA-CBD-CGD-O2D
28	b	710	CLA	C1A-C2A-CAA-CBA
28	b	710	CLA	C3A-C2A-CAA-CBA
28	b	711	CLA	CHA-CBD-CGD-O1D
28	b	711	CLA	CHA-CBD-CGD-O2D
28	b	711	CLA	CAD-CBD-CGD-O1D
28	b	711	CLA	CBD-CGD-O2D-CED
28	b	714	CLA	C2A-CAA-CBA-CGA
28	b	715	CLA	C1A-C2A-CAA-CBA
28	b	715	CLA	C3A-C2A-CAA-CBA
28	b	715	CLA	C2-C3-C5-C6
28	b	715	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	b	717	CLA	C1A-C2A-CAA-CBA
28	b	717	CLA	C3A-C2A-CAA-CBA
28	b	717	CLA	C14-C13-C15-C16
28	b	719	CLA	CHA-CBD-CGD-O1D
28	b	719	CLA	CHA-CBD-CGD-O2D
28	b	719	CLA	CAD-CBD-CGD-O1D
28	b	720	CLA	CBD-CGD-O2D-CED
28	b	723	CLA	C3A-C2A-CAA-CBA
28	b	723	CLA	CHA-CBD-CGD-O2D
28	b	724	CLA	C1A-C2A-CAA-CBA
28	b	725	CLA	C2-C3-C5-C6
28	b	725	CLA	C4-C3-C5-C6
28	B	308	CLA	C1A-C2A-CAA-CBA
28	B	309	CLA	CHA-CBD-CGD-O1D
28	B	309	CLA	CHA-CBD-CGD-O2D
28	B	311	CLA	CBD-CGD-O2D-CED
28	B	311	CLA	C14-C13-C15-C16
28	B	315	CLA	CHA-CBD-CGD-O1D
28	B	315	CLA	CHA-CBD-CGD-O2D
28	B	315	CLA	CAD-CBD-CGD-O1D
28	B	315	CLA	CAD-CBD-CGD-O2D
28	B	315	CLA	CBD-CGD-O2D-CED
28	B	317	CLA	C1A-C2A-CAA-CBA
28	D	309	CLA	CBA-CGA-O2A-C1
28	D	312	CLA	CBA-CGA-O2A-C1
28	D	314	CLA	CBA-CGA-O2A-C1
28	D	314	CLA	CBD-CGD-O2D-CED
28	F	310	CLA	C1A-C2A-CAA-CBA
28	F	313	CLA	CBD-CGD-O2D-CED
28	F	315	CLA	CHA-CBD-CGD-O2D
28	H	304	CLA	CHA-CBD-CGD-O1D
28	H	304	CLA	CHA-CBD-CGD-O2D
28	H	307	CLA	CBD-CGD-O2D-CED
28	H	308	CLA	CBA-CGA-O2A-C1
28	H	309	CLA	C3A-C2A-CAA-CBA
28	H	309	CLA	CBD-CGD-O2D-CED
28	H	311	CLA	CAD-CBD-CGD-O1D
28	H	311	CLA	CAD-CBD-CGD-O2D
28	H	311	CLA	CBD-CGD-O2D-CED
28	H	312	CLA	C1A-C2A-CAA-CBA
28	H	312	CLA	C3A-C2A-CAA-CBA
28	H	312	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	H	312	CLA	CBD-CGD-O2D-CED
28	J	307	CLA	C1A-C2A-CAA-CBA
28	J	307	CLA	C3A-C2A-CAA-CBA
28	J	307	CLA	C2-C3-C5-C6
28	J	307	CLA	C4-C3-C5-C6
28	J	308	CLA	C2A-CAA-CBA-CGA
28	J	311	CLA	C1A-C2A-CAA-CBA
28	J	311	CLA	C3A-C2A-CAA-CBA
28	J	314	CLA	CHA-CBD-CGD-O1D
28	J	314	CLA	CHA-CBD-CGD-O2D
28	L	308	CLA	C1A-C2A-CAA-CBA
28	L	308	CLA	C3A-C2A-CAA-CBA
28	L	312	CLA	C3A-C2A-CAA-CBA
28	L	312	CLA	CBD-CGD-O2D-CED
28	L	313	CLA	C3A-C2A-CAA-CBA
28	L	317	CLA	C3-C5-C6-C7
28	L	318	CLA	CBD-CGD-O2D-CED
28	M	313	CLA	CHA-CBD-CGD-O1D
28	M	313	CLA	CHA-CBD-CGD-O2D
28	M	317	CLA	CBD-CGD-O2D-CED
28	M	317	CLA	O1D-CGD-O2D-CED
28	M	318	CLA	C1A-C2A-CAA-CBA
28	M	318	CLA	C3A-C2A-CAA-CBA
28	M	318	CLA	C2A-CAA-CBA-CGA
28	M	318	CLA	CAD-CBD-CGD-O1D
28	M	318	CLA	CAD-CBD-CGD-O2D
28	N	305	CLA	CHA-CBD-CGD-O1D
28	N	305	CLA	CHA-CBD-CGD-O2D
28	N	309	CLA	C1A-C2A-CAA-CBA
28	N	310	CLA	C1A-C2A-CAA-CBA
28	N	310	CLA	CBD-CGD-O2D-CED
29	I	314	KC1	C2B-C3B-CAB-CBB
29	I	314	KC1	C4B-C3B-CAB-CBB
29	I	314	KC1	C2A-CAA-CBA-CGA
29	I	314	KC1	CHA-CBD-CGD-O2D
29	K	314	KC1	C1A-C2A-CAA-CBA
29	K	314	KC1	C2B-C3B-CAB-CBB
29	K	314	KC1	C4B-C3B-CAB-CBB
29	K	314	KC1	CAA-CBA-CGA-O1A
29	G	515	KC1	C4B-C3B-CAB-CBB
29	A	306	KC1	C1A-C2A-CAA-CBA
29	A	306	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	A	306	KC1	C4B-C3B-CAB-CBB
29	A	306	KC1	CHA-CBD-CGD-O2D
29	A	314	KC1	C2B-C3B-CAB-CBB
29	A	314	KC1	C4B-C3B-CAB-CBB
29	A	314	KC1	C2A-CAA-CBA-CGA
29	A	314	KC1	CHA-CBD-CGD-O1D
29	B	314	KC1	C2B-C3B-CAB-CBB
29	B	314	KC1	C4B-C3B-CAB-CBB
29	B	314	KC1	CBD-CGD-O2D-CED
29	D	310	KC1	C1A-C2A-CAA-CBA
29	D	310	KC1	C3A-C2A-CAA-CBA
29	D	310	KC1	C2B-C3B-CAB-CBB
29	D	310	KC1	C4B-C3B-CAB-CBB
29	D	310	KC1	C2A-CAA-CBA-CGA
29	D	310	KC1	CAA-CBA-CGA-O2A
29	D	310	KC1	CHA-CBD-CGD-O2D
29	F	309	KC1	C2B-C3B-CAB-CBB
29	F	309	KC1	C4B-C3B-CAB-CBB
29	F	309	KC1	CHA-CBD-CGD-O1D
29	F	309	KC1	CHA-CBD-CGD-O2D
29	F	314	KC1	C2B-C3B-CAB-CBB
29	F	314	KC1	C4B-C3B-CAB-CBB
29	F	314	KC1	CHA-CBD-CGD-O2D
29	H	306	KC1	C1A-C2A-CAA-CBA
29	H	306	KC1	C3A-C2A-CAA-CBA
29	H	306	KC1	C2B-C3B-CAB-CBB
29	H	306	KC1	C4B-C3B-CAB-CBB
29	H	310	KC1	C3A-C2A-CAA-CBA
29	H	310	KC1	C2B-C3B-CAB-CBB
29	H	310	KC1	C4B-C3B-CAB-CBB
29	H	310	KC1	CBD-CGD-O2D-CED
29	J	313	KC1	C1A-C2A-CAA-CBA
29	J	313	KC1	C2B-C3B-CAB-CBB
29	J	313	KC1	C4B-C3B-CAB-CBB
29	L	307	KC1	CHA-CBD-CGD-O1D
29	L	307	KC1	CHA-CBD-CGD-O2D
29	L	315	KC1	C1A-C2A-CAA-CBA
29	L	315	KC1	C2B-C3B-CAB-CBB
29	L	315	KC1	C4B-C3B-CAB-CBB
29	L	315	KC1	C2A-CAA-CBA-CGA
29	L	315	KC1	CBD-CGD-O2D-CED
29	M	307	KC1	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	M	307	KC1	C4B-C3B-CAB-CBB
29	M	314	KC1	C3A-C2A-CAA-CBA
29	M	314	KC1	C2B-C3B-CAB-CBB
29	M	314	KC1	C4B-C3B-CAB-CBB
29	M	314	KC1	CBD-CGD-O2D-CED
29	N	306	KC1	C1A-C2A-CAA-CBA
29	N	306	KC1	C3A-C2A-CAA-CBA
29	N	306	KC1	C2B-C3B-CAB-CBB
29	N	306	KC1	C4B-C3B-CAB-CBB
29	N	308	KC1	C2B-C3B-CAB-CBB
29	N	308	KC1	C2A-CAA-CBA-CGA
29	N	311	KC1	C1A-C2A-CAA-CBA
29	N	311	KC1	C3A-C2A-CAA-CBA
29	N	311	KC1	C2B-C3B-CAB-CBB
29	N	311	KC1	C4B-C3B-CAB-CBB
29	N	311	KC1	CBD-CGD-O2D-CED
30	G	521	DGD	C2E-C1E-O5D-C6D
30	G	521	DGD	O6E-C1E-O5D-C6D
30	j	103	DGD	C2B-C1B-O2G-C2G
31	I	318	LMG	O6-C1-O1-C7
31	K	317	LMG	C2-C1-O1-C7
31	K	317	LMG	O6-C1-O1-C7
31	K	317	LMG	C11-C10-O7-C8
31	K	318	LMG	O7-C8-C9-O8
31	K	318	LMG	C11-C10-O7-C8
31	j	101	LMG	O9-C10-O7-C8
31	j	101	LMG	C11-C10-O7-C8
31	b	734	LMG	C2-C1-O1-C7
31	b	734	LMG	O6-C1-O1-C7
31	b	734	LMG	O1-C7-C8-O7
31	b	734	LMG	C11-C10-O7-C8
31	B	318	LMG	O10-C28-O8-C9
32	G	506	PID	O1-C6-C7-C8
32	j	105	PID	C20-C21-C22-C23
32	j	105	PID	CM5-C21-C22-C23
32	D	301	PID	O1-C6-C7-C8
32	D	301	PID	O4-C12-C13-C14
32	D	302	PID	C26-C27-O6-C30
32	D	306	PID	O1-C6-C7-C8
32	D	307	PID	O1-C6-C7-C8
32	F	304	PID	O7-C30-O6-C27
32	F	305	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
32	H	301	PID	O1-C6-C7-C8
32	N	301	PID	O4-C12-C13-C14
32	N	301	PID	C12-C13-C14-CM4
32	N	301	PID	O7-C30-O6-C27
32	N	302	PID	O7-C30-O6-C27
33	A	318	SQD	C46-C45-O47-C7
33	A	318	SQD	C8-C7-O47-C45
35	i	201	BCR	C5-C6-C7-C8
35	i	201	BCR	C7-C8-C9-C10
35	i	201	BCR	C7-C8-C9-C34
35	i	201	BCR	C21-C22-C23-C24
35	i	201	BCR	C37-C22-C23-C24
35	i	201	BCR	C23-C24-C25-C26
35	i	201	BCR	C23-C24-C25-C30
35	j	102	BCR	C7-C8-C9-C10
35	j	102	BCR	C7-C8-C9-C34
35	m	201	BCR	C7-C8-C9-C10
35	m	201	BCR	C7-C8-C9-C34
35	a	734	BCR	C7-C8-C9-C10
35	a	734	BCR	C7-C8-C9-C34
35	a	736	BCR	C7-C8-C9-C10
35	a	736	BCR	C7-C8-C9-C34
35	b	730	BCR	C21-C22-C23-C24
35	b	730	BCR	C37-C22-C23-C24
36	a	732	PQN	C12-C13-C15-C16
36	a	732	PQN	C14-C13-C15-C16
27	h	201	UIX	C31-C27-O2-C18
32	j	105	PID	O7-C30-O6-C27
32	F	304	PID	C31-C30-O6-C27
32	F	305	PID	C31-C30-O6-C27
32	H	302	PID	C31-C30-O6-C27
32	N	301	PID	C31-C30-O6-C27
32	N	302	PID	C31-C30-O6-C27
28	a	722	CLA	O1D-CGD-O2D-CED
28	a	731	CLA	O1D-CGD-O2D-CED
28	H	309	CLA	O1D-CGD-O2D-CED
28	H	311	CLA	O1D-CGD-O2D-CED
29	I	314	KC1	O1D-CGD-O2D-CED
29	H	310	KC1	O1D-CGD-O2D-CED
29	L	315	KC1	O1D-CGD-O2D-CED
29	M	314	KC1	O1D-CGD-O2D-CED
29	N	311	KC1	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	G	503	UIX	O4-C27-O2-C18
27	J	305	UIX	C31-C27-O2-C18
32	j	105	PID	C31-C30-O6-C27
28	K	312	CLA	O1D-CGD-O2D-CED
28	a	712	CLA	O1D-CGD-O2D-CED
28	a	715	CLA	O1D-CGD-O2D-CED
28	B	311	CLA	O1D-CGD-O2D-CED
28	F	312	CLA	O1D-CGD-O2D-CED
28	L	312	CLA	O1D-CGD-O2D-CED
28	N	310	CLA	O1D-CGD-O2D-CED
29	B	314	KC1	O1D-CGD-O2D-CED
28	I	309	CLA	CBD-CGD-O2D-CED
28	I	316	CLA	CBD-CGD-O2D-CED
28	K	312	CLA	CBD-CGD-O2D-CED
28	A	313	CLA	CBD-CGD-O2D-CED
28	A	319	CLA	CBD-CGD-O2D-CED
28	j	106	CLA	CBD-CGD-O2D-CED
28	a	704	CLA	CBD-CGD-O2D-CED
28	a	712	CLA	CBD-CGD-O2D-CED
28	a	714	CLA	CBD-CGD-O2D-CED
28	a	730	CLA	CBD-CGD-O2D-CED
28	B	317	CLA	CBD-CGD-O2D-CED
28	D	313	CLA	CBD-CGD-O2D-CED
28	F	310	CLA	CBD-CGD-O2D-CED
28	F	312	CLA	CBD-CGD-O2D-CED
28	L	316	CLA	CBD-CGD-O2D-CED
28	M	315	CLA	CBD-CGD-O2D-CED
28	M	316	CLA	CBD-CGD-O2D-CED
28	M	318	CLA	CBD-CGD-O2D-CED
28	N	307	CLA	CBD-CGD-O2D-CED
29	I	314	KC1	CBD-CGD-O2D-CED
28	b	701	CLA	O1A-CGA-O2A-C1
28	H	304	CLA	O1A-CGA-O2A-C1
28	J	307	CLA	O1A-CGA-O2A-C1
28	J	311	CLA	O1A-CGA-O2A-C1
28	N	310	CLA	O1A-CGA-O2A-C1
28	A	311	CLA	O1A-CGA-O2A-C1
28	A	320	CLA	O1A-CGA-O2A-C1
28	D	312	CLA	O1A-CGA-O2A-C1
28	D	314	CLA	O1A-CGA-O2A-C1
28	H	308	CLA	O1A-CGA-O2A-C1
32	H	302	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
28	I	309	CLA	O1D-CGD-O2D-CED
28	D	313	CLA	O1D-CGD-O2D-CED
28	D	314	CLA	O1D-CGD-O2D-CED
28	H	312	CLA	O1D-CGD-O2D-CED
28	M	318	CLA	O1D-CGD-O2D-CED
28	N	307	CLA	O1D-CGD-O2D-CED
28	G	518	CLA	CBA-CGA-O2A-C1
28	F	311	CLA	CBA-CGA-O2A-C1
28	J	310	CLA	CBA-CGA-O2A-C1
27	J	305	UIX	C19-C18-O2-C27
28	I	313	CLA	O1D-CGD-O2D-CED
28	I	316	CLA	O1D-CGD-O2D-CED
28	K	308	CLA	O1D-CGD-O2D-CED
28	f	301	CLA	O1D-CGD-O2D-CED
28	a	702	CLA	O1D-CGD-O2D-CED
28	a	707	CLA	O1D-CGD-O2D-CED
28	b	701	CLA	O1D-CGD-O2D-CED
28	b	711	CLA	O1D-CGD-O2D-CED
28	B	315	CLA	O1D-CGD-O2D-CED
28	F	313	CLA	O1D-CGD-O2D-CED
28	b	701	CLA	CBA-CGA-O2A-C1
28	H	304	CLA	CBA-CGA-O2A-C1
28	J	307	CLA	CBA-CGA-O2A-C1
28	J	311	CLA	CBA-CGA-O2A-C1
30	G	521	DGD	C2A-C1A-O1G-C1G
31	K	318	LMG	C29-C28-O8-C9
31	j	101	LMG	C29-C28-O8-C9
28	I	319	CLA	CBD-CGD-O2D-CED
28	I	321	CLA	CBD-CGD-O2D-CED
28	A	315	CLA	CBD-CGD-O2D-CED
28	l	308	CLA	CBD-CGD-O2D-CED
28	m	202	CLA	CBD-CGD-O2D-CED
28	a	711	CLA	CBD-CGD-O2D-CED
28	a	725	CLA	CBD-CGD-O2D-CED
28	a	726	CLA	CBD-CGD-O2D-CED
28	b	707	CLA	CBD-CGD-O2D-CED
28	b	713	CLA	CBD-CGD-O2D-CED
28	H	304	CLA	CBD-CGD-O2D-CED
28	H	308	CLA	CBD-CGD-O2D-CED
28	J	306	CLA	CBD-CGD-O2D-CED
28	J	307	CLA	CBD-CGD-O2D-CED
28	J	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	J	315	CLA	CBD-CGD-O2D-CED
28	L	313	CLA	CBD-CGD-O2D-CED
28	M	308	CLA	CBD-CGD-O2D-CED
28	M	309	CLA	CBD-CGD-O2D-CED
28	M	310	CLA	CBD-CGD-O2D-CED
28	I	308	CLA	O1A-CGA-O2A-C1
28	I	315	CLA	O1A-CGA-O2A-C1
28	K	308	CLA	O1A-CGA-O2A-C1
28	G	513	CLA	O1A-CGA-O2A-C1
28	a	706	CLA	O1A-CGA-O2A-C1
28	a	721	CLA	O1A-CGA-O2A-C1
28	b	707	CLA	O1A-CGA-O2A-C1
28	b	717	CLA	O1A-CGA-O2A-C1
28	B	311	CLA	O1A-CGA-O2A-C1
28	H	309	CLA	O1A-CGA-O2A-C1
28	L	313	CLA	O1A-CGA-O2A-C1
30	G	521	DGD	O1A-C1A-O1G-C1G
31	I	318	LMG	O10-C28-O8-C9
31	K	318	LMG	O10-C28-O8-C9
31	j	101	LMG	O10-C28-O8-C9
31	b	733	LMG	O10-C28-O8-C9
28	G	517	CLA	O1A-CGA-O2A-C1
28	f	302	CLA	O1A-CGA-O2A-C1
28	F	311	CLA	O1A-CGA-O2A-C1
28	K	315	CLA	O1D-CGD-O2D-CED
28	l	312	CLA	O1D-CGD-O2D-CED
28	b	703	CLA	O1D-CGD-O2D-CED
28	H	307	CLA	O1D-CGD-O2D-CED
29	B	314	KC1	CAA-CBA-CGA-O1A
28	b	720	CLA	O1D-CGD-O2D-CED
28	L	318	CLA	O1D-CGD-O2D-CED
27	I	304	UIX	O4-C27-O2-C18
32	G	506	PID	C31-C30-O6-C27
28	A	312	CLA	CBD-CGD-O2D-CED
28	b	715	CLA	CBD-CGD-O2D-CED
28	J	311	CLA	CBD-CGD-O2D-CED
28	M	311	CLA	CBD-CGD-O2D-CED
28	G	516	CLA	O1D-CGD-O2D-CED
28	l	310	CLA	O1D-CGD-O2D-CED
28	a	713	CLA	O1D-CGD-O2D-CED
28	a	721	CLA	O1D-CGD-O2D-CED
28	b	704	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	F	310	CLA	O1D-CGD-O2D-CED
28	M	315	CLA	O1D-CGD-O2D-CED
30	j	103	DGD	O1B-C1B-O2G-C2G
31	I	318	LMG	O9-C10-O7-C8
31	I	320	LMG	O9-C10-O7-C8
31	K	318	LMG	O9-C10-O7-C8
31	b	734	LMG	O9-C10-O7-C8
31	B	318	LMG	O9-C10-O7-C8
33	A	318	SQD	O49-C7-O47-C45
28	F	313	CLA	CBA-CGA-O2A-C1
28	a	718	CLA	O1A-CGA-O2A-C1
28	F	310	CLA	O1A-CGA-O2A-C1
28	I	311	CLA	C3-C5-C6-C7
28	I	312	CLA	C3-C5-C6-C7
28	I	316	CLA	C3-C5-C6-C7
28	K	313	CLA	C3-C5-C6-C7
28	G	514	CLA	C3-C5-C6-C7
28	G	519	CLA	C3-C5-C6-C7
28	j	104	CLA	C3-C5-C6-C7
28	l	305	CLA	C3-C5-C6-C7
28	a	702	CLA	C3-C5-C6-C7
28	a	705	CLA	C3-C5-C6-C7
28	a	706	CLA	C3-C5-C6-C7
28	b	701	CLA	C3-C5-C6-C7
28	b	707	CLA	C3-C5-C6-C7
28	b	717	CLA	C3-C5-C6-C7
28	B	310	CLA	C3-C5-C6-C7
28	J	307	CLA	C3-C5-C6-C7
28	L	309	CLA	C3-C5-C6-C7
28	I	315	CLA	CBA-CGA-O2A-C1
28	K	308	CLA	CBA-CGA-O2A-C1
28	G	513	CLA	CBA-CGA-O2A-C1
28	a	706	CLA	CBA-CGA-O2A-C1
28	a	728	CLA	CBA-CGA-O2A-C1
28	b	720	CLA	CBA-CGA-O2A-C1
28	B	310	CLA	CBA-CGA-O2A-C1
28	H	309	CLA	CBA-CGA-O2A-C1
28	L	314	CLA	CBA-CGA-O2A-C1
28	L	317	CLA	CBA-CGA-O2A-C1
28	N	310	CLA	CBA-CGA-O2A-C1
31	b	733	LMG	C29-C28-O8-C9
32	G	506	PID	O7-C30-O6-C27

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Mol	Chain	Res	Type	Atoms
31	I	318	LMG	C11-C10-O7-C8
31	I	320	LMG	C11-C10-O7-C8
31	B	318	LMG	C11-C10-O7-C8
28	G	512	CLA	CBD-CGD-O2D-CED
28	L	314	CLA	CBD-CGD-O2D-CED
29	M	307	KC1	CBD-CGD-O2D-CED
32	D	305	PID	C31-C30-O6-C27
32	D	305	PID	O7-C30-O6-C27
28	N	304	CLA	O1A-CGA-O2A-C1
28	D	309	CLA	O1A-CGA-O2A-C1
28	F	313	CLA	O1A-CGA-O2A-C1
29	F	309	KC1	CAA-CBA-CGA-O2A
28	a	718	CLA	CBA-CGA-O2A-C1
28	F	307	CLA	CBA-CGA-O2A-C1
28	F	310	CLA	CBA-CGA-O2A-C1
28	M	316	CLA	C3-C5-C6-C7
28	I	308	CLA	C4-C3-C5-C6
28	A	313	CLA	C4-C3-C5-C6
28	l	305	CLA	C4-C3-C5-C6
28	l	311	CLA	C4-C3-C5-C6
28	a	731	CLA	C4-C3-C5-C6
28	L	309	CLA	C4-C3-C5-C6
28	L	317	CLA	C4-C3-C5-C6
28	M	308	CLA	C4-C3-C5-C6
28	M	316	CLA	C4-C3-C5-C6
28	a	713	CLA	C2-C3-C5-C6
28	a	724	CLA	C2-C3-C5-C6
28	a	731	CLA	C2-C3-C5-C6
28	a	735	CLA	C2-C3-C5-C6
28	M	308	CLA	C2-C3-C5-C6
28	a	723	CLA	CBD-CGD-O2D-CED
28	B	312	CLA	CBD-CGD-O2D-CED
28	K	308	CLA	C2A-CAA-CBA-CGA
28	G	513	CLA	C2A-CAA-CBA-CGA
28	G	520	CLA	C2A-CAA-CBA-CGA
28	A	319	CLA	C2A-CAA-CBA-CGA
28	a	709	CLA	C2A-CAA-CBA-CGA
28	a	719	CLA	C2A-CAA-CBA-CGA
28	N	305	CLA	C2A-CAA-CBA-CGA
28	G	518	CLA	O1A-CGA-O2A-C1
28	J	310	CLA	O1A-CGA-O2A-C1
28	A	308	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	A	312	CLA	C3-C5-C6-C7
28	h	202	CLA	C3-C5-C6-C7
28	I	308	CLA	CBA-CGA-O2A-C1
28	G	514	CLA	CBA-CGA-O2A-C1
28	a	721	CLA	CBA-CGA-O2A-C1
28	b	707	CLA	CBA-CGA-O2A-C1
28	b	717	CLA	CBA-CGA-O2A-C1
28	B	311	CLA	CBA-CGA-O2A-C1
28	L	313	CLA	CBA-CGA-O2A-C1
28	N	304	CLA	CBA-CGA-O2A-C1
31	I	318	LMG	C29-C28-O8-C9
31	B	318	LMG	C29-C28-O8-C9
28	j	106	CLA	O1D-CGD-O2D-CED
28	B	317	CLA	O1D-CGD-O2D-CED
27	J	305	UIX	O4-C27-O2-C18
28	A	313	CLA	O1D-CGD-O2D-CED
28	A	319	CLA	O1D-CGD-O2D-CED
28	a	714	CLA	O1D-CGD-O2D-CED
28	a	730	CLA	O1D-CGD-O2D-CED
31	B	318	LMG	C4-C5-C6-O5
28	G	514	CLA	O1A-CGA-O2A-C1
28	l	313	CLA	O1A-CGA-O2A-C1
28	a	728	CLA	O1A-CGA-O2A-C1
28	b	720	CLA	O1A-CGA-O2A-C1
28	L	317	CLA	O1A-CGA-O2A-C1
28	l	310	CLA	O1A-CGA-O2A-C1
28	F	307	CLA	O1A-CGA-O2A-C1
28	M	316	CLA	O1D-CGD-O2D-CED
26	I	301	DD6	C24-C25-C26-C27
26	G	502	DD6	C24-C25-C26-C27
26	M	302	DD6	C1-C2-C3-C4
32	F	305	PID	C14-C15-C16-C17
32	F	305	PID	C18-C19-C20-C21
28	I	306	CLA	CBD-CGD-O2D-CED
28	I	311	CLA	CBD-CGD-O2D-CED
28	A	308	CLA	CBD-CGD-O2D-CED
28	A	320	CLA	CBD-CGD-O2D-CED
28	f	303	CLA	CBD-CGD-O2D-CED
28	l	313	CLA	CBD-CGD-O2D-CED
28	a	705	CLA	CBD-CGD-O2D-CED
28	a	709	CLA	CBD-CGD-O2D-CED
28	b	712	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	b	727	CLA	CBD-CGD-O2D-CED
28	J	301	CLA	CBD-CGD-O2D-CED
28	J	314	CLA	CBD-CGD-O2D-CED
28	L	317	CLA	CBD-CGD-O2D-CED
29	D	310	KC1	CBD-CGD-O2D-CED
28	G	511	CLA	C3-C5-C6-C7
28	A	309	CLA	C3-C5-C6-C7
28	J	301	CLA	CBA-CGA-O2A-C1
27	B	305	UIX	C31-C27-O2-C18
32	F	302	PID	C31-C30-O6-C27
32	H	301	PID	C31-C30-O6-C27
28	B	310	CLA	O1A-CGA-O2A-C1
28	L	314	CLA	O1A-CGA-O2A-C1
28	a	704	CLA	O1D-CGD-O2D-CED
28	L	316	CLA	O1D-CGD-O2D-CED
27	B	305	UIX	O4-C27-O2-C18
32	F	302	PID	O7-C30-O6-C27
32	H	301	PID	O7-C30-O6-C27
28	K	316	CLA	CBA-CGA-O2A-C1
28	H	312	CLA	CBA-CGA-O2A-C1
28	G	519	CLA	CBD-CGD-O2D-CED
28	a	710	CLA	CBD-CGD-O2D-CED
28	B	316	CLA	CBD-CGD-O2D-CED
28	J	309	CLA	CBD-CGD-O2D-CED
29	N	306	KC1	CBD-CGD-O2D-CED
31	K	318	LMG	O6-C5-C6-O5
28	b	703	CLA	C3-C5-C6-C7
28	l	313	CLA	CBA-CGA-O2A-C1
31	K	317	LMG	O6-C5-C6-O5
29	D	315	KC1	CAA-CBA-CGA-O2A
29	F	309	KC1	CAA-CBA-CGA-O1A
29	J	313	KC1	CAA-CBA-CGA-O2A
28	b	704	CLA	C2C-C3C-CAC-CBC
28	J	301	CLA	O1A-CGA-O2A-C1
28	G	510	CLA	C4-C3-C5-C6
28	b	703	CLA	C4-C3-C5-C6
28	G	510	CLA	C2-C3-C5-C6
28	b	703	CLA	C2-C3-C5-C6
28	a	735	CLA	CBD-CGD-O2D-CED
28	a	722	CLA	C2A-CAA-CBA-CGA
28	b	727	CLA	C2A-CAA-CBA-CGA
31	B	318	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
30	G	501	DGD	O6E-C1E-O5D-C6D
31	D	317	LMG	O6-C1-O1-C7
28	a	708	CLA	CBA-CGA-O2A-C1
28	a	709	CLA	CBA-CGA-O2A-C1
28	b	723	CLA	CBA-CGA-O2A-C1
28	B	309	CLA	CBA-CGA-O2A-C1
28	M	308	CLA	CBA-CGA-O2A-C1
28	G	514	CLA	CBD-CGD-O2D-CED
29	B	314	KC1	CAA-CBA-CGA-O2A
28	b	707	CLA	O1D-CGD-O2D-CED
28	H	308	CLA	O1D-CGD-O2D-CED
28	J	308	CLA	O1D-CGD-O2D-CED
28	M	309	CLA	O1D-CGD-O2D-CED
28	a	708	CLA	O1A-CGA-O2A-C1
28	b	723	CLA	O1A-CGA-O2A-C1
28	M	308	CLA	O1A-CGA-O2A-C1
28	b	728	CLA	C3-C5-C6-C7
28	M	308	CLA	C3-C5-C6-C7
28	I	319	CLA	O1D-CGD-O2D-CED
28	b	713	CLA	O1D-CGD-O2D-CED
28	J	307	CLA	O1D-CGD-O2D-CED
28	I	321	CLA	CBA-CGA-O2A-C1
28	G	519	CLA	CBA-CGA-O2A-C1
28	A	313	CLA	CBA-CGA-O2A-C1
28	l	311	CLA	CBA-CGA-O2A-C1
28	a	707	CLA	CBA-CGA-O2A-C1
28	a	712	CLA	CBA-CGA-O2A-C1
28	M	312	CLA	CBA-CGA-O2A-C1
28	F	315	CLA	CBD-CGD-O2D-CED
28	K	316	CLA	O1A-CGA-O2A-C1
28	H	312	CLA	O1A-CGA-O2A-C1
28	b	717	CLA	C5-C6-C7-C8
29	K	314	KC1	CAA-CBA-CGA-O2A
29	A	314	KC1	CAA-CBA-CGA-O2A
29	N	308	KC1	CAA-CBA-CGA-O2A
28	a	721	CLA	C10-C11-C12-C13
28	a	730	CLA	C5-C6-C7-C8
28	b	719	CLA	CBA-CGA-O2A-C1
28	M	317	CLA	CBA-CGA-O2A-C1
30	y	201	DGD	C1B-C2B-C3B-C4B
33	A	318	SQD	C2-C1-O6-C44
30	y	201	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	a	707	CLA	O1A-CGA-O2A-C1
28	I	308	CLA	C2-C3-C5-C6
28	A	313	CLA	C2-C3-C5-C6
28	L	309	CLA	C2-C3-C5-C6
28	M	316	CLA	C2-C3-C5-C6
28	I	312	CLA	C14-C13-C15-C16
28	l	303	CLA	C11-C12-C13-C14
28	l	304	CLA	C11-C10-C8-C9
28	l	305	CLA	C11-C12-C13-C14
28	a	707	CLA	C11-C10-C8-C9
28	a	720	CLA	C11-C12-C13-C14
28	a	721	CLA	C14-C13-C15-C16
28	a	722	CLA	C6-C7-C8-C9
28	a	724	CLA	C6-C7-C8-C9
28	a	731	CLA	C11-C12-C13-C14
28	b	704	CLA	C6-C7-C8-C9
28	b	708	CLA	C6-C7-C8-C9
28	B	311	CLA	C6-C7-C8-C9
28	A	315	CLA	O1D-CGD-O2D-CED
28	J	306	CLA	O1D-CGD-O2D-CED
28	J	315	CLA	O1D-CGD-O2D-CED
28	L	313	CLA	O1D-CGD-O2D-CED
28	B	313	CLA	CBD-CGD-O2D-CED
28	J	310	CLA	CBD-CGD-O2D-CED
28	b	713	CLA	C10-C11-C12-C13
28	B	313	CLA	C10-C11-C12-C13
28	f	303	CLA	C2A-CAA-CBA-CGA
28	a	717	CLA	C2A-CAA-CBA-CGA
28	B	309	CLA	C2A-CAA-CBA-CGA
28	F	311	CLA	C2A-CAA-CBA-CGA
28	J	315	CLA	C2A-CAA-CBA-CGA
26	I	305	DD6	C7-C6-C8-C9
26	K	305	DD6	C12-C11-C13-C14
26	G	502	DD6	C12-C11-C13-C14
26	b	731	DD6	C12-C11-C13-C14
26	D	303	DD6	C12-C11-C13-C14
26	L	302	DD6	C12-C11-C13-C14
35	l	306	BCR	C37-C22-C23-C24
35	b	702	BCR	C37-C22-C23-C24
35	b	730	BCR	C7-C8-C9-C34
26	K	301	DD6	C10-C11-C13-C14
26	B	302	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	D	303	DD6	C10-C11-C13-C14
26	L	302	DD6	C10-C11-C13-C14
35	l	306	BCR	C21-C22-C23-C24
35	b	702	BCR	C21-C22-C23-C24
35	b	730	BCR	C7-C8-C9-C10
31	I	318	LMG	C28-C29-C30-C31
28	G	519	CLA	O1A-CGA-O2A-C1
28	A	313	CLA	O1A-CGA-O2A-C1
28	M	312	CLA	O1A-CGA-O2A-C1
28	I	312	CLA	C13-C15-C16-C17
28	I	313	CLA	C5-C6-C7-C8
28	j	106	CLA	C5-C6-C7-C8
28	B	313	CLA	C8-C10-C11-C12
28	J	307	CLA	C8-C10-C11-C12
28	a	725	CLA	O1D-CGD-O2D-CED
28	H	304	CLA	O1D-CGD-O2D-CED
28	M	308	CLA	O1D-CGD-O2D-CED
29	L	307	KC1	CAA-CBA-CGA-O2A
29	M	307	KC1	CAA-CBA-CGA-O2A
28	l	308	CLA	O1D-CGD-O2D-CED
28	l	303	CLA	C8-C10-C11-C12
28	a	706	CLA	C5-C6-C7-C8
28	a	713	CLA	C10-C11-C12-C13
28	b	713	CLA	C8-C10-C11-C12
28	J	309	CLA	C5-C6-C7-C8
31	I	318	LMG	C10-C11-C12-C13
28	a	711	CLA	O1D-CGD-O2D-CED
28	a	726	CLA	O1D-CGD-O2D-CED
31	K	317	LMG	C4-C5-C6-O5
29	F	314	KC1	CBD-CGD-O2D-CED
28	I	309	CLA	C5-C6-C7-C8
28	m	202	CLA	C5-C6-C7-C8
28	a	723	CLA	C13-C15-C16-C17
28	a	724	CLA	C15-C16-C17-C18
28	a	726	CLA	C15-C16-C17-C18
28	b	722	CLA	C15-C16-C17-C18
28	B	310	CLA	C5-C6-C7-C8
28	J	307	CLA	C13-C15-C16-C17
28	I	321	CLA	C2C-C3C-CAC-CBC
28	l	311	CLA	O1A-CGA-O2A-C1
31	j	101	LMG	C28-C29-C30-C31
28	I	312	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	a	707	CLA	C5-C6-C7-C8
28	b	707	CLA	C10-C11-C12-C13
28	I	321	CLA	O1D-CGD-O2D-CED
28	m	202	CLA	O1D-CGD-O2D-CED
29	D	310	KC1	CAA-CBA-CGA-O1A
29	N	308	KC1	CAA-CBA-CGA-O1A
28	H	305	CLA	C15-C16-C17-C18
28	A	309	CLA	CBD-CGD-O2D-CED
28	a	706	CLA	CBD-CGD-O2D-CED
28	K	312	CLA	O2A-C1-C2-C3
28	a	735	CLA	C13-C15-C16-C17
28	b	722	CLA	C5-C6-C7-C8
28	B	309	CLA	C13-C15-C16-C17
28	b	715	CLA	O1D-CGD-O2D-CED
28	M	310	CLA	O1D-CGD-O2D-CED
28	a	731	CLA	C11-C12-C13-C15
28	b	708	CLA	C6-C7-C8-C10
28	b	717	CLA	C6-C7-C8-C10
28	b	717	CLA	C12-C13-C15-C16
28	b	724	CLA	C11-C12-C13-C15
26	I	305	DD6	C11-C10-C9-C8
26	M	302	DD6	C24-C25-C26-C27
26	M	306	DD6	C24-C25-C26-C27
28	b	719	CLA	C2A-CAA-CBA-CGA
28	b	724	CLA	C2A-CAA-CBA-CGA
28	H	312	CLA	C2A-CAA-CBA-CGA
28	L	312	CLA	C2A-CAA-CBA-CGA
28	M	310	CLA	C2A-CAA-CBA-CGA
28	J	311	CLA	O1D-CGD-O2D-CED
28	M	311	CLA	O1D-CGD-O2D-CED
28	I	312	CLA	C10-C11-C12-C13
28	G	510	CLA	C5-C6-C7-C8
28	l	305	CLA	C5-C6-C7-C8
28	l	313	CLA	C5-C6-C7-C8
28	a	709	CLA	C5-C6-C7-C8
28	b	705	CLA	C10-C11-C12-C13
28	b	705	CLA	C13-C15-C16-C17
28	I	321	CLA	O1A-CGA-O2A-C1
28	a	712	CLA	O1A-CGA-O2A-C1
30	y	201	DGD	O6D-C1D-O3G-C3G
31	j	101	LMG	O6-C1-O1-C7
33	A	318	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
28	A	312	CLA	O1D-CGD-O2D-CED
28	I	311	CLA	C5-C6-C7-C8
28	l	311	CLA	C8-C10-C11-C12
28	a	723	CLA	C15-C16-C17-C18
28	B	311	CLA	C13-C15-C16-C17
28	K	313	CLA	CBA-CGA-O2A-C1
28	a	709	CLA	O1A-CGA-O2A-C1
28	B	309	CLA	O1A-CGA-O2A-C1
28	I	308	CLA	C8-C10-C11-C12
28	h	202	CLA	C5-C6-C7-C8
28	l	311	CLA	C5-C6-C7-C8
28	a	705	CLA	C5-C6-C7-C8
28	a	723	CLA	C5-C6-C7-C8
28	b	707	CLA	C15-C16-C17-C18
28	B	311	CLA	C10-C11-C12-C13
30	G	521	DGD	C4A-C5A-C6A-C7A
28	L	314	CLA	O1D-CGD-O2D-CED
28	I	312	CLA	C5-C6-C7-C8
28	I	316	CLA	C5-C6-C7-C8
28	A	313	CLA	C3-C5-C6-C7
28	a	716	CLA	CBD-CGD-O2D-CED
28	B	309	CLA	C15-C16-C17-C18
36	b	729	PQN	C20-C21-C22-C23
28	G	512	CLA	O1D-CGD-O2D-CED
30	G	501	DGD	O6D-C5D-C6D-O5D
31	j	101	LMG	O6-C5-C6-O5
30	G	521	DGD	O1B-C1B-O2G-C2G
28	L	317	CLA	C2-C3-C5-C6
28	a	723	CLA	O1D-CGD-O2D-CED
28	I	308	CLA	C2A-CAA-CBA-CGA
28	I	319	CLA	C2A-CAA-CBA-CGA
28	B	317	CLA	C2A-CAA-CBA-CGA
28	D	312	CLA	C2A-CAA-CBA-CGA
28	J	316	CLA	C2A-CAA-CBA-CGA
28	L	308	CLA	C2A-CAA-CBA-CGA
28	M	311	CLA	C2A-CAA-CBA-CGA
28	m	202	CLA	C11-C12-C13-C15
28	b	720	CLA	C3-C5-C6-C7
28	L	313	CLA	C3-C5-C6-C7
28	L	314	CLA	C3-C5-C6-C7
32	F	305	PID	C16-C17-C18-C19
29	I	314	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	I	306	CLA	CBA-CGA-O2A-C1
28	b	716	CLA	CBA-CGA-O2A-C1
28	B	313	CLA	CBA-CGA-O2A-C1
28	L	309	CLA	CBA-CGA-O2A-C1
28	G	513	CLA	C5-C6-C7-C8
30	G	521	DGD	C1A-C2A-C3A-C4A
27	J	305	UIX	C11-C13-C14-C23
29	N	308	KC1	CBD-CGD-O2D-CED
30	G	521	DGD	C2B-C1B-O2G-C2G
28	a	707	CLA	C8-C10-C11-C12
32	D	307	PID	C19-C20-C21-CM5
32	F	305	PID	C19-C20-C21-CM5
28	I	313	CLA	C3-C5-C6-C7
28	b	709	CLA	C3-C5-C6-C7
31	I	318	LMG	C29-C30-C31-C32
28	B	312	CLA	O1D-CGD-O2D-CED
29	K	314	KC1	C2A-CAA-CBA-CGA
29	B	314	KC1	C2A-CAA-CBA-CGA
29	F	314	KC1	C2A-CAA-CBA-CGA
29	J	313	KC1	C2A-CAA-CBA-CGA
28	G	512	CLA	C11-C12-C13-C14
28	b	715	CLA	C11-C12-C13-C15
28	B	311	CLA	C16-C17-C18-C20
30	l	301	DGD	C2B-C3B-C4B-C5B
31	B	318	LMG	C7-C8-O7-C10
31	K	317	LMG	O9-C10-O7-C8
29	M	307	KC1	CAA-CBA-CGA-O1A
28	D	309	CLA	CBD-CGD-O2D-CED
31	D	317	LMG	C32-C33-C34-C35
31	K	318	LMG	C32-C33-C34-C35
31	D	317	LMG	C15-C16-C17-C18
31	K	318	LMG	C4-C5-C6-O5
28	I	311	CLA	O1D-CGD-O2D-CED
30	G	521	DGD	C2D-C1D-O3G-C3G
31	I	318	LMG	C2-C1-O1-C7
31	j	101	LMG	C2-C1-O1-C7
32	D	306	PID	C19-C20-C21-C22
32	D	307	PID	C19-C20-C21-C22
32	F	305	PID	C19-C20-C21-C22
28	b	704	CLA	C4C-C3C-CAC-CBC
31	b	733	LMG	C33-C34-C35-C36
28	I	316	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	h	202	CLA	C6-C7-C8-C9
28	j	104	CLA	C6-C7-C8-C10
28	b	708	CLA	C16-C17-C18-C20
28	b	717	CLA	C16-C17-C18-C20
28	J	307	CLA	C16-C17-C18-C19
31	K	318	LMG	C34-C35-C36-C37
31	B	318	LMG	C31-C32-C33-C34
28	l	305	CLA	C2-C3-C5-C6
28	l	311	CLA	C2-C3-C5-C6
28	a	702	CLA	C11-C12-C13-C14
28	a	723	CLA	C11-C12-C13-C14
28	b	701	CLA	C11-C12-C13-C14
28	b	717	CLA	C6-C7-C8-C9
28	b	717	CLA	C11-C12-C13-C14
28	b	727	CLA	C14-C13-C15-C16
30	I	317	DGD	C1B-C2B-C3B-C4B
31	K	318	LMG	C31-C32-C33-C34
28	f	302	CLA	C2A-CAA-CBA-CGA
28	j	106	CLA	C2A-CAA-CBA-CGA
28	b	701	CLA	C2A-CAA-CBA-CGA
28	B	308	CLA	C2A-CAA-CBA-CGA
28	N	310	CLA	C2A-CAA-CBA-CGA
26	K	319	DD6	C12-C11-C13-C14
26	A	301	DD6	C12-C11-C13-C14
26	B	302	DD6	C12-C11-C13-C14
26	J	304	DD6	C12-C11-C13-C14
26	M	303	DD6	C12-C11-C13-C14
27	J	305	UIX	C7-C10-C11-C12
31	b	733	LMG	C36-C37-C38-C39
26	K	319	DD6	C10-C11-C13-C14
26	A	301	DD6	C10-C11-C13-C14
26	M	303	DD6	C10-C11-C13-C14
27	J	305	UIX	C7-C10-C11-C13
28	I	309	CLA	C3-C5-C6-C7
36	a	732	PQN	C13-C15-C16-C17
28	j	104	CLA	C5-C6-C7-C8
28	a	702	CLA	C8-C10-C11-C12
31	b	733	LMG	C32-C33-C34-C35
28	a	709	CLA	O1D-CGD-O2D-CED
28	G	512	CLA	C11-C12-C13-C15
28	l	311	CLA	C16-C17-C18-C20
28	B	301	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	B	311	CLA	C16-C17-C18-C19
28	J	307	CLA	C16-C17-C18-C20
28	L	313	CLA	C6-C7-C8-C10
36	a	732	PQN	C26-C27-C28-C29
36	a	732	PQN	C26-C27-C28-C30
30	G	521	DGD	O6D-C1D-O3G-C3G
28	A	312	CLA	C5-C6-C7-C8
28	a	735	CLA	C15-C16-C17-C18
36	a	732	PQN	C18-C20-C21-C22
28	J	301	CLA	O1D-CGD-O2D-CED
28	L	317	CLA	O1D-CGD-O2D-CED
28	L	308	CLA	C2C-C3C-CAC-CBC
31	D	317	LMG	C30-C31-C32-C33
28	b	717	CLA	CBD-CGD-O2D-CED
28	a	705	CLA	O1D-CGD-O2D-CED
28	J	314	CLA	O1D-CGD-O2D-CED
31	B	318	LMG	C32-C33-C34-C35
29	A	314	KC1	CAA-CBA-CGA-O1A
29	D	315	KC1	CAA-CBA-CGA-O1A
29	L	307	KC1	CAA-CBA-CGA-O1A
29	N	306	KC1	CAA-CBA-CGA-O2A
28	L	309	CLA	O1A-CGA-O2A-C1
30	G	521	DGD	O6D-C5D-C6D-O5D
28	G	519	CLA	O1D-CGD-O2D-CED
28	b	712	CLA	O1D-CGD-O2D-CED
28	f	302	CLA	C3A-C2A-CAA-CBA
28	a	718	CLA	C3A-C2A-CAA-CBA
28	a	719	CLA	C3A-C2A-CAA-CBA
28	a	725	CLA	C3A-C2A-CAA-CBA
28	a	727	CLA	C3A-C2A-CAA-CBA
28	a	735	CLA	C3A-C2A-CAA-CBA
28	B	308	CLA	C3A-C2A-CAA-CBA
28	D	314	CLA	C3A-C2A-CAA-CBA
28	F	310	CLA	C3A-C2A-CAA-CBA
28	J	308	CLA	C3A-C2A-CAA-CBA
28	L	317	CLA	C3A-C2A-CAA-CBA
28	N	310	CLA	C3A-C2A-CAA-CBA
31	D	317	LMG	C33-C34-C35-C36
28	A	308	CLA	O1D-CGD-O2D-CED
28	b	727	CLA	O1D-CGD-O2D-CED
28	K	313	CLA	O1A-CGA-O2A-C1
28	h	202	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	j	104	CLA	C6-C7-C8-C9
28	l	311	CLA	C16-C17-C18-C19
28	b	717	CLA	C16-C17-C18-C19
28	B	301	CLA	C11-C12-C13-C15
28	L	313	CLA	C6-C7-C8-C9
31	b	733	LMG	C37-C38-C39-C40
28	I	310	CLA	O2A-C1-C2-C3
28	I	306	CLA	O1D-CGD-O2D-CED
28	A	320	CLA	O1D-CGD-O2D-CED
28	f	303	CLA	O1D-CGD-O2D-CED
28	B	301	CLA	CBD-CGD-O2D-CED
31	I	318	LMG	C14-C15-C16-C17
31	j	101	LMG	C33-C34-C35-C36
32	D	307	PID	C17-C18-C19-C20
28	l	313	CLA	O1D-CGD-O2D-CED
31	K	318	LMG	C28-C29-C30-C31
31	D	317	LMG	C10-C11-C12-C13
31	I	318	LMG	C30-C31-C32-C33
31	K	318	LMG	C30-C31-C32-C33
28	b	716	CLA	O1A-CGA-O2A-C1
28	B	301	CLA	CBA-CGA-O2A-C1
28	a	707	CLA	C2-C3-C5-C6
28	B	311	CLA	C2-C3-C5-C6
29	J	313	KC1	CAA-CBA-CGA-O1A
30	G	501	DGD	C4D-C5D-C6D-O5D
31	B	318	LMG	C33-C34-C35-C36
28	J	309	CLA	O1D-CGD-O2D-CED
28	a	728	CLA	C6-C7-C8-C9
28	M	317	CLA	O1A-CGA-O2A-C1
28	a	704	CLA	C15-C16-C17-C18
28	b	724	CLA	C3-C5-C6-C7
28	b	725	CLA	C3-C5-C6-C7
30	G	521	DGD	C4D-C5D-C6D-O5D
28	I	306	CLA	O1A-CGA-O2A-C1
28	B	313	CLA	O1A-CGA-O2A-C1
28	l	303	CLA	C10-C11-C12-C13
31	K	318	LMG	C12-C13-C14-C15
37	a	733	LHG	C26-C27-C28-C29
28	b	715	CLA	C11-C12-C13-C14
28	b	719	CLA	O1A-CGA-O2A-C1
28	K	308	CLA	C3-C5-C6-C7
28	J	312	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	i	201	BCR	C1-C6-C7-C8
35	b	730	BCR	C1-C6-C7-C8
35	b	730	BCR	C5-C6-C7-C8
31	D	317	LMG	O6-C5-C6-O5
28	I	313	CLA	CBA-CGA-O2A-C1
28	b	703	CLA	CBA-CGA-O2A-C1
28	l	311	CLA	C10-C11-C12-C13
28	a	712	CLA	C10-C11-C12-C13
28	b	712	CLA	C5-C6-C7-C8
31	D	317	LMG	C13-C14-C15-C16
28	a	707	CLA	C4-C3-C5-C6
28	b	722	CLA	C4-C3-C5-C6
28	a	710	CLA	O1D-CGD-O2D-CED
28	G	513	CLA	C12-C13-C15-C16
28	l	313	CLA	C12-C13-C15-C16
28	a	702	CLA	C11-C12-C13-C15
28	a	707	CLA	C11-C10-C8-C7
28	a	721	CLA	C12-C13-C15-C16
28	a	722	CLA	C6-C7-C8-C10
28	b	701	CLA	C11-C12-C13-C15
28	b	704	CLA	C11-C10-C8-C7
28	b	707	CLA	C11-C10-C8-C7
28	b	709	CLA	C2-C3-C5-C6
28	b	717	CLA	C11-C12-C13-C15
28	b	724	CLA	C12-C13-C15-C16
28	B	311	CLA	C11-C10-C8-C7
28	a	729	CLA	C3-C5-C6-C7
28	I	313	CLA	O1A-CGA-O2A-C1
28	B	301	CLA	O1A-CGA-O2A-C1
36	a	732	PQN	C15-C16-C17-C18
28	I	316	CLA	C6-C7-C8-C10
28	b	708	CLA	C16-C17-C18-C19
28	B	316	CLA	O1D-CGD-O2D-CED
28	K	311	CLA	CBA-CGA-O2A-C1
28	G	510	CLA	CBA-CGA-O2A-C1
28	h	202	CLA	CBA-CGA-O2A-C1
28	a	705	CLA	CBA-CGA-O2A-C1
28	a	735	CLA	CBA-CGA-O2A-C1
30	l	301	DGD	C2A-C1A-O1G-C1G
28	I	316	CLA	C2A-CAA-CBA-CGA
28	G	510	CLA	C2A-CAA-CBA-CGA
28	G	514	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	m	202	CLA	C2A-CAA-CBA-CGA
28	b	708	CLA	C2A-CAA-CBA-CGA
28	b	718	CLA	C2A-CAA-CBA-CGA
28	b	723	CLA	C2A-CAA-CBA-CGA
28	D	309	CLA	C2A-CAA-CBA-CGA
28	J	312	CLA	C2A-CAA-CBA-CGA
28	b	704	CLA	C13-C15-C16-C17
28	b	722	CLA	CBD-CGD-O2D-CED
29	G	515	KC1	C2C-C3C-CAC-CBC
28	B	311	CLA	C5-C6-C7-C8
29	G	515	KC1	C2B-C3B-CAB-CBB
29	L	307	KC1	C2B-C3B-CAB-CBB
29	M	314	KC1	CAA-CBA-CGA-O2A
31	D	317	LMG	C14-C15-C16-C17
28	f	301	CLA	CBA-CGA-O2A-C1
28	I	313	CLA	C6-C7-C8-C10
31	I	320	LMG	O6-C1-O1-C7
31	b	733	LMG	C15-C16-C17-C18
30	G	501	DGD	C2B-C1B-O2G-C2G
37	a	733	LHG	C8-C7-O7-C5
31	I	320	LMG	C16-C17-C18-C19
29	L	307	KC1	C4B-C3B-CAB-CBB
29	N	308	KC1	C4B-C3B-CAB-CBB
28	l	304	CLA	C8-C10-C11-C12
28	b	701	CLA	C10-C11-C12-C13
28	b	711	CLA	C5-C6-C7-C8
36	b	729	PQN	C23-C25-C26-C27
31	D	317	LMG	C18-C19-C20-C21
28	M	310	CLA	O2A-C1-C2-C3
28	A	310	CLA	C16-C17-C18-C20
31	b	733	LMG	C14-C15-C16-C17
30	L	301	DGD	O6E-C5E-C6E-O5E
28	a	731	CLA	C8-C10-C11-C12
28	b	709	CLA	C4-C3-C5-C6
26	K	301	DD6	C27-C29-C30-C31
26	K	305	DD6	C27-C29-C30-C31
26	K	319	DD6	C27-C29-C30-C31
26	G	502	DD6	C27-C29-C30-C31
26	G	508	DD6	C27-C29-C30-C31
26	B	303	DD6	C27-C29-C30-C31
26	J	302	DD6	C27-C29-C30-C31
26	L	306	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	G	510	CLA	C11-C12-C13-C14
28	G	513	CLA	C14-C13-C15-C16
28	l	313	CLA	C14-C13-C15-C16
28	b	704	CLA	C11-C10-C8-C9
28	b	724	CLA	C11-C12-C13-C14
28	b	724	CLA	C14-C13-C15-C16
28	B	311	CLA	C11-C10-C8-C9
28	B	313	CLA	C11-C10-C8-C9
28	I	310	CLA	CBD-CGD-O2D-CED
28	I	307	CLA	C2A-CAA-CBA-CGA
28	I	313	CLA	C2A-CAA-CBA-CGA
28	I	315	CLA	C2A-CAA-CBA-CGA
28	A	310	CLA	C2A-CAA-CBA-CGA
28	A	311	CLA	C2A-CAA-CBA-CGA
28	H	307	CLA	C2A-CAA-CBA-CGA
28	J	301	CLA	C2A-CAA-CBA-CGA
28	M	316	CLA	C2A-CAA-CBA-CGA
26	I	301	DD6	C12-C11-C13-C14
35	j	102	BCR	C36-C18-C19-C20
26	I	301	DD6	C10-C11-C13-C14
26	I	305	DD6	C5-C6-C8-C9
28	a	705	CLA	O1A-CGA-O2A-C1
28	b	703	CLA	O1A-CGA-O2A-C1
28	I	315	CLA	C1A-C2A-CAA-CBA
28	A	319	CLA	C1A-C2A-CAA-CBA
28	f	302	CLA	C1A-C2A-CAA-CBA
28	l	312	CLA	C1A-C2A-CAA-CBA
28	a	707	CLA	C1A-C2A-CAA-CBA
28	a	711	CLA	C1A-C2A-CAA-CBA
28	a	712	CLA	C1A-C2A-CAA-CBA
28	a	715	CLA	C1A-C2A-CAA-CBA
28	a	717	CLA	C1A-C2A-CAA-CBA
28	a	719	CLA	C1A-C2A-CAA-CBA
28	a	720	CLA	C1A-C2A-CAA-CBA
28	a	725	CLA	C1A-C2A-CAA-CBA
28	a	727	CLA	C1A-C2A-CAA-CBA
28	a	735	CLA	C1A-C2A-CAA-CBA
28	b	706	CLA	C1A-C2A-CAA-CBA
28	b	720	CLA	C1A-C2A-CAA-CBA
28	b	721	CLA	C1A-C2A-CAA-CBA
28	b	723	CLA	C1A-C2A-CAA-CBA
28	D	314	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	F	308	CLA	C1A-C2A-CAA-CBA
28	H	309	CLA	C1A-C2A-CAA-CBA
28	J	301	CLA	C1A-C2A-CAA-CBA
28	J	308	CLA	C1A-C2A-CAA-CBA
28	L	312	CLA	C1A-C2A-CAA-CBA
28	L	313	CLA	C1A-C2A-CAA-CBA
28	L	317	CLA	C1A-C2A-CAA-CBA
28	M	313	CLA	C1A-C2A-CAA-CBA
28	N	305	CLA	C1A-C2A-CAA-CBA
28	I	313	CLA	C6-C7-C8-C9
28	m	202	CLA	C11-C12-C13-C14
28	a	728	CLA	C6-C7-C8-C10
28	a	735	CLA	C16-C17-C18-C20
28	b	712	CLA	C6-C7-C8-C10
30	G	501	DGD	O1B-C1B-O2G-C2G
29	A	306	KC1	CAA-CBA-CGA-O2A
31	K	318	LMG	C29-C30-C31-C32
28	G	514	CLA	O1D-CGD-O2D-CED
28	G	512	CLA	C5-C6-C7-C8
28	a	731	CLA	C15-C16-C17-C18
28	b	701	CLA	C5-C6-C7-C8
28	b	707	CLA	C5-C6-C7-C8
27	J	305	UIX	C17-C18-O2-C27
28	a	735	CLA	O1D-CGD-O2D-CED
28	a	721	CLA	C8-C10-C11-C12
28	b	704	CLA	C10-C11-C12-C13
28	b	717	CLA	C13-C15-C16-C17
30	l	301	DGD	C3B-C4B-C5B-C6B
28	A	310	CLA	C8-C10-C11-C12
28	l	304	CLA	C3-C5-C6-C7
30	I	317	DGD	O6E-C5E-C6E-O5E
28	D	311	CLA	CBA-CGA-O2A-C1
28	B	311	CLA	C4-C3-C5-C6
28	G	510	CLA	O1A-CGA-O2A-C1
28	h	202	CLA	O1A-CGA-O2A-C1
28	l	303	CLA	C16-C17-C18-C20
28	a	735	CLA	C3-C5-C6-C7
30	G	501	DGD	C1G-C2G-C3G-O3G
31	K	318	LMG	C7-C8-C9-O8
31	b	734	LMG	O1-C7-C8-C9
31	B	318	LMG	C7-C8-C9-O8
28	a	729	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	I	318	LMG	C15-C16-C17-C18
30	l	301	DGD	O1A-C1A-O1G-C1G
31	I	320	LMG	C32-C33-C34-C35
31	b	734	LMG	O6-C5-C6-O5
30	G	521	DGD	C1B-C2B-C3B-C4B
28	K	311	CLA	O1A-CGA-O2A-C1
28	f	301	CLA	O1A-CGA-O2A-C1
28	a	735	CLA	O1A-CGA-O2A-C1
28	f	303	CLA	CBA-CGA-O2A-C1
28	b	712	CLA	C6-C7-C8-C9
28	l	311	CLA	C13-C15-C16-C17
28	b	706	CLA	O2A-C1-C2-C3
28	J	306	CLA	CBA-CGA-O2A-C1
28	F	315	CLA	O1D-CGD-O2D-CED
32	D	306	PID	C19-C20-C21-CM5
28	a	721	CLA	C16-C17-C18-C19
28	L	308	CLA	CBA-CGA-O2A-C1
28	l	303	CLA	CBD-CGD-O2D-CED
28	K	308	CLA	C6-C7-C8-C9
28	B	313	CLA	O1D-CGD-O2D-CED
28	a	723	CLA	C2A-CAA-CBA-CGA
28	K	310	CLA	C5-C6-C7-C8
28	b	704	CLA	C15-C16-C17-C18
28	K	311	CLA	C2-C1-O2A-CGA
28	J	310	CLA	O1D-CGD-O2D-CED
28	A	309	CLA	O1D-CGD-O2D-CED
31	I	320	LMG	C17-C18-C19-C20
28	A	312	CLA	CBA-CGA-O2A-C1
28	b	704	CLA	CBA-CGA-O2A-C1
28	b	705	CLA	CBA-CGA-O2A-C1
31	b	734	LMG	C29-C28-O8-C9
28	L	318	CLA	CAA-CBA-CGA-O2A
28	b	711	CLA	C6-C7-C8-C9
28	A	311	CLA	CBD-CGD-O2D-CED
28	l	313	CLA	C15-C16-C17-C18
28	a	713	CLA	C8-C10-C11-C12
28	a	731	CLA	C5-C6-C7-C8
30	G	521	DGD	O2G-C2G-C3G-O3G
28	A	310	CLA	C16-C17-C18-C19
31	b	733	LMG	C38-C39-C40-C41
28	I	312	CLA	C12-C13-C15-C16
28	G	510	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	G	519	CLA	C6-C7-C8-C10
28	G	519	CLA	C11-C10-C8-C7
28	A	310	CLA	C11-C12-C13-C15
28	l	313	CLA	C6-C7-C8-C10
28	a	702	CLA	C12-C13-C15-C16
28	a	709	CLA	C12-C13-C15-C16
28	a	717	CLA	C11-C10-C8-C7
28	b	703	CLA	C11-C10-C8-C7
28	b	709	CLA	C11-C10-C8-C7
28	B	301	CLA	C11-C10-C8-C7
28	B	309	CLA	C6-C7-C8-C10
28	B	309	CLA	C11-C12-C13-C15
28	B	311	CLA	C11-C12-C13-C15
28	B	311	CLA	C12-C13-C15-C16
28	B	313	CLA	C11-C10-C8-C7
28	J	307	CLA	C11-C10-C8-C7
28	J	309	CLA	C6-C7-C8-C10
28	N	305	CLA	C11-C12-C13-C15
28	b	714	CLA	CAA-CBA-CGA-O2A
28	I	312	CLA	C11-C12-C13-C14
28	G	510	CLA	C6-C7-C8-C9
28	G	512	CLA	C11-C10-C8-C9
28	A	310	CLA	C11-C12-C13-C14
28	A	310	CLA	C14-C13-C15-C16
28	l	313	CLA	C6-C7-C8-C9
28	a	707	CLA	C11-C12-C13-C14
28	a	709	CLA	C14-C13-C15-C16
28	a	717	CLA	C11-C10-C8-C9
28	a	724	CLA	C14-C13-C15-C16
28	b	703	CLA	C11-C10-C8-C9
28	b	705	CLA	C14-C13-C15-C16
28	b	709	CLA	C11-C10-C8-C9
28	B	309	CLA	C6-C7-C8-C9
28	B	309	CLA	C11-C12-C13-C14
28	N	305	CLA	C11-C12-C13-C14
36	a	732	PQN	C21-C22-C23-C24
35	l	306	BCR	C13-C14-C15-C16
28	I	312	CLA	CBA-CGA-O2A-C1
28	I	310	CLA	C2A-CAA-CBA-CGA
26	G	505	DD6	C12-C11-C13-C14
26	L	305	DD6	C12-C11-C13-C14
28	l	303	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	a	721	CLA	C16-C17-C18-C20
26	I	303	DD6	C10-C11-C13-C14
26	G	504	DD6	C5-C6-C8-C9
26	G	505	DD6	C10-C11-C13-C14
28	L	308	CLA	O1A-CGA-O2A-C1
28	a	723	CLA	C10-C11-C12-C13
28	b	711	CLA	C3-C5-C6-C7
31	b	733	LMG	C28-C29-C30-C31
28	a	724	CLA	C5-C6-C7-C8
28	a	716	CLA	O1D-CGD-O2D-CED
28	B	309	CLA	C4-C3-C5-C6
28	D	309	CLA	O1D-CGD-O2D-CED
29	G	515	KC1	CAA-CBA-CGA-O2A
28	I	311	CLA	C6-C7-C8-C10
28	f	301	CLA	C6-C7-C8-C10
31	j	101	LMG	C31-C32-C33-C34
28	a	720	CLA	C10-C11-C12-C13
28	K	306	CLA	CBA-CGA-O2A-C1
28	a	724	CLA	CBA-CGA-O2A-C1
28	a	726	CLA	CBA-CGA-O2A-C1
28	b	712	CLA	CBA-CGA-O2A-C1
37	a	733	LHG	C2-C3-O3-P
28	I	310	CLA	C3A-C2A-CAA-CBA
28	b	706	CLA	C3A-C2A-CAA-CBA
28	b	724	CLA	C3A-C2A-CAA-CBA
28	B	317	CLA	C3A-C2A-CAA-CBA
31	I	318	LMG	C12-C13-C14-C15
28	a	735	CLA	C16-C17-C18-C19
28	b	728	CLA	CBA-CGA-O2A-C1
28	a	721	CLA	C5-C6-C7-C8
30	y	201	DGD	C1G-C2G-C3G-O3G
31	I	318	LMG	O1-C7-C8-C9
31	I	318	LMG	C7-C8-C9-O8
31	D	317	LMG	C7-C8-C9-O8
31	I	318	LMG	C32-C33-C34-C35
28	a	726	CLA	C3-C5-C6-C7
28	a	706	CLA	O1D-CGD-O2D-CED
28	b	704	CLA	O1A-CGA-O2A-C1
28	H	305	CLA	C4-C3-C5-C6
31	I	320	LMG	C31-C32-C33-C34
28	A	312	CLA	O1A-CGA-O2A-C1
28	b	705	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	D	315	KC1	C3A-C2A-CAA-CBA
29	F	309	KC1	C3A-C2A-CAA-CBA
29	L	315	KC1	C3A-C2A-CAA-CBA
28	B	310	CLA	C6-C7-C8-C9
28	b	708	CLA	C5-C6-C7-C8
28	B	316	CLA	CBA-CGA-O2A-C1
28	b	717	CLA	O1D-CGD-O2D-CED
31	b	734	LMG	C11-C12-C13-C14
28	I	312	CLA	O1A-CGA-O2A-C1
30	G	521	DGD	O1G-C1G-C2G-O2G
30	j	103	DGD	O1G-C1G-C2G-O2G
30	l	301	DGD	O2G-C2G-C3G-O3G
31	I	318	LMG	O1-C7-C8-O7
31	I	318	LMG	O7-C8-C9-O8
31	j	101	LMG	O7-C8-C9-O8
31	b	734	LMG	O7-C8-C9-O8
28	l	313	CLA	C2C-C3C-CAC-CBC
28	b	711	CLA	C6-C7-C8-C10
28	a	704	CLA	C5-C6-C7-C8
28	I	307	CLA	CBD-CGD-O2D-CED
28	b	719	CLA	CBD-CGD-O2D-CED
28	f	301	CLA	C2-C1-O2A-CGA
28	a	703	CLA	C2-C1-O2A-CGA
28	b	725	CLA	C2-C1-O2A-CGA
28	B	301	CLA	O1D-CGD-O2D-CED
28	G	510	CLA	C14-C13-C15-C16
28	G	519	CLA	C6-C7-C8-C9
28	m	202	CLA	C6-C7-C8-C9
28	b	704	CLA	C11-C12-C13-C14
28	b	727	CLA	C11-C12-C13-C14
28	a	724	CLA	C13-C15-C16-C17
29	M	314	KC1	C1A-C2A-CAA-CBA
31	I	318	LMG	C31-C32-C33-C34
28	l	310	CLA	C2A-CAA-CBA-CGA
28	b	712	CLA	C2A-CAA-CBA-CGA
28	I	311	CLA	C6-C7-C8-C9
35	j	102	BCR	C23-C24-C25-C30
35	l	306	BCR	C1-C6-C7-C8
35	l	306	BCR	C5-C6-C7-C8
35	l	306	BCR	C23-C24-C25-C26
35	l	306	BCR	C23-C24-C25-C30
26	I	303	DD6	C12-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
26	A	302	DD6	C7-C6-C8-C9
26	K	305	DD6	C10-C11-C13-C14
26	b	731	DD6	C10-C11-C13-C14
26	L	305	DD6	C10-C11-C13-C14
35	j	102	BCR	C17-C18-C19-C20
35	m	201	BCR	C11-C12-C13-C14
28	b	722	CLA	O1D-CGD-O2D-CED
32	D	306	PID	C15-C16-C17-C18
28	I	321	CLA	C4C-C3C-CAC-CBC
28	M	312	CLA	O2A-C1-C2-C3
29	L	315	KC1	C2C-C3C-CAC-CBC
28	G	510	CLA	C6-C7-C8-C10
28	G	512	CLA	C11-C10-C8-C7
28	A	310	CLA	C11-C10-C8-C7
28	A	310	CLA	C12-C13-C15-C16
28	l	305	CLA	C11-C12-C13-C15
28	l	313	CLA	C11-C12-C13-C15
28	m	202	CLA	C6-C7-C8-C10
28	a	709	CLA	C11-C10-C8-C7
28	a	713	CLA	C11-C10-C8-C7
28	a	717	CLA	C6-C7-C8-C10
28	a	725	CLA	C11-C10-C8-C7
28	b	704	CLA	C6-C7-C8-C10
28	b	704	CLA	C12-C13-C15-C16
28	b	705	CLA	C11-C12-C13-C15
28	b	707	CLA	C6-C7-C8-C10
28	b	722	CLA	C2-C3-C5-C6
28	b	727	CLA	C12-C13-C15-C16
28	b	728	CLA	C6-C7-C8-C10
28	B	309	CLA	C12-C13-C15-C16
28	H	305	CLA	C11-C12-C13-C15
28	a	702	CLA	C15-C16-C17-C18
26	I	305	DD6	C1-C2-C3-C4
26	I	305	DD6	C3-C4-C5-C6
28	f	301	CLA	C6-C7-C8-C9
28	G	519	CLA	C10-C11-C12-C13
28	K	310	CLA	C2A-CAA-CBA-CGA
28	L	309	CLA	C2A-CAA-CBA-CGA
28	a	722	CLA	C5-C6-C7-C8
32	D	306	PID	CM4-C14-C15-C16
28	a	713	CLA	C3-C5-C6-C7
28	J	308	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	I	310	CLA	CAD-CBD-CGD-O2D
28	I	315	CLA	CAD-CBD-CGD-O2D
28	K	311	CLA	CAD-CBD-CGD-O2D
28	K	315	CLA	CAD-CBD-CGD-O2D
28	G	513	CLA	CAD-CBD-CGD-O2D
28	G	517	CLA	CAD-CBD-CGD-O2D
28	G	519	CLA	CAD-CBD-CGD-O2D
28	f	302	CLA	CAD-CBD-CGD-O2D
28	l	305	CLA	CAD-CBD-CGD-O2D
28	l	309	CLA	CAD-CBD-CGD-O2D
28	a	705	CLA	CAD-CBD-CGD-O2D
28	a	708	CLA	CAD-CBD-CGD-O2D
28	a	735	CLA	CAD-CBD-CGD-O2D
28	b	708	CLA	CAD-CBD-CGD-O2D
28	b	714	CLA	CAD-CBD-CGD-O2D
28	b	715	CLA	CAD-CBD-CGD-O2D
28	b	719	CLA	CAD-CBD-CGD-O2D
28	B	316	CLA	CAD-CBD-CGD-O2D
28	D	311	CLA	CAD-CBD-CGD-O2D
28	D	312	CLA	CAD-CBD-CGD-O2D
28	D	313	CLA	CAD-CBD-CGD-O2D
28	J	315	CLA	CAD-CBD-CGD-O2D
28	L	318	CLA	CAD-CBD-CGD-O2D
29	N	308	KC1	CAD-CBD-CGD-O2D
30	G	521	DGD	C1G-C2G-O2G-C1B
31	I	320	LMG	C14-C15-C16-C17
28	a	717	CLA	CBA-CGA-O2A-C1
28	a	720	CLA	CBA-CGA-O2A-C1
30	G	521	DGD	O1G-C1G-C2G-C3G
30	j	103	DGD	O1G-C1G-C2G-C3G
30	l	301	DGD	C1G-C2G-C3G-O3G
31	b	734	LMG	C7-C8-C9-O8
31	I	318	LMG	C11-C12-C13-C14
37	a	733	LHG	C24-C25-C26-C27
28	a	704	CLA	C2A-CAA-CBA-CGA
28	b	705	CLA	C2A-CAA-CBA-CGA
28	b	712	CLA	O1A-CGA-O2A-C1
37	a	733	LHG	O9-C7-O7-C5
28	I	306	CLA	CHA-CBD-CGD-O1D
28	I	306	CLA	CHA-CBD-CGD-O2D
28	K	310	CLA	CHA-CBD-CGD-O2D
28	G	512	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	G	512	CLA	CHA-CBD-CGD-O2D
28	A	315	CLA	CHA-CBD-CGD-O1D
28	A	320	CLA	CHA-CBD-CGD-O1D
28	f	303	CLA	CHA-CBD-CGD-O2D
28	l	304	CLA	CHA-CBD-CGD-O1D
28	l	304	CLA	CHA-CBD-CGD-O2D
28	a	703	CLA	CHA-CBD-CGD-O2D
28	a	714	CLA	CHA-CBD-CGD-O1D
28	a	714	CLA	CHA-CBD-CGD-O2D
28	a	722	CLA	CHA-CBD-CGD-O2D
28	a	724	CLA	CHA-CBD-CGD-O1D
28	a	724	CLA	CHA-CBD-CGD-O2D
28	a	727	CLA	CHA-CBD-CGD-O1D
28	a	727	CLA	CHA-CBD-CGD-O2D
28	a	729	CLA	CHA-CBD-CGD-O1D
28	a	729	CLA	CHA-CBD-CGD-O2D
28	b	705	CLA	CHA-CBD-CGD-O1D
28	b	723	CLA	CHA-CBD-CGD-O1D
28	F	310	CLA	CHA-CBD-CGD-O1D
28	F	310	CLA	CHA-CBD-CGD-O2D
28	F	315	CLA	CHA-CBD-CGD-O1D
28	H	312	CLA	CHA-CBD-CGD-O2D
28	J	301	CLA	CHA-CBD-CGD-O1D
28	J	301	CLA	CHA-CBD-CGD-O2D
28	J	312	CLA	CHA-CBD-CGD-O1D
28	J	312	CLA	CHA-CBD-CGD-O2D
28	L	316	CLA	CHA-CBD-CGD-O1D
28	L	316	CLA	CHA-CBD-CGD-O2D
28	N	307	CLA	CHA-CBD-CGD-O1D
29	I	314	KC1	CHA-CBD-CGD-O1D
29	K	314	KC1	CHA-CBD-CGD-O1D
29	K	314	KC1	CHA-CBD-CGD-O2D
29	A	306	KC1	CHA-CBD-CGD-O1D
29	D	310	KC1	CHA-CBD-CGD-O1D
29	N	308	KC1	CHA-CBD-CGD-O1D
32	N	301	PID	C12-C13-C14-C15
28	b	728	CLA	O1A-CGA-O2A-C1
32	D	306	PID	C13-C14-C15-C16
30	G	501	DGD	O2G-C2G-C3G-O3G
31	B	318	LMG	O7-C8-C9-O8
28	K	306	CLA	O1A-CGA-O2A-C1
28	a	724	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	726	CLA	O1A-CGA-O2A-C1
28	B	310	CLA	C6-C7-C8-C10
31	b	733	LMG	C35-C36-C37-C38
31	K	317	LMG	C28-C29-C30-C31
36	b	729	PQN	C14-C13-C15-C16
26	I	302	DD6	C27-C29-C30-C31
26	K	304	DD6	C27-C29-C30-C31
26	h	203	DD6	C27-C29-C30-C31
26	b	731	DD6	C27-C29-C30-C31
26	B	302	DD6	C27-C29-C30-C31
26	B	306	DD6	C27-C29-C30-C31
26	F	303	DD6	C27-C29-C30-C31
26	H	303	DD6	C27-C29-C30-C31
26	L	302	DD6	C27-C29-C30-C31
28	a	721	CLA	C13-C15-C16-C17
28	a	725	CLA	C5-C6-C7-C8
28	G	513	CLA	C6-C7-C8-C9
28	l	304	CLA	C6-C7-C8-C9
28	l	311	CLA	C14-C13-C15-C16
28	a	709	CLA	C11-C10-C8-C9
28	a	713	CLA	C11-C10-C8-C9
28	a	725	CLA	C11-C10-C8-C9
28	b	715	CLA	C6-C7-C8-C9
28	b	728	CLA	C6-C7-C8-C9
28	J	301	CLA	C11-C10-C8-C9
28	I	310	CLA	O1D-CGD-O2D-CED
28	A	319	CLA	CAA-CBA-CGA-O2A
28	b	703	CLA	CAA-CBA-CGA-O2A
28	a	709	CLA	C8-C10-C11-C12
28	b	720	CLA	C5-C6-C7-C8
26	L	306	DD6	C12-C11-C13-C14
27	K	302	UIX	C7-C10-C11-C12
35	m	201	BCR	C11-C12-C13-C35
28	A	311	CLA	O1D-CGD-O2D-CED
26	G	502	DD6	C10-C11-C13-C14
26	L	306	DD6	C10-C11-C13-C14
27	K	302	UIX	C7-C10-C11-C13
28	a	703	CLA	C3-C5-C6-C7
28	N	305	CLA	C3-C5-C6-C7
28	l	303	CLA	O1D-CGD-O2D-CED
28	a	724	CLA	C1A-C2A-CAA-CBA
28	H	305	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	D	317	LMG	C28-C29-C30-C31
28	b	709	CLA	C11-C12-C13-C14
28	b	707	CLA	C2-C1-O2A-CGA
28	K	311	CLA	C4-C3-C5-C6
28	K	313	CLA	C6-C7-C8-C10
29	M	314	KC1	C2C-C3C-CAC-CBC
37	a	733	LHG	C24-C23-O8-C6
28	F	312	CLA	C2C-C3C-CAC-CBC
28	A	313	CLA	C6-C7-C8-C9
28	N	305	CLA	C16-C17-C18-C20
31	b	733	LMG	C31-C32-C33-C34
28	K	310	CLA	CAD-CBD-CGD-O1D
28	G	512	CLA	CAD-CBD-CGD-O1D
28	a	708	CLA	C2-C3-C5-C6
28	a	718	CLA	CAD-CBD-CGD-O1D
28	a	721	CLA	CAD-CBD-CGD-O1D
28	a	729	CLA	CAD-CBD-CGD-O1D
28	F	311	CLA	CAD-CBD-CGD-O1D
28	H	312	CLA	CAD-CBD-CGD-O1D
28	J	307	CLA	CAD-CBD-CGD-O1D
28	l	312	CLA	CBA-CGA-O2A-C1
28	J	301	CLA	C8-C10-C11-C12
28	a	717	CLA	O1A-CGA-O2A-C1
28	a	720	CLA	O1A-CGA-O2A-C1
28	b	725	CLA	CBA-CGA-O2A-C1
28	b	704	CLA	C16-C17-C18-C20
28	b	707	CLA	C4-C3-C5-C6
28	A	310	CLA	C6-C7-C8-C10
28	l	303	CLA	C11-C12-C13-C15
28	a	706	CLA	C3A-C2A-CAA-CBA
28	a	722	CLA	C11-C10-C8-C7
28	a	724	CLA	C6-C7-C8-C10
28	b	708	CLA	C11-C10-C8-C7
28	B	301	CLA	C6-C7-C8-C10
28	B	311	CLA	C6-C7-C8-C10
28	J	301	CLA	C11-C10-C8-C7
28	N	305	CLA	C12-C13-C15-C16
28	a	703	CLA	C6-C7-C8-C9
28	A	316	CLA	CAA-CBA-CGA-O2A
28	M	317	CLA	CAA-CBA-CGA-O2A
30	G	521	DGD	C1G-C2G-C3G-O3G
32	D	306	PID	O4-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	H	301	PID	O4-C12-C13-C14
31	D	317	LMG	O7-C8-C9-O8
28	a	702	CLA	CAA-CBA-CGA-O2A
28	l	303	CLA	C15-C16-C17-C18
28	b	724	CLA	C5-C6-C7-C8
28	b	712	CLA	C3-C5-C6-C7
28	b	719	CLA	O1D-CGD-O2D-CED
28	B	309	CLA	C10-C11-C12-C13
28	A	310	CLA	C11-C10-C8-C9
28	l	311	CLA	C11-C12-C13-C14
28	l	313	CLA	C11-C12-C13-C14
28	a	723	CLA	C14-C13-C15-C16
28	a	726	CLA	C14-C13-C15-C16
28	b	705	CLA	C11-C12-C13-C14
28	b	707	CLA	C6-C7-C8-C9
28	B	309	CLA	C14-C13-C15-C16
28	H	305	CLA	C11-C12-C13-C14
28	J	309	CLA	C6-C7-C8-C9
31	b	733	LMG	C34-C35-C36-C37
26	I	302	DD6	C6-C8-C9-C10
26	D	303	DD6	C11-C10-C9-C8
31	K	317	LMG	C10-C11-C12-C13
28	l	313	CLA	C13-C15-C16-C17
28	b	725	CLA	O1A-CGA-O2A-C1
37	a	733	LHG	C23-C24-C25-C26
28	f	303	CLA	CAA-CBA-CGA-O2A
28	K	311	CLA	C2-C3-C5-C6
29	F	309	KC1	C2A-CAA-CBA-CGA
28	A	313	CLA	C6-C7-C8-C10
28	a	726	CLA	C13-C15-C16-C17
28	G	520	CLA	C1-C2-C3-C4
29	M	314	KC1	C4C-C3C-CAC-CBC
31	I	318	LMG	C9-C8-O7-C10
28	G	512	CLA	C2A-CAA-CBA-CGA
28	M	310	CLA	CBA-CGA-O2A-C1
28	I	308	CLA	C2-C1-O2A-CGA
28	j	106	CLA	C2-C1-O2A-CGA
28	L	313	CLA	C2-C1-O2A-CGA
28	M	308	CLA	C2-C1-O2A-CGA
28	M	309	CLA	C2-C1-O2A-CGA
32	D	306	PID	C17-C18-C19-C20
28	D	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	B	318	LMG	C34-C35-C36-C37
28	b	710	CLA	O1A-CGA-O2A-C1
28	M	310	CLA	O1A-CGA-O2A-C1
28	f	303	CLA	O1A-CGA-O2A-C1
28	G	513	CLA	C8-C10-C11-C12
28	b	710	CLA	CBA-CGA-O2A-C1
28	M	316	CLA	CBA-CGA-O2A-C1
31	D	317	LMG	C29-C28-O8-C9
28	M	316	CLA	O1A-CGA-O2A-C1
30	y	201	DGD	C9B-CAB-CBB-CCB
31	B	318	LMG	C36-C37-C38-C39
35	j	102	BCR	C23-C24-C25-C26
36	b	729	PQN	C12-C13-C15-C16
28	l	304	CLA	C11-C12-C13-C14
31	b	733	LMG	C11-C10-O7-C8
28	J	307	CLA	C10-C11-C12-C13
28	L	318	CLA	C2A-CAA-CBA-CGA
31	I	320	LMG	C2-C1-O1-C7
32	D	304	PID	C19-C20-C21-C22
28	L	308	CLA	C4C-C3C-CAC-CBC
31	b	733	LMG	C29-C30-C31-C32
37	a	733	LHG	C3-O3-P-O6
37	a	733	LHG	C4-O6-P-O3
28	N	305	CLA	C16-C17-C18-C19
28	I	307	CLA	O1D-CGD-O2D-CED
28	G	510	CLA	C12-C13-C15-C16
28	G	513	CLA	C6-C7-C8-C10
28	l	304	CLA	C11-C10-C8-C7
28	a	707	CLA	C11-C12-C13-C15
28	a	724	CLA	C12-C13-C15-C16
28	B	309	CLA	C11-C10-C8-C7
28	a	722	CLA	C11-C10-C8-C9
28	B	301	CLA	C6-C7-C8-C9
31	b	733	LMG	C30-C31-C32-C33
37	a	733	LHG	C32-C33-C34-C35
28	l	305	CLA	C10-C11-C12-C13
28	B	309	CLA	C2-C3-C5-C6
28	J	306	CLA	O1A-CGA-O2A-C1
28	G	518	CLA	C2A-CAA-CBA-CGA
28	L	311	CLA	C2A-CAA-CBA-CGA
31	b	734	LMG	C14-C15-C16-C17
28	a	717	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	b	728	CLA	C5-C6-C7-C8
37	a	733	LHG	O2-C2-C3-O3
28	K	313	CLA	C6-C7-C8-C9
28	b	707	CLA	C16-C17-C18-C20
28	a	728	CLA	C2A-CAA-CBA-CGA
28	D	311	CLA	C2A-CAA-CBA-CGA
28	b	716	CLA	C3A-C2A-CAA-CBA
28	b	719	CLA	C3A-C2A-CAA-CBA
28	B	307	CLA	C3A-C2A-CAA-CBA
28	F	313	CLA	C3A-C2A-CAA-CBA
37	a	733	LHG	C29-C30-C31-C32
28	l	303	CLA	C14-C13-C15-C16
28	a	721	CLA	C11-C12-C13-C14
28	b	724	CLA	C11-C10-C8-C9
28	b	727	CLA	C6-C7-C8-C9
28	N	305	CLA	C14-C13-C15-C16
28	D	308	CLA	CBA-CGA-O2A-C1
30	G	501	DGD	C3A-C4A-C5A-C6A
26	I	302	DD6	C9-C10-C11-C12
30	G	501	DGD	O1G-C1G-C2G-C3G
32	D	304	PID	C19-C20-C21-CM5
35	f	304	BCR	C35-C13-C14-C15
35	l	302	BCR	C20-C21-C22-C37
28	I	315	CLA	C4C-C3C-CAC-CBC
28	l	304	CLA	C11-C12-C13-C15
28	b	727	CLA	C16-C17-C18-C20
27	G	503	UIX	C36-C38-C40-C41
31	I	320	LMG	C7-C8-O7-C10
37	a	733	LHG	C4-C5-O7-C7
37	a	733	LHG	C6-C5-O7-C7
28	I	308	CLA	C1A-C2A-CAA-CBA
28	I	310	CLA	C1A-C2A-CAA-CBA
28	a	706	CLA	C1A-C2A-CAA-CBA
28	b	716	CLA	C1A-C2A-CAA-CBA
28	B	313	CLA	C1A-C2A-CAA-CBA
28	H	305	CLA	C16-C17-C18-C20
28	B	316	CLA	O1A-CGA-O2A-C1
28	a	709	CLA	C6-C7-C8-C10
28	a	735	CLA	C12-C13-C15-C16
28	b	713	CLA	C11-C10-C8-C7
28	a	723	CLA	C3-C5-C6-C7
28	L	318	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	F	303	DD6	C11-C10-C9-C8
28	D	308	CLA	O1A-CGA-O2A-C1
28	A	308	CLA	C2A-CAA-CBA-CGA
28	b	725	CLA	C2A-CAA-CBA-CGA
28	L	314	CLA	C2A-CAA-CBA-CGA
30	j	103	DGD	C2A-C3A-C4A-C5A
28	b	715	CLA	CBA-CGA-O2A-C1
29	G	515	KC1	C4C-C3C-CAC-CBC
26	I	302	DD6	C9-C10-C11-C13
35	f	304	BCR	C12-C13-C14-C15
35	l	302	BCR	C20-C21-C22-C23
28	I	308	CLA	C10-C11-C12-C13
26	G	504	DD6	C24-C25-C26-C27
26	M	302	DD6	C3-C4-C5-C6
28	I	321	CLA	C2-C1-O2A-CGA
28	G	514	CLA	C2-C1-O2A-CGA
28	A	309	CLA	C2-C1-O2A-CGA
28	I	312	CLA	C6-C7-C8-C9
28	b	707	CLA	C11-C10-C8-C9
28	b	725	CLA	C6-C7-C8-C9
28	J	307	CLA	C14-C13-C15-C16
28	B	316	CLA	C2C-C3C-CAC-CBC
29	G	515	KC1	C1A-C2A-CAA-CBA
29	A	314	KC1	C1A-C2A-CAA-CBA
29	F	314	KC1	C1A-C2A-CAA-CBA
29	H	310	KC1	C1A-C2A-CAA-CBA
29	M	307	KC1	C1A-C2A-CAA-CBA
28	I	316	CLA	O1A-CGA-O2A-C1
28	a	710	CLA	C2A-CAA-CBA-CGA
28	b	720	CLA	C2A-CAA-CBA-CGA
28	J	309	CLA	C2A-CAA-CBA-CGA
28	b	715	CLA	O1A-CGA-O2A-C1
37	a	733	LHG	O10-C23-O8-C6
35	f	304	BCR	C23-C24-C25-C30
35	a	734	BCR	C23-C24-C25-C30
35	a	736	BCR	C5-C6-C7-C8
35	b	730	BCR	C23-C24-C25-C30
35	b	732	BCR	C1-C6-C7-C8
28	a	727	CLA	O1D-CGD-O2D-CED
28	l	305	CLA	CAA-CBA-CGA-O2A
28	a	729	CLA	CAA-CBA-CGA-O2A
28	A	310	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	a	728	CLA	C5-C6-C7-C8
28	B	309	CLA	C5-C6-C7-C8
28	A	316	CLA	O1A-CGA-O2A-C1
26	A	302	DD6	C5-C6-C8-C9
28	b	714	CLA	CAA-CBA-CGA-O1A
33	A	318	SQD	C45-C44-O6-C1
28	a	725	CLA	CBA-CGA-O2A-C1
28	b	707	CLA	C16-C17-C18-C19
28	G	517	CLA	C2A-CAA-CBA-CGA
28	b	722	CLA	C2A-CAA-CBA-CGA
31	j	101	LMG	C4-C5-C6-O5
28	l	312	CLA	O1A-CGA-O2A-C1
28	a	710	CLA	C6-C7-C8-C10
31	b	733	LMG	C17-C18-C19-C20
28	G	509	CLA	O1A-CGA-O2A-C1
28	a	725	CLA	O1A-CGA-O2A-C1
28	L	311	CLA	C4-C3-C5-C6
28	l	311	CLA	C11-C12-C13-C15
28	a	704	CLA	C11-C10-C8-C7
28	b	725	CLA	C6-C7-C8-C10
28	H	305	CLA	C2-C3-C5-C6
28	B	308	CLA	CAA-CBA-CGA-O2A
26	K	301	DD6	C24-C25-C26-C27
27	J	305	UIX	C26-C30-C34-C37
28	G	509	CLA	CBA-CGA-O2A-C1
28	A	316	CLA	CBA-CGA-O2A-C1
31	D	317	LMG	C16-C17-C18-C19
32	D	304	PID	CM4-C14-C15-C16
28	b	720	CLA	C4-C3-C5-C6
28	L	313	CLA	C4-C3-C5-C6
28	l	303	CLA	C13-C15-C16-C17
29	N	311	KC1	C2A-CAA-CBA-CGA
31	K	318	LMG	C18-C19-C20-C21
28	m	202	CLA	CAA-CBA-CGA-O2A
28	B	310	CLA	CAA-CBA-CGA-O2A
28	a	729	CLA	C11-C10-C8-C7
28	A	310	CLA	C6-C7-C8-C9
28	a	723	CLA	C11-C10-C8-C9
28	a	729	CLA	C6-C7-C8-C9
28	a	735	CLA	C14-C13-C15-C16
28	b	708	CLA	C11-C10-C8-C9
28	B	309	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	B	311	CLA	C11-C12-C13-C14
28	J	307	CLA	C11-C10-C8-C9
31	D	317	LMG	C20-C21-C22-C23
28	l	311	CLA	C3A-C2A-CAA-CBA
28	H	307	CLA	C3A-C2A-CAA-CBA
28	L	318	CLA	C3A-C2A-CAA-CBA
28	M	311	CLA	C3A-C2A-CAA-CBA
28	b	713	CLA	CAA-CBA-CGA-O2A
28	b	724	CLA	CAA-CBA-CGA-O2A
28	L	317	CLA	CAA-CBA-CGA-O2A
28	J	312	CLA	CBD-CGD-O2D-CED
28	a	715	CLA	CAA-CBA-CGA-O2A
28	I	312	CLA	CAD-CBD-CGD-O2D
28	I	313	CLA	CAD-CBD-CGD-O2D
28	I	316	CLA	CAD-CBD-CGD-O2D
28	K	312	CLA	CAD-CBD-CGD-O2D
28	G	510	CLA	CAD-CBD-CGD-O2D
28	G	518	CLA	CAD-CBD-CGD-O2D
28	G	520	CLA	CAD-CBD-CGD-O2D
28	A	309	CLA	CAD-CBD-CGD-O2D
28	j	106	CLA	CAD-CBD-CGD-O2D
28	l	303	CLA	CAD-CBD-CGD-O2D
28	l	311	CLA	CAD-CBD-CGD-O2D
28	a	706	CLA	CAD-CBD-CGD-O2D
28	a	713	CLA	CAD-CBD-CGD-O2D
28	b	722	CLA	CAD-CBD-CGD-O2D
28	b	724	CLA	CAD-CBD-CGD-O2D
28	b	725	CLA	CAD-CBD-CGD-O2D
28	b	726	CLA	CAD-CBD-CGD-O2D
28	B	301	CLA	CAD-CBD-CGD-O2D
28	B	311	CLA	CAD-CBD-CGD-O2D
28	F	312	CLA	CAD-CBD-CGD-O2D
28	H	309	CLA	CAD-CBD-CGD-O2D
28	J	311	CLA	CAD-CBD-CGD-O2D
28	M	311	CLA	CAD-CBD-CGD-O2D
28	M	312	CLA	CAD-CBD-CGD-O2D
28	M	316	CLA	CAD-CBD-CGD-O2D
28	N	309	CLA	CAD-CBD-CGD-O2D
28	N	310	CLA	CAD-CBD-CGD-O2D
29	G	515	KC1	CAD-CBD-CGD-O2D
31	I	320	LMG	C9-C8-O7-C10
28	a	703	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	j	101	LMG	C10-C11-C12-C13
28	l	310	CLA	CAA-CBA-CGA-O2A
28	a	723	CLA	CAA-CBA-CGA-O2A
28	I	315	CLA	C2C-C3C-CAC-CBC
28	I	308	CLA	CAA-CBA-CGA-O2A
28	I	316	CLA	CAA-CBA-CGA-O2A
28	a	717	CLA	CAA-CBA-CGA-O2A
31	I	320	LMG	O8-C28-C29-C30
27	G	503	UIX	C36-C38-C40-C39
26	K	301	DD6	C13-C14-C15-O1
26	K	305	DD6	C13-C14-C15-O1
26	K	319	DD6	C13-C14-C15-O1
26	A	302	DD6	C13-C14-C15-O1
26	M	306	DD6	C13-C14-C15-O1
27	I	304	UIX	O-C-C7-C10
31	j	101	LMG	O1-C7-C8-C9
32	F	305	PID	O1-C6-C7-C8
32	M	301	PID	O1-C6-C7-C8
32	N	301	PID	O1-C6-C7-C8
28	G	511	CLA	CAA-CBA-CGA-O2A
28	A	310	CLA	CAA-CBA-CGA-O2A
28	a	706	CLA	CAA-CBA-CGA-O2A
28	B	307	CLA	O2A-C1-C2-C3
28	I	309	CLA	O2A-C1-C2-C3
28	G	510	CLA	O2A-C1-C2-C3
28	l	304	CLA	O2A-C1-C2-C3
28	l	313	CLA	O2A-C1-C2-C3
28	a	723	CLA	O2A-C1-C2-C3
28	b	716	CLA	O2A-C1-C2-C3
28	b	717	CLA	O2A-C1-C2-C3
28	B	309	CLA	O2A-C1-C2-C3
28	B	311	CLA	O2A-C1-C2-C3
28	J	307	CLA	O2A-C1-C2-C3
28	L	309	CLA	O2A-C1-C2-C3
28	L	310	CLA	O2A-C1-C2-C3
28	b	708	CLA	CAA-CBA-CGA-O2A
28	b	711	CLA	CAA-CBA-CGA-O2A
28	a	711	CLA	CAA-CBA-CGA-O2A
28	a	715	CLA	CAA-CBA-CGA-O1A
28	I	308	CLA	C11-C12-C13-C15
28	a	731	CLA	C16-C17-C18-C19
28	H	305	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	I	321	CLA	CHA-CBD-CGD-O2D
28	K	308	CLA	CHA-CBD-CGD-O1D
28	K	308	CLA	CHA-CBD-CGD-O2D
28	A	315	CLA	CHA-CBD-CGD-O2D
28	A	320	CLA	CHA-CBD-CGD-O2D
28	j	104	CLA	CHA-CBD-CGD-O1D
28	l	303	CLA	CHA-CBD-CGD-O1D
28	l	312	CLA	CHA-CBD-CGD-O1D
28	l	312	CLA	CHA-CBD-CGD-O2D
28	a	702	CLA	CHA-CBD-CGD-O2D
28	a	707	CLA	CHA-CBD-CGD-O1D
28	a	707	CLA	CHA-CBD-CGD-O2D
28	a	709	CLA	CHA-CBD-CGD-O1D
28	a	709	CLA	CHA-CBD-CGD-O2D
28	a	719	CLA	CHA-CBD-CGD-O2D
28	b	705	CLA	CHA-CBD-CGD-O2D
28	b	710	CLA	CHA-CBD-CGD-O1D
28	b	710	CLA	CHA-CBD-CGD-O2D
28	b	714	CLA	CHA-CBD-CGD-O2D
28	b	721	CLA	CHA-CBD-CGD-O1D
28	b	721	CLA	CHA-CBD-CGD-O2D
28	b	727	CLA	CHA-CBD-CGD-O1D
28	b	727	CLA	CHA-CBD-CGD-O2D
28	B	313	CLA	CHA-CBD-CGD-O1D
28	B	313	CLA	CHA-CBD-CGD-O2D
28	D	308	CLA	CHA-CBD-CGD-O1D
28	D	308	CLA	CHA-CBD-CGD-O2D
28	F	307	CLA	CHA-CBD-CGD-O1D
28	F	307	CLA	CHA-CBD-CGD-O2D
28	H	311	CLA	CHA-CBD-CGD-O1D
28	H	311	CLA	CHA-CBD-CGD-O2D
28	J	308	CLA	CHA-CBD-CGD-O1D
28	J	308	CLA	CHA-CBD-CGD-O2D
28	J	309	CLA	CHA-CBD-CGD-O1D
28	J	309	CLA	CHA-CBD-CGD-O2D
28	L	309	CLA	CHA-CBD-CGD-O1D
28	L	309	CLA	CHA-CBD-CGD-O2D
28	L	311	CLA	CHA-CBD-CGD-O1D
28	M	310	CLA	CHA-CBD-CGD-O1D
28	M	315	CLA	CHA-CBD-CGD-O1D
28	M	315	CLA	CHA-CBD-CGD-O2D
28	M	318	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	M	318	CLA	CHA-CBD-CGD-O2D
28	N	307	CLA	CHA-CBD-CGD-O2D
29	G	515	KC1	CHA-CBD-CGD-O1D
29	F	314	KC1	CHA-CBD-CGD-O1D
29	M	307	KC1	CHA-CBD-CGD-O2D
28	a	711	CLA	CAA-CBA-CGA-O1A
28	D	309	CLA	CAA-CBA-CGA-O2A
28	J	310	CLA	CAA-CBA-CGA-O2A
28	M	316	CLA	CAA-CBA-CGA-O2A
30	l	301	DGD	C3A-C4A-C5A-C6A
28	l	305	CLA	C15-C16-C17-C18
31	K	318	LMG	C19-C20-C21-C22
28	G	514	CLA	CAA-CBA-CGA-O2A
28	l	305	CLA	O1A-CGA-O2A-C1
28	B	308	CLA	CAA-CBA-CGA-O1A
31	D	317	LMG	C36-C37-C38-C39
28	a	706	CLA	C10-C11-C12-C13
28	I	309	CLA	O1A-CGA-O2A-C1
28	M	317	CLA	C2A-CAA-CBA-CGA
28	I	319	CLA	CAA-CBA-CGA-O2A
28	L	309	CLA	C5-C6-C7-C8
28	I	309	CLA	CBA-CGA-O2A-C1
28	l	305	CLA	CBA-CGA-O2A-C1
28	K	309	CLA	CAA-CBA-CGA-O2A
28	b	707	CLA	C2-C3-C5-C6
30	j	103	DGD	O6D-C5D-C6D-O5D
28	J	312	CLA	O1D-CGD-O2D-CED
28	b	725	CLA	C16-C17-C18-C20
26	M	306	DD6	C27-C29-C30-C31
28	a	724	CLA	C11-C10-C8-C9
28	a	725	CLA	C6-C7-C8-C9
28	B	301	CLA	C11-C10-C8-C9
28	G	520	CLA	O2A-C1-C2-C3
30	j	103	DGD	C1A-C2A-C3A-C4A
28	A	313	CLA	C2A-CAA-CBA-CGA
28	a	735	CLA	C2A-CAA-CBA-CGA
28	a	727	CLA	CBD-CGD-O2D-CED
28	A	310	CLA	CAA-CBA-CGA-O1A
28	a	717	CLA	CAA-CBA-CGA-O1A
28	B	316	CLA	C4C-C3C-CAC-CBC
28	I	316	CLA	CBA-CGA-O2A-C1
35	m	201	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
28	I	308	CLA	CAA-CBA-CGA-O1A
28	m	202	CLA	CAA-CBA-CGA-O1A
28	a	706	CLA	CAA-CBA-CGA-O1A
28	b	724	CLA	CAA-CBA-CGA-O1A
28	B	310	CLA	CAA-CBA-CGA-O1A
35	l	302	BCR	C17-C18-C19-C20
30	G	501	DGD	C2A-C3A-C4A-C5A
28	I	307	CLA	C1A-C2A-CAA-CBA
28	b	713	CLA	C1A-C2A-CAA-CBA
28	b	719	CLA	C1A-C2A-CAA-CBA
28	b	728	CLA	C1A-C2A-CAA-CBA
28	B	307	CLA	C1A-C2A-CAA-CBA
28	B	309	CLA	C1A-C2A-CAA-CBA
28	H	307	CLA	C1A-C2A-CAA-CBA
28	L	318	CLA	C1A-C2A-CAA-CBA
28	M	311	CLA	C1A-C2A-CAA-CBA
28	G	511	CLA	C6-C7-C8-C10
28	b	713	CLA	CAA-CBA-CGA-O1A
32	D	302	PID	C28-C27-O6-C30
28	L	310	CLA	C2-C1-O2A-CGA
28	I	316	CLA	CAA-CBA-CGA-O1A
28	J	312	CLA	CAA-CBA-CGA-O2A
28	I	321	CLA	C2A-CAA-CBA-CGA
28	l	305	CLA	C2A-CAA-CBA-CGA
28	J	307	CLA	C2A-CAA-CBA-CGA
28	M	313	CLA	C2A-CAA-CBA-CGA
28	D	312	CLA	CBD-CGD-O2D-CED
28	b	724	CLA	C16-C17-C18-C20
28	a	723	CLA	CAA-CBA-CGA-O1A
28	J	310	CLA	CAA-CBA-CGA-O1A
28	M	316	CLA	CAA-CBA-CGA-O1A
29	F	314	KC1	CAA-CBA-CGA-O2A
28	K	308	CLA	CAA-CBA-CGA-O2A
28	l	313	CLA	C3-C5-C6-C7
28	a	730	CLA	C3-C5-C6-C7
28	D	309	CLA	CAA-CBA-CGA-O1A
30	y	201	DGD	C2A-C3A-C4A-C5A
37	a	733	LHG	C3-O3-P-O5
37	a	733	LHG	C4-O6-P-O5
28	B	309	CLA	C16-C17-C18-C19
28	G	514	CLA	CAA-CBA-CGA-O1A
28	b	708	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	L	317	CLA	CAA-CBA-CGA-O1A
31	B	318	LMG	O9-C10-C11-C12
28	a	718	CLA	CAA-CBA-CGA-O2A
28	L	311	CLA	CAA-CBA-CGA-O2A
35	a	734	BCR	C23-C24-C25-C26
35	b	730	BCR	C23-C24-C25-C26
35	b	732	BCR	C5-C6-C7-C8
28	G	519	CLA	C11-C12-C13-C14
28	b	705	CLA	C5-C6-C7-C8
26	I	302	DD6	C11-C13-C14-C15
26	D	303	DD6	C11-C13-C14-C15
32	F	304	PID	C6-C7-C8-C9
28	l	310	CLA	CAA-CBA-CGA-O1A
28	j	106	CLA	O1A-CGA-O2A-C1
30	I	317	DGD	O6D-C5D-C6D-O5D
28	G	511	CLA	CAA-CBA-CGA-O1A
28	b	711	CLA	CAA-CBA-CGA-O1A
31	I	320	LMG	O9-C10-C11-C12
28	b	713	CLA	C13-C15-C16-C17
28	I	319	CLA	CAA-CBA-CGA-O1A
28	K	310	CLA	CAA-CBA-CGA-O2A
28	M	309	CLA	CAA-CBA-CGA-O2A
28	D	312	CLA	O1D-CGD-O2D-CED
28	b	701	CLA	C8-C10-C11-C12
28	I	319	CLA	CAD-CBD-CGD-O1D
28	b	705	CLA	CAD-CBD-CGD-O1D
28	b	713	CLA	CAD-CBD-CGD-O1D
28	b	721	CLA	CAD-CBD-CGD-O1D
28	F	307	CLA	CAD-CBD-CGD-O1D
28	H	307	CLA	CAD-CBD-CGD-O1D
28	J	316	CLA	CAD-CBD-CGD-O1D
28	L	309	CLA	CAD-CBD-CGD-O1D
28	N	304	CLA	CAD-CBD-CGD-O1D
28	N	307	CLA	CAD-CBD-CGD-O1D
28	N	307	CLA	C2-C3-C5-C6
31	I	320	LMG	O10-C28-C29-C30
28	a	726	CLA	C5-C6-C7-C8
28	a	702	CLA	C14-C13-C15-C16
28	a	709	CLA	C6-C7-C8-C9
28	b	713	CLA	C14-C13-C15-C16
37	a	733	LHG	C31-C32-C33-C34
31	b	733	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	J	308	CLA	CAA-CBA-CGA-O1A
28	J	312	CLA	CAA-CBA-CGA-O1A
28	A	309	CLA	CAA-CBA-CGA-O2A
28	a	729	CLA	CBD-CGD-O2D-CED
28	l	303	CLA	C2A-CAA-CBA-CGA
28	l	311	CLA	C2A-CAA-CBA-CGA
28	a	703	CLA	C2A-CAA-CBA-CGA
28	M	309	CLA	C2A-CAA-CBA-CGA
28	G	512	CLA	CAA-CBA-CGA-O2A
28	h	202	CLA	CAA-CBA-CGA-O2A
28	a	703	CLA	CAA-CBA-CGA-O2A
28	b	705	CLA	CAA-CBA-CGA-O2A
28	b	706	CLA	CAA-CBA-CGA-O2A
28	b	716	CLA	CAA-CBA-CGA-O2A
28	b	725	CLA	CAA-CBA-CGA-O2A
28	K	309	CLA	CAA-CBA-CGA-O1A
28	l	313	CLA	C4-C3-C5-C6
30	y	201	DGD	C2B-C3B-C4B-C5B
28	l	304	CLA	C6-C7-C8-C10
28	a	717	CLA	C2-C3-C5-C6
28	a	721	CLA	C11-C12-C13-C15
28	a	725	CLA	C6-C7-C8-C10
28	J	307	CLA	C12-C13-C15-C16
28	N	309	CLA	C3A-C2A-CAA-CBA
28	K	308	CLA	CAA-CBA-CGA-O1A
28	I	309	CLA	CAA-CBA-CGA-O2A
28	I	306	CLA	O2A-C1-C2-C3
28	J	311	CLA	C2-C1-O2A-CGA
35	l	302	BCR	C21-C22-C23-C24
28	b	725	CLA	CAA-CBA-CGA-O1A
28	G	518	CLA	CAA-CBA-CGA-O2A
28	j	104	CLA	CAA-CBA-CGA-O2A
28	b	715	CLA	CAA-CBA-CGA-O2A
28	N	307	CLA	CAA-CBA-CGA-O2A
28	b	715	CLA	C8-C10-C11-C12
28	M	315	CLA	C2C-C3C-CAC-CBC
28	G	512	CLA	CAA-CBA-CGA-O1A
28	a	703	CLA	CAA-CBA-CGA-O1A
28	j	106	CLA	CBA-CGA-O2A-C1
28	N	310	CLA	C2-C1-O2A-CGA
31	K	318	LMG	C16-C17-C18-C19
28	a	731	CLA	CAA-CBA-CGA-O2A

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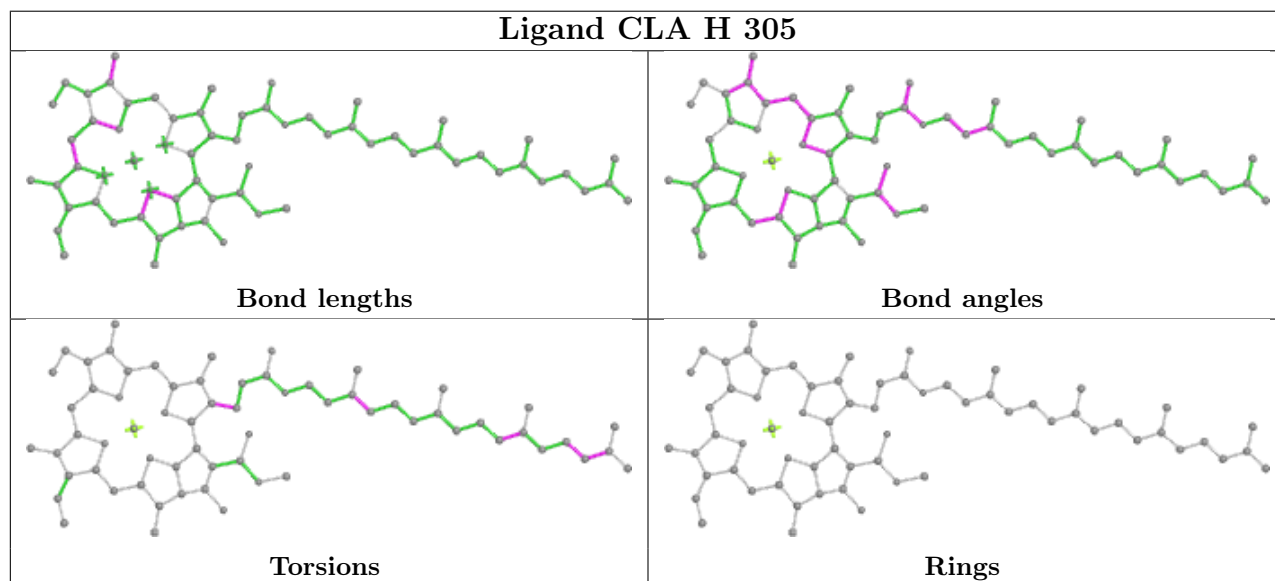
Mol	Chain	Res	Type	Atoms
28	b	721	CLA	CAA-CBA-CGA-O2A
28	H	307	CLA	CAA-CBA-CGA-O2A
30	L	301	DGD	O2G-C1B-C2B-C3B
28	A	309	CLA	CAA-CBA-CGA-O1A
28	b	705	CLA	CAA-CBA-CGA-O1A
28	b	716	CLA	CAA-CBA-CGA-O1A

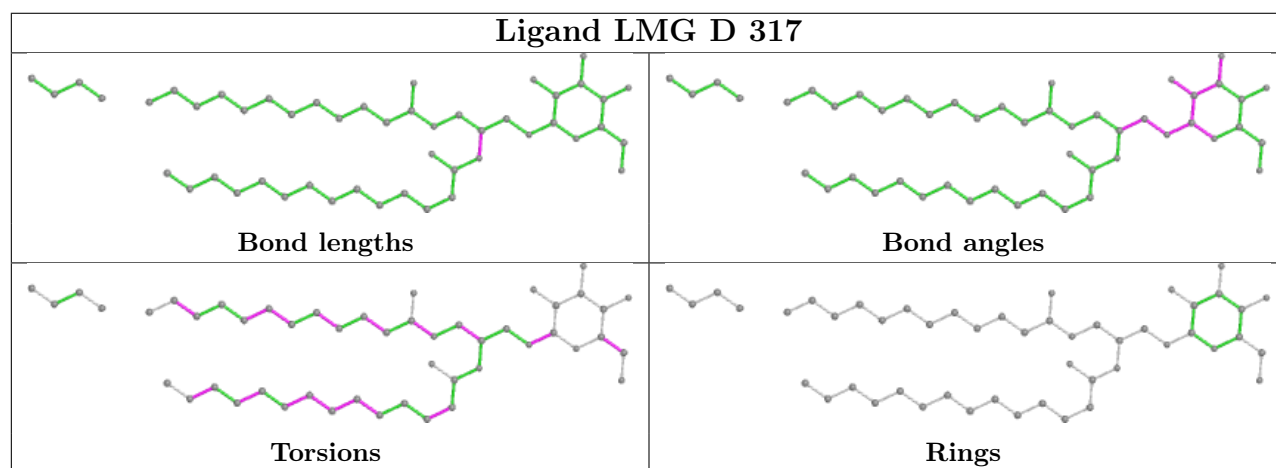
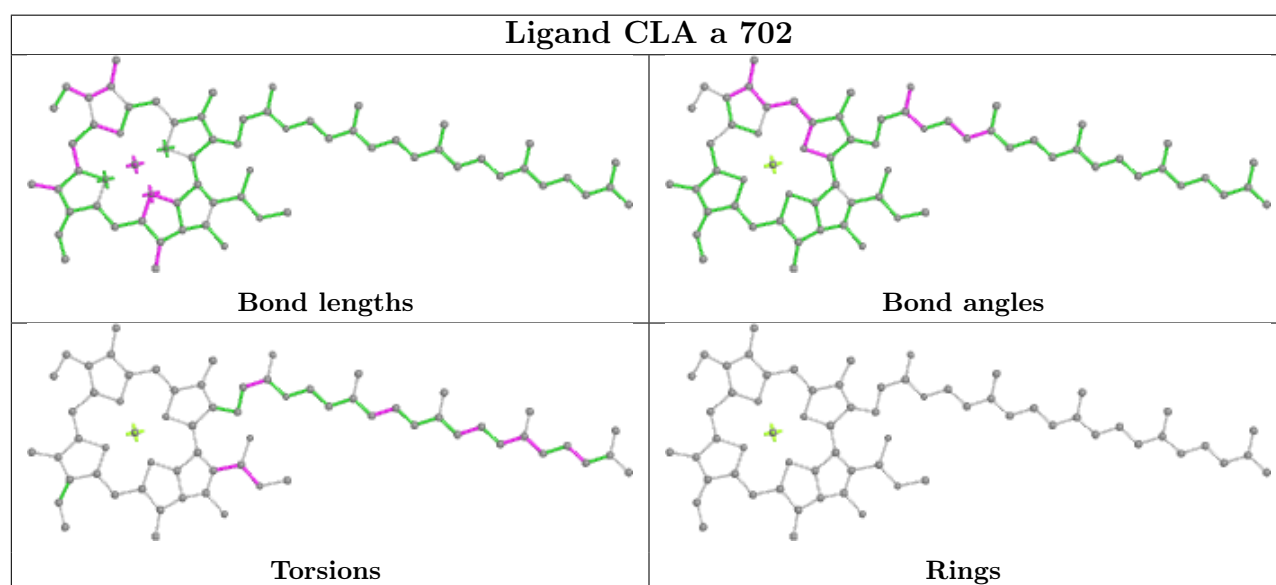
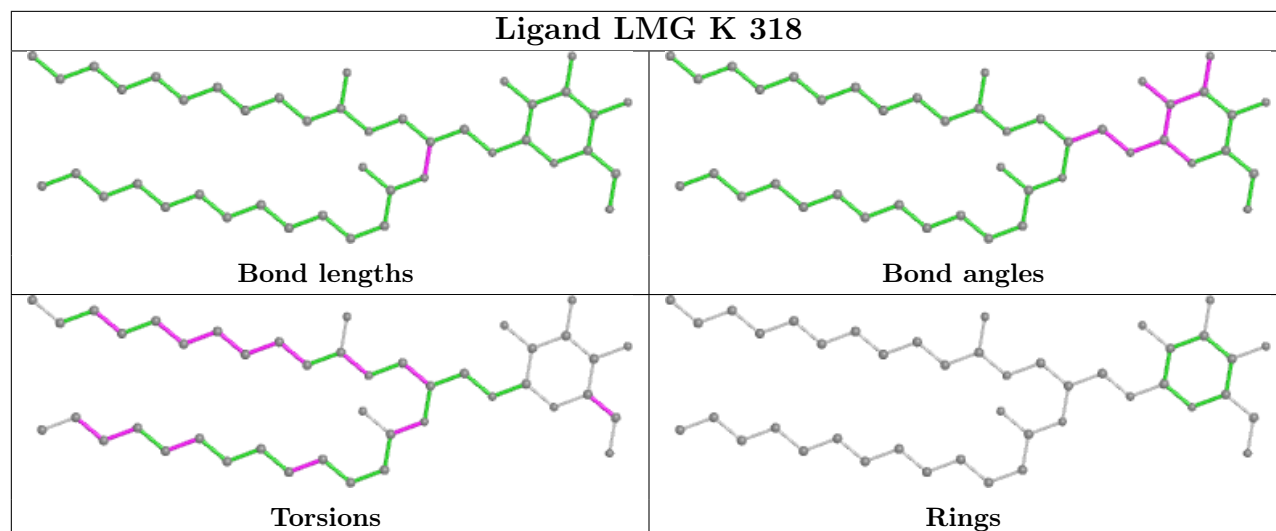
All (1) ring outliers are listed below:

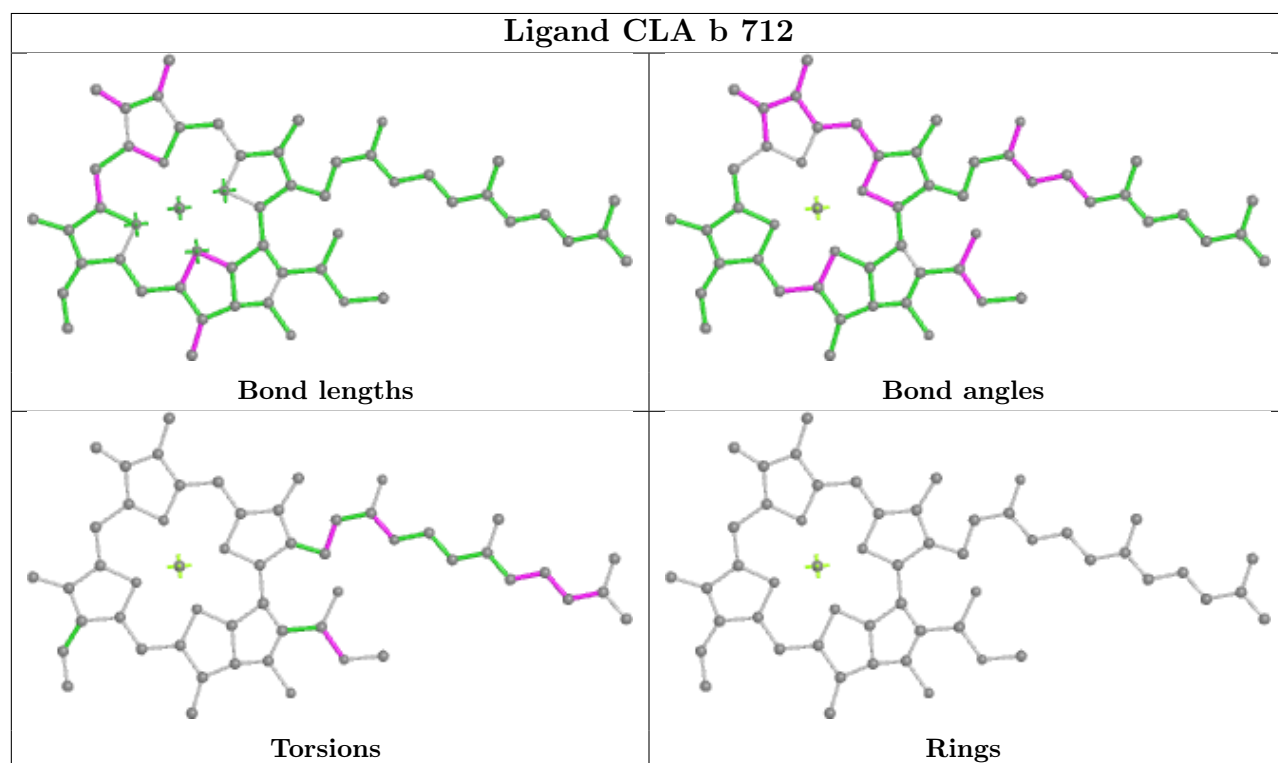
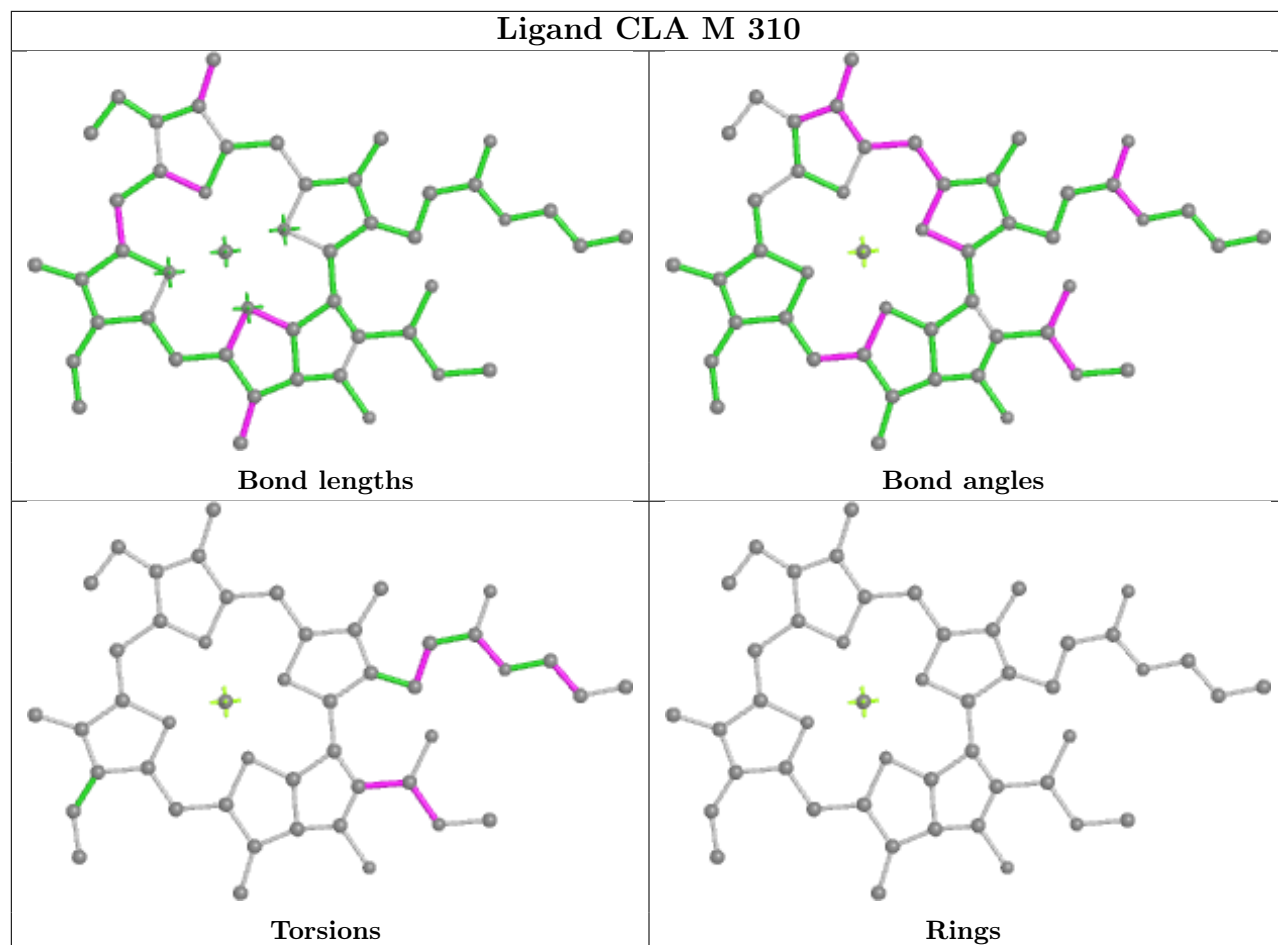
Mol	Chain	Res	Type	Atoms
32	G	507	PID	C24-C25-C26-C27-C28-C29

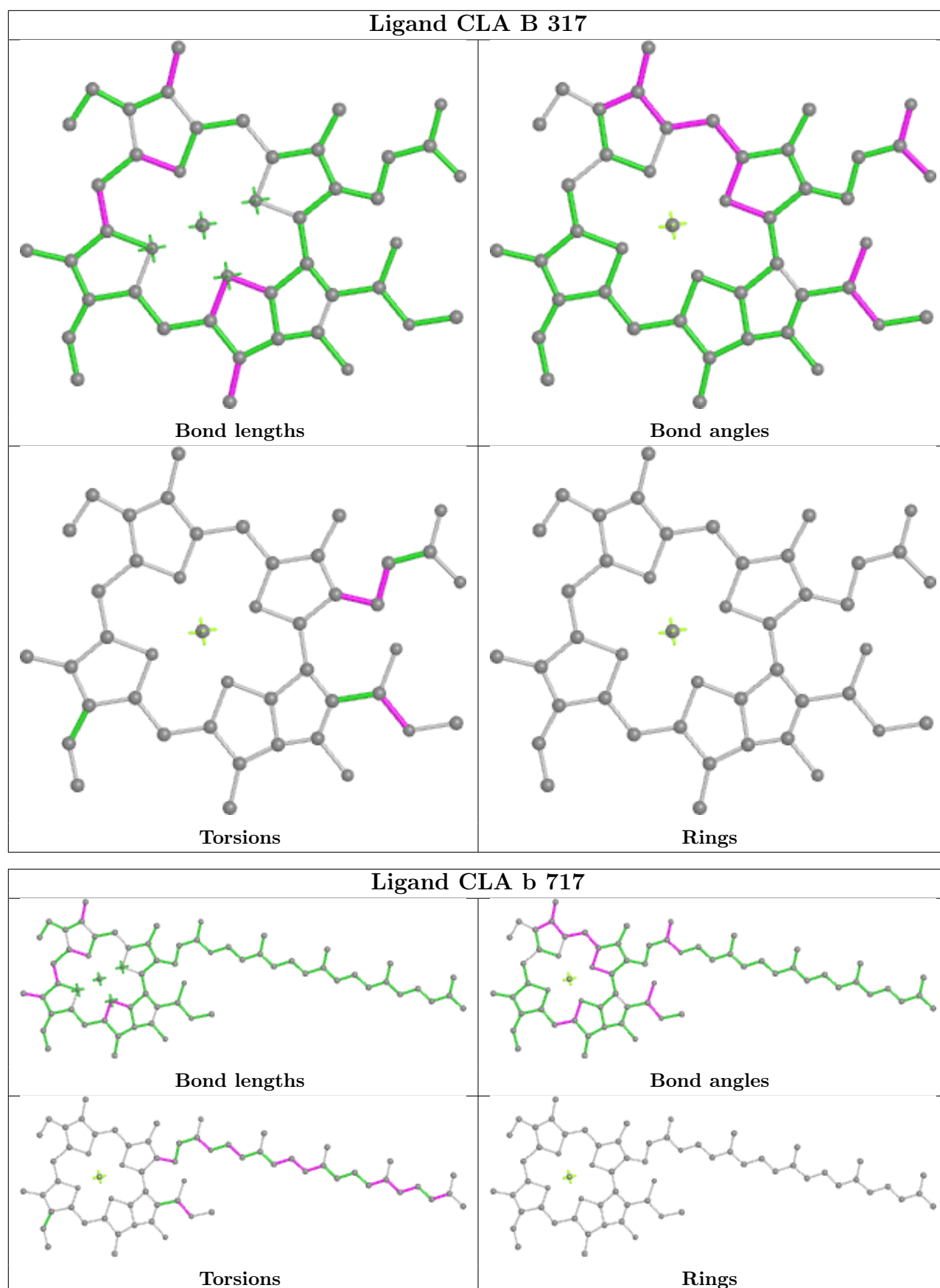
No monomer is involved in short contacts.

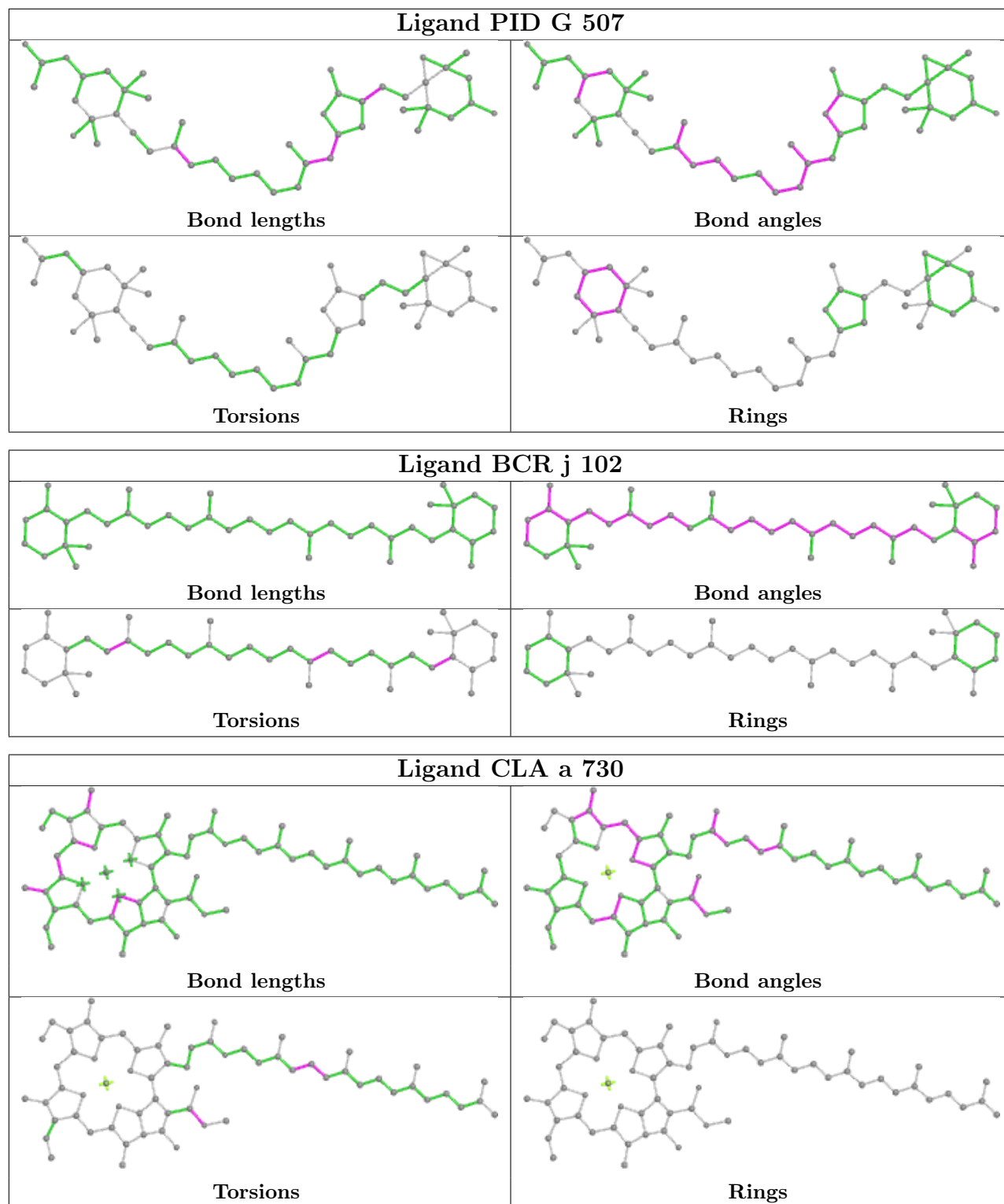
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

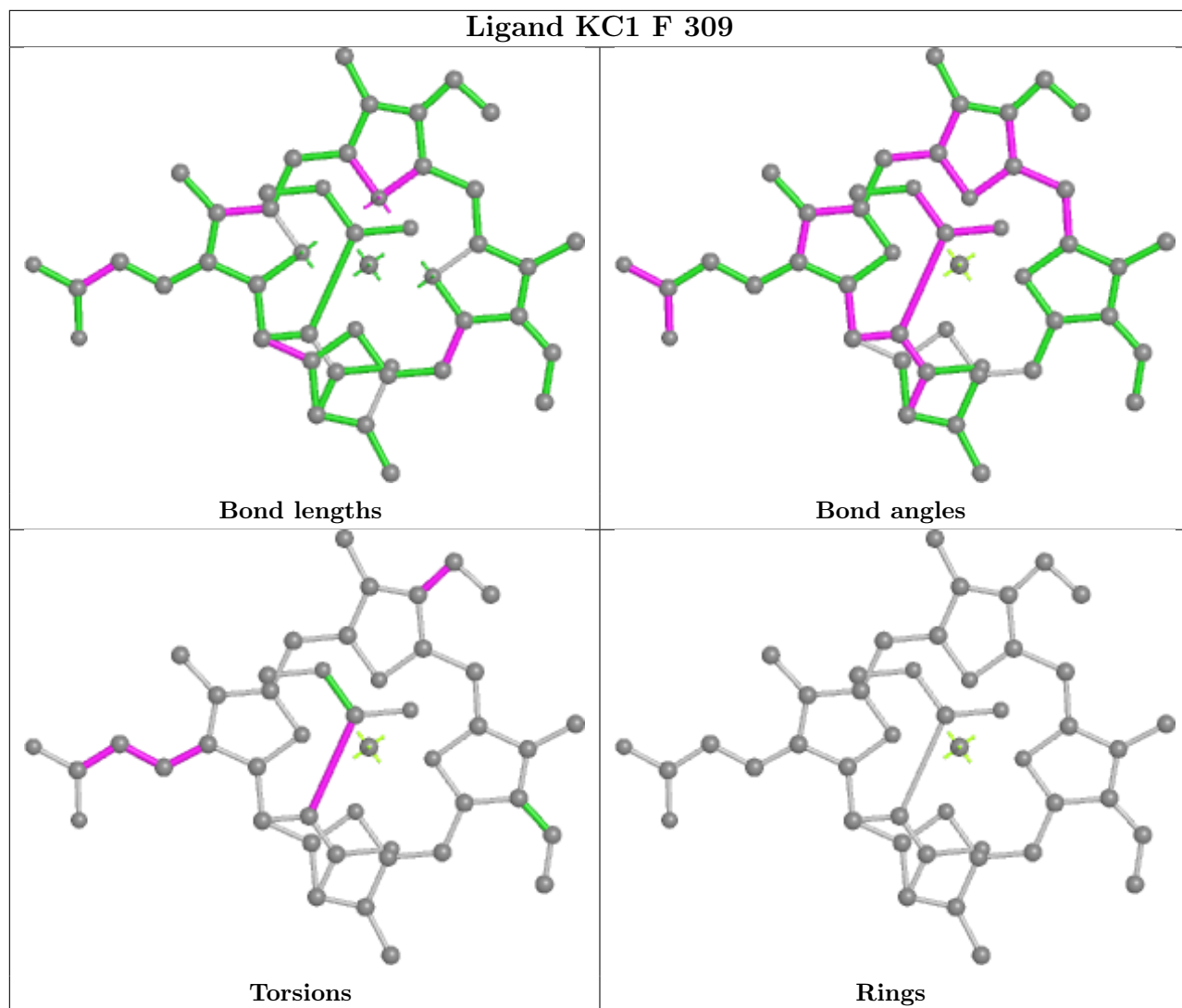


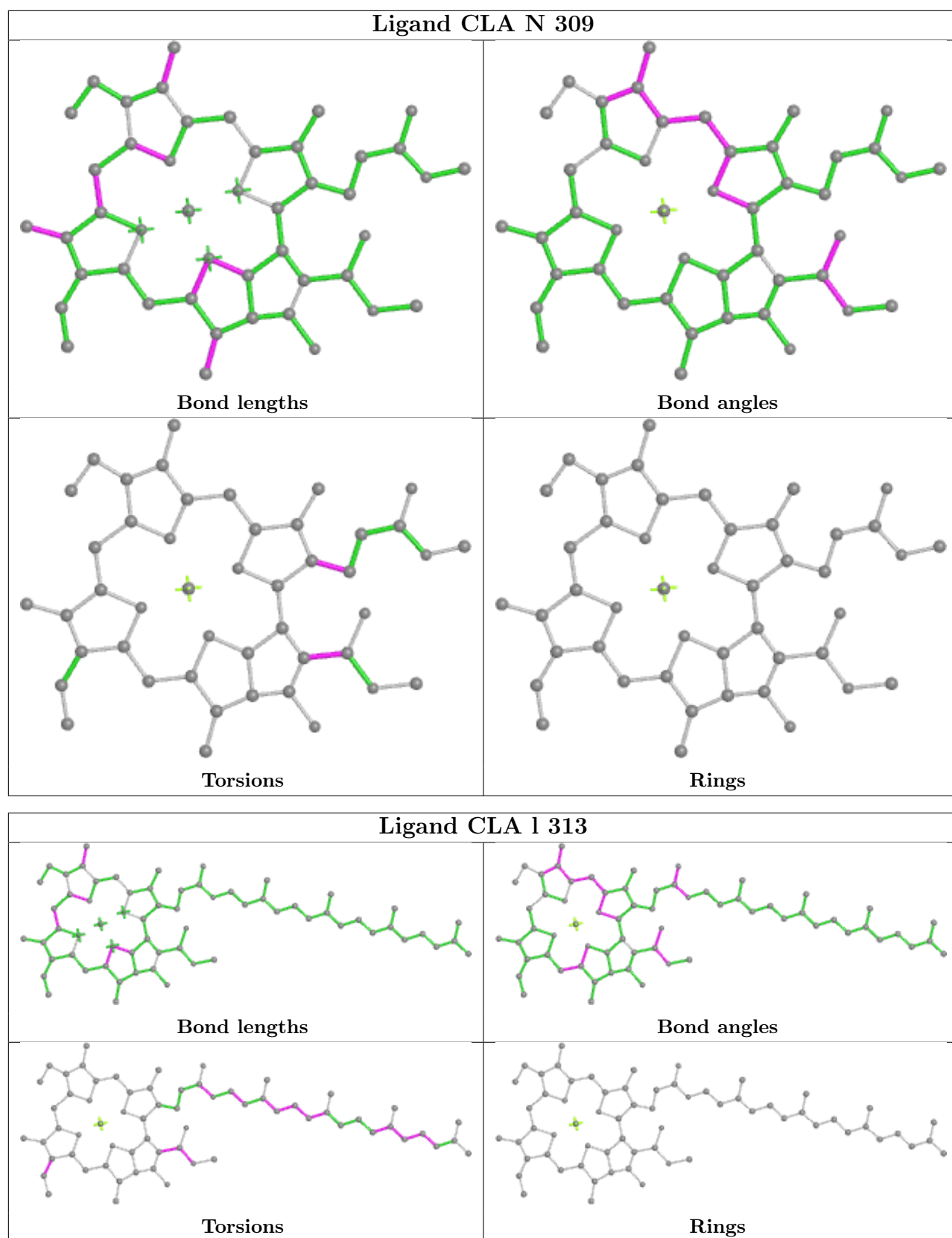


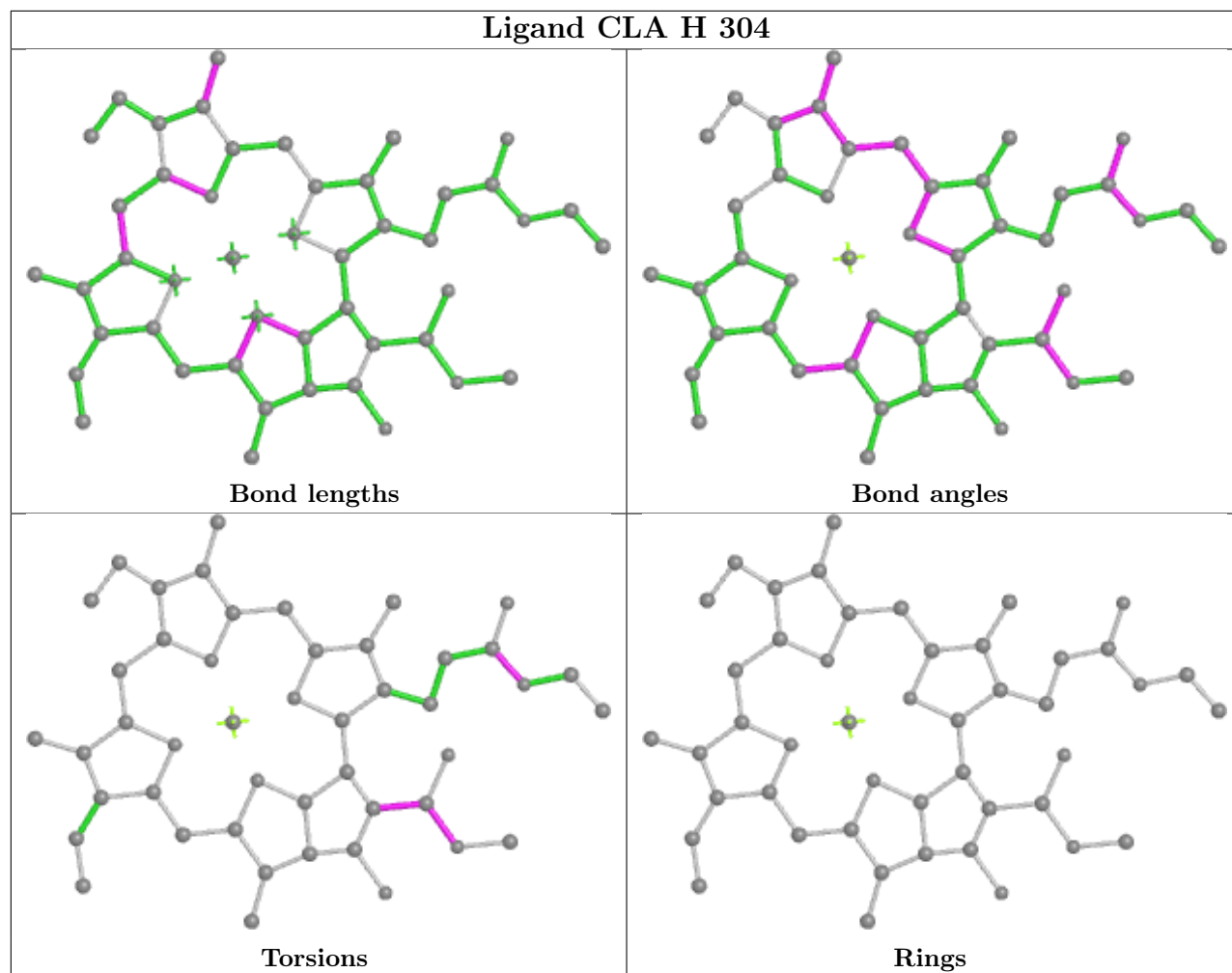


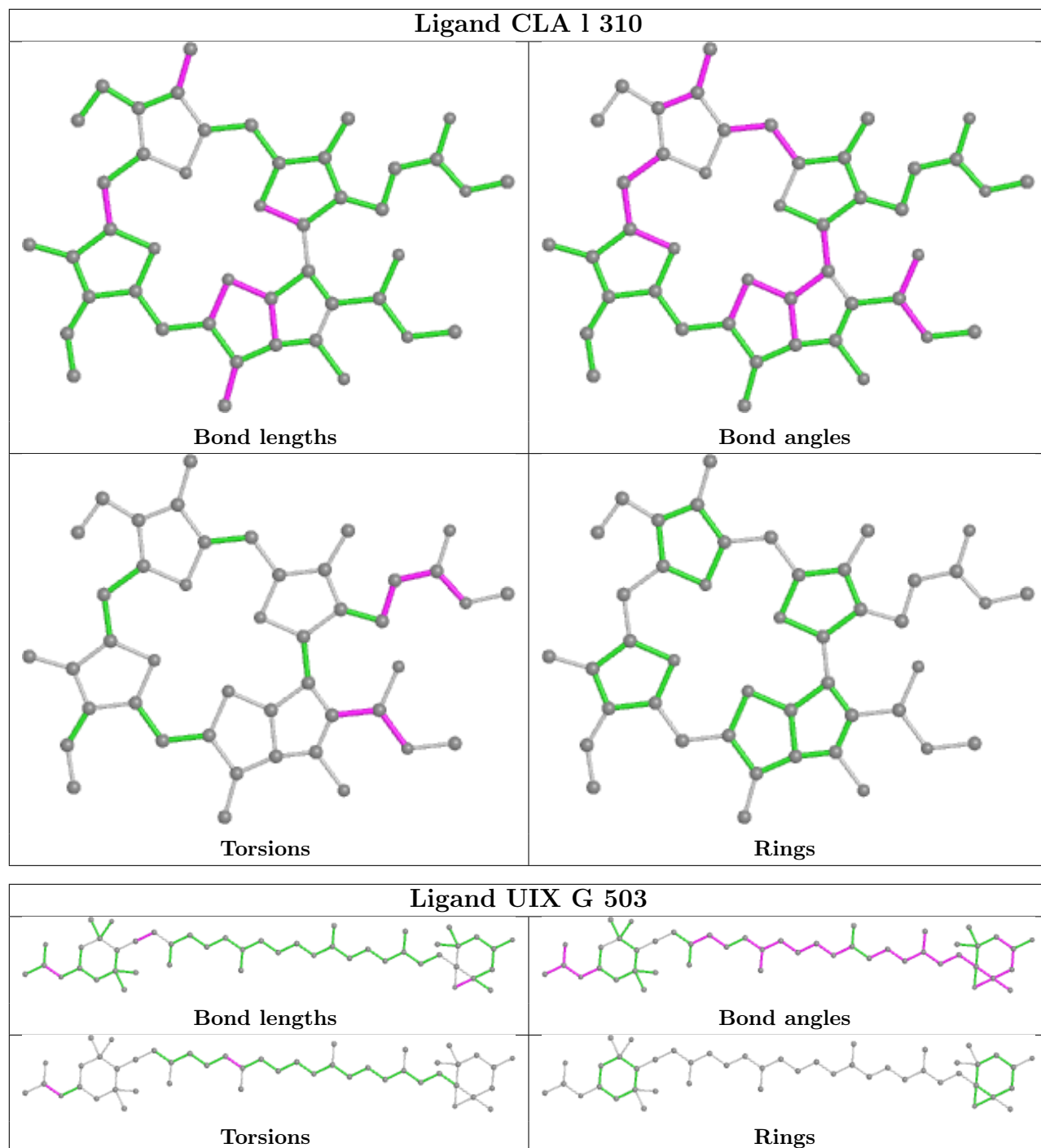


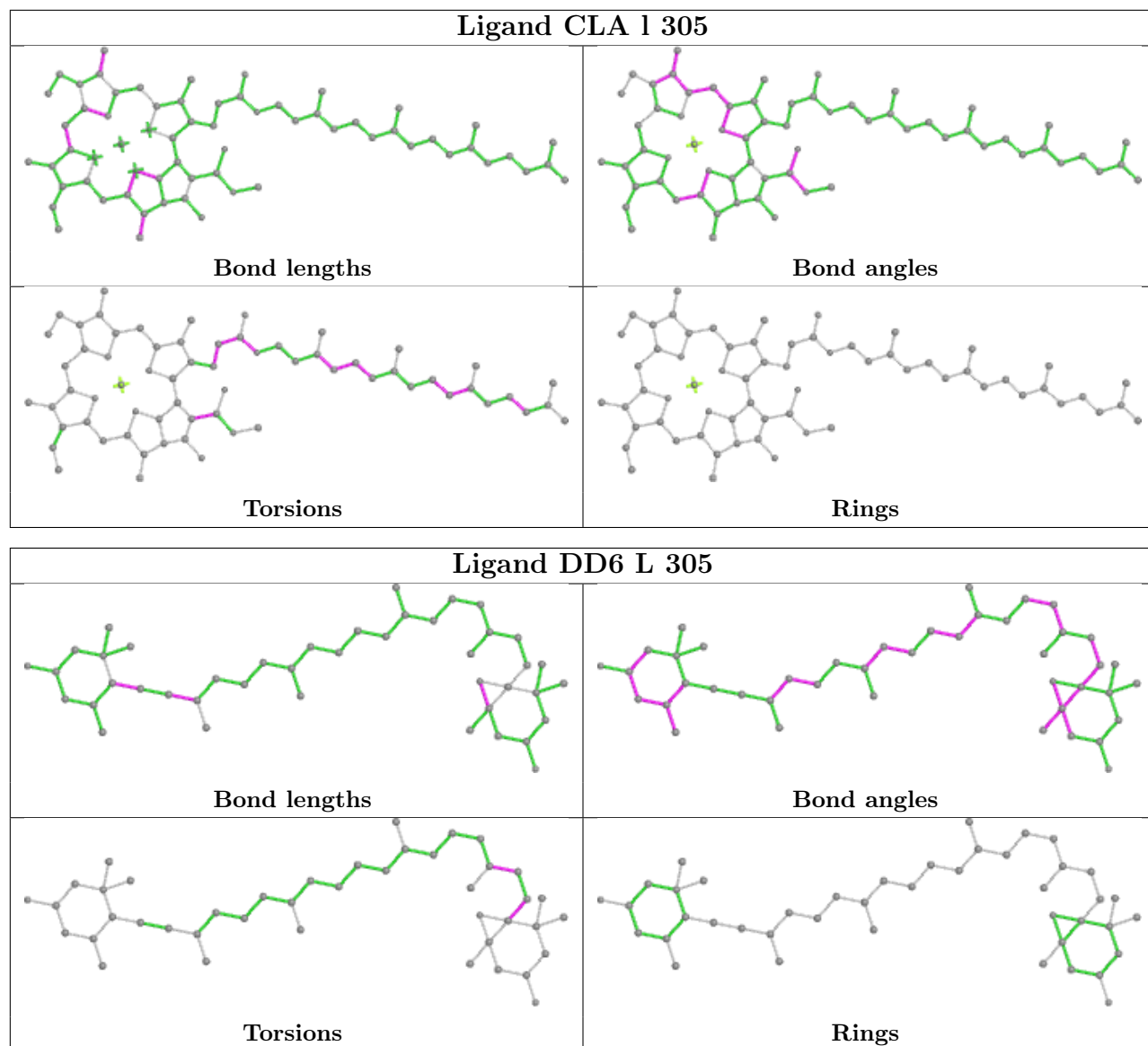


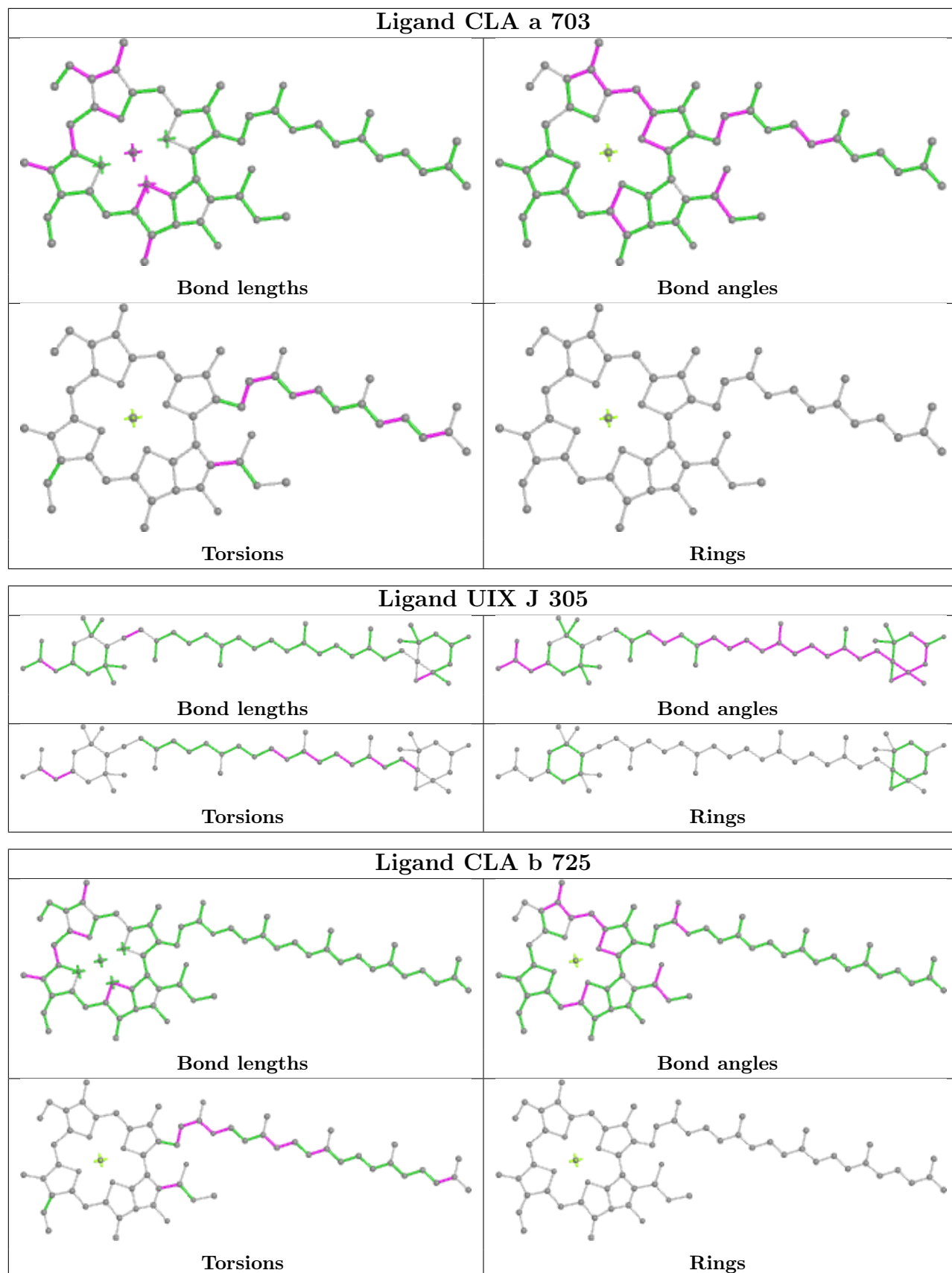


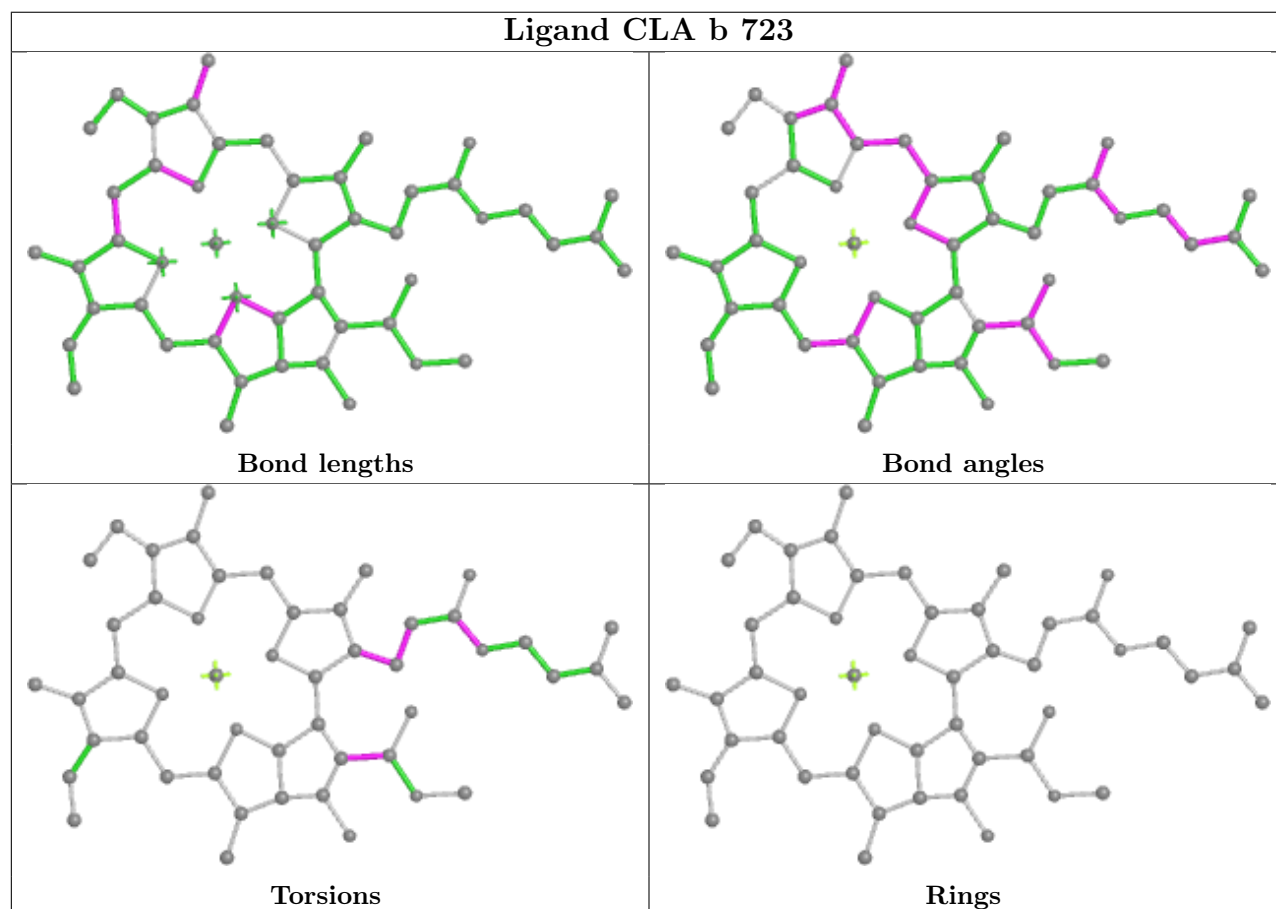
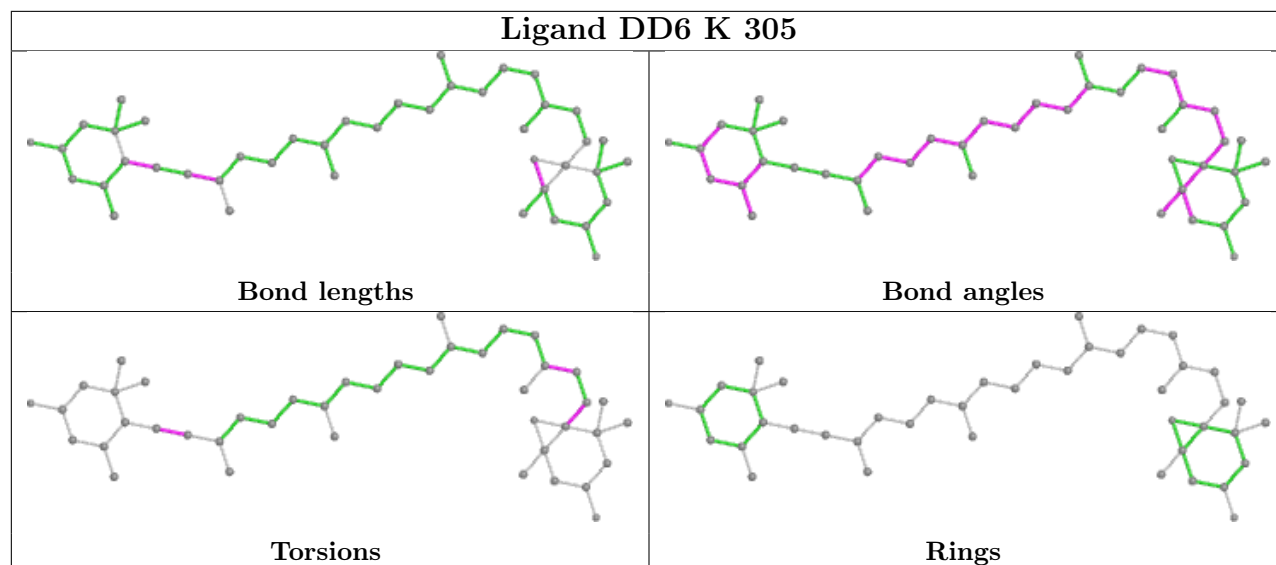


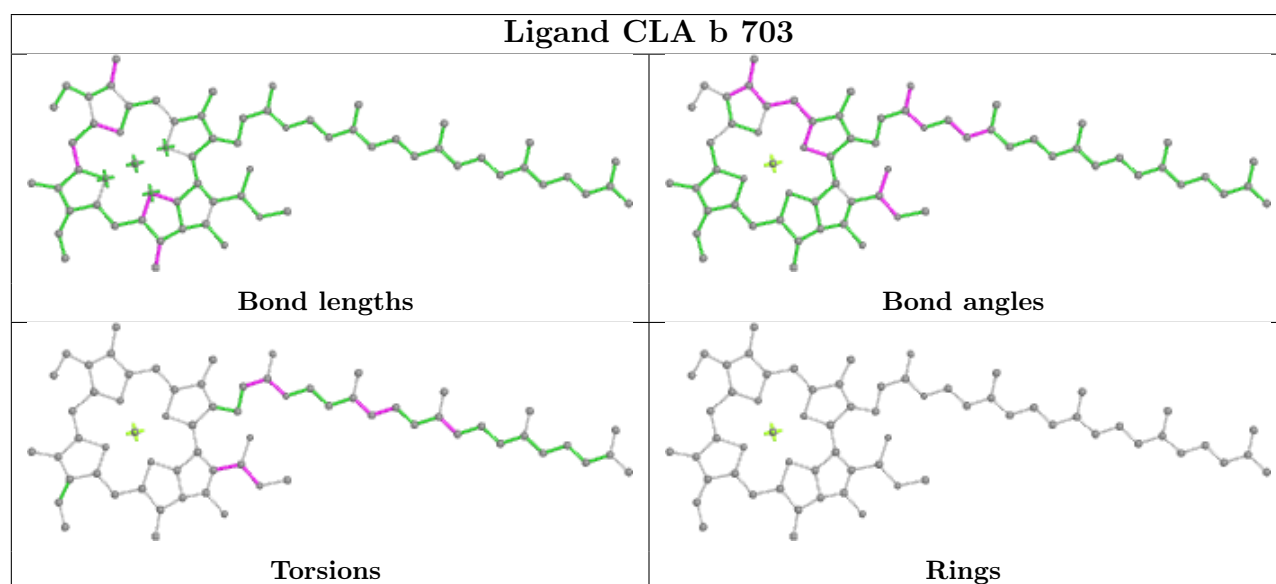
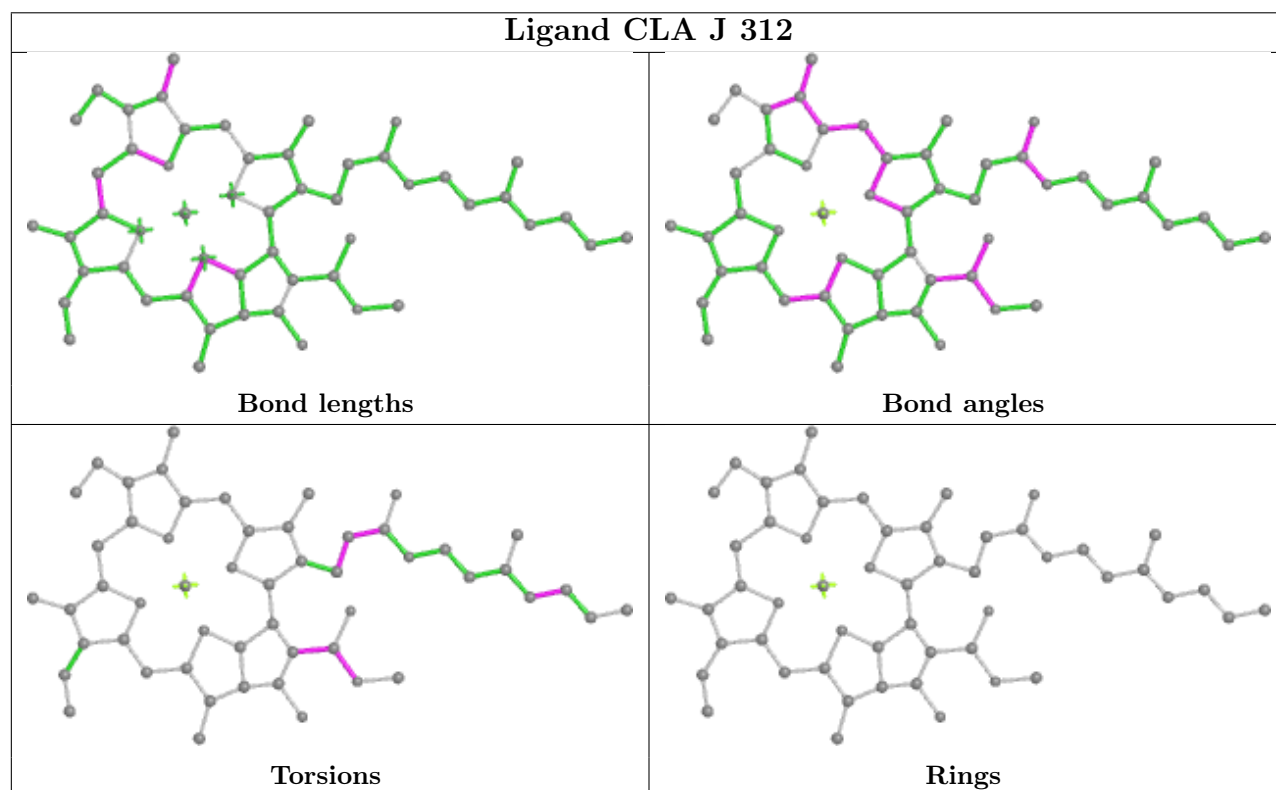
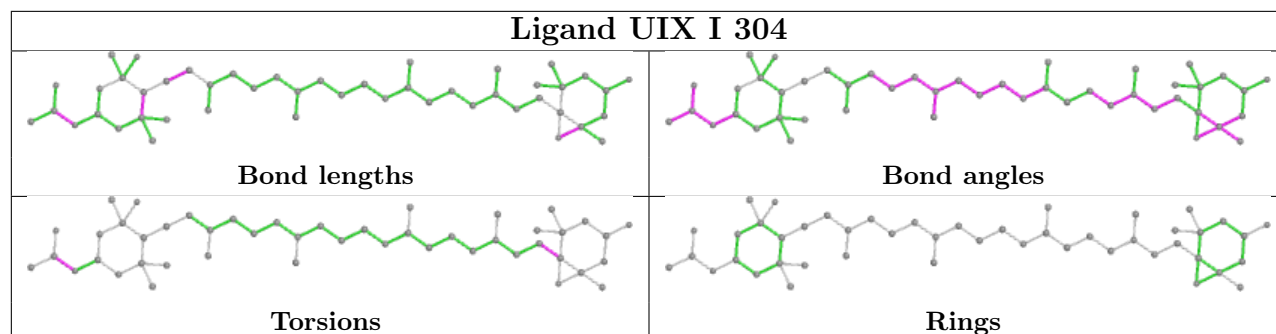


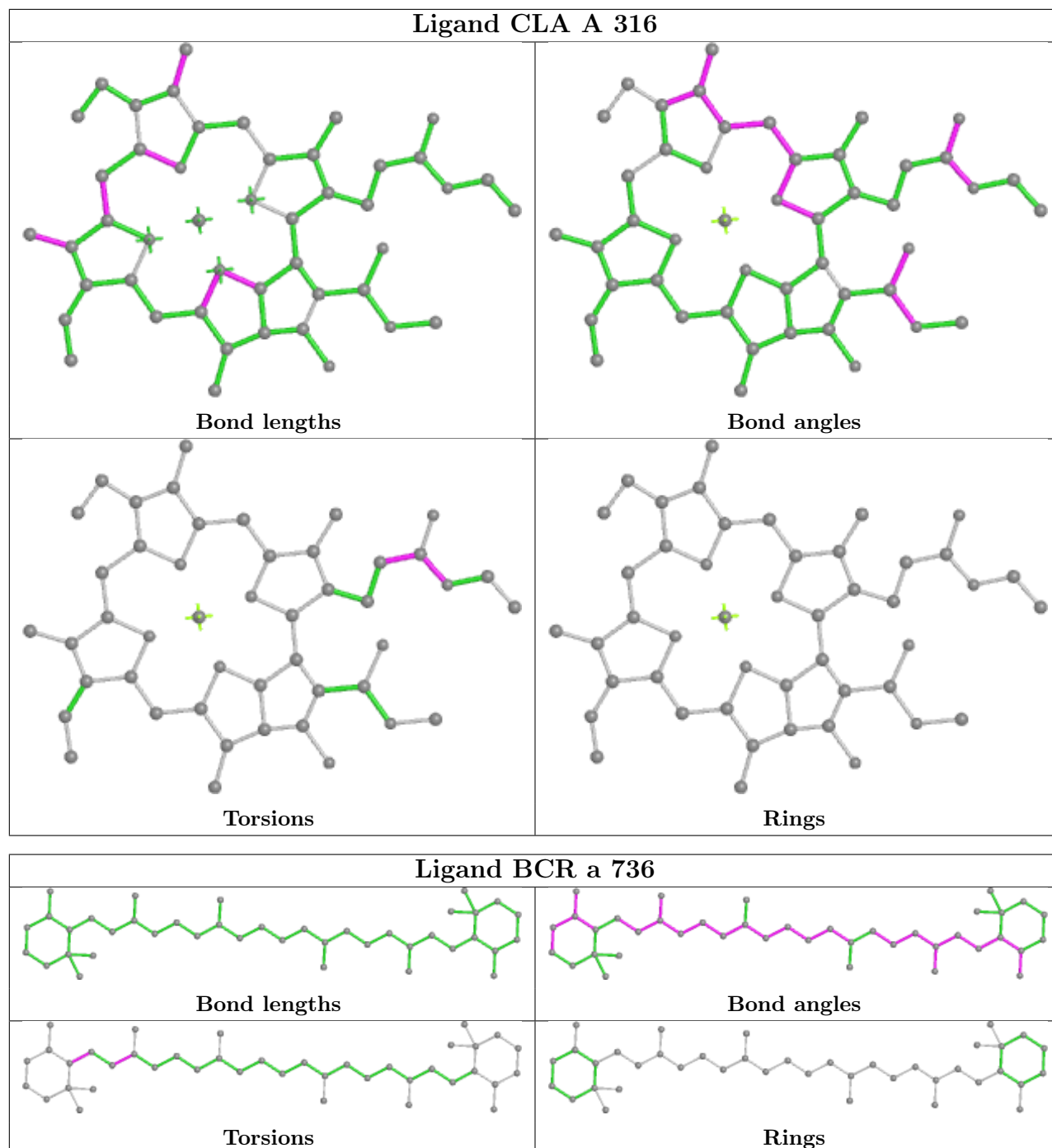


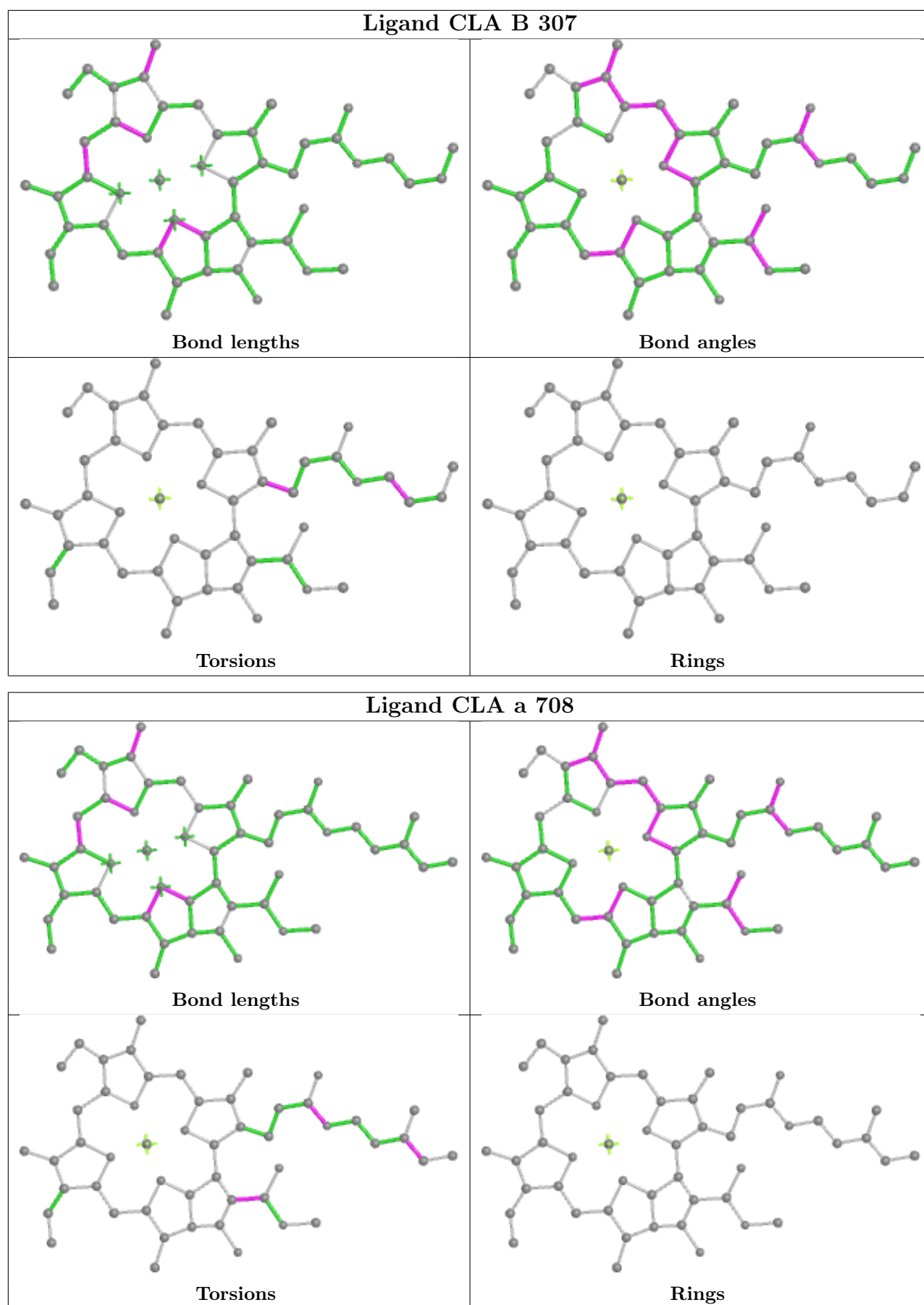


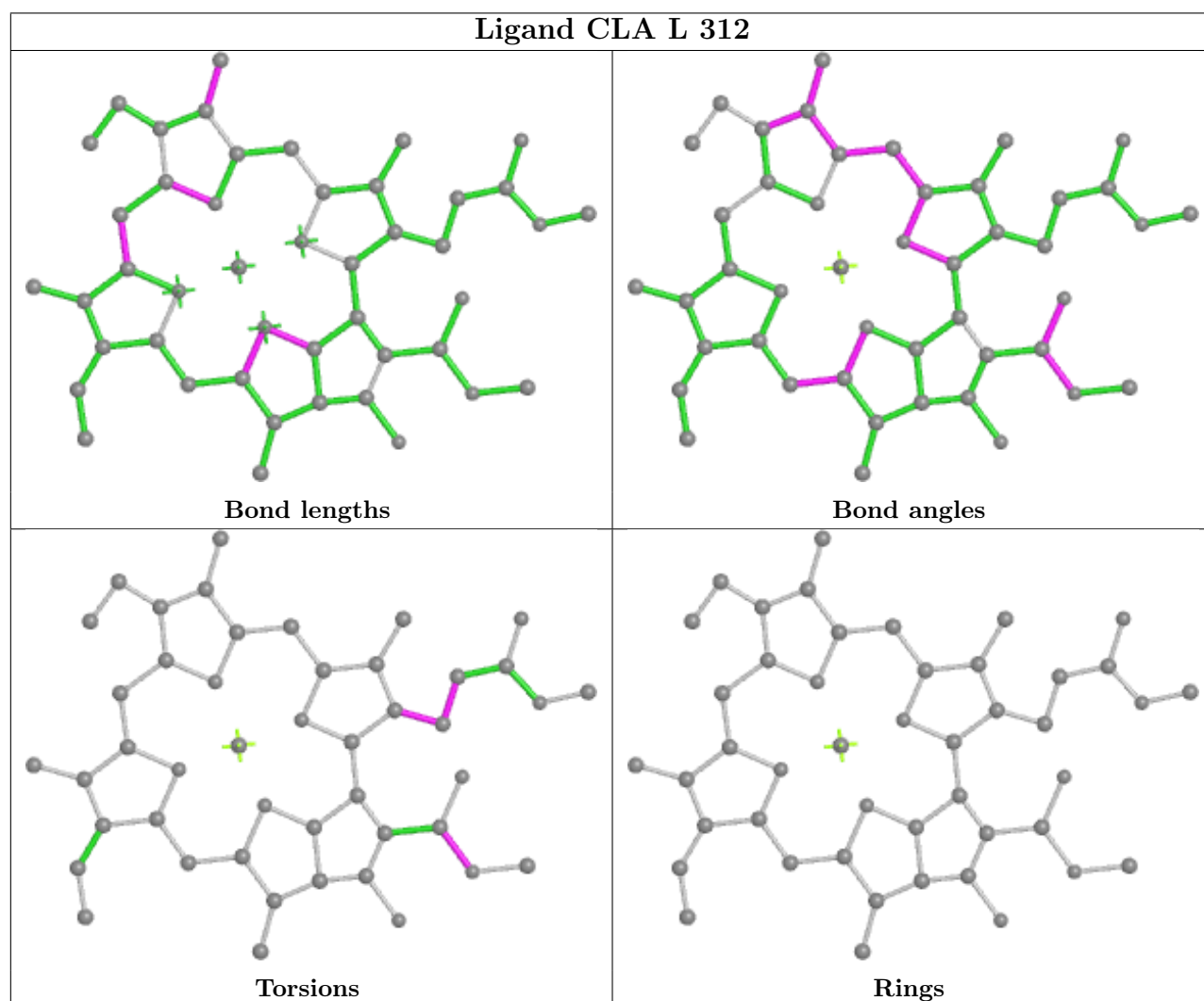
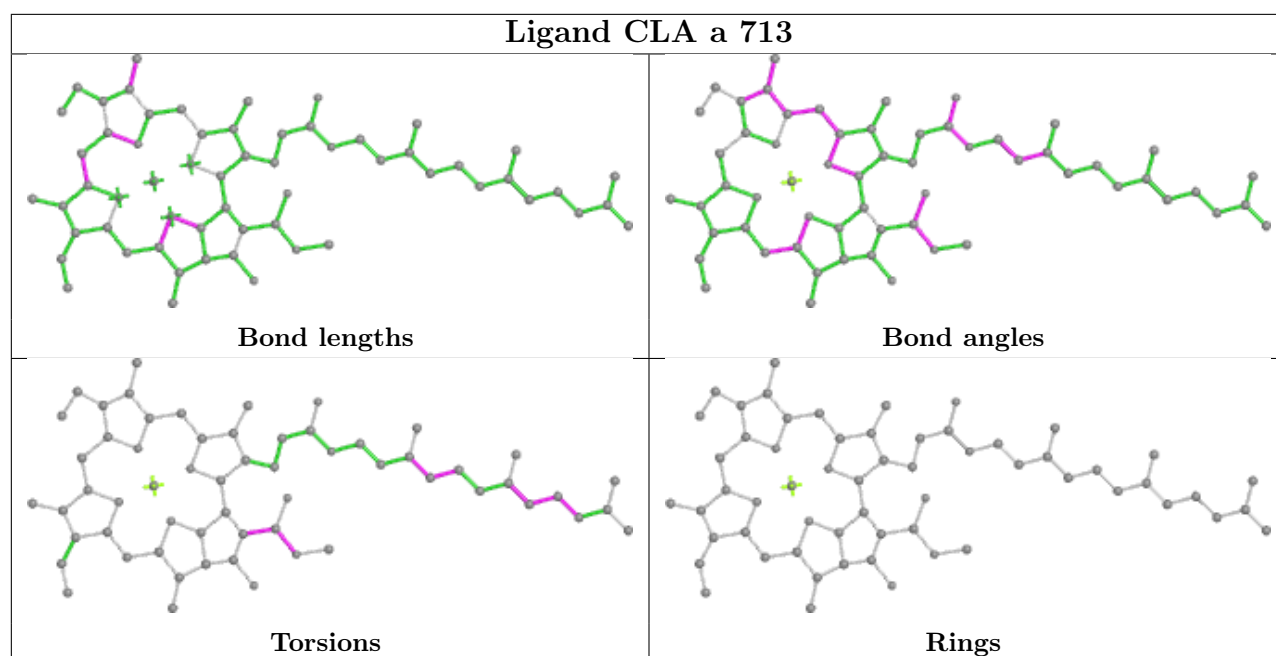


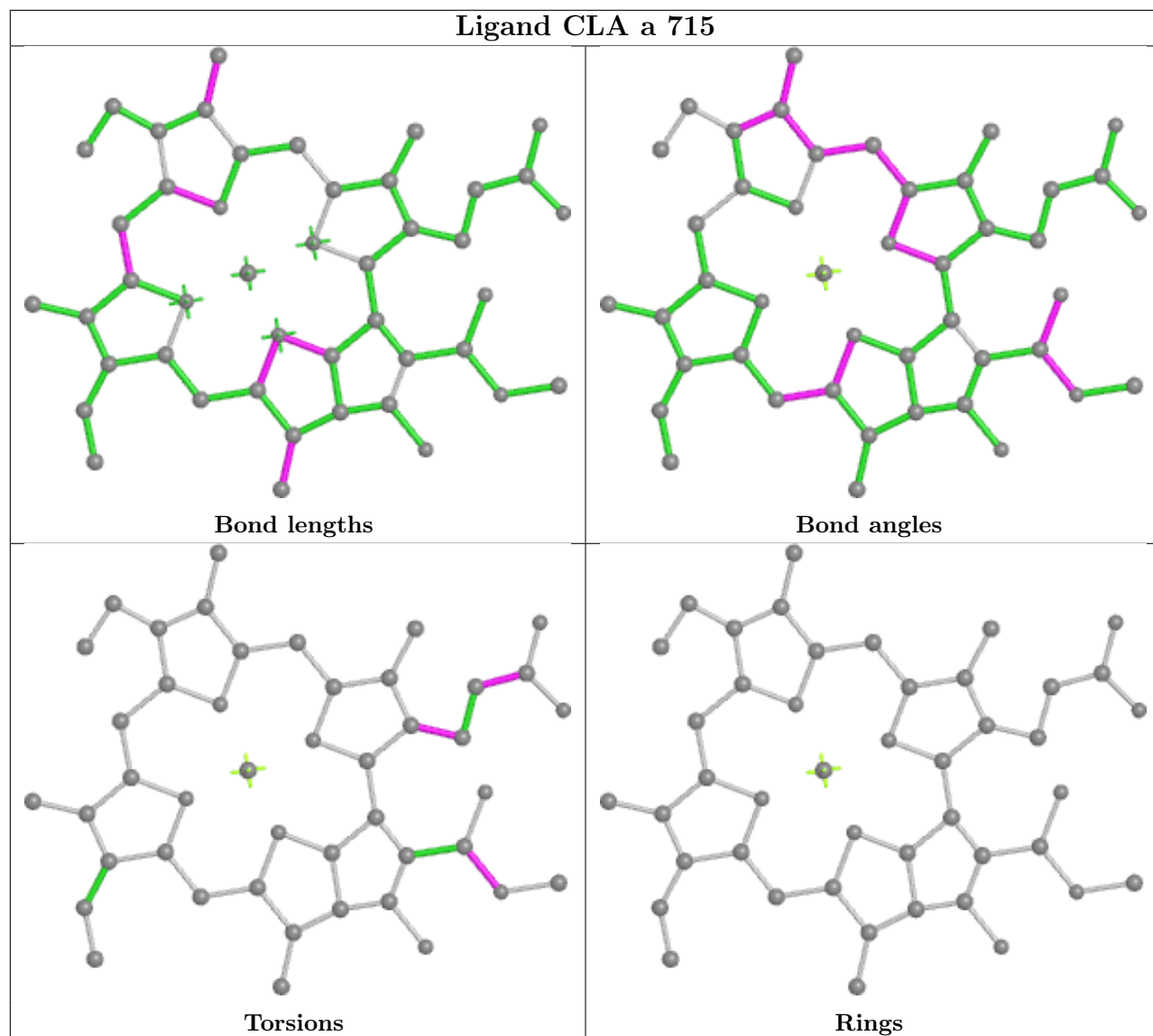


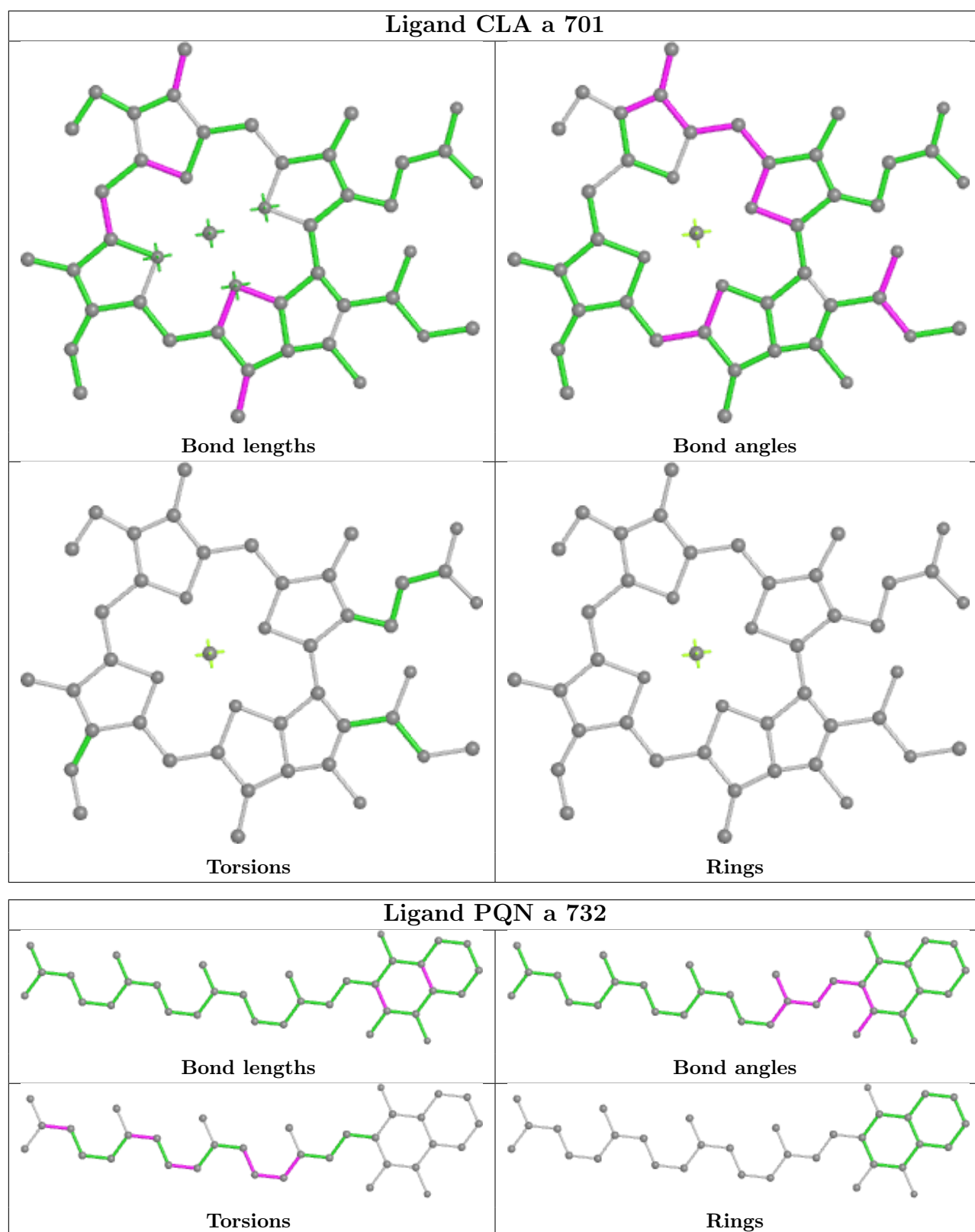


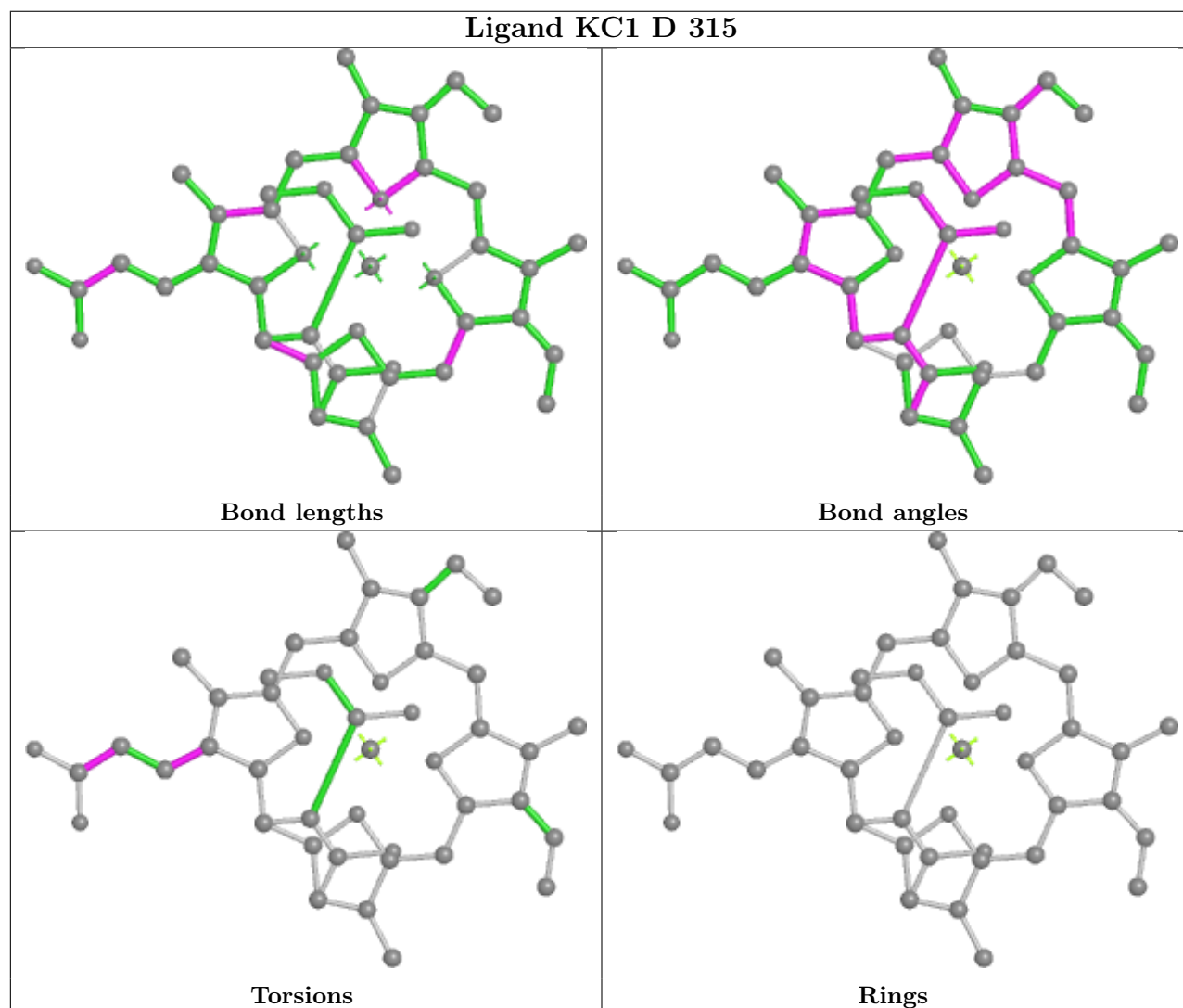
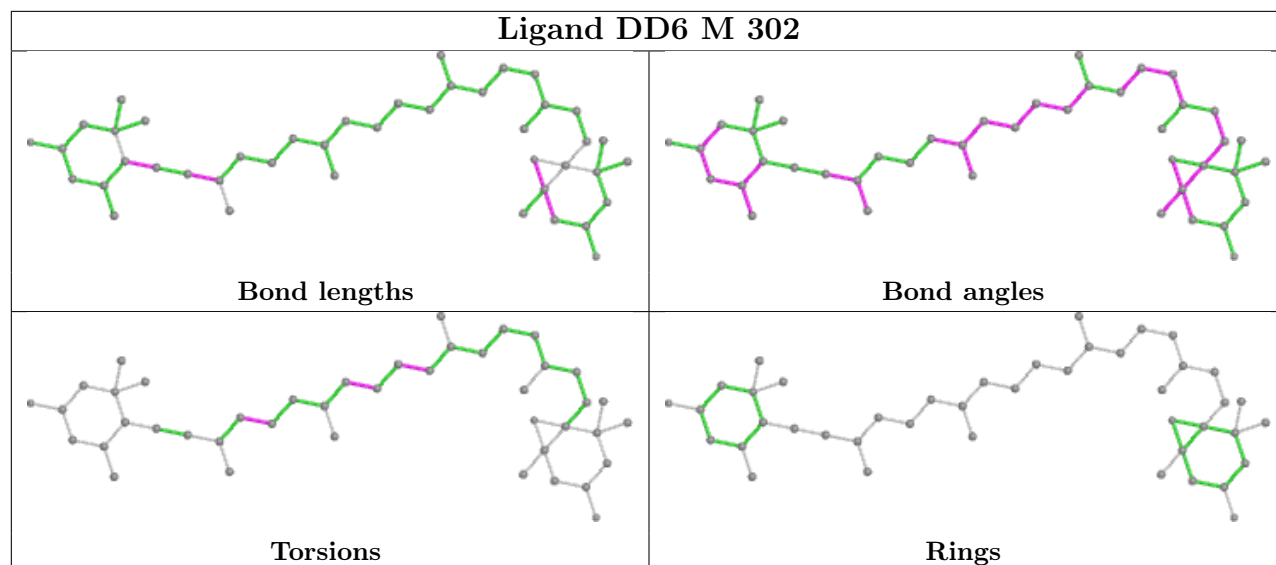


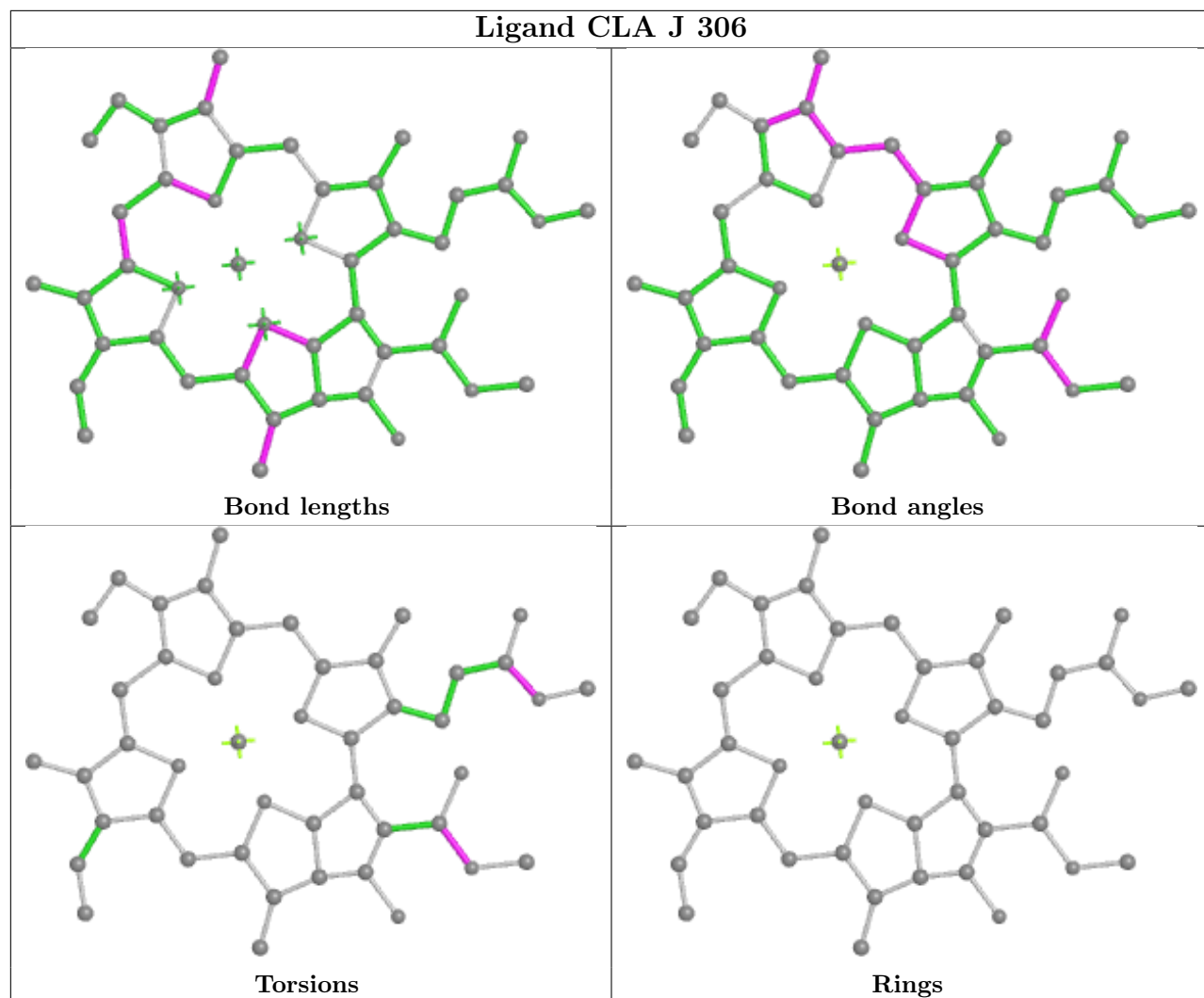


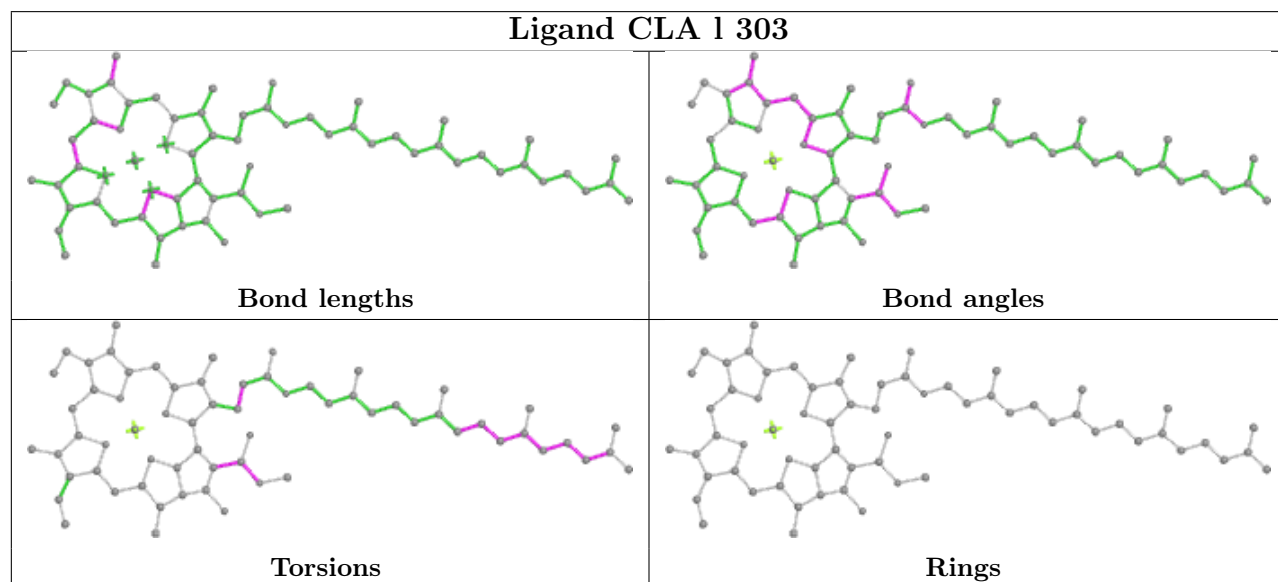
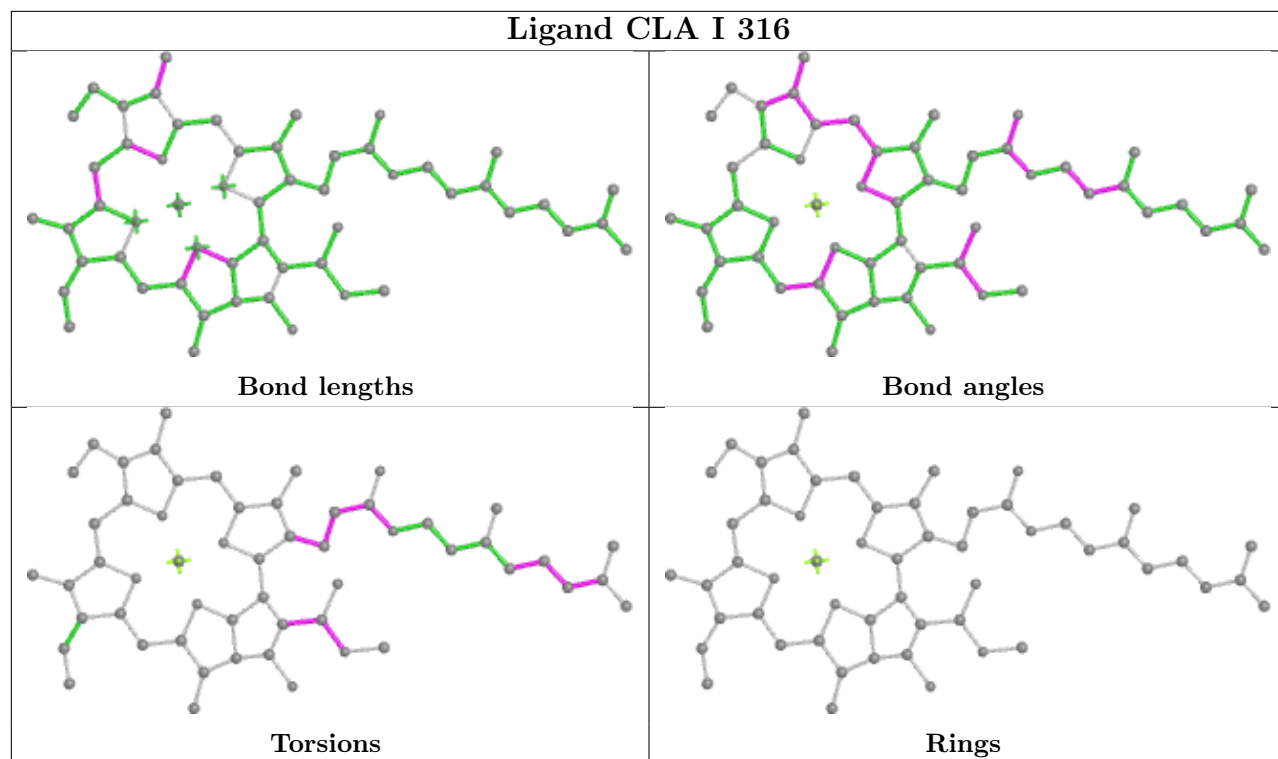


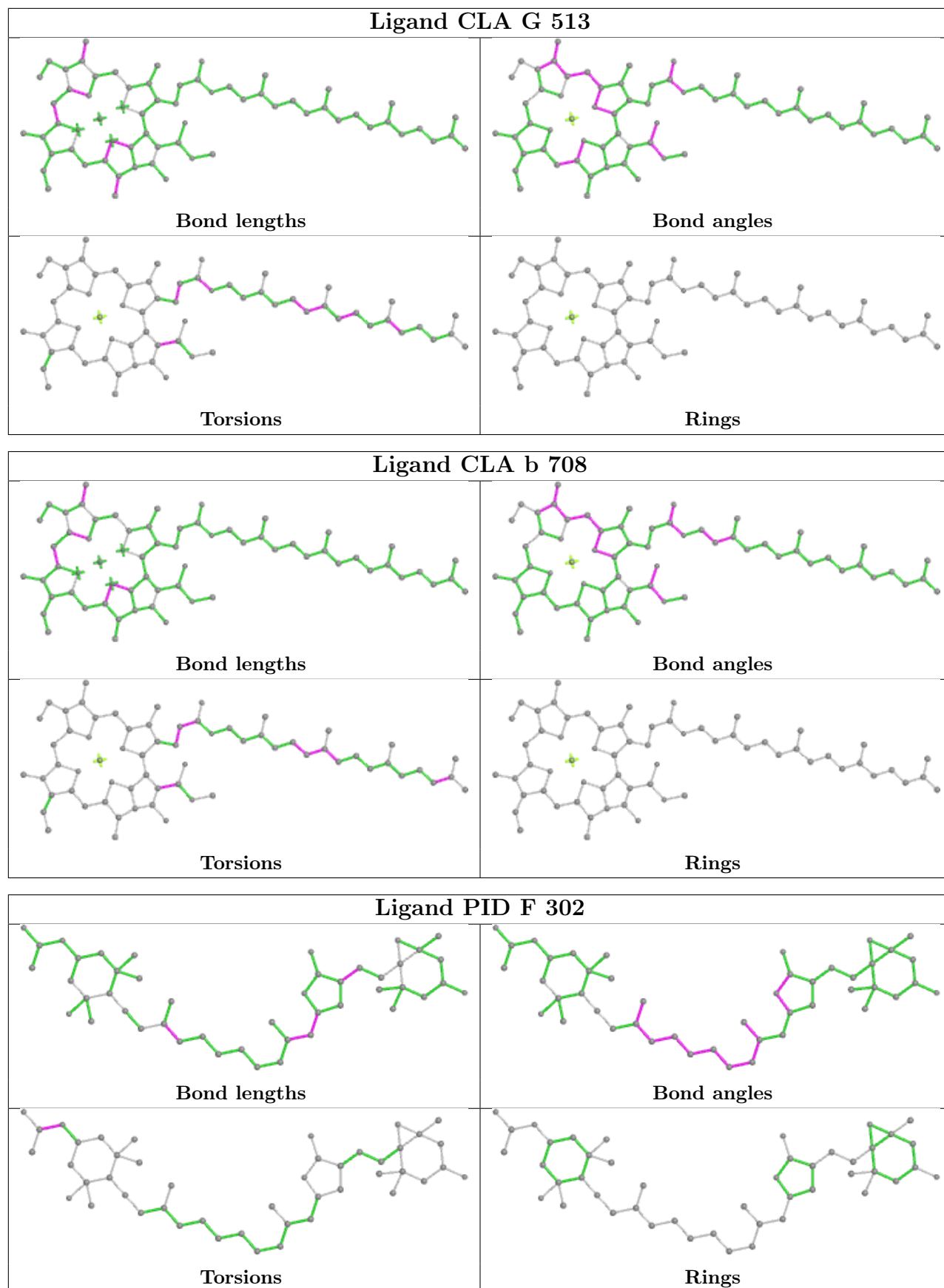


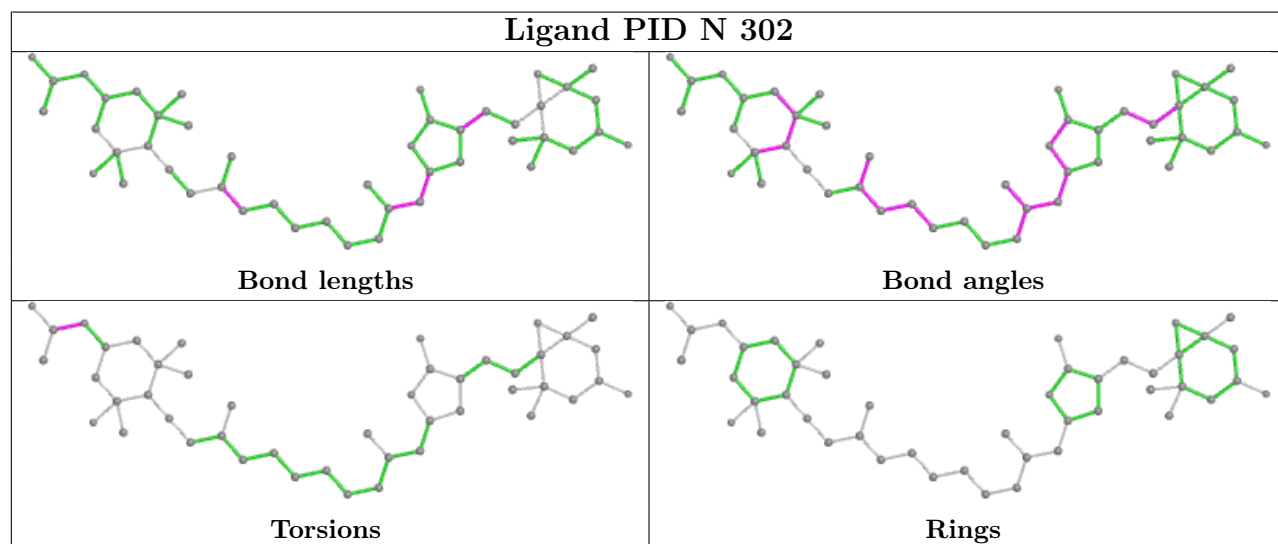
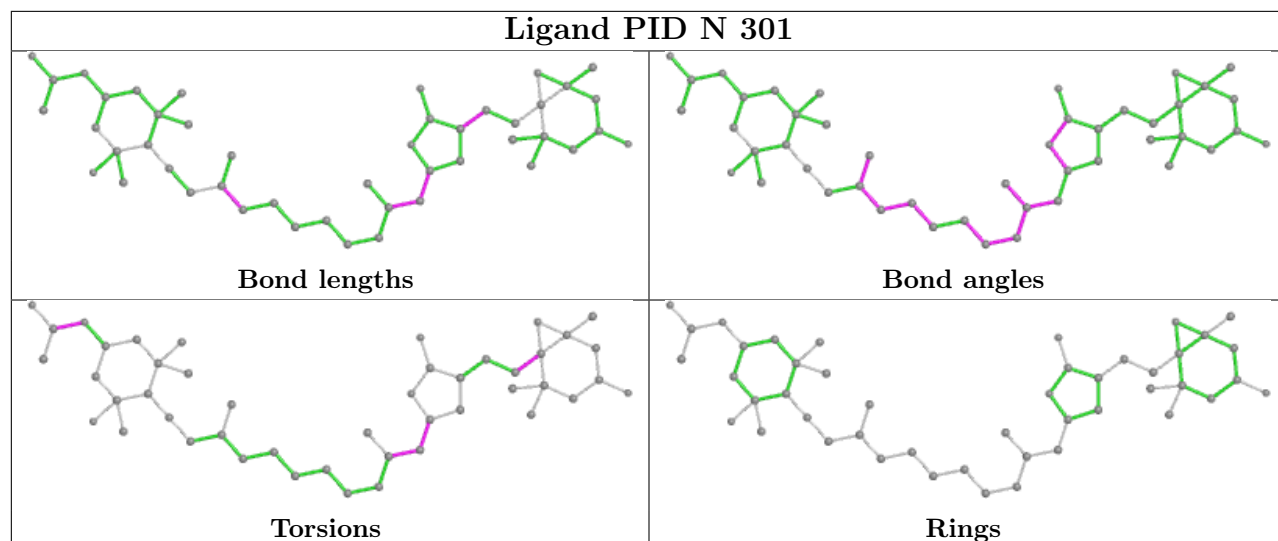


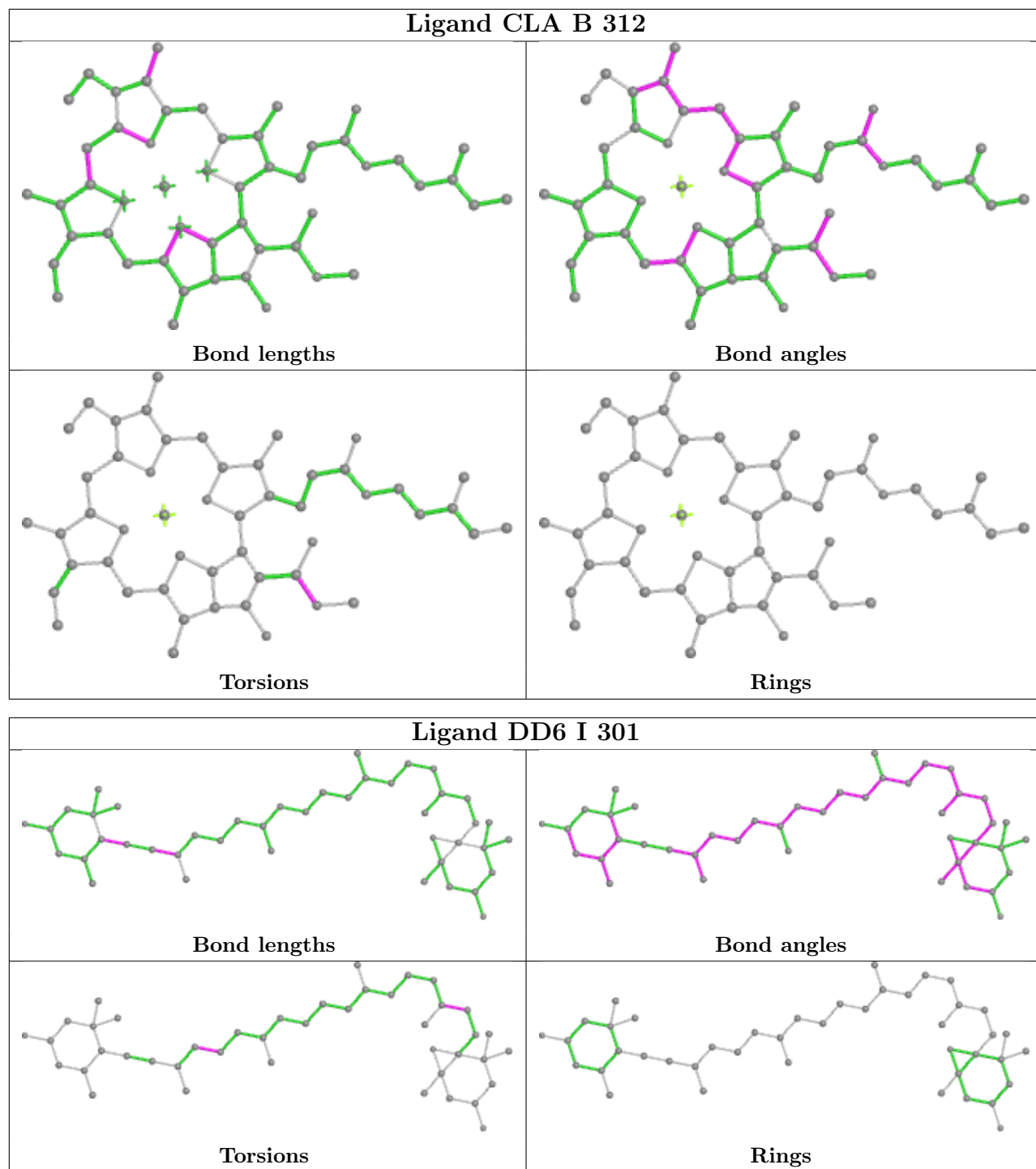


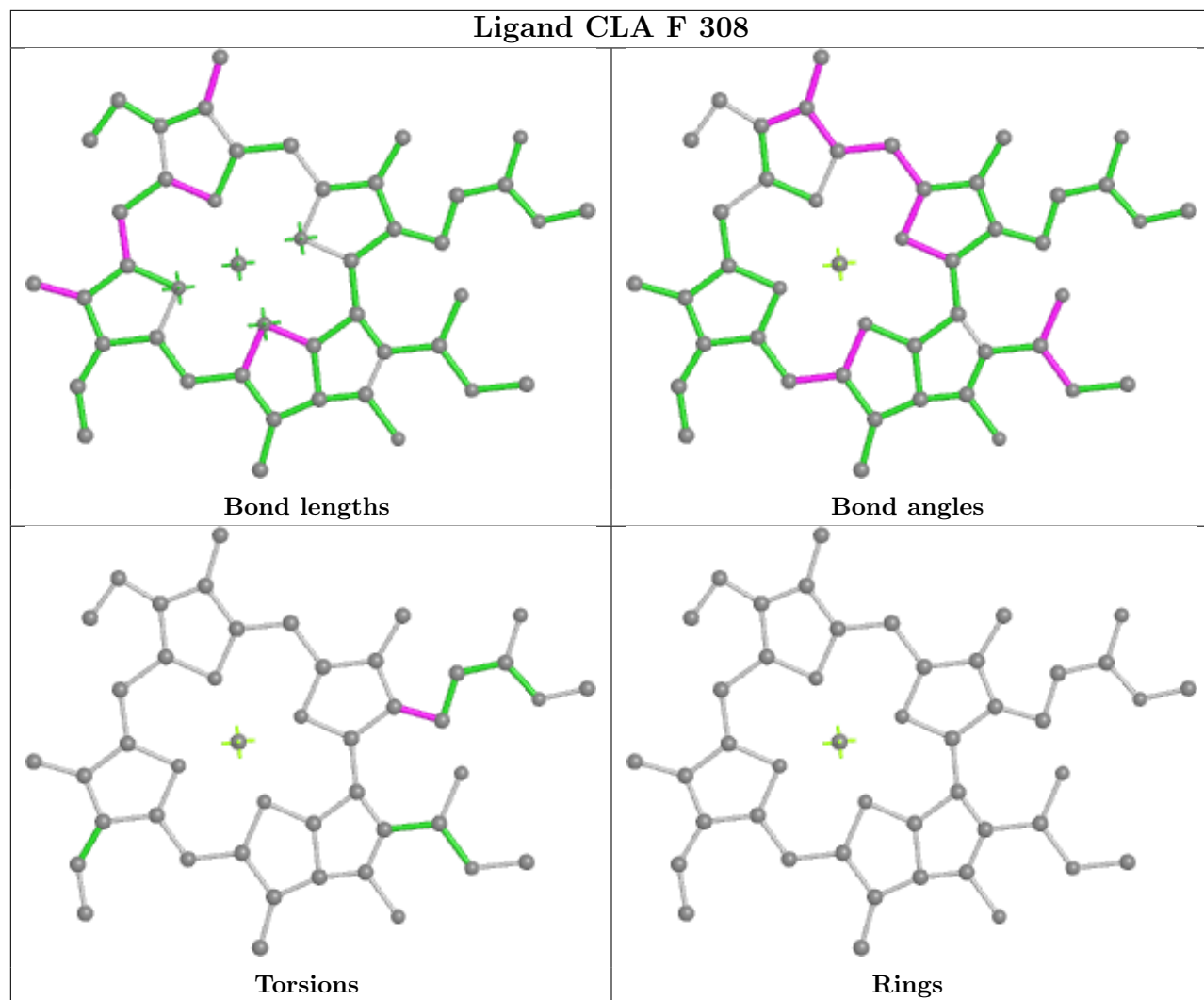


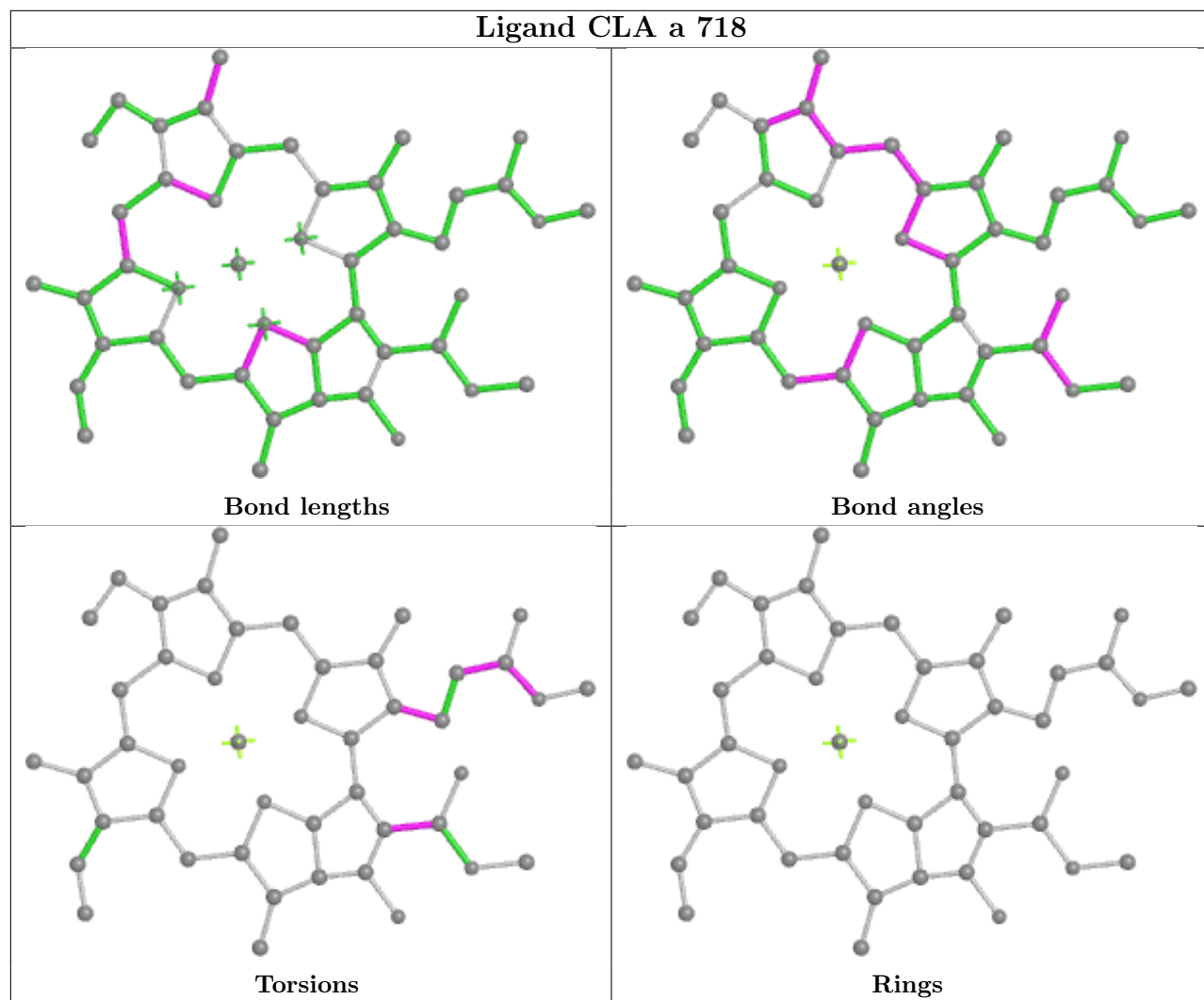


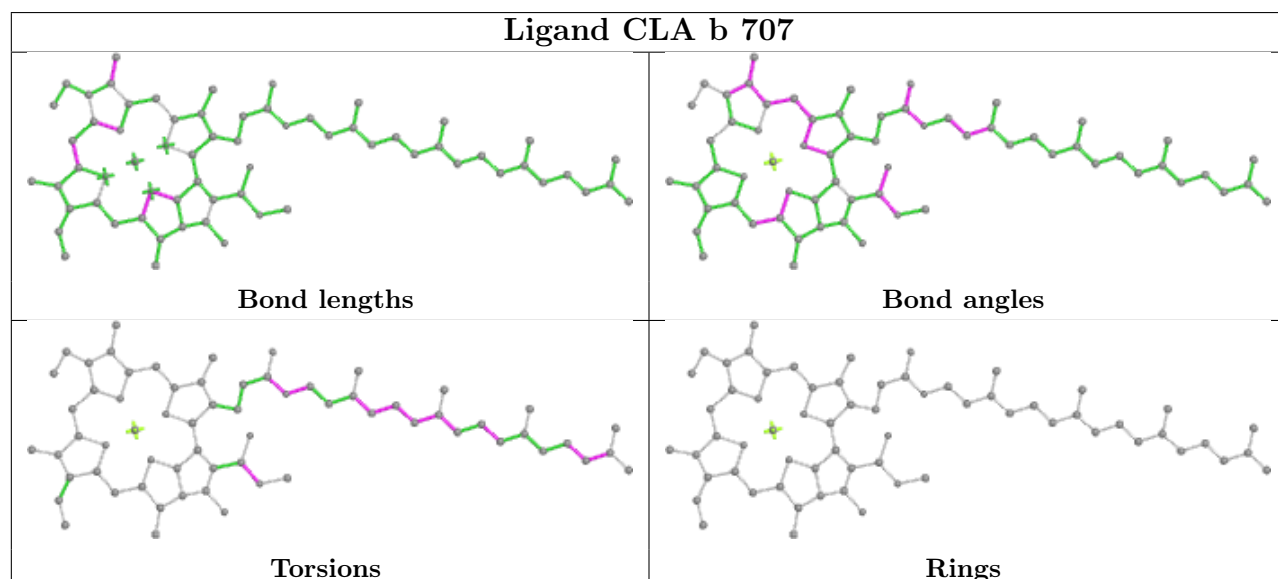
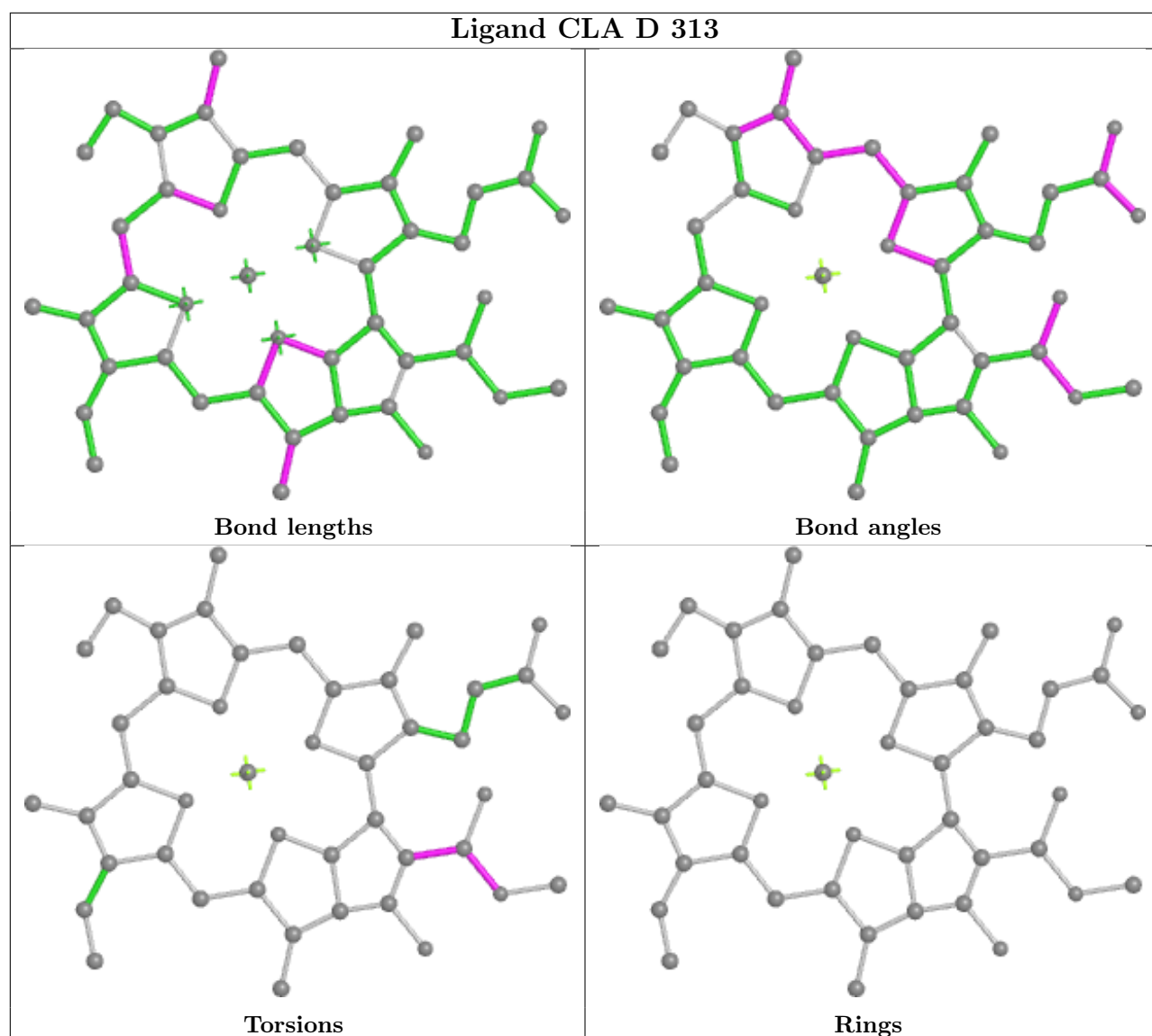


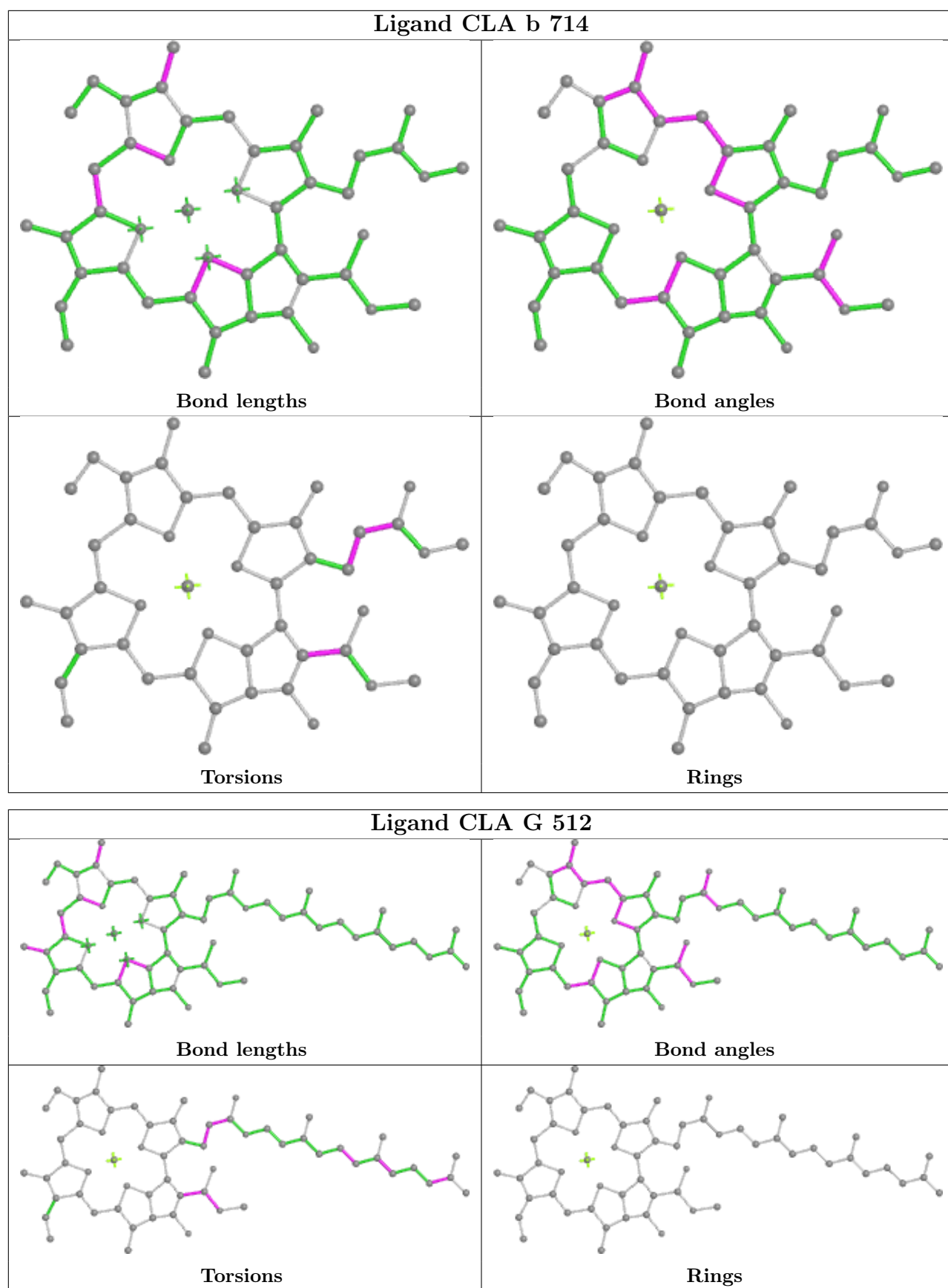


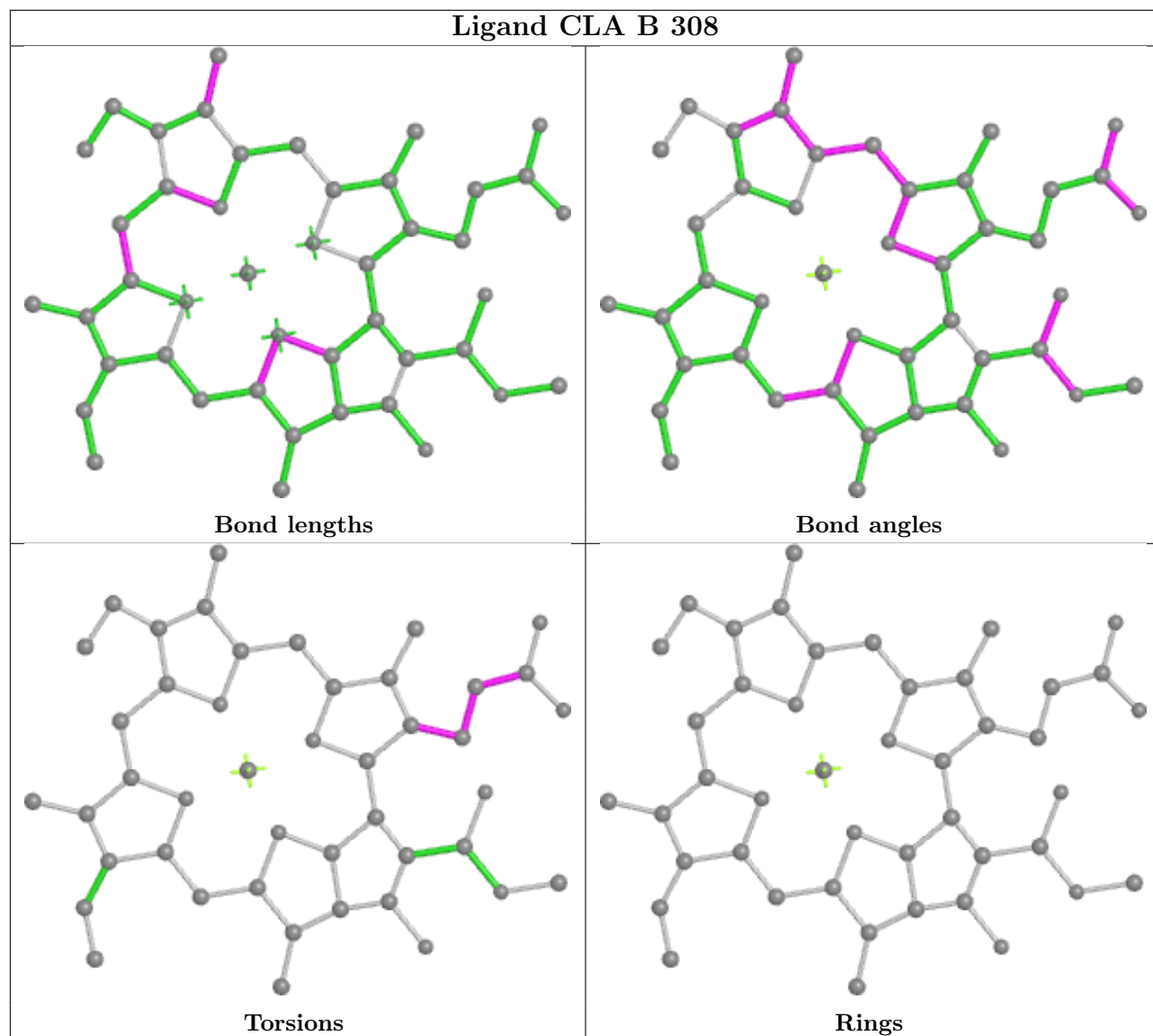


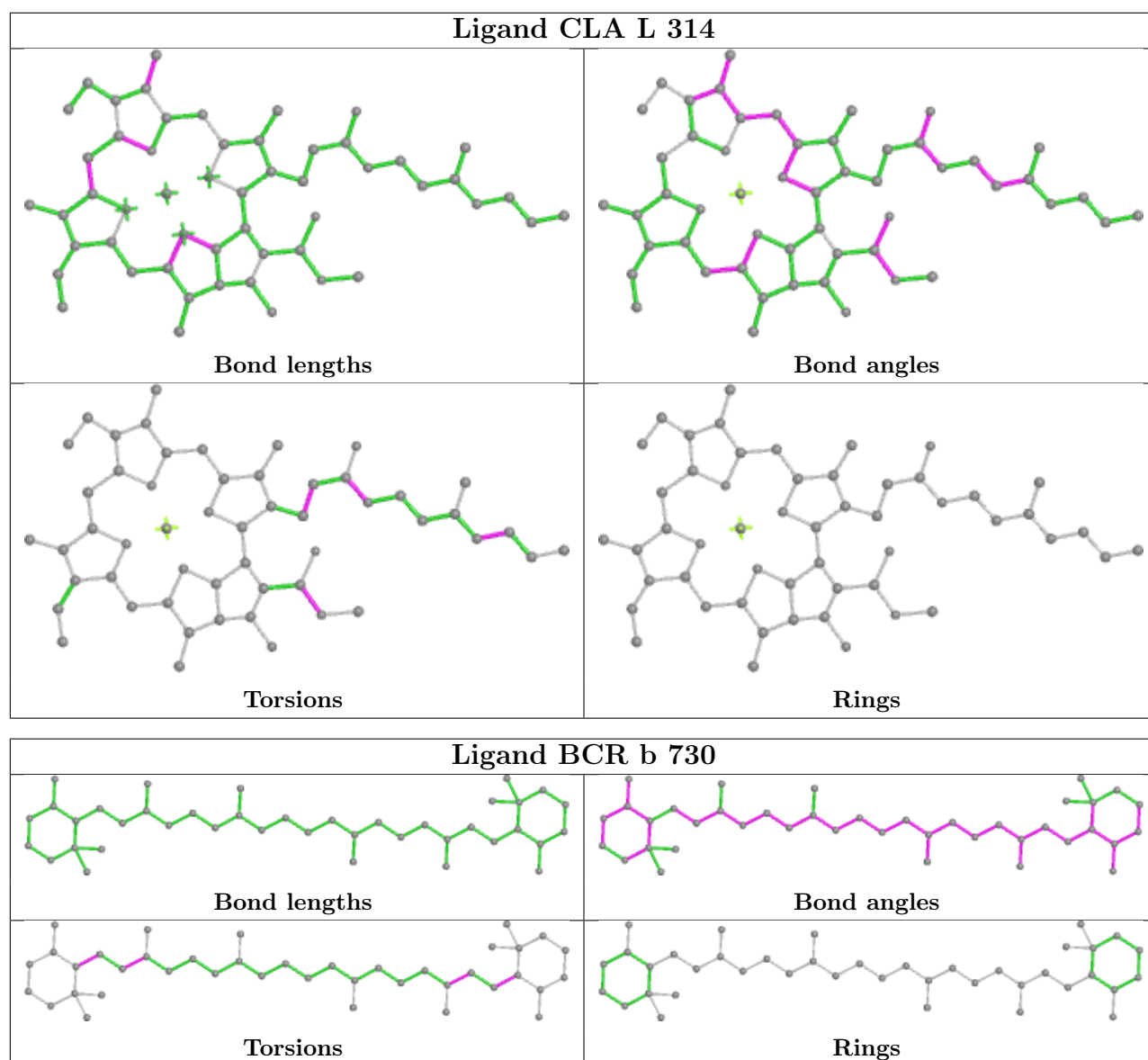


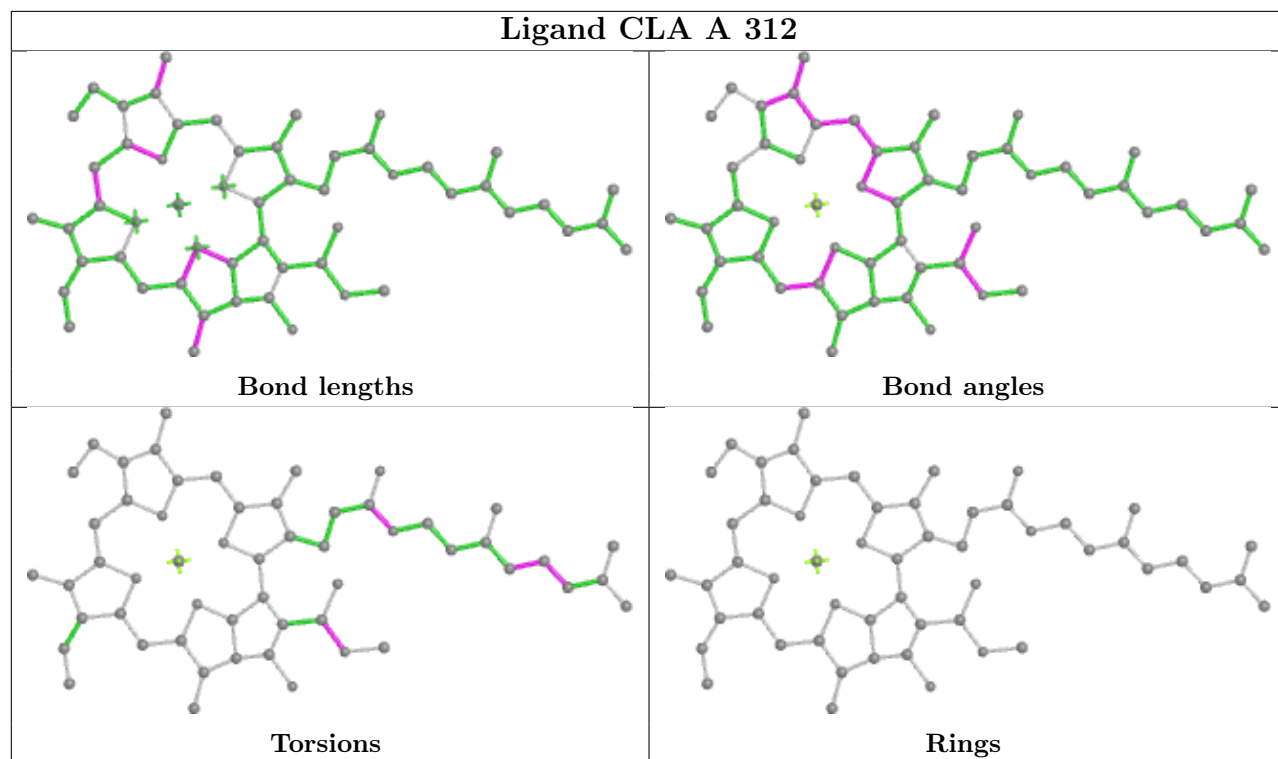


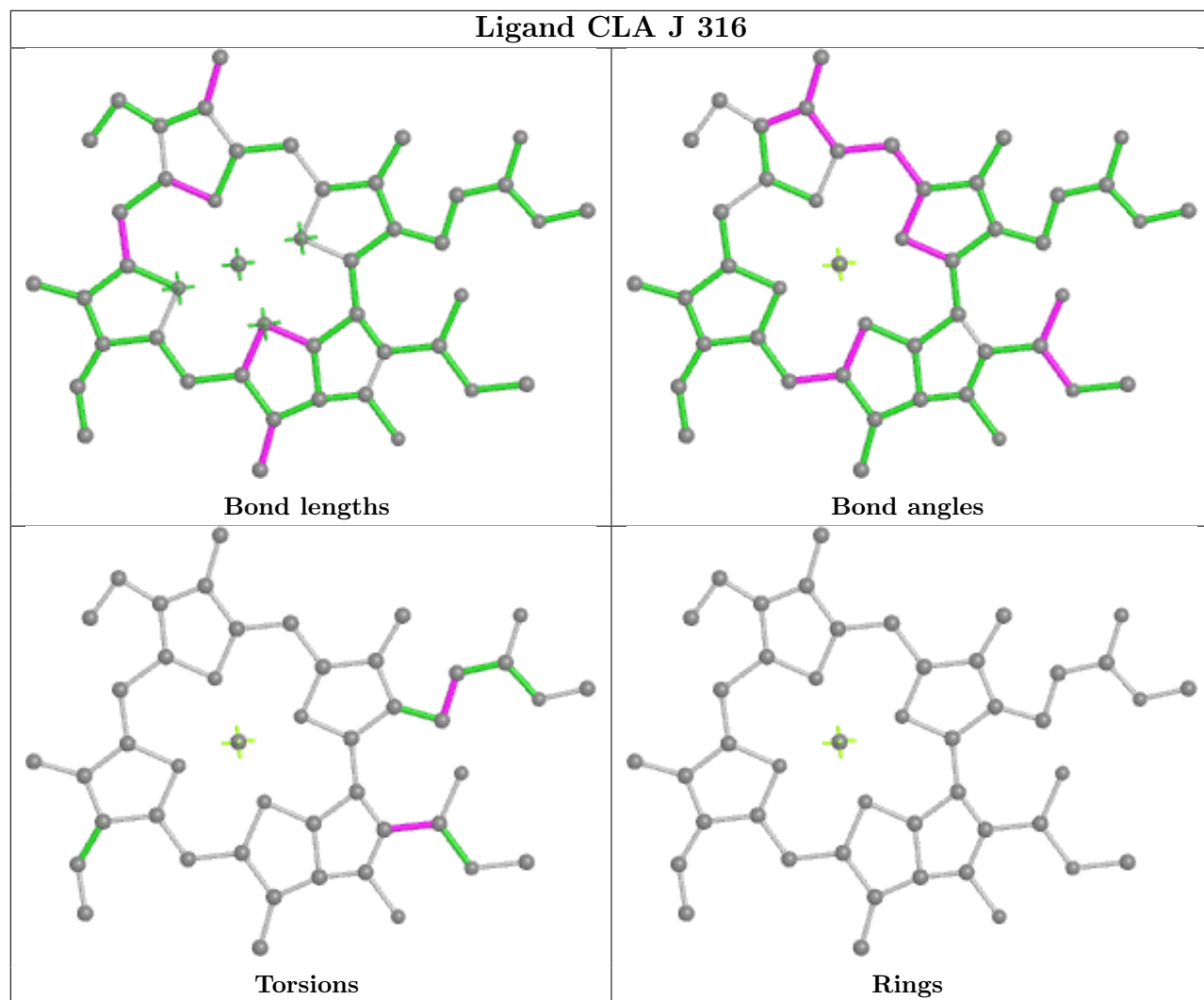


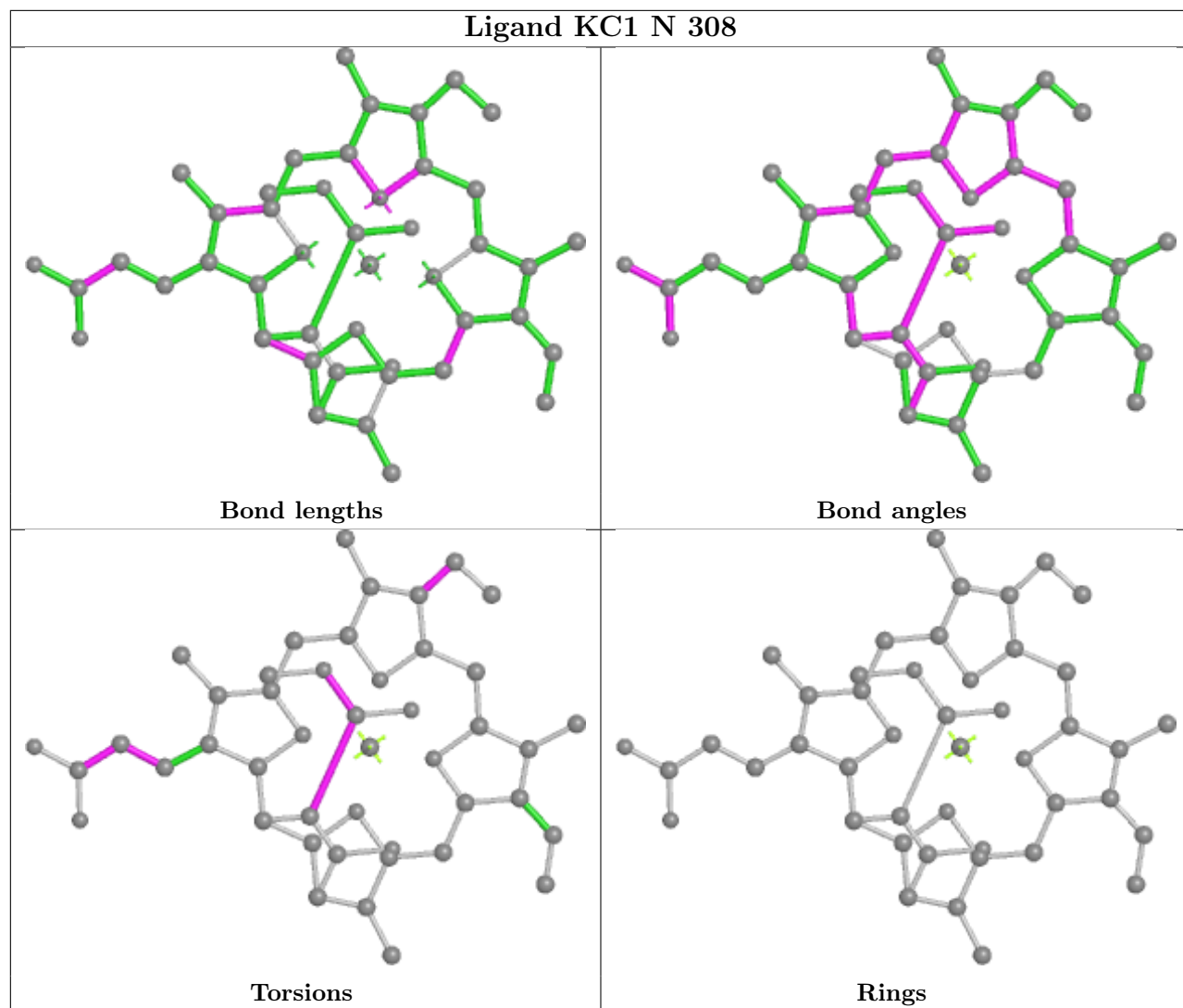


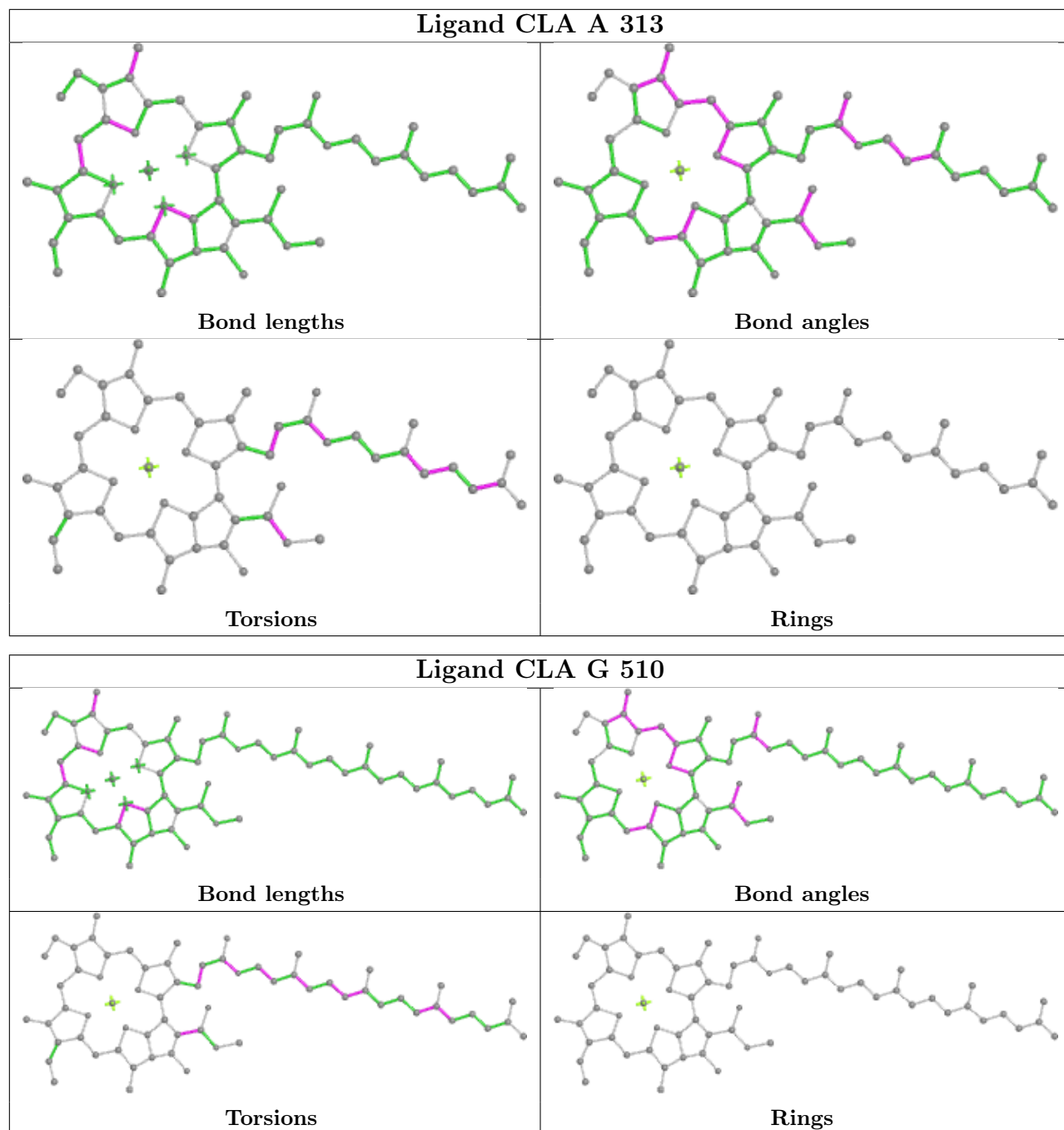


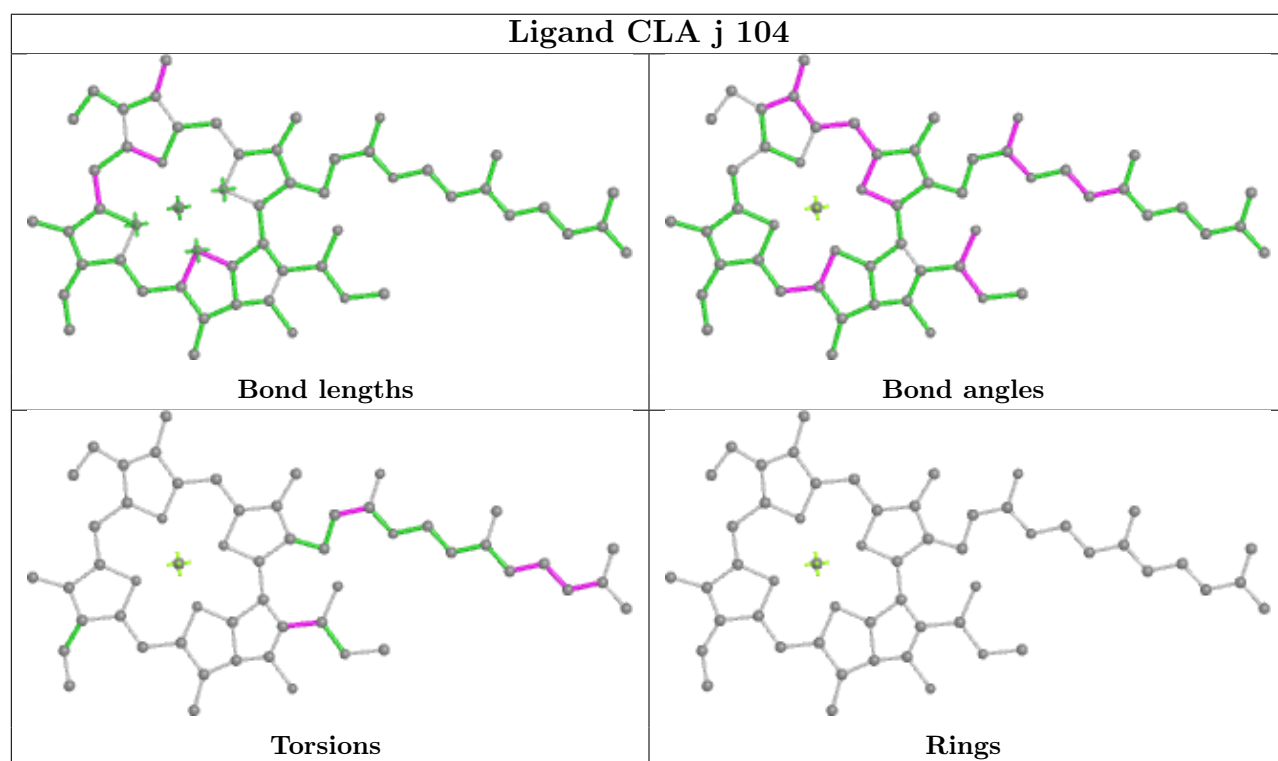
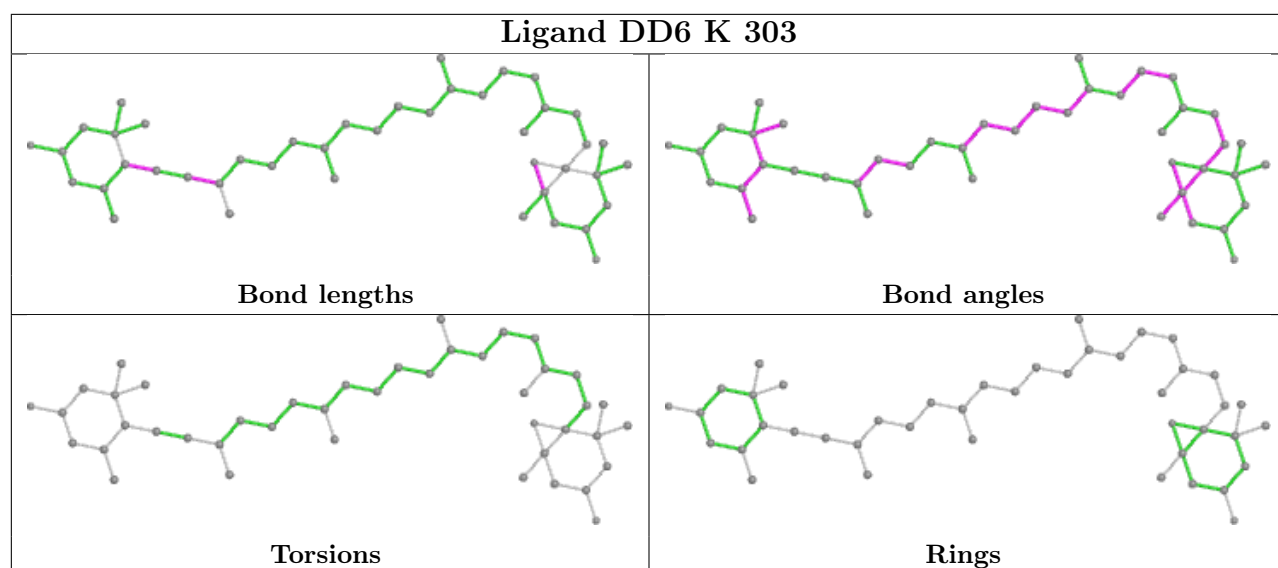


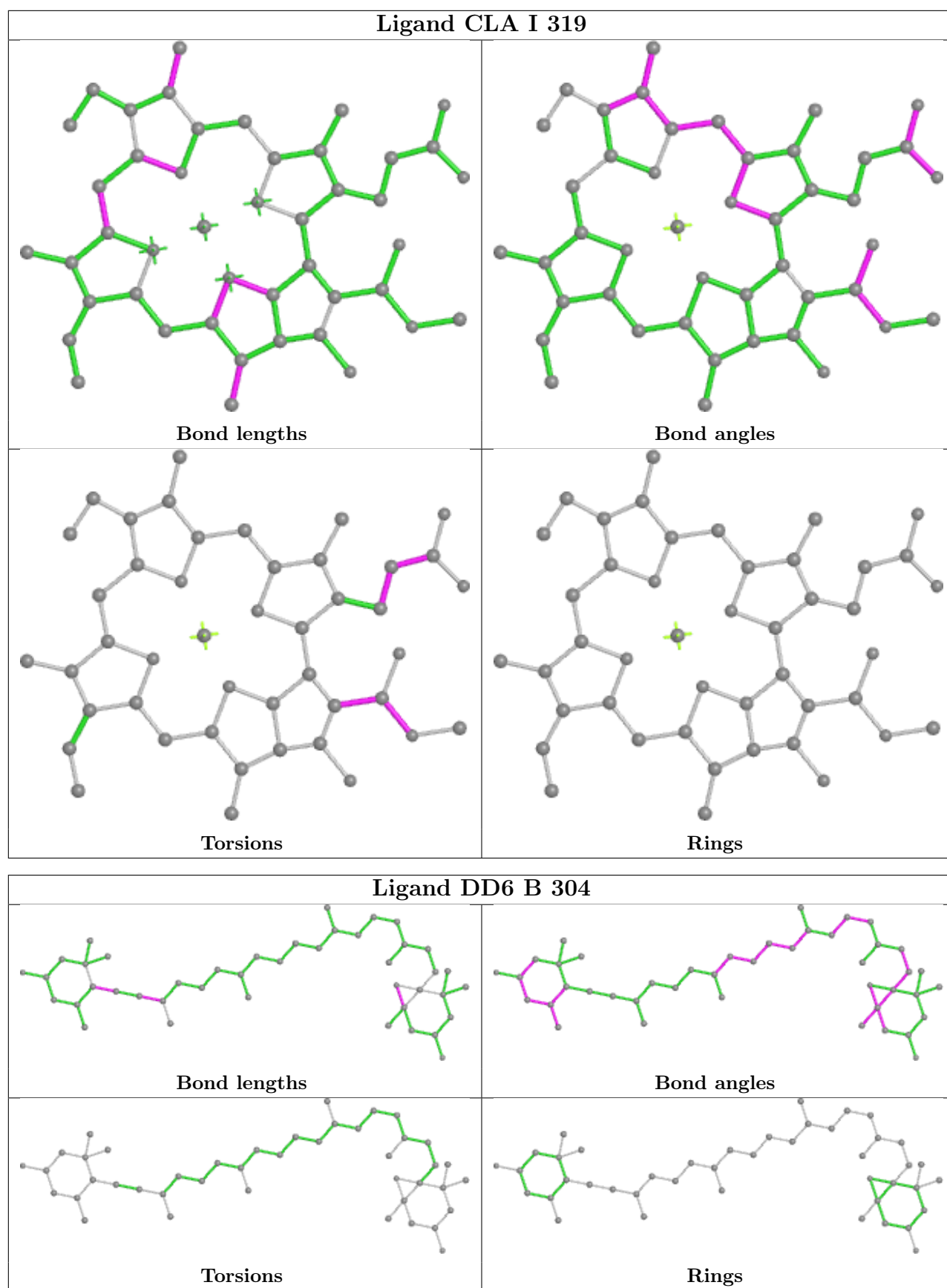


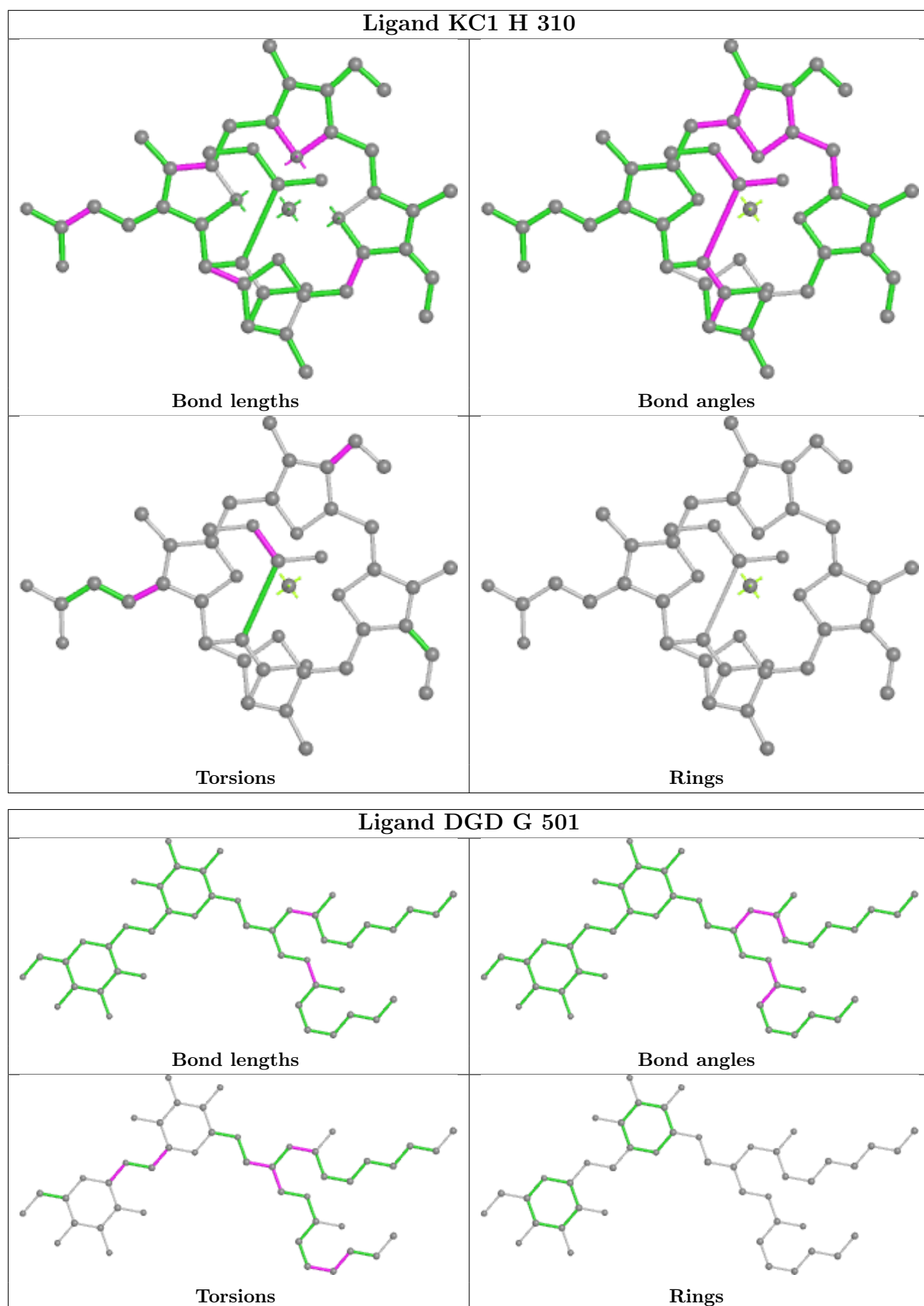


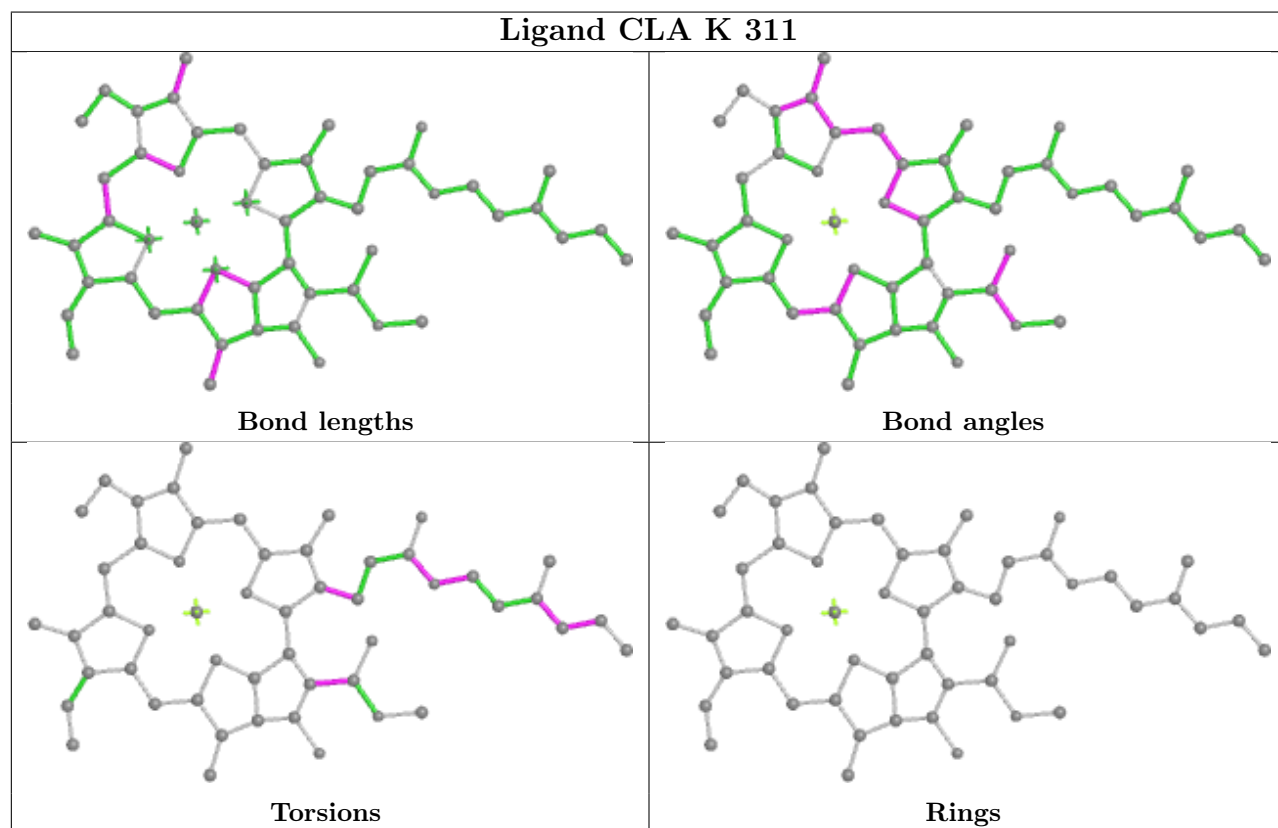
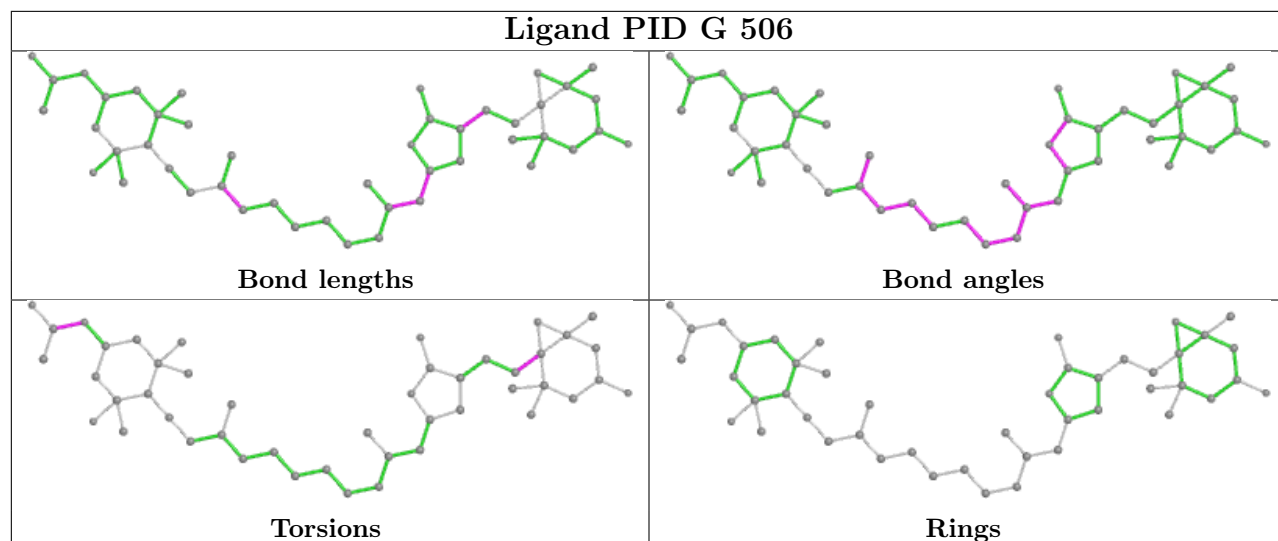


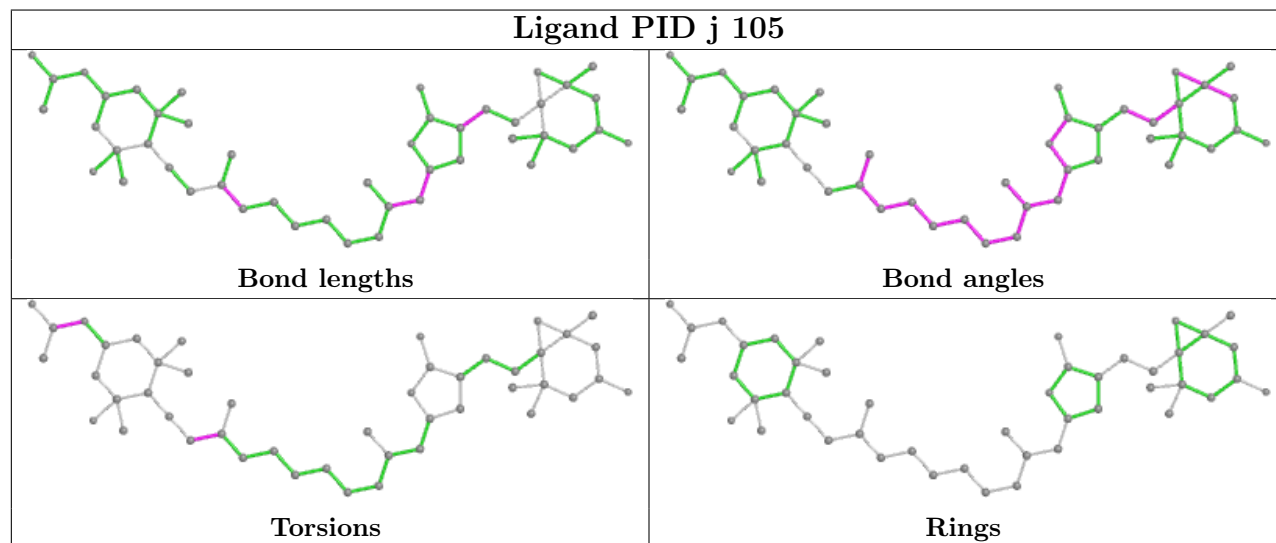
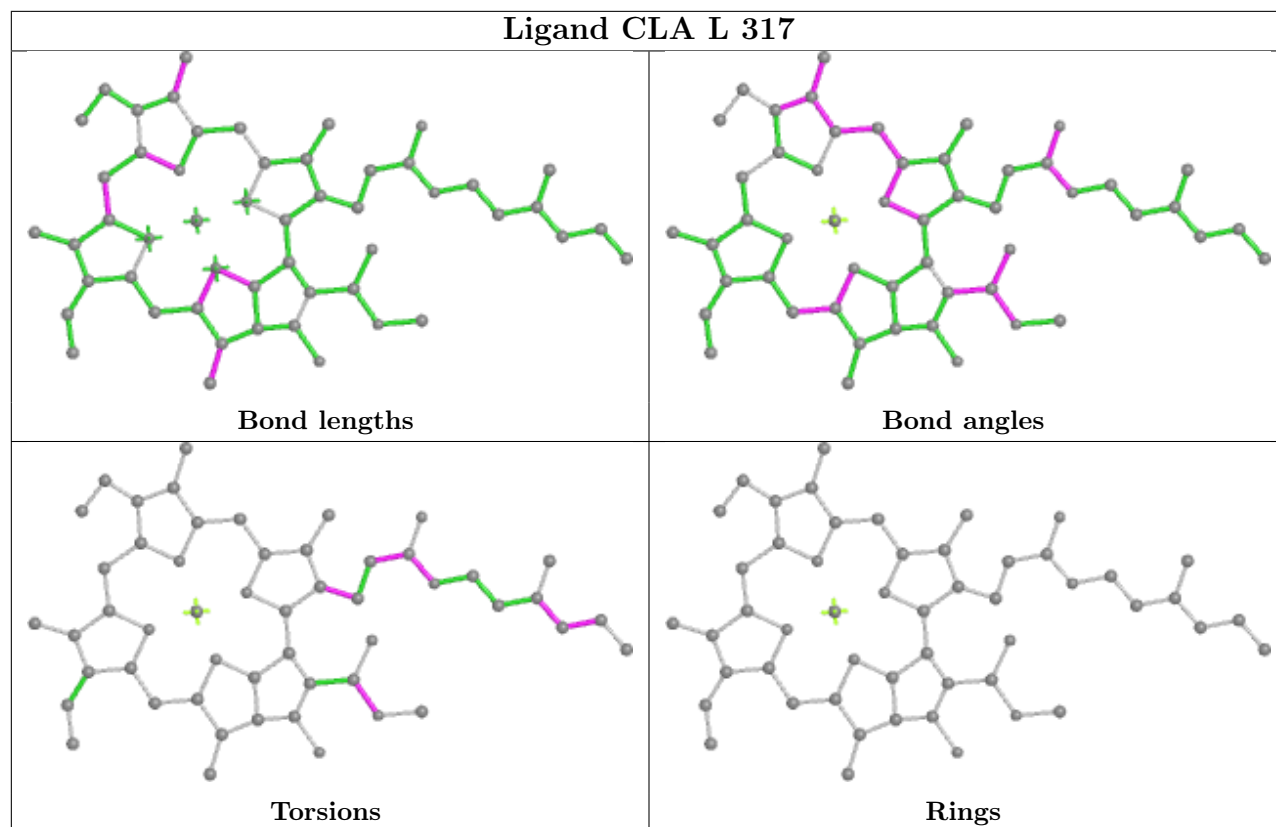


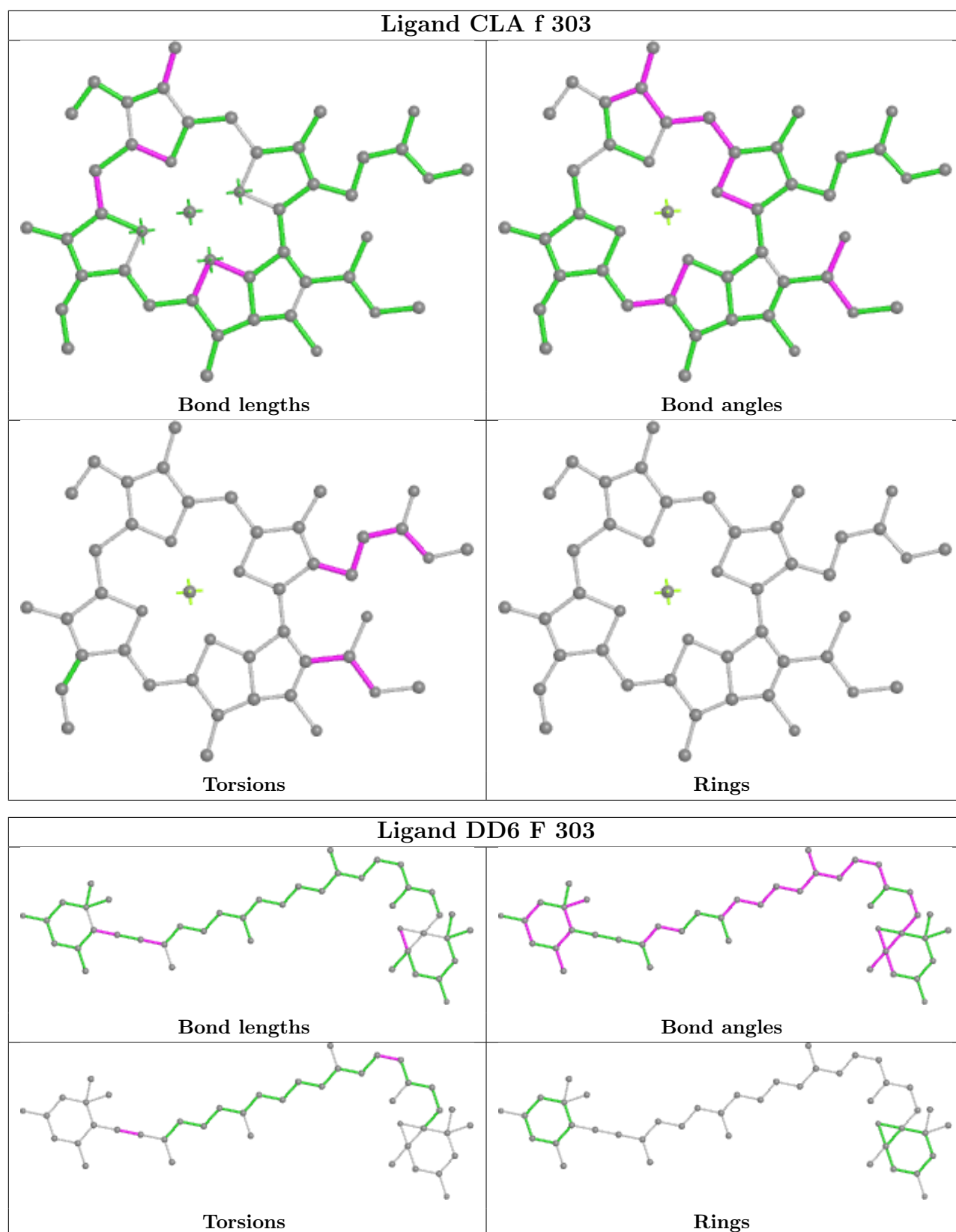


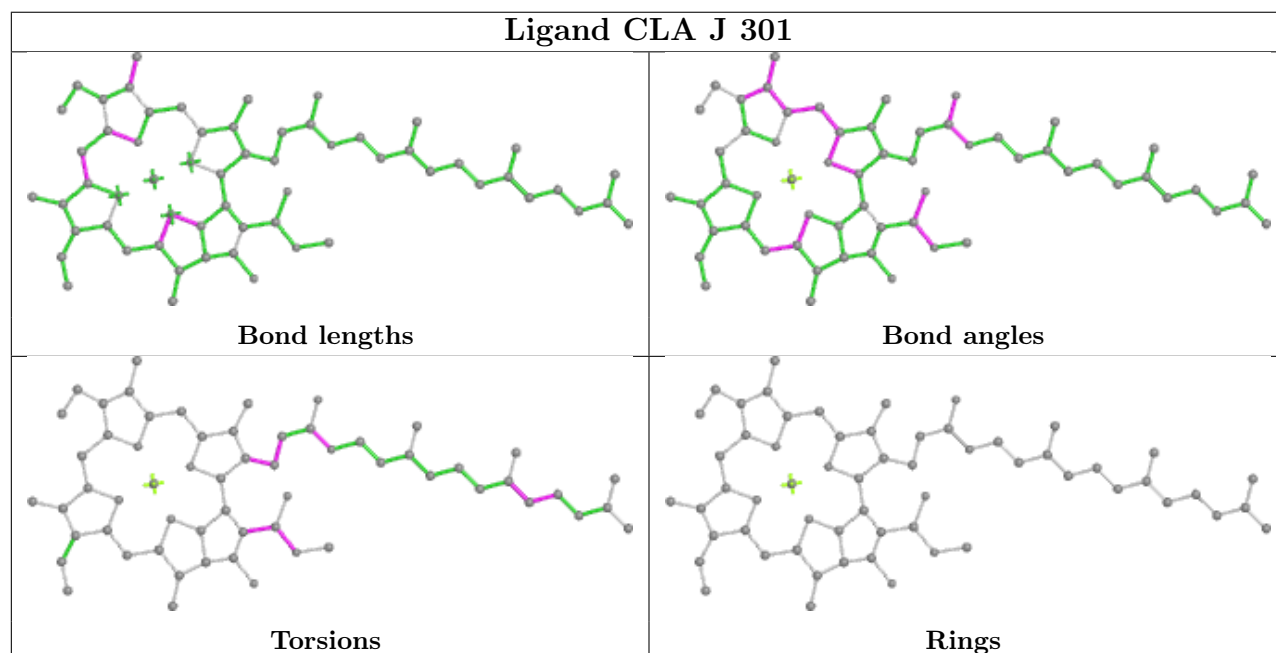
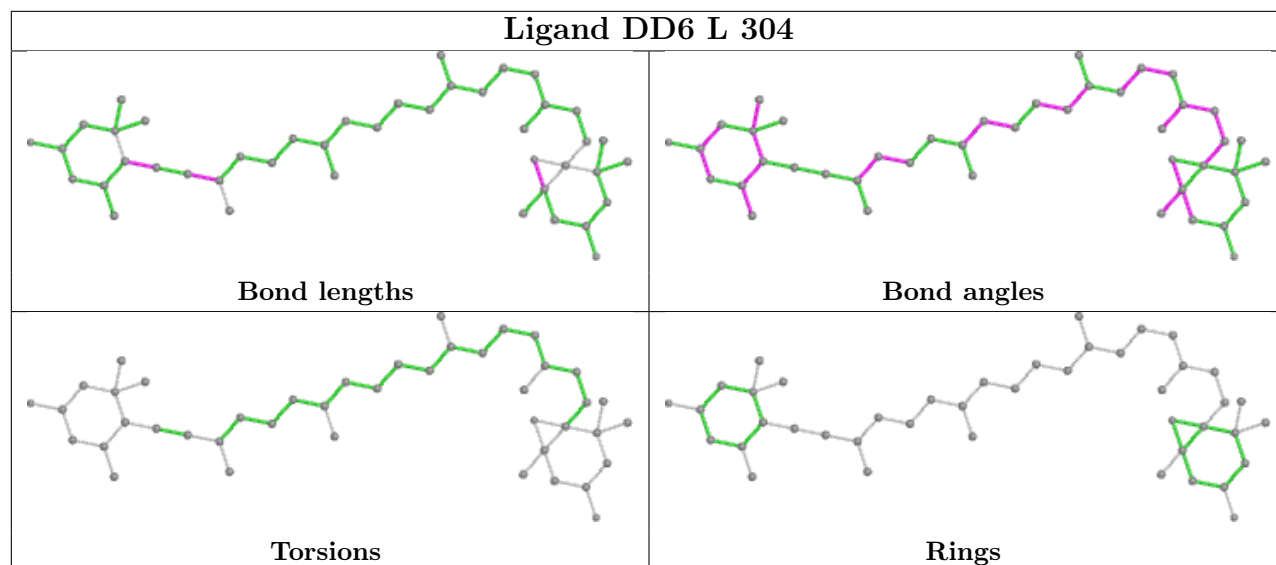


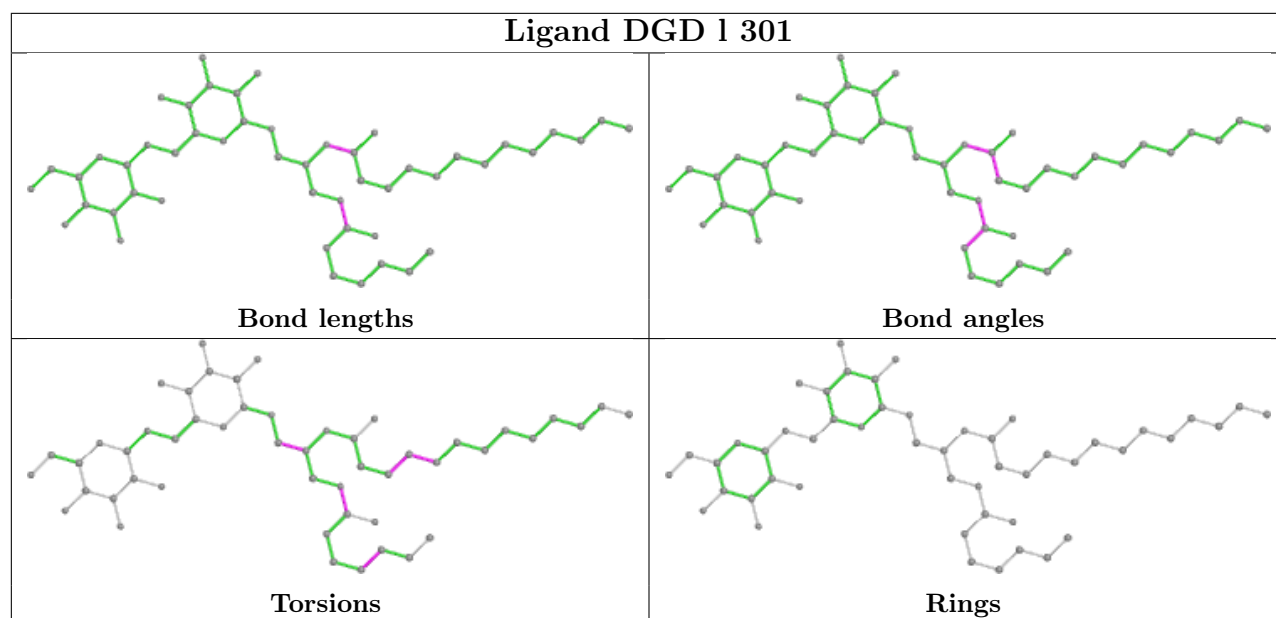
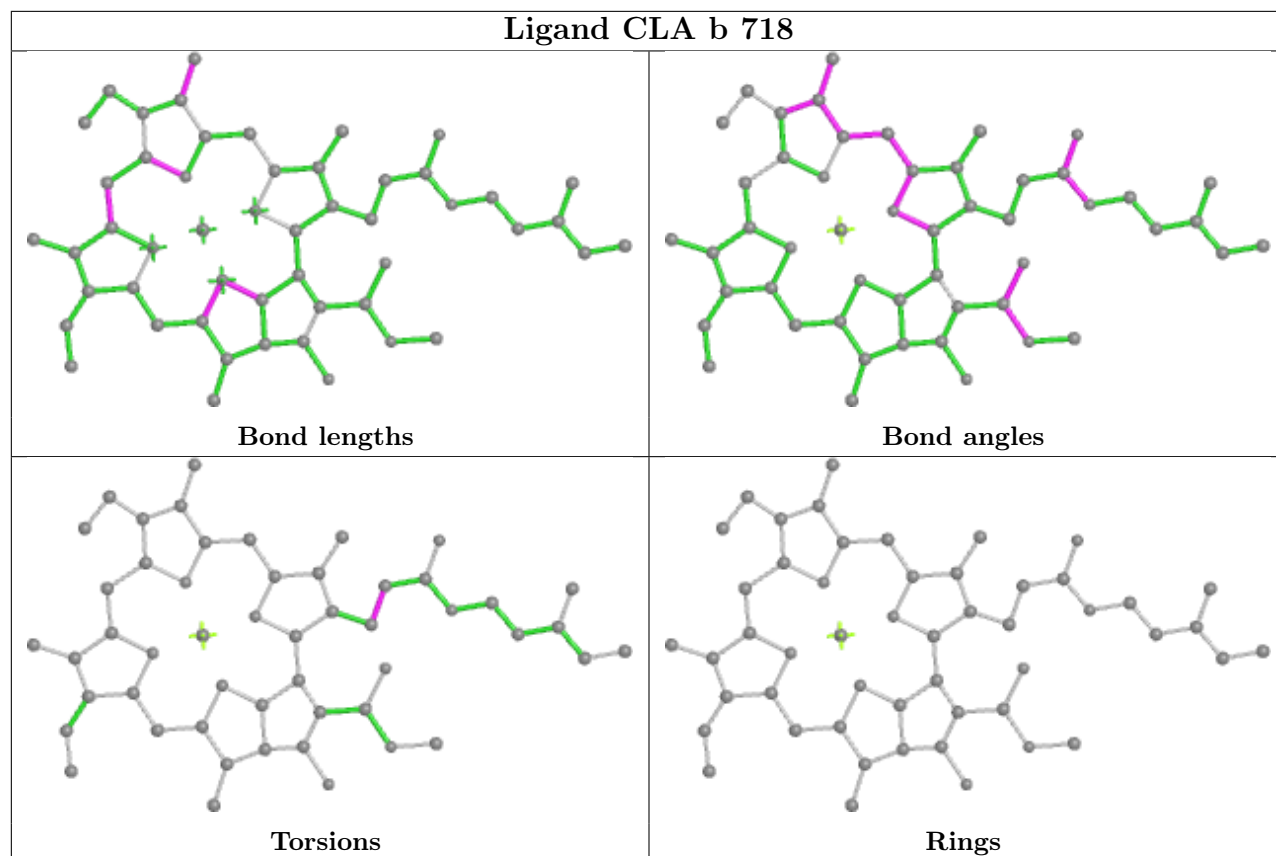


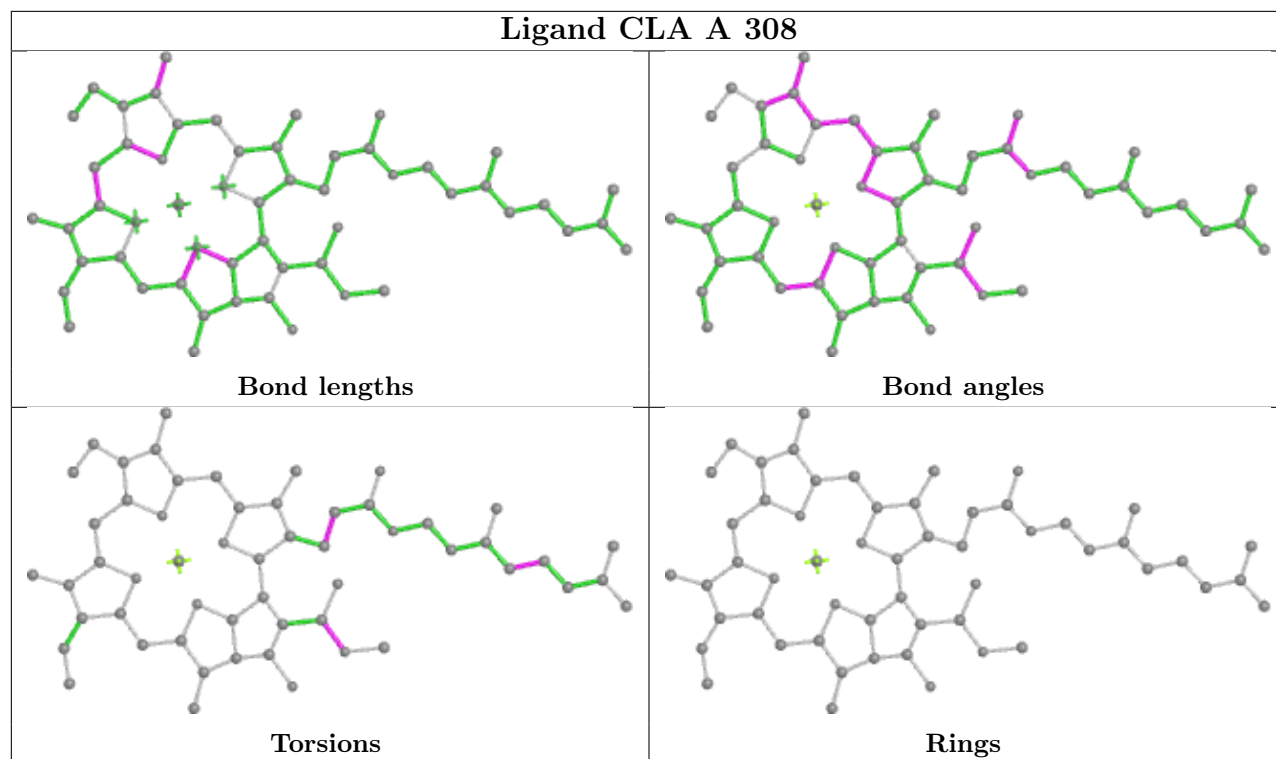


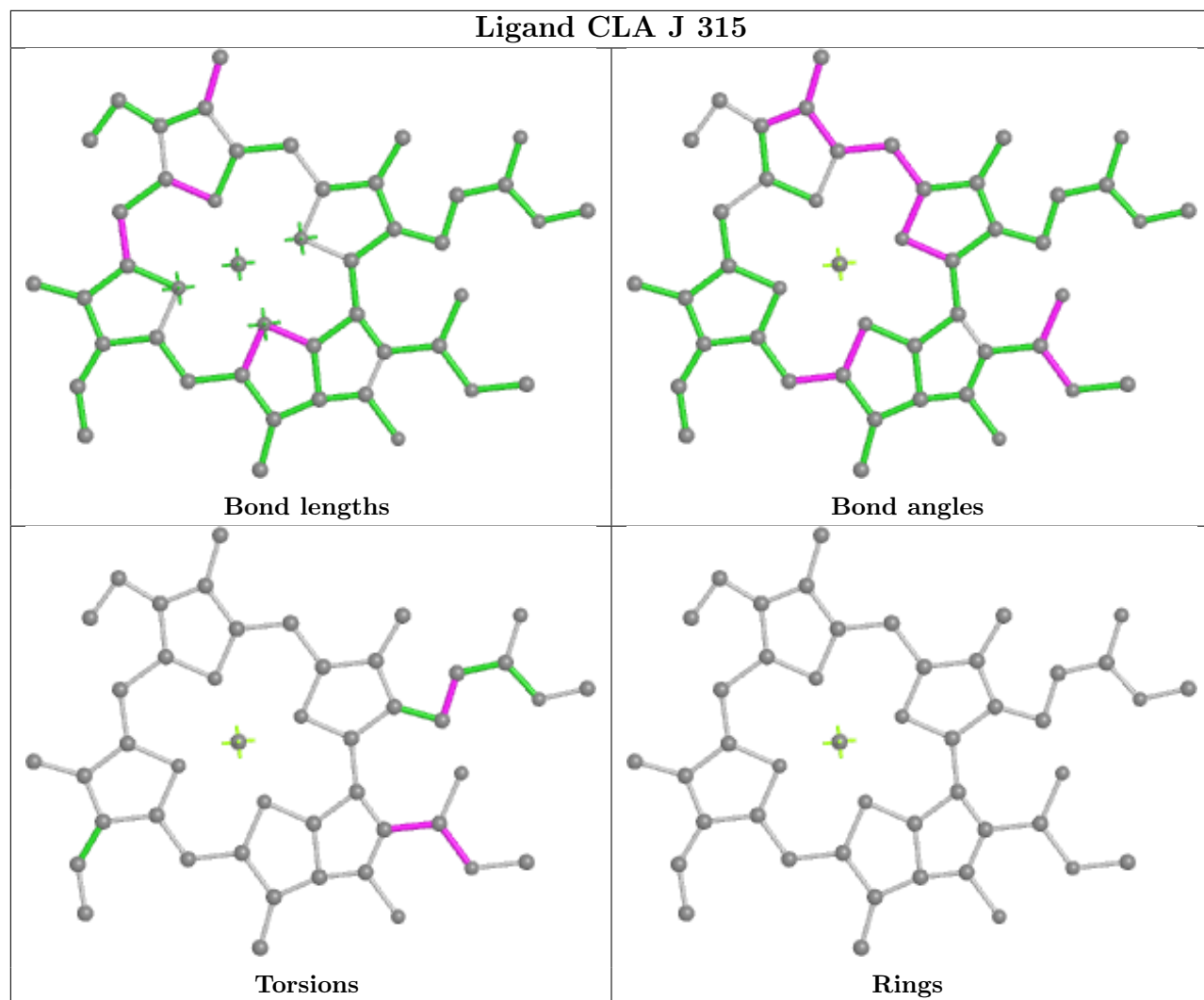


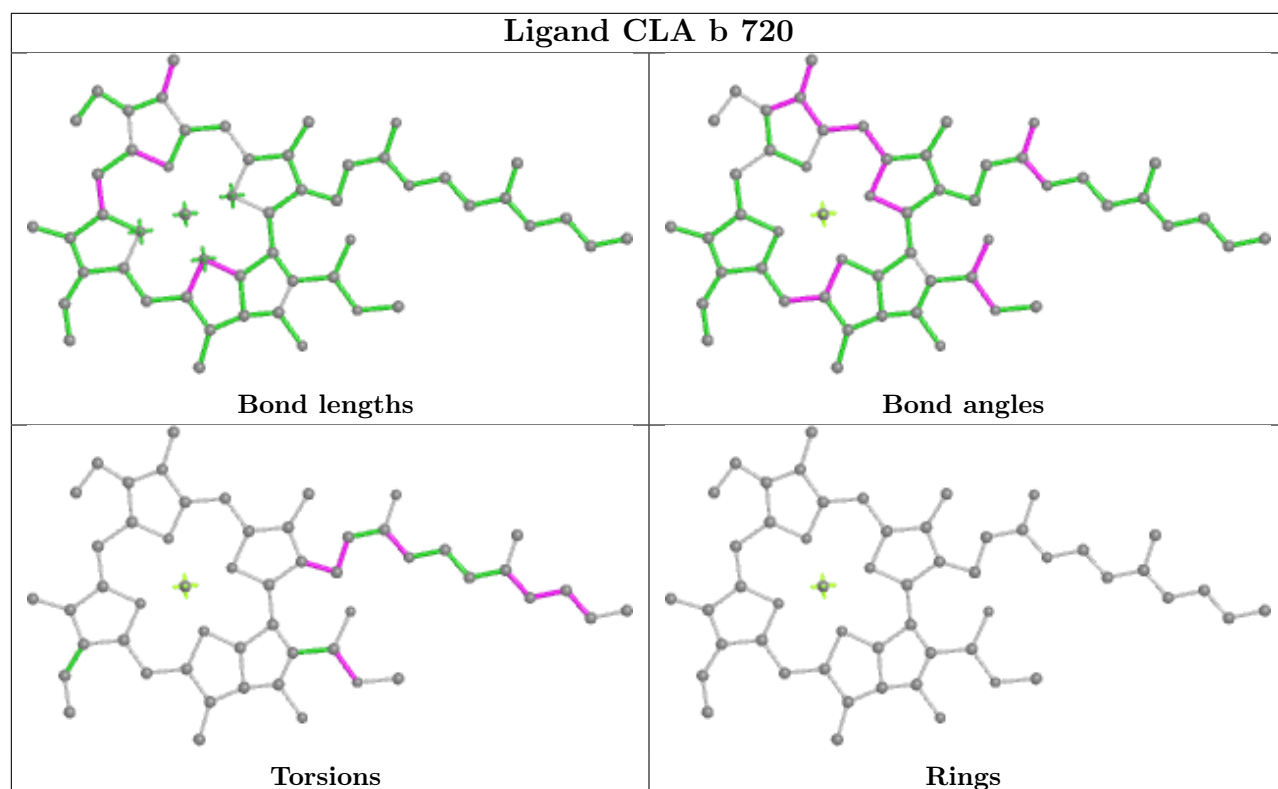
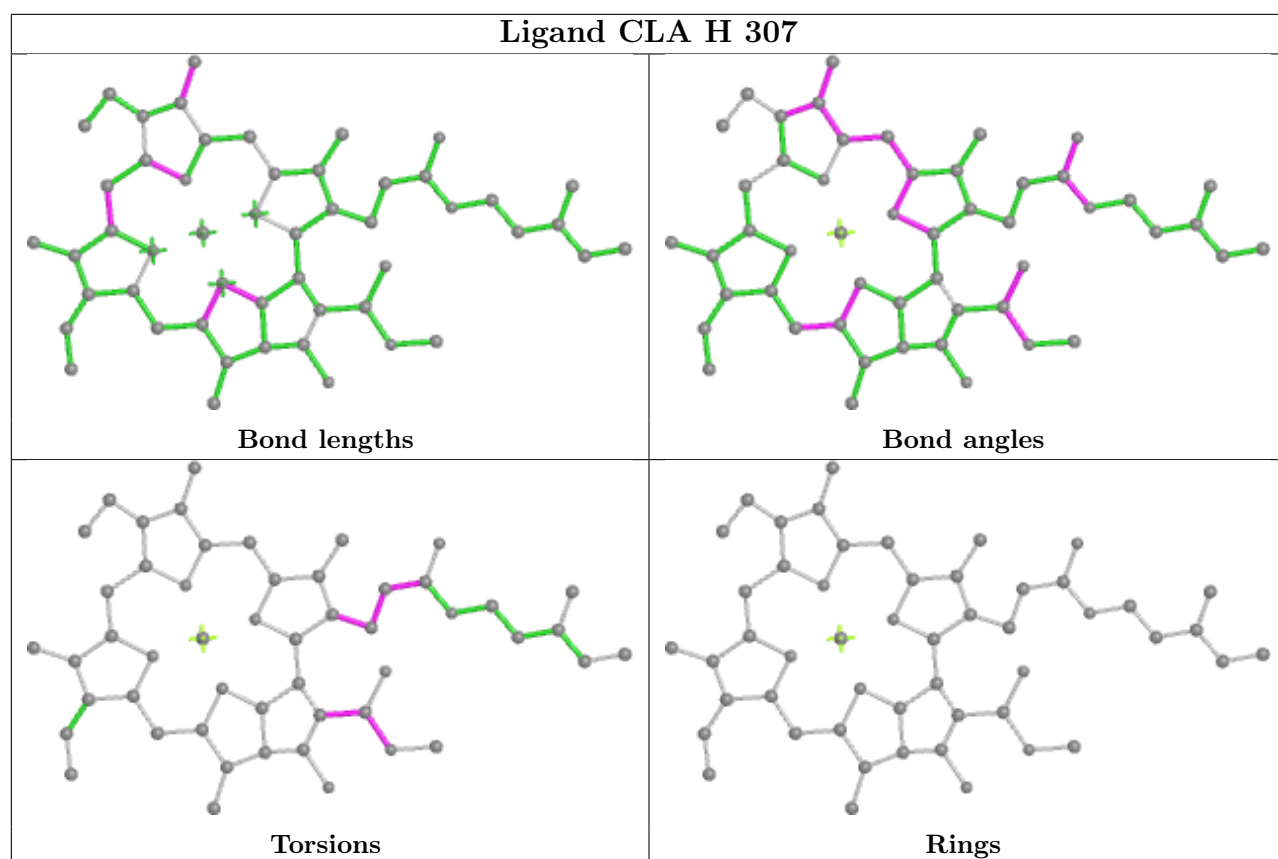


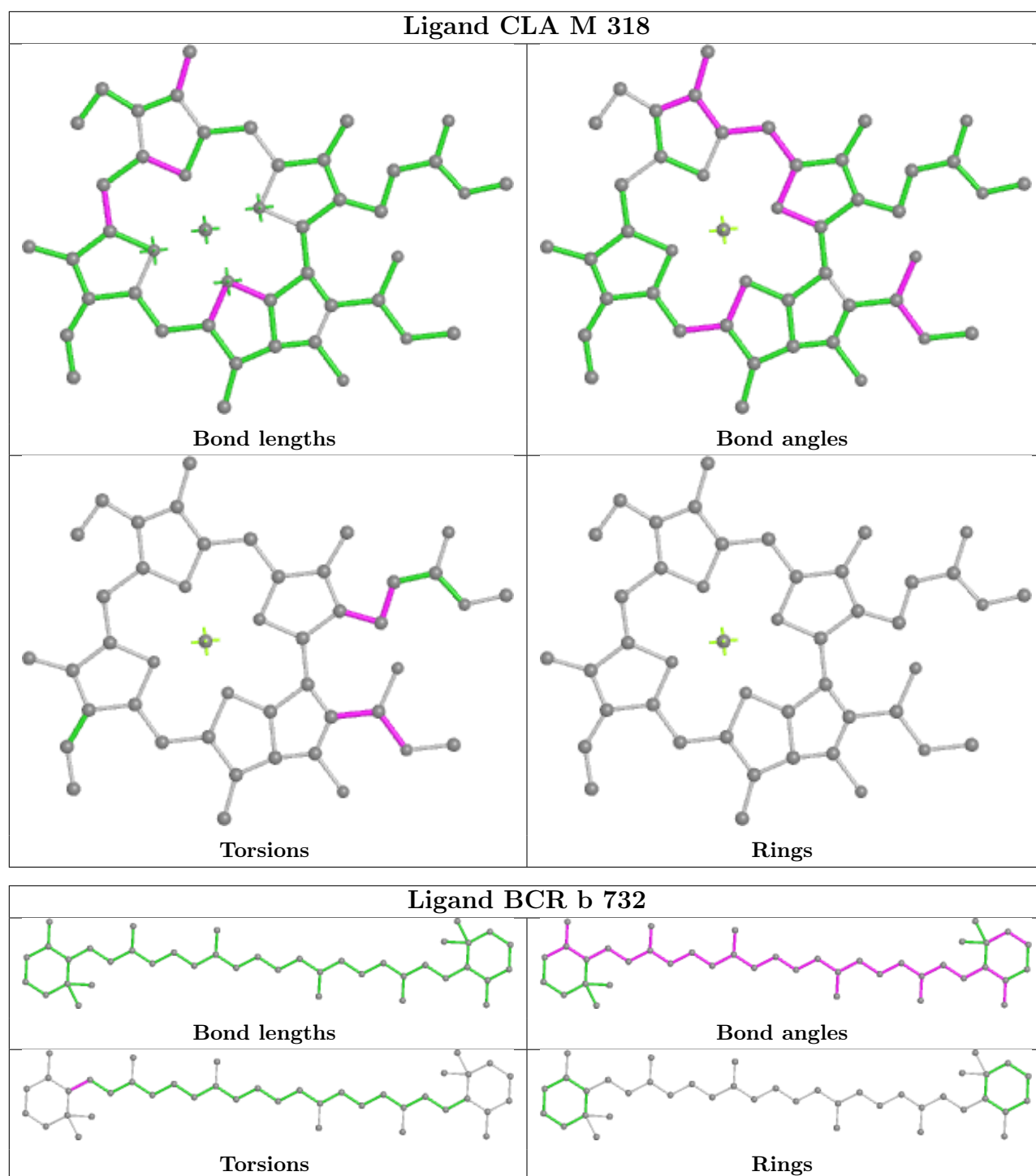


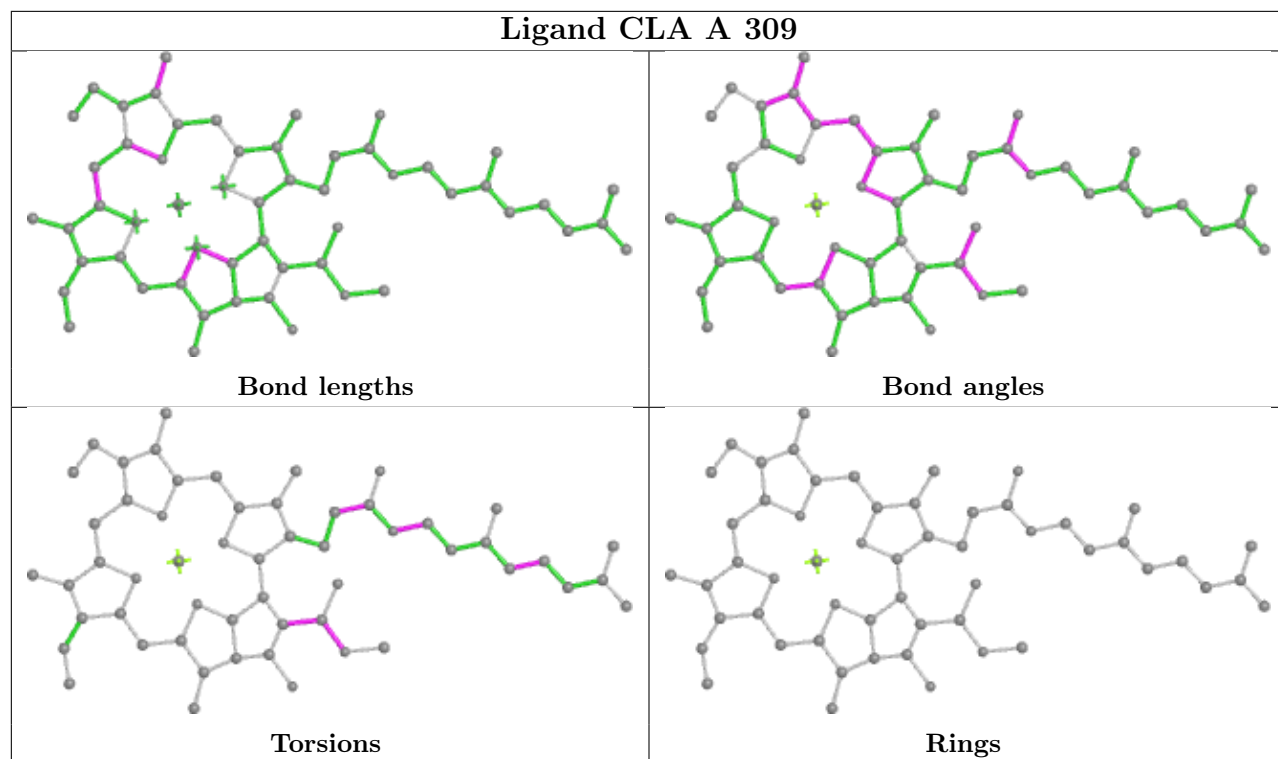


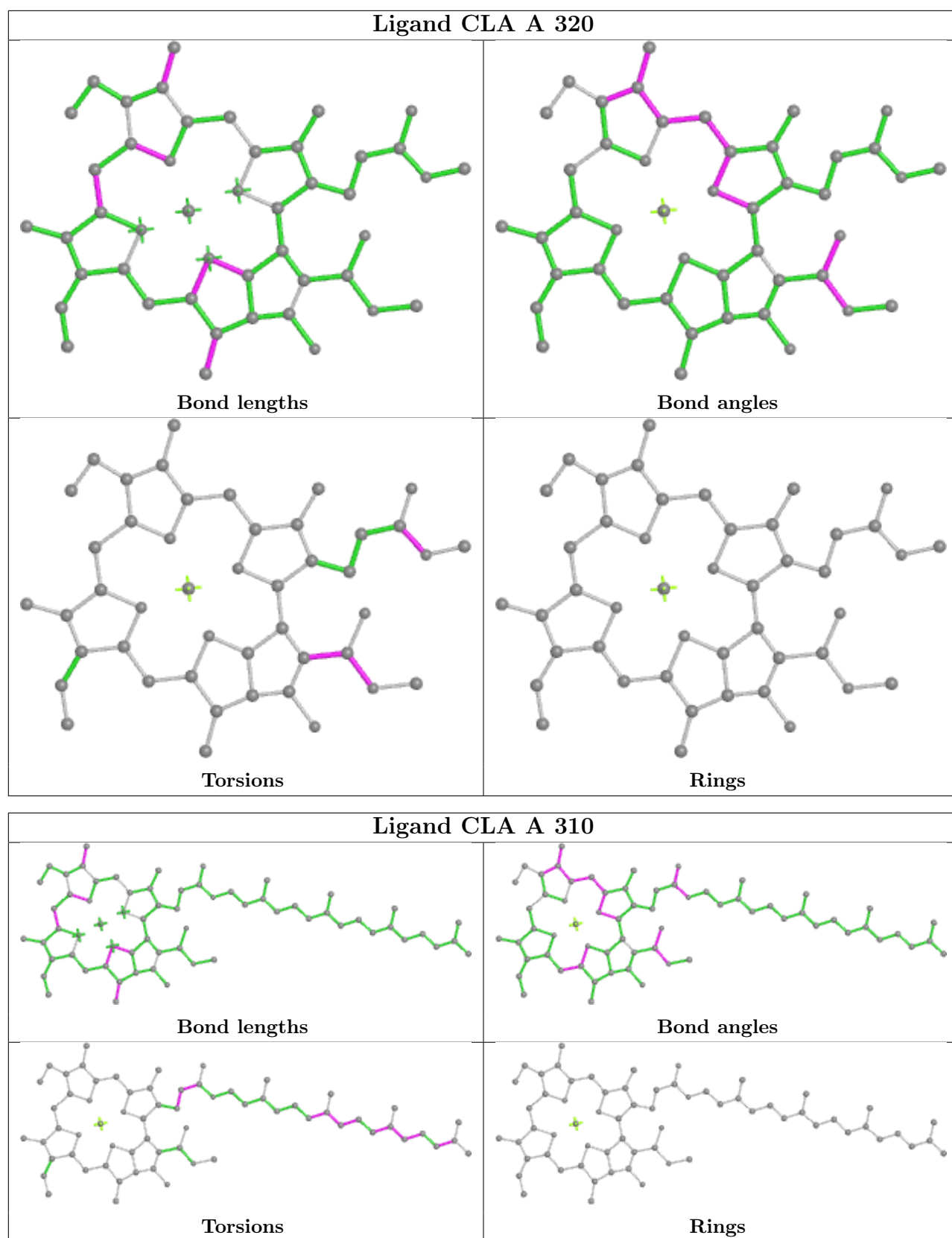


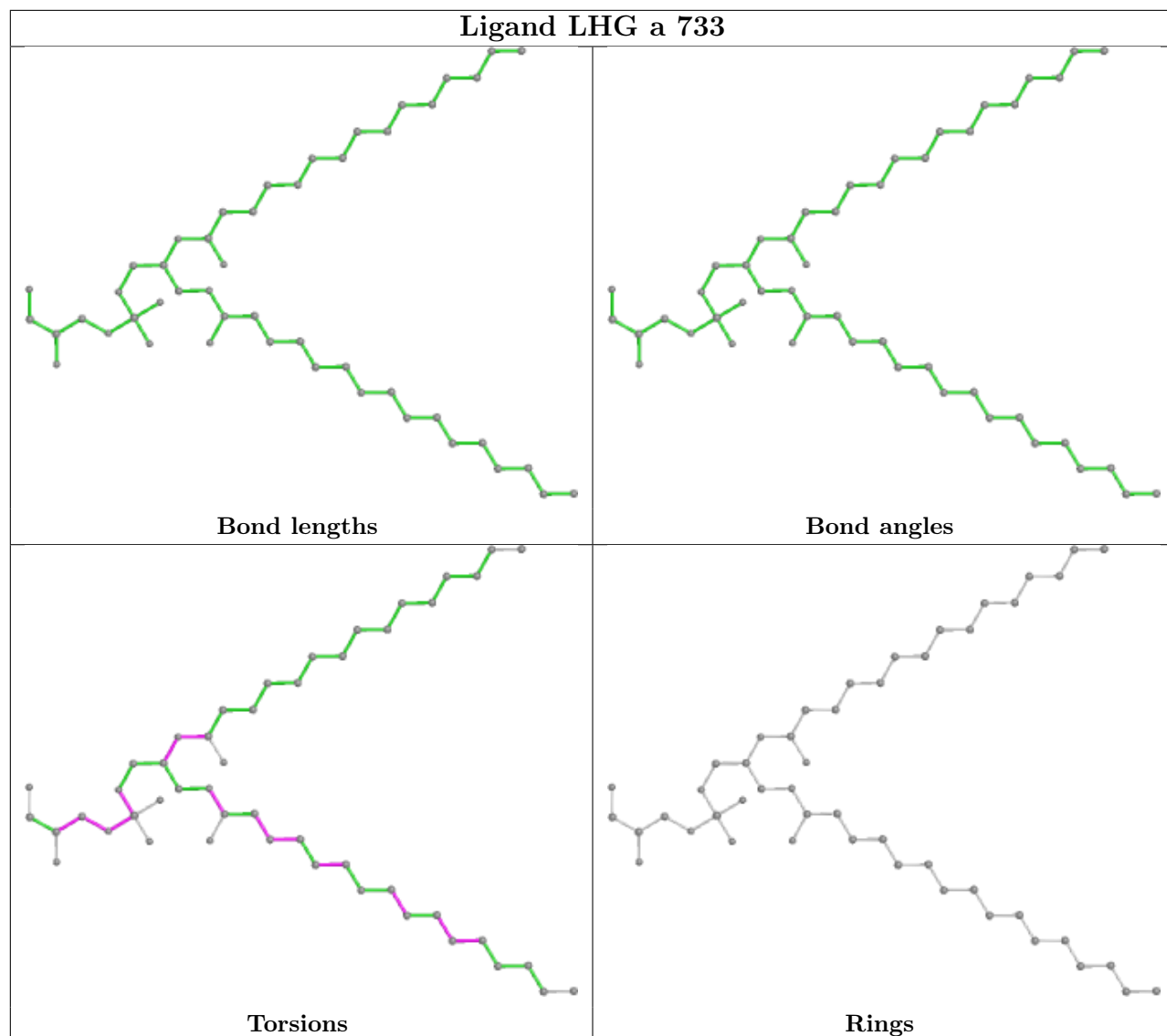


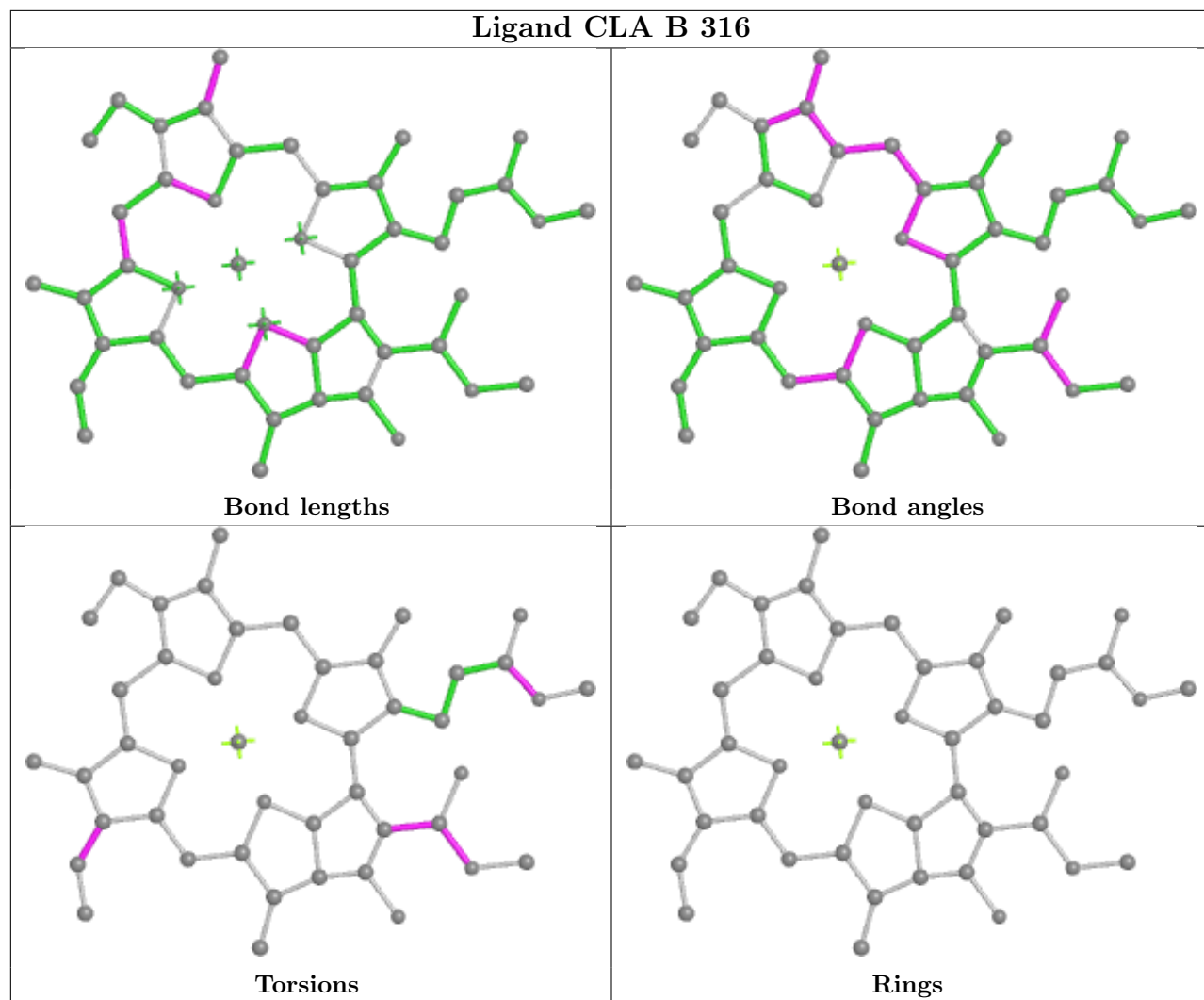


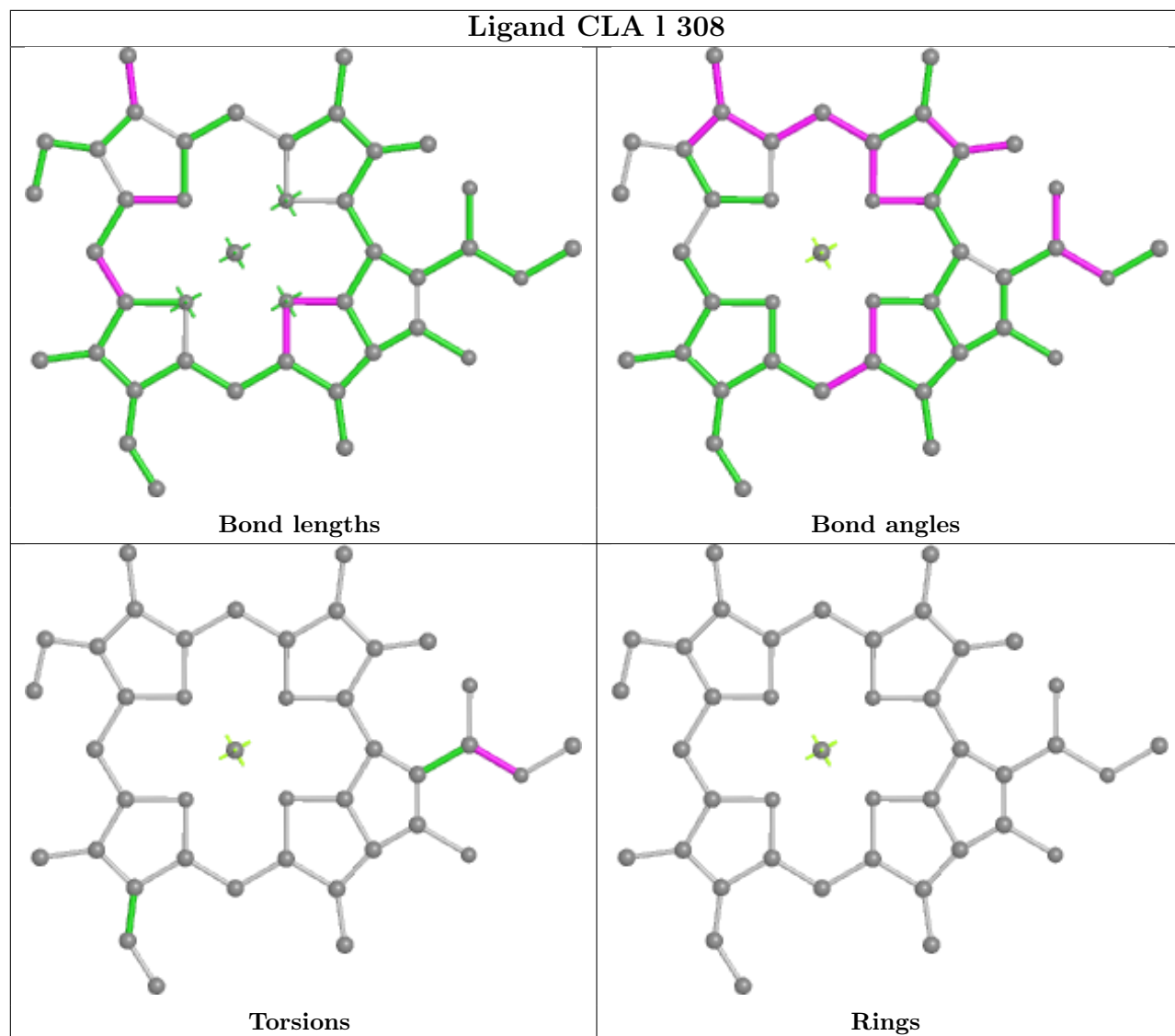


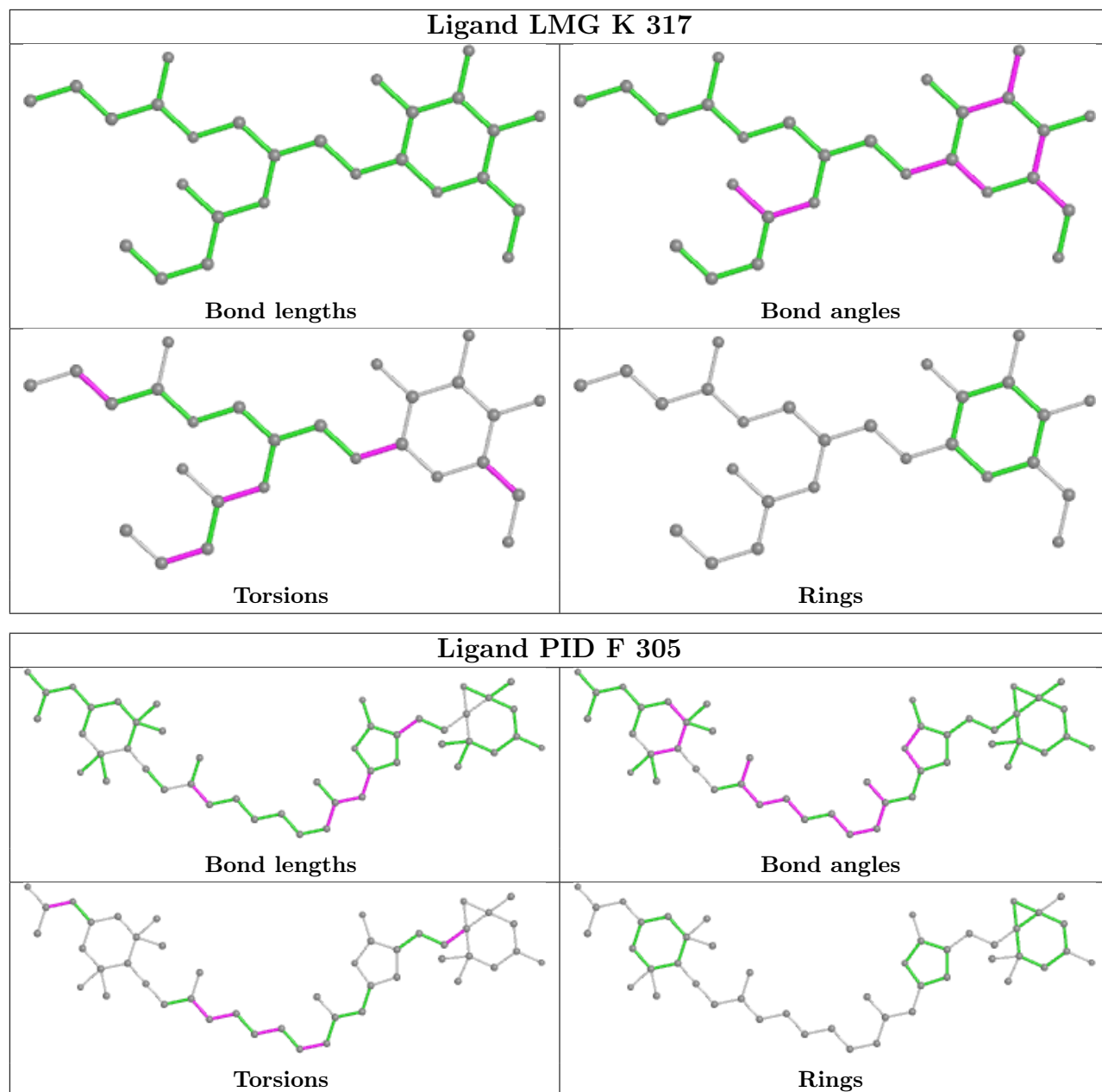


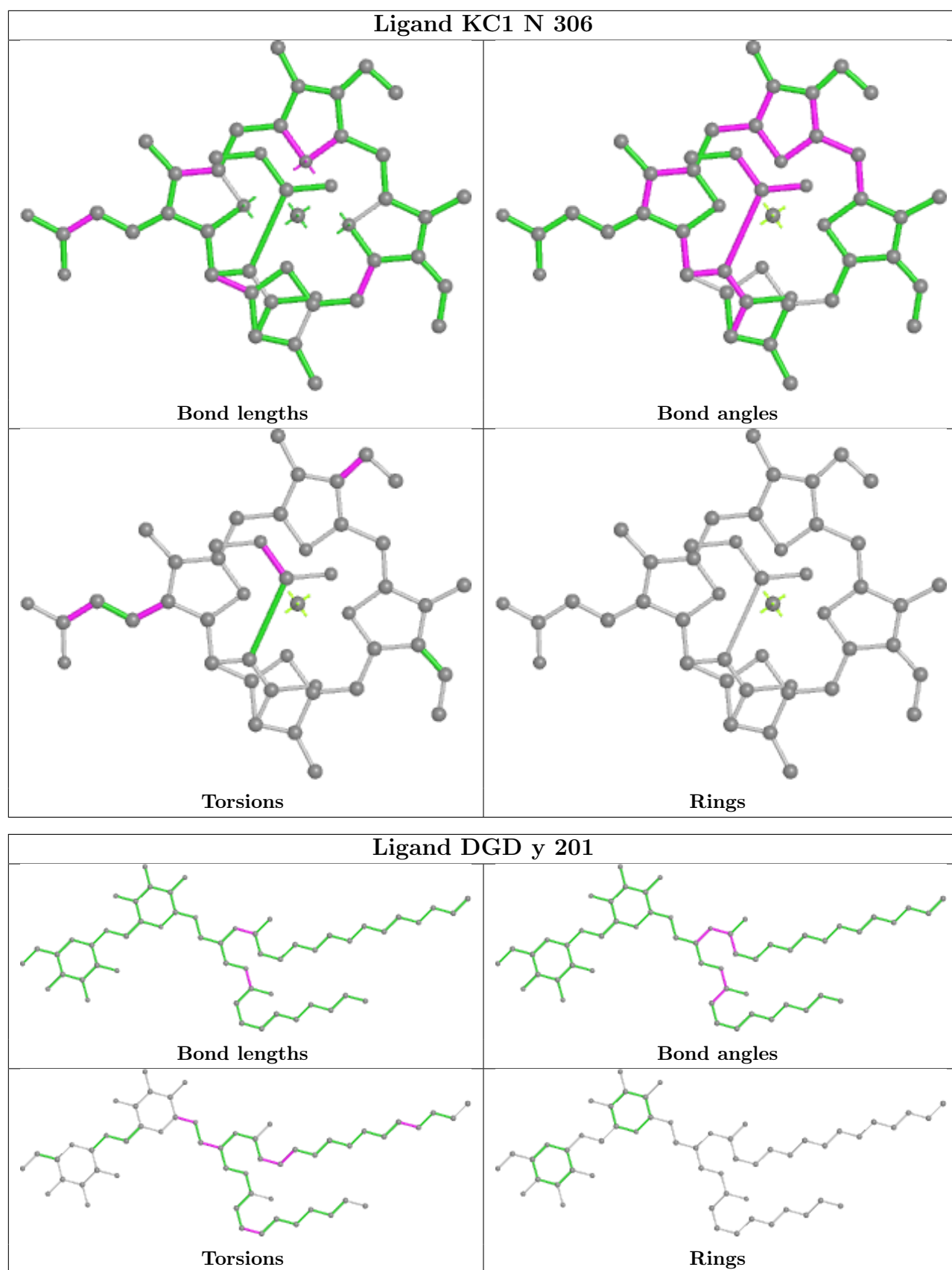


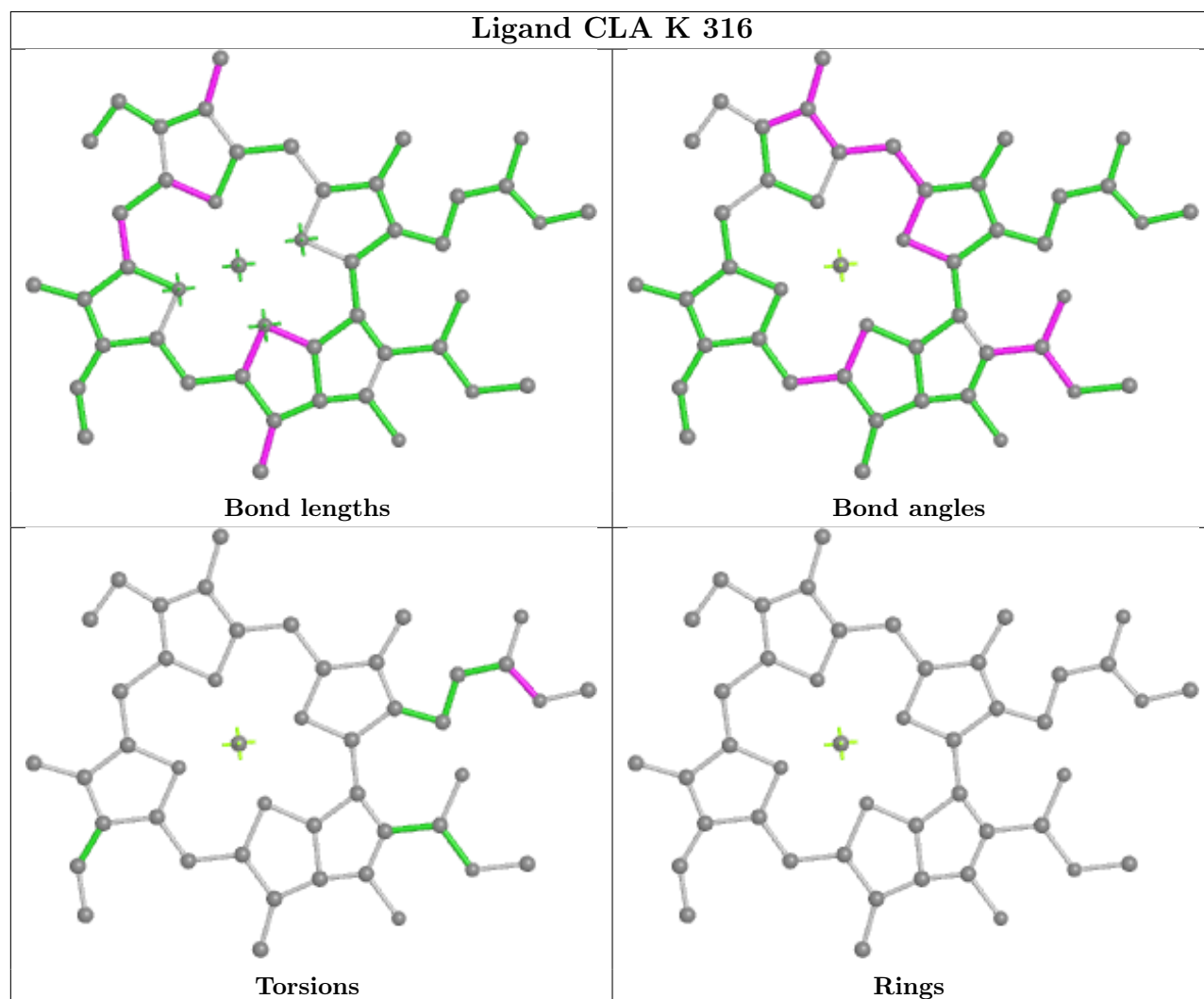
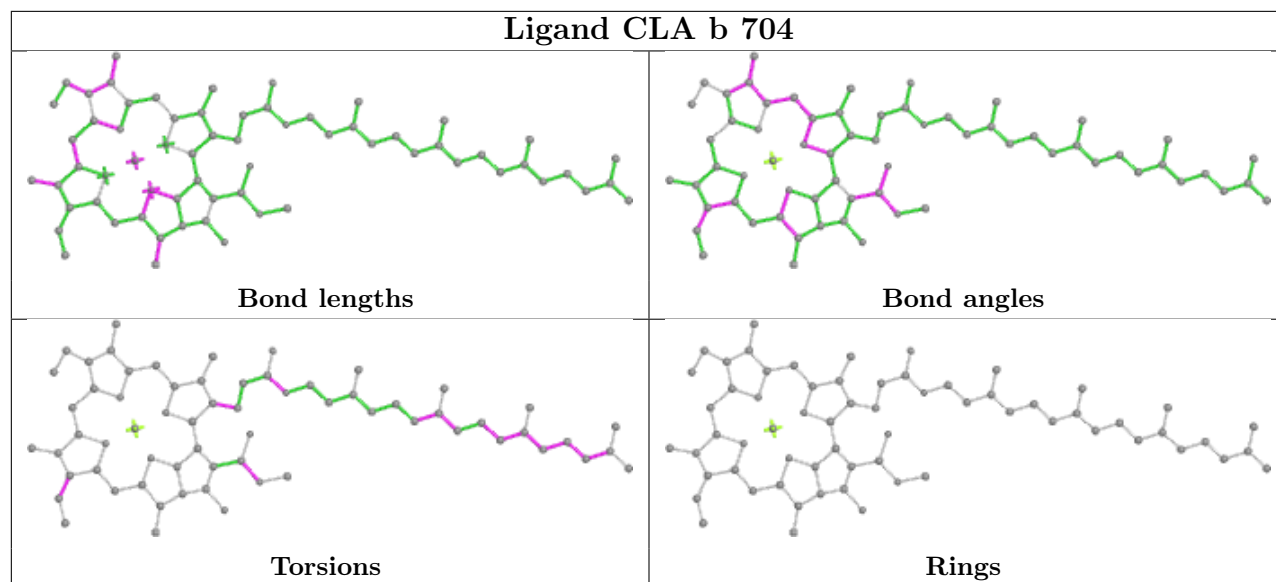


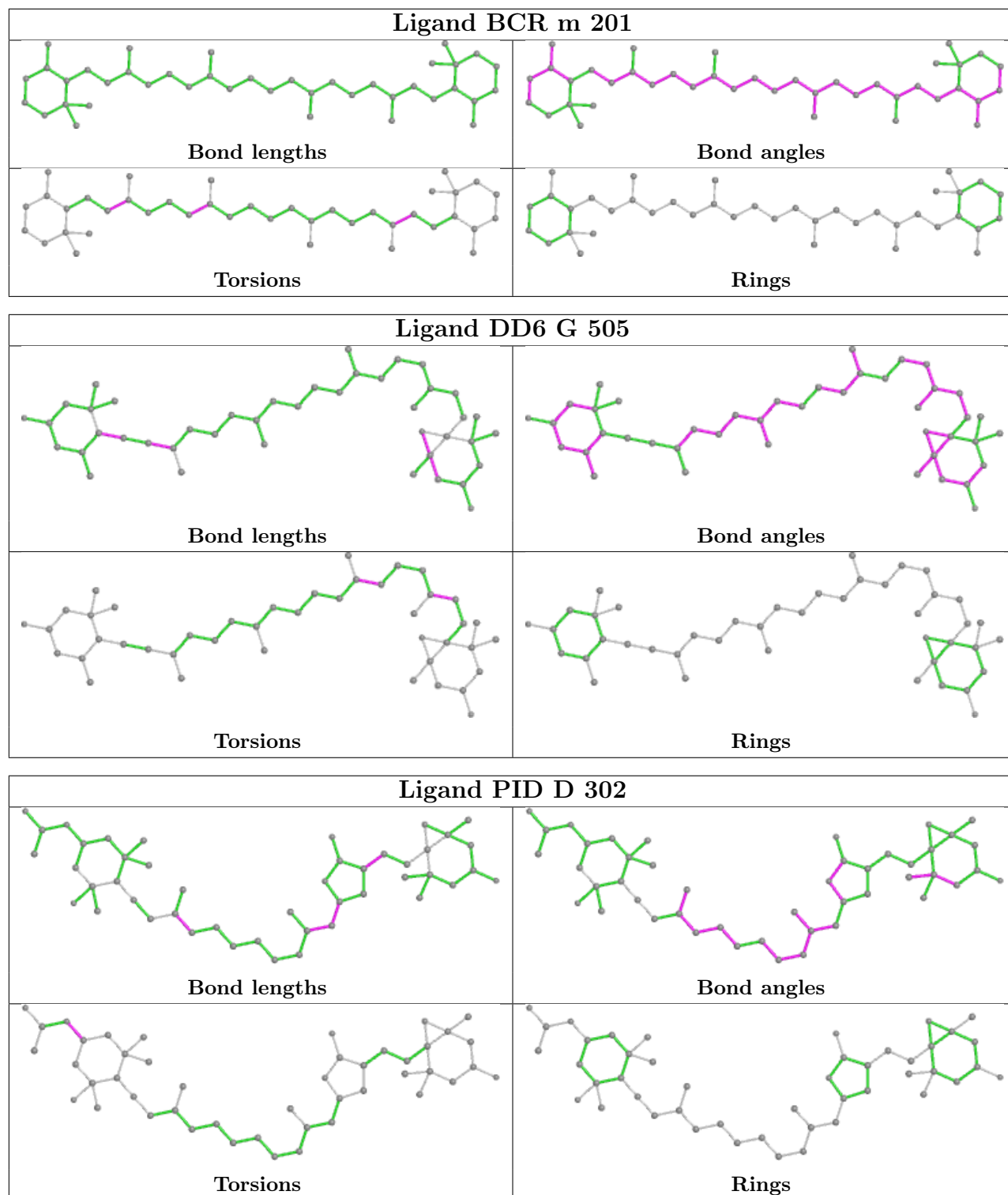


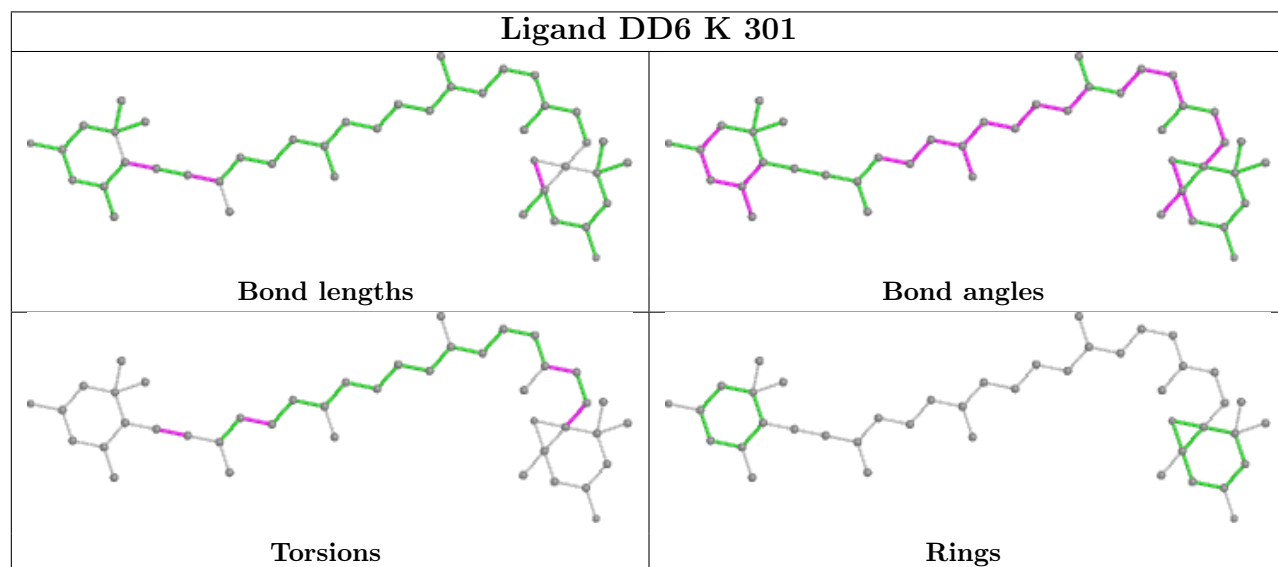
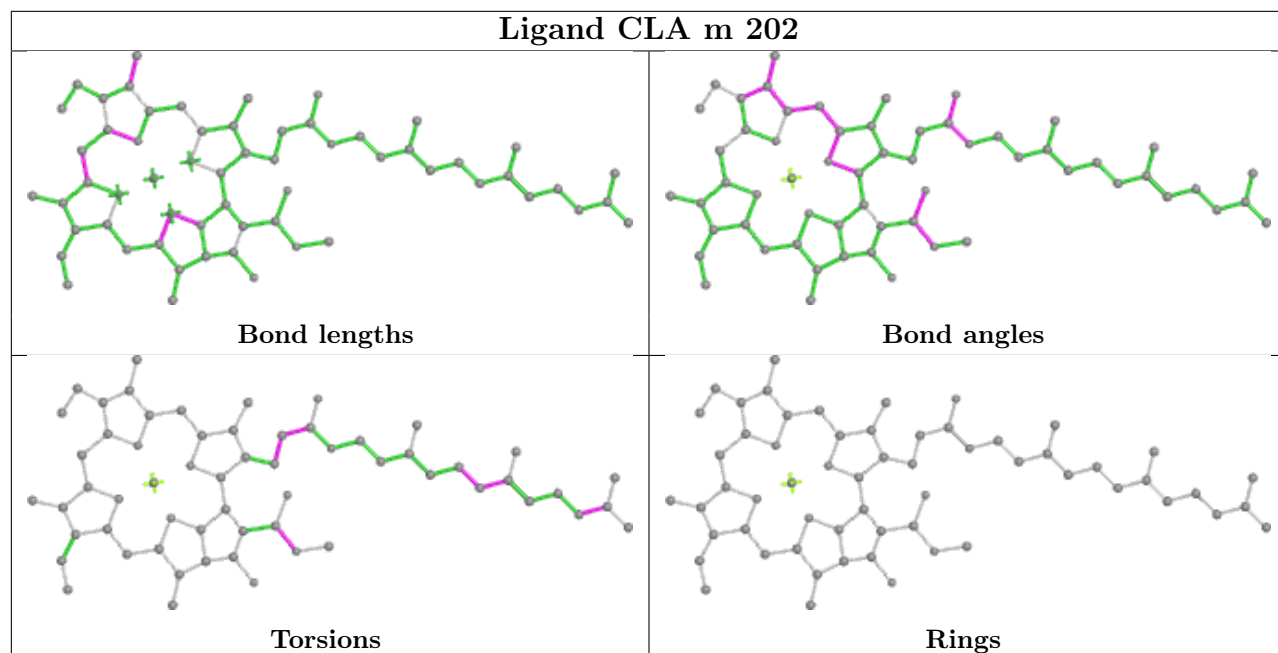


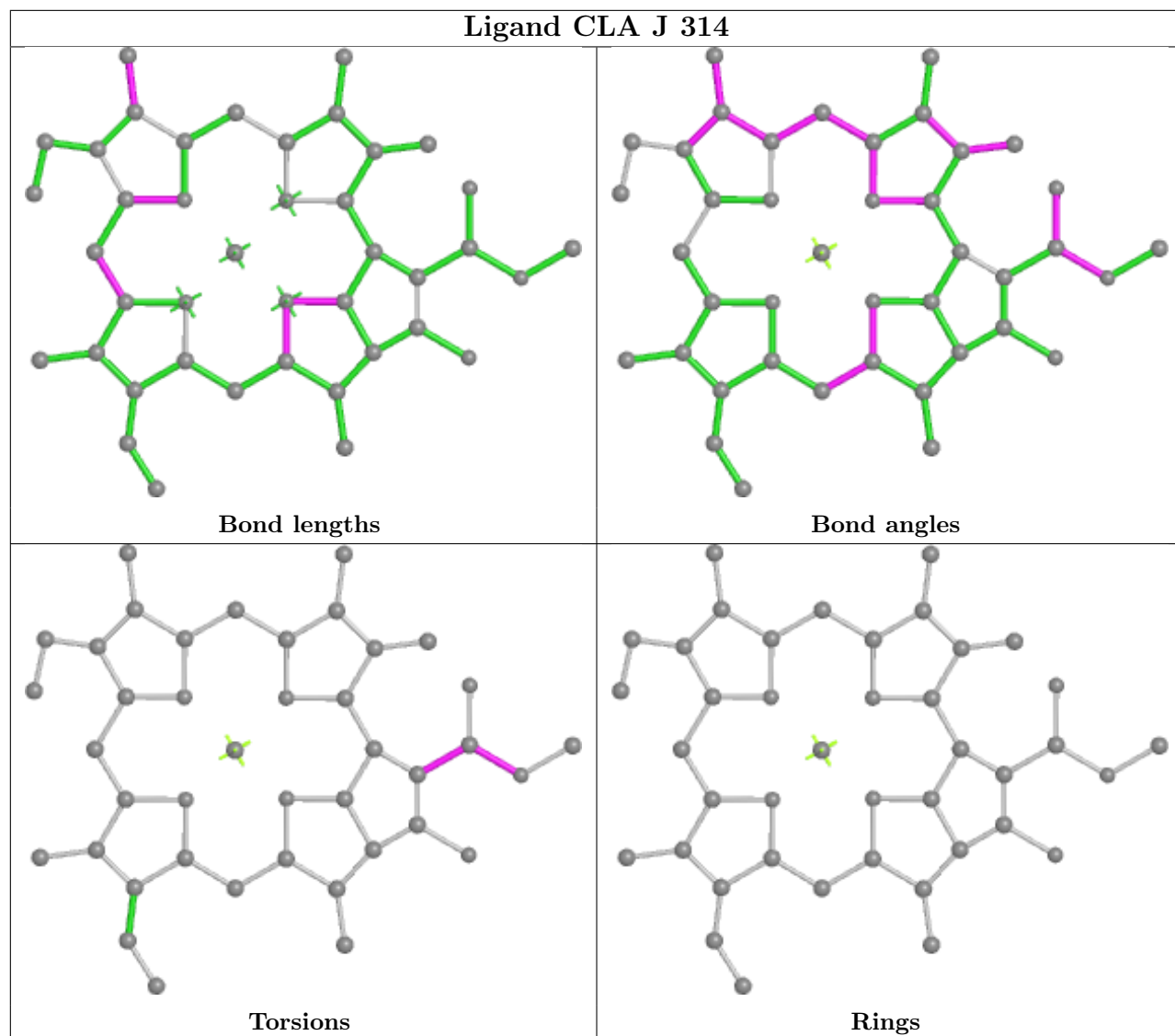


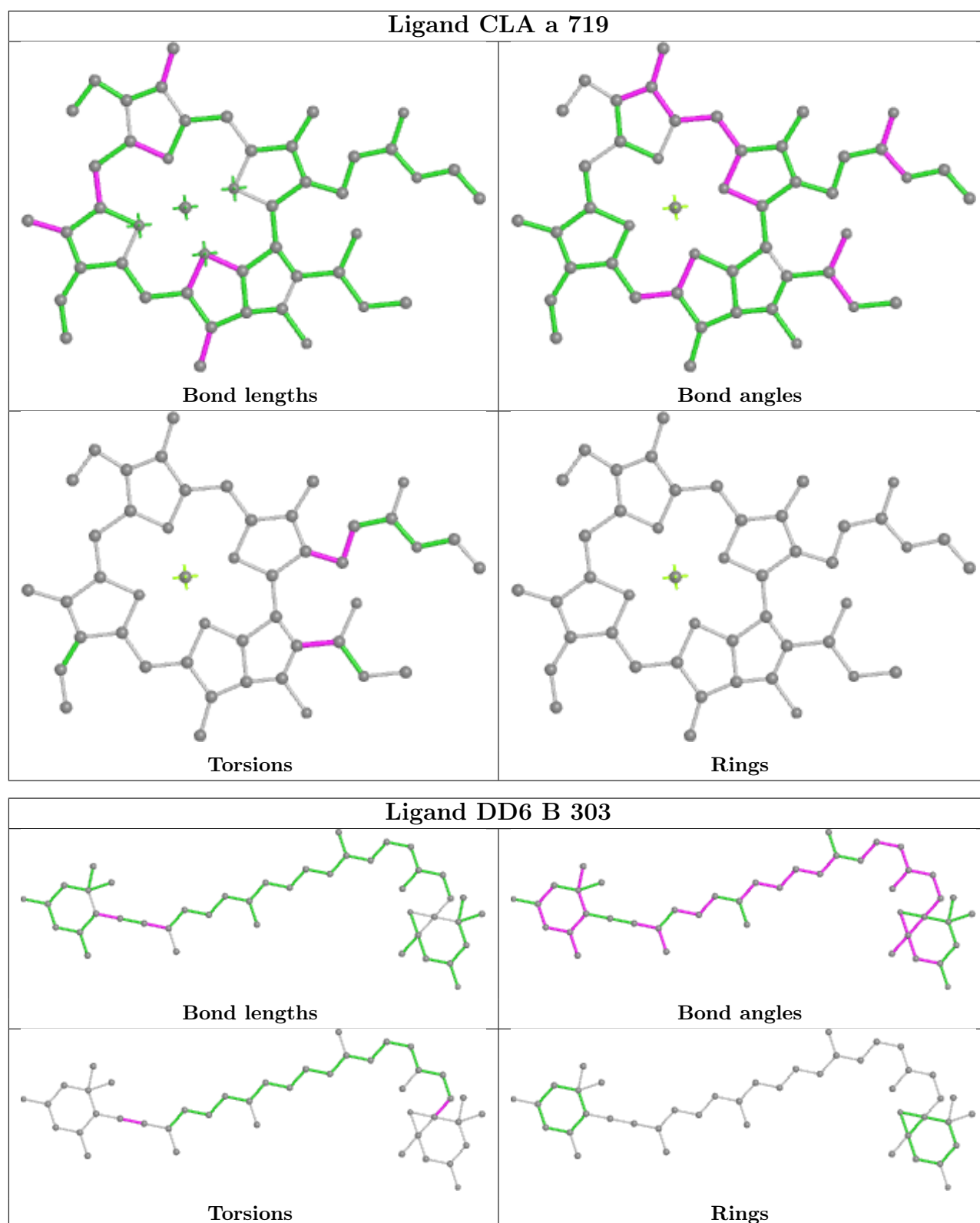


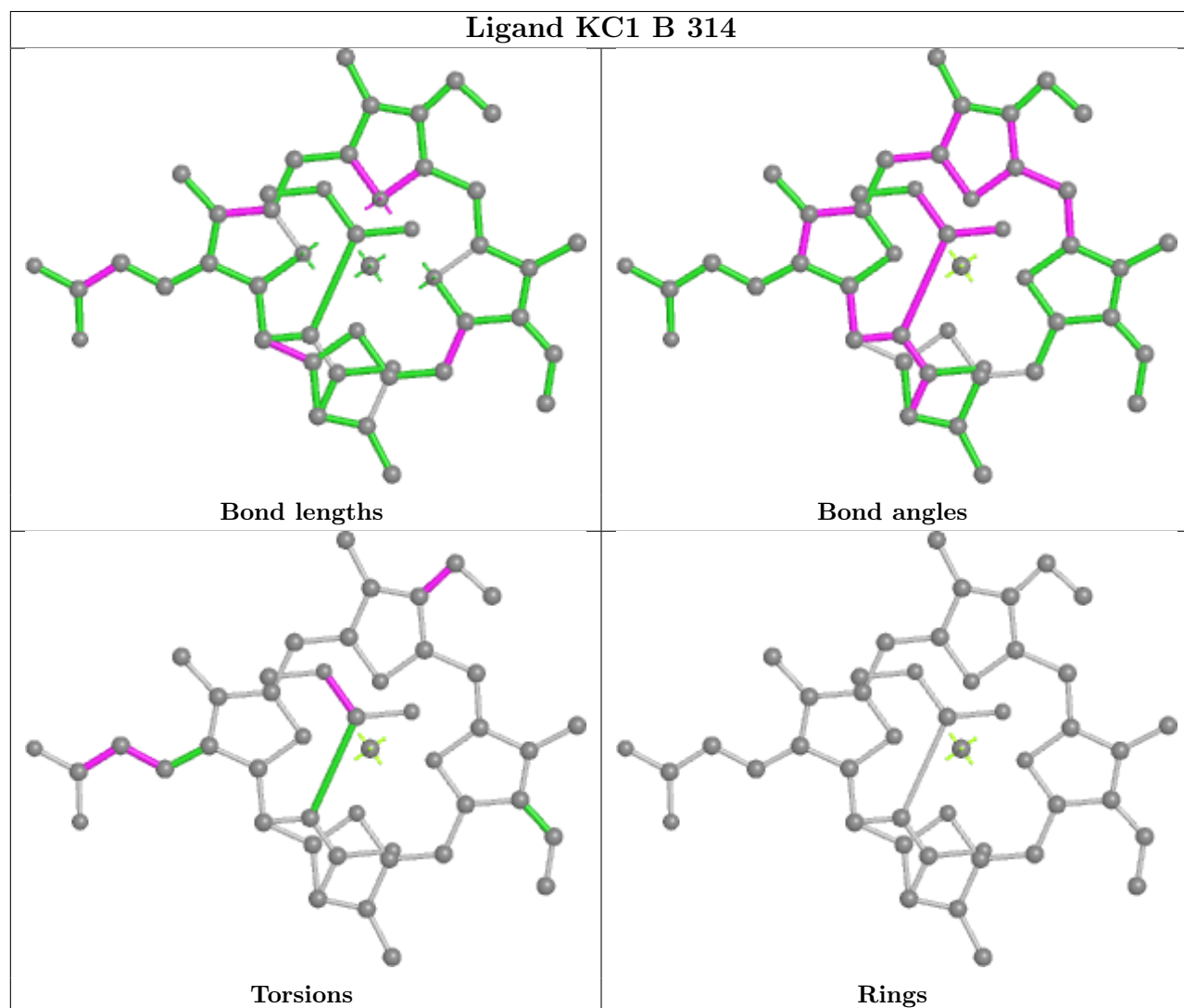
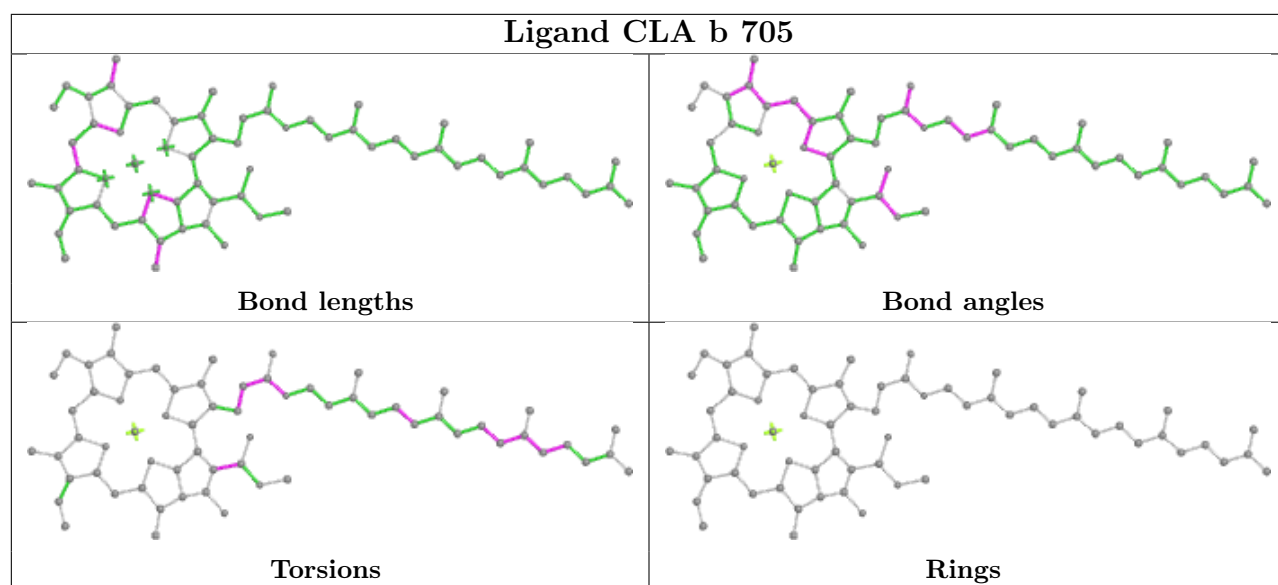


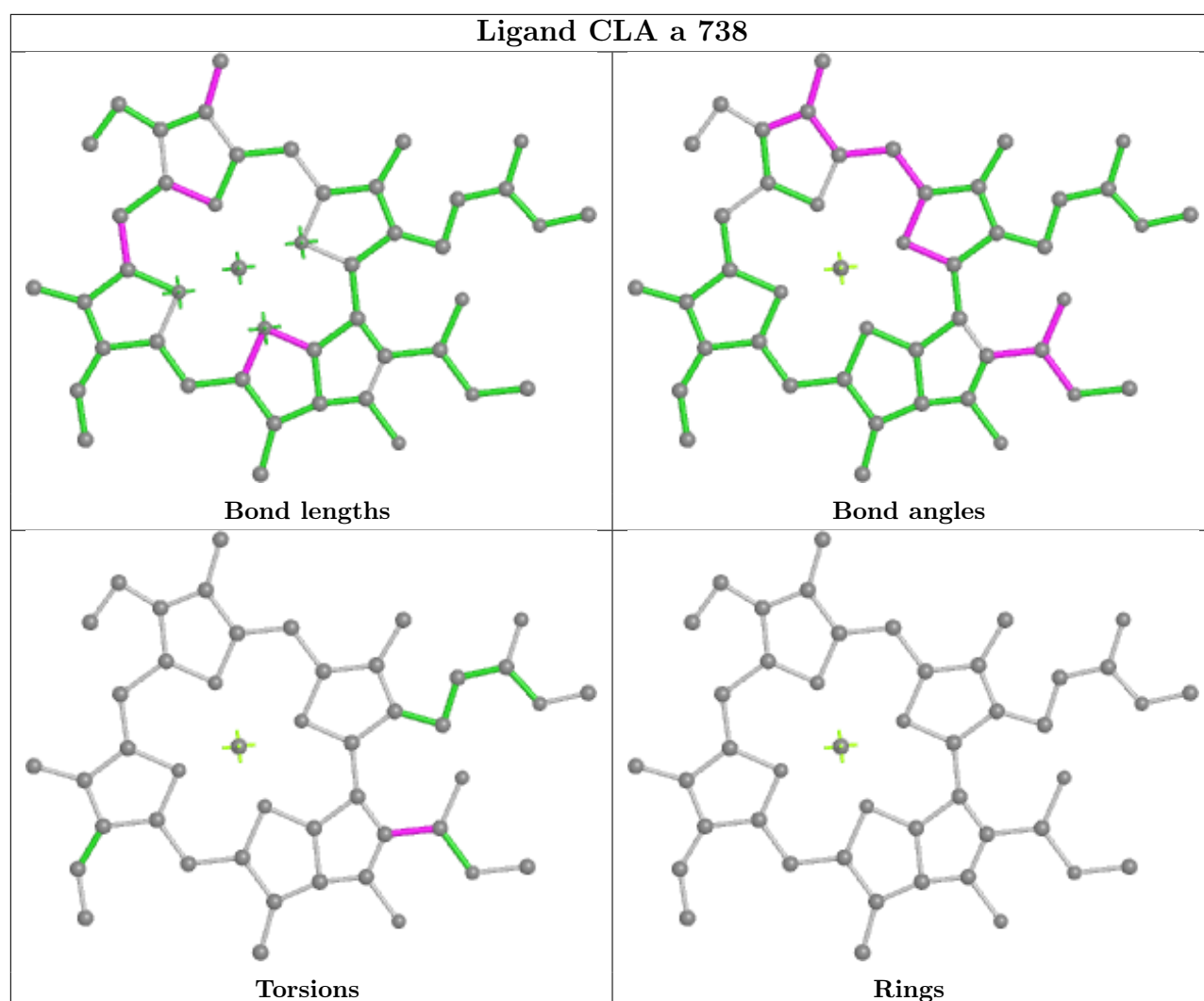
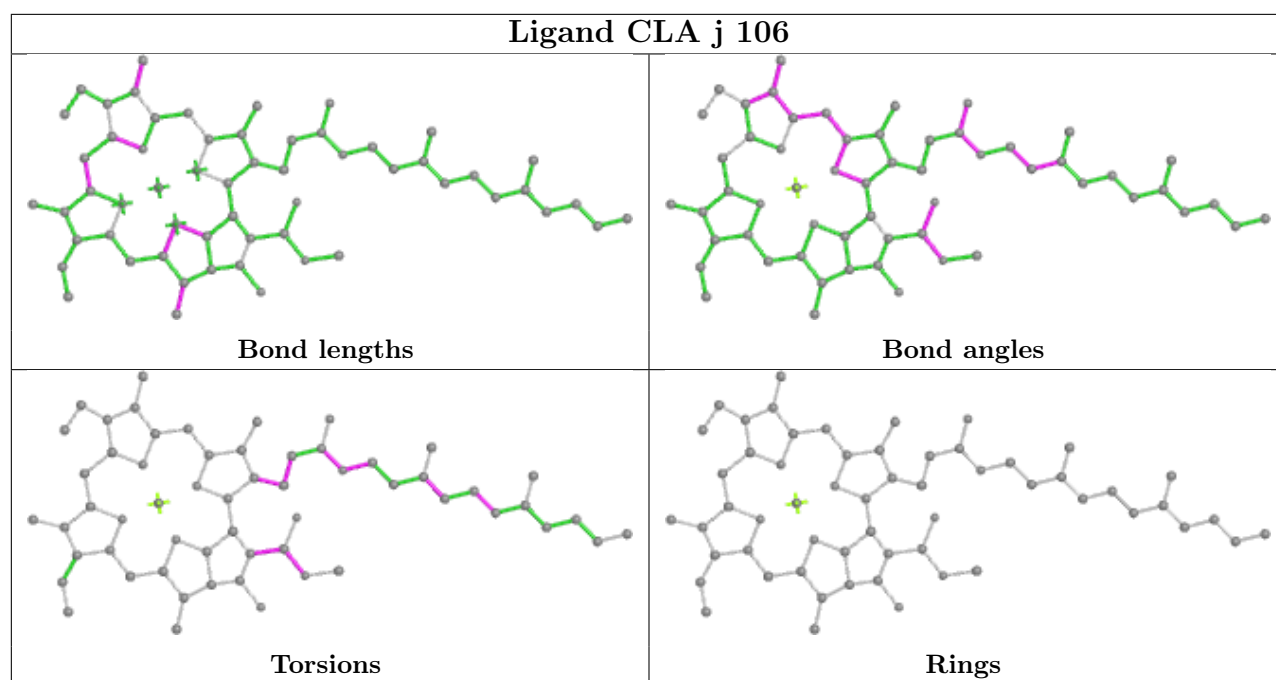


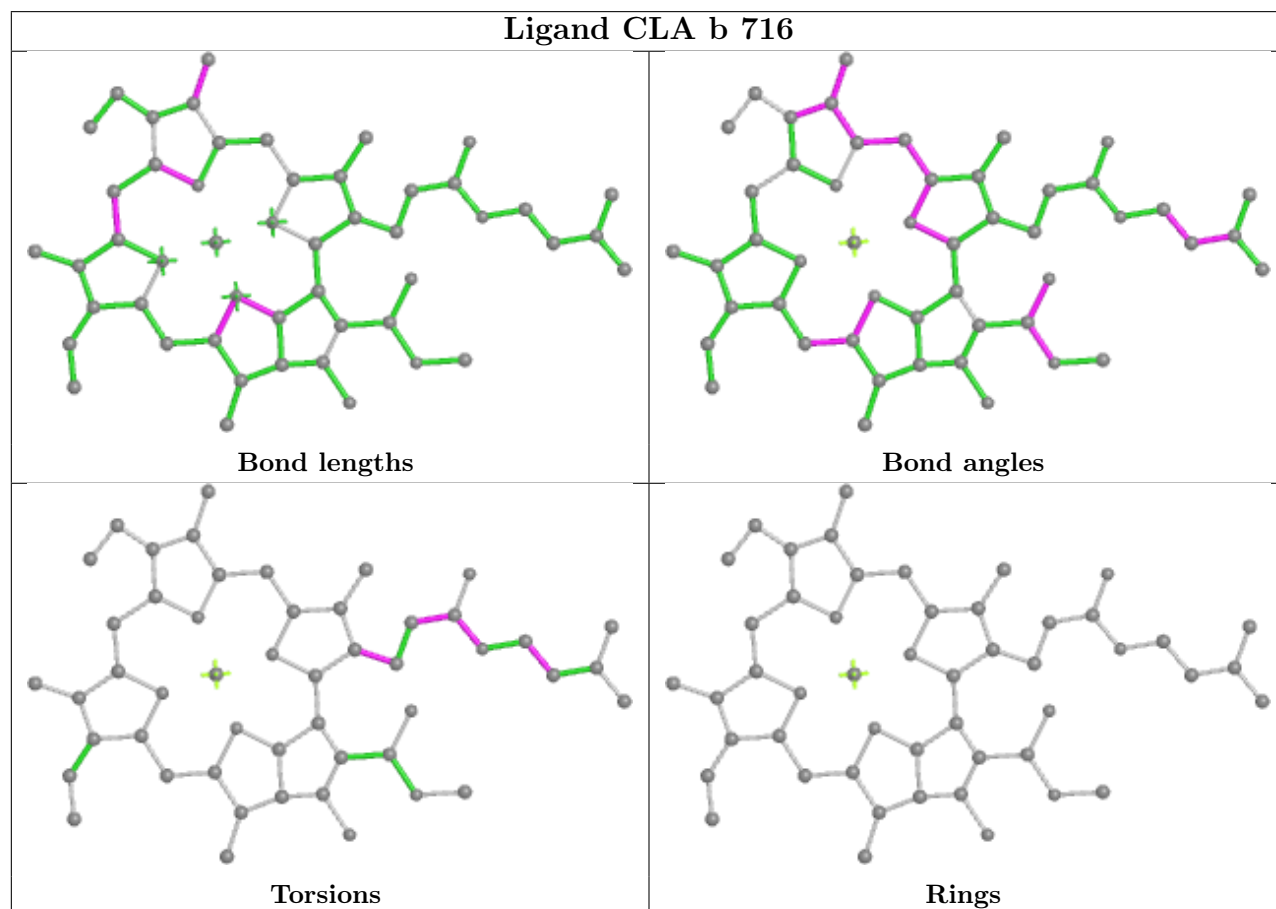
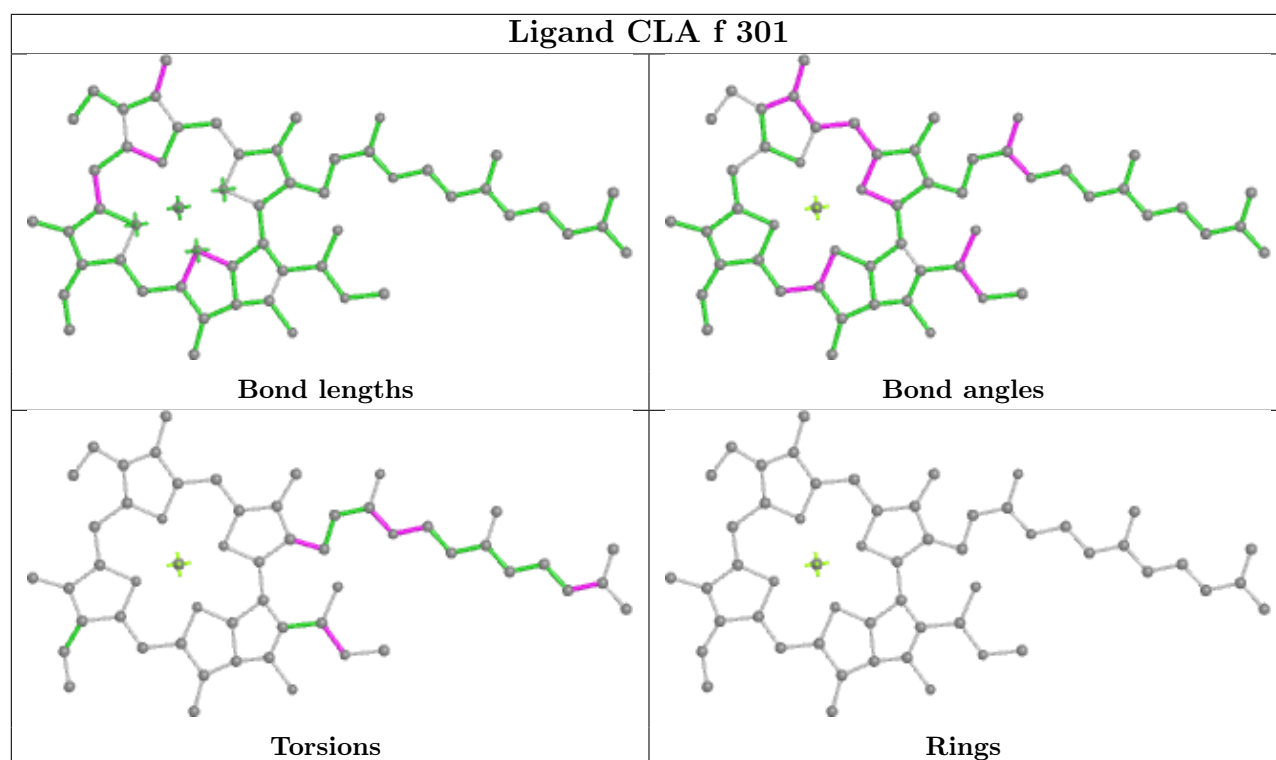




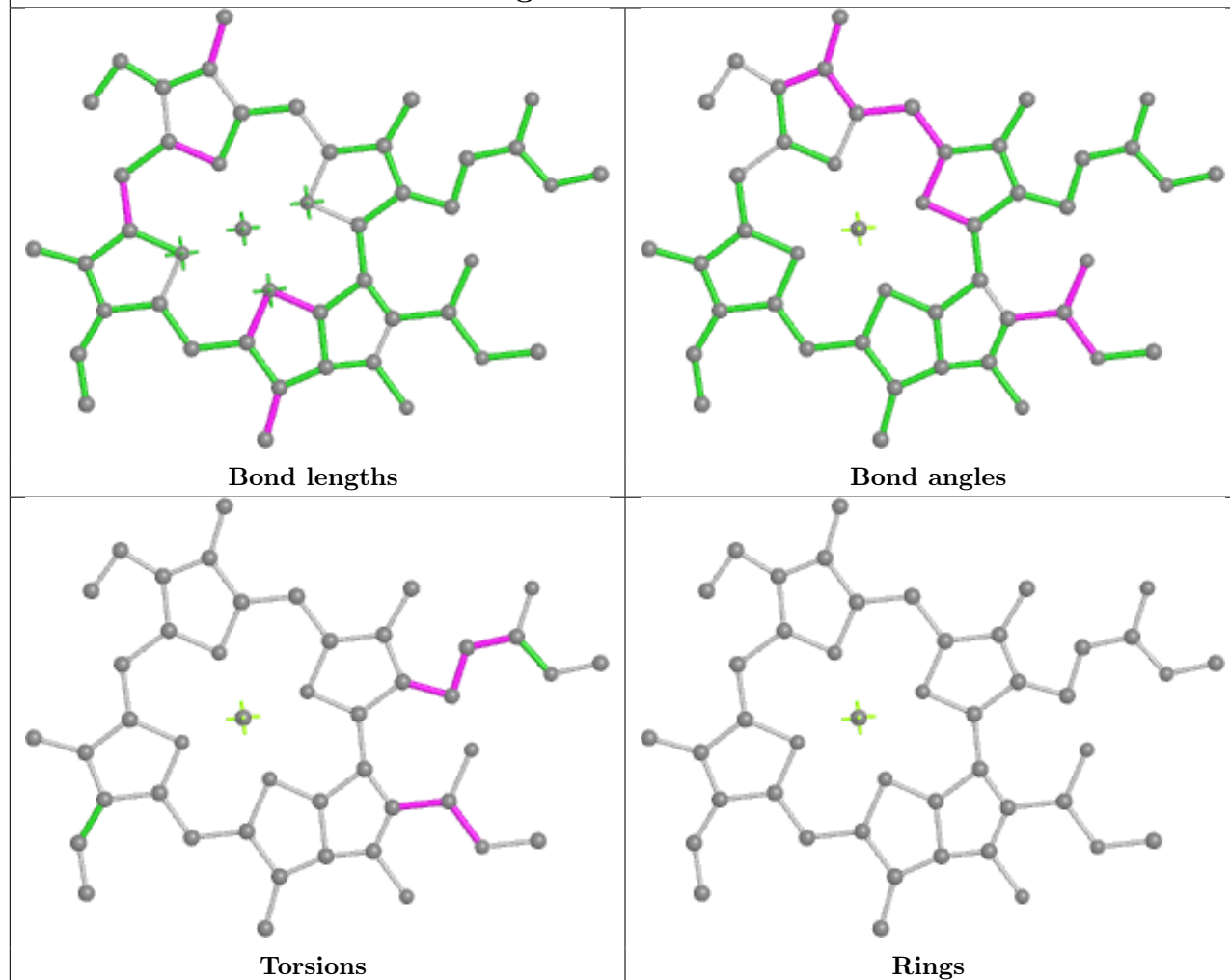




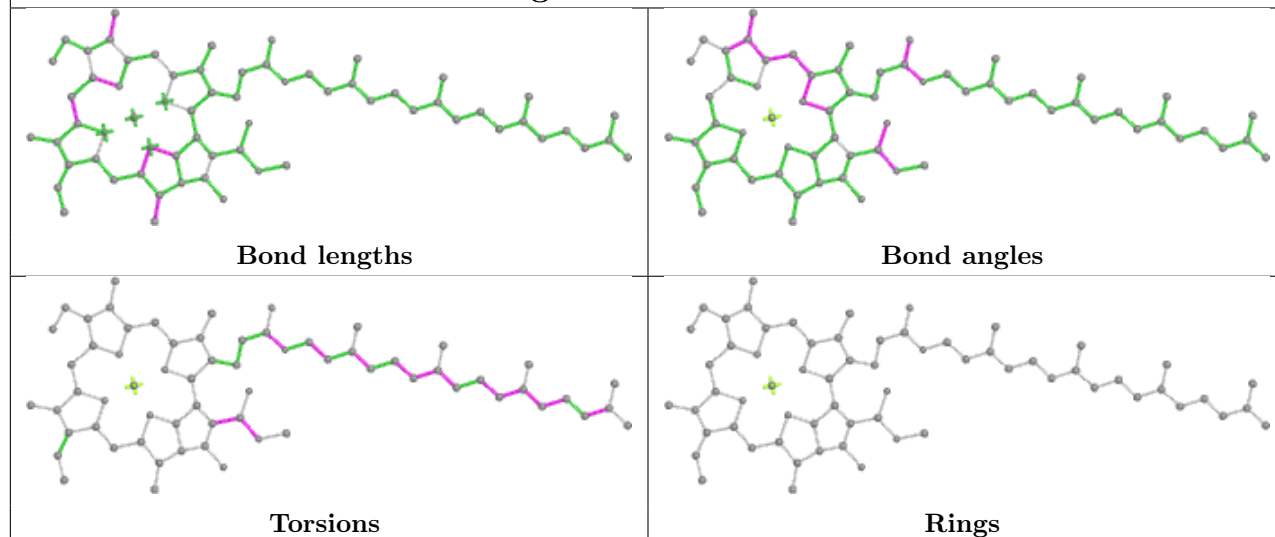


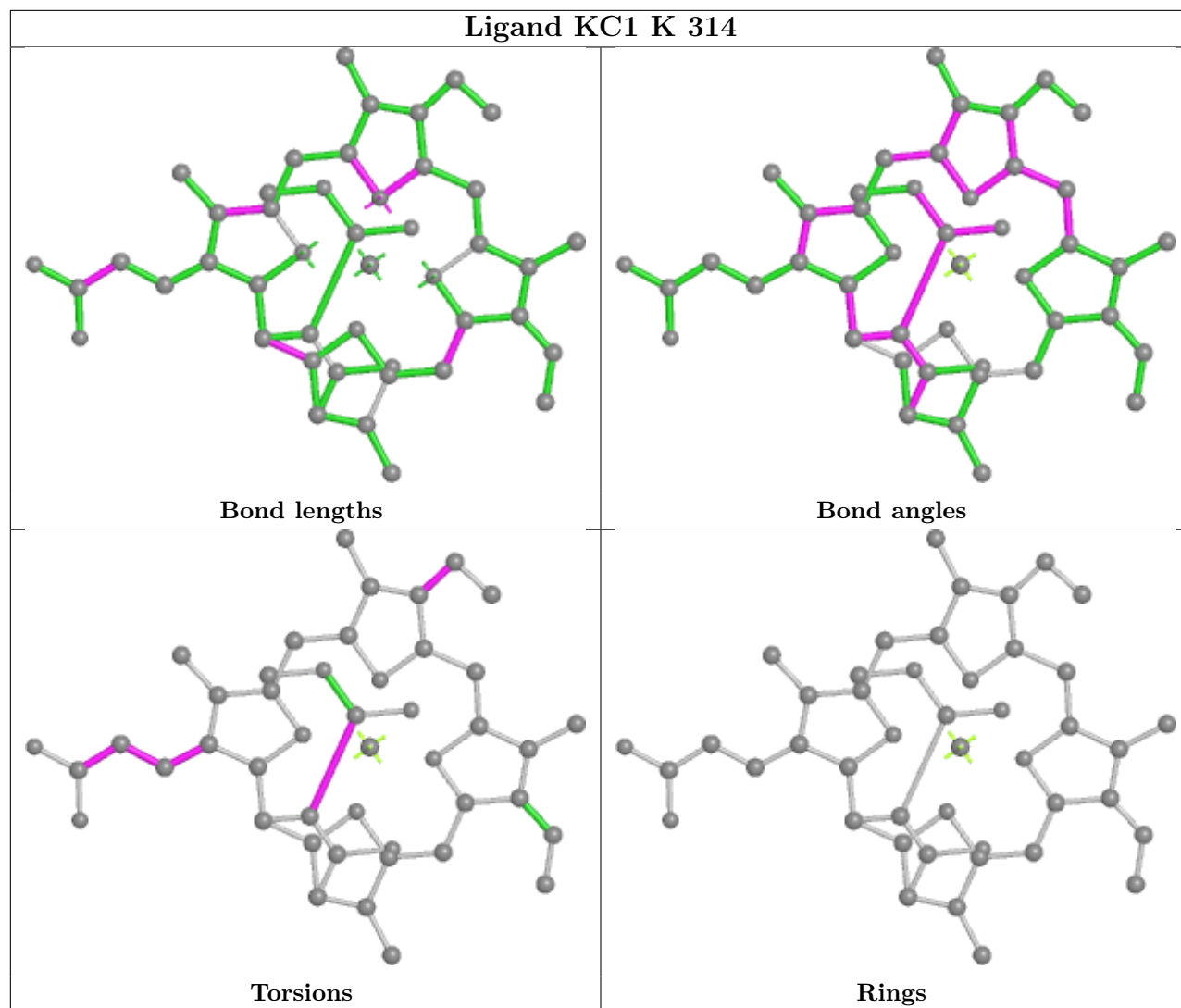


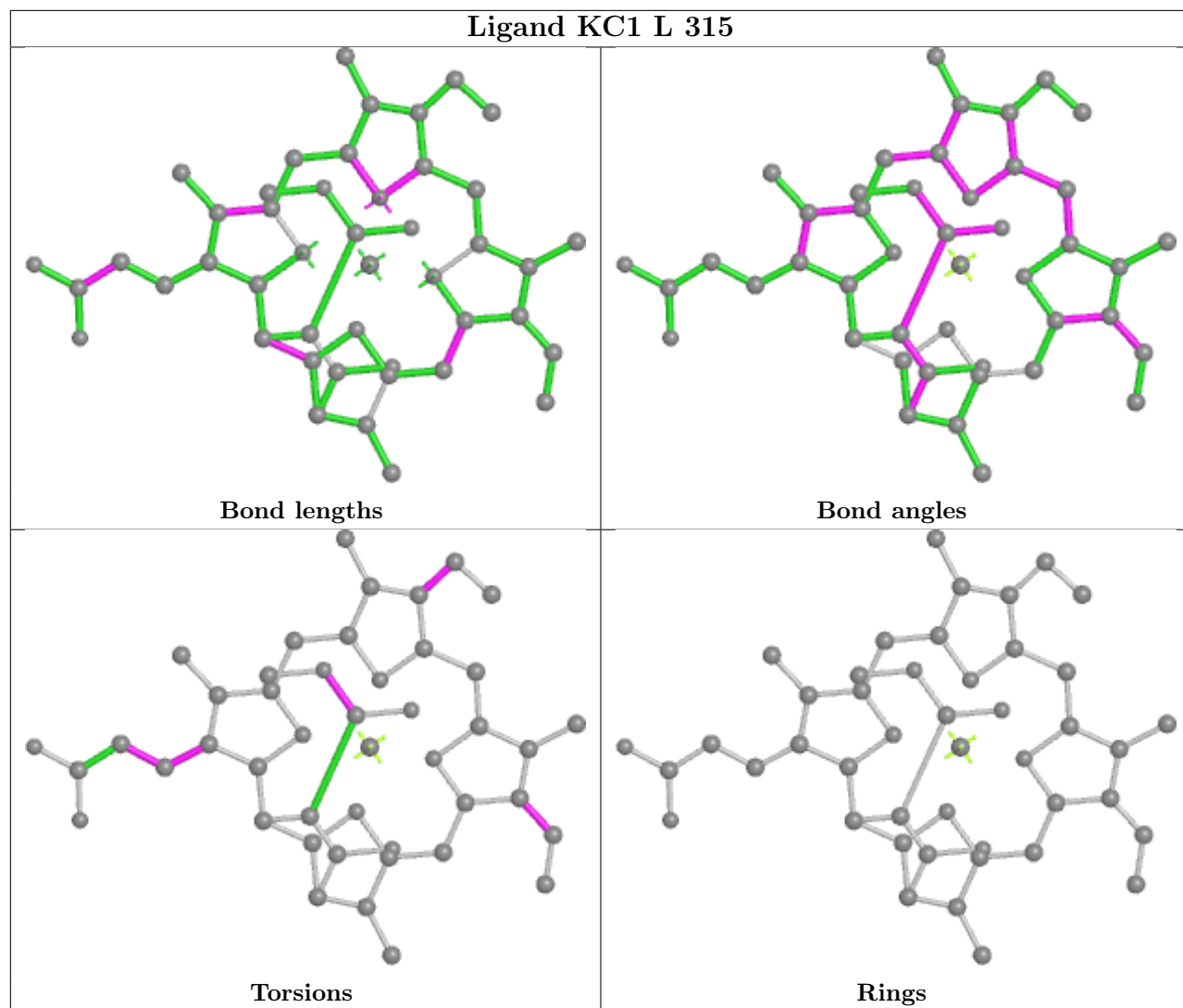
Ligand CLA J 308

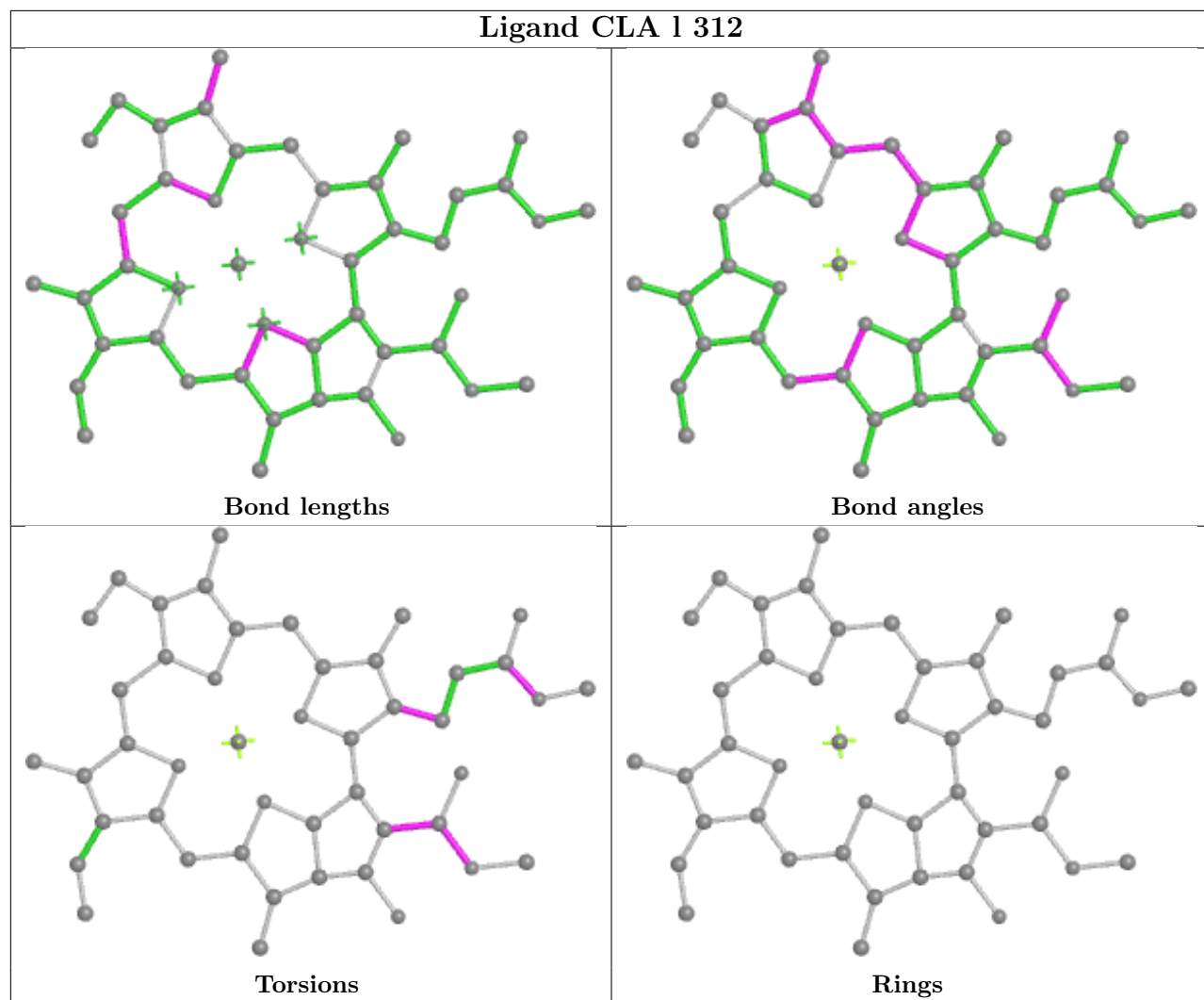


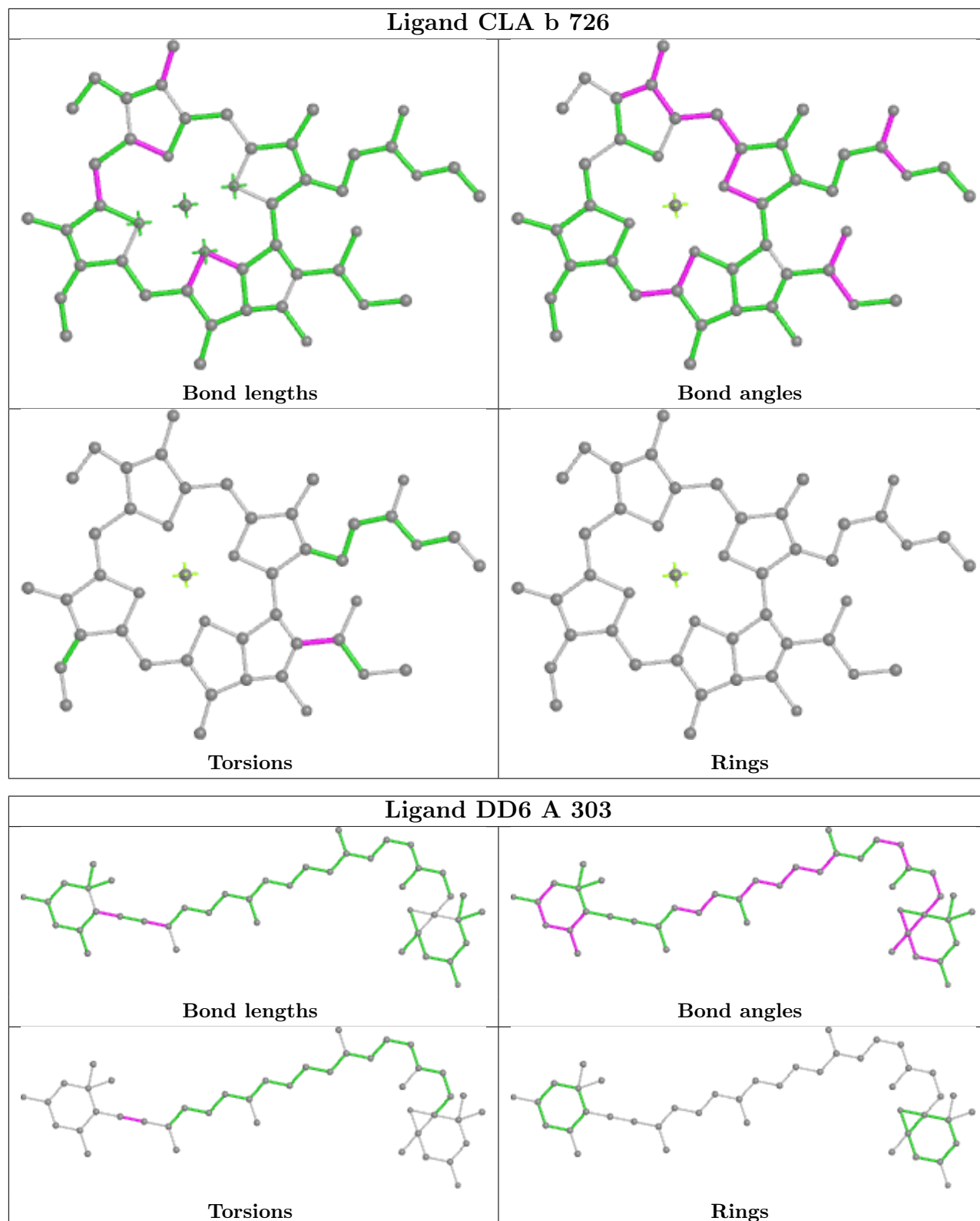
Ligand CLA B 311

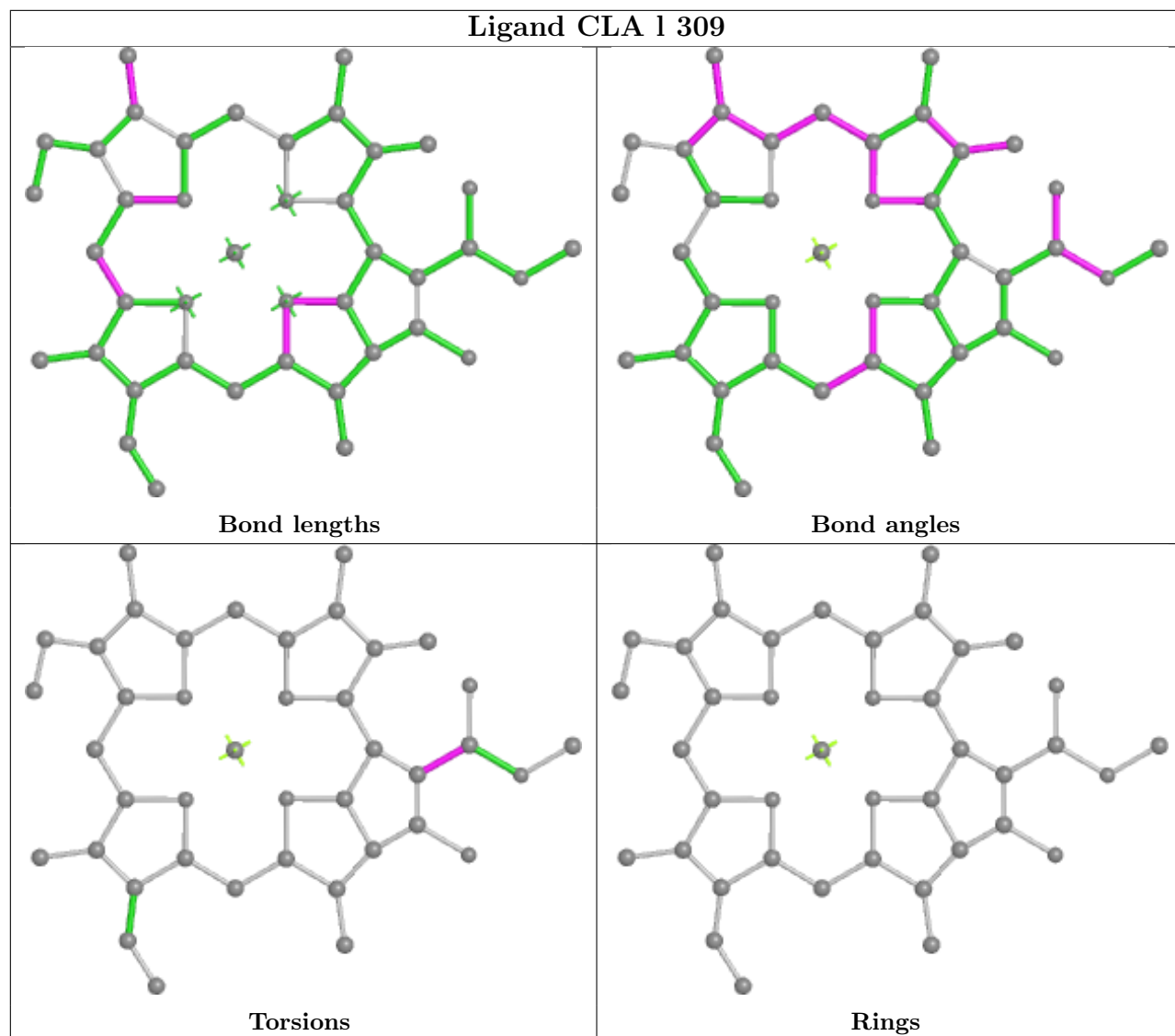


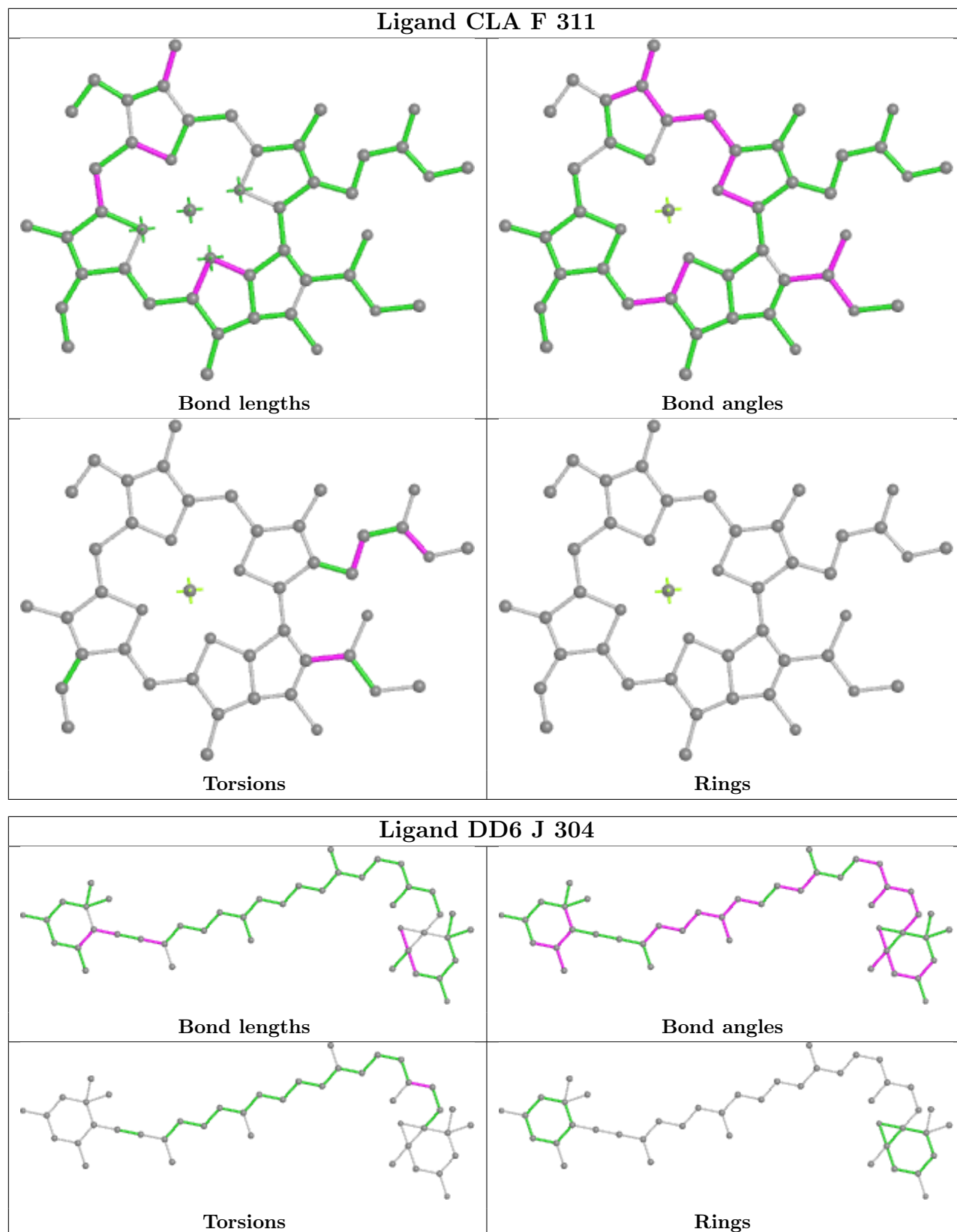


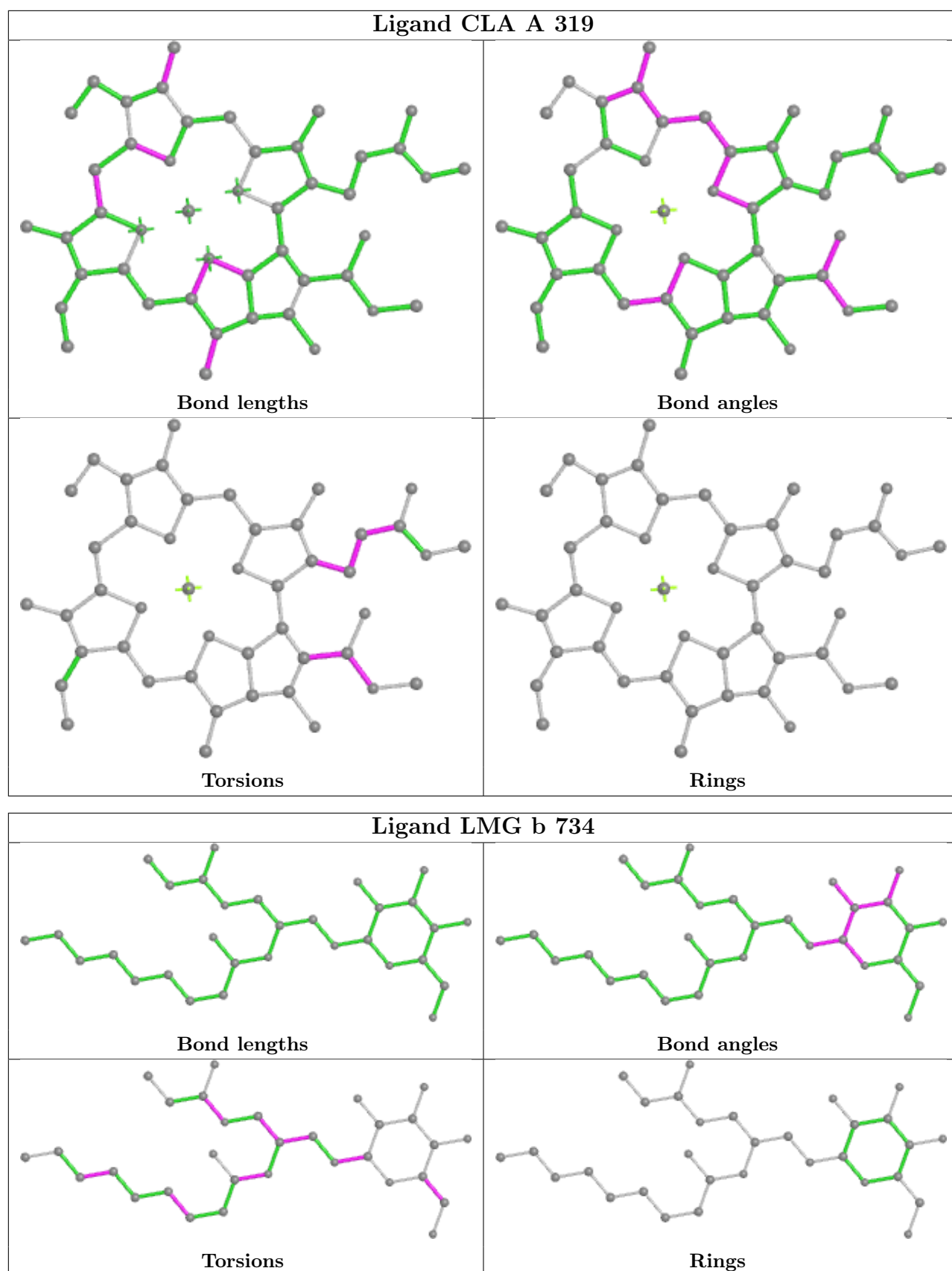


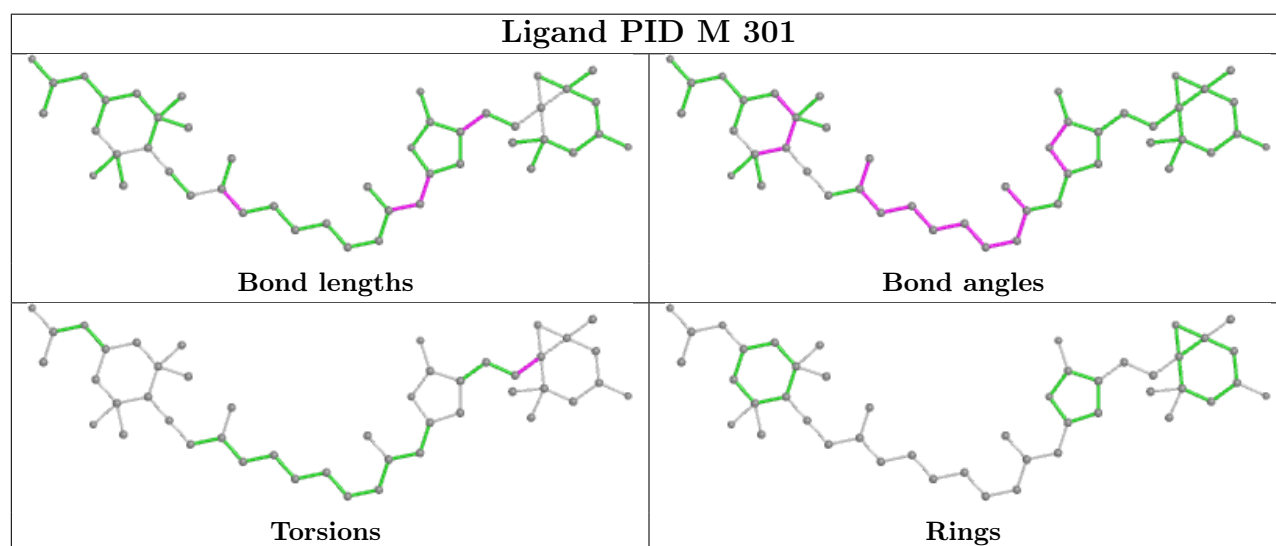
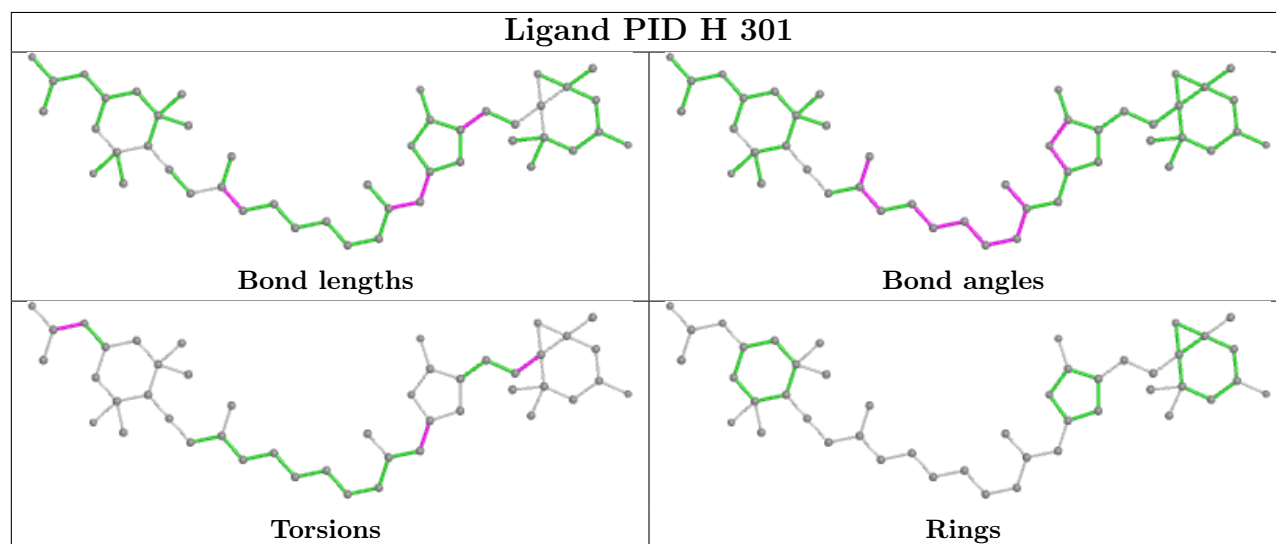
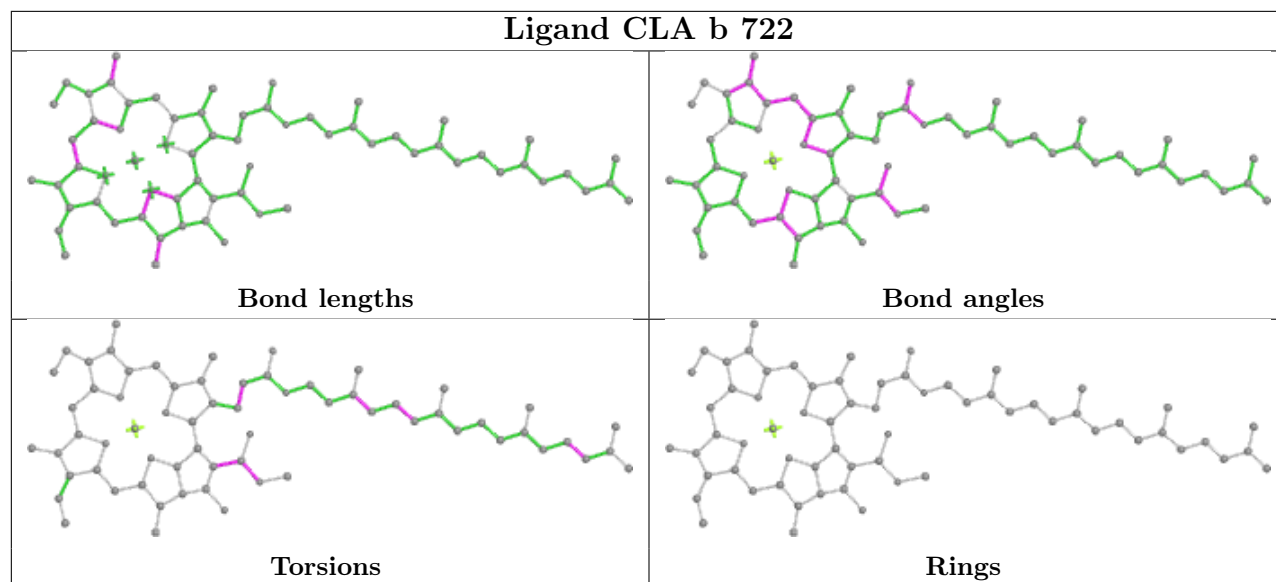


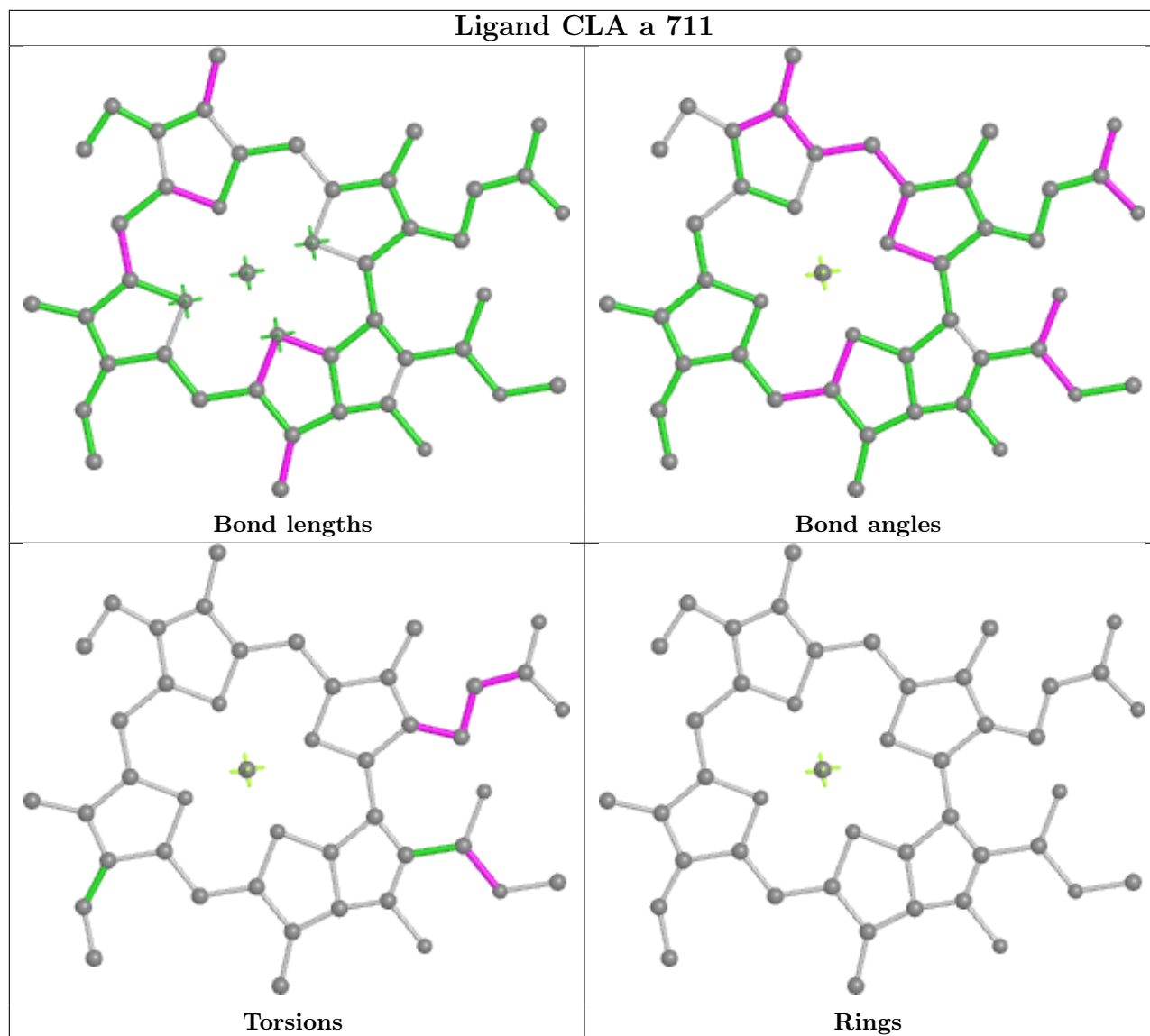
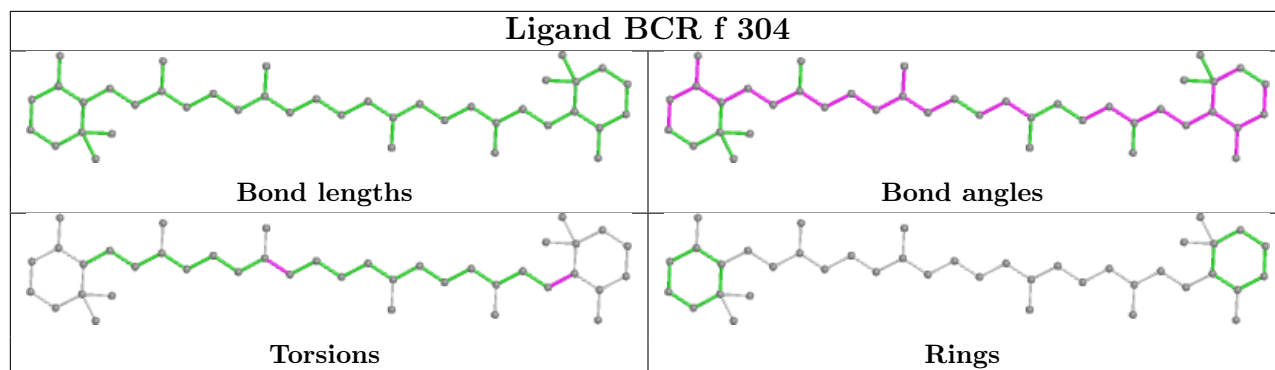


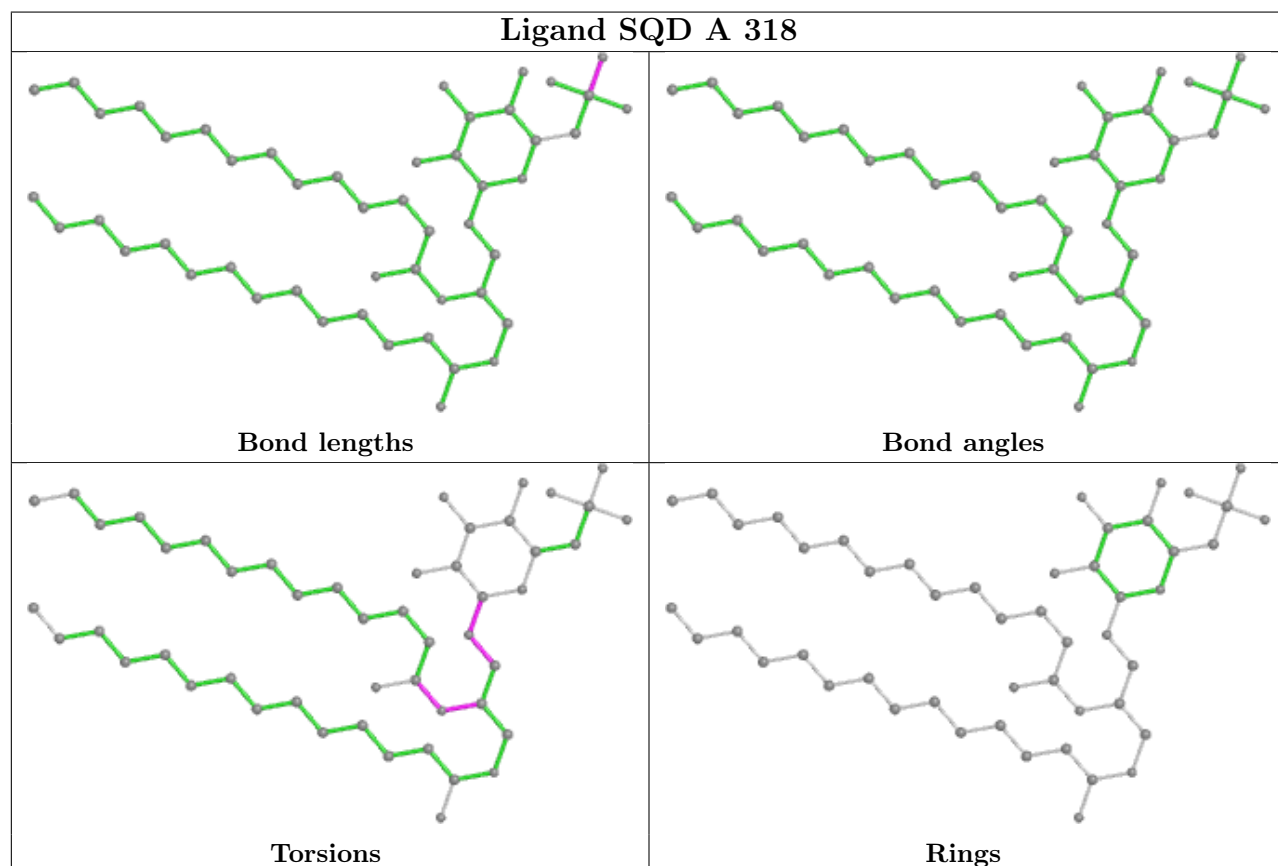
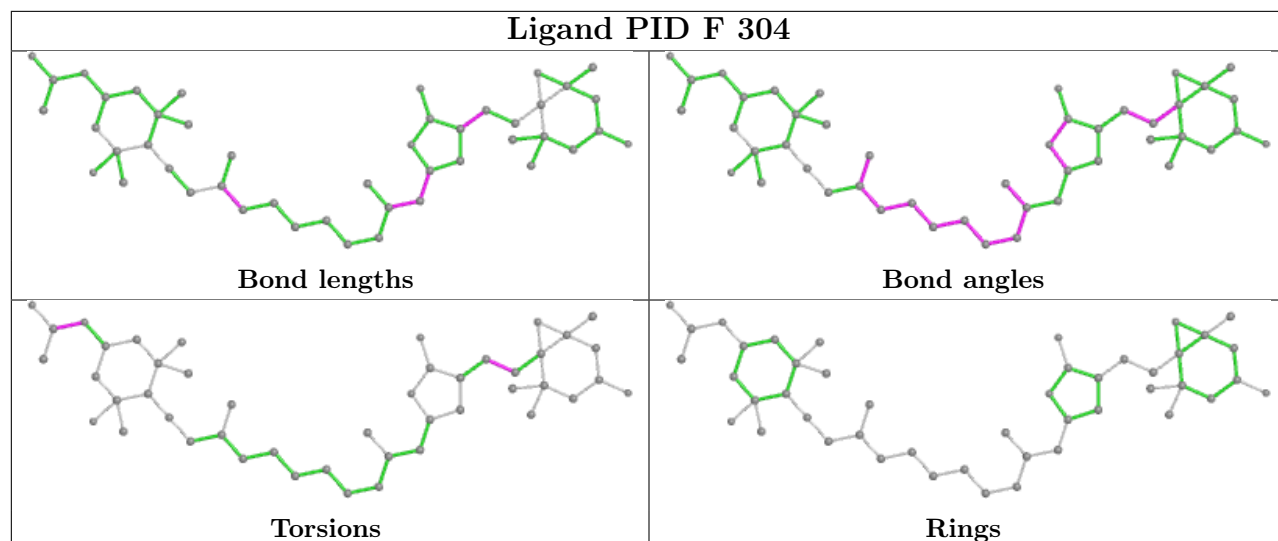


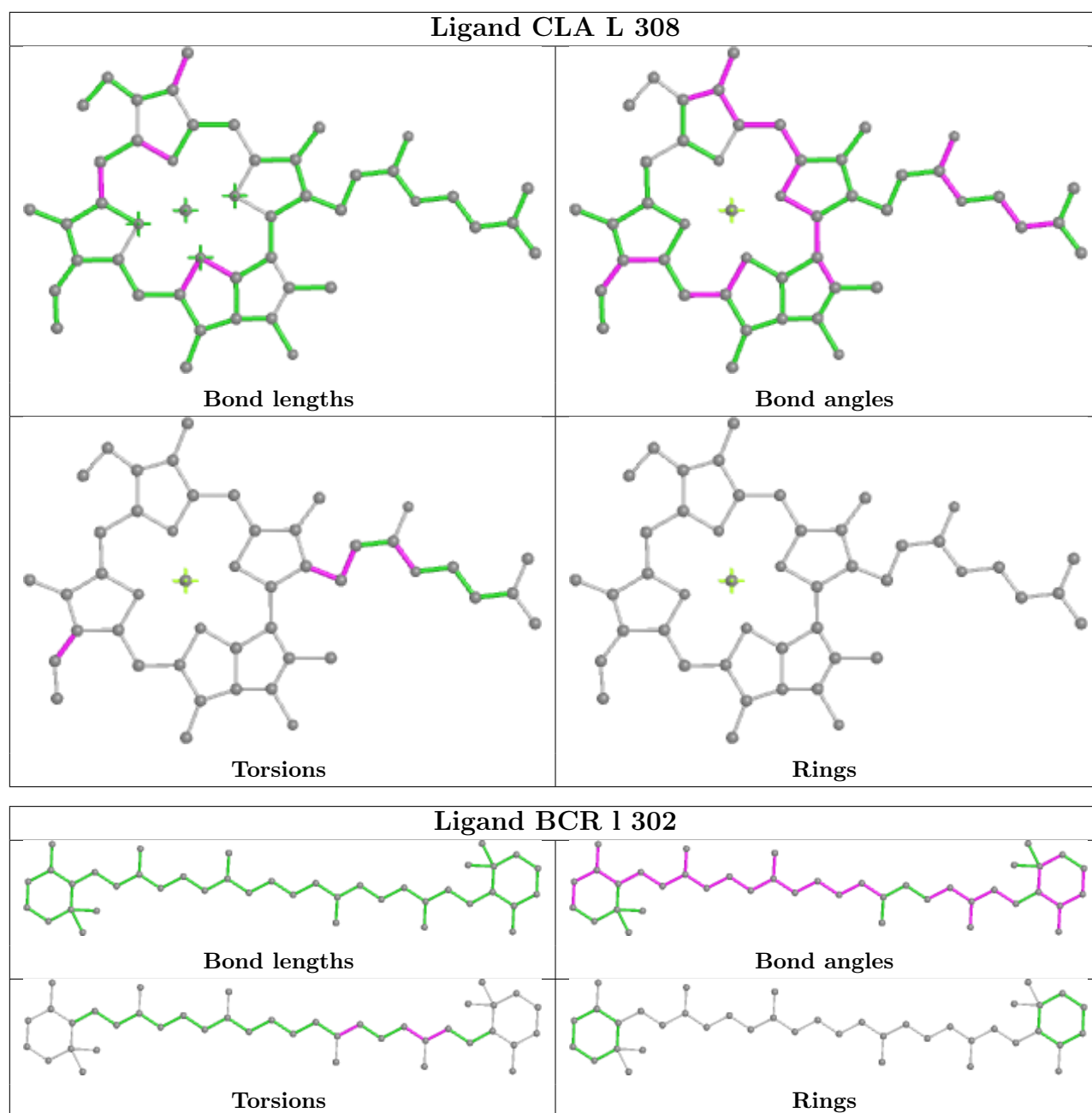


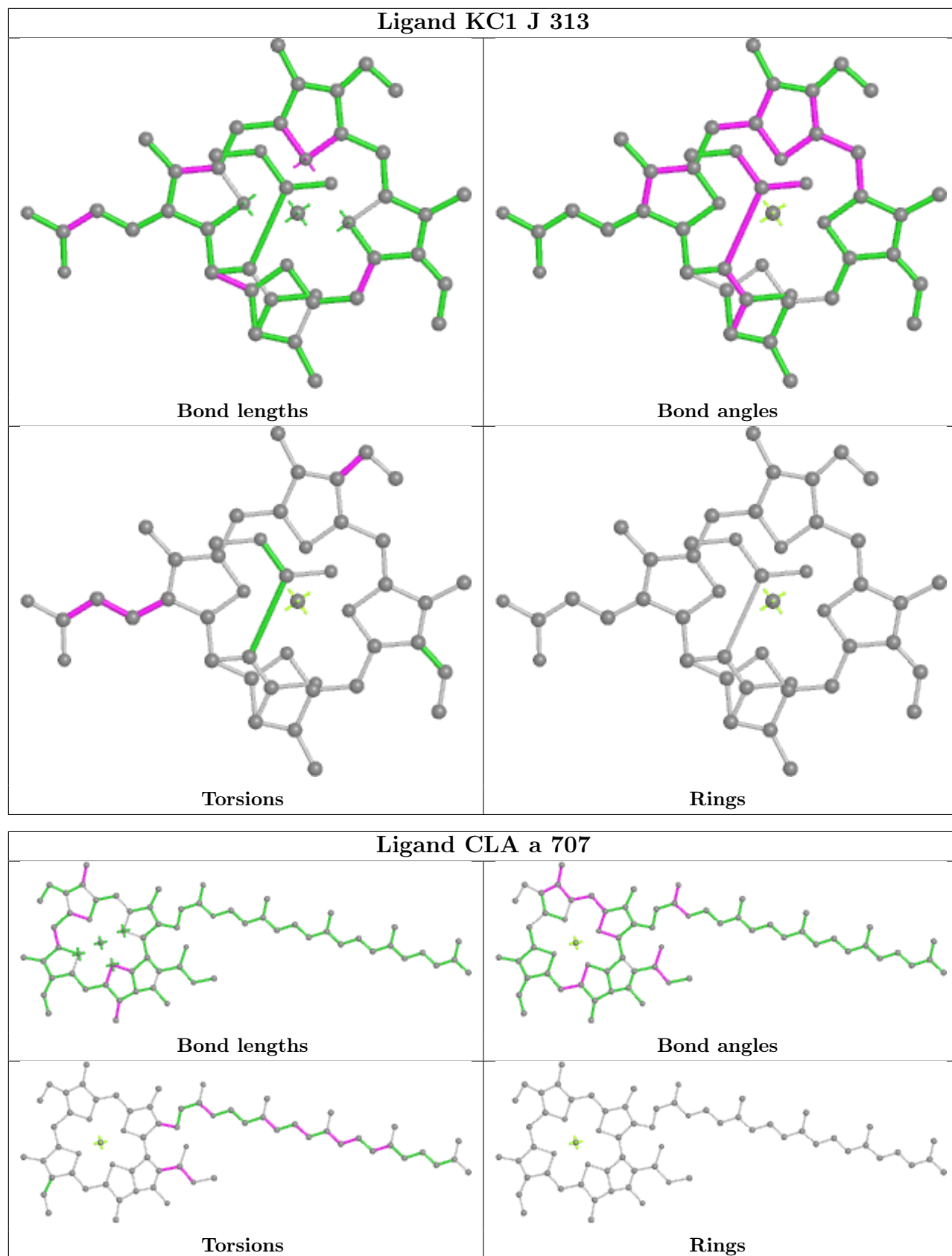


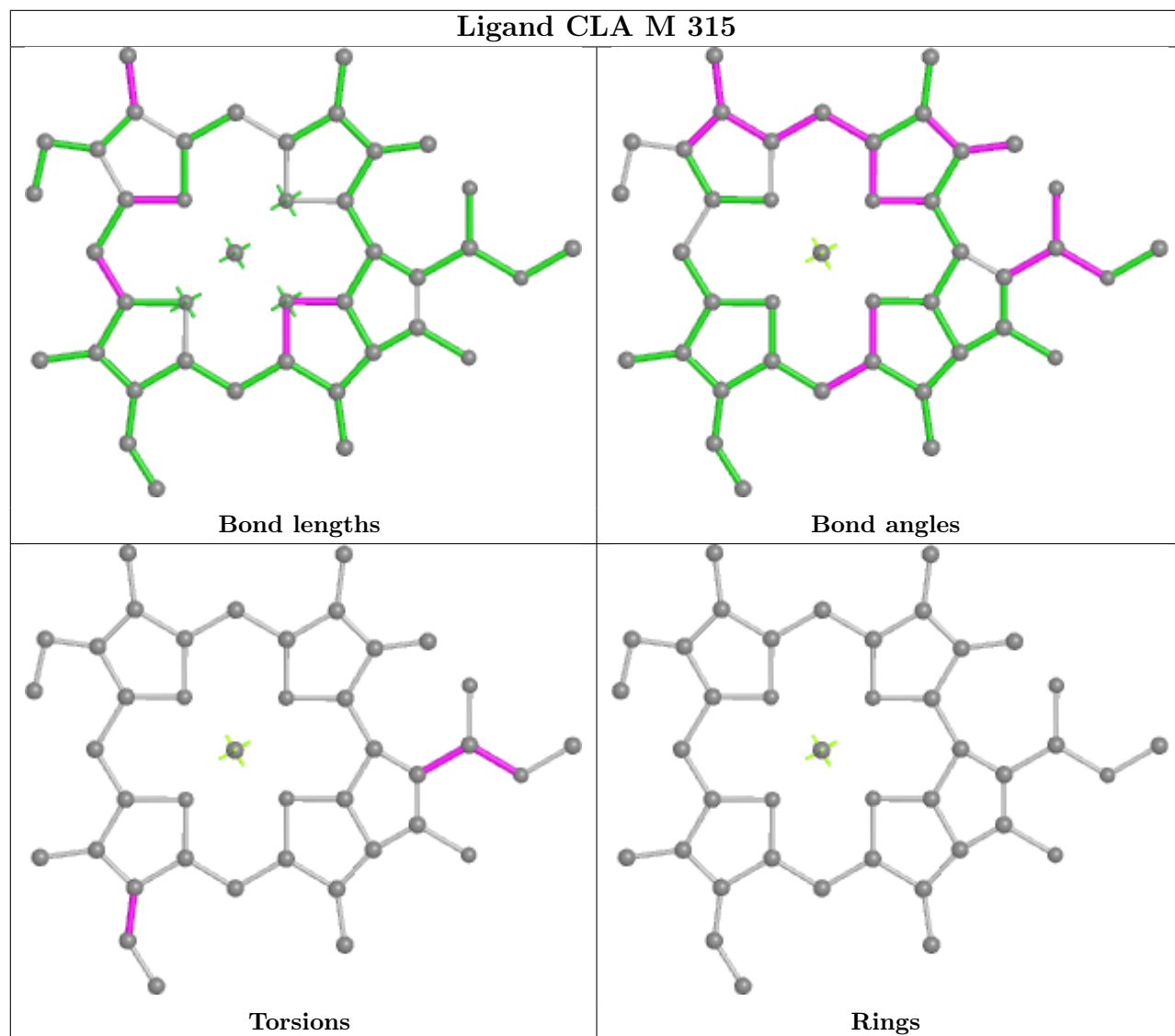


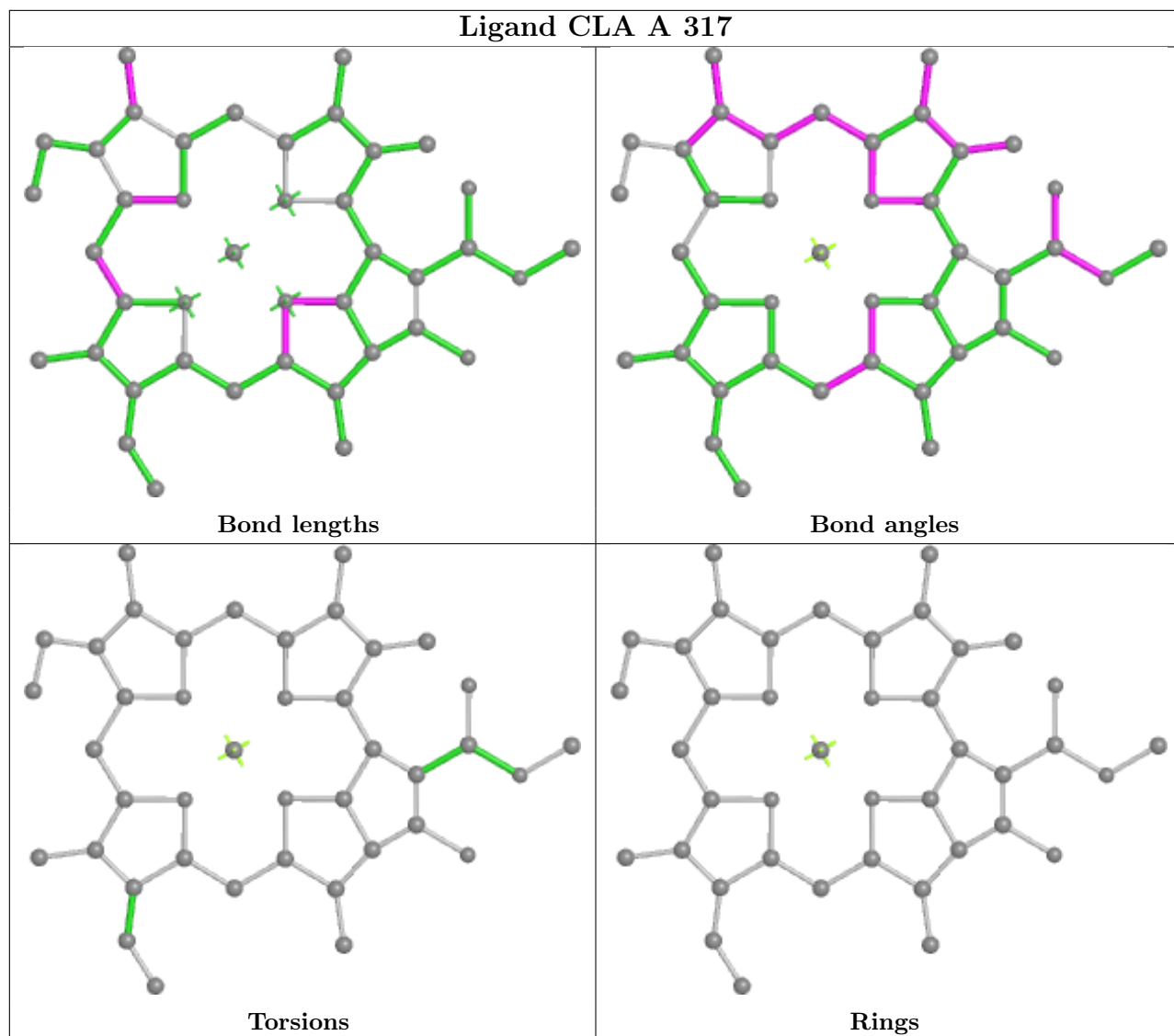


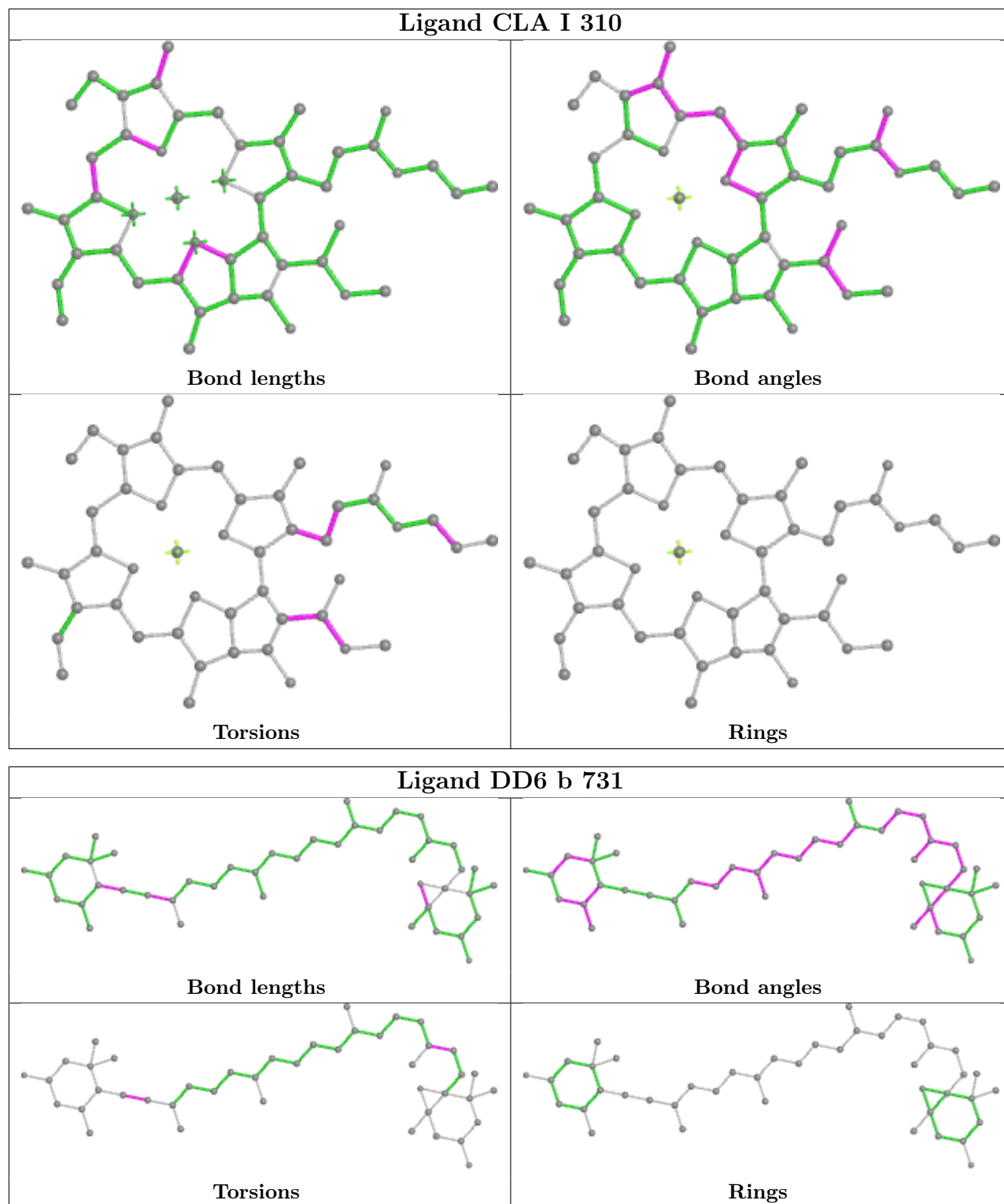


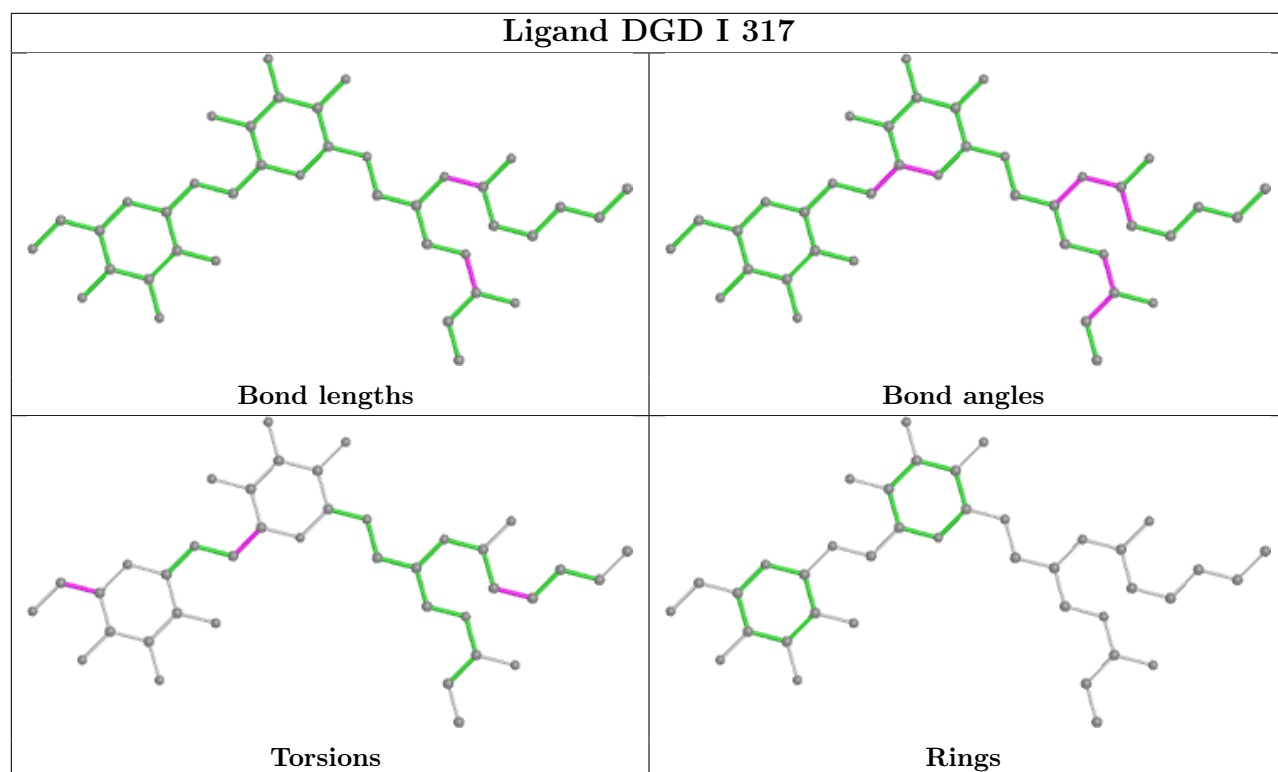
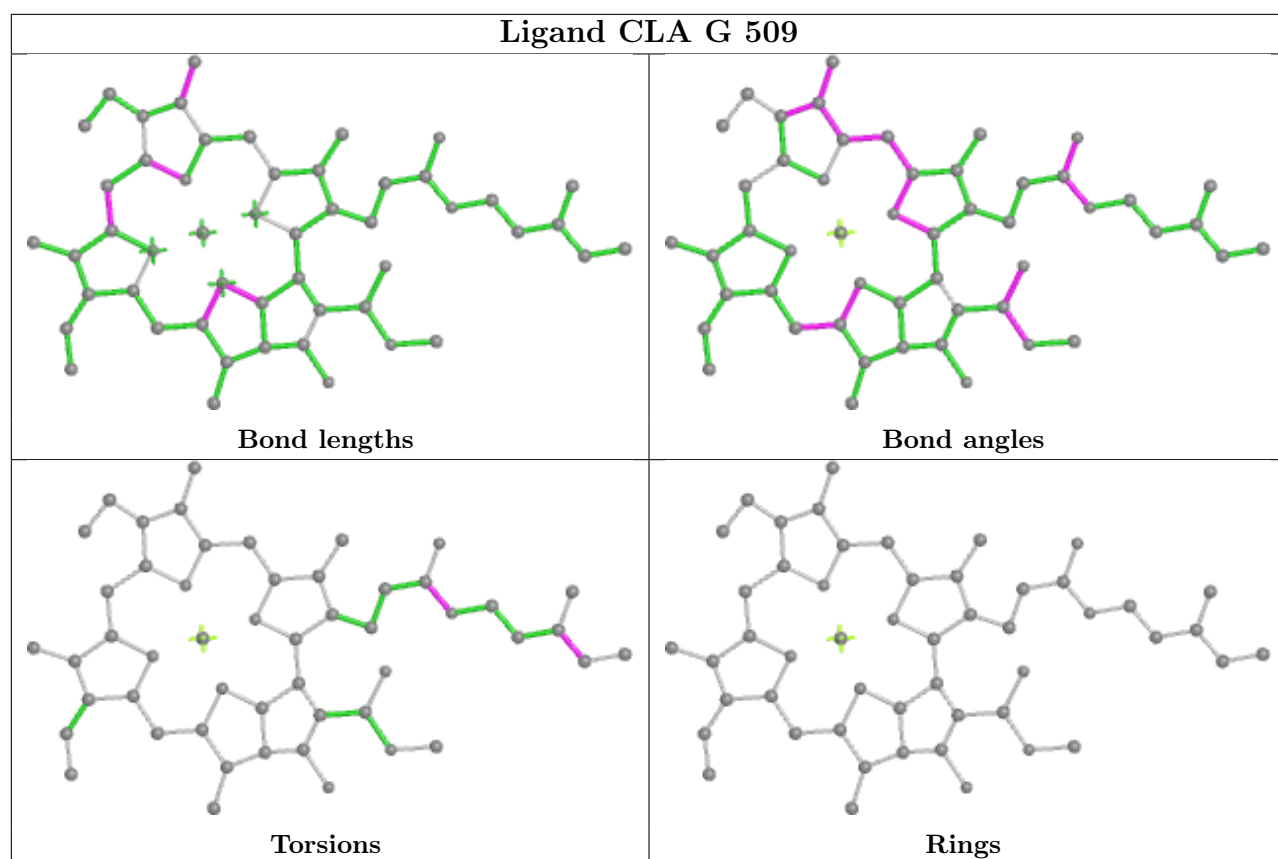


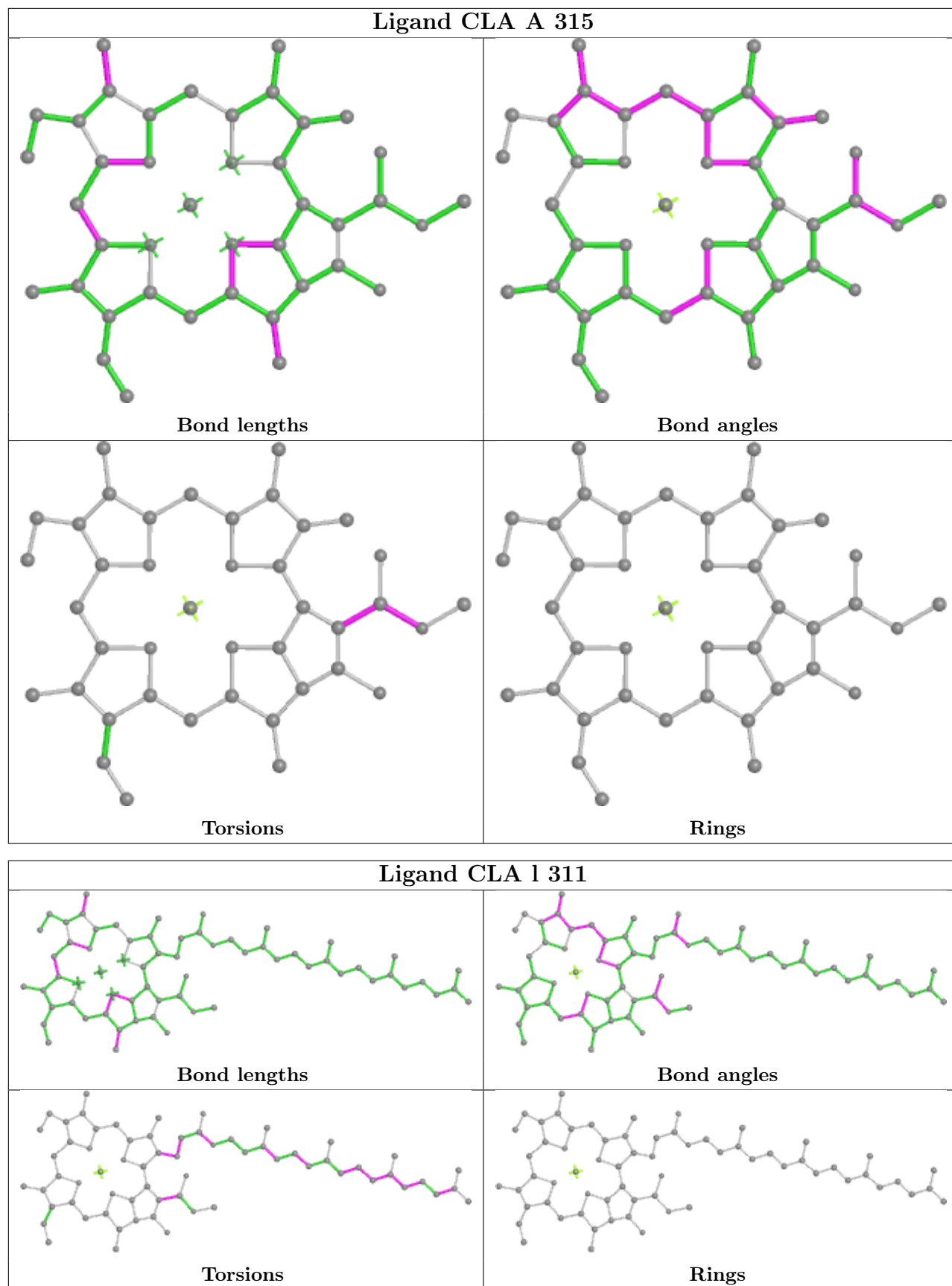


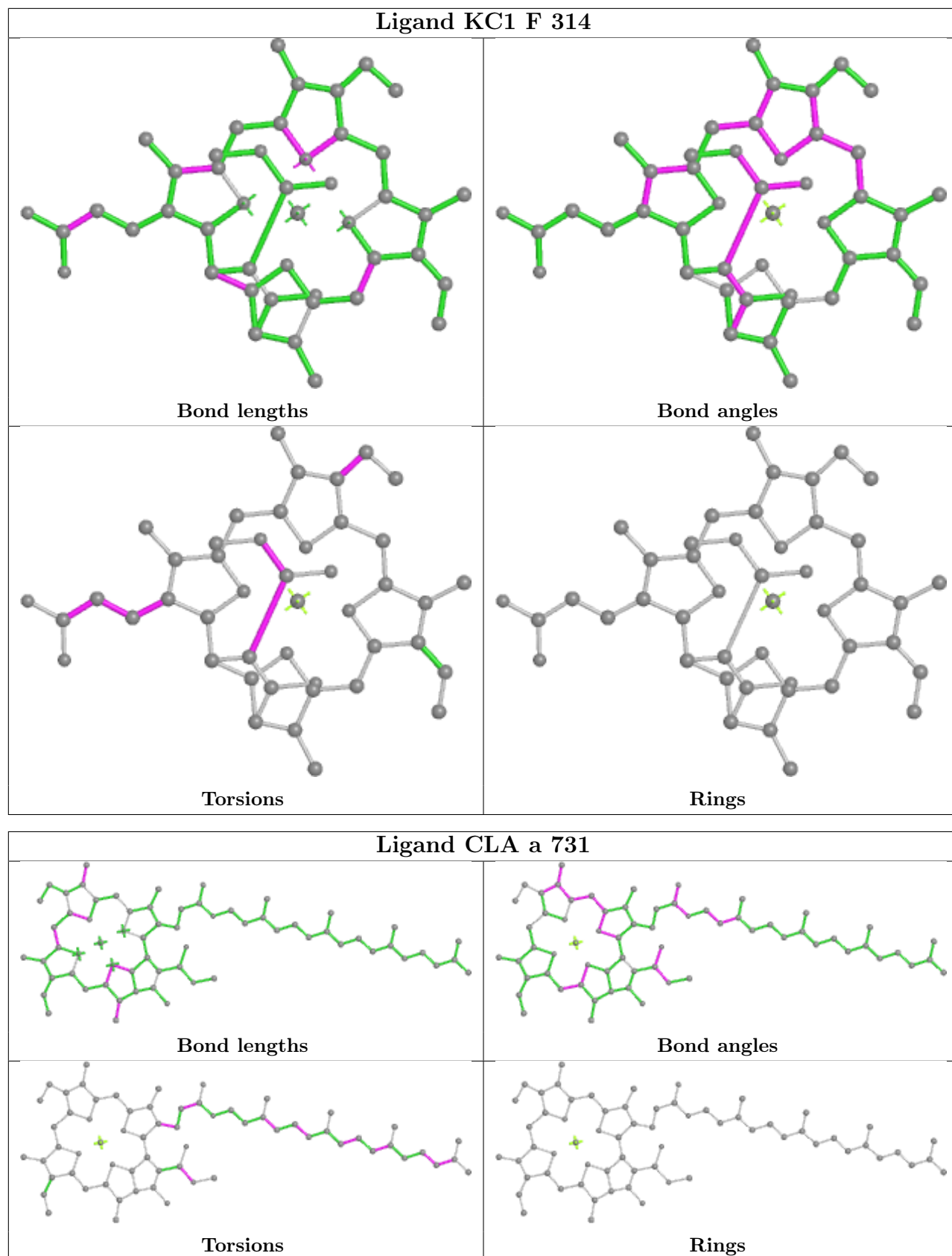


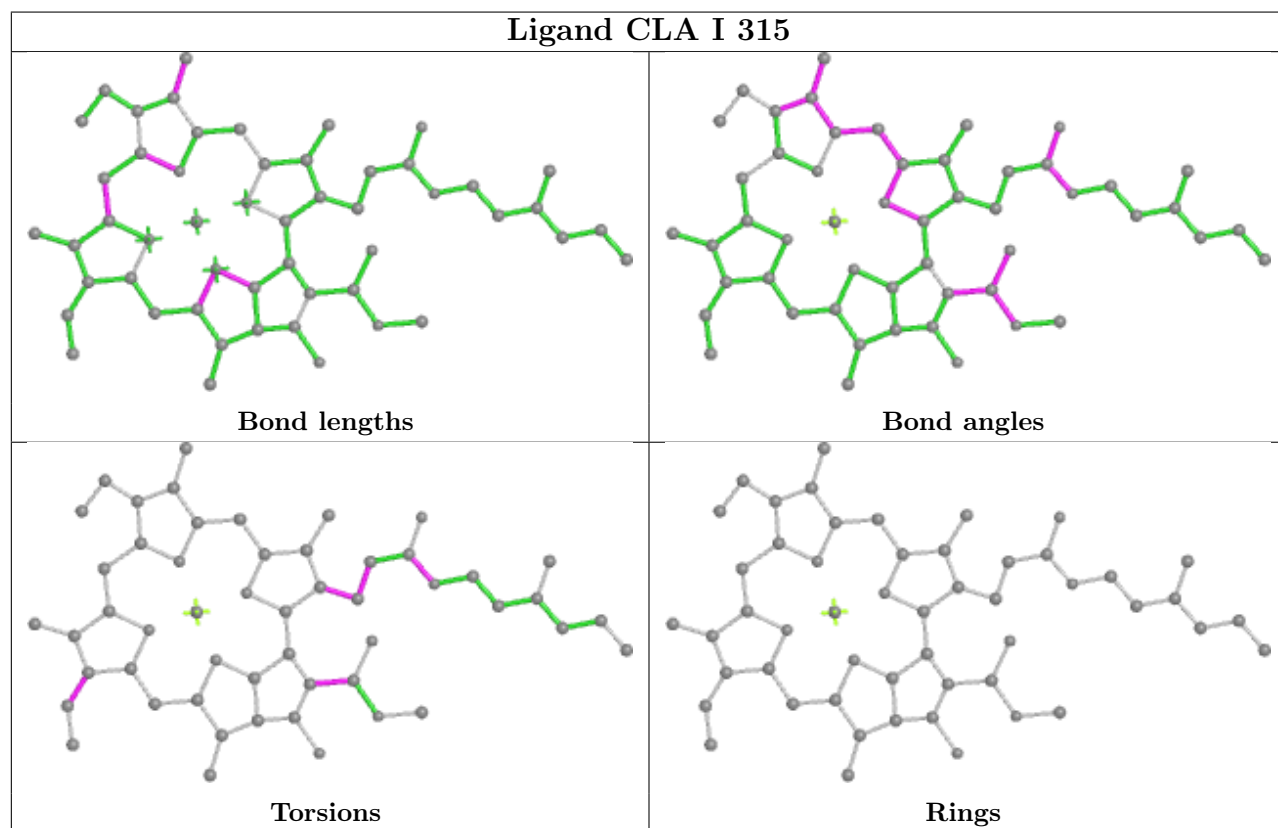
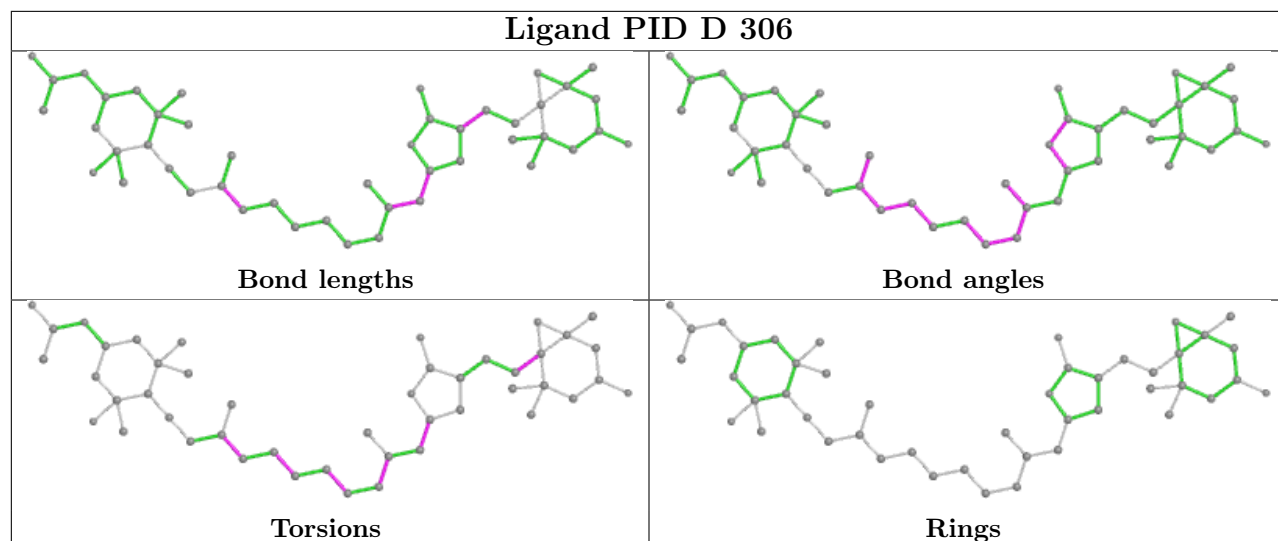


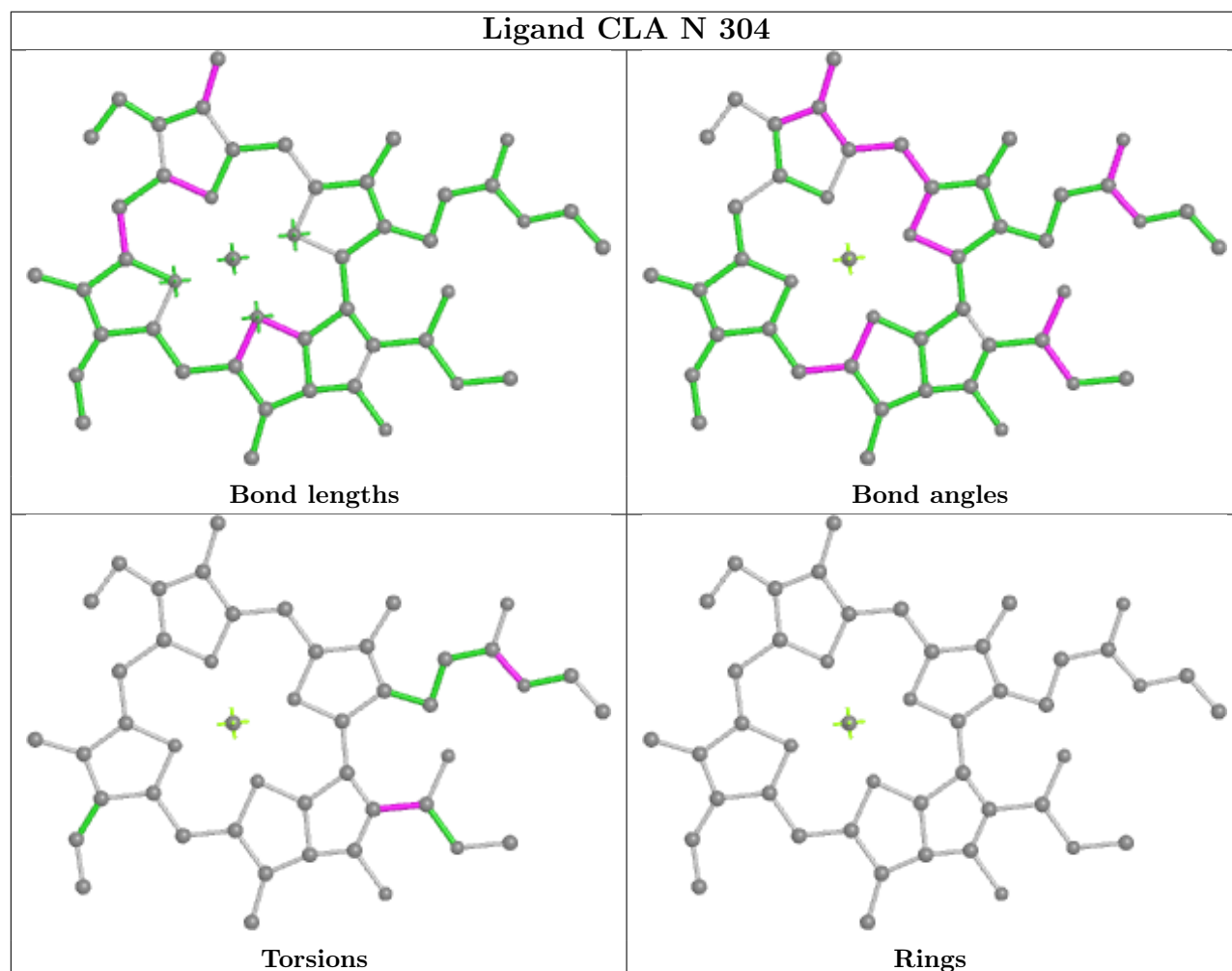
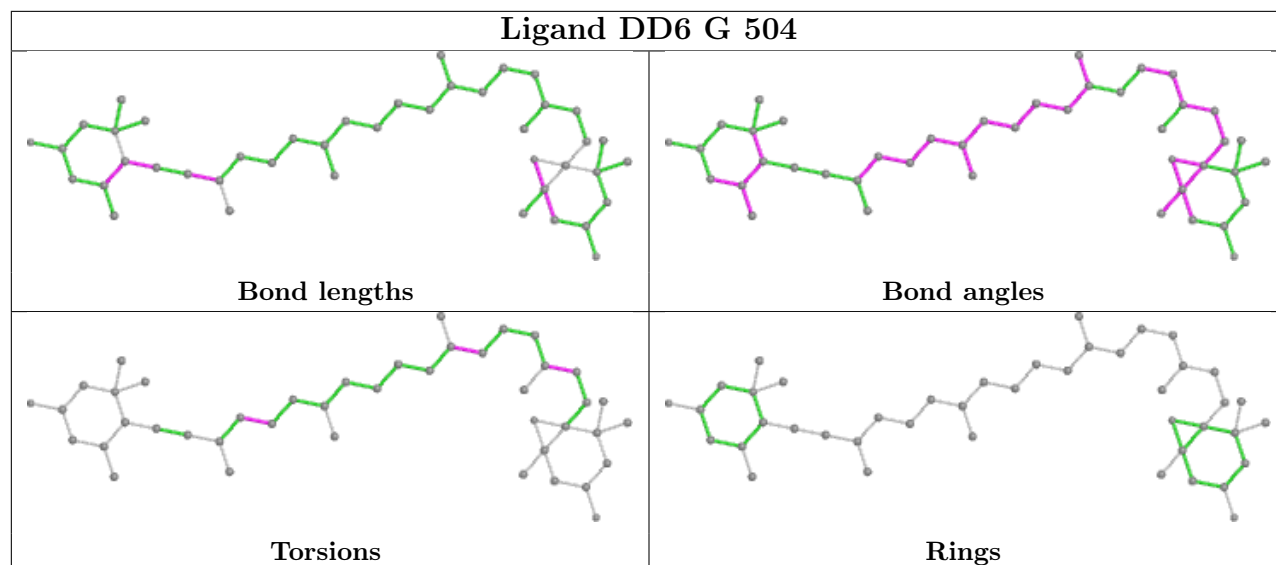


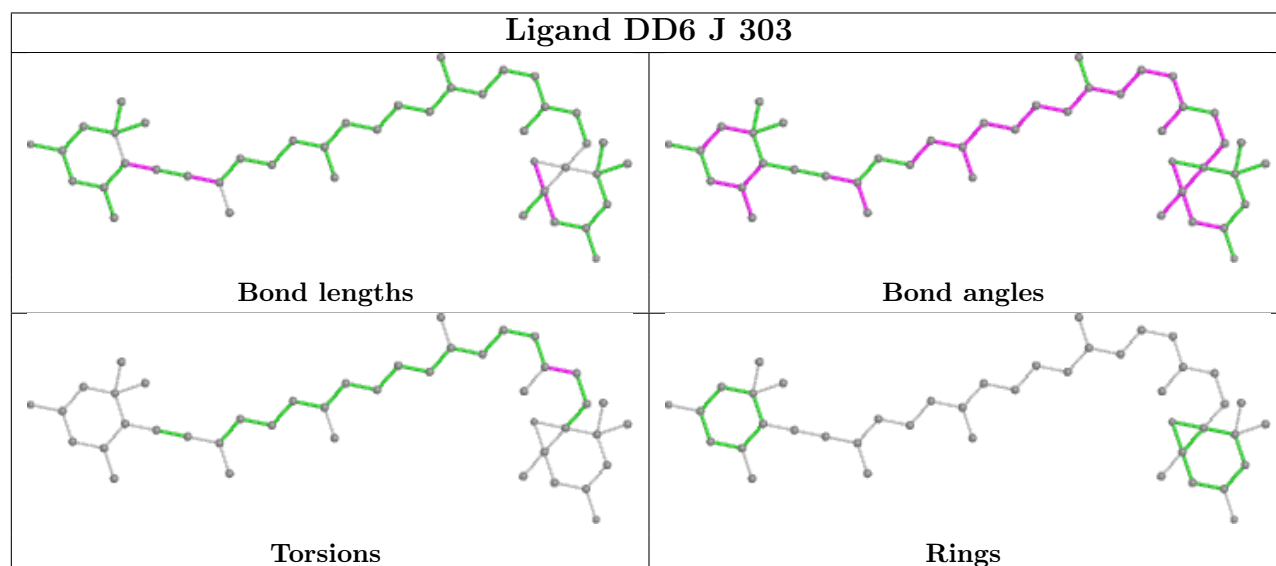
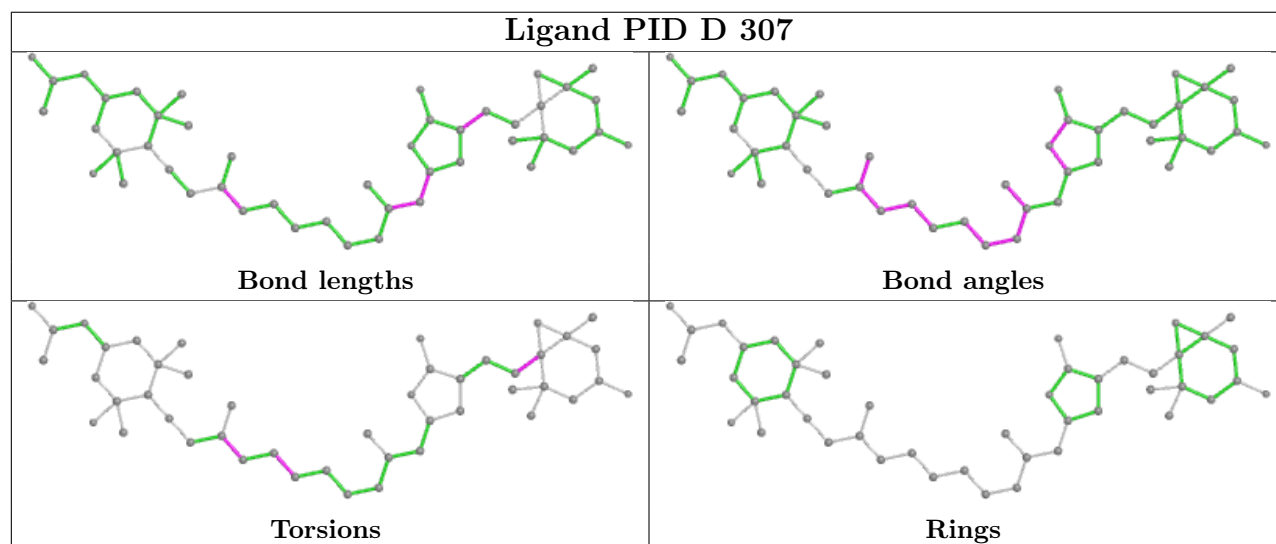
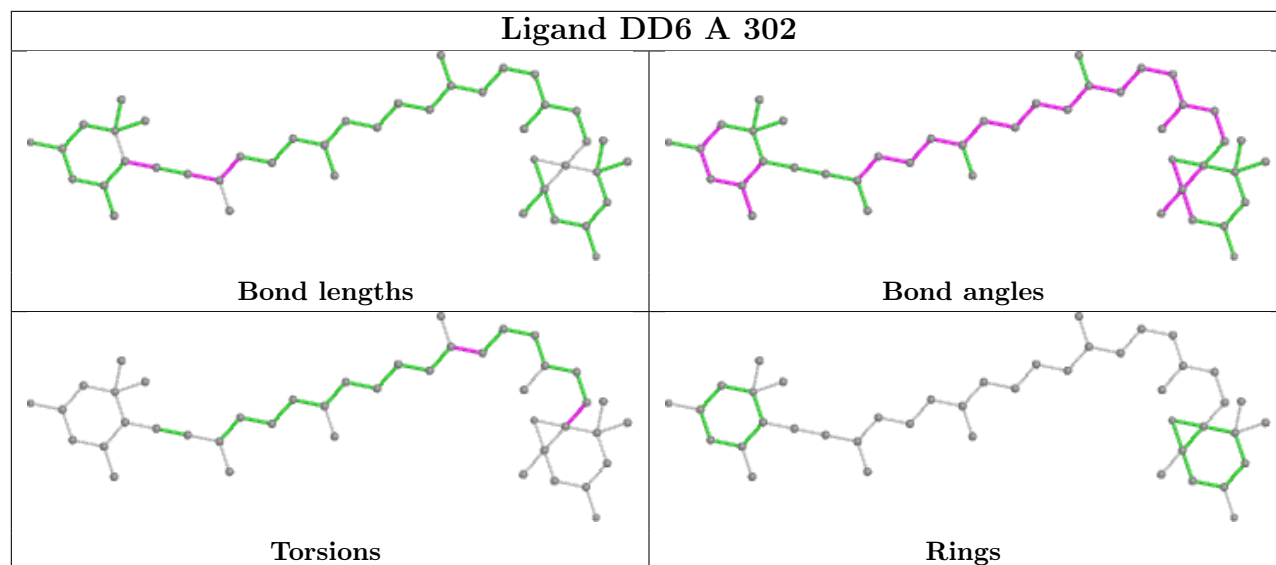


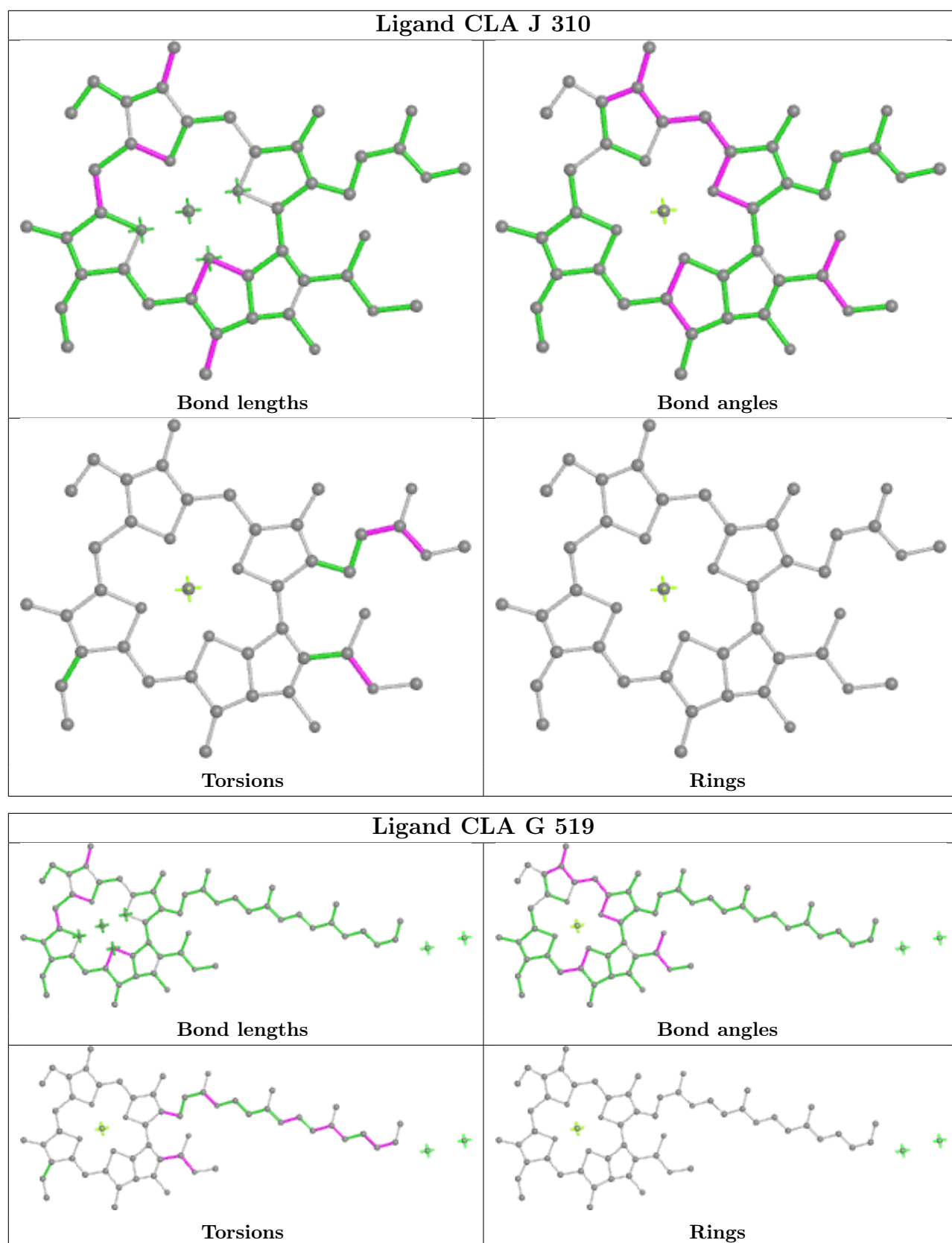


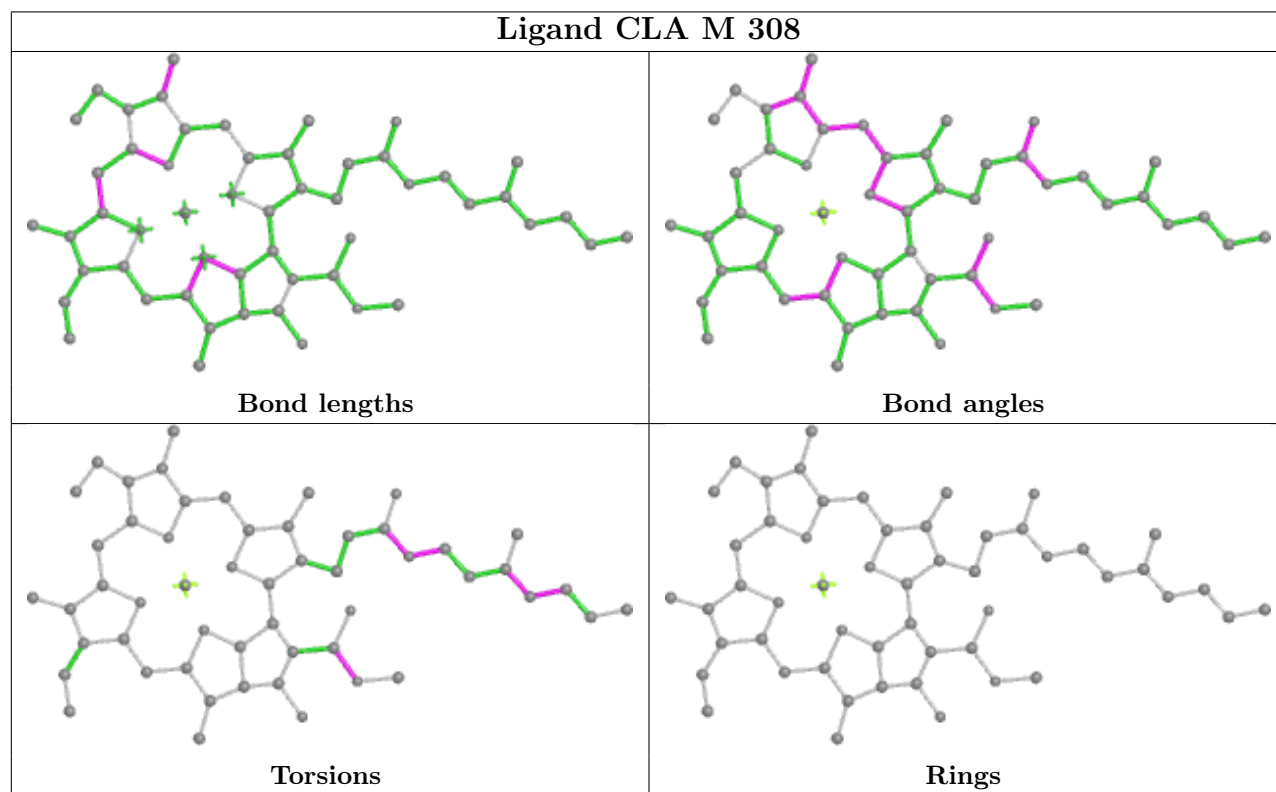
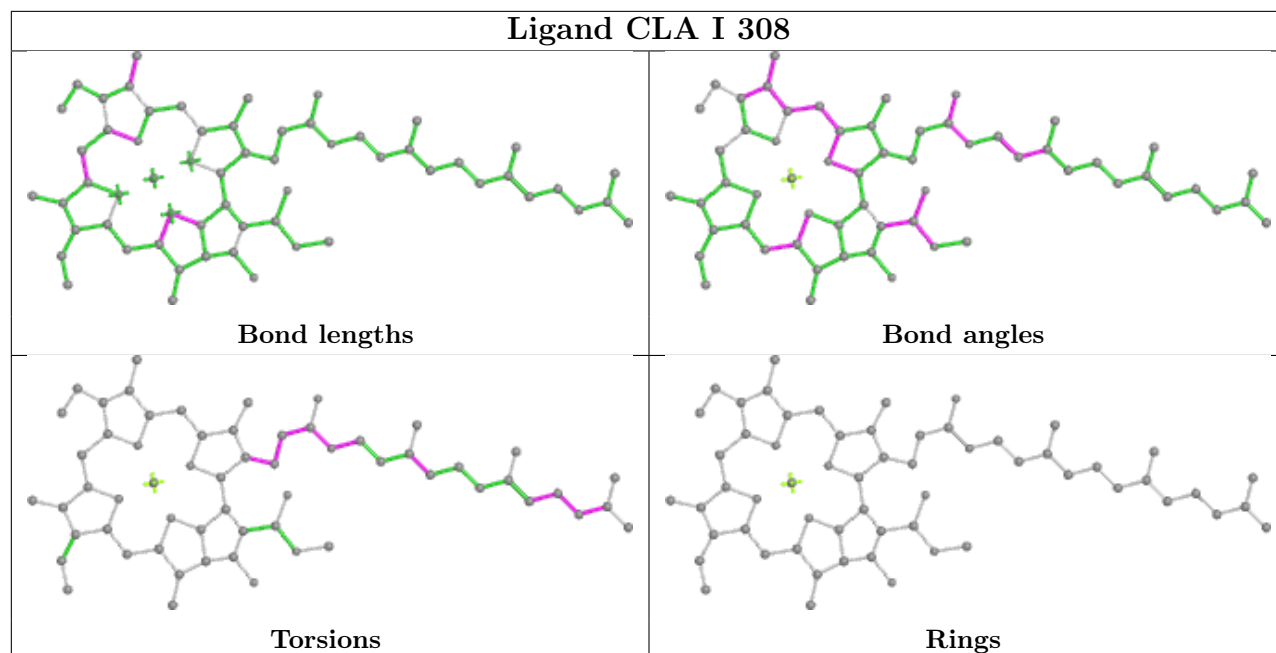


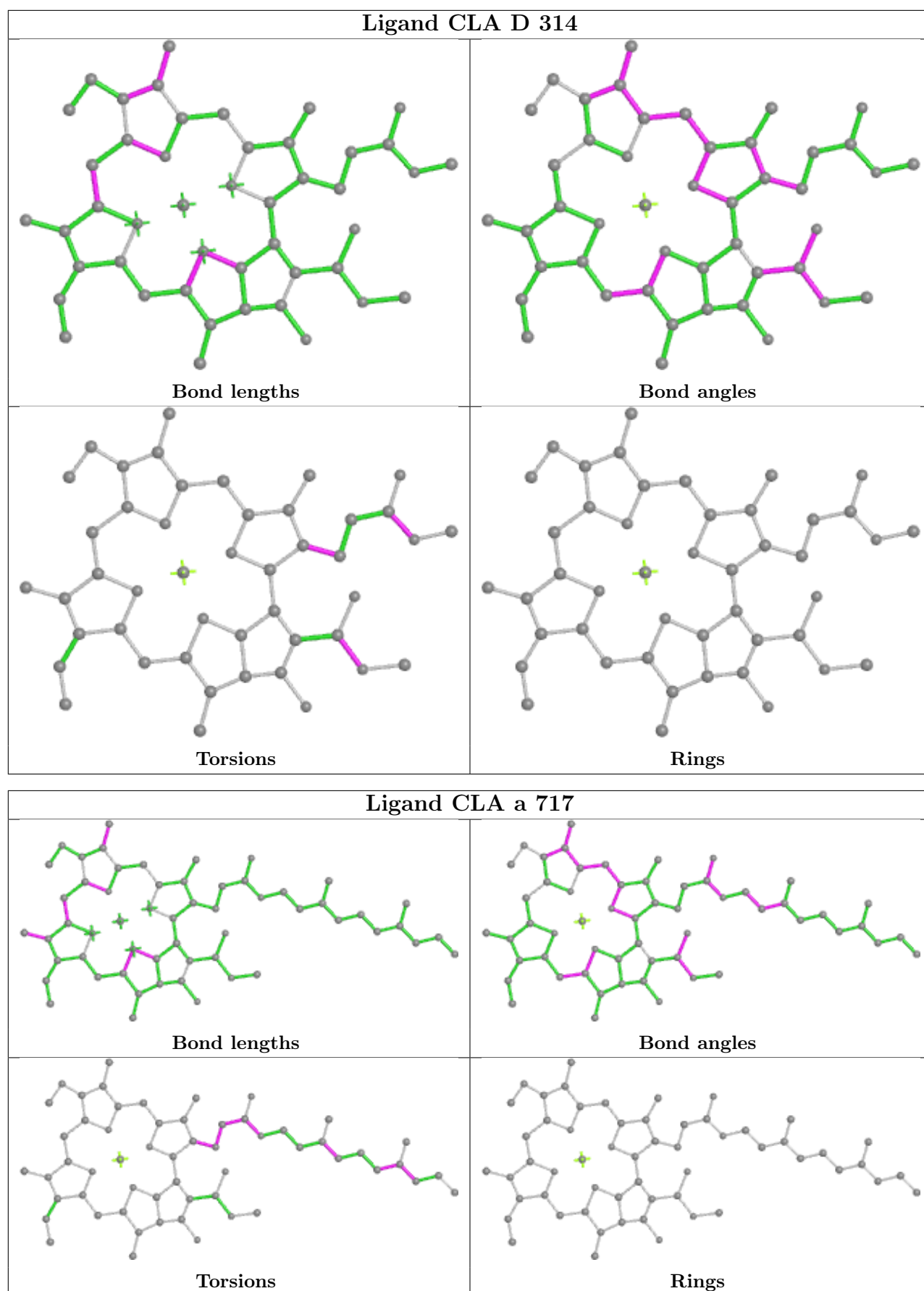


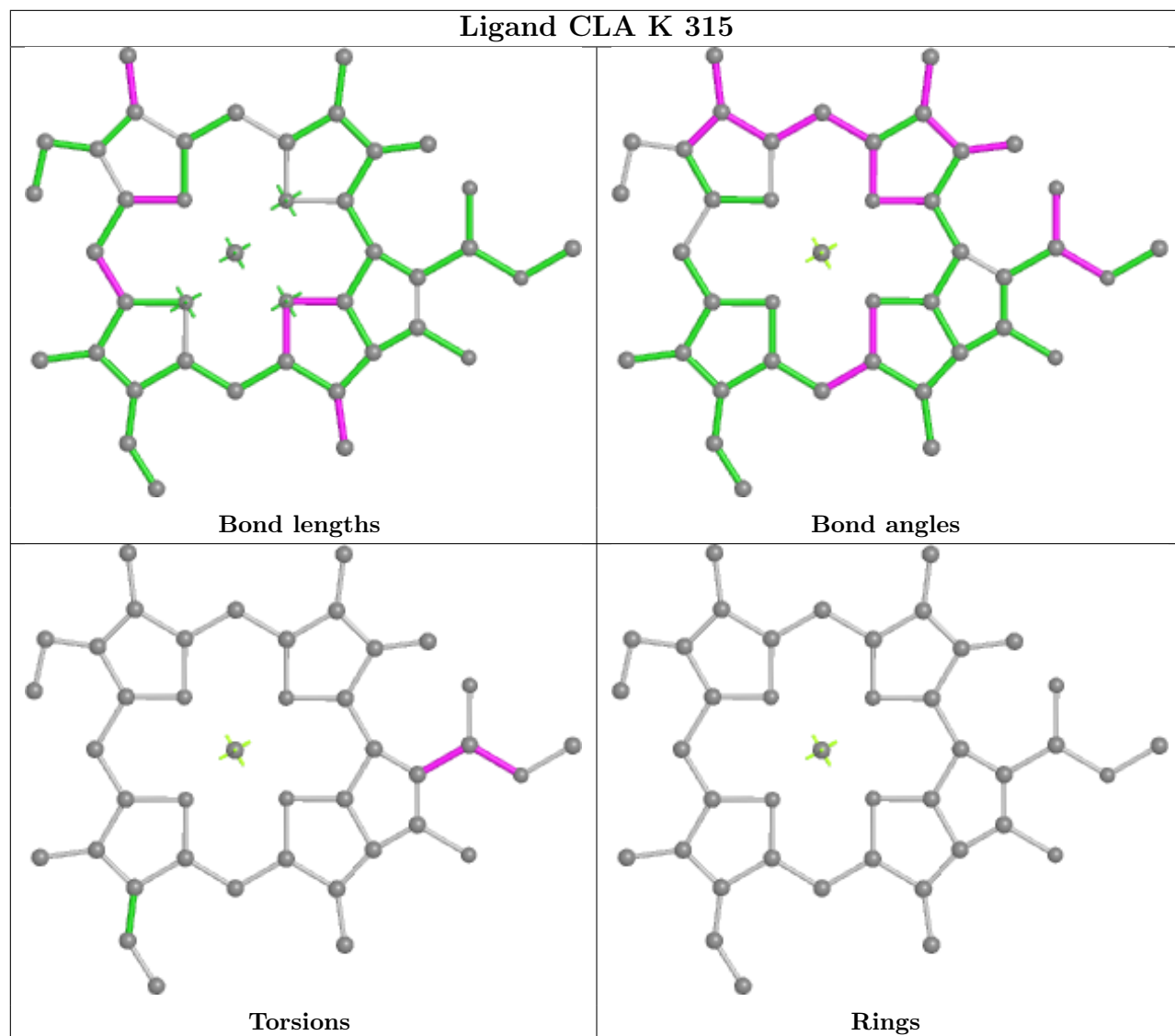


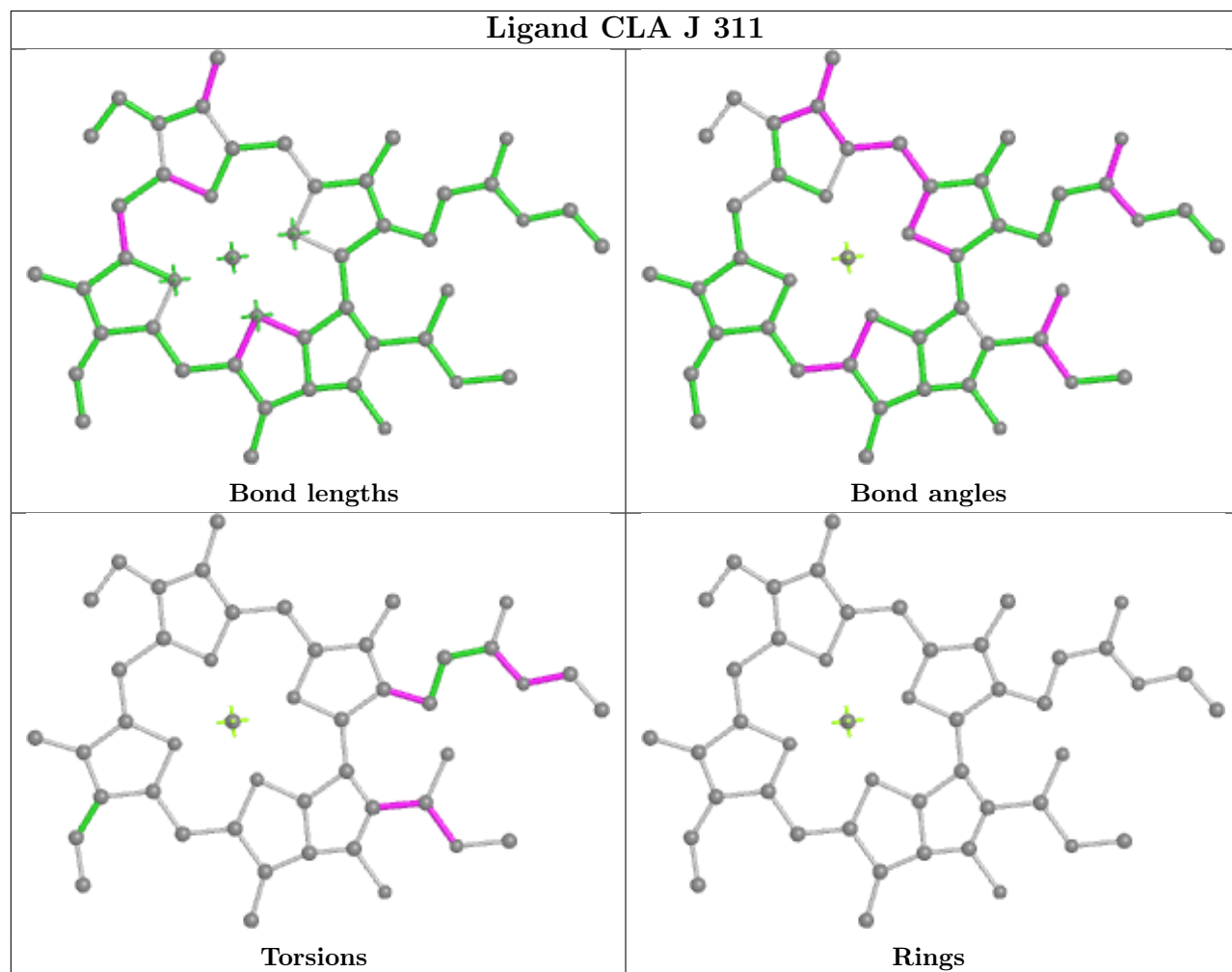


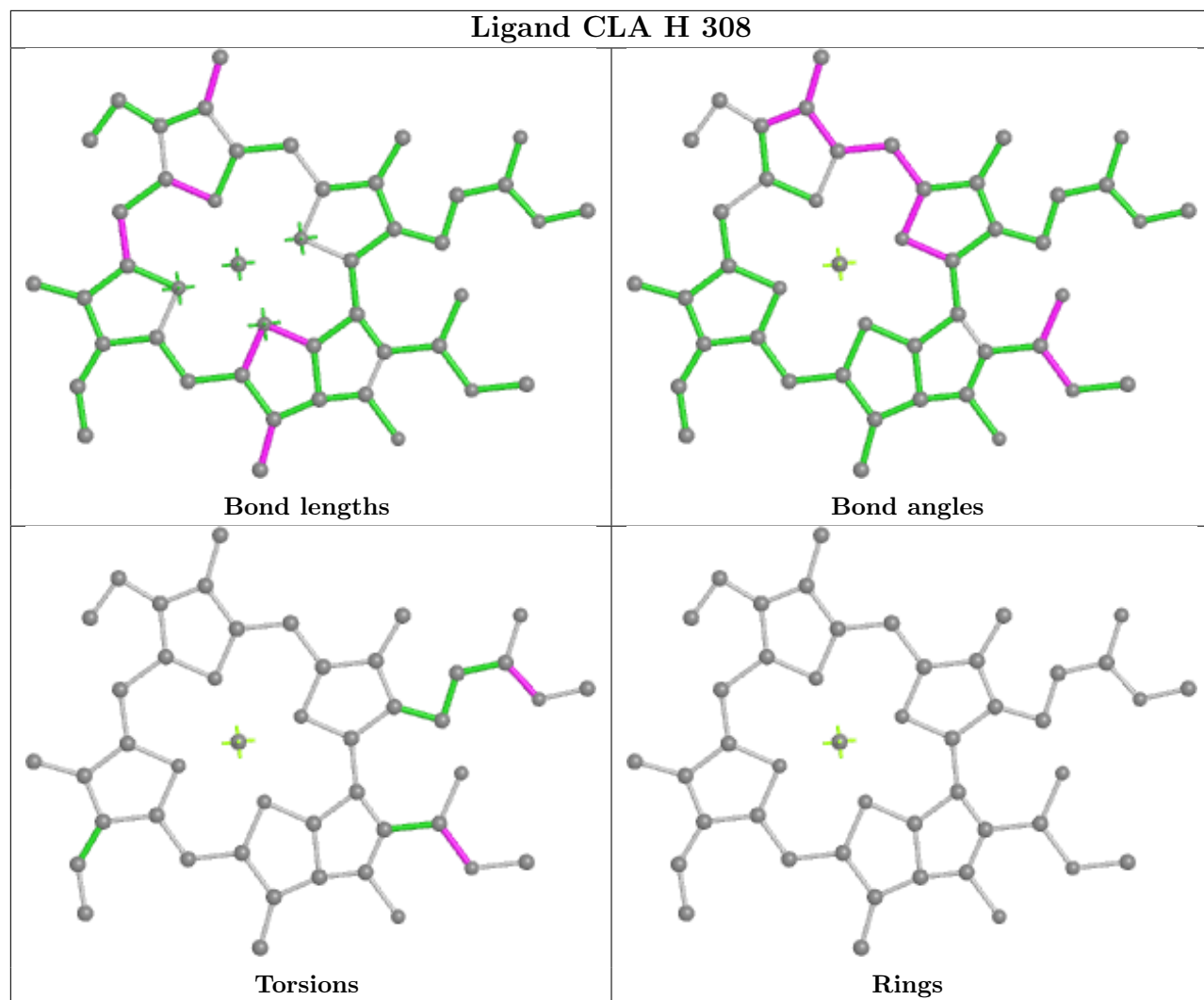


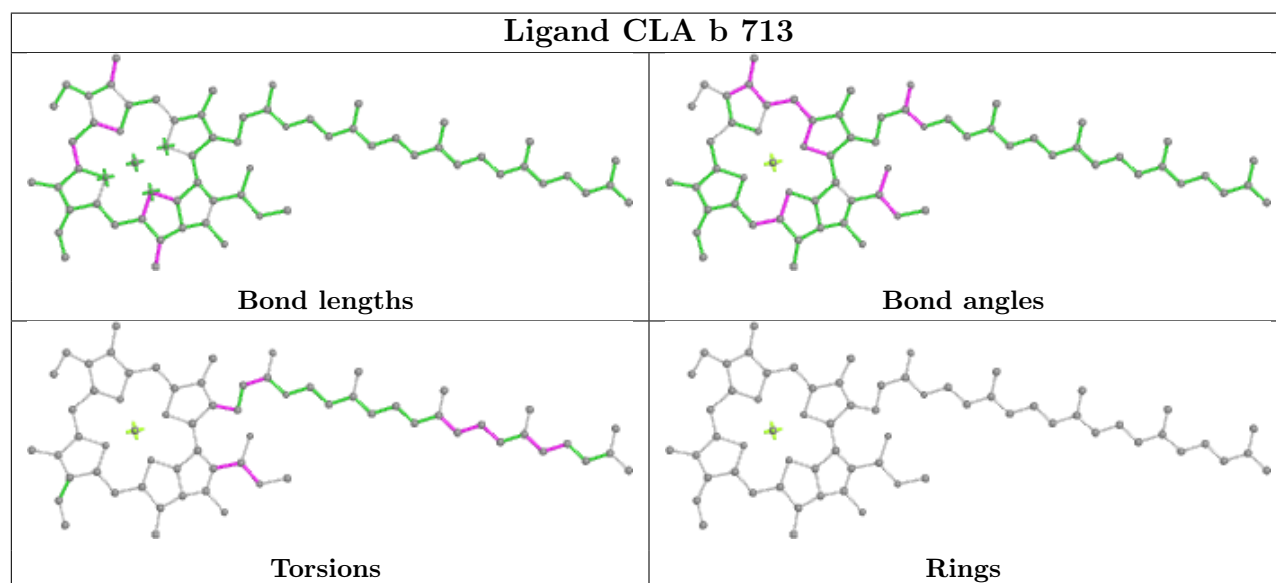
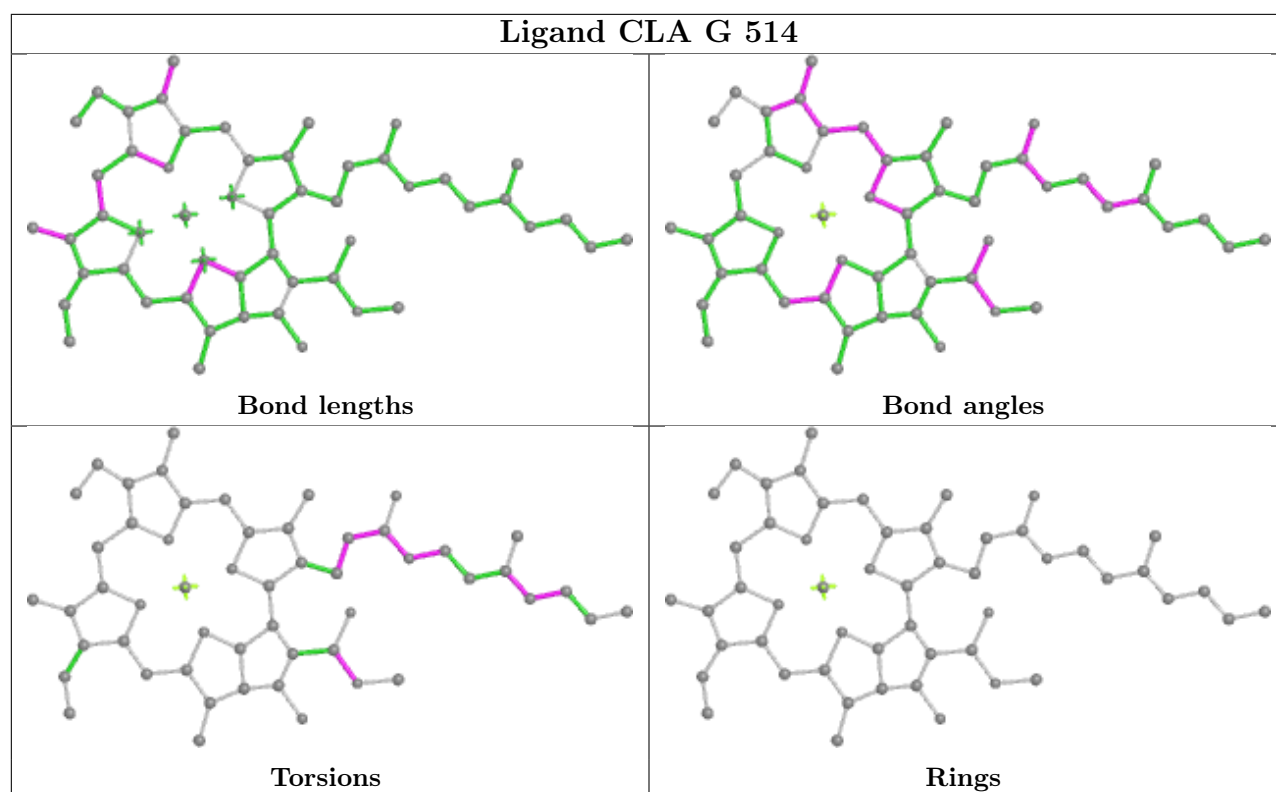


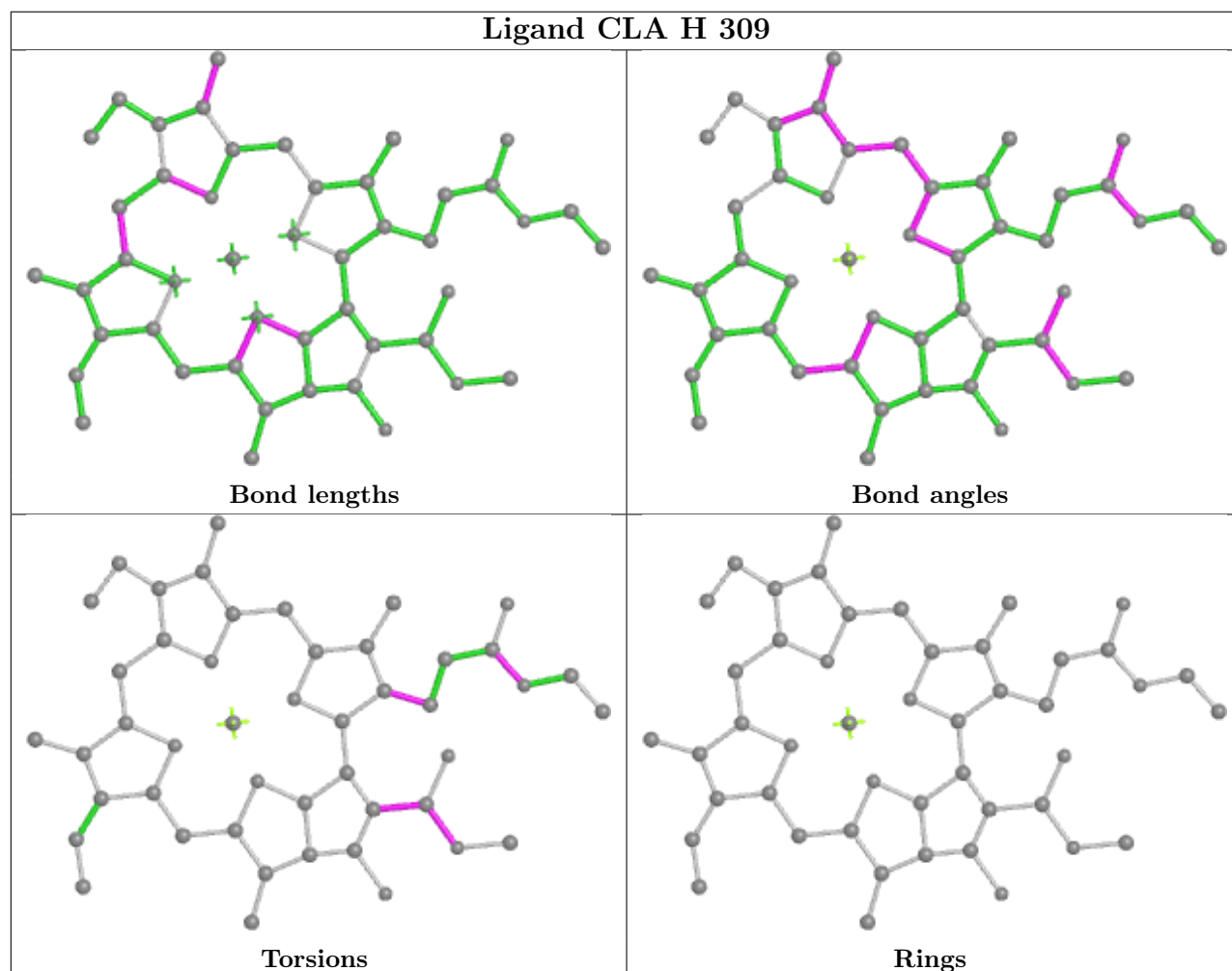
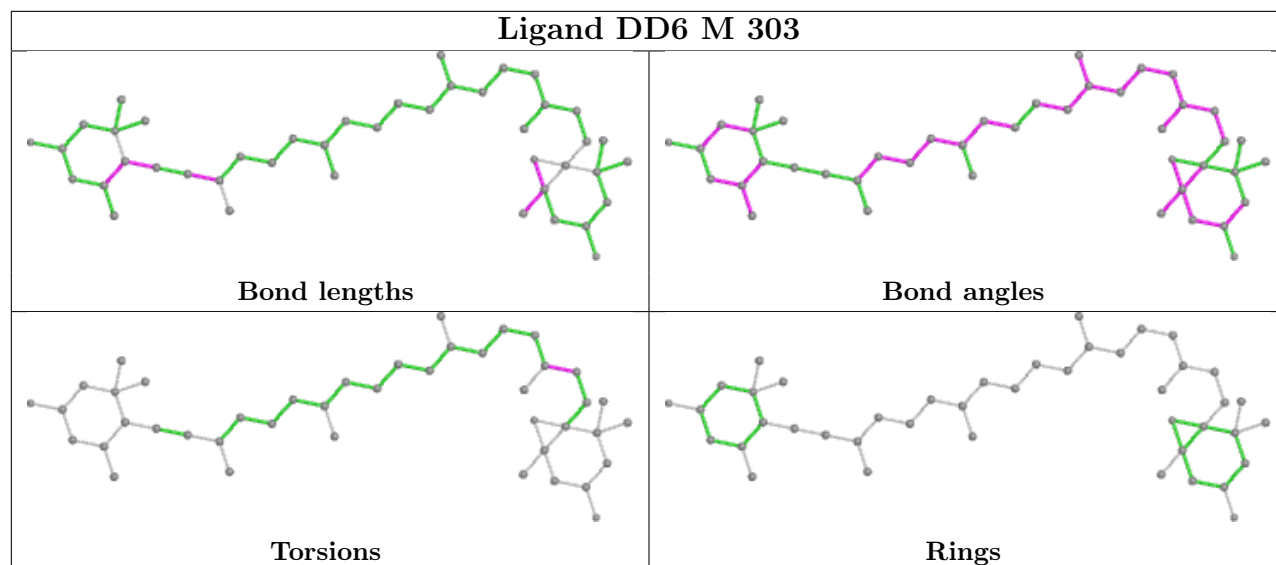


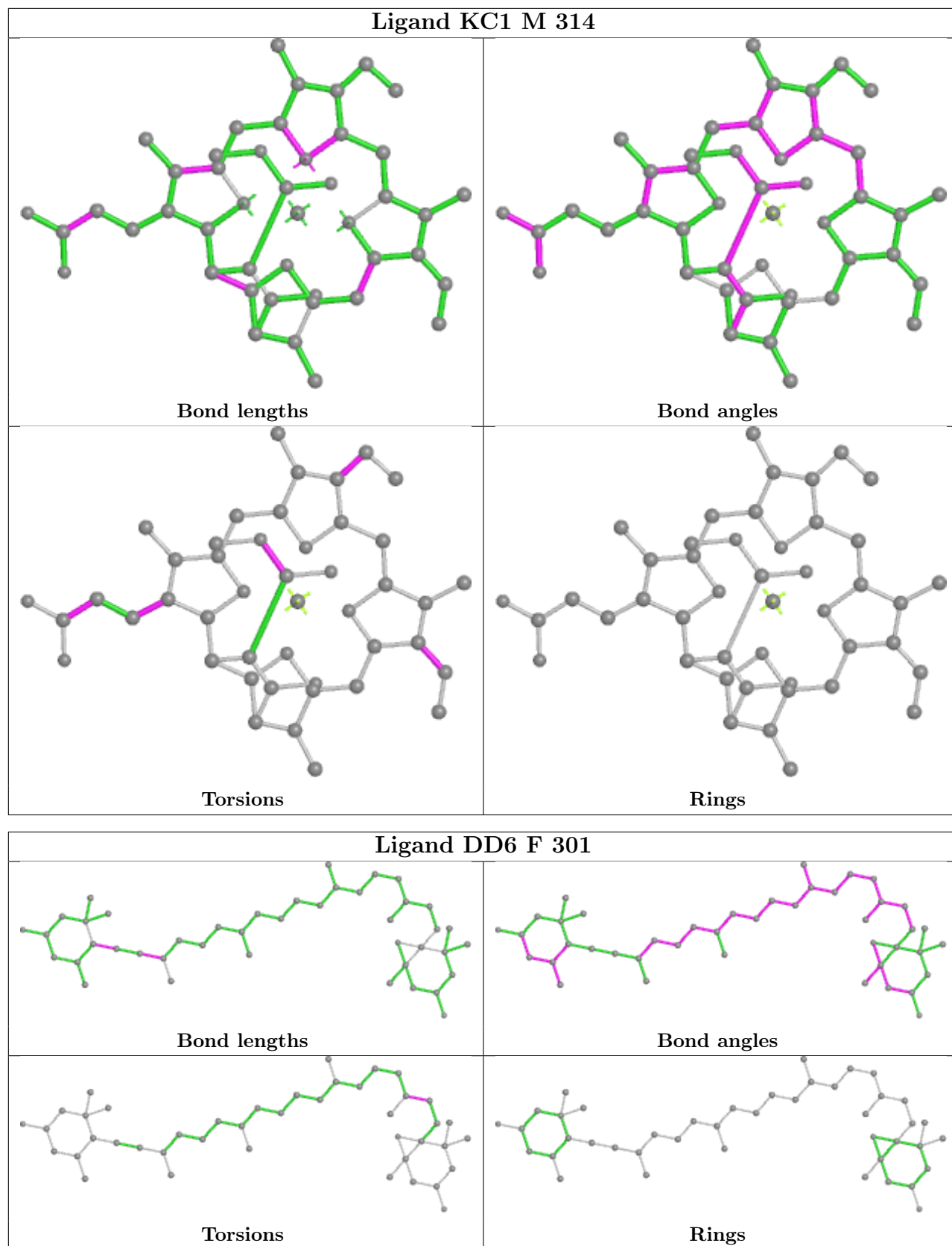


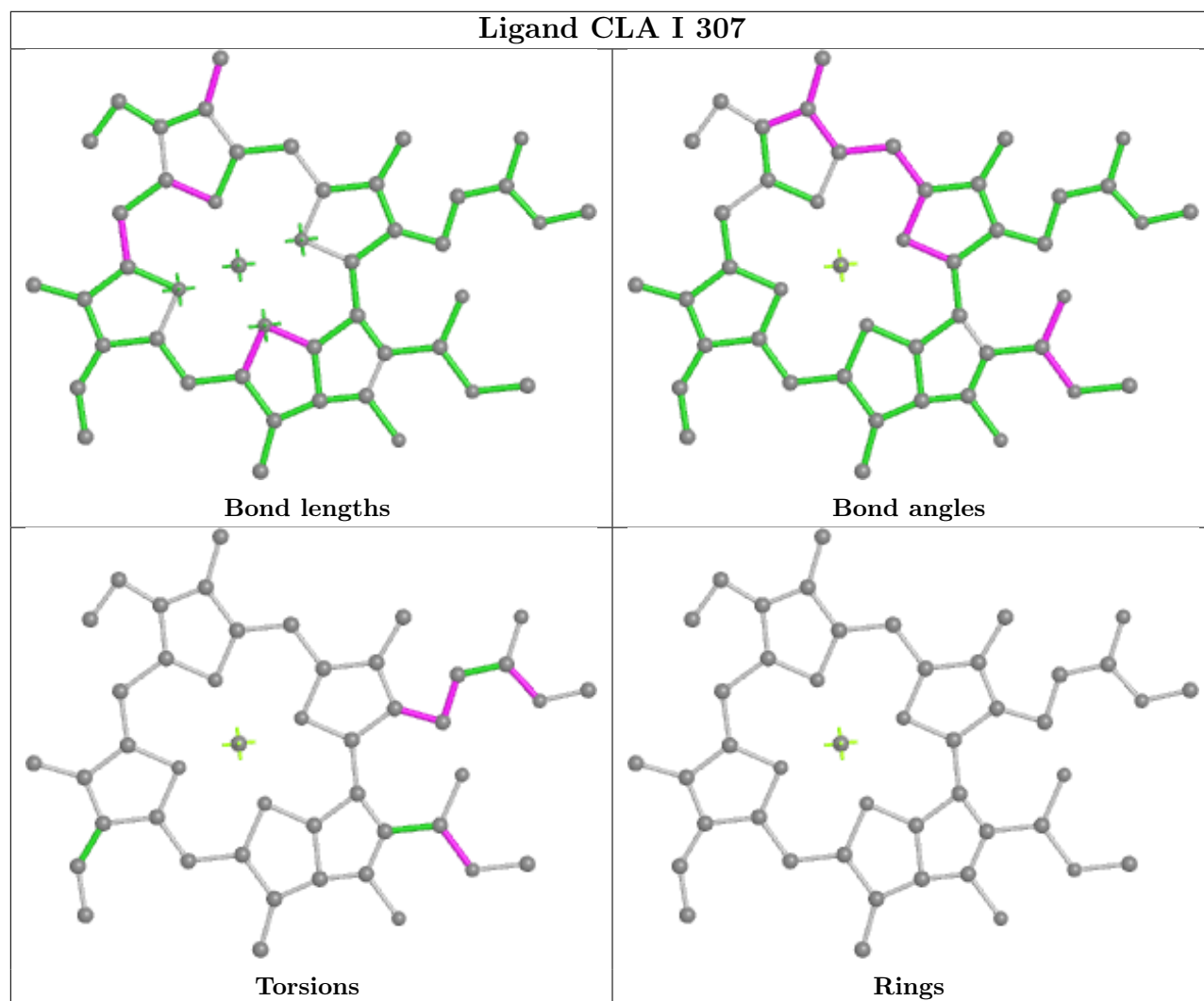
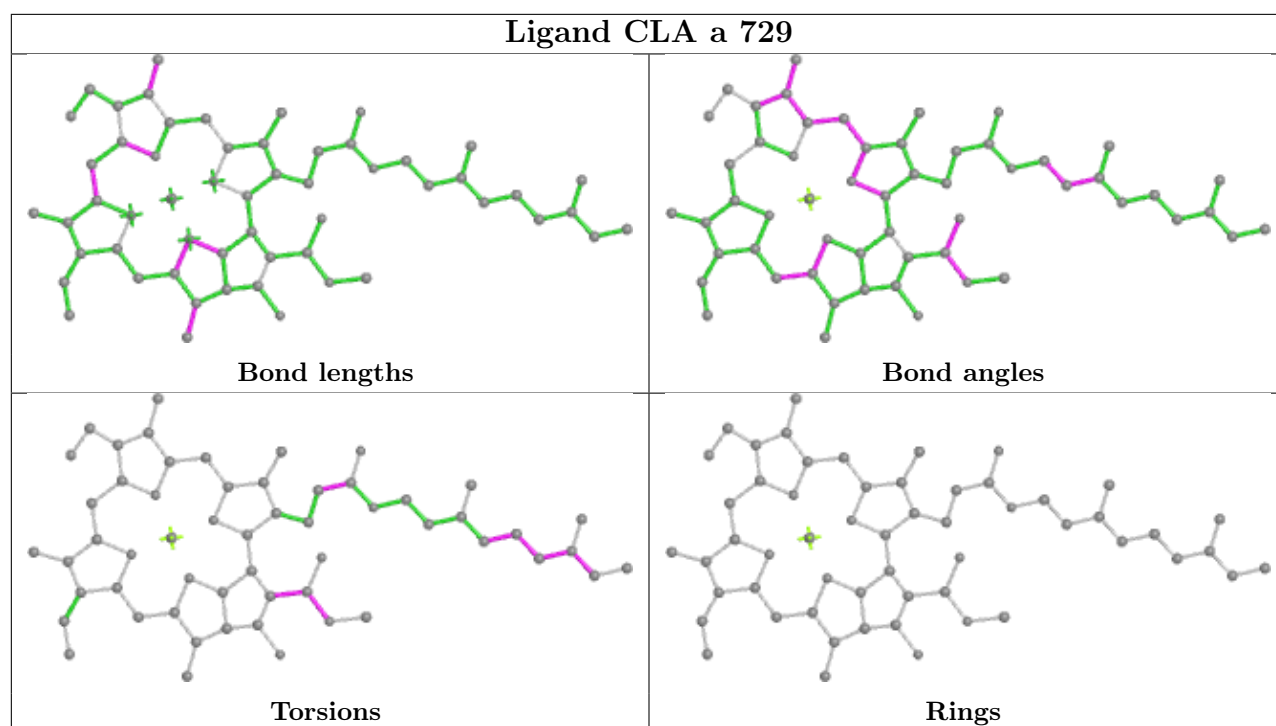


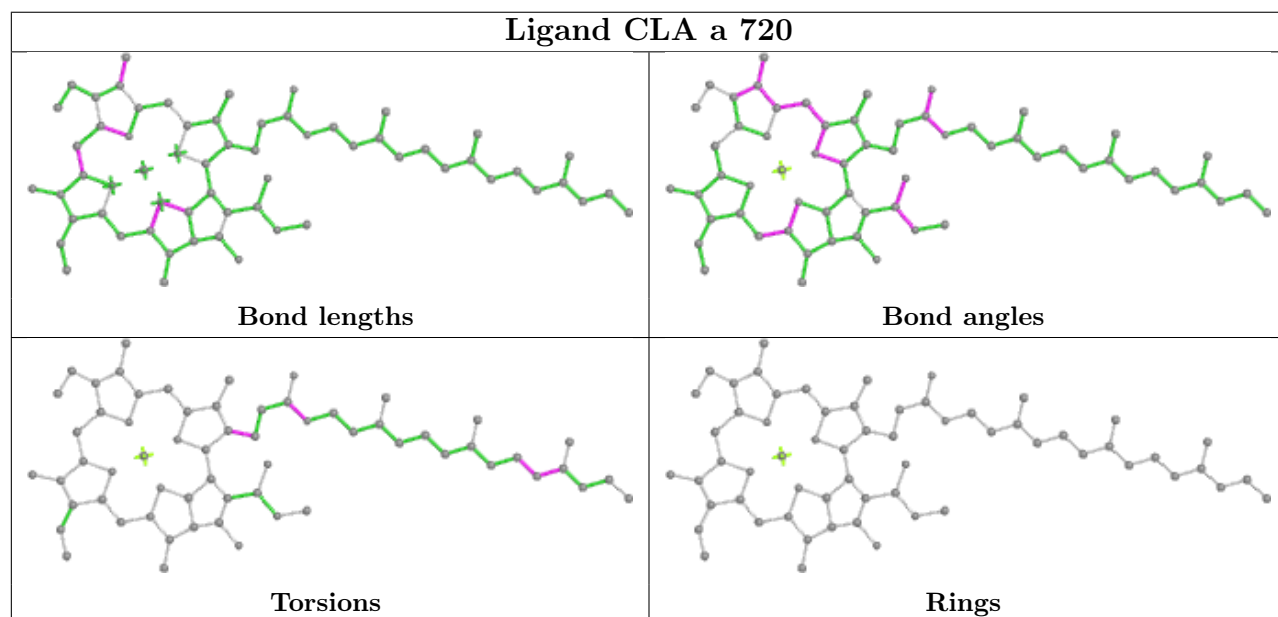
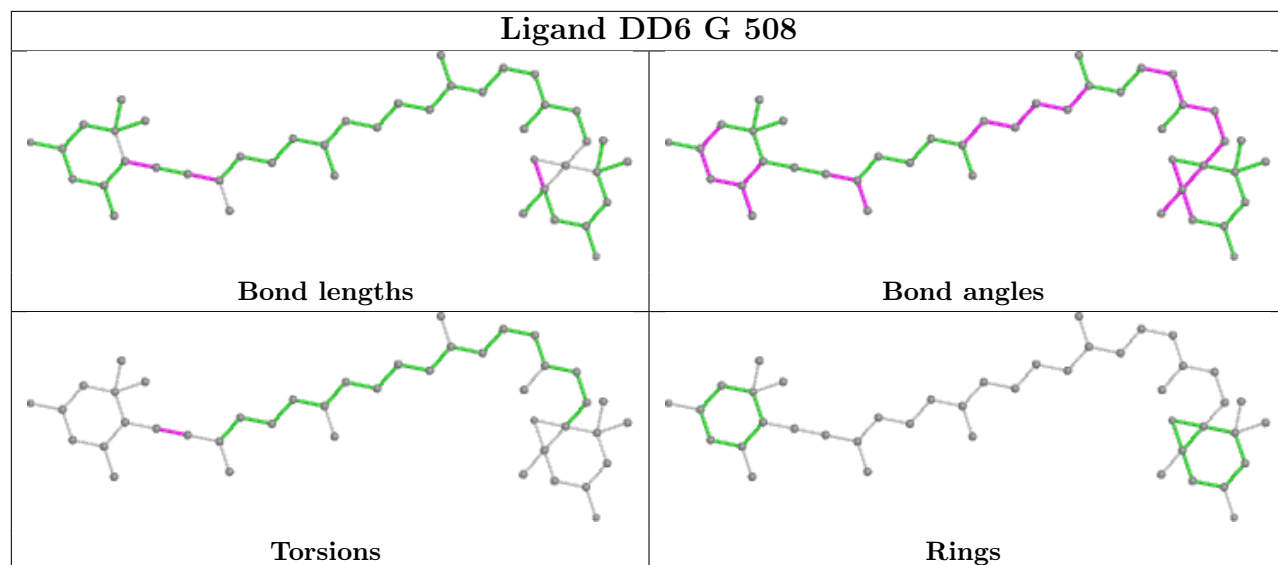


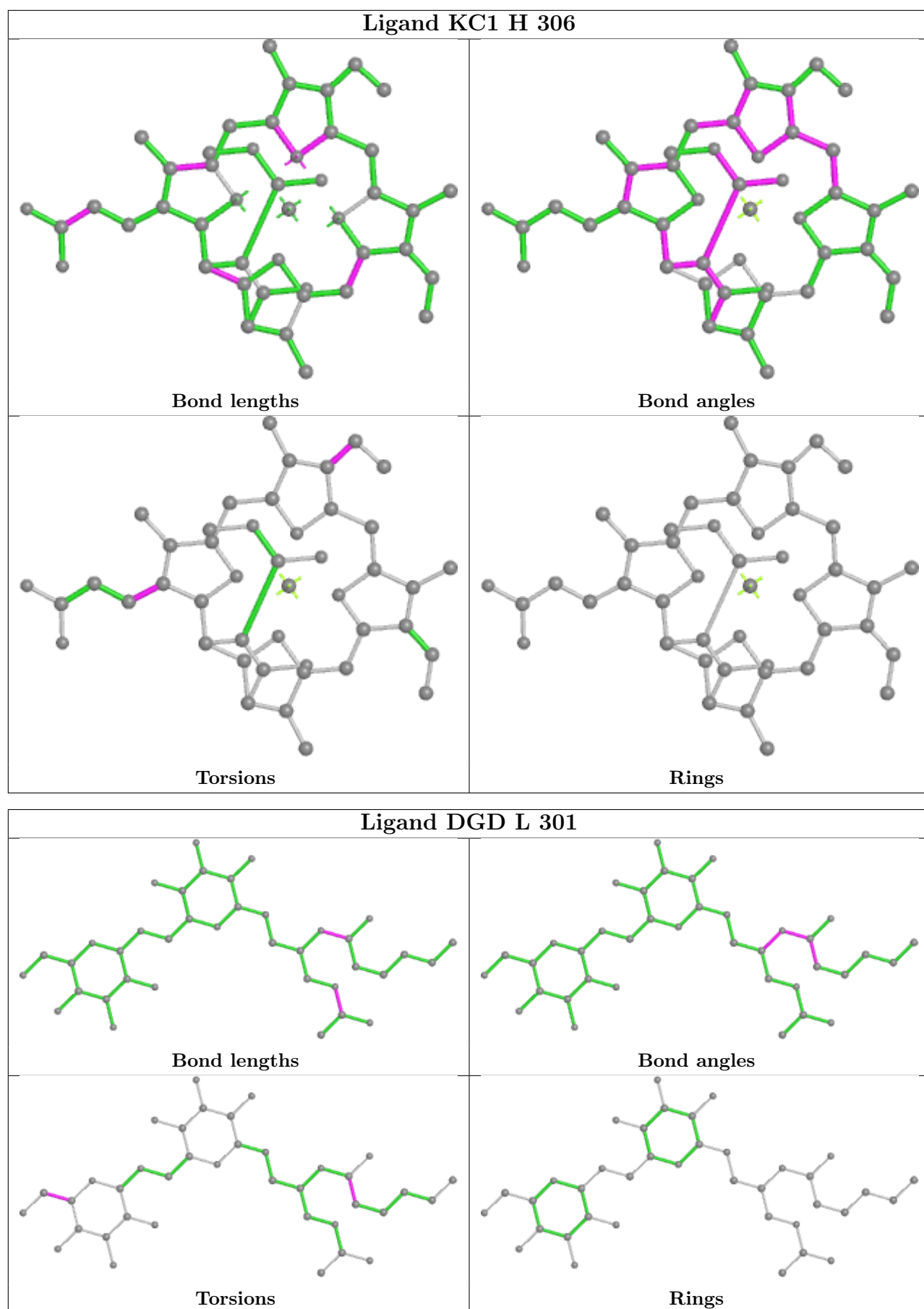


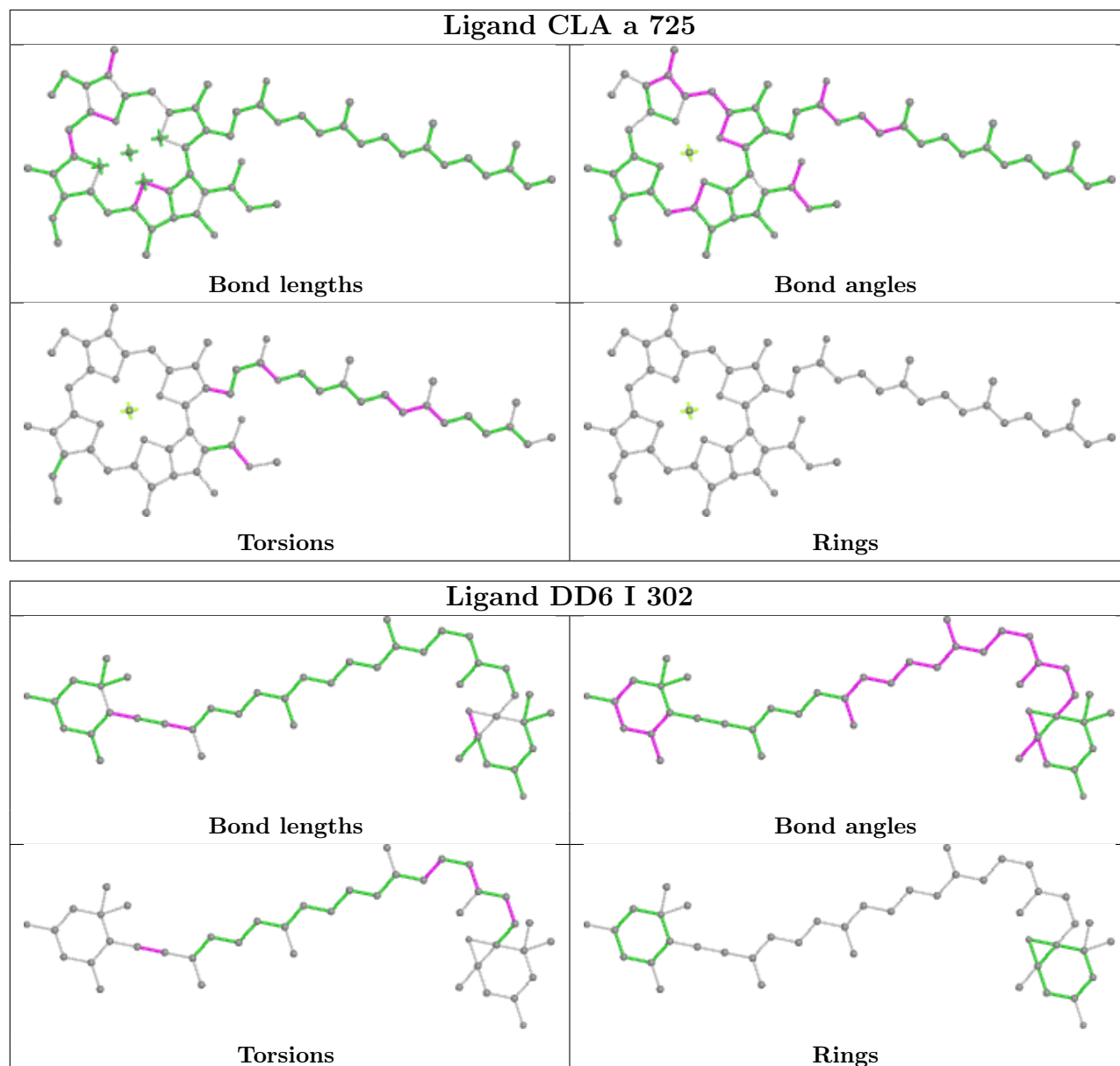


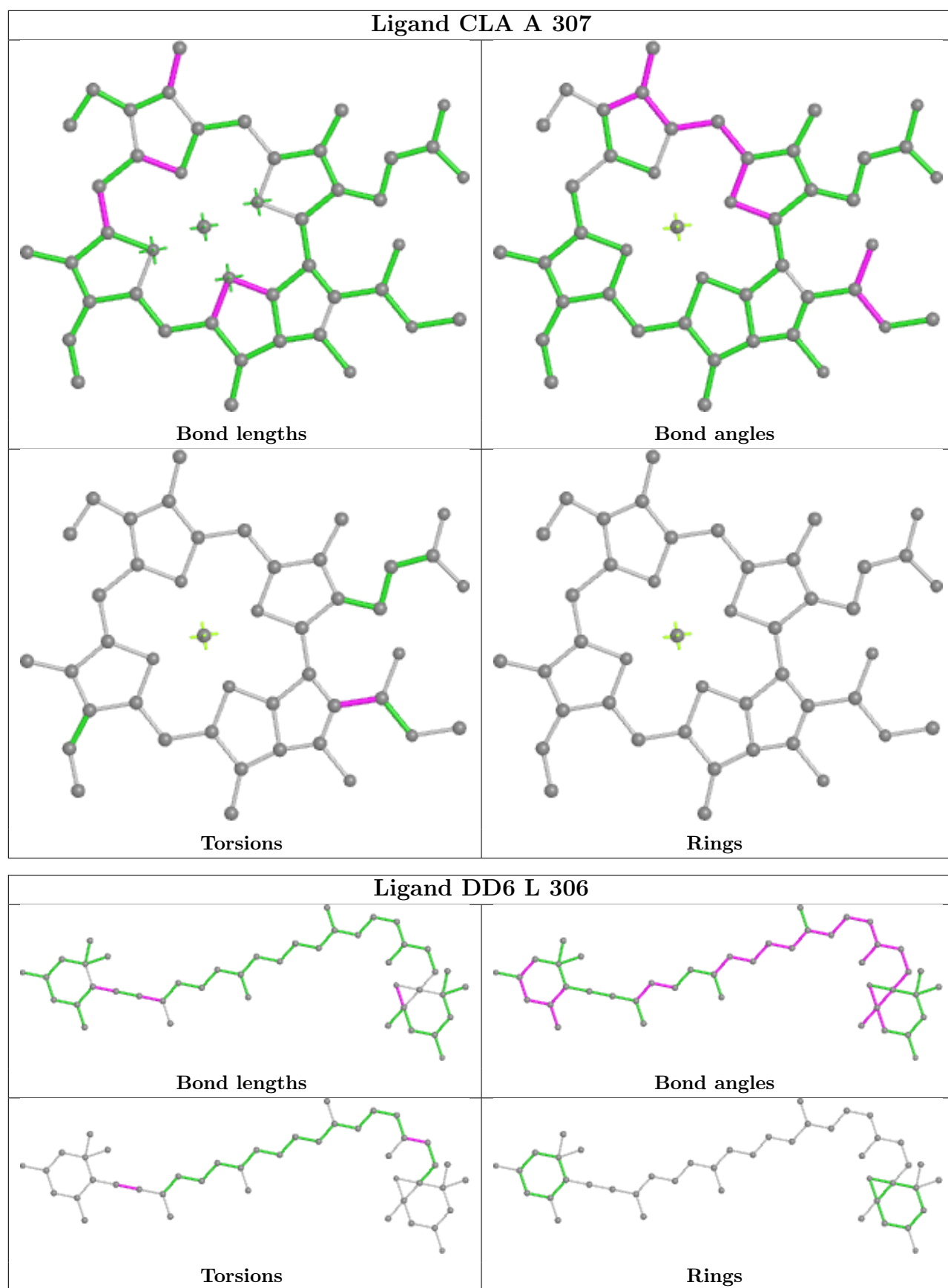


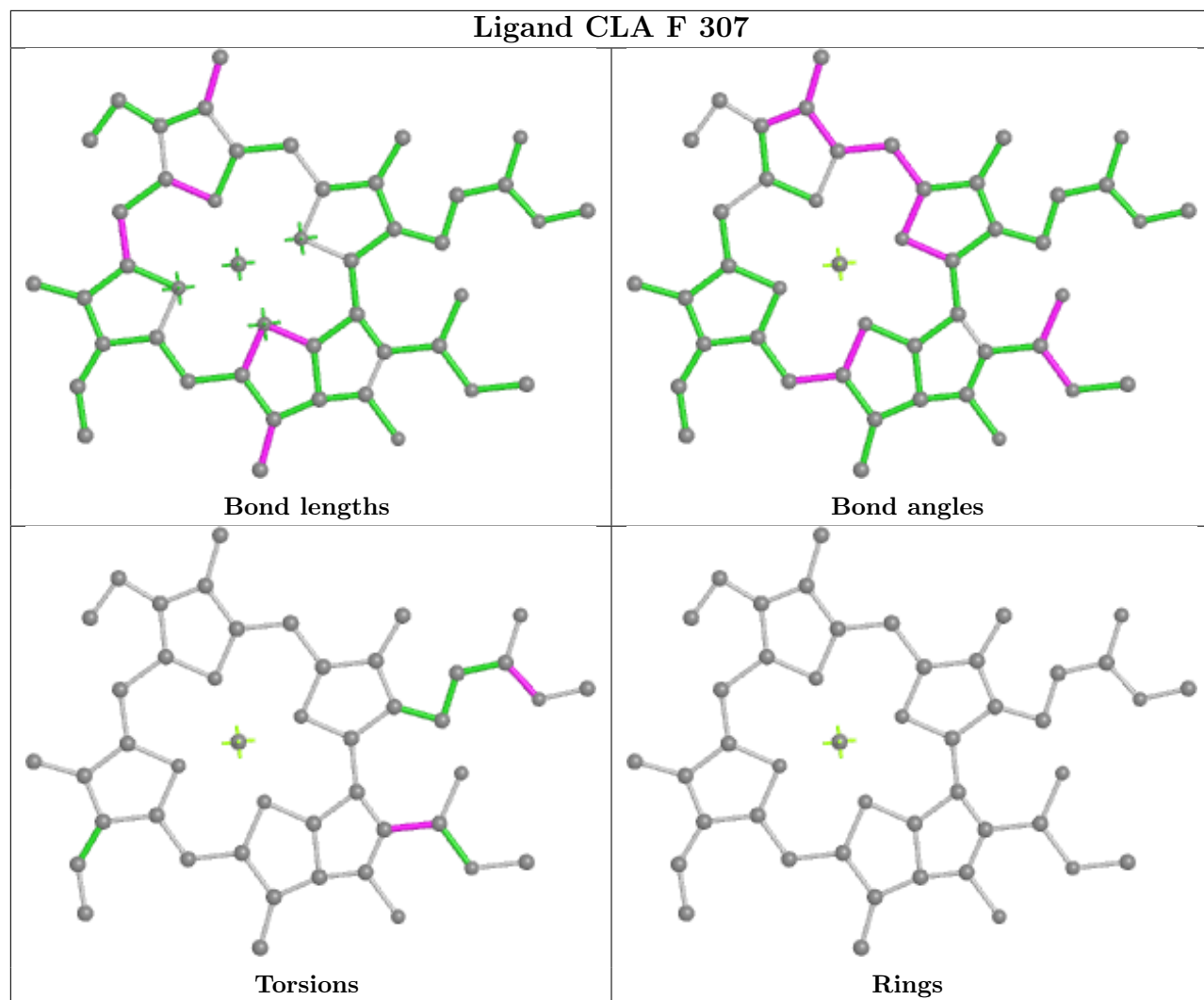


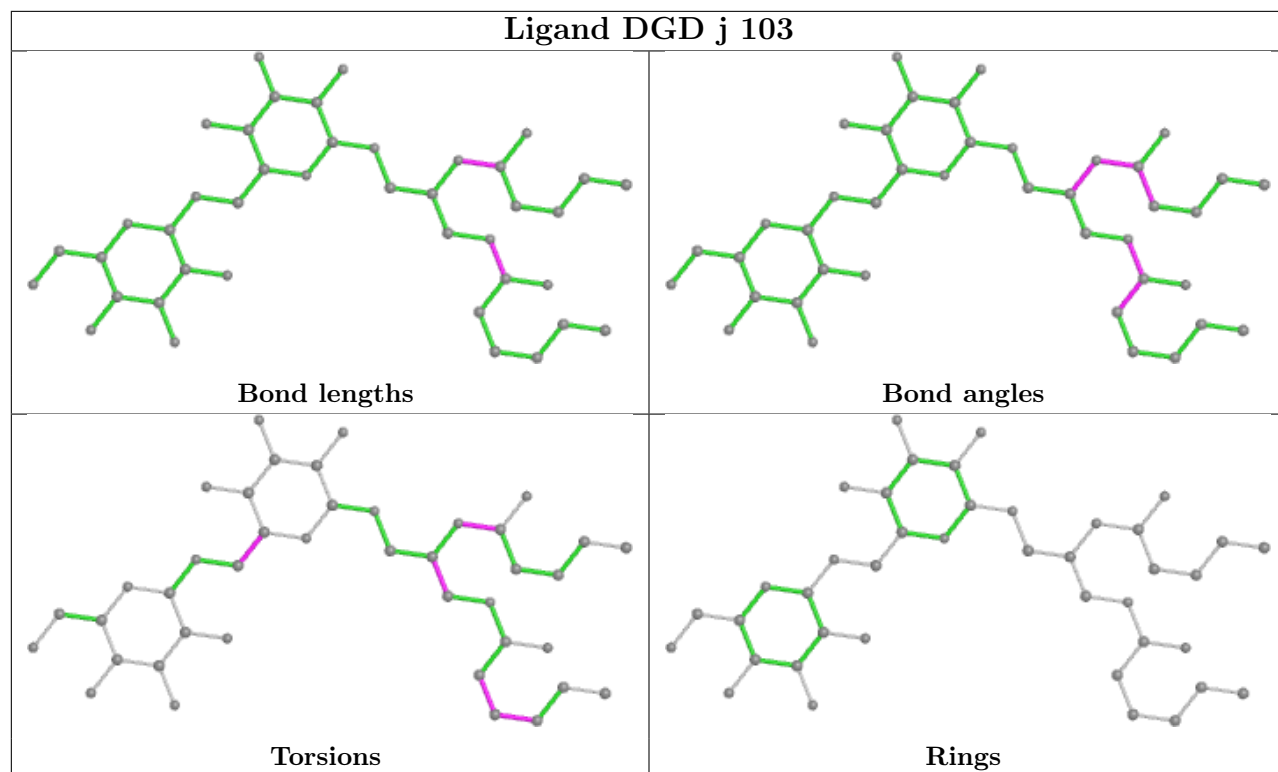


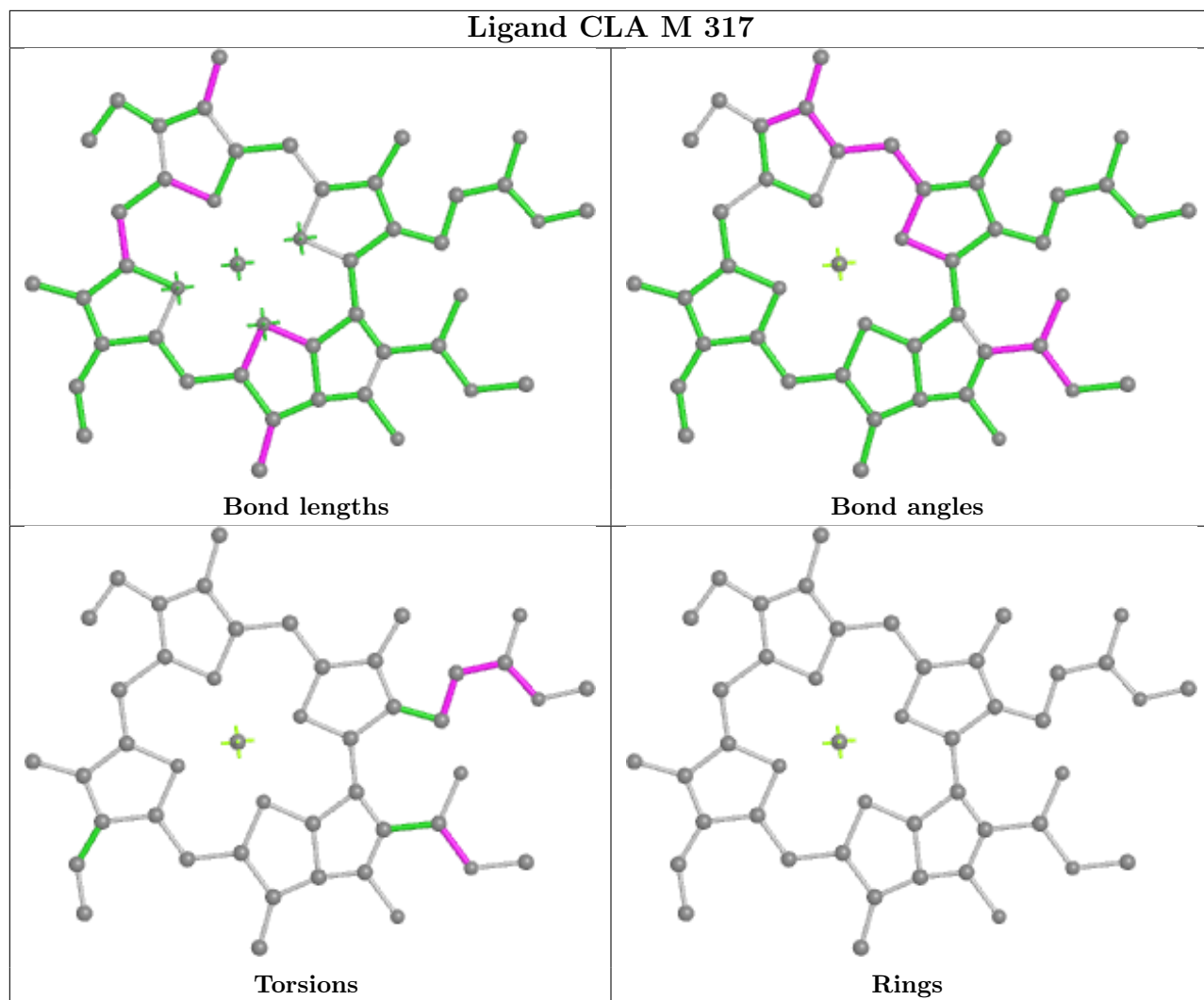


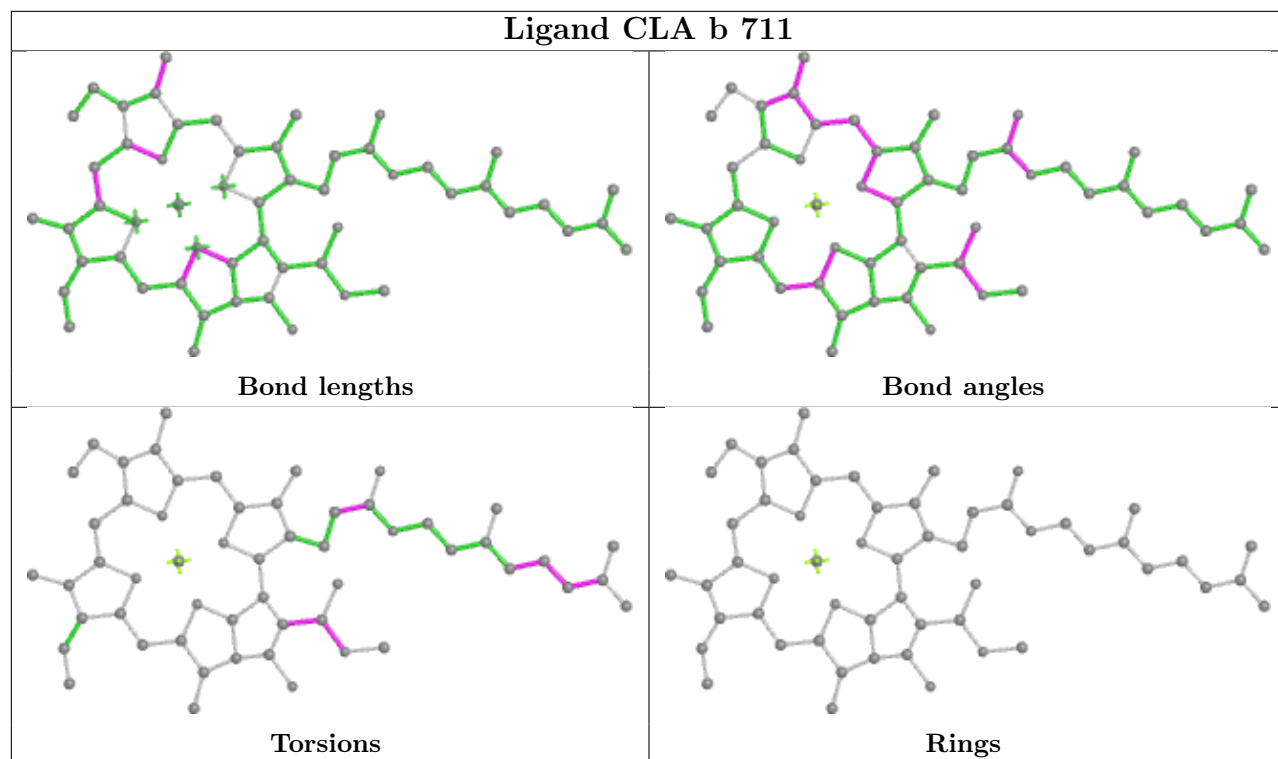


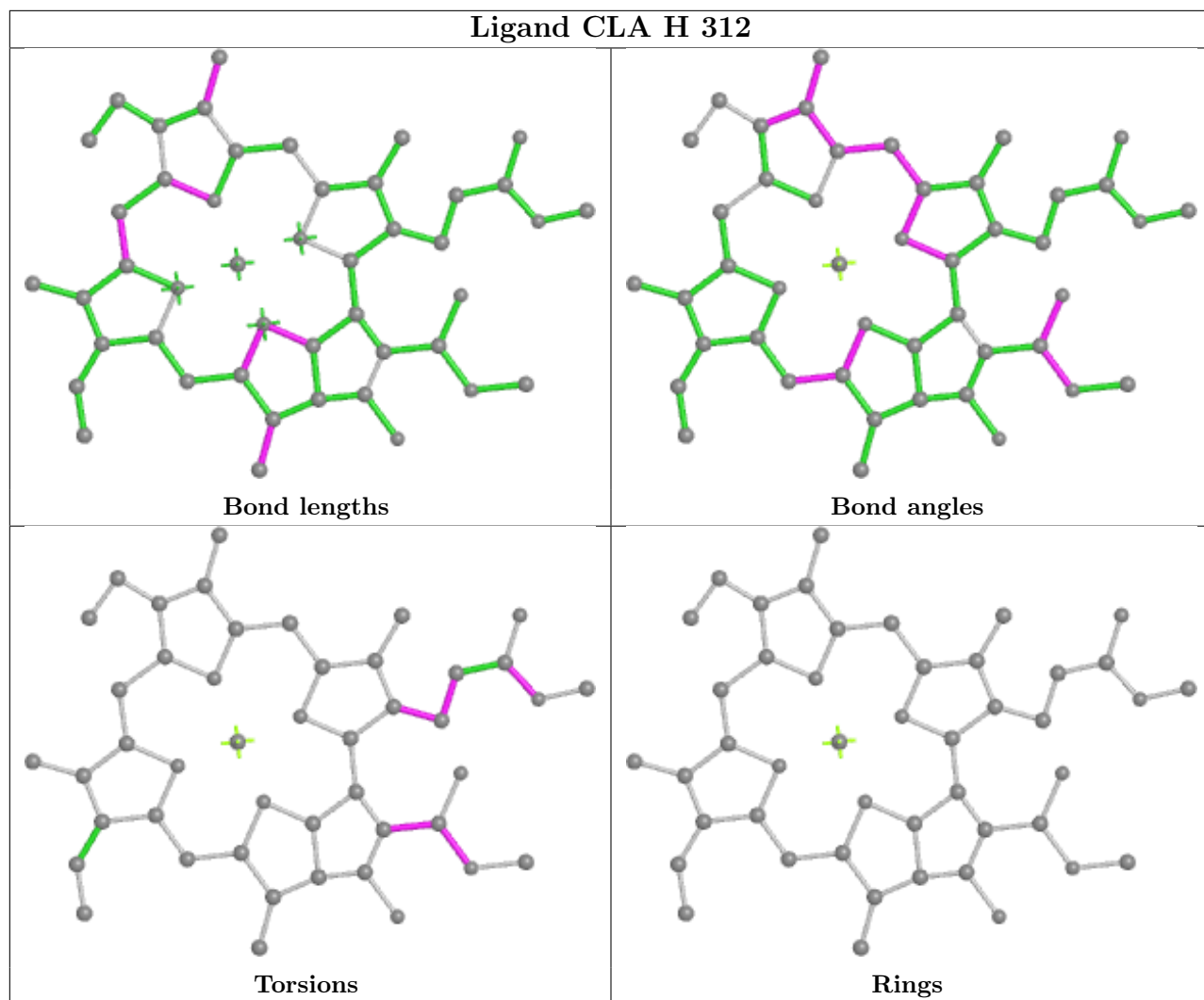


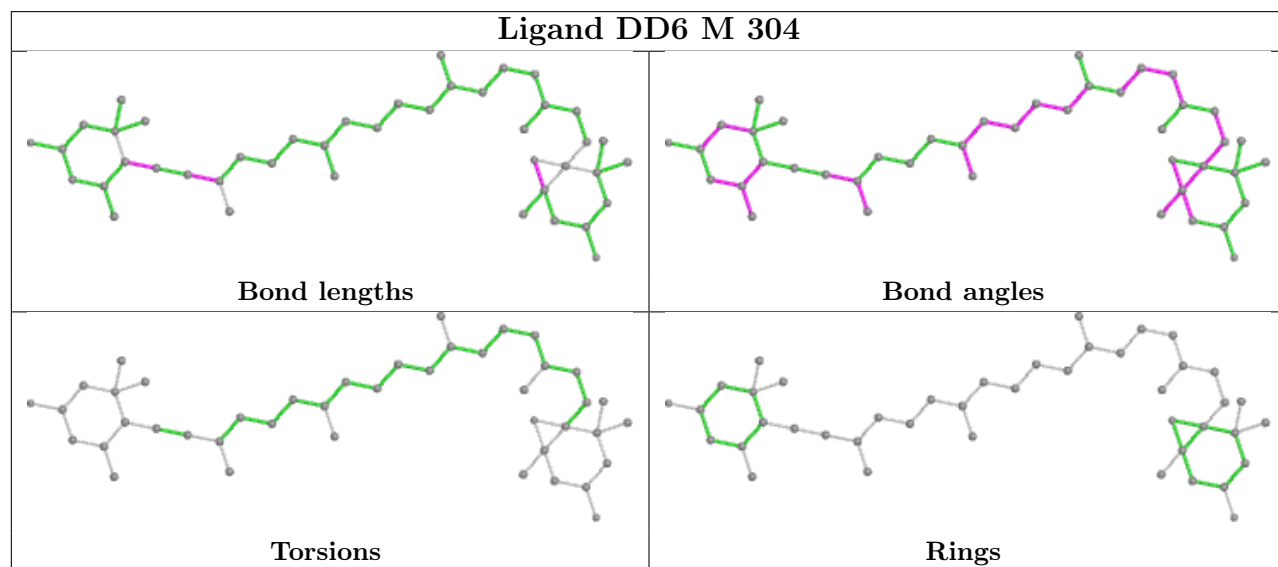
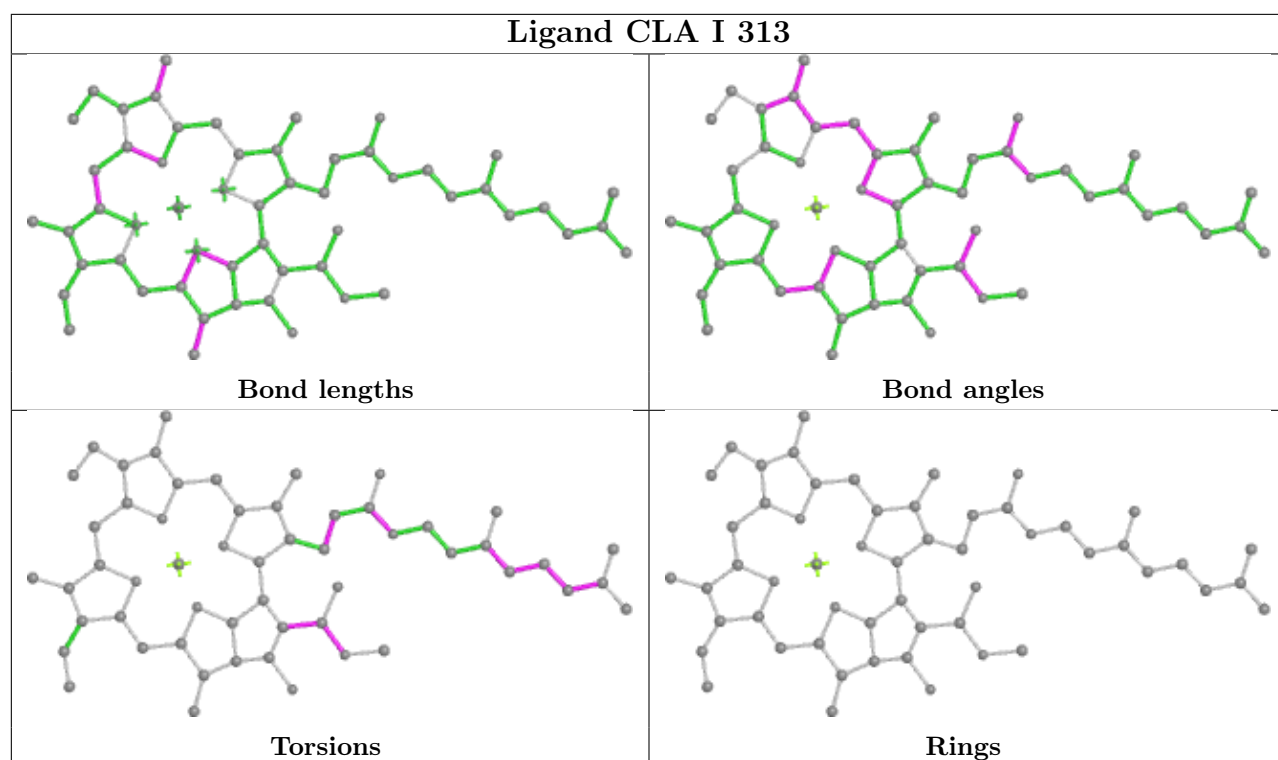


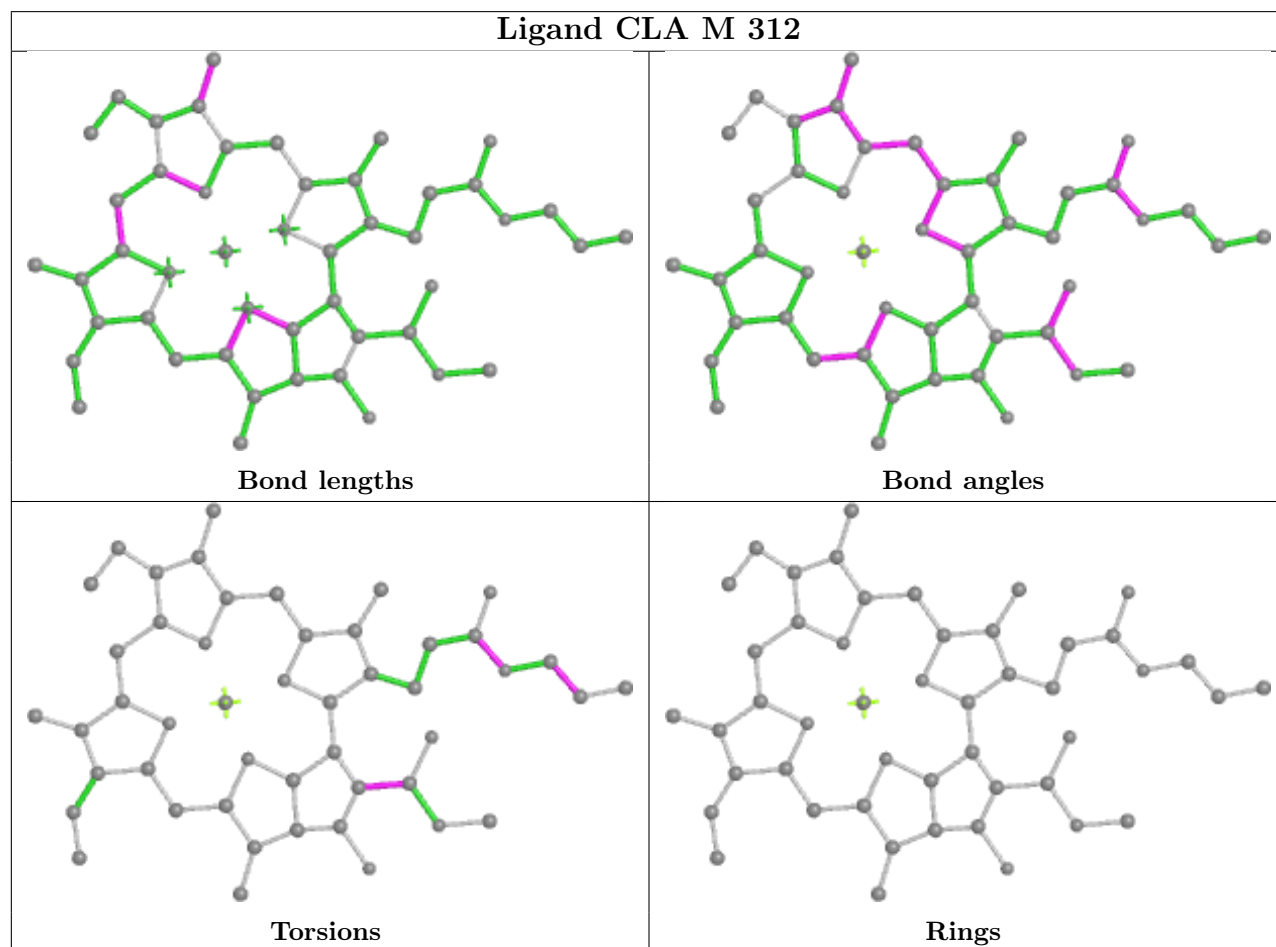
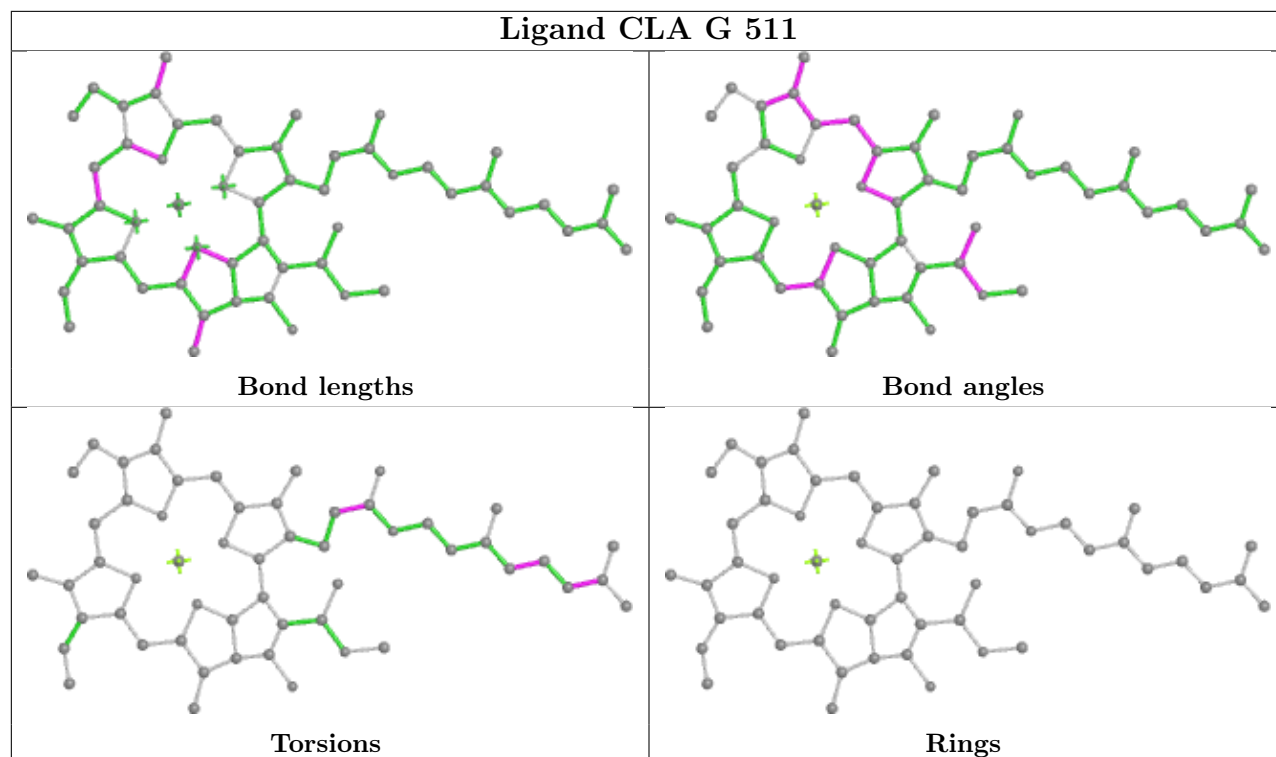


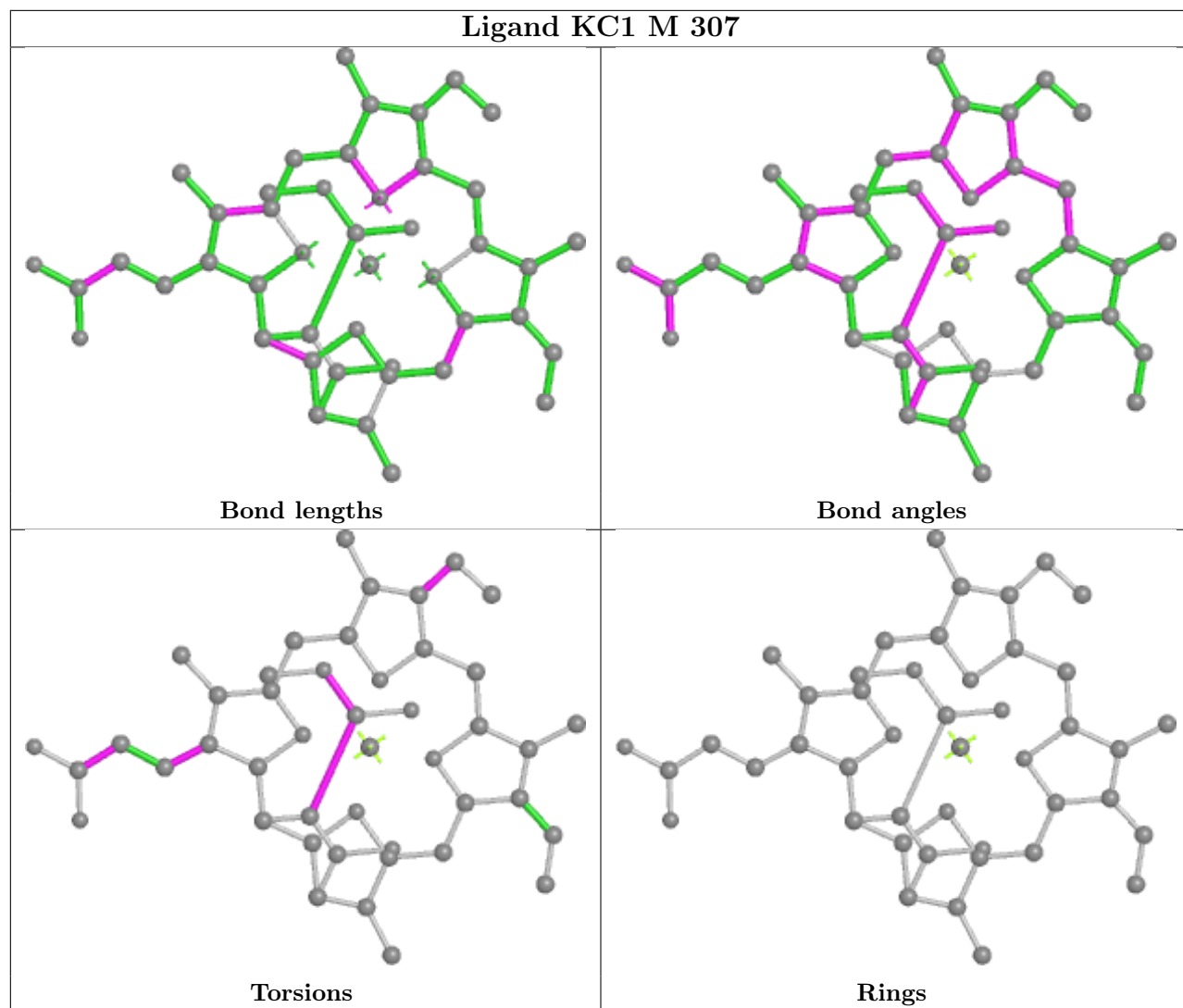


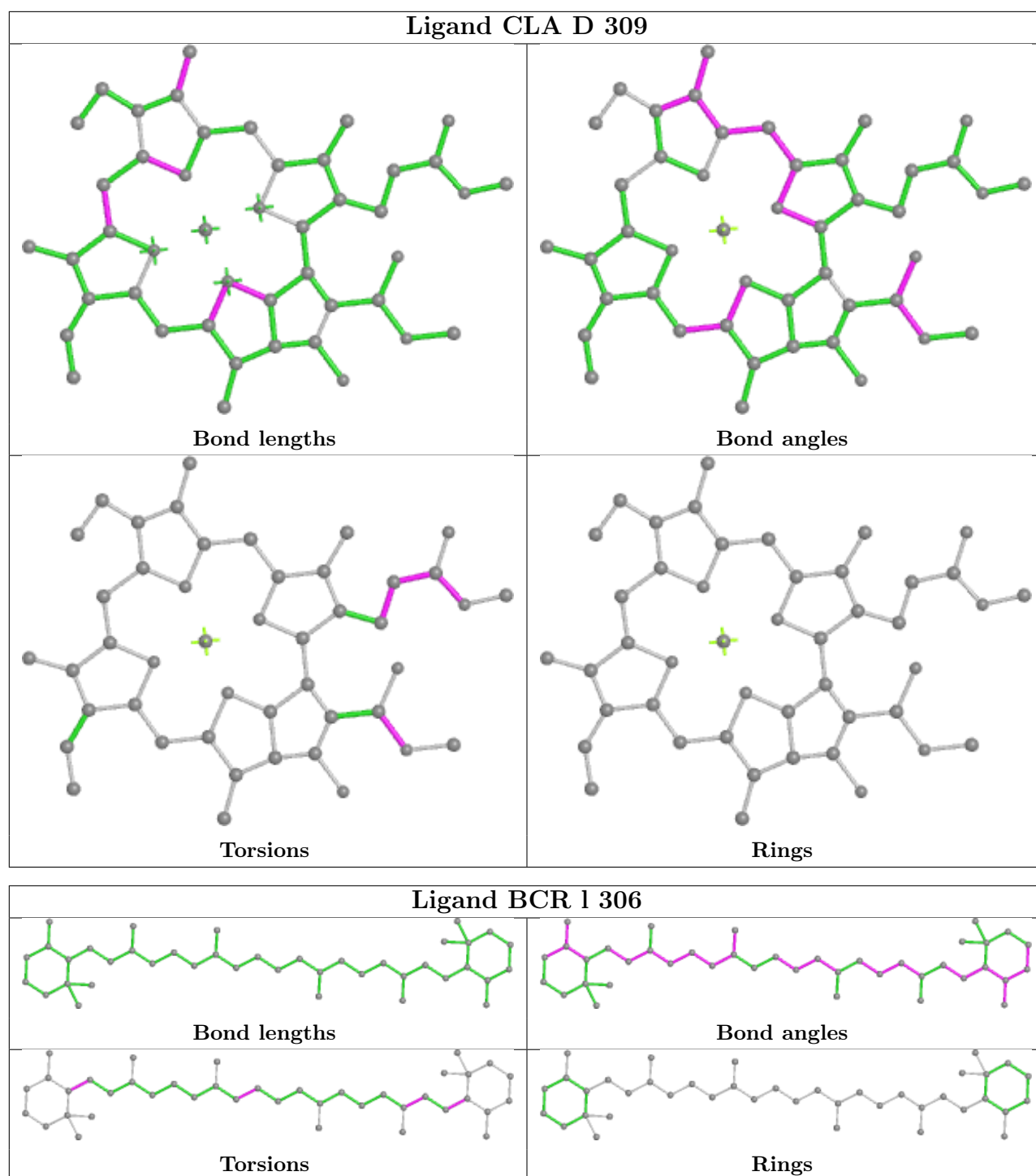


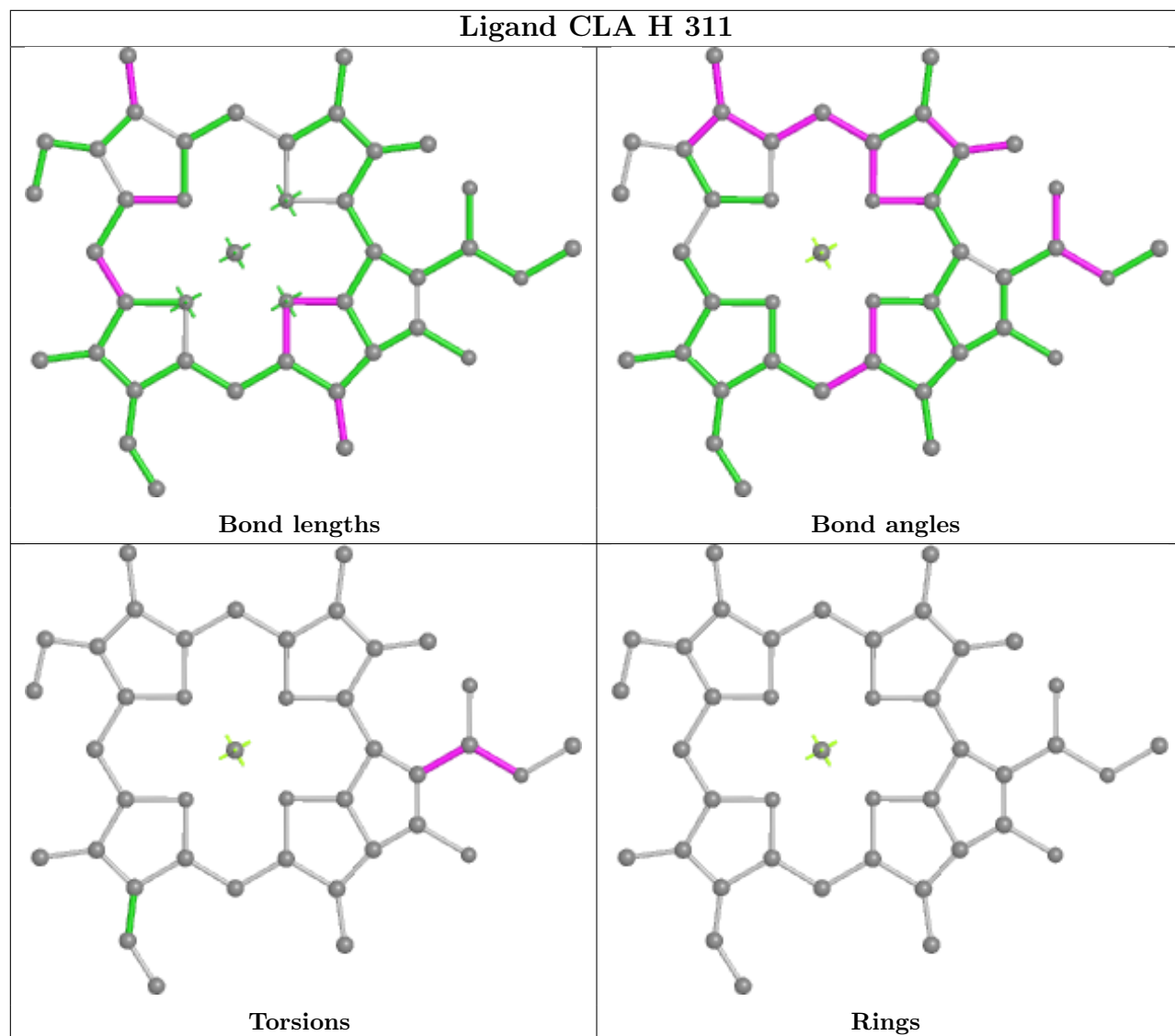


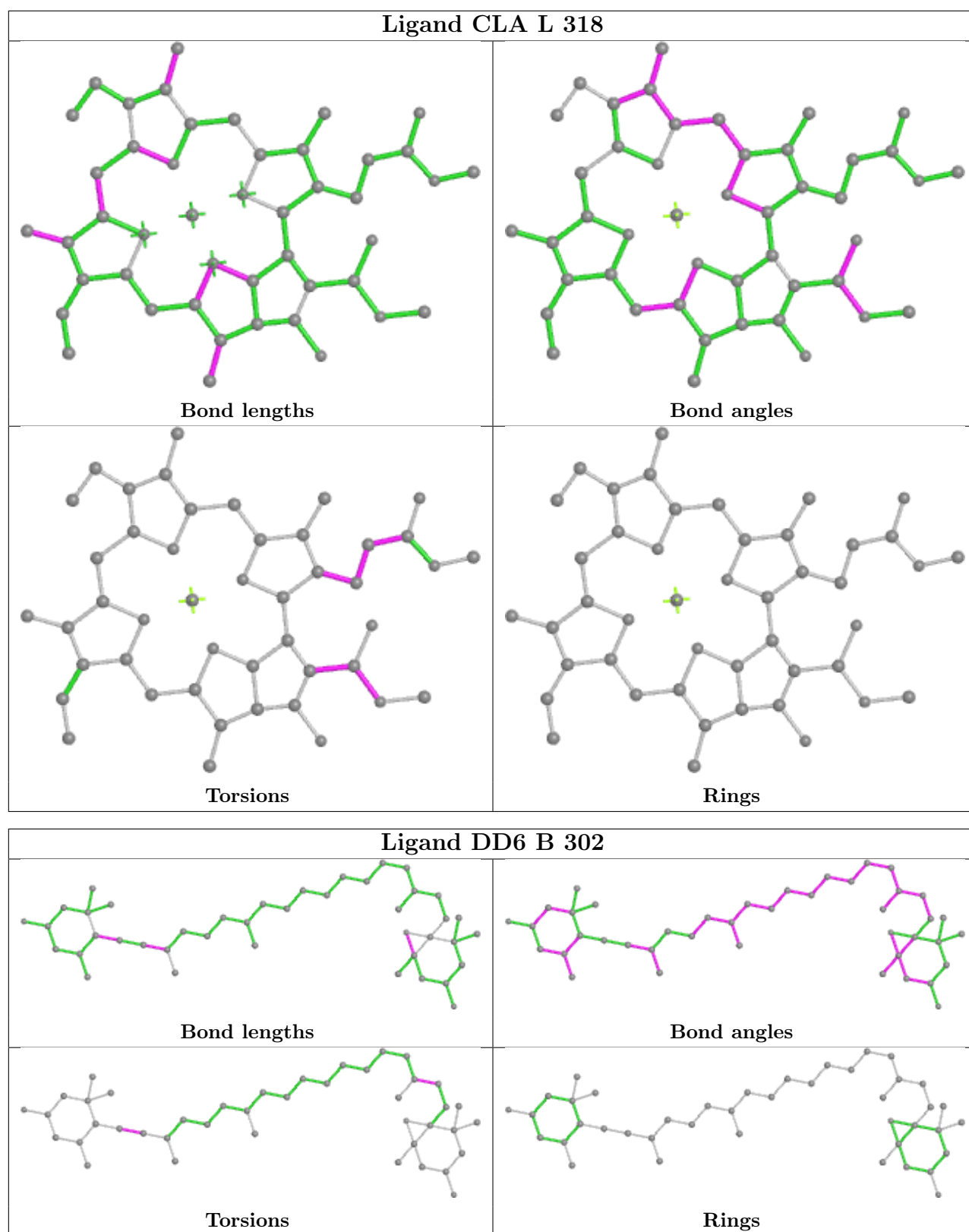


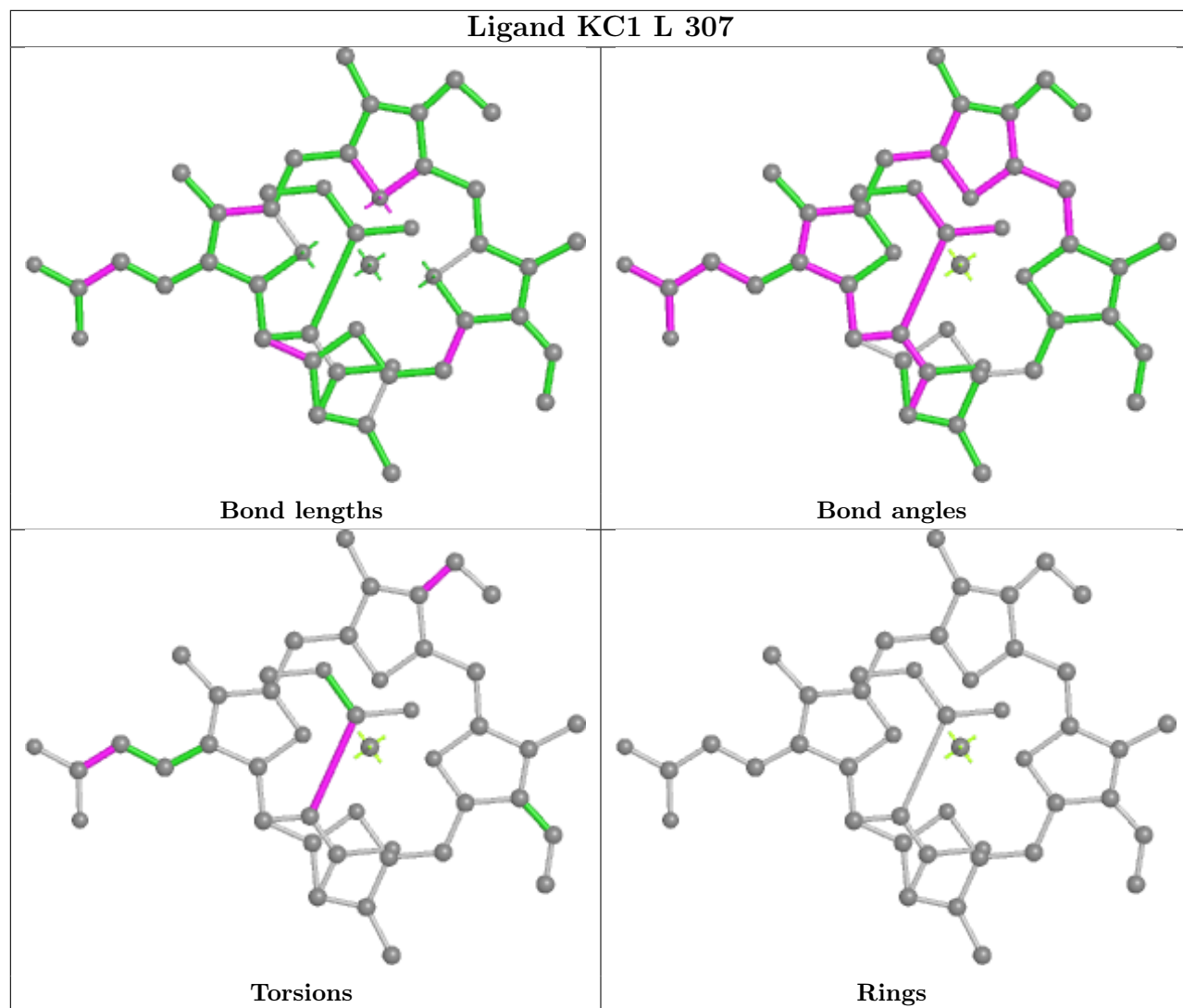


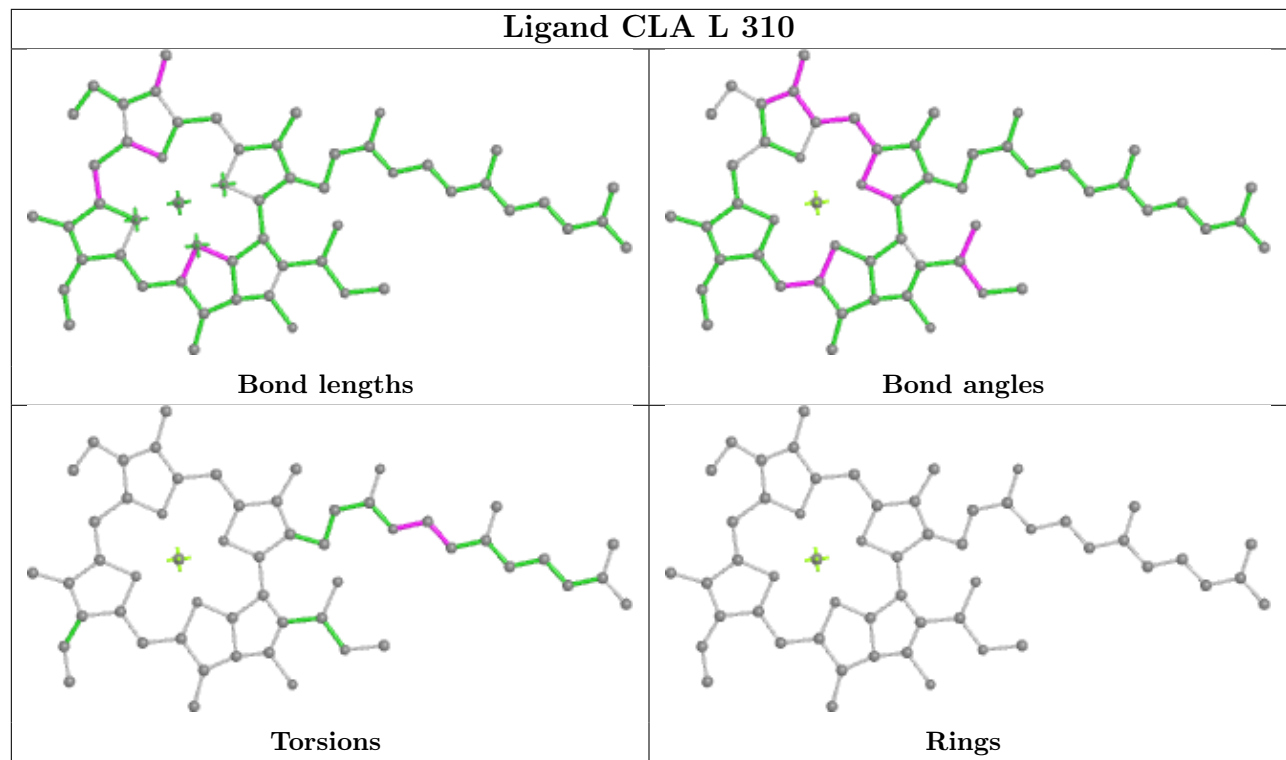


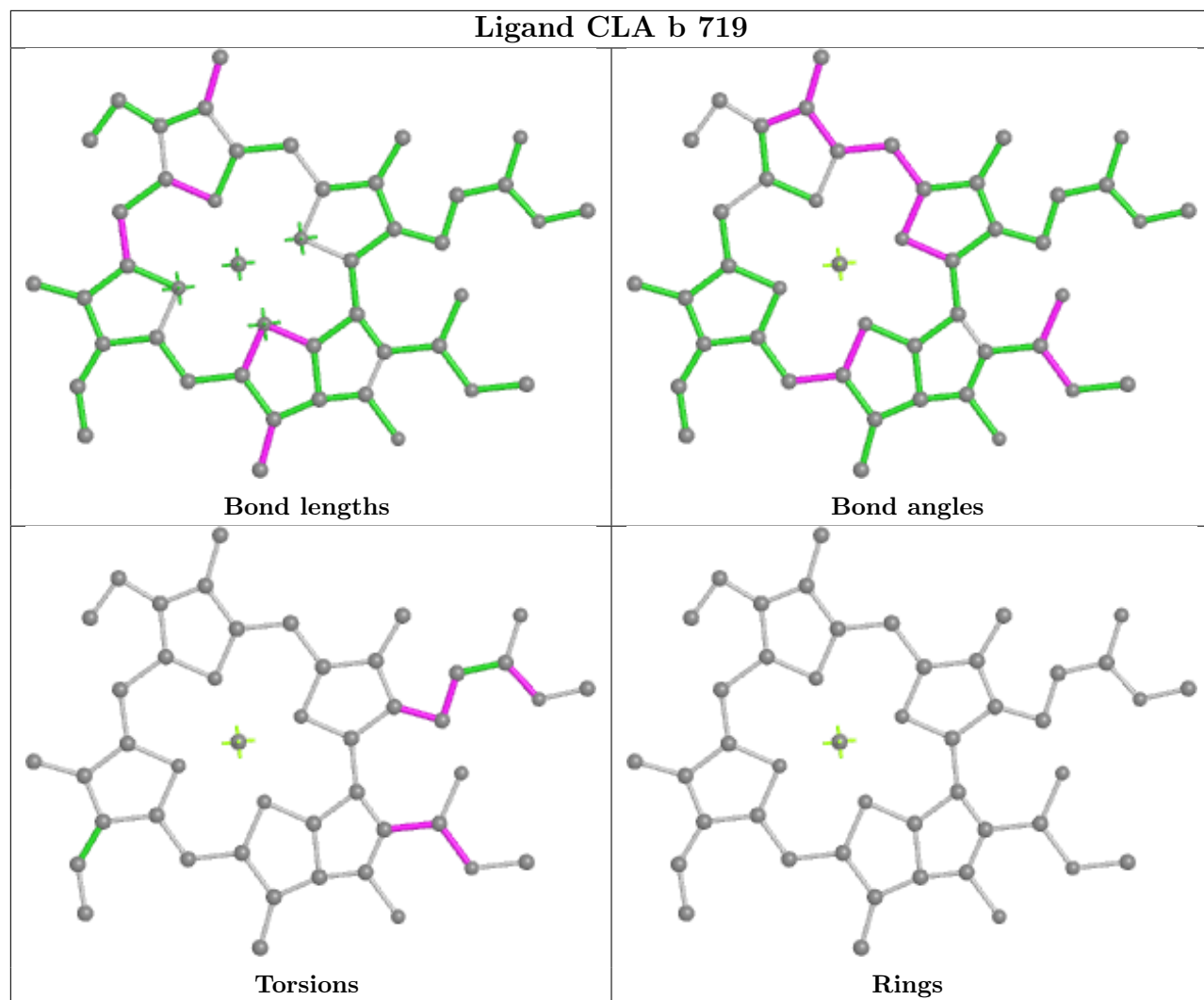


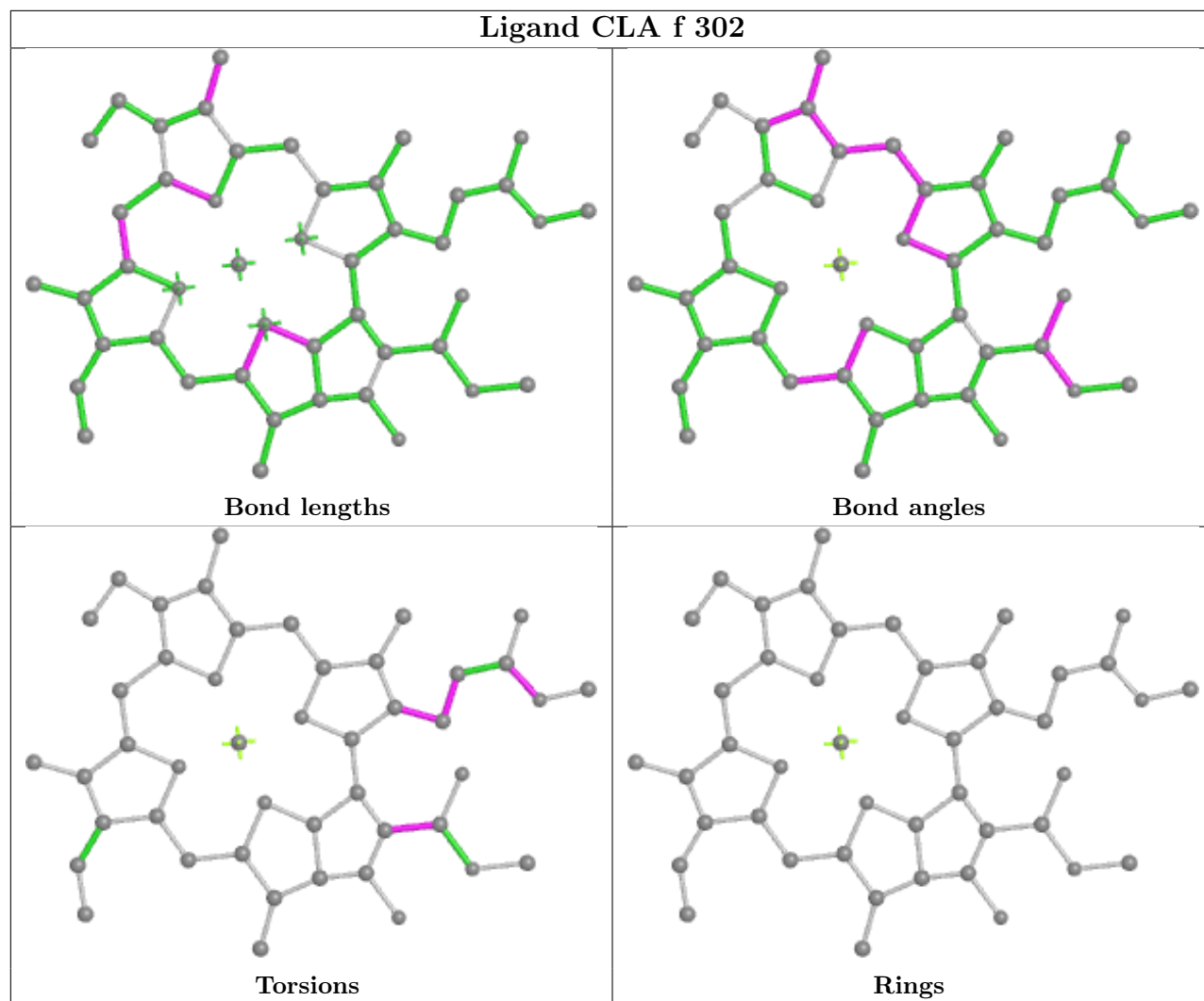




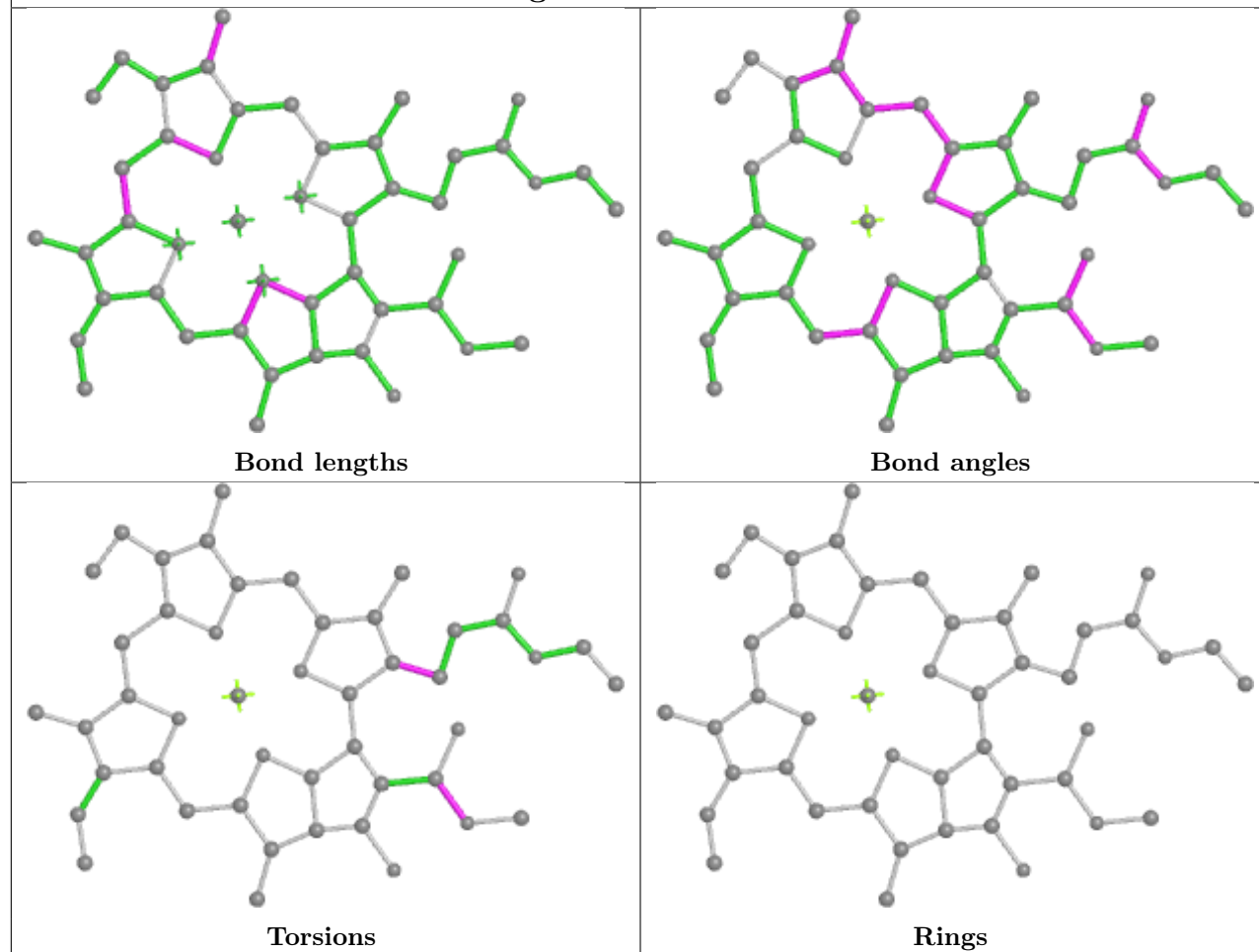




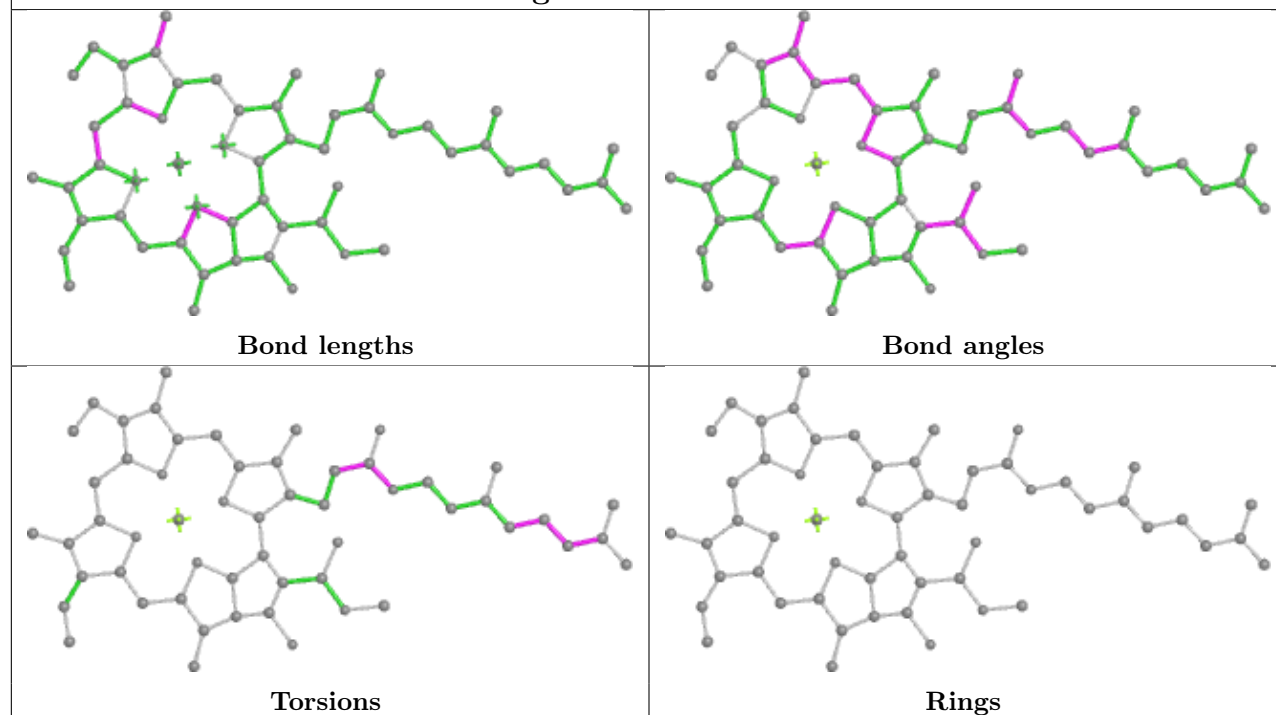


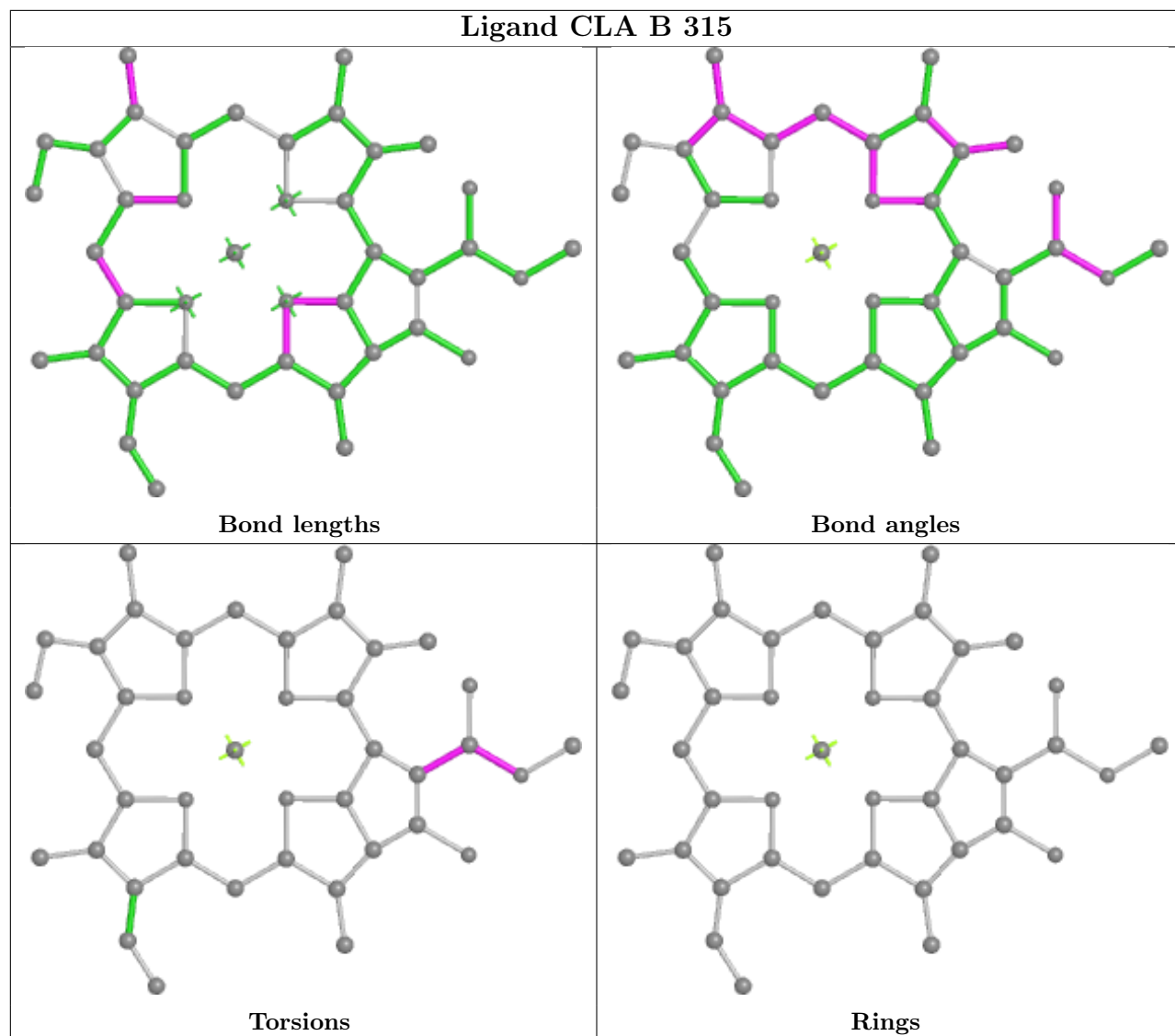


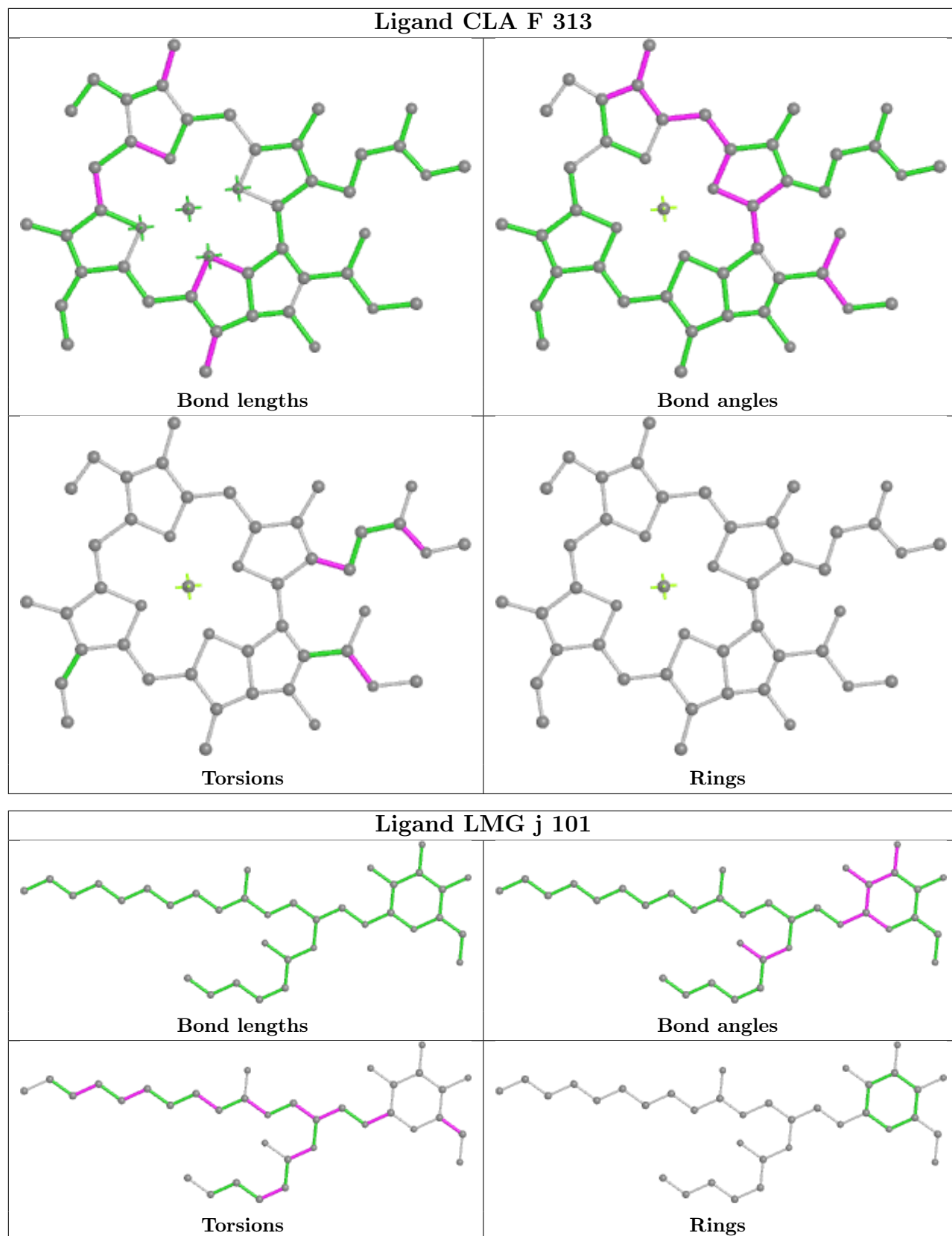
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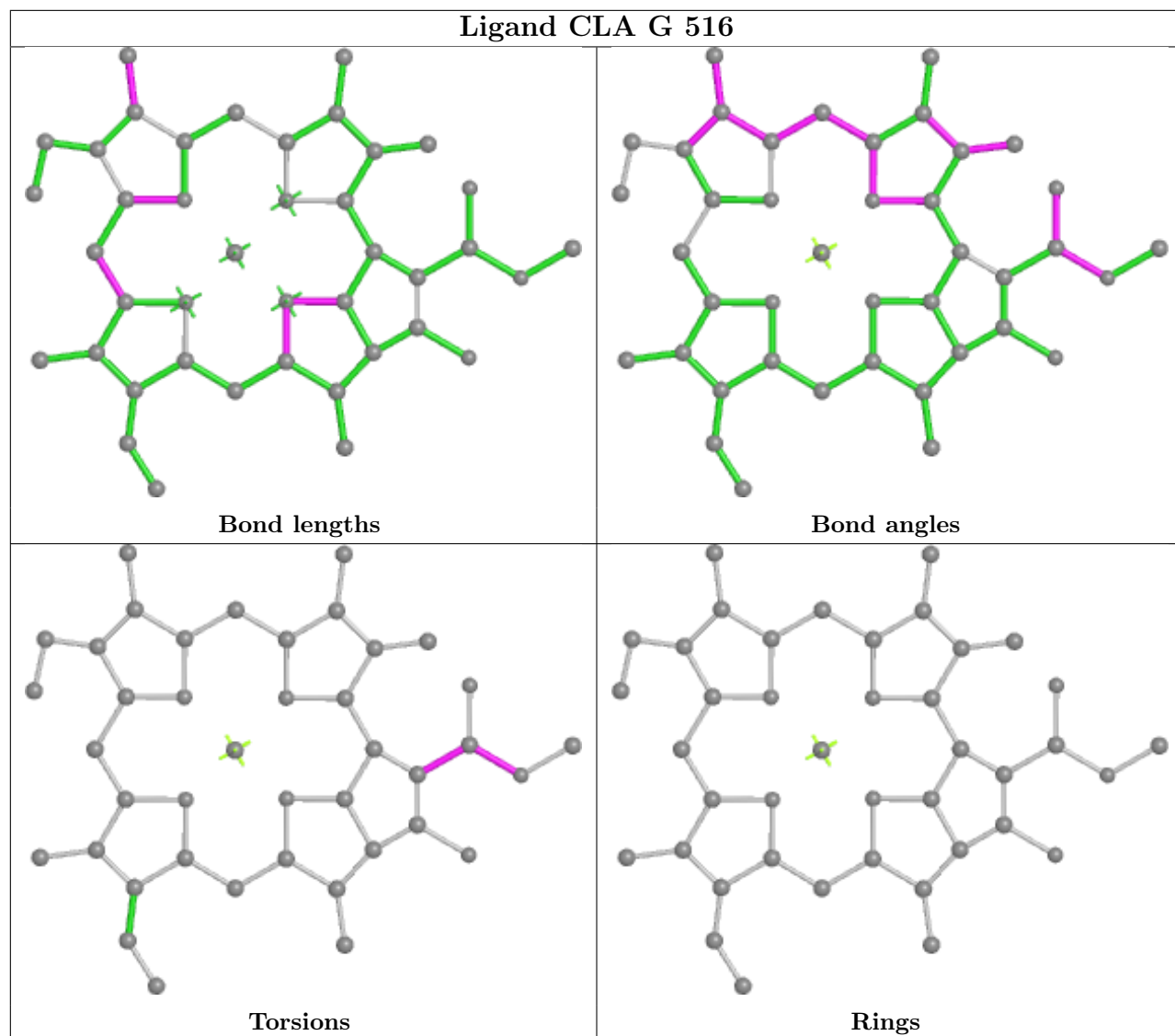


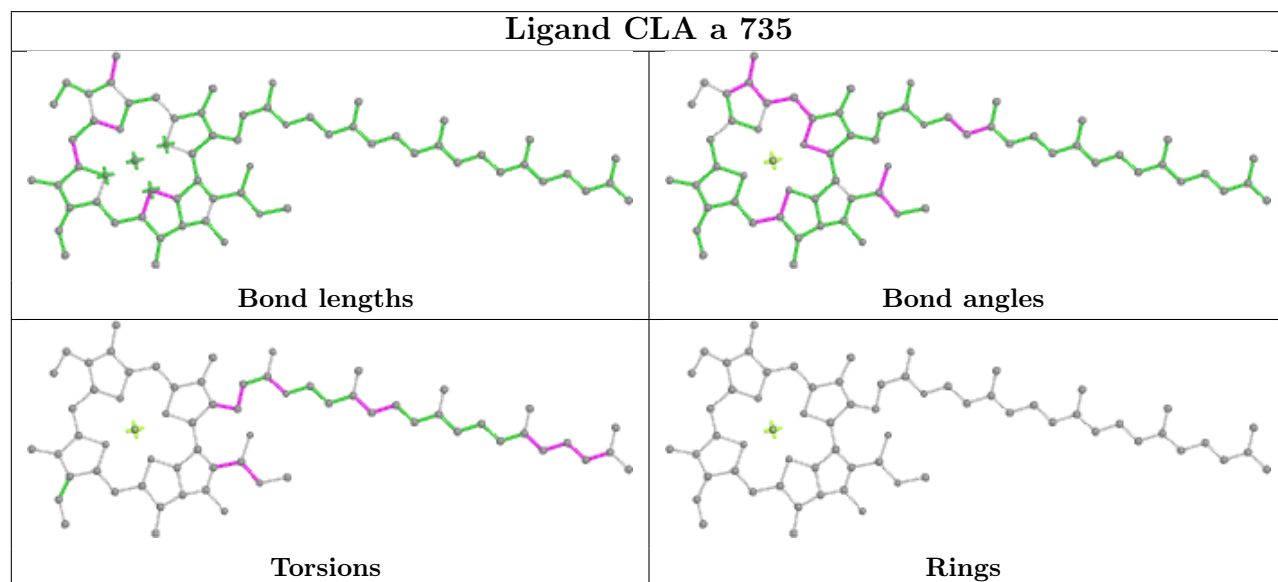
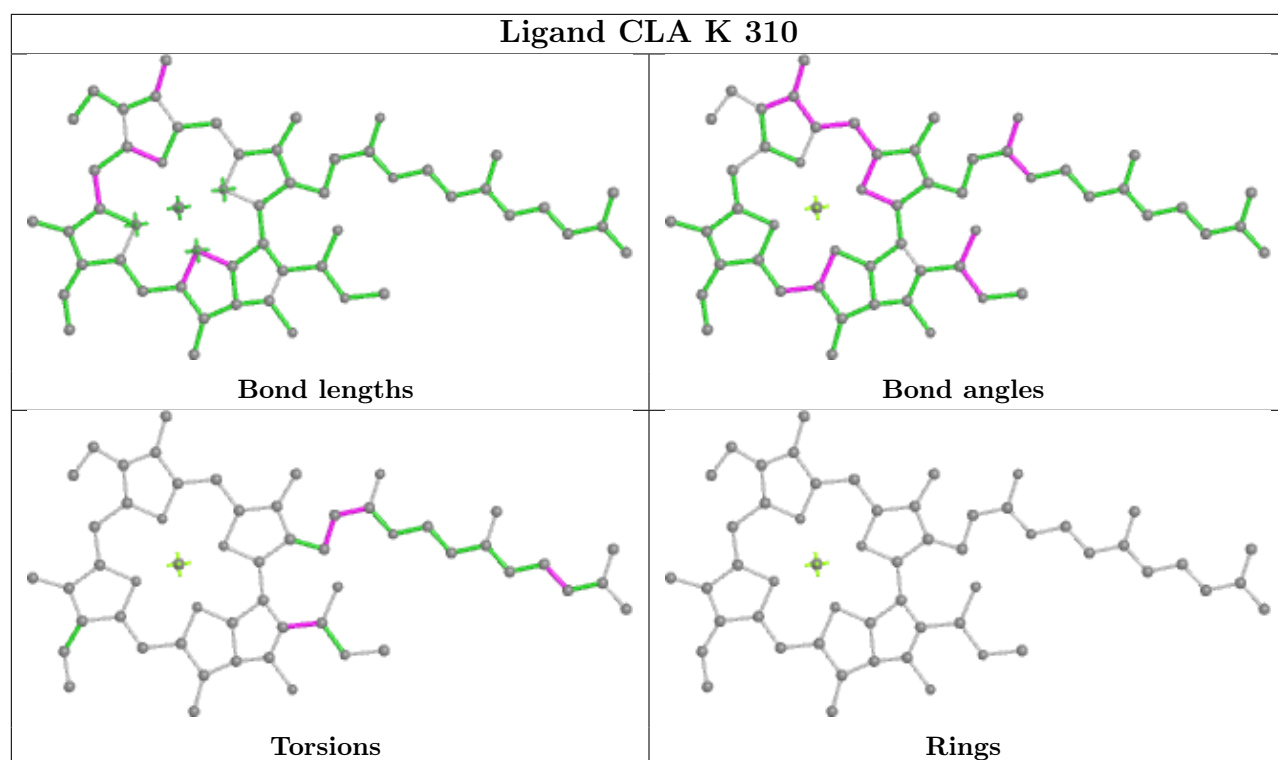
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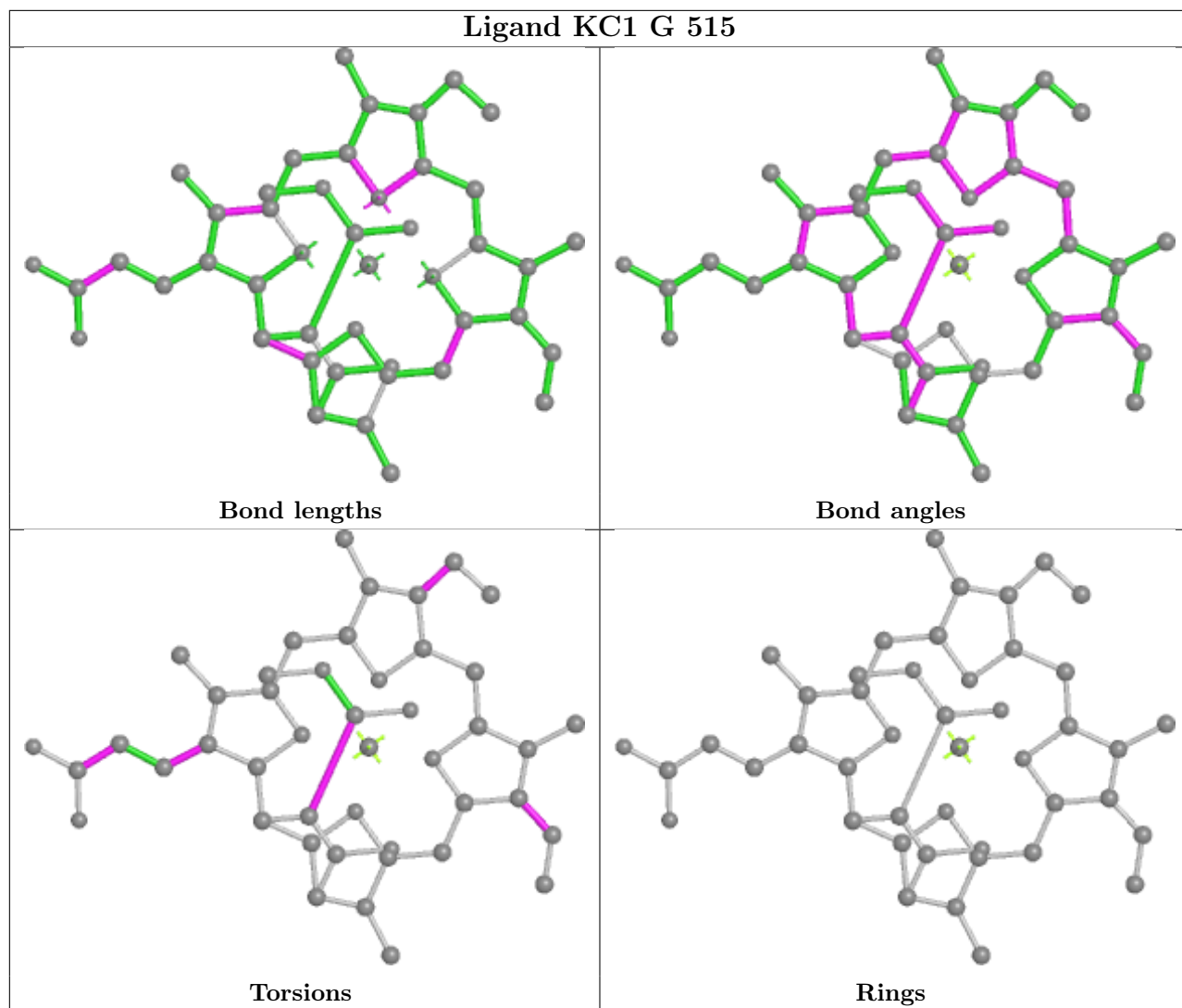


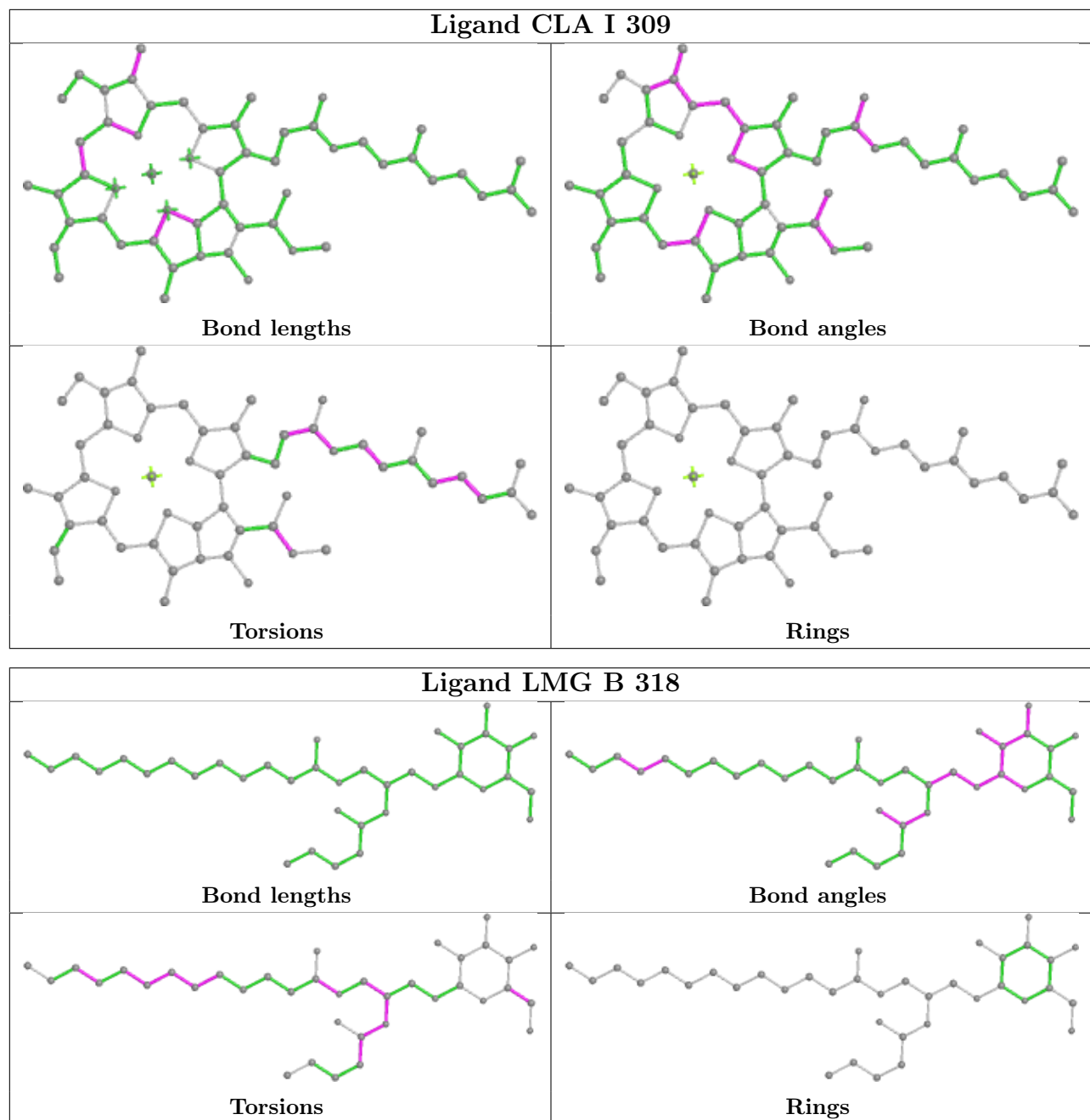


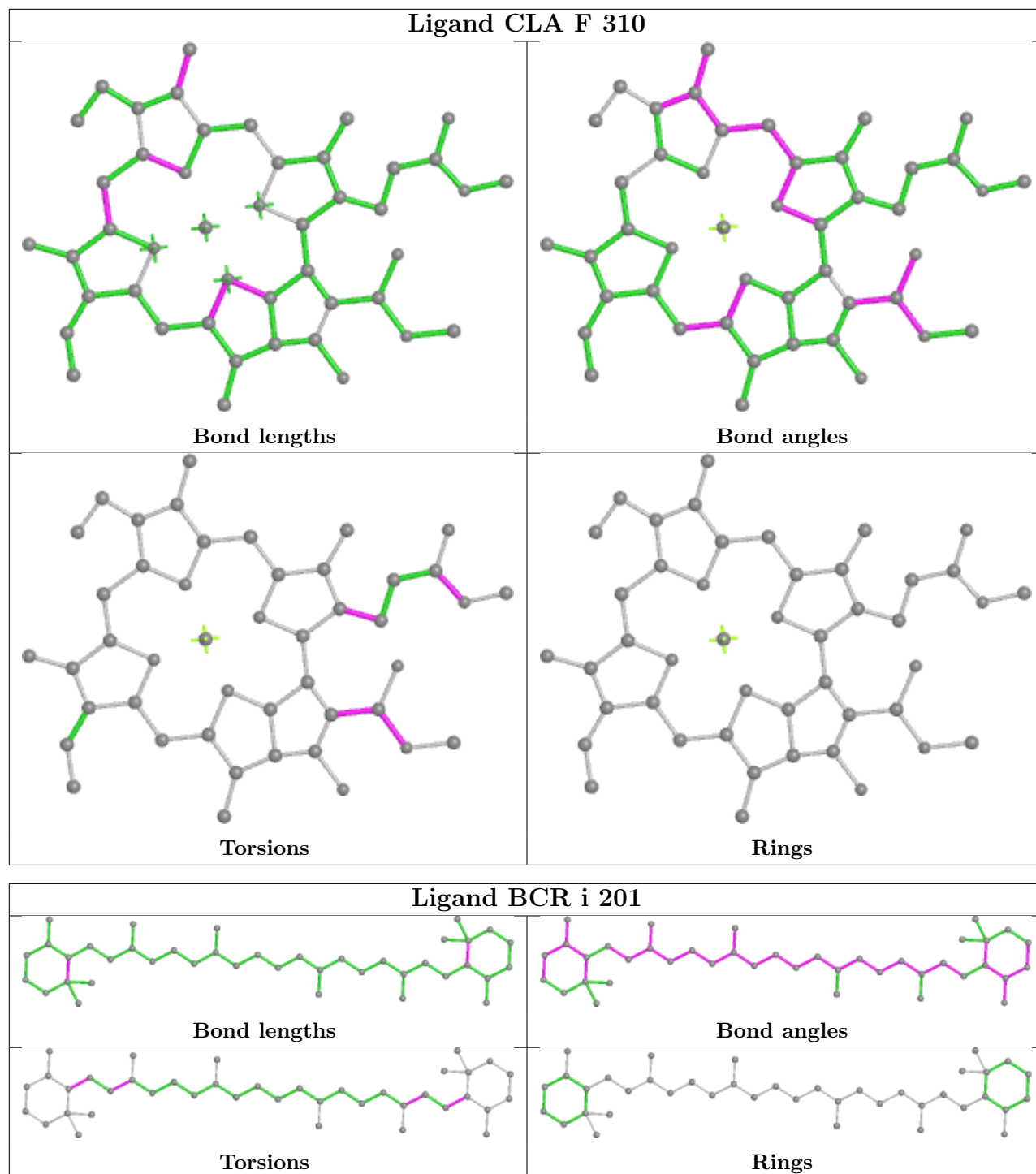


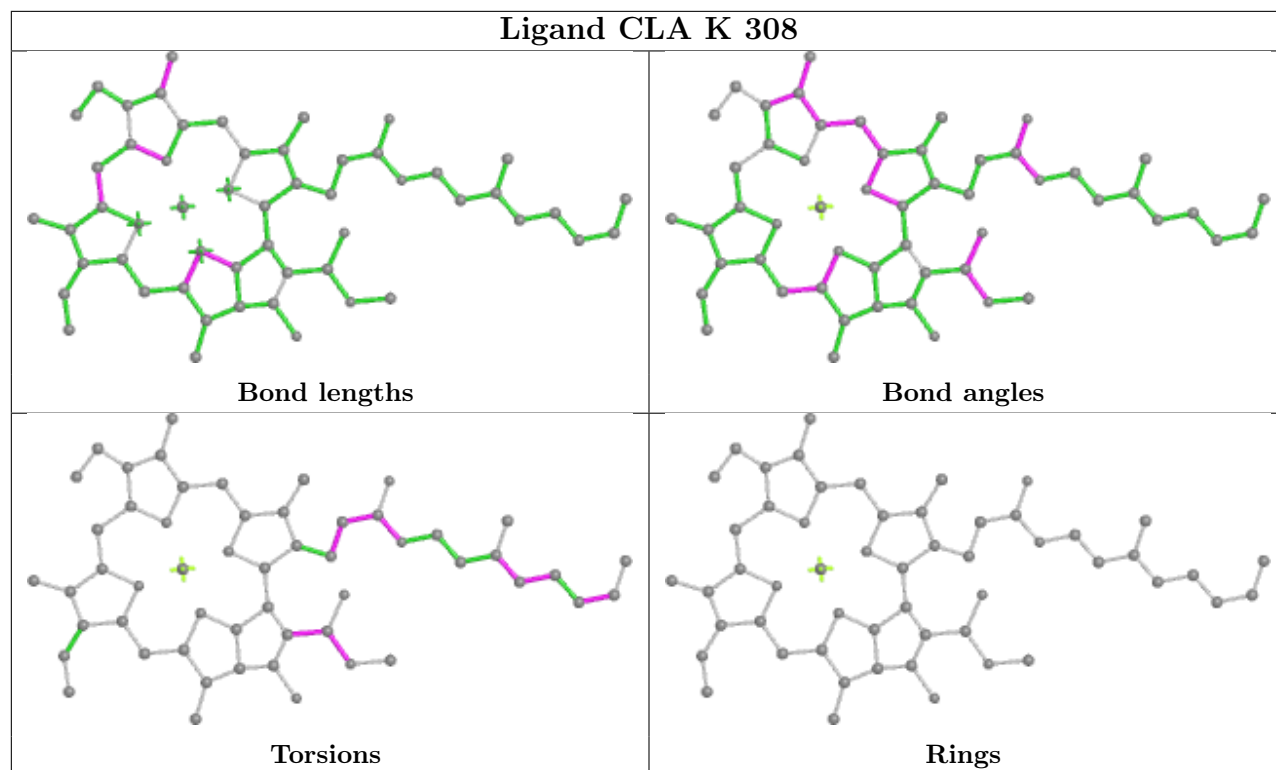


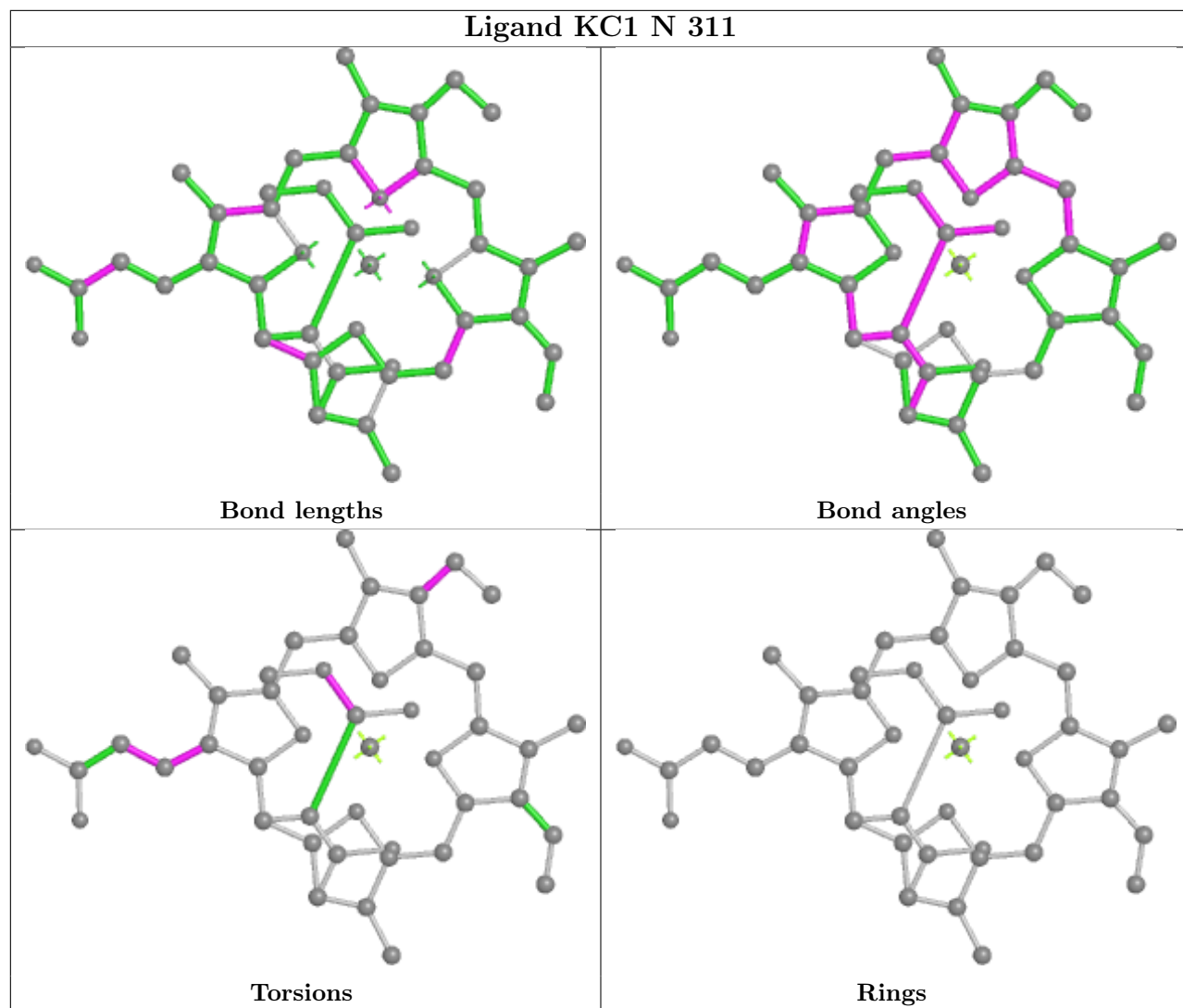


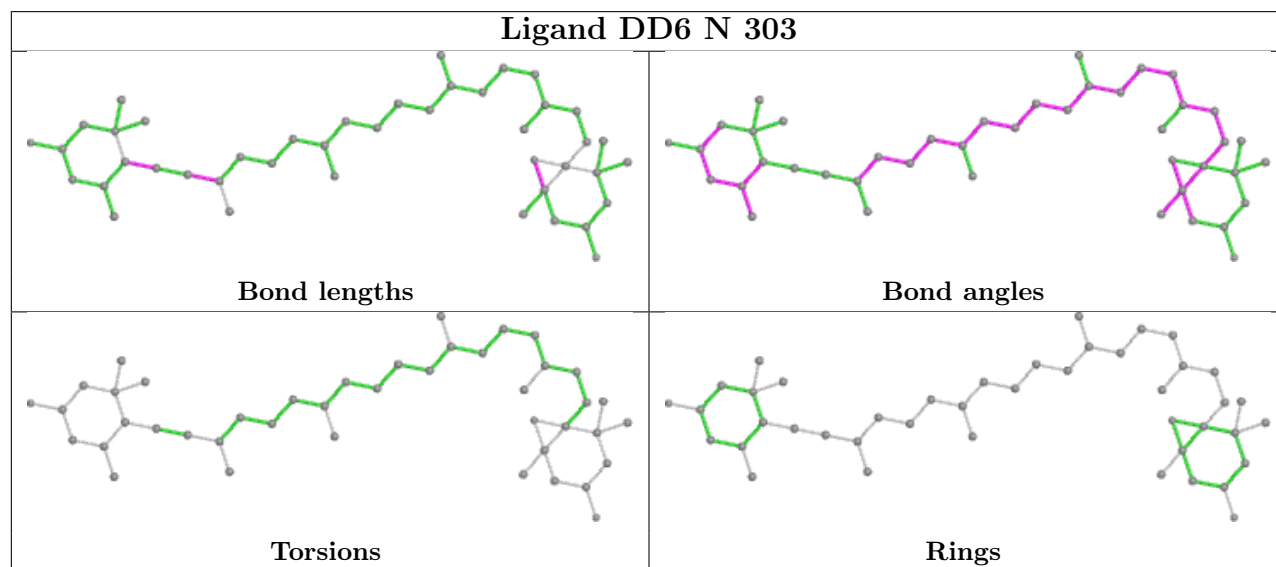
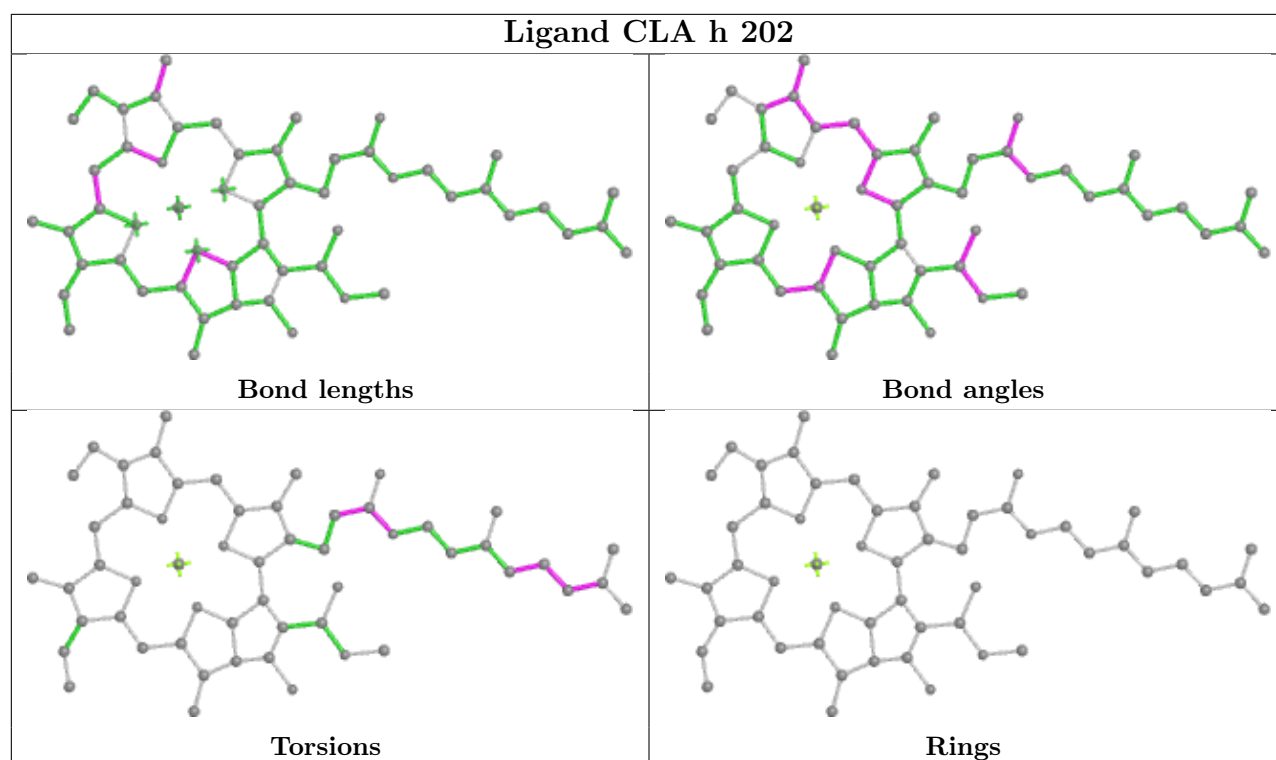


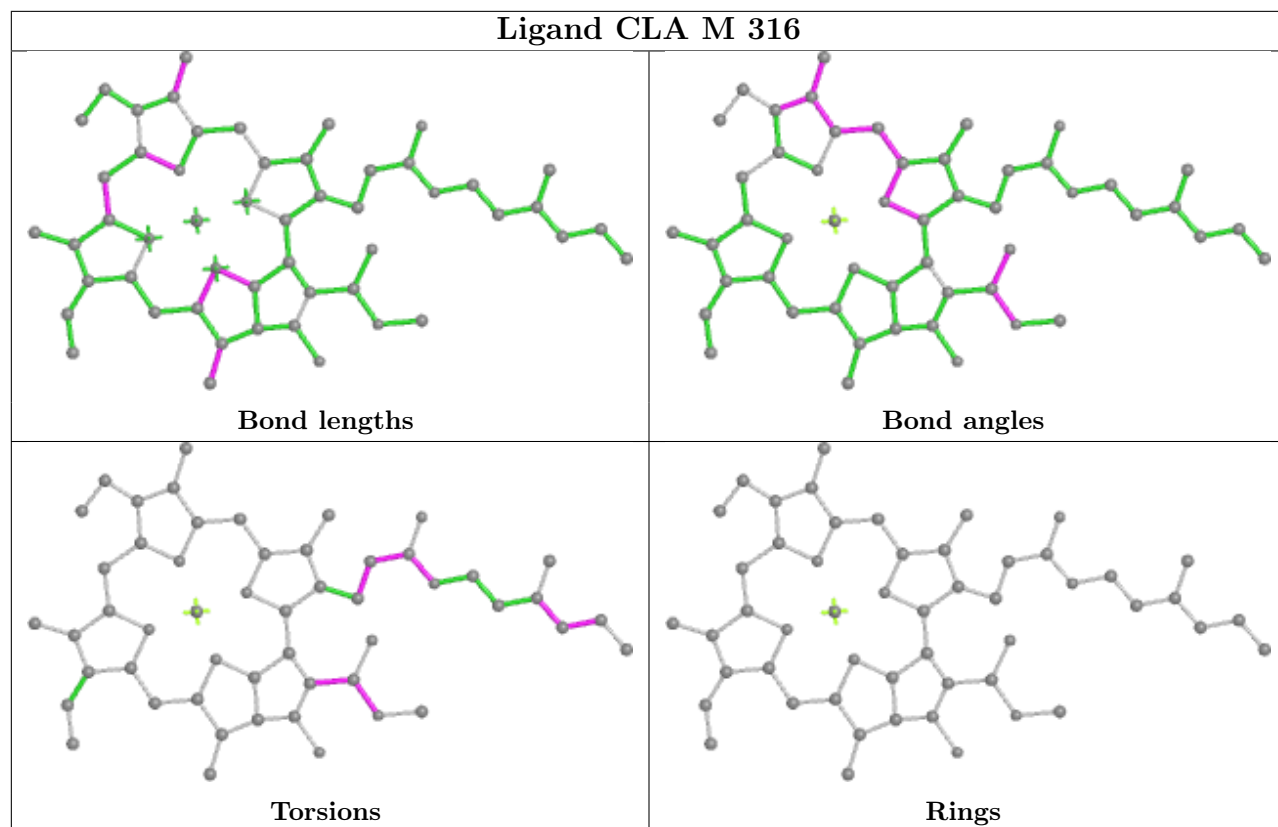


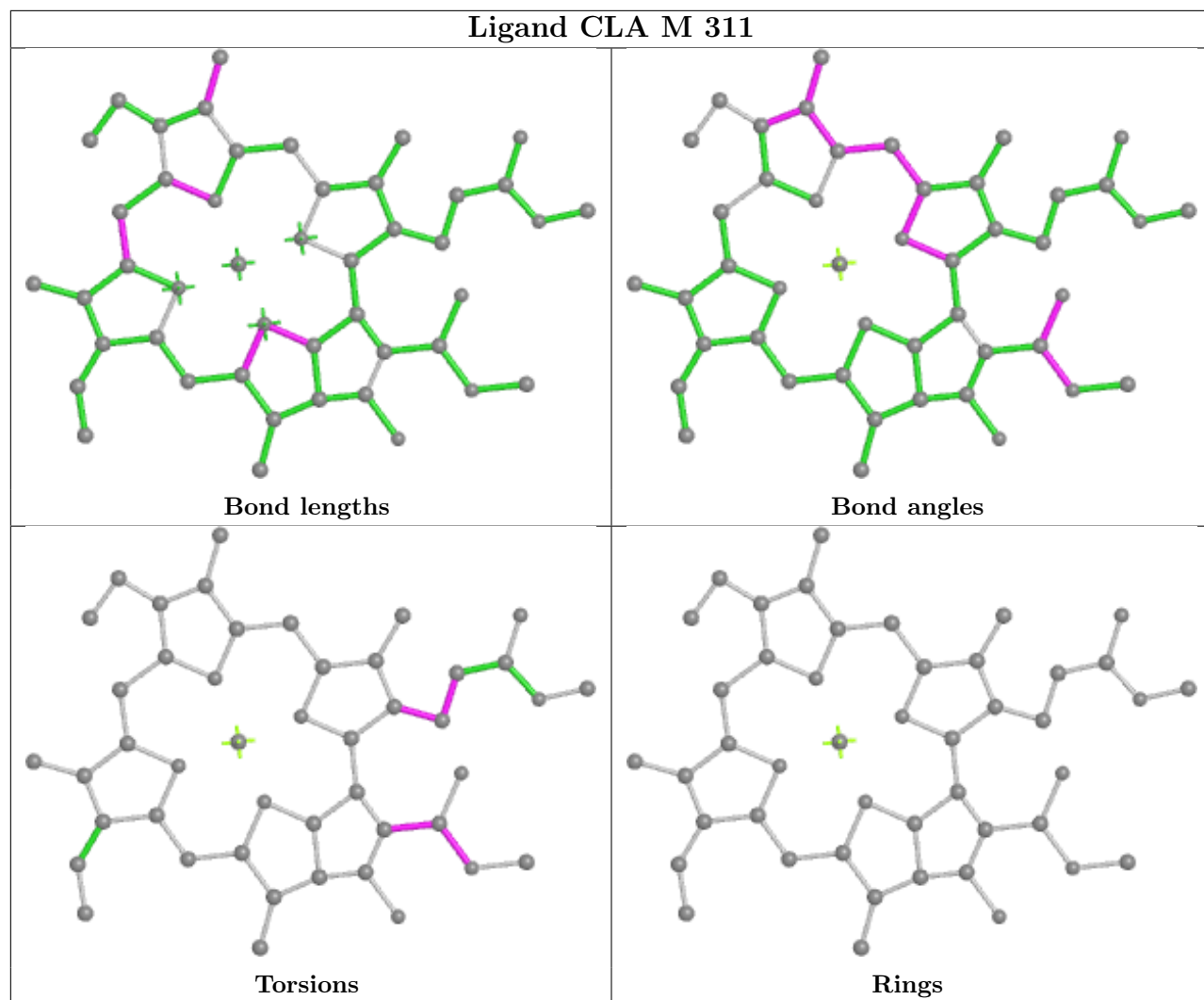


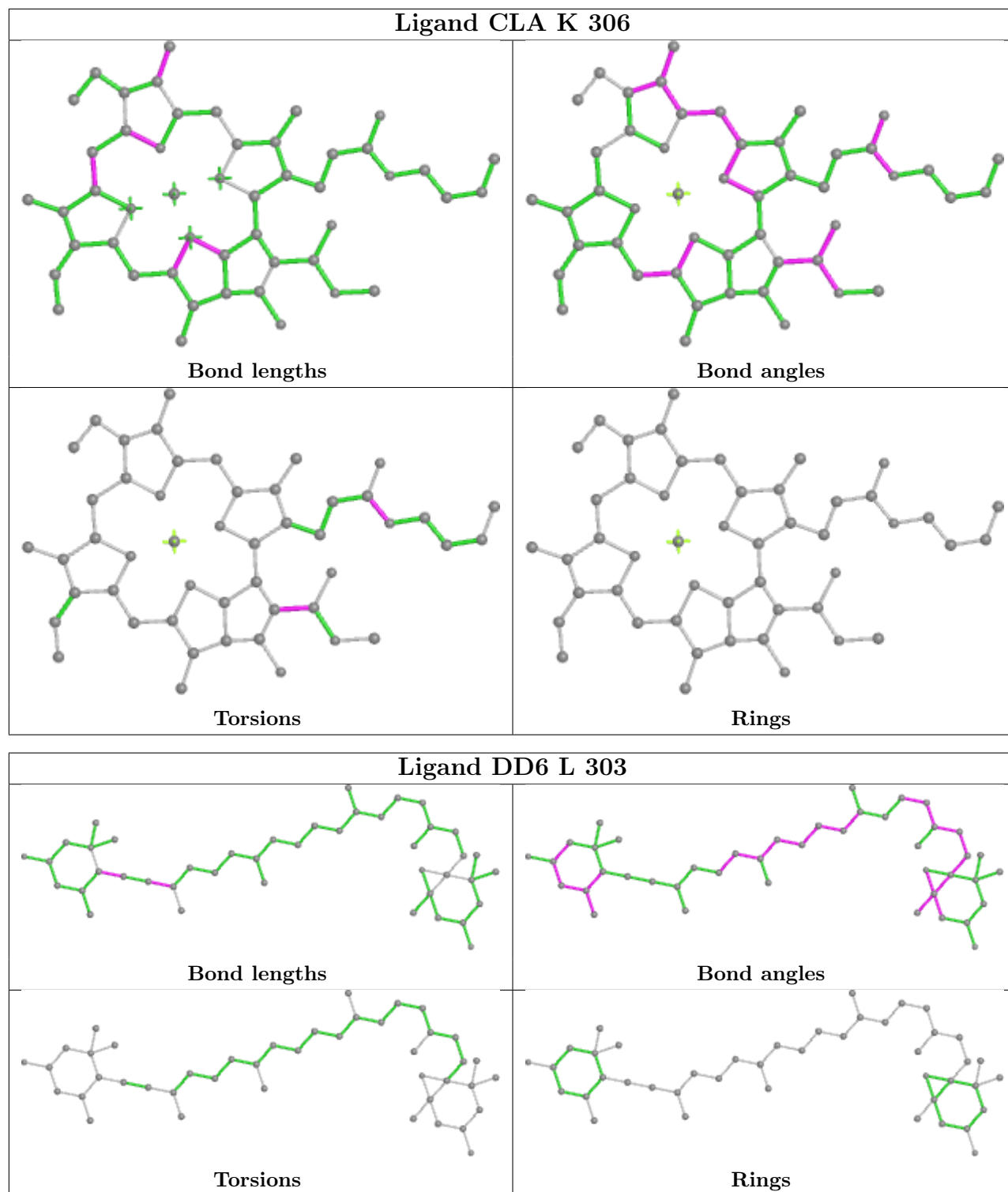


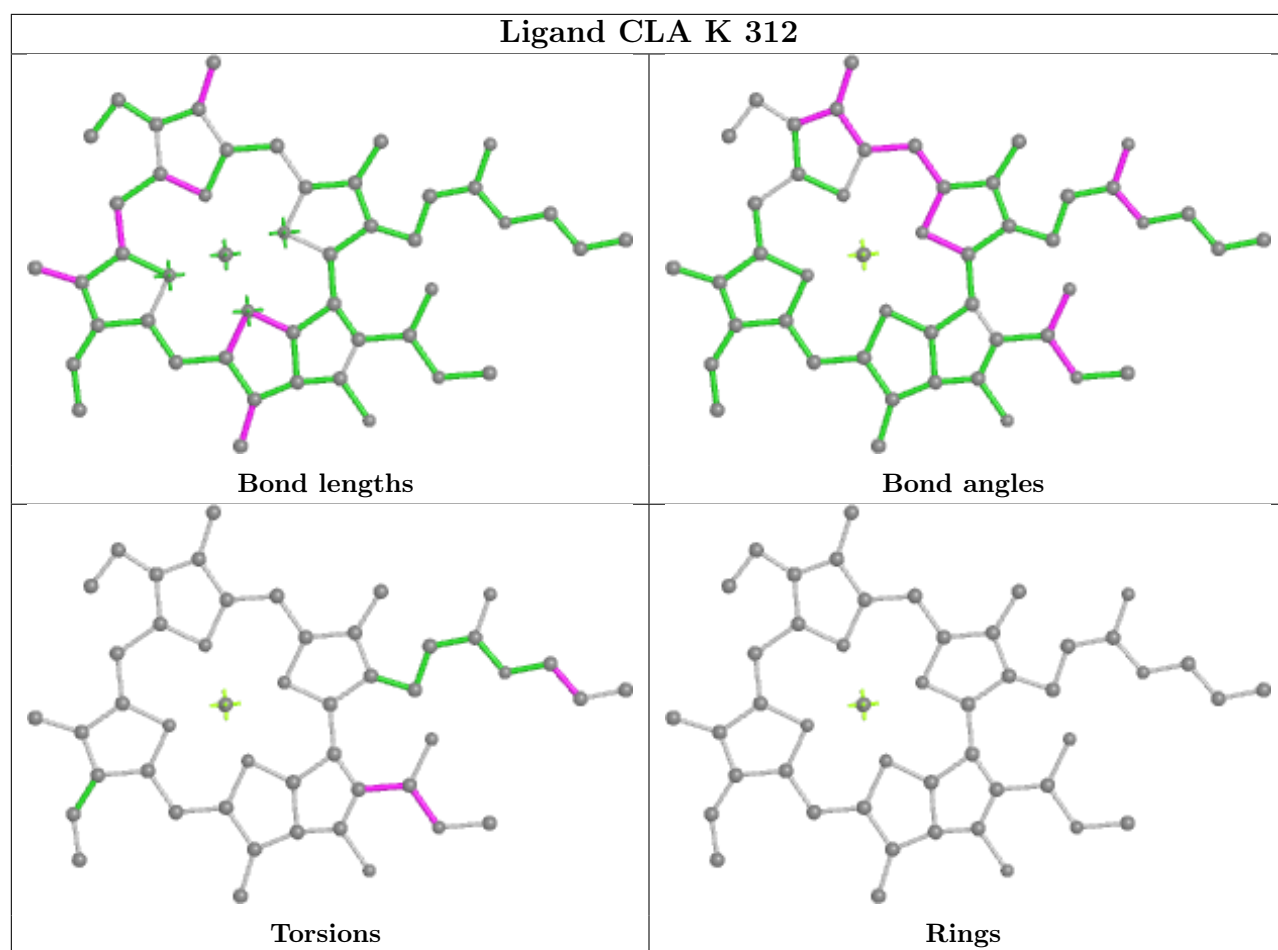


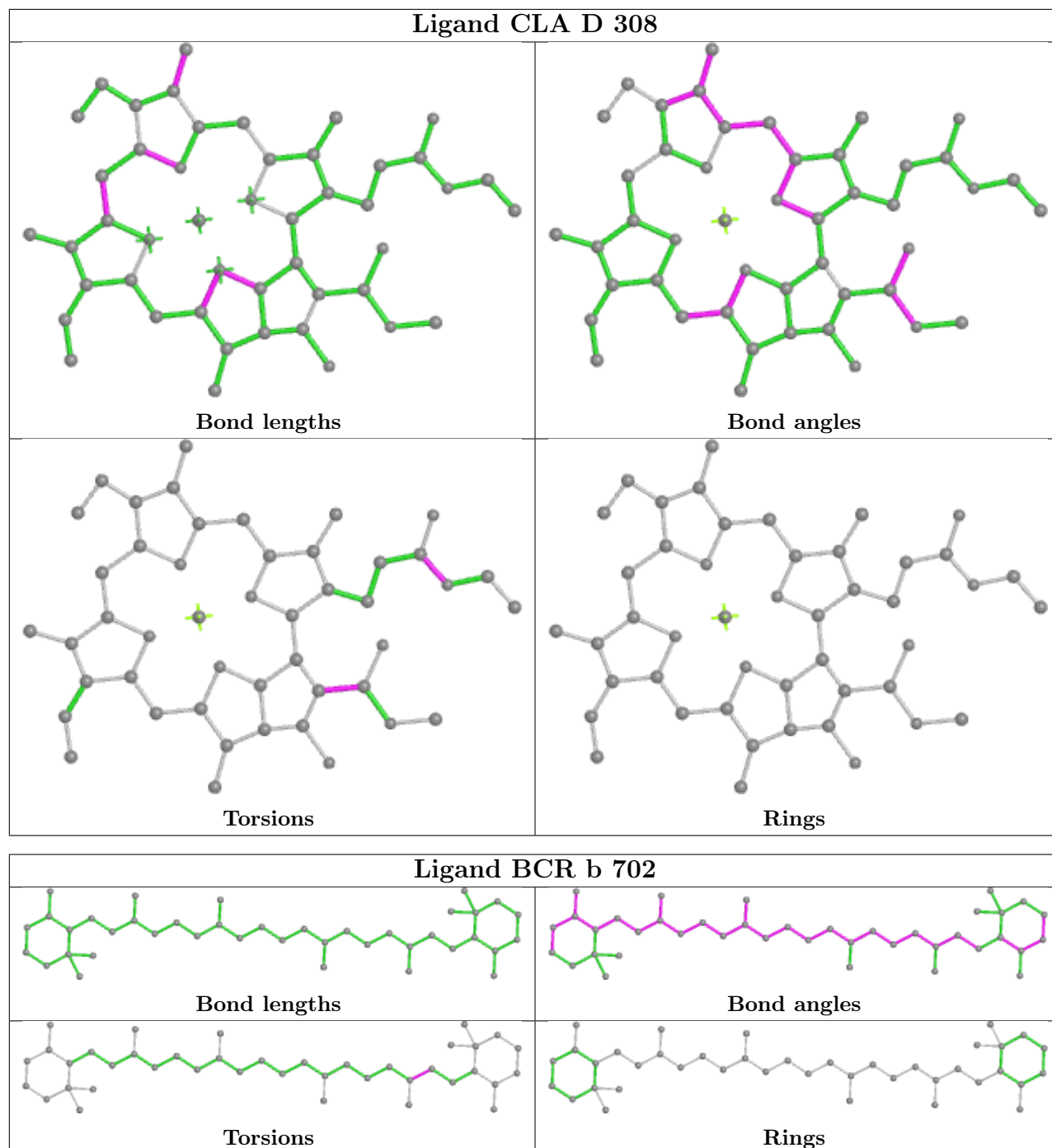


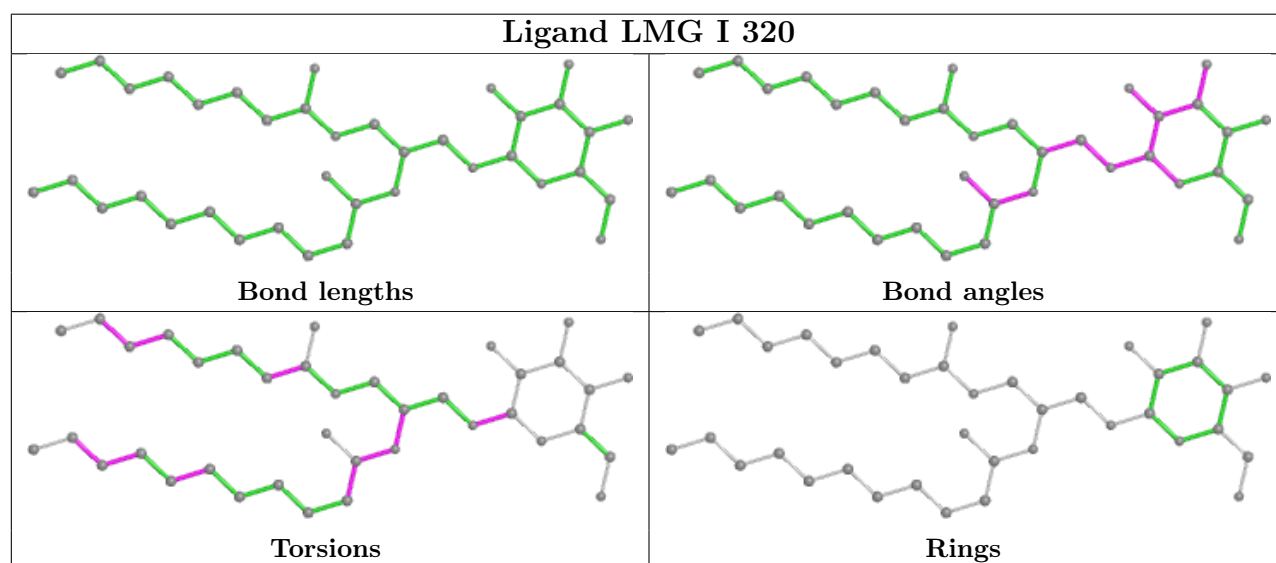
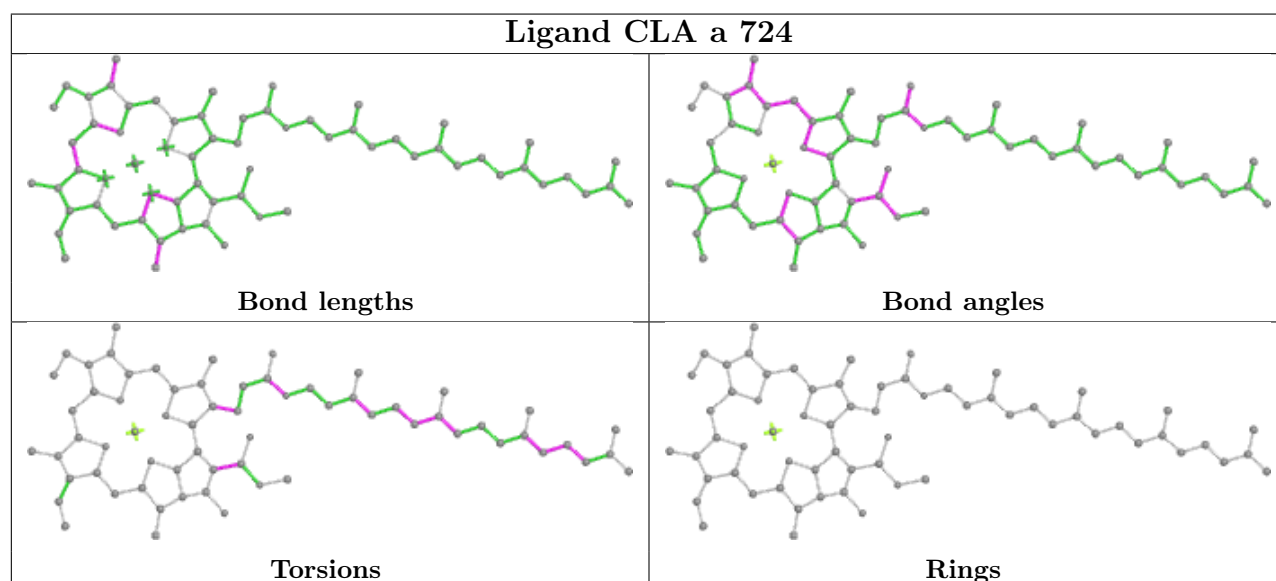
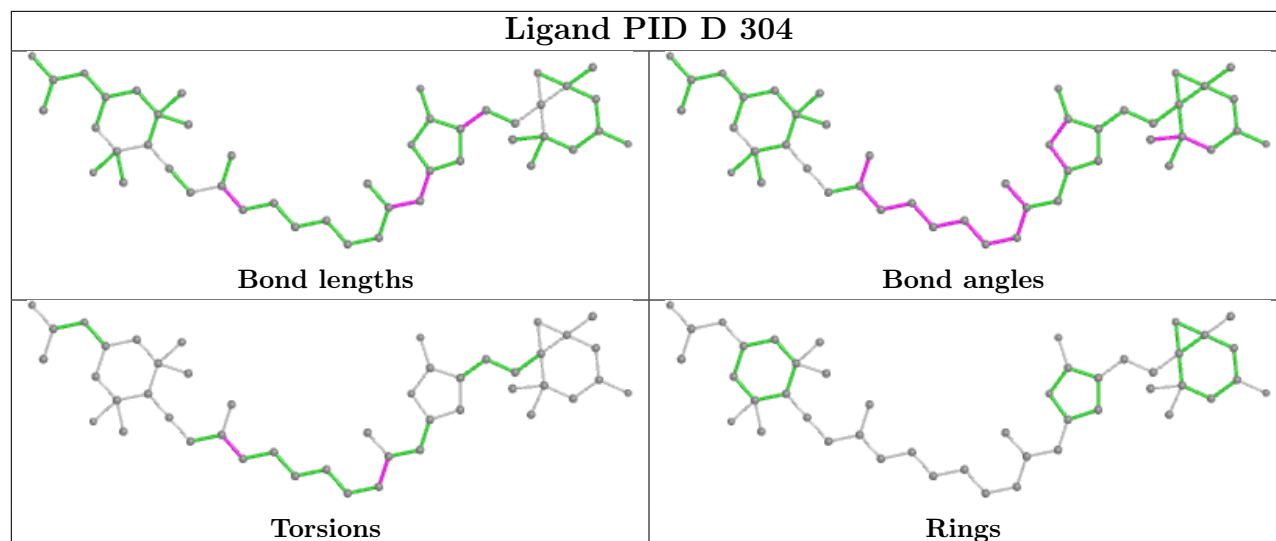


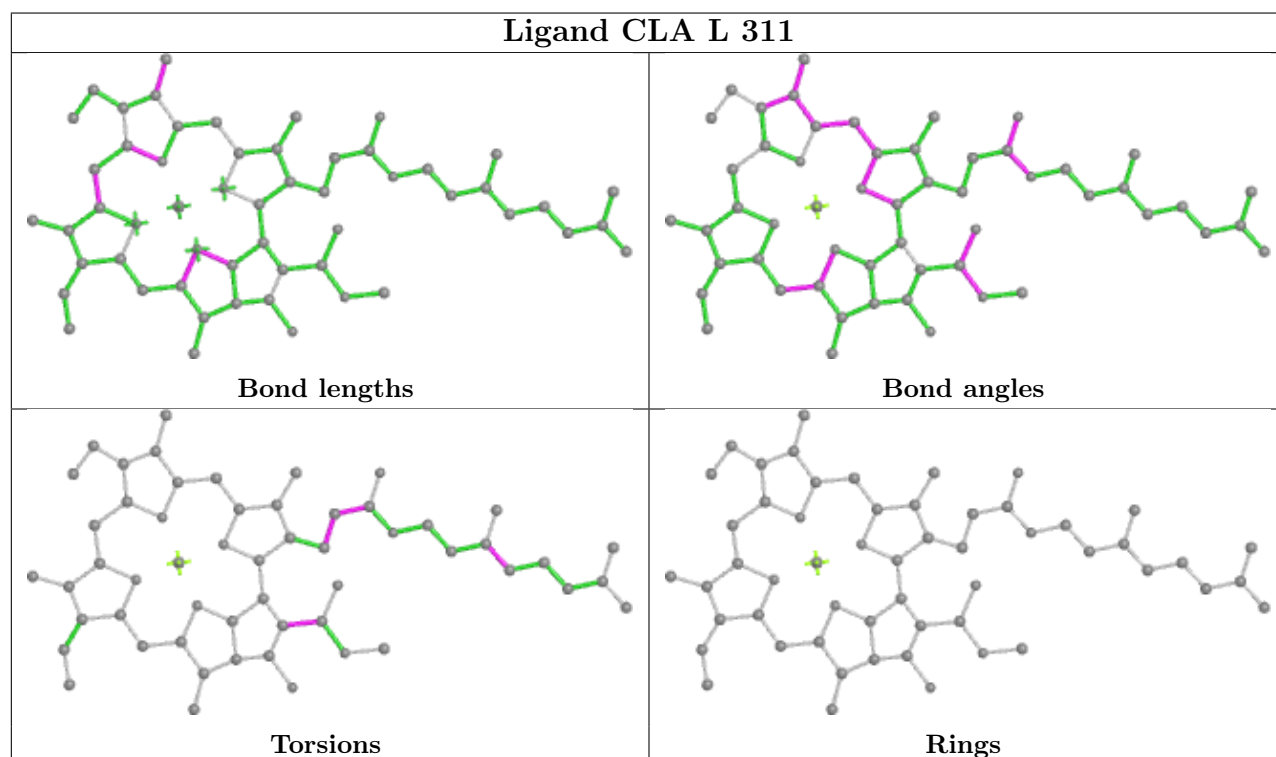
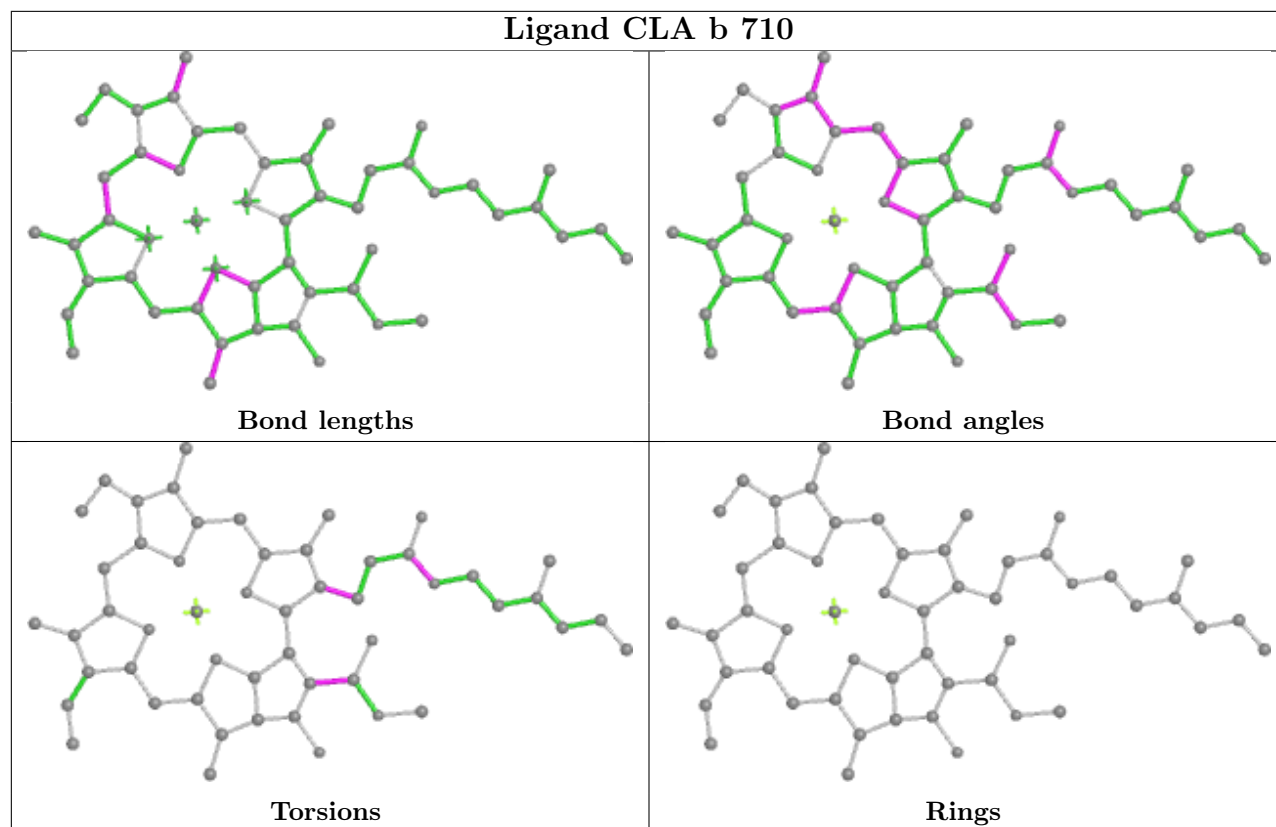


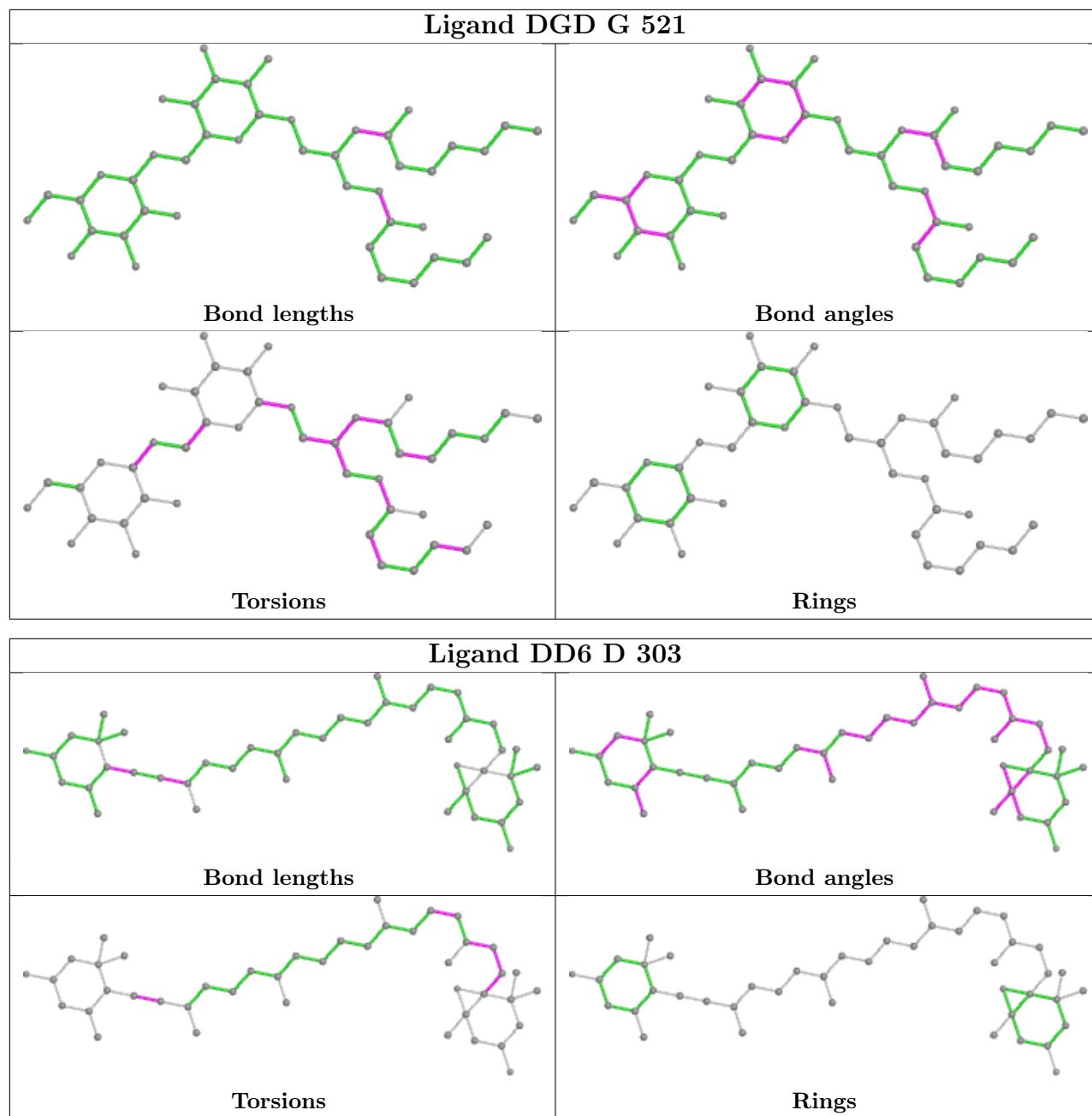


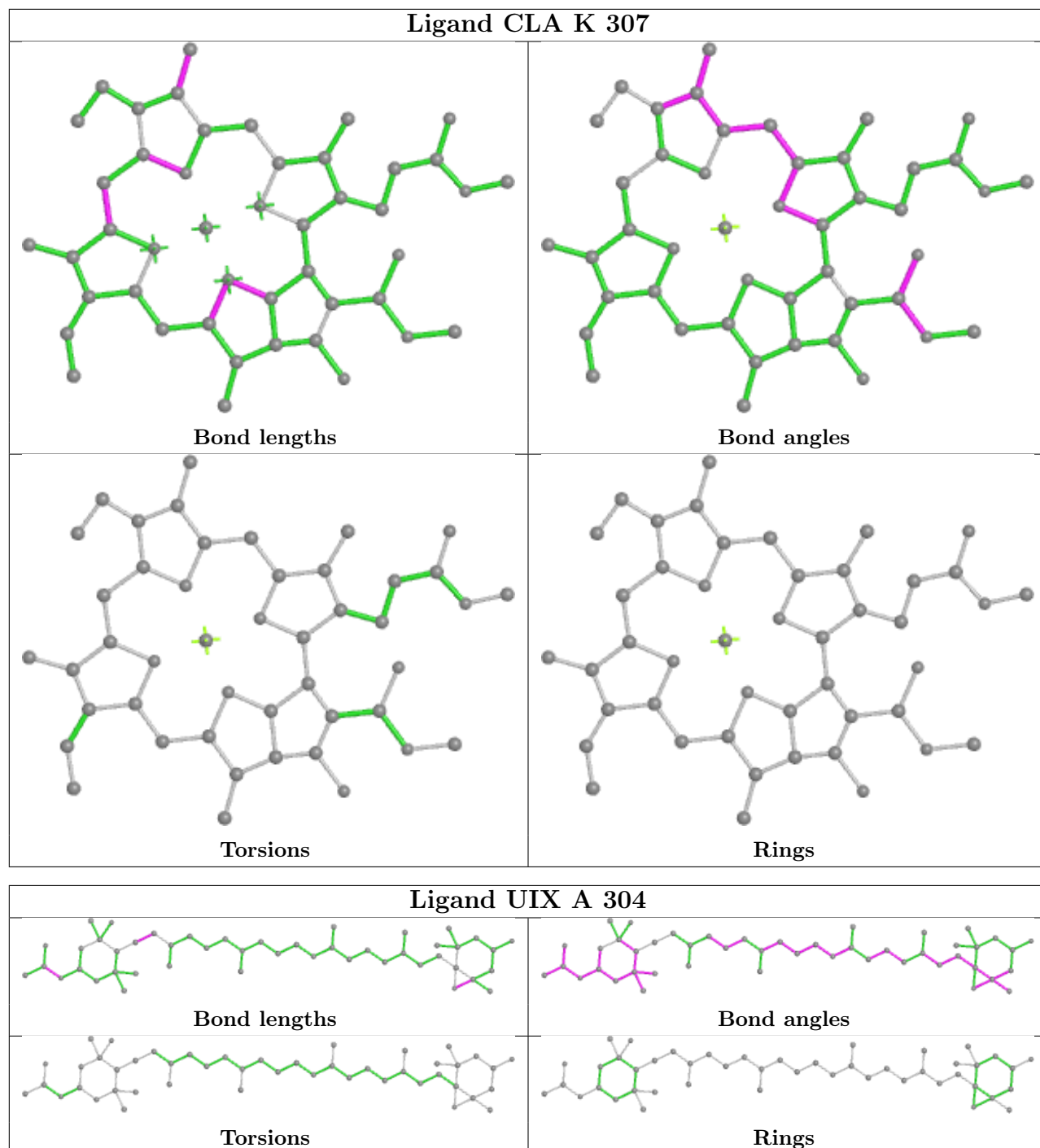


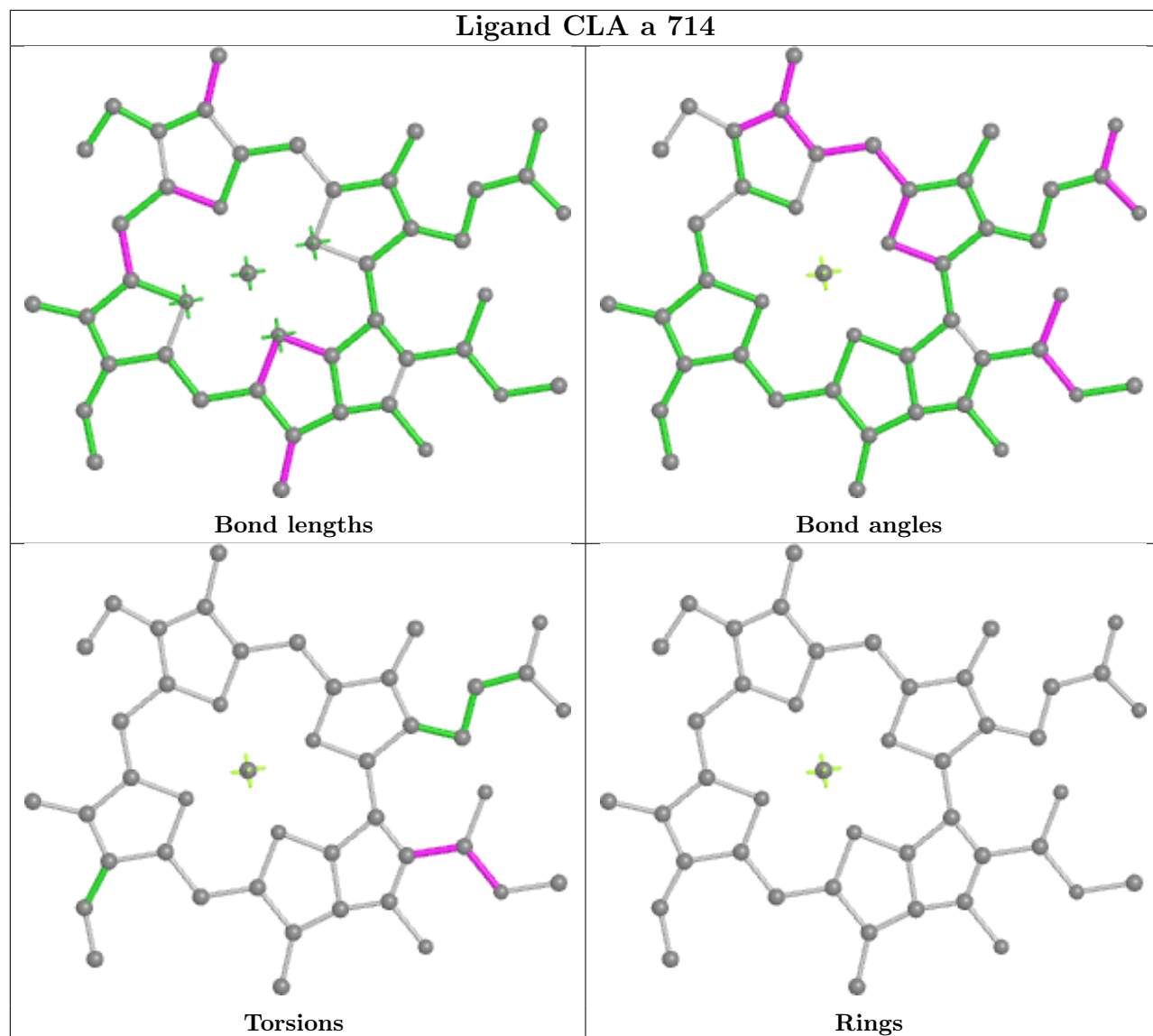


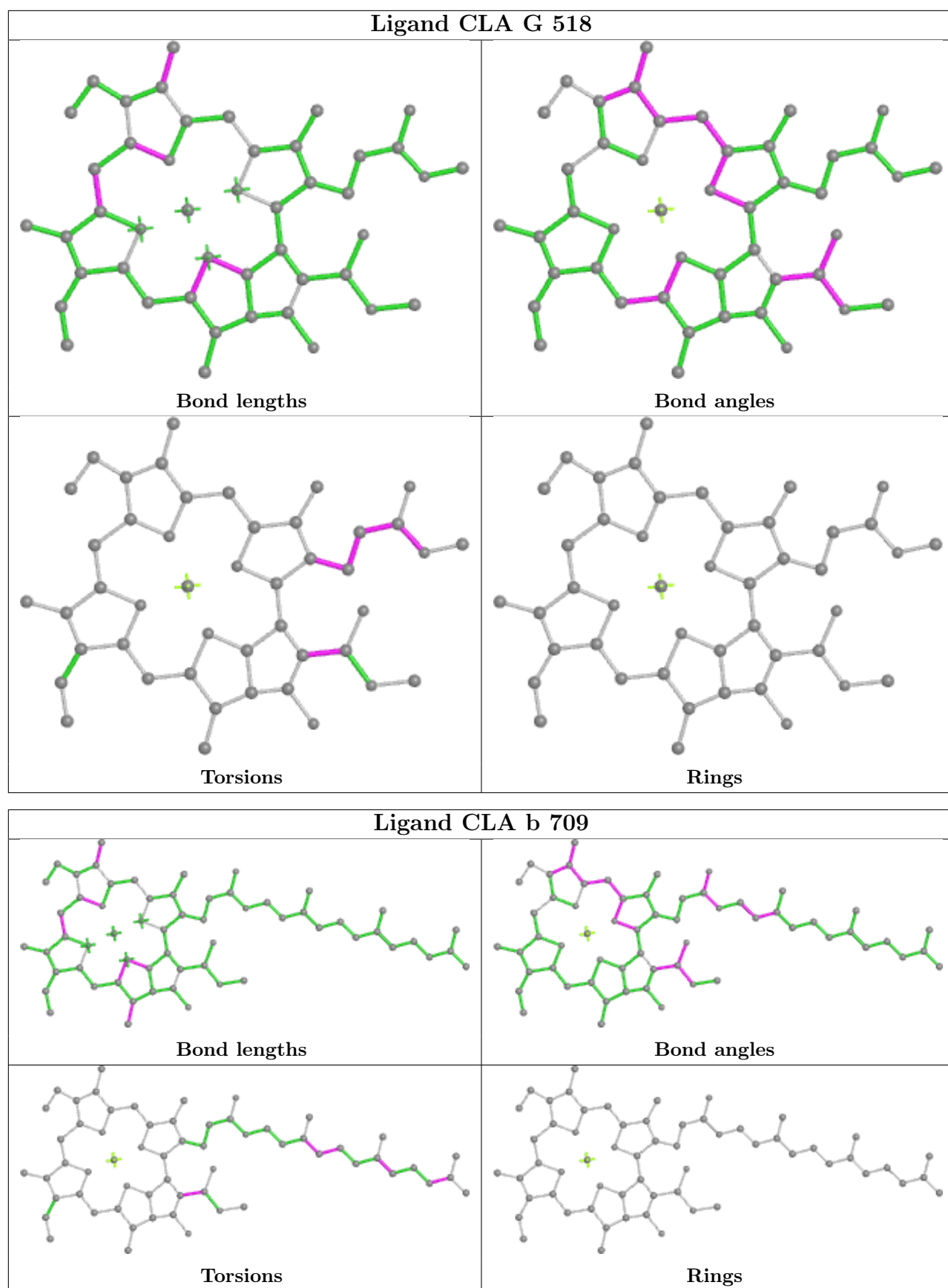


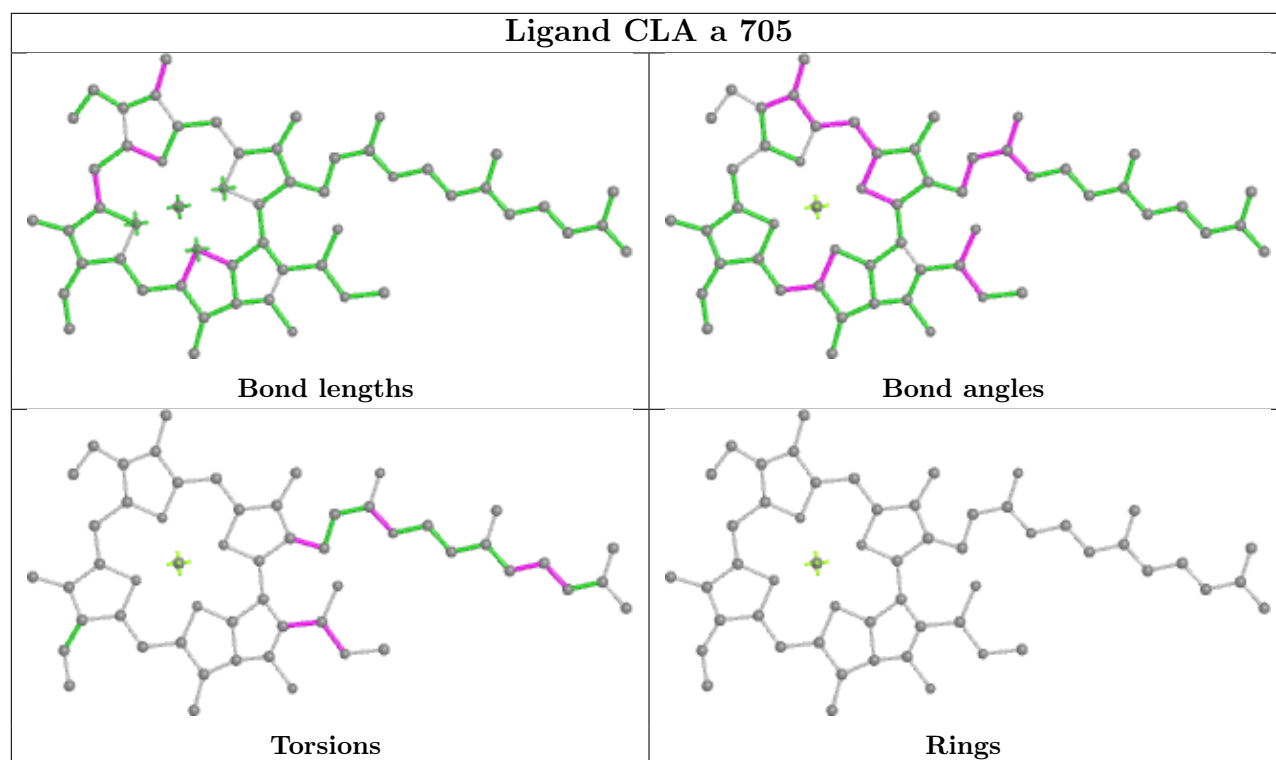
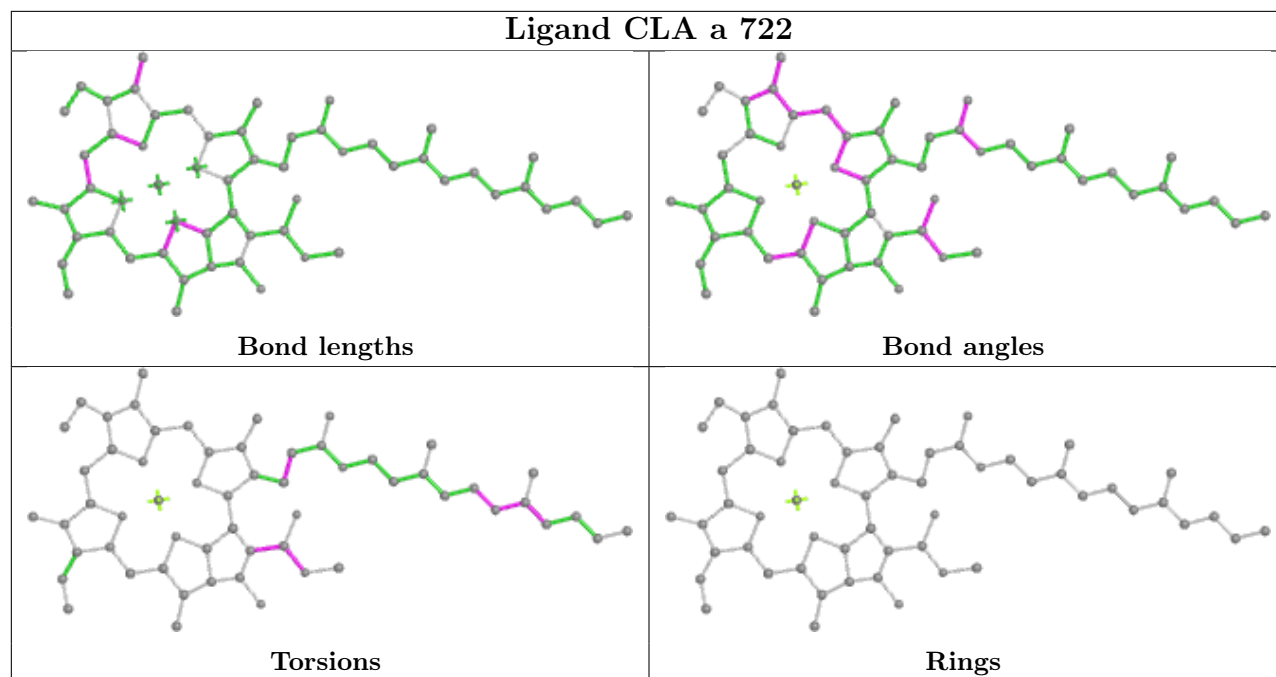


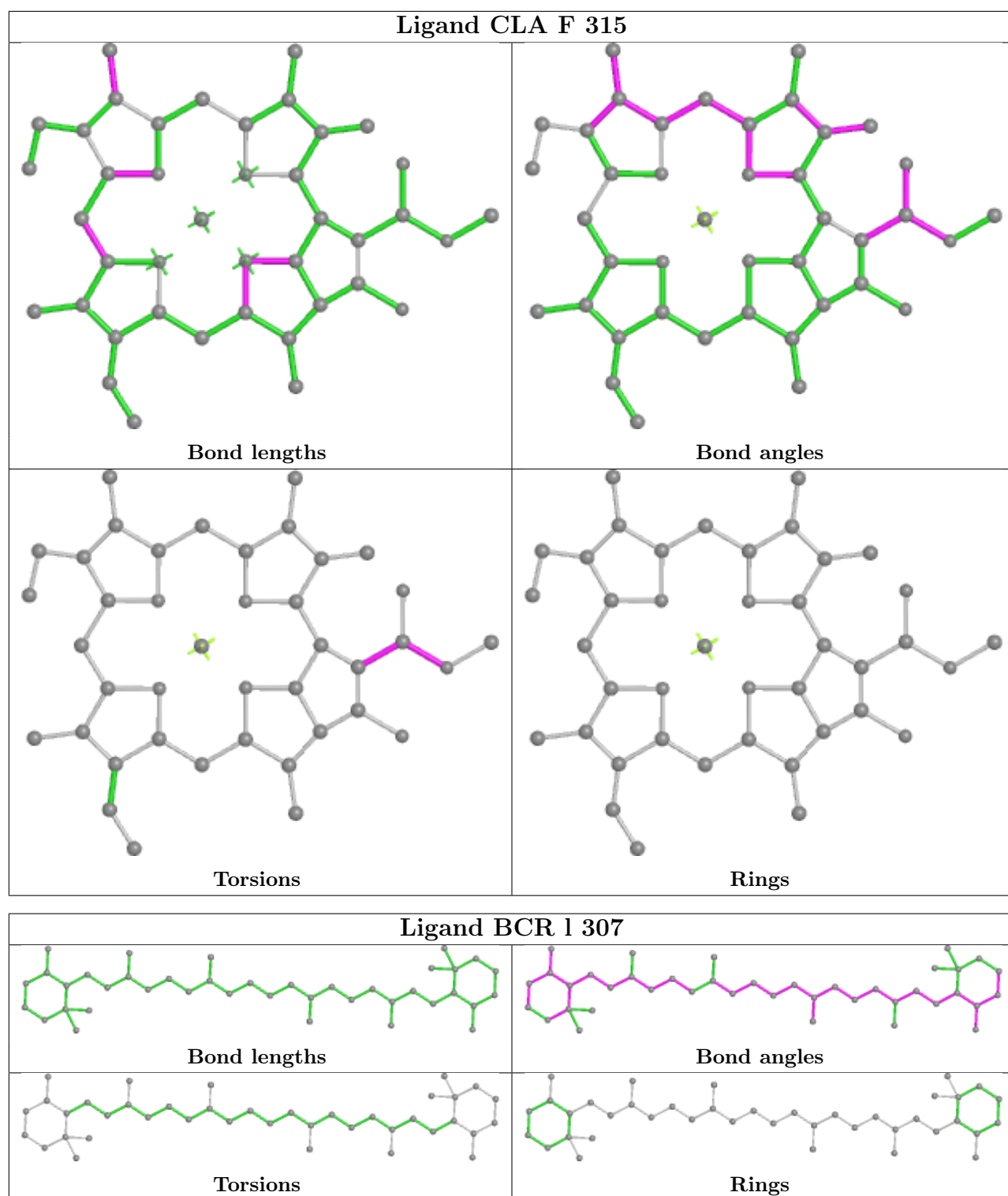


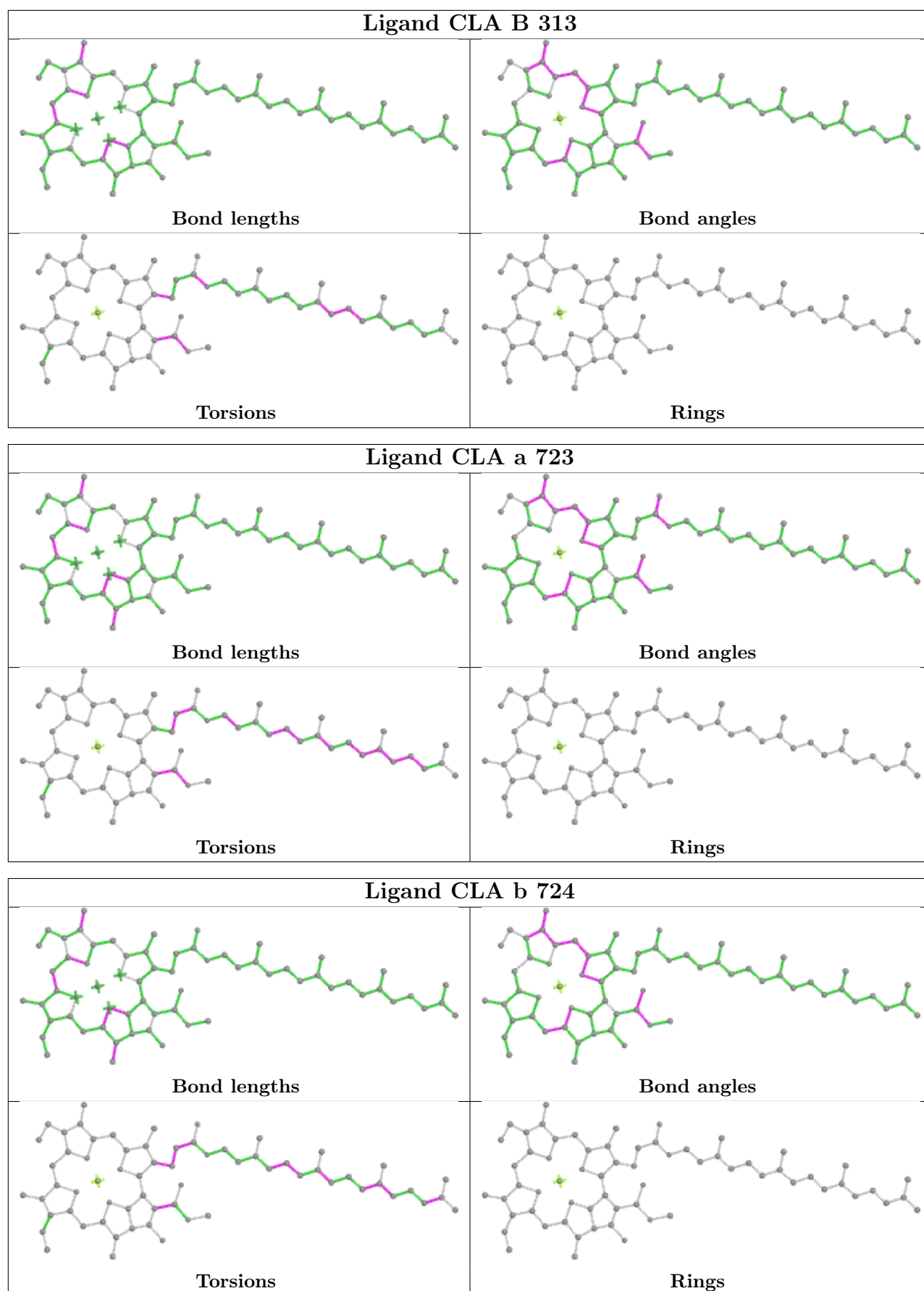


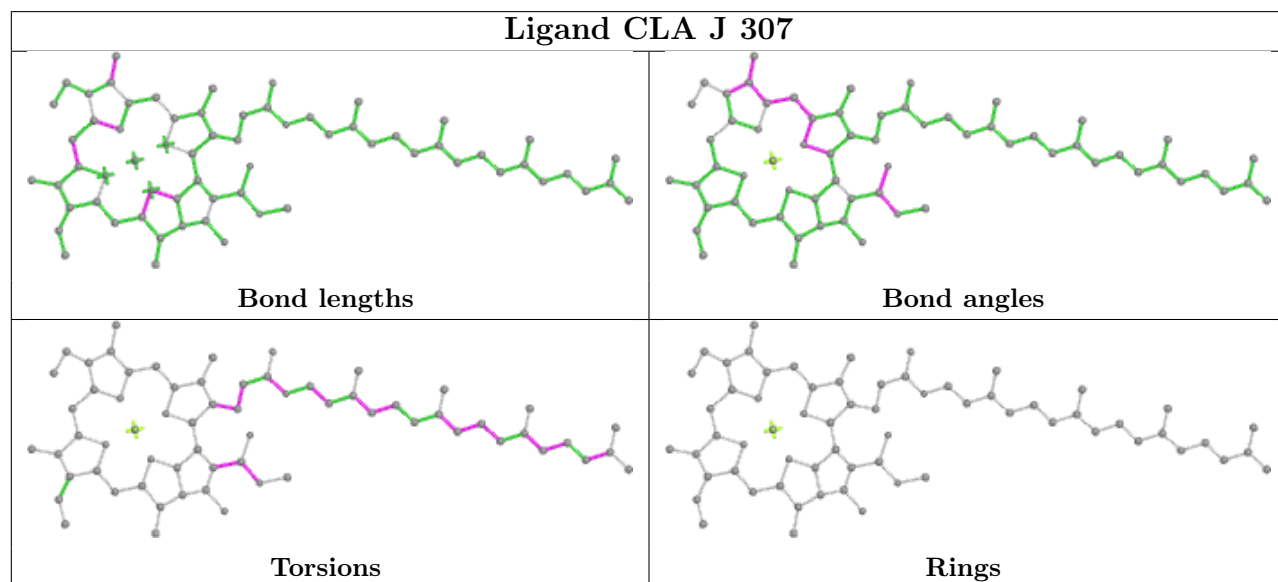
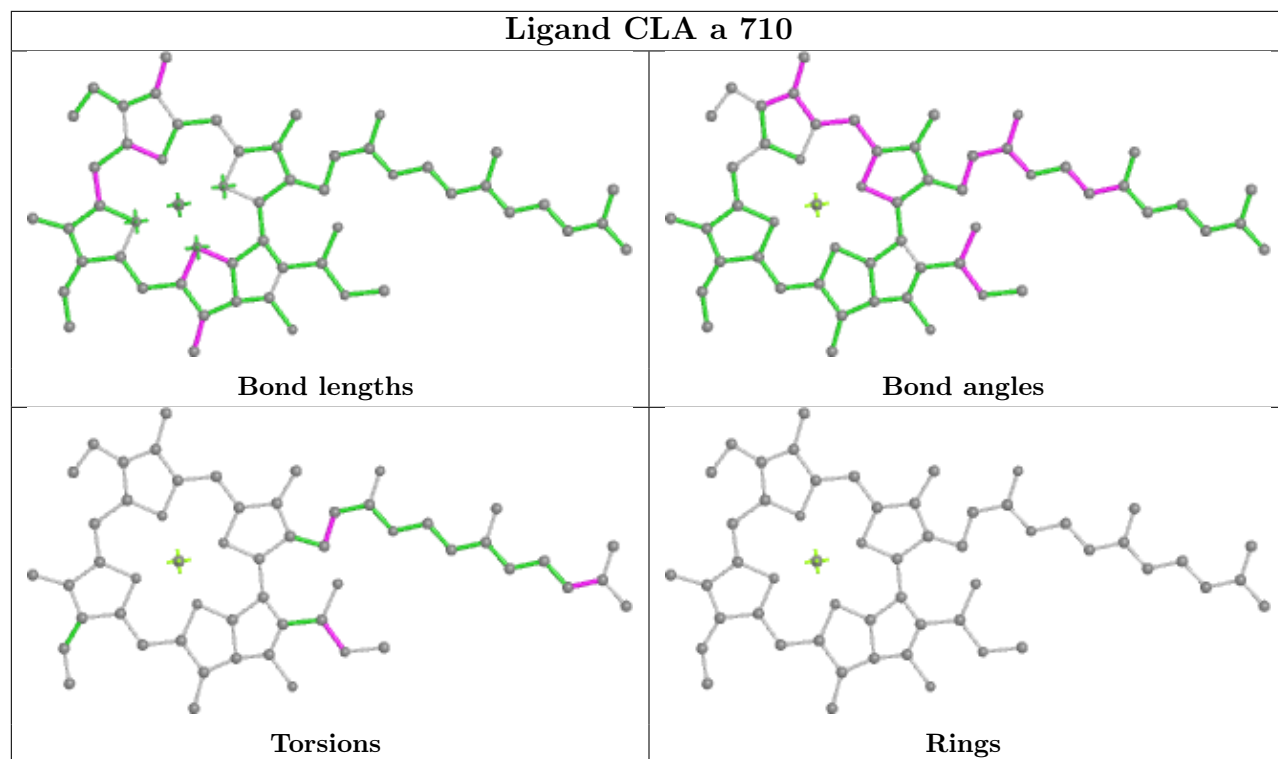


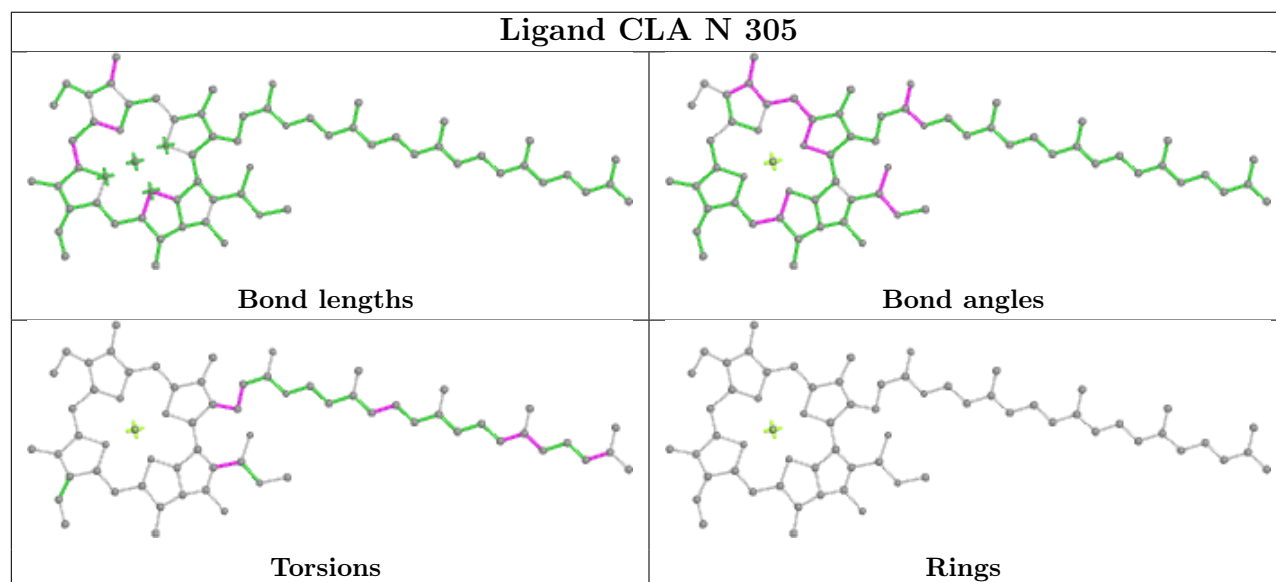
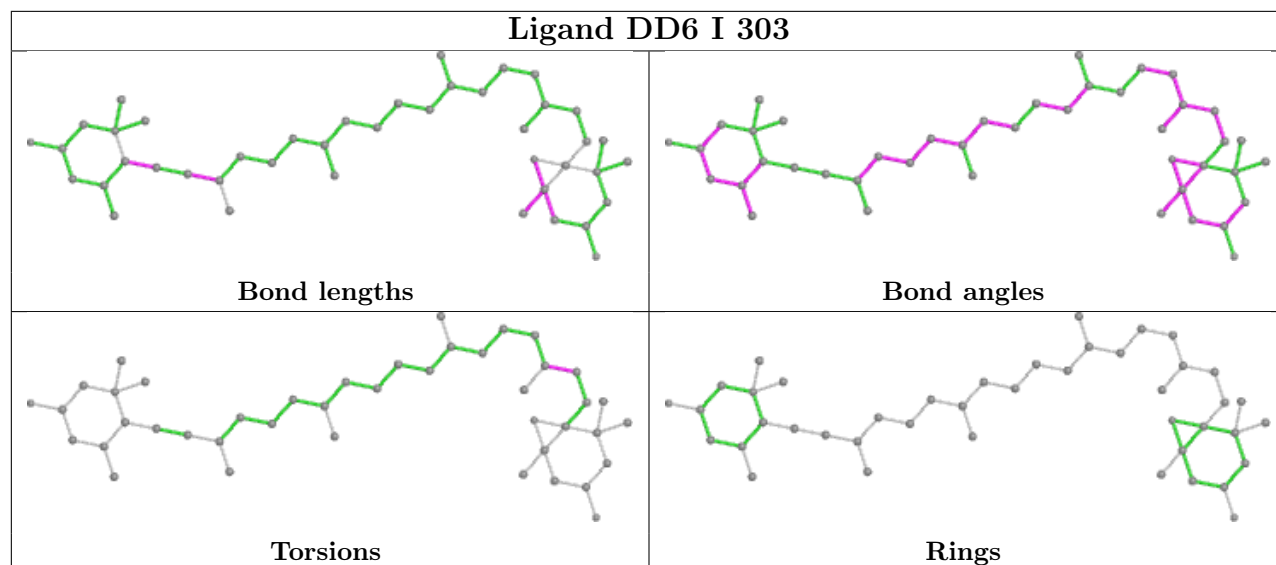


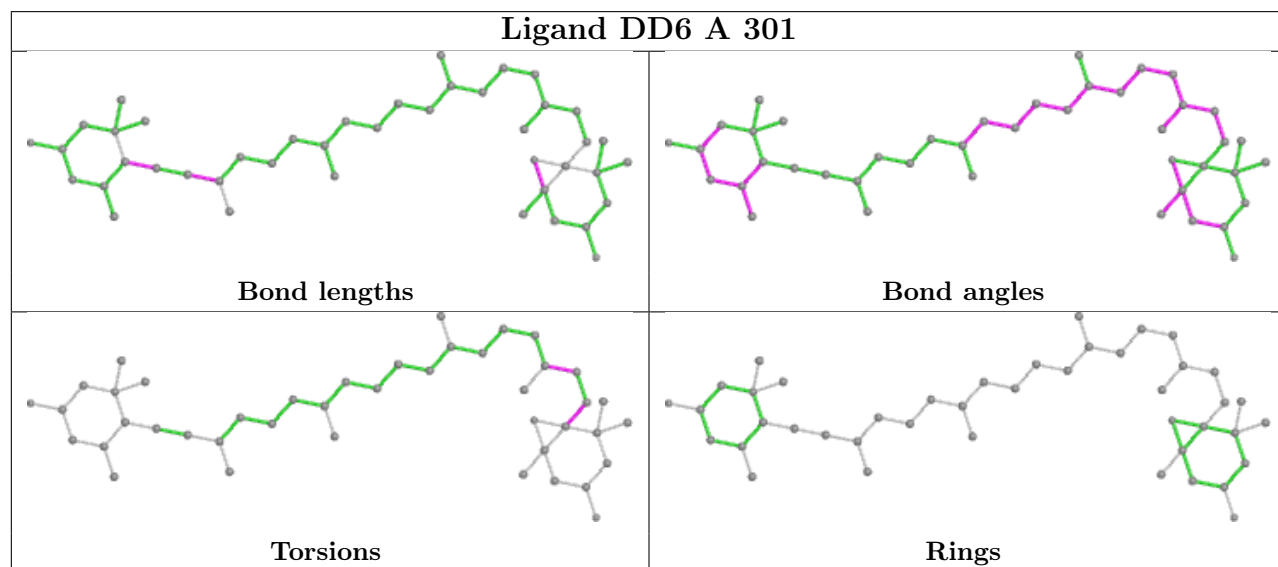
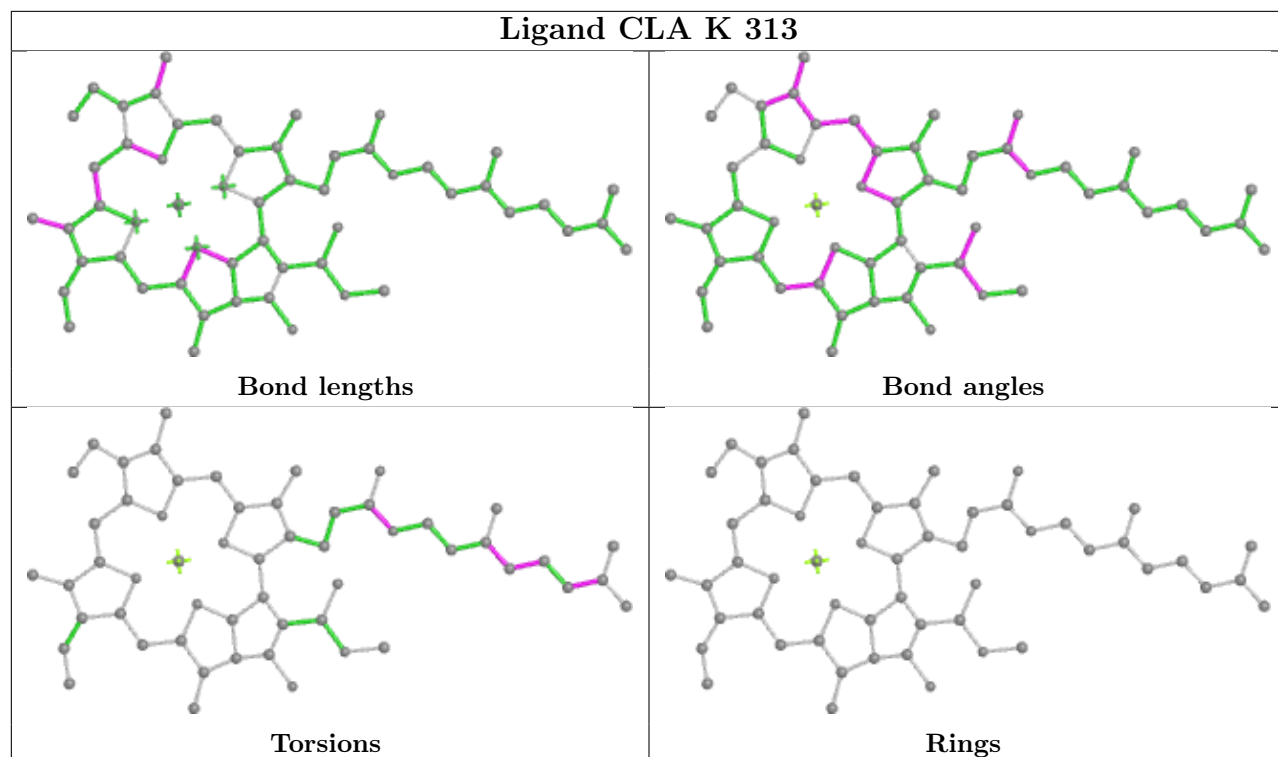


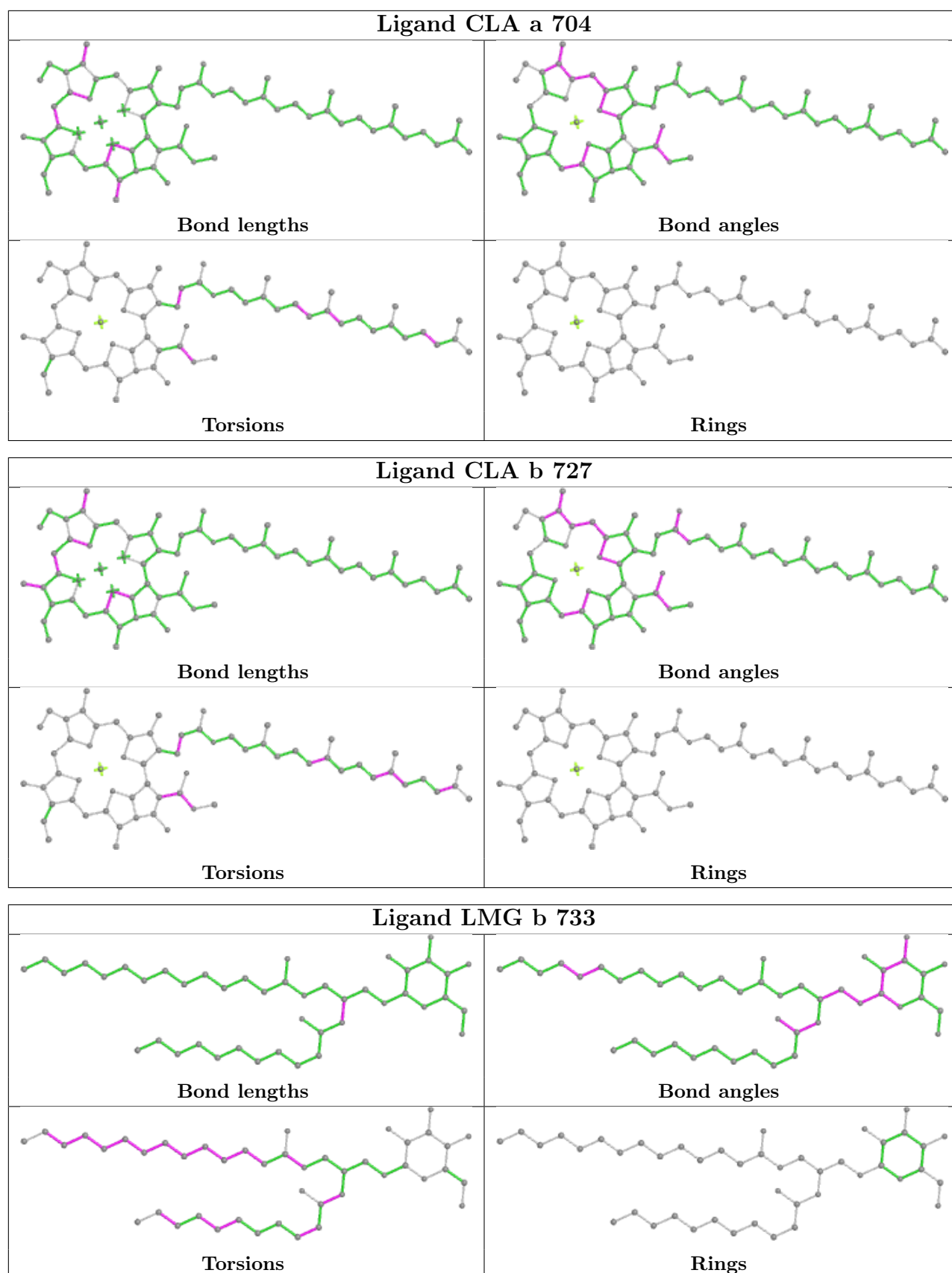


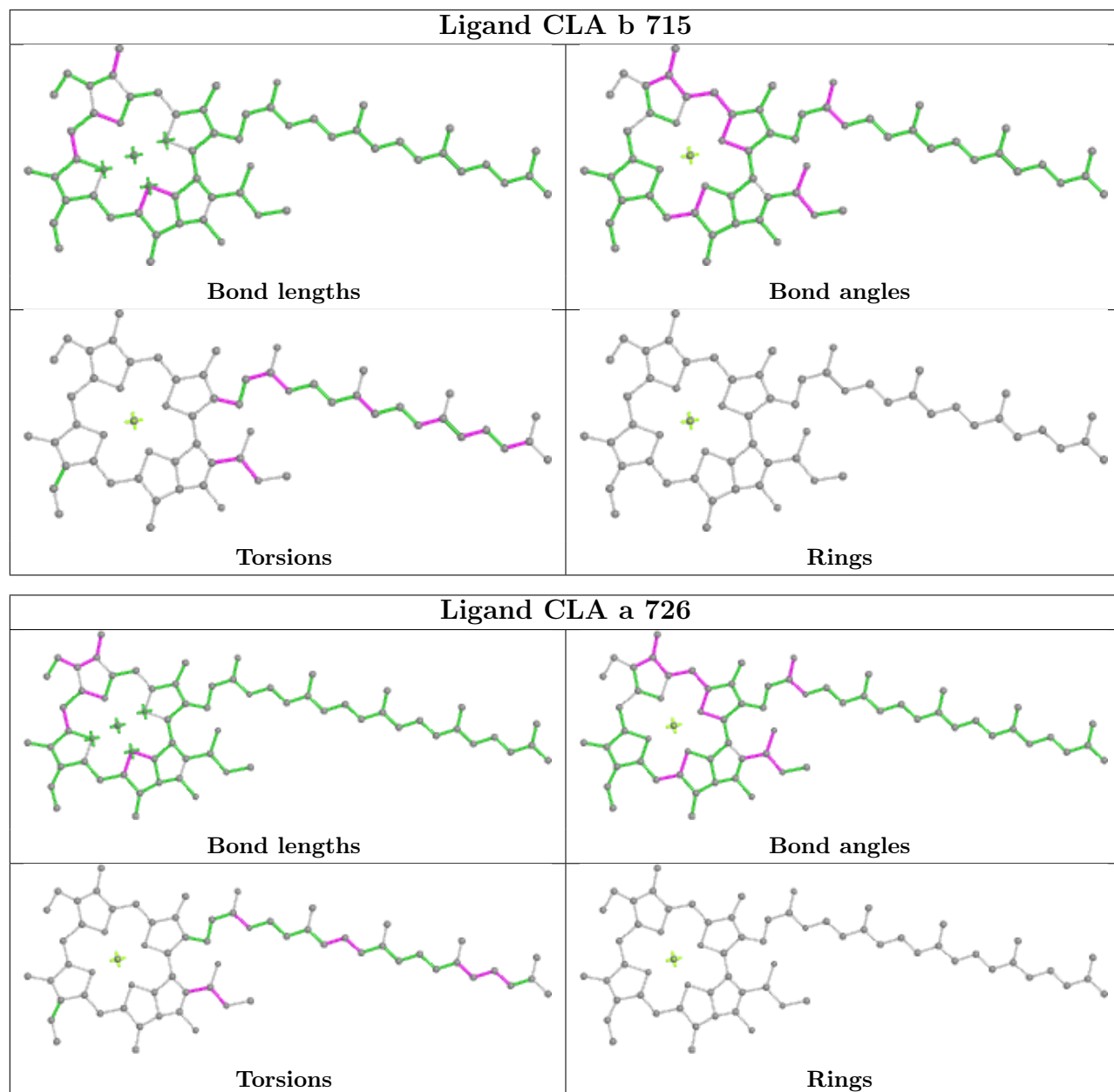


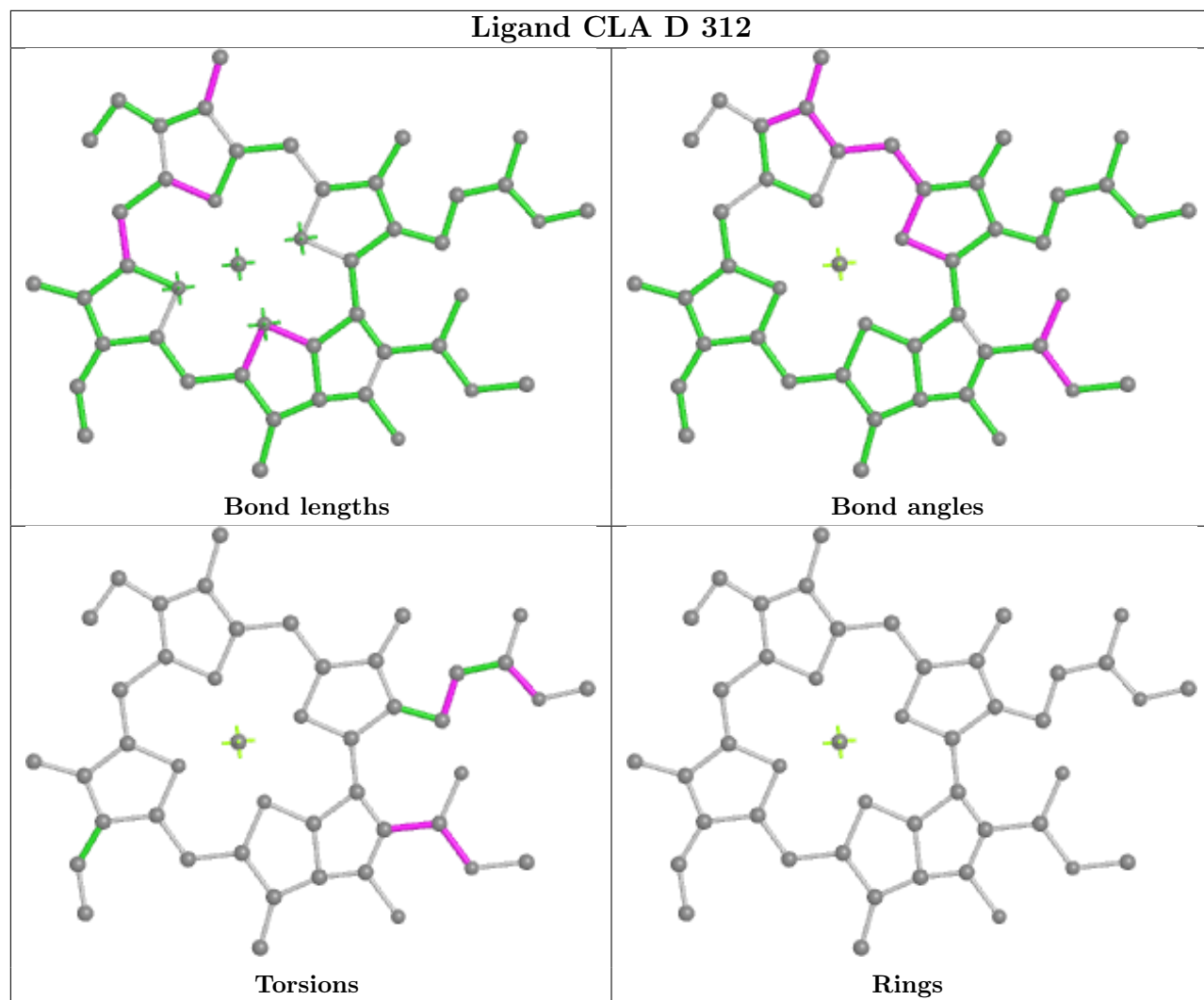


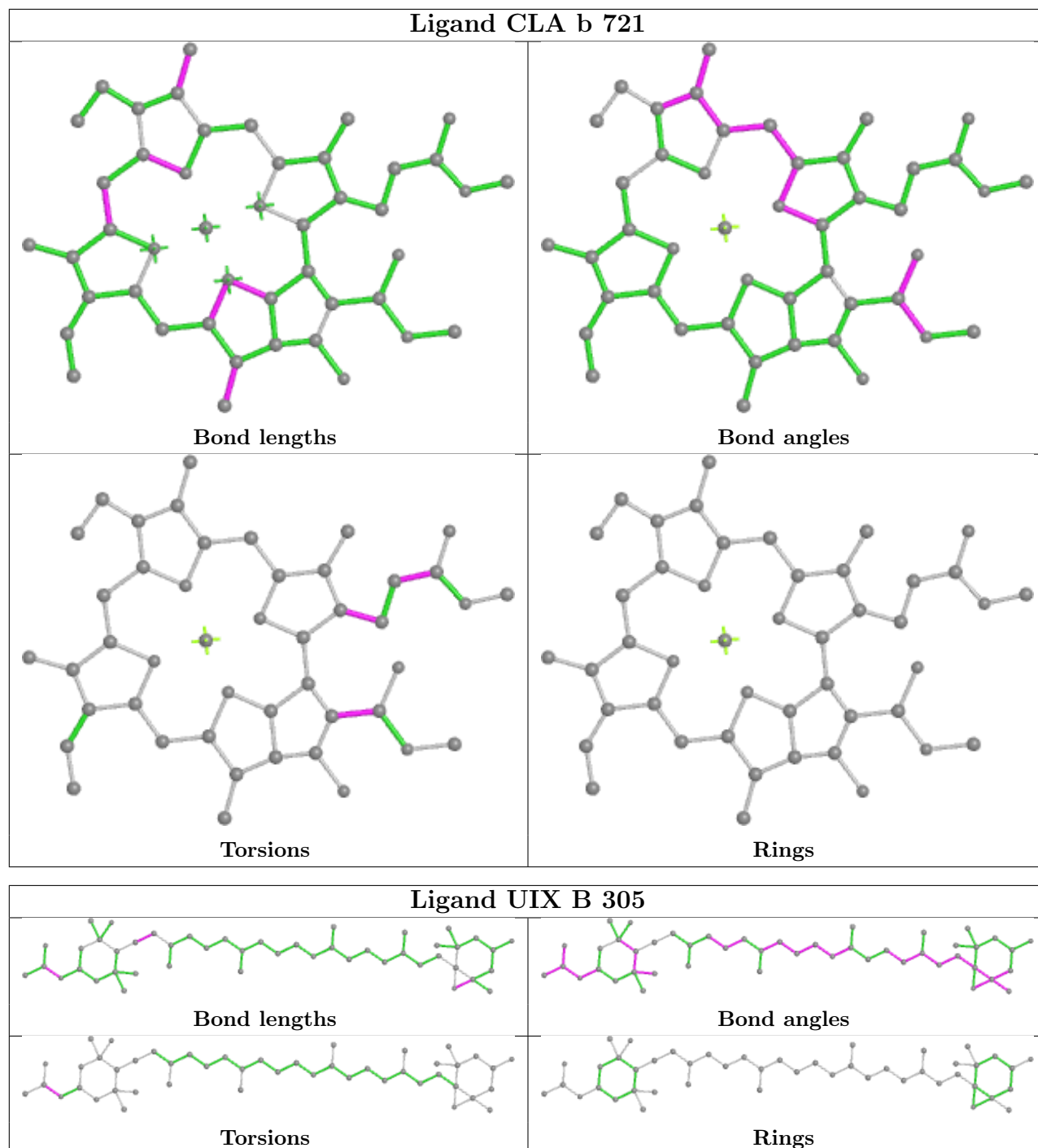


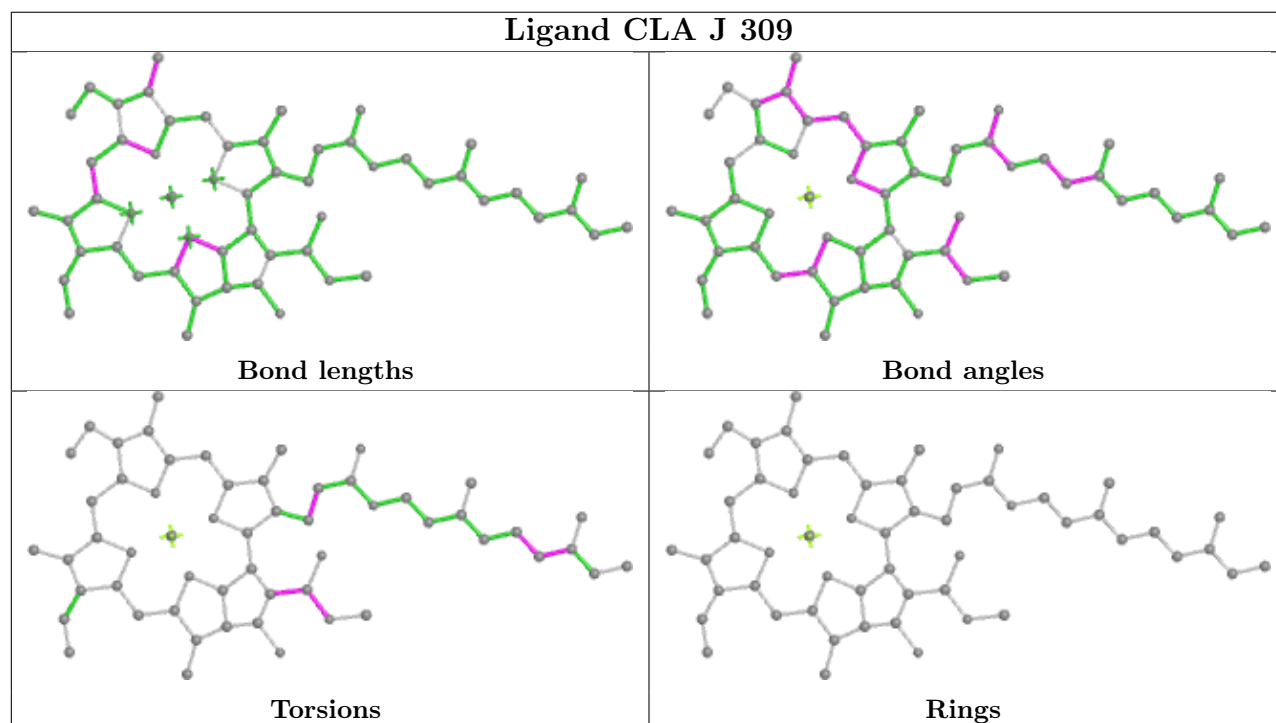
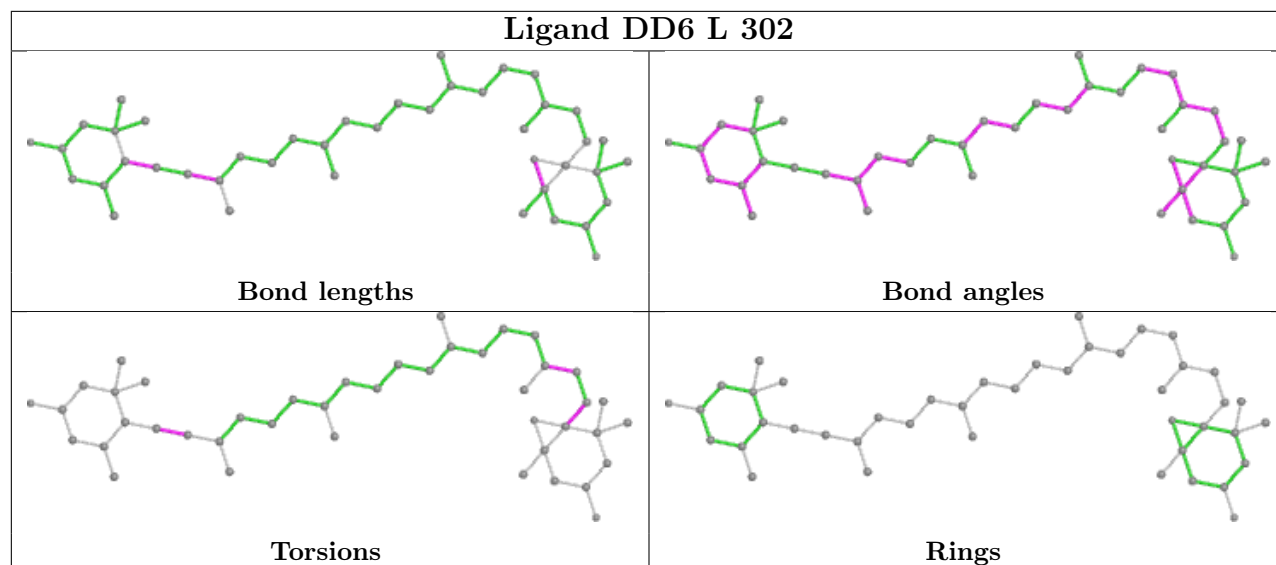


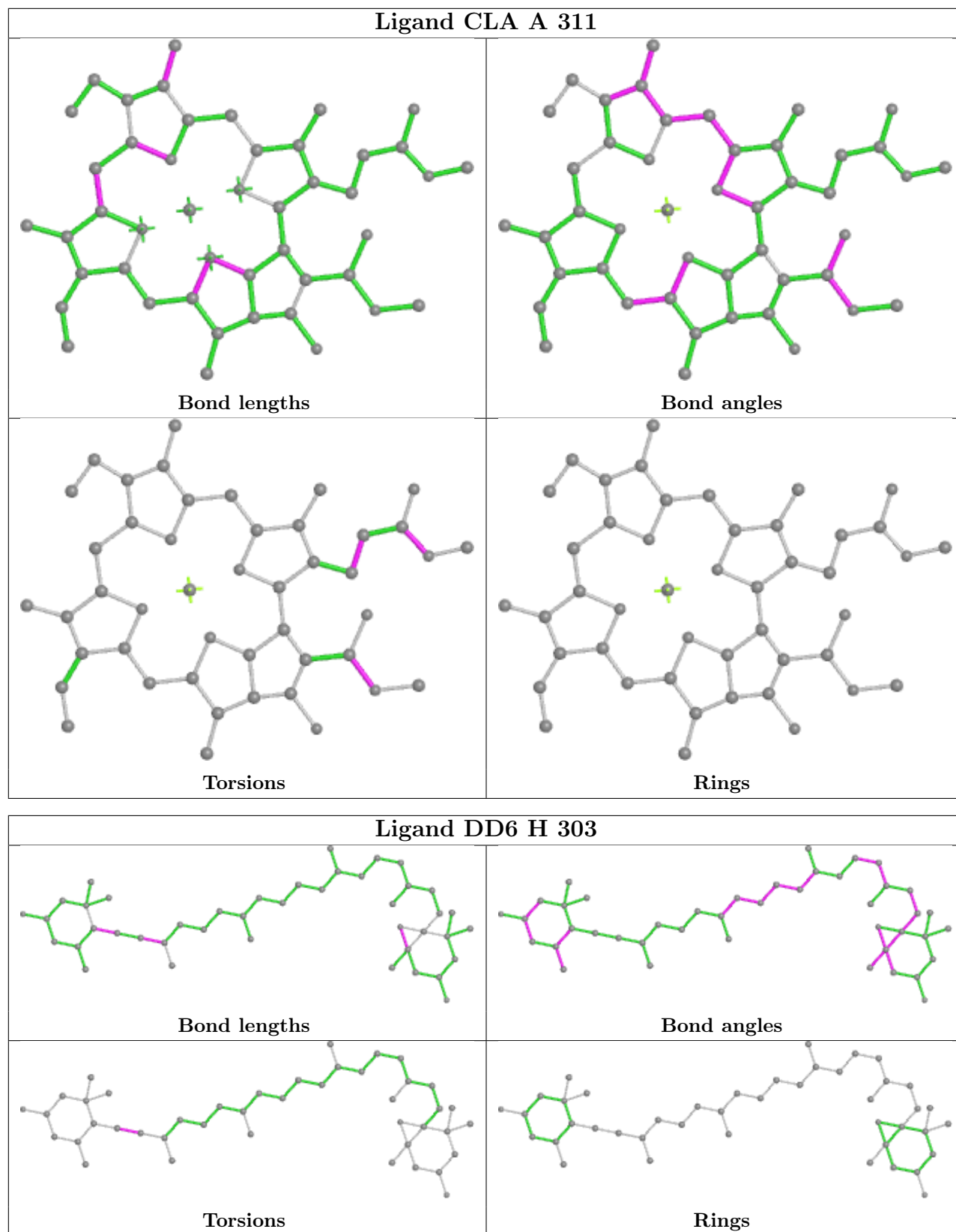


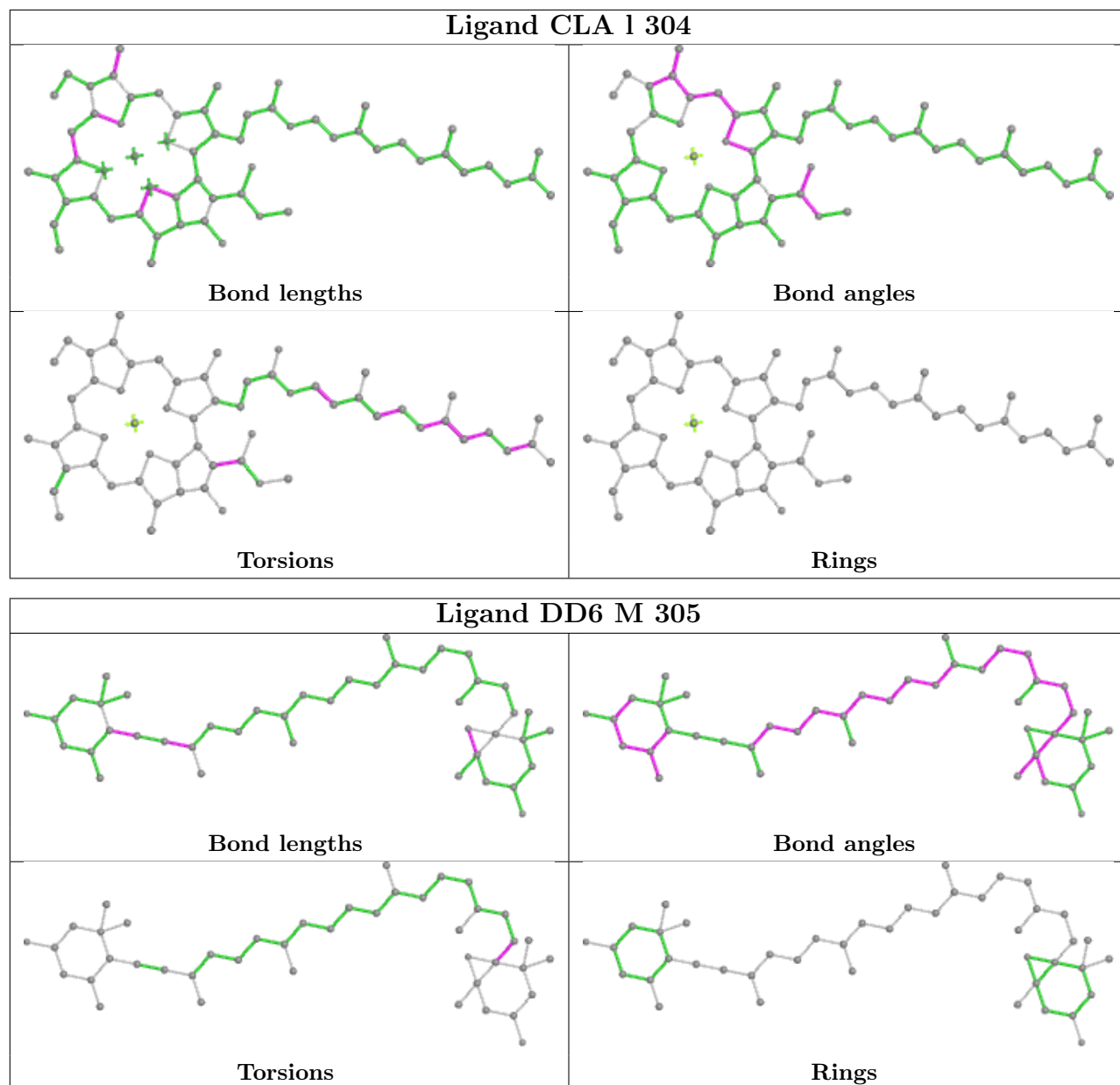


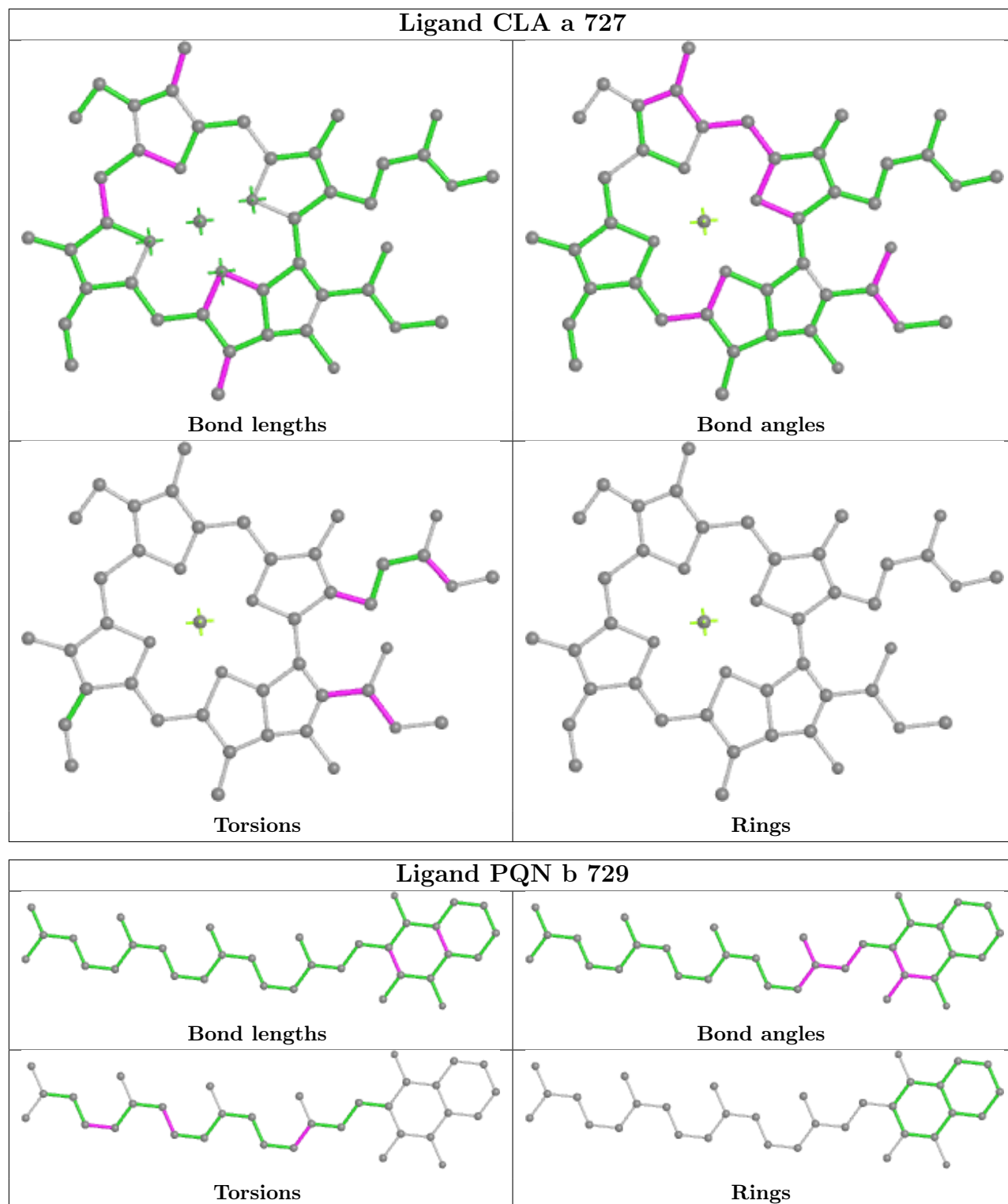


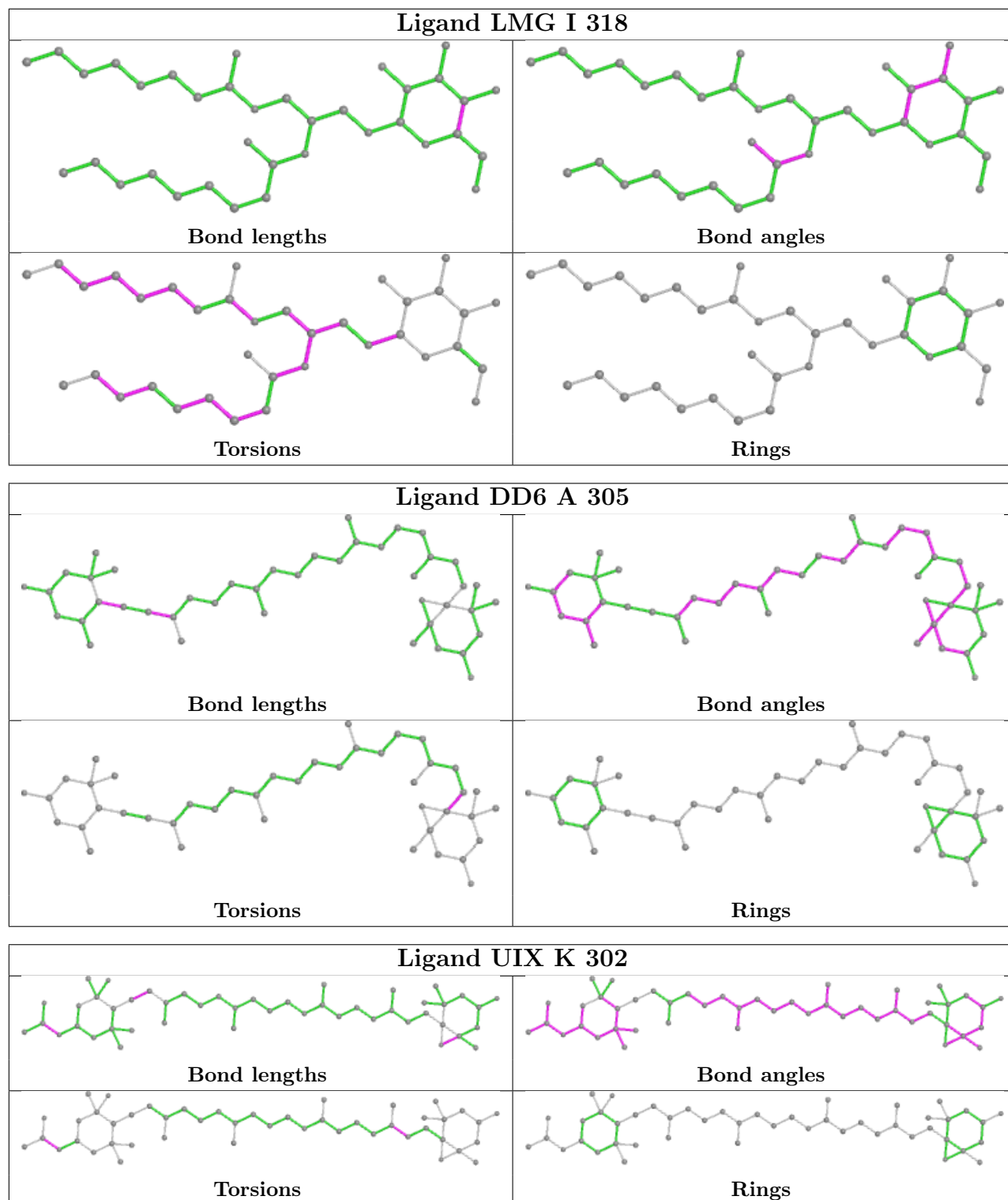


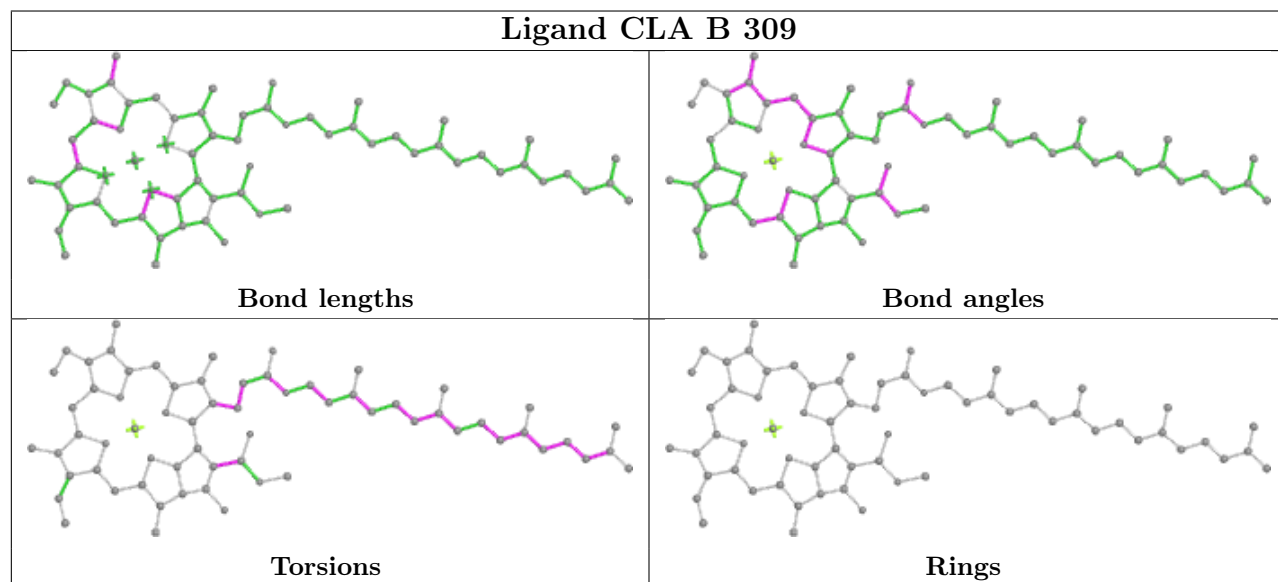
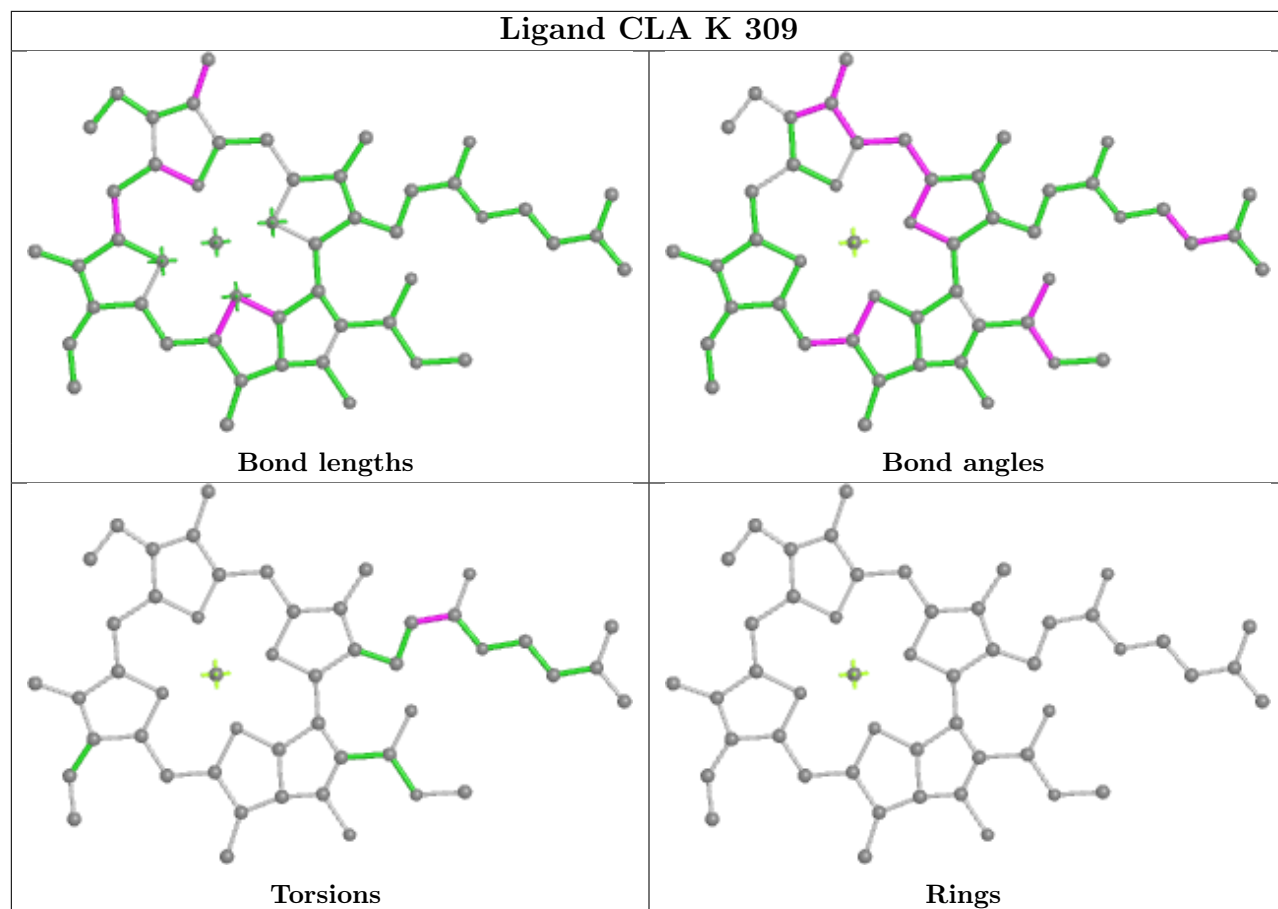


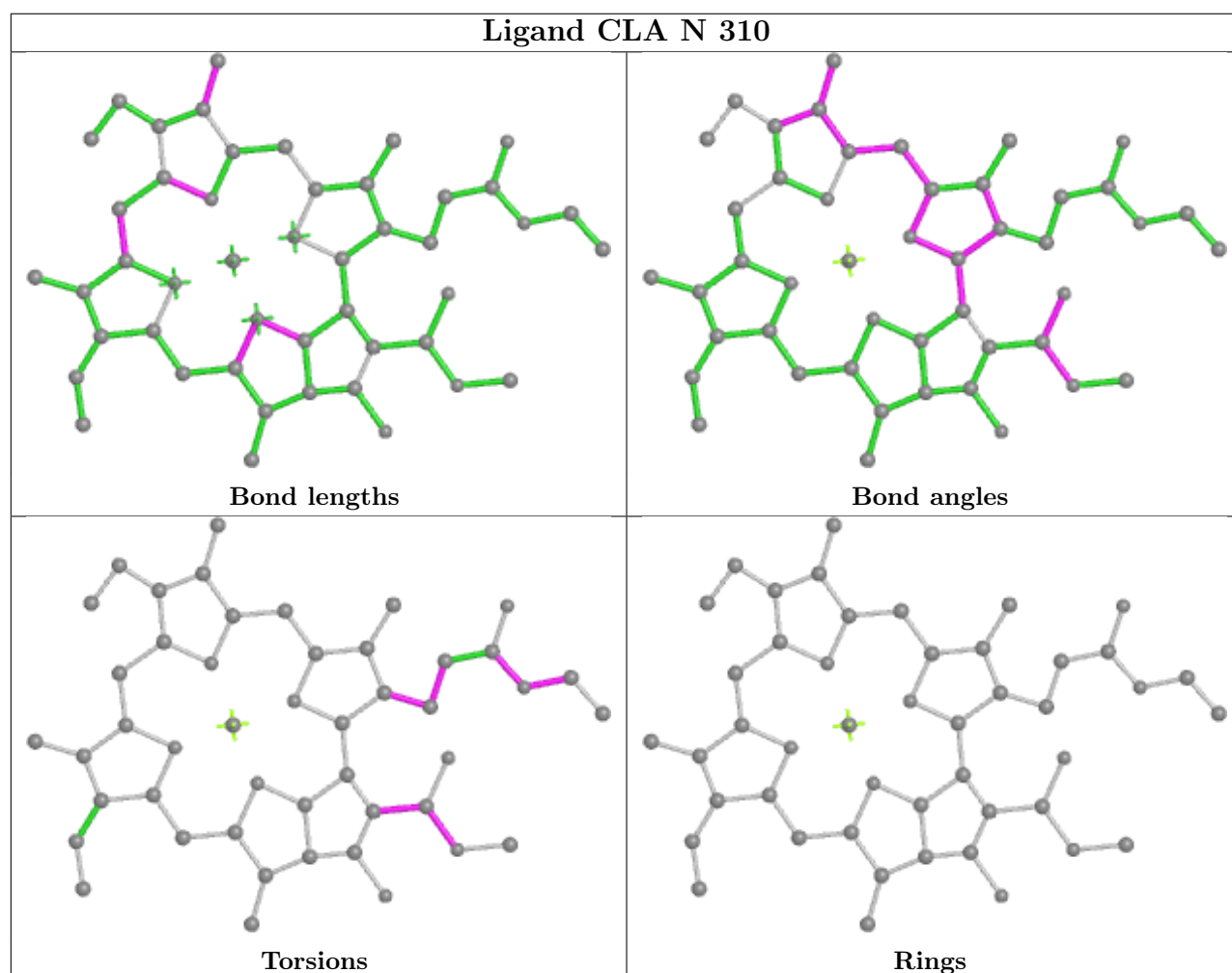
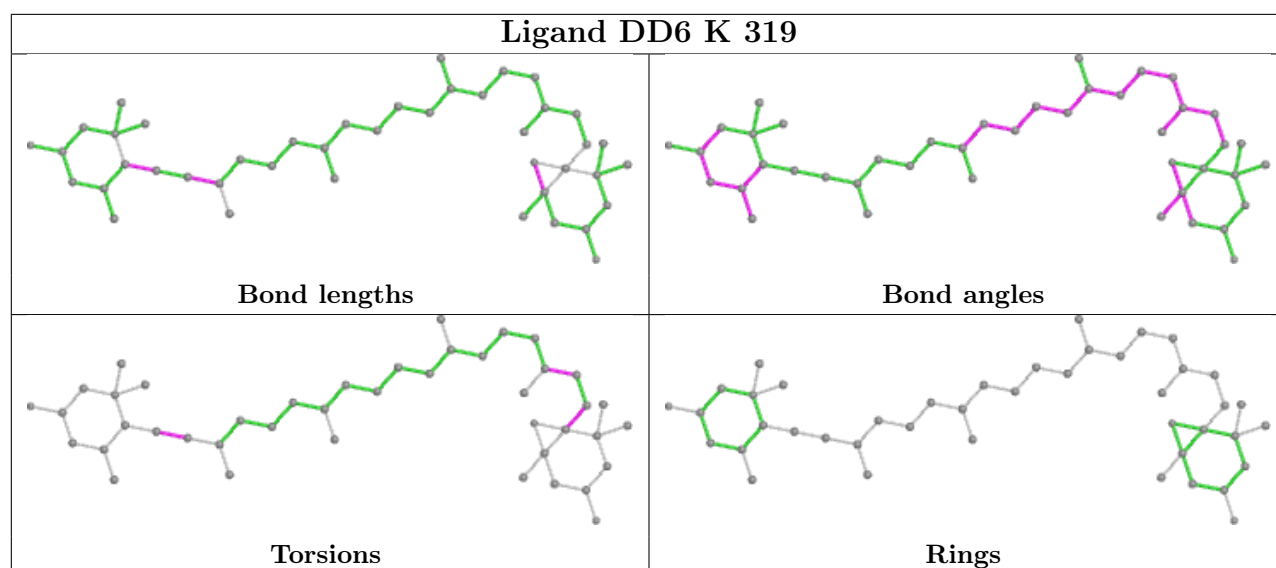


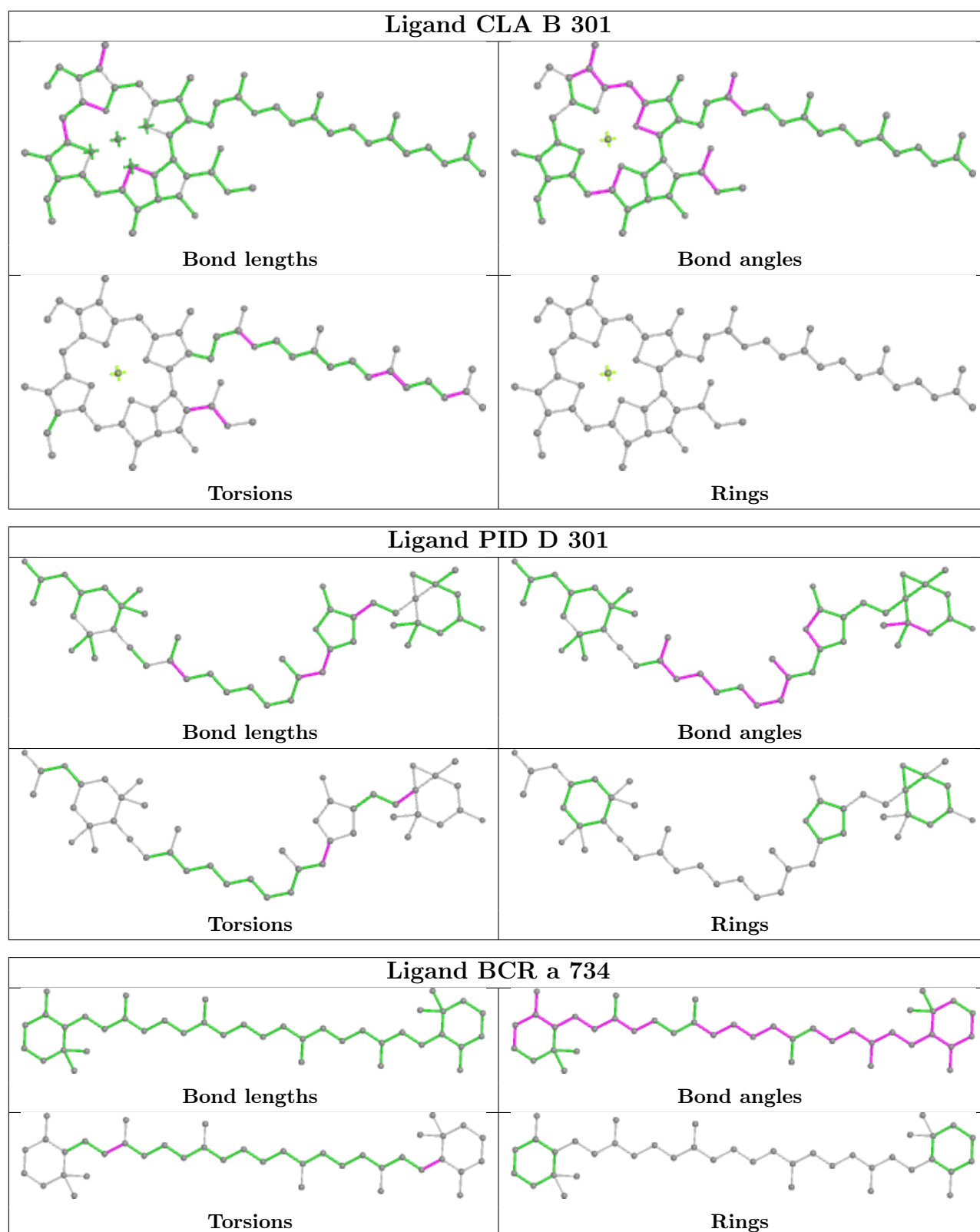


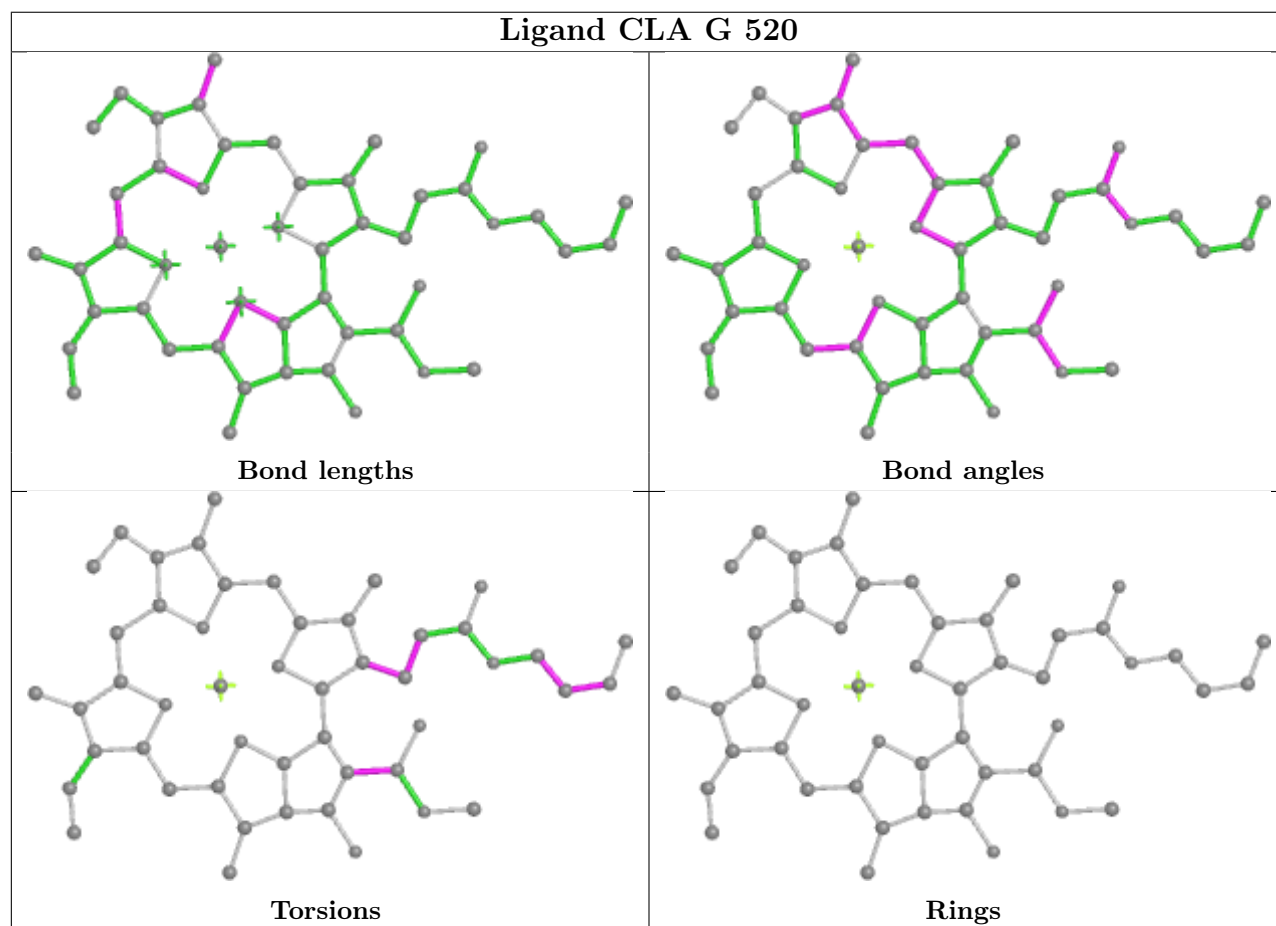
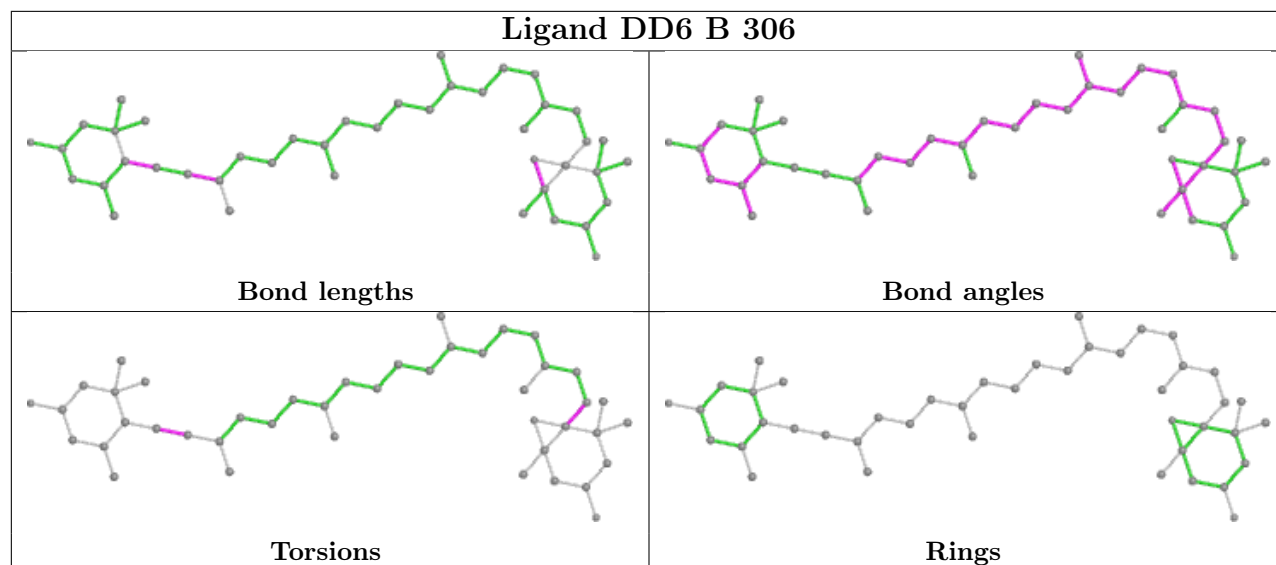


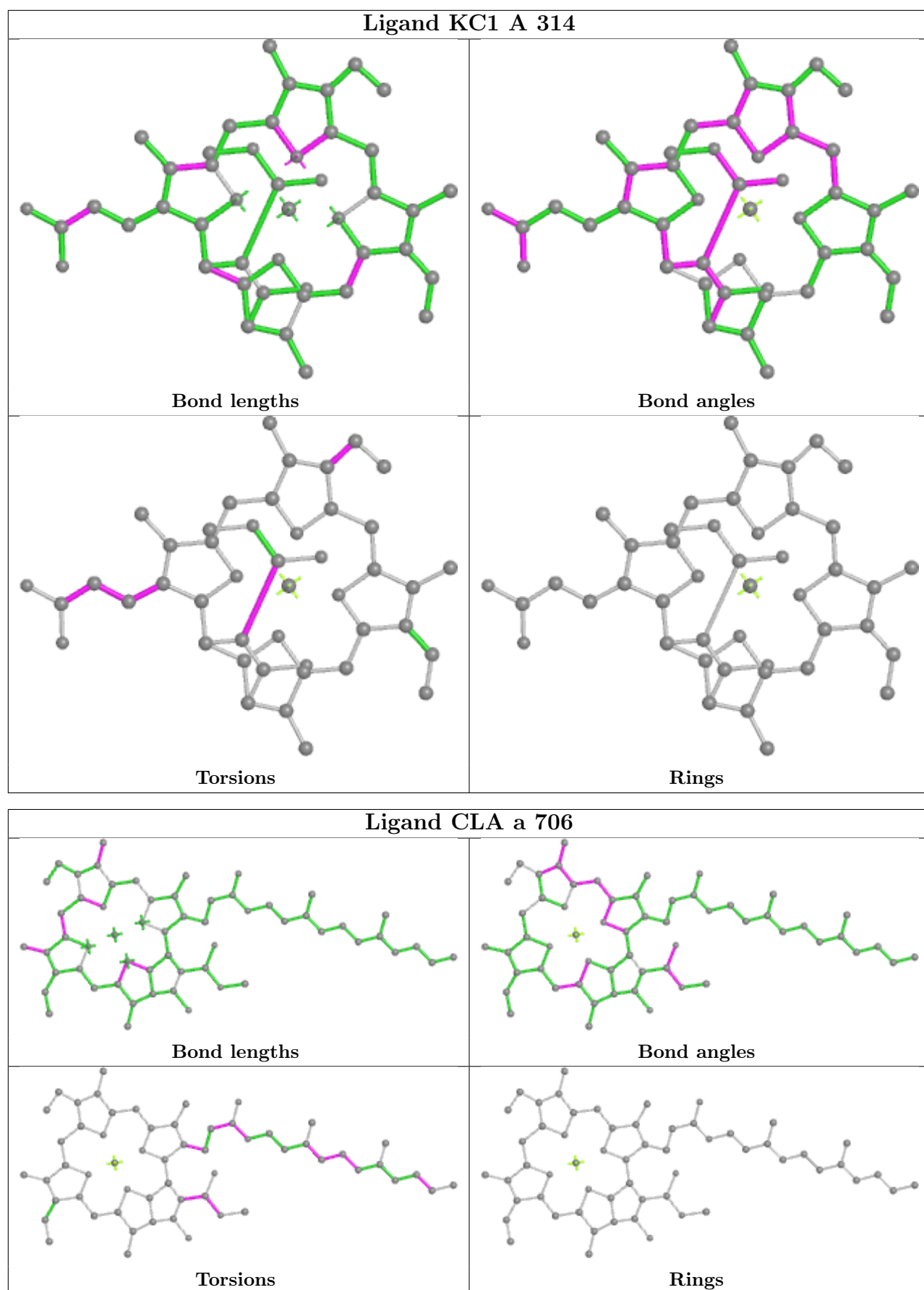


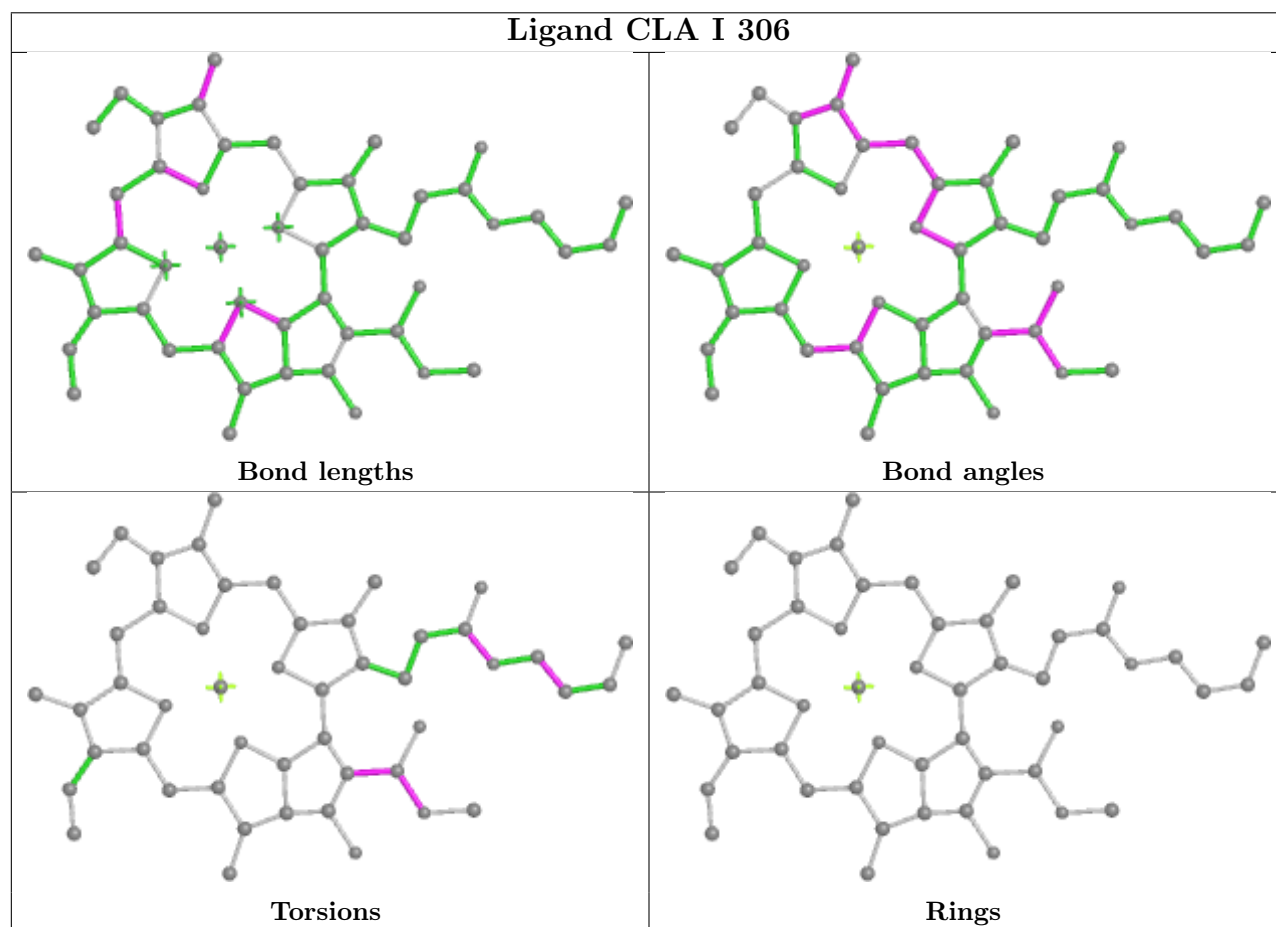
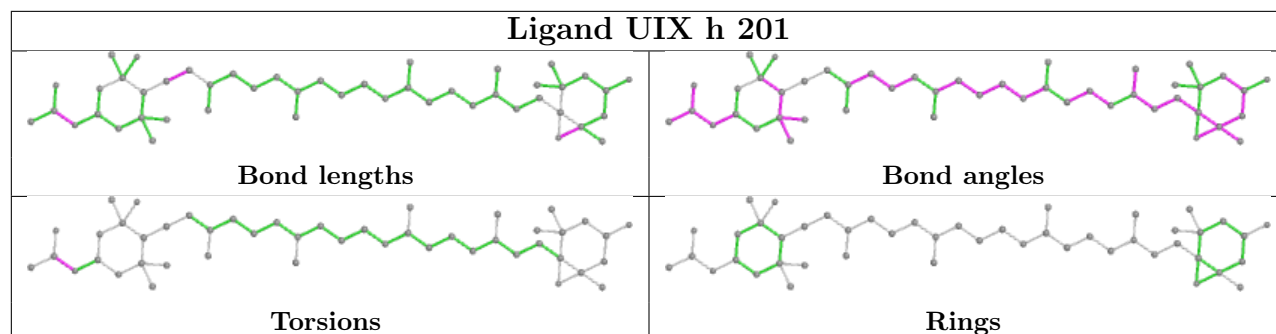


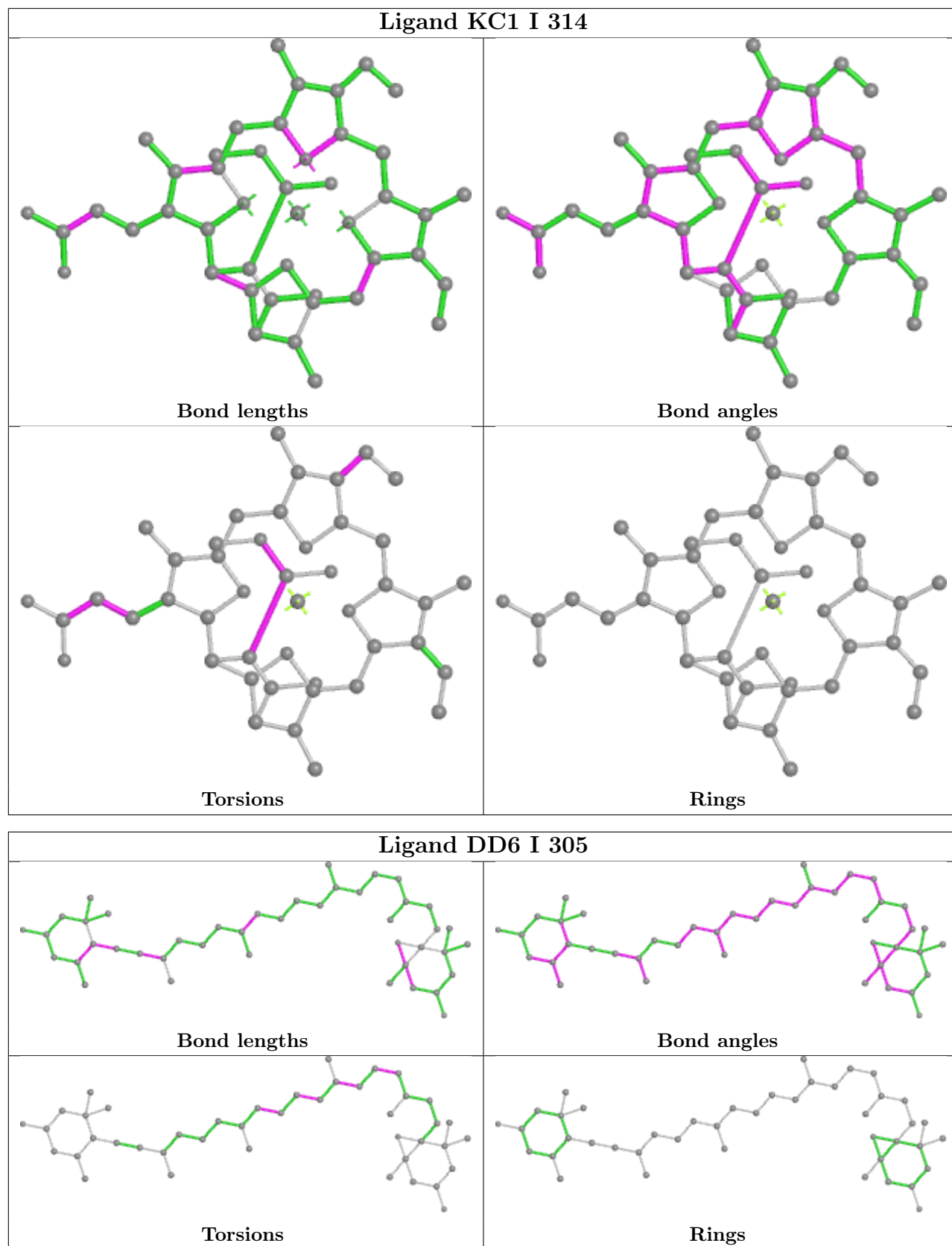


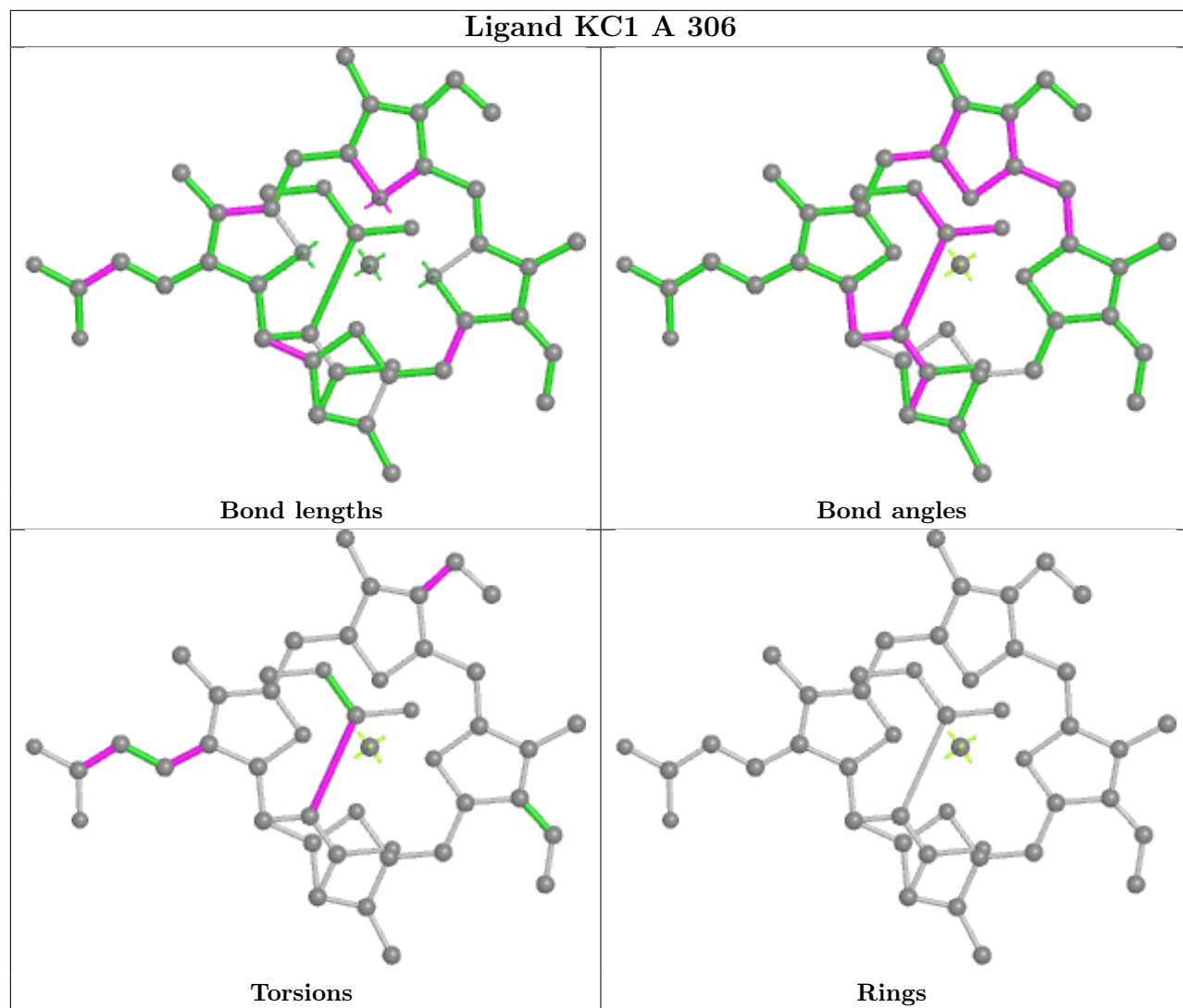


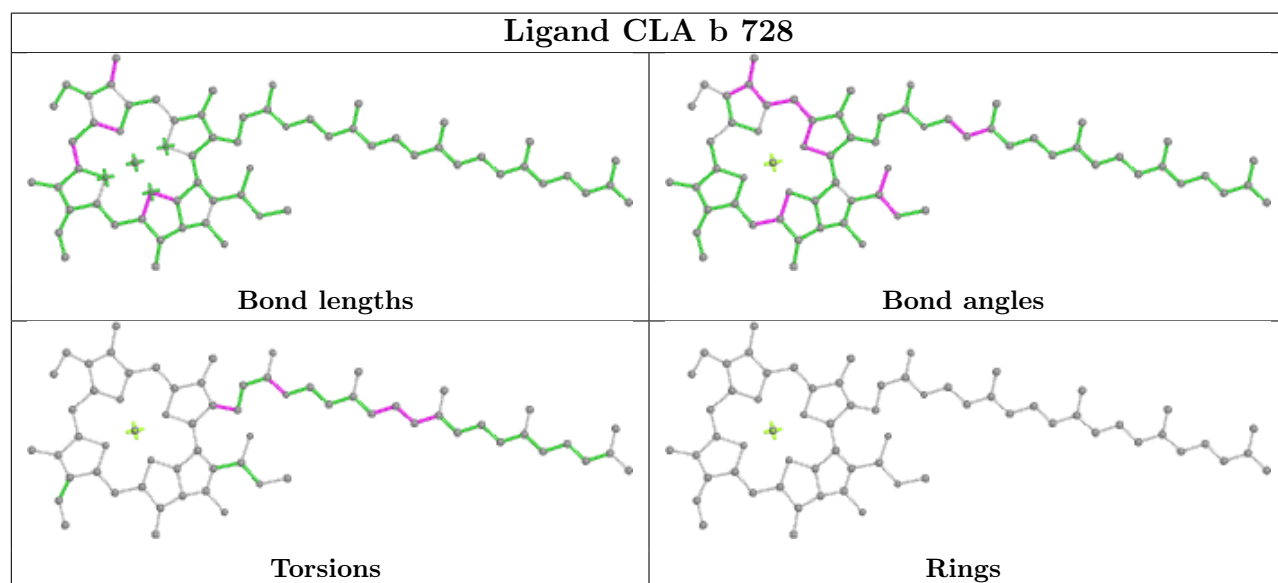
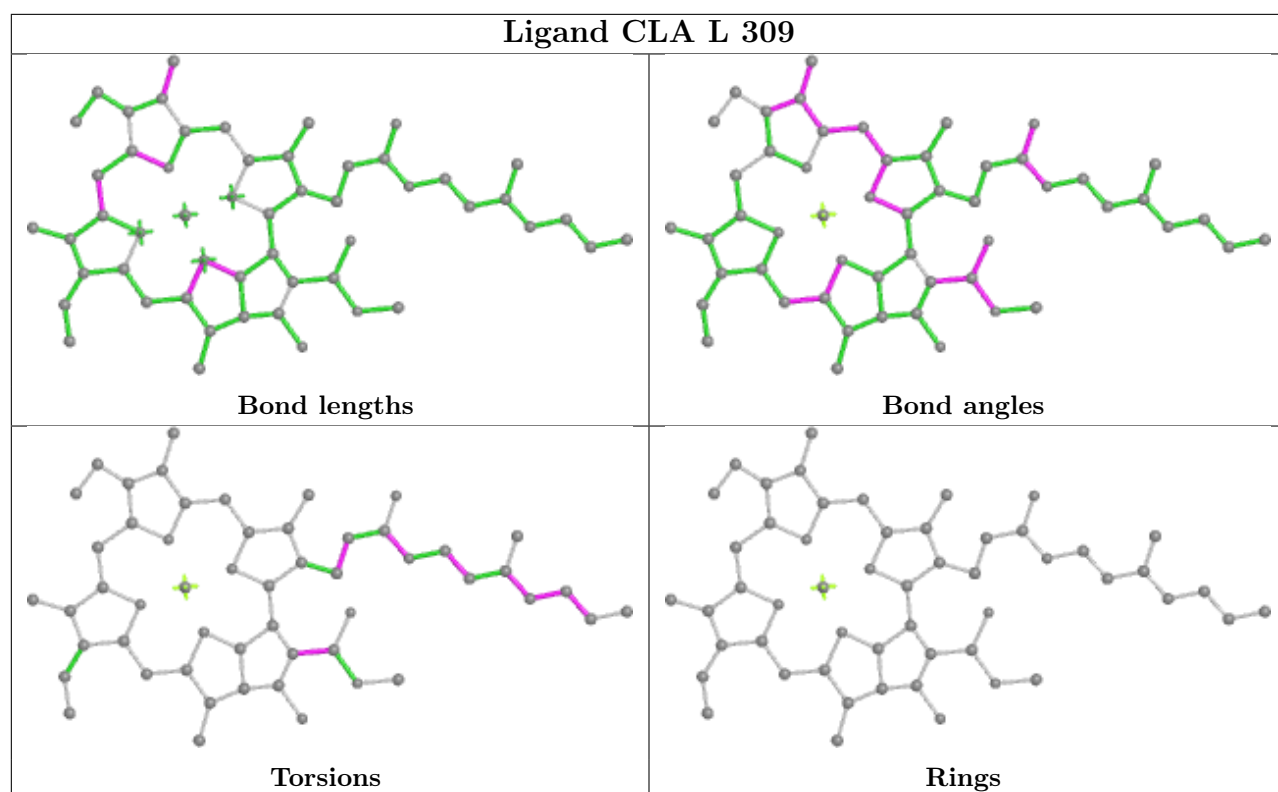


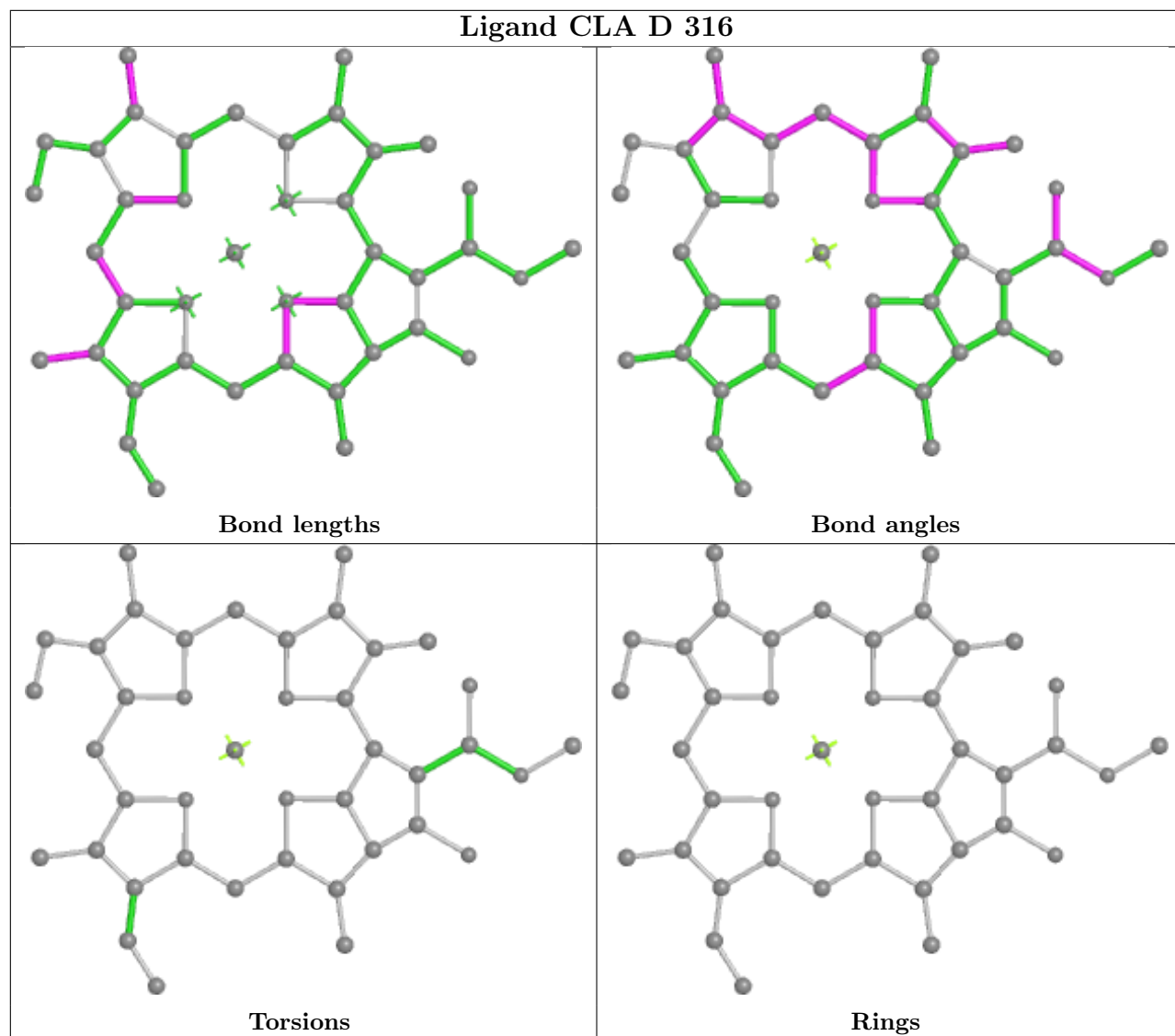


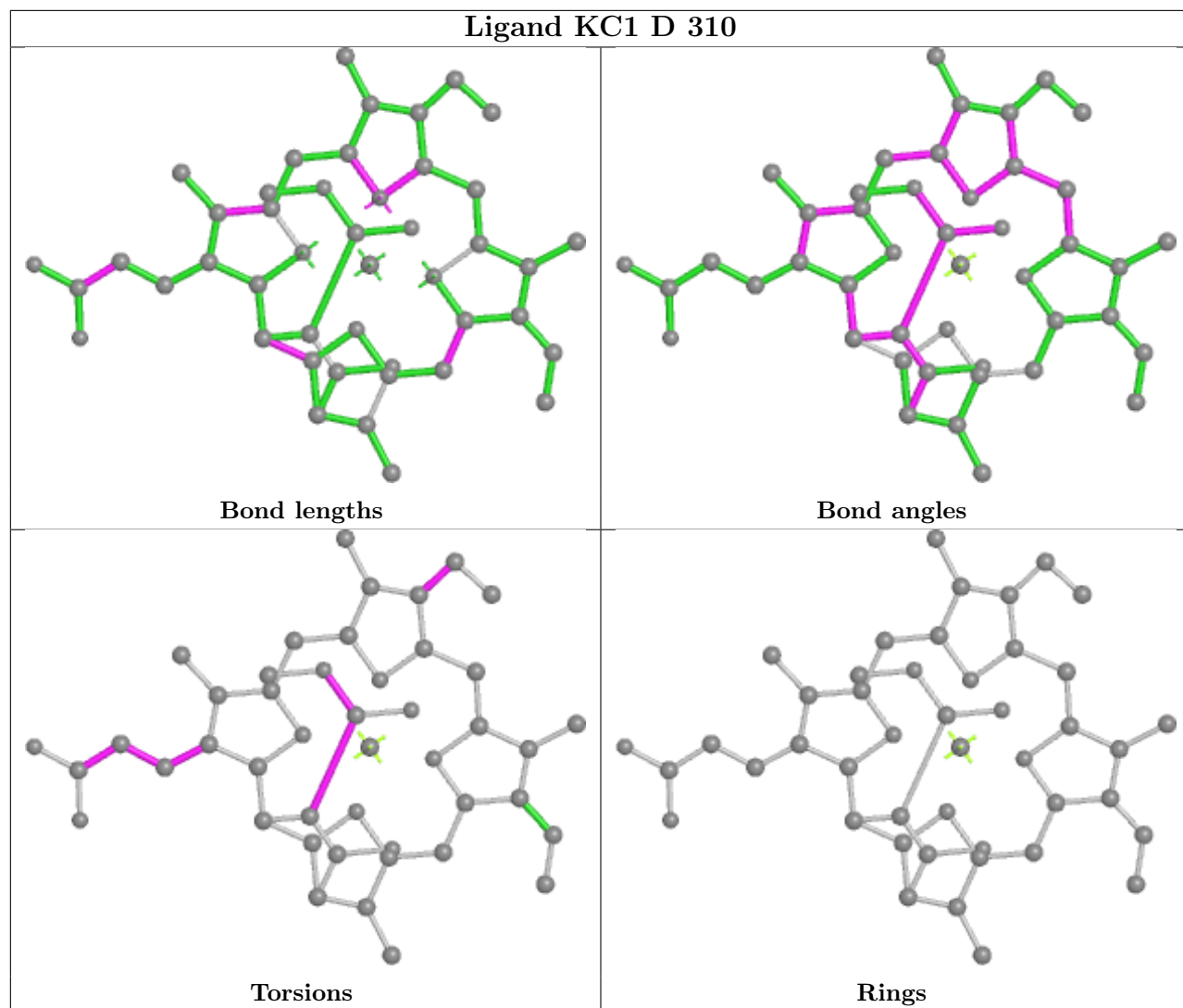


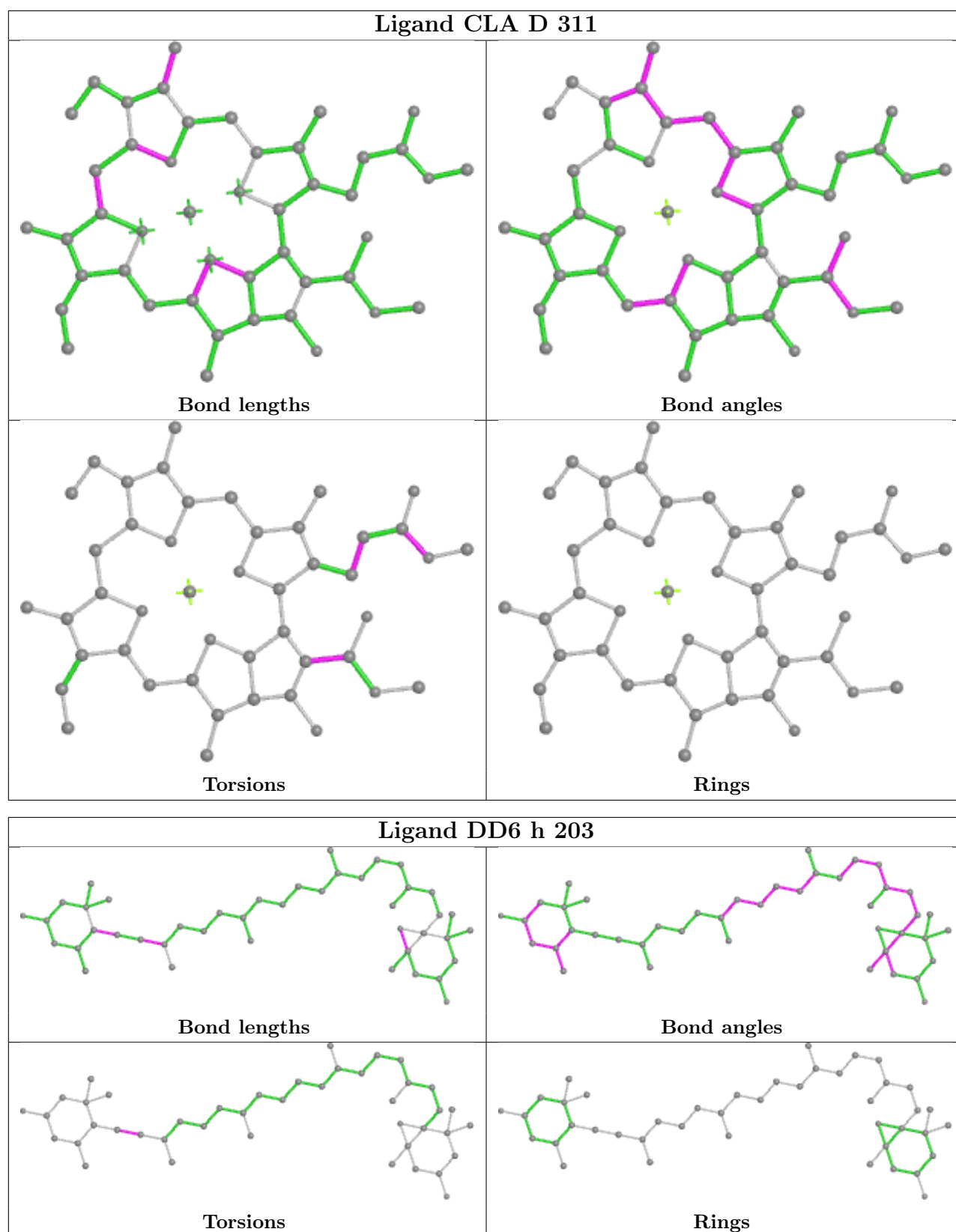


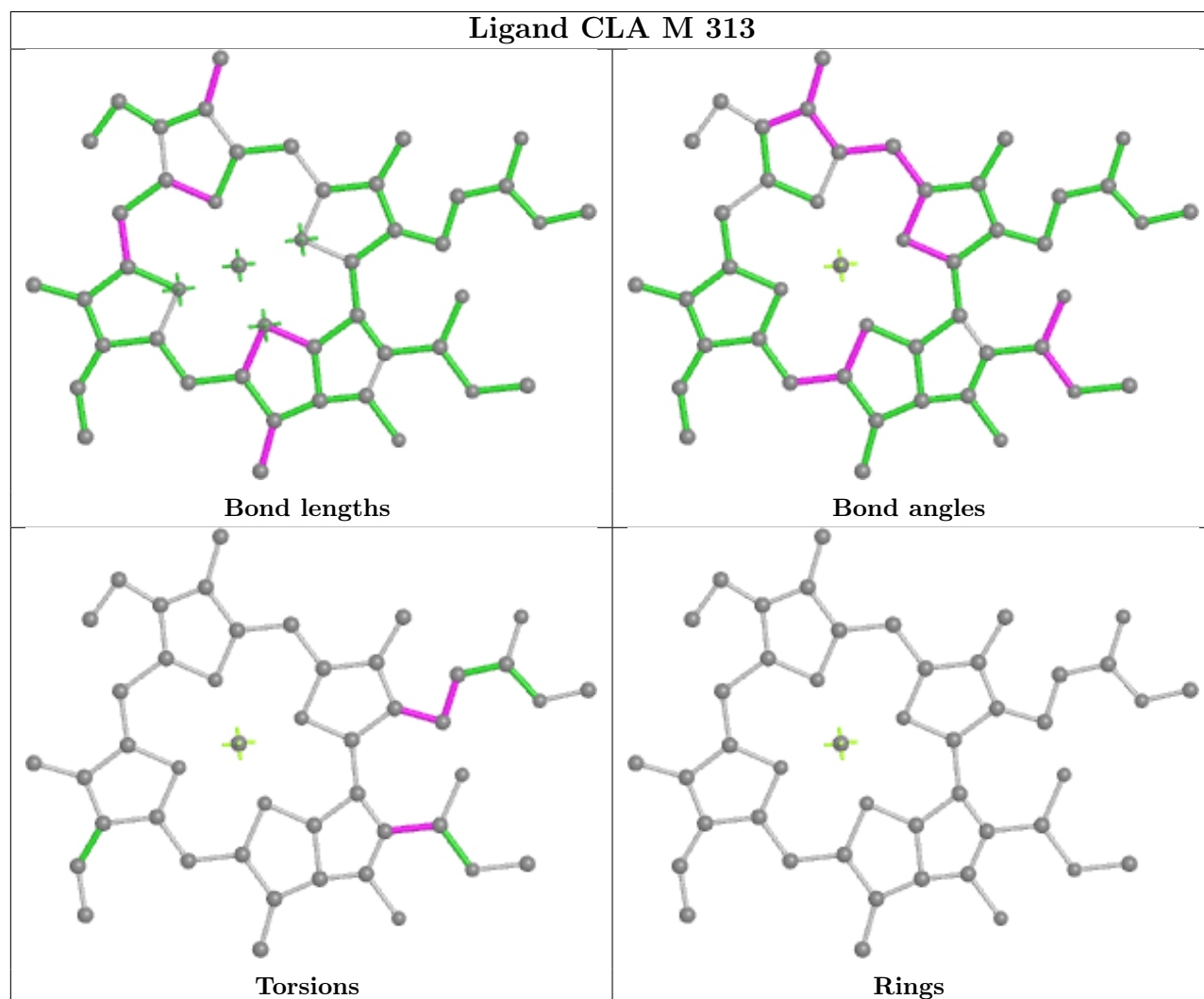
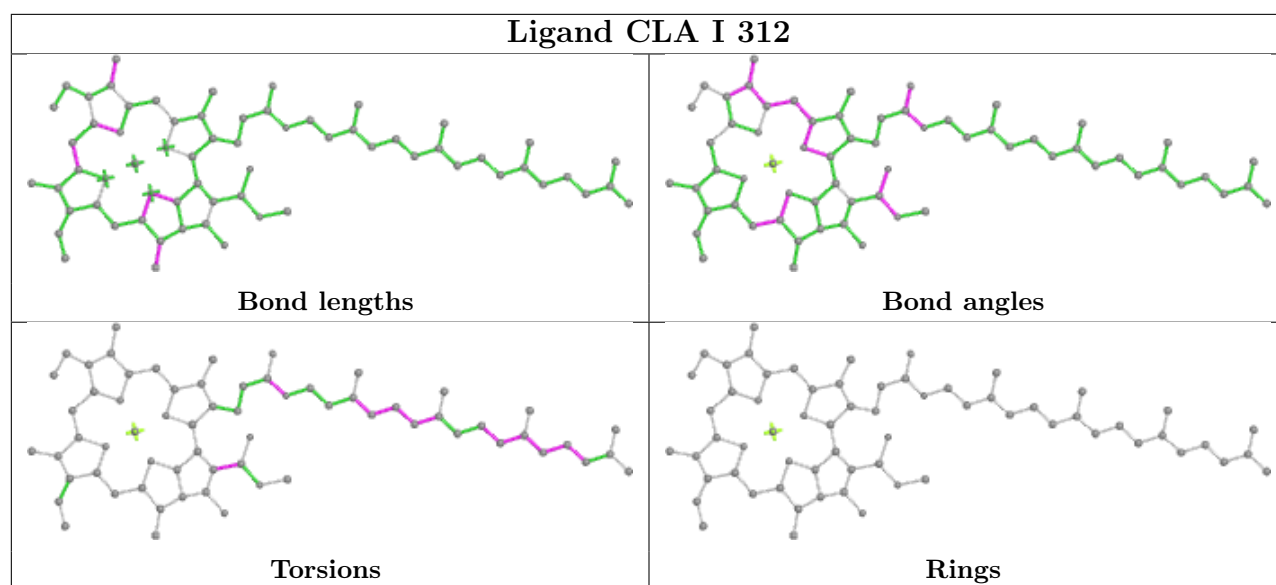


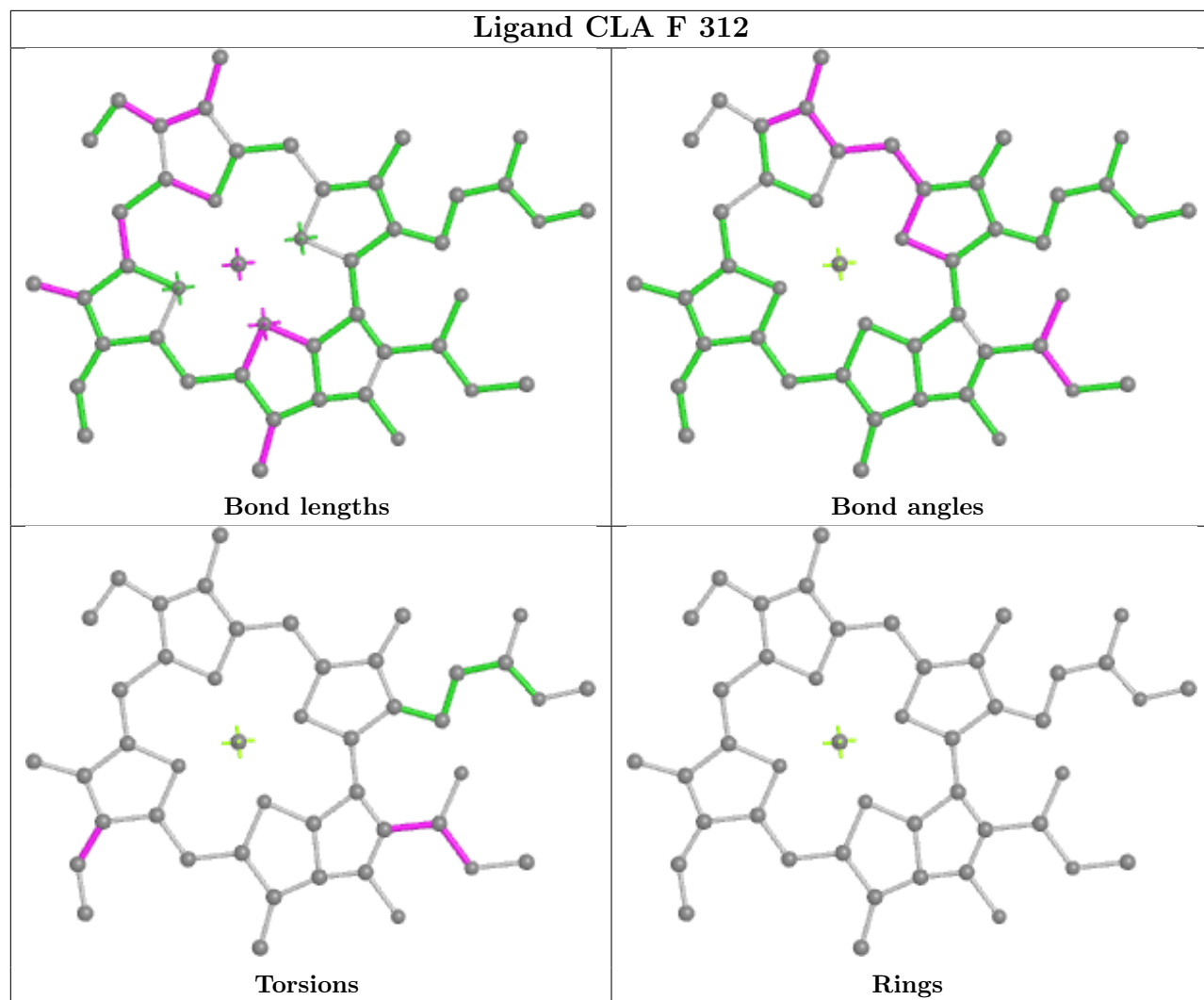


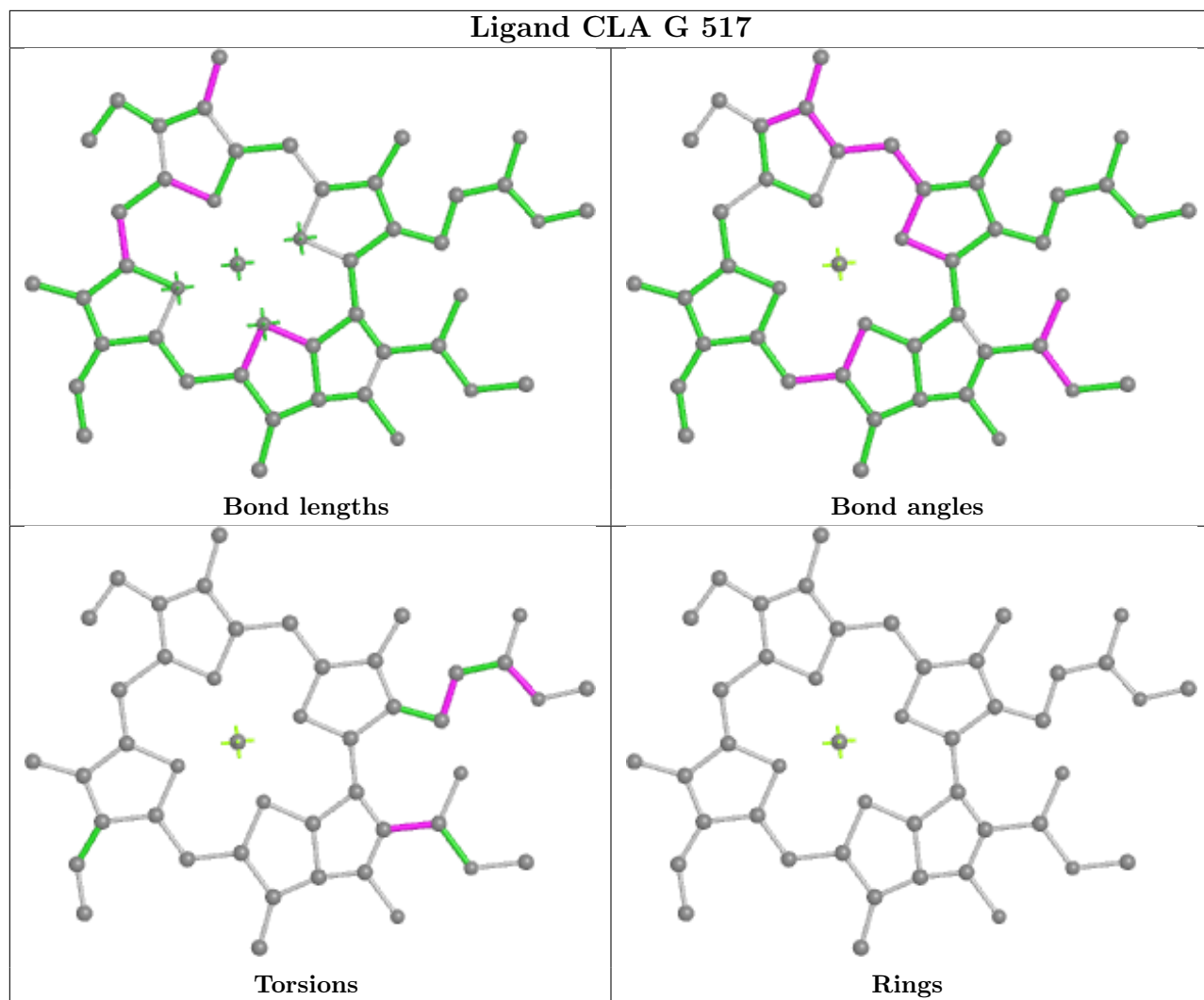


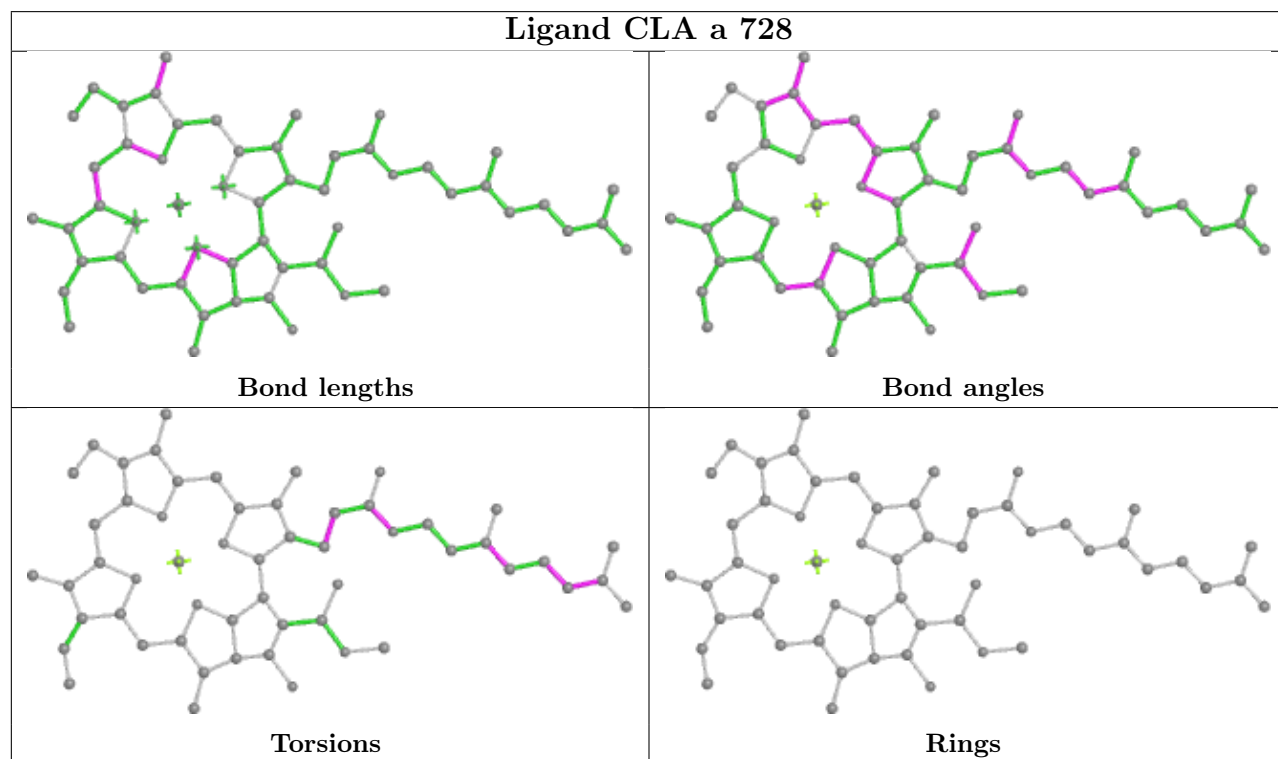
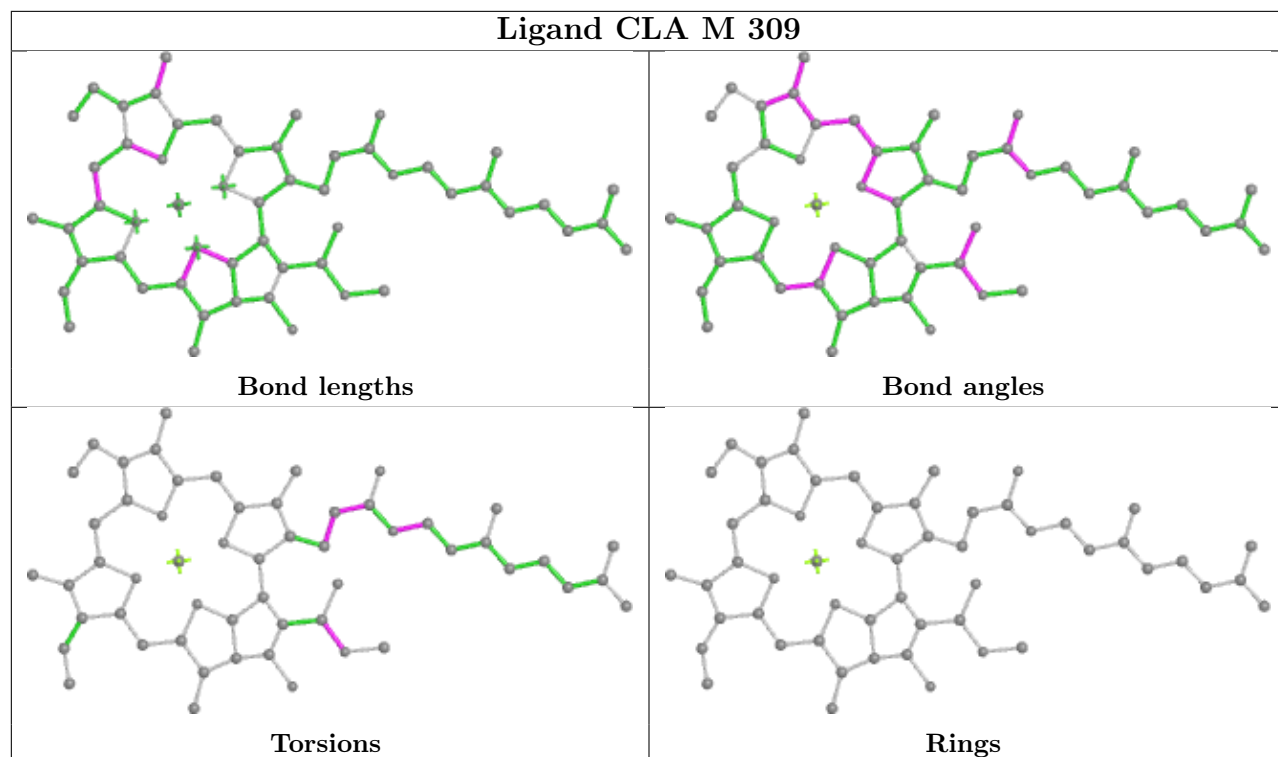


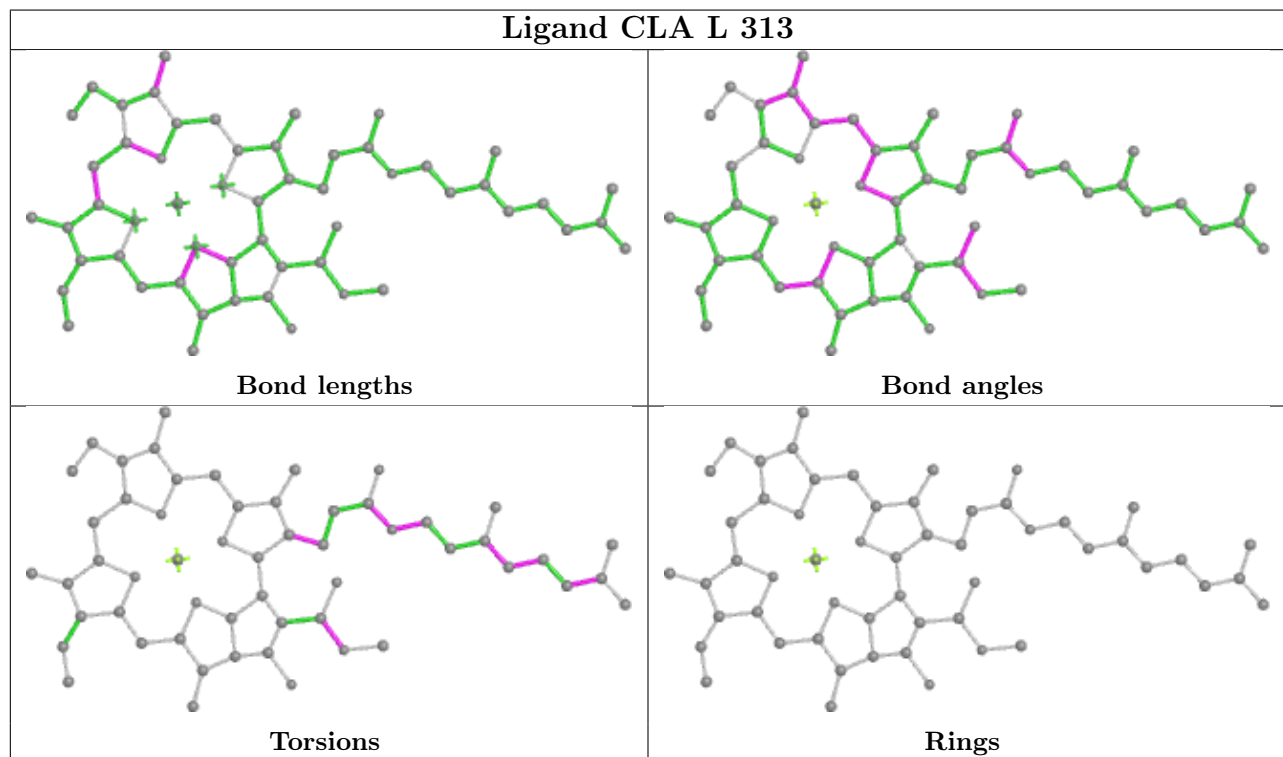
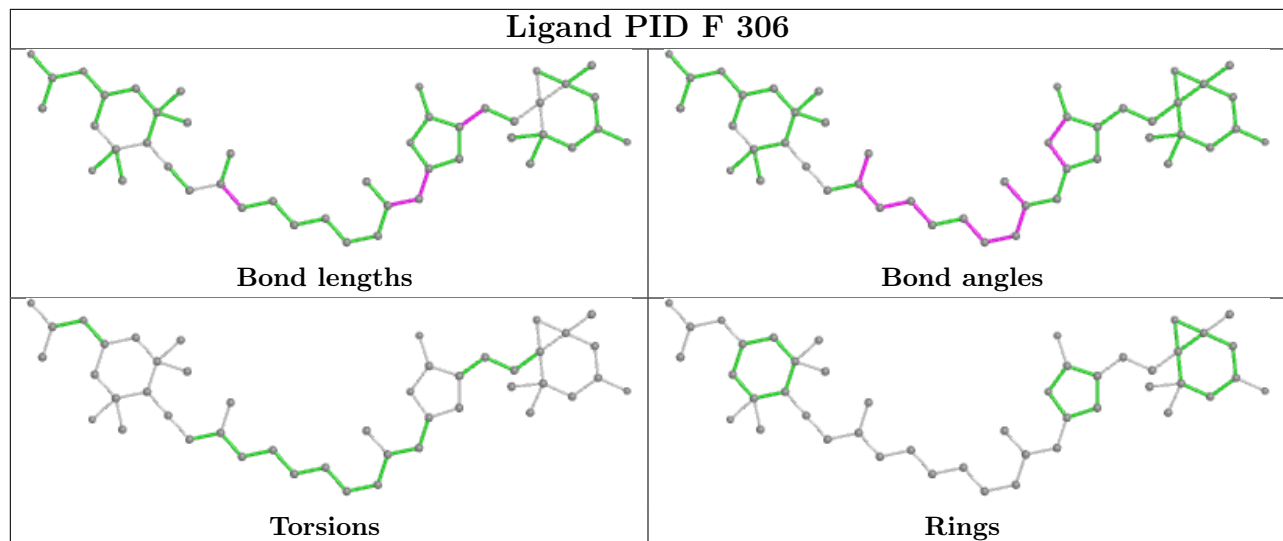


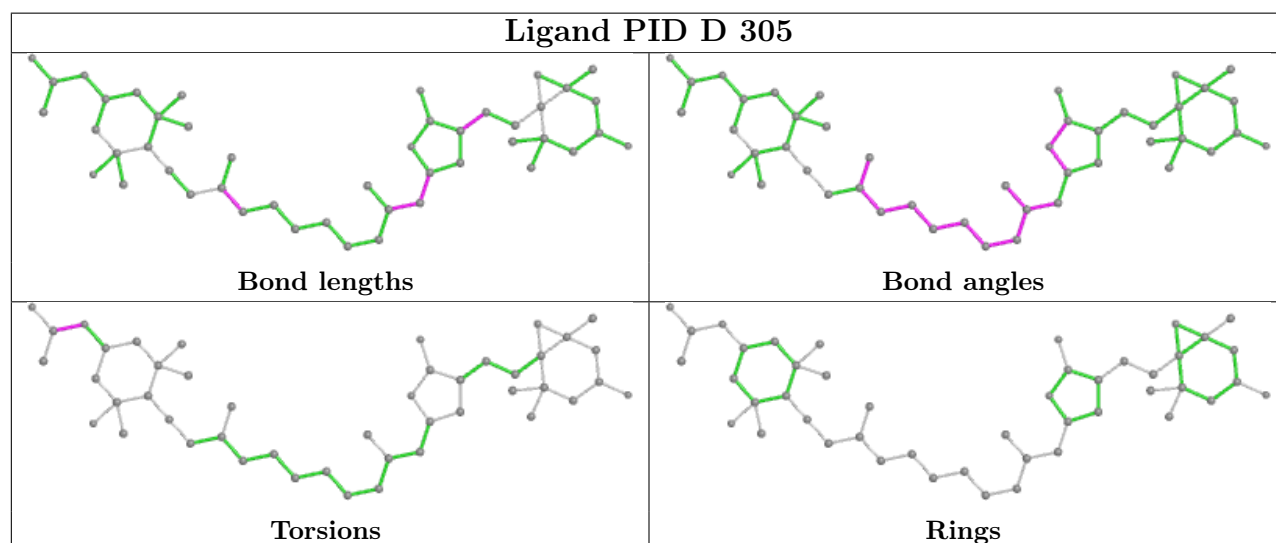
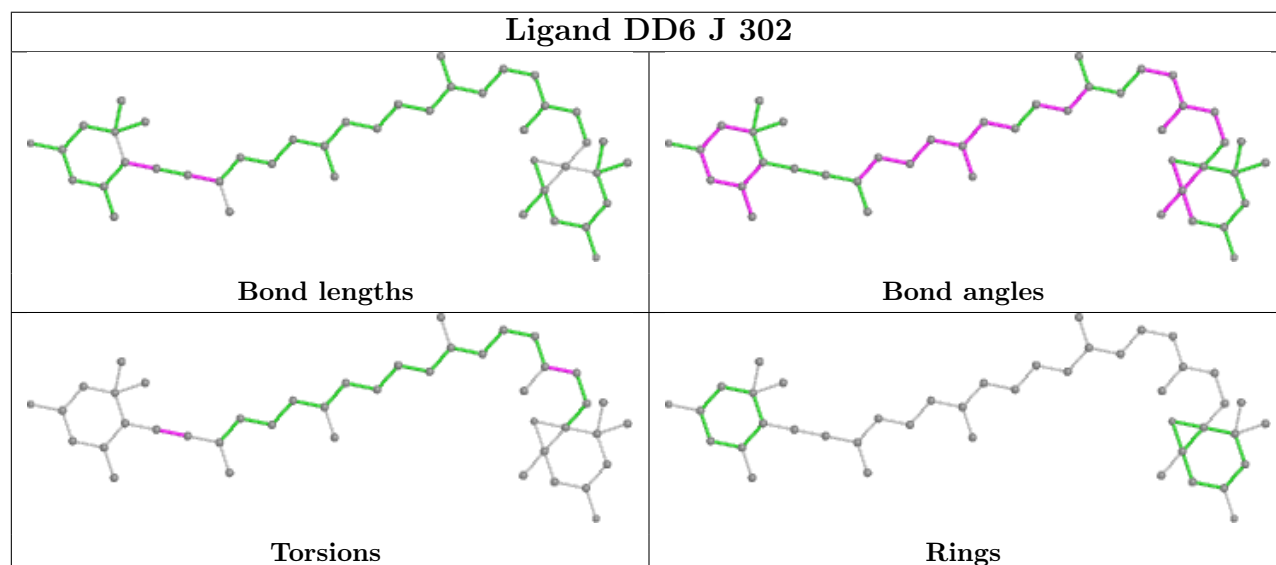
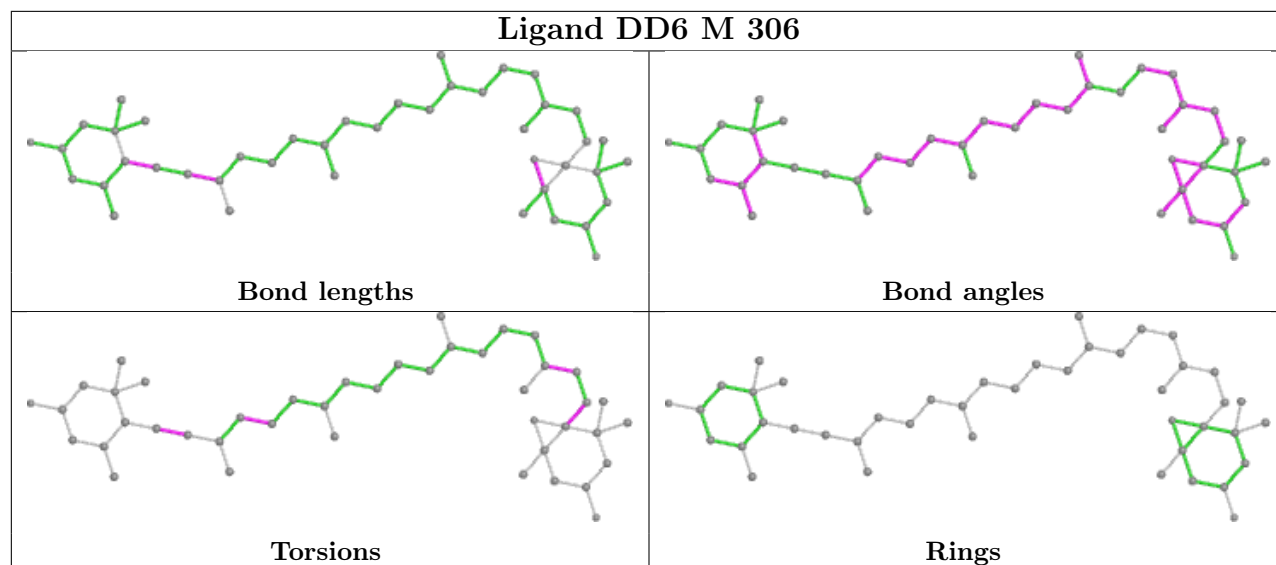


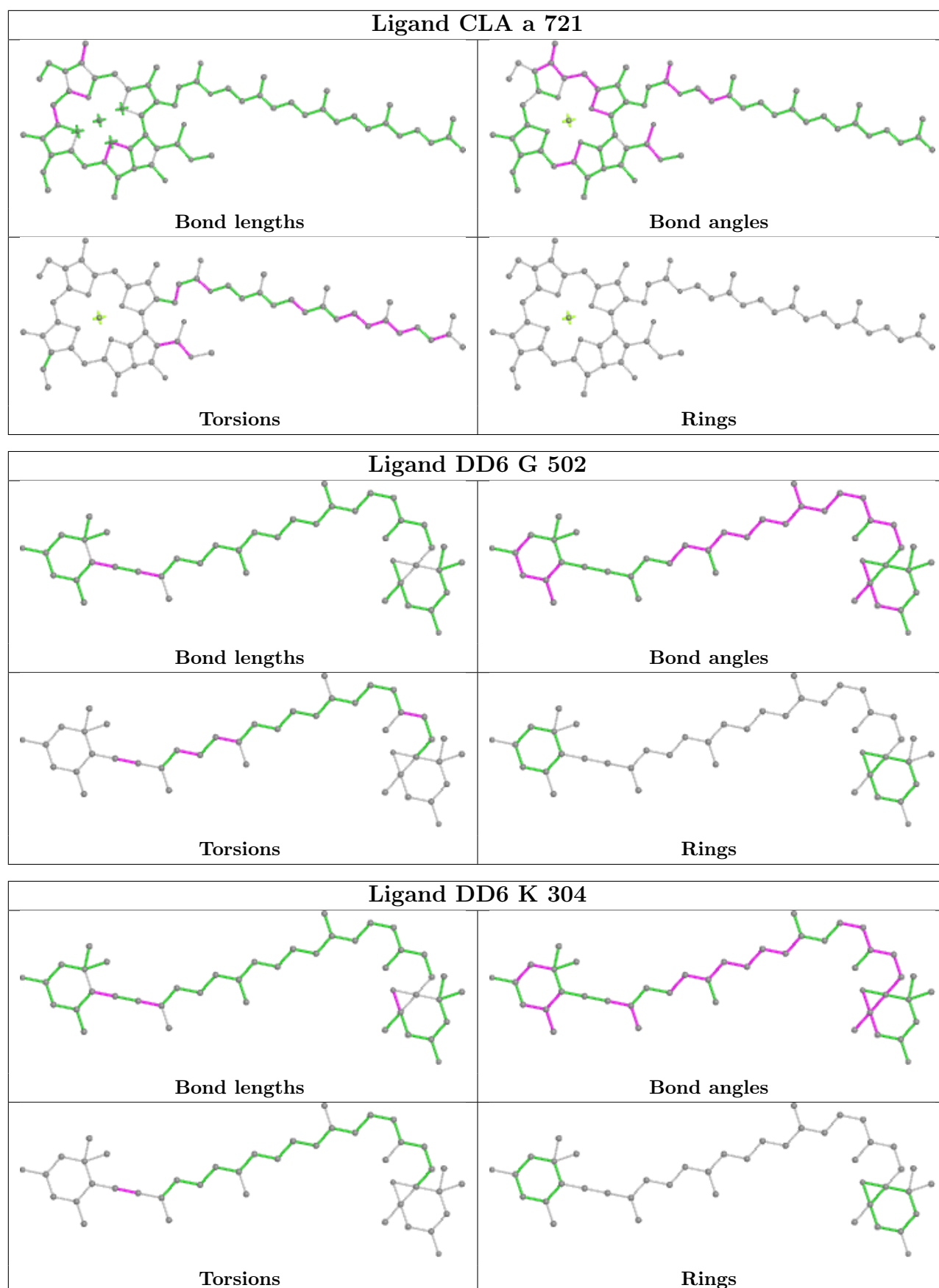


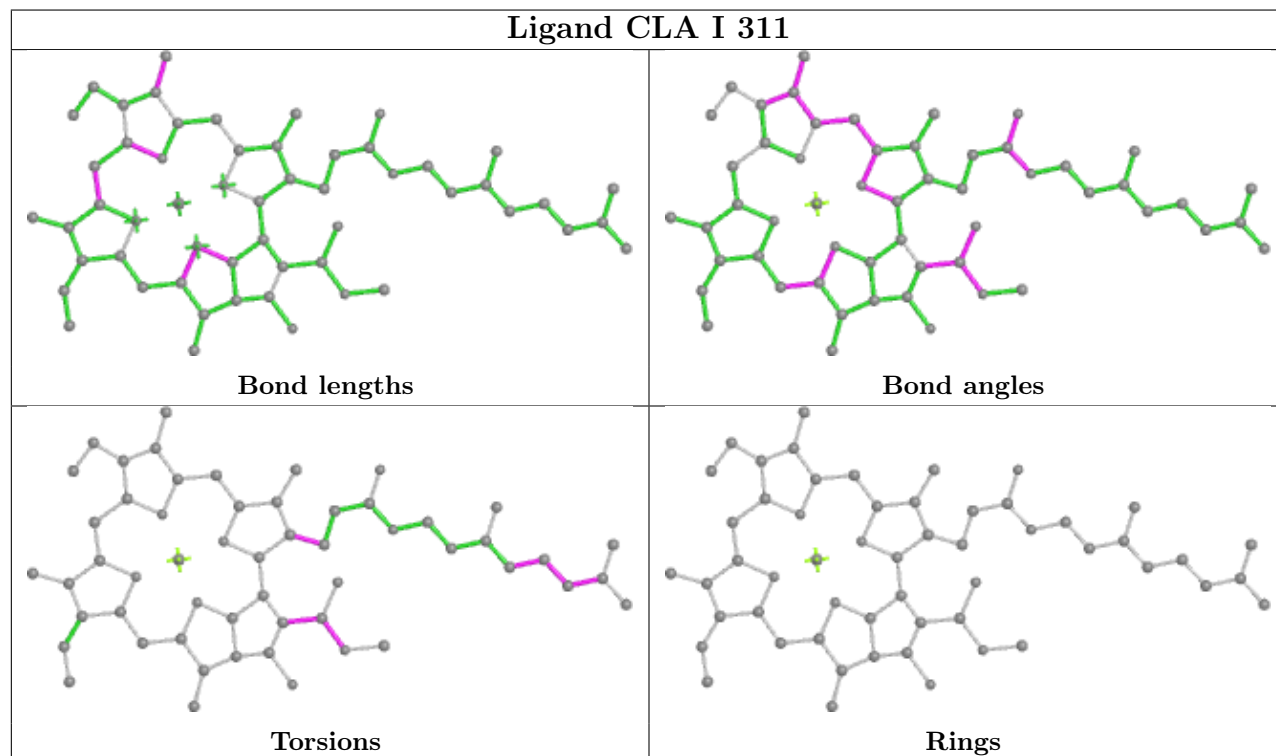
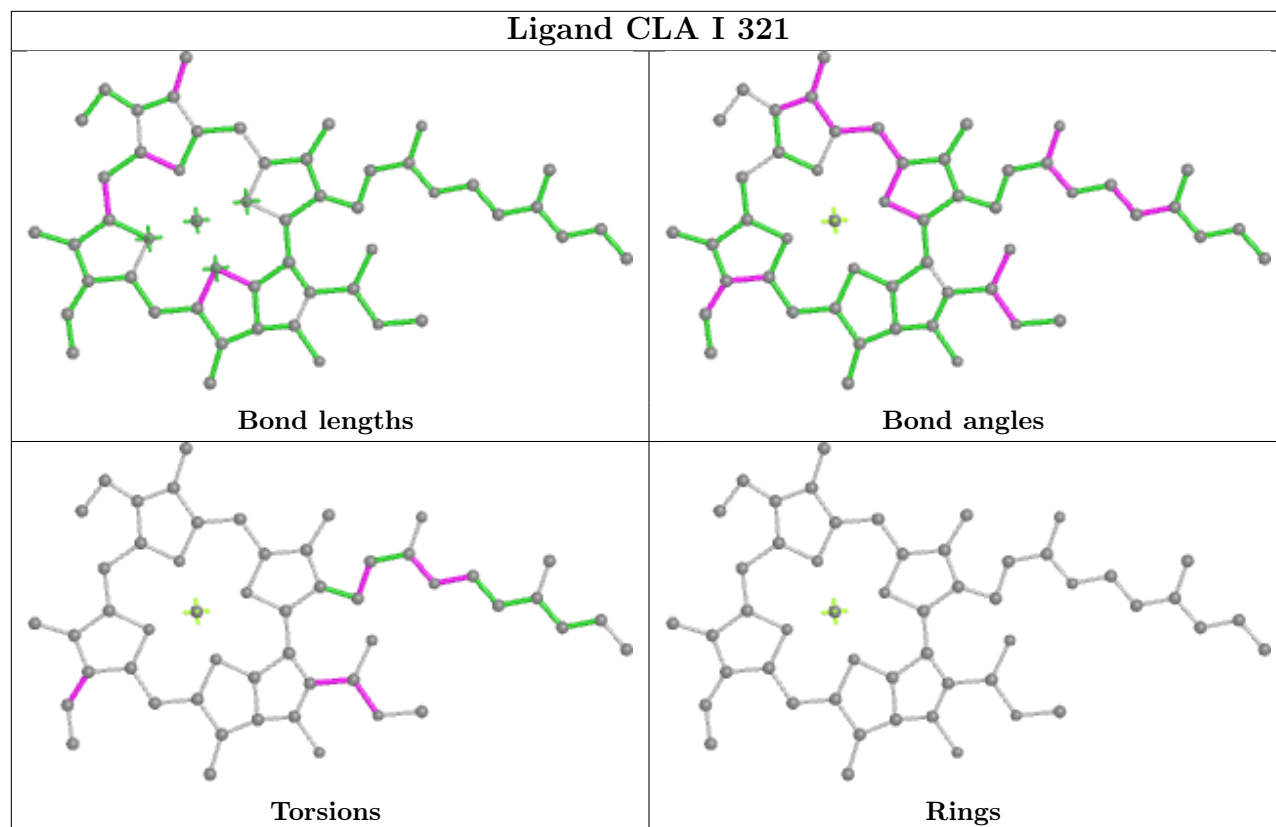


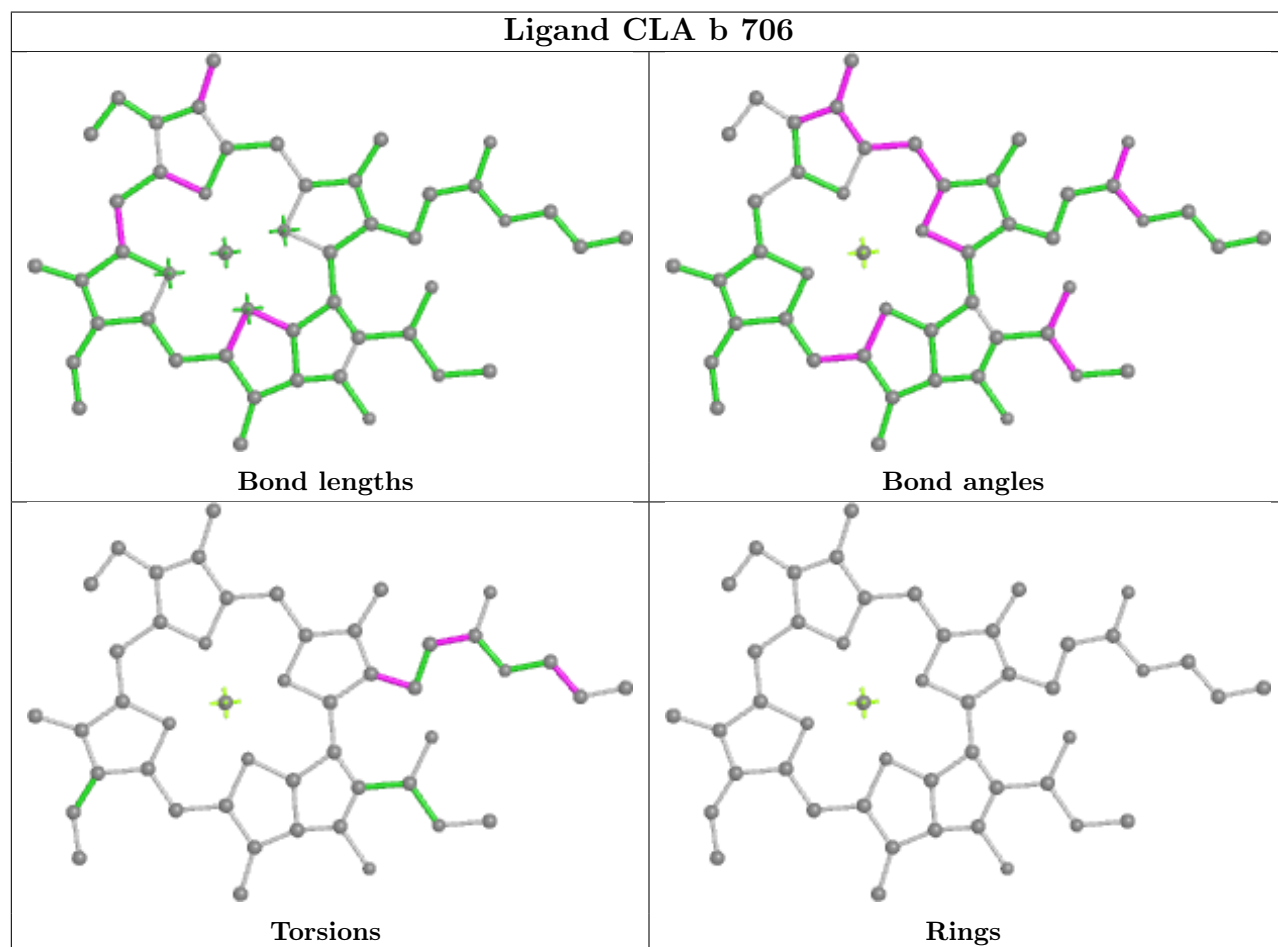
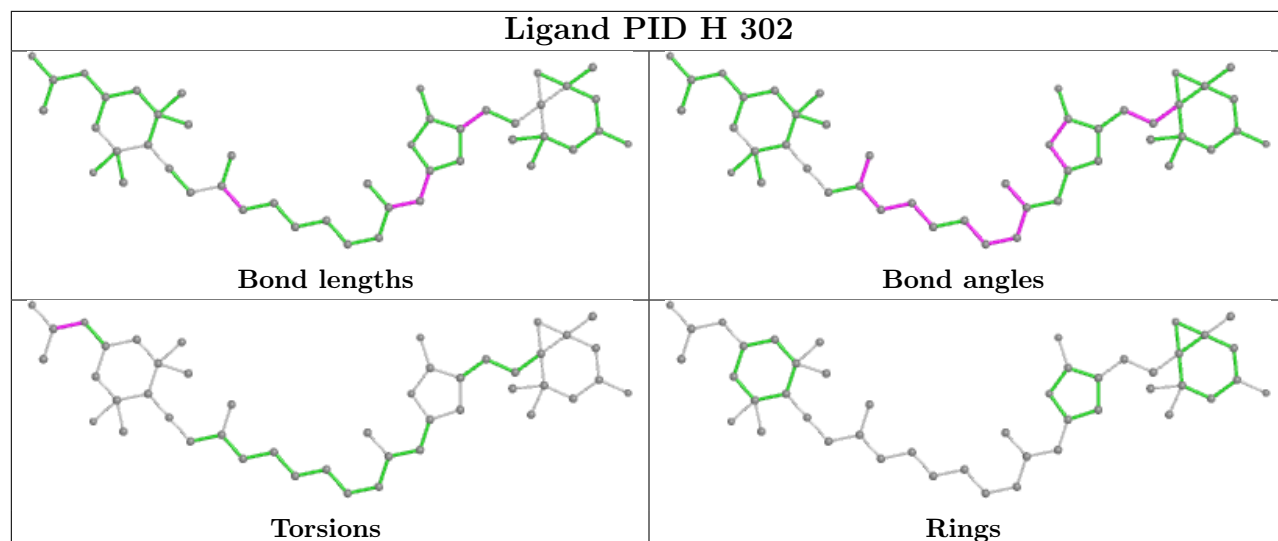


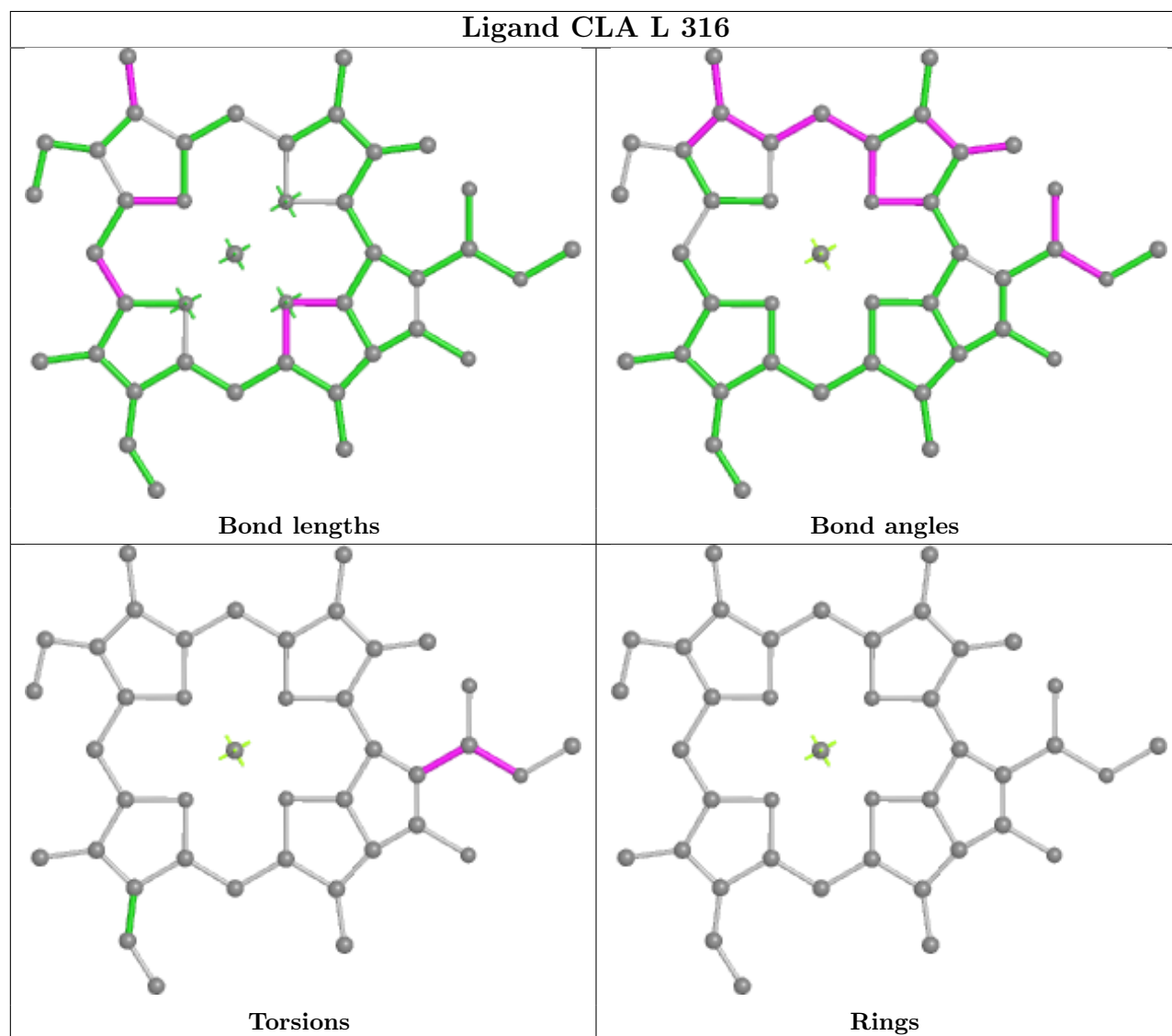
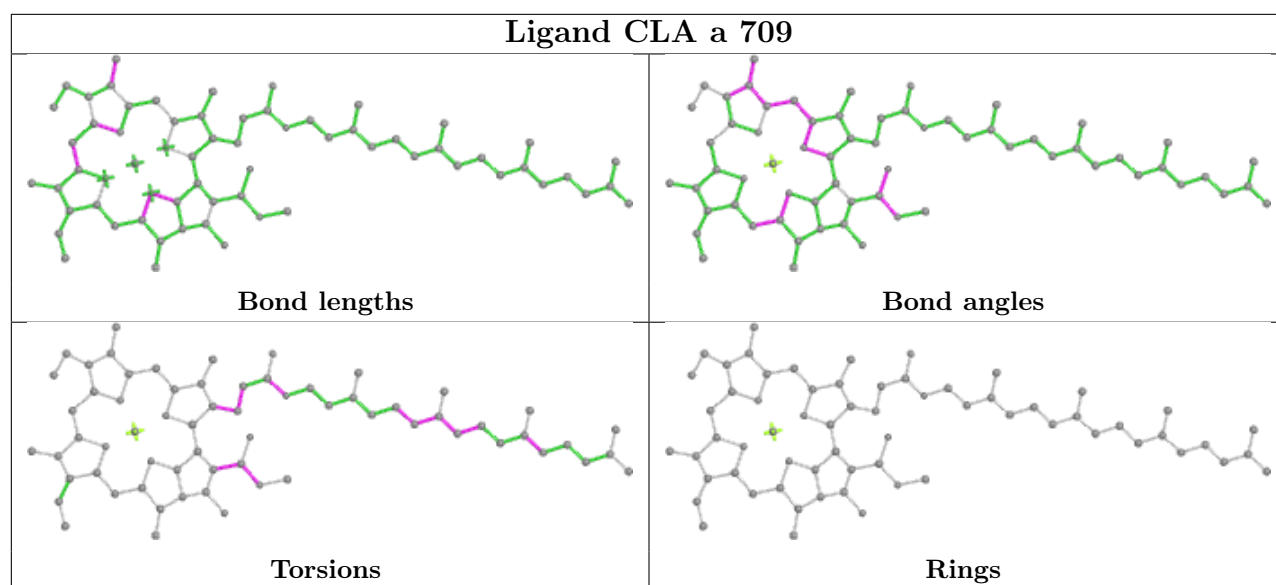


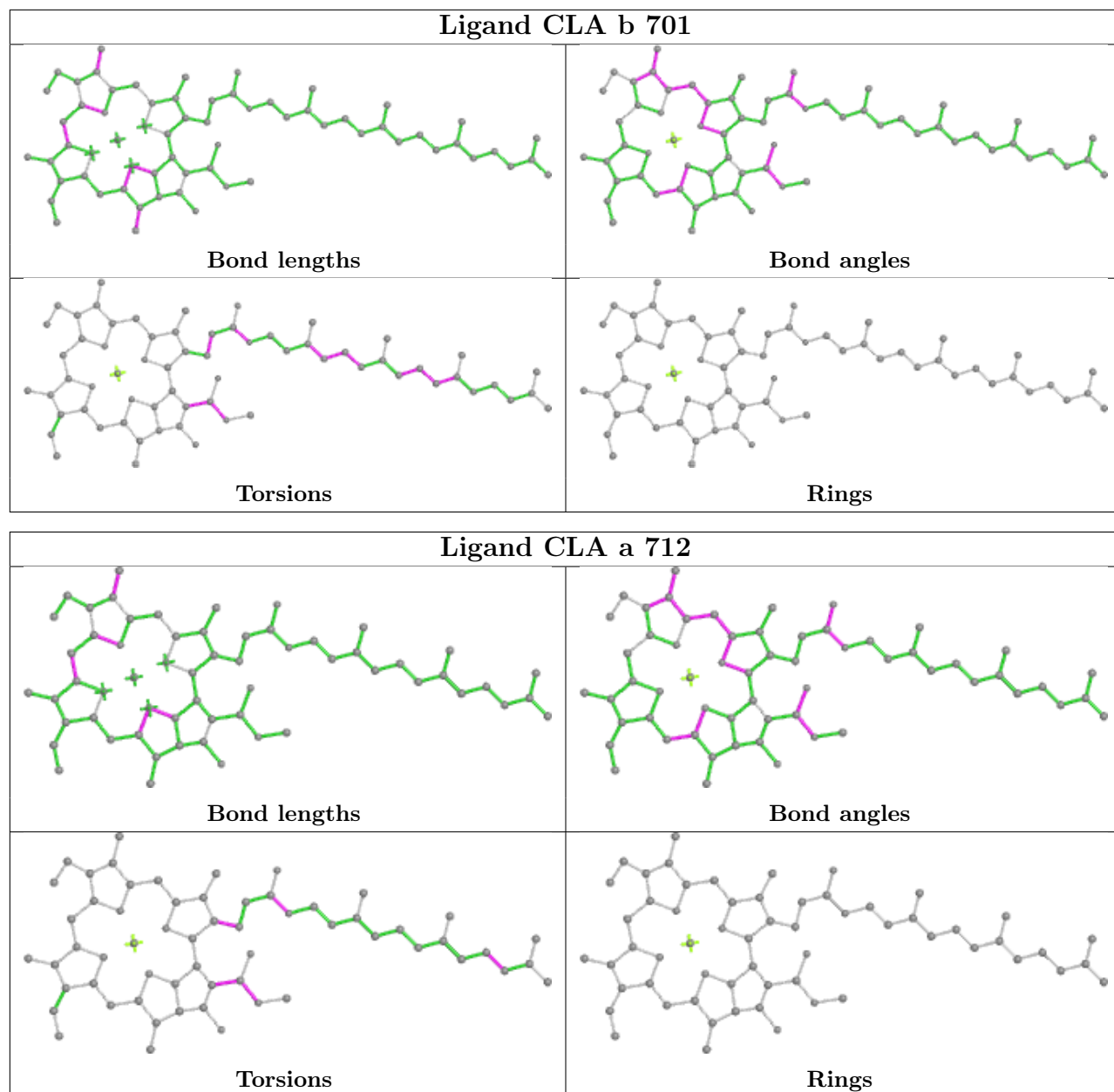


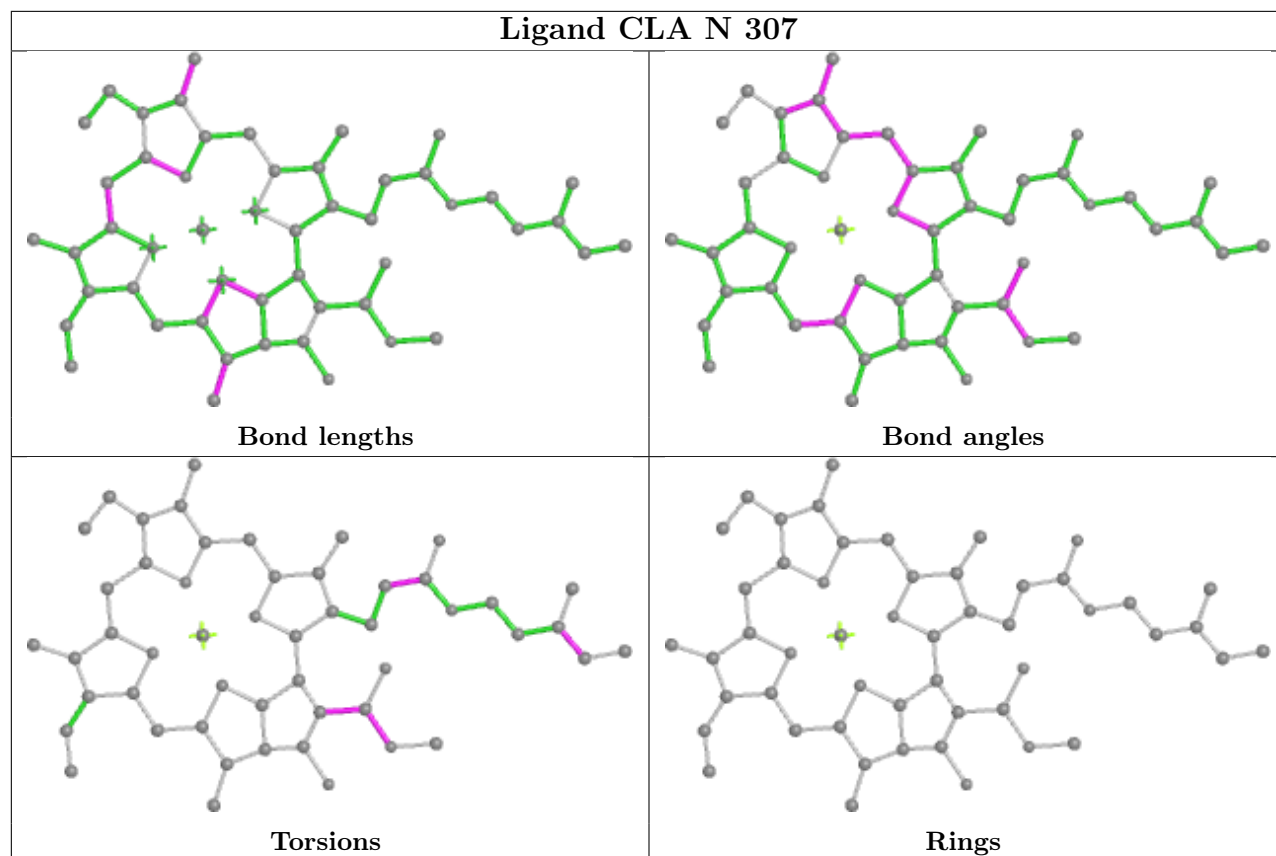












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

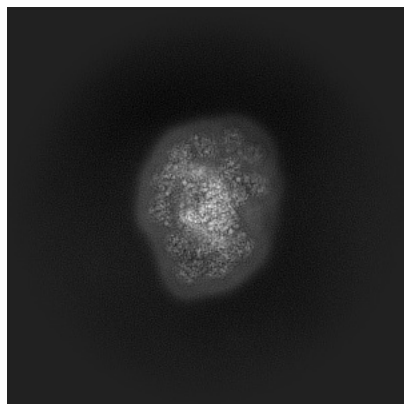
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36743. These allow visual inspection of the internal detail of the map and identification of artifacts.

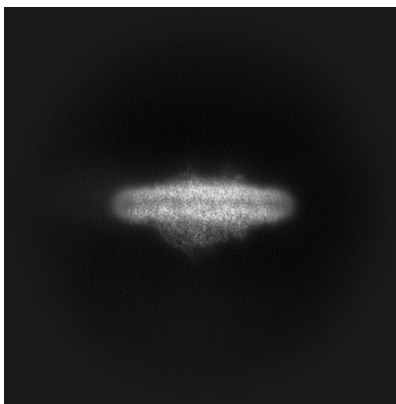
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

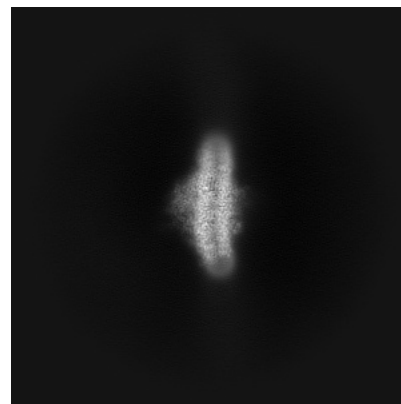
6.1.1 Primary map



X

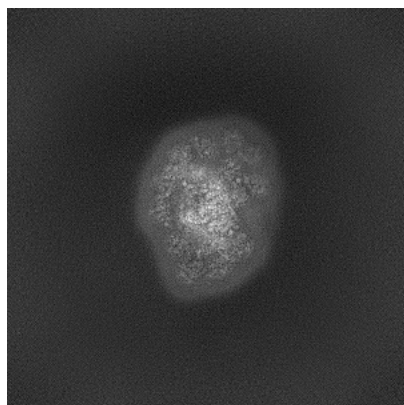


Y

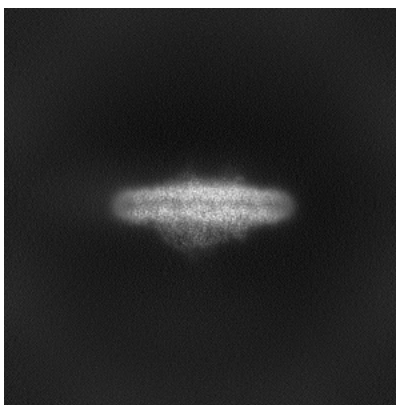


Z

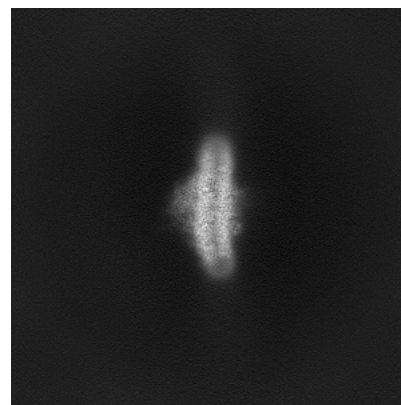
6.1.2 Raw map



X



Y

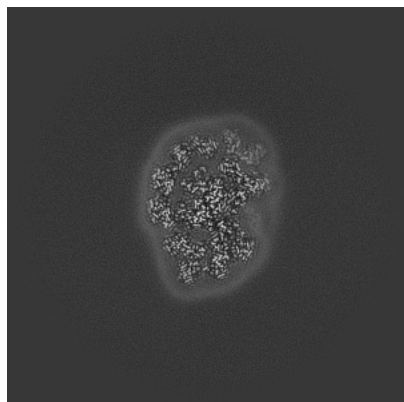


Z

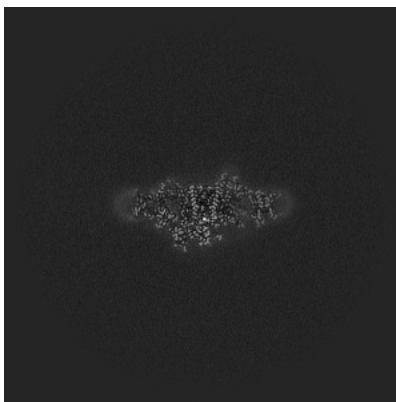
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

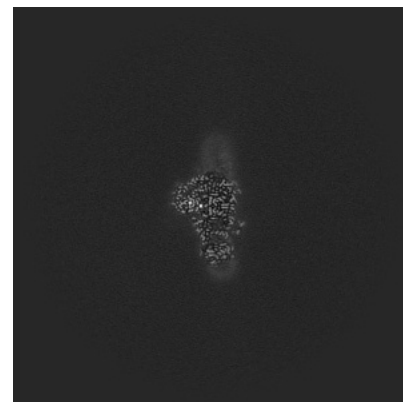
6.2.1 Primary map



X Index: 256

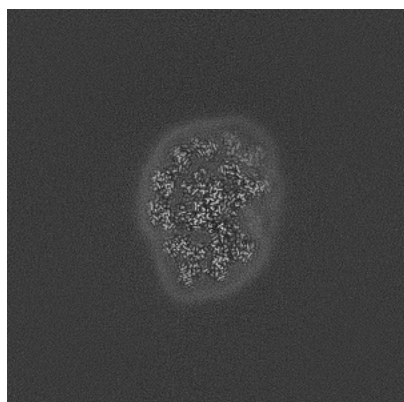


Y Index: 256

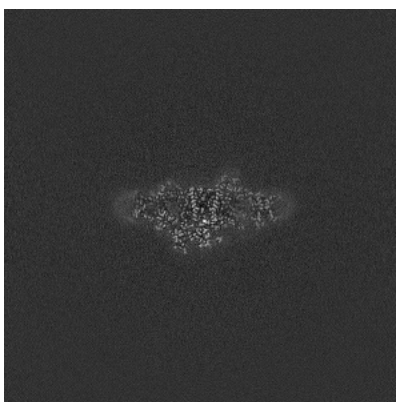


Z Index: 256

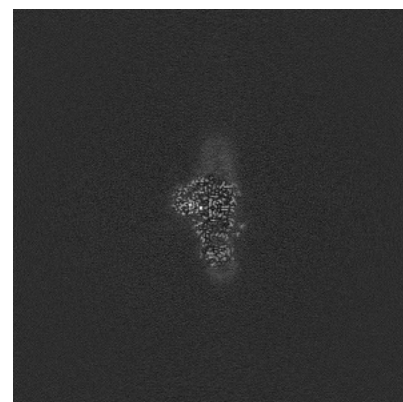
6.2.2 Raw map



X Index: 256



Y Index: 256

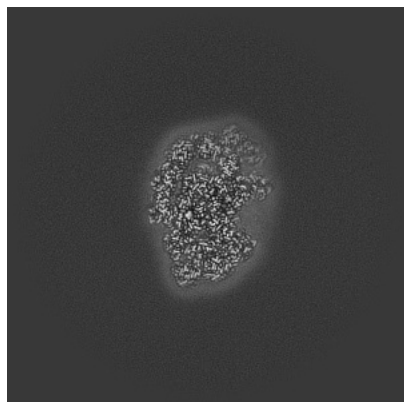


Z Index: 256

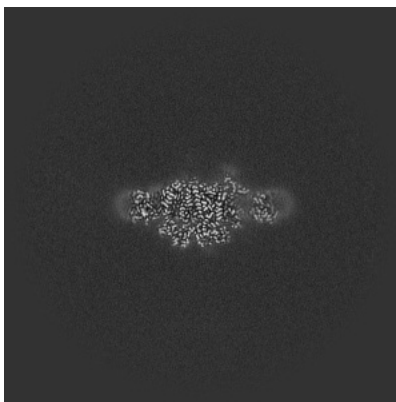
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

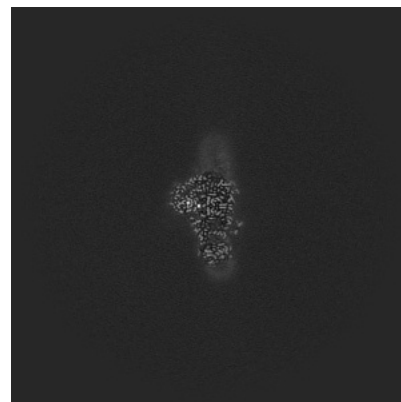
6.3.1 Primary map



X Index: 248

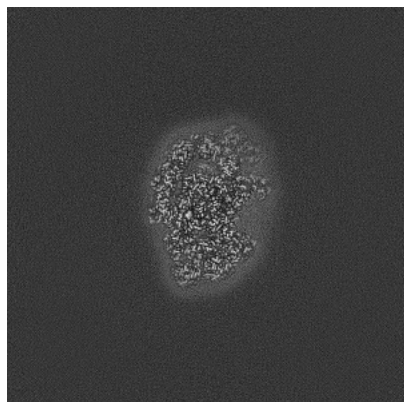


Y Index: 263

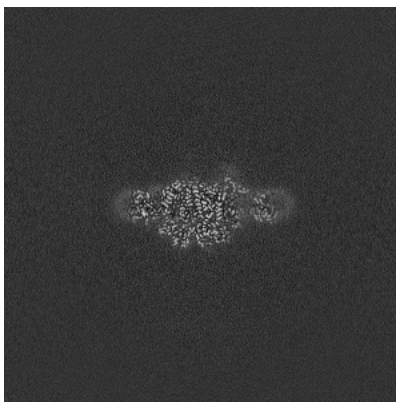


Z Index: 256

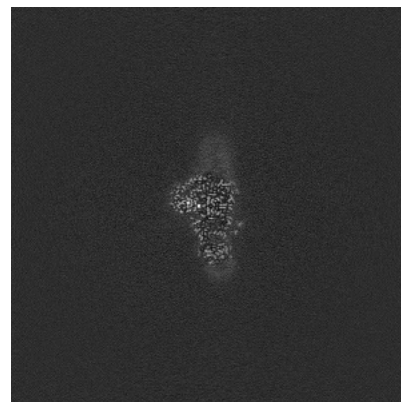
6.3.2 Raw map



X Index: 248



Y Index: 263

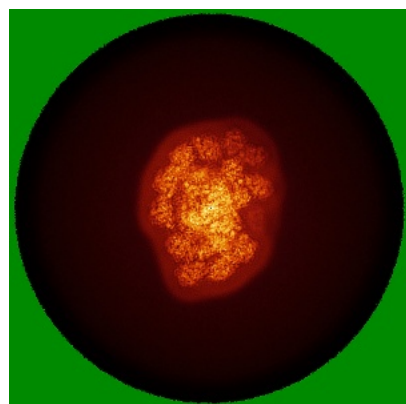


Z Index: 256

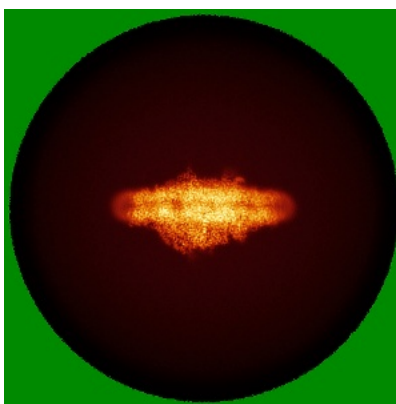
The images above show the largest variance slices of the map in three orthogonal directions.

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

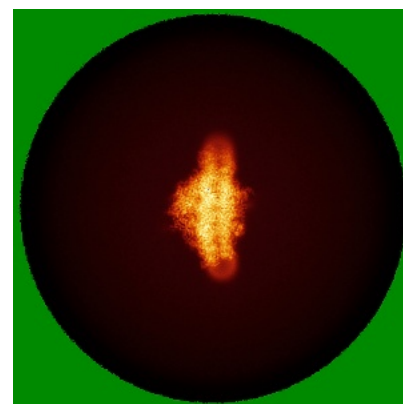
6.4.1 Primary map



X

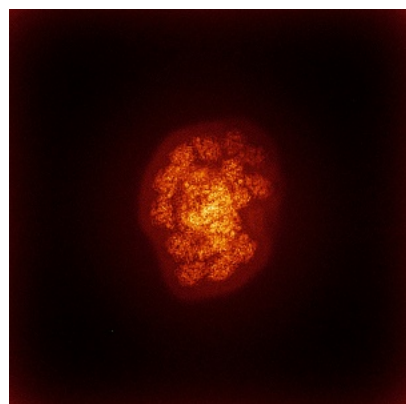


Y

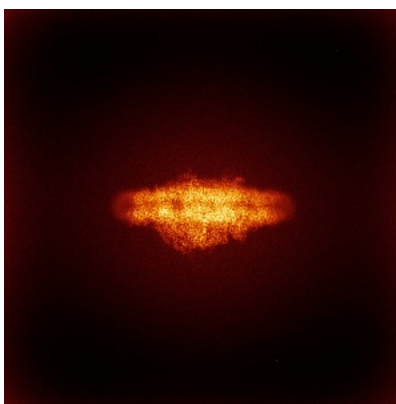


Z

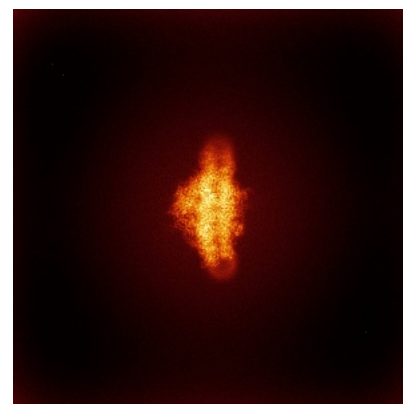
6.4.2 Raw map



X



Y

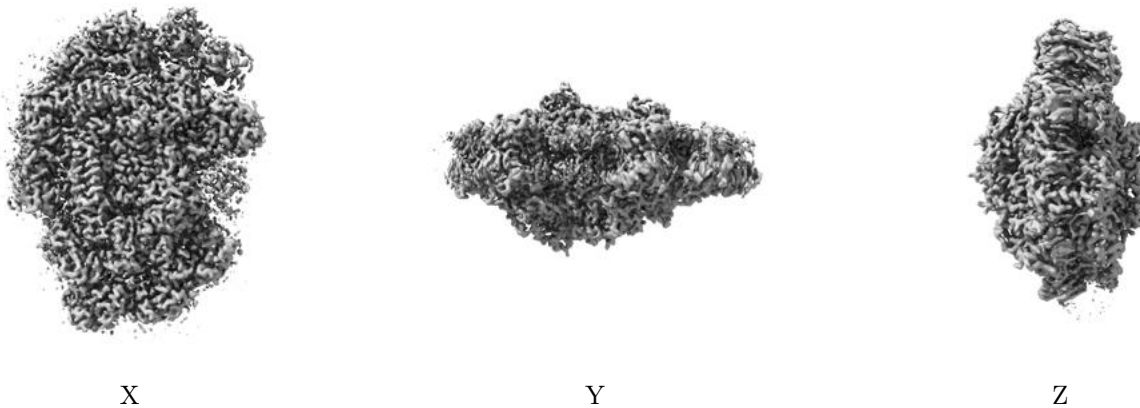


Z

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.

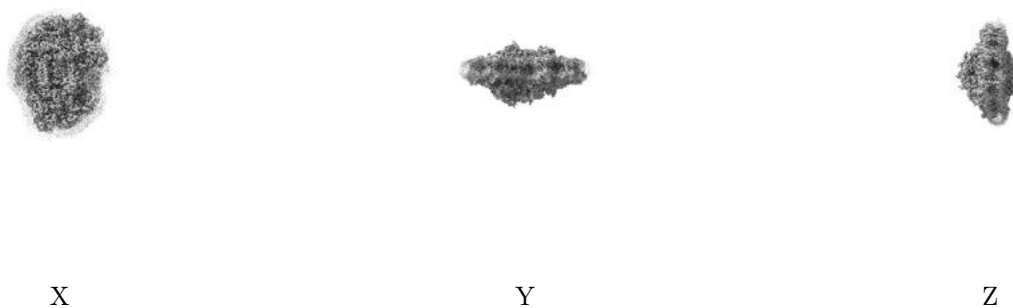
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. 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.

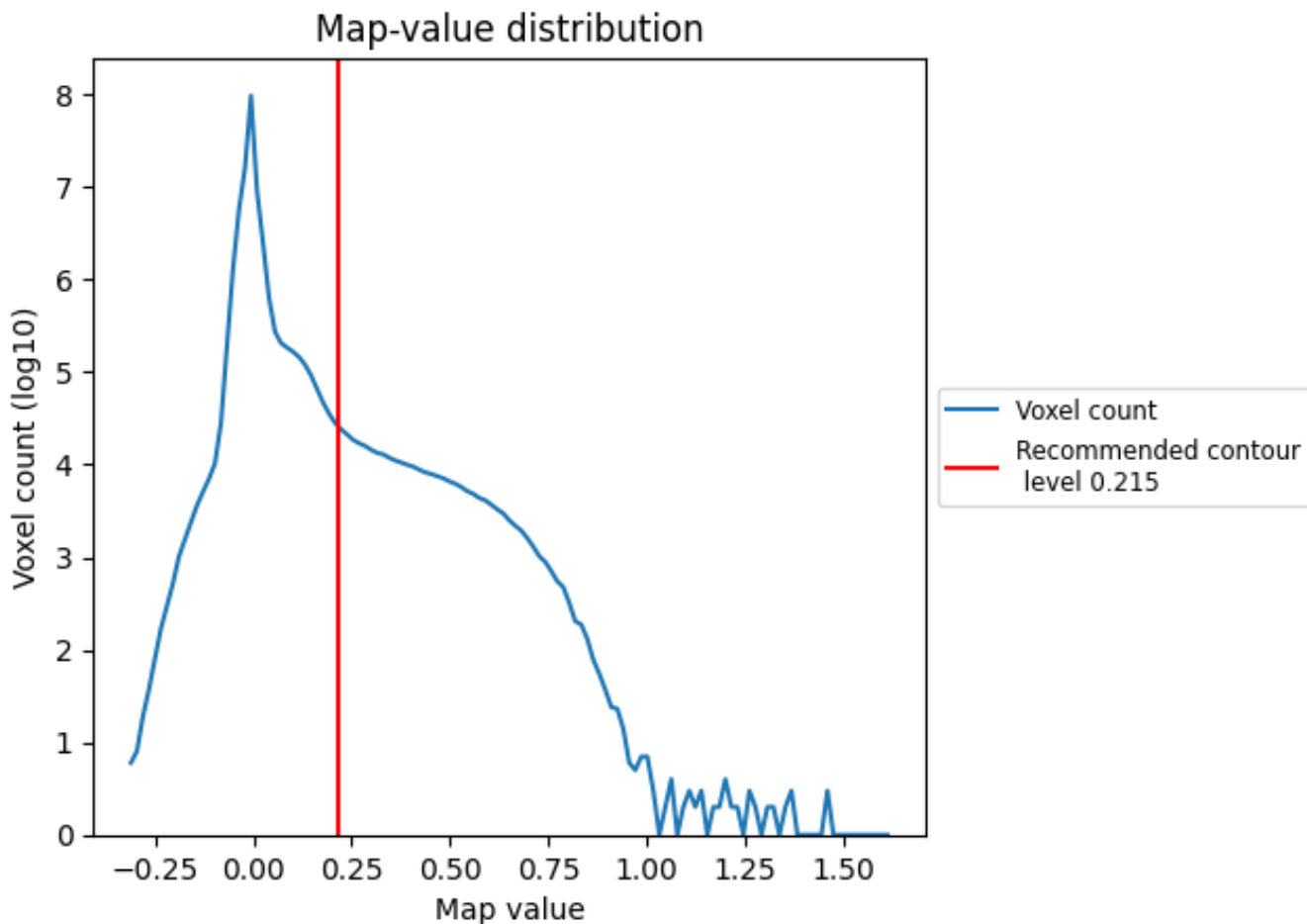
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

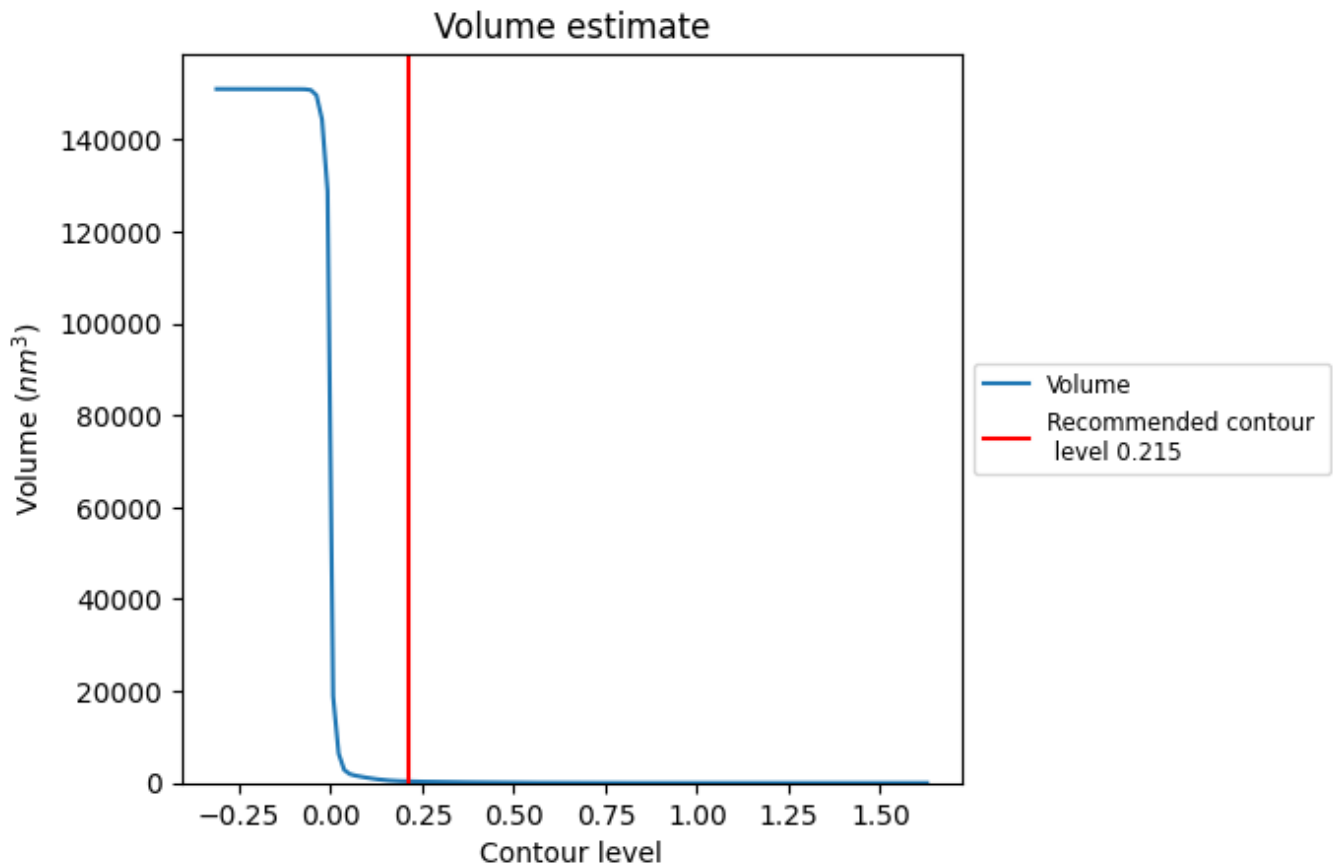
This section contains the results of statistical analysis of the map.

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.

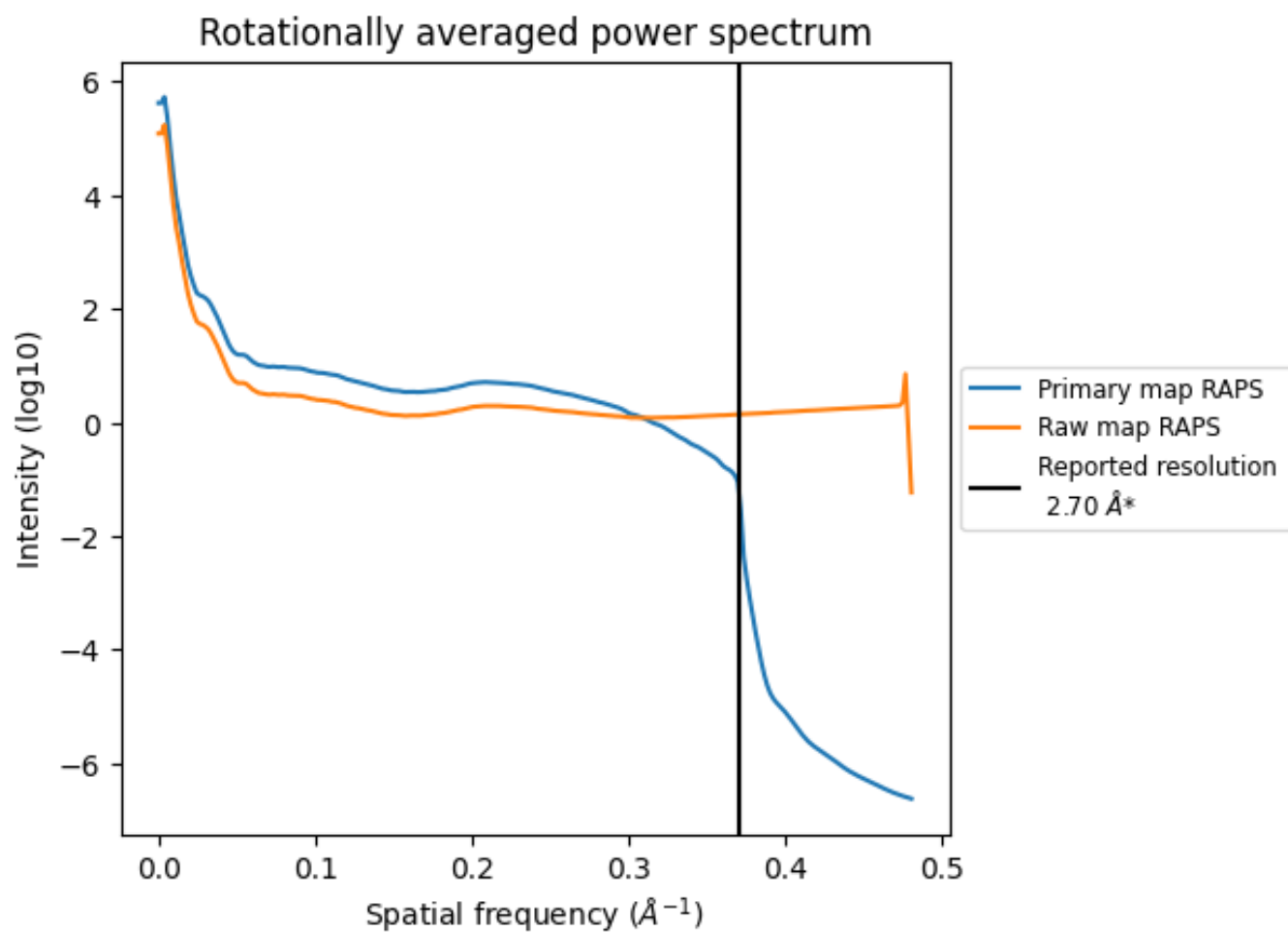
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 344 nm^3 ; this corresponds to an approximate mass of 311 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

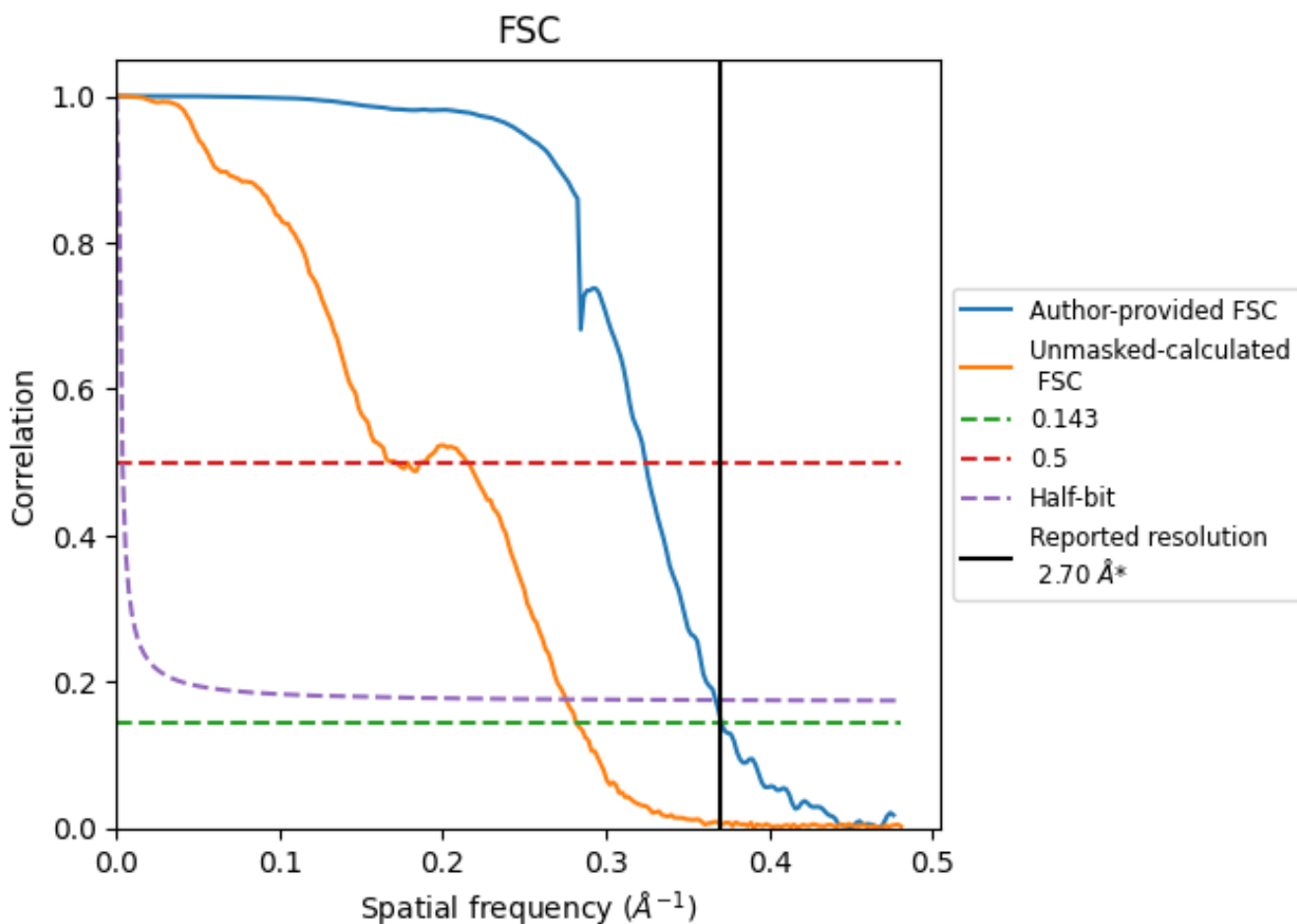


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

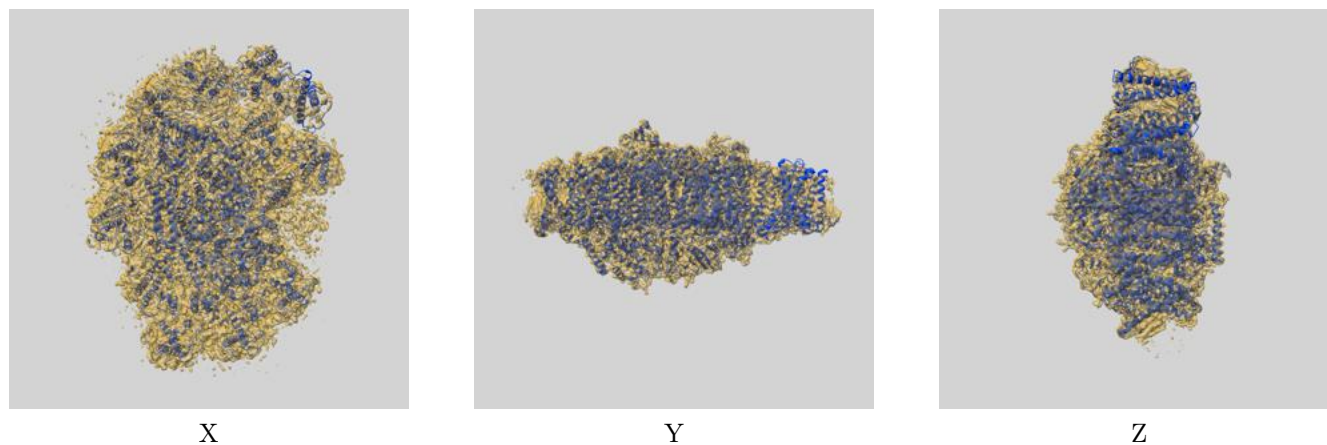
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.09	2.72
Unmasked-calculated*	3.55	5.84	3.63

*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 3.55 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

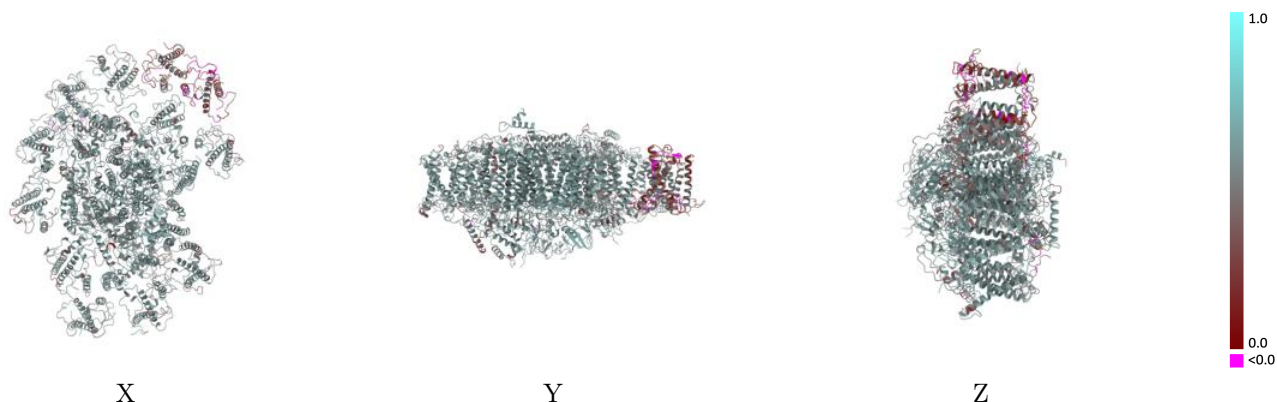
This section contains information regarding the fit between EMDB map EMD-36743 and PDB model 8JZF. Per-residue inclusion information can be found in section 3 on page 34.

9.1 Map-model overlay [i](#)



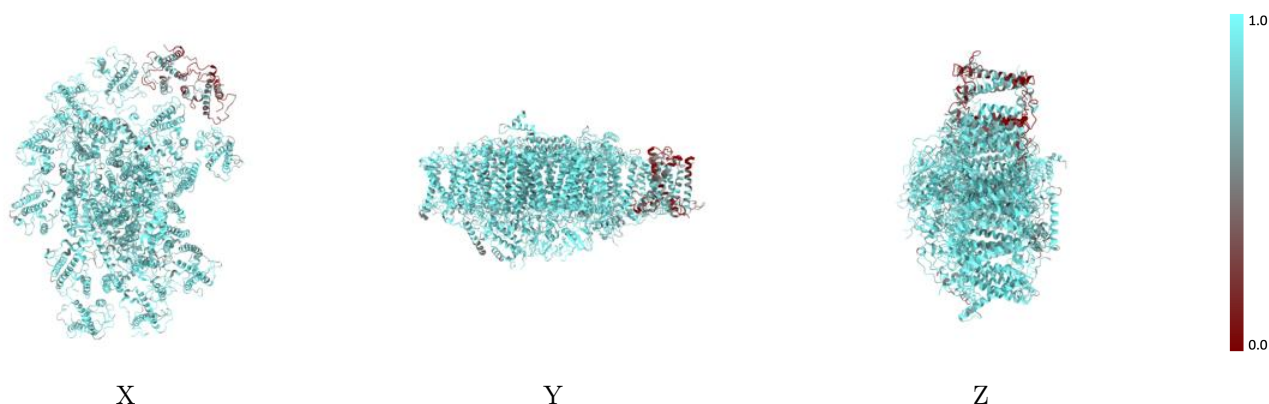
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



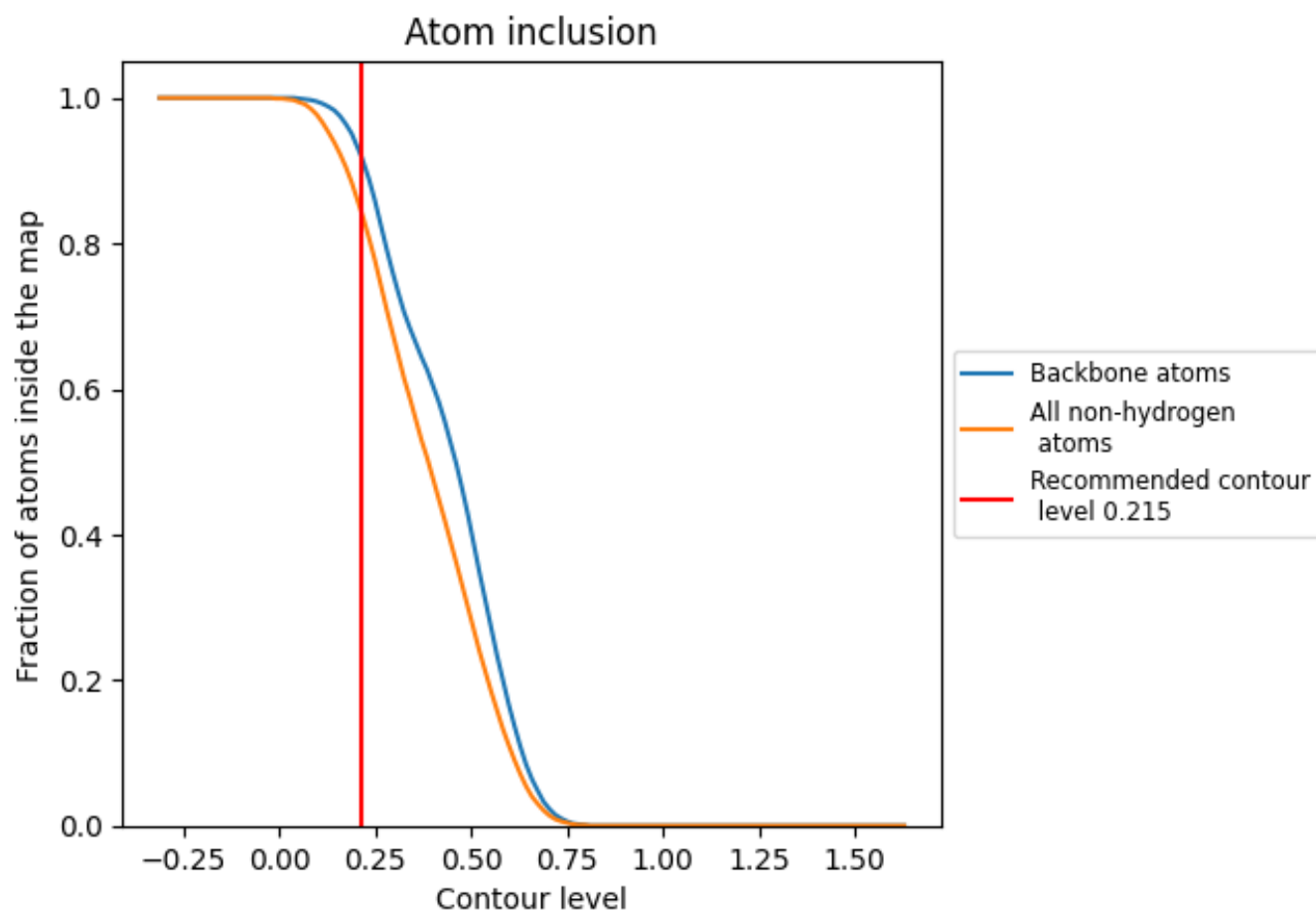
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.215).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5370
A	 0.8820	 0.5560
B	 0.8450	 0.5390
D	 0.8150	 0.5140
F	 0.7870	 0.5140
G	 0.8470	 0.5260
H	 0.3050	 0.2360
I	 0.8220	 0.5280
J	 0.8630	 0.5390
K	 0.8900	 0.5620
L	 0.8750	 0.5590
M	 0.8060	 0.5270
N	 0.4790	 0.3450
a	 0.8860	 0.5680
b	 0.9240	 0.5820
c	 0.9440	 0.5790
d	 0.8820	 0.5540
e	 0.9230	 0.5830
f	 0.8710	 0.5580
h	 0.9130	 0.5770
i	 0.8730	 0.5480
j	 0.8130	 0.5390
l	 0.9020	 0.5690
m	 0.8750	 0.5550
y	 0.8730	 0.5410
z	 0.9050	 0.5070

