



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:19 AM UTC

PDB ID : 9LUU / pdb_00009luu
EMDB ID : EMD-63405
Title : PSI-4 LHCI dimer supercomplex from M. polymorpha
Authors : Tsai, P.-C.; La Rocca, R.; Shen, J.-R.; Akita, F.
Deposited on : 2025-02-10
Resolution : 2.52 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:

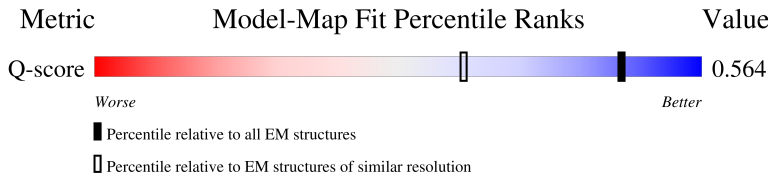
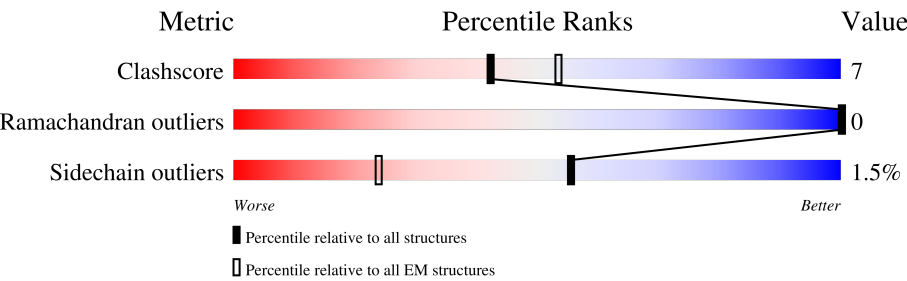
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.52 Å.

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






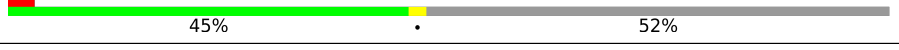


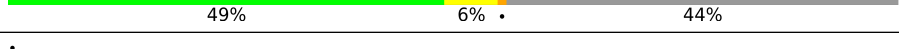
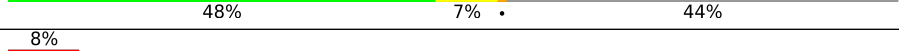
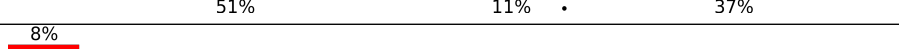
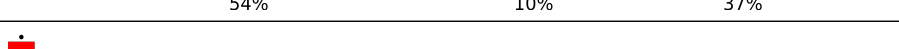
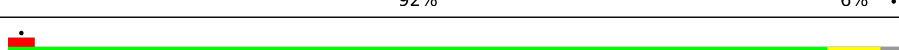
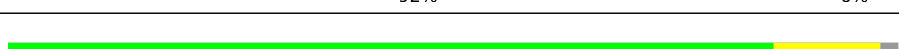
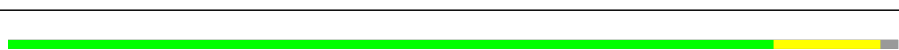

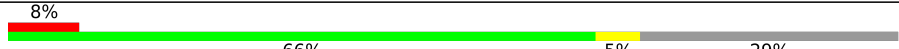





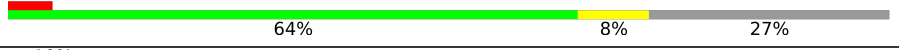
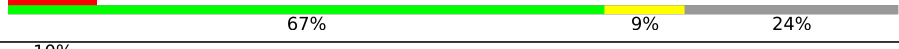



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

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	B	734	90% 10%
1	b	734	91% 9%
2	C	81	89% 10% .
2	c	81	89% 10% .






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Mol	Chain	Length	Quality of chain
3	D	215	
3	d	215	
4	E	132	
4	e	132	
5	F	246	
5	f	246	
6	G	161	
6	g	161	
7	H	142	
7	h	142	
8	I	36	
8	i	36	
9	J	42	
9	j	42	
10	L	221	
10	l	221	
11	M	32	
11	m	32	
12	A	750	
12	a	750	
13	2a	267	
13	2b	267	
14	3a	279	
14	3b	279	
15	5a	249	

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Mol	Chain	Length	Quality of chain
15	5b	249	
16	6a	243	
16	6b	243	
17	K	135	
17	k	135	

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
18	CLA	2a	301	X	-	-	-
18	CLA	2a	302	X	-	-	-
18	CLA	2a	303	X	-	-	-
18	CLA	2a	307	X	-	-	-
18	CLA	2a	308	X	-	-	-
18	CLA	2a	309	X	-	-	-
18	CLA	2a	310	X	-	-	-
18	CLA	2a	312	X	-	-	-
18	CLA	2b	301	X	-	-	-
18	CLA	2b	302	X	-	-	-
18	CLA	2b	303	X	-	-	-
18	CLA	2b	307	X	-	-	-
18	CLA	2b	308	X	-	-	-
18	CLA	2b	309	X	-	-	-
18	CLA	2b	310	X	-	-	-
18	CLA	2b	312	X	-	-	-
18	CLA	3a	303	X	-	-	-
18	CLA	3a	304	X	-	-	-
18	CLA	3a	306	X	-	-	-
18	CLA	3a	308	X	-	-	-
18	CLA	3a	310	X	-	-	-
18	CLA	3a	311	X	-	-	-
18	CLA	3a	313	X	-	-	-
18	CLA	3a	314	X	-	-	-
18	CLA	3b	303	X	-	-	-
18	CLA	3b	304	X	-	-	-
18	CLA	3b	306	X	-	-	-
18	CLA	3b	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3b	310	X	-	-	-
18	CLA	3b	311	X	-	-	-
18	CLA	3b	313	X	-	-	-
18	CLA	3b	314	X	-	-	-
18	CLA	5a	303	X	-	-	-
18	CLA	5a	308	X	-	-	-
18	CLA	5a	310	X	-	-	-
18	CLA	5a	311	X	-	-	-
18	CLA	5a	313	X	-	-	-
18	CLA	5b	303	X	-	-	-
18	CLA	5b	308	X	-	-	-
18	CLA	5b	310	X	-	-	-
18	CLA	5b	311	X	-	-	-
18	CLA	5b	313	X	-	-	-
18	CLA	6a	306	X	-	-	-
18	CLA	6a	308	X	-	-	-
18	CLA	6a	310	X	-	-	-
18	CLA	6a	311	X	-	-	-
18	CLA	6a	313	X	-	-	-
18	CLA	6a	314	X	-	-	-
18	CLA	6a	315	X	-	-	-
18	CLA	6a	317	X	-	-	-
18	CLA	6b	306	X	-	-	-
18	CLA	6b	308	X	-	-	-
18	CLA	6b	310	X	-	-	-
18	CLA	6b	311	X	-	-	-
18	CLA	6b	313	X	-	-	-
18	CLA	6b	314	X	-	-	-
18	CLA	6b	315	X	-	-	-
18	CLA	6b	317	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	818	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	853	X	-	-	-
18	CLA	B	854	X	-	-	-
18	CLA	F	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	F	303	X	-	-	-
18	CLA	F	305	X	-	-	-
18	CLA	G	202	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	L	301	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	a	803	X	-	-	-
18	CLA	a	804	X	-	-	-
18	CLA	a	805	X	-	-	-
18	CLA	a	806	X	-	-	-
18	CLA	a	807	X	-	-	-
18	CLA	a	808	X	-	-	-
18	CLA	a	809	X	-	-	-
18	CLA	a	811	X	-	-	-
18	CLA	a	812	X	-	-	-
18	CLA	a	813	X	-	-	-
18	CLA	a	814	X	-	-	-
18	CLA	a	817	X	-	-	-
18	CLA	a	818	X	-	-	-
18	CLA	a	822	X	-	-	-
18	CLA	a	824	X	-	-	-
18	CLA	a	825	X	-	-	-
18	CLA	a	826	X	-	-	-
18	CLA	a	827	X	-	-	-
18	CLA	a	831	X	-	-	-
18	CLA	a	832	X	-	-	-
18	CLA	a	835	X	-	-	-
18	CLA	a	836	X	-	-	-
18	CLA	a	837	X	-	-	-
18	CLA	a	838	X	-	-	-
18	CLA	a	840	X	-	-	-
18	CLA	a	841	X	-	-	-
18	CLA	b	801	X	-	-	-
18	CLA	b	802	X	-	-	-
18	CLA	b	803	X	-	-	-
18	CLA	b	804	X	-	-	-
18	CLA	b	805	X	-	-	-
18	CLA	b	807	X	-	-	-
18	CLA	b	808	X	-	-	-
18	CLA	b	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	b	812	X	-	-	-
18	CLA	b	816	X	-	-	-
18	CLA	b	817	X	-	-	-
18	CLA	b	819	X	-	-	-
18	CLA	b	821	X	-	-	-
18	CLA	b	823	X	-	-	-
18	CLA	b	824	X	-	-	-
18	CLA	b	825	X	-	-	-
18	CLA	b	826	X	-	-	-
18	CLA	b	830	X	-	-	-
18	CLA	b	831	X	-	-	-
18	CLA	b	833	X	-	-	-
18	CLA	b	834	X	-	-	-
18	CLA	b	835	X	-	-	-
18	CLA	b	836	X	-	-	-
18	CLA	b	837	X	-	-	-
18	CLA	b	840	X	-	-	-
18	CLA	b	853	X	-	-	-
18	CLA	b	854	X	-	-	-
18	CLA	f	302	X	-	-	-
18	CLA	f	303	X	-	-	-
18	CLA	f	305	X	-	-	-
18	CLA	g	202	X	-	-	-
18	CLA	g	203	X	-	-	-
18	CLA	j	101	X	-	-	-
18	CLA	k	201	X	-	-	-
18	CLA	l	301	X	-	-	-
18	CLA	l	303	X	-	-	-
29	CHL	2a	304	X	-	-	-
29	CHL	2a	305	X	-	-	-
29	CHL	2a	306	X	-	-	-
29	CHL	2a	313	X	-	-	-
29	CHL	2b	304	X	-	-	-
29	CHL	2b	305	X	-	-	-
29	CHL	2b	306	X	-	-	-
29	CHL	2b	313	X	-	-	-
29	CHL	3a	301	X	-	-	-
29	CHL	3a	307	X	-	-	-
29	CHL	3a	315	X	-	-	-
29	CHL	3b	301	X	-	-	-
29	CHL	3b	307	X	-	-	-
29	CHL	3b	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	5a	301	X	-	-	-
29	CHL	5a	305	X	-	-	-
29	CHL	5a	306	X	-	-	-
29	CHL	5a	307	X	-	-	-
29	CHL	5a	314	X	-	-	-
29	CHL	5b	301	X	-	-	-
29	CHL	5b	305	X	-	-	-
29	CHL	5b	306	X	-	-	-
29	CHL	5b	307	X	-	-	-
29	CHL	5b	314	X	-	-	-
29	CHL	6a	304	X	-	-	-
29	CHL	6a	309	X	-	-	-
29	CHL	6b	304	X	-	-	-
29	CHL	6b	309	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 70242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		
1	b	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	80	Total	C	N	O	S	0	0
			602	368	104	119	11		
2	c	80	Total	C	N	O	S	0	0
			602	368	104	119	11		

- Molecule 3 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	140	Total	C	N	O	S	0	0
			1094	706	189	196	3		
3	d	140	Total	C	N	O	S	0	0
			1094	706	189	196	3		

- Molecule 4 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	63	Total	C	N	O	S	0	0
			495	314	85	94	2		
4	e	63	Total	C	N	O	S	0	0
			495	314	85	94	2		

- Molecule 5 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		
5	f	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		

- Molecule 6 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	90	Total	C	N	O	S	0	0
			673	432	117	123	1		
6	g	90	Total	C	N	O	S	0	0
			673	432	117	123	1		

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	90	Total	C	N	O	S	0	0
			680	438	113	127	2		
7	h	90	Total	C	N	O	S	0	0
			680	438	113	127	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			274	187	36	49	2		
8	i	35	Total	C	N	O	S	0	0
			274	187	36	49	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			328	225	48	54	1		
9	j	41	Total	C	N	O	S	0	0
			328	225	48	54	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	158	Total	C	N	O	S	0	0
			1180	781	188	209	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	158	Total	C	N	O	S	0	0
			1180	781	188	209	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O		0	0
			242	159	37	46			
11	m	31	Total	C	N	O		0	0
			242	159	37	46			

- Molecule 12 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	737	Total	C	N	O	S	0	0
			5810	3818	983	992	17		
12	a	737	Total	C	N	O	S	0	0
			5810	3818	983	992	17		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2a	194	Total	C	N	O	S	0	0
			1520	1003	245	267	5		
13	2b	194	Total	C	N	O	S	0	0
			1520	1003	245	267	5		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3a	212	Total	C	N	O	S	0	0
			1633	1072	261	294	6		
14	3b	212	Total	C	N	O	S	0	0
			1633	1072	261	294	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5a	193	Total	C	N	O	S	0	0
			1516	1001	242	269	4		
15	5b	193	Total	C	N	O	S	0	0
			1516	1001	242	269	4		

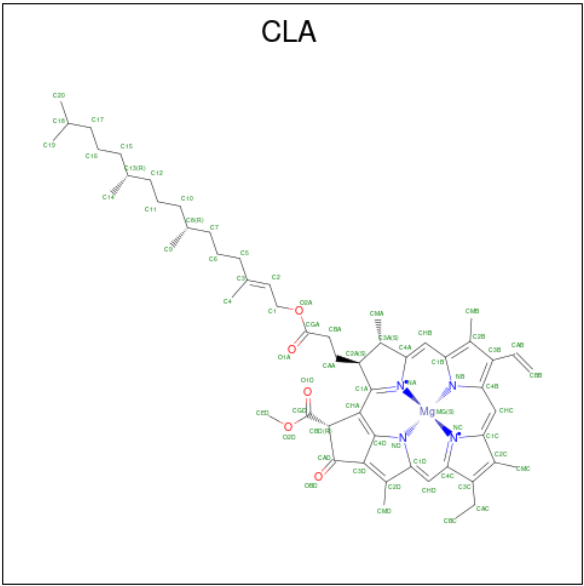
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6a	193	Total	C	N	O	S	0	0
			1491	973	249	266	3		
16	6b	193	Total	C	N	O	S	0	0
			1491	973	249	266	3		

- Molecule 17 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	64	Total	C	N	O	S	0	0
			441	280	73	84	4		
17	k	64	Total	C	N	O	S	0	0
			441	280	73	84	4		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	f	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	l	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	3a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	5a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	5a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	5a	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	5a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5a	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	6a	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6a	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	a	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	2b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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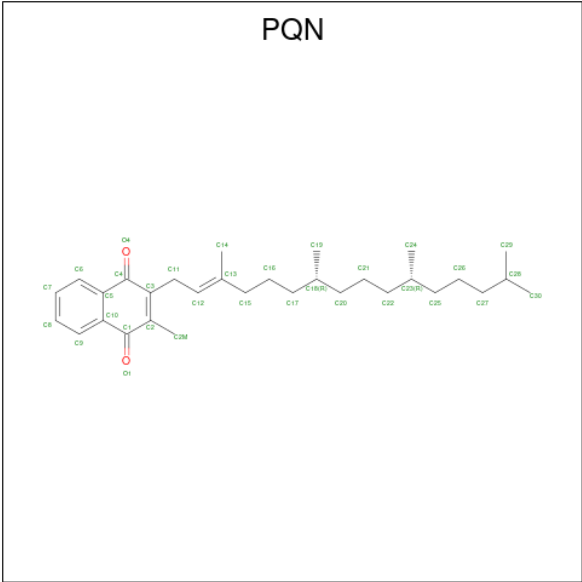
Mol	Chain	Residues	Atoms					AltConf
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3b	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	3b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3b	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	3b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	5b	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	5b	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	5b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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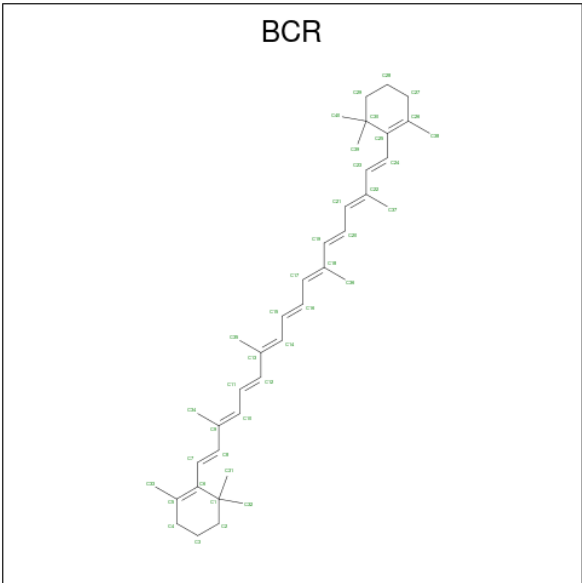
Mol	Chain	Residues	Atoms					AltConf
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	k	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			33	31	2	
19	b	1	Total	C	O	0
			33	31	2	
19	A	1	Total	C	O	0
			33	31	2	
19	a	1	Total	C	O	0
			33	31	2	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



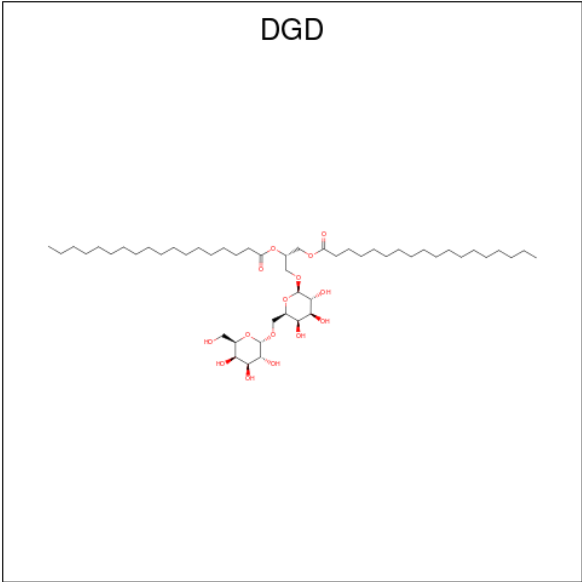
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	G	1	Total C 40 40	0
20	G	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	M	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0

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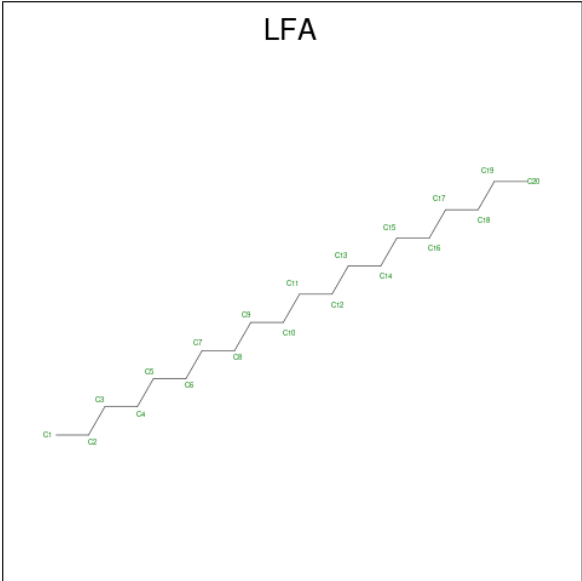
Mol	Chain	Residues	Atoms	AltConf
20	f	1	Total C 40 40	0
20	f	1	Total C 40 40	0
20	g	1	Total C 40 40	0
20	g	1	Total C 40 40	0
20	i	1	Total C 40 40	0
20	j	1	Total C 40 40	0
20	l	1	Total C 40 40	0
20	m	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	k	1	Total C 40 40	0

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			59	44	15	
21	b	1	Total	C	O	0
			59	44	15	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂) (labeled as "Ligand of Interest" by depositor).



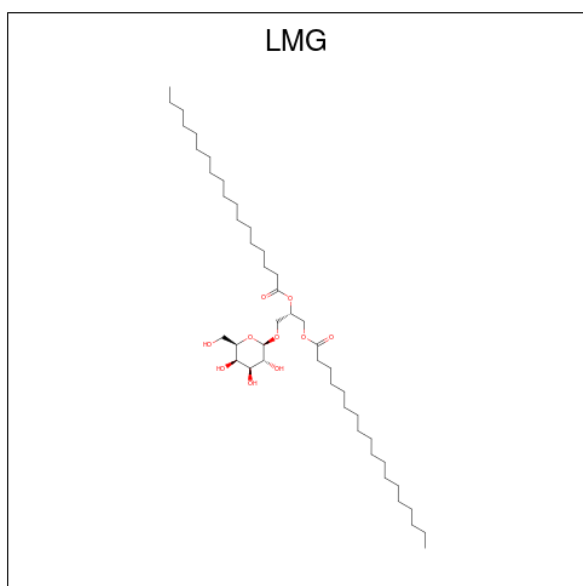
Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			12	12	

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Mol	Chain	Residues	Atoms		AltConf
22	M	1	Total	C	0
			12	12	
22	b	1	Total	C	0
			12	12	
22	m	1	Total	C	0
			12	12	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



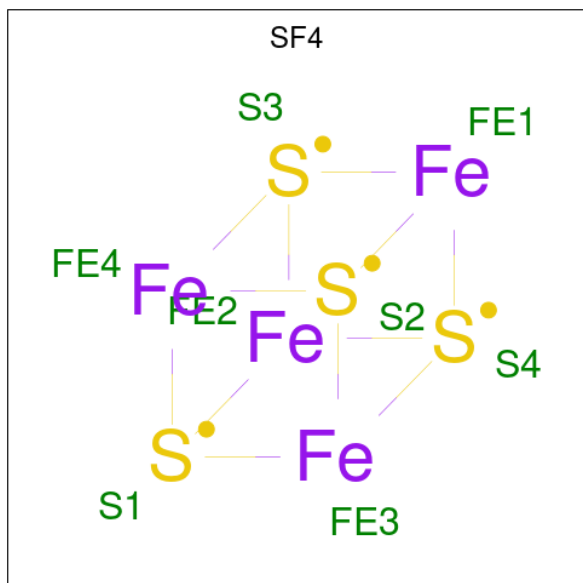
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			42	32	10	
23	I	1	Total	C	O	0
			31	21	10	
23	J	1	Total	C	O	0
			30	20	10	
23	J	1	Total	C	O	0
			41	31	10	
23	b	1	Total	C	O	0
			42	32	10	
23	i	1	Total	C	O	0
			31	21	10	
23	j	1	Total	C	O	0
			30	20	10	
23	j	1	Total	C	O	0
			41	31	10	

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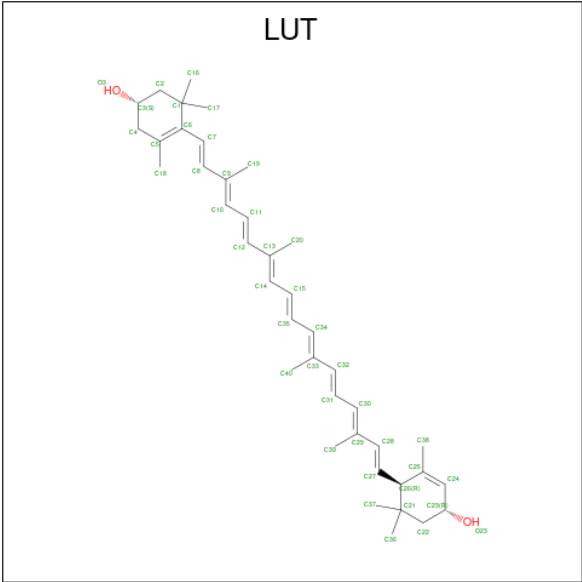
Mol	Chain	Residues	Atoms			AltConf
23	5a	1	Total	C	O	0
			35	25	10	
23	5b	1	Total	C	O	0
			35	25	10	

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total	Fe	S	0
			8	4	4	
24	C	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	A	1	Total	Fe	S	0
			8	4	4	
24	a	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $\text{C}_{40}\text{H}_{56}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



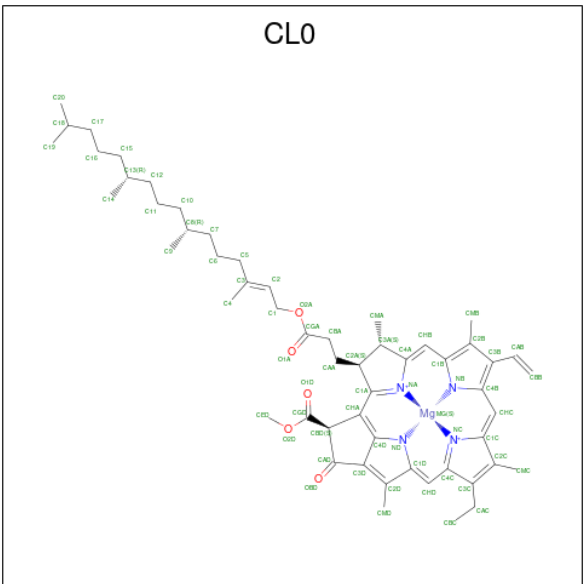
Mol	Chain	Residues	Atoms			AltConf
25	J	1	Total	C	O	0
			42	40	2	
25	j	1	Total	C	O	0
			42	40	2	
25	2a	1	Total	C	O	0
			42	40	2	
25	2a	1	Total	C	O	0
			42	40	2	
25	3a	1	Total	C	O	0
			42	40	2	
25	3a	1	Total	C	O	0
			42	40	2	
25	5a	1	Total	C	O	0
			42	40	2	
25	5a	1	Total	C	O	0
			42	40	2	
25	6a	1	Total	C	O	0
			42	40	2	
25	6a	1	Total	C	O	0
			42	40	2	
25	2b	1	Total	C	O	0
			42	40	2	
25	2b	1	Total	C	O	0
			42	40	2	
25	3b	1	Total	C	O	0
			42	40	2	

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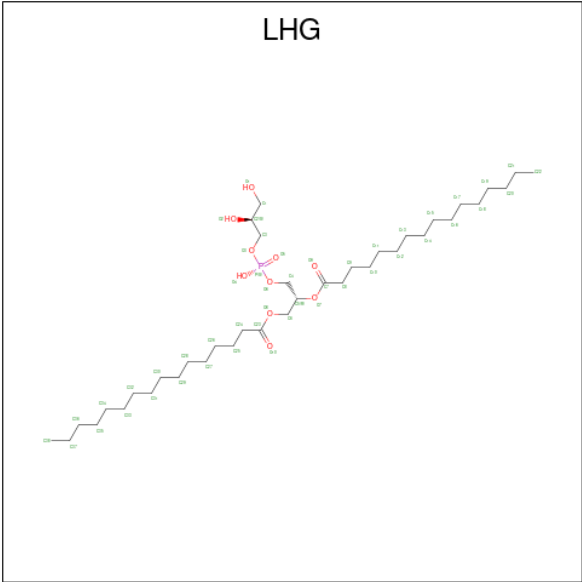
Mol	Chain	Residues	Atoms			AltConf
25	3b	1	Total	C	O	0
			42	40	2	
25	5b	1	Total	C	O	0
			42	40	2	
25	5b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	
25	6b	1	Total	C	O	0
			42	40	2	

- Molecule 26 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

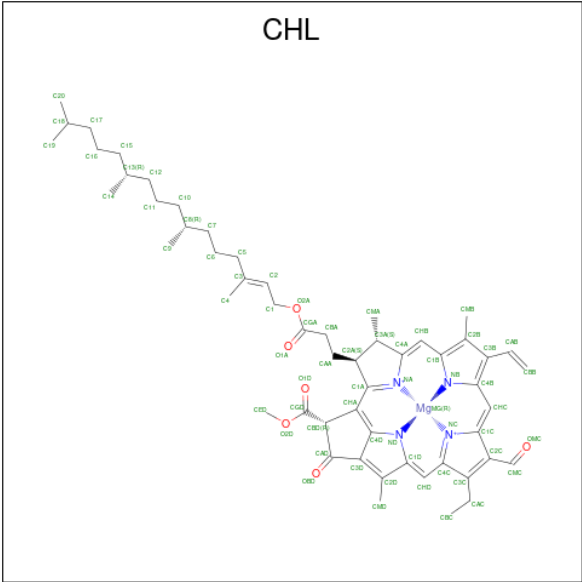


Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			34	23	10	1	
27	2a	1	Total	C	O	P	0
			32	21	10	1	
27	5a	1	Total	C	O	P	0
			32	21	10	1	
27	5a	1	Total	C	O	P	0
			37	26	10	1	
27	6a	1	Total	C	O	P	0
			39	28	10	1	
27	a	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			34	23	10	1	
27	2b	1	Total	C	O	P	0
			32	21	10	1	
27	5b	1	Total	C	O	P	0
			32	21	10	1	
27	5b	1	Total	C	O	P	0
			37	26	10	1	
27	6b	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	2a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	2a	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	2a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	2a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	3a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5a	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	5a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5a	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	6a	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6a	1	Total 41	C 32	Mg 1	N 4	O 4	0

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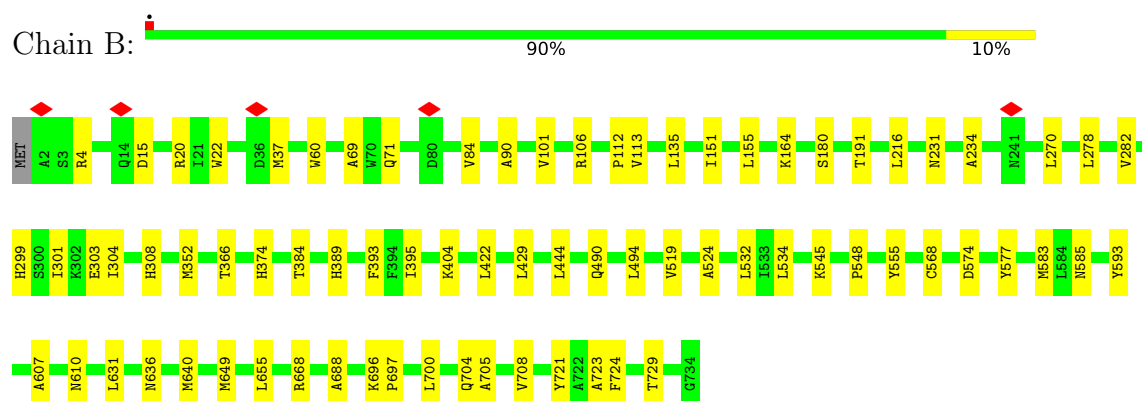
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Mol	Chain	Residues	Atoms					AltConf
29	2b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2b	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	2b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	3b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	3b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	3b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5b	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	5b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5b	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6b	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

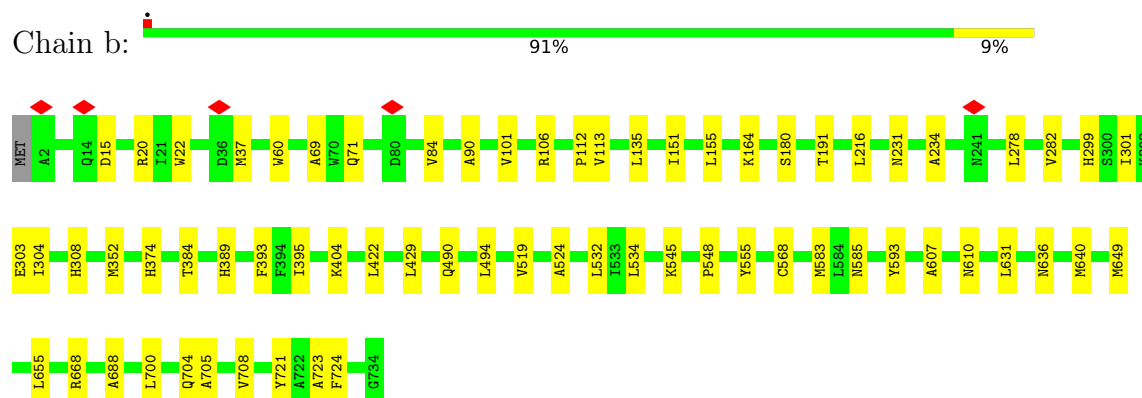
3 Residue-property plots [i](#)

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.

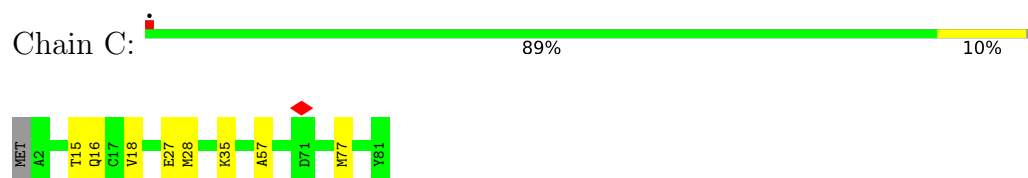
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I iron-sulfur center



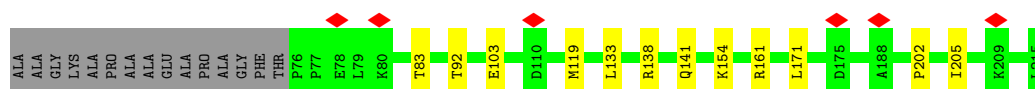
- Molecule 2: Photosystem I iron-sulfur center



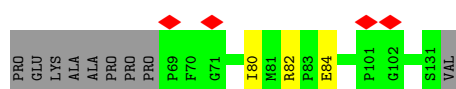
- Molecule 3: Photosystem I reaction center subunit II, chloroplastic



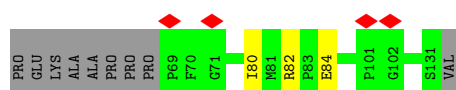
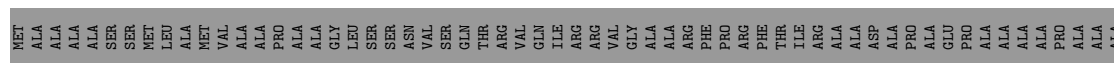
- Molecule 3: Photosystem I reaction center subunit II, chloroplastic



- Molecule 4: Photosystem I reaction centre subunit IV

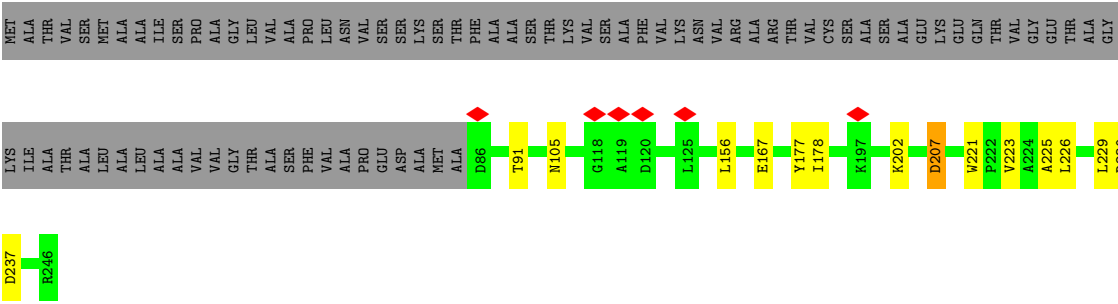


- Molecule 4: Photosystem I reaction centre subunit IV

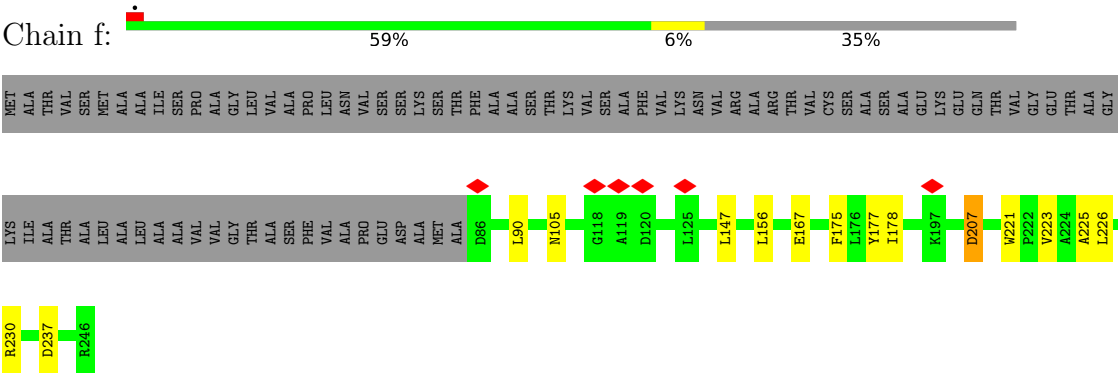


- Molecule 5: Photosystem I reaction center subunit III

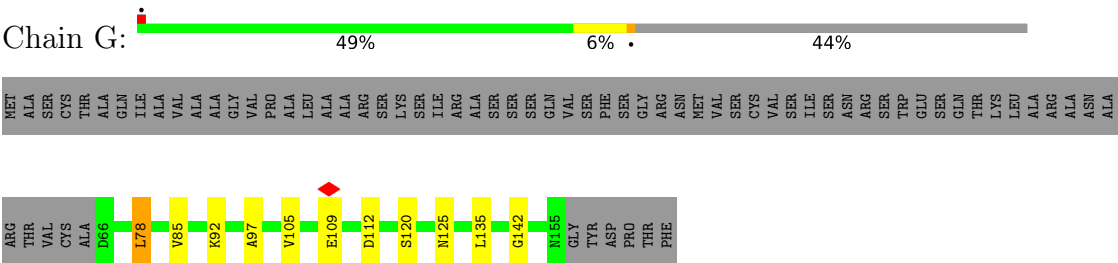




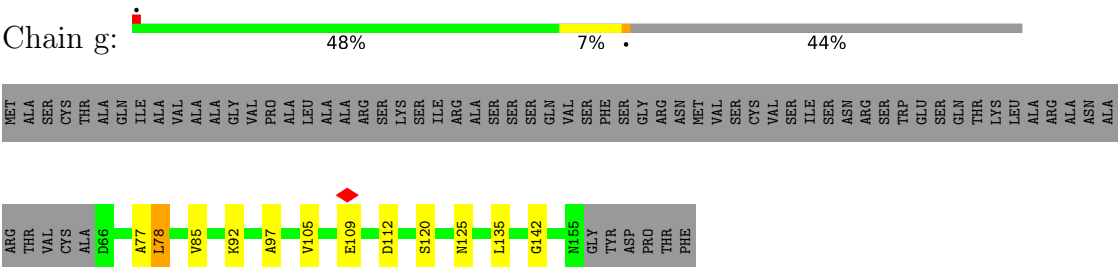
• Molecule 5: Photosystem I reaction center subunit III



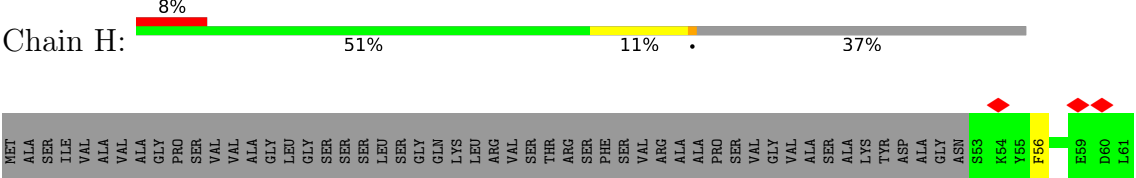
• Molecule 6: Photosystem I reaction center subunit V, chloroplastic

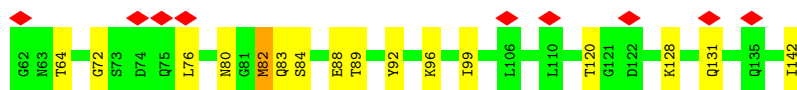


• Molecule 6: Photosystem I reaction center subunit V, chloroplastic

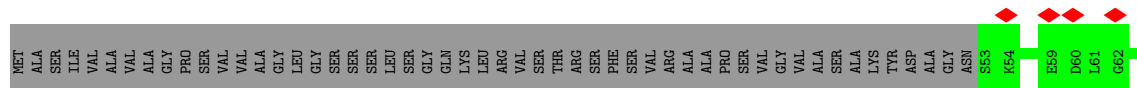


• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic

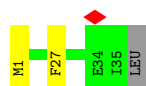




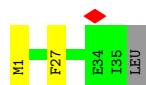
- Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



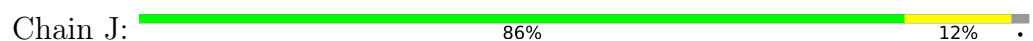
- Molecule 8: Photosystem I reaction center subunit VIII



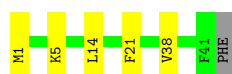
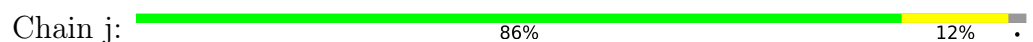
- Molecule 8: Photosystem I reaction center subunit VIII



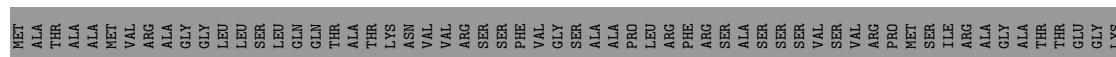
- Molecule 9: Photosystem I reaction center subunit IX

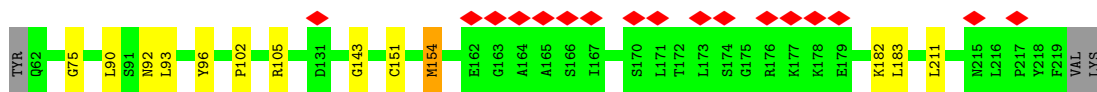


- Molecule 9: Photosystem I reaction center subunit IX

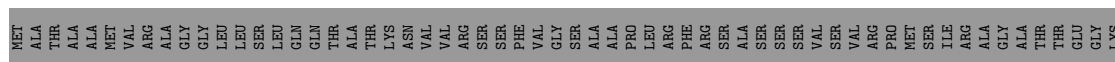


- Molecule 10: PSI subunit V

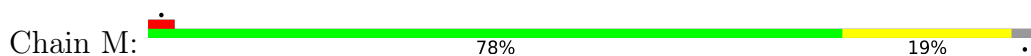




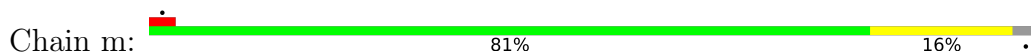
• Molecule 10: PSI subunit V



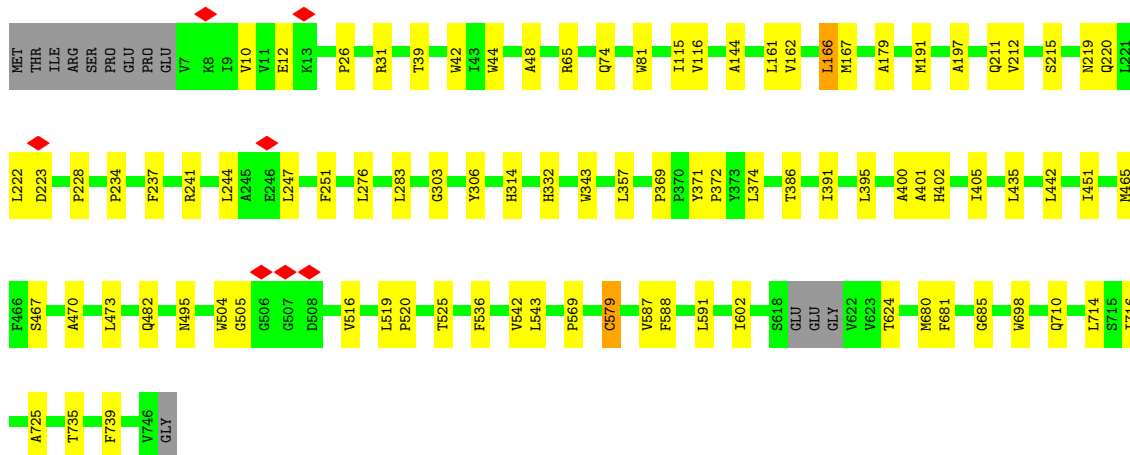
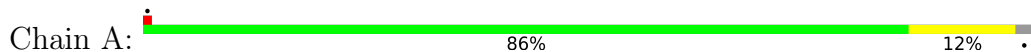
• Molecule 11: Photosystem I reaction center subunit XII



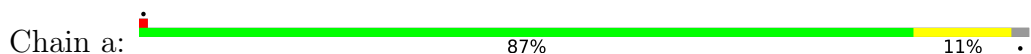
• Molecule 11: Photosystem I reaction center subunit XII

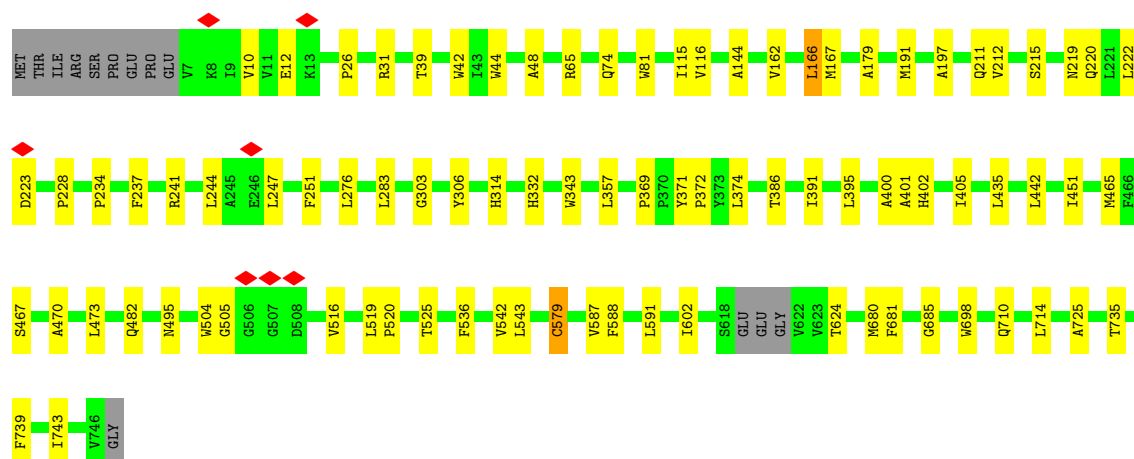


• Molecule 12: Photosystem I P700 chlorophyll a apoprotein A1

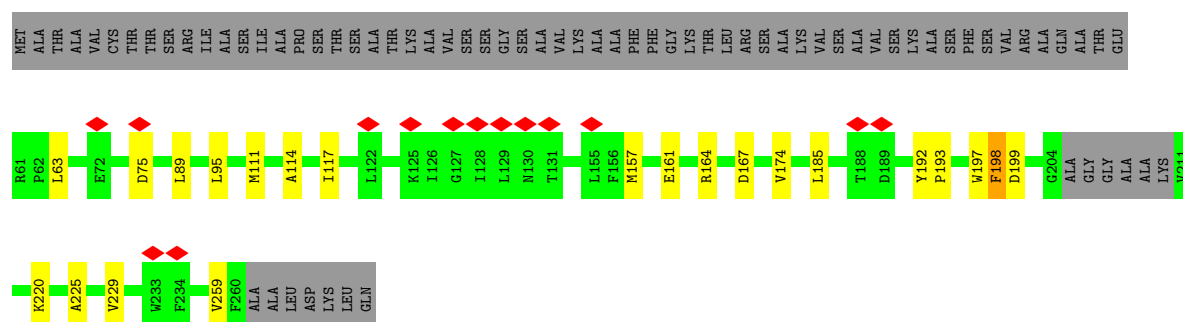


• Molecule 12: Photosystem I P700 chlorophyll a apoprotein A1

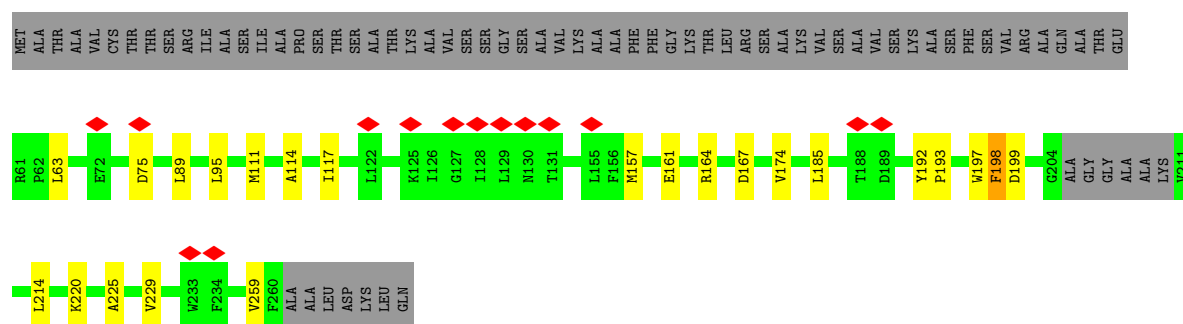




- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

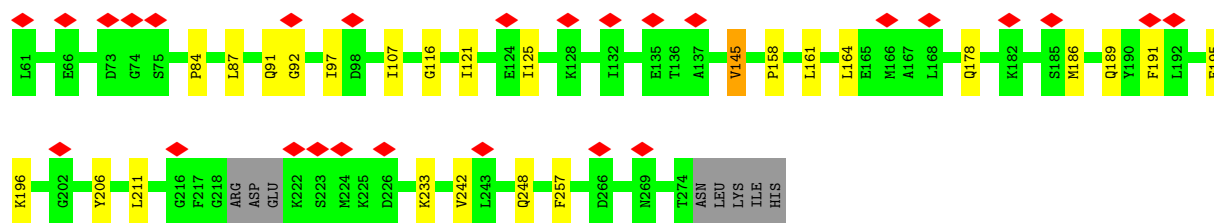


- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

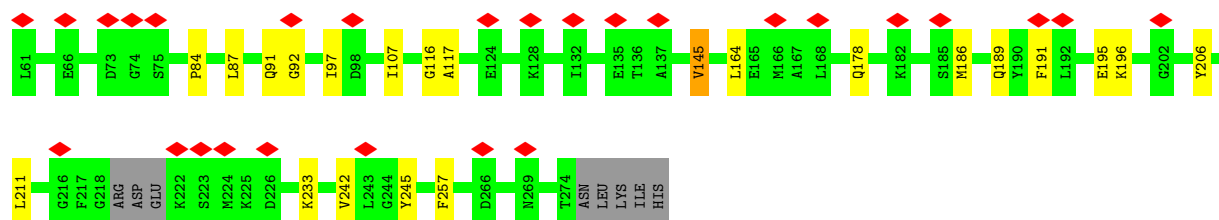


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

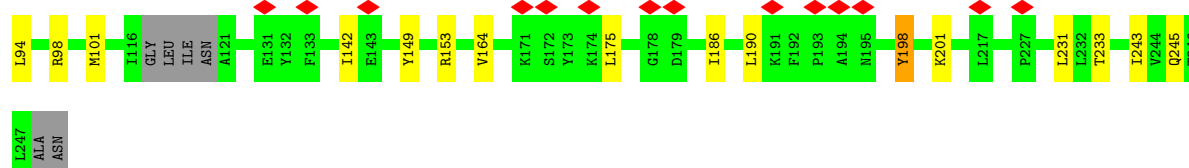
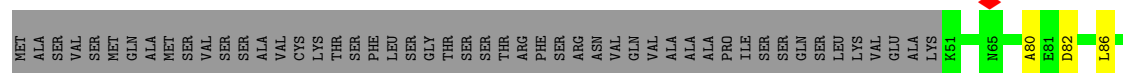
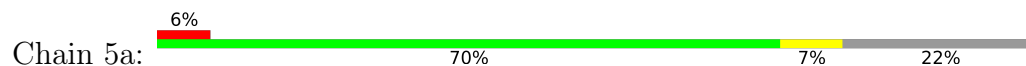




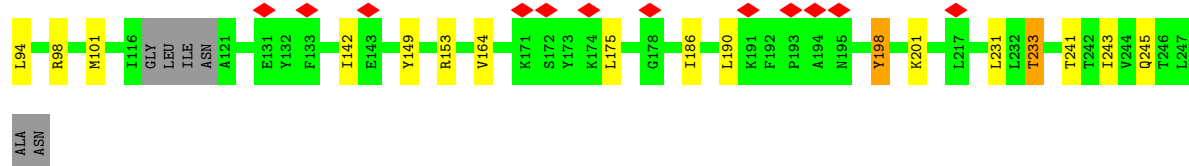
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



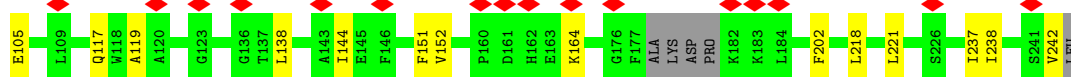
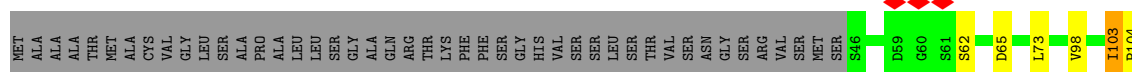
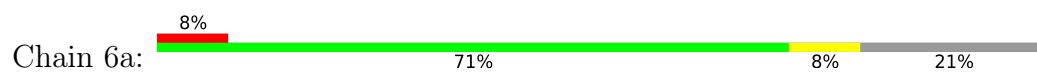
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



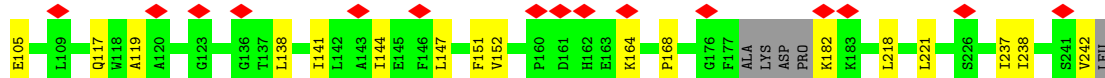
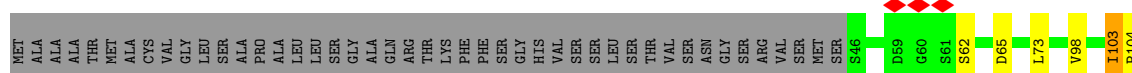
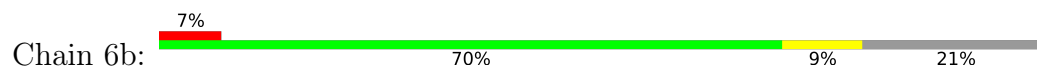
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



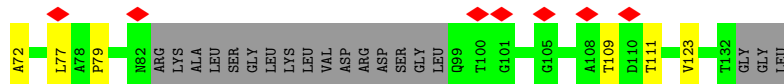
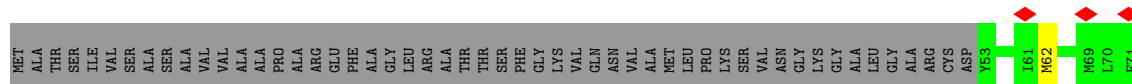
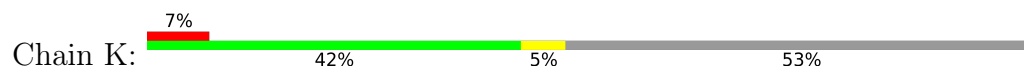
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



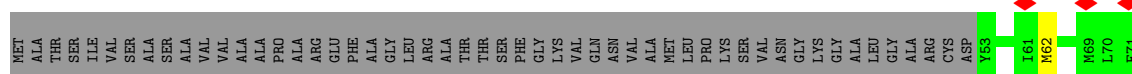
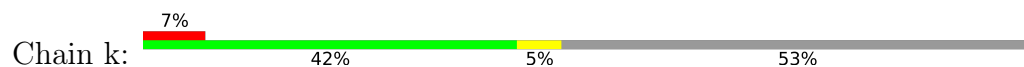
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: PSI-K



- Molecule 17: PSI-K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	465.28, 465.28, 465.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, DGD, CHL, SF4, LMU, LMG, LUT, CLA, LFA, BCR, LHG, CLO

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	B	0.21	0/6066	0.44	0/8277
1	b	0.21	0/6066	0.44	0/8277
2	C	0.23	0/612	0.56	0/829
2	c	0.23	0/612	0.56	0/829
3	D	0.21	0/1122	0.56	0/1511
3	d	0.21	0/1122	0.56	0/1511
4	E	0.21	0/508	0.49	0/691
4	e	0.22	0/508	0.49	0/691
5	F	0.21	0/1275	0.47	2/1725 (0.1%)
5	f	0.21	0/1275	0.47	2/1725 (0.1%)
6	G	0.25	0/686	0.51	0/931
6	g	0.26	0/686	0.51	0/931
7	H	0.22	0/696	0.55	0/939
7	h	0.22	0/696	0.55	0/939
8	I	0.31	0/281	0.70	0/384
8	i	0.31	0/281	0.70	0/384
9	J	0.24	0/338	0.57	0/462
9	j	0.24	0/338	0.57	0/462
10	L	0.23	0/1215	0.58	0/1660
10	l	0.23	0/1215	0.58	0/1660
11	M	0.30	0/243	0.56	0/327
11	m	0.30	0/243	0.56	0/327
12	A	0.21	0/6007	0.46	2/8198 (0.0%)
12	a	0.21	0/6007	0.46	2/8198 (0.0%)
13	2a	0.21	0/1574	0.56	2/2151 (0.1%)
13	2b	0.21	0/1574	0.56	2/2151 (0.1%)
14	3a	0.24	0/1682	0.59	0/2281
14	3b	0.24	0/1682	0.59	0/2281
15	5a	0.19	0/1566	0.49	1/2137 (0.0%)
15	5b	0.19	0/1566	0.49	1/2137 (0.0%)
16	6a	0.22	0/1539	0.56	2/2100 (0.1%)
16	6b	0.23	0/1539	0.56	2/2100 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	K	0.26	0/446	0.58	0/604
17	k	0.26	0/446	0.58	0/604
All	All	0.22	0/51712	0.51	18/70414 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2a	198	PHE	CA-CB-CG	-6.88	106.92	113.80
13	2b	198	PHE	CA-CB-CG	-6.88	106.92	113.80
5	F	207	ASP	CA-C-N	6.41	124.28	120.24
5	F	207	ASP	C-N-CA	6.41	124.28	120.24
5	f	207	ASP	CA-C-N	6.41	124.28	120.24
5	f	207	ASP	C-N-CA	6.41	124.28	120.24
13	2b	199	ASP	CB-CA-C	6.32	117.95	109.42
13	2a	199	ASP	CB-CA-C	6.32	117.95	109.42
12	a	166	LEU	CA-CB-CG	5.50	135.53	116.30
12	A	166	LEU	CA-CB-CG	5.49	135.53	116.30
16	6b	164	LYS	CA-CB-CG	5.40	124.91	114.10
16	6a	164	LYS	CA-CB-CG	5.40	124.90	114.10
15	5b	245	GLN	CA-CB-CG	5.38	124.86	114.10
15	5a	245	GLN	CA-CB-CG	5.37	124.85	114.10
12	A	167	MET	CB-CG-SD	5.32	128.66	112.70
12	a	167	MET	CB-CG-SD	5.32	128.66	112.70
16	6a	103	ILE	CA-CB-CG1	5.07	119.02	110.40
16	6b	103	ILE	CA-CB-CG1	5.07	119.02	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5854	0	5632	55	0
1	b	5854	0	5632	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	602	0	575	6	0
2	c	602	0	575	6	0
3	D	1094	0	1113	6	0
3	d	1094	0	1113	7	0
4	E	495	0	481	2	0
4	e	495	0	481	2	0
5	F	1248	0	1291	10	0
5	f	1248	0	1291	11	0
6	G	673	0	678	17	0
6	g	673	0	678	18	0
7	H	680	0	680	20	0
7	h	680	0	680	18	0
8	I	274	0	285	2	0
8	i	274	0	285	2	0
9	J	328	0	339	3	0
9	j	328	0	339	3	0
10	L	1180	0	1186	12	0
10	l	1180	0	1186	12	0
11	M	242	0	266	6	0
11	m	242	0	266	5	0
12	A	5810	0	5687	61	0
12	a	5810	0	5687	59	0
13	2a	1520	0	1470	18	0
13	2b	1520	0	1470	18	0
14	3a	1633	0	1594	17	0
14	3b	1633	0	1594	14	0
15	5a	1516	0	1491	12	0
15	5b	1516	0	1491	13	0
16	6a	1491	0	1471	13	0
16	6b	1491	0	1471	16	0
17	K	441	0	446	4	0
17	k	441	0	446	4	0
18	2a	425	0	329	14	0
18	2b	425	0	329	14	0
18	3a	566	0	438	13	0
18	3b	566	0	438	11	0
18	5a	479	0	367	14	0
18	5b	479	0	367	14	0
18	6a	590	0	478	21	0
18	6b	590	0	478	22	0
18	A	2387	0	2303	72	0
18	B	2483	0	2431	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	146	0	121	6	0
18	G	95	0	72	4	0
18	J	45	0	33	2	0
18	K	44	0	30	0	0
18	L	147	0	123	5	0
18	a	2387	0	2303	72	0
18	b	2483	0	2431	84	0
18	f	146	0	121	6	0
18	g	95	0	72	4	0
18	j	45	0	33	2	0
18	k	44	0	30	0	0
18	l	147	0	123	5	0
19	A	33	0	46	1	0
19	B	33	0	46	3	0
19	a	33	0	46	1	0
19	b	33	0	46	3	0
20	A	200	0	280	15	0
20	B	280	0	392	19	0
20	F	80	0	112	3	0
20	G	80	0	112	5	0
20	I	40	0	56	3	0
20	J	40	0	56	4	0
20	K	40	0	56	3	0
20	L	40	0	56	2	0
20	M	40	0	56	4	0
20	a	200	0	280	16	0
20	b	280	0	392	18	0
20	f	80	0	112	5	0
20	g	80	0	112	6	0
20	i	40	0	56	3	0
20	j	40	0	56	5	0
20	k	40	0	56	2	0
20	l	40	0	56	2	0
20	m	40	0	56	3	0
21	B	59	0	79	3	0
21	b	59	0	79	3	0
22	B	12	0	23	0	0
22	M	12	0	23	0	0
22	b	12	0	23	0	0
22	m	12	0	23	0	0
23	5a	35	0	40	1	0
23	5b	35	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	42	0	54	1	0
23	I	31	0	32	1	0
23	J	71	0	85	2	0
23	b	42	0	54	1	0
23	i	31	0	32	1	0
23	j	71	0	85	2	0
24	A	8	0	0	1	0
24	C	16	0	0	0	0
24	a	8	0	0	1	0
24	c	16	0	0	0	0
25	2a	84	0	112	11	0
25	2b	84	0	112	11	0
25	3a	84	0	112	8	0
25	3b	84	0	112	8	0
25	5a	84	0	112	8	0
25	5b	84	0	112	5	0
25	6a	126	0	168	14	0
25	6b	126	0	168	12	0
25	J	42	0	56	4	0
25	j	42	0	56	3	0
26	A	65	0	72	3	0
26	a	65	0	72	3	0
27	2a	32	0	34	0	0
27	2b	32	0	34	0	0
27	5a	69	0	78	3	0
27	5b	69	0	78	3	0
27	6a	39	0	51	1	0
27	6b	39	0	51	1	0
27	A	83	0	112	7	0
27	a	83	0	112	7	0
28	6a	68	0	85	0	0
28	6b	68	0	85	0	0
28	A	35	0	46	0	0
28	a	35	0	46	0	0
29	2a	181	0	122	9	0
29	2b	181	0	122	8	0
29	3a	138	0	93	4	0
29	3b	138	0	93	4	0
29	5a	224	0	151	6	0
29	5b	224	0	151	6	0
29	6a	87	0	55	3	0
29	6b	87	0	55	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	70242	0	68946	937	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (937) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:92:TYR:CD1	6:g:125:ASN:ND2	1.83	1.41
6:G:125:ASN:ND2	7:h:92:TYR:CD1	1.81	1.40
7:H:92:TYR:CE1	6:g:125:ASN:ND2	1.83	1.39
6:G:125:ASN:ND2	7:h:92:TYR:CE1	1.83	1.37
6:G:120:SER:HB2	7:h:96:LYS:HE2	1.41	1.00
7:H:96:LYS:HE2	6:g:120:SER:HB2	1.42	1.00
6:G:125:ASN:CG	7:h:92:TYR:CE1	2.52	0.87
7:H:92:TYR:CE1	6:g:125:ASN:CG	2.53	0.86
13:2b:229:VAL:HG11	25:2b:315:LUT:H30	1.70	0.73
13:2a:229:VAL:HG11	25:2a:315:LUT:H30	1.69	0.72
16:6a:98:VAL:HG11	25:6a:318:LUT:H12	1.73	0.71
6:G:125:ASN:ND2	7:h:92:TYR:CZ	2.57	0.70
7:H:92:TYR:CG	6:g:125:ASN:ND2	2.58	0.70
6:G:125:ASN:ND2	7:h:92:TYR:CG	2.57	0.69
16:6a:103:ILE:HD12	16:6a:104:PRO:HD3	1.74	0.69
16:6b:103:ILE:HD12	16:6b:104:PRO:HD3	1.74	0.69
16:6b:98:VAL:HG11	25:6b:318:LUT:H12	1.73	0.69
20:B:851:BCR:H17C	18:B:854:CLA:H151	1.75	0.68
20:b:851:BCR:H17C	18:b:854:CLA:H151	1.75	0.68
6:G:135:LEU:HD11	20:G:204:BCR:H19C	1.75	0.68
18:5b:308:CLA:HBB	18:5b:315:CLA:HBC2	1.76	0.68
18:5a:308:CLA:HBB	18:5a:315:CLA:HBC2	1.76	0.67
7:H:92:TYR:CZ	6:g:125:ASN:ND2	2.57	0.67
6:g:135:LEU:HD11	20:g:204:BCR:H19C	1.75	0.67
18:2a:310:CLA:HMC2	25:2a:314:LUT:H30	1.76	0.67
18:b:810:CLA:HBB2	18:b:812:CLA:HMA3	1.78	0.66
18:6a:308:CLA:HBA1	25:6a:319:LUT:H31	1.76	0.66
27:5b:320:LHG:O4	18:6b:313:CLA:MG	1.38	0.66
18:6b:308:CLA:HBA1	25:6b:319:LUT:H31	1.76	0.66
27:5a:320:LHG:O4	18:6a:313:CLA:NB	2.29	0.66
27:5b:320:LHG:O4	18:6b:313:CLA:NB	2.29	0.66
18:A:809:CLA:HBB2	18:A:812:CLA:HMA3	1.78	0.65
18:2b:310:CLA:HMC2	25:2b:314:LUT:H30	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:805:CLA:H2	18:B:805:CLA:HED3	1.79	0.65
18:B:810:CLA:HBB2	18:B:812:CLA:HMA3	1.78	0.64
18:a:809:CLA:HBB2	18:a:812:CLA:HMA3	1.78	0.64
27:5a:320:LHG:O4	18:6a:313:CLA:MG	1.38	0.64
6:G:120:SER:CB	7:h:96:LYS:HE2	2.23	0.63
13:2a:111:MET:HG2	25:2a:314:LUT:H35	1.80	0.63
15:5a:94:LEU:HD22	15:5a:98:ARG:HH21	1.63	0.63
18:b:805:CLA:HED3	18:b:805:CLA:H2	1.79	0.63
20:G:201:BCR:H362	20:G:204:BCR:H312	1.80	0.63
13:2b:111:MET:HG2	25:2b:314:LUT:H35	1.80	0.63
18:2b:301:CLA:HAB	25:2b:315:LUT:H12	1.80	0.62
15:5b:94:LEU:HD22	15:5b:98:ARG:HH21	1.63	0.62
18:2a:301:CLA:HAB	25:2a:315:LUT:H12	1.80	0.62
20:g:201:BCR:H362	20:g:204:BCR:H312	1.80	0.62
18:b:806:CLA:HHB	18:b:807:CLA:HHB	1.82	0.62
12:A:473:LEU:HB2	12:A:525:THR:HG23	1.81	0.62
12:a:473:LEU:HB2	12:a:525:THR:HG23	1.81	0.62
12:a:579:CYS:HB3	24:a:844:SF4:S4	2.40	0.62
7:H:96:LYS:HE2	6:g:120:SER:CB	2.24	0.62
6:G:125:ASN:CG	7:h:92:TYR:CZ	2.77	0.61
20:f:301:BCR:H19C	18:a:839:CLA:H52	1.81	0.61
18:B:806:CLA:HHB	18:B:807:CLA:HHB	1.82	0.61
12:A:579:CYS:HB3	24:A:844:SF4:S4	2.40	0.61
20:F:301:BCR:H19C	18:A:839:CLA:H52	1.81	0.61
7:H:92:TYR:CZ	6:g:125:ASN:CG	2.78	0.60
4:E:80:ILE:HG22	4:E:82:ARG:H	1.66	0.60
5:F:178:ILE:HG23	18:F:302:CLA:HAA1	1.82	0.60
12:A:442:LEU:HB3	12:A:536:PHE:HB2	1.84	0.60
14:3b:195:GLU:HG2	14:3b:196:LYS:HD3	1.83	0.60
25:2a:314:LUT:H181	25:2a:314:LUT:H8	1.83	0.60
12:a:211:GLN:HA	12:a:215:SER:HB3	1.82	0.60
4:e:80:ILE:HG22	4:e:82:ARG:H	1.66	0.60
12:A:211:GLN:HA	12:A:215:SER:HB3	1.82	0.60
5:f:178:ILE:HG23	18:f:302:CLA:HAA1	1.82	0.60
25:2b:314:LUT:H181	25:2b:314:LUT:H8	1.83	0.60
23:B:850:LMG:H161	23:B:850:LMG:H301	1.83	0.60
14:3a:195:GLU:HG2	14:3a:196:LYS:HD3	1.83	0.60
12:a:442:LEU:HB3	12:a:536:PHE:HB2	1.84	0.60
11:m:7:SER:HA	11:m:10:ILE:HD12	1.84	0.59
1:b:303:GLU:HG2	6:g:97:ALA:HA	1.85	0.59
23:b:850:LMG:H161	23:b:850:LMG:H301	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:HB3	1:B:304:ILE:HD11	1.85	0.59
11:M:7:SER:HA	11:M:10:ILE:HD12	1.84	0.59
1:B:585:ASN:HB2	18:A:841:CLA:HBC2	1.84	0.59
1:b:180:SER:HB3	18:b:819:CLA:HAC2	1.86	0.58
1:B:303:GLU:HG2	6:G:97:ALA:HA	1.85	0.58
1:b:585:ASN:HB2	18:a:841:CLA:HBC2	1.84	0.58
11:M:16:VAL:HG23	20:M:101:BCR:H14C	1.86	0.57
1:b:299:HIS:HB3	1:b:304:ILE:HD11	1.85	0.57
18:B:821:CLA:HBC2	18:B:822:CLA:HBA1	1.86	0.57
27:5b:320:LHG:HC61	29:6b:304:CHL:HBC3	1.86	0.57
18:b:821:CLA:HBC2	18:b:822:CLA:HBA1	1.86	0.57
27:5a:320:LHG:HC61	29:6a:304:CHL:HBC3	1.86	0.57
18:a:821:CLA:HAA1	17:k:79:PRO:HG2	1.87	0.57
1:B:180:SER:HB3	18:B:819:CLA:HAC2	1.86	0.57
11:m:16:VAL:HG23	20:m:101:BCR:H14C	1.86	0.57
7:h:80:ASN:HB3	7:h:83:GLN:HB2	1.87	0.56
12:A:241:ARG:HG3	18:A:814:CLA:HED3	1.86	0.56
18:B:832:CLA:H42	23:J:104:LMG:H291	1.87	0.56
18:B:839:CLA:H143	20:L:304:BCR:H17C	1.88	0.56
10:l:102:PRO:HB3	10:l:183:LEU:HD12	1.87	0.56
15:5b:243:ILE:HD11	18:5b:312:CLA:H11	1.86	0.56
15:5a:243:ILE:HD11	18:5a:312:CLA:H11	1.86	0.56
7:H:80:ASN:HB3	7:H:83:GLN:HB2	1.87	0.56
18:A:821:CLA:HAA1	17:K:79:PRO:HG2	1.87	0.56
12:a:241:ARG:HG3	18:a:814:CLA:HED3	1.86	0.56
18:B:817:CLA:H142	18:B:823:CLA:H171	1.88	0.56
5:F:156:LEU:HD22	5:F:167:GLU:HG2	1.88	0.55
18:b:817:CLA:H142	18:b:823:CLA:H171	1.88	0.55
10:L:102:PRO:HB3	10:L:183:LEU:HD12	1.87	0.55
18:b:839:CLA:H143	20:l:304:BCR:H17C	1.88	0.55
5:f:156:LEU:HD22	5:f:167:GLU:HG2	1.88	0.55
18:b:838:CLA:HBB2	19:b:841:PQN:H141	1.89	0.55
18:b:832:CLA:H42	23:j:104:LMG:H291	1.87	0.55
14:3b:242:VAL:HG11	25:3b:317:LUT:H32	1.88	0.55
18:2a:312:CLA:HAA2	14:3a:164:LEU:HG	1.89	0.55
18:6a:310:CLA:HAB	25:6a:319:LUT:H193	1.89	0.55
18:b:813:CLA:H62	20:b:843:BCR:H16C	1.89	0.55
18:2b:312:CLA:HAA2	14:3b:164:LEU:HG	1.89	0.55
27:6b:301:LHG:H351	27:6b:301:LHG:H262	1.88	0.54
18:A:806:CLA:HED2	18:A:806:CLA:H62	1.89	0.54
14:3a:242:VAL:HG11	25:3a:317:LUT:H32	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:39:THR:HG22	12:A:710:GLN:HB2	1.89	0.54
18:A:820:CLA:H122	18:A:823:CLA:H93	1.90	0.54
12:a:39:THR:HG22	12:a:710:GLN:HB2	1.89	0.54
18:B:838:CLA:HBB2	19:B:841:PQN:H141	1.89	0.54
25:j:105:LUT:H32	18:a:801:CLA:HBA2	1.90	0.54
18:a:806:CLA:HED2	18:a:806:CLA:H62	1.89	0.54
27:6a:301:LHG:H351	27:6a:301:LHG:H262	1.88	0.54
18:a:820:CLA:H122	18:a:823:CLA:H93	1.90	0.54
1:b:164:LYS:HE2	6:g:112:ASP:HA	1.89	0.54
18:A:817:CLA:H102	18:A:835:CLA:HBA2	1.90	0.54
12:A:391:ILE:HD12	18:A:806:CLA:H143	1.90	0.53
18:B:813:CLA:H62	20:B:843:BCR:H16C	1.89	0.53
18:b:826:CLA:HBC3	21:b:847:DGD:HBV1	1.91	0.53
18:6b:310:CLA:HAB	25:6b:319:LUT:H193	1.89	0.53
18:B:826:CLA:HBC3	21:B:847:DGD:HBV1	1.91	0.53
9:J:5:LYS:HE2	13:2a:95:LEU:HD22	1.90	0.53
12:a:391:ILE:HD12	18:a:806:CLA:H143	1.90	0.53
1:B:164:LYS:HE2	6:G:112:ASP:HA	1.89	0.53
5:F:207:ASP:HA	23:J:103:LMG:HC61	1.91	0.53
12:A:495:ASN:HB2	18:A:835:CLA:HED2	1.90	0.53
25:J:105:LUT:H32	18:A:801:CLA:HBA2	1.90	0.53
18:a:823:CLA:H151	27:a:846:LHG:H172	1.91	0.53
3:d:161:ARG:HB2	3:d:171:LEU:HD11	1.91	0.53
18:A:823:CLA:H151	27:A:846:LHG:H172	1.91	0.53
9:j:5:LYS:HE2	13:2b:95:LEU:HD22	1.90	0.52
12:A:234:PRO:HA	12:A:237:PHE:HD2	1.75	0.52
16:6a:237:ILE:HG22	16:6a:238:ILE:HD12	1.91	0.52
18:a:817:CLA:H102	18:a:835:CLA:HBA2	1.90	0.52
9:J:21:PHE:HA	18:J:101:CLA:HBB2	1.92	0.52
12:a:234:PRO:HA	12:a:237:PHE:HD2	1.75	0.52
1:B:374:HIS:HE1	18:B:826:CLA:ND	2.08	0.52
1:b:700:LEU:HB3	1:b:704:GLN:HG2	1.91	0.52
15:5a:231:LEU:HD13	25:5a:316:LUT:H163	1.92	0.52
12:a:495:ASN:HB2	18:a:835:CLA:HED2	1.90	0.52
16:6b:237:ILE:HG22	16:6b:238:ILE:HD12	1.91	0.52
6:G:125:ASN:OD1	7:h:92:TYR:CE1	2.62	0.52
15:5b:175:LEU:HD21	15:5b:186:ILE:HG22	1.90	0.52
1:B:649:MET:HG2	1:B:723:ALA:HB2	1.91	0.52
5:f:207:ASP:HA	23:j:103:LMG:HC61	1.91	0.52
15:5a:231:LEU:HD22	25:5a:316:LUT:H172	1.92	0.52
1:B:700:LEU:HB3	1:B:704:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:ARG:HB2	3:D:171:LEU:HD11	1.91	0.52
18:A:839:CLA:H111	18:A:839:CLA:HAB	1.92	0.52
13:2a:225:ALA:HB2	25:2a:314:LUT:H34	1.92	0.52
12:A:10:VAL:HA	14:3a:92:GLY:HA3	1.91	0.52
12:A:191:MET:HG2	18:A:824:CLA:HMD3	1.92	0.52
16:6b:105:GLU:HB2	16:6b:218:LEU:HD12	1.91	0.52
15:5b:231:LEU:HD22	25:5b:316:LUT:H172	1.92	0.52
18:b:838:CLA:H93	20:i:202:BCR:H382	1.93	0.51
14:3a:191:PHE:HE2	29:3a:307:CHL:HBB2	1.74	0.51
15:5b:80:ALA:HB1	15:5b:86:LEU:HD23	1.91	0.51
15:5a:175:LEU:HD21	15:5a:186:ILE:HG22	1.90	0.51
12:a:10:VAL:HA	14:3b:92:GLY:HA3	1.91	0.51
18:B:801:CLA:H172	18:A:841:CLA:HMA1	1.93	0.51
12:a:588:PHE:HA	12:a:591:LEU:HD12	1.92	0.51
18:a:805:CLA:H51	18:a:812:CLA:H12	1.93	0.51
1:b:649:MET:HG2	1:b:723:ALA:HB2	1.91	0.51
16:6a:105:GLU:HB2	16:6a:218:LEU:HD12	1.91	0.51
13:2b:225:ALA:HB2	25:2b:314:LUT:H34	1.92	0.51
20:B:844:BCR:H383	20:B:845:BCR:H402	1.93	0.51
14:3b:116:GLY:HA2	25:3b:317:LUT:H381	1.91	0.51
18:6b:305:CLA:H13	25:6b:320:LUT:H193	1.93	0.51
18:B:838:CLA:H93	20:I:202:BCR:H382	1.93	0.51
18:b:854:CLA:HAA2	18:a:831:CLA:HBB1	1.92	0.51
12:A:26:PRO:HB3	18:A:803:CLA:HAC1	1.93	0.51
18:A:824:CLA:H42	18:A:828:CLA:H193	1.93	0.51
1:b:374:HIS:HE1	18:b:826:CLA:ND	2.08	0.51
18:2a:308:CLA:HBB1	25:2a:314:LUT:H12	1.93	0.51
1:B:234:ALA:HB2	18:B:815:CLA:HMA2	1.94	0.51
18:b:801:CLA:H172	18:a:841:CLA:HMA1	1.93	0.51
18:6a:305:CLA:H13	25:6a:320:LUT:H193	1.93	0.51
9:j:21:PHE:HA	18:j:101:CLA:HBB2	1.91	0.50
12:A:588:PHE:HA	12:A:591:LEU:HD12	1.92	0.50
14:3a:116:GLY:HA2	25:3a:317:LUT:H381	1.91	0.50
15:5b:231:LEU:HD13	25:5b:316:LUT:H163	1.92	0.50
1:B:15:ASP:HB3	1:B:20:ARG:HB2	1.93	0.50
1:B:721:TYR:HB2	18:B:801:CLA:HED2	1.93	0.50
12:A:435:LEU:HG	12:A:543:LEU:HB2	1.93	0.50
16:6a:152:VAL:HG11	25:6a:319:LUT:H35	1.94	0.50
12:a:191:MET:HG2	18:a:824:CLA:HMD3	1.92	0.50
12:a:283:LEU:HD13	18:a:817:CLA:HMA2	1.93	0.50
12:a:435:LEU:HG	12:a:543:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3b:191:PHE:HE2	29:3b:307:CHL:HBB2	1.74	0.50
1:B:71:GLN:HE21	8:I:1:MET:HE1	1.77	0.50
6:G:125:ASN:OD1	7:h:92:TYR:CZ	2.64	0.50
18:a:835:CLA:HAB	20:a:850:BCR:H282	1.94	0.50
18:a:839:CLA:HAB	18:a:839:CLA:H111	1.92	0.50
1:b:721:TYR:HB2	18:b:801:CLA:HED2	1.93	0.50
15:5a:80:ALA:HB1	15:5a:86:LEU:HD23	1.91	0.50
18:A:805:CLA:H51	18:A:812:CLA:H12	1.93	0.50
7:H:92:TYR:CE1	6:g:125:ASN:OD1	2.64	0.50
14:3a:178:GLN:HB2	14:3a:186:MET:HE3	1.94	0.50
18:a:824:CLA:H42	18:a:828:CLA:H193	1.93	0.50
18:B:854:CLA:HAA2	18:A:831:CLA:HBB1	1.92	0.50
20:b:844:BCR:H383	20:b:845:BCR:H402	1.93	0.50
18:2b:308:CLA:HBB1	25:2b:314:LUT:H12	1.93	0.50
1:b:22:TRP:CG	1:b:704:GLN:HE22	2.30	0.49
13:2a:193:PRO:HB3	29:2a:306:CHL:HBC2	1.94	0.49
1:b:234:ALA:HB2	18:b:815:CLA:HMA2	1.94	0.49
1:B:22:TRP:CG	1:B:704:GLN:HE22	2.30	0.49
7:H:92:TYR:CZ	6:g:125:ASN:OD1	2.66	0.49
10:L:90:LEU:HD13	10:L:93:LEU:HD12	1.95	0.49
14:3a:87:LEU:HD22	18:3a:302:CLA:H42	1.95	0.49
18:A:835:CLA:HAB	20:A:850:BCR:H282	1.94	0.49
12:a:26:PRO:HB3	18:a:803:CLA:HAC1	1.93	0.49
1:B:191:THR:HG21	1:B:278:LEU:HB2	1.95	0.49
18:a:823:CLA:H172	27:a:846:LHG:H191	1.94	0.49
1:B:490:GLN:HA	1:B:494:LEU:HB2	1.95	0.49
18:B:806:CLA:HMB2	18:B:807:CLA:H3A	1.95	0.49
1:b:15:ASP:HB3	1:b:20:ARG:HB2	1.93	0.49
18:f:305:CLA:HBB1	12:a:44:TRP:HE1	1.78	0.49
12:A:191:MET:HB2	18:A:812:CLA:HBC2	1.95	0.49
12:a:191:MET:HB2	18:a:812:CLA:HBC2	1.95	0.49
18:b:804:CLA:HBC2	18:b:828:CLA:HMA1	1.95	0.49
12:A:283:LEU:HD13	18:A:817:CLA:HMA2	1.93	0.49
12:a:197:ALA:HB2	12:a:303:GLY:HA3	1.95	0.49
12:a:395:LEU:HD21	18:a:806:CLA:H142	1.93	0.49
10:L:92:ASN:HB3	18:L:301:CLA:HAC1	1.94	0.49
10:L:102:PRO:HA	10:L:105:ARG:HD3	1.95	0.49
3:d:138:ARG:HB2	3:d:141:GLN:HG3	1.95	0.49
12:A:395:LEU:HD21	18:A:806:CLA:H142	1.93	0.49
1:B:69:ALA:HB2	1:B:135:LEU:HB2	1.95	0.49
1:B:384:THR:HG22	1:B:534:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:607:ALA:HA	1:b:610:ASN:HB2	1.95	0.49
18:A:803:CLA:HBB2	18:A:810:CLA:H72	1.95	0.48
14:3b:178:GLN:HB2	14:3b:186:MET:HE3	1.94	0.48
16:6b:152:VAL:HG11	25:6b:319:LUT:H35	1.94	0.48
1:B:607:ALA:HA	1:B:610:ASN:HB2	1.95	0.48
18:B:804:CLA:HBC2	18:B:828:CLA:HMA1	1.95	0.48
1:b:71:GLN:HE21	8:i:1:MET:HE1	1.77	0.48
1:b:490:GLN:HA	1:b:494:LEU:HB2	1.95	0.48
20:b:848:BCR:H21C	20:b:848:BCR:H361	1.94	0.48
13:2b:193:PRO:HB3	29:2b:306:CHL:HBC2	1.94	0.48
29:5b:301:CHL:HBB2	18:5b:302:CLA:HHD	1.95	0.48
1:b:69:ALA:HB2	1:b:135:LEU:HB2	1.95	0.48
1:b:191:THR:HG21	1:b:278:LEU:HB2	1.95	0.48
1:b:384:THR:HG22	1:b:534:LEU:HD11	1.94	0.48
12:A:451:ILE:HG22	18:A:833:CLA:HBC2	1.96	0.48
18:F:305:CLA:HBB1	12:A:44:TRP:HE1	1.78	0.48
12:a:357:LEU:HD21	18:a:818:CLA:H93	1.96	0.48
18:A:823:CLA:H172	27:A:846:LHG:H191	1.94	0.48
14:3b:87:LEU:HD22	18:3b:302:CLA:H42	1.95	0.48
2:c:15:THR:HG22	2:c:28:MET:HE2	1.96	0.48
10:l:90:LEU:HD13	10:l:93:LEU:HD12	1.95	0.48
25:2a:315:LUT:H201	25:2a:315:LUT:H35	1.96	0.48
15:5b:153:ARG:HB3	29:5b:307:CHL:CMC	2.44	0.48
29:5b:301:CHL:HHC	29:5b:301:CHL:HBB1	1.95	0.48
20:j:102:BCR:H343	18:a:808:CLA:H71	1.96	0.48
18:A:805:CLA:H203	20:A:847:BCR:H10C	1.95	0.48
3:D:138:ARG:HB2	3:D:141:GLN:HG3	1.95	0.48
10:l:92:ASN:HB3	18:l:301:CLA:HAC1	1.94	0.48
20:B:848:BCR:H21C	20:B:848:BCR:H361	1.94	0.48
12:A:48:ALA:HB2	27:A:845:LHG:HC91	1.94	0.48
12:A:725:ALA:HA	27:A:845:LHG:H342	1.96	0.48
25:3b:316:LUT:H171	25:3b:316:LUT:H8	1.96	0.48
18:B:808:CLA:H11	18:B:808:CLA:HBA2	1.58	0.48
29:2a:306:CHL:H3A	29:2a:306:CHL:HBA1	1.60	0.48
25:2b:315:LUT:H201	25:2b:315:LUT:H35	1.96	0.48
1:B:352:MET:HE2	1:B:352:MET:HB3	1.80	0.47
23:I:201:LMG:H141	23:I:201:LMG:H301	1.95	0.47
29:5a:301:CHL:HBB2	18:5a:302:CLA:HHD	1.96	0.47
23:i:201:LMG:H141	23:i:201:LMG:H301	1.95	0.47
10:l:102:PRO:HA	10:l:105:ARG:HD3	1.95	0.47
1:B:90:ALA:HA	1:B:113:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:725:ALA:HA	27:a:845:LHG:H342	1.96	0.47
12:A:197:ALA:HB2	12:A:303:GLY:HA3	1.95	0.47
15:5a:153:ARG:HB3	29:5a:307:CHL:CMC	2.44	0.47
20:J:102:BCR:H343	18:A:808:CLA:H71	1.96	0.47
13:2a:197:TRP:HZ3	29:2a:306:CHL:HAB	1.79	0.47
12:a:48:ALA:HB2	27:a:845:LHG:HC91	1.94	0.47
18:B:838:CLA:HHC	18:B:838:CLA:HBB1	1.97	0.47
1:b:90:ALA:HA	1:b:113:VAL:HG12	1.97	0.47
18:b:802:CLA:HHC	18:b:802:CLA:HBB1	1.97	0.47
18:b:806:CLA:HMB2	18:b:807:CLA:H3A	1.95	0.47
18:b:838:CLA:HHC	18:b:838:CLA:HBB1	1.97	0.47
2:C:15:THR:HG22	2:C:28:MET:HE2	1.96	0.47
5:F:223:VAL:HG22	18:5a:303:CLA:H2	1.96	0.47
12:A:357:LEU:HD21	18:A:818:CLA:H93	1.96	0.47
29:5a:301:CHL:HHC	29:5a:301:CHL:HBB1	1.96	0.47
16:6a:221:LEU:HB2	25:6a:318:LUT:H22	1.97	0.47
18:a:803:CLA:HBB2	18:a:810:CLA:H72	1.95	0.47
18:a:805:CLA:H203	20:a:847:BCR:H10C	1.96	0.47
1:B:216:LEU:HD12	18:B:814:CLA:HED3	1.97	0.47
12:a:220:GLN:HG2	12:a:247:LEU:HD22	1.97	0.47
13:2b:197:TRP:HZ3	29:2b:306:CHL:HAB	1.79	0.47
16:6b:221:LEU:HB2	25:6b:318:LUT:H22	1.97	0.47
1:B:688:ALA:HB2	20:B:851:BCR:HC22	1.97	0.47
18:B:830:CLA:H72	5:F:229:LEU:HD22	1.97	0.47
1:b:688:ALA:HB2	20:b:851:BCR:HC22	1.97	0.47
18:b:830:CLA:H72	5:f:229:LEU:HD22	1.97	0.47
25:3a:316:LUT:H171	25:3a:316:LUT:H8	1.96	0.47
12:a:451:ILE:HG22	18:a:833:CLA:HBC2	1.96	0.47
27:a:846:LHG:H241	27:a:846:LHG:HC61	1.42	0.47
16:6b:221:LEU:HD22	25:6b:318:LUT:H172	1.97	0.47
3:D:83:THR:HB	3:D:133:LEU:HB2	1.96	0.47
3:d:83:THR:HB	3:d:133:LEU:HB2	1.96	0.47
12:A:516:VAL:HG11	12:A:519:LEU:HD23	1.98	0.47
25:5b:317:LUT:H15	25:5b:317:LUT:H201	1.79	0.47
18:L:302:CLA:H43	18:A:831:CLA:H43	1.97	0.46
18:l:302:CLA:H43	18:a:831:CLA:H43	1.97	0.46
12:A:343:TRP:HB3	18:A:805:CLA:HAC1	1.97	0.46
12:a:343:TRP:HB3	18:a:805:CLA:HAC1	1.97	0.46
12:a:435:LEU:HD21	12:a:542:VAL:HG12	1.97	0.46
18:A:837:CLA:H12	18:A:837:CLA:HBA2	1.72	0.46
5:f:226:LEU:HD22	18:5b:303:CLA:H42	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:435:LEU:HD21	12:A:542:VAL:HG12	1.97	0.46
12:A:482:GLN:HG2	12:A:504:TRP:HA	1.97	0.46
18:B:802:CLA:HHC	18:B:802:CLA:HBB1	1.97	0.46
1:b:216:LEU:HD12	18:b:814:CLA:HED3	1.97	0.46
25:3a:317:LUT:H191	25:3a:317:LUT:H12	1.98	0.46
12:a:516:VAL:HG11	12:a:519:LEU:HD23	1.98	0.46
18:B:832:CLA:H12	20:F:301:BCR:HC42	1.98	0.46
1:b:352:MET:HE2	1:b:352:MET:HB3	1.80	0.46
3:d:119:MET:HE3	3:d:119:MET:HB3	1.77	0.46
18:6a:311:CLA:HHC	18:6a:311:CLA:HBB1	1.98	0.46
18:A:819:CLA:HAA2	17:K:109:THR:HG23	1.98	0.46
13:2a:157:MET:HE2	13:2a:161:GLU:HG2	1.98	0.46
25:3a:317:LUT:H201	25:3a:317:LUT:H15	1.75	0.46
12:a:222:LEU:HD21	12:a:228:PRO:HG3	1.98	0.46
18:a:817:CLA:HHC	18:a:817:CLA:HBB1	1.98	0.46
14:3b:206:TYR:HB3	18:3b:309:CLA:HED2	1.98	0.46
29:3b:301:CHL:HHC	29:3b:301:CHL:HBB1	1.98	0.46
18:A:817:CLA:HHC	18:A:817:CLA:HBB1	1.98	0.46
13:2b:167:ASP:HB3	13:2b:174:VAL:HG11	1.98	0.46
7:H:96:LYS:HE3	7:H:99:ILE:HG23	1.98	0.46
25:J:105:LUT:H31	25:J:105:LUT:H28	1.78	0.46
18:b:830:CLA:HED3	12:a:698:TRP:HH2	1.81	0.46
6:g:92:LYS:HB2	6:g:92:LYS:HE3	1.79	0.46
12:A:115:ILE:HG13	12:A:116:VAL:HG13	1.98	0.46
12:A:306:TYR:HA	12:A:314:HIS:H	1.81	0.46
26:A:802:CL0:H51	26:A:802:CL0:H43	1.79	0.46
12:a:115:ILE:HG13	12:a:116:VAL:HG13	1.98	0.46
12:a:306:TYR:HA	12:a:314:HIS:H	1.81	0.46
12:a:482:GLN:HG2	12:a:504:TRP:HA	1.97	0.46
25:3b:317:LUT:H12	25:3b:317:LUT:H191	1.98	0.46
1:B:308:HIS:HE1	18:B:821:CLA:ND	2.13	0.46
18:B:801:CLA:H62	18:B:801:CLA:H102	1.81	0.46
6:G:92:LYS:HB2	6:G:92:LYS:HE3	1.79	0.46
18:b:809:CLA:HHC	18:b:809:CLA:HBB1	1.98	0.46
18:b:832:CLA:H12	20:f:301:BCR:HC42	1.98	0.46
5:f:223:VAL:HG22	18:5b:303:CLA:H2	1.96	0.46
7:h:96:LYS:HE3	7:h:99:ILE:HG23	1.98	0.46
16:6a:73:LEU:HD12	18:6a:305:CLA:H11	1.98	0.46
18:a:819:CLA:HAA2	17:k:109:THR:HG23	1.98	0.46
18:3b:306:CLA:HHC	18:3b:306:CLA:HBB1	1.98	0.46
1:B:301:ILE:HG23	18:B:818:CLA:HED3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:811:CLA:HHC	18:B:811:CLA:HBB1	1.98	0.46
18:b:806:CLA:HHC	18:b:806:CLA:HBB1	1.98	0.46
18:b:831:CLA:HMA1	20:a:851:BCR:H391	1.98	0.46
12:A:467:SER:HB3	12:A:470:ALA:HB3	1.98	0.46
18:a:815:CLA:C4C	18:3b:306:CLA:HBB2	2.46	0.46
18:6b:311:CLA:HHC	18:6b:311:CLA:HBB1	1.98	0.46
1:b:301:ILE:HG23	18:b:818:CLA:HED3	1.98	0.45
18:A:808:CLA:HBB2	18:A:827:CLA:H171	1.98	0.45
18:A:815:CLA:C4C	18:3a:306:CLA:HBB2	2.46	0.45
13:2a:167:ASP:HB3	13:2a:174:VAL:HG11	1.98	0.45
1:B:84:VAL:HA	7:H:142:ILE:HG22	1.99	0.45
25:J:105:LUT:H201	25:J:105:LUT:H15	1.57	0.45
18:6a:313:CLA:HBB1	18:6a:313:CLA:HHC	1.98	0.45
18:B:830:CLA:HED3	12:A:698:TRP:HH2	1.81	0.45
18:B:840:CLA:HBA2	18:B:840:CLA:H12	1.67	0.45
20:b:845:BCR:H11C	20:b:845:BCR:H341	1.83	0.45
20:j:102:BCR:H11C	20:j:102:BCR:H341	1.84	0.45
18:2a:308:CLA:HBB1	18:2a:308:CLA:HHC	1.98	0.45
14:3a:206:TYR:HB3	18:3a:309:CLA:HED2	1.98	0.45
18:6b:313:CLA:HHC	18:6b:313:CLA:HBB1	1.98	0.45
2:C:35:LYS:HA	2:C:35:LYS:HD2	1.72	0.45
20:J:102:BCR:H11C	20:J:102:BCR:H341	1.84	0.45
1:b:231:ASN:HA	18:b:815:CLA:HAA2	1.98	0.45
12:A:220:GLN:HG2	12:A:247:LEU:HD22	1.97	0.45
12:A:222:LEU:HD21	12:A:228:PRO:HG3	1.98	0.45
15:5a:190:LEU:HD12	25:5a:316:LUT:H222	1.98	0.45
18:a:808:CLA:HBB2	18:a:827:CLA:H171	1.98	0.45
1:B:37:MET:HE2	1:B:37:MET:HB2	1.89	0.45
1:b:84:VAL:HA	7:h:142:ILE:HG22	1.99	0.45
18:b:811:CLA:HHC	18:b:811:CLA:HBB1	1.98	0.45
18:b:830:CLA:H91	5:f:225:ALA:HB1	1.98	0.45
6:g:85:VAL:HG22	16:6b:151:PHE:HD1	1.81	0.45
12:a:400:ALA:HB2	20:a:850:BCR:H323	1.98	0.45
18:6b:310:CLA:HHC	18:6b:310:CLA:HBB1	1.98	0.45
5:F:226:LEU:HD22	18:5a:303:CLA:H42	1.98	0.45
6:G:85:VAL:HG22	16:6a:151:PHE:HD1	1.81	0.45
1:b:308:HIS:HE1	18:b:821:CLA:ND	2.14	0.45
20:A:849:BCR:H11C	20:A:849:BCR:H341	1.84	0.45
29:3a:301:CHL:HHC	29:3a:301:CHL:HBB1	1.98	0.45
18:a:806:CLA:H92	18:a:806:CLA:H61	1.87	0.45
18:a:853:CLA:HHC	18:a:853:CLA:HBB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6b:317:CLA:HBB1	18:6b:317:CLA:HHC	1.99	0.45
10:l:90:LEU:HD21	18:a:831:CLA:H42	1.99	0.45
12:A:400:ALA:HB2	20:A:850:BCR:H323	1.98	0.45
14:3a:84:PRO:HD2	25:3a:317:LUT:H3	1.99	0.45
18:B:825:CLA:HHC	18:B:825:CLA:HBB1	1.99	0.45
18:J:101:CLA:HBB1	18:J:101:CLA:HHC	1.99	0.45
18:A:833:CLA:HHC	18:A:833:CLA:HBB1	1.99	0.45
18:A:840:CLA:HHC	18:A:840:CLA:HBB1	1.99	0.45
18:3a:314:CLA:HHC	18:3a:314:CLA:HBB1	1.99	0.45
12:a:467:SER:HB3	12:a:470:ALA:HB3	1.98	0.45
25:6b:320:LUT:H11	25:6b:320:LUT:H191	1.86	0.45
18:B:831:CLA:HMA1	20:A:851:BCR:H391	1.98	0.45
18:G:203:CLA:HMD2	7:h:89:THR:HG21	1.98	0.45
18:b:806:CLA:H122	20:i:202:BCR:H323	1.99	0.45
18:b:825:CLA:HHC	18:b:825:CLA:HBB1	1.99	0.45
18:a:803:CLA:HHC	18:a:803:CLA:HBB1	1.99	0.45
18:3b:313:CLA:HBB1	18:3b:313:CLA:HHC	1.99	0.45
16:6b:73:LEU:HD12	18:6b:305:CLA:H11	1.98	0.45
1:B:668:ARG:HB2	19:B:841:PQN:H7	1.98	0.45
18:B:809:CLA:HHC	18:B:809:CLA:HBB1	1.98	0.45
18:B:840:CLA:HBB2	18:6a:305:CLA:H42	1.99	0.45
7:H:89:THR:HG21	18:g:203:CLA:HMD2	1.99	0.45
5:f:177:TYR:HA	5:f:221:TRP:HE1	1.81	0.45
18:A:853:CLA:HHC	18:A:853:CLA:HBB1	1.99	0.45
29:2a:313:CHL:HHC	29:2a:313:CHL:HBB1	1.99	0.45
16:6a:221:LEU:HD22	25:6a:318:LUT:H172	1.97	0.45
18:6a:317:CLA:HHC	18:6a:317:CLA:HBB1	1.99	0.45
18:a:807:CLA:HHC	18:a:807:CLA:HBB1	1.99	0.45
18:a:833:CLA:HBB1	18:a:833:CLA:HHC	1.99	0.45
13:2b:157:MET:HE2	13:2b:161:GLU:HG2	1.98	0.45
18:2b:303:CLA:HHC	18:2b:303:CLA:HBB1	1.99	0.45
14:3b:145:VAL:HG11	25:3b:317:LUT:H372	1.99	0.45
18:B:814:CLA:HHC	18:B:814:CLA:HBB1	1.99	0.44
20:B:848:BCR:H331	20:B:848:BCR:HC7	1.67	0.44
18:b:806:CLA:H102	20:i:202:BCR:HC21	1.99	0.44
18:b:840:CLA:HBB2	18:6b:305:CLA:H42	1.99	0.44
12:A:386:THR:HG23	12:A:602:ILE:HG21	2.00	0.44
12:A:505:GLY:HA2	12:A:520:PRO:HB3	1.99	0.44
18:2a:307:CLA:HHC	18:2a:307:CLA:HBB1	1.99	0.44
18:5a:308:CLA:HHC	18:5a:308:CLA:HBB1	1.99	0.44
18:5a:310:CLA:HHC	18:5a:310:CLA:HBB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6a:308:CLA:HMC2	25:6a:320:LUT:H363	2.00	0.44
18:3b:310:CLA:HHC	18:3b:310:CLA:HBB1	1.99	0.44
20:B:845:BCR:H341	20:B:845:BCR:H11C	1.83	0.44
5:F:177:TYR:HA	5:F:221:TRP:HE1	1.81	0.44
6:g:78:LEU:HD13	6:g:142:GLY:HA2	1.99	0.44
18:A:835:CLA:HHC	18:A:835:CLA:HBB1	1.99	0.44
18:3a:312:CLA:HHC	18:3a:312:CLA:HBB1	1.99	0.44
16:6a:62:SER:HB2	16:6a:65:ASP:HB2	1.99	0.44
12:a:386:THR:HG23	12:a:602:ILE:HG21	1.99	0.44
12:a:505:GLY:HA2	12:a:520:PRO:HB3	1.99	0.44
18:a:816:CLA:H62	18:a:816:CLA:H41	1.69	0.44
18:a:819:CLA:HHC	18:a:819:CLA:HBB1	1.99	0.44
29:2b:313:CHL:HHC	29:2b:313:CHL:HBB1	1.99	0.44
1:B:429:LEU:HD11	18:B:836:CLA:HMB2	2.00	0.44
1:B:545:LYS:HE3	1:B:545:LYS:HB3	1.81	0.44
18:B:806:CLA:HHC	18:B:806:CLA:HBB1	1.98	0.44
2:c:35:LYS:HD2	2:c:35:LYS:HA	1.72	0.44
18:3a:306:CLA:HHC	18:3a:306:CLA:HBB1	1.98	0.44
18:6a:316:CLA:HHC	18:6a:316:CLA:HBB1	2.00	0.44
12:a:12:GLU:HB2	12:a:65:ARG:HH22	1.82	0.44
29:2b:304:CHL:HHC	29:2b:304:CHL:HBB1	1.99	0.44
18:2b:308:CLA:H3A	18:2b:308:CLA:HBA2	1.77	0.44
18:2b:309:CLA:HHC	18:2b:309:CLA:HBB1	1.99	0.44
18:3b:314:CLA:HHC	18:3b:314:CLA:HBB1	1.99	0.44
18:5b:310:CLA:HHC	18:5b:310:CLA:HBB1	1.99	0.44
18:5b:311:CLA:HHC	18:5b:311:CLA:HBB1	1.99	0.44
18:b:808:CLA:H11	18:b:808:CLA:HBA2	1.58	0.44
12:A:735:THR:O	12:A:739:PHE:HB2	2.17	0.44
18:2a:312:CLA:HHC	18:2a:312:CLA:HBB1	2.00	0.44
29:5a:305:CHL:HBB2	29:5a:306:CHL:HAB	2.00	0.44
18:6a:308:CLA:HHC	18:6a:308:CLA:HBB1	1.99	0.44
18:6a:310:CLA:HHC	18:6a:310:CLA:HBB1	1.98	0.44
18:2b:311:CLA:HHC	18:2b:311:CLA:HBB1	2.00	0.44
25:2b:315:LUT:H401	25:2b:315:LUT:H15	1.99	0.44
15:5b:190:LEU:HD12	25:5b:316:LUT:H222	1.98	0.44
18:6b:316:CLA:HHC	18:6b:316:CLA:HBB1	2.00	0.44
1:B:393:PHE:CD2	20:B:845:BCR:H282	2.52	0.44
13:2a:185:LEU:HD23	29:2a:306:CHL:HBC3	1.99	0.44
18:a:815:CLA:HHC	18:a:815:CLA:HBB1	2.00	0.44
18:a:841:CLA:H42	20:a:851:BCR:H362	1.99	0.44
18:2b:308:CLA:HBB1	18:2b:308:CLA:HHC	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6b:314:CLA:HHC	18:6b:314:CLA:HBB1	2.00	0.44
1:B:151:ILE:HD13	11:M:22:LEU:HD13	2.00	0.44
18:B:806:CLA:H102	20:I:202:BCR:HC21	1.99	0.44
18:B:830:CLA:H91	5:F:225:ALA:HB1	1.98	0.44
20:G:201:BCR:H311	20:G:201:BCR:HC7	1.76	0.44
25:J:105:LUT:H7	25:J:105:LUT:H161	1.74	0.44
10:L:90:LEU:HD21	18:A:831:CLA:H42	1.99	0.44
1:b:583:MET:HE3	1:b:583:MET:HB3	1.91	0.44
18:b:854:CLA:H3A	18:b:854:CLA:HBA2	1.83	0.44
10:l:211:LEU:HG	18:l:303:CLA:HED3	1.99	0.44
18:A:803:CLA:HHC	18:A:803:CLA:HBB1	1.99	0.44
18:A:834:CLA:HHC	18:A:834:CLA:HBB1	2.00	0.44
18:A:841:CLA:H42	20:A:851:BCR:H362	1.99	0.44
18:3a:310:CLA:HHC	18:3a:310:CLA:HBB1	1.99	0.44
18:5a:311:CLA:HHC	18:5a:311:CLA:HBB1	1.99	0.44
12:a:735:THR:O	12:a:739:PHE:HB2	2.17	0.44
18:2b:307:CLA:HHC	18:2b:307:CLA:HBB1	1.99	0.44
18:5b:315:CLA:HHC	18:5b:315:CLA:HBB1	1.99	0.44
18:6b:308:CLA:HHC	18:6b:308:CLA:HBB1	1.99	0.44
7:H:72:GLY:HA2	10:L:96:TYR:HB3	1.99	0.44
1:b:545:LYS:HE3	1:b:545:LYS:HB3	1.81	0.44
18:b:819:CLA:HHC	18:b:819:CLA:HBB1	1.99	0.44
20:b:844:BCR:H11C	20:b:844:BCR:H341	1.89	0.44
12:A:12:GLU:HB2	12:A:65:ARG:HH22	1.82	0.44
18:A:819:CLA:HBB1	18:A:819:CLA:HHC	1.99	0.44
18:A:831:CLA:HBC2	18:A:838:CLA:HAC2	2.00	0.44
18:6a:306:CLA:HHC	18:6a:306:CLA:HBB1	2.00	0.44
18:6a:307:CLA:HBB1	18:6a:307:CLA:HHC	2.00	0.44
18:6a:314:CLA:HHC	18:6a:314:CLA:HBB1	2.00	0.44
20:K:202:BCR:H311	20:K:202:BCR:HC7	1.74	0.44
12:a:212:VAL:HG22	12:a:251:PHE:HZ	1.83	0.44
18:a:834:CLA:H51	18:a:834:CLA:H8	1.86	0.44
18:2b:312:CLA:HHC	18:2b:312:CLA:HBB1	2.00	0.44
29:5b:314:CHL:HHC	29:5b:314:CHL:HBB1	2.00	0.44
18:6b:308:CLA:HMC2	25:6b:320:LUT:H363	1.99	0.44
1:B:231:ASN:HA	18:B:815:CLA:HAA2	1.98	0.44
1:b:429:LEU:HD11	18:b:836:CLA:HMB2	2.00	0.44
7:h:72:GLY:HA2	10:l:96:TYR:HB3	1.99	0.44
18:2a:309:CLA:HHC	18:2a:309:CLA:HBB1	1.99	0.44
25:2a:315:LUT:H401	25:2a:315:LUT:H15	1.99	0.44
15:5a:142:ILE:HG12	18:6a:316:CLA:HED1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5a:231:LEU:HB2	25:5a:316:LUT:H22	2.00	0.44
13:2b:114:ALA:HA	13:2b:117:ILE:HG22	2.00	0.44
14:3b:84:PRO:HD2	25:3b:317:LUT:H3	1.99	0.44
29:5b:305:CHL:HBB2	29:5b:306:CHL:HAB	2.00	0.44
2:C:28:MET:HE3	2:C:28:MET:HB3	1.92	0.44
1:b:37:MET:HE2	1:b:37:MET:HB2	1.89	0.44
1:b:393:PHE:CD2	20:b:845:BCR:H282	2.52	0.44
18:b:804:CLA:HBA1	18:b:804:CLA:H3A	1.73	0.44
3:d:202:PRO:HA	3:d:205:ILE:HG12	2.00	0.44
25:j:105:LUT:H7	25:j:105:LUT:H161	1.74	0.44
18:5a:303:CLA:HHC	18:5a:303:CLA:HBB1	2.00	0.44
16:6a:103:ILE:HD11	18:6a:307:CLA:HAC2	2.00	0.44
12:a:237:PHE:HD1	12:a:244:LEU:HB2	1.82	0.44
18:B:831:CLA:HBA2	18:B:831:CLA:HBD	2.00	0.43
18:f:303:CLA:HHC	18:f:303:CLA:HBB1	2.00	0.43
18:j:101:CLA:HHC	18:j:101:CLA:HBB1	1.99	0.43
18:A:810:CLA:HHC	18:A:810:CLA:HBB1	2.00	0.43
13:2a:114:ALA:HA	13:2a:117:ILE:HG22	2.00	0.43
18:2a:303:CLA:HHC	18:2a:303:CLA:HBB1	1.99	0.43
14:3a:145:VAL:HG11	25:3a:317:LUT:H372	1.99	0.43
18:a:816:CLA:H12	18:a:816:CLA:HBA2	1.70	0.43
18:a:840:CLA:HHC	18:a:840:CLA:HBB1	1.99	0.43
18:5b:308:CLA:HHC	18:5b:308:CLA:HBB1	1.99	0.43
18:6b:307:CLA:HHC	18:6b:307:CLA:HBB1	2.00	0.43
18:6b:315:CLA:HHC	18:6b:315:CLA:HBB1	2.00	0.43
18:B:801:CLA:H142	18:B:801:CLA:H112	1.82	0.43
18:B:806:CLA:H122	20:I:202:BCR:H323	1.99	0.43
1:b:101:VAL:HG13	1:b:112:PRO:HG3	2.00	0.43
18:b:814:CLA:HHC	18:b:814:CLA:HBB1	1.99	0.43
12:A:212:VAL:HG22	12:A:251:PHE:HZ	1.83	0.43
18:A:807:CLA:HHC	18:A:807:CLA:HBB1	1.99	0.43
18:A:815:CLA:HHC	18:A:815:CLA:HBB1	2.00	0.43
18:5a:315:CLA:HHC	18:5a:315:CLA:HBB1	1.99	0.43
18:6a:315:CLA:HHC	18:6a:315:CLA:HBB1	2.00	0.43
20:a:849:BCR:H15C	20:a:849:BCR:H351	1.84	0.43
18:3b:303:CLA:HHC	18:3b:303:CLA:HBB1	2.00	0.43
1:B:101:VAL:HG13	1:B:112:PRO:HG3	2.00	0.43
18:B:832:CLA:H91	18:F:302:CLA:HMA1	2.00	0.43
1:b:151:ILE:HD13	11:m:22:LEU:HD13	2.00	0.43
12:a:402:HIS:HA	12:a:405:ILE:HD12	2.01	0.43
12:a:402:HIS:HE1	18:a:829:CLA:NA	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2b:197:TRP:CZ3	29:2b:306:CHL:HAB	2.54	0.43
18:B:804:CLA:HBA1	18:B:804:CLA:H3A	1.73	0.43
20:G:201:BCR:H11C	20:G:201:BCR:H341	1.87	0.43
18:b:801:CLA:H142	18:b:801:CLA:H112	1.82	0.43
20:b:842:BCR:H331	20:b:842:BCR:HC7	1.71	0.43
2:c:28:MET:HE3	2:c:28:MET:HB3	1.91	0.43
12:A:237:PHE:HD1	12:A:244:LEU:HB2	1.82	0.43
12:A:402:HIS:HA	12:A:405:ILE:HD12	2.01	0.43
18:A:822:CLA:HHC	18:A:822:CLA:HBB1	2.00	0.43
18:2a:311:CLA:HHC	18:2a:311:CLA:HBB1	2.00	0.43
18:3a:303:CLA:HHC	18:3a:303:CLA:HBB1	2.00	0.43
29:5a:314:CHL:HHC	29:5a:314:CHL:HBB1	2.00	0.43
18:a:831:CLA:HBC2	18:a:838:CLA:HAC2	2.00	0.43
18:6b:306:CLA:HHC	18:6b:306:CLA:HBB1	2.00	0.43
1:B:519:VAL:HG21	1:B:593:TYR:HB2	2.01	0.43
1:b:668:ARG:HB2	19:b:841:PQN:H7	1.98	0.43
18:g:202:CLA:HHC	18:g:202:CLA:HBB1	2.00	0.43
25:j:105:LUT:H201	25:j:105:LUT:H15	1.57	0.43
12:A:276:LEU:HD21	12:A:369:PRO:HD2	2.00	0.43
18:a:834:CLA:HHC	18:a:834:CLA:HBB1	2.00	0.43
25:3b:316:LUT:H35	25:3b:316:LUT:H401	1.92	0.43
18:B:801:CLA:HBB1	18:B:801:CLA:HHC	2.00	0.43
18:G:203:CLA:CED	7:h:89:THR:O	2.67	0.43
1:b:519:VAL:HG21	1:b:593:TYR:HB2	2.01	0.43
18:b:801:CLA:HHC	18:b:801:CLA:HBB1	2.00	0.43
12:A:402:HIS:HE1	18:A:829:CLA:NA	2.15	0.43
29:2a:304:CHL:HHC	29:2a:304:CHL:HBB1	1.99	0.43
18:a:835:CLA:HHC	18:a:835:CLA:HBB1	1.99	0.43
16:6b:62:SER:HB2	16:6b:65:ASP:HB2	1.99	0.43
1:B:282:VAL:HG21	18:B:815:CLA:HBB1	2.01	0.43
3:D:202:PRO:HA	3:D:205:ILE:HG12	2.00	0.43
1:b:395:ILE:HD13	1:b:555:TYR:HA	2.00	0.43
25:6a:319:LUT:H8	25:6a:319:LUT:H181	2.01	0.43
17:K:72:ALA:HA	17:K:77:LEU:HB3	2.01	0.43
12:a:74:GLN:HG2	18:a:805:CLA:H3A	2.01	0.43
12:a:276:LEU:HD21	12:a:369:PRO:HD2	2.00	0.43
18:a:810:CLA:HHC	18:a:810:CLA:HBB1	2.00	0.43
15:5b:231:LEU:HB2	25:5b:316:LUT:H22	2.00	0.43
18:B:833:CLA:HHC	18:B:833:CLA:HBB1	2.00	0.43
1:b:422:LEU:HD13	1:b:532:LEU:HA	2.00	0.43
18:b:832:CLA:H61	18:b:832:CLA:H41	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:840:CLA:HBA2	18:b:840:CLA:H12	1.66	0.43
7:h:128:LYS:HG3	7:h:131:GLN:HE22	1.84	0.43
18:A:804:CLA:H2	18:A:810:CLA:H92	2.01	0.43
18:3a:313:CLA:HHC	18:3a:313:CLA:HBB1	1.99	0.43
26:a:802:CL0:H43	26:a:802:CL0:H51	1.79	0.43
20:a:847:BCR:H362	20:a:848:BCR:H21C	2.00	0.43
13:2b:185:LEU:HD23	29:2b:306:CHL:HBC3	1.99	0.43
18:5b:312:CLA:HHC	18:5b:312:CLA:HBB1	2.00	0.43
29:6b:304:CHL:HHC	29:6b:304:CHL:HBB1	2.00	0.43
1:B:395:ILE:HD13	1:B:555:TYR:HA	2.00	0.43
18:B:819:CLA:HHC	18:B:819:CLA:HBB1	1.99	0.43
18:F:302:CLA:HHC	18:F:302:CLA:HBB1	2.00	0.43
20:J:102:BCR:H403	20:J:102:BCR:H24C	1.86	0.43
18:L:301:CLA:HHC	18:L:301:CLA:HBB1	2.00	0.43
20:b:845:BCR:H403	20:b:845:BCR:H23C	2.01	0.43
18:l:301:CLA:HHC	18:l:301:CLA:HBB1	2.00	0.43
12:A:681:PHE:HZ	18:A:840:CLA:HBC3	1.84	0.43
18:A:823:CLA:HHC	18:A:823:CLA:HBB1	2.01	0.43
18:a:801:CLA:HHC	18:a:801:CLA:HBB1	2.01	0.43
20:a:847:BCR:HC7	20:a:847:BCR:H331	1.80	0.43
13:2b:192:TYR:HB3	18:2b:308:CLA:HED2	2.01	0.43
1:B:422:LEU:HD13	1:B:532:LEU:HA	2.00	0.43
18:B:801:CLA:H71	18:A:841:CLA:HMA3	2.01	0.43
20:B:842:BCR:H11C	20:B:842:BCR:H341	1.92	0.43
11:M:21:ILE:HD13	11:M:21:ILE:HA	1.90	0.43
18:b:832:CLA:H91	18:f:302:CLA:HMA1	2.00	0.43
12:A:74:GLN:HG2	18:A:805:CLA:H3A	2.01	0.43
29:3a:315:CHL:HHC	29:3a:315:CHL:HBB1	2.00	0.43
13:2b:63:LEU:H	14:3b:189:GLN:HE22	1.66	0.43
13:2b:220:LYS:HE2	13:2b:220:LYS:HB3	1.90	0.43
16:6b:119:ALA:HB1	16:6b:138:LEU:HD13	2.01	0.43
18:6b:315:CLA:H11	18:6b:315:CLA:H51	1.85	0.43
19:B:841:PQN:H301	21:B:847:DGD:HAT1	2.00	0.42
2:C:18:VAL:HG21	2:C:28:MET:HG2	2.01	0.42
18:F:303:CLA:HHC	18:F:303:CLA:HBB1	2.01	0.42
18:b:808:CLA:HBA1	18:b:808:CLA:H3A	1.85	0.42
19:b:841:PQN:H301	21:b:847:DGD:HAT1	2.00	0.42
18:f:302:CLA:HHC	18:f:302:CLA:HBB1	2.00	0.42
27:A:846:LHG:HC61	27:A:846:LHG:H241	1.42	0.42
13:2a:63:LEU:H	14:3a:189:GLN:HE22	1.66	0.42
13:2a:197:TRP:CZ3	29:2a:306:CHL:HAB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2a:220:LYS:HE2	13:2a:220:LYS:HB3	1.90	0.42
18:5a:312:CLA:HHC	18:5a:312:CLA:HBB1	2.00	0.42
25:6a:318:LUT:H35	25:6a:318:LUT:H401	1.87	0.42
18:3b:312:CLA:HHC	18:3b:312:CLA:HBB1	1.99	0.42
15:5b:142:ILE:HG12	18:6b:316:CLA:HED1	2.00	0.42
18:B:820:CLA:HHC	18:B:820:CLA:HBB1	2.01	0.42
6:G:78:LEU:HD13	6:G:142:GLY:HA2	2.00	0.42
18:G:203:CLA:HHC	18:G:203:CLA:HBB1	2.01	0.42
10:L:211:LEU:HG	18:L:303:CLA:HED3	1.99	0.42
18:b:833:CLA:HHC	18:b:833:CLA:HBB1	2.00	0.42
20:A:847:BCR:H362	20:A:848:BCR:H21C	2.00	0.42
18:3a:311:CLA:HHC	18:3a:311:CLA:HBB1	2.00	0.42
12:a:65:ARG:HG2	12:a:179:ALA:HB1	2.01	0.42
16:6b:103:ILE:HD11	18:6b:307:CLA:HAC2	2.00	0.42
29:6b:309:CHL:HHC	29:6b:309:CHL:HBB1	2.01	0.42
18:B:839:CLA:HBB1	18:B:839:CLA:HHC	2.01	0.42
20:J:102:BCR:HC7	20:J:102:BCR:H331	1.71	0.42
20:L:304:BCR:H15C	20:L:304:BCR:H351	1.94	0.42
18:b:804:CLA:HHC	18:b:804:CLA:HBB1	2.01	0.42
18:b:820:CLA:HHC	18:b:820:CLA:HBB1	2.01	0.42
20:g:204:BCR:H311	20:g:204:BCR:HC7	1.88	0.42
20:A:849:BCR:H351	20:A:849:BCR:H15C	1.84	0.42
12:a:215:SER:O	12:a:219:ASN:HB2	2.19	0.42
18:5b:303:CLA:HHC	18:5b:303:CLA:HBB1	2.00	0.42
18:B:805:CLA:H151	18:B:827:CLA:HBB2	2.02	0.42
20:B:844:BCR:H20C	20:B:844:BCR:H361	1.86	0.42
20:B:845:BCR:H403	20:B:845:BCR:H23C	2.00	0.42
18:G:202:CLA:HHC	18:G:202:CLA:HBB1	2.00	0.42
18:b:812:CLA:H51	18:b:817:CLA:HBC3	2.01	0.42
2:c:61:ASP:HA	2:c:62:PHE:HA	1.87	0.42
8:i:27:PHE:HD2	10:l:154:MET:HG2	1.84	0.42
12:A:215:SER:O	12:A:219:ASN:HB2	2.19	0.42
12:A:401:ALA:HB2	12:A:587:VAL:HG11	2.02	0.42
18:A:801:CLA:HHC	18:A:801:CLA:HBB1	2.01	0.42
29:6a:304:CHL:HHC	29:6a:304:CHL:HBB1	2.00	0.42
18:2b:302:CLA:HHC	18:2b:302:CLA:HBB1	2.01	0.42
1:B:404:LYS:HE3	1:B:404:LYS:HB2	1.87	0.42
1:B:696:LYS:HA	1:B:697:PRO:HD3	1.94	0.42
6:G:105:VAL:HB	6:G:109:GLU:HG3	2.01	0.42
20:b:844:BCR:H15C	20:b:844:BCR:H351	1.90	0.42
20:b:851:BCR:H15C	20:b:851:BCR:H351	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:101:BCR:H11C	20:m:101:BCR:H341	1.89	0.42
13:2a:192:TYR:HB3	18:2a:308:CLA:HED2	2.01	0.42
25:2a:315:LUT:H7	25:2a:315:LUT:H161	1.78	0.42
25:6a:319:LUT:H30	25:6a:319:LUT:H26	2.01	0.42
18:a:821:CLA:HHC	18:a:821:CLA:HBB1	2.02	0.42
18:a:823:CLA:HHC	18:a:823:CLA:HBB1	2.01	0.42
20:a:851:BCR:H361	20:a:851:BCR:H20C	1.80	0.42
25:2b:315:LUT:H11	25:2b:315:LUT:H191	1.93	0.42
18:B:804:CLA:HHC	18:B:804:CLA:HBB1	2.00	0.42
20:j:102:BCR:H15C	20:j:102:BCR:H351	1.90	0.42
20:l:304:BCR:H11C	20:l:304:BCR:H341	1.90	0.42
12:A:332:HIS:CE1	27:A:846:LHG:HC12	2.55	0.42
18:A:816:CLA:H62	18:A:816:CLA:H41	1.69	0.42
18:A:821:CLA:HHC	18:A:821:CLA:HBB1	2.02	0.42
20:A:850:BCR:H321	20:A:850:BCR:HC7	1.89	0.42
25:5a:317:LUT:H181	25:5a:317:LUT:H7	1.66	0.42
18:2b:310:CLA:HHC	18:2b:310:CLA:HBB1	2.02	0.42
15:5b:198:TYR:HA	15:5b:201:LYS:HG3	2.02	0.42
25:6b:319:LUT:H7	25:6b:319:LUT:H171	1.80	0.42
1:B:4:ARG:HA	1:B:4:ARG:HD2	1.88	0.42
7:H:89:THR:O	18:g:203:CLA:CED	2.67	0.42
8:I:27:PHE:HD2	10:L:154:MET:HG2	1.84	0.42
1:b:705:ALA:HA	1:b:708:VAL:HB	2.01	0.42
18:b:839:CLA:HHC	18:b:839:CLA:HBB1	2.00	0.42
10:l:182:LYS:HD2	10:l:182:LYS:HA	1.82	0.42
12:A:26:PRO:HB2	12:A:42:TRP:HH2	1.84	0.42
18:a:804:CLA:H2	18:a:810:CLA:H92	2.01	0.42
25:2b:315:LUT:H7	25:2b:315:LUT:H161	1.78	0.42
14:3b:191:PHE:CE2	29:3b:307:CHL:HBB2	2.53	0.42
18:3b:309:CLA:HHC	18:3b:309:CLA:HBB1	2.02	0.42
18:3b:311:CLA:HHC	18:3b:311:CLA:HBB1	2.00	0.42
29:3b:315:CHL:HHC	29:3b:315:CHL:HBB1	2.00	0.42
3:D:134:LEU:HD12	3:D:134:LEU:HA	1.88	0.42
18:b:828:CLA:HHC	18:b:828:CLA:HBB1	2.02	0.42
12:A:65:ARG:HG2	12:A:179:ALA:HB1	2.01	0.42
18:5a:313:CLA:HHC	18:5a:313:CLA:HBB1	2.01	0.42
18:a:822:CLA:HHC	18:a:822:CLA:HBB1	2.00	0.42
13:2b:164:ARG:HG3	29:2b:306:CHL:C1D	2.50	0.42
18:b:831:CLA:HBA2	18:b:831:CLA:HBD	2.00	0.42
7:h:84:SER:O	7:h:88:GLU:HB2	2.20	0.42
20:A:851:BCR:H20C	20:A:851:BCR:H361	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2a:310:CLA:HBB1	18:2a:310:CLA:HHC	2.02	0.42
12:a:26:PRO:HB2	12:a:42:TRP:HH2	1.84	0.42
18:a:829:CLA:HHC	18:a:829:CLA:HBB1	2.02	0.42
25:3b:316:LUT:H7	25:3b:316:LUT:H181	1.82	0.42
18:5b:313:CLA:HHC	18:5b:313:CLA:HBB1	2.01	0.42
18:B:838:CLA:H12	18:B:854:CLA:H93	2.01	0.42
7:H:128:LYS:HG3	7:H:131:GLN:HE22	1.83	0.42
2:c:18:VAL:HG21	2:c:28:MET:HG2	2.01	0.42
18:A:808:CLA:H201	27:A:845:LHG:H171	2.01	0.42
20:A:851:BCR:H403	20:A:851:BCR:H24C	1.86	0.42
17:K:62:MET:HE1	17:K:123:VAL:HG23	2.02	0.42
12:a:714:LEU:HD21	19:a:843:PQN:H151	2.01	0.42
18:B:806:CLA:HBC1	11:M:12:ILE:HG12	2.02	0.41
20:G:204:BCR:H15C	20:G:204:BCR:H351	1.92	0.41
1:b:60:TRP:HA	18:b:806:CLA:HBB2	2.02	0.41
18:b:805:CLA:H151	18:b:827:CLA:HBB2	2.02	0.41
20:b:851:BCR:H352	18:l:302:CLA:HAB	2.02	0.41
18:A:805:CLA:H151	20:A:847:BCR:H323	2.01	0.41
18:A:806:CLA:H92	18:A:806:CLA:H61	1.87	0.41
18:A:817:CLA:H62	18:A:817:CLA:H41	1.79	0.41
14:3a:158:PRO:HA	14:3a:161:LEU:HD12	2.02	0.41
25:5a:317:LUT:H201	25:5a:317:LUT:H15	1.79	0.41
29:6a:309:CHL:HHC	29:6a:309:CHL:HBB1	2.01	0.41
12:a:144:ALA:HB2	12:a:372:PRO:HD2	2.02	0.41
12:a:681:PHE:HZ	18:a:840:CLA:HBC3	1.84	0.41
18:a:805:CLA:H151	20:a:847:BCR:H323	2.01	0.41
20:a:848:BCR:H15C	20:a:848:BCR:H351	1.90	0.41
1:B:705:ALA:HA	1:B:708:VAL:HB	2.01	0.41
18:B:812:CLA:H51	18:B:817:CLA:HBC3	2.01	0.41
18:B:828:CLA:HHC	18:B:828:CLA:HBB1	2.02	0.41
20:B:851:BCR:H352	18:L:302:CLA:HAB	2.02	0.41
7:H:82:MET:HE3	7:H:82:MET:HB2	1.99	0.41
10:L:182:LYS:HD2	10:L:182:LYS:HA	1.82	0.41
11:M:10:ILE:HG23	20:M:101:BCR:H332	2.03	0.41
5:f:230:ARG:HH12	23:5b:319:LMG:HC91	1.85	0.41
20:f:301:BCR:H381	18:f:305:CLA:HMC2	2.02	0.41
18:2a:302:CLA:HHC	18:2a:302:CLA:HBB1	2.01	0.41
13:2b:214:LEU:HD23	13:2b:214:LEU:HA	1.94	0.41
25:6b:319:LUT:H181	25:6b:319:LUT:H8	2.01	0.41
17:k:72:ALA:HA	17:k:77:LEU:HB3	2.01	0.41
1:B:631:LEU:HD22	1:B:724:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:816:CLA:HBB1	18:B:816:CLA:HHC	2.02	0.41
18:B:824:CLA:HMA1	20:B:845:BCR:H15C	2.02	0.41
20:B:844:BCR:H11C	20:B:844:BCR:H341	1.89	0.41
5:F:202:LYS:HD3	5:F:207:ASP:HB2	2.03	0.41
1:b:649:MET:HE2	20:b:846:BCR:H333	2.02	0.41
18:b:816:CLA:HHC	18:b:816:CLA:HBB1	2.02	0.41
18:b:822:CLA:HBB2	18:b:840:CLA:H62	2.02	0.41
12:A:714:LEU:HD21	19:A:843:PQN:H151	2.01	0.41
13:2a:95:LEU:HD12	13:2a:95:LEU:HA	1.94	0.41
13:2a:164:ARG:HG3	29:2a:306:CHL:C1D	2.50	0.41
18:3a:309:CLA:HHC	18:3a:309:CLA:HBB1	2.02	0.41
25:5a:317:LUT:H11	25:5a:317:LUT:H191	1.84	0.41
20:K:202:BCR:H11C	20:K:202:BCR:H341	1.87	0.41
18:a:823:CLA:H52	18:a:823:CLA:H8	1.88	0.41
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.95	0.41
1:B:301:ILE:HG21	18:B:823:CLA:HAC1	2.02	0.41
18:b:801:CLA:H71	18:a:841:CLA:HMA3	2.01	0.41
18:b:824:CLA:HBB1	18:b:824:CLA:HHC	2.02	0.41
18:b:838:CLA:H12	18:b:854:CLA:H93	2.01	0.41
6:g:105:VAL:HB	6:g:109:GLU:HG3	2.01	0.41
12:A:371:TYR:HB2	12:A:374:LEU:HD13	2.03	0.41
18:3a:312:CLA:HHB	18:3a:313:CLA:HBC3	2.03	0.41
12:a:162:VAL:O	12:a:166:LEU:HD23	2.20	0.41
12:a:332:HIS:CE1	27:a:846:LHG:HC12	2.55	0.41
20:a:847:BCR:H321	20:a:847:BCR:HC8	2.02	0.41
29:2b:313:CHL:HBD	29:2b:313:CHL:HBA1	2.02	0.41
1:B:574:ASP:HA	1:B:577:TYR:HB3	2.03	0.41
1:B:583:MET:HE3	1:B:583:MET:HB3	1.91	0.41
1:B:649:MET:HE2	20:B:846:BCR:H333	2.02	0.41
18:b:809:CLA:H112	20:b:851:BCR:H271	2.03	0.41
10:l:151:CYS:HA	10:l:154:MET:HE2	2.03	0.41
12:A:81:TRP:HZ3	20:A:848:BCR:H322	1.86	0.41
18:A:820:CLA:HHC	18:A:820:CLA:HBB1	2.02	0.41
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	2.02	0.41
20:A:851:BCR:HC7	20:A:851:BCR:H321	1.89	0.41
18:a:820:CLA:HHC	18:a:820:CLA:HBB1	2.02	0.41
20:M:101:BCR:H15C	20:M:101:BCR:H351	1.88	0.41
1:b:301:ILE:HG21	18:b:823:CLA:HAC1	2.02	0.41
18:b:829:CLA:HHC	18:b:829:CLA:HBB1	2.03	0.41
20:g:201:BCR:H311	20:g:201:BCR:HC7	1.76	0.41
18:g:203:CLA:HHC	18:g:203:CLA:HBB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:93:LEU:HD23	10:l:93:LEU:HA	1.93	0.41
12:A:162:VAL:O	12:A:166:LEU:HD23	2.20	0.41
16:6a:119:ALA:HB1	16:6a:138:LEU:HD13	2.01	0.41
12:a:401:ALA:HB2	12:a:587:VAL:HG11	2.02	0.41
18:a:837:CLA:H12	18:a:837:CLA:HBA2	1.72	0.41
20:a:851:BCR:H403	20:a:851:BCR:H24C	1.86	0.41
15:5b:149:TYR:HE2	29:5b:307:CHL:HAB	1.85	0.41
18:5b:309:CLA:HHC	18:5b:309:CLA:HBB1	2.02	0.41
1:B:60:TRP:HA	18:B:806:CLA:HBB2	2.02	0.41
18:B:801:CLA:H62	18:B:801:CLA:H41	1.77	0.41
18:B:809:CLA:H112	20:B:851:BCR:H271	2.03	0.41
2:C:77:MET:HE3	2:C:77:MET:HB3	1.97	0.41
7:H:84:SER:O	7:H:88:GLU:HB2	2.20	0.41
1:b:548:PRO:HB2	4:e:84:GLU:HB2	2.02	0.41
18:b:809:CLA:H143	18:b:809:CLA:H111	1.91	0.41
18:b:831:CLA:H201	20:f:304:BCR:H17C	2.03	0.41
20:j:102:BCR:HC7	20:j:102:BCR:H331	1.71	0.41
20:j:102:BCR:H361	20:j:102:BCR:H20C	1.86	0.41
12:A:332:HIS:CD2	18:A:823:CLA:ND	2.88	0.41
18:2a:301:CLA:H62	18:2a:301:CLA:H41	1.94	0.41
18:a:841:CLA:H152	18:a:841:CLA:H111	1.83	0.41
1:B:655:LEU:HD13	18:B:853:CLA:HAA1	2.02	0.41
10:L:151:CYS:HA	10:L:154:MET:HE2	2.03	0.41
1:b:282:VAL:HG21	18:b:815:CLA:HBB1	2.01	0.41
20:b:842:BCR:H15C	20:b:842:BCR:H351	1.88	0.41
12:A:144:ALA:HB2	12:A:372:PRO:HD2	2.02	0.41
18:A:829:CLA:HHC	18:A:829:CLA:HBB1	2.02	0.41
18:3a:303:CLA:HED2	18:3a:303:CLA:HBD	1.95	0.41
18:a:808:CLA:H201	27:a:845:LHG:H171	2.01	0.41
25:6b:319:LUT:H30	25:6b:319:LUT:H26	2.01	0.41
17:k:62:MET:HE1	17:k:123:VAL:HG23	2.02	0.41
1:B:389:HIS:HE1	18:B:828:CLA:NA	2.18	0.41
18:B:804:CLA:H8	18:B:823:CLA:HBA2	2.03	0.41
20:B:851:BCR:H351	20:B:851:BCR:H15C	1.88	0.41
3:D:92:THR:HA	10:L:75:GLY:H	1.85	0.41
20:F:301:BCR:H381	18:F:305:CLA:HMC2	2.02	0.41
20:M:101:BCR:H11C	20:M:101:BCR:H341	1.89	0.41
1:b:389:HIS:HE1	18:b:828:CLA:NA	2.18	0.41
1:b:404:LYS:HE3	1:b:404:LYS:HB2	1.87	0.41
18:b:801:CLA:HAB	26:a:802:CLO:H7	2.03	0.41
3:d:92:THR:HA	10:l:75:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:154:LYS:HE2	3:d:154:LYS:HB2	1.81	0.41
20:g:204:BCR:H11C	20:g:204:BCR:H341	1.95	0.41
15:5a:149:TYR:HE2	29:5a:307:CHL:HAB	1.85	0.41
18:6a:315:CLA:H11	18:6a:315:CLA:H51	1.85	0.41
25:6a:320:LUT:H31	25:6a:320:LUT:H391	1.98	0.41
12:a:743:ILE:HD12	12:a:743:ILE:HA	1.92	0.41
18:a:817:CLA:H62	18:a:817:CLA:H41	1.79	0.41
18:a:820:CLA:H101	20:a:850:BCR:H12C	2.03	0.41
13:2b:185:LEU:HD21	13:2b:198:PHE:CE2	2.56	0.41
16:6b:141:ILE:HD13	16:6b:141:ILE:HA	1.91	0.41
20:k:202:BCR:H20C	20:k:202:BCR:H361	1.93	0.41
1:B:524:ALA:HB2	18:B:836:CLA:HMA1	2.03	0.41
1:B:568:CYS:HB2	12:A:685:GLY:HA3	2.03	0.41
18:B:829:CLA:HBB1	18:B:829:CLA:HHC	2.03	0.41
1:b:524:ALA:HB2	18:b:836:CLA:HMA1	2.03	0.41
18:b:801:CLA:HBB2	26:a:802:CL0:O1D	2.21	0.41
18:b:824:CLA:HMA1	20:b:845:BCR:H15C	2.02	0.41
20:g:204:BCR:H20C	20:g:204:BCR:H361	1.96	0.41
9:j:1:MET:HE3	13:2b:89:LEU:HA	2.02	0.41
12:A:161:LEU:HD23	12:A:161:LEU:HA	1.95	0.41
13:2a:185:LEU:HD21	13:2a:198:PHE:CE2	2.56	0.41
29:2a:313:CHL:HBA1	29:2a:313:CHL:HBD	2.02	0.41
14:3a:125:ILE:HD13	14:3a:125:ILE:HA	1.96	0.41
12:a:81:TRP:HZ3	20:a:848:BCR:H322	1.86	0.41
18:5b:312:CLA:C1C	18:5b:312:CLA:H51	2.51	0.41
18:B:801:CLA:HBB2	26:A:802:CL0:O1D	2.21	0.40
2:C:16:GLN:HB3	2:C:57:ALA:HB1	2.04	0.40
1:b:631:LEU:HD22	1:b:724:PHE:HA	2.03	0.40
18:b:810:CLA:H13	20:b:842:BCR:H333	2.03	0.40
11:m:10:ILE:HG23	20:m:101:BCR:H332	2.03	0.40
12:A:357:LEU:HD11	18:A:818:CLA:H71	2.03	0.40
18:A:834:CLA:H51	18:A:834:CLA:H8	1.86	0.40
15:5a:198:TYR:HA	15:5a:201:LYS:HG3	2.01	0.40
12:a:357:LEU:HD11	18:a:818:CLA:H71	2.03	0.40
1:B:366:THR:HG23	1:B:729:THR:HB	2.04	0.40
1:B:444:LEU:HD13	1:B:444:LEU:HA	1.93	0.40
18:B:809:CLA:H111	10:L:143:GLY:HA3	2.04	0.40
18:B:810:CLA:H13	20:B:842:BCR:H333	2.03	0.40
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	2.03	0.40
18:B:824:CLA:HHC	18:B:824:CLA:HBB1	2.01	0.40
1:b:568:CYS:HB2	12:a:685:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:806:CLA:HBC1	11:m:12:ILE:HG12	2.02	0.40
18:b:823:CLA:HBB1	18:b:823:CLA:HHC	2.04	0.40
26:A:802:CL0:H2	26:A:802:CL0:H14	1.88	0.40
25:2a:314:LUT:H7	25:2a:314:LUT:H171	1.88	0.40
16:6a:202:PHE:CE1	25:6a:320:LUT:H28	2.57	0.40
20:k:202:BCR:H15C	20:k:202:BCR:H351	1.86	0.40
18:B:802:CLA:H52	18:B:802:CLA:HMB1	2.04	0.40
18:B:852:CLA:C1C	12:A:680:MET:HB2	2.52	0.40
1:b:374:HIS:HE2	18:b:827:CLA:C1B	2.35	0.40
18:b:803:CLA:HBC1	21:b:847:DGD:HA81	2.03	0.40
18:b:835:CLA:HHC	18:b:835:CLA:HBB1	2.04	0.40
18:b:852:CLA:HBC2	12:a:680:MET:HA	2.03	0.40
5:f:175:PHE:HB2	20:f:301:BCR:H321	2.03	0.40
12:A:569:PRO:HB3	12:A:716:ILE:HB	2.02	0.40
20:A:849:BCR:H20C	20:A:849:BCR:H361	1.90	0.40
14:3a:191:PHE:CE2	29:3a:307:CHL:HBB2	2.53	0.40
20:K:202:BCR:H351	20:K:202:BCR:H15C	1.86	0.40
20:a:848:BCR:H11C	20:a:848:BCR:H341	1.91	0.40
16:6b:168:PRO:HB3	18:6b:310:CLA:HBC2	2.04	0.40
1:B:548:PRO:HB2	4:E:84:GLU:HB2	2.03	0.40
18:B:811:CLA:HMD2	20:B:848:BCR:H19C	2.03	0.40
5:F:230:ARG:HH12	23:5a:319:LMG:HC91	1.85	0.40
1:b:655:LEU:HD13	18:b:853:CLA:HAA1	2.02	0.40
2:c:66:ARG:HD2	2:c:66:ARG:HA	1.92	0.40
5:f:90:LEU:HB2	5:f:147:LEU:HD13	2.04	0.40
6:g:77:ALA:HB1	16:6b:147:LEU:HD21	2.04	0.40
18:A:841:CLA:H152	18:A:841:CLA:H111	1.83	0.40
14:3a:248:GLN:HE22	25:3a:316:LUT:H41	1.87	0.40
18:5a:309:CLA:HHC	18:5a:309:CLA:HBB1	2.02	0.40
25:6a:320:LUT:H15	25:6a:320:LUT:H201	1.90	0.40
12:a:371:TYR:HB2	12:a:374:LEU:HD13	2.03	0.40
18:a:816:CLA:HBB1	18:a:816:CLA:HHC	2.03	0.40
16:6b:182:LYS:HE3	16:6b:182:LYS:HB3	1.89	0.40
18:B:803:CLA:HBC1	21:B:847:DGD:HA81	2.03	0.40
7:H:56:PHE:HD1	7:H:64:THR:HG21	1.87	0.40
9:J:1:MET:HE3	13:2a:89:LEU:HA	2.02	0.40
18:b:805:CLA:HBB	18:b:828:CLA:CBB	2.52	0.40
18:A:811:CLA:HAC2	18:A:812:CLA:H143	2.03	0.40
18:A:816:CLA:HHC	18:A:816:CLA:HBB1	2.03	0.40
14:3a:121:ILE:HD12	14:3a:121:ILE:HA	1.89	0.40
18:5a:309:CLA:H52	25:5a:316:LUT:H30	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3b:117:ALA:HA	14:3b:245:TYR:HE2	1.87	0.40
15:5b:233:THR:HG22	15:5b:241:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
1	b	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
2	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	138/215 (64%)	132 (96%)	6 (4%)	0	100	100
3	d	138/215 (64%)	132 (96%)	6 (4%)	0	100	100
4	E	61/132 (46%)	57 (93%)	4 (7%)	0	100	100
4	e	61/132 (46%)	57 (93%)	4 (7%)	0	100	100
5	F	159/246 (65%)	157 (99%)	2 (1%)	0	100	100
5	f	159/246 (65%)	157 (99%)	2 (1%)	0	100	100
6	G	88/161 (55%)	86 (98%)	2 (2%)	0	100	100
6	g	88/161 (55%)	86 (98%)	2 (2%)	0	100	100
7	H	88/142 (62%)	84 (96%)	4 (4%)	0	100	100
7	h	88/142 (62%)	84 (96%)	4 (4%)	0	100	100
8	I	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
8	i	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
9	J	39/42 (93%)	37 (95%)	2 (5%)	0	100	100
9	j	39/42 (93%)	37 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	156/221 (71%)	147 (94%)	9 (6%)	0	100	100
10	l	156/221 (71%)	147 (94%)	9 (6%)	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	m	29/32 (91%)	29 (100%)	0	0	100	100
12	A	733/750 (98%)	716 (98%)	17 (2%)	0	100	100
12	a	733/750 (98%)	716 (98%)	17 (2%)	0	100	100
13	2a	190/267 (71%)	182 (96%)	8 (4%)	0	100	100
13	2b	190/267 (71%)	182 (96%)	8 (4%)	0	100	100
14	3a	208/279 (75%)	200 (96%)	8 (4%)	0	100	100
14	3b	208/279 (75%)	200 (96%)	8 (4%)	0	100	100
15	5a	189/249 (76%)	184 (97%)	5 (3%)	0	100	100
15	5b	189/249 (76%)	184 (97%)	5 (3%)	0	100	100
16	6a	189/243 (78%)	180 (95%)	9 (5%)	0	100	100
16	6b	189/243 (78%)	180 (95%)	9 (5%)	0	100	100
17	K	60/135 (44%)	58 (97%)	2 (3%)	0	100	100
17	k	60/135 (44%)	58 (97%)	2 (3%)	0	100	100
All	All	6338/7930 (80%)	6126 (97%)	212 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	597/598 (100%)	593 (99%)	4 (1%)	76	89
1	b	597/598 (100%)	593 (99%)	4 (1%)	76	89
2	C	68/69 (99%)	67 (98%)	1 (2%)	57	79
2	c	68/69 (99%)	67 (98%)	1 (2%)	57	79
3	D	114/161 (71%)	113 (99%)	1 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	114/161 (71%)	113 (99%)	1 (1%)	70	86
4	E	56/99 (57%)	56 (100%)	0	100	100
4	e	56/99 (57%)	56 (100%)	0	100	100
5	F	129/189 (68%)	126 (98%)	3 (2%)	44	70
5	f	129/189 (68%)	127 (98%)	2 (2%)	55	78
6	G	70/125 (56%)	69 (99%)	1 (1%)	59	80
6	g	70/125 (56%)	69 (99%)	1 (1%)	59	80
7	H	70/107 (65%)	67 (96%)	3 (4%)	26	49
7	h	70/107 (65%)	68 (97%)	2 (3%)	37	63
8	I	31/32 (97%)	31 (100%)	0	100	100
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	35/36 (97%)	33 (94%)	2 (6%)	18	36
9	j	35/36 (97%)	33 (94%)	2 (6%)	18	36
10	L	121/169 (72%)	120 (99%)	1 (1%)	73	88
10	l	121/169 (72%)	120 (99%)	1 (1%)	73	88
11	M	29/30 (97%)	29 (100%)	0	100	100
11	m	29/30 (97%)	29 (100%)	0	100	100
12	A	600/611 (98%)	595 (99%)	5 (1%)	73	88
12	a	600/611 (98%)	595 (99%)	5 (1%)	73	88
13	2a	154/204 (76%)	152 (99%)	2 (1%)	61	81
13	2b	154/204 (76%)	152 (99%)	2 (1%)	61	81
14	3a	165/216 (76%)	158 (96%)	7 (4%)	26	49
14	3b	165/216 (76%)	158 (96%)	7 (4%)	26	49
15	5a	156/202 (77%)	151 (97%)	5 (3%)	34	60
15	5b	156/202 (77%)	151 (97%)	5 (3%)	34	60
16	6a	152/190 (80%)	149 (98%)	3 (2%)	48	73
16	6b	152/190 (80%)	149 (98%)	3 (2%)	48	73
17	K	45/96 (47%)	44 (98%)	1 (2%)	45	71
17	k	45/96 (47%)	44 (98%)	1 (2%)	45	71
All	All	5184/6268 (83%)	5108 (98%)	76 (2%)	55	79

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	106	ARG
1	B	155	LEU
1	B	636	ASN
1	B	640	MET
2	C	27	GLU
3	D	103	GLU
5	F	91	THR
5	F	105	ASN
5	F	237	ASP
6	G	78	LEU
7	H	76	LEU
7	H	82	MET
7	H	120	THR
9	J	14	LEU
9	J	38	VAL
10	L	154	MET
1	b	106	ARG
1	b	155	LEU
1	b	636	ASN
1	b	640	MET
2	c	27	GLU
3	d	103	GLU
5	f	105	ASN
5	f	237	ASP
6	g	78	LEU
7	h	76	LEU
7	h	120	THR
9	j	14	LEU
9	j	38	VAL
10	l	154	MET
12	A	31	ARG
12	A	223	ASP
12	A	465	MET
12	A	579	CYS
12	A	624	THR
13	2a	75	ASP
13	2a	259	VAL
14	3a	91	GLN
14	3a	97	ILE
14	3a	107	ILE
14	3a	145	VAL
14	3a	211	LEU
14	3a	233	LYS

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Mol	Chain	Res	Type
14	3a	257	PHE
15	5a	82	ASP
15	5a	101	MET
15	5a	164	VAL
15	5a	198	TYR
15	5a	233	THR
16	6a	117	GLN
16	6a	144	ILE
16	6a	242	VAL
17	K	111	THR
12	a	31	ARG
12	a	223	ASP
12	a	465	MET
12	a	579	CYS
12	a	624	THR
13	2b	75	ASP
13	2b	259	VAL
14	3b	91	GLN
14	3b	97	ILE
14	3b	107	ILE
14	3b	145	VAL
14	3b	211	LEU
14	3b	233	LYS
14	3b	257	PHE
15	5b	82	ASP
15	5b	101	MET
15	5b	164	VAL
15	5b	198	TYR
15	5b	233	THR
16	6b	117	GLN
16	6b	144	ILE
16	6b	242	VAL
17	k	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	HIS
1	B	350	GLN
1	B	399	ASN
3	D	100	GLN
3	D	132	ASN

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Mol	Chain	Res	Type
3	D	141	GLN
4	E	122	ASN
5	F	162	GLN
5	F	164	HIS
5	F	240	ASN
6	G	155	ASN
7	H	83	GLN
7	H	131	GLN
7	H	140	ASN
9	J	2	GLN
10	L	62	GLN
10	L	129	ASN
10	L	215	ASN
1	b	248	GLN
1	b	331	HIS
1	b	350	GLN
1	b	399	ASN
3	d	100	GLN
3	d	132	ASN
3	d	141	GLN
3	d	172	HIS
4	e	122	ASN
5	f	162	GLN
5	f	164	HIS
5	f	240	ASN
6	g	155	ASN
7	h	131	GLN
7	h	140	ASN
9	j	2	GLN
10	l	62	GLN
10	l	129	ASN
10	l	215	ASN
12	A	186	GLN
12	A	220	GLN
12	A	235	HIS
12	A	483	ASN
12	A	718	GLN
13	2a	183	ASN
13	2a	221	ASN
14	3a	189	GLN
15	5a	65	ASN
15	5a	156	GLN

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Mol	Chain	Res	Type
15	5a	240	HIS
17	K	59	ASN
12	a	186	GLN
12	a	220	GLN
12	a	235	HIS
12	a	483	ASN
12	a	718	GLN
13	2b	183	ASN
13	2b	221	ASN
14	3b	189	GLN
15	5b	65	ASN
15	5b	156	GLN
15	5b	240	HIS
17	k	59	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

412 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
18	CLA	B	822	1	49,53,73	1.35	6 (12%)	58,89,113	1.10	5 (8%)
20	BCR	k	202	-	41,41,41	1.45	7 (17%)	56,56,56	1.78	16 (28%)
20	BCR	f	304	-	41,41,41	1.44	8 (19%)	56,56,56	1.76	15 (26%)
18	CLA	b	808	1	51,55,73	1.38	8 (15%)	60,91,113	1.12	4 (6%)
18	CLA	b	813	1	59,63,73	1.26	6 (10%)	70,101,113	0.93	3 (4%)
18	CLA	3b	312	14	59,63,73	1.25	7 (11%)	70,101,113	1.11	5 (7%)
29	CHL	5a	305	-	40,54,74	1.15	3 (7%)	34,90,114	2.77	10 (29%)
18	CLA	a	840	12	69,73,73	1.19	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	B	823	-	69,73,73	1.17	6 (8%)	82,113,113	1.05	6 (7%)
18	CLA	a	823	12	69,73,73	1.20	8 (11%)	82,113,113	1.01	5 (6%)
18	CLA	3b	306	14	49,53,73	1.38	7 (14%)	58,89,113	1.15	4 (6%)
20	BCR	A	847	-	41,41,41	1.45	9 (21%)	56,56,56	1.86	17 (30%)
20	BCR	i	202	-	41,41,41	1.45	4 (9%)	56,56,56	1.62	13 (23%)
18	CLA	5a	311	15	48,52,73	1.38	7 (14%)	57,88,113	1.13	4 (7%)
29	CHL	2a	305	-	37,51,74	1.16	3 (8%)	30,86,114	2.93	10 (33%)
18	CLA	b	812	1	69,73,73	1.17	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	a	806	12	69,73,73	1.19	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	5a	310	-	49,53,73	1.39	7 (14%)	58,89,113	1.09	3 (5%)
18	CLA	5a	312	15	56,60,73	1.27	6 (10%)	65,97,113	1.15	6 (9%)
23	LMG	b	850	-	42,42,55	0.54	0	50,50,63	0.67	0
25	LUT	3a	317	-	42,43,43	1.36	8 (19%)	51,60,60	2.02	11 (21%)
18	CLA	2b	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.20	4 (6%)
18	CLA	5b	302	15	60,64,73	1.22	6 (10%)	71,102,113	1.01	4 (5%)
18	CLA	6b	315	16	59,63,73	1.28	7 (11%)	70,101,113	1.04	4 (5%)
18	CLA	B	803	1	49,53,73	1.40	7 (14%)	58,89,113	1.04	4 (6%)
18	CLA	a	803	12	65,69,73	1.19	6 (9%)	77,108,113	1.00	4 (5%)
18	CLA	a	839	12	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	b	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.94	3 (3%)
18	CLA	B	854	-	69,73,73	1.20	7 (10%)	82,113,113	1.00	6 (7%)
25	LUT	3b	316	-	42,43,43	1.31	6 (14%)	51,60,60	1.81	15 (29%)
18	CLA	A	840	12	69,73,73	1.19	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	5b	312	15	56,60,73	1.27	6 (10%)	65,97,113	1.16	6 (9%)
18	CLA	6b	308	16	49,53,73	1.47	7 (14%)	58,89,113	1.05	4 (6%)
20	BCR	A	849	-	41,41,41	1.45	8 (19%)	56,56,56	1.71	17 (30%)
18	CLA	5a	315	15	50,54,73	1.39	7 (14%)	59,90,113	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	g	201	-	41,41,41	1.48	4 (9%)	56,56,56	1.74	17 (30%)
18	CLA	B	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.01	4 (4%)
18	CLA	b	822	1	49,53,73	1.35	6 (12%)	58,89,113	1.10	5 (8%)
18	CLA	b	802	-	69,73,73	1.13	6 (8%)	82,113,113	0.98	6 (7%)
20	BCR	G	204	-	41,41,41	1.46	7 (17%)	56,56,56	1.68	15 (26%)
20	BCR	B	848	-	41,41,41	1.40	10 (24%)	56,56,56	2.23	22 (39%)
20	BCR	a	848	-	41,41,41	1.46	7 (17%)	56,56,56	1.72	16 (28%)
18	CLA	B	807	1	65,69,73	1.19	7 (10%)	77,108,113	0.92	3 (3%)
18	CLA	A	804	12	59,63,73	1.25	6 (10%)	70,101,113	1.05	5 (7%)
18	CLA	B	828	1	59,63,73	1.27	7 (11%)	70,101,113	1.05	4 (5%)
18	CLA	B	829	1	49,53,73	1.37	6 (12%)	58,89,113	1.12	5 (8%)
18	CLA	5a	302	15	60,64,73	1.22	6 (10%)	71,102,113	1.01	4 (5%)
18	CLA	a	828	12	69,73,73	1.31	8 (11%)	82,113,113	0.92	3 (3%)
18	CLA	B	809	1	69,73,73	1.17	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	a	820	-	69,73,73	1.19	6 (8%)	82,113,113	0.97	4 (4%)
18	CLA	b	816	1	66,70,73	1.25	7 (10%)	78,109,113	1.06	5 (6%)
20	BCR	B	846	-	41,41,41	1.46	7 (17%)	56,56,56	1.67	13 (23%)
20	BCR	B	843	-	41,41,41	1.46	8 (19%)	56,56,56	2.16	13 (23%)
27	LHG	5b	318	-	31,31,48	0.32	0	34,37,54	0.42	0
25	LUT	6b	318	-	42,43,43	1.29	8 (19%)	51,60,60	1.76	12 (23%)
18	CLA	A	813	12	54,58,73	1.27	5 (9%)	64,95,113	1.10	5 (7%)
18	CLA	b	801	1	69,73,73	1.20	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	6a	305	16	65,69,73	1.17	6 (9%)	77,108,113	0.98	4 (5%)
18	CLA	A	825	-	59,63,73	1.25	7 (11%)	70,101,113	0.97	4 (5%)
28	LMU	6a	302	-	36,36,36	0.26	0	47,47,47	0.67	0
18	CLA	A	822	12	49,53,73	1.41	7 (14%)	58,89,113	1.14	6 (10%)
22	LFA	M	102	-	11,11,19	0.11	0	10,10,18	0.13	0
18	CLA	k	201	17	48,52,73	1.44	8 (16%)	59,88,113	1.06	4 (6%)
18	CLA	b	817	1	69,73,73	1.15	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	3a	305	14	50,54,73	1.36	6 (12%)	59,90,113	1.09	5 (8%)
25	LUT	2a	314	-	42,43,43	1.30	7 (16%)	51,60,60	2.29	15 (29%)
18	CLA	5b	310	-	49,53,73	1.39	7 (14%)	58,89,113	1.09	3 (5%)
18	CLA	6b	317	16	49,53,73	1.39	7 (14%)	58,89,113	1.08	3 (5%)
25	LUT	j	105	-	42,43,43	1.29	7 (16%)	51,60,60	3.07	21 (41%)
18	CLA	B	835	1	54,58,73	1.42	7 (12%)	64,95,113	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	807	1	65,69,73	1.20	7 (10%)	77,108,113	0.92	3 (3%)
18	CLA	6a	310	-	49,53,73	1.40	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	A	811	12	49,53,73	1.36	5 (10%)	58,89,113	1.03	4 (6%)
18	CLA	b	814	1	54,58,73	1.33	6 (11%)	64,95,113	1.04	4 (6%)
18	CLA	2b	309	27	49,53,73	1.39	7 (14%)	58,89,113	1.03	3 (5%)
20	BCR	b	848	-	41,41,41	1.40	10 (24%)	56,56,56	2.23	22 (39%)
20	BCR	a	847	-	41,41,41	1.45	9 (21%)	56,56,56	1.86	17 (30%)
28	LMU	6a	303	-	34,34,36	0.29	0	45,45,47	0.51	0
29	CHL	5b	306	-	37,51,74	1.19	3 (8%)	30,86,114	3.07	12 (40%)
18	CLA	5b	315	15	50,54,73	1.39	7 (14%)	59,90,113	1.03	3 (5%)
20	BCR	B	844	-	41,41,41	1.44	8 (19%)	56,56,56	1.81	17 (30%)
18	CLA	b	824	-	54,58,73	1.28	6 (11%)	64,95,113	1.07	5 (7%)
18	CLA	6a	315	16	59,63,73	1.28	7 (11%)	70,101,113	1.04	4 (5%)
27	LHG	A	846	-	33,33,48	0.34	0	36,39,54	0.47	0
18	CLA	3b	309	14	54,58,73	1.26	6 (11%)	64,95,113	1.07	4 (6%)
18	CLA	2b	308	13	59,63,73	1.22	6 (10%)	70,101,113	1.02	4 (5%)
18	CLA	a	810	12	69,73,73	1.19	6 (8%)	82,113,113	0.89	3 (3%)
20	BCR	A	850	-	41,41,41	1.47	5 (12%)	56,56,56	1.67	15 (26%)
18	CLA	5a	313	15	49,53,73	1.39	7 (14%)	58,89,113	1.04	3 (5%)
18	CLA	a	842	-	49,53,73	1.38	7 (14%)	58,89,113	1.10	5 (8%)
18	CLA	b	837	1	51,55,73	1.35	7 (13%)	60,91,113	1.02	4 (6%)
18	CLA	B	840	27	69,73,73	1.14	6 (8%)	82,113,113	1.03	6 (7%)
20	BCR	j	102	-	41,41,41	1.45	10 (24%)	56,56,56	2.15	21 (37%)
20	BCR	F	304	-	41,41,41	1.44	8 (19%)	56,56,56	1.76	14 (25%)
20	BCR	J	102	-	41,41,41	1.45	10 (24%)	56,56,56	2.15	21 (37%)
27	LHG	5b	320	-	36,36,48	0.31	0	39,42,54	0.47	0
18	CLA	A	853	-	55,59,73	1.29	6 (10%)	64,96,113	1.06	5 (7%)
18	CLA	6a	311	16	49,53,73	1.36	6 (12%)	58,89,113	1.11	3 (5%)
18	CLA	A	831	12	54,58,73	1.33	6 (11%)	64,95,113	0.96	4 (6%)
18	CLA	B	808	1	51,55,73	1.38	8 (15%)	60,91,113	1.11	4 (6%)
18	CLA	a	808	12	69,73,73	1.11	7 (10%)	82,113,113	0.90	4 (4%)
28	LMU	6b	303	-	34,34,36	0.29	0	45,45,47	0.51	0
18	CLA	b	835	1	54,58,73	1.42	7 (12%)	64,95,113	1.10	4 (6%)
25	LUT	6a	320	-	42,43,43	1.31	8 (19%)	51,60,60	1.69	14 (27%)
18	CLA	a	801	12	56,60,73	1.28	6 (10%)	65,97,113	1.05	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	6b	305	16	65,69,73	1.17	6 (9%)	77,108,113	0.98	4 (5%)
29	CHL	3b	301	13	40,54,74	1.11	2 (5%)	34,90,114	2.98	10 (29%)
18	CLA	A	821	12	49,53,73	1.39	7 (14%)	58,89,113	1.09	5 (8%)
25	LUT	2b	315	-	42,43,43	1.36	8 (19%)	51,60,60	2.44	14 (27%)
18	CLA	f	305	-	64,68,73	1.22	7 (10%)	76,107,113	1.02	7 (9%)
18	CLA	3a	312	14	59,63,73	1.25	7 (11%)	70,101,113	1.10	5 (7%)
18	CLA	B	830	1	64,68,73	1.22	7 (10%)	76,107,113	1.07	5 (6%)
18	CLA	b	832	1	64,68,73	1.22	7 (10%)	76,107,113	1.05	5 (6%)
18	CLA	A	824	-	69,73,73	1.24	8 (11%)	82,113,113	0.94	5 (6%)
18	CLA	A	830	12	54,58,73	1.33	7 (12%)	64,95,113	1.17	5 (7%)
18	CLA	g	203	6	49,53,73	1.38	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	b	818	-	57,61,73	1.30	6 (10%)	67,98,113	1.05	4 (5%)
18	CLA	2a	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.14	5 (8%)
18	CLA	a	813	12	54,58,73	1.27	5 (9%)	64,95,113	1.11	5 (7%)
20	BCR	B	842	-	41,41,41	1.45	8 (19%)	56,56,56	1.83	18 (32%)
18	CLA	3b	311	14	47,51,73	1.44	7 (14%)	55,86,113	1.14	4 (7%)
18	CLA	A	829	12	69,73,73	1.20	7 (10%)	82,113,113	0.96	3 (3%)
25	LUT	2a	315	-	42,43,43	1.36	8 (19%)	51,60,60	2.44	14 (27%)
18	CLA	2a	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.20	4 (6%)
18	CLA	3a	302	14	59,63,73	1.23	7 (11%)	70,101,113	0.96	3 (4%)
29	CHL	2b	305	-	37,51,74	1.16	3 (8%)	30,86,114	2.93	10 (33%)
18	CLA	A	837	12	59,63,73	1.26	7 (11%)	70,101,113	1.04	5 (7%)
18	CLA	a	825	-	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
29	CHL	2a	313	13	40,54,74	1.16	2 (5%)	34,90,114	2.91	11 (32%)
18	CLA	3a	314	-	49,53,73	1.36	7 (14%)	58,89,113	1.08	4 (6%)
18	CLA	b	827	1	64,68,73	1.24	7 (10%)	75,106,113	0.90	4 (5%)
24	SF4	c	101	2	0,12,12	-	-	-	-	-
18	CLA	6a	307	-	53,57,73	1.33	7 (13%)	61,93,113	1.07	5 (8%)
18	CLA	B	806	1	64,68,73	1.22	7 (10%)	76,107,113	1.03	4 (5%)
20	BCR	M	101	-	41,41,41	1.45	8 (19%)	56,56,56	1.69	14 (25%)
23	LMG	B	850	-	42,42,55	0.54	0	50,50,63	0.67	0
18	CLA	3b	308	14	49,53,73	1.38	7 (14%)	58,89,113	1.01	3 (5%)
18	CLA	B	816	1	66,70,73	1.25	7 (10%)	78,109,113	1.06	5 (6%)
18	CLA	b	830	1	64,68,73	1.22	6 (9%)	76,107,113	1.07	5 (6%)
18	CLA	f	302	-	49,53,73	1.39	6 (12%)	58,89,113	1.09	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	838	-	69,73,73	1.14	6 (8%)	82,113,113	1.01	7 (8%)
18	CLA	2b	302	13	49,53,73	1.42	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	5a	304	-	49,53,73	1.43	7 (14%)	58,89,113	1.11	5 (8%)
20	BCR	F	301	-	41,41,41	1.45	5 (12%)	56,56,56	1.79	16 (28%)
27	LHG	a	846	-	33,33,48	0.34	0	36,39,54	0.46	0
29	CHL	5a	301	15	40,54,74	1.13	2 (5%)	34,90,114	2.82	10 (29%)
18	CLA	b	805	1	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
27	LHG	2b	316	18	31,31,48	0.33	0	34,37,54	0.46	0
25	LUT	6b	319	-	42,43,43	1.34	8 (19%)	51,60,60	2.66	20 (39%)
20	BCR	a	849	-	41,41,41	1.45	7 (17%)	56,56,56	1.71	17 (30%)
18	CLA	2b	312	13	49,53,73	1.40	7 (14%)	58,89,113	1.12	5 (8%)
18	CLA	B	821	1	59,63,73	1.25	7 (11%)	70,101,113	0.93	5 (7%)
25	LUT	6a	319	-	42,43,43	1.34	8 (19%)	51,60,60	2.66	20 (39%)
18	CLA	A	835	12	49,53,73	1.35	6 (12%)	58,89,113	1.13	4 (6%)
18	CLA	3b	302	14	59,63,73	1.23	7 (11%)	70,101,113	0.96	3 (4%)
18	CLA	b	804	1	69,73,73	1.17	6 (8%)	82,113,113	0.96	4 (4%)
18	CLA	B	833	1	69,73,73	1.13	6 (8%)	82,113,113	0.95	4 (4%)
18	CLA	3a	303	14	54,58,73	1.40	7 (12%)	64,95,113	1.10	5 (7%)
18	CLA	a	811	12	49,53,73	1.36	5 (10%)	58,89,113	1.03	4 (6%)
18	CLA	g	202	6	54,58,73	1.34	8 (14%)	64,95,113	1.04	3 (4%)
18	CLA	5b	308	15	49,53,73	1.34	6 (12%)	58,89,113	1.14	4 (6%)
18	CLA	a	814	12	46,50,73	1.40	7 (15%)	53,85,113	1.08	4 (7%)
18	CLA	6a	308	16	49,53,73	1.47	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	B	853	-	69,73,73	1.17	7 (10%)	82,113,113	0.93	4 (4%)
18	CLA	a	809	12	59,63,73	1.29	6 (10%)	70,101,113	1.09	5 (7%)
18	CLA	a	853	-	55,59,73	1.29	6 (10%)	64,96,113	1.06	5 (7%)
29	CHL	2a	306	-	40,54,74	1.13	4 (10%)	34,90,114	2.40	8 (23%)
18	CLA	a	831	12	54,58,73	1.33	6 (11%)	64,95,113	0.96	4 (6%)
18	CLA	b	811	1	49,53,73	1.39	6 (12%)	58,89,113	1.10	4 (6%)
18	CLA	5a	308	15	49,53,73	1.34	6 (12%)	58,89,113	1.14	4 (6%)
18	CLA	B	811	1	49,53,73	1.39	6 (12%)	58,89,113	1.10	4 (6%)
20	BCR	A	851	-	41,41,41	1.49	7 (17%)	56,56,56	1.78	13 (23%)
18	CLA	L	302	10	64,68,73	1.22	7 (10%)	76,107,113	0.86	3 (3%)
29	CHL	5a	307	-	40,54,74	1.16	3 (7%)	34,90,114	1.99	9 (26%)
18	CLA	j	101	-	49,53,73	1.39	7 (14%)	58,89,113	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	827	12	69,73,73	1.21	7 (10%)	82,113,113	0.94	4 (4%)
18	CLA	J	101	-	49,53,73	1.39	7 (14%)	58,89,113	1.11	4 (6%)
18	CLA	B	839	1	69,73,73	1.24	8 (11%)	82,113,113	0.97	5 (6%)
27	LHG	2a	316	18	31,31,48	0.33	0	34,37,54	0.46	0
27	LHG	5a	320	-	36,36,48	0.31	0	39,42,54	0.47	0
18	CLA	a	821	12	49,53,73	1.39	7 (14%)	58,89,113	1.08	5 (8%)
18	CLA	A	838	12	54,58,73	1.37	7 (12%)	64,95,113	1.03	4 (6%)
20	BCR	a	850	-	41,41,41	1.47	5 (12%)	56,56,56	1.67	15 (26%)
18	CLA	B	820	1	49,53,73	1.41	7 (14%)	58,89,113	1.09	4 (6%)
20	BCR	l	304	-	41,41,41	1.48	9 (21%)	56,56,56	1.93	16 (28%)
18	CLA	6a	314	16	49,53,73	1.42	7 (14%)	58,89,113	1.10	3 (5%)
18	CLA	b	803	1	49,53,73	1.41	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	3a	313	14	46,50,73	1.45	7 (15%)	53,85,113	1.14	4 (7%)
18	CLA	b	834	-	49,53,73	1.41	8 (16%)	58,89,113	1.09	5 (8%)
18	CLA	l	301	10	49,53,73	1.40	7 (14%)	58,89,113	1.18	5 (8%)
18	CLA	a	804	12	59,63,73	1.25	6 (10%)	70,101,113	1.05	5 (7%)
18	CLA	5a	309	15	55,59,73	1.28	6 (10%)	64,96,113	1.11	3 (4%)
18	CLA	G	203	6	49,53,73	1.38	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	5b	304	-	49,53,73	1.43	7 (14%)	58,89,113	1.12	5 (8%)
20	BCR	b	846	-	41,41,41	1.45	7 (17%)	56,56,56	1.66	13 (23%)
18	CLA	A	814	12	46,50,73	1.40	7 (15%)	53,85,113	1.08	4 (7%)
28	LMU	6b	302	-	36,36,36	0.26	0	47,47,47	0.67	0
29	CHL	3a	307	-	40,54,74	1.13	3 (7%)	34,90,114	3.08	12 (35%)
18	CLA	5a	303	15	54,58,73	1.39	7 (12%)	64,95,113	1.03	4 (6%)
18	CLA	2b	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.14	5 (8%)
18	CLA	3a	309	14	54,58,73	1.26	6 (11%)	64,95,113	1.07	4 (6%)
18	CLA	a	818	12	69,73,73	1.17	5 (7%)	82,113,113	1.00	4 (4%)
18	CLA	b	823	-	69,73,73	1.17	6 (8%)	82,113,113	1.05	6 (7%)
22	LFA	m	102	-	11,11,19	0.11	0	10,10,18	0.13	0
19	PQN	B	841	-	34,34,34	0.45	0	43,45,45	0.73	0
18	CLA	2a	312	13	49,53,73	1.40	7 (14%)	58,89,113	1.12	5 (8%)
18	CLA	b	828	1	59,63,73	1.27	7 (11%)	70,101,113	1.05	4 (5%)
23	LMG	5b	319	-	35,35,55	0.58	0	43,43,63	0.72	0
29	CHL	2b	313	13	40,54,74	1.16	2 (5%)	34,90,114	2.91	11 (32%)
18	CLA	L	303	-	46,50,73	1.42	7 (15%)	53,85,113	1.12	4 (7%)
18	CLA	2a	308	13	59,63,73	1.22	6 (10%)	70,101,113	1.02	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PQN	A	843	-	34,34,34	0.37	0	43,45,45	0.64	1 (2%)
18	CLA	b	809	1	69,73,73	1.17	7 (10%)	82,113,113	0.92	3 (3%)
18	CLA	b	806	1	64,68,73	1.22	7 (10%)	76,107,113	1.03	4 (5%)
24	SF4	A	844	12,1	0,12,12	-	-	-		
18	CLA	F	303	5	45,49,73	1.47	7 (15%)	54,84,113	1.19	5 (9%)
18	CLA	A	805	12	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
18	CLA	3b	313	14	46,50,73	1.46	7 (15%)	53,85,113	1.14	4 (7%)
18	CLA	B	810	1	64,68,73	1.25	7 (10%)	76,107,113	0.89	3 (3%)
18	CLA	a	841	-	69,73,73	1.18	7 (10%)	82,113,113	0.90	2 (2%)
22	LFA	b	849	-	11,11,19	0.10	0	10,10,18	0.08	0
27	LHG	5a	318	-	31,31,48	0.32	0	34,37,54	0.42	0
25	LUT	2b	314	-	42,43,43	1.30	7 (16%)	51,60,60	2.30	15 (29%)
18	CLA	A	816	12	64,68,73	1.26	8 (12%)	76,107,113	1.07	6 (7%)
18	CLA	a	805	12	69,73,73	1.14	7 (10%)	82,113,113	0.92	4 (4%)
18	CLA	B	832	1	64,68,73	1.22	7 (10%)	76,107,113	1.05	5 (6%)
20	BCR	G	201	-	41,41,41	1.48	4 (9%)	56,56,56	1.74	17 (30%)
18	CLA	A	841	-	69,73,73	1.18	7 (10%)	82,113,113	0.90	2 (2%)
18	CLA	A	803	12	65,69,73	1.19	6 (9%)	77,108,113	1.00	4 (5%)
20	BCR	B	845	-	41,41,41	1.49	7 (17%)	56,56,56	1.79	18 (32%)
18	CLA	K	201	17	48,52,73	1.44	8 (16%)	59,88,113	1.05	4 (6%)
18	CLA	b	819	1	47,51,73	1.39	6 (12%)	55,86,113	1.12	4 (7%)
18	CLA	A	832	12	69,73,73	1.22	6 (8%)	82,113,113	0.87	2 (2%)
18	CLA	3b	305	14	50,54,73	1.36	6 (12%)	59,90,113	1.09	5 (8%)
20	BCR	I	202	-	41,41,41	1.45	4 (9%)	56,56,56	1.62	13 (23%)
18	CLA	6b	306	16	59,63,73	1.28	7 (11%)	70,101,113	0.98	4 (5%)
28	LMU	A	852	-	36,36,36	0.29	0	47,47,47	0.72	1 (2%)
18	CLA	b	815	1	61,65,73	1.30	7 (11%)	72,103,113	0.99	5 (6%)
25	LUT	5a	316	-	42,43,43	1.32	8 (19%)	51,60,60	1.57	12 (23%)
29	CHL	5b	314	15	37,51,74	1.16	2 (5%)	30,86,114	3.17	11 (36%)
18	CLA	A	815	-	49,53,73	1.37	5 (10%)	58,89,113	1.20	5 (8%)
18	CLA	a	835	12	49,53,73	1.35	6 (12%)	58,89,113	1.13	4 (6%)
18	CLA	5b	313	15	49,53,73	1.39	7 (14%)	58,89,113	1.04	3 (5%)
18	CLA	6a	306	16	59,63,73	1.28	7 (11%)	70,101,113	0.98	4 (5%)
18	CLA	6b	312	16	59,63,73	1.25	6 (10%)	70,101,113	1.12	7 (10%)
26	CL0	a	802	12	58,73,73	0.85	4 (6%)	60,113,113	1.69	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	6b	301	18	38,38,48	0.29	0	41,44,54	0.38	0
18	CLA	A	817	12	61,65,73	1.26	7 (11%)	72,103,113	0.98	4 (5%)
18	CLA	2b	307	13	49,53,73	1.37	6 (12%)	58,89,113	1.09	3 (5%)
22	LFA	B	849	-	11,11,19	0.10	0	10,10,18	0.08	0
29	CHL	3a	315	14	40,54,74	1.12	2 (5%)	34,90,114	2.63	9 (26%)
18	CLA	6a	312	16	59,63,73	1.24	6 (10%)	70,101,113	1.12	8 (11%)
18	CLA	3a	304	-	49,53,73	1.36	7 (14%)	58,89,113	1.07	5 (8%)
20	BCR	m	101	-	41,41,41	1.45	8 (19%)	56,56,56	1.69	14 (25%)
18	CLA	b	836	1	69,73,73	1.14	6 (8%)	82,113,113	0.95	5 (6%)
18	CLA	a	832	12	69,73,73	1.22	6 (8%)	82,113,113	0.87	2 (2%)
18	CLA	a	807	12	52,56,73	1.37	7 (13%)	61,92,113	1.05	3 (4%)
21	DGD	b	847	-	60,60,67	0.56	0	74,74,81	0.74	1 (1%)
18	CLA	B	826	1	62,66,73	1.24	7 (11%)	73,104,113	0.93	3 (4%)
18	CLA	B	824	-	54,58,73	1.28	6 (11%)	64,95,113	1.07	5 (7%)
18	CLA	B	827	1	64,68,73	1.24	7 (10%)	75,106,113	0.90	4 (5%)
18	CLA	a	827	12	69,73,73	1.21	7 (10%)	82,113,113	0.94	4 (4%)
23	LMG	I	201	-	31,31,55	0.59	0	39,39,63	0.82	1 (2%)
18	CLA	A	834	12	64,68,73	1.20	6 (9%)	76,107,113	0.95	3 (3%)
18	CLA	a	830	12	54,58,73	1.33	7 (12%)	64,95,113	1.17	6 (9%)
18	CLA	b	810	1	64,68,73	1.25	7 (10%)	76,107,113	0.89	3 (3%)
25	LUT	6b	320	-	42,43,43	1.31	8 (19%)	51,60,60	1.69	14 (27%)
18	CLA	b	852	-	69,73,73	1.18	8 (11%)	82,113,113	0.85	4 (4%)
18	CLA	a	815	-	49,53,73	1.37	5 (10%)	58,89,113	1.20	5 (8%)
23	LMG	j	103	-	30,30,55	0.64	0	38,38,63	0.74	0
18	CLA	A	801	12	56,60,73	1.28	6 (10%)	65,97,113	1.05	5 (7%)
18	CLA	A	819	12	49,53,73	1.39	7 (14%)	58,89,113	1.06	4 (6%)
29	CHL	2b	304	-	40,54,74	1.13	2 (5%)	34,90,114	2.88	11 (32%)
20	BCR	b	845	-	41,41,41	1.49	7 (17%)	56,56,56	1.79	18 (32%)
29	CHL	5a	306	-	37,51,74	1.19	3 (8%)	30,86,114	3.07	12 (40%)
19	PQN	b	841	-	34,34,34	0.45	0	43,45,45	0.73	0
18	CLA	l	303	-	46,50,73	1.42	7 (15%)	53,85,113	1.12	4 (7%)
18	CLA	B	804	1	69,73,73	1.17	6 (8%)	82,113,113	0.96	4 (4%)
25	LUT	3a	316	-	42,43,43	1.31	6 (14%)	51,60,60	1.81	15 (29%)
29	CHL	3b	315	14	40,54,74	1.12	2 (5%)	34,90,114	2.63	9 (26%)
18	CLA	A	836	12	55,59,73	1.41	7 (12%)	64,96,113	1.12	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LUT	6a	318	-	42,43,43	1.29	8 (19%)	51,60,60	1.76	12 (23%)
18	CLA	5b	303	15	54,58,73	1.39	7 (12%)	64,95,113	1.04	4 (6%)
18	CLA	6b	311	16	49,53,73	1.36	6 (12%)	58,89,113	1.11	3 (5%)
18	CLA	3b	303	14	54,58,73	1.40	7 (12%)	64,95,113	1.10	5 (7%)
18	CLA	6b	313	-	49,53,73	1.36	6 (12%)	58,89,113	1.11	4 (6%)
18	CLA	b	826	1	62,66,73	1.24	7 (11%)	73,104,113	0.93	3 (4%)
29	CHL	2a	304	-	40,54,74	1.14	2 (5%)	34,90,114	2.88	11 (32%)
24	SF4	C	102	2	0,12,12	-	-	-		
18	CLA	B	805	1	69,73,73	1.20	7 (10%)	82,113,113	0.95	4 (4%)
18	CLA	3a	311	14	47,51,73	1.44	7 (14%)	55,86,113	1.14	4 (7%)
26	CL0	A	802	12	58,73,73	0.85	4 (6%)	60,113,113	1.69	8 (13%)
18	CLA	5b	311	15	48,52,73	1.39	7 (14%)	57,88,113	1.13	4 (7%)
18	CLA	A	809	12	59,63,73	1.30	6 (10%)	70,101,113	1.09	5 (7%)
18	CLA	a	816	12	64,68,73	1.26	8 (12%)	76,107,113	1.07	6 (7%)
20	BCR	b	842	-	41,41,41	1.45	8 (19%)	56,56,56	1.83	18 (32%)
18	CLA	3b	314	-	49,53,73	1.36	7 (14%)	58,89,113	1.08	4 (6%)
18	CLA	B	834	-	49,53,73	1.41	8 (16%)	58,89,113	1.09	5 (8%)
29	CHL	5b	307	-	40,54,74	1.16	3 (7%)	34,90,114	2.00	9 (26%)
19	PQN	a	843	-	34,34,34	0.37	0	43,45,45	0.63	1 (2%)
29	CHL	5b	301	15	40,54,74	1.13	2 (5%)	34,90,114	2.82	10 (29%)
18	CLA	l	302	10	64,68,73	1.22	7 (10%)	76,107,113	0.86	3 (3%)
20	BCR	a	851	-	41,41,41	1.49	7 (17%)	56,56,56	1.78	13 (23%)
29	CHL	5b	305	-	40,54,74	1.15	3 (7%)	34,90,114	2.77	10 (29%)
18	CLA	B	802	-	69,73,73	1.13	6 (8%)	82,113,113	0.98	6 (7%)
25	LUT	5b	317	-	42,43,43	1.31	8 (19%)	51,60,60	1.78	14 (27%)
18	CLA	A	808	12	69,73,73	1.11	7 (10%)	82,113,113	0.90	4 (4%)
20	BCR	b	851	-	41,41,41	1.43	8 (19%)	56,56,56	1.78	16 (28%)
18	CLA	a	817	12	61,65,73	1.26	7 (11%)	72,103,113	0.98	4 (5%)
29	CHL	6b	309	16	35,49,74	1.41	2 (5%)	28,84,114	3.04	10 (35%)
18	CLA	A	826	12	69,73,73	1.21	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	5b	309	15	55,59,73	1.28	6 (10%)	64,96,113	1.11	3 (4%)
18	CLA	a	838	12	54,58,73	1.36	7 (12%)	64,95,113	1.03	3 (4%)
18	CLA	B	815	1	61,65,73	1.30	7 (11%)	72,103,113	0.99	5 (6%)
18	CLA	6a	313	-	49,53,73	1.36	6 (12%)	58,89,113	1.11	4 (6%)
18	CLA	b	839	1	69,73,73	1.25	8 (11%)	82,113,113	0.97	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	812	12	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
29	CHL	5a	314	15	37,51,74	1.16	2 (5%)	30,86,114	3.17	11 (36%)
29	CHL	6a	309	16	35,49,74	1.40	2 (5%)	28,84,114	3.05	10 (35%)
18	CLA	A	818	12	69,73,73	1.17	5 (7%)	82,113,113	1.00	4 (4%)
29	CHL	2b	306	-	40,54,74	1.13	4 (10%)	34,90,114	2.40	8 (23%)
24	SF4	c	102	2	0,12,12	-	-	-		
18	CLA	6b	307	-	53,57,73	1.33	7 (13%)	61,93,113	1.07	5 (8%)
18	CLA	F	302	-	49,53,73	1.39	6 (12%)	58,89,113	1.09	3 (5%)
18	CLA	a	834	12	64,68,73	1.20	6 (9%)	76,107,113	0.95	3 (3%)
23	LMG	J	103	-	30,30,55	0.64	0	38,38,63	0.74	0
18	CLA	2a	302	13	49,53,73	1.43	7 (14%)	58,89,113	1.05	4 (6%)
18	CLA	b	821	1	59,63,73	1.25	7 (11%)	70,101,113	0.93	5 (7%)
27	LHG	6a	301	18	38,38,48	0.29	0	41,44,54	0.38	0
18	CLA	6b	316	16	49,53,73	1.37	6 (12%)	58,89,113	1.09	4 (6%)
28	LMU	a	852	-	36,36,36	0.29	0	47,47,47	0.72	1 (2%)
18	CLA	b	854	-	69,73,73	1.20	7 (10%)	82,113,113	1.00	6 (7%)
18	CLA	a	819	12	49,53,73	1.40	7 (14%)	58,89,113	1.06	4 (6%)
18	CLA	b	833	1	69,73,73	1.13	6 (8%)	82,113,113	0.95	4 (4%)
18	CLA	a	826	12	69,73,73	1.21	7 (10%)	82,113,113	0.87	3 (3%)
20	BCR	B	851	-	41,41,41	1.43	8 (19%)	56,56,56	1.78	16 (28%)
18	CLA	a	837	12	59,63,73	1.26	7 (11%)	70,101,113	1.04	5 (7%)
18	CLA	2b	311	13	49,53,73	1.39	8 (16%)	58,89,113	1.12	5 (8%)
18	CLA	b	853	-	69,73,73	1.18	7 (10%)	82,113,113	0.94	4 (4%)
29	CHL	3a	301	13	40,54,74	1.11	2 (5%)	34,90,114	2.98	10 (29%)
24	SF4	C	101	2	0,12,12	-	-	-		
18	CLA	b	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.01	4 (4%)
18	CLA	B	817	1	69,73,73	1.15	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	A	810	12	69,73,73	1.19	6 (8%)	82,113,113	0.89	3 (3%)
18	CLA	B	838	-	69,73,73	1.14	6 (8%)	82,113,113	1.02	7 (8%)
18	CLA	A	823	12	69,73,73	1.20	8 (11%)	82,113,113	1.00	5 (6%)
18	CLA	A	807	12	52,56,73	1.37	7 (13%)	61,92,113	1.05	3 (4%)
29	CHL	6a	304	16	40,54,74	1.19	2 (5%)	34,90,114	2.66	10 (29%)
18	CLA	b	829	1	49,53,73	1.37	6 (12%)	58,89,113	1.12	5 (8%)
18	CLA	B	836	1	69,73,73	1.14	6 (8%)	82,113,113	0.95	5 (6%)
18	CLA	a	836	12	55,59,73	1.41	7 (12%)	64,96,113	1.12	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	a	822	12	49,53,73	1.41	7 (14%)	58,89,113	1.14	6 (10%)
18	CLA	B	814	1	54,58,73	1.33	6 (11%)	64,95,113	1.04	3 (4%)
18	CLA	2b	301	13	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
21	DGD	B	847	-	60,60,67	0.56	0	74,74,81	0.74	1 (1%)
25	LUT	J	105	-	42,43,43	1.30	7 (16%)	51,60,60	3.07	21 (41%)
18	CLA	a	833	12	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
23	LMG	i	201	-	31,31,55	0.59	0	39,39,63	0.82	1 (2%)
18	CLA	b	820	1	49,53,73	1.41	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	2a	311	13	49,53,73	1.39	8 (16%)	58,89,113	1.12	5 (8%)
18	CLA	A	839	12	69,73,73	1.19	7 (10%)	82,113,113	0.87	3 (3%)
18	CLA	f	303	5	45,49,73	1.47	7 (15%)	54,84,113	1.19	5 (9%)
20	BCR	b	843	-	41,41,41	1.46	8 (19%)	56,56,56	2.16	13 (23%)
23	LMG	5a	319	-	35,35,55	0.58	0	43,43,63	0.72	0
18	CLA	a	812	12	69,73,73	1.18	7 (10%)	82,113,113	0.91	3 (3%)
18	CLA	B	819	1	47,51,73	1.39	6 (12%)	55,86,113	1.12	4 (7%)
18	CLA	A	820	-	69,73,73	1.18	6 (8%)	82,113,113	0.97	4 (4%)
18	CLA	6b	314	16	49,53,73	1.43	7 (14%)	58,89,113	1.10	3 (5%)
20	BCR	b	844	-	41,41,41	1.44	8 (19%)	56,56,56	1.81	17 (30%)
18	CLA	3a	306	14	49,53,73	1.38	7 (14%)	58,89,113	1.15	4 (6%)
18	CLA	2a	307	13	49,53,73	1.37	6 (12%)	58,89,113	1.09	3 (5%)
18	CLA	B	852	-	69,73,73	1.18	8 (11%)	82,113,113	0.86	4 (4%)
18	CLA	B	837	1	51,55,73	1.35	7 (13%)	60,91,113	1.02	4 (6%)
20	BCR	f	301	-	41,41,41	1.45	5 (12%)	56,56,56	1.79	16 (28%)
18	CLA	2a	301	13	59,63,73	1.24	7 (11%)	70,101,113	0.97	4 (5%)
29	CHL	6b	304	16	40,54,74	1.19	2 (5%)	34,90,114	2.66	10 (29%)
20	BCR	L	304	-	41,41,41	1.48	9 (21%)	56,56,56	1.93	16 (28%)
18	CLA	3a	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.09	4 (6%)
24	SF4	a	844	12,1	0,12,12	-	-	-	-	-
18	CLA	2a	309	27	49,53,73	1.39	7 (14%)	58,89,113	1.03	3 (5%)
18	CLA	B	813	1	59,63,73	1.26	6 (10%)	70,101,113	0.93	3 (4%)
29	CHL	3b	307	-	40,54,74	1.14	3 (7%)	34,90,114	3.07	12 (35%)
18	CLA	L	301	10	49,53,73	1.40	7 (14%)	58,89,113	1.18	5 (8%)
20	BCR	A	848	-	41,41,41	1.46	7 (17%)	56,56,56	1.72	16 (28%)
25	LUT	5b	316	-	42,43,43	1.32	8 (19%)	51,60,60	1.57	12 (23%)
23	LMG	j	104	-	41,41,55	0.54	0	49,49,63	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	833	12	69,73,73	1.20	7 (10%)	82,113,113	0.90	3 (3%)
18	CLA	A	828	12	69,73,73	1.31	8 (11%)	82,113,113	0.92	3 (3%)
23	LMG	J	104	-	41,41,55	0.54	0	49,49,63	0.63	0
18	CLA	F	305	-	64,68,73	1.22	7 (10%)	76,107,113	1.02	7 (9%)
18	CLA	G	202	6	54,58,73	1.34	8 (14%)	64,95,113	1.03	3 (4%)
18	CLA	A	842	-	49,53,73	1.38	7 (14%)	58,89,113	1.10	5 (8%)
27	LHG	a	845	-	48,48,48	0.28	0	51,54,54	0.35	0
18	CLA	A	806	12	69,73,73	1.19	8 (11%)	82,113,113	0.87	3 (3%)
20	BCR	K	202	-	41,41,41	1.46	7 (17%)	56,56,56	1.78	16 (28%)
18	CLA	6a	317	16	49,53,73	1.39	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	B	812	1	69,73,73	1.18	7 (10%)	82,113,113	0.91	4 (4%)
18	CLA	a	829	12	69,73,73	1.20	7 (10%)	82,113,113	0.96	3 (3%)
25	LUT	5a	317	-	42,43,43	1.31	8 (19%)	51,60,60	1.78	14 (27%)
18	CLA	B	801	1	69,73,73	1.20	8 (11%)	82,113,113	0.88	3 (3%)
18	CLA	6b	310	-	49,53,73	1.40	7 (14%)	58,89,113	1.08	3 (5%)
18	CLA	6a	316	16	49,53,73	1.37	6 (12%)	58,89,113	1.08	4 (6%)
25	LUT	3b	317	-	42,43,43	1.36	8 (19%)	51,60,60	2.02	11 (21%)
18	CLA	B	818	-	57,61,73	1.30	6 (10%)	67,98,113	1.05	4 (5%)
18	CLA	3a	308	14	49,53,73	1.37	7 (14%)	58,89,113	1.01	3 (5%)
18	CLA	b	840	27	69,73,73	1.14	6 (8%)	82,113,113	1.03	6 (7%)
18	CLA	a	824	-	69,73,73	1.24	8 (11%)	82,113,113	0.94	5 (6%)
20	BCR	g	204	-	41,41,41	1.45	7 (17%)	56,56,56	1.68	15 (26%)
18	CLA	3b	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.09	4 (6%)
27	LHG	A	845	-	48,48,48	0.28	0	51,54,54	0.35	0
18	CLA	B	825	1	69,73,73	1.23	7 (10%)	82,113,113	0.94	3 (3%)
18	CLA	3b	304	-	49,53,73	1.36	7 (14%)	58,89,113	1.07	5 (8%)

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
18	CLA	B	822	1	-	2/15/91/115	-
20	BCR	k	202	-	-	3/29/63/63	0/2/2/2
20	BCR	f	304	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	808	1	1/1/11/20	2/18/94/115	-
18	CLA	b	813	1	-	2/27/103/115	-
18	CLA	3b	312	14	-	5/27/103/115	-
29	CHL	5a	305	-	3/3/16/26	2/15/113/137	-
18	CLA	a	840	12	1/1/15/20	0/39/115/115	-
18	CLA	B	823	-	1/1/15/20	8/39/115/115	-
18	CLA	a	823	12	-	1/39/115/115	-
18	CLA	3b	306	14	1/1/11/20	0/15/91/115	-
20	BCR	A	847	-	-	3/29/63/63	0/2/2/2
20	BCR	i	202	-	-	2/29/63/63	0/2/2/2
18	CLA	5a	311	15	1/1/11/20	3/13/89/115	-
29	CHL	2a	305	-	3/3/15/26	2/12/110/137	-
18	CLA	b	812	1	1/1/15/20	5/39/115/115	-
18	CLA	a	806	12	1/1/15/20	8/39/115/115	-
18	CLA	5a	310	-	1/1/11/20	2/15/91/115	-
18	CLA	5a	312	15	-	5/24/100/115	-
23	LMG	b	850	-	-	18/37/57/70	0/1/1/1
25	LUT	3a	317	-	-	4/29/67/67	0/2/2/2
18	CLA	2b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	5b	302	15	-	8/29/105/115	-
18	CLA	6b	315	16	1/1/13/20	2/27/103/115	-
18	CLA	B	803	1	1/1/11/20	2/15/91/115	-
18	CLA	a	803	12	1/1/14/20	3/35/111/115	-
18	CLA	a	839	12	-	3/39/115/115	-
18	CLA	b	825	1	1/1/15/20	0/39/115/115	-
18	CLA	B	854	-	1/1/15/20	6/39/115/115	-
25	LUT	3b	316	-	-	0/29/67/67	0/2/2/2
18	CLA	A	840	12	1/1/15/20	0/39/115/115	-
18	CLA	5b	312	15	-	5/24/100/115	-
18	CLA	6b	308	16	1/1/11/20	2/15/91/115	-
20	BCR	A	849	-	-	3/29/63/63	0/2/2/2
18	CLA	5a	315	15	-	2/17/93/115	-
20	BCR	g	201	-	-	4/29/63/63	0/2/2/2
18	CLA	B	831	1	1/1/15/20	2/39/115/115	-
18	CLA	b	822	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	802	-	1/1/15/20	1/39/115/115	-
20	BCR	G	204	-	-	2/29/63/63	0/2/2/2
20	BCR	B	848	-	-	6/29/63/63	0/2/2/2
20	BCR	a	848	-	-	3/29/63/63	0/2/2/2
18	CLA	B	807	1	1/1/14/20	0/35/111/115	-
18	CLA	A	804	12	1/1/13/20	3/27/103/115	-
18	CLA	a	828	12	-	3/39/115/115	-
18	CLA	B	828	1	-	5/27/103/115	-
18	CLA	B	829	1	-	2/15/91/115	-
18	CLA	5a	302	15	-	8/29/105/115	-
18	CLA	B	809	1	1/1/15/20	8/39/115/115	-
18	CLA	a	820	-	-	3/39/115/115	-
18	CLA	b	816	1	1/1/14/20	6/36/112/115	-
20	BCR	B	846	-	-	1/29/63/63	0/2/2/2
20	BCR	B	843	-	-	11/29/63/63	0/2/2/2
27	LHG	5b	318	-	-	6/36/36/53	-
25	LUT	6b	318	-	-	3/29/67/67	0/2/2/2
18	CLA	A	813	12	1/1/12/20	1/21/97/115	-
18	CLA	b	801	1	1/1/15/20	7/39/115/115	-
18	CLA	6a	305	16	-	4/35/111/115	-
18	CLA	A	825	-	1/1/13/20	0/27/103/115	-
28	LMU	6a	302	-	-	8/21/61/61	0/2/2/2
18	CLA	A	822	12	1/1/11/20	2/15/91/115	-
22	LFA	M	102	-	-	0/9/9/17	-
18	CLA	k	201	17	1/1/11/20	2/13/89/115	-
18	CLA	b	817	1	1/1/15/20	5/39/115/115	-
18	CLA	3a	305	14	-	3/17/93/115	-
25	LUT	2a	314	-	-	8/29/67/67	0/2/2/2
18	CLA	5b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	6b	317	16	1/1/11/20	3/15/91/115	-
25	LUT	j	105	-	-	10/29/67/67	0/2/2/2
18	CLA	B	835	1	1/1/12/20	0/21/97/115	-
18	CLA	b	807	1	1/1/14/20	0/35/111/115	-
18	CLA	6a	310	-	1/1/11/20	2/15/91/115	-
18	CLA	A	811	12	1/1/11/20	4/15/91/115	-
18	CLA	b	814	1	-	1/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2b	309	27	1/1/11/20	2/15/91/115	-
20	BCR	b	848	-	-	6/29/63/63	0/2/2/2
20	BCR	a	847	-	-	3/29/63/63	0/2/2/2
28	LMU	6a	303	-	-	4/19/59/61	0/2/2/2
29	CHL	5b	306	-	3/3/15/26	4/12/110/137	-
18	CLA	5b	315	15	-	2/17/93/115	-
20	BCR	B	844	-	-	3/29/63/63	0/2/2/2
18	CLA	b	824	-	1/1/12/20	2/21/97/115	-
18	CLA	6a	315	16	1/1/13/20	2/27/103/115	-
27	LHG	A	846	-	-	13/38/38/53	-
18	CLA	3b	309	14	-	1/21/97/115	-
18	CLA	2b	308	13	1/1/13/20	6/27/103/115	-
18	CLA	a	810	12	-	4/39/115/115	-
20	BCR	A	850	-	-	0/29/63/63	0/2/2/2
18	CLA	5a	313	15	1/1/11/20	1/15/91/115	-
18	CLA	a	842	-	-	3/15/91/115	-
18	CLA	b	837	1	1/1/11/20	0/18/94/115	-
18	CLA	B	840	27	1/1/15/20	10/39/115/115	-
20	BCR	j	102	-	-	6/29/63/63	0/2/2/2
20	BCR	F	304	-	-	5/29/63/63	0/2/2/2
20	BCR	J	102	-	-	6/29/63/63	0/2/2/2
27	LHG	5b	320	-	-	5/41/41/53	-
18	CLA	A	853	-	-	1/23/99/115	-
18	CLA	6a	311	16	1/1/11/20	0/15/91/115	-
18	CLA	A	831	12	1/1/12/20	0/21/97/115	-
18	CLA	B	808	1	1/1/11/20	2/18/94/115	-
18	CLA	a	808	12	1/1/15/20	3/39/115/115	-
28	LMU	6b	303	-	-	4/19/59/61	0/2/2/2
18	CLA	b	835	1	1/1/12/20	0/21/97/115	-
25	LUT	6a	320	-	-	3/29/67/67	0/2/2/2
18	CLA	a	801	12	-	2/24/100/115	-
18	CLA	6b	305	16	-	4/35/111/115	-
29	CHL	3b	301	13	3/3/16/26	0/15/113/137	-
18	CLA	A	821	12	-	2/15/91/115	-
25	LUT	2b	315	-	-	4/29/67/67	0/2/2/2
18	CLA	f	305	-	1/1/14/20	3/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3a	312	14	-	5/27/103/115	-
18	CLA	B	830	1	1/1/14/20	11/33/109/115	-
18	CLA	A	824	-	1/1/15/20	2/39/115/115	-
18	CLA	b	832	1	-	7/33/109/115	-
18	CLA	A	830	12	-	5/21/97/115	-
18	CLA	g	203	6	1/1/11/20	4/15/91/115	-
18	CLA	b	818	-	-	0/25/101/115	-
18	CLA	2a	303	-	1/1/11/20	2/15/91/115	-
18	CLA	a	813	12	1/1/12/20	1/21/97/115	-
20	BCR	B	842	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	311	14	1/1/10/20	0/13/89/115	-
18	CLA	A	829	12	-	6/39/115/115	-
25	LUT	2a	315	-	-	4/29/67/67	0/2/2/2
18	CLA	2a	310	-	1/1/11/20	2/15/91/115	-
29	CHL	2b	305	-	3/3/15/26	2/12/110/137	-
18	CLA	3a	302	14	-	4/27/103/115	-
18	CLA	A	837	12	1/1/13/20	3/27/103/115	-
18	CLA	a	825	-	1/1/13/20	0/27/103/115	-
29	CHL	2a	313	13	3/3/16/26	6/15/113/137	-
18	CLA	3a	314	-	1/1/11/20	2/15/91/115	-
18	CLA	b	827	1	-	1/33/109/115	-
24	SF4	c	101	2	-	-	0/6/5/5
18	CLA	6a	307	-	-	2/20/96/115	-
18	CLA	B	806	1	-	2/33/109/115	-
20	BCR	M	101	-	-	4/29/63/63	0/2/2/2
23	LMG	B	850	-	-	18/37/57/70	0/1/1/1
18	CLA	3b	308	14	1/1/11/20	0/15/91/115	-
18	CLA	B	816	1	1/1/14/20	6/36/112/115	-
18	CLA	b	830	1	1/1/14/20	11/33/109/115	-
18	CLA	f	302	-	1/1/11/20	2/15/91/115	-
18	CLA	b	838	-	-	6/39/115/115	-
18	CLA	2b	302	13	1/1/11/20	2/15/91/115	-
29	CHL	5a	301	15	3/3/16/26	2/15/113/137	-
18	CLA	5a	304	-	-	2/15/91/115	-
20	BCR	F	301	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	a	846	-	-	13/38/38/53	-
18	CLA	b	805	1	1/1/15/20	10/39/115/115	-
27	LHG	2b	316	18	-	5/36/36/53	-
25	LUT	6b	319	-	-	16/29/67/67	0/2/2/2
20	BCR	a	849	-	-	3/29/63/63	0/2/2/2
18	CLA	2b	312	13	1/1/11/20	2/15/91/115	-
18	CLA	B	821	1	1/1/13/20	4/27/103/115	-
25	LUT	6a	319	-	-	16/29/67/67	0/2/2/2
18	CLA	A	835	12	1/1/11/20	3/15/91/115	-
18	CLA	3b	302	14	-	4/27/103/115	-
18	CLA	b	804	1	1/1/15/20	4/39/115/115	-
18	CLA	B	833	1	1/1/15/20	5/39/115/115	-
18	CLA	3a	303	14	1/1/12/20	4/21/97/115	-
18	CLA	a	811	12	1/1/11/20	4/15/91/115	-
18	CLA	g	202	6	1/1/12/20	1/21/97/115	-
18	CLA	5b	308	15	1/1/11/20	2/15/91/115	-
18	CLA	a	814	12	1/1/10/20	0/12/88/115	-
18	CLA	6a	308	16	1/1/11/20	2/15/91/115	-
18	CLA	a	853	-	-	1/23/99/115	-
18	CLA	B	853	-	1/1/15/20	3/39/115/115	-
18	CLA	a	809	12	1/1/13/20	3/27/103/115	-
29	CHL	2a	306	-	2/2/16/26	10/15/113/137	-
18	CLA	a	831	12	1/1/12/20	0/21/97/115	-
18	CLA	b	811	1	-	3/15/91/115	-
18	CLA	5a	308	15	1/1/11/20	2/15/91/115	-
18	CLA	B	811	1	-	3/15/91/115	-
20	BCR	A	851	-	-	8/29/63/63	0/2/2/2
18	CLA	L	302	10	-	0/33/109/115	-
29	CHL	5a	307	-	2/2/16/26	7/15/113/137	-
18	CLA	j	101	-	1/1/11/20	2/15/91/115	-
18	CLA	A	827	12	1/1/15/20	5/39/115/115	-
18	CLA	J	101	-	1/1/11/20	2/15/91/115	-
18	CLA	B	839	1	-	2/39/115/115	-
27	LHG	2a	316	18	-	5/36/36/53	-
27	LHG	5a	320	-	-	5/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	821	12	-	2/15/91/115	-
18	CLA	A	838	12	1/1/12/20	0/21/97/115	-
20	BCR	a	850	-	-	0/29/63/63	0/2/2/2
18	CLA	B	820	1	-	2/15/91/115	-
20	BCR	l	304	-	-	2/29/63/63	0/2/2/2
18	CLA	6a	314	16	1/1/11/20	2/15/91/115	-
18	CLA	b	803	1	1/1/11/20	2/15/91/115	-
18	CLA	3a	313	14	1/1/10/20	0/12/88/115	-
18	CLA	b	834	-	1/1/11/20	0/15/91/115	-
18	CLA	l	301	10	1/1/11/20	4/15/91/115	-
18	CLA	a	804	12	1/1/13/20	3/27/103/115	-
18	CLA	5a	309	15	-	2/23/99/115	-
18	CLA	G	203	6	1/1/11/20	4/15/91/115	-
18	CLA	5b	304	-	-	2/15/91/115	-
20	BCR	b	846	-	-	1/29/63/63	0/2/2/2
18	CLA	A	814	12	1/1/10/20	0/12/88/115	-
28	LMU	6b	302	-	-	8/21/61/61	0/2/2/2
29	CHL	3a	307	-	3/3/16/26	3/15/113/137	-
18	CLA	5a	303	15	1/1/12/20	6/21/97/115	-
18	CLA	2b	303	-	1/1/11/20	2/15/91/115	-
18	CLA	3a	309	14	-	1/21/97/115	-
18	CLA	a	818	12	1/1/15/20	4/39/115/115	-
18	CLA	b	823	-	1/1/15/20	8/39/115/115	-
22	LFA	m	102	-	-	0/9/9/17	-
19	PQN	B	841	-	-	0/23/43/43	0/2/2/2
18	CLA	2a	312	13	1/1/11/20	2/15/91/115	-
18	CLA	b	828	1	-	4/27/103/115	-
23	LMG	5b	319	-	-	5/30/50/70	0/1/1/1
29	CHL	2b	313	13	3/3/16/26	6/15/113/137	-
18	CLA	L	303	-	1/1/10/20	1/12/88/115	-
18	CLA	2a	308	13	1/1/13/20	6/27/103/115	-
19	PQN	A	843	-	-	4/23/43/43	0/2/2/2
18	CLA	b	809	1	1/1/15/20	8/39/115/115	-
18	CLA	b	806	1	-	2/33/109/115	-
24	SF4	A	844	12,1	-	-	0/6/5/5
18	CLA	F	303	5	1/1/10/20	0/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	805	12	1/1/15/20	5/39/115/115	-
18	CLA	3b	313	14	1/1/10/20	0/12/88/115	-
18	CLA	B	810	1	-	5/33/109/115	-
18	CLA	a	841	-	1/1/15/20	6/39/115/115	-
22	LFA	b	849	-	-	1/9/9/17	-
27	LHG	5a	318	-	-	6/36/36/53	-
25	LUT	2b	314	-	-	8/29/67/67	0/2/2/2
18	CLA	A	816	12	-	6/33/109/115	-
18	CLA	a	805	12	1/1/15/20	5/39/115/115	-
18	CLA	B	832	1	-	7/33/109/115	-
20	BCR	G	201	-	-	4/29/63/63	0/2/2/2
18	CLA	A	841	-	1/1/15/20	6/39/115/115	-
18	CLA	A	803	12	1/1/14/20	3/35/111/115	-
20	BCR	B	845	-	-	4/29/63/63	0/2/2/2
18	CLA	K	201	17	1/1/11/20	2/13/89/115	-
18	CLA	b	819	1	1/1/10/20	1/13/89/115	-
18	CLA	A	832	12	1/1/15/20	2/39/115/115	-
18	CLA	3b	305	14	-	3/17/93/115	-
20	BCR	I	202	-	-	2/29/63/63	0/2/2/2
18	CLA	6b	306	16	1/1/13/20	4/27/103/115	-
28	LMU	A	852	-	-	4/21/61/61	0/2/2/2
18	CLA	b	815	1	-	0/30/106/115	-
25	LUT	5a	316	-	-	0/29/67/67	0/2/2/2
29	CHL	5b	314	15	3/3/15/26	1/12/110/137	-
18	CLA	A	815	-	-	5/15/91/115	-
18	CLA	a	835	12	1/1/11/20	3/15/91/115	-
18	CLA	5b	313	15	1/1/11/20	1/15/91/115	-
18	CLA	6a	306	16	1/1/13/20	4/27/103/115	-
18	CLA	6b	312	16	-	3/27/103/115	-
26	CL0	a	802	12	-	7/37/135/135	-
27	LHG	6b	301	18	-	11/43/43/53	-
18	CLA	A	817	12	1/1/13/20	8/30/106/115	-
18	CLA	2b	307	13	1/1/11/20	0/15/91/115	-
29	CHL	3a	315	14	3/3/16/26	2/15/113/137	-
22	LFA	B	849	-	-	1/9/9/17	-
18	CLA	6a	312	16	-	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3a	304	-	1/1/11/20	1/15/91/115	-
20	BCR	m	101	-	-	4/29/63/63	0/2/2/2
18	CLA	b	836	1	1/1/15/20	5/39/115/115	-
18	CLA	a	832	12	1/1/15/20	2/39/115/115	-
18	CLA	a	807	12	1/1/11/20	0/19/95/115	-
21	DGD	b	847	-	-	19/48/88/95	0/2/2/2
18	CLA	B	826	1	1/1/13/20	1/31/107/115	-
18	CLA	B	824	-	1/1/12/20	2/21/97/115	-
18	CLA	a	827	12	1/1/15/20	5/39/115/115	-
18	CLA	B	827	1	-	1/33/109/115	-
23	LMG	I	201	-	-	16/26/46/70	0/1/1/1
18	CLA	A	834	12	-	4/33/109/115	-
18	CLA	a	830	12	-	5/21/97/115	-
18	CLA	b	810	1	-	5/33/109/115	-
25	LUT	6b	320	-	-	3/29/67/67	0/2/2/2
18	CLA	b	852	-	-	4/39/115/115	-
18	CLA	a	815	-	-	5/15/91/115	-
23	LMG	j	103	-	-	7/25/45/70	0/1/1/1
18	CLA	A	801	12	-	2/24/100/115	-
18	CLA	A	819	12	-	0/15/91/115	-
29	CHL	2b	304	-	3/3/16/26	4/15/113/137	-
20	BCR	b	845	-	-	4/29/63/63	0/2/2/2
29	CHL	5a	306	-	3/3/15/26	4/12/110/137	-
19	PQN	b	841	-	-	0/23/43/43	0/2/2/2
18	CLA	l	303	-	1/1/10/20	1/12/88/115	-
18	CLA	B	804	1	1/1/15/20	4/39/115/115	-
25	LUT	3a	316	-	-	0/29/67/67	0/2/2/2
29	CHL	3b	315	14	3/3/16/26	2/15/113/137	-
18	CLA	A	836	12	1/1/12/20	4/23/99/115	-
25	LUT	6a	318	-	-	3/29/67/67	0/2/2/2
18	CLA	5b	303	15	1/1/12/20	6/21/97/115	-
18	CLA	6b	311	16	1/1/11/20	0/15/91/115	-
18	CLA	3b	303	14	1/1/12/20	4/21/97/115	-
18	CLA	6b	313	-	1/1/11/20	4/15/91/115	-
18	CLA	b	826	1	1/1/13/20	1/31/107/115	-
29	CHL	2a	304	-	3/3/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	SF4	C	102	2	-	-	0/6/5/5
18	CLA	B	805	1	1/1/15/20	10/39/115/115	-
18	CLA	3a	311	14	1/1/10/20	0/13/89/115	-
26	CL0	A	802	12	-	7/37/135/135	-
18	CLA	5b	311	15	1/1/11/20	3/13/89/115	-
18	CLA	A	809	12	1/1/13/20	3/27/103/115	-
18	CLA	a	816	12	-	6/33/109/115	-
20	BCR	b	842	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	314	-	1/1/11/20	2/15/91/115	-
18	CLA	B	834	-	1/1/11/20	0/15/91/115	-
29	CHL	5b	307	-	2/2/16/26	7/15/113/137	-
19	PQN	a	843	-	-	4/23/43/43	0/2/2/2
29	CHL	5b	301	15	3/3/16/26	2/15/113/137	-
18	CLA	l	302	10	-	0/33/109/115	-
20	BCR	a	851	-	-	8/29/63/63	0/2/2/2
29	CHL	5b	305	-	3/3/16/26	2/15/113/137	-
18	CLA	B	802	-	1/1/15/20	1/39/115/115	-
25	LUT	5b	317	-	-	2/29/67/67	0/2/2/2
18	CLA	A	808	12	1/1/15/20	3/39/115/115	-
20	BCR	b	851	-	-	8/29/63/63	0/2/2/2
18	CLA	a	817	12	1/1/13/20	8/30/106/115	-
29	CHL	6b	309	16	3/3/15/26	2/8/106/137	-
18	CLA	A	826	12	1/1/15/20	2/39/115/115	-
18	CLA	5b	309	15	-	2/23/99/115	-
18	CLA	a	838	12	1/1/12/20	0/21/97/115	-
18	CLA	B	815	1	-	0/30/106/115	-
18	CLA	6a	313	-	1/1/11/20	4/15/91/115	-
18	CLA	b	839	1	-	2/39/115/115	-
18	CLA	A	812	12	1/1/15/20	6/39/115/115	-
29	CHL	5a	314	15	3/3/15/26	1/12/110/137	-
29	CHL	6a	309	16	3/3/15/26	2/8/106/137	-
18	CLA	A	818	12	1/1/15/20	4/39/115/115	-
29	CHL	2b	306	-	2/2/16/26	10/15/113/137	-
24	SF4	c	102	2	-	-	0/6/5/5
18	CLA	6b	307	-	-	2/20/96/115	-
18	CLA	F	302	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	834	12	-	4/33/109/115	-
23	LMG	J	103	-	-	7/25/45/70	0/1/1/1
18	CLA	2a	302	13	1/1/11/20	2/15/91/115	-
18	CLA	b	821	1	1/1/13/20	4/27/103/115	-
27	LHG	6a	301	18	-	11/43/43/53	-
18	CLA	6b	316	16	-	2/15/91/115	-
28	LMU	a	852	-	-	4/21/61/61	0/2/2/2
18	CLA	b	854	-	1/1/15/20	6/39/115/115	-
18	CLA	a	819	12	-	0/15/91/115	-
18	CLA	b	833	1	1/1/15/20	5/39/115/115	-
18	CLA	a	826	12	1/1/15/20	2/39/115/115	-
20	BCR	B	851	-	-	8/29/63/63	0/2/2/2
18	CLA	a	837	12	1/1/13/20	3/27/103/115	-
18	CLA	2b	311	13	-	3/15/91/115	-
18	CLA	b	853	-	1/1/15/20	3/39/115/115	-
29	CHL	3a	301	13	3/3/16/26	0/15/113/137	-
24	SF4	C	101	2	-	-	0/6/5/5
18	CLA	b	831	1	1/1/15/20	2/39/115/115	-
18	CLA	B	817	1	1/1/15/20	5/39/115/115	-
18	CLA	A	810	12	-	4/39/115/115	-
18	CLA	B	838	-	-	6/39/115/115	-
18	CLA	A	823	12	-	1/39/115/115	-
18	CLA	A	807	12	1/1/11/20	0/19/95/115	-
29	CHL	6a	304	16	3/3/16/26	4/15/113/137	-
18	CLA	b	829	1	-	2/15/91/115	-
18	CLA	B	836	1	1/1/15/20	5/39/115/115	-
18	CLA	a	836	12	1/1/12/20	4/23/99/115	-
18	CLA	a	822	12	1/1/11/20	2/15/91/115	-
18	CLA	B	814	1	-	1/21/97/115	-
18	CLA	2b	301	13	1/1/13/20	6/27/103/115	-
21	DGD	B	847	-	-	19/48/88/95	0/2/2/2
25	LUT	J	105	-	-	10/29/67/67	0/2/2/2
18	CLA	a	833	12	-	6/39/115/115	-
23	LMG	i	201	-	-	16/26/46/70	0/1/1/1
18	CLA	b	820	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2a	311	13	-	3/15/91/115	-
18	CLA	A	839	12	-	3/39/115/115	-
18	CLA	f	303	5	1/1/10/20	0/10/86/115	-
20	BCR	b	843	-	-	11/29/63/63	0/2/2/2
23	LMG	5a	319	-	-	5/30/50/70	0/1/1/1
18	CLA	a	812	12	1/1/15/20	6/39/115/115	-
18	CLA	B	819	1	1/1/10/20	1/13/89/115	-
18	CLA	6b	314	16	1/1/11/20	2/15/91/115	-
18	CLA	A	820	-	-	3/39/115/115	-
20	BCR	b	844	-	-	3/29/63/63	0/2/2/2
18	CLA	3a	306	14	1/1/11/20	0/15/91/115	-
18	CLA	2a	307	13	1/1/11/20	0/15/91/115	-
18	CLA	B	852	-	-	4/39/115/115	-
18	CLA	B	837	1	1/1/11/20	0/18/94/115	-
20	BCR	f	301	-	-	3/29/63/63	0/2/2/2
18	CLA	2a	301	13	1/1/13/20	6/27/103/115	-
29	CHL	6b	304	16	3/3/16/26	4/15/113/137	-
20	BCR	L	304	-	-	2/29/63/63	0/2/2/2
18	CLA	3a	310	-	1/1/11/20	2/15/91/115	-
24	SF4	a	844	12,1	-	-	0/6/5/5
18	CLA	2a	309	27	1/1/11/20	2/15/91/115	-
29	CHL	3b	307	-	3/3/16/26	3/15/113/137	-
18	CLA	B	813	1	-	2/27/103/115	-
18	CLA	L	301	10	1/1/11/20	4/15/91/115	-
20	BCR	A	848	-	-	3/29/63/63	0/2/2/2
25	LUT	5b	316	-	-	0/29/67/67	0/2/2/2
23	LMG	j	104	-	-	7/36/56/70	0/1/1/1
18	CLA	A	833	12	-	6/39/115/115	-
18	CLA	A	828	12	-	3/39/115/115	-
23	LMG	J	104	-	-	7/36/56/70	0/1/1/1
18	CLA	F	305	-	1/1/14/20	3/33/109/115	-
18	CLA	G	202	6	1/1/12/20	1/21/97/115	-
18	CLA	A	842	-	-	3/15/91/115	-
27	LHG	a	845	-	-	4/53/53/53	-
18	CLA	A	806	12	1/1/15/20	8/39/115/115	-
20	BCR	K	202	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	6a	317	16	1/1/11/20	3/15/91/115	-
18	CLA	B	812	1	1/1/15/20	5/39/115/115	-
18	CLA	a	829	12	-	6/39/115/115	-
25	LUT	5a	317	-	-	2/29/67/67	0/2/2/2
18	CLA	B	801	1	1/1/15/20	7/39/115/115	-
18	CLA	6b	310	-	1/1/11/20	2/15/91/115	-
18	CLA	6a	316	16	-	2/15/91/115	-
25	LUT	3b	317	-	-	4/29/67/67	0/2/2/2
18	CLA	B	818	-	-	0/25/101/115	-
18	CLA	3a	308	14	1/1/11/20	0/15/91/115	-
18	CLA	b	840	27	1/1/15/20	10/39/115/115	-
18	CLA	a	824	-	1/1/15/20	2/39/115/115	-
20	BCR	g	204	-	-	2/29/63/63	0/2/2/2
18	CLA	3b	310	-	1/1/11/20	2/15/91/115	-
27	LHG	A	845	-	-	4/53/53/53	-
18	CLA	B	825	1	1/1/15/20	0/39/115/115	-
18	CLA	3b	304	-	1/1/11/20	1/15/91/115	-

All (2398) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6b	309	CHL	C2C-C3C	5.68	1.41	1.36
29	6a	309	CHL	C2C-C3C	5.65	1.41	1.36
18	A	828	CLA	MG-NA	5.28	2.18	2.06
18	a	828	CLA	MG-NA	5.28	2.18	2.06
18	B	835	CLA	MG-NA	5.26	2.18	2.06
18	b	835	CLA	MG-NA	5.26	2.18	2.06
18	A	836	CLA	MG-NA	5.02	2.18	2.06
18	a	836	CLA	MG-NA	5.02	2.18	2.06
18	5a	303	CLA	C4C-C3C	-4.78	1.36	1.45
18	5b	303	CLA	C4C-C3C	-4.78	1.36	1.45
18	B	827	CLA	C4C-C3C	-4.74	1.37	1.45
18	b	827	CLA	C4C-C3C	-4.73	1.37	1.45
18	A	826	CLA	C4C-C3C	-4.66	1.37	1.45
18	a	826	CLA	C4C-C3C	-4.66	1.37	1.45
18	B	805	CLA	C4C-C3C	-4.65	1.37	1.45
18	b	805	CLA	C4C-C3C	-4.65	1.37	1.45
18	5a	309	CLA	C4C-C3C	-4.64	1.37	1.45
18	5b	309	CLA	C4C-C3C	-4.63	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	829	CLA	C4C-C3C	-4.63	1.37	1.45
18	b	829	CLA	C4C-C3C	-4.63	1.37	1.45
18	A	804	CLA	C4C-C3C	-4.62	1.37	1.45
18	a	804	CLA	C4C-C3C	-4.62	1.37	1.45
18	B	819	CLA	C4C-C3C	-4.62	1.37	1.45
18	b	819	CLA	C4C-C3C	-4.62	1.37	1.45
18	B	817	CLA	C4C-C3C	-4.62	1.37	1.45
18	B	836	CLA	C4C-C3C	-4.62	1.37	1.45
18	b	836	CLA	C4C-C3C	-4.62	1.37	1.45
18	B	825	CLA	C4C-C3C	-4.61	1.37	1.45
18	b	825	CLA	C4C-C3C	-4.61	1.37	1.45
18	B	852	CLA	C4C-C3C	-4.61	1.37	1.45
18	b	852	CLA	C4C-C3C	-4.61	1.37	1.45
18	B	802	CLA	C4C-C3C	-4.61	1.37	1.45
18	b	802	CLA	C4C-C3C	-4.61	1.37	1.45
18	B	801	CLA	C4C-C3C	-4.61	1.37	1.45
18	b	801	CLA	C4C-C3C	-4.61	1.37	1.45
18	b	817	CLA	C4C-C3C	-4.59	1.37	1.45
18	b	808	CLA	C4C-C3C	-4.59	1.37	1.45
18	A	801	CLA	C4C-C3C	-4.59	1.37	1.45
18	a	801	CLA	C4C-C3C	-4.58	1.37	1.45
18	B	806	CLA	C4C-C3C	-4.58	1.37	1.45
18	b	806	CLA	C4C-C3C	-4.58	1.37	1.45
18	6a	308	CLA	MG-NA	4.58	2.17	2.06
18	3b	311	CLA	C4C-C3C	-4.56	1.37	1.45
18	A	817	CLA	C4C-C3C	-4.56	1.37	1.45
18	a	817	CLA	C4C-C3C	-4.56	1.37	1.45
18	6b	308	CLA	MG-NA	4.56	2.17	2.06
18	A	806	CLA	C4C-C3C	-4.55	1.37	1.45
18	a	806	CLA	C4C-C3C	-4.55	1.37	1.45
18	B	839	CLA	C4C-C3C	-4.55	1.37	1.45
18	b	839	CLA	C4C-C3C	-4.55	1.37	1.45
18	b	840	CLA	C4C-C3C	-4.55	1.37	1.45
18	A	840	CLA	C4C-C3C	-4.55	1.37	1.45
18	a	840	CLA	C4C-C3C	-4.55	1.37	1.45
18	a	832	CLA	C4C-C3C	-4.55	1.37	1.45
18	6a	308	CLA	C4C-C3C	-4.54	1.37	1.45
18	6b	308	CLA	C4C-C3C	-4.54	1.37	1.45
18	6b	316	CLA	C4C-C3C	-4.54	1.37	1.45
18	3a	309	CLA	C4C-C3C	-4.54	1.37	1.45
18	B	837	CLA	C4C-C3C	-4.54	1.37	1.45
18	B	840	CLA	C4C-C3C	-4.54	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	837	CLA	C4C-C3C	-4.54	1.37	1.45
18	A	819	CLA	C4C-C3C	-4.54	1.37	1.45
18	a	819	CLA	C4C-C3C	-4.54	1.37	1.45
18	3a	303	CLA	MG-NA	4.54	2.17	2.06
18	3b	303	CLA	MG-NA	4.54	2.17	2.06
18	A	832	CLA	C4C-C3C	-4.54	1.37	1.45
18	6a	315	CLA	C4C-C3C	-4.54	1.37	1.45
18	6b	315	CLA	C4C-C3C	-4.54	1.37	1.45
18	B	854	CLA	C4C-C3C	-4.54	1.37	1.45
18	b	854	CLA	C4C-C3C	-4.54	1.37	1.45
18	B	815	CLA	C4C-C3C	-4.53	1.37	1.45
18	b	815	CLA	C4C-C3C	-4.53	1.37	1.45
18	3b	309	CLA	C4C-C3C	-4.53	1.37	1.45
18	B	808	CLA	C4C-C3C	-4.53	1.37	1.45
18	3a	305	CLA	C4C-C3C	-4.53	1.37	1.45
18	3b	305	CLA	C4C-C3C	-4.53	1.37	1.45
18	B	822	CLA	C4C-C3C	-4.53	1.37	1.45
18	b	822	CLA	C4C-C3C	-4.53	1.37	1.45
18	A	805	CLA	C4C-C3C	-4.53	1.37	1.45
18	a	805	CLA	C4C-C3C	-4.53	1.37	1.45
18	A	803	CLA	C4C-C3C	-4.53	1.37	1.45
18	a	803	CLA	C4C-C3C	-4.53	1.37	1.45
18	A	827	CLA	C4C-C3C	-4.53	1.37	1.45
18	a	827	CLA	C4C-C3C	-4.53	1.37	1.45
18	b	807	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	825	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	810	CLA	C4C-C3C	-4.52	1.37	1.45
18	a	810	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	821	CLA	C4C-C3C	-4.52	1.37	1.45
18	a	821	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	830	CLA	C4C-C3C	-4.52	1.37	1.45
18	a	830	CLA	C4C-C3C	-4.52	1.37	1.45
18	a	834	CLA	C4C-C3C	-4.52	1.37	1.45
18	B	804	CLA	C4C-C3C	-4.52	1.37	1.45
18	b	804	CLA	C4C-C3C	-4.52	1.37	1.45
18	2a	308	CLA	C4C-C3C	-4.52	1.37	1.45
18	2b	308	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	853	CLA	C4C-C3C	-4.52	1.37	1.45
18	a	853	CLA	C4C-C3C	-4.52	1.37	1.45
18	2b	302	CLA	C4C-C3C	-4.52	1.37	1.45
18	A	816	CLA	C4C-C3C	-4.51	1.37	1.45
18	a	816	CLA	C4C-C3C	-4.51	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	820	CLA	C4C-C3C	-4.51	1.37	1.45
18	b	820	CLA	C4C-C3C	-4.51	1.37	1.45
18	2a	302	CLA	C4C-C3C	-4.51	1.37	1.45
18	a	825	CLA	C4C-C3C	-4.51	1.37	1.45
18	B	838	CLA	C4C-C3C	-4.51	1.37	1.45
18	b	838	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	834	CLA	C4C-C3C	-4.51	1.37	1.45
18	3a	311	CLA	C4C-C3C	-4.51	1.37	1.45
18	A	838	CLA	C4C-C3C	-4.50	1.37	1.45
18	B	816	CLA	C4C-C3C	-4.50	1.37	1.45
18	b	816	CLA	C4C-C3C	-4.50	1.37	1.45
18	B	833	CLA	C4C-C3C	-4.50	1.37	1.45
18	b	833	CLA	C4C-C3C	-4.50	1.37	1.45
18	6a	316	CLA	C4C-C3C	-4.50	1.37	1.45
18	b	813	CLA	C4C-C3C	-4.49	1.37	1.45
18	A	824	CLA	C4C-C3C	-4.49	1.37	1.45
18	a	824	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	832	CLA	C4C-C3C	-4.49	1.37	1.45
18	b	832	CLA	C4C-C3C	-4.49	1.37	1.45
18	A	820	CLA	C4C-C3C	-4.49	1.37	1.45
18	A	831	CLA	C4C-C3C	-4.49	1.37	1.45
18	a	820	CLA	C4C-C3C	-4.49	1.37	1.45
18	a	831	CLA	C4C-C3C	-4.49	1.37	1.45
18	G	203	CLA	C4C-C3C	-4.49	1.37	1.45
18	g	203	CLA	C4C-C3C	-4.49	1.37	1.45
18	L	302	CLA	C4C-C3C	-4.49	1.37	1.45
18	l	302	CLA	C4C-C3C	-4.49	1.37	1.45
18	A	808	CLA	C4C-C3C	-4.49	1.37	1.45
18	a	808	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	811	CLA	C4C-C3C	-4.49	1.37	1.45
18	B	823	CLA	C4C-C3C	-4.49	1.37	1.45
18	b	811	CLA	C4C-C3C	-4.49	1.37	1.45
18	b	823	CLA	C4C-C3C	-4.49	1.37	1.45
18	A	837	CLA	C4C-C3C	-4.48	1.37	1.45
18	a	837	CLA	C4C-C3C	-4.48	1.37	1.45
18	2a	301	CLA	C4C-C3C	-4.48	1.37	1.45
18	2b	301	CLA	C4C-C3C	-4.48	1.37	1.45
18	B	807	CLA	C4C-C3C	-4.48	1.37	1.45
18	B	809	CLA	C4C-C3C	-4.48	1.37	1.45
18	b	809	CLA	C4C-C3C	-4.48	1.37	1.45
18	B	826	CLA	C4C-C3C	-4.48	1.37	1.45
18	b	826	CLA	C4C-C3C	-4.48	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	824	CLA	C4C-C3C	-4.48	1.37	1.45
18	b	824	CLA	C4C-C3C	-4.48	1.37	1.45
18	B	813	CLA	C4C-C3C	-4.48	1.37	1.45
18	a	814	CLA	C4C-C3C	-4.48	1.37	1.45
18	6b	314	CLA	C4C-C3C	-4.48	1.37	1.45
18	F	302	CLA	C4C-C3C	-4.47	1.37	1.45
18	f	302	CLA	C4C-C3C	-4.47	1.37	1.45
18	6a	310	CLA	C4C-C3C	-4.47	1.37	1.45
18	6b	310	CLA	C4C-C3C	-4.47	1.37	1.45
18	6a	317	CLA	C4C-C3C	-4.47	1.37	1.45
18	6b	317	CLA	C4C-C3C	-4.47	1.37	1.45
18	G	202	CLA	C4C-C3C	-4.47	1.37	1.45
18	6a	306	CLA	C4C-C3C	-4.47	1.37	1.45
18	6b	306	CLA	C4C-C3C	-4.47	1.37	1.45
18	a	838	CLA	C4C-C3C	-4.47	1.37	1.45
18	A	813	CLA	C4C-C3C	-4.47	1.37	1.45
18	a	813	CLA	C4C-C3C	-4.47	1.37	1.45
18	3a	303	CLA	C4C-C3C	-4.47	1.37	1.45
18	5a	310	CLA	C4C-C3C	-4.47	1.37	1.45
18	5b	310	CLA	C4C-C3C	-4.47	1.37	1.45
18	A	814	CLA	C4C-C3C	-4.47	1.37	1.45
18	3a	302	CLA	C4C-C3C	-4.46	1.37	1.45
18	3b	302	CLA	C4C-C3C	-4.46	1.37	1.45
18	6a	312	CLA	C4C-C3C	-4.46	1.37	1.45
18	6b	312	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	829	CLA	C4C-C3C	-4.46	1.37	1.45
18	a	829	CLA	C4C-C3C	-4.46	1.37	1.45
18	5a	315	CLA	C4C-C3C	-4.46	1.37	1.45
18	5b	315	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	835	CLA	C4C-C3C	-4.46	1.37	1.45
18	a	835	CLA	C4C-C3C	-4.46	1.37	1.45
18	A	824	CLA	MG-NA	4.45	2.16	2.06
18	a	824	CLA	MG-NA	4.45	2.16	2.06
18	B	831	CLA	C4C-C3C	-4.45	1.37	1.45
18	b	831	CLA	C4C-C3C	-4.45	1.37	1.45
18	A	811	CLA	C4C-C3C	-4.45	1.37	1.45
18	a	811	CLA	C4C-C3C	-4.45	1.37	1.45
18	2a	311	CLA	C4C-C3C	-4.45	1.37	1.45
18	2b	311	CLA	C4C-C3C	-4.45	1.37	1.45
18	2a	310	CLA	C4C-C3C	-4.45	1.37	1.45
18	6a	314	CLA	C4C-C3C	-4.45	1.37	1.45
18	2b	310	CLA	C4C-C3C	-4.45	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	839	CLA	C4C-C3C	-4.45	1.37	1.45
18	a	839	CLA	C4C-C3C	-4.45	1.37	1.45
18	A	809	CLA	C4C-C3C	-4.45	1.37	1.45
18	6a	307	CLA	C4C-C3C	-4.45	1.37	1.45
18	a	809	CLA	C4C-C3C	-4.45	1.37	1.45
18	L	303	CLA	C4C-C3C	-4.45	1.37	1.45
18	l	303	CLA	C4C-C3C	-4.45	1.37	1.45
18	3a	314	CLA	C4C-C3C	-4.44	1.37	1.45
18	3b	314	CLA	C4C-C3C	-4.44	1.37	1.45
18	B	810	CLA	C4C-C3C	-4.44	1.37	1.45
18	b	810	CLA	C4C-C3C	-4.44	1.37	1.45
18	A	807	CLA	C4C-C3C	-4.44	1.37	1.45
18	a	807	CLA	C4C-C3C	-4.44	1.37	1.45
18	L	301	CLA	C4C-C3C	-4.44	1.37	1.45
18	l	301	CLA	C4C-C3C	-4.44	1.37	1.45
18	J	101	CLA	C4C-C3C	-4.44	1.37	1.45
18	j	101	CLA	C4C-C3C	-4.44	1.37	1.45
18	B	803	CLA	C4C-C3C	-4.44	1.37	1.45
18	B	834	CLA	C4C-C3C	-4.44	1.37	1.45
18	b	803	CLA	C4C-C3C	-4.44	1.37	1.45
18	b	834	CLA	C4C-C3C	-4.44	1.37	1.45
18	3a	304	CLA	C4C-C3C	-4.43	1.37	1.45
18	3a	313	CLA	C4C-C3C	-4.43	1.37	1.45
18	3b	304	CLA	C4C-C3C	-4.43	1.37	1.45
18	3b	313	CLA	C4C-C3C	-4.43	1.37	1.45
18	5a	304	CLA	C4C-C3C	-4.43	1.37	1.45
18	5b	304	CLA	C4C-C3C	-4.43	1.37	1.45
18	B	814	CLA	C4C-C3C	-4.43	1.37	1.45
18	b	814	CLA	C4C-C3C	-4.43	1.37	1.45
18	6b	307	CLA	C4C-C3C	-4.43	1.37	1.45
18	6a	311	CLA	C4C-C3C	-4.43	1.37	1.45
18	6b	311	CLA	C4C-C3C	-4.43	1.37	1.45
18	A	836	CLA	C4C-C3C	-4.42	1.37	1.45
18	a	836	CLA	C4C-C3C	-4.42	1.37	1.45
18	g	202	CLA	C4C-C3C	-4.42	1.37	1.45
18	5b	304	CLA	MG-NA	4.41	2.16	2.06
18	2a	309	CLA	C4C-C3C	-4.41	1.37	1.45
18	2b	309	CLA	C4C-C3C	-4.41	1.37	1.45
18	5a	304	CLA	MG-NA	4.41	2.16	2.06
18	3b	306	CLA	C4C-C3C	-4.41	1.37	1.45
18	3a	306	CLA	C4C-C3C	-4.41	1.37	1.45
18	3b	303	CLA	C4C-C3C	-4.41	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	C4C-C3C	-4.40	1.37	1.45
18	f	303	CLA	C4C-C3C	-4.40	1.37	1.45
18	A	826	CLA	MG-NA	4.40	2.16	2.06
18	a	826	CLA	MG-NA	4.40	2.16	2.06
18	2a	307	CLA	C4C-C3C	-4.40	1.37	1.45
18	2b	307	CLA	C4C-C3C	-4.40	1.37	1.45
18	F	305	CLA	C4C-C3C	-4.40	1.37	1.45
18	f	305	CLA	C4C-C3C	-4.40	1.37	1.45
18	3a	312	CLA	C4C-C3C	-4.40	1.37	1.45
18	3b	312	CLA	C4C-C3C	-4.40	1.37	1.45
18	3a	310	CLA	C4C-C3C	-4.40	1.37	1.45
18	3b	310	CLA	C4C-C3C	-4.40	1.37	1.45
18	B	853	CLA	C4C-C3C	-4.39	1.37	1.45
18	b	853	CLA	C4C-C3C	-4.39	1.37	1.45
18	5a	313	CLA	C4C-C3C	-4.39	1.37	1.45
18	5b	313	CLA	C4C-C3C	-4.39	1.37	1.45
18	A	841	CLA	C4C-C3C	-4.39	1.37	1.45
18	a	841	CLA	C4C-C3C	-4.39	1.37	1.45
18	2a	312	CLA	C4C-C3C	-4.39	1.37	1.45
18	2b	312	CLA	C4C-C3C	-4.39	1.37	1.45
18	B	830	CLA	C4C-C3C	-4.39	1.37	1.45
18	b	830	CLA	C4C-C3C	-4.39	1.37	1.45
18	2a	303	CLA	C4C-C3C	-4.39	1.37	1.45
18	2b	303	CLA	C4C-C3C	-4.39	1.37	1.45
18	B	816	CLA	MG-NA	4.38	2.16	2.06
18	b	816	CLA	MG-NA	4.38	2.16	2.06
18	A	833	CLA	C4C-C3C	-4.38	1.37	1.45
18	a	833	CLA	C4C-C3C	-4.38	1.37	1.45
18	5a	302	CLA	C4C-C3C	-4.38	1.37	1.45
18	5b	302	CLA	C4C-C3C	-4.38	1.37	1.45
18	B	818	CLA	C4C-C3C	-4.38	1.37	1.45
18	b	818	CLA	C4C-C3C	-4.38	1.37	1.45
18	k	201	CLA	C4C-C3C	-4.38	1.37	1.45
18	6b	313	CLA	C4C-C3C	-4.38	1.37	1.45
18	5a	312	CLA	C4C-C3C	-4.37	1.37	1.45
18	5b	312	CLA	C4C-C3C	-4.37	1.37	1.45
18	B	821	CLA	C4C-C3C	-4.37	1.37	1.45
18	b	821	CLA	C4C-C3C	-4.37	1.37	1.45
18	3a	308	CLA	C4C-C3C	-4.37	1.37	1.45
18	3b	308	CLA	C4C-C3C	-4.37	1.37	1.45
18	B	807	CLA	C1C-C2C	-4.37	1.35	1.44
18	b	807	CLA	C1C-C2C	-4.37	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6a	313	CLA	C4C-C3C	-4.37	1.37	1.45
18	5a	308	CLA	C4C-C3C	-4.36	1.37	1.45
18	5b	308	CLA	C4C-C3C	-4.36	1.37	1.45
18	A	812	CLA	C4C-C3C	-4.35	1.37	1.45
18	a	812	CLA	C4C-C3C	-4.35	1.37	1.45
18	A	823	CLA	C4C-C3C	-4.35	1.37	1.45
18	K	201	CLA	C4C-C3C	-4.35	1.37	1.45
18	a	823	CLA	C4C-C3C	-4.35	1.37	1.45
18	B	808	CLA	C1C-C2C	-4.35	1.35	1.44
18	b	808	CLA	C1C-C2C	-4.35	1.35	1.44
18	b	828	CLA	C4C-C3C	-4.34	1.37	1.45
18	b	835	CLA	C4C-C3C	-4.34	1.37	1.45
18	A	818	CLA	C4C-C3C	-4.34	1.37	1.45
18	a	818	CLA	C4C-C3C	-4.34	1.37	1.45
18	B	828	CLA	C4C-C3C	-4.33	1.37	1.45
18	B	835	CLA	C4C-C3C	-4.33	1.37	1.45
18	B	825	CLA	MG-NA	4.33	2.16	2.06
18	b	825	CLA	MG-NA	4.33	2.16	2.06
18	A	822	CLA	C4C-C3C	-4.31	1.37	1.45
18	5a	303	CLA	MG-NA	4.31	2.16	2.06
18	5b	303	CLA	MG-NA	4.31	2.16	2.06
18	5b	309	CLA	C1C-C2C	-4.30	1.35	1.44
18	5a	309	CLA	C1C-C2C	-4.30	1.35	1.44
18	6a	305	CLA	C4C-C3C	-4.29	1.37	1.45
18	A	842	CLA	C4C-C3C	-4.29	1.37	1.45
18	a	842	CLA	C4C-C3C	-4.29	1.37	1.45
18	a	822	CLA	C4C-C3C	-4.28	1.37	1.45
18	B	815	CLA	MG-NA	4.28	2.16	2.06
18	b	815	CLA	MG-NA	4.28	2.16	2.06
18	b	839	CLA	C1C-C2C	-4.28	1.35	1.44
18	3a	311	CLA	MG-NA	4.28	2.16	2.06
18	3b	311	CLA	MG-NA	4.28	2.16	2.06
18	A	828	CLA	C4C-C3C	-4.27	1.37	1.45
18	a	828	CLA	C4C-C3C	-4.27	1.37	1.45
18	3b	313	CLA	MG-NA	4.27	2.16	2.06
18	B	802	CLA	C1C-C2C	-4.26	1.35	1.44
18	b	802	CLA	C1C-C2C	-4.26	1.35	1.44
18	B	839	CLA	C1C-C2C	-4.25	1.35	1.44
29	6a	304	CHL	C2C-C3C	4.25	1.40	1.36
29	6b	304	CHL	C2C-C3C	4.25	1.40	1.36
18	3a	313	CLA	MG-NA	4.24	2.16	2.06
18	A	809	CLA	MG-NA	4.24	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	809	CLA	MG-NA	4.24	2.16	2.06
18	B	812	CLA	C4C-C3C	-4.23	1.37	1.45
18	b	812	CLA	C4C-C3C	-4.23	1.37	1.45
18	A	815	CLA	C4C-C3C	-4.23	1.37	1.45
18	a	815	CLA	C4C-C3C	-4.23	1.37	1.45
18	6b	305	CLA	C4C-C3C	-4.23	1.37	1.45
18	A	803	CLA	C1C-C2C	-4.23	1.35	1.44
18	a	803	CLA	C1C-C2C	-4.23	1.35	1.44
18	5a	311	CLA	MG-NA	4.21	2.16	2.06
18	5b	311	CLA	MG-NA	4.21	2.16	2.06
18	B	827	CLA	C1C-C2C	-4.21	1.36	1.44
18	b	827	CLA	C1C-C2C	-4.21	1.36	1.44
29	2a	305	CHL	C2C-C3C	4.21	1.40	1.36
29	2b	305	CHL	C2C-C3C	4.21	1.40	1.36
18	A	832	CLA	MG-NA	4.20	2.16	2.06
18	a	832	CLA	MG-NA	4.20	2.16	2.06
18	A	812	CLA	C1C-C2C	-4.20	1.36	1.44
18	a	812	CLA	C1C-C2C	-4.20	1.36	1.44
18	B	810	CLA	MG-NA	4.20	2.16	2.06
18	b	810	CLA	MG-NA	4.20	2.16	2.06
18	b	814	CLA	C1C-C2C	-4.19	1.36	1.44
18	B	832	CLA	C1C-C2C	-4.18	1.36	1.44
18	b	832	CLA	C1C-C2C	-4.18	1.36	1.44
18	B	806	CLA	C1C-C2C	-4.18	1.36	1.44
18	b	806	CLA	C1C-C2C	-4.18	1.36	1.44
18	a	832	CLA	C1C-C2C	-4.18	1.36	1.44
18	A	833	CLA	C1C-C2C	-4.18	1.36	1.44
18	a	833	CLA	C1C-C2C	-4.18	1.36	1.44
18	A	815	CLA	C1C-C2C	-4.18	1.36	1.44
18	a	815	CLA	C1C-C2C	-4.18	1.36	1.44
18	A	811	CLA	C1C-C2C	-4.18	1.36	1.44
18	a	811	CLA	C1C-C2C	-4.18	1.36	1.44
18	a	828	CLA	C1C-C2C	-4.18	1.36	1.44
18	A	823	CLA	C1C-C2C	-4.17	1.36	1.44
18	a	823	CLA	C1C-C2C	-4.17	1.36	1.44
18	A	838	CLA	MG-NA	4.17	2.16	2.06
18	a	838	CLA	MG-NA	4.17	2.16	2.06
18	B	814	CLA	C1C-C2C	-4.16	1.36	1.44
18	A	832	CLA	C1C-C2C	-4.16	1.36	1.44
18	A	805	CLA	C1C-C2C	-4.15	1.36	1.44
18	a	805	CLA	C1C-C2C	-4.15	1.36	1.44
18	B	825	CLA	C1C-C2C	-4.15	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	825	CLA	C1C-C2C	-4.15	1.36	1.44
18	b	853	CLA	C1C-C2C	-4.15	1.36	1.44
18	6b	305	CLA	C1C-C2C	-4.15	1.36	1.44
18	B	853	CLA	C1C-C2C	-4.14	1.36	1.44
18	F	302	CLA	C1C-C2C	-4.14	1.36	1.44
18	f	302	CLA	C1C-C2C	-4.14	1.36	1.44
18	A	828	CLA	C1C-C2C	-4.14	1.36	1.44
18	B	854	CLA	MG-NA	4.14	2.16	2.06
18	b	854	CLA	MG-NA	4.14	2.16	2.06
18	A	853	CLA	C1C-C2C	-4.14	1.36	1.44
18	6b	314	CLA	MG-NA	4.13	2.16	2.06
18	a	818	CLA	C1C-C2C	-4.13	1.36	1.44
18	6a	305	CLA	C1C-C2C	-4.13	1.36	1.44
18	6b	307	CLA	C1C-C2C	-4.13	1.36	1.44
18	a	853	CLA	C1C-C2C	-4.13	1.36	1.44
18	3a	308	CLA	C1C-C2C	-4.13	1.36	1.44
18	3b	308	CLA	C1C-C2C	-4.13	1.36	1.44
18	A	818	CLA	C1C-C2C	-4.12	1.36	1.44
18	A	829	CLA	C1C-C2C	-4.12	1.36	1.44
18	a	829	CLA	C1C-C2C	-4.12	1.36	1.44
18	B	830	CLA	C1C-C2C	-4.12	1.36	1.44
18	b	830	CLA	C1C-C2C	-4.12	1.36	1.44
18	B	812	CLA	C1C-C2C	-4.12	1.36	1.44
18	b	812	CLA	C1C-C2C	-4.12	1.36	1.44
18	5a	308	CLA	C1C-C2C	-4.12	1.36	1.44
18	5b	308	CLA	C1C-C2C	-4.12	1.36	1.44
18	A	822	CLA	C1C-C2C	-4.12	1.36	1.44
18	a	822	CLA	C1C-C2C	-4.12	1.36	1.44
18	A	822	CLA	MG-NA	4.12	2.16	2.06
18	a	822	CLA	MG-NA	4.12	2.16	2.06
18	F	305	CLA	C1C-C2C	-4.11	1.36	1.44
18	f	305	CLA	C1C-C2C	-4.11	1.36	1.44
18	6a	311	CLA	C1C-C2C	-4.11	1.36	1.44
18	6b	311	CLA	C1C-C2C	-4.11	1.36	1.44
18	B	817	CLA	C1C-C2C	-4.11	1.36	1.44
18	b	817	CLA	C1C-C2C	-4.11	1.36	1.44
18	3b	303	CLA	C1C-C2C	-4.11	1.36	1.44
18	2a	302	CLA	MG-NA	4.11	2.16	2.06
18	2b	302	CLA	MG-NA	4.11	2.16	2.06
18	G	202	CLA	MG-NA	4.11	2.16	2.06
18	g	202	CLA	MG-NA	4.11	2.16	2.06
18	A	807	CLA	MG-NA	4.11	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	807	CLA	MG-NA	4.11	2.16	2.06
18	B	834	CLA	C1C-C2C	-4.11	1.36	1.44
18	b	834	CLA	C1C-C2C	-4.11	1.36	1.44
18	6a	314	CLA	MG-NA	4.11	2.16	2.06
18	B	803	CLA	MG-NA	4.11	2.16	2.06
18	b	803	CLA	MG-NA	4.11	2.16	2.06
18	A	839	CLA	C1C-C2C	-4.10	1.36	1.44
18	a	839	CLA	C1C-C2C	-4.10	1.36	1.44
18	A	831	CLA	C1C-C2C	-4.10	1.36	1.44
18	3a	305	CLA	C1C-C2C	-4.10	1.36	1.44
18	a	831	CLA	C1C-C2C	-4.10	1.36	1.44
18	3b	305	CLA	C1C-C2C	-4.10	1.36	1.44
18	6a	307	CLA	C1C-C2C	-4.10	1.36	1.44
18	3a	303	CLA	C1C-C2C	-4.09	1.36	1.44
18	B	822	CLA	C1C-C2C	-4.09	1.36	1.44
18	b	822	CLA	C1C-C2C	-4.09	1.36	1.44
18	6a	314	CLA	C1C-C2C	-4.09	1.36	1.44
18	6b	314	CLA	C1C-C2C	-4.09	1.36	1.44
18	6a	310	CLA	C1C-C2C	-4.09	1.36	1.44
18	6b	310	CLA	C1C-C2C	-4.09	1.36	1.44
18	B	809	CLA	C1C-C2C	-4.09	1.36	1.44
18	b	809	CLA	C1C-C2C	-4.09	1.36	1.44
18	B	821	CLA	C1C-C2C	-4.09	1.36	1.44
18	b	821	CLA	C1C-C2C	-4.09	1.36	1.44
18	B	801	CLA	C1C-C2C	-4.08	1.36	1.44
18	b	801	CLA	C1C-C2C	-4.08	1.36	1.44
18	A	835	CLA	C1C-C2C	-4.08	1.36	1.44
18	a	835	CLA	C1C-C2C	-4.08	1.36	1.44
29	2b	313	CHL	C2C-C3C	4.08	1.40	1.36
18	A	814	CLA	C1C-C2C	-4.08	1.36	1.44
18	A	823	CLA	MG-NA	4.07	2.15	2.06
18	a	823	CLA	MG-NA	4.07	2.15	2.06
18	A	810	CLA	C1C-C2C	-4.07	1.36	1.44
18	a	810	CLA	C1C-C2C	-4.07	1.36	1.44
18	A	840	CLA	C1C-C2C	-4.07	1.36	1.44
18	6a	315	CLA	C1C-C2C	-4.07	1.36	1.44
18	a	840	CLA	C1C-C2C	-4.07	1.36	1.44
18	B	811	CLA	C1C-C2C	-4.07	1.36	1.44
18	b	811	CLA	C1C-C2C	-4.07	1.36	1.44
18	2a	307	CLA	C1C-C2C	-4.07	1.36	1.44
18	2b	307	CLA	C1C-C2C	-4.07	1.36	1.44
18	A	834	CLA	C1C-C2C	-4.07	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5a	302	CLA	C1C-C2C	-4.07	1.36	1.44
18	5b	302	CLA	C1C-C2C	-4.07	1.36	1.44
18	b	830	CLA	MG-NA	4.07	2.15	2.06
18	A	817	CLA	C1C-C2C	-4.07	1.36	1.44
18	a	817	CLA	C1C-C2C	-4.07	1.36	1.44
18	6b	315	CLA	C1C-C2C	-4.06	1.36	1.44
18	B	805	CLA	C1C-C2C	-4.06	1.36	1.44
18	b	805	CLA	C1C-C2C	-4.06	1.36	1.44
18	A	816	CLA	C1C-C2C	-4.06	1.36	1.44
18	5a	303	CLA	C1C-C2C	-4.06	1.36	1.44
18	a	816	CLA	C1C-C2C	-4.06	1.36	1.44
18	5b	303	CLA	C1C-C2C	-4.06	1.36	1.44
18	B	810	CLA	C1C-C2C	-4.06	1.36	1.44
18	b	810	CLA	C1C-C2C	-4.06	1.36	1.44
29	5b	307	CHL	C2C-C3C	4.06	1.40	1.36
18	B	834	CLA	MG-NA	4.06	2.15	2.06
18	A	837	CLA	C1C-C2C	-4.06	1.36	1.44
18	6a	317	CLA	C1C-C2C	-4.06	1.36	1.44
18	6b	317	CLA	C1C-C2C	-4.06	1.36	1.44
18	5b	311	CLA	C1C-C2C	-4.06	1.36	1.44
18	5a	310	CLA	C1C-C2C	-4.05	1.36	1.44
18	5b	310	CLA	C1C-C2C	-4.05	1.36	1.44
18	B	823	CLA	C1C-C2C	-4.05	1.36	1.44
18	b	823	CLA	C1C-C2C	-4.05	1.36	1.44
18	6a	306	CLA	C1C-C2C	-4.05	1.36	1.44
18	6b	306	CLA	C1C-C2C	-4.05	1.36	1.44
29	2a	313	CHL	C2C-C3C	4.05	1.40	1.36
18	B	816	CLA	C1C-C2C	-4.05	1.36	1.44
18	b	816	CLA	C1C-C2C	-4.05	1.36	1.44
18	A	842	CLA	C1C-C2C	-4.05	1.36	1.44
18	a	842	CLA	C1C-C2C	-4.05	1.36	1.44
18	B	830	CLA	MG-NA	4.05	2.15	2.06
18	B	852	CLA	C1C-C2C	-4.05	1.36	1.44
18	b	852	CLA	C1C-C2C	-4.05	1.36	1.44
18	a	801	CLA	C1C-C2C	-4.05	1.36	1.44
18	A	820	CLA	C1C-C2C	-4.04	1.36	1.44
18	a	820	CLA	C1C-C2C	-4.04	1.36	1.44
18	L	302	CLA	C1C-C2C	-4.04	1.36	1.44
18	l	302	CLA	C1C-C2C	-4.04	1.36	1.44
18	A	819	CLA	C1C-C2C	-4.04	1.36	1.44
18	a	819	CLA	C1C-C2C	-4.04	1.36	1.44
18	A	808	CLA	C1C-C2C	-4.04	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	808	CLA	C1C-C2C	-4.04	1.36	1.44
18	B	828	CLA	C1C-C2C	-4.04	1.36	1.44
18	b	828	CLA	C1C-C2C	-4.04	1.36	1.44
18	A	809	CLA	C1C-C2C	-4.04	1.36	1.44
18	a	809	CLA	C1C-C2C	-4.04	1.36	1.44
18	2b	312	CLA	C1C-C2C	-4.04	1.36	1.44
18	2a	302	CLA	C1C-C2C	-4.04	1.36	1.44
18	a	834	CLA	C1C-C2C	-4.04	1.36	1.44
18	2b	302	CLA	C1C-C2C	-4.04	1.36	1.44
18	b	834	CLA	MG-NA	4.04	2.15	2.06
18	a	814	CLA	C1C-C2C	-4.04	1.36	1.44
18	A	813	CLA	C1C-C2C	-4.04	1.36	1.44
18	a	813	CLA	C1C-C2C	-4.04	1.36	1.44
18	2a	312	CLA	C1C-C2C	-4.03	1.36	1.44
18	5a	311	CLA	C1C-C2C	-4.03	1.36	1.44
18	A	827	CLA	MG-NA	4.03	2.15	2.06
18	B	824	CLA	C1C-C2C	-4.03	1.36	1.44
18	b	824	CLA	C1C-C2C	-4.03	1.36	1.44
18	3a	313	CLA	C1C-C2C	-4.03	1.36	1.44
18	3b	313	CLA	C1C-C2C	-4.03	1.36	1.44
18	B	837	CLA	C1C-C2C	-4.03	1.36	1.44
18	b	837	CLA	C1C-C2C	-4.03	1.36	1.44
18	B	803	CLA	C1C-C2C	-4.03	1.36	1.44
18	b	803	CLA	C1C-C2C	-4.03	1.36	1.44
18	A	824	CLA	C1C-C2C	-4.03	1.36	1.44
18	a	824	CLA	C1C-C2C	-4.03	1.36	1.44
18	L	303	CLA	C1C-C2C	-4.02	1.36	1.44
18	l	303	CLA	C1C-C2C	-4.02	1.36	1.44
18	B	839	CLA	MG-NA	4.02	2.15	2.06
18	b	839	CLA	MG-NA	4.02	2.15	2.06
18	a	816	CLA	MG-NA	4.02	2.15	2.06
18	A	801	CLA	C1C-C2C	-4.02	1.36	1.44
18	A	821	CLA	C1C-C2C	-4.02	1.36	1.44
18	a	821	CLA	C1C-C2C	-4.02	1.36	1.44
18	3a	312	CLA	C1C-C2C	-4.02	1.36	1.44
18	3b	312	CLA	C1C-C2C	-4.02	1.36	1.44
18	2b	312	CLA	MG-NA	4.02	2.15	2.06
18	6b	310	CLA	MG-NA	4.02	2.15	2.06
18	2b	303	CLA	C1C-C2C	-4.02	1.36	1.44
18	A	806	CLA	C1C-C2C	-4.02	1.36	1.44
18	a	806	CLA	C1C-C2C	-4.02	1.36	1.44
18	B	826	CLA	C1C-C2C	-4.02	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	826	CLA	C1C-C2C	-4.02	1.36	1.44
18	2a	311	CLA	C1C-C2C	-4.02	1.36	1.44
18	2b	311	CLA	C1C-C2C	-4.02	1.36	1.44
18	B	831	CLA	C1C-C2C	-4.02	1.36	1.44
18	b	831	CLA	C1C-C2C	-4.02	1.36	1.44
18	G	203	CLA	C1C-C2C	-4.02	1.36	1.44
18	g	203	CLA	C1C-C2C	-4.02	1.36	1.44
18	2a	310	CLA	C1C-C2C	-4.02	1.36	1.44
18	2b	310	CLA	C1C-C2C	-4.02	1.36	1.44
29	5a	307	CHL	C2C-C3C	4.02	1.40	1.36
18	B	820	CLA	C1C-C2C	-4.02	1.36	1.44
18	b	820	CLA	C1C-C2C	-4.02	1.36	1.44
18	a	837	CLA	C1C-C2C	-4.02	1.36	1.44
18	B	833	CLA	C1C-C2C	-4.01	1.36	1.44
18	b	833	CLA	C1C-C2C	-4.01	1.36	1.44
18	G	202	CLA	C1C-C2C	-4.01	1.36	1.44
18	g	202	CLA	C1C-C2C	-4.01	1.36	1.44
18	2a	303	CLA	C1C-C2C	-4.01	1.36	1.44
18	3a	310	CLA	C1C-C2C	-4.01	1.36	1.44
18	3b	310	CLA	C1C-C2C	-4.01	1.36	1.44
18	5a	315	CLA	C1C-C2C	-4.01	1.36	1.44
18	5b	315	CLA	C1C-C2C	-4.01	1.36	1.44
18	2a	312	CLA	MG-NA	4.01	2.15	2.06
29	5a	301	CHL	C2C-C3C	4.01	1.40	1.36
29	5b	301	CHL	C2C-C3C	4.01	1.40	1.36
29	5a	305	CHL	C2C-C3C	4.01	1.40	1.36
29	5b	305	CHL	C2C-C3C	4.01	1.40	1.36
18	2b	301	CLA	C1C-C2C	-4.01	1.36	1.44
18	L	301	CLA	MG-NA	4.01	2.15	2.06
18	l	301	CLA	MG-NA	4.01	2.15	2.06
18	B	836	CLA	C1C-C2C	-4.01	1.36	1.44
18	b	836	CLA	C1C-C2C	-4.01	1.36	1.44
18	6a	316	CLA	C1C-C2C	-4.01	1.36	1.44
18	a	827	CLA	MG-NA	4.01	2.15	2.06
18	L	301	CLA	C1C-C2C	-4.01	1.36	1.44
18	l	301	CLA	C1C-C2C	-4.01	1.36	1.44
18	6b	313	CLA	C1C-C2C	-4.01	1.36	1.44
18	6a	313	CLA	C1C-C2C	-4.01	1.36	1.44
18	A	816	CLA	MG-NA	4.01	2.15	2.06
18	A	826	CLA	C1C-C2C	-4.01	1.36	1.44
18	a	826	CLA	C1C-C2C	-4.01	1.36	1.44
18	B	831	CLA	MG-NA	4.01	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	831	CLA	MG-NA	4.01	2.15	2.06
18	5b	315	CLA	MG-NA	4.00	2.15	2.06
18	F	303	CLA	C1C-C2C	-4.00	1.36	1.44
18	f	303	CLA	C1C-C2C	-4.00	1.36	1.44
18	2a	308	CLA	C1C-C2C	-4.00	1.36	1.44
18	2b	308	CLA	C1C-C2C	-4.00	1.36	1.44
18	B	819	CLA	C1C-C2C	-4.00	1.36	1.44
18	B	838	CLA	C1C-C2C	-4.00	1.36	1.44
18	b	819	CLA	C1C-C2C	-4.00	1.36	1.44
18	b	838	CLA	C1C-C2C	-4.00	1.36	1.44
18	B	854	CLA	C1C-C2C	-3.99	1.36	1.44
18	b	854	CLA	C1C-C2C	-3.99	1.36	1.44
18	B	804	CLA	C1C-C2C	-3.99	1.36	1.44
18	b	804	CLA	C1C-C2C	-3.99	1.36	1.44
29	2a	304	CHL	C2C-C3C	3.99	1.40	1.36
29	2b	304	CHL	C2C-C3C	3.99	1.40	1.36
18	5a	315	CLA	MG-NA	3.99	2.15	2.06
18	3a	309	CLA	C1C-C2C	-3.99	1.36	1.44
18	5a	312	CLA	C1C-C2C	-3.99	1.36	1.44
18	3b	309	CLA	C1C-C2C	-3.99	1.36	1.44
18	5b	312	CLA	C1C-C2C	-3.99	1.36	1.44
18	6b	316	CLA	C1C-C2C	-3.99	1.36	1.44
18	J	101	CLA	C1C-C2C	-3.99	1.36	1.44
18	j	101	CLA	C1C-C2C	-3.99	1.36	1.44
18	A	830	CLA	C1C-C2C	-3.99	1.36	1.44
18	a	830	CLA	C1C-C2C	-3.99	1.36	1.44
18	6a	310	CLA	MG-NA	3.99	2.15	2.06
29	5a	306	CHL	C2C-C3C	3.99	1.40	1.36
29	5b	306	CHL	C2C-C3C	3.99	1.40	1.36
18	3a	314	CLA	C1C-C2C	-3.99	1.36	1.44
18	3b	314	CLA	C1C-C2C	-3.99	1.36	1.44
18	B	835	CLA	C1C-C2C	-3.98	1.36	1.44
18	b	835	CLA	C1C-C2C	-3.98	1.36	1.44
18	3a	306	CLA	C1C-C2C	-3.98	1.36	1.44
18	2a	309	CLA	C1C-C2C	-3.98	1.36	1.44
18	2b	309	CLA	C1C-C2C	-3.98	1.36	1.44
18	K	201	CLA	C1C-C2C	-3.98	1.36	1.44
18	k	201	CLA	C1C-C2C	-3.98	1.36	1.44
18	2a	301	CLA	C1C-C2C	-3.98	1.36	1.44
18	3a	311	CLA	C1C-C2C	-3.98	1.36	1.44
18	3b	306	CLA	C1C-C2C	-3.98	1.36	1.44
18	J	101	CLA	MG-NA	3.97	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	j	101	CLA	MG-NA	3.97	2.15	2.06
18	a	841	CLA	MG-NA	3.97	2.15	2.06
18	F	303	CLA	MG-NA	3.97	2.15	2.06
18	f	303	CLA	MG-NA	3.97	2.15	2.06
18	3a	304	CLA	C1C-C2C	-3.97	1.36	1.44
18	3b	304	CLA	C1C-C2C	-3.97	1.36	1.44
18	A	839	CLA	MG-NA	3.97	2.15	2.06
18	3a	302	CLA	C1C-C2C	-3.97	1.36	1.44
18	3b	302	CLA	C1C-C2C	-3.97	1.36	1.44
18	A	838	CLA	C1C-C2C	-3.96	1.36	1.44
18	a	838	CLA	C1C-C2C	-3.96	1.36	1.44
18	B	818	CLA	C1C-C2C	-3.96	1.36	1.44
18	b	818	CLA	C1C-C2C	-3.96	1.36	1.44
18	B	812	CLA	MG-NA	3.96	2.15	2.06
18	B	837	CLA	MG-NA	3.96	2.15	2.06
18	6a	312	CLA	C1C-C2C	-3.96	1.36	1.44
18	6b	312	CLA	C1C-C2C	-3.96	1.36	1.44
18	6a	315	CLA	MG-NA	3.96	2.15	2.06
18	6b	315	CLA	MG-NA	3.96	2.15	2.06
18	A	833	CLA	MG-NA	3.96	2.15	2.06
18	a	833	CLA	MG-NA	3.96	2.15	2.06
18	5a	304	CLA	C1C-C2C	-3.96	1.36	1.44
18	6a	308	CLA	C1C-C2C	-3.96	1.36	1.44
18	5b	304	CLA	C1C-C2C	-3.96	1.36	1.44
18	6b	308	CLA	C1C-C2C	-3.96	1.36	1.44
18	B	813	CLA	C1C-C2C	-3.95	1.36	1.44
18	b	813	CLA	C1C-C2C	-3.95	1.36	1.44
18	3b	311	CLA	C1C-C2C	-3.95	1.36	1.44
18	A	825	CLA	C1C-C2C	-3.95	1.36	1.44
18	a	825	CLA	C1C-C2C	-3.95	1.36	1.44
18	A	827	CLA	C1C-C2C	-3.95	1.36	1.44
18	a	827	CLA	C1C-C2C	-3.95	1.36	1.44
18	5a	313	CLA	C1C-C2C	-3.95	1.36	1.44
18	5b	313	CLA	C1C-C2C	-3.95	1.36	1.44
18	b	812	CLA	MG-NA	3.95	2.15	2.06
18	b	837	CLA	MG-NA	3.95	2.15	2.06
18	A	841	CLA	C1C-C2C	-3.95	1.36	1.44
18	a	841	CLA	C1C-C2C	-3.95	1.36	1.44
18	a	839	CLA	MG-NA	3.95	2.15	2.06
18	A	841	CLA	MG-NA	3.95	2.15	2.06
18	B	829	CLA	C1C-C2C	-3.94	1.36	1.44
18	b	829	CLA	C1C-C2C	-3.94	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	MG-NA	3.94	2.15	2.06
18	a	840	CLA	MG-NA	3.94	2.15	2.06
18	A	806	CLA	MG-NA	3.94	2.15	2.06
18	a	806	CLA	MG-NA	3.94	2.15	2.06
18	5b	313	CLA	MG-NA	3.94	2.15	2.06
18	A	836	CLA	C1C-C2C	-3.93	1.36	1.44
18	l	303	CLA	MG-NA	3.93	2.15	2.06
18	A	804	CLA	C1C-C2C	-3.93	1.36	1.44
18	a	804	CLA	C1C-C2C	-3.93	1.36	1.44
18	B	832	CLA	MG-NA	3.93	2.15	2.06
18	b	832	CLA	MG-NA	3.93	2.15	2.06
18	A	807	CLA	C1C-C2C	-3.92	1.36	1.44
18	a	807	CLA	C1C-C2C	-3.92	1.36	1.44
18	b	815	CLA	C1C-C2C	-3.92	1.36	1.44
18	A	831	CLA	MG-NA	3.92	2.15	2.06
18	a	831	CLA	MG-NA	3.92	2.15	2.06
18	3a	306	CLA	MG-NA	3.92	2.15	2.06
18	3b	306	CLA	MG-NA	3.92	2.15	2.06
18	5a	313	CLA	MG-NA	3.92	2.15	2.06
18	B	815	CLA	C1C-C2C	-3.92	1.36	1.44
18	L	303	CLA	MG-NA	3.91	2.15	2.06
18	L	302	CLA	MG-NA	3.91	2.15	2.06
18	A	810	CLA	MG-NA	3.91	2.15	2.06
18	a	810	CLA	MG-NA	3.91	2.15	2.06
18	B	805	CLA	MG-NA	3.91	2.15	2.06
18	b	805	CLA	MG-NA	3.91	2.15	2.06
18	a	836	CLA	C1C-C2C	-3.90	1.36	1.44
18	B	820	CLA	MG-NA	3.90	2.15	2.06
18	b	820	CLA	MG-NA	3.90	2.15	2.06
18	l	302	CLA	MG-NA	3.90	2.15	2.06
18	B	814	CLA	MG-NA	3.89	2.15	2.06
18	b	814	CLA	MG-NA	3.89	2.15	2.06
29	3a	301	CHL	C2C-C3C	3.89	1.40	1.36
29	3b	301	CHL	C2C-C3C	3.89	1.40	1.36
18	B	840	CLA	C1C-C2C	-3.89	1.36	1.44
18	b	840	CLA	C1C-C2C	-3.89	1.36	1.44
18	2a	303	CLA	MG-NA	3.87	2.15	2.06
18	2b	303	CLA	MG-NA	3.87	2.15	2.06
18	B	853	CLA	MG-NA	3.86	2.15	2.06
18	b	853	CLA	MG-NA	3.86	2.15	2.06
18	a	829	CLA	MG-NA	3.86	2.15	2.06
18	B	813	CLA	MG-NA	3.85	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	813	CLA	MG-NA	3.85	2.15	2.06
18	6a	306	CLA	MG-NA	3.85	2.15	2.06
18	6b	306	CLA	MG-NA	3.85	2.15	2.06
18	B	827	CLA	MG-NA	3.84	2.15	2.06
18	B	823	CLA	MG-NA	3.84	2.15	2.06
18	b	823	CLA	MG-NA	3.84	2.15	2.06
18	A	829	CLA	MG-NA	3.84	2.15	2.06
18	a	830	CLA	MG-NA	3.84	2.15	2.06
18	2a	310	CLA	MG-NA	3.83	2.15	2.06
18	2b	310	CLA	MG-NA	3.83	2.15	2.06
18	b	827	CLA	MG-NA	3.82	2.15	2.06
29	2a	306	CHL	C2C-C3C	3.82	1.40	1.36
29	2b	306	CHL	C2C-C3C	3.82	1.40	1.36
18	A	817	CLA	MG-NA	3.82	2.15	2.06
18	a	817	CLA	MG-NA	3.82	2.15	2.06
18	B	828	CLA	MG-NA	3.81	2.15	2.06
18	b	828	CLA	MG-NA	3.81	2.15	2.06
18	f	305	CLA	MG-NA	3.81	2.15	2.06
18	6a	307	CLA	MG-NA	3.81	2.15	2.06
29	5a	314	CHL	C2C-C3C	3.81	1.40	1.36
29	5b	314	CHL	C2C-C3C	3.81	1.40	1.36
18	A	818	CLA	MG-NA	3.81	2.15	2.06
18	a	818	CLA	MG-NA	3.81	2.15	2.06
18	F	305	CLA	MG-NA	3.81	2.15	2.06
18	B	821	CLA	MG-NA	3.80	2.15	2.06
18	b	821	CLA	MG-NA	3.80	2.15	2.06
18	A	830	CLA	MG-NA	3.80	2.15	2.06
18	A	842	CLA	MG-NA	3.79	2.15	2.06
18	a	842	CLA	MG-NA	3.79	2.15	2.06
29	3a	315	CHL	C2C-C3C	3.79	1.40	1.36
29	3b	315	CHL	C2C-C3C	3.79	1.40	1.36
18	2b	311	CLA	MG-NA	3.78	2.15	2.06
18	B	818	CLA	MG-NA	3.78	2.15	2.06
18	b	818	CLA	MG-NA	3.78	2.15	2.06
18	6b	307	CLA	MG-NA	3.78	2.15	2.06
18	k	201	CLA	MG-NA	3.78	2.15	2.06
18	A	821	CLA	MG-NA	3.78	2.15	2.06
18	B	826	CLA	MG-NA	3.77	2.15	2.06
18	b	826	CLA	MG-NA	3.77	2.15	2.06
18	A	812	CLA	MG-NA	3.77	2.15	2.06
18	2a	311	CLA	MG-NA	3.77	2.15	2.06
18	a	812	CLA	MG-NA	3.77	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	819	CLA	MG-NA	3.77	2.15	2.06
18	a	819	CLA	MG-NA	3.77	2.15	2.06
18	B	811	CLA	MG-NA	3.76	2.15	2.06
18	6a	317	CLA	MG-NA	3.76	2.15	2.06
18	6b	317	CLA	MG-NA	3.76	2.15	2.06
18	G	203	CLA	MG-NA	3.76	2.15	2.06
18	5b	310	CLA	MG-NA	3.76	2.15	2.06
18	2a	309	CLA	MG-NA	3.76	2.15	2.06
18	2b	309	CLA	MG-NA	3.76	2.15	2.06
18	b	811	CLA	MG-NA	3.76	2.15	2.06
18	g	203	CLA	MG-NA	3.75	2.15	2.06
18	5a	310	CLA	MG-NA	3.75	2.15	2.06
18	K	201	CLA	MG-NA	3.75	2.15	2.06
18	a	821	CLA	MG-NA	3.74	2.15	2.06
18	A	837	CLA	MG-NA	3.73	2.15	2.06
18	a	837	CLA	MG-NA	3.73	2.15	2.06
18	A	820	CLA	MG-NA	3.72	2.15	2.06
18	a	820	CLA	MG-NA	3.72	2.15	2.06
18	3a	305	CLA	MG-NA	3.70	2.15	2.06
29	3b	307	CHL	C2C-C3C	3.69	1.40	1.36
18	3b	305	CLA	MG-NA	3.67	2.15	2.06
18	f	302	CLA	MG-NA	3.66	2.15	2.06
18	3a	304	CLA	MG-NA	3.65	2.14	2.06
18	3b	304	CLA	MG-NA	3.65	2.14	2.06
29	3a	307	CHL	C2C-C3C	3.65	1.39	1.36
18	A	815	CLA	MG-NA	3.65	2.14	2.06
18	F	302	CLA	MG-NA	3.64	2.14	2.06
18	B	804	CLA	MG-NA	3.64	2.14	2.06
18	B	806	CLA	MG-NA	3.64	2.14	2.06
18	b	804	CLA	MG-NA	3.64	2.14	2.06
18	b	806	CLA	MG-NA	3.63	2.14	2.06
18	a	815	CLA	MG-NA	3.63	2.14	2.06
18	A	825	CLA	MG-NA	3.62	2.14	2.06
18	2b	301	CLA	MG-NA	3.62	2.14	2.06
18	2a	301	CLA	MG-NA	3.61	2.14	2.06
18	6a	312	CLA	MG-NA	3.61	2.14	2.06
18	6b	312	CLA	MG-NA	3.61	2.14	2.06
18	a	825	CLA	MG-NA	3.60	2.14	2.06
18	B	808	CLA	MG-NA	3.60	2.14	2.06
18	3a	310	CLA	MG-NA	3.59	2.14	2.06
18	3b	310	CLA	MG-NA	3.59	2.14	2.06
18	B	809	CLA	MG-NA	3.59	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	809	CLA	MG-NA	3.59	2.14	2.06
18	b	808	CLA	MG-NA	3.57	2.14	2.06
18	3a	312	CLA	MG-NA	3.54	2.14	2.06
18	3b	308	CLA	MG-NA	3.53	2.14	2.06
18	a	804	CLA	MG-NA	3.53	2.14	2.06
18	3a	308	CLA	MG-NA	3.53	2.14	2.06
18	3a	302	CLA	MG-NA	3.53	2.14	2.06
18	b	819	CLA	MG-NA	3.52	2.14	2.06
18	A	804	CLA	MG-NA	3.52	2.14	2.06
18	5b	311	CLA	C4C-C3C	-3.52	1.37	1.44
18	3b	312	CLA	MG-NA	3.51	2.14	2.06
18	5a	311	CLA	C4C-C3C	-3.51	1.37	1.44
18	2a	307	CLA	MG-NA	3.51	2.14	2.06
18	2b	307	CLA	MG-NA	3.51	2.14	2.06
18	B	817	CLA	MG-NA	3.51	2.14	2.06
18	b	817	CLA	MG-NA	3.51	2.14	2.06
18	A	834	CLA	MG-NA	3.51	2.14	2.06
18	a	834	CLA	MG-NA	3.51	2.14	2.06
18	6a	313	CLA	MG-NA	3.51	2.14	2.06
18	6b	313	CLA	MG-NA	3.51	2.14	2.06
18	3b	302	CLA	MG-NA	3.50	2.14	2.06
18	B	819	CLA	MG-NA	3.50	2.14	2.06
18	6a	305	CLA	MG-NA	3.50	2.14	2.06
18	6b	305	CLA	MG-NA	3.50	2.14	2.06
18	B	801	CLA	MG-NA	3.50	2.14	2.06
18	b	801	CLA	MG-NA	3.50	2.14	2.06
18	6a	316	CLA	MG-NA	3.49	2.14	2.06
18	6b	316	CLA	MG-NA	3.49	2.14	2.06
18	B	836	CLA	MG-NA	3.49	2.14	2.06
18	b	836	CLA	MG-NA	3.49	2.14	2.06
18	A	814	CLA	MG-NA	3.49	2.14	2.06
18	a	814	CLA	MG-NA	3.49	2.14	2.06
18	A	853	CLA	MG-NA	3.48	2.14	2.06
18	a	853	CLA	MG-NA	3.48	2.14	2.06
18	5b	312	CLA	MG-NA	3.48	2.14	2.06
18	b	852	CLA	MG-NA	3.47	2.14	2.06
18	3a	314	CLA	MG-NA	3.47	2.14	2.06
18	3b	314	CLA	MG-NA	3.47	2.14	2.06
18	5a	312	CLA	MG-NA	3.47	2.14	2.06
18	B	852	CLA	MG-NA	3.46	2.14	2.06
18	5a	302	CLA	MG-NA	3.45	2.14	2.06
18	5b	302	CLA	MG-NA	3.45	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	845	BCR	C8-C9	-3.43	1.38	1.46
20	b	845	BCR	C8-C9	-3.43	1.38	1.46
18	B	829	CLA	MG-NA	3.43	2.14	2.06
18	b	829	CLA	MG-NA	3.43	2.14	2.06
18	A	801	CLA	MG-NA	3.39	2.14	2.06
18	6a	311	CLA	MG-NA	3.39	2.14	2.06
18	a	801	CLA	MG-NA	3.39	2.14	2.06
20	B	845	BCR	C23-C22	-3.39	1.38	1.46
20	b	845	BCR	C23-C22	-3.39	1.38	1.46
18	A	811	CLA	MG-NA	3.38	2.14	2.06
18	a	811	CLA	MG-NA	3.38	2.14	2.06
18	b	807	CLA	MG-NA	3.38	2.14	2.06
18	6b	311	CLA	MG-NA	3.37	2.14	2.06
18	B	807	CLA	MG-NA	3.35	2.14	2.06
18	A	813	CLA	MG-NA	3.34	2.14	2.06
18	a	813	CLA	MG-NA	3.34	2.14	2.06
20	A	851	BCR	C23-C22	-3.34	1.38	1.46
18	A	835	CLA	MG-NA	3.34	2.14	2.06
18	a	835	CLA	MG-NA	3.34	2.14	2.06
20	a	851	BCR	C23-C22	-3.32	1.38	1.46
18	A	803	CLA	MG-NA	3.31	2.14	2.06
18	a	803	CLA	MG-NA	3.31	2.14	2.06
25	3a	317	LUT	C8-C9	-3.30	1.38	1.46
25	3b	317	LUT	C8-C9	-3.30	1.38	1.46
20	A	850	BCR	C8-C9	-3.27	1.38	1.46
20	G	201	BCR	C23-C22	-3.27	1.39	1.46
20	g	201	BCR	C23-C22	-3.27	1.39	1.46
20	a	850	BCR	C8-C9	-3.26	1.39	1.46
18	B	840	CLA	MG-NA	3.24	2.14	2.06
18	b	840	CLA	MG-NA	3.24	2.14	2.06
20	A	849	BCR	C23-C22	-3.23	1.39	1.46
20	I	202	BCR	C23-C22	-3.21	1.39	1.46
20	i	202	BCR	C23-C22	-3.21	1.39	1.46
18	B	838	CLA	MG-NA	3.21	2.13	2.06
18	b	838	CLA	MG-NA	3.21	2.13	2.06
20	a	849	BCR	C23-C22	-3.19	1.39	1.46
20	A	848	BCR	C8-C9	-3.19	1.39	1.46
18	B	833	CLA	MG-NA	3.18	2.13	2.06
18	b	833	CLA	MG-NA	3.18	2.13	2.06
20	L	304	BCR	C8-C9	-3.17	1.39	1.46
20	l	304	BCR	C8-C9	-3.17	1.39	1.46
20	a	848	BCR	C8-C9	-3.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	304	BCR	C23-C22	-3.15	1.39	1.46
20	l	304	BCR	C23-C22	-3.15	1.39	1.46
25	5a	316	LUT	C8-C9	-3.15	1.39	1.46
25	5b	316	LUT	C8-C9	-3.15	1.39	1.46
18	2b	308	CLA	MG-NA	3.15	2.13	2.06
20	G	201	BCR	C8-C9	-3.15	1.39	1.46
20	g	201	BCR	C8-C9	-3.15	1.39	1.46
20	A	851	BCR	C8-C9	-3.15	1.39	1.46
20	a	851	BCR	C8-C9	-3.15	1.39	1.46
18	2a	308	CLA	MG-NA	3.13	2.13	2.06
18	B	824	CLA	MG-NA	3.13	2.13	2.06
18	b	824	CLA	MG-NA	3.12	2.13	2.06
20	F	301	BCR	C23-C22	-3.12	1.39	1.46
20	f	301	BCR	C23-C22	-3.12	1.39	1.46
20	A	850	BCR	C23-C22	-3.12	1.39	1.46
18	A	805	CLA	MG-NA	3.11	2.13	2.06
18	a	805	CLA	MG-NA	3.11	2.13	2.06
20	a	850	BCR	C23-C22	-3.11	1.39	1.46
20	M	101	BCR	C23-C22	-3.10	1.39	1.46
20	m	101	BCR	C23-C22	-3.10	1.39	1.46
25	2a	315	LUT	C14-C13	3.09	1.43	1.35
25	2b	315	LUT	C14-C13	3.09	1.42	1.35
18	5a	308	CLA	MG-NA	3.08	2.13	2.06
18	5b	308	CLA	MG-NA	3.08	2.13	2.06
20	B	846	BCR	C8-C9	-3.08	1.39	1.46
18	B	822	CLA	MG-NA	3.07	2.13	2.06
18	b	822	CLA	MG-NA	3.07	2.13	2.06
18	A	828	CLA	MG-NC	3.06	2.13	2.06
18	a	828	CLA	MG-NC	3.06	2.13	2.06
20	G	204	BCR	C8-C9	-3.06	1.39	1.46
20	g	204	BCR	C8-C9	-3.06	1.39	1.46
20	B	842	BCR	C23-C22	-3.05	1.39	1.46
20	b	842	BCR	C23-C22	-3.05	1.39	1.46
20	A	847	BCR	C8-C9	-3.04	1.39	1.46
20	a	847	BCR	C8-C9	-3.04	1.39	1.46
20	b	851	BCR	C8-C9	-3.04	1.39	1.46
20	B	851	BCR	C8-C9	-3.04	1.39	1.46
25	3a	317	LUT	C10-C9	3.03	1.42	1.35
25	3b	317	LUT	C10-C9	3.03	1.42	1.35
18	3a	309	CLA	MG-NA	3.03	2.13	2.06
18	3b	309	CLA	MG-NA	3.03	2.13	2.06
20	I	202	BCR	C8-C9	-3.03	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	846	BCR	C8-C9	-3.03	1.39	1.46
20	i	202	BCR	C8-C9	-3.03	1.39	1.46
20	F	304	BCR	C23-C22	-3.02	1.39	1.46
20	f	304	BCR	C23-C22	-3.02	1.39	1.46
20	F	301	BCR	C8-C9	-3.02	1.39	1.46
20	f	301	BCR	C8-C9	-3.02	1.39	1.46
18	6a	308	CLA	MG-NC	3.01	2.13	2.06
18	6b	308	CLA	MG-NC	3.01	2.13	2.06
20	F	304	BCR	C8-C9	-3.01	1.39	1.46
20	f	304	BCR	C8-C9	-3.01	1.39	1.46
25	2a	315	LUT	C34-C33	3.00	1.42	1.35
25	2b	315	LUT	C34-C33	3.00	1.42	1.35
18	b	839	CLA	MG-NC	3.00	2.13	2.06
25	3a	316	LUT	C8-C9	-2.99	1.39	1.46
25	3b	316	LUT	C8-C9	-2.99	1.39	1.46
25	5a	317	LUT	C8-C9	-2.98	1.39	1.46
25	5b	317	LUT	C8-C9	-2.98	1.39	1.46
25	6a	319	LUT	C30-C29	2.97	1.42	1.35
18	A	832	CLA	MG-NC	2.97	2.13	2.06
18	a	832	CLA	MG-NC	2.97	2.13	2.06
18	A	824	CLA	MG-NC	2.97	2.13	2.06
18	a	824	CLA	MG-NC	2.97	2.13	2.06
20	B	844	BCR	C8-C9	-2.97	1.39	1.46
20	b	844	BCR	C8-C9	-2.97	1.39	1.46
20	K	202	BCR	C8-C9	-2.97	1.39	1.46
25	6b	319	LUT	C30-C29	2.97	1.42	1.35
18	B	839	CLA	MG-NC	2.97	2.13	2.06
18	A	808	CLA	MG-NA	2.97	2.13	2.06
18	a	808	CLA	MG-NA	2.97	2.13	2.06
20	A	848	BCR	C23-C22	-2.96	1.39	1.46
20	a	848	BCR	C23-C22	-2.96	1.39	1.46
20	A	851	BCR	C19-C18	-2.96	1.39	1.46
20	a	851	BCR	C19-C18	-2.96	1.39	1.46
20	B	846	BCR	C23-C22	-2.96	1.39	1.46
20	b	846	BCR	C23-C22	-2.96	1.39	1.46
20	B	851	BCR	C23-C22	-2.96	1.39	1.46
20	b	851	BCR	C23-C22	-2.96	1.39	1.46
20	K	202	BCR	C23-C22	-2.94	1.39	1.46
20	k	202	BCR	C23-C22	-2.94	1.39	1.46
20	k	202	BCR	C8-C9	-2.93	1.39	1.46
20	A	849	BCR	C8-C9	-2.91	1.39	1.46
20	a	849	BCR	C8-C9	-2.91	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	847	BCR	C23-C22	-2.91	1.39	1.46
20	a	847	BCR	C23-C22	-2.91	1.39	1.46
20	A	850	BCR	C12-C13	-2.91	1.39	1.46
20	a	850	BCR	C12-C13	-2.91	1.39	1.46
20	G	204	BCR	C23-C22	-2.90	1.39	1.46
20	g	204	BCR	C23-C22	-2.90	1.39	1.46
20	J	102	BCR	C23-C22	-2.90	1.39	1.46
20	j	102	BCR	C23-C22	-2.90	1.39	1.46
20	B	843	BCR	C8-C9	-2.89	1.39	1.46
20	b	843	BCR	C8-C9	-2.89	1.39	1.46
18	5a	309	CLA	MG-NA	2.87	2.13	2.06
18	5b	309	CLA	MG-NA	2.87	2.13	2.06
20	B	842	BCR	C8-C9	-2.87	1.39	1.46
18	A	828	CLA	C1D-C2D	-2.87	1.39	1.45
18	a	828	CLA	C1D-C2D	-2.87	1.39	1.45
25	6a	320	LUT	C8-C9	-2.86	1.39	1.46
25	6b	320	LUT	C8-C9	-2.86	1.39	1.46
20	G	201	BCR	C19-C18	-2.86	1.39	1.46
20	g	201	BCR	C19-C18	-2.86	1.39	1.46
20	b	842	BCR	C8-C9	-2.85	1.39	1.46
20	B	844	BCR	C23-C22	-2.85	1.39	1.46
20	b	844	BCR	C23-C22	-2.85	1.39	1.46
18	A	827	CLA	MG-NC	2.84	2.13	2.06
18	a	827	CLA	MG-NC	2.84	2.13	2.06
20	B	845	BCR	C12-C13	-2.83	1.39	1.46
20	b	845	BCR	C12-C13	-2.83	1.39	1.46
18	A	836	CLA	MG-NC	2.83	2.13	2.06
18	a	836	CLA	MG-NC	2.83	2.13	2.06
20	M	101	BCR	C8-C9	-2.82	1.39	1.46
20	m	101	BCR	C8-C9	-2.82	1.39	1.46
18	A	809	CLA	MG-NC	2.82	2.13	2.06
18	a	809	CLA	MG-NC	2.82	2.13	2.06
20	B	848	BCR	C23-C22	-2.80	1.40	1.46
20	b	848	BCR	C23-C22	-2.80	1.40	1.46
25	2b	315	LUT	C8-C9	-2.80	1.40	1.46
20	B	843	BCR	C23-C22	-2.80	1.40	1.46
20	b	843	BCR	C23-C22	-2.80	1.40	1.46
18	3a	303	CLA	MG-NC	2.80	2.12	2.06
18	3b	303	CLA	MG-NC	2.80	2.12	2.06
26	A	802	CL0	C3B-C4B	-2.80	1.38	1.41
26	a	802	CL0	C3B-C4B	-2.80	1.38	1.41
20	I	202	BCR	C19-C18	-2.79	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2a	315	LUT	C8-C9	-2.79	1.40	1.46
25	2a	314	LUT	C8-C9	-2.79	1.40	1.46
25	2b	314	LUT	C8-C9	-2.79	1.40	1.46
18	A	824	CLA	C1D-C2D	-2.78	1.39	1.45
18	a	824	CLA	C1D-C2D	-2.78	1.39	1.45
18	B	818	CLA	C1B-C2B	-2.77	1.36	1.43
20	G	201	BCR	C12-C13	-2.77	1.40	1.46
20	g	201	BCR	C12-C13	-2.77	1.40	1.46
20	i	202	BCR	C19-C18	-2.77	1.40	1.46
18	b	801	CLA	MG-NC	2.76	2.12	2.06
20	J	102	BCR	C8-C9	-2.76	1.40	1.46
20	j	102	BCR	C8-C9	-2.76	1.40	1.46
20	B	846	BCR	C12-C13	-2.76	1.40	1.46
18	B	801	CLA	MG-NC	2.75	2.12	2.06
18	A	839	CLA	MG-NC	2.75	2.12	2.06
18	a	839	CLA	MG-NC	2.75	2.12	2.06
18	b	818	CLA	C1B-C2B	-2.74	1.36	1.43
25	6b	318	LUT	C8-C9	-2.74	1.40	1.46
25	6a	318	LUT	C8-C9	-2.74	1.40	1.46
20	B	848	BCR	C8-C9	-2.73	1.40	1.46
20	b	848	BCR	C8-C9	-2.73	1.40	1.46
18	B	828	CLA	C3D-C4D	-2.73	1.38	1.44
18	b	828	CLA	C3D-C4D	-2.73	1.38	1.44
25	3a	317	LUT	C12-C13	-2.72	1.40	1.46
25	3b	317	LUT	C12-C13	-2.72	1.40	1.46
20	B	845	BCR	C19-C18	-2.72	1.40	1.46
20	b	845	BCR	C19-C18	-2.72	1.40	1.46
20	B	842	BCR	C19-C18	-2.72	1.40	1.46
20	b	842	BCR	C19-C18	-2.72	1.40	1.46
20	b	846	BCR	C12-C13	-2.71	1.40	1.46
25	6a	319	LUT	C8-C9	-2.70	1.40	1.46
25	6b	319	LUT	C8-C9	-2.70	1.40	1.46
18	A	818	CLA	C1B-C2B	-2.69	1.36	1.43
18	a	818	CLA	C1B-C2B	-2.69	1.36	1.43
18	5b	304	CLA	C1B-C2B	-2.68	1.36	1.43
20	A	850	BCR	C19-C18	-2.67	1.40	1.46
20	a	850	BCR	C19-C18	-2.67	1.40	1.46
18	5a	304	CLA	C1B-C2B	-2.66	1.36	1.43
25	3a	316	LUT	C12-C13	-2.66	1.40	1.46
25	3b	316	LUT	C12-C13	-2.66	1.40	1.46
20	F	301	BCR	C19-C18	-2.66	1.40	1.46
20	f	301	BCR	C19-C18	-2.66	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	838	CLA	MG-NC	2.65	2.12	2.06
18	A	836	CLA	C1B-C2B	-2.65	1.36	1.43
18	a	836	CLA	C1B-C2B	-2.65	1.36	1.43
18	B	835	CLA	MG-NC	2.65	2.12	2.06
18	b	835	CLA	MG-NC	2.65	2.12	2.06
18	B	824	CLA	C1B-C2B	-2.65	1.36	1.43
18	b	824	CLA	C1B-C2B	-2.65	1.36	1.43
20	L	304	BCR	C19-C18	-2.65	1.40	1.46
20	l	304	BCR	C19-C18	-2.65	1.40	1.46
29	2a	306	CHL	C3B-C4B	-2.65	1.38	1.41
29	2b	306	CHL	C3B-C4B	-2.65	1.38	1.41
18	b	835	CLA	C1B-C2B	-2.64	1.36	1.43
18	B	810	CLA	MG-NC	2.64	2.12	2.06
18	b	810	CLA	MG-NC	2.64	2.12	2.06
18	B	825	CLA	C1D-C2D	-2.64	1.40	1.45
18	b	825	CLA	C1D-C2D	-2.64	1.40	1.45
18	B	852	CLA	C1D-C2D	-2.64	1.40	1.45
18	b	852	CLA	C1D-C2D	-2.64	1.40	1.45
18	a	839	CLA	C3D-C4D	-2.64	1.38	1.44
18	B	823	CLA	C1B-C2B	-2.64	1.36	1.43
25	5a	316	LUT	C32-C33	-2.63	1.40	1.46
25	5b	316	LUT	C32-C33	-2.63	1.40	1.46
20	A	848	BCR	C12-C13	-2.63	1.40	1.46
20	a	848	BCR	C12-C13	-2.63	1.40	1.46
18	A	839	CLA	C3D-C4D	-2.63	1.38	1.44
18	a	838	CLA	MG-NC	2.63	2.12	2.06
18	A	825	CLA	C3D-C4D	-2.62	1.38	1.44
18	a	825	CLA	C3D-C4D	-2.62	1.38	1.44
29	5a	305	CHL	CHB-C1B	2.62	1.43	1.39
25	3a	316	LUT	C32-C33	-2.62	1.40	1.46
25	3b	316	LUT	C32-C33	-2.62	1.40	1.46
18	B	824	CLA	C3D-C4D	-2.62	1.38	1.44
18	b	824	CLA	C3D-C4D	-2.62	1.38	1.44
25	5a	316	LUT	C12-C13	-2.62	1.40	1.46
25	5b	316	LUT	C12-C13	-2.62	1.40	1.46
18	B	835	CLA	C1B-C2B	-2.62	1.37	1.43
18	B	827	CLA	C3D-C4D	-2.62	1.38	1.44
18	b	827	CLA	C3D-C4D	-2.62	1.38	1.44
18	A	820	CLA	C1B-C2B	-2.61	1.37	1.43
18	a	820	CLA	C1B-C2B	-2.61	1.37	1.43
20	G	204	BCR	C19-C18	-2.61	1.40	1.46
20	g	204	BCR	C19-C18	-2.61	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	846	BCR	C19-C18	-2.61	1.40	1.46
20	L	304	BCR	C12-C13	-2.61	1.40	1.46
20	l	304	BCR	C12-C13	-2.61	1.40	1.46
26	A	802	CL0	CHB-C1B	2.60	1.43	1.39
26	a	802	CL0	CHB-C1B	2.60	1.43	1.39
18	b	823	CLA	C1B-C2B	-2.60	1.37	1.43
20	F	301	BCR	C12-C13	-2.60	1.40	1.46
20	f	301	BCR	C12-C13	-2.60	1.40	1.46
29	5b	305	CHL	CHB-C1B	2.60	1.43	1.39
29	2b	313	CHL	CHB-C1B	2.60	1.43	1.39
18	B	829	CLA	C3D-C4D	-2.60	1.38	1.44
18	b	829	CLA	C3D-C4D	-2.60	1.38	1.44
18	B	838	CLA	C1B-C2B	-2.59	1.37	1.43
29	2a	313	CHL	CHB-C1B	2.59	1.43	1.39
18	B	836	CLA	C3D-C4D	-2.59	1.38	1.44
18	b	836	CLA	C3D-C4D	-2.59	1.38	1.44
18	A	820	CLA	C3D-C4D	-2.59	1.38	1.44
18	a	820	CLA	C3D-C4D	-2.59	1.38	1.44
18	B	825	CLA	C3D-C4D	-2.58	1.38	1.44
18	b	825	CLA	C3D-C4D	-2.58	1.38	1.44
18	6b	305	CLA	C3D-C4D	-2.58	1.38	1.44
18	b	853	CLA	MG-NC	2.58	2.12	2.06
18	A	806	CLA	C3D-C4D	-2.58	1.38	1.44
18	b	818	CLA	C3D-C4D	-2.58	1.38	1.44
18	B	818	CLA	C3D-C4D	-2.58	1.38	1.44
18	6a	305	CLA	C3D-C4D	-2.58	1.38	1.44
18	a	806	CLA	C3D-C4D	-2.57	1.38	1.44
20	K	202	BCR	C12-C13	-2.57	1.40	1.46
18	b	838	CLA	C1B-C2B	-2.57	1.37	1.43
18	B	805	CLA	C3D-C4D	-2.57	1.38	1.44
20	B	843	BCR	C17-C18	2.57	1.41	1.35
20	b	843	BCR	C17-C18	2.57	1.41	1.35
18	B	853	CLA	MG-NC	2.57	2.12	2.06
20	A	849	BCR	C19-C18	-2.57	1.40	1.46
18	A	841	CLA	MG-NC	2.57	2.12	2.06
18	B	801	CLA	C1D-C2D	-2.57	1.40	1.45
20	I	202	BCR	C12-C13	-2.57	1.40	1.46
20	i	202	BCR	C12-C13	-2.57	1.40	1.46
18	B	806	CLA	C3D-C4D	-2.57	1.38	1.44
18	b	806	CLA	C3D-C4D	-2.57	1.38	1.44
20	K	202	BCR	C19-C18	-2.56	1.40	1.46
20	k	202	BCR	C19-C18	-2.56	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	846	BCR	C19-C18	-2.56	1.40	1.46
20	f	304	BCR	C19-C18	-2.56	1.40	1.46
18	a	841	CLA	MG-NC	2.56	2.12	2.06
18	A	801	CLA	C3D-C4D	-2.56	1.38	1.44
18	a	801	CLA	C3D-C4D	-2.56	1.38	1.44
18	b	805	CLA	C3D-C4D	-2.56	1.38	1.44
18	A	801	CLA	C1B-C2B	-2.56	1.37	1.43
18	a	801	CLA	C1B-C2B	-2.56	1.37	1.43
18	B	839	CLA	C3D-C4D	-2.56	1.38	1.44
18	b	839	CLA	C3D-C4D	-2.56	1.38	1.44
29	5a	314	CHL	CHB-C1B	2.55	1.43	1.39
29	5b	314	CHL	CHB-C1B	2.55	1.43	1.39
29	5a	307	CHL	CHB-C1B	2.55	1.43	1.39
29	5b	307	CHL	CHB-C1B	2.55	1.43	1.39
18	B	826	CLA	MG-NC	2.55	2.12	2.06
18	b	826	CLA	MG-NC	2.55	2.12	2.06
20	G	204	BCR	C12-C13	-2.55	1.40	1.46
20	g	204	BCR	C12-C13	-2.55	1.40	1.46
18	K	201	CLA	C3D-C4D	-2.55	1.38	1.44
18	k	201	CLA	C3D-C4D	-2.55	1.38	1.44
18	A	804	CLA	C1B-C2B	-2.54	1.37	1.43
18	a	804	CLA	C1B-C2B	-2.54	1.37	1.43
18	3a	302	CLA	C3D-C4D	-2.54	1.38	1.44
18	3b	302	CLA	C3D-C4D	-2.54	1.38	1.44
18	B	838	CLA	C3D-C4D	-2.54	1.38	1.44
18	b	838	CLA	C3D-C4D	-2.54	1.38	1.44
20	k	202	BCR	C12-C13	-2.54	1.40	1.46
29	6a	309	CHL	CHB-C1B	2.54	1.43	1.39
29	6b	309	CHL	CHB-C1B	2.54	1.43	1.39
18	b	821	CLA	C3D-C4D	-2.54	1.38	1.44
18	l	302	CLA	C3D-C4D	-2.53	1.38	1.44
20	a	849	BCR	C19-C18	-2.53	1.40	1.46
18	B	833	CLA	C3D-C4D	-2.53	1.38	1.44
18	b	833	CLA	C3D-C4D	-2.53	1.38	1.44
18	A	813	CLA	C3D-C4D	-2.53	1.38	1.44
18	a	813	CLA	C3D-C4D	-2.53	1.38	1.44
20	m	101	BCR	C19-C18	-2.53	1.40	1.46
20	F	304	BCR	C19-C18	-2.53	1.40	1.46
25	3a	316	LUT	C28-C29	-2.53	1.40	1.46
25	3b	316	LUT	C28-C29	-2.53	1.40	1.46
18	B	822	CLA	C3D-C4D	-2.53	1.38	1.44
18	B	821	CLA	C3D-C4D	-2.53	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3a	301	CHL	CHB-C1B	2.53	1.43	1.39
29	3b	301	CHL	CHB-C1B	2.53	1.43	1.39
18	A	826	CLA	C3D-C4D	-2.53	1.38	1.44
18	A	833	CLA	C3D-C4D	-2.53	1.38	1.44
18	a	833	CLA	C3D-C4D	-2.53	1.38	1.44
18	b	801	CLA	C1D-C2D	-2.53	1.40	1.45
18	5b	315	CLA	C3D-C4D	-2.53	1.38	1.44
20	M	101	BCR	C19-C18	-2.52	1.40	1.46
18	A	822	CLA	C3D-C4D	-2.52	1.38	1.44
18	a	822	CLA	C3D-C4D	-2.52	1.38	1.44
18	B	809	CLA	C3D-C4D	-2.52	1.38	1.44
18	b	809	CLA	C3D-C4D	-2.52	1.38	1.44
20	B	844	BCR	C12-C13	-2.52	1.40	1.46
20	b	844	BCR	C12-C13	-2.52	1.40	1.46
18	B	831	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	817	CLA	C3D-C4D	-2.52	1.38	1.44
18	a	817	CLA	C3D-C4D	-2.52	1.38	1.44
18	A	835	CLA	C1B-C2B	-2.52	1.37	1.43
18	B	816	CLA	C3D-C4D	-2.52	1.38	1.44
18	b	816	CLA	C3D-C4D	-2.52	1.38	1.44
20	B	843	BCR	C19-C18	-2.52	1.40	1.46
20	b	843	BCR	C19-C18	-2.52	1.40	1.46
18	5a	315	CLA	C3D-C4D	-2.52	1.38	1.44
18	B	815	CLA	C1B-C2B	-2.52	1.37	1.43
18	A	830	CLA	C3D-C4D	-2.52	1.38	1.44
18	2a	302	CLA	C3D-C4D	-2.52	1.38	1.44
18	a	830	CLA	C3D-C4D	-2.52	1.38	1.44
18	2b	302	CLA	C3D-C4D	-2.52	1.38	1.44
20	B	851	BCR	C19-C18	-2.52	1.40	1.46
20	b	851	BCR	C19-C18	-2.52	1.40	1.46
18	B	802	CLA	MG-NA	2.51	2.12	2.06
18	b	802	CLA	MG-NA	2.51	2.12	2.06
18	A	840	CLA	C3D-C4D	-2.51	1.38	1.44
18	a	840	CLA	C3D-C4D	-2.51	1.38	1.44
18	5a	302	CLA	C3D-C4D	-2.51	1.38	1.44
18	5b	302	CLA	C3D-C4D	-2.51	1.38	1.44
18	L	302	CLA	C3D-C4D	-2.51	1.38	1.44
18	A	812	CLA	MG-NC	2.51	2.12	2.06
18	a	812	CLA	MG-NC	2.51	2.12	2.06
29	5a	301	CHL	CHB-C1B	2.51	1.43	1.39
29	5b	301	CHL	CHB-C1B	2.51	1.43	1.39
18	3a	308	CLA	C3D-C4D	-2.51	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	826	CLA	C3D-C4D	-2.51	1.38	1.44
18	3b	308	CLA	C3D-C4D	-2.51	1.38	1.44
18	a	835	CLA	C1B-C2B	-2.51	1.37	1.43
18	A	815	CLA	C3D-C4D	-2.51	1.38	1.44
18	a	815	CLA	C3D-C4D	-2.51	1.38	1.44
29	2a	306	CHL	CHB-C1B	2.51	1.43	1.39
29	2b	306	CHL	CHB-C1B	2.51	1.43	1.39
18	A	836	CLA	C3D-C4D	-2.50	1.38	1.44
18	a	836	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	803	CLA	C3D-C4D	-2.50	1.38	1.44
18	a	803	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	805	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	836	CLA	C1D-C2D	-2.50	1.40	1.45
18	a	836	CLA	C1D-C2D	-2.50	1.40	1.45
18	B	807	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	807	CLA	C3D-C4D	-2.50	1.38	1.44
18	B	854	CLA	C1B-C2B	-2.50	1.37	1.43
18	b	854	CLA	C1B-C2B	-2.50	1.37	1.43
18	B	813	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	813	CLA	C3D-C4D	-2.50	1.38	1.44
18	B	832	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	832	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	829	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	835	CLA	C3D-C4D	-2.50	1.38	1.44
18	a	835	CLA	C3D-C4D	-2.50	1.38	1.44
18	6a	306	CLA	C3D-C4D	-2.50	1.38	1.44
18	6b	306	CLA	C3D-C4D	-2.50	1.38	1.44
18	L	302	CLA	C1D-C2D	-2.50	1.40	1.45
18	l	302	CLA	C1D-C2D	-2.50	1.40	1.45
25	5a	316	LUT	C28-C29	-2.50	1.40	1.46
25	5b	316	LUT	C28-C29	-2.50	1.40	1.46
18	A	811	CLA	C3D-C4D	-2.50	1.38	1.44
18	a	811	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	822	CLA	C3D-C4D	-2.50	1.38	1.44
18	B	815	CLA	C3D-C4D	-2.50	1.38	1.44
18	B	826	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	815	CLA	C3D-C4D	-2.50	1.38	1.44
18	b	826	CLA	C3D-C4D	-2.50	1.38	1.44
18	a	805	CLA	C3D-C4D	-2.50	1.38	1.44
18	A	804	CLA	C3D-C4D	-2.49	1.38	1.44
18	a	804	CLA	C3D-C4D	-2.49	1.38	1.44
20	F	304	BCR	C12-C13	-2.49	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	847	BCR	C19-C18	-2.49	1.40	1.46
18	B	815	CLA	MG-NC	2.49	2.12	2.06
18	b	815	CLA	MG-NC	2.49	2.12	2.06
18	B	837	CLA	C3D-C4D	-2.49	1.38	1.44
18	b	837	CLA	C3D-C4D	-2.49	1.38	1.44
18	2a	308	CLA	C3D-C4D	-2.49	1.38	1.44
18	2b	308	CLA	C3D-C4D	-2.49	1.38	1.44
18	f	303	CLA	C3D-C4D	-2.49	1.38	1.44
25	J	105	LUT	C8-C9	-2.49	1.40	1.46
18	b	831	CLA	C3D-C4D	-2.49	1.38	1.44
25	j	105	LUT	C8-C9	-2.49	1.40	1.46
18	a	829	CLA	C3D-C4D	-2.49	1.38	1.44
20	B	842	BCR	C12-C13	-2.49	1.40	1.46
20	b	842	BCR	C12-C13	-2.49	1.40	1.46
18	B	812	CLA	MG-NC	2.49	2.12	2.06
18	b	812	CLA	MG-NC	2.49	2.12	2.06
18	A	832	CLA	C1D-C2D	-2.49	1.40	1.45
18	a	832	CLA	C1D-C2D	-2.49	1.40	1.45
18	3a	303	CLA	C3D-C4D	-2.49	1.38	1.44
29	3b	307	CHL	C3B-C4B	-2.49	1.39	1.41
18	b	829	CLA	C1B-C2B	-2.48	1.37	1.43
20	f	304	BCR	C12-C13	-2.48	1.40	1.46
18	B	835	CLA	C3D-C4D	-2.48	1.38	1.44
18	G	202	CLA	C3D-C4D	-2.48	1.38	1.44
18	b	835	CLA	C3D-C4D	-2.48	1.38	1.44
18	g	202	CLA	C3D-C4D	-2.48	1.38	1.44
18	A	812	CLA	C3D-C4D	-2.48	1.38	1.44
18	a	812	CLA	C3D-C4D	-2.48	1.38	1.44
18	b	815	CLA	C1B-C2B	-2.48	1.37	1.43
18	3b	303	CLA	C3D-C4D	-2.48	1.38	1.44
18	A	828	CLA	C3D-C4D	-2.48	1.38	1.44
18	a	828	CLA	C3D-C4D	-2.48	1.38	1.44
18	a	819	CLA	C3D-C4D	-2.48	1.38	1.44
18	A	832	CLA	C3D-C4D	-2.48	1.38	1.44
18	a	832	CLA	C3D-C4D	-2.48	1.38	1.44
25	6a	319	LUT	C14-C13	2.47	1.41	1.35
25	6a	319	LUT	C34-C33	2.47	1.41	1.35
25	6b	319	LUT	C14-C13	2.47	1.41	1.35
25	6b	319	LUT	C34-C33	2.47	1.41	1.35
20	A	847	BCR	C12-C13	-2.47	1.40	1.46
20	a	847	BCR	C12-C13	-2.47	1.40	1.46
18	F	303	CLA	C3D-C4D	-2.47	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	850	BCR	C29-C28	-2.47	1.46	1.52
18	B	823	CLA	C3D-C4D	-2.47	1.38	1.44
18	b	823	CLA	C3D-C4D	-2.47	1.38	1.44
18	B	810	CLA	C3D-C4D	-2.47	1.38	1.44
18	b	810	CLA	C3D-C4D	-2.47	1.38	1.44
18	B	802	CLA	C1B-C2B	-2.47	1.37	1.43
18	b	802	CLA	C1B-C2B	-2.47	1.37	1.43
18	B	804	CLA	C3D-C4D	-2.47	1.38	1.44
18	b	804	CLA	C3D-C4D	-2.47	1.38	1.44
18	6b	312	CLA	C3D-C4D	-2.47	1.38	1.44
25	J	105	LUT	C34-C33	2.47	1.41	1.35
25	j	105	LUT	C34-C33	2.47	1.41	1.35
18	A	814	CLA	C3D-C4D	-2.47	1.38	1.44
18	a	814	CLA	C3D-C4D	-2.47	1.38	1.44
29	5a	306	CHL	CHB-C1B	2.47	1.43	1.39
29	5b	306	CHL	CHB-C1B	2.47	1.43	1.39
18	5a	308	CLA	C3D-C4D	-2.47	1.38	1.44
18	5b	308	CLA	C3D-C4D	-2.47	1.38	1.44
20	A	847	BCR	C19-C18	-2.47	1.40	1.46
20	B	848	BCR	C20-C19	2.46	1.41	1.34
20	b	848	BCR	C20-C19	2.46	1.41	1.34
25	J	105	LUT	C14-C13	2.46	1.41	1.35
25	j	105	LUT	C14-C13	2.46	1.41	1.35
18	A	818	CLA	C3D-C4D	-2.46	1.38	1.44
18	A	842	CLA	C3D-C4D	-2.46	1.38	1.44
18	a	818	CLA	C3D-C4D	-2.46	1.38	1.44
18	a	842	CLA	C3D-C4D	-2.46	1.38	1.44
18	6a	316	CLA	C3D-C4D	-2.46	1.38	1.44
18	6b	316	CLA	C3D-C4D	-2.46	1.38	1.44
20	B	851	BCR	C12-C13	-2.46	1.40	1.46
20	b	851	BCR	C12-C13	-2.46	1.40	1.46
18	A	834	CLA	C3D-C4D	-2.46	1.38	1.44
18	a	834	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	819	CLA	C3D-C4D	-2.46	1.38	1.44
18	b	819	CLA	C3D-C4D	-2.46	1.38	1.44
18	5a	309	CLA	C3D-C4D	-2.46	1.38	1.44
18	5b	309	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	828	CLA	C1B-C2B	-2.46	1.37	1.43
18	b	828	CLA	C1B-C2B	-2.46	1.37	1.43
18	6a	311	CLA	C3D-C4D	-2.46	1.38	1.44
18	6b	311	CLA	C3D-C4D	-2.46	1.38	1.44
18	B	829	CLA	C1B-C2B	-2.45	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	105	LUT	C30-C29	2.45	1.41	1.35
25	j	105	LUT	C30-C29	2.45	1.41	1.35
18	A	808	CLA	C3D-C4D	-2.45	1.38	1.44
18	a	808	CLA	C3D-C4D	-2.45	1.38	1.44
18	A	819	CLA	C3D-C4D	-2.45	1.38	1.44
18	2b	312	CLA	C3D-C4D	-2.45	1.38	1.44
18	5b	303	CLA	C3D-C4D	-2.45	1.38	1.44
18	5a	303	CLA	C3D-C4D	-2.45	1.38	1.44
18	B	812	CLA	C3D-C4D	-2.45	1.38	1.44
18	b	812	CLA	C3D-C4D	-2.45	1.38	1.44
18	J	101	CLA	C3D-C4D	-2.45	1.38	1.44
18	j	101	CLA	C3D-C4D	-2.45	1.38	1.44
18	6b	317	CLA	C3D-C4D	-2.45	1.38	1.44
20	A	850	BCR	C29-C28	-2.45	1.46	1.52
18	G	203	CLA	C3D-C4D	-2.45	1.38	1.44
18	g	203	CLA	C3D-C4D	-2.45	1.38	1.44
18	6a	312	CLA	C3D-C4D	-2.45	1.38	1.44
25	2a	315	LUT	C32-C33	-2.45	1.40	1.46
25	2b	315	LUT	C32-C33	-2.45	1.40	1.46
18	B	811	CLA	C3D-C4D	-2.45	1.38	1.44
18	b	811	CLA	C3D-C4D	-2.45	1.38	1.44
18	5a	304	CLA	C3D-C4D	-2.45	1.38	1.44
18	5b	304	CLA	C3D-C4D	-2.45	1.38	1.44
18	A	828	CLA	C1B-C2B	-2.44	1.37	1.43
18	a	828	CLA	C1B-C2B	-2.44	1.37	1.43
18	B	834	CLA	C3D-C4D	-2.44	1.38	1.44
18	b	834	CLA	C3D-C4D	-2.44	1.38	1.44
29	5a	306	CHL	C3B-C4B	-2.44	1.39	1.41
29	5b	306	CHL	C3B-C4B	-2.44	1.39	1.41
18	A	807	CLA	C3D-C4D	-2.44	1.38	1.44
18	a	807	CLA	C3D-C4D	-2.44	1.38	1.44
18	2b	311	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	830	CLA	C1B-C2B	-2.44	1.37	1.43
18	a	830	CLA	C1B-C2B	-2.44	1.37	1.43
18	B	816	CLA	C1B-C2B	-2.44	1.37	1.43
18	b	816	CLA	C1B-C2B	-2.44	1.37	1.43
18	6a	310	CLA	C3D-C4D	-2.44	1.38	1.44
18	6b	310	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	816	CLA	C3D-C4D	-2.44	1.38	1.44
18	6a	317	CLA	C3D-C4D	-2.44	1.38	1.44
18	a	816	CLA	C3D-C4D	-2.44	1.38	1.44
18	B	808	CLA	C1D-C2D	-2.44	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	808	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	827	CLA	C1D-C2D	-2.44	1.40	1.45
18	a	827	CLA	C1D-C2D	-2.44	1.40	1.45
18	L	301	CLA	C3D-C4D	-2.44	1.38	1.44
18	l	301	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	853	CLA	C3D-C4D	-2.44	1.38	1.44
18	a	853	CLA	C3D-C4D	-2.44	1.38	1.44
18	a	827	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	809	CLA	C3D-C4D	-2.44	1.38	1.44
18	a	809	CLA	C3D-C4D	-2.44	1.38	1.44
20	A	848	BCR	C19-C18	-2.44	1.40	1.46
18	2a	307	CLA	C3D-C4D	-2.44	1.38	1.44
18	2b	307	CLA	C3D-C4D	-2.44	1.38	1.44
18	A	816	CLA	MG-NC	2.44	2.12	2.06
18	B	840	CLA	C3D-C4D	-2.44	1.38	1.44
18	b	840	CLA	C3D-C4D	-2.44	1.38	1.44
18	F	305	CLA	C3D-C4D	-2.43	1.38	1.44
18	f	305	CLA	C3D-C4D	-2.43	1.38	1.44
20	J	102	BCR	C10-C9	2.43	1.41	1.35
20	j	102	BCR	C10-C9	2.43	1.41	1.35
18	5a	303	CLA	C1D-C2D	-2.43	1.40	1.45
18	5b	303	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	820	CLA	C3D-C4D	-2.43	1.38	1.44
18	b	820	CLA	C3D-C4D	-2.43	1.38	1.44
18	B	802	CLA	C1D-C2D	-2.43	1.40	1.45
18	b	802	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	818	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	837	CLA	C3D-C4D	-2.43	1.38	1.44
18	2a	311	CLA	C3D-C4D	-2.43	1.38	1.44
18	a	837	CLA	C3D-C4D	-2.43	1.38	1.44
18	a	819	CLA	C1D-C2D	-2.43	1.40	1.45
29	3a	307	CHL	CHB-C1B	2.43	1.43	1.39
29	3b	307	CHL	CHB-C1B	2.43	1.43	1.39
18	6a	312	CLA	C1B-C2B	-2.43	1.37	1.43
18	6b	312	CLA	C1B-C2B	-2.43	1.37	1.43
25	6a	318	LUT	C34-C33	2.43	1.41	1.35
25	6b	318	LUT	C34-C33	2.43	1.41	1.35
18	B	808	CLA	C3D-C4D	-2.42	1.38	1.44
18	b	808	CLA	C3D-C4D	-2.42	1.38	1.44
18	b	813	CLA	MG-NC	2.42	2.12	2.06
18	2a	309	CLA	C3D-C4D	-2.42	1.38	1.44
18	3a	312	CLA	C3D-C4D	-2.42	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2b	309	CLA	C3D-C4D	-2.42	1.38	1.44
18	3b	312	CLA	C3D-C4D	-2.42	1.38	1.44
18	A	831	CLA	MG-NC	2.42	2.12	2.06
18	a	831	CLA	MG-NC	2.42	2.12	2.06
18	A	827	CLA	C3D-C4D	-2.42	1.38	1.44
18	a	816	CLA	MG-NC	2.42	2.12	2.06
29	6a	304	CHL	CHB-C1B	2.42	1.43	1.39
29	6b	304	CHL	CHB-C1B	2.42	1.43	1.39
18	B	803	CLA	C3D-C4D	-2.42	1.38	1.44
18	b	803	CLA	C3D-C4D	-2.42	1.38	1.44
18	A	841	CLA	C1D-C2D	-2.42	1.40	1.45
18	F	302	CLA	C3D-C4D	-2.42	1.38	1.44
18	f	302	CLA	C3D-C4D	-2.42	1.38	1.44
18	a	810	CLA	C3D-C4D	-2.42	1.38	1.44
18	b	818	CLA	C1D-C2D	-2.42	1.40	1.45
25	2a	315	LUT	C28-C29	-2.42	1.40	1.46
25	2b	315	LUT	C28-C29	-2.42	1.40	1.46
25	2b	314	LUT	C34-C33	2.42	1.41	1.35
18	B	854	CLA	C1D-C2D	-2.42	1.40	1.45
18	b	854	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	817	CLA	C3D-C4D	-2.42	1.38	1.44
18	b	817	CLA	C3D-C4D	-2.42	1.38	1.44
20	a	848	BCR	C19-C18	-2.42	1.40	1.46
29	3a	307	CHL	C3B-C4B	-2.42	1.39	1.41
18	L	303	CLA	C3D-C4D	-2.42	1.38	1.44
18	l	303	CLA	C3D-C4D	-2.42	1.38	1.44
18	B	805	CLA	C1D-C2D	-2.42	1.40	1.45
18	b	805	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	821	CLA	C3D-C4D	-2.41	1.38	1.44
18	3a	314	CLA	C3D-C4D	-2.41	1.38	1.44
18	a	821	CLA	C3D-C4D	-2.41	1.38	1.44
18	3b	314	CLA	C3D-C4D	-2.41	1.38	1.44
18	2a	312	CLA	C3D-C4D	-2.41	1.38	1.44
18	2a	301	CLA	C3D-C4D	-2.41	1.38	1.44
18	2b	301	CLA	C3D-C4D	-2.41	1.38	1.44
18	B	852	CLA	C3D-C4D	-2.41	1.38	1.44
18	b	852	CLA	C3D-C4D	-2.41	1.38	1.44
20	B	844	BCR	C19-C18	-2.41	1.40	1.46
20	b	844	BCR	C19-C18	-2.41	1.40	1.46
25	2a	315	LUT	C12-C13	-2.41	1.40	1.46
25	2b	315	LUT	C12-C13	-2.41	1.40	1.46
18	5a	311	CLA	MG-NC	2.41	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5b	311	CLA	MG-NC	2.41	2.12	2.06
18	A	831	CLA	C1D-C2D	-2.41	1.40	1.45
18	a	831	CLA	C1D-C2D	-2.41	1.40	1.45
18	a	823	CLA	MG-NC	2.41	2.12	2.06
18	A	829	CLA	C1B-C2B	-2.41	1.37	1.43
18	a	829	CLA	C1B-C2B	-2.41	1.37	1.43
18	3b	305	CLA	C3D-C4D	-2.41	1.38	1.44
20	M	101	BCR	C12-C13	-2.41	1.40	1.46
20	m	101	BCR	C12-C13	-2.41	1.40	1.46
18	5a	312	CLA	C3D-C4D	-2.40	1.38	1.44
18	5b	312	CLA	C3D-C4D	-2.40	1.38	1.44
25	6a	319	LUT	C10-C9	2.40	1.41	1.35
25	6b	319	LUT	C10-C9	2.40	1.41	1.35
18	B	826	CLA	C1D-C2D	-2.40	1.40	1.45
18	b	826	CLA	C1D-C2D	-2.40	1.40	1.45
18	b	837	CLA	MG-NC	2.40	2.12	2.06
18	B	854	CLA	C3D-C4D	-2.40	1.38	1.44
18	b	854	CLA	C3D-C4D	-2.40	1.38	1.44
29	2a	304	CHL	CHB-C1B	2.40	1.43	1.39
29	2b	304	CHL	CHB-C1B	2.40	1.43	1.39
18	B	852	CLA	C1B-C2B	-2.40	1.37	1.43
18	b	852	CLA	C1B-C2B	-2.40	1.37	1.43
25	6a	320	LUT	C12-C13	-2.40	1.40	1.46
25	6b	320	LUT	C12-C13	-2.40	1.40	1.46
18	A	819	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	833	CLA	MG-NC	2.40	2.12	2.06
29	5a	307	CHL	C3B-C4B	-2.40	1.39	1.41
29	5b	307	CHL	C3B-C4B	-2.40	1.39	1.41
18	A	823	CLA	C3D-C4D	-2.40	1.38	1.44
18	B	830	CLA	C3D-C4D	-2.40	1.38	1.44
18	b	830	CLA	C3D-C4D	-2.40	1.38	1.44
18	a	833	CLA	MG-NC	2.40	2.12	2.06
18	a	806	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	823	CLA	MG-NC	2.40	2.12	2.06
25	5a	317	LUT	C12-C13	-2.40	1.40	1.46
25	5b	317	LUT	C12-C13	-2.40	1.40	1.46
25	2a	314	LUT	C34-C33	2.40	1.41	1.35
18	5a	310	CLA	C3D-C4D	-2.40	1.38	1.44
18	5b	310	CLA	C3D-C4D	-2.40	1.38	1.44
20	A	849	BCR	C12-C13	-2.39	1.40	1.46
20	a	849	BCR	C12-C13	-2.39	1.40	1.46
18	B	827	CLA	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	827	CLA	C1D-C2D	-2.39	1.40	1.45
25	6b	318	LUT	C14-C13	2.39	1.41	1.35
25	3a	317	LUT	C32-C33	-2.39	1.40	1.46
25	5a	317	LUT	C32-C33	-2.39	1.40	1.46
25	5b	317	LUT	C32-C33	-2.39	1.40	1.46
18	3a	305	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	806	CLA	MG-NC	2.39	2.12	2.06
18	3b	308	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	813	CLA	MG-NC	2.39	2.12	2.06
18	B	804	CLA	C1B-C2B	-2.39	1.37	1.43
18	b	804	CLA	C1B-C2B	-2.39	1.37	1.43
18	6a	315	CLA	C3D-C4D	-2.39	1.38	1.44
18	6b	315	CLA	C3D-C4D	-2.39	1.38	1.44
18	a	806	CLA	MG-NC	2.39	2.11	2.06
18	A	806	CLA	C1D-C2D	-2.39	1.40	1.45
18	3a	309	CLA	C3D-C4D	-2.39	1.38	1.44
18	6a	314	CLA	C3D-C4D	-2.39	1.38	1.44
18	3b	309	CLA	C3D-C4D	-2.39	1.38	1.44
18	6b	314	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	810	CLA	C3D-C4D	-2.39	1.38	1.44
18	A	820	CLA	C1D-C2D	-2.39	1.40	1.45
18	a	820	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	840	CLA	C1D-C2D	-2.39	1.40	1.45
18	b	840	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	817	CLA	C1B-C2B	-2.38	1.37	1.43
18	a	817	CLA	C1B-C2B	-2.38	1.37	1.43
25	6a	318	LUT	C14-C13	2.38	1.41	1.35
20	B	845	BCR	C29-C28	-2.38	1.47	1.52
20	b	845	BCR	C29-C28	-2.38	1.47	1.52
18	A	831	CLA	C3D-C4D	-2.38	1.38	1.44
18	a	831	CLA	C3D-C4D	-2.38	1.38	1.44
18	b	816	CLA	MG-NC	2.38	2.11	2.06
18	3a	313	CLA	C3D-C4D	-2.38	1.38	1.44
18	3b	313	CLA	C3D-C4D	-2.38	1.38	1.44
18	3a	304	CLA	C3D-C4D	-2.38	1.38	1.44
18	6a	307	CLA	C3D-C4D	-2.38	1.38	1.44
18	3b	304	CLA	C3D-C4D	-2.38	1.38	1.44
18	6b	307	CLA	C3D-C4D	-2.38	1.38	1.44
25	2a	314	LUT	C28-C29	-2.38	1.40	1.46
25	2b	314	LUT	C28-C29	-2.38	1.40	1.46
18	A	826	CLA	C1D-C2D	-2.38	1.40	1.45
18	6a	313	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6b	313	CLA	C3D-C4D	-2.38	1.38	1.44
18	A	838	CLA	C1B-C2B	-2.38	1.37	1.43
18	a	838	CLA	C1B-C2B	-2.38	1.37	1.43
18	B	837	CLA	MG-NC	2.38	2.11	2.06
18	a	841	CLA	C1D-C2D	-2.37	1.40	1.45
18	6a	308	CLA	C3D-C4D	-2.37	1.38	1.44
18	6b	308	CLA	C3D-C4D	-2.37	1.38	1.44
25	6a	320	LUT	C32-C33	-2.37	1.40	1.46
25	6b	320	LUT	C32-C33	-2.37	1.40	1.46
18	B	801	CLA	C3D-C4D	-2.37	1.38	1.44
18	b	801	CLA	C3D-C4D	-2.37	1.38	1.44
18	B	819	CLA	C1D-C2D	-2.37	1.40	1.45
18	b	819	CLA	C1D-C2D	-2.37	1.40	1.45
18	5a	313	CLA	C3D-C4D	-2.37	1.38	1.44
18	5b	313	CLA	C3D-C4D	-2.37	1.38	1.44
25	5b	317	LUT	C28-C29	-2.37	1.40	1.46
18	l	301	CLA	C1B-C2B	-2.37	1.37	1.43
18	A	809	CLA	C1D-C2D	-2.37	1.40	1.45
18	a	809	CLA	C1D-C2D	-2.37	1.40	1.45
18	3a	310	CLA	C3D-C4D	-2.37	1.38	1.44
18	3b	310	CLA	C3D-C4D	-2.37	1.38	1.44
18	a	823	CLA	C3D-C4D	-2.37	1.38	1.44
29	3a	315	CHL	CHB-C1B	2.37	1.43	1.39
29	3b	315	CHL	CHB-C1B	2.37	1.43	1.39
25	5a	317	LUT	C28-C29	-2.37	1.40	1.46
18	2a	303	CLA	C3D-C4D	-2.37	1.38	1.44
18	2b	303	CLA	C3D-C4D	-2.37	1.38	1.44
18	A	838	CLA	C3D-C4D	-2.37	1.38	1.44
18	a	838	CLA	C3D-C4D	-2.37	1.38	1.44
18	A	833	CLA	C1B-C2B	-2.36	1.37	1.43
18	a	833	CLA	C1B-C2B	-2.36	1.37	1.43
18	a	826	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	839	CLA	C1D-C2D	-2.36	1.40	1.45
18	b	839	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	816	CLA	C1D-C2D	-2.36	1.40	1.45
18	b	816	CLA	C1D-C2D	-2.36	1.40	1.45
18	a	807	CLA	C1B-C2B	-2.36	1.37	1.43
18	A	807	CLA	MG-NC	2.36	2.11	2.06
18	a	807	CLA	MG-NC	2.36	2.11	2.06
18	F	305	CLA	C1D-C2D	-2.36	1.40	1.45
18	f	305	CLA	C1D-C2D	-2.36	1.40	1.45
18	A	823	CLA	C1B-C2B	-2.36	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	823	CLA	C1B-C2B	-2.36	1.37	1.43
25	3b	317	LUT	C32-C33	-2.36	1.40	1.46
18	B	814	CLA	C3D-C4D	-2.35	1.38	1.44
18	b	814	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	816	CLA	MG-NC	2.35	2.11	2.06
18	5a	309	CLA	C1B-C2B	-2.35	1.37	1.43
18	5b	309	CLA	C1B-C2B	-2.35	1.37	1.43
18	3a	309	CLA	C1B-C2B	-2.35	1.37	1.43
18	3b	309	CLA	C1B-C2B	-2.35	1.37	1.43
18	B	820	CLA	C1B-C2B	-2.35	1.37	1.43
18	b	820	CLA	C1B-C2B	-2.35	1.37	1.43
18	B	830	CLA	MG-NC	2.35	2.11	2.06
18	b	830	CLA	MG-NC	2.35	2.11	2.06
18	3a	308	CLA	C1D-C2D	-2.35	1.40	1.45
18	L	301	CLA	C1B-C2B	-2.35	1.37	1.43
18	2a	310	CLA	C1B-C2B	-2.35	1.37	1.43
18	2b	310	CLA	C1B-C2B	-2.35	1.37	1.43
18	B	805	CLA	C1B-C2B	-2.35	1.37	1.43
18	b	805	CLA	C1B-C2B	-2.35	1.37	1.43
18	A	829	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	822	CLA	MG-NC	2.34	2.11	2.06
18	a	822	CLA	MG-NC	2.34	2.11	2.06
18	2a	310	CLA	C3D-C4D	-2.34	1.38	1.44
18	2b	310	CLA	C3D-C4D	-2.34	1.38	1.44
18	A	816	CLA	C1B-C2B	-2.34	1.37	1.43
18	A	839	CLA	C1D-C2D	-2.34	1.40	1.45
18	a	839	CLA	C1D-C2D	-2.34	1.40	1.45
20	J	102	BCR	C21-C22	2.34	1.41	1.35
20	j	102	BCR	C21-C22	2.34	1.41	1.35
18	A	801	CLA	C1D-C2D	-2.34	1.40	1.45
18	a	801	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	802	CLA	C3D-C4D	-2.33	1.38	1.44
18	b	802	CLA	C3D-C4D	-2.33	1.38	1.44
18	A	825	CLA	C1D-C2D	-2.33	1.40	1.45
18	a	825	CLA	C1D-C2D	-2.33	1.40	1.45
18	5a	311	CLA	C3D-C4D	-2.33	1.38	1.44
18	5b	311	CLA	C3D-C4D	-2.33	1.38	1.44
25	3a	317	LUT	C28-C29	-2.33	1.41	1.46
25	3b	317	LUT	C28-C29	-2.33	1.41	1.46
18	6a	306	CLA	MG-NC	2.33	2.11	2.06
18	6b	306	CLA	MG-NC	2.33	2.11	2.06
18	A	807	CLA	C1B-C2B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	822	CLA	C1B-C2B	-2.33	1.37	1.43
18	b	822	CLA	C1B-C2B	-2.33	1.37	1.43
18	5a	303	CLA	MG-NC	2.33	2.11	2.06
18	5b	303	CLA	MG-NC	2.33	2.11	2.06
18	3a	306	CLA	C3D-C4D	-2.33	1.39	1.44
18	3b	306	CLA	C3D-C4D	-2.33	1.39	1.44
18	B	811	CLA	C1D-C2D	-2.33	1.40	1.45
18	b	811	CLA	C1D-C2D	-2.33	1.40	1.45
18	B	835	CLA	C1D-C2D	-2.33	1.40	1.45
18	b	835	CLA	C1D-C2D	-2.33	1.40	1.45
18	a	829	CLA	C1D-C2D	-2.33	1.40	1.45
18	B	803	CLA	MG-NC	2.32	2.11	2.06
18	b	803	CLA	MG-NC	2.32	2.11	2.06
25	2a	314	LUT	C12-C13	-2.32	1.41	1.46
25	2b	314	LUT	C12-C13	-2.32	1.41	1.46
25	6a	320	LUT	C30-C29	2.32	1.41	1.35
25	6b	320	LUT	C30-C29	2.32	1.41	1.35
18	A	841	CLA	C3D-C4D	-2.32	1.39	1.44
18	a	841	CLA	C3D-C4D	-2.32	1.39	1.44
18	A	821	CLA	C1B-C2B	-2.32	1.37	1.43
18	a	821	CLA	C1B-C2B	-2.32	1.37	1.43
18	A	830	CLA	MG-NC	2.32	2.11	2.06
18	a	830	CLA	MG-NC	2.32	2.11	2.06
18	6a	308	CLA	C1B-C2B	-2.32	1.37	1.43
18	6b	308	CLA	C1B-C2B	-2.32	1.37	1.43
18	3a	311	CLA	C3D-C4D	-2.32	1.39	1.44
18	3b	311	CLA	C3D-C4D	-2.32	1.39	1.44
18	B	834	CLA	C1B-C2B	-2.32	1.37	1.43
18	b	834	CLA	C1B-C2B	-2.32	1.37	1.43
18	5a	303	CLA	C1B-C2B	-2.32	1.37	1.43
18	5b	303	CLA	C1B-C2B	-2.32	1.37	1.43
18	B	806	CLA	C1D-C2D	-2.32	1.40	1.45
18	b	806	CLA	C1D-C2D	-2.32	1.40	1.45
20	A	851	BCR	C12-C13	-2.32	1.41	1.46
20	J	102	BCR	C17-C18	2.32	1.41	1.35
20	j	102	BCR	C17-C18	2.32	1.41	1.35
29	2a	305	CHL	CHB-C1B	2.31	1.43	1.39
18	B	807	CLA	C1D-C2D	-2.31	1.40	1.45
18	b	807	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	810	CLA	C1B-C2B	-2.31	1.37	1.43
18	a	810	CLA	C1B-C2B	-2.31	1.37	1.43
18	B	812	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	812	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	824	CLA	C3D-C4D	-2.31	1.39	1.44
18	a	824	CLA	C3D-C4D	-2.31	1.39	1.44
18	A	837	CLA	MG-NC	2.31	2.11	2.06
18	3a	311	CLA	MG-NC	2.31	2.11	2.06
18	3b	311	CLA	MG-NC	2.31	2.11	2.06
18	a	816	CLA	C1B-C2B	-2.31	1.37	1.43
18	K	201	CLA	CAB-C3B	-2.31	1.46	1.50
18	k	201	CLA	CAB-C3B	-2.31	1.46	1.50
29	2b	305	CHL	CHB-C1B	2.31	1.43	1.39
18	3a	303	CLA	C1B-C2B	-2.31	1.37	1.43
18	6a	314	CLA	MG-NC	2.31	2.11	2.06
18	6b	314	CLA	MG-NC	2.31	2.11	2.06
20	a	851	BCR	C12-C13	-2.30	1.41	1.46
18	F	305	CLA	MG-NC	2.30	2.11	2.06
18	f	305	CLA	MG-NC	2.30	2.11	2.06
18	A	840	CLA	C1D-C2D	-2.30	1.40	1.45
18	a	840	CLA	C1D-C2D	-2.30	1.40	1.45
18	A	810	CLA	C1D-C2D	-2.30	1.40	1.45
18	a	810	CLA	C1D-C2D	-2.30	1.40	1.45
18	6a	308	CLA	C1D-C2D	-2.30	1.40	1.45
18	6b	308	CLA	C1D-C2D	-2.30	1.40	1.45
18	5a	309	CLA	C1D-C2D	-2.30	1.40	1.45
18	5b	309	CLA	C1D-C2D	-2.30	1.40	1.45
18	B	831	CLA	MG-NC	2.30	2.11	2.06
18	b	831	CLA	MG-NC	2.30	2.11	2.06
18	3b	303	CLA	C1B-C2B	-2.30	1.37	1.43
18	A	812	CLA	C1D-C2D	-2.30	1.40	1.45
18	a	812	CLA	C1D-C2D	-2.30	1.40	1.45
18	2a	307	CLA	C1B-C2B	-2.30	1.37	1.43
18	2b	307	CLA	C1B-C2B	-2.30	1.37	1.43
18	b	852	CLA	C1B-NB	-2.30	1.34	1.37
18	A	815	CLA	C1B-C2B	-2.30	1.37	1.43
18	a	815	CLA	C1B-C2B	-2.30	1.37	1.43
25	6a	320	LUT	C34-C33	2.30	1.41	1.35
25	6b	320	LUT	C34-C33	2.30	1.41	1.35
18	l	303	CLA	MG-NC	2.30	2.11	2.06
18	B	814	CLA	C1B-C2B	-2.30	1.37	1.43
18	b	814	CLA	C1B-C2B	-2.30	1.37	1.43
20	B	843	BCR	C12-C13	-2.30	1.41	1.46
20	b	843	BCR	C12-C13	-2.30	1.41	1.46
18	B	814	CLA	C1D-C2D	-2.30	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	814	CLA	C1D-C2D	-2.30	1.40	1.45
18	A	817	CLA	C1D-C2D	-2.30	1.40	1.45
18	a	817	CLA	C1D-C2D	-2.30	1.40	1.45
25	6b	320	LUT	C28-C29	-2.29	1.41	1.46
18	g	203	CLA	C1B-C2B	-2.29	1.37	1.43
18	A	834	CLA	C1B-C2B	-2.29	1.37	1.43
18	a	834	CLA	C1B-C2B	-2.29	1.37	1.43
18	B	820	CLA	C1D-C2D	-2.29	1.40	1.45
18	b	820	CLA	C1D-C2D	-2.29	1.40	1.45
18	L	303	CLA	MG-NC	2.29	2.11	2.06
25	6a	320	LUT	C28-C29	-2.29	1.41	1.46
18	a	837	CLA	MG-NC	2.29	2.11	2.06
18	5a	315	CLA	MG-NC	2.29	2.11	2.06
18	5b	315	CLA	MG-NC	2.29	2.11	2.06
29	2a	305	CHL	C3B-C4B	-2.29	1.39	1.41
29	2b	305	CHL	C3B-C4B	-2.29	1.39	1.41
20	J	102	BCR	C14-C13	2.29	1.41	1.35
20	j	102	BCR	C14-C13	2.29	1.41	1.35
25	6a	318	LUT	C10-C9	2.28	1.41	1.35
25	6b	318	LUT	C10-C9	2.28	1.41	1.35
18	f	302	CLA	C1D-C2D	-2.28	1.40	1.45
18	B	838	CLA	C1D-C2D	-2.28	1.40	1.45
18	b	838	CLA	C1D-C2D	-2.28	1.40	1.45
20	A	851	BCR	C14-C13	2.28	1.41	1.35
20	a	851	BCR	C14-C13	2.28	1.41	1.35
18	L	302	CLA	MG-NC	2.28	2.11	2.06
18	l	302	CLA	MG-NC	2.28	2.11	2.06
18	G	203	CLA	C1B-C2B	-2.28	1.37	1.43
18	6a	307	CLA	C1B-C2B	-2.28	1.37	1.43
18	6b	307	CLA	C1B-C2B	-2.28	1.37	1.43
18	A	803	CLA	C1B-C2B	-2.28	1.37	1.43
18	a	803	CLA	C1B-C2B	-2.28	1.37	1.43
25	6a	318	LUT	C12-C13	-2.28	1.41	1.46
25	6b	318	LUT	C12-C13	-2.28	1.41	1.46
18	A	840	CLA	C1B-C2B	-2.28	1.37	1.43
18	a	840	CLA	C1B-C2B	-2.28	1.37	1.43
20	A	849	BCR	C10-C9	2.28	1.41	1.35
20	a	849	BCR	C10-C9	2.28	1.41	1.35
18	b	809	CLA	C1D-C2D	-2.27	1.40	1.45
25	J	105	LUT	C12-C13	-2.27	1.41	1.46
25	j	105	LUT	C12-C13	-2.27	1.41	1.46
18	a	814	CLA	MG-NC	2.27	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	825	CLA	C1B-C2B	-2.27	1.37	1.43
18	J	101	CLA	C1B-C2B	-2.27	1.37	1.43
18	b	825	CLA	C1B-C2B	-2.27	1.37	1.43
18	j	101	CLA	C1B-C2B	-2.27	1.37	1.43
18	2a	302	CLA	MG-NC	2.27	2.11	2.06
18	2b	302	CLA	MG-NC	2.27	2.11	2.06
18	B	831	CLA	C1D-C2D	-2.27	1.40	1.45
20	B	848	BCR	C10-C9	2.27	1.41	1.35
20	b	848	BCR	C10-C9	2.27	1.41	1.35
18	F	302	CLA	C1D-C2D	-2.27	1.40	1.45
20	A	847	BCR	C21-C22	2.27	1.41	1.35
20	a	847	BCR	C21-C22	2.27	1.41	1.35
25	5b	317	LUT	C14-C13	2.26	1.41	1.35
18	6a	306	CLA	C1B-C2B	-2.26	1.37	1.43
18	6b	306	CLA	C1B-C2B	-2.26	1.37	1.43
18	G	202	CLA	MG-NC	2.26	2.11	2.06
18	g	202	CLA	MG-NC	2.26	2.11	2.06
18	B	852	CLA	C1B-NB	-2.26	1.34	1.37
18	B	821	CLA	MG-NC	2.26	2.11	2.06
18	F	303	CLA	C1B-C2B	-2.26	1.37	1.43
18	f	303	CLA	C1B-C2B	-2.26	1.37	1.43
18	3a	302	CLA	C1D-C2D	-2.26	1.40	1.45
18	3b	302	CLA	C1D-C2D	-2.26	1.40	1.45
18	3a	313	CLA	MG-NC	2.26	2.11	2.06
18	3b	313	CLA	MG-NC	2.26	2.11	2.06
18	g	202	CLA	C1D-C2D	-2.26	1.40	1.45
20	L	304	BCR	C29-C28	-2.26	1.47	1.52
20	l	304	BCR	C29-C28	-2.26	1.47	1.52
18	B	834	CLA	C1D-C2D	-2.26	1.40	1.45
18	b	834	CLA	C1D-C2D	-2.26	1.40	1.45
25	6a	318	LUT	C30-C29	2.25	1.41	1.35
18	b	831	CLA	C1D-C2D	-2.25	1.40	1.45
18	b	821	CLA	MG-NC	2.25	2.11	2.06
18	B	811	CLA	C1B-C2B	-2.25	1.37	1.43
18	b	811	CLA	C1B-C2B	-2.25	1.37	1.43
18	2a	309	CLA	C1D-C2D	-2.25	1.40	1.45
18	2b	309	CLA	C1D-C2D	-2.25	1.40	1.45
18	6a	314	CLA	C1B-C2B	-2.25	1.37	1.43
18	5a	312	CLA	C1B-C2B	-2.25	1.37	1.43
18	5b	312	CLA	C1B-C2B	-2.25	1.37	1.43
18	B	833	CLA	C1B-C2B	-2.25	1.37	1.43
18	b	833	CLA	C1B-C2B	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	MG-NC	2.25	2.11	2.06
18	a	840	CLA	MG-NC	2.25	2.11	2.06
18	A	819	CLA	C1B-C2B	-2.25	1.37	1.43
18	B	806	CLA	C1B-C2B	-2.25	1.37	1.43
18	b	806	CLA	C1B-C2B	-2.25	1.37	1.43
18	3b	303	CLA	C1D-C2D	-2.25	1.40	1.45
18	B	809	CLA	C1D-C2D	-2.25	1.40	1.45
18	B	822	CLA	C1D-C2D	-2.25	1.40	1.45
18	b	822	CLA	C1D-C2D	-2.25	1.40	1.45
18	6a	310	CLA	C1D-C2D	-2.25	1.40	1.45
18	6b	310	CLA	C1D-C2D	-2.25	1.40	1.45
18	2a	302	CLA	C1B-C2B	-2.25	1.37	1.43
18	2b	302	CLA	C1B-C2B	-2.25	1.37	1.43
18	B	819	CLA	C1B-C2B	-2.25	1.37	1.43
18	b	819	CLA	C1B-C2B	-2.25	1.37	1.43
18	A	853	CLA	C1D-C2D	-2.25	1.40	1.45
18	a	853	CLA	C1D-C2D	-2.25	1.40	1.45
18	B	853	CLA	C1B-C2B	-2.25	1.37	1.43
18	b	853	CLA	C1B-C2B	-2.25	1.37	1.43
18	B	804	CLA	C1D-C2D	-2.25	1.40	1.45
18	b	804	CLA	C1D-C2D	-2.25	1.40	1.45
18	6a	310	CLA	C1B-C2B	-2.25	1.37	1.43
18	6b	310	CLA	C1B-C2B	-2.25	1.37	1.43
18	B	832	CLA	C1D-C2D	-2.25	1.40	1.45
18	b	832	CLA	C1D-C2D	-2.25	1.40	1.45
25	6b	318	LUT	C31-C32	2.24	1.40	1.34
18	2a	309	CLA	C1B-C2B	-2.24	1.37	1.43
18	2b	309	CLA	C1B-C2B	-2.24	1.37	1.43
20	B	848	BCR	C12-C13	-2.24	1.41	1.46
20	b	848	BCR	C12-C13	-2.24	1.41	1.46
20	B	848	BCR	C17-C18	2.24	1.41	1.35
20	b	848	BCR	C17-C18	2.24	1.41	1.35
18	6b	315	CLA	MG-NC	2.24	2.11	2.06
20	B	848	BCR	C14-C13	2.24	1.41	1.35
20	b	848	BCR	C14-C13	2.24	1.41	1.35
18	2a	303	CLA	C1B-C2B	-2.24	1.37	1.43
18	2b	303	CLA	C1B-C2B	-2.24	1.37	1.43
25	3a	317	LUT	C14-C13	2.24	1.41	1.35
25	3b	317	LUT	C14-C13	2.24	1.41	1.35
18	2a	308	CLA	C1B-C2B	-2.24	1.37	1.43
18	2b	308	CLA	C1B-C2B	-2.24	1.37	1.43
25	6a	318	LUT	C28-C29	-2.24	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6b	318	LUT	C28-C29	-2.24	1.41	1.46
18	3a	303	CLA	C1D-C2D	-2.24	1.40	1.45
18	2b	301	CLA	C1D-C2D	-2.24	1.40	1.45
18	A	807	CLA	C1D-C2D	-2.24	1.40	1.45
18	a	807	CLA	C1D-C2D	-2.24	1.40	1.45
29	5a	305	CHL	C3B-C4B	-2.24	1.39	1.41
29	5b	305	CHL	C3B-C4B	-2.24	1.39	1.41
18	A	814	CLA	MG-NC	2.24	2.11	2.06
18	6a	315	CLA	MG-NC	2.24	2.11	2.06
18	2a	311	CLA	C1B-C2B	-2.23	1.37	1.43
18	2b	311	CLA	C1B-C2B	-2.23	1.37	1.43
18	6b	314	CLA	C1B-C2B	-2.23	1.37	1.43
18	b	834	CLA	MG-NC	2.23	2.11	2.06
18	a	819	CLA	C1B-C2B	-2.23	1.37	1.43
18	B	837	CLA	C1D-C2D	-2.23	1.40	1.45
18	b	837	CLA	C1D-C2D	-2.23	1.40	1.45
18	F	302	CLA	C1B-C2B	-2.23	1.37	1.43
18	f	302	CLA	C1B-C2B	-2.23	1.37	1.43
18	5b	310	CLA	C1B-C2B	-2.23	1.37	1.43
18	5b	310	CLA	C1D-C2D	-2.23	1.40	1.45
25	5a	317	LUT	C14-C13	2.23	1.41	1.35
18	2a	307	CLA	C1D-C2D	-2.23	1.40	1.45
18	2b	307	CLA	C1D-C2D	-2.23	1.40	1.45
18	A	822	CLA	C1B-C2B	-2.23	1.37	1.43
18	a	822	CLA	C1B-C2B	-2.23	1.37	1.43
25	6a	318	LUT	C31-C32	2.23	1.40	1.34
18	5a	311	CLA	C1B-C2B	-2.23	1.37	1.43
18	5b	311	CLA	C1B-C2B	-2.23	1.37	1.43
18	F	303	CLA	MG-NC	2.23	2.11	2.06
18	f	303	CLA	MG-NC	2.23	2.11	2.06
18	G	202	CLA	C1D-C2D	-2.23	1.40	1.45
18	5a	311	CLA	C1D-C2D	-2.23	1.40	1.45
18	5b	311	CLA	C1D-C2D	-2.23	1.40	1.45
25	5a	317	LUT	C34-C33	2.23	1.40	1.35
25	5b	317	LUT	C34-C33	2.23	1.40	1.35
18	B	809	CLA	C1B-C2B	-2.22	1.37	1.43
18	b	809	CLA	C1B-C2B	-2.22	1.37	1.43
18	5a	308	CLA	C1B-C2B	-2.22	1.37	1.43
20	M	101	BCR	C10-C9	2.22	1.40	1.35
20	m	101	BCR	C10-C9	2.22	1.40	1.35
18	3a	306	CLA	C1B-C2B	-2.22	1.37	1.43
18	3b	306	CLA	C1B-C2B	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5a	317	LUT	C10-C9	2.22	1.40	1.35
25	5b	317	LUT	C10-C9	2.22	1.40	1.35
25	2a	314	LUT	C10-C9	2.22	1.40	1.35
25	2b	314	LUT	C10-C9	2.22	1.40	1.35
18	A	808	CLA	C1D-C2D	-2.22	1.40	1.45
18	a	808	CLA	C1D-C2D	-2.22	1.40	1.45
18	2a	301	CLA	C1D-C2D	-2.22	1.40	1.45
18	2a	311	CLA	C1D-C2D	-2.22	1.40	1.45
18	2b	311	CLA	C1D-C2D	-2.22	1.40	1.45
18	2b	309	CLA	MG-NC	2.22	2.11	2.06
18	A	834	CLA	C1D-C2D	-2.22	1.40	1.45
18	a	834	CLA	C1D-C2D	-2.22	1.40	1.45
18	3a	313	CLA	C1B-C2B	-2.22	1.37	1.43
18	3b	313	CLA	C1B-C2B	-2.22	1.37	1.43
25	J	105	LUT	C10-C9	2.22	1.40	1.35
18	b	839	CLA	C1B-C2B	-2.22	1.37	1.43
25	6b	318	LUT	C30-C29	2.22	1.40	1.35
18	A	842	CLA	C1D-C2D	-2.22	1.41	1.45
18	a	842	CLA	C1D-C2D	-2.22	1.41	1.45
18	2a	309	CLA	MG-NC	2.22	2.11	2.06
18	6a	317	CLA	C1D-C2D	-2.22	1.41	1.45
18	6b	317	CLA	C1D-C2D	-2.22	1.41	1.45
25	5b	317	LUT	C30-C29	2.21	1.40	1.35
18	3a	314	CLA	C1B-C2B	-2.21	1.37	1.43
18	3b	314	CLA	C1B-C2B	-2.21	1.37	1.43
18	A	829	CLA	MG-NC	2.21	2.11	2.06
18	5a	313	CLA	C1D-C2D	-2.21	1.41	1.45
18	5b	313	CLA	C1D-C2D	-2.21	1.41	1.45
20	a	847	BCR	C14-C13	2.21	1.40	1.35
18	5b	308	CLA	C1B-C2B	-2.21	1.37	1.43
18	2a	308	CLA	C1D-C2D	-2.21	1.41	1.45
18	2b	308	CLA	C1D-C2D	-2.21	1.41	1.45
18	6a	313	CLA	C1B-C2B	-2.21	1.37	1.43
18	6b	313	CLA	C1B-C2B	-2.21	1.37	1.43
18	6a	316	CLA	C1B-C2B	-2.21	1.37	1.43
18	6b	316	CLA	C1B-C2B	-2.21	1.37	1.43
18	B	817	CLA	C1D-C2D	-2.21	1.41	1.45
18	b	817	CLA	C1D-C2D	-2.21	1.41	1.45
18	6a	307	CLA	C1D-C2D	-2.21	1.41	1.45
18	6b	307	CLA	C1D-C2D	-2.21	1.41	1.45
18	5a	315	CLA	C1B-C2B	-2.21	1.37	1.43
18	5b	315	CLA	C1B-C2B	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	810	CLA	C1D-C2D	-2.21	1.41	1.45
18	b	810	CLA	C1D-C2D	-2.21	1.41	1.45
25	j	105	LUT	C10-C9	2.21	1.40	1.35
18	3a	313	CLA	C1D-C2D	-2.21	1.41	1.45
18	B	813	CLA	C1D-C2D	-2.21	1.41	1.45
18	b	813	CLA	C1D-C2D	-2.21	1.41	1.45
18	6a	315	CLA	C1B-C2B	-2.21	1.38	1.43
18	6b	315	CLA	C1B-C2B	-2.21	1.38	1.43
18	B	854	CLA	MG-NC	2.20	2.11	2.06
18	B	821	CLA	C1D-C2D	-2.20	1.41	1.45
18	b	821	CLA	C1D-C2D	-2.20	1.41	1.45
18	5b	315	CLA	C1D-C2D	-2.20	1.41	1.45
26	A	802	CL0	MG-NB	-2.20	2.01	2.05
26	a	802	CL0	MG-NB	-2.20	2.01	2.05
18	B	839	CLA	C1B-C2B	-2.20	1.38	1.43
18	B	834	CLA	MG-NC	2.20	2.11	2.06
18	6a	317	CLA	C1B-C2B	-2.20	1.38	1.43
18	6b	317	CLA	C1B-C2B	-2.20	1.38	1.43
18	K	201	CLA	MG-NC	2.20	2.11	2.06
18	k	201	CLA	MG-NC	2.20	2.11	2.06
20	B	843	BCR	C10-C9	2.20	1.40	1.35
20	b	843	BCR	C10-C9	2.20	1.40	1.35
25	3a	317	LUT	C30-C29	2.20	1.40	1.35
25	3b	317	LUT	C30-C29	2.20	1.40	1.35
18	B	808	CLA	C1B-NB	-2.20	1.35	1.37
18	b	808	CLA	C1B-NB	-2.20	1.35	1.37
18	6a	314	CLA	C1D-C2D	-2.20	1.41	1.45
18	6b	314	CLA	C1D-C2D	-2.20	1.41	1.45
18	B	853	CLA	C1D-C2D	-2.20	1.41	1.45
18	b	853	CLA	C1D-C2D	-2.20	1.41	1.45
18	5a	315	CLA	C1D-C2D	-2.20	1.41	1.45
18	J	101	CLA	MG-NC	2.20	2.11	2.06
18	j	101	CLA	MG-NC	2.20	2.11	2.06
18	A	837	CLA	C1D-C2D	-2.20	1.41	1.45
18	a	837	CLA	C1D-C2D	-2.20	1.41	1.45
18	3b	305	CLA	C1D-C2D	-2.20	1.41	1.45
18	A	821	CLA	C1D-C2D	-2.20	1.41	1.45
18	a	821	CLA	C1D-C2D	-2.20	1.41	1.45
18	B	840	CLA	C1B-C2B	-2.20	1.38	1.43
18	2a	312	CLA	C1B-C2B	-2.19	1.38	1.43
18	5a	310	CLA	C1B-C2B	-2.19	1.38	1.43
18	2b	312	CLA	C1B-C2B	-2.19	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	202	CLA	C1B-C2B	-2.19	1.38	1.43
18	g	202	CLA	C1B-C2B	-2.19	1.38	1.43
18	3b	313	CLA	C1D-C2D	-2.19	1.41	1.45
18	B	853	CLA	C3D-C4D	-2.19	1.39	1.44
18	b	853	CLA	C3D-C4D	-2.19	1.39	1.44
18	B	824	CLA	C1D-C2D	-2.19	1.41	1.45
18	b	824	CLA	C1D-C2D	-2.19	1.41	1.45
18	5a	310	CLA	C1D-C2D	-2.19	1.41	1.45
18	B	834	CLA	C1B-NB	-2.19	1.35	1.37
18	b	834	CLA	C1B-NB	-2.19	1.35	1.37
18	A	833	CLA	C1D-C2D	-2.19	1.41	1.45
18	6a	313	CLA	C1D-C2D	-2.19	1.41	1.45
18	6b	313	CLA	C1D-C2D	-2.19	1.41	1.45
18	A	805	CLA	C1B-C2B	-2.19	1.38	1.43
18	a	805	CLA	C1B-C2B	-2.19	1.38	1.43
18	5a	313	CLA	MG-NC	2.19	2.11	2.06
18	5b	313	CLA	MG-NC	2.19	2.11	2.06
18	A	842	CLA	MG-NC	2.19	2.11	2.06
18	6a	315	CLA	C1D-C2D	-2.19	1.41	1.45
18	6b	315	CLA	C1D-C2D	-2.19	1.41	1.45
20	A	847	BCR	C14-C13	2.19	1.40	1.35
18	2a	302	CLA	C1D-C2D	-2.19	1.41	1.45
18	2b	302	CLA	C1D-C2D	-2.19	1.41	1.45
18	A	805	CLA	C1D-C2D	-2.19	1.41	1.45
18	a	805	CLA	C1D-C2D	-2.19	1.41	1.45
18	b	854	CLA	MG-NC	2.19	2.11	2.06
25	5a	316	LUT	C34-C33	2.19	1.40	1.35
25	5b	316	LUT	C34-C33	2.19	1.40	1.35
18	3a	311	CLA	C1B-C2B	-2.18	1.38	1.43
18	3b	311	CLA	C1B-C2B	-2.18	1.38	1.43
25	6a	319	LUT	C31-C32	2.18	1.40	1.34
25	6b	319	LUT	C31-C32	2.18	1.40	1.34
18	B	828	CLA	C1D-C2D	-2.18	1.41	1.45
18	b	828	CLA	C1D-C2D	-2.18	1.41	1.45
25	5a	317	LUT	C30-C29	2.18	1.40	1.35
18	B	817	CLA	C1B-C2B	-2.18	1.38	1.43
18	b	817	CLA	C1B-C2B	-2.18	1.38	1.43
18	B	852	CLA	MG-NC	2.18	2.11	2.06
18	3a	306	CLA	C1D-C2D	-2.18	1.41	1.45
18	3b	306	CLA	C1D-C2D	-2.18	1.41	1.45
18	b	840	CLA	C1B-C2B	-2.18	1.38	1.43
25	2b	314	LUT	C14-C13	2.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	848	BCR	C21-C22	2.18	1.40	1.35
18	3a	312	CLA	C1B-C2B	-2.18	1.38	1.43
18	3b	312	CLA	C1B-C2B	-2.18	1.38	1.43
18	6a	311	CLA	C1B-C2B	-2.18	1.38	1.43
18	6b	311	CLA	C1B-C2B	-2.18	1.38	1.43
18	L	303	CLA	C1D-C2D	-2.18	1.41	1.45
18	l	303	CLA	C1D-C2D	-2.18	1.41	1.45
18	6a	311	CLA	C1D-C2D	-2.18	1.41	1.45
18	3a	304	CLA	C1B-C2B	-2.18	1.38	1.43
18	3b	304	CLA	C1B-C2B	-2.18	1.38	1.43
20	B	843	BCR	C21-C22	2.18	1.40	1.35
20	b	843	BCR	C21-C22	2.18	1.40	1.35
18	A	803	CLA	C1D-C2D	-2.18	1.41	1.45
18	a	803	CLA	C1D-C2D	-2.18	1.41	1.45
18	A	830	CLA	C1D-C2D	-2.18	1.41	1.45
18	a	830	CLA	C1D-C2D	-2.18	1.41	1.45
25	3a	317	LUT	C34-C33	2.18	1.40	1.35
25	3b	317	LUT	C34-C33	2.18	1.40	1.35
20	B	848	BCR	C21-C22	2.18	1.40	1.35
18	A	826	CLA	MG-NC	2.18	2.11	2.06
18	a	826	CLA	MG-NC	2.18	2.11	2.06
18	J	101	CLA	C1D-C2D	-2.18	1.41	1.45
18	a	829	CLA	MG-NC	2.18	2.11	2.06
18	A	838	CLA	C1D-C2D	-2.17	1.41	1.45
18	a	838	CLA	C1D-C2D	-2.17	1.41	1.45
18	b	852	CLA	MG-NC	2.17	2.11	2.06
18	a	842	CLA	MG-NC	2.17	2.11	2.06
25	2a	314	LUT	C14-C13	2.17	1.40	1.35
18	j	101	CLA	C1D-C2D	-2.17	1.41	1.45
18	6a	310	CLA	MG-NC	2.17	2.11	2.06
18	6b	310	CLA	MG-NC	2.17	2.11	2.06
20	A	847	BCR	C17-C18	2.17	1.40	1.35
20	a	847	BCR	C17-C18	2.17	1.40	1.35
18	B	820	CLA	MG-NC	2.17	2.11	2.06
18	b	820	CLA	MG-NC	2.17	2.11	2.06
18	A	853	CLA	C1B-C2B	-2.17	1.38	1.43
18	a	853	CLA	C1B-C2B	-2.17	1.38	1.43
18	B	803	CLA	C1D-C2D	-2.17	1.41	1.45
18	b	803	CLA	C1D-C2D	-2.17	1.41	1.45
18	3a	305	CLA	C1D-C2D	-2.17	1.41	1.45
25	6a	320	LUT	C14-C13	2.17	1.40	1.35
25	6b	320	LUT	C14-C13	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	C1D-C2D	-2.17	1.41	1.45
18	f	303	CLA	C1D-C2D	-2.17	1.41	1.45
18	B	808	CLA	C1B-C2B	-2.17	1.38	1.43
18	b	808	CLA	C1B-C2B	-2.17	1.38	1.43
20	M	101	BCR	C17-C18	2.17	1.40	1.35
20	m	101	BCR	C17-C18	2.17	1.40	1.35
20	l	304	BCR	C17-C18	2.16	1.40	1.35
18	6b	312	CLA	C1D-C2D	-2.16	1.41	1.45
18	B	831	CLA	C1B-C2B	-2.16	1.38	1.43
18	b	831	CLA	C1B-C2B	-2.16	1.38	1.43
18	B	825	CLA	MG-NC	2.16	2.11	2.06
18	3a	308	CLA	MG-NC	2.16	2.11	2.06
18	3b	308	CLA	MG-NC	2.16	2.11	2.06
18	B	837	CLA	C1B-C2B	-2.16	1.38	1.43
18	b	837	CLA	C1B-C2B	-2.16	1.38	1.43
20	m	101	BCR	C14-C13	2.16	1.40	1.35
18	6b	311	CLA	C1D-C2D	-2.16	1.41	1.45
18	5a	313	CLA	C1B-C2B	-2.16	1.38	1.43
18	5b	313	CLA	C1B-C2B	-2.16	1.38	1.43
20	B	851	BCR	C21-C22	2.16	1.40	1.35
20	b	851	BCR	C21-C22	2.16	1.40	1.35
18	6a	312	CLA	C1D-C2D	-2.16	1.41	1.45
20	b	842	BCR	C17-C18	2.16	1.40	1.35
18	3a	310	CLA	C1B-C2B	-2.16	1.38	1.43
18	3b	310	CLA	C1B-C2B	-2.16	1.38	1.43
20	M	101	BCR	C14-C13	2.15	1.40	1.35
18	2a	312	CLA	MG-NC	2.15	2.11	2.06
18	2b	312	CLA	MG-NC	2.15	2.11	2.06
20	A	849	BCR	C14-C13	2.15	1.40	1.35
20	a	849	BCR	C14-C13	2.15	1.40	1.35
18	B	833	CLA	C1D-C2D	-2.15	1.41	1.45
18	b	833	CLA	C1D-C2D	-2.15	1.41	1.45
18	A	811	CLA	C1D-C2D	-2.15	1.41	1.45
18	a	811	CLA	C1D-C2D	-2.15	1.41	1.45
18	L	301	CLA	C1D-C2D	-2.15	1.41	1.45
18	l	301	CLA	C1D-C2D	-2.15	1.41	1.45
26	A	802	CL0	MG-ND	-2.15	2.01	2.05
26	a	802	CL0	MG-ND	-2.15	2.01	2.05
18	a	833	CLA	C1D-C2D	-2.15	1.41	1.45
18	b	825	CLA	MG-NC	2.15	2.11	2.06
20	J	102	BCR	C19-C18	-2.15	1.41	1.46
25	6a	319	LUT	C12-C13	-2.14	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6b	319	LUT	C12-C13	-2.14	1.41	1.46
18	A	839	CLA	C1B-C2B	-2.14	1.38	1.43
18	a	839	CLA	C1B-C2B	-2.14	1.38	1.43
18	2a	310	CLA	C1D-C2D	-2.14	1.41	1.45
18	2b	310	CLA	C1D-C2D	-2.14	1.41	1.45
18	B	836	CLA	C1B-C2B	-2.14	1.38	1.43
18	b	836	CLA	C1B-C2B	-2.14	1.38	1.43
18	B	836	CLA	C1D-C2D	-2.14	1.41	1.45
18	b	836	CLA	C1D-C2D	-2.14	1.41	1.45
18	3a	309	CLA	C1D-C2D	-2.14	1.41	1.45
18	3b	309	CLA	C1D-C2D	-2.14	1.41	1.45
18	B	815	CLA	C1D-C2D	-2.14	1.41	1.45
18	b	815	CLA	C1D-C2D	-2.14	1.41	1.45
18	A	828	CLA	MG-NB	2.14	2.10	2.05
18	a	828	CLA	MG-NB	2.14	2.10	2.05
20	A	851	BCR	C17-C18	2.14	1.40	1.35
20	a	851	BCR	C17-C18	2.14	1.40	1.35
20	L	304	BCR	C17-C18	2.14	1.40	1.35
20	G	204	BCR	C21-C22	2.13	1.40	1.35
20	g	204	BCR	C21-C22	2.13	1.40	1.35
25	2a	315	LUT	C10-C9	2.13	1.40	1.35
25	2b	315	LUT	C10-C9	2.13	1.40	1.35
18	6a	305	CLA	C1D-C2D	-2.13	1.41	1.45
20	A	849	BCR	C17-C18	2.13	1.40	1.35
18	A	841	CLA	C1B-C2B	-2.13	1.38	1.43
18	a	841	CLA	C1B-C2B	-2.13	1.38	1.43
18	5a	310	CLA	MG-NC	2.13	2.11	2.06
18	5b	310	CLA	MG-NC	2.13	2.11	2.06
25	6a	320	LUT	C10-C9	2.13	1.40	1.35
25	6b	320	LUT	C10-C9	2.13	1.40	1.35
18	A	837	CLA	C1B-C2B	-2.13	1.38	1.43
18	a	837	CLA	C1B-C2B	-2.13	1.38	1.43
20	b	842	BCR	C10-C9	2.13	1.40	1.35
18	B	828	CLA	MG-NC	2.13	2.11	2.06
18	2a	301	CLA	MG-NC	2.13	2.11	2.06
18	2b	301	CLA	MG-NC	2.13	2.11	2.06
18	3b	304	CLA	C1D-C2D	-2.13	1.41	1.45
18	B	817	CLA	C1B-NB	-2.13	1.35	1.37
18	b	817	CLA	C1B-NB	-2.13	1.35	1.37
18	a	804	CLA	C1D-C2D	-2.12	1.41	1.45
20	b	851	BCR	C2-C3	-2.12	1.47	1.52
20	B	843	BCR	C14-C13	2.12	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	843	BCR	C14-C13	2.12	1.40	1.35
18	A	813	CLA	C1B-C2B	-2.12	1.38	1.43
18	a	813	CLA	C1B-C2B	-2.12	1.38	1.43
20	A	851	BCR	C10-C9	2.12	1.40	1.35
20	a	851	BCR	C10-C9	2.12	1.40	1.35
18	B	830	CLA	C1D-C2D	-2.12	1.41	1.45
18	b	830	CLA	C1D-C2D	-2.12	1.41	1.45
20	A	848	BCR	C17-C18	2.12	1.40	1.35
20	a	848	BCR	C17-C18	2.12	1.40	1.35
18	B	827	CLA	C1B-C2B	-2.12	1.38	1.43
18	b	827	CLA	C1B-C2B	-2.12	1.38	1.43
18	2b	303	CLA	MG-NC	2.12	2.11	2.06
20	B	842	BCR	C17-C18	2.12	1.40	1.35
20	A	848	BCR	C21-C22	2.12	1.40	1.35
20	a	848	BCR	C21-C22	2.12	1.40	1.35
20	B	844	BCR	C17-C18	2.12	1.40	1.35
20	b	844	BCR	C17-C18	2.12	1.40	1.35
20	B	851	BCR	C2-C3	-2.12	1.47	1.52
18	3a	311	CLA	C1D-C2D	-2.12	1.41	1.45
20	j	102	BCR	C19-C18	-2.12	1.41	1.46
18	5a	304	CLA	C1D-C2D	-2.11	1.41	1.45
18	5b	304	CLA	C1D-C2D	-2.11	1.41	1.45
20	G	204	BCR	C17-C18	2.11	1.40	1.35
20	g	204	BCR	C17-C18	2.11	1.40	1.35
18	B	829	CLA	C1D-C2D	-2.11	1.41	1.45
18	b	829	CLA	C1D-C2D	-2.11	1.41	1.45
20	A	847	BCR	C29-C28	-2.11	1.47	1.52
20	a	847	BCR	C29-C28	-2.11	1.47	1.52
20	B	842	BCR	C14-C13	2.11	1.40	1.35
20	b	842	BCR	C14-C13	2.11	1.40	1.35
20	a	849	BCR	C17-C18	2.11	1.40	1.35
18	B	806	CLA	MG-NC	2.11	2.11	2.06
18	b	806	CLA	MG-NC	2.11	2.11	2.06
18	5a	302	CLA	C1D-C2D	-2.11	1.41	1.45
18	5b	302	CLA	C1D-C2D	-2.11	1.41	1.45
18	6b	305	CLA	C1D-C2D	-2.11	1.41	1.45
18	b	828	CLA	MG-NC	2.11	2.11	2.06
18	k	201	CLA	C1D-C2D	-2.11	1.41	1.45
18	A	806	CLA	C1B-C2B	-2.10	1.38	1.43
18	a	806	CLA	C1B-C2B	-2.10	1.38	1.43
18	a	825	CLA	C1B-C2B	-2.10	1.38	1.43
18	B	808	CLA	MG-NC	2.10	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	808	CLA	MG-NC	2.10	2.11	2.06
18	b	827	CLA	MG-NC	2.10	2.11	2.06
18	B	809	CLA	MG-NC	2.10	2.11	2.06
18	b	809	CLA	MG-NC	2.10	2.11	2.06
18	3a	304	CLA	C1D-C2D	-2.10	1.41	1.45
18	A	812	CLA	C1B-NB	-2.10	1.35	1.37
18	a	812	CLA	C1B-NB	-2.10	1.35	1.37
18	3a	312	CLA	C1D-C2D	-2.10	1.41	1.45
18	3b	312	CLA	C1D-C2D	-2.10	1.41	1.45
25	2a	315	LUT	C30-C29	2.10	1.40	1.35
18	B	801	CLA	C1B-C2B	-2.10	1.38	1.43
18	b	801	CLA	C1B-C2B	-2.10	1.38	1.43
18	G	203	CLA	C1D-C2D	-2.10	1.41	1.45
18	g	203	CLA	C1D-C2D	-2.10	1.41	1.45
18	2a	303	CLA	MG-NC	2.10	2.11	2.06
25	3b	316	LUT	C34-C33	2.10	1.40	1.35
18	A	825	CLA	C1B-C2B	-2.10	1.38	1.43
18	a	823	CLA	C1D-C2D	-2.10	1.41	1.45
18	3a	314	CLA	C1D-C2D	-2.09	1.41	1.45
18	3b	314	CLA	C1D-C2D	-2.09	1.41	1.45
20	B	848	BCR	C2-C3	-2.09	1.47	1.52
20	b	848	BCR	C2-C3	-2.09	1.47	1.52
18	A	823	CLA	C1D-C2D	-2.09	1.41	1.45
20	B	844	BCR	C14-C13	2.09	1.40	1.35
20	F	304	BCR	C10-C9	2.09	1.40	1.35
20	b	844	BCR	C14-C13	2.09	1.40	1.35
20	f	304	BCR	C10-C9	2.09	1.40	1.35
18	6a	306	CLA	C1D-C2D	-2.09	1.41	1.45
18	6b	306	CLA	C1D-C2D	-2.09	1.41	1.45
20	f	304	BCR	C17-C18	2.09	1.40	1.35
18	A	814	CLA	C1B-C2B	-2.09	1.38	1.43
18	a	814	CLA	C1B-C2B	-2.09	1.38	1.43
20	B	842	BCR	C10-C9	2.09	1.40	1.35
18	B	832	CLA	MG-NC	2.09	2.11	2.06
18	b	832	CLA	MG-NC	2.09	2.11	2.06
20	F	304	BCR	C17-C18	2.09	1.40	1.35
20	A	848	BCR	C14-C13	2.09	1.40	1.35
20	a	848	BCR	C14-C13	2.09	1.40	1.35
18	A	808	CLA	C1B-C2B	-2.09	1.38	1.43
18	a	808	CLA	C1B-C2B	-2.09	1.38	1.43
18	A	842	CLA	C1B-C2B	-2.09	1.38	1.43
18	a	842	CLA	C1B-C2B	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5a	316	LUT	C14-C13	2.09	1.40	1.35
25	5b	316	LUT	C14-C13	2.09	1.40	1.35
18	A	817	CLA	MG-NC	2.08	2.11	2.06
18	a	817	CLA	MG-NC	2.08	2.11	2.06
20	J	102	BCR	C2-C3	-2.08	1.47	1.52
20	j	102	BCR	C2-C3	-2.08	1.47	1.52
18	A	804	CLA	C1D-C2D	-2.08	1.41	1.45
18	b	801	CLA	CHB-C1B	2.08	1.44	1.39
18	B	803	CLA	C1B-C2B	-2.08	1.38	1.43
18	b	803	CLA	C1B-C2B	-2.08	1.38	1.43
18	A	821	CLA	MG-NC	2.08	2.11	2.06
18	a	821	CLA	MG-NC	2.08	2.11	2.06
25	J	105	LUT	C31-C32	2.08	1.40	1.34
20	B	844	BCR	C10-C9	2.08	1.40	1.35
20	b	844	BCR	C10-C9	2.08	1.40	1.35
18	K	201	CLA	C1D-C2D	-2.08	1.41	1.45
20	B	842	BCR	C2-C3	-2.08	1.47	1.52
20	b	842	BCR	C2-C3	-2.08	1.47	1.52
18	3a	302	CLA	C1B-C2B	-2.08	1.38	1.43
18	3b	302	CLA	C1B-C2B	-2.08	1.38	1.43
18	3b	311	CLA	C1D-C2D	-2.08	1.41	1.45
18	A	816	CLA	C1D-C2D	-2.08	1.41	1.45
18	a	816	CLA	C1D-C2D	-2.08	1.41	1.45
18	B	827	CLA	MG-NC	2.08	2.11	2.06
18	B	812	CLA	C1B-C2B	-2.08	1.38	1.43
18	b	812	CLA	C1B-C2B	-2.08	1.38	1.43
18	L	302	CLA	C1B-C2B	-2.07	1.38	1.43
18	l	302	CLA	C1B-C2B	-2.07	1.38	1.43
25	3a	316	LUT	C34-C33	2.07	1.40	1.35
18	K	201	CLA	C1B-C2B	-2.07	1.38	1.43
18	B	805	CLA	MG-NC	2.07	2.11	2.06
18	b	805	CLA	MG-NC	2.07	2.11	2.06
18	B	807	CLA	MG-NC	2.07	2.11	2.06
18	b	807	CLA	MG-NC	2.07	2.11	2.06
18	B	821	CLA	C1B-C2B	-2.07	1.38	1.43
18	b	821	CLA	C1B-C2B	-2.07	1.38	1.43
20	K	202	BCR	C10-C9	2.07	1.40	1.35
18	B	807	CLA	C1B-C2B	-2.07	1.38	1.43
18	b	807	CLA	C1B-C2B	-2.07	1.38	1.43
20	F	304	BCR	C14-C13	2.07	1.40	1.35
20	F	304	BCR	C21-C22	2.07	1.40	1.35
20	f	304	BCR	C14-C13	2.07	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	f	304	BCR	C21-C22	2.07	1.40	1.35
18	B	832	CLA	C1B-C2B	-2.07	1.38	1.43
20	f	301	BCR	C17-C18	2.07	1.40	1.35
18	A	814	CLA	C1D-C2D	-2.07	1.41	1.45
18	a	814	CLA	C1D-C2D	-2.07	1.41	1.45
18	3b	312	CLA	CHB-C1B	2.07	1.44	1.39
20	b	845	BCR	C14-C13	2.07	1.40	1.35
18	2a	311	CLA	MG-NC	2.06	2.11	2.06
18	5a	304	CLA	MG-NC	2.06	2.11	2.06
18	2b	311	CLA	MG-NC	2.06	2.11	2.06
18	5b	304	CLA	MG-NC	2.06	2.11	2.06
18	A	826	CLA	C1B-C2B	-2.06	1.38	1.43
18	a	826	CLA	C1B-C2B	-2.06	1.38	1.43
18	3a	310	CLA	C1D-C2D	-2.06	1.41	1.45
18	3a	306	CLA	MG-NC	2.06	2.11	2.06
18	3b	306	CLA	MG-NC	2.06	2.11	2.06
25	j	105	LUT	C31-C32	2.06	1.40	1.34
18	a	816	CLA	MG-NB	2.06	2.09	2.05
20	k	202	BCR	C10-C9	2.06	1.40	1.35
18	b	832	CLA	C1B-C2B	-2.06	1.38	1.43
18	3a	312	CLA	CHB-C1B	2.06	1.44	1.39
18	2a	303	CLA	C1D-C2D	-2.06	1.41	1.45
18	2b	303	CLA	C1D-C2D	-2.06	1.41	1.45
18	B	801	CLA	CHB-C1B	2.06	1.44	1.39
25	2b	315	LUT	C30-C29	2.06	1.40	1.35
18	L	301	CLA	MG-NC	2.06	2.11	2.06
18	l	301	CLA	MG-NC	2.06	2.11	2.06
18	6b	317	CLA	MG-NC	2.06	2.11	2.06
18	A	806	CLA	C1B-NB	-2.06	1.35	1.37
18	a	806	CLA	C1B-NB	-2.06	1.35	1.37
18	3a	304	CLA	MG-NC	2.06	2.11	2.06
18	3b	304	CLA	MG-NC	2.06	2.11	2.06
18	6a	317	CLA	MG-NC	2.06	2.11	2.06
25	3a	316	LUT	C14-C13	2.06	1.40	1.35
25	3b	316	LUT	C14-C13	2.06	1.40	1.35
20	B	848	BCR	C29-C28	-2.05	1.47	1.52
20	b	848	BCR	C29-C28	-2.05	1.47	1.52
18	b	839	CLA	CHB-C1B	2.05	1.44	1.39
18	A	825	CLA	MG-NC	2.05	2.11	2.06
18	a	825	CLA	MG-NC	2.05	2.11	2.06
20	B	845	BCR	C14-C13	2.05	1.40	1.35
18	3b	305	CLA	MG-NC	2.05	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	303	CLA	C1B-C2B	-2.05	1.38	1.43
18	l	303	CLA	C1B-C2B	-2.05	1.38	1.43
25	2a	314	LUT	C30-C29	2.05	1.40	1.35
25	2b	314	LUT	C30-C29	2.05	1.40	1.35
20	G	204	BCR	C10-C9	2.05	1.40	1.35
25	5a	316	LUT	C10-C9	2.05	1.40	1.35
25	5b	316	LUT	C10-C9	2.05	1.40	1.35
18	5a	308	CLA	C1D-C2D	-2.04	1.41	1.45
18	5b	308	CLA	C1D-C2D	-2.04	1.41	1.45
18	3a	308	CLA	CHB-C1B	2.04	1.44	1.39
18	A	805	CLA	C1B-NB	-2.04	1.35	1.37
18	a	805	CLA	C1B-NB	-2.04	1.35	1.37
18	3b	310	CLA	C1D-C2D	-2.04	1.41	1.45
18	A	824	CLA	C1B-NB	-2.04	1.35	1.37
18	a	824	CLA	C1B-NB	-2.04	1.35	1.37
18	A	823	CLA	MG-NB	2.04	2.09	2.05
18	F	305	CLA	C1B-C2B	-2.04	1.38	1.43
18	2a	301	CLA	C1B-C2B	-2.04	1.38	1.43
18	2b	301	CLA	C1B-C2B	-2.04	1.38	1.43
29	2a	306	CHL	C3D-C4D	-2.04	1.38	1.41
29	2b	306	CHL	C3D-C4D	-2.04	1.38	1.41
20	B	846	BCR	C14-C13	2.04	1.40	1.35
20	F	301	BCR	C17-C18	2.04	1.40	1.35
18	3a	302	CLA	MG-NC	2.04	2.11	2.06
18	3b	302	CLA	MG-NC	2.04	2.11	2.06
20	B	851	BCR	C17-C18	2.04	1.40	1.35
20	b	851	BCR	C17-C18	2.04	1.40	1.35
18	6a	316	CLA	C1D-C2D	-2.04	1.41	1.45
18	6b	316	CLA	C1D-C2D	-2.04	1.41	1.45
18	k	201	CLA	C1B-C2B	-2.04	1.38	1.43
20	B	845	BCR	C17-C18	2.04	1.40	1.35
20	b	845	BCR	C17-C18	2.04	1.40	1.35
18	3a	314	CLA	CHB-C1B	2.04	1.44	1.39
18	3b	314	CLA	CHB-C1B	2.04	1.44	1.39
20	B	846	BCR	C17-C18	2.04	1.40	1.35
18	3a	305	CLA	MG-NC	2.04	2.11	2.06
18	b	810	CLA	C1B-C2B	-2.04	1.38	1.43
18	A	835	CLA	C1D-C2D	-2.03	1.41	1.45
18	a	835	CLA	C1D-C2D	-2.03	1.41	1.45
18	B	826	CLA	CHB-C1B	2.03	1.44	1.39
18	b	826	CLA	CHB-C1B	2.03	1.44	1.39
18	A	808	CLA	C1B-NB	-2.03	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	808	CLA	C1B-NB	-2.03	1.35	1.37
20	j	102	BCR	C12-C13	-2.03	1.41	1.46
18	B	810	CLA	C1B-C2B	-2.03	1.38	1.43
20	B	844	BCR	C21-C22	2.03	1.40	1.35
20	b	844	BCR	C21-C22	2.03	1.40	1.35
18	G	203	CLA	MG-NC	2.03	2.11	2.06
18	g	203	CLA	MG-NC	2.03	2.11	2.06
25	5a	316	LUT	C30-C29	2.03	1.40	1.35
25	5b	316	LUT	C30-C29	2.03	1.40	1.35
20	a	847	BCR	C2-C3	-2.03	1.47	1.52
18	G	202	CLA	CHB-C1B	2.03	1.44	1.39
18	g	202	CLA	CHB-C1B	2.03	1.44	1.39
18	6a	307	CLA	MG-NC	2.03	2.11	2.06
18	6b	307	CLA	MG-NC	2.03	2.11	2.06
20	L	304	BCR	C21-C22	2.03	1.40	1.35
20	l	304	BCR	C21-C22	2.03	1.40	1.35
18	B	823	CLA	C1D-C2D	-2.03	1.41	1.45
18	f	305	CLA	C1B-C2B	-2.03	1.38	1.43
20	b	846	BCR	C17-C18	2.03	1.40	1.35
18	5a	302	CLA	C1B-C2B	-2.03	1.38	1.43
18	5b	302	CLA	C1B-C2B	-2.03	1.38	1.43
18	3b	308	CLA	CHB-C1B	2.03	1.44	1.39
20	b	846	BCR	C14-C13	2.03	1.40	1.35
18	5a	312	CLA	C1D-C2D	-2.02	1.41	1.45
18	5b	312	CLA	C1D-C2D	-2.02	1.41	1.45
18	A	816	CLA	MG-NB	2.02	2.09	2.05
20	K	202	BCR	C14-C13	2.02	1.40	1.35
18	A	824	CLA	CHB-C1B	2.02	1.44	1.39
18	a	824	CLA	CHB-C1B	2.02	1.44	1.39
20	A	847	BCR	C2-C3	-2.02	1.47	1.52
18	a	823	CLA	MG-NB	2.02	2.09	2.05
18	B	839	CLA	CHB-C1B	2.02	1.43	1.39
20	B	851	BCR	C14-C13	2.02	1.40	1.35
20	b	851	BCR	C14-C13	2.02	1.40	1.35
18	A	819	CLA	C1B-NB	-2.02	1.35	1.37
18	a	819	CLA	C1B-NB	-2.02	1.35	1.37
18	6a	305	CLA	CHB-C1B	2.02	1.43	1.39
18	6b	305	CLA	CHB-C1B	2.02	1.43	1.39
18	2a	311	CLA	CHB-C1B	2.02	1.43	1.39
18	2b	311	CLA	CHB-C1B	2.02	1.43	1.39
20	K	202	BCR	C17-C18	2.02	1.40	1.35
20	k	202	BCR	C17-C18	2.02	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	101	BCR	C21-C22	2.02	1.40	1.35
20	m	101	BCR	C21-C22	2.02	1.40	1.35
20	A	849	BCR	C21-C22	2.02	1.40	1.35
20	k	202	BCR	C14-C13	2.02	1.40	1.35
20	B	846	BCR	C29-C28	-2.01	1.47	1.52
20	b	846	BCR	C29-C28	-2.01	1.47	1.52
25	6a	319	LUT	C32-C33	-2.01	1.41	1.46
25	6b	319	LUT	C32-C33	-2.01	1.41	1.46
18	A	827	CLA	C1B-C2B	-2.01	1.38	1.43
18	a	827	CLA	C1B-C2B	-2.01	1.38	1.43
20	J	102	BCR	C29-C28	-2.01	1.47	1.52
20	j	102	BCR	C29-C28	-2.01	1.47	1.52
20	g	204	BCR	C10-C9	2.01	1.40	1.35
18	b	823	CLA	C1B-NB	-2.01	1.35	1.37
18	A	822	CLA	C1D-C2D	-2.01	1.41	1.45
18	a	822	CLA	C1D-C2D	-2.01	1.41	1.45
18	2a	310	CLA	MG-NC	2.01	2.11	2.06
18	2b	310	CLA	MG-NC	2.01	2.11	2.06
18	B	830	CLA	C1B-C2B	-2.01	1.38	1.43
18	2a	312	CLA	C1D-C2D	-2.01	1.41	1.45
18	2b	312	CLA	C1D-C2D	-2.01	1.41	1.45
20	L	304	BCR	C10-C9	2.01	1.40	1.35
20	l	304	BCR	C10-C9	2.01	1.40	1.35
18	2a	303	CLA	CHB-C1B	2.00	1.43	1.39
18	2b	303	CLA	CHB-C1B	2.00	1.43	1.39
20	L	304	BCR	C14-C13	2.00	1.40	1.35
20	l	304	BCR	C14-C13	2.00	1.40	1.35
20	J	102	BCR	C12-C13	-2.00	1.41	1.46

All (2426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3a	301	CHL	C1B-CHB-C4A	13.84	130.22	121.32
29	3b	301	CHL	C1B-CHB-C4A	13.84	130.22	121.32
29	5b	314	CHL	C1B-CHB-C4A	13.76	130.17	121.32
29	5a	314	CHL	C1B-CHB-C4A	13.75	130.17	121.32
29	2a	313	CHL	C1B-CHB-C4A	13.42	129.96	121.32
29	2b	313	CHL	C1B-CHB-C4A	13.37	129.93	121.32
29	3a	307	CHL	C1B-CHB-C4A	13.26	129.85	121.32
29	3b	307	CHL	C1B-CHB-C4A	13.23	129.83	121.32
29	2a	304	CHL	C1B-CHB-C4A	13.16	129.79	121.32
29	2b	304	CHL	C1B-CHB-C4A	13.16	129.79	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5a	301	CHL	C1B-CHB-C4A	12.60	129.43	121.32
29	5b	301	CHL	C1B-CHB-C4A	12.60	129.43	121.32
29	6a	309	CHL	C1B-CHB-C4A	12.41	129.31	121.32
29	5a	305	CHL	C1B-CHB-C4A	12.35	129.27	121.32
29	5b	305	CHL	C1B-CHB-C4A	12.35	129.26	121.32
29	6b	309	CHL	C1B-CHB-C4A	12.35	129.26	121.32
29	2b	305	CHL	C1B-CHB-C4A	12.27	129.21	121.32
29	2a	305	CHL	C1B-CHB-C4A	12.24	129.20	121.32
29	5a	306	CHL	C1B-CHB-C4A	12.20	129.17	121.32
29	5b	306	CHL	C1B-CHB-C4A	12.20	129.17	121.32
29	3a	315	CHL	C1B-CHB-C4A	11.39	128.65	121.32
29	3b	315	CHL	C1B-CHB-C4A	11.39	128.65	121.32
29	6a	304	CHL	C1B-CHB-C4A	11.33	128.61	121.32
29	6b	304	CHL	C1B-CHB-C4A	11.33	128.61	121.32
29	2a	306	CHL	C1B-CHB-C4A	10.27	127.93	121.32
29	2b	306	CHL	C1B-CHB-C4A	10.27	127.93	121.32
25	2a	314	LUT	C15-C35-C34	9.93	143.83	123.52
25	2b	314	LUT	C15-C35-C34	9.93	143.83	123.52
20	B	843	BCR	C15-C16-C17	9.83	143.64	123.52
20	b	843	BCR	C15-C16-C17	9.81	143.60	123.52
25	J	105	LUT	C35-C15-C14	9.65	143.26	123.52
25	j	105	LUT	C35-C15-C14	9.65	143.26	123.52
26	A	802	CL0	C1B-CHB-C4A	9.54	127.46	121.32
26	a	802	CL0	C1B-CHB-C4A	9.54	127.46	121.32
25	2a	315	LUT	C15-C35-C34	8.31	140.53	123.52
25	2b	315	LUT	C15-C35-C34	8.31	140.53	123.52
25	2a	315	LUT	C35-C15-C14	8.11	140.11	123.52
25	2b	315	LUT	C35-C15-C14	8.11	140.11	123.52
25	6a	319	LUT	C15-C35-C34	7.88	139.64	123.52
25	6b	319	LUT	C15-C35-C34	7.88	139.64	123.52
25	6b	319	LUT	C30-C31-C32	7.49	144.90	123.20
25	6a	319	LUT	C30-C31-C32	7.48	144.87	123.20
25	J	105	LUT	C27-C28-C29	6.98	141.33	126.32
25	j	105	LUT	C27-C28-C29	6.98	141.33	126.32
29	5a	307	CHL	C1B-CHB-C4A	6.47	125.48	121.32
29	5b	307	CHL	C1B-CHB-C4A	6.47	125.48	121.32
25	3b	317	LUT	C35-C15-C14	6.45	136.72	123.52
25	3a	317	LUT	C35-C15-C14	6.44	136.69	123.52
25	J	105	LUT	C12-C13-C14	6.29	128.90	119.01
25	j	105	LUT	C12-C13-C14	6.29	128.90	119.01
25	j	105	LUT	C30-C31-C32	6.00	140.59	123.20
25	J	105	LUT	C30-C31-C32	6.00	140.58	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3a	317	LUT	C11-C10-C9	5.78	135.39	127.28
25	3b	317	LUT	C11-C10-C9	5.78	135.39	127.28
20	A	851	BCR	C15-C16-C17	5.74	135.27	123.52
20	a	851	BCR	C15-C16-C17	5.72	135.23	123.52
25	6a	318	LUT	C30-C31-C32	5.72	139.78	123.20
25	6b	318	LUT	C30-C31-C32	5.71	139.73	123.20
25	j	105	LUT	C8-C9-C10	5.60	127.81	119.01
25	J	105	LUT	C8-C9-C10	5.59	127.80	119.01
25	5a	317	LUT	C35-C15-C14	5.52	134.82	123.52
25	5b	317	LUT	C35-C15-C14	5.52	134.81	123.52
25	6a	319	LUT	C27-C28-C29	5.41	137.96	126.32
25	6b	319	LUT	C27-C28-C29	5.41	137.96	126.32
25	2b	315	LUT	C15-C14-C13	5.27	134.67	127.28
25	2a	315	LUT	C15-C14-C13	5.25	134.65	127.28
25	3a	317	LUT	C10-C11-C12	5.23	138.35	123.20
25	3b	317	LUT	C10-C11-C12	5.23	138.35	123.20
25	6a	319	LUT	C28-C29-C30	5.21	127.21	119.01
25	6b	319	LUT	C28-C29-C30	5.21	127.20	119.01
25	2a	315	LUT	C35-C34-C33	5.18	134.55	127.28
25	2b	315	LUT	C35-C34-C33	5.18	134.55	127.28
20	J	102	BCR	C23-C22-C21	4.96	126.82	119.01
20	j	102	BCR	C23-C22-C21	4.96	126.82	119.01
25	J	105	LUT	C11-C10-C9	4.93	134.19	127.28
25	j	105	LUT	C11-C10-C9	4.91	134.17	127.28
25	6a	319	LUT	C31-C30-C29	4.75	133.94	127.28
25	j	105	LUT	C19-C9-C10	-4.74	115.14	122.82
25	J	105	LUT	C19-C9-C10	-4.73	115.15	122.82
25	6b	319	LUT	C31-C30-C29	4.71	133.89	127.28
25	6a	318	LUT	C15-C35-C34	4.71	133.15	123.52
25	6b	318	LUT	C15-C35-C34	4.71	133.15	123.52
20	B	843	BCR	C16-C17-C18	4.71	133.88	127.28
20	b	843	BCR	C16-C17-C18	4.71	133.88	127.28
20	B	848	BCR	C21-C20-C19	4.70	136.82	123.20
20	b	848	BCR	C21-C20-C19	4.70	136.82	123.20
20	A	847	BCR	C15-C16-C17	4.69	133.12	123.52
20	a	847	BCR	C15-C16-C17	4.69	133.12	123.52
25	2a	314	LUT	C30-C31-C32	4.66	136.70	123.20
20	B	848	BCR	C16-C15-C14	4.65	133.03	123.52
25	2b	314	LUT	C30-C31-C32	4.64	136.66	123.20
20	b	848	BCR	C16-C15-C14	4.64	133.01	123.52
29	3a	307	CHL	O2D-CGD-CBD	4.63	116.03	110.95
29	3b	307	CHL	O2D-CGD-CBD	4.63	116.03	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	304	BCR	C16-C15-C14	4.62	132.97	123.52
20	f	304	BCR	C16-C15-C14	4.62	132.97	123.52
25	2b	314	LUT	C35-C34-C33	4.61	133.74	127.28
25	2a	314	LUT	C35-C34-C33	4.59	133.71	127.28
20	B	848	BCR	C15-C16-C17	4.52	132.76	123.52
20	b	848	BCR	C15-C16-C17	4.50	132.73	123.52
25	J	105	LUT	C39-C29-C28	4.48	124.93	118.09
25	j	105	LUT	C39-C29-C28	4.47	124.92	118.09
25	J	105	LUT	C26-C27-C28	4.46	131.52	124.58
25	j	105	LUT	C26-C27-C28	4.46	131.52	124.58
20	l	304	BCR	C15-C16-C17	4.44	132.59	123.52
20	L	304	BCR	C15-C16-C17	4.43	132.58	123.52
20	L	304	BCR	C24-C23-C22	4.34	132.66	126.23
20	l	304	BCR	C24-C23-C22	4.34	132.66	126.23
25	2a	314	LUT	C18-C5-C6	4.34	129.22	124.48
25	2b	314	LUT	C18-C5-C6	4.34	129.22	124.48
20	K	202	BCR	C38-C26-C25	4.32	129.20	124.48
20	k	202	BCR	C38-C26-C25	4.32	129.20	124.48
25	J	105	LUT	C20-C13-C14	-4.29	115.87	122.82
25	j	105	LUT	C20-C13-C14	-4.29	115.87	122.82
29	5a	301	CHL	C1C-CHC-C4B	4.27	131.35	116.07
29	5b	301	CHL	C1C-CHC-C4B	4.26	131.33	116.07
20	B	846	BCR	C15-C16-C17	4.22	132.16	123.52
29	5b	307	CHL	C3D-C4D-CHA	4.20	114.93	108.54
20	b	846	BCR	C15-C16-C17	4.20	132.10	123.52
20	J	102	BCR	C24-C23-C22	4.18	132.42	126.23
20	j	102	BCR	C24-C23-C22	4.18	132.42	126.23
29	5a	307	CHL	C3D-C4D-CHA	4.17	114.87	108.54
29	5b	306	CHL	O2D-CGD-CBD	4.16	115.52	110.95
29	2b	304	CHL	C1C-CHC-C4B	4.14	130.90	116.07
25	J	105	LUT	C7-C8-C9	-4.14	120.11	126.23
29	6a	309	CHL	C3D-C4D-CHA	4.14	114.83	108.54
29	6b	309	CHL	C3D-C4D-CHA	4.14	114.83	108.54
25	j	105	LUT	C7-C8-C9	-4.13	120.12	126.23
29	6b	304	CHL	C1C-CHC-C4B	4.13	130.86	116.07
29	2a	304	CHL	C1C-CHC-C4B	4.13	130.86	116.07
29	5a	306	CHL	O2D-CGD-CBD	4.13	115.49	110.95
29	6a	304	CHL	C3D-C4D-CHA	4.13	114.82	108.54
29	6a	304	CHL	C1C-CHC-C4B	4.13	130.84	116.07
20	F	301	BCR	C15-C16-C17	4.13	131.97	123.52
20	f	301	BCR	C15-C16-C17	4.13	131.97	123.52
18	B	831	CLA	CAA-C2A-C3A	-4.13	101.85	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	831	CLA	CAA-C2A-C3A	-4.13	101.85	113.00
29	5a	301	CHL	C3D-C4D-CHA	4.12	114.81	108.54
29	5b	301	CHL	C3D-C4D-CHA	4.12	114.81	108.54
29	6b	304	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	2b	313	CHL	C1C-CHC-C4B	4.12	130.81	116.07
29	5a	314	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	5b	314	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	3a	301	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	3b	301	CHL	C3D-C4D-CHA	4.12	114.80	108.54
29	2a	313	CHL	C1C-CHC-C4B	4.11	130.78	116.07
25	2a	315	LUT	C39-C29-C28	4.11	124.37	118.09
29	2a	304	CHL	C3D-C4D-CHA	4.10	114.77	108.54
29	2b	304	CHL	C3D-C4D-CHA	4.10	114.77	108.54
25	2b	315	LUT	C39-C29-C28	4.10	124.34	118.09
29	2a	305	CHL	C3D-C4D-CHA	4.10	114.77	108.54
29	2b	305	CHL	C3D-C4D-CHA	4.10	114.77	108.54
29	3a	307	CHL	C1A-CHA-C4D	4.09	125.81	118.98
29	3b	307	CHL	C1A-CHA-C4D	4.09	125.81	118.98
25	3a	316	LUT	C19-C9-C8	4.09	124.33	118.09
25	3b	316	LUT	C19-C9-C8	4.09	124.33	118.09
29	3a	315	CHL	C1C-CHC-C4B	4.09	130.70	116.07
29	3b	315	CHL	C1C-CHC-C4B	4.09	130.70	116.07
20	G	201	BCR	C38-C26-C25	4.08	128.94	124.48
20	g	201	BCR	C38-C26-C25	4.08	128.94	124.48
29	3a	301	CHL	C1C-CHC-C4B	4.08	130.66	116.07
29	3a	315	CHL	C3D-C4D-CHA	4.08	114.74	108.54
29	3b	315	CHL	C3D-C4D-CHA	4.08	114.74	108.54
20	A	849	BCR	C16-C15-C14	4.08	131.86	123.52
20	a	849	BCR	C16-C15-C14	4.08	131.86	123.52
18	b	853	CLA	C4D-CHA-C1A	4.08	126.11	121.24
29	5a	306	CHL	C3D-C4D-CHA	4.07	114.73	108.54
29	5b	306	CHL	C3D-C4D-CHA	4.07	114.73	108.54
29	2a	313	CHL	C3D-C4D-CHA	4.07	114.73	108.54
29	2b	313	CHL	C3D-C4D-CHA	4.07	114.73	108.54
18	A	809	CLA	C1-O2A-CGA	4.07	126.51	116.65
29	3b	301	CHL	C1C-CHC-C4B	4.07	130.62	116.07
29	6a	304	CHL	C1A-CHA-C4D	4.07	125.77	118.98
29	6b	304	CHL	C1A-CHA-C4D	4.07	125.77	118.98
20	B	845	BCR	C1-C6-C5	-4.06	117.08	122.64
18	a	809	CLA	C1-O2A-CGA	4.06	126.49	116.65
20	b	845	BCR	C1-C6-C5	-4.06	117.08	122.64
18	B	853	CLA	C4D-CHA-C1A	4.06	126.09	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6a	320	LUT	C15-C35-C34	4.06	131.82	123.52
18	B	830	CLA	C1-O2A-CGA	4.05	126.45	116.65
18	b	830	CLA	C1-O2A-CGA	4.05	126.45	116.65
25	6b	320	LUT	C15-C35-C34	4.05	131.80	123.52
29	5a	314	CHL	C1C-CHC-C4B	4.04	130.51	116.07
29	5b	314	CHL	C1C-CHC-C4B	4.04	130.51	116.07
29	6a	309	CHL	C1C-CHC-C4B	4.03	130.47	116.07
29	3a	307	CHL	C3D-C4D-CHA	4.02	114.66	108.54
29	3b	307	CHL	C3D-C4D-CHA	4.02	114.66	108.54
29	6b	309	CHL	C1C-CHC-C4B	4.02	130.46	116.07
20	F	301	BCR	C38-C26-C25	4.02	128.87	124.48
20	f	301	BCR	C38-C26-C25	4.02	128.87	124.48
25	J	105	LUT	C39-C29-C30	-4.01	116.32	122.82
25	j	105	LUT	C39-C29-C30	-4.00	116.33	122.82
29	5a	306	CHL	C1A-CHA-C4D	4.00	125.65	118.98
29	5b	306	CHL	C1A-CHA-C4D	4.00	125.65	118.98
20	G	204	BCR	C15-C16-C17	3.99	131.69	123.52
29	2a	306	CHL	C3D-C4D-CHA	3.99	114.60	108.54
29	2b	306	CHL	C3D-C4D-CHA	3.99	114.60	108.54
29	5a	305	CHL	C3D-C4D-CHA	3.99	114.60	108.54
29	5b	305	CHL	C3D-C4D-CHA	3.99	114.60	108.54
20	g	204	BCR	C15-C16-C17	3.98	131.66	123.52
18	B	817	CLA	C4D-CHA-C1A	3.97	125.98	121.24
18	b	817	CLA	C4D-CHA-C1A	3.97	125.98	121.24
25	3a	316	LUT	C7-C8-C9	3.97	132.10	126.23
25	3b	316	LUT	C7-C8-C9	3.97	132.10	126.23
18	B	837	CLA	C4D-CHA-C1A	3.96	125.97	121.24
18	b	837	CLA	C4D-CHA-C1A	3.95	125.96	121.24
18	a	814	CLA	C4D-CHA-C1A	3.93	125.93	121.24
20	B	851	BCR	C16-C15-C14	3.92	131.54	123.52
20	b	851	BCR	C16-C15-C14	3.92	131.54	123.52
20	J	102	BCR	C8-C9-C10	3.90	125.14	119.01
20	j	102	BCR	C8-C9-C10	3.90	125.14	119.01
18	A	814	CLA	C4D-CHA-C1A	3.89	125.89	121.24
20	G	204	BCR	C38-C26-C25	3.89	128.73	124.48
20	g	204	BCR	C38-C26-C25	3.89	128.73	124.48
20	B	844	BCR	C37-C22-C21	-3.89	116.52	122.82
20	b	844	BCR	C37-C22-C21	-3.89	116.52	122.82
29	6b	309	CHL	C1A-CHA-C4D	3.87	125.44	118.98
20	j	102	BCR	C37-C22-C21	-3.87	116.55	122.82
20	b	842	BCR	C38-C26-C25	3.87	128.70	124.48
18	B	806	CLA	C4D-CHA-C1A	3.86	125.85	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6a	309	CHL	C1A-CHA-C4D	3.86	125.42	118.98
29	2a	305	CHL	C1C-CHC-C4B	3.85	129.86	116.07
29	2b	305	CHL	C1C-CHC-C4B	3.85	129.86	116.07
25	5a	316	LUT	C15-C35-C34	3.85	131.40	123.52
25	5b	316	LUT	C15-C35-C34	3.85	131.40	123.52
18	2b	310	CLA	C4D-CHA-C1A	3.85	125.83	121.24
20	J	102	BCR	C37-C22-C21	-3.84	116.59	122.82
20	B	842	BCR	C38-C26-C25	3.84	128.67	124.48
18	b	806	CLA	C4D-CHA-C1A	3.84	125.82	121.24
18	2a	310	CLA	C4D-CHA-C1A	3.84	125.82	121.24
29	5a	301	CHL	C1A-CHA-C4D	3.83	125.37	118.98
29	5a	306	CHL	C1C-CHC-C4B	3.83	129.78	116.07
29	5b	306	CHL	C1C-CHC-C4B	3.83	129.78	116.07
29	5b	301	CHL	C1A-CHA-C4D	3.83	125.37	118.98
29	5a	305	CHL	C1C-CHC-C4B	3.83	129.76	116.07
29	5b	305	CHL	C1C-CHC-C4B	3.83	129.76	116.07
25	6a	319	LUT	C19-C9-C10	-3.81	116.64	122.82
25	6b	319	LUT	C19-C9-C10	-3.81	116.64	122.82
29	5a	314	CHL	C1A-CHA-C4D	3.81	125.33	118.98
29	5b	314	CHL	C1A-CHA-C4D	3.81	125.33	118.98
18	3a	311	CLA	C4D-CHA-C1A	3.80	125.78	121.24
18	3b	311	CLA	C4D-CHA-C1A	3.80	125.78	121.24
18	A	803	CLA	C4D-CHA-C1A	3.79	125.77	121.24
18	a	803	CLA	C4D-CHA-C1A	3.79	125.77	121.24
25	J	105	LUT	C35-C34-C33	3.78	132.58	127.28
25	j	105	LUT	C35-C34-C33	3.78	132.58	127.28
18	B	835	CLA	C4D-CHA-C1A	3.78	125.75	121.24
18	b	835	CLA	C4D-CHA-C1A	3.78	125.75	121.24
29	5a	305	CHL	C1A-CHA-C4D	3.78	125.29	118.98
29	5b	305	CHL	C1A-CHA-C4D	3.78	125.29	118.98
18	A	830	CLA	C1-O2A-CGA	3.77	125.77	116.65
18	a	830	CLA	C1-O2A-CGA	3.77	125.77	116.65
18	a	825	CLA	C4D-CHA-C1A	3.76	125.73	121.24
25	3a	317	LUT	C12-C13-C14	3.76	124.92	119.01
25	3b	317	LUT	C12-C13-C14	3.76	124.92	119.01
29	2b	304	CHL	C1A-CHA-C4D	3.75	125.23	118.98
20	B	842	BCR	C1-C6-C7	3.74	125.78	115.65
20	b	842	BCR	C1-C6-C7	3.74	125.78	115.65
20	A	851	BCR	C38-C26-C25	3.73	128.55	124.48
18	A	825	CLA	C4D-CHA-C1A	3.73	125.69	121.24
18	A	805	CLA	C4D-CHA-C1A	3.73	125.69	121.24
18	a	805	CLA	C4D-CHA-C1A	3.73	125.69	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2a	304	CHL	C1A-CHA-C4D	3.72	125.20	118.98
29	2a	313	CHL	C1A-CHA-C4D	3.72	125.20	118.98
29	2b	313	CHL	C1A-CHA-C4D	3.72	125.20	118.98
18	a	853	CLA	C4D-CHA-C1A	3.72	125.68	121.24
20	a	851	BCR	C38-C26-C25	3.72	128.54	124.48
18	a	813	CLA	C4D-CHA-C1A	3.71	125.67	121.24
18	6a	314	CLA	C4D-CHA-C1A	3.71	125.67	121.24
20	J	102	BCR	C1-C6-C7	3.71	125.72	115.65
20	j	102	BCR	C1-C6-C7	3.71	125.72	115.65
18	a	837	CLA	C4D-CHA-C1A	3.71	125.67	121.24
20	B	842	BCR	C16-C15-C14	3.71	131.10	123.52
20	b	842	BCR	C16-C15-C14	3.71	131.10	123.52
18	6b	314	CLA	C4D-CHA-C1A	3.70	125.66	121.24
18	5a	311	CLA	C4D-CHA-C1A	3.70	125.65	121.24
18	5b	311	CLA	C4D-CHA-C1A	3.70	125.65	121.24
29	3a	307	CHL	C1C-CHC-C4B	3.70	129.29	116.07
29	3b	307	CHL	C1C-CHC-C4B	3.70	129.29	116.07
20	B	848	BCR	C12-C13-C14	3.69	124.82	119.01
20	b	848	BCR	C12-C13-C14	3.69	124.82	119.01
18	A	853	CLA	C4D-CHA-C1A	3.69	125.65	121.24
20	a	847	BCR	C30-C25-C24	3.69	125.66	115.65
18	A	835	CLA	C4D-CHA-C1A	3.69	125.64	121.24
18	A	813	CLA	C4D-CHA-C1A	3.68	125.64	121.24
20	J	102	BCR	C15-C16-C17	3.68	131.06	123.52
20	j	102	BCR	C15-C16-C17	3.68	131.06	123.52
20	B	848	BCR	C1-C6-C7	3.68	125.63	115.65
18	A	811	CLA	C4D-CHA-C1A	3.68	125.63	121.24
18	A	837	CLA	C4D-CHA-C1A	3.68	125.63	121.24
18	a	811	CLA	C4D-CHA-C1A	3.68	125.63	121.24
20	A	847	BCR	C30-C25-C24	3.68	125.62	115.65
25	6a	319	LUT	C40-C33-C34	-3.67	116.86	122.82
25	6b	319	LUT	C40-C33-C34	-3.67	116.86	122.82
20	A	850	BCR	C30-C25-C24	3.67	125.60	115.65
20	a	850	BCR	C30-C25-C24	3.67	125.60	115.65
20	b	848	BCR	C1-C6-C7	3.67	125.60	115.65
18	a	835	CLA	C4D-CHA-C1A	3.66	125.61	121.24
20	J	102	BCR	C34-C9-C10	-3.65	116.91	122.82
20	j	102	BCR	C34-C9-C10	-3.65	116.91	122.82
18	2b	303	CLA	C4D-CHA-C1A	3.64	125.59	121.24
29	2a	306	CHL	C1A-CHA-C4D	3.64	125.06	118.98
29	2b	306	CHL	C1A-CHA-C4D	3.64	125.06	118.98
18	F	303	CLA	C4D-CHA-C1A	3.63	125.58	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5a	316	LUT	C39-C29-C28	3.63	123.64	118.09
25	5b	316	LUT	C39-C29-C28	3.63	123.64	118.09
18	A	837	CLA	C1-O2A-CGA	3.63	125.45	116.65
18	a	837	CLA	C1-O2A-CGA	3.63	125.45	116.65
20	K	202	BCR	C16-C15-C14	3.63	130.95	123.52
20	l	304	BCR	C30-C25-C24	3.63	125.49	115.65
20	L	304	BCR	C30-C25-C24	3.63	125.49	115.65
18	3a	302	CLA	C4D-CHA-C1A	3.62	125.57	121.24
20	L	304	BCR	C29-C30-C25	3.62	115.70	110.44
20	l	304	BCR	C29-C30-C25	3.62	115.70	110.44
18	B	831	CLA	C4D-CHA-C1A	3.62	125.56	121.24
18	b	831	CLA	C4D-CHA-C1A	3.62	125.56	121.24
18	5a	315	CLA	C4D-CHA-C1A	3.62	125.56	121.24
18	5b	315	CLA	C4D-CHA-C1A	3.62	125.56	121.24
18	f	303	CLA	C4D-CHA-C1A	3.62	125.56	121.24
29	3a	307	CHL	C4D-CHA-CBD	-3.62	105.32	108.97
29	3b	307	CHL	C4D-CHA-CBD	-3.62	105.32	108.97
25	3a	316	LUT	C1-C6-C7	3.62	125.46	115.65
25	3b	316	LUT	C1-C6-C7	3.62	125.46	115.65
18	2a	303	CLA	C4D-CHA-C1A	3.62	125.56	121.24
18	6a	307	CLA	C4D-CHA-C1A	3.62	125.56	121.24
20	k	202	BCR	C16-C15-C14	3.62	130.92	123.52
25	6a	320	LUT	C19-C9-C10	-3.62	116.96	122.82
25	6b	320	LUT	C19-C9-C10	-3.62	116.96	122.82
18	3b	302	CLA	C4D-CHA-C1A	3.62	125.56	121.24
20	B	851	BCR	C38-C26-C25	3.61	128.42	124.48
20	b	851	BCR	C38-C26-C25	3.61	128.42	124.48
20	L	304	BCR	C33-C5-C6	3.61	128.42	124.48
20	l	304	BCR	C33-C5-C6	3.61	128.42	124.48
18	B	832	CLA	C4D-CHA-C1A	3.60	125.54	121.24
18	b	832	CLA	C4D-CHA-C1A	3.60	125.54	121.24
20	L	304	BCR	C37-C22-C23	3.60	123.59	118.09
20	l	304	BCR	C37-C22-C23	3.60	123.59	118.09
18	6b	307	CLA	C4D-CHA-C1A	3.60	125.54	121.24
25	6a	320	LUT	C35-C15-C14	3.60	130.88	123.52
25	6b	320	LUT	C35-C15-C14	3.60	130.88	123.52
18	a	818	CLA	C4D-CHA-C1A	3.60	125.53	121.24
18	A	818	CLA	C4D-CHA-C1A	3.59	125.53	121.24
25	6a	319	LUT	C26-C27-C28	3.59	130.17	124.58
25	6b	319	LUT	C26-C27-C28	3.59	130.17	124.58
18	3a	306	CLA	C4D-CHA-C1A	3.58	125.52	121.24
18	3b	306	CLA	C4D-CHA-C1A	3.58	125.52	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	807	CLA	C4D-CHA-C1A	3.57	125.51	121.24
25	6a	319	LUT	C18-C5-C6	3.57	128.37	124.48
25	6b	319	LUT	C18-C5-C6	3.57	128.37	124.48
20	B	848	BCR	C36-C18-C17	-3.56	117.05	122.82
20	b	848	BCR	C36-C18-C17	-3.56	117.05	122.82
20	J	102	BCR	C16-C15-C14	3.56	130.80	123.52
20	j	102	BCR	C16-C15-C14	3.56	130.80	123.52
18	3a	305	CLA	C4D-CHA-C1A	3.56	125.49	121.24
18	3b	305	CLA	C4D-CHA-C1A	3.56	125.49	121.24
20	b	844	BCR	C15-C16-C17	3.55	130.79	123.52
29	5b	307	CHL	C1A-CHA-C4D	3.55	124.91	118.98
29	2a	305	CHL	C1A-CHA-C4D	3.55	124.91	118.98
29	2b	305	CHL	C1A-CHA-C4D	3.55	124.91	118.98
18	B	836	CLA	C4D-CHA-C1A	3.55	125.48	121.24
18	B	809	CLA	C4D-CHA-C1A	3.55	125.47	121.24
18	b	809	CLA	C4D-CHA-C1A	3.55	125.47	121.24
18	B	807	CLA	C4D-CHA-C1A	3.54	125.47	121.24
18	b	836	CLA	C4D-CHA-C1A	3.54	125.47	121.24
20	B	844	BCR	C15-C16-C17	3.54	130.75	123.52
20	J	102	BCR	C1-C6-C5	-3.54	117.80	122.64
20	j	102	BCR	C1-C6-C5	-3.54	117.80	122.64
29	3a	315	CHL	C1A-CHA-C4D	3.54	124.88	118.98
29	3b	315	CHL	C1A-CHA-C4D	3.53	124.88	118.98
18	A	809	CLA	C4D-CHA-C1A	3.53	125.46	121.24
18	a	809	CLA	C4D-CHA-C1A	3.53	125.46	121.24
20	K	202	BCR	C37-C22-C21	-3.53	117.10	122.82
20	k	202	BCR	C37-C22-C21	-3.53	117.10	122.82
20	B	842	BCR	C1-C6-C5	-3.53	117.82	122.64
20	b	842	BCR	C1-C6-C5	-3.53	117.82	122.64
20	B	844	BCR	C38-C26-C25	3.53	128.33	124.48
20	b	844	BCR	C38-C26-C25	3.53	128.33	124.48
20	M	101	BCR	C16-C15-C14	3.52	130.73	123.52
20	m	101	BCR	C16-C15-C14	3.52	130.73	123.52
18	6a	317	CLA	C4D-CHA-C1A	3.52	125.44	121.24
18	6b	317	CLA	C4D-CHA-C1A	3.52	125.44	121.24
29	5a	307	CHL	C1A-CHA-C4D	3.52	124.85	118.98
25	3a	316	LUT	C39-C29-C28	3.52	123.46	118.09
25	3b	316	LUT	C39-C29-C28	3.52	123.46	118.09
18	5b	303	CLA	C4D-CHA-C1A	3.51	125.44	121.24
18	B	820	CLA	C4D-CHA-C1A	3.51	125.43	121.24
18	b	820	CLA	C4D-CHA-C1A	3.51	125.43	121.24
18	L	303	CLA	C4D-CHA-C1A	3.51	125.43	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	l	303	CLA	C4D-CHA-C1A	3.51	125.43	121.24
18	B	832	CLA	C1-O2A-CGA	3.50	125.14	116.65
18	B	834	CLA	C4D-CHA-C1A	3.50	125.42	121.24
20	A	850	BCR	C15-C16-C17	3.50	130.69	123.52
20	a	850	BCR	C15-C16-C17	3.50	130.69	123.52
20	A	847	BCR	C34-C9-C10	-3.50	117.14	122.82
20	a	847	BCR	C34-C9-C10	-3.50	117.14	122.82
20	F	304	BCR	C34-C9-C10	-3.50	117.14	122.82
20	f	304	BCR	C34-C9-C10	-3.50	117.14	122.82
18	b	832	CLA	C1-O2A-CGA	3.50	125.12	116.65
25	5b	317	LUT	C12-C13-C14	3.50	124.51	119.01
18	A	831	CLA	C4D-CHA-C1A	3.50	125.42	121.24
18	A	839	CLA	C4D-CHA-C1A	3.50	125.42	121.24
18	a	831	CLA	C4D-CHA-C1A	3.50	125.42	121.24
20	G	201	BCR	C34-C9-C10	-3.50	117.15	122.82
20	g	201	BCR	C34-C9-C10	-3.50	117.15	122.82
18	a	801	CLA	C4D-CHA-C1A	3.50	125.41	121.24
25	5a	317	LUT	C12-C13-C14	3.49	124.51	119.01
18	2b	301	CLA	C4D-CHA-C1A	3.49	125.41	121.24
18	5a	310	CLA	C4D-CHA-C1A	3.49	125.41	121.24
18	5b	310	CLA	C4D-CHA-C1A	3.49	125.41	121.24
18	a	816	CLA	C1-O2A-CGA	3.49	125.10	116.65
20	A	849	BCR	C34-C9-C10	-3.49	117.16	122.82
20	a	849	BCR	C34-C9-C10	-3.49	117.16	122.82
20	b	845	BCR	C12-C13-C14	3.49	124.50	119.01
18	5a	303	CLA	C4D-CHA-C1A	3.49	125.40	121.24
20	A	848	BCR	C37-C22-C21	-3.48	117.17	122.82
20	a	848	BCR	C37-C22-C21	-3.48	117.17	122.82
18	G	202	CLA	C4D-CHA-C1A	3.48	125.40	121.24
18	g	202	CLA	C4D-CHA-C1A	3.48	125.40	121.24
29	2a	306	CHL	C1C-CHC-C4B	3.48	128.53	116.07
18	b	834	CLA	C4D-CHA-C1A	3.48	125.40	121.24
18	3a	310	CLA	C4D-CHA-C1A	3.48	125.39	121.24
18	2a	301	CLA	C4D-CHA-C1A	3.48	125.39	121.24
18	A	816	CLA	C1-O2A-CGA	3.47	125.06	116.65
29	2b	306	CHL	C1C-CHC-C4B	3.47	128.50	116.07
18	b	823	CLA	C4D-CHA-C1A	3.47	125.39	121.24
18	a	839	CLA	C4D-CHA-C1A	3.47	125.38	121.24
18	A	815	CLA	C4D-CHA-C1A	3.47	125.38	121.24
20	F	304	BCR	C38-C26-C25	3.47	128.27	124.48
20	f	304	BCR	C38-C26-C25	3.47	128.27	124.48
25	5a	317	LUT	C19-C9-C10	-3.47	117.20	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5b	317	LUT	C19-C9-C10	-3.47	117.20	122.82
20	B	845	BCR	C12-C13-C14	3.46	124.46	119.01
29	3a	301	CHL	C1A-CHA-C4D	3.46	124.76	118.98
29	3b	301	CHL	C1A-CHA-C4D	3.46	124.76	118.98
25	2a	314	LUT	C39-C29-C30	-3.46	117.20	122.82
25	2b	314	LUT	C39-C29-C30	-3.46	117.20	122.82
18	A	801	CLA	C4D-CHA-C1A	3.46	125.38	121.24
20	K	202	BCR	C34-C9-C10	-3.46	117.21	122.82
18	3a	314	CLA	C4D-CHA-C1A	3.46	125.37	121.24
18	3b	310	CLA	C4D-CHA-C1A	3.46	125.37	121.24
18	3b	314	CLA	C4D-CHA-C1A	3.46	125.37	121.24
20	B	844	BCR	C34-C9-C10	-3.46	117.22	122.82
20	b	844	BCR	C34-C9-C10	-3.46	117.22	122.82
25	6a	319	LUT	C8-C9-C10	3.45	124.44	119.01
25	6b	319	LUT	C8-C9-C10	3.45	124.44	119.01
18	a	815	CLA	C4D-CHA-C1A	3.45	125.36	121.24
20	A	847	BCR	C37-C22-C21	-3.45	117.23	122.82
20	a	847	BCR	C37-C22-C21	-3.45	117.23	122.82
18	6a	306	CLA	C4D-CHA-C1A	3.45	125.36	121.24
18	B	823	CLA	C4D-CHA-C1A	3.45	125.35	121.24
18	A	840	CLA	C4D-CHA-C1A	3.44	125.35	121.24
18	a	840	CLA	C4D-CHA-C1A	3.44	125.35	121.24
18	2a	312	CLA	C4D-CHA-C1A	3.44	125.35	121.24
18	2b	312	CLA	C4D-CHA-C1A	3.44	125.35	121.24
18	K	201	CLA	C4D-CHA-C1A	3.44	125.35	121.24
20	k	202	BCR	C34-C9-C10	-3.44	117.25	122.82
20	B	843	BCR	C37-C22-C21	-3.44	117.25	122.82
20	b	843	BCR	C37-C22-C21	-3.44	117.25	122.82
18	F	302	CLA	C4D-CHA-C1A	3.44	125.34	121.24
18	f	302	CLA	C4D-CHA-C1A	3.44	125.34	121.24
18	6b	306	CLA	C4D-CHA-C1A	3.43	125.34	121.24
20	A	848	BCR	C16-C15-C14	3.43	130.55	123.52
20	a	848	BCR	C16-C15-C14	3.43	130.55	123.52
18	k	201	CLA	C4D-CHA-C1A	3.43	125.34	121.24
20	B	848	BCR	C1-C6-C5	-3.43	117.95	122.64
18	6b	315	CLA	C4D-CHA-C1A	3.43	125.33	121.24
18	B	840	CLA	C1-O2A-CGA	3.42	124.94	116.65
20	b	848	BCR	C1-C6-C5	-3.42	117.96	122.64
18	6a	315	CLA	C4D-CHA-C1A	3.42	125.32	121.24
18	b	840	CLA	C1-O2A-CGA	3.41	124.91	116.65
25	5a	317	LUT	C1-C6-C7	3.41	124.89	115.65
25	2b	315	LUT	C31-C30-C29	3.41	132.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2b	315	LUT	C18-C5-C6	3.40	128.20	124.48
18	6b	316	CLA	C4D-CHA-C1A	3.40	125.30	121.24
20	L	304	BCR	C30-C25-C26	-3.40	117.99	122.64
20	l	304	BCR	C30-C25-C26	-3.40	117.99	122.64
20	B	843	BCR	C38-C26-C25	3.40	128.19	124.48
20	b	843	BCR	C38-C26-C25	3.40	128.19	124.48
25	J	105	LUT	C10-C11-C12	-3.40	113.36	123.20
25	j	105	LUT	C10-C11-C12	-3.40	113.36	123.20
18	a	830	CLA	C4D-CHA-C1A	3.40	125.30	121.24
18	3a	304	CLA	C4D-CHA-C1A	3.40	125.29	121.24
18	3b	304	CLA	C4D-CHA-C1A	3.40	125.29	121.24
25	5b	317	LUT	C1-C6-C7	3.40	124.86	115.65
20	A	851	BCR	C33-C5-C6	3.39	128.19	124.48
20	a	851	BCR	C33-C5-C6	3.39	128.19	124.48
25	2a	315	LUT	C19-C9-C10	-3.39	117.32	122.82
25	2b	315	LUT	C19-C9-C10	-3.39	117.32	122.82
20	B	848	BCR	C37-C22-C23	3.39	123.27	118.09
20	b	848	BCR	C37-C22-C23	3.39	123.27	118.09
25	2a	315	LUT	C31-C30-C29	3.39	132.04	127.28
25	6a	318	LUT	C39-C29-C30	-3.39	117.32	122.82
18	l	302	CLA	C4D-CHA-C1A	3.39	125.29	121.24
25	6b	318	LUT	C39-C29-C30	-3.39	117.32	122.82
20	F	304	BCR	C1-C6-C5	-3.39	118.00	122.64
18	5b	304	CLA	C4D-CHA-C1A	3.39	125.29	121.24
20	A	850	BCR	C34-C9-C10	-3.39	117.33	122.82
20	a	850	BCR	C34-C9-C10	-3.39	117.33	122.82
25	2a	315	LUT	C18-C5-C6	3.38	128.18	124.48
18	6a	316	CLA	C4D-CHA-C1A	3.38	125.28	121.24
18	B	830	CLA	C4D-CHA-C1A	3.38	125.28	121.24
18	b	830	CLA	C4D-CHA-C1A	3.38	125.28	121.24
26	A	802	CL0	C1C-CHC-C4B	3.38	128.17	116.07
26	a	802	CL0	C1C-CHC-C4B	3.38	128.17	116.07
18	5b	302	CLA	C4D-CHA-C1A	3.38	125.28	121.24
18	5a	302	CLA	C4D-CHA-C1A	3.38	125.27	121.24
18	A	812	CLA	C4D-CHA-C1A	3.37	125.27	121.24
18	a	812	CLA	C4D-CHA-C1A	3.37	125.27	121.24
20	G	204	BCR	C37-C22-C21	-3.37	117.35	122.82
20	g	204	BCR	C37-C22-C21	-3.37	117.35	122.82
20	J	102	BCR	C38-C26-C25	3.37	128.16	124.48
20	j	102	BCR	C38-C26-C25	3.37	128.16	124.48
18	5a	304	CLA	C4D-CHA-C1A	3.37	125.27	121.24
20	M	101	BCR	C38-C26-C25	3.37	128.16	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	m	101	BCR	C38-C26-C25	3.37	128.16	124.48
18	A	823	CLA	C4D-CHA-C1A	3.37	125.26	121.24
18	a	823	CLA	C4D-CHA-C1A	3.37	125.26	121.24
25	3a	316	LUT	C15-C35-C34	3.37	130.41	123.52
25	3b	316	LUT	C15-C35-C34	3.37	130.41	123.52
20	f	304	BCR	C1-C6-C5	-3.36	118.04	122.64
26	A	802	CL0	C3D-C4D-CHA	3.36	113.65	108.54
25	j	105	LUT	C31-C32-C33	3.36	135.58	126.36
18	A	807	CLA	C4D-CHA-C1A	3.36	125.25	121.24
18	a	807	CLA	C4D-CHA-C1A	3.36	125.25	121.24
18	3a	313	CLA	C4D-CHA-C1A	3.36	125.25	121.24
20	I	202	BCR	C15-C16-C17	3.36	130.39	123.52
20	i	202	BCR	C15-C16-C17	3.36	130.39	123.52
18	L	302	CLA	C4D-CHA-C1A	3.36	125.25	121.24
20	M	101	BCR	C34-C9-C10	-3.36	117.38	122.82
20	m	101	BCR	C34-C9-C10	-3.36	117.38	122.82
18	B	839	CLA	C4D-CHA-C1A	3.35	125.25	121.24
18	b	839	CLA	C4D-CHA-C1A	3.35	125.25	121.24
18	a	817	CLA	C4D-CHA-C1A	3.35	125.25	121.24
18	6a	305	CLA	C4D-CHA-C1A	3.35	125.24	121.24
18	a	816	CLA	C4D-CHA-C1A	3.35	125.24	121.24
18	6b	305	CLA	C4D-CHA-C1A	3.35	125.24	121.24
20	F	304	BCR	C37-C22-C21	-3.35	117.39	122.82
20	f	304	BCR	C37-C22-C21	-3.35	117.39	122.82
18	B	812	CLA	C4D-CHA-C1A	3.35	125.24	121.24
18	b	812	CLA	C4D-CHA-C1A	3.35	125.24	121.24
18	A	830	CLA	C4D-CHA-C1A	3.35	125.24	121.24
26	a	802	CL0	C3D-C4D-CHA	3.35	113.63	108.54
25	J	105	LUT	C31-C32-C33	3.35	135.55	126.36
20	A	849	BCR	C33-C5-C6	3.35	128.14	124.48
20	a	849	BCR	C33-C5-C6	3.35	128.14	124.48
18	B	829	CLA	C4D-CHA-C1A	3.35	125.23	121.24
18	A	817	CLA	C4D-CHA-C1A	3.34	125.23	121.24
20	B	848	BCR	C10-C11-C12	3.34	132.88	123.20
20	b	848	BCR	C10-C11-C12	3.34	132.88	123.20
18	A	816	CLA	C4D-CHA-C1A	3.34	125.23	121.24
20	B	846	BCR	C37-C22-C21	-3.34	117.41	122.82
20	A	847	BCR	C30-C25-C26	-3.34	118.08	122.64
20	a	847	BCR	C30-C25-C26	-3.34	118.08	122.64
18	B	813	CLA	C4D-CHA-C1A	3.33	125.22	121.24
18	b	813	CLA	C4D-CHA-C1A	3.33	125.22	121.24
20	b	846	BCR	C37-C22-C21	-3.33	117.42	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	822	CLA	C4D-CHA-C1A	3.33	125.22	121.24
18	A	821	CLA	C4D-CHA-C1A	3.33	125.21	121.24
18	b	829	CLA	C4D-CHA-C1A	3.32	125.21	121.24
18	a	822	CLA	C4D-CHA-C1A	3.32	125.21	121.24
20	A	851	BCR	C37-C22-C21	-3.32	117.43	122.82
20	G	201	BCR	C33-C5-C6	3.32	128.11	124.48
18	3b	313	CLA	C4D-CHA-C1A	3.32	125.20	121.24
25	3a	317	LUT	C39-C29-C28	3.32	123.16	118.09
25	3b	317	LUT	C39-C29-C28	3.32	123.16	118.09
29	5a	307	CHL	C4D-ND-C1D	3.32	107.74	105.22
29	5b	307	CHL	C4D-ND-C1D	3.32	107.74	105.22
20	a	851	BCR	C37-C22-C21	-3.32	117.44	122.82
18	A	842	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	a	842	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	2a	307	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	2b	307	CLA	C4D-CHA-C1A	3.31	125.19	121.24
20	L	304	BCR	C34-C9-C10	-3.31	117.45	122.82
20	l	304	BCR	C34-C9-C10	-3.31	117.45	122.82
20	A	848	BCR	C34-C9-C10	-3.31	117.45	122.82
20	a	848	BCR	C34-C9-C10	-3.31	117.45	122.82
25	2b	314	LUT	C19-C9-C10	-3.31	117.45	122.82
18	2a	302	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	2b	302	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	a	821	CLA	C4D-CHA-C1A	3.31	125.19	121.24
18	5a	313	CLA	C4D-CHA-C1A	3.30	125.19	121.24
20	B	843	BCR	C34-C9-C10	-3.30	117.46	122.82
20	b	843	BCR	C34-C9-C10	-3.30	117.46	122.82
20	a	849	BCR	C1-C6-C5	-3.30	118.12	122.64
18	B	818	CLA	C4D-CHA-C1A	3.30	125.18	121.24
18	b	818	CLA	C4D-CHA-C1A	3.30	125.18	121.24
20	a	848	BCR	C38-C26-C25	3.30	128.09	124.48
20	B	851	BCR	C37-C22-C21	-3.30	117.47	122.82
20	b	851	BCR	C37-C22-C21	-3.30	117.47	122.82
18	A	826	CLA	C4D-CHA-C1A	3.30	125.18	121.24
18	a	826	CLA	C4D-CHA-C1A	3.30	125.18	121.24
18	B	804	CLA	C4D-CHA-C1A	3.30	125.18	121.24
18	b	804	CLA	C4D-CHA-C1A	3.30	125.18	121.24
20	B	842	BCR	C34-C9-C10	-3.30	117.48	122.82
18	A	820	CLA	C4D-CHA-C1A	3.29	125.17	121.24
18	a	820	CLA	C4D-CHA-C1A	3.29	125.17	121.24
20	B	845	BCR	C29-C30-C25	3.29	115.22	110.44
18	6a	310	CLA	C4D-CHA-C1A	3.29	125.17	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6b	310	CLA	C4D-CHA-C1A	3.29	125.17	121.24
20	A	851	BCR	C34-C9-C10	-3.29	117.48	122.82
20	a	851	BCR	C34-C9-C10	-3.29	117.48	122.82
20	B	843	BCR	C33-C5-C6	3.29	128.07	124.48
20	G	201	BCR	C15-C16-C17	3.29	130.25	123.52
20	g	201	BCR	C15-C16-C17	3.29	130.25	123.52
25	2a	314	LUT	C19-C9-C10	-3.29	117.49	122.82
18	F	305	CLA	C4D-CHA-C1A	3.29	125.17	121.24
18	f	305	CLA	C4D-CHA-C1A	3.29	125.17	121.24
20	b	845	BCR	C29-C30-C25	3.29	115.21	110.44
20	M	101	BCR	C33-C5-C6	3.28	128.07	124.48
20	m	101	BCR	C33-C5-C6	3.28	128.07	124.48
20	b	842	BCR	C34-C9-C10	-3.28	117.50	122.82
18	5b	313	CLA	C4D-CHA-C1A	3.28	125.16	121.24
20	A	848	BCR	C38-C26-C25	3.28	128.06	124.48
20	b	843	BCR	C33-C5-C6	3.28	128.06	124.48
18	6a	313	CLA	C4D-CHA-C1A	3.28	125.15	121.24
18	6b	313	CLA	C4D-CHA-C1A	3.28	125.15	121.24
18	B	815	CLA	C4D-CHA-C1A	3.27	125.15	121.24
18	b	815	CLA	C4D-CHA-C1A	3.27	125.15	121.24
20	g	201	BCR	C33-C5-C6	3.27	128.06	124.48
20	A	849	BCR	C37-C22-C21	-3.27	117.52	122.82
20	B	851	BCR	C1-C6-C7	3.27	124.52	115.65
20	b	851	BCR	C1-C6-C7	3.27	124.52	115.65
20	b	844	BCR	C33-C5-C6	3.27	128.05	124.48
18	5b	312	CLA	CAA-C2A-C3A	-3.27	104.16	113.00
20	I	202	BCR	C37-C22-C21	-3.27	117.52	122.82
20	i	202	BCR	C37-C22-C21	-3.27	117.52	122.82
18	B	854	CLA	C4D-CHA-C1A	3.27	125.14	121.24
18	b	854	CLA	C4D-CHA-C1A	3.27	125.14	121.24
18	b	811	CLA	C4D-CHA-C1A	3.27	125.14	121.24
18	B	811	CLA	C4D-CHA-C1A	3.26	125.14	121.24
18	B	808	CLA	C4D-CHA-C1A	3.26	125.14	121.24
18	b	808	CLA	C4D-CHA-C1A	3.26	125.14	121.24
20	A	849	BCR	C1-C6-C5	-3.26	118.18	122.64
18	B	810	CLA	C4D-CHA-C1A	3.26	125.14	121.24
18	5a	308	CLA	C4D-CHA-C1A	3.26	125.13	121.24
18	5b	308	CLA	C4D-CHA-C1A	3.26	125.13	121.24
18	5a	312	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
20	B	845	BCR	C34-C9-C10	-3.26	117.54	122.82
20	b	845	BCR	C34-C9-C10	-3.26	117.54	122.82
18	b	810	CLA	C4D-CHA-C1A	3.25	125.12	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	g	203	CLA	C4D-CHA-C1A	3.25	125.12	121.24
18	6b	308	CLA	C4D-CHA-C1A	3.25	125.12	121.24
20	a	849	BCR	C37-C22-C21	-3.25	117.55	122.82
18	B	833	CLA	C4D-CHA-C1A	3.25	125.12	121.24
18	2a	311	CLA	C4D-CHA-C1A	3.25	125.11	121.24
18	2b	311	CLA	C4D-CHA-C1A	3.25	125.11	121.24
25	6a	319	LUT	C35-C34-C33	3.25	131.83	127.28
25	6b	319	LUT	C35-C34-C33	3.25	131.83	127.28
20	B	844	BCR	C33-C5-C6	3.24	128.02	124.48
20	A	847	BCR	C1-C6-C7	3.24	124.45	115.65
20	a	847	BCR	C1-C6-C7	3.24	124.45	115.65
18	B	816	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	b	816	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	3a	312	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	3b	312	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	j	101	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	G	203	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	3a	303	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	3b	303	CLA	C4D-CHA-C1A	3.24	125.11	121.24
18	A	836	CLA	C4D-CHA-C1A	3.24	125.10	121.24
18	a	836	CLA	C4D-CHA-C1A	3.24	125.10	121.24
18	A	838	CLA	C4D-CHA-C1A	3.23	125.10	121.24
18	a	838	CLA	C4D-CHA-C1A	3.23	125.10	121.24
20	b	846	BCR	C38-C26-C25	3.23	128.01	124.48
18	b	833	CLA	C4D-CHA-C1A	3.23	125.10	121.24
20	G	204	BCR	C34-C9-C10	-3.23	117.59	122.82
20	B	848	BCR	C35-C13-C14	-3.22	117.60	122.82
20	b	848	BCR	C35-C13-C14	-3.22	117.60	122.82
20	g	204	BCR	C34-C9-C10	-3.22	117.60	122.82
18	J	101	CLA	C4D-CHA-C1A	3.22	125.08	121.24
20	B	845	BCR	C30-C25-C24	3.21	124.36	115.65
18	6a	308	CLA	C4D-CHA-C1A	3.21	125.07	121.24
18	a	834	CLA	C4D-CHA-C1A	3.21	125.07	121.24
20	b	845	BCR	C30-C25-C24	3.21	124.35	115.65
18	5b	312	CLA	C4D-CHA-C1A	3.21	125.07	121.24
20	B	846	BCR	C38-C26-C25	3.21	127.98	124.48
20	M	101	BCR	C37-C22-C21	-3.21	117.62	122.82
25	6b	318	LUT	C31-C32-C33	3.21	135.15	126.36
18	5a	312	CLA	C4D-CHA-C1A	3.20	125.06	121.24
20	G	201	BCR	C37-C22-C21	-3.20	117.63	122.82
20	g	201	BCR	C37-C22-C21	-3.20	117.63	122.82
20	m	101	BCR	C37-C22-C21	-3.20	117.64	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	838	CLA	C4D-CHA-C1A	3.20	125.06	121.24
18	b	838	CLA	C4D-CHA-C1A	3.20	125.06	121.24
20	k	202	BCR	C33-C5-C6	3.19	127.97	124.48
25	5b	317	LUT	C39-C29-C28	3.19	122.96	118.09
25	6a	318	LUT	C31-C32-C33	3.19	135.10	126.36
20	b	848	BCR	C37-C22-C21	-3.18	117.66	122.82
20	B	848	BCR	C20-C19-C18	3.18	135.08	126.36
20	b	848	BCR	C20-C19-C18	3.18	135.08	126.36
20	A	850	BCR	C37-C22-C21	-3.18	117.66	122.82
20	a	850	BCR	C37-C22-C21	-3.18	117.66	122.82
18	A	834	CLA	C4D-CHA-C1A	3.18	125.03	121.24
20	K	202	BCR	C33-C5-C6	3.18	127.95	124.48
18	b	819	CLA	C4D-CHA-C1A	3.18	125.03	121.24
20	F	301	BCR	C34-C9-C10	-3.18	117.67	122.82
20	f	301	BCR	C34-C9-C10	-3.18	117.67	122.82
18	A	832	CLA	C4D-CHA-C1A	3.17	125.03	121.24
18	a	832	CLA	C4D-CHA-C1A	3.17	125.03	121.24
20	B	846	BCR	C34-C9-C10	-3.17	117.68	122.82
20	F	301	BCR	C37-C22-C21	-3.17	117.68	122.82
20	f	301	BCR	C37-C22-C21	-3.17	117.68	122.82
20	a	847	BCR	C19-C18-C17	3.17	124.00	119.01
25	5a	317	LUT	C39-C29-C28	3.17	122.93	118.09
20	B	848	BCR	C34-C9-C10	-3.17	117.69	122.82
20	b	848	BCR	C34-C9-C10	-3.17	117.69	122.82
20	B	848	BCR	C37-C22-C21	-3.16	117.69	122.82
20	I	202	BCR	C34-C9-C10	-3.16	117.69	122.82
18	B	819	CLA	C4D-CHA-C1A	3.16	125.02	121.24
20	A	850	BCR	C30-C25-C26	-3.16	118.32	122.64
20	a	850	BCR	C30-C25-C26	-3.16	118.32	122.64
20	B	842	BCR	C24-C25-C26	3.16	128.83	121.56
20	B	851	BCR	C34-C9-C10	-3.15	117.71	122.82
20	b	851	BCR	C34-C9-C10	-3.15	117.71	122.82
18	B	827	CLA	C4D-CHA-C1A	3.15	125.01	121.24
18	b	827	CLA	C4D-CHA-C1A	3.15	125.01	121.24
20	b	846	BCR	C34-C9-C10	-3.15	117.71	122.82
20	B	845	BCR	C33-C5-C6	3.15	127.92	124.48
20	b	845	BCR	C33-C5-C6	3.15	127.92	124.48
25	6a	318	LUT	C19-C9-C10	-3.15	117.71	122.82
25	6b	318	LUT	C19-C9-C10	-3.15	117.71	122.82
20	A	847	BCR	C19-C18-C17	3.15	123.97	119.01
25	3a	317	LUT	C20-C13-C14	-3.15	117.71	122.82
25	3b	317	LUT	C20-C13-C14	-3.15	117.71	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3a	301	CHL	C4D-ND-C1D	3.15	107.61	105.22
20	m	101	BCR	C15-C16-C17	3.15	129.96	123.52
20	M	101	BCR	C15-C16-C17	3.14	129.95	123.52
20	i	202	BCR	C34-C9-C10	-3.14	117.72	122.82
29	3a	301	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
29	3b	301	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
20	b	842	BCR	C24-C25-C26	3.14	128.79	121.56
18	a	827	CLA	C4D-CHA-C1A	3.14	124.99	121.24
20	j	102	BCR	C19-C18-C17	3.14	123.95	119.01
20	B	844	BCR	C16-C15-C14	3.13	129.93	123.52
20	b	844	BCR	C16-C15-C14	3.13	129.93	123.52
18	A	824	CLA	CHA-C1A-NA	-3.13	119.30	126.39
18	a	824	CLA	CHA-C1A-NA	-3.13	119.30	126.39
25	6a	320	LUT	C39-C29-C30	-3.13	117.74	122.82
25	6b	320	LUT	C39-C29-C30	-3.13	117.74	122.82
18	L	301	CLA	C4D-CHA-C1A	3.13	124.98	121.24
18	l	301	CLA	C4D-CHA-C1A	3.13	124.98	121.24
25	6a	320	LUT	C39-C29-C28	3.13	122.87	118.09
18	B	808	CLA	C1-O2A-CGA	3.13	125.56	116.67
18	b	808	CLA	C1-O2A-CGA	3.13	125.56	116.67
18	A	827	CLA	C4D-CHA-C1A	3.13	124.97	121.24
25	5a	316	LUT	C19-C9-C8	3.13	122.86	118.09
25	5b	316	LUT	C19-C9-C8	3.13	122.86	118.09
20	B	848	BCR	C30-C25-C24	3.13	124.13	115.65
20	b	848	BCR	C30-C25-C24	3.13	124.13	115.65
29	3b	301	CHL	C4D-ND-C1D	3.12	107.59	105.22
18	B	826	CLA	C4D-CHA-C1A	3.12	124.97	121.24
18	b	826	CLA	C4D-CHA-C1A	3.12	124.97	121.24
25	3b	317	LUT	C1-C6-C5	-3.12	118.37	122.64
20	J	102	BCR	C19-C18-C17	3.12	123.92	119.01
18	B	814	CLA	C4D-CHA-C1A	3.12	124.96	121.24
18	b	814	CLA	C4D-CHA-C1A	3.12	124.96	121.24
18	A	824	CLA	C4A-NA-C1A	3.11	108.10	106.68
18	a	824	CLA	C4A-NA-C1A	3.11	108.10	106.68
20	A	848	BCR	C15-C16-C17	3.11	129.89	123.52
20	a	848	BCR	C15-C16-C17	3.11	129.89	123.52
20	A	848	BCR	C33-C5-C6	3.11	127.88	124.48
20	a	848	BCR	C33-C5-C6	3.11	127.88	124.48
25	5a	317	LUT	C39-C29-C30	-3.11	117.78	122.82
25	6b	320	LUT	C39-C29-C28	3.10	122.83	118.09
20	F	301	BCR	C33-C5-C6	3.10	127.87	124.48
20	f	301	BCR	C33-C5-C6	3.10	127.87	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6a	319	LUT	C39-C29-C30	-3.10	117.79	122.82
25	5b	317	LUT	C39-C29-C30	-3.10	117.79	122.82
25	2a	314	LUT	C7-C6-C5	3.10	128.69	121.56
25	2b	314	LUT	C7-C6-C5	3.10	128.69	121.56
25	6b	319	LUT	C39-C29-C30	-3.10	117.80	122.82
20	A	849	BCR	C12-C13-C14	3.10	123.88	119.01
20	a	849	BCR	C12-C13-C14	3.10	123.88	119.01
25	J	105	LUT	C11-C12-C13	3.09	134.85	126.36
25	j	105	LUT	C11-C12-C13	3.09	134.85	126.36
25	3a	317	LUT	C1-C6-C5	-3.09	118.41	122.64
29	2a	305	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
29	2b	305	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
18	B	829	CLA	CHD-C1D-ND	-3.09	120.46	124.80
18	2a	309	CLA	C4D-CHA-C1A	3.09	124.92	121.24
20	B	845	BCR	C37-C22-C21	-3.08	117.82	122.82
20	b	845	BCR	C37-C22-C21	-3.08	117.82	122.82
25	6a	319	LUT	C32-C33-C34	3.08	123.86	119.01
25	6b	319	LUT	C32-C33-C34	3.08	123.86	119.01
20	K	202	BCR	C24-C25-C26	3.08	128.64	121.56
20	k	202	BCR	C24-C25-C26	3.08	128.64	121.56
18	A	804	CLA	C4D-CHA-C1A	3.07	124.91	121.24
18	a	804	CLA	C4D-CHA-C1A	3.07	124.91	121.24
25	5b	317	LUT	C20-C13-C14	-3.07	117.84	122.82
25	5a	317	LUT	C20-C13-C14	-3.07	117.85	122.82
20	B	842	BCR	C37-C22-C21	-3.07	117.85	122.82
20	b	851	BCR	C1-C6-C5	-3.06	118.46	122.64
18	b	829	CLA	CHD-C1D-ND	-3.06	120.50	124.80
18	B	840	CLA	C4D-CHA-C1A	3.06	124.89	121.24
18	2b	309	CLA	C4D-CHA-C1A	3.06	124.89	121.24
18	A	823	CLA	CHD-C1D-ND	-3.06	120.50	124.80
18	a	823	CLA	CHD-C1D-ND	-3.06	120.50	124.80
20	B	844	BCR	C23-C22-C21	3.06	123.82	119.01
20	b	844	BCR	C23-C22-C21	3.06	123.82	119.01
25	3a	317	LUT	C39-C29-C30	-3.06	117.87	122.82
25	3b	317	LUT	C39-C29-C30	-3.06	117.87	122.82
18	A	833	CLA	C4D-CHA-C1A	3.06	124.89	121.24
18	a	833	CLA	C4D-CHA-C1A	3.06	124.89	121.24
20	b	842	BCR	C37-C22-C21	-3.05	117.87	122.82
20	I	202	BCR	C37-C22-C23	3.05	122.74	118.09
20	i	202	BCR	C37-C22-C23	3.05	122.74	118.09
18	A	808	CLA	C4D-CHA-C1A	3.05	124.88	121.24
18	a	808	CLA	C4D-CHA-C1A	3.05	124.88	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6b	319	LUT	C10-C11-C12	3.04	132.02	123.20
20	I	202	BCR	C38-C26-C25	3.04	127.80	124.48
20	i	202	BCR	C38-C26-C25	3.04	127.80	124.48
29	5b	314	CHL	C4D-CHA-CBD	-3.04	105.90	108.97
20	B	845	BCR	C30-C25-C26	-3.04	118.48	122.64
20	A	847	BCR	C1-C6-C5	-3.04	118.48	122.64
20	a	847	BCR	C1-C6-C5	-3.04	118.48	122.64
18	6a	311	CLA	C4D-CHA-C1A	3.04	124.87	121.24
18	6b	311	CLA	C4D-CHA-C1A	3.04	124.87	121.24
20	B	851	BCR	C1-C6-C5	-3.04	118.49	122.64
20	B	848	BCR	C24-C23-C22	3.03	130.72	126.23
20	b	848	BCR	C24-C23-C22	3.03	130.72	126.23
29	5a	314	CHL	C4D-CHA-CBD	-3.03	105.91	108.97
25	6a	319	LUT	C10-C11-C12	3.03	131.99	123.20
20	F	304	BCR	C33-C5-C6	3.03	127.79	124.48
20	f	304	BCR	C33-C5-C6	3.03	127.79	124.48
29	2a	305	CHL	C4D-ND-C1D	3.03	107.52	105.22
20	B	848	BCR	C30-C25-C26	-3.03	118.49	122.64
20	b	848	BCR	C30-C25-C26	-3.03	118.49	122.64
20	b	845	BCR	C30-C25-C26	-3.03	118.50	122.64
18	b	840	CLA	C4D-CHA-C1A	3.03	124.86	121.24
20	j	102	BCR	C35-C13-C14	-3.02	117.92	122.82
20	J	102	BCR	C35-C13-C14	-3.02	117.93	122.82
20	B	846	BCR	C34-C9-C8	3.02	122.69	118.09
29	2a	306	CHL	CHA-C1A-C2A	-3.02	126.23	133.31
29	2b	306	CHL	CHA-C1A-C2A	-3.02	126.23	133.31
29	2b	305	CHL	C4D-ND-C1D	3.01	107.50	105.22
20	b	846	BCR	C34-C9-C8	3.01	122.69	118.09
20	j	102	BCR	C12-C13-C14	3.01	123.74	119.01
18	5a	309	CLA	C4D-CHA-C1A	3.00	124.83	121.24
18	5b	309	CLA	C4D-CHA-C1A	3.00	124.83	121.24
18	A	813	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	a	813	CLA	CHD-C1D-ND	-3.00	120.58	124.80
18	b	822	CLA	C4D-CHA-C1A	3.00	124.83	121.24
25	6a	320	LUT	C18-C5-C6	3.00	127.76	124.48
25	6b	320	LUT	C18-C5-C6	3.00	127.76	124.48
18	3a	308	CLA	C4D-CHA-C1A	3.00	124.82	121.24
18	3b	308	CLA	C4D-CHA-C1A	3.00	124.82	121.24
18	a	841	CLA	CHA-C1A-NA	-3.00	119.60	126.39
18	A	836	CLA	CHA-C1A-NA	-3.00	119.60	126.39
18	a	836	CLA	CHA-C1A-NA	-3.00	119.60	126.39
18	A	841	CLA	CHA-C1A-NA	-2.99	119.61	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3a	316	LUT	C39-C29-C30	-2.99	117.97	122.82
25	3b	316	LUT	C39-C29-C30	-2.99	117.97	122.82
20	J	102	BCR	C12-C13-C14	2.99	123.71	119.01
18	B	822	CLA	C4D-CHA-C1A	2.99	124.81	121.24
25	5a	316	LUT	C39-C29-C30	-2.98	117.98	122.82
25	5b	316	LUT	C39-C29-C30	-2.98	117.98	122.82
29	5a	301	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
29	5b	301	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
18	A	828	CLA	CHA-C1A-NA	-2.98	119.64	126.39
18	a	828	CLA	CHA-C1A-NA	-2.98	119.64	126.39
18	B	803	CLA	C4D-CHA-C1A	2.98	124.80	121.24
18	b	803	CLA	C4D-CHA-C1A	2.98	124.80	121.24
20	I	202	BCR	C33-C5-C6	2.98	127.73	124.48
25	6a	318	LUT	C40-C33-C34	-2.98	118.00	122.82
20	A	847	BCR	C36-C18-C17	-2.97	118.00	122.82
20	a	847	BCR	C36-C18-C17	-2.97	118.00	122.82
29	6a	304	CHL	CHA-C1A-C2A	-2.97	126.33	133.31
25	6b	318	LUT	C40-C33-C34	-2.97	118.01	122.82
18	3a	312	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
18	3b	312	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
18	B	838	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
18	b	838	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
18	b	836	CLA	CHD-C1D-ND	-2.96	120.63	124.80
20	J	102	BCR	C36-C18-C17	-2.96	118.02	122.82
20	j	102	BCR	C36-C18-C17	-2.96	118.02	122.82
18	a	813	CLA	CAA-C2A-C1A	-2.96	102.26	111.97
29	5a	306	CHL	CHA-C1A-C2A	-2.96	126.36	133.31
29	5b	306	CHL	CHA-C1A-C2A	-2.96	126.36	133.31
29	6b	304	CHL	CHA-C1A-C2A	-2.96	126.36	133.31
18	A	813	CLA	CAA-C2A-C1A	-2.96	102.28	111.97
20	i	202	BCR	C33-C5-C6	2.96	127.71	124.48
29	2b	304	CHL	C4D-CHA-CBD	-2.95	105.99	108.97
20	A	849	BCR	C35-C13-C14	-2.95	118.04	122.82
20	a	849	BCR	C35-C13-C14	-2.95	118.04	122.82
29	2a	304	CHL	C4D-CHA-CBD	-2.95	106.00	108.97
18	B	836	CLA	CHD-C1D-ND	-2.94	120.66	124.80
20	L	304	BCR	C37-C22-C21	-2.94	118.06	122.82
20	l	304	BCR	C37-C22-C21	-2.94	118.06	122.82
29	3a	307	CHL	C4D-ND-C1D	2.93	107.45	105.22
20	A	851	BCR	C24-C25-C26	2.93	128.31	121.56
20	a	851	BCR	C24-C25-C26	2.93	128.31	121.56
20	I	202	BCR	C34-C9-C8	2.93	122.57	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	i	202	BCR	C34-C9-C8	2.93	122.57	118.09
18	A	832	CLA	CHA-C1A-NA	-2.93	119.75	126.39
18	a	832	CLA	CHA-C1A-NA	-2.93	119.75	126.39
18	a	829	CLA	C4D-CHA-C1A	2.93	124.74	121.24
18	b	823	CLA	CHA-C1A-NA	-2.93	119.76	126.39
18	3a	309	CLA	C4D-CHA-C1A	2.93	124.73	121.24
18	3b	309	CLA	C4D-CHA-C1A	2.93	124.73	121.24
29	5a	305	CHL	CHA-C1A-C2A	-2.93	126.44	133.31
29	5b	305	CHL	CHA-C1A-C2A	-2.93	126.44	133.31
18	a	841	CLA	C4D-CHA-C1A	2.93	124.73	121.24
18	A	819	CLA	C4D-CHA-C1A	2.92	124.73	121.24
18	a	819	CLA	C4D-CHA-C1A	2.92	124.73	121.24
29	2a	313	CHL	C4D-CHA-CBD	-2.92	106.02	108.97
29	2b	313	CHL	C4D-CHA-CBD	-2.92	106.02	108.97
18	2b	310	CLA	CHA-C1A-NA	-2.92	119.78	126.39
29	3b	307	CHL	CHA-C1A-C2A	-2.92	126.45	133.31
18	2a	310	CLA	CHA-C1A-NA	-2.92	119.79	126.39
18	B	823	CLA	CHA-C1A-NA	-2.92	119.79	126.39
20	A	849	BCR	C15-C16-C17	2.92	129.48	123.52
20	a	849	BCR	C15-C16-C17	2.92	129.48	123.52
18	A	829	CLA	C4D-CHA-C1A	2.91	124.72	121.24
18	L	301	CLA	CHA-C1A-NA	-2.91	119.79	126.39
18	l	301	CLA	CHA-C1A-NA	-2.91	119.79	126.39
29	3b	307	CHL	C4D-ND-C1D	2.91	107.43	105.22
20	B	846	BCR	C37-C22-C23	2.91	122.53	118.09
20	b	846	BCR	C37-C22-C23	2.91	122.53	118.09
29	5a	306	CHL	C4D-CHA-CBD	-2.91	106.04	108.97
29	5b	306	CHL	C4D-CHA-CBD	-2.91	106.04	108.97
25	5a	316	LUT	C19-C9-C10	-2.90	118.11	122.82
25	5b	316	LUT	C19-C9-C10	-2.90	118.11	122.82
29	3a	307	CHL	CHA-C1A-C2A	-2.90	126.49	133.31
18	B	805	CLA	C4D-CHA-C1A	2.90	124.71	121.24
18	b	805	CLA	C4D-CHA-C1A	2.90	124.71	121.24
18	A	841	CLA	C4D-CHA-C1A	2.90	124.70	121.24
29	3a	315	CHL	C4D-CHA-CBD	-2.90	106.04	108.97
29	3b	315	CHL	C4D-CHA-CBD	-2.90	106.04	108.97
29	5a	301	CHL	C4D-ND-C1D	2.90	107.42	105.22
29	5b	301	CHL	C4D-ND-C1D	2.90	107.42	105.22
18	B	837	CLA	CHD-C1D-ND	-2.90	120.73	124.80
18	b	835	CLA	CHA-C1A-NA	-2.89	119.84	126.39
18	B	835	CLA	CHA-C1A-NA	-2.89	119.84	126.39
25	3a	316	LUT	C19-C9-C10	-2.89	118.13	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3b	316	LUT	C19-C9-C10	-2.89	118.13	122.82
25	3a	316	LUT	C1-C6-C5	-2.89	118.69	122.64
25	3b	316	LUT	C1-C6-C5	-2.89	118.69	122.64
18	6b	312	CLA	C1-O2A-CGA	2.89	123.64	116.65
18	B	826	CLA	CHA-C1A-NA	-2.89	119.86	126.39
18	b	826	CLA	CHA-C1A-NA	-2.89	119.86	126.39
18	B	825	CLA	CHA-C1A-NA	-2.89	119.86	126.39
18	b	825	CLA	CHA-C1A-NA	-2.89	119.86	126.39
18	B	853	CLA	CHA-C1A-NA	-2.88	119.86	126.39
18	b	853	CLA	CHA-C1A-NA	-2.88	119.86	126.39
18	b	837	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	A	815	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	a	815	CLA	CHD-C1D-ND	-2.88	120.75	124.80
18	a	806	CLA	C4D-CHA-C1A	2.88	124.68	121.24
20	A	848	BCR	C34-C9-C8	2.88	122.48	118.09
18	6a	312	CLA	C1-O2A-CGA	2.87	123.61	116.65
18	6b	316	CLA	CHD-C1D-ND	-2.87	120.76	124.80
29	5b	301	CHL	CHA-C1A-C2A	-2.87	126.57	133.31
20	G	204	BCR	C19-C18-C17	2.87	123.52	119.01
20	g	204	BCR	C19-C18-C17	2.87	123.52	119.01
18	B	825	CLA	C4D-CHA-C1A	2.87	124.66	121.24
18	b	825	CLA	C4D-CHA-C1A	2.87	124.66	121.24
29	5a	301	CHL	CHA-C1A-C2A	-2.86	126.58	133.31
18	B	816	CLA	CHA-C1A-NA	-2.86	119.91	126.39
18	b	816	CLA	CHA-C1A-NA	-2.86	119.91	126.39
20	a	848	BCR	C34-C9-C8	2.86	122.46	118.09
18	A	806	CLA	C4D-CHA-C1A	2.86	124.66	121.24
20	b	851	BCR	C34-C9-C8	2.86	122.45	118.09
29	5a	305	CHL	C4D-ND-C1D	2.86	107.39	105.22
18	A	809	CLA	CHA-C1A-NA	-2.86	119.92	126.39
18	a	809	CLA	CHA-C1A-NA	-2.86	119.92	126.39
18	a	827	CLA	CHA-C1A-NA	-2.86	119.92	126.39
20	G	204	BCR	C36-C18-C17	-2.86	118.19	122.82
20	g	204	BCR	C36-C18-C17	-2.86	118.19	122.82
18	A	819	CLA	CHA-C1A-NA	-2.86	119.92	126.39
18	a	819	CLA	CHA-C1A-NA	-2.86	119.92	126.39
29	6a	309	CHL	C4D-CHA-CBD	-2.86	106.09	108.97
29	6b	309	CHL	C4D-CHA-CBD	-2.86	106.09	108.97
20	F	301	BCR	C24-C25-C26	2.85	128.13	121.56
20	f	301	BCR	C24-C25-C26	2.85	128.13	121.56
18	A	827	CLA	CHA-C1A-NA	-2.85	119.93	126.39
18	6a	316	CLA	CHD-C1D-ND	-2.85	120.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	839	CLA	CHA-C1A-NA	-2.85	119.93	126.39
18	b	839	CLA	CHA-C1A-NA	-2.85	119.93	126.39
29	5a	314	CHL	C4D-ND-C1D	2.85	107.38	105.22
29	5b	314	CHL	C4D-ND-C1D	2.85	107.38	105.22
18	A	838	CLA	CHA-C1A-NA	-2.85	119.94	126.39
18	a	838	CLA	CHA-C1A-NA	-2.85	119.94	126.39
18	a	804	CLA	CHD-C1D-ND	-2.85	120.80	124.80
20	B	844	BCR	C19-C18-C17	2.85	123.48	119.01
20	b	844	BCR	C19-C18-C17	2.85	123.48	119.01
29	5b	305	CHL	C4D-ND-C1D	2.84	107.38	105.22
29	5b	307	CHL	C4D-CHA-CBD	-2.84	106.10	108.97
20	B	851	BCR	C34-C9-C8	2.84	122.43	118.09
18	j	101	CLA	CHA-C1A-NA	-2.84	119.96	126.39
25	J	105	LUT	C18-C5-C6	2.84	127.58	124.48
25	j	105	LUT	C18-C5-C6	2.84	127.58	124.48
18	B	805	CLA	CHA-C1A-NA	-2.84	119.97	126.39
18	b	805	CLA	CHA-C1A-NA	-2.84	119.97	126.39
20	b	845	BCR	C35-C13-C14	-2.83	118.22	122.82
18	A	835	CLA	CHD-C1D-ND	-2.83	120.81	124.80
18	a	835	CLA	CHD-C1D-ND	-2.83	120.81	124.80
25	3b	316	LUT	C11-C10-C9	2.83	131.25	127.28
18	6a	312	CLA	C4D-CHA-C1A	2.83	124.62	121.24
18	6b	312	CLA	C4D-CHA-C1A	2.83	124.62	121.24
29	2b	313	CHL	C4D-ND-C1D	2.83	107.37	105.22
20	A	850	BCR	C37-C22-C23	2.83	122.41	118.09
18	l	303	CLA	CHA-C1A-NA	-2.83	119.98	126.39
20	j	102	BCR	C21-C20-C19	2.83	131.40	123.20
18	B	801	CLA	CHA-C1A-NA	-2.83	119.99	126.39
18	b	801	CLA	CHA-C1A-NA	-2.83	119.99	126.39
18	J	101	CLA	CHA-C1A-NA	-2.83	119.99	126.39
18	2a	310	CLA	C4A-NA-C1A	2.83	107.97	106.68
25	2a	315	LUT	C39-C29-C30	-2.83	118.24	122.82
25	2b	315	LUT	C39-C29-C30	-2.83	118.24	122.82
20	F	301	BCR	C34-C9-C8	2.83	122.41	118.09
20	f	301	BCR	C34-C9-C8	2.83	122.41	118.09
25	6a	319	LUT	C7-C6-C5	2.83	128.06	121.56
18	L	303	CLA	CHA-C1A-NA	-2.82	120.00	126.39
18	6a	310	CLA	CHA-C1A-NA	-2.82	120.00	126.39
18	6b	310	CLA	CHA-C1A-NA	-2.82	120.00	126.39
18	3a	306	CLA	CHA-C1A-NA	-2.82	120.00	126.39
18	3b	306	CLA	CHA-C1A-NA	-2.82	120.00	126.39
29	2a	313	CHL	C4C-CHD-C1D	2.82	126.17	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	824	CLA	C4D-CHA-C1A	2.82	124.61	121.24
18	2b	308	CLA	C4D-CHA-C1A	2.82	124.61	121.24
18	B	823	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
18	A	818	CLA	CHD-C1D-ND	-2.82	120.83	124.80
18	a	818	CLA	CHD-C1D-ND	-2.82	120.83	124.80
18	b	823	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
20	B	844	BCR	C36-C18-C17	-2.82	118.25	122.82
26	A	802	CL0	C1A-CHA-C4D	2.82	123.69	118.98
26	a	802	CL0	C1A-CHA-C4D	2.82	123.69	118.98
20	F	301	BCR	C37-C22-C23	2.82	122.40	118.09
20	f	301	BCR	C37-C22-C23	2.82	122.40	118.09
18	B	823	CLA	CHD-C1D-ND	-2.82	120.83	124.80
18	A	804	CLA	CHD-C1D-ND	-2.82	120.83	124.80
29	5a	314	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
29	5b	314	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
29	2a	304	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
18	B	834	CLA	CHA-C1A-NA	-2.82	120.01	126.39
18	b	834	CLA	CHA-C1A-NA	-2.82	120.01	126.39
18	b	824	CLA	C4D-CHA-C1A	2.82	124.60	121.24
25	6b	319	LUT	C7-C6-C5	2.82	128.04	121.56
25	3a	317	LUT	C35-C34-C33	2.81	131.22	127.28
25	3b	317	LUT	C35-C34-C33	2.81	131.22	127.28
29	2b	313	CHL	C4C-CHD-C1D	2.81	126.14	116.07
18	B	854	CLA	CHA-C1A-NA	-2.81	120.02	126.39
18	b	854	CLA	CHA-C1A-NA	-2.81	120.02	126.39
20	b	844	BCR	C36-C18-C17	-2.81	118.26	122.82
20	B	845	BCR	C35-C13-C14	-2.81	118.26	122.82
25	3a	316	LUT	C11-C10-C9	2.81	131.22	127.28
20	J	102	BCR	C21-C20-C19	2.81	131.34	123.20
18	6b	315	CLA	CHA-C1A-NA	-2.81	120.03	126.39
18	2b	310	CLA	C4A-NA-C1A	2.81	107.96	106.68
29	5a	307	CHL	C4D-CHA-CBD	-2.80	106.14	108.97
18	5a	311	CLA	CHA-C1A-NA	-2.80	120.04	126.39
18	5b	311	CLA	CHA-C1A-NA	-2.80	120.04	126.39
29	2b	304	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
20	a	850	BCR	C37-C22-C23	2.80	122.37	118.09
25	2b	315	LUT	C27-C28-C29	2.80	132.35	126.32
18	b	820	CLA	CHA-C1A-NA	-2.80	120.05	126.39
18	b	823	CLA	CHD-C1D-ND	-2.80	120.86	124.80
29	5a	306	CHL	C4D-ND-C1D	2.80	107.34	105.22
29	5b	306	CHL	C4D-ND-C1D	2.80	107.34	105.22
20	B	848	BCR	C34-C9-C8	2.80	122.36	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	848	BCR	C34-C9-C8	2.80	122.36	118.09
18	6a	315	CLA	CHA-C1A-NA	-2.80	120.05	126.39
18	B	814	CLA	CHA-C1A-NA	-2.80	120.05	126.39
18	b	814	CLA	CHA-C1A-NA	-2.80	120.05	126.39
18	A	814	CLA	CHD-C1D-ND	-2.80	120.87	124.80
18	a	814	CLA	CHD-C1D-ND	-2.80	120.87	124.80
18	3a	305	CLA	C1-O2A-CGA	2.80	125.03	116.07
29	2a	304	CHL	C4D-ND-C1D	2.80	107.34	105.22
29	2b	304	CHL	C4D-ND-C1D	2.80	107.34	105.22
18	A	822	CLA	CHA-C1A-NA	-2.80	120.06	126.39
18	a	822	CLA	CHA-C1A-NA	-2.80	120.06	126.39
18	2a	308	CLA	C4D-CHA-C1A	2.80	124.58	121.24
29	5a	305	CHL	C4D-CHA-CBD	-2.79	106.15	108.97
29	5b	305	CHL	C4D-CHA-CBD	-2.79	106.15	108.97
18	3a	313	CLA	CHA-C1A-NA	-2.79	120.06	126.39
18	5a	310	CLA	CHA-C1A-NA	-2.79	120.06	126.39
18	5b	310	CLA	CHA-C1A-NA	-2.79	120.06	126.39
25	2a	315	LUT	C27-C28-C29	2.79	132.33	126.32
18	A	823	CLA	CHA-C1A-NA	-2.79	120.07	126.39
18	a	823	CLA	CHA-C1A-NA	-2.79	120.07	126.39
20	K	202	BCR	C12-C13-C14	2.79	123.40	119.01
18	B	820	CLA	CHA-C1A-NA	-2.79	120.08	126.39
18	3b	305	CLA	C1-O2A-CGA	2.79	125.00	116.07
20	K	202	BCR	C35-C13-C14	-2.79	118.30	122.82
18	5a	308	CLA	CHD-C1D-ND	-2.79	120.88	124.80
18	5b	308	CLA	CHD-C1D-ND	-2.79	120.88	124.80
29	6a	309	CHL	C4D-ND-C1D	2.79	107.33	105.22
29	6b	309	CHL	C4D-ND-C1D	2.79	107.33	105.22
18	B	819	CLA	CHA-C1A-NA	-2.78	120.08	126.39
18	b	822	CLA	CHD-C1D-ND	-2.78	120.88	124.80
18	B	808	CLA	CHA-C1A-NA	-2.78	120.09	126.39
18	b	808	CLA	CHA-C1A-NA	-2.78	120.09	126.39
18	A	822	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	a	822	CLA	CHD-C1D-ND	-2.78	120.89	124.80
29	2a	313	CHL	CHA-C1A-C2A	-2.78	126.77	133.31
29	2b	313	CHL	CHA-C1A-C2A	-2.78	126.77	133.31
18	2a	312	CLA	CHD-C1D-ND	-2.78	120.89	124.80
18	2b	312	CLA	CHD-C1D-ND	-2.78	120.89	124.80
29	2a	313	CHL	C4D-ND-C1D	2.78	107.33	105.22
18	A	812	CLA	CHA-C1A-NA	-2.78	120.10	126.39
18	a	812	CLA	CHA-C1A-NA	-2.78	120.10	126.39
29	6a	309	CHL	C4C-CHD-C1D	2.78	126.00	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6b	309	CHL	C4C-CHD-C1D	2.78	126.00	116.07
18	b	819	CLA	CHA-C1A-NA	-2.78	120.11	126.39
18	6b	308	CLA	CHA-C1A-NA	-2.78	120.11	126.39
29	6a	304	CHL	C4D-CHA-CBD	-2.78	106.17	108.97
18	B	852	CLA	CHA-C1A-NA	-2.77	120.11	126.39
18	b	852	CLA	CHA-C1A-NA	-2.77	120.11	126.39
18	3a	311	CLA	CHA-C1A-NA	-2.77	120.11	126.39
18	3b	311	CLA	CHA-C1A-NA	-2.77	120.11	126.39
18	6a	305	CLA	CHD-C1D-ND	-2.77	120.90	124.80
18	a	806	CLA	CHA-C1A-NA	-2.77	120.11	126.39
20	B	846	BCR	C36-C18-C17	-2.77	118.32	122.82
20	G	204	BCR	C35-C13-C14	-2.77	118.33	122.82
20	g	204	BCR	C35-C13-C14	-2.77	118.33	122.82
18	B	802	CLA	C4D-CHA-C1A	2.77	124.55	121.24
18	b	802	CLA	C4D-CHA-C1A	2.77	124.55	121.24
18	3a	303	CLA	CHA-C1A-NA	-2.77	120.12	126.39
18	3b	303	CLA	CHA-C1A-NA	-2.77	120.12	126.39
18	3b	313	CLA	CHA-C1A-NA	-2.77	120.12	126.39
20	B	848	BCR	C2-C1-C6	2.77	114.46	110.44
20	B	851	BCR	C35-C13-C14	-2.77	118.33	122.82
20	b	851	BCR	C35-C13-C14	-2.77	118.33	122.82
29	5a	314	CHL	C4C-CHD-C1D	2.77	125.97	116.07
18	B	802	CLA	CHA-C1A-NA	-2.77	120.12	126.39
18	b	802	CLA	CHA-C1A-NA	-2.77	120.12	126.39
18	B	830	CLA	CHA-C1A-NA	-2.76	120.13	126.39
18	b	830	CLA	CHA-C1A-NA	-2.76	120.13	126.39
18	A	806	CLA	CHA-C1A-NA	-2.76	120.13	126.39
18	B	815	CLA	CHA-C1A-NA	-2.76	120.13	126.39
18	b	815	CLA	CHA-C1A-NA	-2.76	120.13	126.39
18	B	811	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	A	815	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	a	815	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	b	811	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	f	302	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	A	820	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	a	820	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	6a	308	CLA	CHA-C1A-NA	-2.76	120.14	126.39
18	5b	304	CLA	CHA-C1A-NA	-2.76	120.14	126.39
29	5b	314	CHL	C4C-CHD-C1D	2.76	125.94	116.07
29	6a	304	CHL	C4C-CHD-C1D	2.76	125.94	116.07
29	6b	304	CHL	C4C-CHD-C1D	2.76	125.94	116.07
18	B	831	CLA	CHA-C1A-NA	-2.76	120.15	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	831	CLA	CHA-C1A-NA	-2.76	120.15	126.39
20	G	201	BCR	C24-C25-C26	2.76	127.91	121.56
20	g	201	BCR	C24-C25-C26	2.76	127.91	121.56
18	B	828	CLA	C4D-CHA-C1A	2.76	124.53	121.24
18	b	828	CLA	C4D-CHA-C1A	2.76	124.53	121.24
18	B	822	CLA	CHD-C1D-ND	-2.76	120.92	124.80
18	F	302	CLA	CHA-C1A-NA	-2.76	120.15	126.39
18	A	816	CLA	CHD-C1D-ND	-2.76	120.92	124.80
18	a	816	CLA	CHD-C1D-ND	-2.76	120.92	124.80
29	6b	304	CHL	C4D-CHA-CBD	-2.76	106.19	108.97
18	3a	304	CLA	CHA-C1A-NA	-2.76	120.15	126.39
18	3b	304	CLA	CHA-C1A-NA	-2.76	120.15	126.39
18	2a	311	CLA	CHA-C1A-NA	-2.75	120.15	126.39
18	2b	311	CLA	CHA-C1A-NA	-2.75	120.15	126.39
20	B	846	BCR	C19-C18-C17	2.75	123.34	119.01
28	A	852	LMU	O1B-C4'-C3'	-2.75	100.24	107.23
28	a	852	LMU	O1B-C4'-C3'	-2.75	100.24	107.23
20	L	304	BCR	C36-C18-C17	-2.75	118.36	122.82
18	B	818	CLA	CHA-C1A-NA	-2.75	120.16	126.39
18	b	818	CLA	CHA-C1A-NA	-2.75	120.16	126.39
18	A	831	CLA	CHA-C1A-NA	-2.75	120.17	126.39
18	a	831	CLA	CHA-C1A-NA	-2.75	120.17	126.39
20	b	848	BCR	C2-C1-C6	2.75	114.43	110.44
18	6a	307	CLA	CHA-C1A-NA	-2.75	120.17	126.39
18	5a	304	CLA	CHA-C1A-NA	-2.75	120.17	126.39
18	3a	309	CLA	CHD-C1D-ND	-2.75	120.94	124.80
18	3b	309	CLA	CHD-C1D-ND	-2.75	120.94	124.80
20	k	202	BCR	C35-C13-C14	-2.74	118.37	122.82
18	A	828	CLA	C4D-CHA-C1A	2.74	124.52	121.24
18	6a	313	CLA	CHA-C1A-NA	-2.74	120.18	126.39
18	6b	313	CLA	CHA-C1A-NA	-2.74	120.18	126.39
20	k	202	BCR	C12-C13-C14	2.74	123.32	119.01
18	6b	307	CLA	CHA-C1A-NA	-2.74	120.19	126.39
18	6b	305	CLA	CHD-C1D-ND	-2.74	120.95	124.80
20	m	101	BCR	C12-C13-C14	2.74	123.32	119.01
20	G	204	BCR	C24-C25-C26	2.74	127.87	121.56
20	g	204	BCR	C24-C25-C26	2.74	127.87	121.56
20	G	201	BCR	C16-C15-C14	2.74	129.12	123.52
20	g	201	BCR	C16-C15-C14	2.74	129.12	123.52
29	5a	307	CHL	C1C-CHC-C4B	2.74	125.86	116.07
29	5b	307	CHL	C1C-CHC-C4B	2.74	125.86	116.07
20	b	846	BCR	C36-C18-C17	-2.74	118.38	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	m	101	BCR	C35-C13-C14	-2.73	118.39	122.82
29	2a	304	CHL	C4C-CHD-C1D	2.73	125.85	116.07
29	2b	304	CHL	C4C-CHD-C1D	2.73	125.85	116.07
18	a	817	CLA	CHA-C1A-NA	-2.73	120.20	126.39
18	a	828	CLA	CAC-C3C-C4C	2.73	128.34	124.79
18	B	832	CLA	CHD-C1D-ND	-2.73	120.96	124.80
18	A	840	CLA	CHA-C1A-NA	-2.73	120.21	126.39
18	a	840	CLA	CHA-C1A-NA	-2.73	120.21	126.39
18	a	828	CLA	C4D-CHA-C1A	2.73	124.50	121.24
18	B	813	CLA	CHA-C1A-NA	-2.73	120.21	126.39
18	b	813	CLA	CHA-C1A-NA	-2.73	120.21	126.39
18	F	305	CLA	CHA-C1A-NA	-2.73	120.21	126.39
18	f	305	CLA	CHA-C1A-NA	-2.73	120.21	126.39
20	l	304	BCR	C36-C18-C17	-2.73	118.39	122.82
20	B	842	BCR	C37-C22-C23	2.73	122.26	118.09
20	b	842	BCR	C37-C22-C23	2.73	122.26	118.09
20	a	849	BCR	C19-C18-C17	2.73	123.30	119.01
18	A	808	CLA	CHD-C1D-ND	-2.73	120.97	124.80
18	a	808	CLA	CHD-C1D-ND	-2.73	120.97	124.80
20	L	304	BCR	C19-C18-C17	2.73	123.30	119.01
18	A	817	CLA	CHA-C1A-NA	-2.73	120.22	126.39
20	F	301	BCR	C29-C30-C25	2.73	114.40	110.44
18	b	810	CLA	CHA-C1A-NA	-2.73	120.22	126.39
20	B	848	BCR	C7-C8-C9	2.72	130.27	126.23
20	b	848	BCR	C7-C8-C9	2.72	130.27	126.23
18	6a	312	CLA	CHA-C1A-NA	-2.72	120.22	126.39
18	6b	312	CLA	CHA-C1A-NA	-2.72	120.22	126.39
18	B	837	CLA	CHA-C1A-NA	-2.72	120.22	126.39
18	a	816	CLA	CHA-C1A-NA	-2.72	120.23	126.39
18	2b	303	CLA	CHA-C1A-NA	-2.72	120.23	126.39
18	B	810	CLA	CHA-C1A-NA	-2.72	120.23	126.39
18	A	807	CLA	CHA-C1A-NA	-2.72	120.23	126.39
18	a	807	CLA	CHA-C1A-NA	-2.72	120.23	126.39
20	M	101	BCR	C12-C13-C14	2.72	123.29	119.01
20	b	846	BCR	C19-C18-C17	2.72	123.29	119.01
18	a	810	CLA	C4D-CHA-C1A	2.72	124.49	121.24
18	b	837	CLA	CHA-C1A-NA	-2.72	120.24	126.39
18	2a	303	CLA	CHA-C1A-NA	-2.72	120.24	126.39
20	f	301	BCR	C29-C30-C25	2.72	114.39	110.44
20	A	849	BCR	C19-C18-C17	2.72	123.28	119.01
18	B	812	CLA	CHA-C1A-NA	-2.72	120.24	126.39
18	b	812	CLA	CHA-C1A-NA	-2.72	120.24	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	l	302	CLA	CHA-C1A-NA	-2.72	120.24	126.39
20	M	101	BCR	C35-C13-C14	-2.72	118.41	122.82
18	f	303	CLA	CHA-C1A-NA	-2.72	120.24	126.39
25	6a	320	LUT	C20-C13-C14	-2.72	118.42	122.82
29	5a	305	CHL	C4C-CHD-C1D	2.72	125.78	116.07
29	5b	305	CHL	C4C-CHD-C1D	2.72	125.78	116.07
18	B	827	CLA	CHA-C1A-NA	-2.71	120.24	126.39
18	b	827	CLA	CHA-C1A-NA	-2.71	120.24	126.39
18	A	805	CLA	CHD-C1D-ND	-2.71	120.98	124.80
18	a	805	CLA	CHD-C1D-ND	-2.71	120.98	124.80
18	A	816	CLA	CHA-C1A-NA	-2.71	120.25	126.39
18	5b	303	CLA	CHA-C1A-NA	-2.71	120.25	126.39
18	F	303	CLA	CHA-C1A-NA	-2.71	120.25	126.39
18	a	834	CLA	CHA-C1A-NA	-2.71	120.25	126.39
18	b	832	CLA	CHD-C1D-ND	-2.71	120.99	124.80
18	a	803	CLA	CHD-C1D-ND	-2.71	120.99	124.80
18	A	821	CLA	CHA-C1A-NA	-2.71	120.25	126.39
25	6b	320	LUT	C20-C13-C14	-2.71	118.43	122.82
29	3a	307	CHL	C4C-CHD-C1D	2.71	125.76	116.07
29	3b	307	CHL	C4C-CHD-C1D	2.71	125.76	116.07
20	l	304	BCR	C19-C18-C17	2.71	123.27	119.01
18	A	810	CLA	C4D-CHA-C1A	2.71	124.47	121.24
18	A	828	CLA	CAC-C3C-C4C	2.71	128.31	124.79
18	a	826	CLA	CHA-C1A-NA	-2.71	120.26	126.39
18	A	853	CLA	CHD-C1D-ND	-2.71	121.00	124.80
18	a	853	CLA	CHD-C1D-ND	-2.71	121.00	124.80
18	b	821	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	B	840	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	b	840	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	2a	301	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	2b	301	CLA	CHA-C1A-NA	-2.70	120.27	126.39
20	A	848	BCR	C36-C18-C17	-2.70	118.44	122.82
20	a	848	BCR	C36-C18-C17	-2.70	118.44	122.82
18	G	202	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	g	202	CLA	CHA-C1A-NA	-2.70	120.27	126.39
18	B	828	CLA	CHD-C1D-ND	-2.70	121.00	124.80
18	B	803	CLA	CHA-C1A-NA	-2.70	120.28	126.39
18	b	803	CLA	CHA-C1A-NA	-2.70	120.28	126.39
18	5a	303	CLA	CHA-C1A-NA	-2.70	120.28	126.39
18	6b	311	CLA	CHA-C1A-NA	-2.70	120.28	126.39
18	L	302	CLA	CHA-C1A-NA	-2.70	120.28	126.39
20	G	201	BCR	C37-C22-C23	2.70	122.21	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	g	201	BCR	C37-C22-C23	2.70	122.21	118.09
18	a	821	CLA	CHA-C1A-NA	-2.70	120.28	126.39
20	g	201	BCR	C35-C13-C14	-2.70	118.45	122.82
18	b	828	CLA	CHD-C1D-ND	-2.70	121.01	124.80
18	A	842	CLA	CHA-C1A-NA	-2.70	120.29	126.39
18	a	842	CLA	CHA-C1A-NA	-2.70	120.29	126.39
29	3a	301	CHL	C4C-CHD-C1D	2.70	125.71	116.07
29	3b	301	CHL	C4C-CHD-C1D	2.70	125.71	116.07
18	A	826	CLA	CHA-C1A-NA	-2.69	120.29	126.39
18	2a	312	CLA	CHA-C1A-NA	-2.69	120.29	126.39
18	2b	312	CLA	CHA-C1A-NA	-2.69	120.29	126.39
18	A	834	CLA	CHA-C1A-NA	-2.69	120.29	126.39
25	6a	320	LUT	C12-C13-C14	2.69	123.24	119.01
25	6b	320	LUT	C12-C13-C14	2.69	123.24	119.01
18	6a	311	CLA	CHA-C1A-NA	-2.69	120.30	126.39
18	6a	314	CLA	CHA-C1A-NA	-2.69	120.30	126.39
18	6b	314	CLA	CHA-C1A-NA	-2.69	120.30	126.39
18	B	804	CLA	CHA-C1A-NA	-2.69	120.30	126.39
18	B	821	CLA	CHA-C1A-NA	-2.69	120.30	126.39
18	b	804	CLA	CHA-C1A-NA	-2.69	120.30	126.39
20	J	102	BCR	C2-C1-C6	2.69	114.34	110.44
20	j	102	BCR	C2-C1-C6	2.69	114.34	110.44
25	2a	315	LUT	C7-C6-C5	2.69	127.75	121.56
20	G	201	BCR	C35-C13-C14	-2.69	118.46	122.82
18	a	853	CLA	CHA-C1A-NA	-2.69	120.31	126.39
18	5a	304	CLA	CHD-C1D-ND	-2.69	121.02	124.80
18	5b	304	CLA	CHD-C1D-ND	-2.69	121.02	124.80
25	2b	315	LUT	C7-C6-C5	2.69	127.74	121.56
29	5a	314	CHL	C1C-C2C-CMC	2.69	131.64	126.80
29	5b	314	CHL	C1C-C2C-CMC	2.69	131.64	126.80
25	3a	317	LUT	C31-C30-C29	2.68	131.04	127.28
25	3b	317	LUT	C31-C30-C29	2.68	131.04	127.28
18	a	830	CLA	CHA-C1A-NA	-2.68	120.32	126.39
18	A	804	CLA	C3B-C4B-NB	-2.68	108.14	110.53
18	a	804	CLA	C3B-C4B-NB	-2.68	108.14	110.53
20	J	102	BCR	C24-C25-C26	2.68	127.73	121.56
20	j	102	BCR	C24-C25-C26	2.68	127.73	121.56
18	3a	312	CLA	CHA-C1A-NA	-2.68	120.32	126.39
18	3b	312	CLA	CHA-C1A-NA	-2.68	120.32	126.39
18	5a	312	CLA	CHA-C1A-NA	-2.68	120.32	126.39
20	B	842	BCR	C35-C13-C14	-2.68	118.47	122.82
20	b	842	BCR	C35-C13-C14	-2.68	118.47	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5b	312	CLA	CHA-C1A-NA	-2.68	120.33	126.39
18	A	824	CLA	C4D-CHA-C1A	2.68	124.44	121.24
18	a	824	CLA	C4D-CHA-C1A	2.68	124.44	121.24
18	2a	302	CLA	CHD-C1D-ND	-2.68	121.03	124.80
18	2b	302	CLA	CHD-C1D-ND	-2.68	121.03	124.80
18	A	853	CLA	CHA-C1A-NA	-2.68	120.33	126.39
20	A	849	BCR	C36-C18-C17	-2.68	118.48	122.82
20	A	850	BCR	C29-C30-C25	2.68	114.33	110.44
20	a	850	BCR	C29-C30-C25	2.68	114.33	110.44
18	L	301	CLA	C4A-NA-C1A	2.67	107.90	106.68
18	l	301	CLA	C4A-NA-C1A	2.67	107.90	106.68
29	2a	305	CHL	C4C-CHD-C1D	2.67	125.64	116.07
29	2b	305	CHL	C4C-CHD-C1D	2.67	125.64	116.07
18	B	824	CLA	CHD-C1D-ND	-2.67	121.04	124.80
18	b	824	CLA	CHD-C1D-ND	-2.67	121.04	124.80
25	6a	320	LUT	C40-C33-C34	-2.67	118.48	122.82
25	6b	320	LUT	C40-C33-C34	-2.67	118.48	122.82
19	A	843	PQN	C11-C3-C4	-2.67	115.76	118.58
19	a	843	PQN	C11-C3-C4	-2.67	115.76	118.58
18	6a	317	CLA	CHA-C1A-NA	-2.67	120.34	126.39
18	6b	317	CLA	CHA-C1A-NA	-2.67	120.34	126.39
20	k	202	BCR	C36-C18-C17	-2.67	118.49	122.82
18	b	828	CLA	CHA-C1A-NA	-2.67	120.34	126.39
18	3a	310	CLA	CHD-C1D-ND	-2.67	121.05	124.80
18	3b	310	CLA	CHD-C1D-ND	-2.67	121.05	124.80
18	A	830	CLA	CHA-C1A-NA	-2.67	120.34	126.39
18	A	803	CLA	CHD-C1D-ND	-2.67	121.05	124.80
20	B	851	BCR	C36-C18-C17	-2.67	118.50	122.82
20	b	851	BCR	C36-C18-C17	-2.67	118.50	122.82
20	L	304	BCR	C7-C6-C5	2.66	127.69	121.56
20	K	202	BCR	C36-C18-C17	-2.66	118.50	122.82
20	B	842	BCR	C2-C1-C6	2.66	114.30	110.44
20	b	842	BCR	C2-C1-C6	2.66	114.30	110.44
18	B	833	CLA	CHA-C1A-NA	-2.66	120.37	126.39
18	b	833	CLA	CHA-C1A-NA	-2.66	120.37	126.39
20	a	849	BCR	C36-C18-C17	-2.66	118.51	122.82
29	2a	305	CHL	CHA-C1A-C2A	-2.66	127.06	133.31
29	2b	305	CHL	CHA-C1A-C2A	-2.66	127.06	133.31
20	A	850	BCR	C35-C13-C14	-2.66	118.51	122.82
18	B	815	CLA	CHD-C1D-ND	-2.66	121.06	124.80
18	b	815	CLA	CHD-C1D-ND	-2.66	121.06	124.80
18	A	810	CLA	CHA-C1A-NA	-2.66	120.37	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3a	317	LUT	C18-C5-C6	2.66	127.38	124.48
25	3b	317	LUT	C18-C5-C6	2.66	127.38	124.48
20	l	304	BCR	C7-C6-C5	2.66	127.67	121.56
18	2a	309	CLA	CHA-C1A-NA	-2.66	120.38	126.39
18	5a	302	CLA	CHA-C1A-NA	-2.66	120.38	126.39
18	5b	302	CLA	CHA-C1A-NA	-2.66	120.38	126.39
18	3b	309	CLA	CHA-C1A-NA	-2.65	120.38	126.39
20	F	301	BCR	C7-C8-C9	2.65	130.16	126.23
20	f	301	BCR	C7-C8-C9	2.65	130.16	126.23
18	k	201	CLA	CHD-C1D-ND	-2.65	121.07	124.80
18	B	828	CLA	CHA-C1A-NA	-2.65	120.38	126.39
18	5a	313	CLA	CHA-C1A-NA	-2.65	120.38	126.39
29	3b	315	CHL	C4D-ND-C1D	2.65	107.23	105.22
18	a	810	CLA	CHA-C1A-NA	-2.65	120.39	126.39
29	5a	307	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
20	B	844	BCR	C35-C13-C14	-2.65	118.52	122.82
20	b	844	BCR	C35-C13-C14	-2.65	118.52	122.82
18	3a	308	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	3b	308	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	a	837	CLA	CHA-C1A-NA	-2.65	120.39	126.39
20	B	843	BCR	C35-C13-C14	-2.65	118.52	122.82
20	b	843	BCR	C35-C13-C14	-2.65	118.52	122.82
18	B	817	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	b	817	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	3a	305	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	3b	305	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	6a	305	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	6b	305	CLA	CHA-C1A-NA	-2.65	120.39	126.39
18	2a	307	CLA	CHA-C1A-NA	-2.65	120.40	126.39
18	3a	309	CLA	CHA-C1A-NA	-2.65	120.40	126.39
18	2b	307	CLA	CHA-C1A-NA	-2.65	120.40	126.39
20	f	301	BCR	C36-C18-C17	-2.65	118.53	122.82
20	B	851	BCR	C12-C13-C14	2.65	123.17	119.01
20	b	851	BCR	C12-C13-C14	2.65	123.17	119.01
29	3a	301	CHL	CHA-C1A-C2A	-2.65	127.09	133.31
29	3b	301	CHL	CHA-C1A-C2A	-2.65	127.09	133.31
18	5b	313	CLA	CHA-C1A-NA	-2.64	120.40	126.39
18	3a	302	CLA	CHA-C1A-NA	-2.64	120.41	126.39
18	K	201	CLA	CHD-C1D-ND	-2.64	121.08	124.80
18	2b	309	CLA	CHA-C1A-NA	-2.64	120.41	126.39
20	F	301	BCR	C36-C18-C17	-2.64	118.54	122.82
29	3a	315	CHL	C4D-ND-C1D	2.64	107.22	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6a	319	LUT	C20-C13-C14	-2.64	118.54	122.82
25	6b	319	LUT	C20-C13-C14	-2.64	118.54	122.82
18	3a	304	CLA	CHD-C1D-ND	-2.64	121.09	124.80
18	3b	304	CLA	CHD-C1D-ND	-2.64	121.09	124.80
29	5b	307	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
18	3b	312	CLA	CHD-C1D-ND	-2.64	121.09	124.80
18	3b	302	CLA	CHA-C1A-NA	-2.64	120.42	126.39
18	A	801	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	a	801	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	A	837	CLA	CHA-C1A-NA	-2.63	120.43	126.39
18	5a	312	CLA	CHD-C1D-ND	-2.63	121.10	124.80
18	5b	312	CLA	CHD-C1D-ND	-2.63	121.10	124.80
20	g	201	BCR	C7-C6-C5	2.63	127.62	121.56
18	G	203	CLA	CHA-C1A-NA	-2.63	120.43	126.39
20	G	201	BCR	C36-C18-C17	-2.63	118.55	122.82
20	g	201	BCR	C36-C18-C17	-2.63	118.55	122.82
20	G	201	BCR	C29-C30-C25	2.63	114.26	110.44
20	g	201	BCR	C29-C30-C25	2.63	114.26	110.44
18	g	203	CLA	CHA-C1A-NA	-2.63	120.43	126.39
18	A	839	CLA	CHA-C1A-NA	-2.63	120.43	126.39
18	B	832	CLA	CHA-C1A-NA	-2.63	120.44	126.39
18	b	832	CLA	CHA-C1A-NA	-2.63	120.44	126.39
20	a	851	BCR	C37-C22-C23	2.63	122.10	118.09
18	6b	312	CLA	CHD-C1D-ND	-2.63	121.10	124.80
29	2a	306	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
29	2b	306	CHL	C4D-CHA-CBD	-2.63	106.32	108.97
25	5a	316	LUT	C31-C30-C29	2.63	130.96	127.28
20	a	848	BCR	C7-C8-C9	2.63	130.12	126.23
20	A	851	BCR	C37-C22-C23	2.63	122.10	118.09
18	B	806	CLA	CHA-C1A-NA	-2.63	120.44	126.39
18	b	806	CLA	CHA-C1A-NA	-2.63	120.44	126.39
20	I	202	BCR	C36-C18-C17	-2.63	118.56	122.82
20	a	850	BCR	C35-C13-C14	-2.63	118.56	122.82
18	3a	310	CLA	CHA-C1A-NA	-2.62	120.45	126.39
18	2a	308	CLA	CHA-C1A-NA	-2.62	120.45	126.39
18	2b	308	CLA	CHA-C1A-NA	-2.62	120.45	126.39
29	5a	306	CHL	C4C-CHD-C1D	2.62	125.44	116.07
29	5b	306	CHL	C4C-CHD-C1D	2.62	125.44	116.07
18	B	816	CLA	CAA-C2A-C1A	2.62	120.56	111.97
20	G	201	BCR	C7-C6-C5	2.62	127.59	121.56
18	B	817	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	b	817	CLA	CHD-C1D-ND	-2.62	121.12	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	801	CLA	CHA-C1A-NA	-2.62	120.46	126.39
18	B	818	CLA	C3B-C4B-NB	-2.62	108.19	110.53
18	b	818	CLA	C3B-C4B-NB	-2.62	108.19	110.53
18	5a	315	CLA	CHA-C1A-NA	-2.62	120.46	126.39
18	a	839	CLA	CHA-C1A-NA	-2.62	120.46	126.39
18	5b	315	CLA	CHA-C1A-NA	-2.62	120.46	126.39
18	B	833	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	b	806	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	b	833	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	A	805	CLA	CHA-C1A-NA	-2.62	120.47	126.39
18	a	805	CLA	CHA-C1A-NA	-2.62	120.47	126.39
18	3a	312	CLA	CHD-C1D-ND	-2.62	121.12	124.80
18	a	818	CLA	CHA-C1A-NA	-2.62	120.47	126.39
29	3a	315	CHL	C1C-C2C-CMC	2.61	131.51	126.80
29	3b	315	CHL	C1C-C2C-CMC	2.61	131.51	126.80
20	g	201	BCR	C12-C13-C14	2.61	123.12	119.01
20	A	848	BCR	C7-C8-C9	2.61	130.10	126.23
18	3b	310	CLA	CHA-C1A-NA	-2.61	120.47	126.39
18	A	818	CLA	CHA-C1A-NA	-2.61	120.48	126.39
18	B	831	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	b	831	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	3a	314	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	3b	314	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	A	811	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	a	811	CLA	CHD-C1D-ND	-2.61	121.13	124.80
18	6a	312	CLA	CHD-C1D-ND	-2.61	121.13	124.80
20	B	844	BCR	C29-C30-C25	2.61	114.23	110.44
18	b	816	CLA	CAA-C2A-C1A	2.61	120.52	111.97
20	M	101	BCR	C24-C25-C26	2.61	127.56	121.56
20	m	101	BCR	C24-C25-C26	2.61	127.56	121.56
25	5b	316	LUT	C31-C30-C29	2.61	130.93	127.28
18	A	830	CLA	CHD-C1D-ND	-2.61	121.14	124.80
18	a	830	CLA	CHD-C1D-ND	-2.61	121.14	124.80
18	K	201	CLA	CHA-C1A-NA	-2.61	120.49	126.39
20	i	202	BCR	C36-C18-C17	-2.60	118.60	122.82
18	3a	314	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	3b	314	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	A	801	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	k	201	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	6b	306	CLA	CHD-C1D-ND	-2.60	121.14	124.80
20	F	304	BCR	C35-C13-C14	-2.60	118.60	122.82
20	f	304	BCR	C35-C13-C14	-2.60	118.60	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	840	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
18	b	840	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
20	a	848	BCR	C19-C18-C17	2.60	123.10	119.01
18	B	824	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	5a	309	CLA	CHA-C1A-NA	-2.60	120.50	126.39
18	5b	309	CLA	CHA-C1A-NA	-2.60	120.50	126.39
20	b	846	BCR	C24-C25-C26	2.60	127.54	121.56
20	A	850	BCR	C36-C18-C17	-2.60	118.61	122.82
20	a	850	BCR	C36-C18-C17	-2.60	118.61	122.82
18	b	824	CLA	CHA-C1A-NA	-2.60	120.51	126.39
20	B	846	BCR	C24-C25-C26	2.60	127.54	121.56
20	A	848	BCR	C19-C18-C17	2.60	123.09	119.01
18	F	303	CLA	CHD-C1D-ND	-2.60	121.15	124.80
18	f	303	CLA	CHD-C1D-ND	-2.60	121.15	124.80
18	B	854	CLA	CAA-CBA-CGA	2.59	120.58	113.21
18	b	854	CLA	CAA-CBA-CGA	2.59	120.58	113.21
18	B	806	CLA	CHD-C1D-ND	-2.59	121.15	124.80
18	2a	302	CLA	CHA-C1A-NA	-2.59	120.52	126.39
18	2b	302	CLA	CHA-C1A-NA	-2.59	120.52	126.39
18	B	829	CLA	CHA-C1A-NA	-2.59	120.53	126.39
20	G	201	BCR	C12-C13-C14	2.59	123.08	119.01
20	G	204	BCR	C12-C13-C14	2.59	123.08	119.01
20	g	204	BCR	C12-C13-C14	2.59	123.08	119.01
18	A	825	CLA	CHA-C1A-NA	-2.59	120.53	126.39
18	a	825	CLA	CHA-C1A-NA	-2.59	120.53	126.39
18	A	803	CLA	CHA-C1A-NA	-2.59	120.53	126.39
20	A	848	BCR	C35-C13-C14	-2.59	118.63	122.82
20	a	848	BCR	C35-C13-C14	-2.59	118.63	122.82
29	5a	301	CHL	C4C-CHD-C1D	2.59	125.32	116.07
18	F	305	CLA	O2D-CGD-CBD	2.59	115.75	111.23
18	f	305	CLA	O2D-CGD-CBD	2.59	115.75	111.23
20	A	850	BCR	C34-C9-C8	2.59	122.04	118.09
18	a	838	CLA	CHD-C1D-ND	-2.58	121.17	124.80
18	6a	306	CLA	CHD-C1D-ND	-2.58	121.17	124.80
20	K	202	BCR	C15-C16-C17	2.58	128.79	123.52
18	b	829	CLA	CHA-C1A-NA	-2.58	120.56	126.39
29	5b	301	CHL	C4C-CHD-C1D	2.58	125.29	116.07
20	L	304	BCR	C35-C13-C14	-2.58	118.64	122.82
20	l	304	BCR	C35-C13-C14	-2.58	118.64	122.82
18	a	803	CLA	CHA-C1A-NA	-2.58	120.56	126.39
18	B	825	CLA	C4A-NA-C1A	2.58	107.85	106.68
18	b	809	CLA	CHA-C1A-NA	-2.57	120.56	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	844	BCR	C29-C30-C25	2.57	114.18	110.44
18	a	814	CLA	CHA-C1A-NA	-2.57	120.56	126.39
20	k	202	BCR	C15-C16-C17	2.57	128.78	123.52
18	b	822	CLA	CHA-C1A-NA	-2.57	120.57	126.39
20	A	851	BCR	C19-C18-C17	2.57	123.06	119.01
20	a	851	BCR	C19-C18-C17	2.57	123.06	119.01
20	A	848	BCR	C24-C25-C26	2.57	127.48	121.56
20	a	848	BCR	C24-C25-C26	2.57	127.48	121.56
18	b	825	CLA	C4A-NA-C1A	2.57	107.85	106.68
18	5a	308	CLA	CHA-C1A-NA	-2.57	120.57	126.39
18	5b	308	CLA	CHA-C1A-NA	-2.57	120.57	126.39
20	A	847	BCR	C35-C13-C14	-2.57	118.65	122.82
18	A	837	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	a	811	CLA	CHA-C1A-NA	-2.57	120.57	126.39
25	6a	320	LUT	C8-C9-C10	2.57	123.05	119.01
25	6b	320	LUT	C8-C9-C10	2.57	123.05	119.01
18	A	811	CLA	CHA-C1A-NA	-2.57	120.58	126.39
18	3b	305	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	A	838	CLA	CHD-C1D-ND	-2.57	121.19	124.80
18	B	838	CLA	CHD-C1D-ND	-2.56	121.19	124.80
18	A	825	CLA	CHD-C1D-ND	-2.56	121.19	124.80
18	a	825	CLA	CHD-C1D-ND	-2.56	121.19	124.80
25	3a	316	LUT	C7-C6-C5	-2.56	115.65	121.56
25	3b	316	LUT	C7-C6-C5	-2.56	115.65	121.56
18	B	836	CLA	CHA-C1A-NA	-2.56	120.59	126.39
18	b	836	CLA	CHA-C1A-NA	-2.56	120.59	126.39
25	2b	314	LUT	C31-C32-C33	2.56	133.39	126.36
18	B	838	CLA	CHA-C1A-NA	-2.56	120.59	126.39
18	b	838	CLA	CHA-C1A-NA	-2.56	120.59	126.39
18	B	822	CLA	CHA-C1A-NA	-2.56	120.59	126.39
18	2a	311	CLA	CHD-C1D-ND	-2.56	121.20	124.80
18	2b	311	CLA	CHD-C1D-ND	-2.56	121.20	124.80
20	a	850	BCR	C34-C9-C8	2.56	122.00	118.09
25	5a	317	LUT	C1-C6-C5	-2.56	119.14	122.64
25	5b	317	LUT	C1-C6-C5	-2.56	119.14	122.64
18	B	809	CLA	CHA-C1A-NA	-2.56	120.60	126.39
29	3b	315	CHL	C4C-CHD-C1D	2.56	125.22	116.07
20	a	847	BCR	C35-C13-C14	-2.56	118.67	122.82
29	3a	315	CHL	C4C-CHD-C1D	2.56	125.22	116.07
18	b	821	CLA	CHD-C1D-ND	-2.56	121.20	124.80
18	A	835	CLA	CHA-C1A-NA	-2.56	120.60	126.39
18	a	835	CLA	CHA-C1A-NA	-2.56	120.60	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	814	CLA	CHA-C1A-NA	-2.56	120.60	126.39
29	3a	307	CHL	C1C-C2C-CMC	2.56	131.41	126.80
29	3b	307	CHL	C1C-C2C-CMC	2.56	131.41	126.80
18	5a	302	CLA	CHD-C1D-ND	-2.56	121.21	124.80
18	5b	302	CLA	CHD-C1D-ND	-2.56	121.21	124.80
29	2b	306	CHL	C4D-ND-C1D	2.56	107.16	105.22
29	5b	306	CHL	C1C-C2C-CMC	2.55	131.41	126.80
18	6a	306	CLA	CHA-C1A-NA	-2.55	120.61	126.39
18	a	813	CLA	CHA-C1A-NA	-2.55	120.61	126.39
18	6a	307	CLA	CHD-C1D-ND	-2.55	121.21	124.80
18	6b	307	CLA	CHD-C1D-ND	-2.55	121.21	124.80
29	3a	315	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
29	5a	306	CHL	C1C-C2C-CMC	2.55	131.40	126.80
29	3b	315	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
18	a	837	CLA	CHD-C1D-ND	-2.55	121.21	124.80
20	f	304	BCR	C12-C13-C14	2.55	123.02	119.01
25	2a	314	LUT	C31-C32-C33	2.55	133.35	126.36
18	B	827	CLA	CHD-C1D-ND	-2.55	121.22	124.80
18	b	827	CLA	CHD-C1D-ND	-2.55	121.22	124.80
20	M	101	BCR	C36-C18-C17	-2.55	118.69	122.82
20	m	101	BCR	C36-C18-C17	-2.55	118.69	122.82
18	6b	306	CLA	CHA-C1A-NA	-2.55	120.63	126.39
20	F	304	BCR	C12-C13-C14	2.54	123.01	119.01
25	5a	316	LUT	C11-C10-C9	2.54	130.85	127.28
25	5b	316	LUT	C11-C10-C9	2.54	130.85	127.28
20	B	851	BCR	C15-C16-C17	2.54	128.72	123.52
20	b	851	BCR	C15-C16-C17	2.54	128.72	123.52
25	6a	320	LUT	C32-C33-C34	2.54	123.01	119.01
25	6b	320	LUT	C32-C33-C34	2.54	123.01	119.01
18	g	203	CLA	CHD-C1D-ND	-2.54	121.23	124.80
20	A	850	BCR	C12-C13-C14	2.54	123.00	119.01
20	b	843	BCR	C7-C6-C5	2.54	127.40	121.56
18	A	813	CLA	CHA-C1A-NA	-2.54	120.64	126.39
18	b	838	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	A	821	CLA	CHD-C1D-ND	-2.54	121.23	124.80
18	a	821	CLA	CHD-C1D-ND	-2.54	121.23	124.80
20	G	204	BCR	C16-C15-C14	2.54	128.71	123.52
20	g	204	BCR	C16-C15-C14	2.54	128.71	123.52
20	B	843	BCR	C7-C6-C5	2.53	127.39	121.56
18	A	808	CLA	CHA-C1A-NA	-2.53	120.65	126.39
18	a	808	CLA	CHA-C1A-NA	-2.53	120.65	126.39
18	B	821	CLA	CHD-C1D-ND	-2.53	121.24	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	301	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	l	301	CLA	CHD-C1D-ND	-2.53	121.24	124.80
20	B	846	BCR	C33-C5-C6	2.53	127.25	124.48
29	2b	304	CHL	C1C-C2C-CMC	2.53	131.36	126.80
18	B	830	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	b	830	CLA	CHD-C1D-ND	-2.53	121.24	124.80
18	3a	305	CLA	CHD-C1D-ND	-2.53	121.25	124.80
20	G	201	BCR	C19-C18-C17	2.53	122.98	119.01
20	g	201	BCR	C19-C18-C17	2.53	122.98	119.01
29	2a	304	CHL	C1C-C2C-CMC	2.53	131.35	126.80
29	3a	301	CHL	C1C-C2C-CMC	2.52	131.35	126.80
29	3b	301	CHL	C1C-C2C-CMC	2.52	131.35	126.80
18	6a	316	CLA	CHA-C1A-NA	-2.52	120.68	126.39
18	6b	316	CLA	CHA-C1A-NA	-2.52	120.68	126.39
20	I	202	BCR	C19-C18-C17	2.52	122.98	119.01
18	A	836	CLA	C3B-C4B-NB	-2.52	108.28	110.53
18	a	836	CLA	C3B-C4B-NB	-2.52	108.28	110.53
20	A	848	BCR	C12-C13-C14	2.52	122.98	119.01
20	a	848	BCR	C12-C13-C14	2.52	122.98	119.01
18	G	203	CLA	CHD-C1D-ND	-2.52	121.25	124.80
18	6b	317	CLA	CHD-C1D-ND	-2.52	121.25	124.80
20	i	202	BCR	C19-C18-C17	2.52	122.97	119.01
20	M	101	BCR	C37-C22-C23	2.52	121.94	118.09
25	6a	319	LUT	C12-C13-C14	2.52	122.97	119.01
25	6b	319	LUT	C12-C13-C14	2.52	122.97	119.01
18	B	824	CLA	C3B-C4B-NB	-2.51	108.29	110.53
18	b	824	CLA	C3B-C4B-NB	-2.51	108.29	110.53
29	5a	305	CHL	C1C-C2C-CMC	2.51	131.33	126.80
29	5b	305	CHL	C1C-C2C-CMC	2.51	131.33	126.80
18	A	833	CLA	CHA-C1A-NA	-2.51	120.70	126.39
18	a	833	CLA	CHA-C1A-NA	-2.51	120.70	126.39
20	b	851	BCR	C37-C22-C23	2.51	121.93	118.09
29	6a	304	CHL	C4D-ND-C1D	2.51	107.12	105.22
29	6b	304	CHL	C4D-ND-C1D	2.51	107.12	105.22
20	a	850	BCR	C12-C13-C14	2.51	122.95	119.01
20	m	101	BCR	C37-C22-C23	2.51	121.92	118.09
29	2a	306	CHL	C4D-ND-C1D	2.51	107.12	105.22
29	5a	307	CHL	C4C-CHD-C1D	2.51	125.03	116.07
29	5b	307	CHL	C4C-CHD-C1D	2.51	125.03	116.07
20	a	847	BCR	C29-C30-C25	2.50	114.08	110.44
18	B	803	CLA	CHD-C1D-ND	-2.50	121.28	124.80
18	b	803	CLA	CHD-C1D-ND	-2.50	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	810	CLA	CHD-C1D-ND	-2.50	121.28	124.80
18	b	810	CLA	CHD-C1D-ND	-2.50	121.28	124.80
20	A	847	BCR	C29-C30-C25	2.50	114.07	110.44
20	B	844	BCR	C12-C13-C14	2.50	122.94	119.01
20	b	844	BCR	C12-C13-C14	2.50	122.94	119.01
18	g	202	CLA	CHD-C1D-ND	-2.50	121.29	124.80
18	A	807	CLA	CHD-C1D-ND	-2.50	121.29	124.80
18	6a	317	CLA	CHD-C1D-ND	-2.50	121.29	124.80
18	a	807	CLA	CHD-C1D-ND	-2.50	121.29	124.80
20	A	851	BCR	C35-C13-C14	-2.50	118.77	122.82
20	a	851	BCR	C35-C13-C14	-2.50	118.77	122.82
18	2a	303	CLA	CHD-C1D-ND	-2.50	121.29	124.80
18	3a	311	CLA	CHD-C1D-ND	-2.50	121.29	124.80
18	2b	303	CLA	CHD-C1D-ND	-2.50	121.29	124.80
20	K	202	BCR	C7-C6-C5	2.49	127.30	121.56
20	k	202	BCR	C7-C6-C5	2.49	127.30	121.56
18	A	827	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	a	827	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	b	807	CLA	CHA-C1A-NA	-2.49	120.75	126.39
18	2b	301	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	L	303	CLA	C4A-NA-C1A	2.49	107.81	106.68
20	B	842	BCR	C12-C13-C14	2.49	122.92	119.01
20	b	842	BCR	C12-C13-C14	2.49	122.92	119.01
18	5a	315	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	5b	315	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	G	202	CLA	CHD-C1D-ND	-2.49	121.30	124.80
20	f	304	BCR	C36-C18-C17	-2.49	118.78	122.82
20	B	851	BCR	C37-C22-C23	2.49	121.89	118.09
20	b	846	BCR	C33-C5-C6	2.49	127.20	124.48
18	2a	307	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	2b	307	CLA	CHD-C1D-ND	-2.49	121.30	124.80
18	A	804	CLA	CHA-C1A-NA	-2.49	120.76	126.39
18	a	804	CLA	CHA-C1A-NA	-2.49	120.76	126.39
25	6a	318	LUT	C11-C10-C9	2.48	130.76	127.28
25	6b	318	LUT	C11-C10-C9	2.48	130.76	127.28
20	F	304	BCR	C36-C18-C17	-2.48	118.79	122.82
20	a	851	BCR	C7-C6-C5	2.48	127.27	121.56
18	3b	311	CLA	CHD-C1D-ND	-2.48	121.31	124.80
20	J	102	BCR	C7-C8-C9	2.48	129.90	126.23
20	j	102	BCR	C7-C8-C9	2.48	129.90	126.23
20	A	851	BCR	C7-C6-C5	2.47	127.25	121.56
20	B	851	BCR	C24-C25-C26	2.47	127.25	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	301	BCR	C19-C18-C17	2.47	122.90	119.01
18	B	807	CLA	CHA-C1A-NA	-2.47	120.79	126.39
20	B	843	BCR	C24-C25-C26	2.47	127.25	121.56
20	b	843	BCR	C24-C25-C26	2.47	127.25	121.56
18	A	833	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	B	820	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	b	802	CLA	C3B-C4B-NB	-2.47	108.33	110.53
18	2a	301	CLA	CHD-C1D-ND	-2.47	121.33	124.80
20	K	202	BCR	C19-C18-C17	2.47	122.89	119.01
20	k	202	BCR	C19-C18-C17	2.47	122.89	119.01
20	A	849	BCR	C38-C26-C25	2.47	127.18	124.48
20	a	849	BCR	C38-C26-C25	2.47	127.18	124.48
20	F	301	BCR	C19-C18-C17	2.47	122.89	119.01
18	3a	303	CLA	O2D-CGD-CBD	2.47	115.54	111.23
18	3b	303	CLA	O2D-CGD-CBD	2.47	115.54	111.23
18	2a	310	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	2b	310	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	B	853	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	b	853	CLA	CHD-C1D-ND	-2.47	121.33	124.80
18	A	836	CLA	CAA-C2A-C1A	2.47	120.05	111.97
18	6a	312	CLA	O2A-C1-C2	2.46	117.59	108.11
18	6b	312	CLA	O2A-C1-C2	2.46	117.59	108.11
18	B	804	CLA	CHD-C1D-ND	-2.46	121.33	124.80
18	b	804	CLA	CHD-C1D-ND	-2.46	121.33	124.80
18	l	303	CLA	C4A-NA-C1A	2.46	107.80	106.68
18	5a	309	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	5b	309	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	a	836	CLA	CAA-C2A-C1A	2.46	120.04	111.97
18	a	823	CLA	CHD-C1D-C2D	2.46	130.60	125.49
18	A	842	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	a	842	CLA	CHD-C1D-ND	-2.46	121.34	124.80
18	b	820	CLA	CHD-C1D-ND	-2.46	121.34	124.80
20	b	851	BCR	C24-C25-C26	2.46	127.22	121.56
26	A	802	CL0	CHA-C1A-C2A	-2.46	127.54	133.31
26	a	802	CL0	CHA-C1A-C2A	-2.46	127.54	133.31
20	K	202	BCR	C29-C30-C25	2.45	114.00	110.44
20	k	202	BCR	C29-C30-C25	2.45	114.00	110.44
25	5a	317	LUT	C7-C6-C5	-2.45	115.90	121.56
18	B	807	CLA	CHD-C1D-ND	-2.45	121.35	124.80
18	b	807	CLA	CHD-C1D-ND	-2.45	121.35	124.80
20	B	844	BCR	C7-C6-C5	2.45	127.20	121.56
20	b	844	BCR	C7-C6-C5	2.45	127.20	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	833	CLA	CHD-C1D-ND	-2.45	121.35	124.80
18	2b	308	CLA	CHD-C1D-ND	-2.45	121.35	124.80
20	B	843	BCR	C12-C13-C14	2.45	122.86	119.01
20	b	843	BCR	C12-C13-C14	2.45	122.86	119.01
18	A	823	CLA	CHD-C1D-C2D	2.45	130.58	125.49
18	B	834	CLA	CHD-C1D-ND	-2.45	121.36	124.80
18	b	834	CLA	CHD-C1D-ND	-2.45	121.36	124.80
20	M	101	BCR	C19-C18-C17	2.45	122.86	119.01
25	6b	319	LUT	C39-C29-C28	-2.45	114.35	118.09
18	A	815	CLA	CHD-C1D-C2D	2.44	130.57	125.49
18	a	815	CLA	CHD-C1D-C2D	2.44	130.57	125.49
20	B	846	BCR	C35-C13-C14	-2.44	118.86	122.82
25	6a	319	LUT	C39-C29-C28	-2.44	114.36	118.09
25	5b	317	LUT	C7-C6-C5	-2.44	115.94	121.56
18	A	829	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	a	829	CLA	CHD-C1D-ND	-2.44	121.37	124.80
18	3a	306	CLA	CHD-C1D-ND	-2.44	121.38	124.80
18	3b	306	CLA	CHD-C1D-ND	-2.44	121.38	124.80
20	A	847	BCR	C12-C13-C14	2.43	122.84	119.01
18	A	829	CLA	CHA-C1A-NA	-2.43	120.89	126.39
18	a	829	CLA	CHA-C1A-NA	-2.43	120.89	126.39
18	B	821	CLA	C4D-CHA-C1A	2.43	124.14	121.24
18	b	821	CLA	C4D-CHA-C1A	2.43	124.14	121.24
25	5a	316	LUT	C40-C33-C34	-2.43	118.88	122.82
25	5b	316	LUT	C40-C33-C34	-2.43	118.88	122.82
18	L	303	CLA	CHD-C1D-ND	-2.43	121.39	124.80
18	l	303	CLA	CHD-C1D-ND	-2.43	121.39	124.80
25	3b	316	LUT	C40-C33-C34	-2.43	118.89	122.82
18	A	813	CLA	CHD-C1D-C2D	2.43	130.53	125.49
18	a	813	CLA	CHD-C1D-C2D	2.43	130.53	125.49
20	m	101	BCR	C19-C18-C17	2.42	122.82	119.01
25	3a	316	LUT	C40-C33-C34	-2.42	118.89	122.82
18	B	802	CLA	C3B-C4B-NB	-2.42	108.37	110.53
20	A	850	BCR	C16-C15-C14	2.42	128.47	123.52
20	a	850	BCR	C16-C15-C14	2.42	128.47	123.52
20	B	851	BCR	C19-C18-C17	2.42	122.82	119.01
20	b	851	BCR	C19-C18-C17	2.42	122.82	119.01
20	a	847	BCR	C12-C13-C14	2.42	122.82	119.01
18	A	820	CLA	CHD-C1D-ND	-2.42	121.40	124.80
18	a	820	CLA	CHD-C1D-ND	-2.42	121.40	124.80
20	b	846	BCR	C35-C13-C14	-2.42	118.90	122.82
25	5a	316	LUT	C7-C8-C9	2.42	129.81	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5b	316	LUT	C7-C8-C9	2.42	129.81	126.23
18	a	810	CLA	CHD-C1D-ND	-2.42	121.40	124.80
18	2a	311	CLA	C4A-NA-C1A	2.41	107.78	106.68
18	2b	311	CLA	C4A-NA-C1A	2.41	107.78	106.68
18	A	834	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	2a	308	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	a	834	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	B	813	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	A	817	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	a	817	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	B	809	CLA	CHD-C1D-ND	-2.41	121.41	124.80
18	b	809	CLA	CHD-C1D-ND	-2.41	121.41	124.80
25	2b	314	LUT	C20-C13-C14	-2.40	118.92	122.82
18	B	836	CLA	CAA-CBA-CGA	2.40	120.03	113.21
18	b	836	CLA	CAA-CBA-CGA	2.40	120.03	113.21
18	b	818	CLA	CHD-C1D-ND	-2.40	121.42	124.80
18	B	838	CLA	C3B-C4B-NB	-2.40	108.39	110.53
20	F	304	BCR	C37-C22-C23	2.40	121.75	118.09
20	f	304	BCR	C37-C22-C23	2.40	121.75	118.09
25	6a	319	LUT	C31-C32-C33	2.40	132.94	126.36
25	6b	319	LUT	C31-C32-C33	2.40	132.94	126.36
18	5b	310	CLA	CHD-C1D-ND	-2.40	121.43	124.80
20	M	101	BCR	C7-C6-C5	2.40	127.08	121.56
20	m	101	BCR	C7-C6-C5	2.40	127.08	121.56
20	A	848	BCR	C1-C6-C5	-2.40	119.36	122.64
20	a	848	BCR	C1-C6-C5	-2.40	119.36	122.64
18	b	819	CLA	C4A-NA-C1A	2.40	107.77	106.68
18	b	838	CLA	C3B-C4B-NB	-2.39	108.39	110.53
18	6a	315	CLA	C4A-NA-C1A	2.39	107.77	106.68
18	6b	315	CLA	C4A-NA-C1A	2.39	107.77	106.68
18	A	810	CLA	CHD-C1D-ND	-2.39	121.44	124.80
20	L	304	BCR	C12-C13-C14	2.39	122.77	119.01
20	l	304	BCR	C12-C13-C14	2.39	122.77	119.01
18	A	819	CLA	C4A-NA-C1A	2.39	107.77	106.68
18	a	819	CLA	C4A-NA-C1A	2.39	107.77	106.68
18	b	813	CLA	CHD-C1D-ND	-2.39	121.44	124.80
25	5a	317	LUT	C31-C30-C29	2.39	130.63	127.28
25	2a	314	LUT	C20-C13-C14	-2.39	118.95	122.82
25	2a	314	LUT	C8-C7-C6	2.39	133.38	127.00
18	B	811	CLA	C4A-NA-C1A	2.39	107.77	106.68
18	b	811	CLA	C4A-NA-C1A	2.39	107.77	106.68
29	2a	305	CHL	C1C-C2C-CMC	2.39	131.10	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2b	305	CHL	C1C-C2C-CMC	2.39	131.10	126.80
18	J	101	CLA	C4A-NA-C1A	2.38	107.77	106.68
18	j	101	CLA	C4A-NA-C1A	2.38	107.77	106.68
25	2b	314	LUT	C8-C7-C6	2.38	133.36	127.00
25	2a	314	LUT	C15-C14-C13	2.38	130.62	127.28
18	A	839	CLA	CHD-C1D-ND	-2.38	121.45	124.80
29	6a	304	CHL	C1C-C2C-CMC	2.38	131.09	126.80
29	6b	304	CHL	C1C-C2C-CMC	2.38	131.09	126.80
18	B	802	CLA	CHD-C1D-ND	-2.38	121.45	124.80
18	b	802	CLA	CHD-C1D-ND	-2.38	121.45	124.80
18	5a	310	CLA	CHD-C1D-ND	-2.38	121.45	124.80
18	b	814	CLA	CHD-C1D-ND	-2.38	121.46	124.80
20	A	850	BCR	C24-C25-C26	-2.38	116.08	121.56
20	a	850	BCR	C24-C25-C26	-2.38	116.08	121.56
20	F	304	BCR	C24-C25-C26	2.37	127.02	121.56
20	f	304	BCR	C24-C25-C26	2.37	127.02	121.56
25	2b	314	LUT	C15-C14-C13	2.37	130.60	127.28
18	B	819	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	b	819	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	6a	311	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	6b	311	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	6a	314	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	6b	314	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	a	839	CLA	CHD-C1D-ND	-2.37	121.47	124.80
18	5a	312	CLA	O2A-C1-C2	2.37	117.22	108.11
20	A	850	BCR	C19-C18-C17	2.37	122.73	119.01
20	a	850	BCR	C19-C18-C17	2.37	122.73	119.01
18	B	814	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	2b	314	LUT	C1-C6-C7	-2.37	109.23	115.65
20	G	204	BCR	C29-C30-C25	2.37	113.88	110.44
18	B	819	CLA	C4A-NA-C1A	2.37	107.76	106.68
18	6a	315	CLA	CHD-C1D-ND	-2.36	121.48	124.80
18	6b	315	CLA	CHD-C1D-ND	-2.36	121.48	124.80
18	5b	312	CLA	O2A-C1-C2	2.36	117.20	108.11
20	B	845	BCR	C37-C22-C23	2.36	121.70	118.09
20	b	845	BCR	C37-C22-C23	2.36	121.70	118.09
25	5b	317	LUT	C31-C30-C29	2.36	130.59	127.28
18	B	818	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	I	202	BCR	C35-C13-C14	-2.36	119.00	122.82
20	i	202	BCR	C35-C13-C14	-2.36	119.00	122.82
20	I	202	BCR	C24-C25-C26	2.36	126.98	121.56
20	i	202	BCR	C24-C25-C26	2.36	126.98	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2a	314	LUT	C1-C6-C7	-2.35	109.27	115.65
18	B	829	CLA	CHD-C1D-C2D	2.35	130.38	125.49
18	3a	313	CLA	CHD-C1D-ND	-2.35	121.49	124.80
18	3b	313	CLA	CHD-C1D-ND	-2.35	121.49	124.80
20	B	851	BCR	C29-C30-C25	2.35	113.85	110.44
18	6a	305	CLA	CHD-C1D-C2D	2.34	130.36	125.49
29	5a	301	CHL	C1C-C2C-CMC	2.34	131.03	126.80
29	5b	301	CHL	C1C-C2C-CMC	2.34	131.03	126.80
18	3a	306	CLA	C4A-NA-C1A	2.34	107.75	106.68
18	3b	306	CLA	C4A-NA-C1A	2.34	107.75	106.68
20	g	204	BCR	C29-C30-C25	2.34	113.84	110.44
18	A	826	CLA	CHD-C1D-ND	-2.34	121.51	124.80
18	5a	313	CLA	CHD-C1D-ND	-2.34	121.51	124.80
18	5b	313	CLA	CHD-C1D-ND	-2.34	121.51	124.80
20	A	847	BCR	C16-C15-C14	2.34	128.30	123.52
20	a	847	BCR	C16-C15-C14	2.34	128.30	123.52
29	2b	313	CHL	C1C-C2C-CMC	2.34	131.01	126.80
29	2a	313	CHL	C1C-C2C-CMC	2.34	131.01	126.80
18	L	302	CLA	CHD-C1D-ND	-2.34	121.52	124.80
18	l	302	CLA	CHD-C1D-ND	-2.34	121.52	124.80
18	a	826	CLA	CHD-C1D-ND	-2.33	121.52	124.80
25	6b	320	LUT	C27-C28-C29	2.33	131.34	126.32
18	b	829	CLA	CHD-C1D-C2D	2.33	130.34	125.49
18	f	303	CLA	CAA-C2A-C3A	-2.33	110.88	116.23
18	B	828	CLA	CHD-C1D-C2D	2.33	130.34	125.49
18	6b	305	CLA	CHD-C1D-C2D	2.33	130.34	125.49
25	6b	319	LUT	C8-C7-C6	2.33	133.22	127.00
18	3a	302	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	3b	302	CLA	CHD-C1D-ND	-2.33	121.52	124.80
18	b	828	CLA	CHD-C1D-C2D	2.33	130.33	125.49
20	F	304	BCR	C2-C1-C6	2.33	113.82	110.44
20	b	851	BCR	C29-C30-C25	2.33	113.82	110.44
20	f	304	BCR	C2-C1-C6	2.33	113.82	110.44
18	F	303	CLA	CAA-C2A-C3A	-2.32	110.90	116.23
20	b	844	BCR	C21-C20-C19	2.32	129.93	123.20
18	B	840	CLA	CHD-C1D-ND	-2.32	121.54	124.80
18	b	840	CLA	CHD-C1D-ND	-2.32	121.54	124.80
25	6a	319	LUT	C8-C7-C6	2.32	133.20	127.00
20	B	844	BCR	C21-C20-C19	2.32	129.92	123.20
20	B	845	BCR	C36-C18-C17	-2.32	119.06	122.82
20	b	845	BCR	C36-C18-C17	-2.32	119.06	122.82
18	b	802	CLA	C2A-C1A-CHA	2.32	127.89	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6a	320	LUT	C27-C28-C29	2.32	131.31	126.32
18	A	823	CLA	C4A-NA-C1A	2.31	107.73	106.68
18	5a	311	CLA	C4A-NA-C1A	2.31	107.73	106.68
18	a	823	CLA	C4A-NA-C1A	2.31	107.73	106.68
18	5b	311	CLA	C4A-NA-C1A	2.31	107.73	106.68
18	6a	310	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	6a	320	LUT	C7-C6-C5	2.31	126.88	121.56
25	2b	314	LUT	C19-C9-C8	2.31	121.62	118.09
20	B	842	BCR	C15-C16-C17	2.31	128.25	123.52
20	b	842	BCR	C15-C16-C17	2.31	128.25	123.52
25	6b	318	LUT	C15-C14-C13	2.31	130.51	127.28
18	B	802	CLA	C2A-C1A-CHA	2.31	127.87	123.87
20	B	842	BCR	C20-C21-C22	2.31	130.51	127.28
25	6a	320	LUT	C31-C30-C29	2.30	130.51	127.28
25	6b	320	LUT	C31-C30-C29	2.30	130.51	127.28
18	B	816	CLA	CHD-C1D-ND	-2.30	121.56	124.80
18	b	816	CLA	CHD-C1D-ND	-2.30	121.56	124.80
25	6b	320	LUT	C7-C6-C5	2.30	126.86	121.56
20	K	202	BCR	C23-C24-C25	2.30	133.15	127.00
18	J	101	CLA	CHD-C1D-ND	-2.30	121.57	124.80
18	j	101	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	6a	318	LUT	C15-C14-C13	2.30	130.50	127.28
20	a	847	BCR	C24-C25-C26	-2.30	116.26	121.56
18	6b	310	CLA	CHD-C1D-ND	-2.29	121.57	124.80
18	A	835	CLA	CHD-C1D-C2D	2.29	130.26	125.49
18	a	835	CLA	CHD-C1D-C2D	2.29	130.26	125.49
20	k	202	BCR	C23-C24-C25	2.29	133.13	127.00
20	b	842	BCR	C20-C21-C22	2.29	130.49	127.28
25	2a	314	LUT	C19-C9-C8	2.29	121.58	118.09
18	A	818	CLA	CHD-C1D-C2D	2.29	130.24	125.49
18	a	818	CLA	CHD-C1D-C2D	2.29	130.24	125.49
20	A	849	BCR	C8-C9-C10	2.29	122.60	119.01
20	a	849	BCR	C8-C9-C10	2.29	122.60	119.01
20	b	842	BCR	C34-C9-C8	2.28	121.58	118.09
20	i	202	BCR	C7-C6-C5	2.28	126.81	121.56
25	5a	317	LUT	C35-C34-C33	2.28	130.48	127.28
25	5b	317	LUT	C35-C34-C33	2.28	130.48	127.28
25	3a	316	LUT	C31-C30-C29	2.28	130.48	127.28
25	3b	316	LUT	C31-C30-C29	2.28	130.48	127.28
20	A	847	BCR	C24-C25-C26	-2.28	116.30	121.56
18	B	835	CLA	CHD-C1D-ND	-2.28	121.59	124.80
18	b	835	CLA	CHD-C1D-ND	-2.28	121.59	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5a	317	LUT	C8-C9-C10	2.28	122.60	119.01
25	5b	317	LUT	C8-C9-C10	2.28	122.60	119.01
18	B	823	CLA	CHD-C1D-C2D	2.28	130.23	125.49
18	A	822	CLA	CHD-C1D-C2D	2.28	130.23	125.49
18	a	822	CLA	CHD-C1D-C2D	2.28	130.23	125.49
20	a	851	BCR	C12-C13-C14	2.28	122.59	119.01
20	m	101	BCR	C1-C6-C5	-2.28	119.52	122.64
18	5a	311	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	5b	311	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	b	835	CLA	C3B-C4B-NB	-2.28	108.50	110.53
20	A	850	BCR	C33-C5-C6	2.28	126.97	124.48
20	a	850	BCR	C33-C5-C6	2.28	126.97	124.48
18	f	302	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	6a	313	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	6b	313	CLA	CHD-C1D-ND	-2.28	121.60	124.80
18	B	839	CLA	C4A-NA-C1A	2.27	107.72	106.68
18	b	839	CLA	C4A-NA-C1A	2.27	107.72	106.68
26	a	802	CL0	C4C-CHD-C1D	2.27	124.20	116.07
26	A	802	CL0	C4C-CHD-C1D	2.27	124.19	116.07
20	I	202	BCR	C7-C6-C5	2.27	126.78	121.56
18	B	836	CLA	CHD-C1D-C2D	2.27	130.20	125.49
18	b	836	CLA	CHD-C1D-C2D	2.27	130.20	125.49
18	5a	308	CLA	CHD-C1D-C2D	2.27	130.20	125.49
18	5b	308	CLA	CHD-C1D-C2D	2.27	130.20	125.49
18	F	302	CLA	CHD-C1D-ND	-2.26	121.62	124.80
20	K	202	BCR	C30-C25-C24	-2.26	109.52	115.65
20	k	202	BCR	C30-C25-C24	-2.26	109.52	115.65
20	B	842	BCR	C34-C9-C8	2.26	121.54	118.09
18	b	823	CLA	CHD-C1D-C2D	2.26	130.18	125.49
20	M	101	BCR	C1-C6-C5	-2.26	119.55	122.64
18	5b	303	CLA	CHD-C1D-ND	-2.26	121.63	124.80
20	A	851	BCR	C12-C13-C14	2.26	122.56	119.01
20	b	848	BCR	C20-C21-C22	2.26	130.44	127.28
29	6a	309	CHL	CAA-C2A-C3A	-2.25	111.06	116.23
29	6b	309	CHL	CAA-C2A-C3A	-2.25	111.06	116.23
18	A	809	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	a	809	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	F	305	CLA	CHD-C1D-ND	-2.25	121.63	124.80
18	f	305	CLA	CHD-C1D-ND	-2.25	121.63	124.80
20	b	842	BCR	C36-C18-C17	-2.25	119.17	122.82
20	I	202	BCR	C16-C15-C14	2.25	128.12	123.52
20	i	202	BCR	C16-C15-C14	2.25	128.12	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	842	BCR	C7-C6-C5	-2.25	116.38	121.56
20	b	842	BCR	C7-C6-C5	-2.25	116.38	121.56
20	B	842	BCR	C36-C18-C17	-2.25	119.18	122.82
29	2a	306	CHL	C4C-CHD-C1D	2.25	124.10	116.07
29	2b	306	CHL	C4C-CHD-C1D	2.25	124.10	116.07
20	B	846	BCR	C12-C13-C14	2.24	122.54	119.01
18	2a	312	CLA	CHD-C1D-C2D	2.24	130.15	125.49
18	2b	312	CLA	CHD-C1D-C2D	2.24	130.15	125.49
20	B	842	BCR	C30-C25-C24	-2.24	109.57	115.65
18	B	811	CLA	CHD-C1D-ND	-2.24	121.65	124.80
18	b	811	CLA	CHD-C1D-ND	-2.24	121.65	124.80
18	5a	303	CLA	CHD-C1D-ND	-2.24	121.65	124.80
18	B	852	CLA	C2A-C1A-CHA	2.24	127.75	123.87
18	b	852	CLA	C2A-C1A-CHA	2.24	127.75	123.87
25	5a	317	LUT	C40-C33-C34	-2.24	119.19	122.82
25	5b	317	LUT	C40-C33-C34	-2.24	119.19	122.82
20	B	845	BCR	C34-C9-C8	2.24	121.50	118.09
20	b	845	BCR	C34-C9-C8	2.24	121.50	118.09
20	B	848	BCR	C20-C21-C22	2.24	130.41	127.28
18	b	801	CLA	C2A-C1A-CHA	2.23	127.75	123.87
18	6b	316	CLA	CHD-C1D-C2D	2.23	130.13	125.49
18	A	824	CLA	C2A-C1A-CHA	2.23	127.74	123.87
18	a	824	CLA	C2A-C1A-CHA	2.23	127.74	123.87
26	a	802	CL0	C4D-CHA-CBD	-2.23	106.72	108.97
18	B	826	CLA	CHD-C1D-ND	-2.23	121.66	124.80
18	b	826	CLA	CHD-C1D-ND	-2.23	121.66	124.80
20	G	204	BCR	C33-C5-C6	2.23	126.92	124.48
20	g	204	BCR	C33-C5-C6	2.23	126.92	124.48
20	A	849	BCR	C7-C6-C5	2.23	126.69	121.56
26	A	802	CL0	C4D-CHA-CBD	-2.23	106.72	108.97
18	B	839	CLA	CHD-C1D-ND	-2.23	121.66	124.80
18	b	839	CLA	CHD-C1D-ND	-2.23	121.66	124.80
25	J	105	LUT	C8-C7-C6	2.23	132.95	127.00
18	3b	308	CLA	CHD-C1D-ND	-2.23	121.67	124.80
20	B	848	BCR	C7-C6-C5	-2.23	116.42	121.56
20	b	842	BCR	C30-C25-C24	-2.23	109.61	115.65
18	B	835	CLA	C3B-C4B-NB	-2.23	108.54	110.53
25	J	105	LUT	C15-C14-C13	-2.23	124.16	127.28
25	j	105	LUT	C15-C14-C13	-2.23	124.16	127.28
18	k	201	CLA	CHD-C1D-C2D	2.22	130.11	125.49
20	B	843	BCR	C34-C9-C8	2.22	121.49	118.09
20	b	843	BCR	C34-C9-C8	2.22	121.49	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	j	105	LUT	C8-C7-C6	2.22	132.94	127.00
18	B	801	CLA	C2A-C1A-CHA	2.22	127.72	123.87
18	A	814	CLA	CHD-C1D-C2D	2.22	130.11	125.49
18	a	814	CLA	CHD-C1D-C2D	2.22	130.11	125.49
18	6a	316	CLA	CHD-C1D-C2D	2.22	130.11	125.49
26	A	802	CL0	C3C-C4C-NC	-2.22	109.22	114.65
26	a	802	CL0	C3C-C4C-NC	-2.22	109.22	114.65
20	b	848	BCR	C7-C6-C5	-2.22	116.44	121.56
18	5b	303	CLA	CGD-CBD-CAD	-2.22	103.66	110.85
18	A	842	CLA	CAA-CBA-CGA	2.22	118.41	112.49
18	a	842	CLA	CAA-CBA-CGA	2.22	118.41	112.49
20	a	849	BCR	C7-C6-C5	2.22	126.67	121.56
18	B	824	CLA	CHD-C1D-C2D	2.22	130.10	125.49
18	b	824	CLA	CHD-C1D-C2D	2.22	130.10	125.49
20	b	846	BCR	C12-C13-C14	2.22	122.50	119.01
25	2b	315	LUT	C1-C6-C7	-2.21	109.64	115.65
18	5a	303	CLA	CGD-CBD-CAD	-2.21	103.69	110.85
20	G	204	BCR	C34-C9-C8	2.21	121.47	118.09
20	J	102	BCR	C7-C6-C5	-2.21	116.46	121.56
20	j	102	BCR	C7-C6-C5	-2.21	116.46	121.56
18	B	852	CLA	CHD-C1D-ND	-2.21	121.69	124.80
18	3a	308	CLA	CHD-C1D-ND	-2.21	121.69	124.80
25	2a	315	LUT	C1-C6-C7	-2.21	109.66	115.65
18	b	852	CLA	CHD-C1D-ND	-2.21	121.69	124.80
18	A	805	CLA	CHD-C1D-C2D	2.21	130.08	125.49
18	a	805	CLA	CHD-C1D-C2D	2.21	130.08	125.49
18	a	806	CLA	CHD-C1D-ND	-2.21	121.70	124.80
18	2a	312	CLA	C4A-NA-C1A	2.21	107.69	106.68
18	2b	312	CLA	C4A-NA-C1A	2.21	107.69	106.68
18	5a	304	CLA	C3B-C4B-NB	-2.20	108.56	110.53
18	5b	304	CLA	C3B-C4B-NB	-2.20	108.56	110.53
20	B	844	BCR	C24-C23-C22	2.20	129.50	126.23
20	b	844	BCR	C24-C23-C22	2.20	129.50	126.23
18	6a	308	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	6b	308	CLA	CHD-C1D-ND	-2.20	121.70	124.80
18	B	815	CLA	C3B-C4B-NB	-2.20	108.56	110.53
18	b	815	CLA	C3B-C4B-NB	-2.20	108.56	110.53
18	K	201	CLA	CHD-C1D-C2D	2.20	130.07	125.49
20	B	845	BCR	C29-C28-C27	-2.20	106.43	111.28
20	b	845	BCR	C29-C28-C27	-2.20	106.43	111.28
20	F	301	BCR	C1-C6-C5	-2.20	119.63	122.64
20	f	301	BCR	C1-C6-C5	-2.20	119.63	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6b	318	LUT	C20-C13-C14	-2.20	119.25	122.82
20	A	848	BCR	C7-C6-C5	2.20	126.62	121.56
20	a	848	BCR	C7-C6-C5	2.20	126.62	121.56
20	B	845	BCR	C4-C5-C6	-2.20	119.73	122.70
20	b	845	BCR	C4-C5-C6	-2.20	119.73	122.70
18	B	805	CLA	CHD-C1D-ND	-2.20	121.71	124.80
18	b	805	CLA	CHD-C1D-ND	-2.20	121.71	124.80
20	g	204	BCR	C34-C9-C8	2.20	121.44	118.09
18	B	840	CLA	C2A-C1A-CHA	2.20	127.68	123.87
18	b	840	CLA	C2A-C1A-CHA	2.20	127.68	123.87
25	6a	318	LUT	C20-C13-C14	-2.19	119.26	122.82
18	B	829	CLA	C3B-C4B-NB	-2.19	108.57	110.53
18	b	829	CLA	C3B-C4B-NB	-2.19	108.57	110.53
20	B	845	BCR	C19-C18-C17	2.19	122.46	119.01
20	b	845	BCR	C19-C18-C17	2.19	122.46	119.01
20	F	301	BCR	C35-C13-C14	-2.19	119.27	122.82
20	f	301	BCR	C35-C13-C14	-2.19	119.27	122.82
20	J	102	BCR	C10-C11-C12	2.19	129.55	123.20
20	j	102	BCR	C10-C11-C12	2.19	129.55	123.20
18	A	801	CLA	CHD-C1D-C2D	2.19	130.04	125.49
18	a	801	CLA	CHD-C1D-C2D	2.19	130.04	125.49
18	A	817	CLA	C3B-C4B-NB	-2.19	108.58	110.53
18	a	817	CLA	C3B-C4B-NB	-2.19	108.58	110.53
20	b	842	BCR	C23-C24-C25	2.19	132.84	127.00
18	A	819	CLA	CHD-C1D-ND	-2.19	121.72	124.80
18	a	819	CLA	CHD-C1D-ND	-2.19	121.72	124.80
20	l	304	BCR	C24-C25-C26	-2.19	116.52	121.56
20	L	304	BCR	C24-C25-C26	-2.19	116.52	121.56
18	b	808	CLA	CHD-C1D-ND	-2.18	121.73	124.80
20	f	304	BCR	C19-C18-C17	2.18	122.44	119.01
25	3a	316	LUT	C20-C13-C14	-2.18	119.28	122.82
25	3b	316	LUT	C20-C13-C14	-2.18	119.28	122.82
18	B	854	CLA	C4A-NA-C1A	2.18	107.67	106.68
18	b	854	CLA	C4A-NA-C1A	2.18	107.67	106.68
18	b	802	CLA	C1D-ND-C4D	2.18	107.84	106.31
18	A	806	CLA	CHD-C1D-ND	-2.18	121.74	124.80
18	A	840	CLA	CHD-C1D-ND	-2.18	121.74	124.80
20	G	201	BCR	C34-C9-C8	2.17	121.41	118.09
20	g	201	BCR	C34-C9-C8	2.17	121.41	118.09
20	B	842	BCR	C23-C24-C25	2.17	132.80	127.00
18	3b	313	CLA	C4A-NA-C1A	2.17	107.67	106.68
18	2b	309	CLA	CHD-C1D-ND	-2.17	121.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	C4A-NA-C1A	2.17	107.67	106.68
18	b	834	CLA	C4A-NA-C1A	2.17	107.67	106.68
18	B	832	CLA	CHD-C1D-C2D	2.16	129.99	125.49
18	b	832	CLA	CHD-C1D-C2D	2.16	129.99	125.49
18	B	808	CLA	CHD-C1D-ND	-2.16	121.76	124.80
18	a	840	CLA	CHD-C1D-ND	-2.16	121.76	124.80
18	3b	310	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	5a	304	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	5b	304	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	B	822	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	b	822	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	5a	312	CLA	CHD-C1D-C2D	2.16	129.97	125.49
18	5b	312	CLA	CHD-C1D-C2D	2.16	129.97	125.49
20	A	851	BCR	C30-C25-C24	-2.16	109.81	115.65
20	a	851	BCR	C30-C25-C24	-2.16	109.81	115.65
20	F	304	BCR	C19-C18-C17	2.15	122.40	119.01
20	F	301	BCR	C11-C10-C9	2.15	130.30	127.28
20	f	301	BCR	C11-C10-C9	2.15	130.30	127.28
18	A	804	CLA	CHD-C1D-C2D	2.15	129.97	125.49
18	3b	304	CLA	CHD-C1D-C2D	2.15	129.96	125.49
18	B	852	CLA	C4D-CHA-C1A	2.15	123.81	121.24
18	b	852	CLA	C4D-CHA-C1A	2.15	123.81	121.24
18	3a	310	CLA	CHD-C1D-C2D	2.15	129.96	125.49
25	J	105	LUT	C40-C33-C34	-2.15	119.34	122.82
18	a	804	CLA	CHD-C1D-C2D	2.15	129.95	125.49
18	3b	312	CLA	CHD-C1D-C2D	2.15	129.95	125.49
18	b	854	CLA	CHD-C1D-ND	-2.15	121.78	124.80
18	2a	303	CLA	C4A-NA-C1A	2.15	107.66	106.68
18	2b	303	CLA	C4A-NA-C1A	2.15	107.66	106.68
20	B	844	BCR	C24-C25-C26	2.15	126.50	121.56
20	b	844	BCR	C24-C25-C26	2.15	126.50	121.56
18	2a	309	CLA	CHD-C1D-ND	-2.14	121.78	124.80
20	B	845	BCR	C10-C11-C12	2.14	129.41	123.20
20	b	845	BCR	C10-C11-C12	2.14	129.41	123.20
20	B	843	BCR	C1-C6-C5	-2.14	119.71	122.64
20	b	843	BCR	C1-C6-C5	-2.14	119.71	122.64
18	B	802	CLA	C1D-ND-C4D	2.14	107.81	106.31
18	3a	304	CLA	CHD-C1D-C2D	2.14	129.94	125.49
25	j	105	LUT	C40-C33-C34	-2.14	119.35	122.82
20	L	304	BCR	C20-C21-C22	2.14	130.27	127.28
20	l	304	BCR	C20-C21-C22	2.14	130.27	127.28
18	A	808	CLA	CHD-C1D-C2D	2.14	129.93	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	808	CLA	CHD-C1D-C2D	2.14	129.93	125.49
18	A	830	CLA	CHD-C1D-C2D	2.13	129.92	125.49
18	a	830	CLA	CHD-C1D-C2D	2.13	129.92	125.49
18	F	305	CLA	C4A-NA-C1A	2.13	107.65	106.68
18	f	305	CLA	C4A-NA-C1A	2.13	107.65	106.68
25	2a	314	LUT	C18-C5-C4	-2.13	110.50	114.42
25	2b	314	LUT	C18-C5-C4	-2.13	110.50	114.42
18	3a	312	CLA	CHD-C1D-C2D	2.13	129.92	125.49
20	a	849	BCR	C2-C1-C6	2.13	113.54	110.44
20	A	847	BCR	C23-C22-C21	2.13	122.36	119.01
20	a	847	BCR	C23-C22-C21	2.13	122.36	119.01
25	2a	314	LUT	C26-C27-C28	2.13	127.89	124.58
25	2b	314	LUT	C26-C27-C28	2.13	127.89	124.58
18	3a	309	CLA	CHD-C1D-C2D	2.13	129.91	125.49
18	3b	309	CLA	CHD-C1D-C2D	2.13	129.91	125.49
20	b	843	BCR	C29-C30-C25	2.13	113.53	110.44
18	5a	302	CLA	CHD-C1D-C2D	2.13	129.91	125.49
18	5b	302	CLA	CHD-C1D-C2D	2.13	129.91	125.49
20	F	301	BCR	C7-C6-C5	2.13	126.45	121.56
20	f	301	BCR	C7-C6-C5	2.13	126.45	121.56
18	A	831	CLA	C4A-NA-C1A	2.12	107.65	106.68
18	a	831	CLA	C4A-NA-C1A	2.12	107.65	106.68
18	B	838	CLA	CHD-C1D-C2D	2.12	129.90	125.49
25	5a	316	LUT	C20-C13-C14	-2.12	119.38	122.82
25	5b	316	LUT	C20-C13-C14	-2.12	119.38	122.82
18	A	853	CLA	C4A-NA-C1A	2.12	107.65	106.68
18	a	853	CLA	C4A-NA-C1A	2.12	107.65	106.68
29	3a	307	CHL	CED-O2D-CGD	2.12	120.73	115.92
29	3b	307	CHL	CED-O2D-CGD	2.12	120.73	115.92
29	3a	307	CHL	C3C-C4C-NC	-2.12	109.47	114.65
18	B	837	CLA	CHD-C1D-C2D	2.12	129.90	125.49
18	A	815	CLA	CMD-C2D-C1D	2.12	128.46	124.73
18	a	815	CLA	CMD-C2D-C1D	2.12	128.46	124.73
18	3a	303	CLA	CED-O2D-CGD	2.12	120.72	115.92
18	3b	303	CLA	CED-O2D-CGD	2.12	120.72	115.92
18	6b	312	CLA	CHD-C1D-C2D	2.12	129.89	125.49
23	I	201	LMG	C7-O1-C1	2.12	118.34	113.80
23	i	201	LMG	C7-O1-C1	2.12	118.34	113.80
18	B	833	CLA	CHD-C1D-C2D	2.12	129.89	125.49
18	b	833	CLA	CHD-C1D-C2D	2.12	129.89	125.49
18	B	854	CLA	CHD-C1D-ND	-2.12	121.82	124.80
20	B	845	BCR	C24-C25-C26	-2.11	116.68	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	845	BCR	C24-C25-C26	-2.11	116.68	121.56
29	3b	307	CHL	C3C-C4C-NC	-2.11	109.48	114.65
25	6b	318	LUT	C19-C9-C8	2.11	121.32	118.09
29	5a	307	CHL	C3C-C4C-NC	-2.11	109.49	114.65
29	5b	307	CHL	C3C-C4C-NC	-2.11	109.49	114.65
18	b	837	CLA	CHD-C1D-C2D	2.11	129.88	125.49
18	2a	308	CLA	CAA-C2A-C1A	-2.11	105.06	111.97
18	2b	308	CLA	CAA-C2A-C1A	-2.11	105.06	111.97
20	B	851	BCR	C7-C6-C5	-2.11	116.69	121.56
18	a	803	CLA	CHD-C1D-C2D	2.11	129.88	125.49
18	3a	303	CLA	CHD-C1D-ND	-2.11	121.83	124.80
20	A	849	BCR	C2-C1-C6	2.11	113.50	110.44
18	6a	312	CLA	CHD-C1D-C2D	2.11	129.87	125.49
20	a	847	BCR	C29-C28-C27	-2.11	106.65	111.28
25	2a	315	LUT	C8-C7-C6	2.10	132.62	127.00
18	b	838	CLA	CHD-C1D-C2D	2.10	129.86	125.49
18	A	821	CLA	C4A-NA-C1A	2.10	107.64	106.68
20	B	843	BCR	C29-C30-C25	2.10	113.50	110.44
18	6a	307	CLA	C4A-NA-C1A	2.10	107.64	106.68
18	6b	307	CLA	C4A-NA-C1A	2.10	107.64	106.68
25	2b	315	LUT	C8-C7-C6	2.10	132.61	127.00
18	A	853	CLA	CHD-C1D-C2D	2.10	129.85	125.49
18	a	853	CLA	CHD-C1D-C2D	2.10	129.85	125.49
20	B	845	BCR	C24-C23-C22	2.10	129.34	126.23
20	b	845	BCR	C24-C23-C22	2.10	129.34	126.23
20	A	851	BCR	C36-C18-C17	-2.10	119.42	122.82
20	a	851	BCR	C36-C18-C17	-2.10	119.42	122.82
29	5a	306	CHL	CED-O2D-CGD	2.10	120.67	115.92
18	3a	314	CLA	CHD-C1D-C2D	2.10	129.85	125.49
18	3b	314	CLA	CHD-C1D-C2D	2.10	129.85	125.49
20	A	847	BCR	C29-C28-C27	-2.10	106.67	111.28
18	A	803	CLA	CHD-C1D-C2D	2.10	129.85	125.49
20	b	851	BCR	C7-C6-C5	-2.10	116.73	121.56
18	A	801	CLA	C3B-C4B-NB	-2.09	108.66	110.53
18	a	801	CLA	C3B-C4B-NB	-2.09	108.66	110.53
20	A	849	BCR	C23-C22-C21	2.09	122.30	119.01
18	B	854	CLA	C3B-C4B-NB	-2.09	108.66	110.53
18	F	305	CLA	CED-O2D-CGD	2.09	120.66	115.92
18	f	305	CLA	CED-O2D-CGD	2.09	120.66	115.92
25	5a	317	LUT	C4-C5-C6	2.09	125.05	120.76
25	5b	317	LUT	C4-C5-C6	2.09	125.05	120.76
18	3b	303	CLA	CHD-C1D-ND	-2.09	121.86	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	j	105	LUT	C7-C6-C5	2.09	126.37	121.56
18	A	822	CLA	CMD-C2D-C1D	2.09	128.41	124.73
18	A	820	CLA	C3B-C4B-NB	-2.09	108.67	110.53
18	a	820	CLA	C3B-C4B-NB	-2.09	108.67	110.53
25	6a	318	LUT	C19-C9-C8	2.09	121.28	118.09
29	5b	306	CHL	CED-O2D-CGD	2.08	120.64	115.92
25	5a	316	LUT	C32-C33-C34	2.08	122.29	119.01
25	5b	316	LUT	C32-C33-C34	2.08	122.29	119.01
18	B	839	CLA	C1-O2A-CGA	2.08	121.69	116.65
18	b	839	CLA	C1-O2A-CGA	2.08	121.69	116.65
18	B	812	CLA	CHD-C1D-ND	-2.08	121.87	124.80
18	b	812	CLA	CHD-C1D-ND	-2.08	121.87	124.80
18	B	816	CLA	C4A-NA-C1A	2.08	107.63	106.68
18	b	816	CLA	C4A-NA-C1A	2.08	107.63	106.68
18	a	822	CLA	CMD-C2D-C1D	2.08	128.40	124.73
18	L	301	CLA	CHD-C1D-C2D	2.08	129.81	125.49
18	l	301	CLA	CHD-C1D-C2D	2.08	129.81	125.49
20	k	202	BCR	C34-C9-C8	2.08	121.26	118.09
25	J	105	LUT	C7-C6-C5	2.08	126.34	121.56
20	a	849	BCR	C23-C22-C21	2.08	122.28	119.01
18	B	812	CLA	C4A-NA-C1A	2.08	107.63	106.68
18	b	812	CLA	C4A-NA-C1A	2.08	107.63	106.68
18	B	821	CLA	CHD-C1D-C2D	2.07	129.80	125.49
18	B	838	CLA	CAA-CBA-CGA	2.07	119.09	113.21
18	b	838	CLA	CAA-CBA-CGA	2.07	119.09	113.21
18	a	809	CLA	CAA-C2A-C1A	2.07	118.77	111.97
20	K	202	BCR	C34-C9-C8	2.07	121.25	118.09
18	B	823	CLA	C3B-C4B-NB	-2.07	108.68	110.53
18	b	823	CLA	C3B-C4B-NB	-2.07	108.68	110.53
18	A	816	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	A	837	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	a	816	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	a	837	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	B	804	CLA	C3B-C4B-NB	-2.07	108.68	110.53
18	2a	311	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	2b	311	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	A	811	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	a	811	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	A	809	CLA	CAA-C2A-C1A	2.07	118.75	111.97
18	A	824	CLA	C1D-ND-C4D	2.07	107.76	106.31
18	a	824	CLA	C1D-ND-C4D	2.07	107.76	106.31
20	B	844	BCR	C34-C9-C8	2.07	121.24	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	844	BCR	C34-C9-C8	2.07	121.24	118.09
29	5a	314	CHL	C3C-C4C-NC	-2.06	109.60	114.65
29	5b	314	CHL	C3C-C4C-NC	-2.06	109.60	114.65
18	b	821	CLA	CHD-C1D-C2D	2.06	129.78	125.49
18	a	827	CLA	C2A-C1A-CHA	2.06	127.45	123.87
18	b	854	CLA	C3B-C4B-NB	-2.06	108.69	110.53
18	A	812	CLA	CHD-C1D-ND	-2.06	121.90	124.80
18	a	812	CLA	CHD-C1D-ND	-2.06	121.90	124.80
18	b	804	CLA	C3B-C4B-NB	-2.06	108.69	110.53
18	g	203	CLA	CHD-C1D-C2D	2.06	129.77	125.49
18	A	822	CLA	C4A-NA-C1A	2.06	107.62	106.68
18	3a	304	CLA	C4A-NA-C1A	2.06	107.62	106.68
18	a	822	CLA	C4A-NA-C1A	2.06	107.62	106.68
18	B	822	CLA	C3B-C4B-NB	-2.06	108.69	110.53
18	b	822	CLA	C3B-C4B-NB	-2.06	108.69	110.53
18	A	825	CLA	CHD-C1D-C2D	2.06	129.77	125.49
18	6a	307	CLA	CHD-C1D-C2D	2.06	129.77	125.49
18	a	825	CLA	CHD-C1D-C2D	2.06	129.77	125.49
18	6b	307	CLA	CHD-C1D-C2D	2.06	129.77	125.49
18	6a	313	CLA	C1D-ND-C4D	2.06	107.75	106.31
18	6b	313	CLA	C1D-ND-C4D	2.06	107.75	106.31
29	3a	301	CHL	C3C-C4C-NC	-2.06	109.62	114.65
29	3b	301	CHL	C3C-C4C-NC	-2.06	109.62	114.65
18	3a	313	CLA	C4A-NA-C1A	2.06	107.62	106.68
18	B	830	CLA	CHD-C1D-C2D	2.05	129.76	125.49
18	b	830	CLA	CHD-C1D-C2D	2.05	129.76	125.49
18	3b	305	CLA	CHD-C1D-C2D	2.05	129.76	125.49
29	5b	306	CHL	C3C-C4C-NC	-2.05	109.64	114.65
18	3a	311	CLA	C4A-NA-C1A	2.05	107.61	106.68
18	3b	311	CLA	C4A-NA-C1A	2.05	107.61	106.68
18	B	817	CLA	CHD-C1D-C2D	2.05	129.75	125.49
18	b	817	CLA	CHD-C1D-C2D	2.05	129.75	125.49
18	6a	308	CLA	C3B-C4B-NB	-2.05	108.70	110.53
18	6b	308	CLA	C3B-C4B-NB	-2.05	108.70	110.53
20	A	849	BCR	C10-C11-C12	2.05	129.14	123.20
29	2a	313	CHL	C3C-C4C-NC	-2.05	109.64	114.65
29	2b	313	CHL	C3C-C4C-NC	-2.05	109.64	114.65
25	3a	316	LUT	C35-C15-C14	2.05	127.71	123.52
25	3b	316	LUT	C35-C15-C14	2.05	127.71	123.52
18	2a	302	CLA	CHD-C1D-C2D	2.05	129.75	125.49
18	2b	302	CLA	CHD-C1D-C2D	2.05	129.75	125.49
18	B	801	CLA	C4D-CHA-C1A	2.05	123.69	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	801	CLA	C4D-CHA-C1A	2.05	123.69	121.24
29	6a	309	CHL	OBD-CAD-CBD	-2.05	122.82	125.82
29	6b	309	CHL	OBD-CAD-CBD	-2.05	122.82	125.82
18	G	203	CLA	CHD-C1D-C2D	2.05	129.74	125.49
18	B	834	CLA	CHD-C1D-C2D	2.05	129.74	125.49
18	b	834	CLA	CHD-C1D-C2D	2.05	129.74	125.49
29	6a	309	CHL	C3C-C4C-NC	-2.05	109.65	114.65
18	B	853	CLA	C1D-ND-C4D	2.05	107.75	106.31
18	b	853	CLA	C1D-ND-C4D	2.05	107.75	106.31
20	G	201	BCR	C27-C26-C25	-2.04	119.94	122.70
20	g	201	BCR	C27-C26-C25	-2.04	119.94	122.70
25	5a	316	LUT	C18-C5-C6	2.04	126.71	124.48
25	5b	316	LUT	C18-C5-C6	2.04	126.71	124.48
29	5b	301	CHL	C3C-C4C-NC	-2.04	109.66	114.65
18	A	827	CLA	C2A-C1A-CHA	2.04	127.41	123.87
25	2b	315	LUT	C18-C5-C4	-2.04	110.67	114.42
29	5a	306	CHL	C3C-C4C-NC	-2.04	109.66	114.65
29	6b	309	CHL	C3C-C4C-NC	-2.04	109.66	114.65
20	a	849	BCR	C10-C11-C12	2.04	129.11	123.20
20	G	201	BCR	C30-C25-C24	-2.04	110.12	115.65
20	g	201	BCR	C30-C25-C24	-2.04	110.12	115.65
18	2b	301	CLA	CHD-C1D-C2D	2.04	129.73	125.49
18	B	821	CLA	C2A-C1A-CHA	2.04	127.41	123.87
18	b	821	CLA	C2A-C1A-CHA	2.04	127.41	123.87
18	2a	303	CLA	CHD-C1D-C2D	2.04	129.73	125.49
18	2b	303	CLA	CHD-C1D-C2D	2.04	129.73	125.49
18	F	305	CLA	CGD-CBD-CAD	-2.04	104.25	110.85
18	f	305	CLA	CGD-CBD-CAD	-2.04	104.25	110.85
29	6a	304	CHL	C3C-C4C-NC	-2.04	109.67	114.65
18	6a	306	CLA	CHD-C1D-C2D	2.04	129.72	125.49
20	G	204	BCR	C23-C24-C25	2.04	132.44	127.00
18	B	820	CLA	C4A-NA-C1A	2.04	107.61	106.68
29	5a	305	CHL	C3C-C4C-NC	-2.04	109.67	114.65
29	5b	305	CHL	C3C-C4C-NC	-2.04	109.67	114.65
20	B	846	BCR	C16-C15-C14	2.04	127.68	123.52
25	6a	318	LUT	C35-C15-C14	2.04	127.68	123.52
25	6b	318	LUT	C35-C15-C14	2.04	127.68	123.52
20	g	204	BCR	C23-C24-C25	2.03	132.43	127.00
18	b	806	CLA	CHD-C1D-C2D	2.03	129.72	125.49
18	6b	306	CLA	CHD-C1D-C2D	2.03	129.72	125.49
18	a	821	CLA	C4A-NA-C1A	2.03	107.61	106.68
21	B	847	DGD	C4D-C3D-C2D	2.03	114.40	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	847	DGD	C4D-C3D-C2D	2.03	114.40	110.83
29	5a	301	CHL	C3C-C4C-NC	-2.03	109.68	114.65
18	B	815	CLA	CHD-C1D-C2D	2.03	129.72	125.49
18	b	815	CLA	CHD-C1D-C2D	2.03	129.72	125.49
25	2a	315	LUT	C18-C5-C4	-2.03	110.69	114.42
18	3a	305	CLA	CHD-C1D-C2D	2.03	129.71	125.49
29	2a	305	CHL	C3C-C4C-NC	-2.03	109.69	114.65
29	2b	305	CHL	C3C-C4C-NC	-2.03	109.69	114.65
18	A	838	CLA	C4A-NA-C1A	2.03	107.61	106.68
25	6a	318	LUT	C39-C29-C28	2.03	121.19	118.09
29	2a	313	CHL	OBD-CAD-CBD	-2.03	122.85	125.82
29	2b	313	CHL	OBD-CAD-CBD	-2.03	122.85	125.82
18	6a	312	CLA	C3B-C4B-NB	-2.03	108.72	110.53
18	B	803	CLA	CHD-C1D-C2D	2.03	129.70	125.49
18	b	803	CLA	CHD-C1D-C2D	2.03	129.70	125.49
29	6b	304	CHL	C3C-C4C-NC	-2.02	109.70	114.65
18	3b	304	CLA	C4A-NA-C1A	2.02	107.60	106.68
20	J	102	BCR	C2-C3-C4	-2.02	106.83	111.28
20	j	102	BCR	C2-C3-C4	-2.02	106.83	111.28
18	A	836	CLA	CHD-C1D-ND	-2.02	121.96	124.80
18	a	836	CLA	CHD-C1D-ND	-2.02	121.96	124.80
20	f	304	BCR	C4-C5-C6	-2.02	119.97	122.70
20	A	849	BCR	C4-C5-C6	-2.02	119.97	122.70
18	b	814	CLA	C4A-NA-C1A	2.02	107.60	106.68
18	B	806	CLA	CHD-C1D-C2D	2.02	129.69	125.49
29	2b	304	CHL	C3C-C4C-NC	-2.02	109.72	114.65
18	B	805	CLA	C3B-C4B-NB	-2.02	108.73	110.53
18	b	805	CLA	C3B-C4B-NB	-2.02	108.73	110.53
25	3b	316	LUT	C32-C33-C34	2.02	122.18	119.01
18	a	830	CLA	C3B-C4B-NB	-2.02	108.73	110.53
29	2a	304	CHL	C3C-C4C-NC	-2.02	109.72	114.65
20	A	848	BCR	C37-C22-C23	2.02	121.17	118.09
20	a	848	BCR	C37-C22-C23	2.02	121.17	118.09
25	3a	316	LUT	C32-C33-C34	2.02	122.18	119.01
29	2b	304	CHL	OBD-CAD-CBD	-2.01	122.87	125.82
18	B	827	CLA	CHD-C1D-C2D	2.01	129.68	125.49
18	b	827	CLA	CHD-C1D-C2D	2.01	129.68	125.49
25	6b	318	LUT	C39-C29-C28	2.01	121.16	118.09
18	A	821	CLA	CHD-C1D-C2D	2.01	129.67	125.49
18	a	821	CLA	CHD-C1D-C2D	2.01	129.67	125.49
18	A	842	CLA	CHD-C1D-C2D	2.01	129.67	125.49
18	2a	301	CLA	CHD-C1D-C2D	2.01	129.67	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	842	CLA	CHD-C1D-C2D	2.01	129.67	125.49
20	G	204	BCR	C37-C22-C23	2.01	121.16	118.09
20	g	204	BCR	C37-C22-C23	2.01	121.16	118.09
18	A	831	CLA	CHD-C1D-ND	-2.01	121.97	124.80
18	a	831	CLA	CHD-C1D-ND	-2.01	121.97	124.80
20	b	846	BCR	C16-C15-C14	2.01	127.63	123.52
18	6a	312	CLA	C2A-C1A-CHA	2.01	127.36	123.87
18	6b	312	CLA	C2A-C1A-CHA	2.01	127.36	123.87
29	2a	304	CHL	OBD-CAD-CBD	-2.01	122.87	125.82
18	A	816	CLA	C4A-NA-C1A	2.01	107.60	106.68
18	a	816	CLA	C4A-NA-C1A	2.01	107.60	106.68
20	a	849	BCR	C4-C5-C6	-2.01	119.99	122.70
20	B	848	BCR	C2-C3-C4	-2.01	106.86	111.28
20	b	848	BCR	C2-C3-C4	-2.01	106.86	111.28
18	F	303	CLA	CHD-C1D-C2D	2.01	129.66	125.49
18	f	303	CLA	CHD-C1D-C2D	2.01	129.66	125.49
20	F	304	BCR	C15-C16-C17	2.01	127.62	123.52
20	f	304	BCR	C15-C16-C17	2.00	127.62	123.52
20	A	847	BCR	C7-C6-C5	-2.00	116.94	121.56
20	a	847	BCR	C7-C6-C5	-2.00	116.94	121.56
29	5a	314	CHL	OBD-CAD-CBD	-2.00	122.89	125.82
29	5b	314	CHL	OBD-CAD-CBD	-2.00	122.89	125.82

All (262) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	B	801	CLA	ND
18	B	802	CLA	ND
18	B	803	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	812	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	819	CLA	ND
18	B	821	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND

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Mol	Chain	Res	Type	Atom
18	B	826	CLA	ND
18	B	830	CLA	ND
18	B	831	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	840	CLA	ND
18	B	853	CLA	ND
18	B	854	CLA	ND
18	F	302	CLA	ND
18	F	303	CLA	ND
18	F	305	CLA	ND
18	G	202	CLA	ND
18	G	203	CLA	ND
18	J	101	CLA	ND
18	L	301	CLA	ND
18	L	303	CLA	ND
18	b	801	CLA	ND
18	b	802	CLA	ND
18	b	803	CLA	ND
18	b	804	CLA	ND
18	b	805	CLA	ND
18	b	807	CLA	ND
18	b	808	CLA	ND
18	b	809	CLA	ND
18	b	812	CLA	ND
18	b	816	CLA	ND
18	b	817	CLA	ND
18	b	819	CLA	ND
18	b	821	CLA	ND
18	b	823	CLA	ND
18	b	824	CLA	ND
18	b	825	CLA	ND
18	b	826	CLA	ND
18	b	830	CLA	ND
18	b	831	CLA	ND
18	b	833	CLA	ND
18	b	834	CLA	ND
18	b	835	CLA	ND
18	b	836	CLA	ND

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Mol	Chain	Res	Type	Atom
18	b	837	CLA	ND
18	b	840	CLA	ND
18	b	853	CLA	ND
18	b	854	CLA	ND
18	f	302	CLA	ND
18	f	303	CLA	ND
18	f	305	CLA	ND
18	g	202	CLA	ND
18	g	203	CLA	ND
18	j	101	CLA	ND
18	l	301	CLA	ND
18	l	303	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND
18	A	806	CLA	ND
18	A	807	CLA	ND
18	A	808	CLA	ND
18	A	809	CLA	ND
18	A	811	CLA	ND
18	A	812	CLA	ND
18	A	813	CLA	ND
18	A	814	CLA	ND
18	A	817	CLA	ND
18	A	818	CLA	ND
18	A	822	CLA	ND
18	A	824	CLA	ND
18	A	825	CLA	ND
18	A	826	CLA	ND
18	A	827	CLA	ND
18	A	831	CLA	ND
18	A	832	CLA	ND
18	A	835	CLA	ND
18	A	836	CLA	ND
18	A	837	CLA	ND
18	A	838	CLA	ND
18	A	840	CLA	ND
18	A	841	CLA	ND
18	2a	301	CLA	ND
18	2a	302	CLA	ND
18	2a	303	CLA	ND
18	2a	307	CLA	ND

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Mol	Chain	Res	Type	Atom
18	2a	308	CLA	ND
18	2a	309	CLA	ND
18	2a	310	CLA	ND
18	2a	312	CLA	ND
18	3a	303	CLA	ND
18	3a	304	CLA	ND
18	3a	306	CLA	ND
18	3a	308	CLA	ND
18	3a	310	CLA	ND
18	3a	311	CLA	ND
18	3a	313	CLA	ND
18	3a	314	CLA	ND
18	5a	303	CLA	ND
18	5a	308	CLA	ND
18	5a	310	CLA	ND
18	5a	311	CLA	ND
18	5a	313	CLA	ND
18	6a	306	CLA	ND
18	6a	308	CLA	ND
18	6a	310	CLA	ND
18	6a	311	CLA	ND
18	6a	313	CLA	ND
18	6a	314	CLA	ND
18	6a	315	CLA	ND
18	6a	317	CLA	ND
18	K	201	CLA	ND
18	a	803	CLA	ND
18	a	804	CLA	ND
18	a	805	CLA	ND
18	a	806	CLA	ND
18	a	807	CLA	ND
18	a	808	CLA	ND
18	a	809	CLA	ND
18	a	811	CLA	ND
18	a	812	CLA	ND
18	a	813	CLA	ND
18	a	814	CLA	ND
18	a	817	CLA	ND
18	a	818	CLA	ND
18	a	822	CLA	ND
18	a	824	CLA	ND
18	a	825	CLA	ND

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Mol	Chain	Res	Type	Atom
18	a	826	CLA	ND
18	a	827	CLA	ND
18	a	831	CLA	ND
18	a	832	CLA	ND
18	a	835	CLA	ND
18	a	836	CLA	ND
18	a	837	CLA	ND
18	a	838	CLA	ND
18	a	840	CLA	ND
18	a	841	CLA	ND
18	2b	301	CLA	ND
18	2b	302	CLA	ND
18	2b	303	CLA	ND
18	2b	307	CLA	ND
18	2b	308	CLA	ND
18	2b	309	CLA	ND
18	2b	310	CLA	ND
18	2b	312	CLA	ND
18	3b	303	CLA	ND
18	3b	304	CLA	ND
18	3b	306	CLA	ND
18	3b	308	CLA	ND
18	3b	310	CLA	ND
18	3b	311	CLA	ND
18	3b	313	CLA	ND
18	3b	314	CLA	ND
18	5b	303	CLA	ND
18	5b	308	CLA	ND
18	5b	310	CLA	ND
18	5b	311	CLA	ND
18	5b	313	CLA	ND
18	6b	306	CLA	ND
18	6b	308	CLA	ND
18	6b	310	CLA	ND
18	6b	311	CLA	ND
18	6b	313	CLA	ND
18	6b	314	CLA	ND
18	6b	315	CLA	ND
18	6b	317	CLA	ND
18	k	201	CLA	ND
29	2a	304	CHL	NC
29	2a	304	CHL	ND

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Mol	Chain	Res	Type	Atom
29	2a	304	CHL	NA
29	2a	305	CHL	NC
29	2a	305	CHL	ND
29	2a	305	CHL	NA
29	2a	306	CHL	NC
29	2a	306	CHL	NA
29	2a	313	CHL	NC
29	2a	313	CHL	ND
29	2a	313	CHL	NA
29	3a	301	CHL	NC
29	3a	301	CHL	ND
29	3a	301	CHL	NA
29	3a	307	CHL	NC
29	3a	307	CHL	ND
29	3a	307	CHL	NA
29	3a	315	CHL	NC
29	3a	315	CHL	ND
29	3a	315	CHL	NA
29	5a	301	CHL	NC
29	5a	301	CHL	ND
29	5a	301	CHL	NA
29	5a	305	CHL	NC
29	5a	305	CHL	ND
29	5a	305	CHL	NA
29	5a	306	CHL	NC
29	5a	306	CHL	ND
29	5a	306	CHL	NA
29	5a	307	CHL	ND
29	5a	307	CHL	NA
29	5a	314	CHL	NC
29	5a	314	CHL	ND
29	5a	314	CHL	NA
29	6a	304	CHL	NC
29	6a	304	CHL	ND
29	6a	304	CHL	NA
29	6a	309	CHL	NC
29	6a	309	CHL	ND
29	6a	309	CHL	NA
29	2b	304	CHL	NC
29	2b	304	CHL	ND
29	2b	304	CHL	NA
29	2b	305	CHL	NC

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Mol	Chain	Res	Type	Atom
29	2b	305	CHL	ND
29	2b	305	CHL	NA
29	2b	306	CHL	NC
29	2b	306	CHL	NA
29	2b	313	CHL	NC
29	2b	313	CHL	ND
29	2b	313	CHL	NA
29	3b	301	CHL	NC
29	3b	301	CHL	ND
29	3b	301	CHL	NA
29	3b	307	CHL	NC
29	3b	307	CHL	ND
29	3b	307	CHL	NA
29	3b	315	CHL	NC
29	3b	315	CHL	ND
29	3b	315	CHL	NA
29	5b	301	CHL	NC
29	5b	301	CHL	ND
29	5b	301	CHL	NA
29	5b	305	CHL	NC
29	5b	305	CHL	ND
29	5b	305	CHL	NA
29	5b	306	CHL	NC
29	5b	306	CHL	ND
29	5b	306	CHL	NA
29	5b	307	CHL	ND
29	5b	307	CHL	NA
29	5b	314	CHL	NC
29	5b	314	CHL	ND
29	5b	314	CHL	NA
29	6b	304	CHL	NC
29	6b	304	CHL	ND
29	6b	304	CHL	NA
29	6b	309	CHL	NC
29	6b	309	CHL	ND
29	6b	309	CHL	NA

All (1475) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	803	CLA	CHA-CBD-CGD-O1D
18	B	803	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	808	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	CAD-CBD-CGD-O1D
18	B	821	CLA	CAD-CBD-CGD-O2D
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C3A-C2A-CAA-CBA
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	830	CLA	CBA-CGA-O2A-C1
18	B	830	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	CBA-CGA-O2A-C1
18	B	832	CLA	O1A-CGA-O2A-C1
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	CBA-CGA-O2A-C1
18	B	840	CLA	O1A-CGA-O2A-C1
18	B	854	CLA	C1A-C2A-CAA-CBA
18	F	305	CLA	CBD-CGD-O2D-CED
18	F	305	CLA	O1D-CGD-O2D-CED
18	b	803	CLA	CHA-CBD-CGD-O1D
18	b	803	CLA	CHA-CBD-CGD-O2D
18	b	808	CLA	CBA-CGA-O2A-C1
18	b	808	CLA	O1A-CGA-O2A-C1
18	b	816	CLA	C1A-C2A-CAA-CBA
18	b	820	CLA	CHA-CBD-CGD-O2D
18	b	821	CLA	C1A-C2A-CAA-CBA
18	b	821	CLA	CAD-CBD-CGD-O1D
18	b	821	CLA	CAD-CBD-CGD-O2D
18	b	823	CLA	C1A-C2A-CAA-CBA
18	b	823	CLA	C3A-C2A-CAA-CBA
18	b	824	CLA	CHA-CBD-CGD-O1D
18	b	824	CLA	CHA-CBD-CGD-O2D
18	b	830	CLA	CBA-CGA-O2A-C1
18	b	830	CLA	O1A-CGA-O2A-C1
18	b	832	CLA	CBA-CGA-O2A-C1
18	b	832	CLA	O1A-CGA-O2A-C1
18	b	832	CLA	CHA-CBD-CGD-O1D
18	b	832	CLA	CHA-CBD-CGD-O2D
18	b	840	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	b	840	CLA	O1A-CGA-O2A-C1
18	b	854	CLA	C1A-C2A-CAA-CBA
18	f	305	CLA	CBD-CGD-O2D-CED
18	f	305	CLA	O1D-CGD-O2D-CED
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CHA-CBD-CGD-O1D
18	A	808	CLA	CHA-CBD-CGD-O2D
18	A	809	CLA	CBA-CGA-O2A-C1
18	A	809	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	CHA-CBD-CGD-O1D
18	A	810	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	CBA-CGA-O2A-C1
18	A	816	CLA	O1A-CGA-O2A-C1
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	821	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	C4-C3-C5-C6
18	A	837	CLA	CBA-CGA-O2A-C1
18	A	837	CLA	O1A-CGA-O2A-C1
18	2a	301	CLA	CHA-CBD-CGD-O1D
18	2a	301	CLA	CHA-CBD-CGD-O2D
18	2a	308	CLA	C1A-C2A-CAA-CBA
18	2a	308	CLA	C3A-C2A-CAA-CBA
18	3a	302	CLA	CHA-CBD-CGD-O1D
18	3a	302	CLA	CHA-CBD-CGD-O2D
18	3a	303	CLA	CBD-CGD-O2D-CED
18	3a	303	CLA	O1D-CGD-O2D-CED
18	3a	312	CLA	C1A-C2A-CAA-CBA
18	5a	302	CLA	CHA-CBD-CGD-O1D
18	5a	302	CLA	CHA-CBD-CGD-O2D
18	5a	303	CLA	CHA-CBD-CGD-O1D
18	5a	303	CLA	CHA-CBD-CGD-O2D
18	6a	312	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	6a	313	CLA	C1A-C2A-CAA-CBA
18	a	804	CLA	CHA-CBD-CGD-O1D
18	a	804	CLA	CHA-CBD-CGD-O2D
18	a	808	CLA	CHA-CBD-CGD-O1D
18	a	808	CLA	CHA-CBD-CGD-O2D
18	a	809	CLA	CBA-CGA-O2A-C1
18	a	809	CLA	O1A-CGA-O2A-C1
18	a	810	CLA	CHA-CBD-CGD-O1D
18	a	810	CLA	CHA-CBD-CGD-O2D
18	a	815	CLA	C1A-C2A-CAA-CBA
18	a	816	CLA	CBA-CGA-O2A-C1
18	a	816	CLA	O1A-CGA-O2A-C1
18	a	817	CLA	C1A-C2A-CAA-CBA
18	a	817	CLA	C3A-C2A-CAA-CBA
18	a	821	CLA	CHA-CBD-CGD-O1D
18	a	821	CLA	CHA-CBD-CGD-O2D
18	a	829	CLA	CHA-CBD-CGD-O1D
18	a	829	CLA	CHA-CBD-CGD-O2D
18	a	830	CLA	CBA-CGA-O2A-C1
18	a	830	CLA	O1A-CGA-O2A-C1
18	a	836	CLA	CHA-CBD-CGD-O1D
18	a	836	CLA	CHA-CBD-CGD-O2D
18	a	836	CLA	C4-C3-C5-C6
18	a	837	CLA	CBA-CGA-O2A-C1
18	a	837	CLA	O1A-CGA-O2A-C1
18	2b	301	CLA	CHA-CBD-CGD-O1D
18	2b	301	CLA	CHA-CBD-CGD-O2D
18	2b	308	CLA	C1A-C2A-CAA-CBA
18	2b	308	CLA	C3A-C2A-CAA-CBA
18	3b	302	CLA	CHA-CBD-CGD-O1D
18	3b	302	CLA	CHA-CBD-CGD-O2D
18	3b	303	CLA	CBD-CGD-O2D-CED
18	3b	303	CLA	O1D-CGD-O2D-CED
18	3b	312	CLA	C1A-C2A-CAA-CBA
18	5b	302	CLA	CHA-CBD-CGD-O1D
18	5b	302	CLA	CHA-CBD-CGD-O2D
18	5b	303	CLA	CHA-CBD-CGD-O1D
18	5b	303	CLA	CHA-CBD-CGD-O2D
18	6b	312	CLA	C1A-C2A-CAA-CBA
18	6b	313	CLA	C1A-C2A-CAA-CBA
20	B	842	BCR	C23-C24-C25-C26
20	B	843	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
20	B	843	BCR	C36-C18-C19-C20
20	b	842	BCR	C23-C24-C25-C26
20	b	843	BCR	C17-C18-C19-C20
20	b	843	BCR	C36-C18-C19-C20
20	K	202	BCR	C23-C24-C25-C26
20	k	202	BCR	C23-C24-C25-C26
21	B	847	DGD	C2B-C1B-O2G-C2G
21	b	847	DGD	C2B-C1B-O2G-C2G
23	I	201	LMG	O6-C1-O1-C7
23	I	201	LMG	C11-C10-O7-C8
23	i	201	LMG	O6-C1-O1-C7
23	i	201	LMG	C11-C10-O7-C8
25	2a	314	LUT	C1-C6-C7-C8
25	2a	314	LUT	C5-C6-C7-C8
25	2a	314	LUT	C30-C31-C32-C33
25	6a	319	LUT	C1-C6-C7-C8
25	6a	319	LUT	C5-C6-C7-C8
25	6a	319	LUT	C29-C30-C31-C32
25	6a	319	LUT	C30-C31-C32-C33
25	2b	314	LUT	C1-C6-C7-C8
25	2b	314	LUT	C5-C6-C7-C8
25	2b	314	LUT	C30-C31-C32-C33
25	6b	319	LUT	C1-C6-C7-C8
25	6b	319	LUT	C5-C6-C7-C8
25	6b	319	LUT	C29-C30-C31-C32
25	6b	319	LUT	C30-C31-C32-C33
27	A	846	LHG	C3-O3-P-O4
27	A	846	LHG	C3-O3-P-O5
27	A	846	LHG	C3-O3-P-O6
27	A	846	LHG	O10-C23-O8-C6
27	A	846	LHG	C24-C23-O8-C6
27	6a	301	LHG	C3-O3-P-O5
27	6a	301	LHG	C4-O6-P-O5
27	a	846	LHG	C3-O3-P-O4
27	a	846	LHG	C3-O3-P-O5
27	a	846	LHG	C3-O3-P-O6
27	a	846	LHG	O10-C23-O8-C6
27	a	846	LHG	C24-C23-O8-C6
27	6b	301	LHG	C3-O3-P-O5
27	6b	301	LHG	C4-O6-P-O5
28	6a	302	LMU	C2'-C1'-O1'-C1
28	6a	302	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	6a	303	LMU	O5'-C1'-O1'-C1
28	6b	302	LMU	C2'-C1'-O1'-C1
28	6b	302	LMU	O5'-C1'-O1'-C1
28	6b	303	LMU	O5'-C1'-O1'-C1
29	2a	306	CHL	C1A-C2A-CAA-CBA
29	2a	306	CHL	C3A-C2A-CAA-CBA
29	2a	306	CHL	C1C-C2C-CMC-OMC
29	2a	306	CHL	C3C-C2C-CMC-OMC
29	3a	307	CHL	CBD-CGD-O2D-CED
29	3a	307	CHL	O1D-CGD-O2D-CED
29	5a	301	CHL	CAD-CBD-CGD-O2D
29	5a	306	CHL	CBD-CGD-O2D-CED
29	5a	306	CHL	O1D-CGD-O2D-CED
29	5a	307	CHL	C1A-C2A-CAA-CBA
29	5a	307	CHL	C1C-C2C-CMC-OMC
29	5a	307	CHL	C3C-C2C-CMC-OMC
29	6a	309	CHL	CHA-CBD-CGD-O2D
29	2b	306	CHL	C1A-C2A-CAA-CBA
29	2b	306	CHL	C3A-C2A-CAA-CBA
29	2b	306	CHL	C1C-C2C-CMC-OMC
29	2b	306	CHL	C3C-C2C-CMC-OMC
29	3b	307	CHL	CBD-CGD-O2D-CED
29	3b	307	CHL	O1D-CGD-O2D-CED
29	5b	301	CHL	CAD-CBD-CGD-O2D
29	5b	306	CHL	CBD-CGD-O2D-CED
29	5b	306	CHL	O1D-CGD-O2D-CED
29	5b	307	CHL	C1A-C2A-CAA-CBA
29	5b	307	CHL	C1C-C2C-CMC-OMC
29	5b	307	CHL	C3C-C2C-CMC-OMC
29	6b	309	CHL	CHA-CBD-CGD-O2D
28	A	852	LMU	O5B-C1B-O1B-C4'
28	a	852	LMU	O5B-C1B-O1B-C4'
29	5a	307	CHL	CBD-CGD-O2D-CED
29	5b	307	CHL	CBD-CGD-O2D-CED
23	I	201	LMG	O10-C28-O8-C9
23	J	103	LMG	O10-C28-O8-C9
23	i	201	LMG	O10-C28-O8-C9
23	j	103	LMG	O10-C28-O8-C9
18	3a	305	CLA	O1A-CGA-O2A-C1
18	3b	305	CLA	O1A-CGA-O2A-C1
28	A	852	LMU	C2B-C1B-O1B-C4'
28	a	852	LMU	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
21	B	847	DGD	O1B-C1B-O2G-C2G
21	b	847	DGD	O1B-C1B-O2G-C2G
23	I	201	LMG	O9-C10-O7-C8
23	i	201	LMG	O9-C10-O7-C8
18	3a	305	CLA	CBA-CGA-O2A-C1
18	3b	305	CLA	CBA-CGA-O2A-C1
18	B	854	CLA	C3-C5-C6-C7
18	b	854	CLA	C3-C5-C6-C7
23	I	201	LMG	C29-C28-O8-C9
23	J	103	LMG	C29-C28-O8-C9
23	i	201	LMG	C29-C28-O8-C9
23	j	103	LMG	C29-C28-O8-C9
18	A	816	CLA	C4-C3-C5-C6
18	2a	301	CLA	C4-C3-C5-C6
18	6a	306	CLA	C4-C3-C5-C6
18	a	816	CLA	C4-C3-C5-C6
18	2b	301	CLA	C4-C3-C5-C6
18	6b	306	CLA	C4-C3-C5-C6
18	2a	301	CLA	C2-C3-C5-C6
18	6a	306	CLA	C2-C3-C5-C6
18	2b	301	CLA	C2-C3-C5-C6
18	6b	306	CLA	C2-C3-C5-C6
28	6a	302	LMU	C3'-C4'-O1B-C1B
28	6b	302	LMU	C3'-C4'-O1B-C1B
20	B	843	BCR	C15-C16-C17-C18
20	b	843	BCR	C15-C16-C17-C18
25	2a	314	LUT	C33-C34-C35-C15
25	2a	315	LUT	C13-C14-C15-C35
25	2a	315	LUT	C33-C34-C35-C15
25	3a	317	LUT	C9-C10-C11-C12
25	6a	319	LUT	C33-C34-C35-C15
25	2b	314	LUT	C33-C34-C35-C15
25	2b	315	LUT	C13-C14-C15-C35
25	2b	315	LUT	C33-C34-C35-C15
25	3b	317	LUT	C9-C10-C11-C12
25	6b	319	LUT	C33-C34-C35-C15
18	A	841	CLA	C3-C5-C6-C7
18	a	841	CLA	C3-C5-C6-C7
29	5a	307	CHL	O1D-CGD-O2D-CED
29	5b	307	CHL	O1D-CGD-O2D-CED
18	A	829	CLA	C4-C3-C5-C6
18	a	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	A	816	CLA	C2-C3-C5-C6
18	A	829	CLA	C2-C3-C5-C6
18	a	816	CLA	C2-C3-C5-C6
18	a	829	CLA	C2-C3-C5-C6
29	2a	306	CHL	CBD-CGD-O2D-CED
29	2b	306	CHL	CBD-CGD-O2D-CED
18	B	823	CLA	C4-C3-C5-C6
18	B	832	CLA	C4-C3-C5-C6
18	b	823	CLA	C4-C3-C5-C6
18	b	832	CLA	C4-C3-C5-C6
18	B	823	CLA	C2-C3-C5-C6
18	B	832	CLA	C2-C3-C5-C6
18	b	823	CLA	C2-C3-C5-C6
18	b	832	CLA	C2-C3-C5-C6
18	B	816	CLA	C3-C5-C6-C7
18	b	816	CLA	C3-C5-C6-C7
20	B	844	BCR	C37-C22-C23-C24
20	J	102	BCR	C37-C22-C23-C24
20	b	844	BCR	C37-C22-C23-C24
20	j	102	BCR	C37-C22-C23-C24
20	A	849	BCR	C7-C8-C9-C34
20	a	849	BCR	C7-C8-C9-C34
25	J	105	LUT	C11-C12-C13-C20
25	j	105	LUT	C11-C12-C13-C20
25	3a	317	LUT	C11-C12-C13-C20
25	6a	319	LUT	C11-C12-C13-C20
25	6a	319	LUT	C27-C28-C29-C39
25	3b	317	LUT	C11-C12-C13-C20
25	6b	319	LUT	C11-C12-C13-C20
25	6b	319	LUT	C27-C28-C29-C39
20	J	102	BCR	C7-C8-C9-C10
20	J	102	BCR	C21-C22-C23-C24
20	j	102	BCR	C7-C8-C9-C10
20	j	102	BCR	C21-C22-C23-C24
20	A	849	BCR	C7-C8-C9-C10
20	a	849	BCR	C7-C8-C9-C10
25	3a	317	LUT	C11-C12-C13-C14
25	5a	317	LUT	C7-C8-C9-C10
25	3b	317	LUT	C11-C12-C13-C14
25	5b	317	LUT	C7-C8-C9-C10
18	A	828	CLA	C2A-CAA-CBA-CGA
18	a	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	B	847	DGD	O2G-C2G-C3G-O3G
21	b	847	DGD	O2G-C2G-C3G-O3G
23	I	201	LMG	O1-C7-C8-O7
23	i	201	LMG	O1-C7-C8-O7
18	B	812	CLA	C13-C15-C16-C17
18	b	812	CLA	C13-C15-C16-C17
23	I	201	LMG	C28-C29-C30-C31
23	i	201	LMG	C28-C29-C30-C31
18	B	832	CLA	C3-C5-C6-C7
18	b	832	CLA	C3-C5-C6-C7
18	A	826	CLA	C5-C6-C7-C8
18	a	826	CLA	C5-C6-C7-C8
18	B	804	CLA	C10-C11-C12-C13
18	B	830	CLA	C10-C11-C12-C13
18	b	804	CLA	C10-C11-C12-C13
18	b	830	CLA	C10-C11-C12-C13
21	B	847	DGD	C1A-C2A-C3A-C4A
21	b	847	DGD	C1A-C2A-C3A-C4A
18	B	817	CLA	C15-C16-C17-C18
18	b	817	CLA	C15-C16-C17-C18
18	B	810	CLA	C10-C11-C12-C13
18	b	810	CLA	C10-C11-C12-C13
18	A	824	CLA	C10-C11-C12-C13
18	a	824	CLA	C10-C11-C12-C13
18	3a	312	CLA	C3-C5-C6-C7
18	3b	312	CLA	C3-C5-C6-C7
20	B	843	BCR	C20-C21-C22-C37
20	b	843	BCR	C20-C21-C22-C37
25	J	105	LUT	C11-C10-C9-C19
25	j	105	LUT	C11-C10-C9-C19
25	2a	314	LUT	C39-C29-C30-C31
25	6a	319	LUT	C11-C10-C9-C19
25	6a	319	LUT	C39-C29-C30-C31
25	6a	319	LUT	C40-C33-C34-C35
25	2b	314	LUT	C39-C29-C30-C31
25	6b	319	LUT	C11-C10-C9-C19
25	6b	319	LUT	C39-C29-C30-C31
25	6b	319	LUT	C40-C33-C34-C35
20	B	851	BCR	C7-C8-C9-C34
20	J	102	BCR	C7-C8-C9-C34
20	b	851	BCR	C7-C8-C9-C34
20	j	102	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
25	5a	317	LUT	C7-C8-C9-C19
25	6a	319	LUT	C31-C32-C33-C40
25	5b	317	LUT	C7-C8-C9-C19
25	6b	319	LUT	C31-C32-C33-C40
20	B	844	BCR	C21-C22-C23-C24
20	b	844	BCR	C21-C22-C23-C24
25	J	105	LUT	C11-C12-C13-C14
25	j	105	LUT	C11-C12-C13-C14
25	6a	319	LUT	C11-C12-C13-C14
25	6a	319	LUT	C27-C28-C29-C30
25	6b	319	LUT	C11-C12-C13-C14
25	6b	319	LUT	C27-C28-C29-C30
18	B	838	CLA	C2A-CAA-CBA-CGA
18	b	838	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	C2A-CAA-CBA-CGA
18	a	823	CLA	C2A-CAA-CBA-CGA
29	3a	307	CHL	C2A-CAA-CBA-CGA
29	5a	307	CHL	C2A-CAA-CBA-CGA
29	3b	307	CHL	C2A-CAA-CBA-CGA
29	5b	307	CHL	C2A-CAA-CBA-CGA
20	B	843	BCR	C20-C21-C22-C23
20	b	843	BCR	C20-C21-C22-C23
25	J	105	LUT	C11-C10-C9-C8
25	j	105	LUT	C11-C10-C9-C8
25	2a	314	LUT	C28-C29-C30-C31
25	2b	314	LUT	C28-C29-C30-C31
18	6a	312	CLA	C2-C1-O2A-CGA
18	6b	312	CLA	C2-C1-O2A-CGA
18	B	828	CLA	C6-C7-C8-C10
18	b	828	CLA	C6-C7-C8-C10
22	B	849	LFA	C16-C17-C18-C19
22	b	849	LFA	C16-C17-C18-C19
27	A	846	LHG	C13-C14-C15-C16
27	a	846	LHG	C13-C14-C15-C16
18	5a	312	CLA	C2A-CAA-CBA-CGA
18	5b	312	CLA	C2A-CAA-CBA-CGA
18	A	827	CLA	C10-C11-C12-C13
18	a	827	CLA	C10-C11-C12-C13
28	6a	302	LMU	C3-C4-C5-C6
28	6b	302	LMU	C3-C4-C5-C6
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	854	CLA	C3A-C2A-CAA-CBA
18	b	812	CLA	C3A-C2A-CAA-CBA
18	b	816	CLA	C3A-C2A-CAA-CBA
18	b	854	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	832	CLA	C3A-C2A-CAA-CBA
18	6a	312	CLA	C3A-C2A-CAA-CBA
18	a	803	CLA	C3A-C2A-CAA-CBA
18	a	832	CLA	C3A-C2A-CAA-CBA
18	6b	312	CLA	C3A-C2A-CAA-CBA
29	2a	313	CHL	C3A-C2A-CAA-CBA
29	5a	307	CHL	C3A-C2A-CAA-CBA
29	2b	313	CHL	C3A-C2A-CAA-CBA
29	5b	307	CHL	C3A-C2A-CAA-CBA
27	2a	316	LHG	C23-C24-C25-C26
27	2b	316	LHG	C23-C24-C25-C26
18	B	828	CLA	C6-C7-C8-C9
18	b	828	CLA	C6-C7-C8-C9
23	B	850	LMG	C7-C8-C9-O8
23	b	850	LMG	C7-C8-C9-O8
19	A	843	PQN	C26-C27-C28-C29
19	a	843	PQN	C26-C27-C28-C29
20	B	842	BCR	C23-C24-C25-C30
20	B	843	BCR	C1-C6-C7-C8
20	B	844	BCR	C1-C6-C7-C8
20	B	851	BCR	C5-C6-C7-C8
20	F	301	BCR	C23-C24-C25-C26
20	F	301	BCR	C23-C24-C25-C30
20	G	201	BCR	C23-C24-C25-C26
20	G	204	BCR	C23-C24-C25-C26
20	G	204	BCR	C23-C24-C25-C30
20	I	202	BCR	C23-C24-C25-C26
20	J	102	BCR	C23-C24-C25-C26
20	L	304	BCR	C1-C6-C7-C8
20	L	304	BCR	C5-C6-C7-C8
20	M	101	BCR	C1-C6-C7-C8
20	M	101	BCR	C23-C24-C25-C26
20	b	842	BCR	C23-C24-C25-C30
20	b	843	BCR	C1-C6-C7-C8
20	b	844	BCR	C1-C6-C7-C8
20	b	851	BCR	C5-C6-C7-C8
20	f	301	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	f	301	BCR	C23-C24-C25-C30
20	g	201	BCR	C23-C24-C25-C26
20	g	204	BCR	C23-C24-C25-C26
20	g	204	BCR	C23-C24-C25-C30
20	i	202	BCR	C23-C24-C25-C26
20	j	102	BCR	C23-C24-C25-C26
20	l	304	BCR	C1-C6-C7-C8
20	l	304	BCR	C5-C6-C7-C8
20	m	101	BCR	C1-C6-C7-C8
20	m	101	BCR	C23-C24-C25-C26
20	A	848	BCR	C23-C24-C25-C26
20	A	849	BCR	C1-C6-C7-C8
20	A	851	BCR	C1-C6-C7-C8
20	A	851	BCR	C23-C24-C25-C26
20	A	851	BCR	C23-C24-C25-C30
20	K	202	BCR	C23-C24-C25-C30
20	a	848	BCR	C23-C24-C25-C26
20	a	849	BCR	C1-C6-C7-C8
20	a	851	BCR	C1-C6-C7-C8
20	a	851	BCR	C23-C24-C25-C26
20	a	851	BCR	C23-C24-C25-C30
20	k	202	BCR	C23-C24-C25-C30
25	2a	315	LUT	C1-C6-C7-C8
25	2b	315	LUT	C1-C6-C7-C8
18	B	801	CLA	C13-C15-C16-C17
18	b	801	CLA	C13-C15-C16-C17
18	A	803	CLA	C3-C5-C6-C7
18	A	805	CLA	C3-C5-C6-C7
18	a	803	CLA	C3-C5-C6-C7
18	a	805	CLA	C3-C5-C6-C7
21	B	847	DGD	C4A-C5A-C6A-C7A
21	b	847	DGD	C4A-C5A-C6A-C7A
18	A	809	CLA	C2A-CAA-CBA-CGA
18	a	809	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C10-C11-C12-C13
18	b	833	CLA	C10-C11-C12-C13
21	B	847	DGD	C3A-C4A-C5A-C6A
21	b	847	DGD	C3A-C4A-C5A-C6A
18	B	801	CLA	C2-C3-C5-C6
18	b	801	CLA	C2-C3-C5-C6
18	B	810	CLA	C6-C7-C8-C9
18	b	810	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	5a	319	LMG	C11-C12-C13-C14
23	5b	319	LMG	C11-C12-C13-C14
23	J	103	LMG	O6-C1-O1-C7
23	j	103	LMG	O6-C1-O1-C7
28	6a	303	LMU	C2'-C1'-O1'-C1
28	6b	303	LMU	C2'-C1'-O1'-C1
20	B	848	BCR	C37-C22-C23-C24
20	b	848	BCR	C37-C22-C23-C24
18	B	801	CLA	C4-C3-C5-C6
18	b	801	CLA	C4-C3-C5-C6
23	J	103	LMG	O6-C5-C6-O5
23	j	103	LMG	O6-C5-C6-O5
28	6a	302	LMU	O5'-C5'-C6'-O6'
28	6b	302	LMU	O5'-C5'-C6'-O6'
23	B	850	LMG	C11-C10-O7-C8
23	b	850	LMG	C11-C10-O7-C8
27	2a	316	LHG	C9-C10-C11-C12
27	2b	316	LHG	C9-C10-C11-C12
27	6a	301	LHG	C29-C30-C31-C32
27	6b	301	LHG	C29-C30-C31-C32
28	6b	303	LMU	O5'-C5'-C6'-O6'
28	6a	303	LMU	O5'-C5'-C6'-O6'
18	A	817	CLA	C2-C3-C5-C6
18	a	817	CLA	C2-C3-C5-C6
18	B	830	CLA	C2A-CAA-CBA-CGA
18	b	830	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C2A-CAA-CBA-CGA
18	a	817	CLA	C2A-CAA-CBA-CGA
29	2a	306	CHL	O1D-CGD-O2D-CED
29	2b	306	CHL	O1D-CGD-O2D-CED
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	b	826	CLA	C1A-C2A-CAA-CBA
18	b	838	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	832	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C1A-C2A-CAA-CBA
18	a	803	CLA	C1A-C2A-CAA-CBA
18	a	810	CLA	C1A-C2A-CAA-CBA
18	a	832	CLA	C1A-C2A-CAA-CBA
18	a	842	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	a	818	CLA	C8-C10-C11-C12
27	5a	318	LHG	C11-C10-C9-C8
27	5b	318	LHG	C11-C10-C9-C8
18	A	818	CLA	C8-C10-C11-C12
18	B	823	CLA	C11-C12-C13-C15
18	b	823	CLA	C11-C12-C13-C15
18	A	817	CLA	C6-C7-C8-C10
18	a	817	CLA	C6-C7-C8-C10
23	5a	319	LMG	C4-C5-C6-O5
23	5b	319	LMG	C4-C5-C6-O5
18	A	817	CLA	C6-C7-C8-C9
18	A	818	CLA	C11-C12-C13-C14
18	A	827	CLA	C6-C7-C8-C9
18	a	817	CLA	C6-C7-C8-C9
18	a	818	CLA	C11-C12-C13-C14
18	a	827	CLA	C6-C7-C8-C9
27	5a	320	LHG	C10-C11-C12-C13
27	5b	320	LHG	C10-C11-C12-C13
23	5b	319	LMG	C13-C14-C15-C16
23	J	104	LMG	C7-C8-C9-O8
23	j	104	LMG	C7-C8-C9-O8
23	5a	319	LMG	C13-C14-C15-C16
23	B	850	LMG	C28-C29-C30-C31
23	b	850	LMG	C28-C29-C30-C31
29	2a	313	CHL	CHA-CBD-CGD-O1D
29	2a	313	CHL	CHA-CBD-CGD-O2D
29	2b	313	CHL	CHA-CBD-CGD-O1D
29	2b	313	CHL	CHA-CBD-CGD-O2D
27	A	845	LHG	C23-C24-C25-C26
27	a	845	LHG	C23-C24-C25-C26
18	B	806	CLA	C4-C3-C5-C6
18	b	806	CLA	C4-C3-C5-C6
18	A	817	CLA	C4-C3-C5-C6
18	a	817	CLA	C4-C3-C5-C6
18	B	806	CLA	C2-C3-C5-C6
18	b	806	CLA	C2-C3-C5-C6
18	B	809	CLA	C8-C10-C11-C12
18	b	809	CLA	C8-C10-C11-C12
18	B	830	CLA	C8-C10-C11-C12
18	b	830	CLA	C8-C10-C11-C12
23	B	850	LMG	C30-C31-C32-C33
23	b	850	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
18	A	806	CLA	C5-C6-C7-C8
18	a	806	CLA	C5-C6-C7-C8
18	B	830	CLA	O2A-C1-C2-C3
18	b	830	CLA	O2A-C1-C2-C3
19	A	843	PQN	C25-C26-C27-C28
19	a	843	PQN	C25-C26-C27-C28
23	I	201	LMG	O7-C8-C9-O8
23	i	201	LMG	O7-C8-C9-O8
18	5a	315	CLA	CAA-CBA-CGA-O2A
18	5b	315	CLA	CAA-CBA-CGA-O2A
21	B	847	DGD	C6B-C7B-C8B-C9B
21	b	847	DGD	C6B-C7B-C8B-C9B
18	B	852	CLA	C3-C5-C6-C7
18	b	852	CLA	C3-C5-C6-C7
18	B	812	CLA	C4-C3-C5-C6
18	b	812	CLA	C4-C3-C5-C6
28	A	852	LMU	C2-C1-O1'-C1'
28	6a	303	LMU	C2-C1-O1'-C1'
28	a	852	LMU	C2-C1-O1'-C1'
28	6b	303	LMU	C2-C1-O1'-C1'
18	B	805	CLA	C14-C13-C15-C16
18	B	823	CLA	C11-C12-C13-C14
18	b	805	CLA	C14-C13-C15-C16
18	b	823	CLA	C11-C12-C13-C14
18	5a	302	CLA	C6-C7-C8-C9
18	5b	302	CLA	C6-C7-C8-C9
21	B	847	DGD	C4E-C5E-C6E-O5E
21	b	847	DGD	C4E-C5E-C6E-O5E
18	B	853	CLA	C2A-CAA-CBA-CGA
18	b	853	CLA	C2A-CAA-CBA-CGA
23	J	103	LMG	C2-C1-O1-C7
23	j	103	LMG	C2-C1-O1-C7
27	6a	301	LHG	O6-C4-C5-C6
27	6b	301	LHG	O6-C4-C5-C6
18	B	805	CLA	C12-C13-C15-C16
18	B	836	CLA	C6-C7-C8-C10
18	b	805	CLA	C12-C13-C15-C16
18	b	836	CLA	C6-C7-C8-C10
18	A	818	CLA	C11-C12-C13-C15
18	5a	302	CLA	C6-C7-C8-C10
18	a	818	CLA	C11-C12-C13-C15
18	5b	302	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	B	850	LMG	C15-C16-C17-C18
23	b	850	LMG	C15-C16-C17-C18
18	A	806	CLA	C4-C3-C5-C6
18	A	833	CLA	C4-C3-C5-C6
18	5a	302	CLA	C4-C3-C5-C6
18	6a	313	CLA	C3A-C2A-CAA-CBA
18	a	806	CLA	C4-C3-C5-C6
18	5b	302	CLA	C4-C3-C5-C6
18	6b	313	CLA	C3A-C2A-CAA-CBA
18	B	812	CLA	C2-C3-C5-C6
18	b	812	CLA	C2-C3-C5-C6
18	A	805	CLA	C2-C3-C5-C6
18	a	805	CLA	C2-C3-C5-C6
21	B	847	DGD	O1G-C1G-C2G-C3G
21	B	847	DGD	C1G-C2G-C3G-O3G
21	b	847	DGD	O1G-C1G-C2G-C3G
21	b	847	DGD	C1G-C2G-C3G-O3G
23	I	201	LMG	O1-C7-C8-C9
23	i	201	LMG	O1-C7-C8-C9
27	A	846	LHG	C4-C5-C6-O8
27	a	846	LHG	C4-C5-C6-O8
19	A	843	PQN	C26-C27-C28-C30
19	a	843	PQN	C26-C27-C28-C30
29	2a	313	CHL	C1A-C2A-CAA-CBA
29	2b	313	CHL	C1A-C2A-CAA-CBA
18	A	805	CLA	C4-C3-C5-C6
18	a	805	CLA	C4-C3-C5-C6
18	a	833	CLA	C4-C3-C5-C6
27	6a	301	LHG	C23-C24-C25-C26
27	6b	301	LHG	C23-C24-C25-C26
18	A	806	CLA	C2-C3-C5-C6
18	5a	302	CLA	C2-C3-C5-C6
18	a	806	CLA	C2-C3-C5-C6
18	5b	302	CLA	C2-C3-C5-C6
18	A	818	CLA	C10-C11-C12-C13
23	I	201	LMG	C30-C31-C32-C33
23	i	201	LMG	C30-C31-C32-C33
20	B	843	BCR	C5-C6-C7-C8
20	B	846	BCR	C23-C24-C25-C26
20	B	848	BCR	C23-C24-C25-C30
20	B	851	BCR	C1-C6-C7-C8
20	B	851	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	F	304	BCR	C23-C24-C25-C26
20	G	201	BCR	C1-C6-C7-C8
20	M	101	BCR	C5-C6-C7-C8
20	b	843	BCR	C5-C6-C7-C8
20	b	846	BCR	C23-C24-C25-C26
20	b	848	BCR	C23-C24-C25-C30
20	b	851	BCR	C1-C6-C7-C8
20	b	851	BCR	C23-C24-C25-C26
20	f	304	BCR	C23-C24-C25-C26
20	g	201	BCR	C1-C6-C7-C8
20	m	101	BCR	C5-C6-C7-C8
20	A	847	BCR	C5-C6-C7-C8
20	A	848	BCR	C23-C24-C25-C30
20	A	851	BCR	C5-C6-C7-C8
20	a	847	BCR	C5-C6-C7-C8
20	a	848	BCR	C23-C24-C25-C30
20	a	851	BCR	C5-C6-C7-C8
25	2a	315	LUT	C5-C6-C7-C8
25	2b	315	LUT	C5-C6-C7-C8
18	a	818	CLA	C10-C11-C12-C13
27	A	846	LHG	O7-C5-C6-O8
27	a	846	LHG	O7-C5-C6-O8
23	B	850	LMG	O9-C10-O7-C8
23	b	850	LMG	O9-C10-O7-C8
23	B	850	LMG	C10-C11-C12-C13
23	b	850	LMG	C10-C11-C12-C13
23	B	850	LMG	C31-C32-C33-C34
23	b	850	LMG	C31-C32-C33-C34
21	B	847	DGD	C7B-C8B-C9B-CAB
21	b	847	DGD	C7B-C8B-C9B-CAB
18	B	805	CLA	C16-C17-C18-C20
18	b	805	CLA	C16-C17-C18-C20
18	B	840	CLA	C14-C13-C15-C16
18	b	840	CLA	C14-C13-C15-C16
23	5a	319	LMG	O6-C5-C6-O5
23	5b	319	LMG	O6-C5-C6-O5
26	A	802	CL0	CAA-CBA-CGA-O2A
26	a	802	CL0	CAA-CBA-CGA-O2A
18	A	833	CLA	C2-C3-C5-C6
18	a	833	CLA	C2-C3-C5-C6
23	I	201	LMG	C4-C5-C6-O5
23	i	201	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
18	A	827	CLA	C6-C7-C8-C10
18	a	827	CLA	C6-C7-C8-C10
20	B	851	BCR	C7-C8-C9-C10
20	b	851	BCR	C7-C8-C9-C10
21	B	847	DGD	C4B-C5B-C6B-C7B
21	b	847	DGD	C4B-C5B-C6B-C7B
18	G	202	CLA	C2A-CAA-CBA-CGA
18	g	202	CLA	C2A-CAA-CBA-CGA
18	A	816	CLA	C2A-CAA-CBA-CGA
18	a	816	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	C3-C5-C6-C7
18	a	834	CLA	C3-C5-C6-C7
27	A	845	LHG	C10-C11-C12-C13
27	a	845	LHG	C10-C11-C12-C13
27	6a	301	LHG	O6-C4-C5-O7
27	6b	301	LHG	O6-C4-C5-O7
27	5a	318	LHG	C4-C5-C6-O8
27	5b	318	LHG	C4-C5-C6-O8
18	A	808	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	C2A-CAA-CBA-CGA
18	a	808	CLA	C2A-CAA-CBA-CGA
18	a	826	CLA	C2A-CAA-CBA-CGA
27	6a	301	LHG	O7-C7-C8-C9
27	6b	301	LHG	O7-C7-C8-C9
21	B	847	DGD	O1G-C1G-C2G-O2G
21	b	847	DGD	O1G-C1G-C2G-O2G
18	B	836	CLA	C6-C7-C8-C9
18	b	836	CLA	C6-C7-C8-C9
23	5a	319	LMG	C10-C11-C12-C13
25	J	105	LUT	C26-C27-C28-C29
25	j	105	LUT	C26-C27-C28-C29
25	6a	319	LUT	C26-C27-C28-C29
25	6b	319	LUT	C26-C27-C28-C29
23	5b	319	LMG	C10-C11-C12-C13
23	I	201	LMG	C2-C1-O1-C7
23	i	201	LMG	C2-C1-O1-C7
23	J	104	LMG	C29-C28-O8-C9
23	j	104	LMG	C29-C28-O8-C9
18	B	817	CLA	C4-C3-C5-C6
18	b	817	CLA	C4-C3-C5-C6
18	3a	312	CLA	C4-C3-C5-C6
18	3b	312	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	6a	302	LMU	C5'-C4'-O1B-C1B
28	6b	302	LMU	C5'-C4'-O1B-C1B
23	B	850	LMG	C4-C5-C6-O5
23	b	850	LMG	C4-C5-C6-O5
20	A	847	BCR	C7-C8-C9-C34
20	a	847	BCR	C7-C8-C9-C34
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	b	812	CLA	C1A-C2A-CAA-CBA
18	b	833	CLA	C1A-C2A-CAA-CBA
18	A	830	CLA	C1A-C2A-CAA-CBA
18	a	830	CLA	C1A-C2A-CAA-CBA
18	B	810	CLA	C4-C3-C5-C6
18	b	810	CLA	C4-C3-C5-C6
18	A	830	CLA	C2A-CAA-CBA-CGA
18	2a	308	CLA	C2A-CAA-CBA-CGA
18	a	830	CLA	C2A-CAA-CBA-CGA
18	2b	308	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2-C3-C5-C6
18	a	836	CLA	C2-C3-C5-C6
23	B	850	LMG	C18-C19-C20-C21
23	b	850	LMG	C18-C19-C20-C21
23	J	104	LMG	O10-C28-O8-C9
23	j	104	LMG	O10-C28-O8-C9
18	B	836	CLA	C4-C3-C5-C6
18	b	836	CLA	C4-C3-C5-C6
18	A	841	CLA	C2A-CAA-CBA-CGA
18	a	841	CLA	C2A-CAA-CBA-CGA
18	6a	307	CLA	C1-C2-C3-C4
18	6b	307	CLA	C1-C2-C3-C4
18	B	840	CLA	C3-C5-C6-C7
18	b	840	CLA	C3-C5-C6-C7
23	B	850	LMG	O7-C8-C9-O8
23	J	104	LMG	O7-C8-C9-O8
23	b	850	LMG	O7-C8-C9-O8
23	j	104	LMG	O7-C8-C9-O8
27	5a	318	LHG	O7-C5-C6-O8
27	5b	318	LHG	O7-C5-C6-O8
18	B	817	CLA	C2-C3-C5-C6
18	b	817	CLA	C2-C3-C5-C6
18	L	301	CLA	CAD-CBD-CGD-O2D
18	l	301	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	805	CLA	CAD-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	841	CLA	CAD-CBD-CGD-O2D
18	a	805	CLA	CAD-CBD-CGD-O2D
18	a	806	CLA	CAD-CBD-CGD-O2D
18	a	841	CLA	CAD-CBD-CGD-O2D
29	6a	304	CHL	CAD-CBD-CGD-O2D
29	6b	304	CHL	CAD-CBD-CGD-O2D
18	6a	305	CLA	C3-C5-C6-C7
18	6b	305	CLA	C3-C5-C6-C7
18	A	820	CLA	C2A-CAA-CBA-CGA
18	a	820	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	CAA-CBA-CGA-O2A
18	a	829	CLA	CAA-CBA-CGA-O2A
18	B	820	CLA	CHA-CBD-CGD-O1D
18	G	203	CLA	CHA-CBD-CGD-O1D
18	G	203	CLA	CHA-CBD-CGD-O2D
18	L	301	CLA	CAD-CBD-CGD-O1D
18	b	820	CLA	CHA-CBD-CGD-O1D
18	g	203	CLA	CHA-CBD-CGD-O1D
18	g	203	CLA	CHA-CBD-CGD-O2D
18	l	301	CLA	CAD-CBD-CGD-O1D
18	A	805	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	833	CLA	CHA-CBD-CGD-O1D
18	A	833	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CAD-CBD-CGD-O1D
18	5a	313	CLA	CHA-CBD-CGD-O1D
18	a	805	CLA	CAD-CBD-CGD-O1D
18	a	806	CLA	CAD-CBD-CGD-O1D
18	a	833	CLA	CHA-CBD-CGD-O1D
18	a	833	CLA	CHA-CBD-CGD-O2D
18	a	841	CLA	CAD-CBD-CGD-O1D
18	5b	313	CLA	CHA-CBD-CGD-O1D
26	A	802	CL0	CHA-CBD-CGD-O2D
26	a	802	CL0	CHA-CBD-CGD-O2D
27	6a	301	LHG	C3-O3-P-O4
27	6a	301	LHG	C3-O3-P-O6
27	6b	301	LHG	C3-O3-P-O4
27	6b	301	LHG	C3-O3-P-O6
29	2a	305	CHL	CHA-CBD-CGD-O1D
29	2a	305	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	3a	315	CHL	CHA-CBD-CGD-O2D
29	5a	301	CHL	CAD-CBD-CGD-O1D
29	5a	306	CHL	CHA-CBD-CGD-O1D
29	5a	306	CHL	CHA-CBD-CGD-O2D
29	6a	304	CHL	CAD-CBD-CGD-O1D
29	6a	309	CHL	CAD-CBD-CGD-O2D
29	2b	305	CHL	CHA-CBD-CGD-O1D
29	2b	305	CHL	CHA-CBD-CGD-O2D
29	3b	315	CHL	CHA-CBD-CGD-O2D
29	5b	301	CHL	CAD-CBD-CGD-O1D
29	5b	306	CHL	CHA-CBD-CGD-O1D
29	5b	306	CHL	CHA-CBD-CGD-O2D
29	6b	304	CHL	CAD-CBD-CGD-O1D
29	6b	309	CHL	CAD-CBD-CGD-O2D
18	A	820	CLA	C4-C3-C5-C6
18	A	828	CLA	C4-C3-C5-C6
18	a	820	CLA	C4-C3-C5-C6
18	a	828	CLA	C4-C3-C5-C6
20	B	845	BCR	C1-C6-C7-C8
20	J	102	BCR	C23-C24-C25-C30
20	b	845	BCR	C1-C6-C7-C8
20	j	102	BCR	C23-C24-C25-C30
20	A	848	BCR	C1-C6-C7-C8
20	K	202	BCR	C1-C6-C7-C8
20	a	848	BCR	C1-C6-C7-C8
20	k	202	BCR	C1-C6-C7-C8
25	3a	317	LUT	C1-C6-C7-C8
25	6a	320	LUT	C1-C6-C7-C8
25	3b	317	LUT	C1-C6-C7-C8
25	6b	320	LUT	C1-C6-C7-C8
21	B	847	DGD	C6A-C7A-C8A-C9A
21	b	847	DGD	C6A-C7A-C8A-C9A
18	B	810	CLA	C2-C3-C5-C6
18	b	810	CLA	C2-C3-C5-C6
18	B	805	CLA	C16-C17-C18-C19
18	b	805	CLA	C16-C17-C18-C19
28	6a	302	LMU	O5B-C1B-O1B-C4'
28	6b	302	LMU	O5B-C1B-O1B-C4'
23	B	850	LMG	C16-C17-C18-C19
23	b	850	LMG	C16-C17-C18-C19
20	B	848	BCR	C18-C19-C20-C21
20	b	848	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	J	105	LUT	C30-C31-C32-C33
25	j	105	LUT	C30-C31-C32-C33
25	6a	318	LUT	C30-C31-C32-C33
25	6b	318	LUT	C30-C31-C32-C33
21	B	847	DGD	CCB-CDB-CEB-CFB
21	b	847	DGD	CCB-CDB-CEB-CFB
25	J	105	LUT	C6-C7-C8-C9
25	j	105	LUT	C6-C7-C8-C9
18	B	839	CLA	C4-C3-C5-C6
18	b	839	CLA	C4-C3-C5-C6
27	2b	316	LHG	C11-C10-C9-C8
27	2a	316	LHG	C11-C10-C9-C8
23	I	201	LMG	C10-C11-C12-C13
23	i	201	LMG	C10-C11-C12-C13
26	A	802	CL0	C4-C3-C5-C6
26	a	802	CL0	C4-C3-C5-C6
23	I	201	LMG	C7-C8-C9-O8
23	i	201	LMG	C7-C8-C9-O8
25	2a	314	LUT	C31-C32-C33-C40
25	2b	314	LUT	C31-C32-C33-C40
18	B	802	CLA	C2A-CAA-CBA-CGA
18	B	811	CLA	C2A-CAA-CBA-CGA
18	B	831	CLA	C2A-CAA-CBA-CGA
18	b	802	CLA	C2A-CAA-CBA-CGA
18	b	811	CLA	C2A-CAA-CBA-CGA
18	b	831	CLA	C2A-CAA-CBA-CGA
20	B	843	BCR	C19-C20-C21-C22
20	b	843	BCR	C19-C20-C21-C22
18	B	805	CLA	C4-C3-C5-C6
18	b	805	CLA	C4-C3-C5-C6
23	I	201	LMG	O6-C5-C6-O5
21	B	847	DGD	O6E-C5E-C6E-O5E
21	b	847	DGD	O6E-C5E-C6E-O5E
23	i	201	LMG	O6-C5-C6-O5
27	5a	320	LHG	C9-C10-C11-C12
27	5b	320	LHG	C9-C10-C11-C12
27	A	846	LHG	O8-C23-C24-C25
27	a	846	LHG	O8-C23-C24-C25
18	B	852	CLA	C8-C10-C11-C12
18	b	852	CLA	C8-C10-C11-C12
18	B	830	CLA	C4-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	b	830	CLA	C4-C3-C5-C6
18	b	833	CLA	C4-C3-C5-C6
18	A	801	CLA	C4-C3-C5-C6
18	A	812	CLA	C4-C3-C5-C6
18	a	801	CLA	C4-C3-C5-C6
18	a	812	CLA	C4-C3-C5-C6
26	A	802	CL0	C2-C3-C5-C6
26	a	802	CL0	C2-C3-C5-C6
18	3a	312	CLA	CAA-CBA-CGA-O2A
18	3b	312	CLA	CAA-CBA-CGA-O2A
28	6a	302	LMU	C2B-C1B-O1B-C4'
28	6b	302	LMU	C2B-C1B-O1B-C4'
18	A	815	CLA	C3A-C2A-CAA-CBA
18	5a	312	CLA	C4-C3-C5-C6
18	a	815	CLA	C3A-C2A-CAA-CBA
18	5b	312	CLA	C4-C3-C5-C6
29	3a	315	CHL	C3A-C2A-CAA-CBA
29	3b	315	CHL	C3A-C2A-CAA-CBA
18	A	828	CLA	C2-C3-C5-C6
18	a	828	CLA	C2-C3-C5-C6
18	A	839	CLA	C8-C10-C11-C12
18	a	839	CLA	C8-C10-C11-C12
18	K	201	CLA	CAA-CBA-CGA-O1A
18	k	201	CLA	CAA-CBA-CGA-O1A
20	B	843	BCR	C11-C10-C9-C34
20	B	845	BCR	C35-C13-C14-C15
20	B	851	BCR	C11-C10-C9-C34
20	F	304	BCR	C35-C13-C14-C15
20	b	843	BCR	C11-C10-C9-C34
20	b	845	BCR	C35-C13-C14-C15
20	b	851	BCR	C11-C10-C9-C34
20	f	304	BCR	C35-C13-C14-C15
20	A	851	BCR	C11-C10-C9-C34
20	A	851	BCR	C16-C17-C18-C36
20	a	851	BCR	C11-C10-C9-C34
20	a	851	BCR	C16-C17-C18-C36
25	J	105	LUT	C39-C29-C30-C31
25	j	105	LUT	C39-C29-C30-C31
25	6a	318	LUT	C39-C29-C30-C31
25	6a	320	LUT	C40-C33-C34-C35
25	6b	318	LUT	C39-C29-C30-C31
25	6b	320	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	J	104	LMG	C23-C24-C25-C26
23	j	104	LMG	C23-C24-C25-C26
18	5a	315	CLA	CAA-CBA-CGA-O1A
18	5b	315	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C5-C6-C7-C8
18	b	805	CLA	C5-C6-C7-C8
18	6a	314	CLA	CAA-CBA-CGA-O1A
18	6b	314	CLA	CAA-CBA-CGA-O1A
29	6a	304	CHL	CAA-CBA-CGA-O1A
29	6b	304	CHL	CAA-CBA-CGA-O1A
18	B	852	CLA	C4-C3-C5-C6
18	B	853	CLA	C4-C3-C5-C6
18	b	852	CLA	C4-C3-C5-C6
18	b	853	CLA	C4-C3-C5-C6
18	B	836	CLA	C2-C3-C5-C6
18	b	836	CLA	C2-C3-C5-C6
18	3a	312	CLA	C2-C3-C5-C6
18	3b	312	CLA	C2-C3-C5-C6
18	5a	311	CLA	CAA-CBA-CGA-O2A
18	5b	311	CLA	CAA-CBA-CGA-O2A
18	3a	314	CLA	CAA-CBA-CGA-O1A
18	6a	308	CLA	CAA-CBA-CGA-O2A
18	3b	314	CLA	CAA-CBA-CGA-O1A
18	6b	308	CLA	CAA-CBA-CGA-O2A
18	B	801	CLA	C11-C10-C8-C9
18	B	830	CLA	C6-C7-C8-C9
18	b	801	CLA	C11-C10-C8-C9
18	b	830	CLA	C6-C7-C8-C9
23	j	104	LMG	C11-C12-C13-C14
21	B	847	DGD	CAB-CBB-CCB-CDB
21	b	847	DGD	CAB-CBB-CCB-CDB
23	J	104	LMG	C11-C12-C13-C14
18	b	801	CLA	C8-C10-C11-C12
18	B	801	CLA	C8-C10-C11-C12
29	6a	304	CHL	CAA-CBA-CGA-O2A
29	6b	304	CHL	CAA-CBA-CGA-O2A
18	5a	312	CLA	CAA-CBA-CGA-O2A
18	5b	312	CLA	CAA-CBA-CGA-O2A
18	B	830	CLA	C2-C3-C5-C6
18	b	830	CLA	C2-C3-C5-C6
18	A	801	CLA	C2-C3-C5-C6
18	A	820	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	5a	312	CLA	C2-C3-C5-C6
18	a	801	CLA	C2-C3-C5-C6
18	a	820	CLA	C2-C3-C5-C6
18	5b	312	CLA	C2-C3-C5-C6
18	2a	303	CLA	CAA-CBA-CGA-O2A
18	2a	309	CLA	CAA-CBA-CGA-O2A
18	2b	303	CLA	CAA-CBA-CGA-O2A
18	2b	309	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	C1A-C2A-CAA-CBA
18	b	840	CLA	C1A-C2A-CAA-CBA
18	5a	303	CLA	C1A-C2A-CAA-CBA
18	6a	316	CLA	C1A-C2A-CAA-CBA
18	5b	303	CLA	C1A-C2A-CAA-CBA
18	6b	316	CLA	C1A-C2A-CAA-CBA
20	B	843	BCR	C11-C10-C9-C8
20	B	845	BCR	C12-C13-C14-C15
20	B	851	BCR	C11-C10-C9-C8
20	F	304	BCR	C12-C13-C14-C15
20	b	843	BCR	C11-C10-C9-C8
20	b	845	BCR	C12-C13-C14-C15
20	b	851	BCR	C11-C10-C9-C8
20	f	304	BCR	C12-C13-C14-C15
20	A	851	BCR	C11-C10-C9-C8
20	A	851	BCR	C16-C17-C18-C19
20	a	851	BCR	C11-C10-C9-C8
20	a	851	BCR	C16-C17-C18-C19
25	J	105	LUT	C28-C29-C30-C31
25	j	105	LUT	C28-C29-C30-C31
25	6a	318	LUT	C28-C29-C30-C31
25	6a	319	LUT	C32-C33-C34-C35
25	6a	320	LUT	C32-C33-C34-C35
25	6b	318	LUT	C28-C29-C30-C31
25	6b	319	LUT	C32-C33-C34-C35
25	6b	320	LUT	C32-C33-C34-C35
20	B	845	BCR	C23-C24-C25-C30
20	G	201	BCR	C5-C6-C7-C8
20	M	101	BCR	C23-C24-C25-C30
20	b	845	BCR	C23-C24-C25-C30
20	g	201	BCR	C5-C6-C7-C8
20	m	101	BCR	C23-C24-C25-C30
18	B	822	CLA	CAA-CBA-CGA-O1A
18	b	822	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	6a	313	CLA	CAA-CBA-CGA-O1A
18	6b	313	CLA	CAA-CBA-CGA-O1A
18	2a	309	CLA	CAA-CBA-CGA-O1A
18	5a	311	CLA	CAA-CBA-CGA-O1A
18	6a	314	CLA	CAA-CBA-CGA-O2A
18	2b	309	CLA	CAA-CBA-CGA-O1A
18	5b	311	CLA	CAA-CBA-CGA-O1A
18	6b	314	CLA	CAA-CBA-CGA-O2A
29	2a	306	CHL	CAA-CBA-CGA-O1A
29	2a	313	CHL	CAA-CBA-CGA-O1A
29	5a	305	CHL	CAA-CBA-CGA-O1A
29	2b	306	CHL	CAA-CBA-CGA-O1A
29	2b	313	CHL	CAA-CBA-CGA-O1A
29	5b	305	CHL	CAA-CBA-CGA-O1A
18	B	809	CLA	C4-C3-C5-C6
18	b	809	CLA	C4-C3-C5-C6
18	2a	308	CLA	C4-C3-C5-C6
18	2b	308	CLA	C4-C3-C5-C6
18	B	839	CLA	C2-C3-C5-C6
18	b	839	CLA	C2-C3-C5-C6
18	G	203	CLA	CAA-CBA-CGA-O2A
18	g	203	CLA	CAA-CBA-CGA-O2A
18	6a	308	CLA	CAA-CBA-CGA-O1A
18	6b	308	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C11-C10-C8-C7
18	B	810	CLA	C6-C7-C8-C10
18	b	809	CLA	C11-C10-C8-C7
18	b	810	CLA	C6-C7-C8-C10
18	A	806	CLA	C12-C13-C15-C16
18	a	806	CLA	C12-C13-C15-C16
18	B	822	CLA	CAA-CBA-CGA-O2A
18	b	822	CLA	CAA-CBA-CGA-O2A
18	6a	313	CLA	CAA-CBA-CGA-O2A
18	6b	313	CLA	CAA-CBA-CGA-O2A
18	K	201	CLA	CAA-CBA-CGA-O2A
18	k	201	CLA	CAA-CBA-CGA-O2A
18	2a	302	CLA	CAA-CBA-CGA-O2A
18	2b	302	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	C2-C3-C5-C6
18	B	833	CLA	C2-C3-C5-C6
18	B	852	CLA	C2-C3-C5-C6
18	B	853	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	b	805	CLA	C2-C3-C5-C6
18	b	833	CLA	C2-C3-C5-C6
18	b	852	CLA	C2-C3-C5-C6
18	b	853	CLA	C2-C3-C5-C6
18	A	812	CLA	C2-C3-C5-C6
18	a	812	CLA	C2-C3-C5-C6
18	2a	303	CLA	CAA-CBA-CGA-O1A
18	2b	303	CLA	CAA-CBA-CGA-O1A
29	2a	306	CHL	CAA-CBA-CGA-O2A
29	2b	306	CHL	CAA-CBA-CGA-O2A
18	A	839	CLA	C11-C10-C8-C9
18	a	839	CLA	C11-C10-C8-C9
27	a	845	LHG	C31-C32-C33-C34
27	A	845	LHG	C31-C32-C33-C34
29	5a	305	CHL	CAA-CBA-CGA-O2A
29	5b	305	CHL	CAA-CBA-CGA-O2A
18	B	840	CLA	C13-C15-C16-C17
18	b	840	CLA	C13-C15-C16-C17
18	2b	311	CLA	CAA-CBA-CGA-O2A
18	A	816	CLA	C3-C5-C6-C7
18	a	816	CLA	C3-C5-C6-C7
18	G	203	CLA	CAA-CBA-CGA-O1A
18	g	203	CLA	CAA-CBA-CGA-O1A
18	2a	311	CLA	CAA-CBA-CGA-O2A
18	A	822	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	CAA-CBA-CGA-O2A
18	a	822	CLA	CAA-CBA-CGA-O2A
18	a	842	CLA	CAA-CBA-CGA-O2A
18	L	301	CLA	CAA-CBA-CGA-O2A
18	l	301	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O2A
27	5a	320	LHG	O6-C4-C5-O7
27	5b	320	LHG	O6-C4-C5-O7
18	A	827	CLA	C4-C3-C5-C6
18	a	827	CLA	C4-C3-C5-C6
18	3a	310	CLA	CAA-CBA-CGA-O2A
18	3a	314	CLA	CAA-CBA-CGA-O2A
18	a	815	CLA	CAA-CBA-CGA-O2A
18	3b	310	CLA	CAA-CBA-CGA-O2A
18	3b	314	CLA	CAA-CBA-CGA-O2A
18	5a	310	CLA	CAA-CBA-CGA-O2A
18	5b	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2a	310	CLA	CAA-CBA-CGA-O2A
18	2b	310	CLA	CAA-CBA-CGA-O2A
29	2a	313	CHL	CAA-CBA-CGA-O2A
29	2b	313	CHL	CAA-CBA-CGA-O2A
20	B	848	BCR	C11-C10-C9-C34
20	b	848	BCR	C11-C10-C9-C34
26	A	802	CL0	CHA-CBD-CGD-O1D
26	a	802	CL0	CHA-CBD-CGD-O1D
29	2a	304	CHL	CHA-CBD-CGD-O1D
29	2a	304	CHL	CHA-CBD-CGD-O2D
29	2a	306	CHL	CHA-CBD-CGD-O1D
29	2a	306	CHL	CHA-CBD-CGD-O2D
29	5a	314	CHL	CHA-CBD-CGD-O2D
29	2b	304	CHL	CHA-CBD-CGD-O1D
29	2b	304	CHL	CHA-CBD-CGD-O2D
29	2b	306	CHL	CHA-CBD-CGD-O1D
29	2b	306	CHL	CHA-CBD-CGD-O2D
29	5b	314	CHL	CHA-CBD-CGD-O2D
18	A	817	CLA	CAA-CBA-CGA-O2A
18	a	817	CLA	CAA-CBA-CGA-O2A
18	2a	302	CLA	CAA-CBA-CGA-O1A
18	2b	302	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	C2-C3-C5-C6
18	b	809	CLA	C2-C3-C5-C6
18	B	804	CLA	C8-C10-C11-C12
18	b	804	CLA	C8-C10-C11-C12
18	2a	310	CLA	CAA-CBA-CGA-O1A
18	3a	310	CLA	CAA-CBA-CGA-O1A
18	5a	304	CLA	CAA-CBA-CGA-O2A
18	6a	317	CLA	CAA-CBA-CGA-O2A
18	2b	310	CLA	CAA-CBA-CGA-O1A
18	3b	310	CLA	CAA-CBA-CGA-O1A
18	5b	304	CLA	CAA-CBA-CGA-O2A
18	6b	317	CLA	CAA-CBA-CGA-O2A
27	A	846	LHG	O10-C23-C24-C25
27	a	846	LHG	O10-C23-C24-C25
23	B	850	LMG	O6-C5-C6-O5
18	A	835	CLA	CAA-CBA-CGA-O2A
18	2a	312	CLA	CAA-CBA-CGA-O2A
18	a	835	CLA	CAA-CBA-CGA-O2A
18	2b	312	CLA	CAA-CBA-CGA-O2A
29	2a	304	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	2b	304	CHL	CAA-CBA-CGA-O2A
18	B	817	CLA	C2A-CAA-CBA-CGA
18	b	817	CLA	C2A-CAA-CBA-CGA
18	B	830	CLA	C2-C1-O2A-CGA
18	b	830	CLA	C2-C1-O2A-CGA
18	B	831	CLA	C3A-C2A-CAA-CBA
18	b	831	CLA	C3A-C2A-CAA-CBA
18	5a	303	CLA	C3A-C2A-CAA-CBA
18	6a	316	CLA	C3A-C2A-CAA-CBA
18	5b	303	CLA	C3A-C2A-CAA-CBA
18	6b	316	CLA	C3A-C2A-CAA-CBA
27	6b	301	LHG	C30-C31-C32-C33
18	B	854	CLA	CAA-CBA-CGA-O2A
18	b	854	CLA	CAA-CBA-CGA-O2A
27	6a	301	LHG	C30-C31-C32-C33
23	b	850	LMG	O6-C5-C6-O5
18	B	829	CLA	CAA-CBA-CGA-O2A
18	b	829	CLA	CAA-CBA-CGA-O2A
18	A	815	CLA	CAA-CBA-CGA-O1A
18	6a	310	CLA	CAA-CBA-CGA-O2A
18	a	815	CLA	CAA-CBA-CGA-O1A
18	6b	310	CLA	CAA-CBA-CGA-O2A
20	B	843	BCR	C18-C19-C20-C21
20	b	843	BCR	C18-C19-C20-C21
18	L	301	CLA	CAA-CBA-CGA-O1A
18	l	301	CLA	CAA-CBA-CGA-O1A
27	a	846	LHG	C10-C11-C12-C13
18	F	302	CLA	CAA-CBA-CGA-O2A
18	f	302	CLA	CAA-CBA-CGA-O2A
18	A	822	CLA	CAA-CBA-CGA-O1A
18	2a	311	CLA	CAA-CBA-CGA-O1A
18	a	822	CLA	CAA-CBA-CGA-O1A
18	2b	311	CLA	CAA-CBA-CGA-O1A
18	5b	310	CLA	CAA-CBA-CGA-O1A
27	A	846	LHG	C10-C11-C12-C13
18	5a	310	CLA	CAA-CBA-CGA-O1A
20	B	848	BCR	C11-C10-C9-C8
20	b	848	BCR	C11-C10-C9-C8
25	2a	314	LUT	C32-C33-C34-C35
25	2b	314	LUT	C32-C33-C34-C35
18	A	842	CLA	CAA-CBA-CGA-O1A
18	6a	317	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	a	842	CLA	CAA-CBA-CGA-O1A
18	6b	317	CLA	CAA-CBA-CGA-O1A
18	2a	312	CLA	CAA-CBA-CGA-O1A
18	6a	310	CLA	CAA-CBA-CGA-O1A
18	2b	312	CLA	CAA-CBA-CGA-O1A
18	6b	310	CLA	CAA-CBA-CGA-O1A
18	5a	304	CLA	CAA-CBA-CGA-O1A
18	5b	304	CLA	CAA-CBA-CGA-O1A
21	B	847	DGD	C5B-C6B-C7B-C8B
21	b	847	DGD	C5B-C6B-C7B-C8B
18	B	829	CLA	CAA-CBA-CGA-O1A
18	b	829	CLA	CAA-CBA-CGA-O1A
26	A	802	CL0	CAA-CBA-CGA-O1A
26	a	802	CL0	CAA-CBA-CGA-O1A
18	F	302	CLA	CAA-CBA-CGA-O1A
18	f	302	CLA	CAA-CBA-CGA-O1A
18	A	812	CLA	CAA-CBA-CGA-O2A
18	a	812	CLA	CAA-CBA-CGA-O2A
18	b	809	CLA	CAA-CBA-CGA-O2A
18	a	835	CLA	CAA-CBA-CGA-O1A
18	B	809	CLA	CAA-CBA-CGA-O2A
18	2a	308	CLA	C2-C3-C5-C6
18	2b	308	CLA	C2-C3-C5-C6
18	A	835	CLA	CAA-CBA-CGA-O1A
29	2b	304	CHL	CAA-CBA-CGA-O1A
18	B	801	CLA	C11-C10-C8-C7
18	B	804	CLA	C11-C12-C13-C15
18	B	830	CLA	C6-C7-C8-C10
18	B	840	CLA	C12-C13-C15-C16
18	b	801	CLA	C11-C10-C8-C7
18	b	804	CLA	C11-C12-C13-C15
18	b	830	CLA	C6-C7-C8-C10
18	b	840	CLA	C12-C13-C15-C16
18	A	839	CLA	C11-C10-C8-C7
18	a	839	CLA	C11-C10-C8-C7
29	2a	304	CHL	CAA-CBA-CGA-O1A
18	B	813	CLA	C2B-C3B-CAB-CBB
18	B	821	CLA	C2B-C3B-CAB-CBB
18	B	827	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	F	305	CLA	C2B-C3B-CAB-CBB
18	L	303	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	b	813	CLA	C2B-C3B-CAB-CBB
18	b	821	CLA	C2B-C3B-CAB-CBB
18	b	827	CLA	C2B-C3B-CAB-CBB
18	b	836	CLA	C2B-C3B-CAB-CBB
18	f	305	CLA	C2B-C3B-CAB-CBB
18	l	303	CLA	C2B-C3B-CAB-CBB
18	A	811	CLA	C2B-C3B-CAB-CBB
18	A	813	CLA	C2B-C3B-CAB-CBB
18	A	837	CLA	C2B-C3B-CAB-CBB
18	A	841	CLA	C2B-C3B-CAB-CBB
18	2a	301	CLA	C2B-C3B-CAB-CBB
18	3a	302	CLA	C2B-C3B-CAB-CBB
18	3a	304	CLA	C2B-C3B-CAB-CBB
18	3a	305	CLA	C2B-C3B-CAB-CBB
18	5a	302	CLA	C2B-C3B-CAB-CBB
18	6a	305	CLA	C2B-C3B-CAB-CBB
18	a	811	CLA	C2B-C3B-CAB-CBB
18	a	813	CLA	C2B-C3B-CAB-CBB
18	a	837	CLA	C2B-C3B-CAB-CBB
18	a	841	CLA	C2B-C3B-CAB-CBB
18	2b	301	CLA	C2B-C3B-CAB-CBB
18	3b	302	CLA	C2B-C3B-CAB-CBB
18	3b	304	CLA	C2B-C3B-CAB-CBB
18	3b	305	CLA	C2B-C3B-CAB-CBB
18	5b	302	CLA	C2B-C3B-CAB-CBB
18	6b	305	CLA	C2B-C3B-CAB-CBB
20	B	848	BCR	C23-C24-C25-C26
20	B	851	BCR	C23-C24-C25-C30
20	F	301	BCR	C1-C6-C7-C8
20	F	304	BCR	C1-C6-C7-C8
20	F	304	BCR	C23-C24-C25-C30
20	G	201	BCR	C23-C24-C25-C30
20	I	202	BCR	C1-C6-C7-C8
20	b	848	BCR	C23-C24-C25-C26
20	b	851	BCR	C23-C24-C25-C30
20	f	301	BCR	C1-C6-C7-C8
20	f	304	BCR	C1-C6-C7-C8
20	f	304	BCR	C23-C24-C25-C30
20	g	201	BCR	C23-C24-C25-C30
20	i	202	BCR	C1-C6-C7-C8
20	A	847	BCR	C1-C6-C7-C8
20	a	847	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	J	105	LUT	C1-C6-C7-C8
25	j	105	LUT	C1-C6-C7-C8
18	B	838	CLA	CAA-CBA-CGA-O2A
18	b	838	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	CAA-CBA-CGA-O2A
18	a	833	CLA	CAA-CBA-CGA-O2A
23	B	850	LMG	O8-C28-C29-C30
23	b	850	LMG	O8-C28-C29-C30
27	A	846	LHG	C9-C10-C11-C12
27	a	846	LHG	C9-C10-C11-C12
23	B	850	LMG	C11-C12-C13-C14
23	b	850	LMG	C11-C12-C13-C14
23	I	201	LMG	C11-C12-C13-C14
23	i	201	LMG	C11-C12-C13-C14
18	B	809	CLA	C10-C11-C12-C13
18	J	101	CLA	CAA-CBA-CGA-O2A
18	j	101	CLA	CAA-CBA-CGA-O2A
18	b	809	CLA	C10-C11-C12-C13
18	5a	303	CLA	CAA-CBA-CGA-O2A
18	6a	306	CLA	CAA-CBA-CGA-O2A
18	6b	306	CLA	CAA-CBA-CGA-O2A
27	A	846	LHG	C11-C12-C13-C14
27	a	846	LHG	C11-C12-C13-C14
18	5b	303	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O2A
18	5a	308	CLA	CAA-CBA-CGA-O1A
18	5b	308	CLA	CAA-CBA-CGA-O1A
18	b	811	CLA	CAA-CBA-CGA-O2A
18	B	809	CLA	C11-C10-C8-C9
18	b	809	CLA	C11-C10-C8-C9
18	B	816	CLA	CAA-CBA-CGA-O2A
18	b	816	CLA	CAA-CBA-CGA-O2A
18	B	801	CLA	C4B-C3B-CAB-CBB
18	B	804	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C4B-C3B-CAB-CBB
18	B	828	CLA	C4B-C3B-CAB-CBB
18	B	833	CLA	C4B-C3B-CAB-CBB
18	B	854	CLA	C4B-C3B-CAB-CBB
18	b	801	CLA	C4B-C3B-CAB-CBB
18	b	804	CLA	C1A-C2A-CAA-CBA
18	b	819	CLA	C4B-C3B-CAB-CBB
18	b	828	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	b	833	CLA	C4B-C3B-CAB-CBB
18	b	854	CLA	C4B-C3B-CAB-CBB
18	A	810	CLA	C4B-C3B-CAB-CBB
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C4B-C3B-CAB-CBB
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	853	CLA	C4B-C3B-CAB-CBB
18	3a	309	CLA	C1A-C2A-CAA-CBA
18	5a	311	CLA	C4B-C3B-CAB-CBB
18	5a	312	CLA	C4B-C3B-CAB-CBB
18	6a	307	CLA	C4B-C3B-CAB-CBB
18	6a	317	CLA	C4B-C3B-CAB-CBB
18	a	810	CLA	C4B-C3B-CAB-CBB
18	a	812	CLA	C1A-C2A-CAA-CBA
18	a	815	CLA	C4B-C3B-CAB-CBB
18	a	834	CLA	C1A-C2A-CAA-CBA
18	a	835	CLA	C4B-C3B-CAB-CBB
18	a	853	CLA	C4B-C3B-CAB-CBB
18	3b	309	CLA	C1A-C2A-CAA-CBA
18	5b	311	CLA	C4B-C3B-CAB-CBB
18	5b	312	CLA	C4B-C3B-CAB-CBB
18	6b	307	CLA	C4B-C3B-CAB-CBB
18	6b	317	CLA	C4B-C3B-CAB-CBB
26	A	802	CL0	C8-C10-C11-C12
26	a	802	CL0	C8-C10-C11-C12
18	A	806	CLA	CAA-CBA-CGA-O2A
18	6a	315	CLA	CAA-CBA-CGA-O2A
18	a	806	CLA	CAA-CBA-CGA-O2A
18	6b	315	CLA	CAA-CBA-CGA-O2A
27	A	845	LHG	O7-C5-C6-O8
27	a	845	LHG	O7-C5-C6-O8
18	A	811	CLA	CAA-CBA-CGA-O1A
18	5a	308	CLA	CAA-CBA-CGA-O2A
18	a	811	CLA	CAA-CBA-CGA-O1A
18	5b	308	CLA	CAA-CBA-CGA-O2A
18	B	823	CLA	CAA-CBA-CGA-O2A
18	b	823	CLA	CAA-CBA-CGA-O2A
23	J	103	LMG	O8-C28-C29-C30
23	j	103	LMG	O8-C28-C29-C30
18	B	854	CLA	C2A-CAA-CBA-CGA
18	b	854	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	b	850	LMG	O7-C10-C11-C12
27	5a	320	LHG	O7-C7-C8-C9
27	5b	320	LHG	O7-C7-C8-C9
18	5a	309	CLA	C2-C3-C5-C6
18	5b	309	CLA	C2-C3-C5-C6
18	A	841	CLA	C2-C1-O2A-CGA
18	a	841	CLA	C2-C1-O2A-CGA
18	B	840	CLA	CAA-CBA-CGA-O2A
18	b	840	CLA	CAA-CBA-CGA-O2A
18	A	834	CLA	CAA-CBA-CGA-O2A
18	a	834	CLA	CAA-CBA-CGA-O2A
23	B	850	LMG	O7-C10-C11-C12
18	B	817	CLA	C11-C12-C13-C15
18	b	817	CLA	C11-C12-C13-C15
18	J	101	CLA	CAA-CBA-CGA-O1A
18	j	101	CLA	CAA-CBA-CGA-O1A
23	J	104	LMG	C22-C23-C24-C25
23	j	104	LMG	C22-C23-C24-C25
18	2a	301	CLA	C2A-CAA-CBA-CGA
18	2a	311	CLA	C2A-CAA-CBA-CGA
18	6a	305	CLA	C2A-CAA-CBA-CGA
18	2b	301	CLA	C2A-CAA-CBA-CGA
18	2b	311	CLA	C2A-CAA-CBA-CGA
18	6b	305	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	B	838	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	b	838	CLA	C3A-C2A-CAA-CBA
18	b	840	CLA	C3A-C2A-CAA-CBA
18	A	811	CLA	C3A-C2A-CAA-CBA
18	A	812	CLA	C3A-C2A-CAA-CBA
18	A	829	CLA	C3A-C2A-CAA-CBA
18	a	811	CLA	C3A-C2A-CAA-CBA
18	a	812	CLA	C3A-C2A-CAA-CBA
18	a	829	CLA	C3A-C2A-CAA-CBA
18	B	838	CLA	CAA-CBA-CGA-O1A
18	b	838	CLA	CAA-CBA-CGA-O1A
25	6a	319	LUT	C11-C10-C9-C8
25	6b	319	LUT	C11-C10-C9-C8
21	B	847	DGD	C7A-C8A-C9A-CAA
21	b	847	DGD	C7A-C8A-C9A-CAA
23	B	850	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	b	850	LMG	O10-C28-C29-C30
27	6a	301	LHG	O9-C7-C8-C9
27	6b	301	LHG	O9-C7-C8-C9
18	A	804	CLA	CAA-CBA-CGA-O2A
18	2a	308	CLA	CAA-CBA-CGA-O2A
18	3a	303	CLA	CAA-CBA-CGA-O2A
18	a	804	CLA	CAA-CBA-CGA-O2A
18	2b	308	CLA	CAA-CBA-CGA-O2A
18	3b	303	CLA	CAA-CBA-CGA-O2A
18	B	811	CLA	CAA-CBA-CGA-O1A
18	a	827	CLA	C2A-CAA-CBA-CGA
18	b	811	CLA	CAA-CBA-CGA-O1A
18	A	806	CLA	CAA-CBA-CGA-O1A
18	A	833	CLA	CAA-CBA-CGA-O1A
18	a	806	CLA	CAA-CBA-CGA-O1A
18	a	833	CLA	CAA-CBA-CGA-O1A
23	J	103	LMG	O10-C28-C29-C30
23	j	103	LMG	O10-C28-C29-C30
18	b	805	CLA	C15-C16-C17-C18
18	B	816	CLA	C4-C3-C5-C6
18	b	816	CLA	C4-C3-C5-C6
18	B	809	CLA	CAA-CBA-CGA-O1A
23	b	850	LMG	O9-C10-C11-C12
18	A	824	CLA	CAA-CBA-CGA-O2A
18	B	805	CLA	C15-C16-C17-C18
18	b	809	CLA	CAA-CBA-CGA-O1A
23	B	850	LMG	O9-C10-C11-C12
18	a	824	CLA	CAA-CBA-CGA-O2A
18	A	811	CLA	CAA-CBA-CGA-O2A
18	a	811	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	CAA-CBA-CGA-O1A
18	b	816	CLA	CAA-CBA-CGA-O1A
27	5a	320	LHG	O9-C7-C8-C9
27	5b	320	LHG	O9-C7-C8-C9
18	B	805	CLA	CAA-CBA-CGA-O2A
18	b	805	CLA	CAA-CBA-CGA-O2A
27	5a	318	LHG	O7-C7-C8-C9
27	5b	318	LHG	O7-C7-C8-C9
18	A	827	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	CAA-CBA-CGA-O1A
18	6a	315	CLA	CAA-CBA-CGA-O1A
18	a	812	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	6b	315	CLA	CAA-CBA-CGA-O1A
19	A	843	PQN	C20-C21-C22-C23
19	a	843	PQN	C20-C21-C22-C23
18	6a	306	CLA	CAA-CBA-CGA-O1A
18	6b	306	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	b	805	CLA	CAD-CBD-CGD-O2D
18	b	813	CLA	CAD-CBD-CGD-O2D
18	b	814	CLA	CAD-CBD-CGD-O2D
18	b	838	CLA	CAD-CBD-CGD-O2D
18	A	830	CLA	CAD-CBD-CGD-O2D
18	5a	309	CLA	CAD-CBD-CGD-O2D
18	6a	305	CLA	CAD-CBD-CGD-O2D
18	a	830	CLA	CAD-CBD-CGD-O2D
18	5b	309	CLA	CAD-CBD-CGD-O2D
18	6b	305	CLA	CAD-CBD-CGD-O2D
18	5a	303	CLA	CAA-CBA-CGA-O1A
18	A	834	CLA	CAA-CBA-CGA-O1A
18	5b	303	CLA	CAA-CBA-CGA-O1A
28	A	852	LMU	C11-C10-C9-C8
28	a	852	LMU	C11-C10-C9-C8
18	3a	302	CLA	C2A-CAA-CBA-CGA
18	5a	302	CLA	C2A-CAA-CBA-CGA
18	3b	302	CLA	C2A-CAA-CBA-CGA
18	5b	302	CLA	C2A-CAA-CBA-CGA
18	B	823	CLA	CAA-CBA-CGA-O1A
18	b	823	CLA	CAA-CBA-CGA-O1A
18	3a	303	CLA	CAA-CBA-CGA-O1A
18	3b	303	CLA	CAA-CBA-CGA-O1A
18	B	828	CLA	CAA-CBA-CGA-O2A
18	b	828	CLA	CAA-CBA-CGA-O2A
27	2a	316	LHG	O8-C23-C24-C25
27	5a	318	LHG	O8-C23-C24-C25
27	2b	316	LHG	O8-C23-C24-C25
27	5b	318	LHG	O8-C23-C24-C25
18	B	840	CLA	CAA-CBA-CGA-O1A
18	b	840	CLA	CAA-CBA-CGA-O1A
18	a	834	CLA	CAA-CBA-CGA-O1A
27	5b	318	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
27	2a	316	LHG	O10-C23-C24-C25
27	5a	318	LHG	O10-C23-C24-C25
27	2b	316	LHG	O10-C23-C24-C25

There are no ring outliers.

360 monomers are involved in 665 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	822	CLA	1	0
20	k	202	BCR	2	0
20	f	304	BCR	1	0
18	b	808	CLA	2	0
18	b	813	CLA	1	0
18	3b	312	CLA	1	0
29	5a	305	CHL	1	0
18	a	840	CLA	2	0
18	B	823	CLA	3	0
18	a	823	CLA	5	0
18	3b	306	CLA	2	0
20	A	847	BCR	3	0
20	i	202	BCR	3	0
18	5a	311	CLA	1	0
18	b	812	CLA	2	0
18	a	806	CLA	4	0
18	5a	310	CLA	1	0
18	5a	312	CLA	2	0
23	b	850	LMG	1	0
25	3a	317	LUT	6	0
18	2b	310	CLA	2	0
18	5b	302	CLA	1	0
18	6b	315	CLA	2	0
18	B	803	CLA	1	0
18	a	803	CLA	3	0
18	a	839	CLA	2	0
18	b	825	CLA	1	0
18	B	854	CLA	3	0
25	3b	316	LUT	3	0
18	A	840	CLA	2	0
18	5b	312	CLA	3	0
18	6b	308	CLA	3	0
20	A	849	BCR	3	0
18	5a	315	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	g	201	BCR	2	0
18	B	831	CLA	2	0
18	b	822	CLA	2	0
18	b	802	CLA	1	0
20	G	204	BCR	3	0
20	B	848	BCR	3	0
20	a	848	BCR	4	0
18	B	807	CLA	2	0
18	A	804	CLA	1	0
18	B	828	CLA	3	0
18	B	829	CLA	1	0
18	5a	302	CLA	1	0
18	a	828	CLA	1	0
18	B	809	CLA	3	0
18	a	820	CLA	3	0
18	b	816	CLA	1	0
20	B	846	BCR	1	0
20	B	843	BCR	1	0
25	6b	318	LUT	3	0
18	b	801	CLA	7	0
18	6a	305	CLA	3	0
18	A	822	CLA	1	0
18	b	817	CLA	2	0
25	2a	314	LUT	6	0
18	5b	310	CLA	1	0
18	6b	317	CLA	1	0
25	j	105	LUT	3	0
18	b	807	CLA	2	0
18	6a	310	CLA	2	0
18	A	811	CLA	1	0
18	b	814	CLA	2	0
18	2b	309	CLA	1	0
20	b	848	BCR	1	0
20	a	847	BCR	5	0
29	5b	306	CHL	1	0
18	5b	315	CLA	2	0
20	B	844	BCR	3	0
18	b	824	CLA	2	0
18	6a	315	CLA	2	0
27	A	846	LHG	4	0
18	3b	309	CLA	2	0
18	2b	308	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	810	CLA	3	0
20	A	850	BCR	3	0
18	5a	313	CLA	1	0
18	B	840	CLA	2	0
20	j	102	BCR	5	0
20	J	102	BCR	4	0
27	5b	320	LHG	3	0
18	A	853	CLA	1	0
18	6a	311	CLA	1	0
18	A	831	CLA	4	0
18	B	808	CLA	1	0
18	a	808	CLA	3	0
18	b	835	CLA	1	0
25	6a	320	LUT	5	0
18	a	801	CLA	2	0
18	6b	305	CLA	3	0
29	3b	301	CHL	1	0
18	A	821	CLA	2	0
25	2b	315	LUT	6	0
18	f	305	CLA	2	0
18	3a	312	CLA	2	0
18	B	830	CLA	3	0
18	b	832	CLA	4	0
18	A	824	CLA	2	0
18	g	203	CLA	3	0
18	b	818	CLA	1	0
18	2a	303	CLA	1	0
20	B	842	BCR	2	0
18	3b	311	CLA	1	0
18	A	829	CLA	2	0
25	2a	315	LUT	5	0
18	2a	310	CLA	2	0
18	3a	302	CLA	1	0
18	A	837	CLA	1	0
29	2a	313	CHL	2	0
18	3a	314	CLA	1	0
18	b	827	CLA	2	0
18	6a	307	CLA	2	0
18	B	806	CLA	7	0
20	M	101	BCR	4	0
23	B	850	LMG	1	0
18	B	816	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	830	CLA	3	0
18	f	302	CLA	3	0
18	b	838	CLA	4	0
18	2b	302	CLA	1	0
20	F	301	BCR	3	0
27	a	846	LHG	4	0
29	5a	301	CHL	2	0
18	b	805	CLA	3	0
25	6b	319	LUT	6	0
20	a	849	BCR	1	0
18	2b	312	CLA	2	0
18	B	821	CLA	3	0
25	6a	319	LUT	5	0
18	A	835	CLA	4	0
18	3b	302	CLA	1	0
18	b	804	CLA	3	0
18	B	833	CLA	1	0
18	3a	303	CLA	2	0
18	g	202	CLA	1	0
18	5b	308	CLA	2	0
18	a	814	CLA	1	0
18	6a	308	CLA	3	0
18	B	853	CLA	1	0
18	a	809	CLA	1	0
18	a	853	CLA	1	0
29	2a	306	CHL	6	0
18	a	831	CLA	4	0
18	b	811	CLA	1	0
18	5a	308	CLA	2	0
18	B	811	CLA	2	0
20	A	851	BCR	5	0
18	L	302	CLA	2	0
29	5a	307	CHL	2	0
18	j	101	CLA	2	0
18	A	827	CLA	1	0
18	J	101	CLA	2	0
18	B	839	CLA	2	0
27	5a	320	LHG	3	0
18	a	821	CLA	2	0
18	A	838	CLA	1	0
20	a	850	BCR	3	0
18	B	820	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	l	304	BCR	2	0
18	6a	314	CLA	1	0
18	b	803	CLA	1	0
18	3a	313	CLA	2	0
18	l	301	CLA	2	0
18	a	804	CLA	1	0
18	5a	309	CLA	2	0
18	G	203	CLA	3	0
20	b	846	BCR	1	0
18	A	814	CLA	1	0
29	3a	307	CHL	2	0
18	5a	303	CLA	3	0
18	2b	303	CLA	1	0
18	3a	309	CLA	2	0
18	a	818	CLA	2	0
18	b	823	CLA	3	0
19	B	841	PQN	3	0
18	2a	312	CLA	2	0
18	b	828	CLA	4	0
23	5b	319	LMG	1	0
29	2b	313	CHL	2	0
18	L	303	CLA	1	0
18	2a	308	CLA	3	0
19	A	843	PQN	1	0
18	b	809	CLA	3	0
18	b	806	CLA	7	0
24	A	844	SF4	1	0
18	F	303	CLA	1	0
18	A	805	CLA	5	0
18	3b	313	CLA	1	0
18	B	810	CLA	2	0
18	a	841	CLA	5	0
25	2b	314	LUT	5	0
18	A	816	CLA	2	0
18	a	805	CLA	5	0
18	B	832	CLA	3	0
20	G	201	BCR	3	0
18	A	841	CLA	5	0
18	A	803	CLA	3	0
20	B	845	BCR	5	0
18	b	819	CLA	2	0
20	I	202	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	6b	306	CLA	1	0
18	b	815	CLA	3	0
25	5a	316	LUT	5	0
29	5b	314	CHL	1	0
18	A	815	CLA	2	0
18	a	835	CLA	4	0
18	5b	313	CLA	1	0
18	6a	306	CLA	1	0
26	a	802	CL0	3	0
27	6b	301	LHG	1	0
18	A	817	CLA	4	0
18	2b	307	CLA	1	0
29	3a	315	CHL	1	0
20	m	101	BCR	3	0
18	b	836	CLA	2	0
18	a	807	CLA	1	0
21	b	847	DGD	3	0
18	B	826	CLA	2	0
18	B	824	CLA	2	0
18	B	827	CLA	1	0
18	a	827	CLA	1	0
23	I	201	LMG	1	0
18	A	834	CLA	2	0
18	b	810	CLA	2	0
25	6b	320	LUT	3	0
18	b	852	CLA	1	0
18	a	815	CLA	2	0
23	j	103	LMG	1	0
18	A	801	CLA	2	0
18	A	819	CLA	2	0
29	2b	304	CHL	1	0
20	b	845	BCR	5	0
29	5a	306	CHL	1	0
19	b	841	PQN	3	0
18	l	303	CLA	1	0
18	B	804	CLA	4	0
25	3a	316	LUT	2	0
29	3b	315	CHL	1	0
18	A	836	CLA	1	0
25	6a	318	LUT	4	0
18	5b	303	CLA	3	0
18	6b	311	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3b	303	CLA	1	0
18	6b	313	CLA	3	0
18	b	826	CLA	2	0
29	2a	304	CHL	1	0
18	B	805	CLA	2	0
18	3a	311	CLA	1	0
26	A	802	CL0	3	0
18	5b	311	CLA	1	0
18	A	809	CLA	1	0
18	a	816	CLA	3	0
20	b	842	BCR	3	0
18	3b	314	CLA	1	0
29	5b	307	CHL	2	0
19	a	843	PQN	1	0
29	5b	301	CHL	2	0
18	l	302	CLA	2	0
20	a	851	BCR	4	0
29	5b	305	CHL	1	0
18	B	802	CLA	2	0
25	5b	317	LUT	1	0
18	A	808	CLA	3	0
20	b	851	BCR	5	0
18	a	817	CLA	4	0
29	6b	309	CHL	1	0
18	5b	309	CLA	1	0
18	a	838	CLA	1	0
18	B	815	CLA	3	0
18	6a	313	CLA	3	0
18	b	839	CLA	2	0
18	A	812	CLA	4	0
29	5a	314	CHL	1	0
29	6a	309	CHL	1	0
18	A	818	CLA	2	0
29	2b	306	CHL	5	0
18	6b	307	CLA	2	0
18	F	302	CLA	3	0
18	a	834	CLA	2	0
23	J	103	LMG	1	0
18	2a	302	CLA	1	0
18	b	821	CLA	2	0
27	6a	301	LHG	1	0
18	6b	316	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	854	CLA	4	0
18	a	819	CLA	2	0
18	b	833	CLA	1	0
20	B	851	BCR	5	0
18	a	837	CLA	1	0
18	2b	311	CLA	1	0
18	b	853	CLA	1	0
29	3a	301	CHL	1	0
18	b	831	CLA	3	0
18	B	817	CLA	2	0
18	A	810	CLA	3	0
18	B	838	CLA	4	0
18	A	823	CLA	5	0
18	A	807	CLA	1	0
29	6a	304	CHL	2	0
18	b	829	CLA	1	0
18	B	836	CLA	2	0
18	a	822	CLA	1	0
18	B	814	CLA	2	0
18	2b	301	CLA	1	0
21	B	847	DGD	3	0
25	J	105	LUT	4	0
18	a	833	CLA	2	0
23	i	201	LMG	1	0
18	b	820	CLA	1	0
18	2a	311	CLA	1	0
18	A	839	CLA	2	0
18	f	303	CLA	1	0
20	b	843	BCR	1	0
23	5a	319	LMG	1	0
18	a	812	CLA	3	0
18	B	819	CLA	2	0
18	A	820	CLA	2	0
18	6b	314	CLA	1	0
20	b	844	BCR	3	0
18	3a	306	CLA	2	0
18	2a	307	CLA	1	0
18	B	852	CLA	1	0
20	f	301	BCR	4	0
18	2a	301	CLA	2	0
29	6b	304	CHL	2	0
20	L	304	BCR	2	0

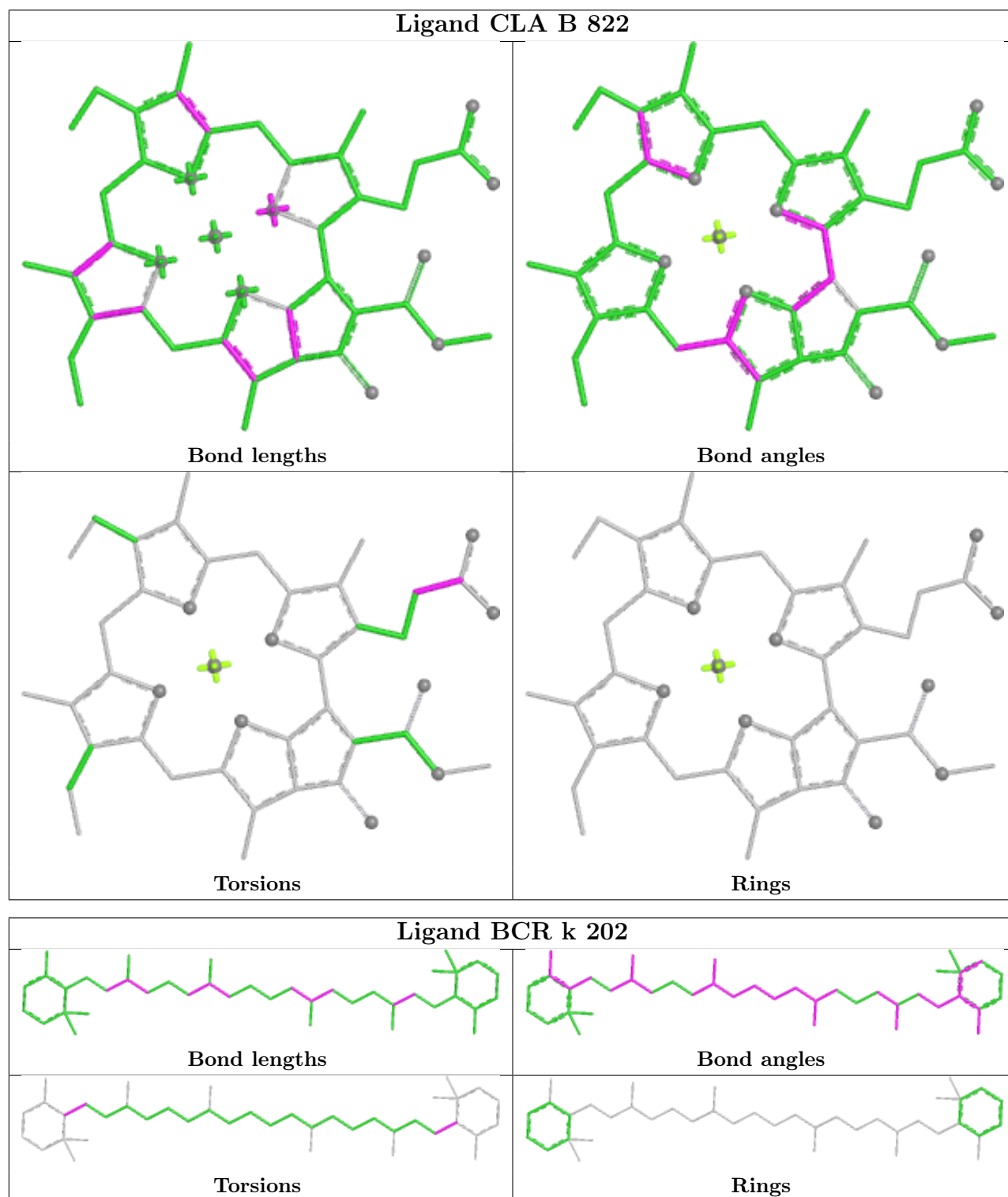
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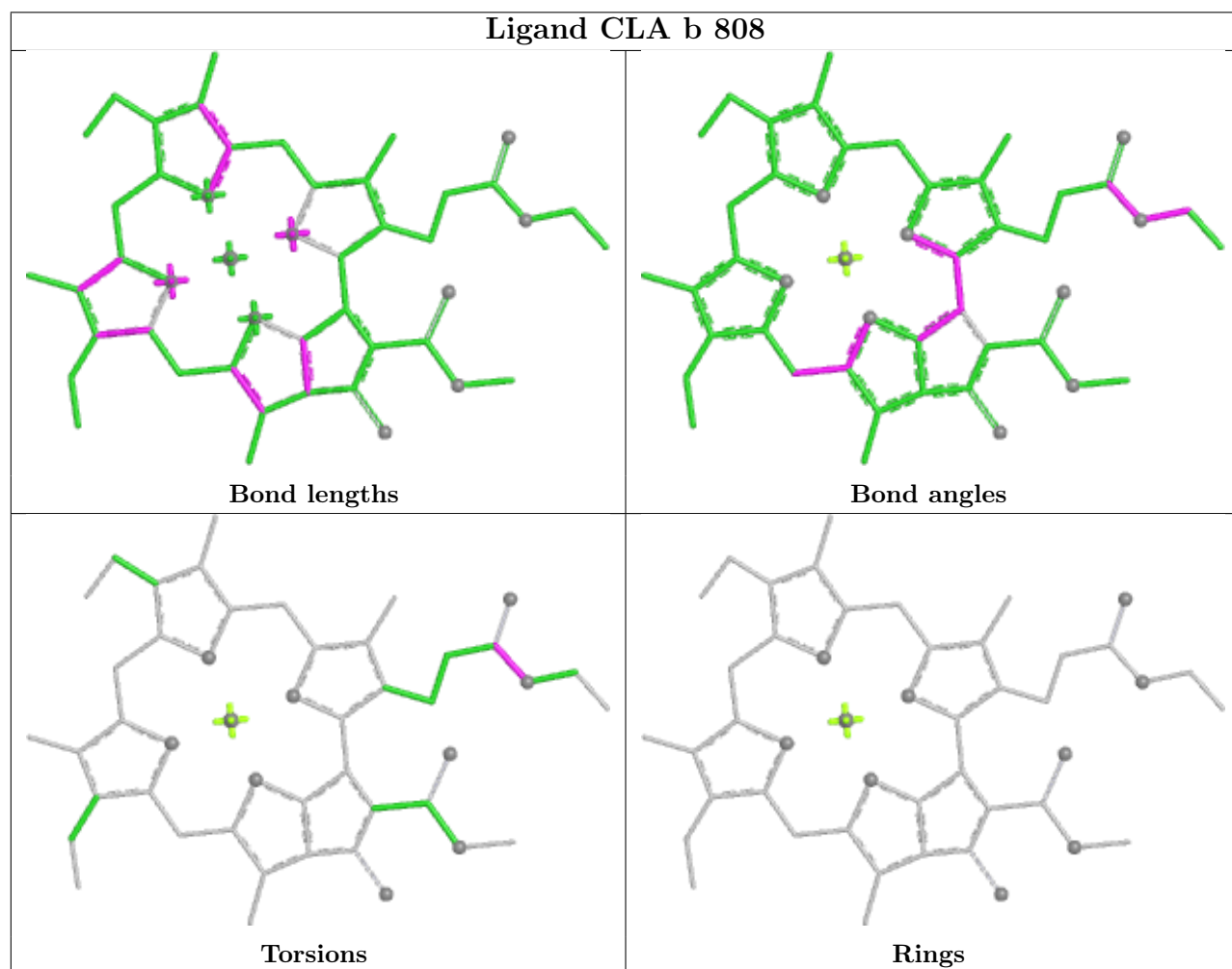
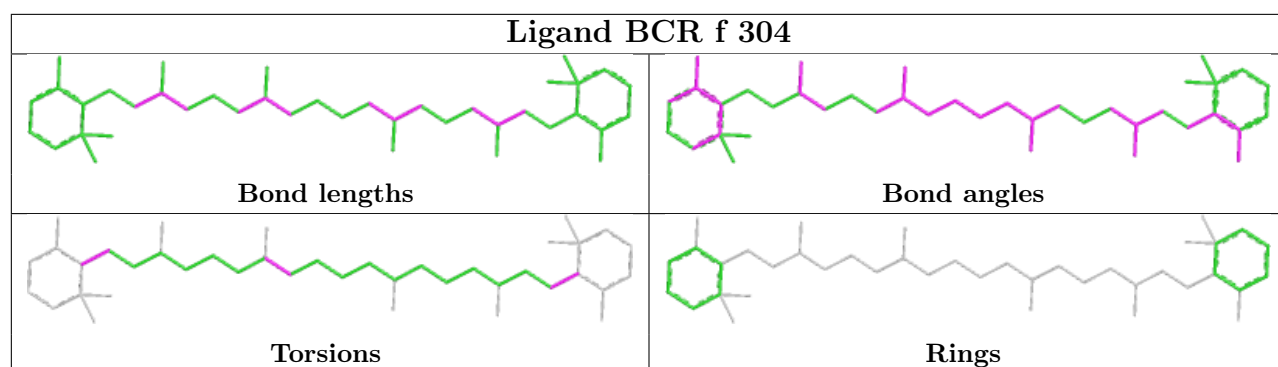
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3a	310	CLA	1	0
24	a	844	SF4	1	0
18	2a	309	CLA	1	0
18	B	813	CLA	1	0
29	3b	307	CHL	2	0
18	L	301	CLA	2	0
20	A	848	BCR	2	0
25	5b	316	LUT	4	0
23	j	104	LMG	1	0
18	A	833	CLA	2	0
18	A	828	CLA	1	0
23	J	104	LMG	1	0
18	F	305	CLA	2	0
18	G	202	CLA	1	0
27	a	845	LHG	3	0
18	A	806	CLA	4	0
20	K	202	BCR	3	0
18	6a	317	CLA	1	0
18	B	812	CLA	2	0
18	a	829	CLA	2	0
25	5a	317	LUT	3	0
18	B	801	CLA	8	0
18	6b	310	CLA	3	0
18	6a	316	CLA	2	0
25	3b	317	LUT	5	0
18	B	818	CLA	1	0
18	b	840	CLA	3	0
18	a	824	CLA	2	0
20	g	204	BCR	5	0
18	3b	310	CLA	1	0
27	A	845	LHG	3	0
18	B	825	CLA	1	0

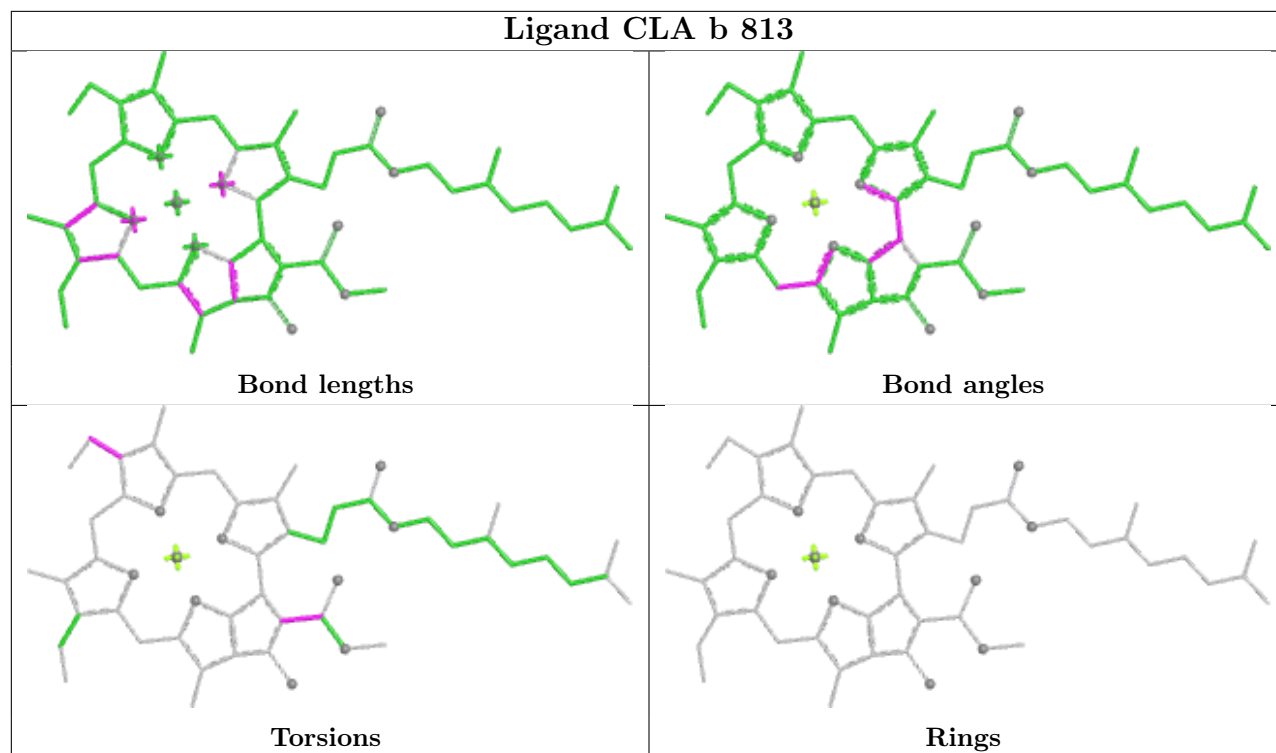
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

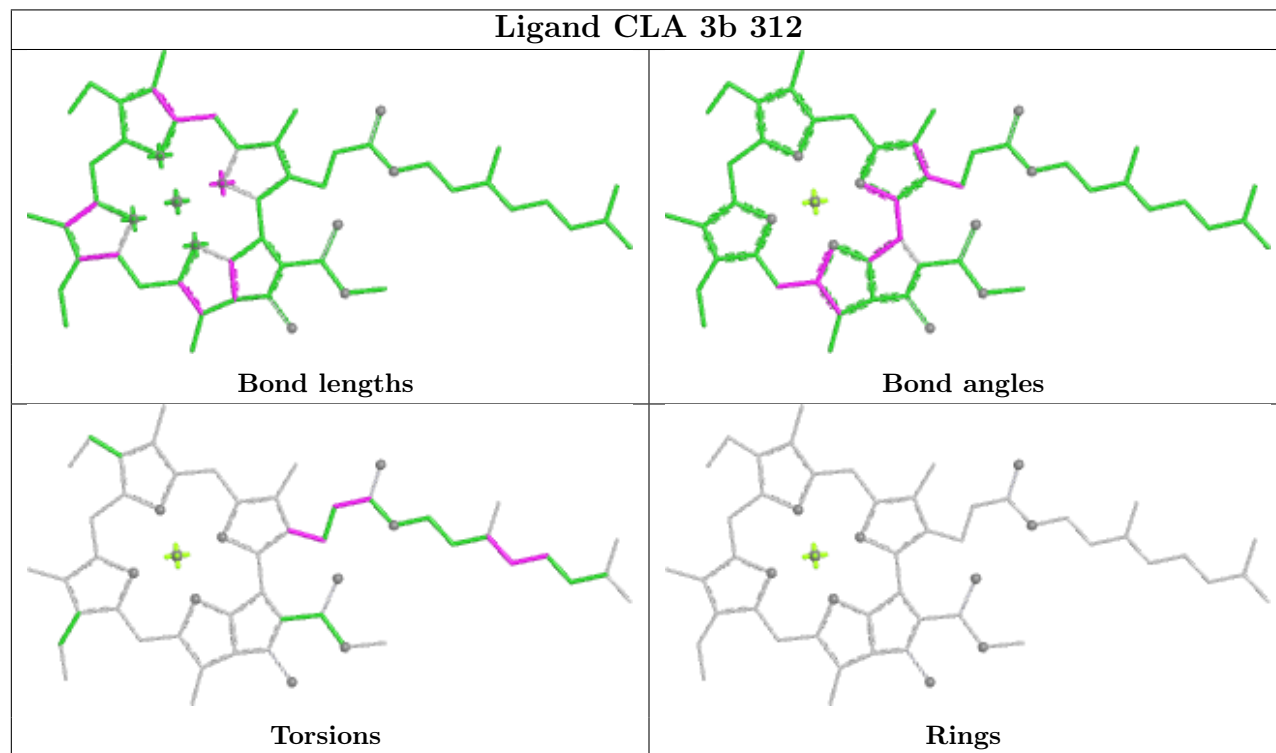


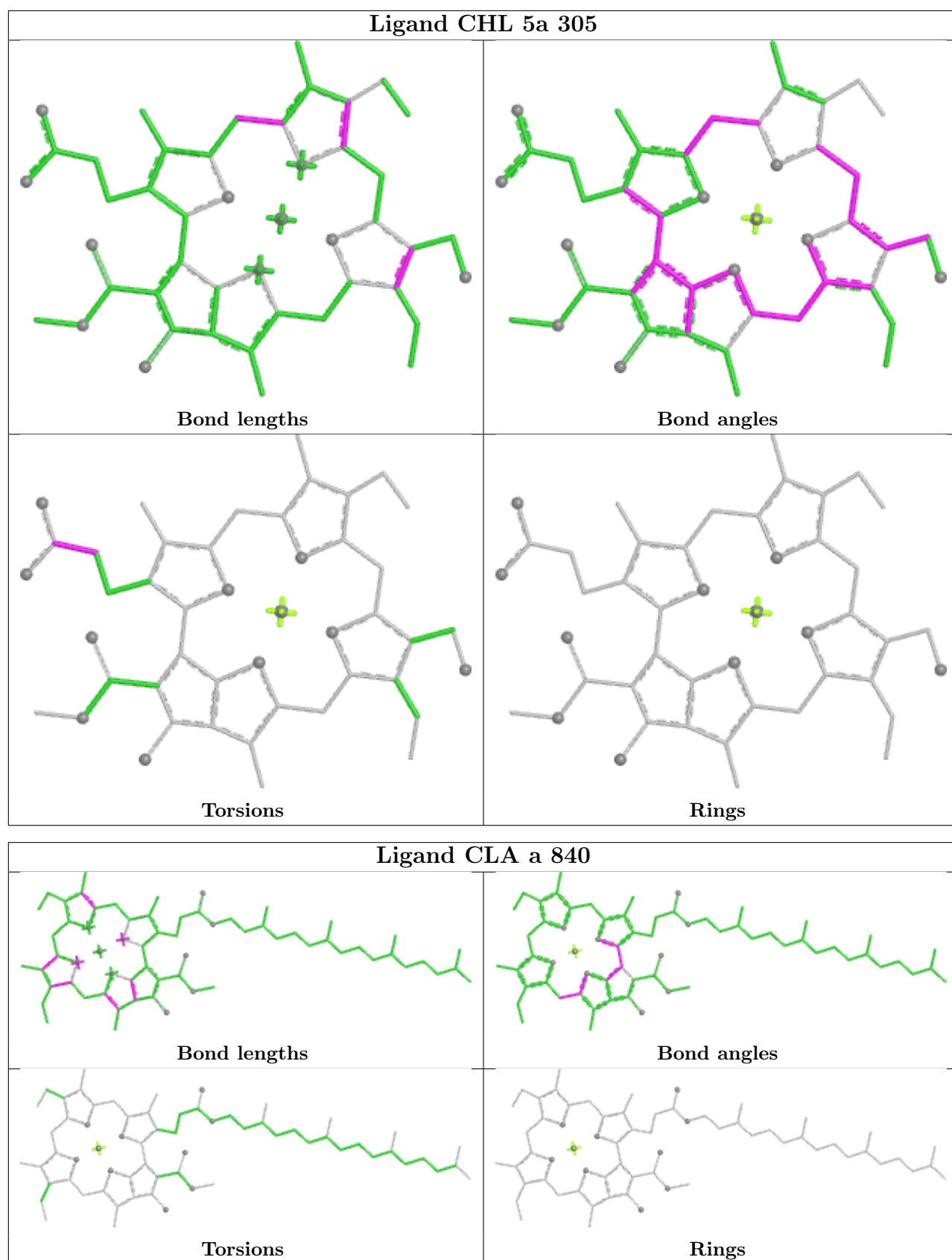


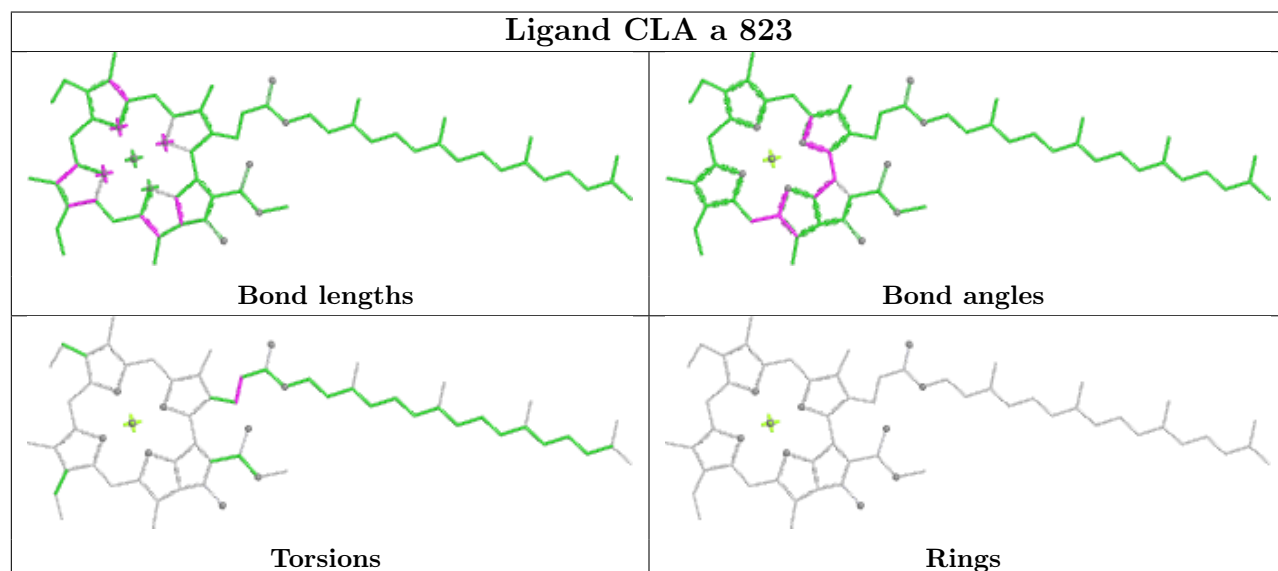
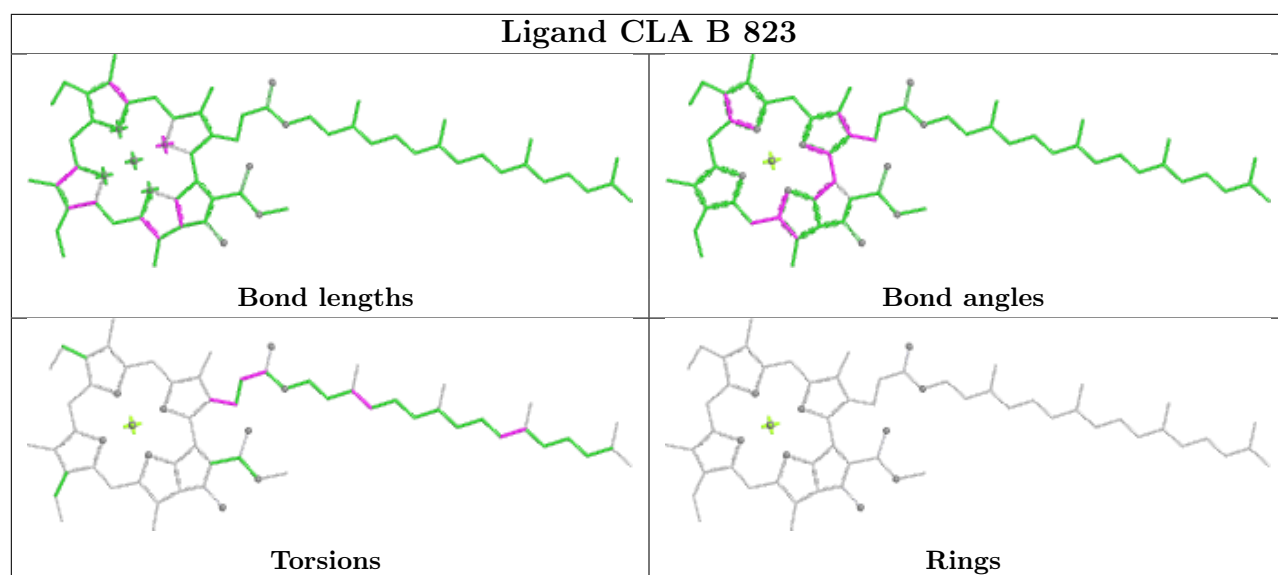
Ligand CLA b 813

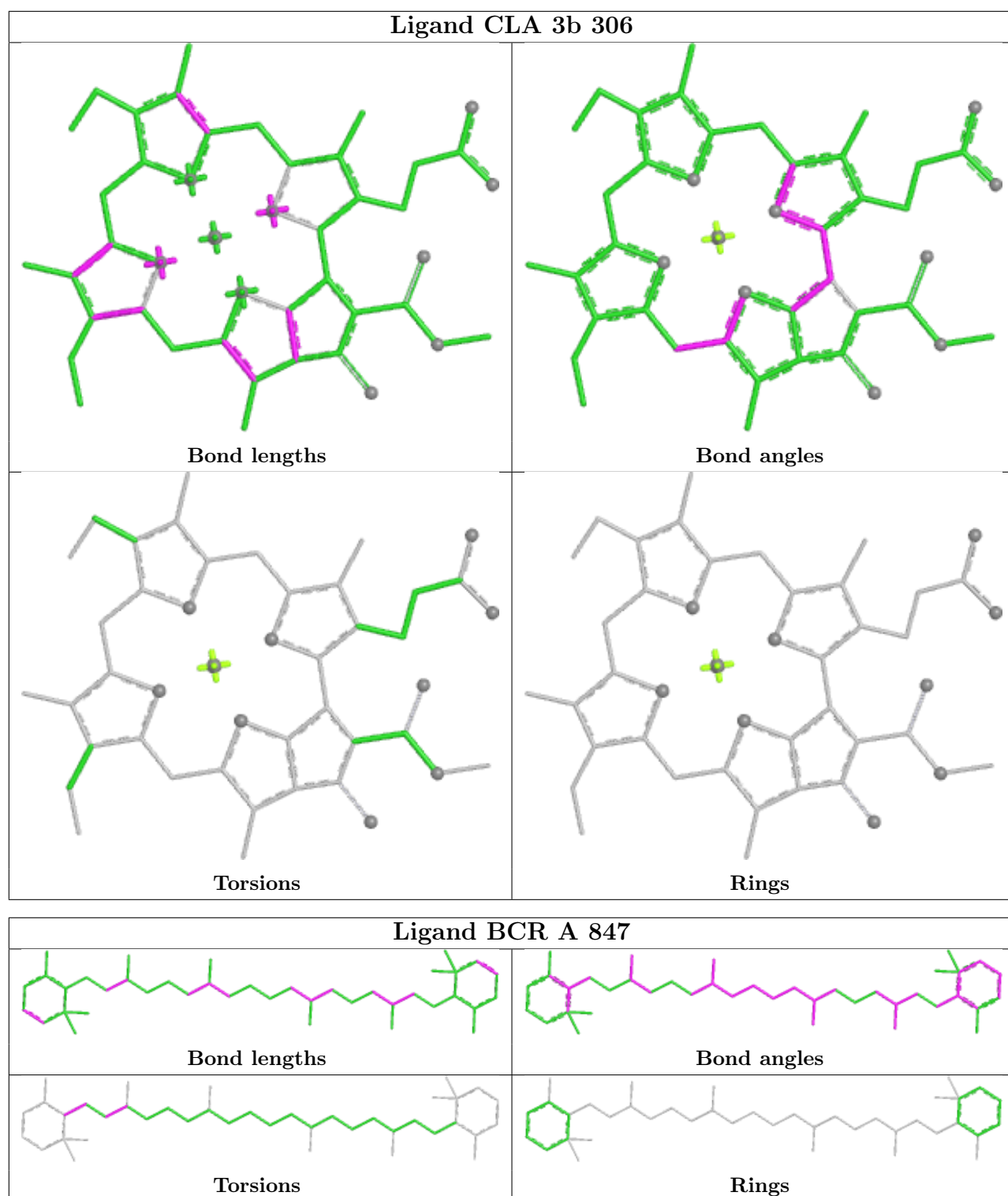


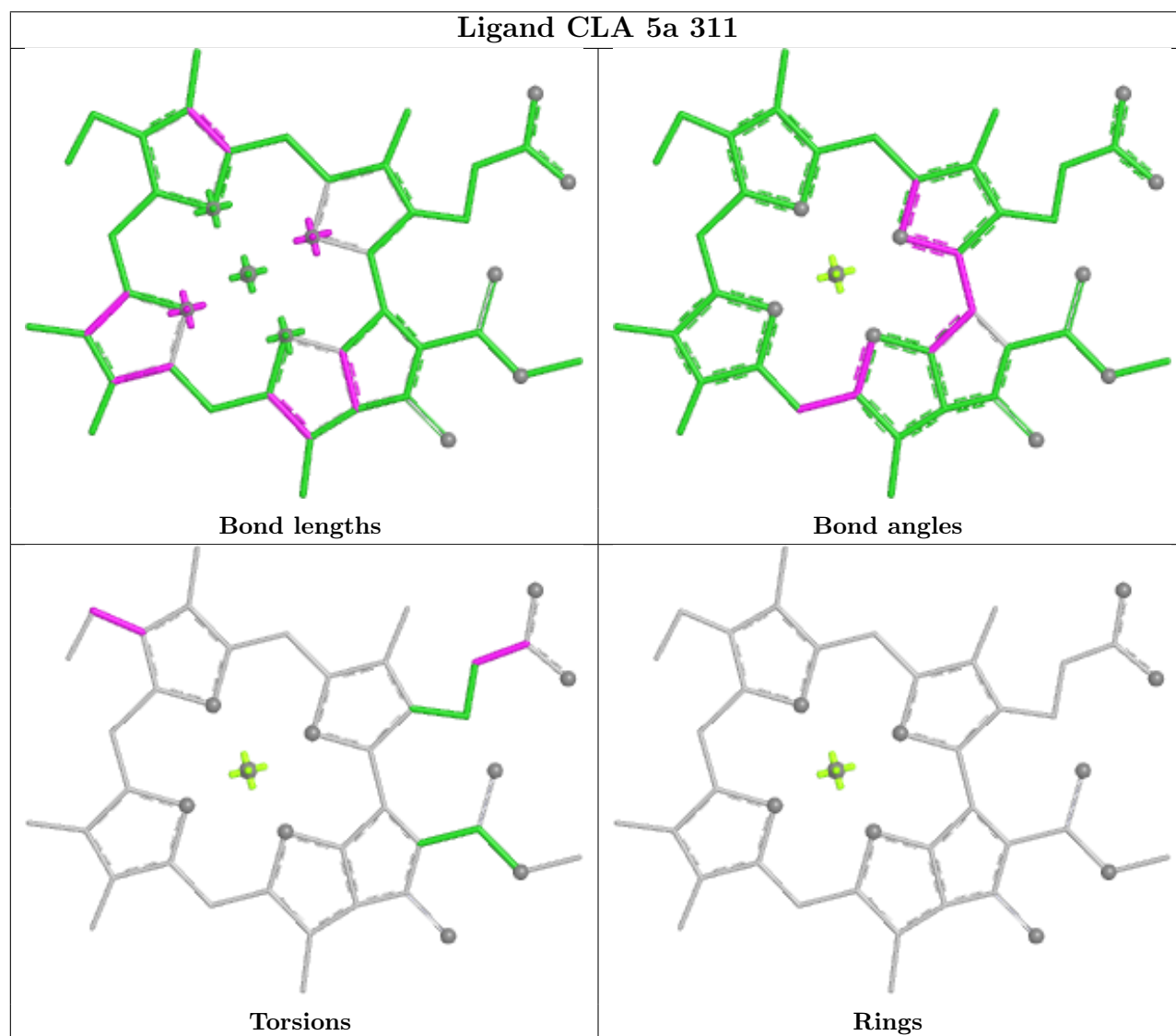
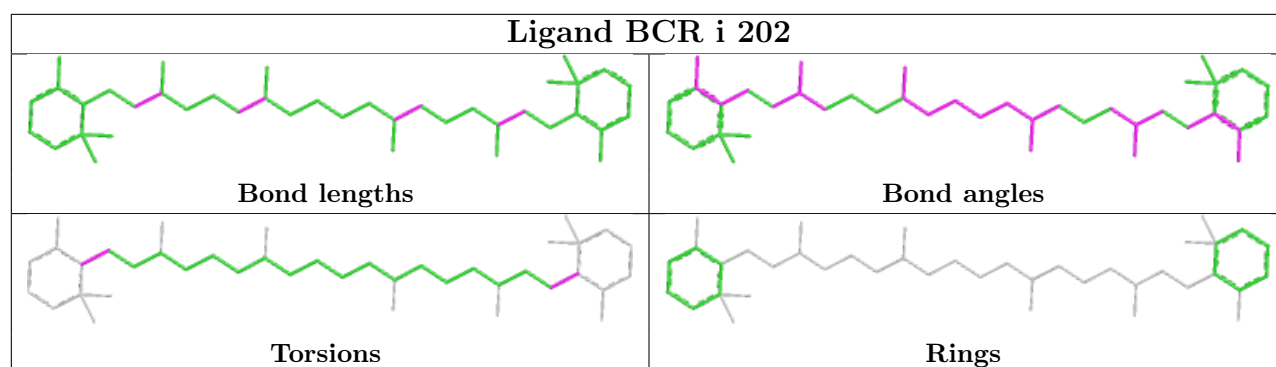
Ligand CLA 3b 312

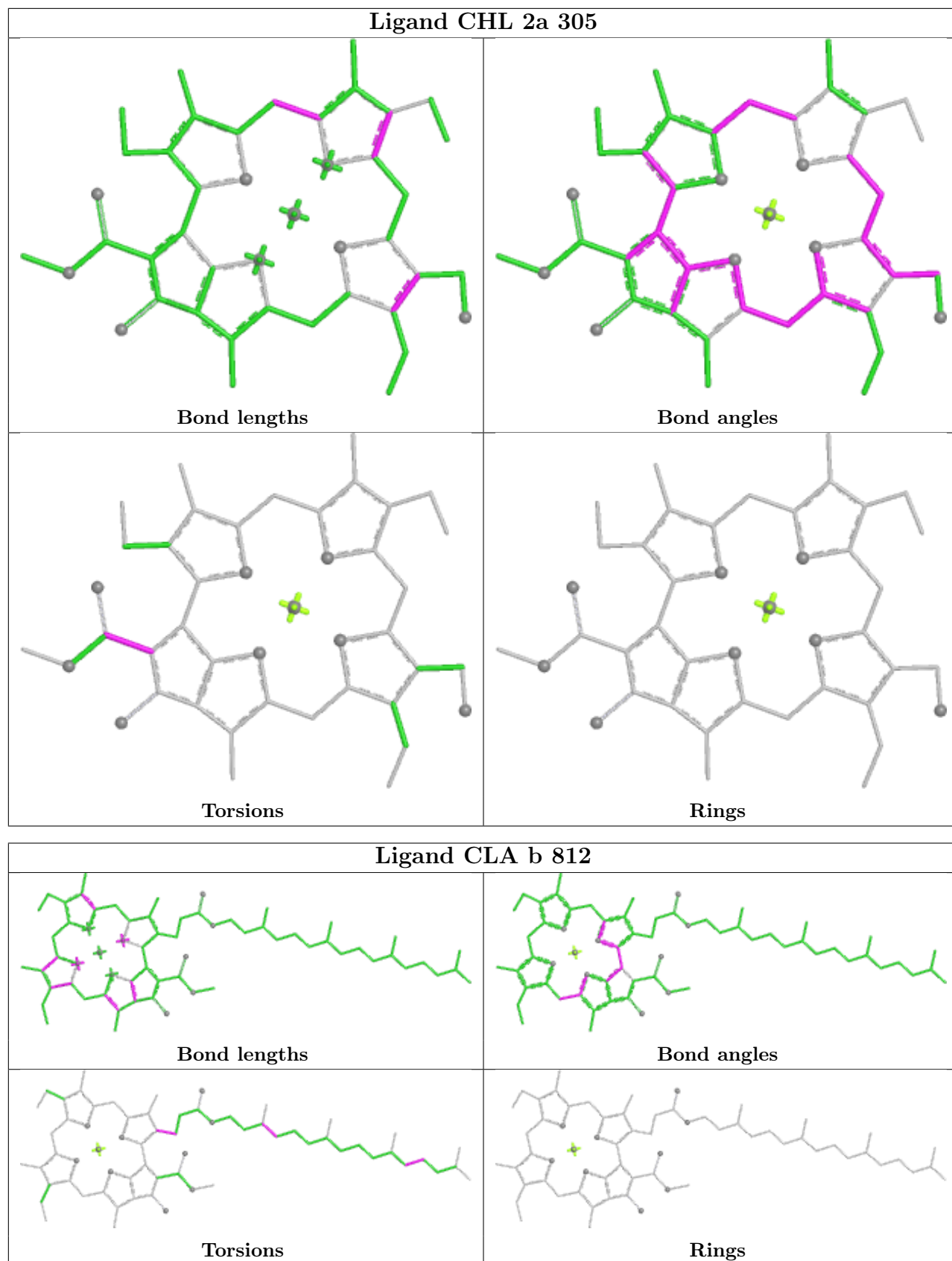


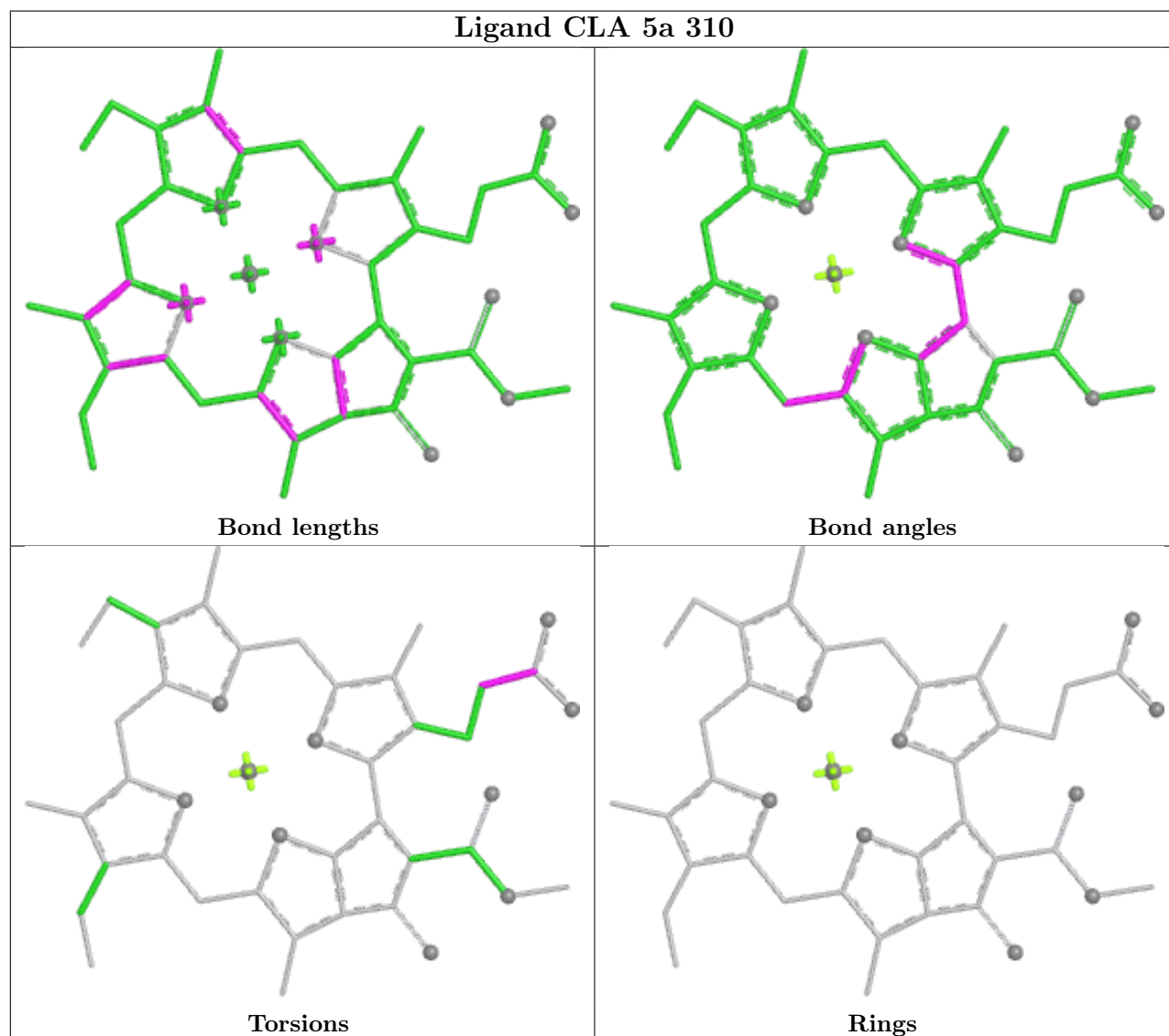
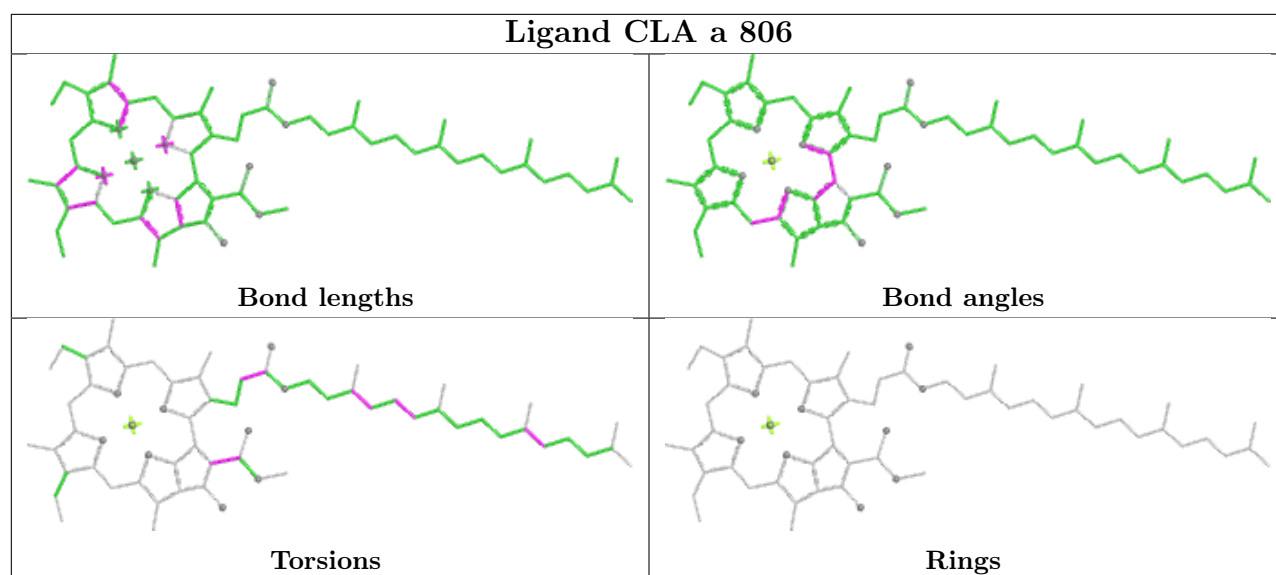


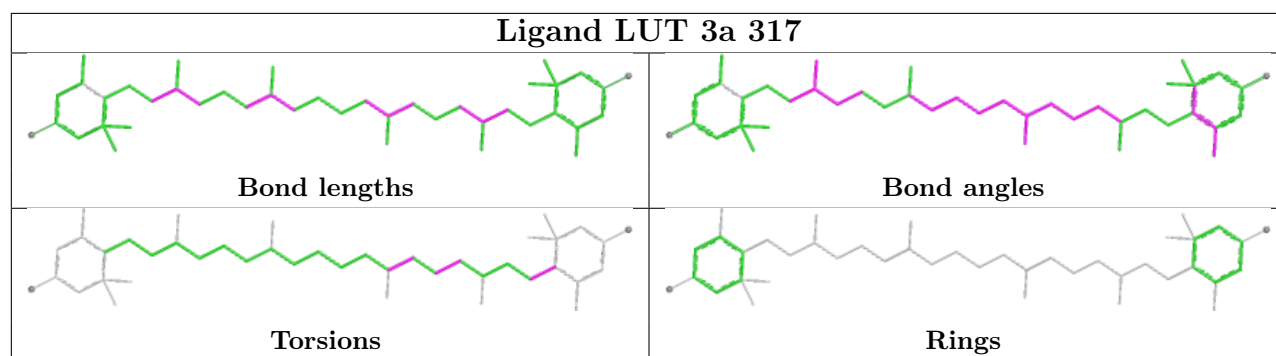
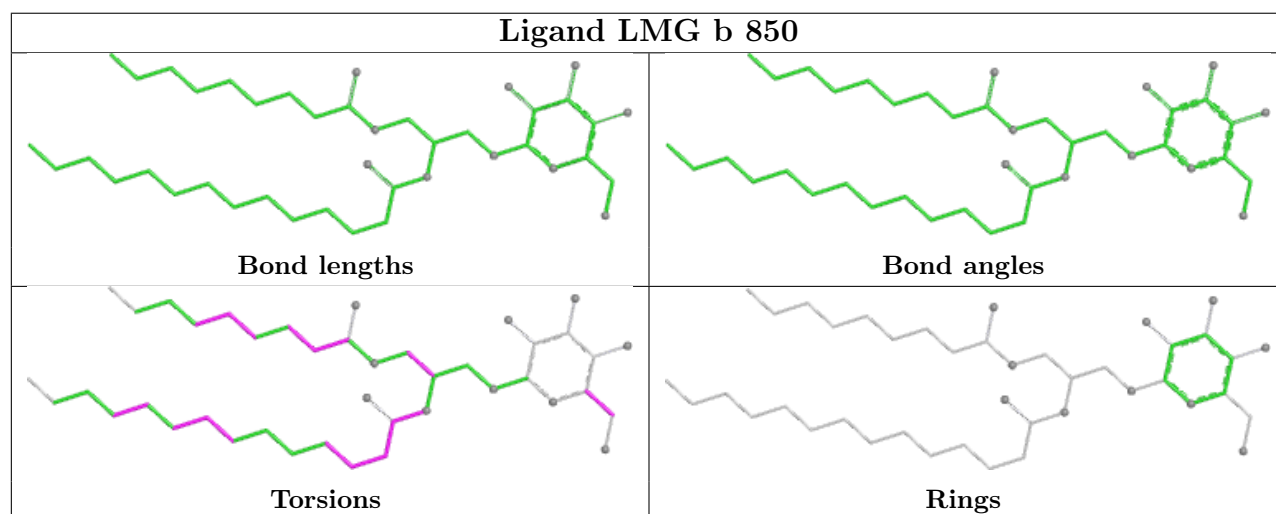
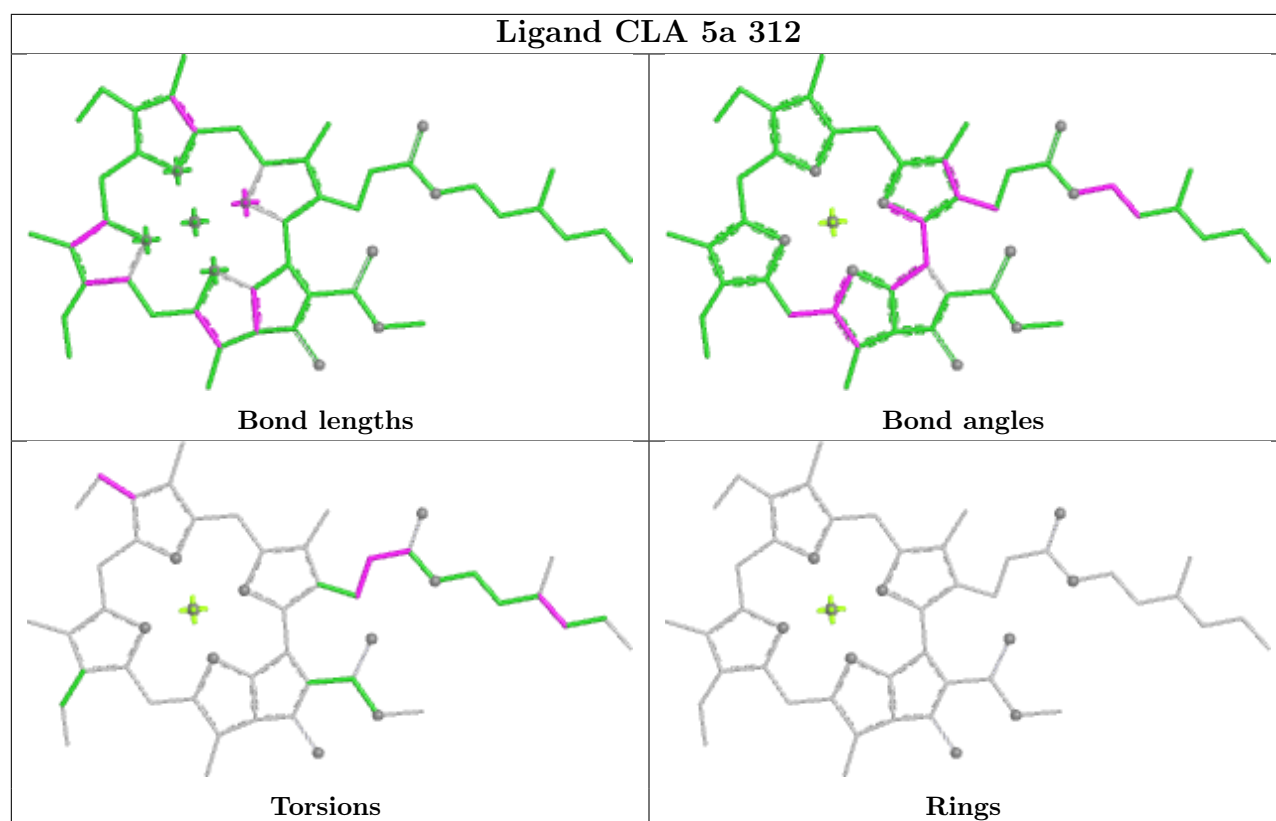


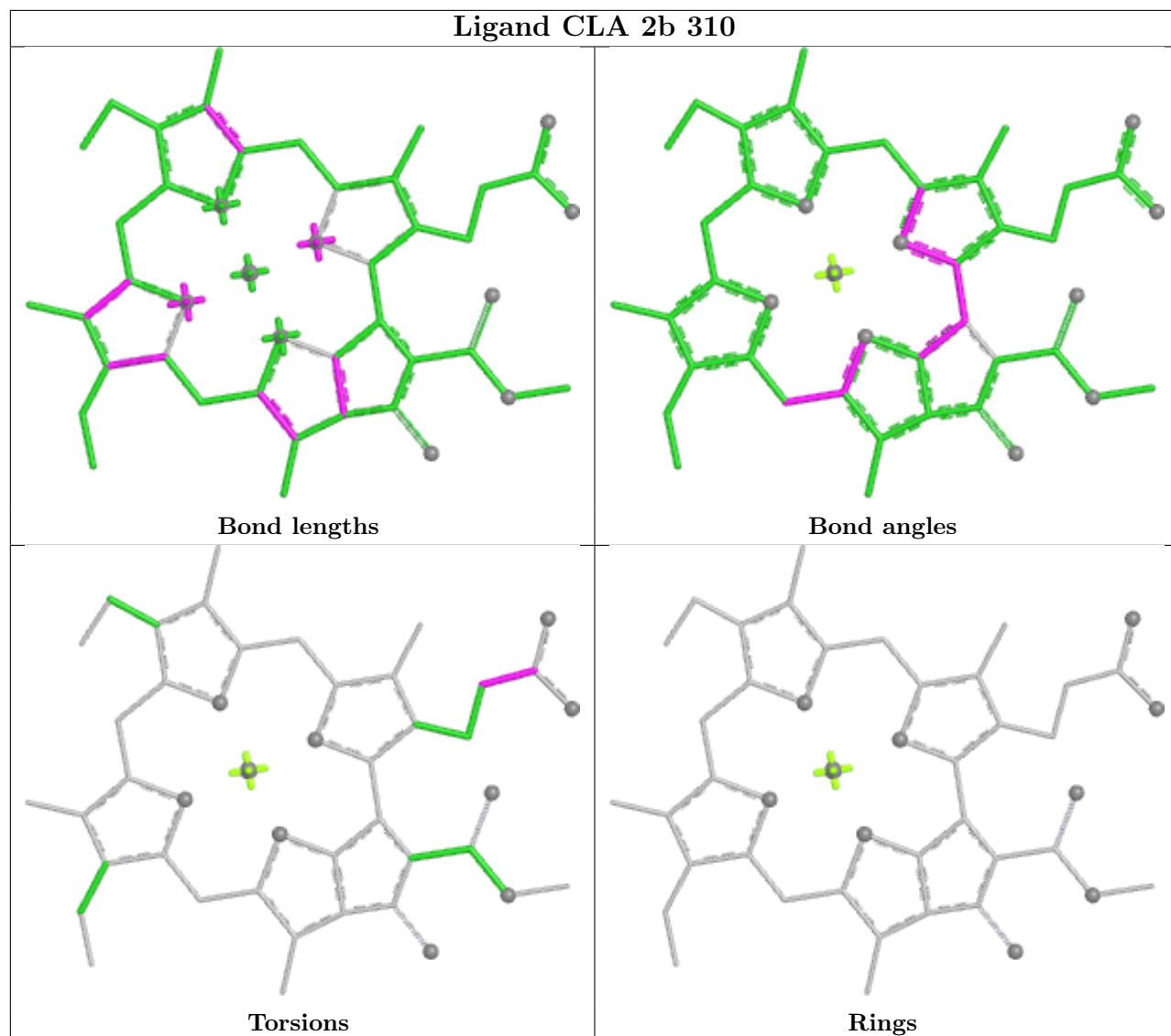


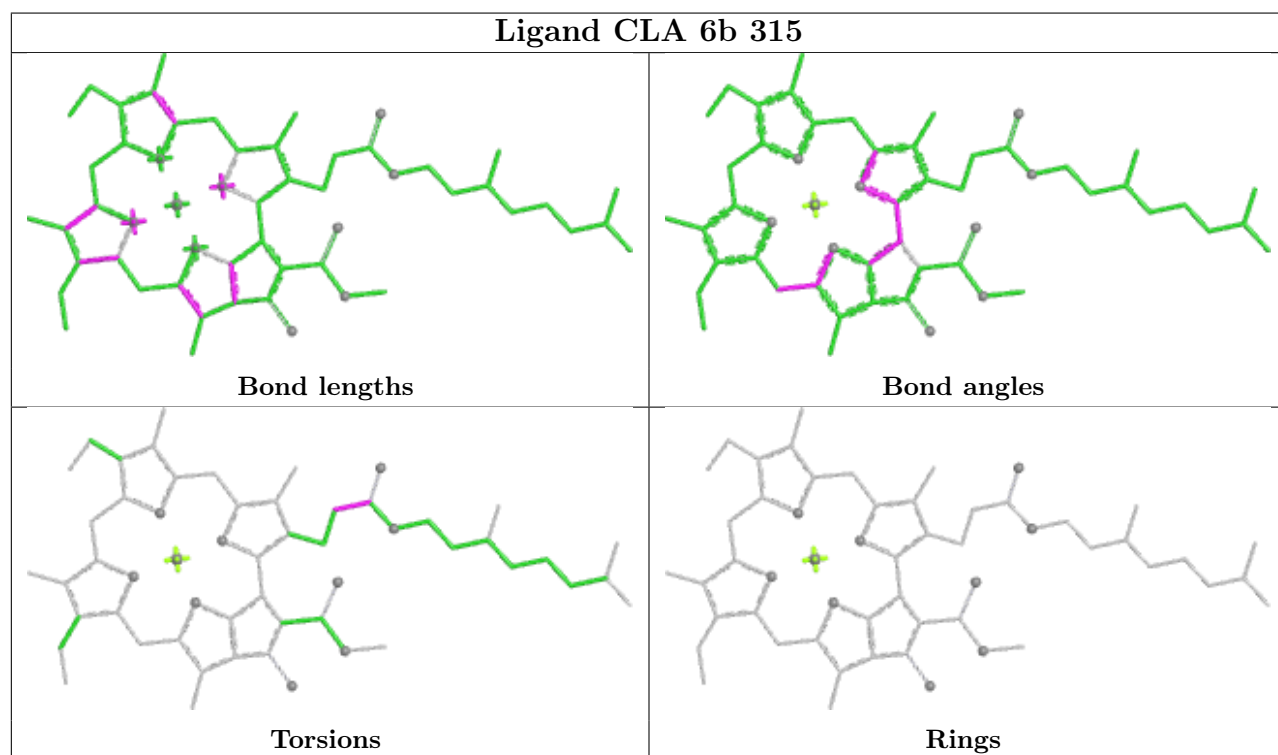
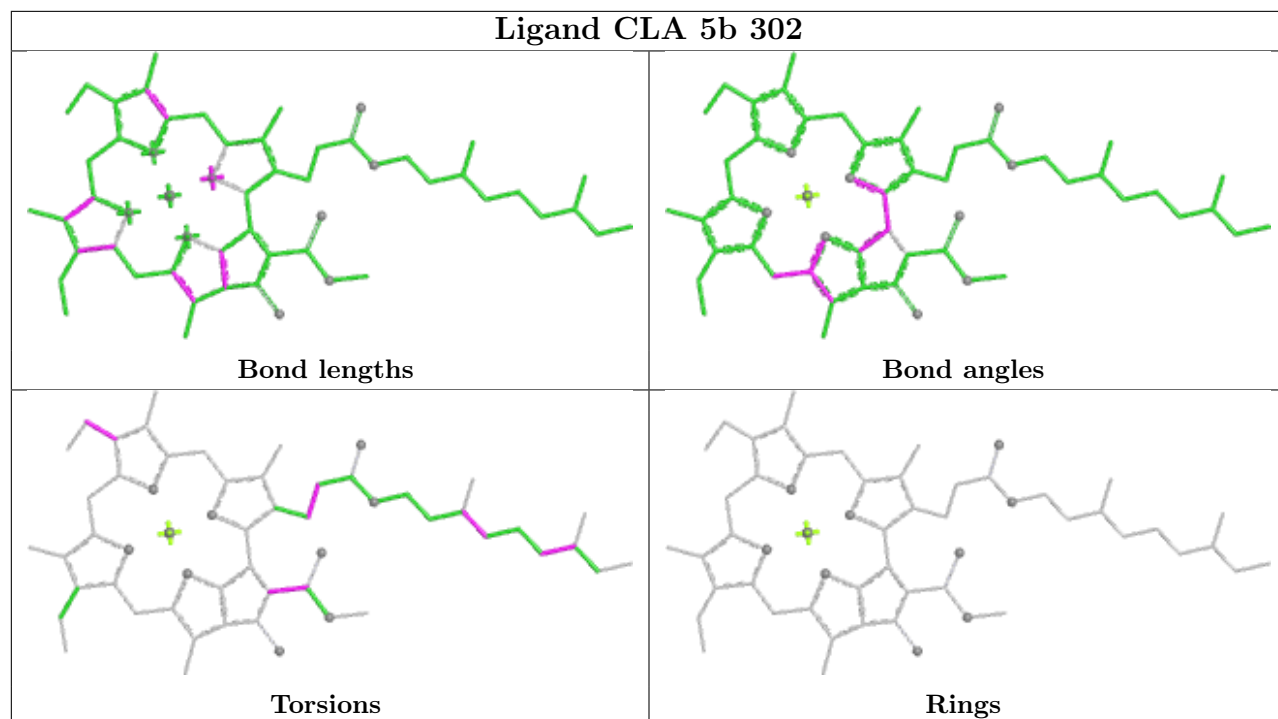




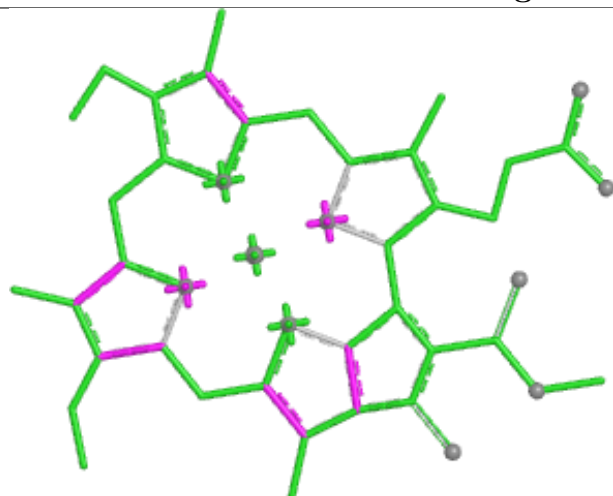




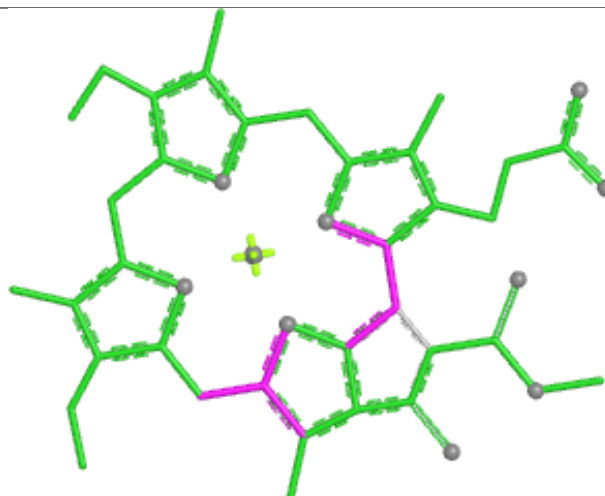




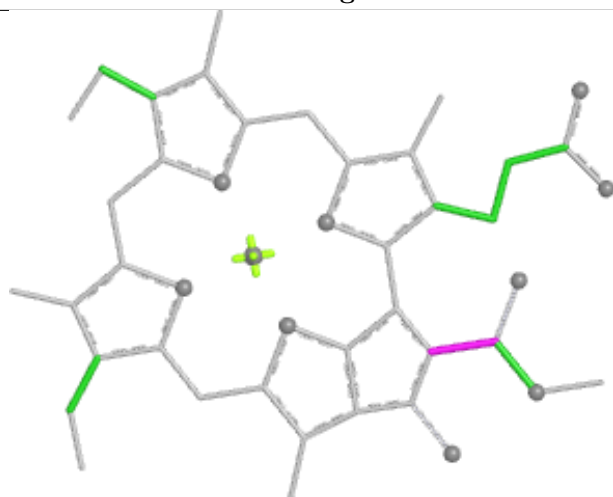
Ligand CLA B 803



Bond lengths



Bond angles

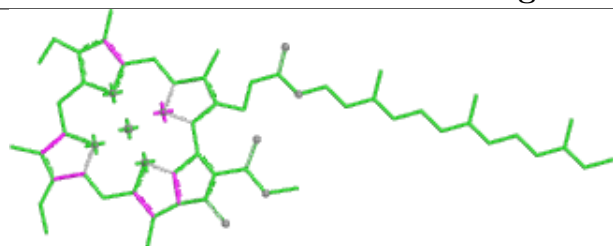


Torsions

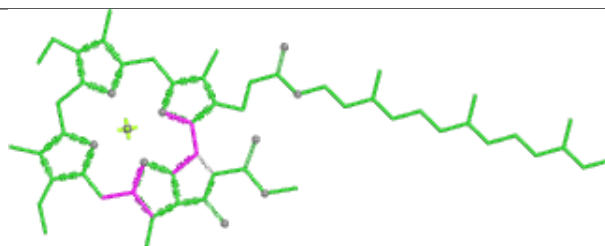


Rings

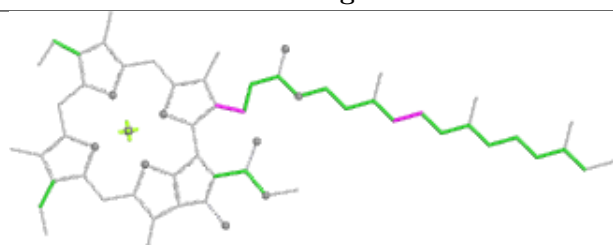
Ligand CLA a 803



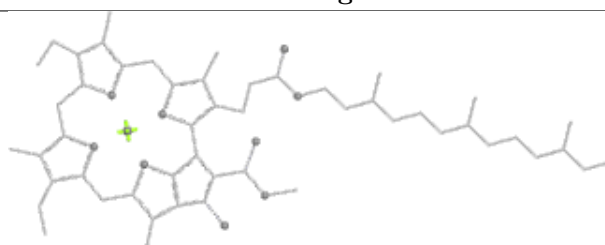
Bond lengths



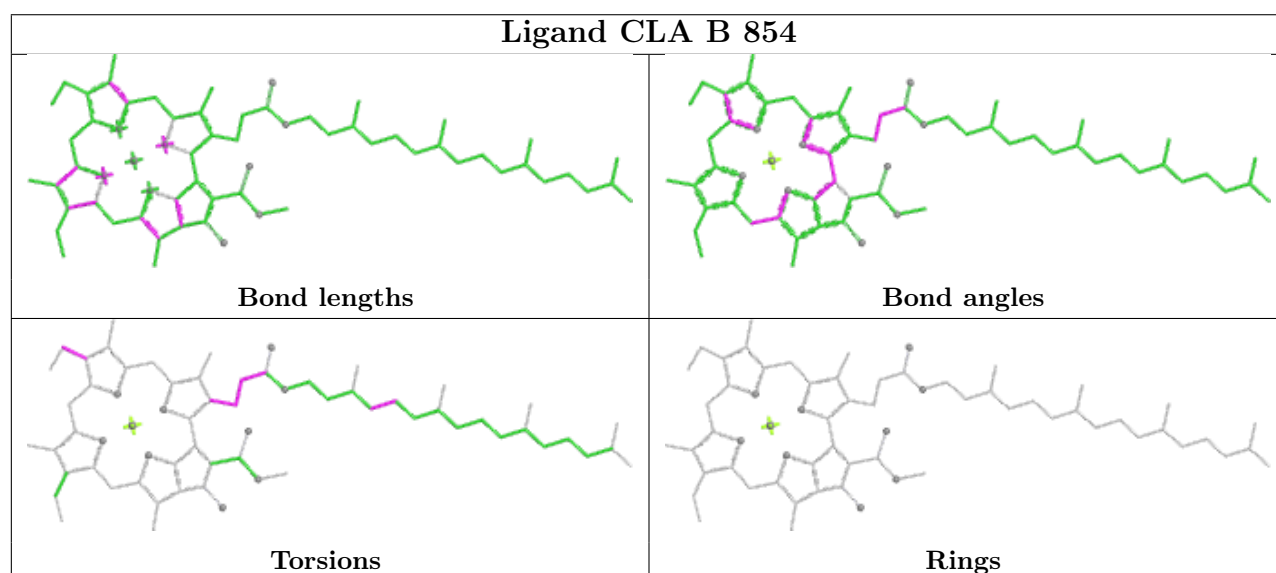
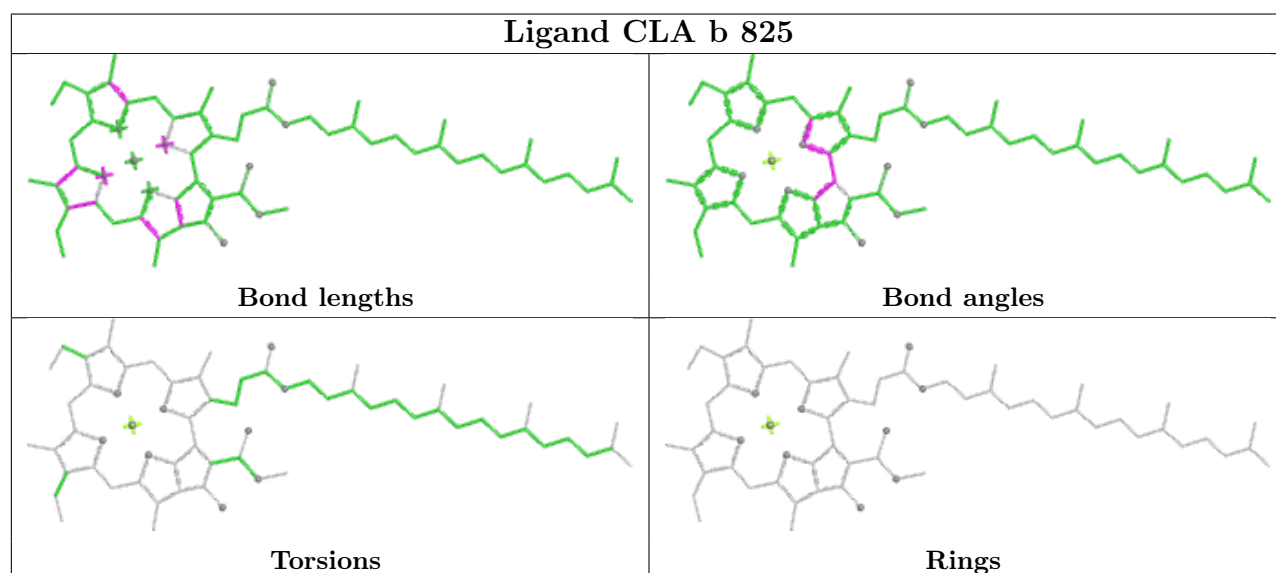
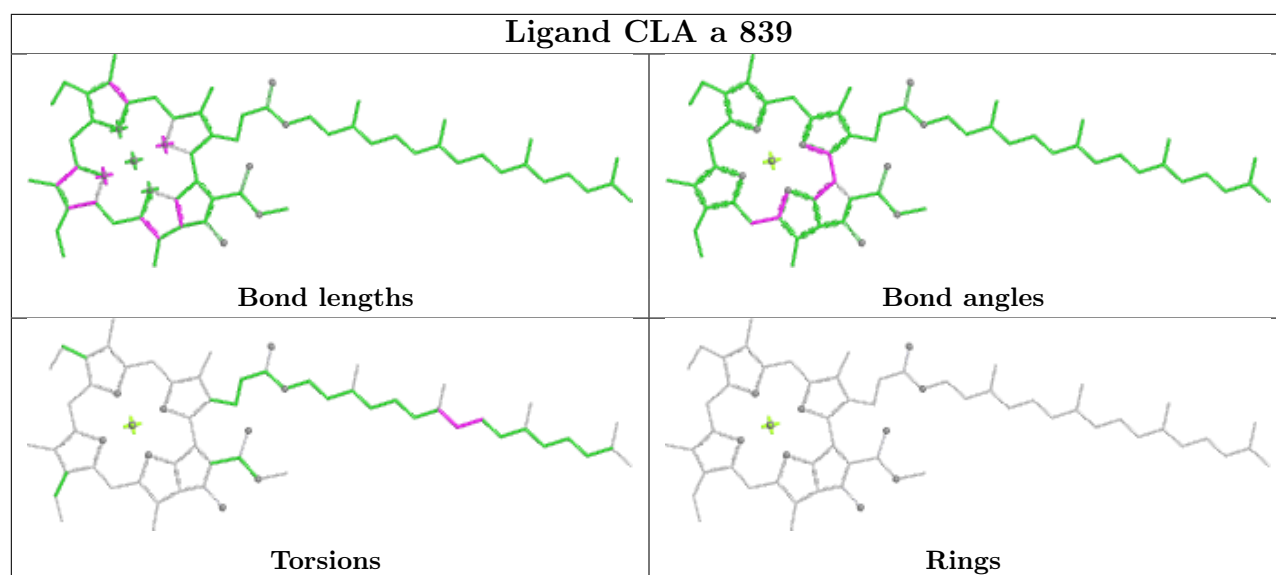
Bond angles

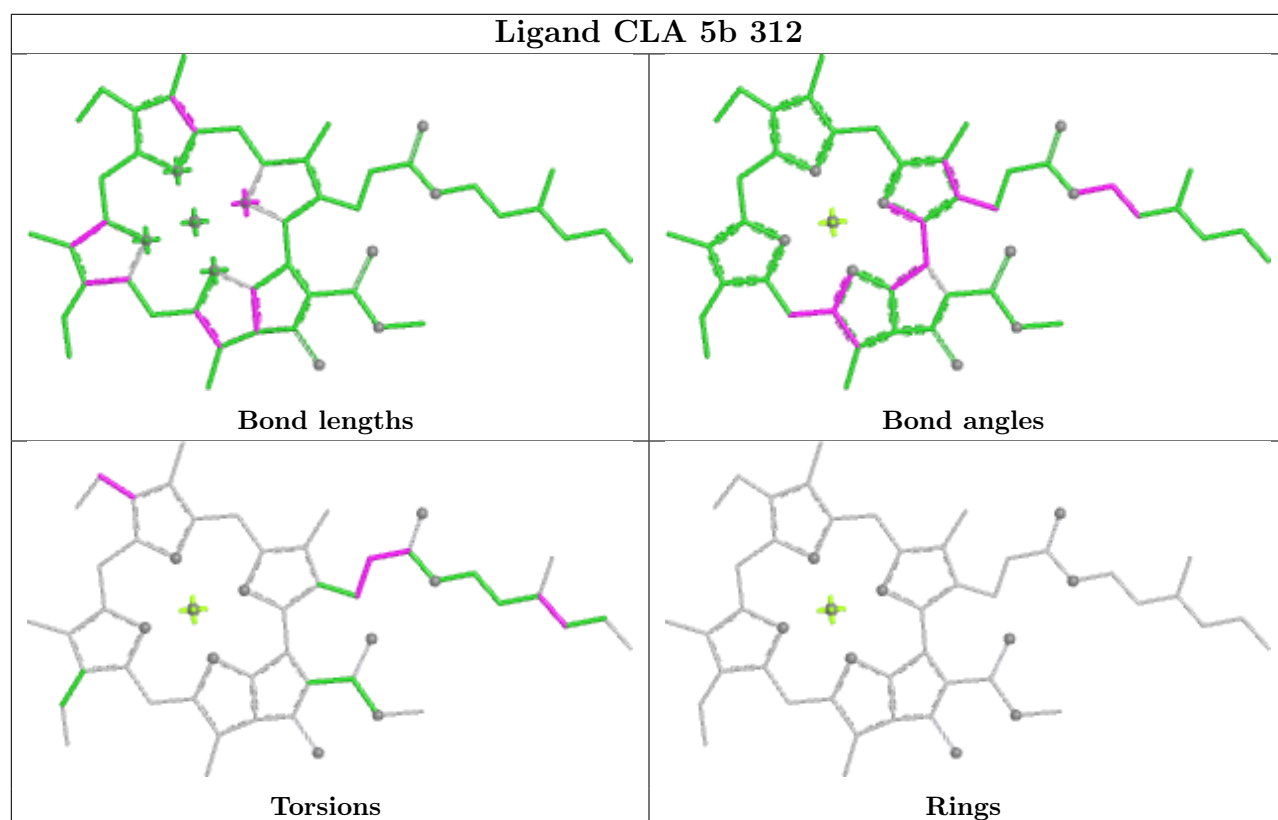
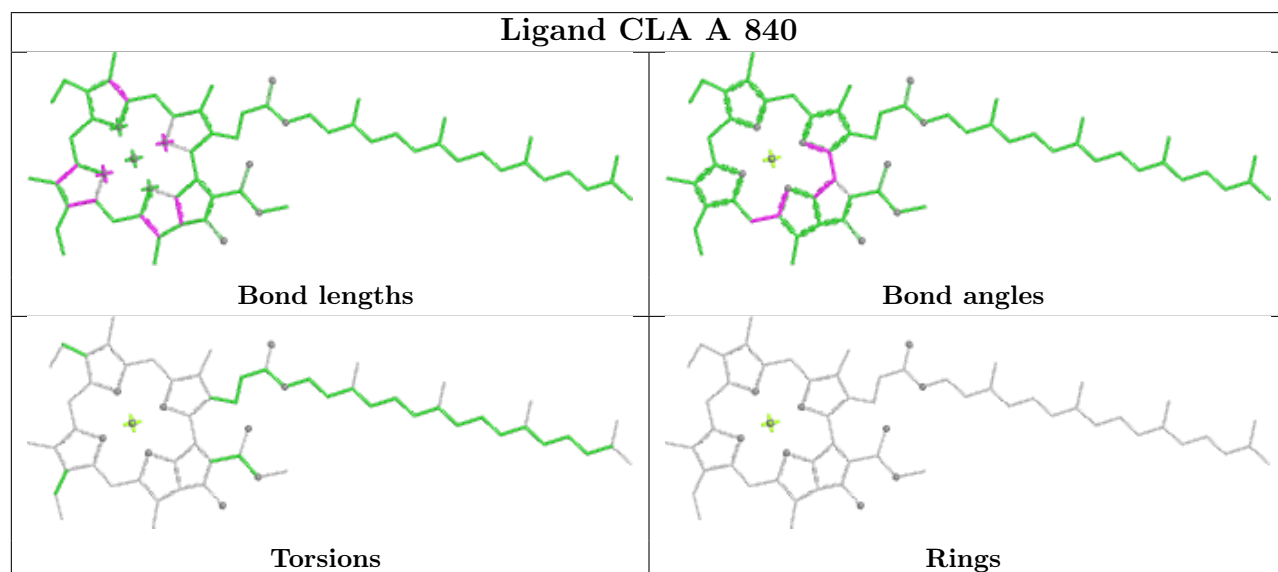
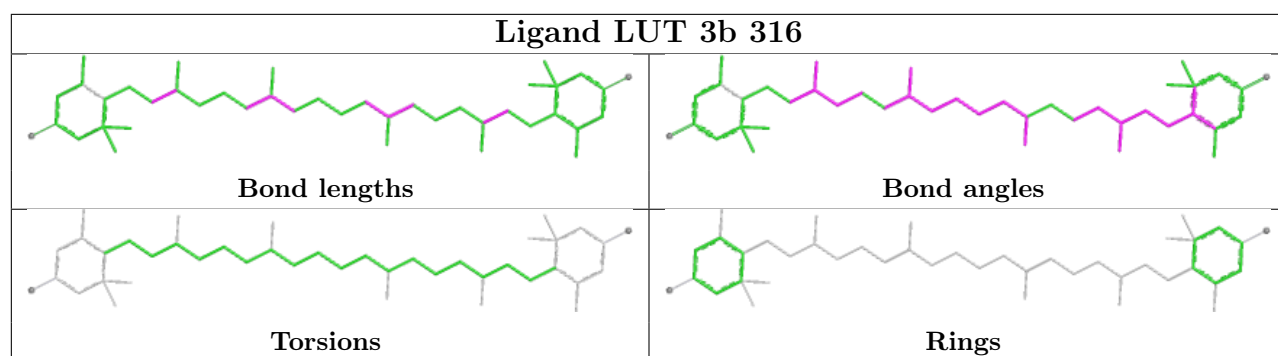


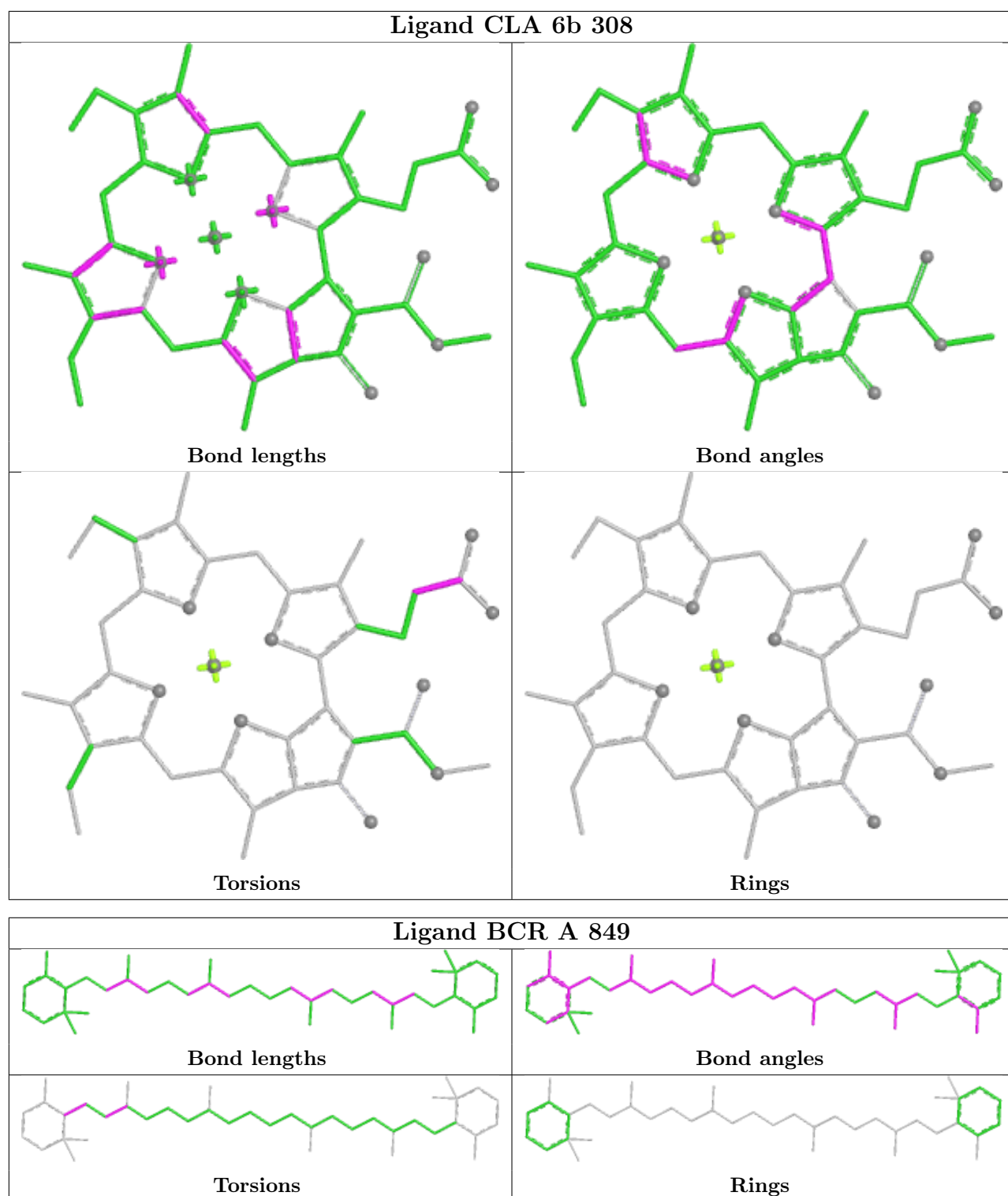
Torsions

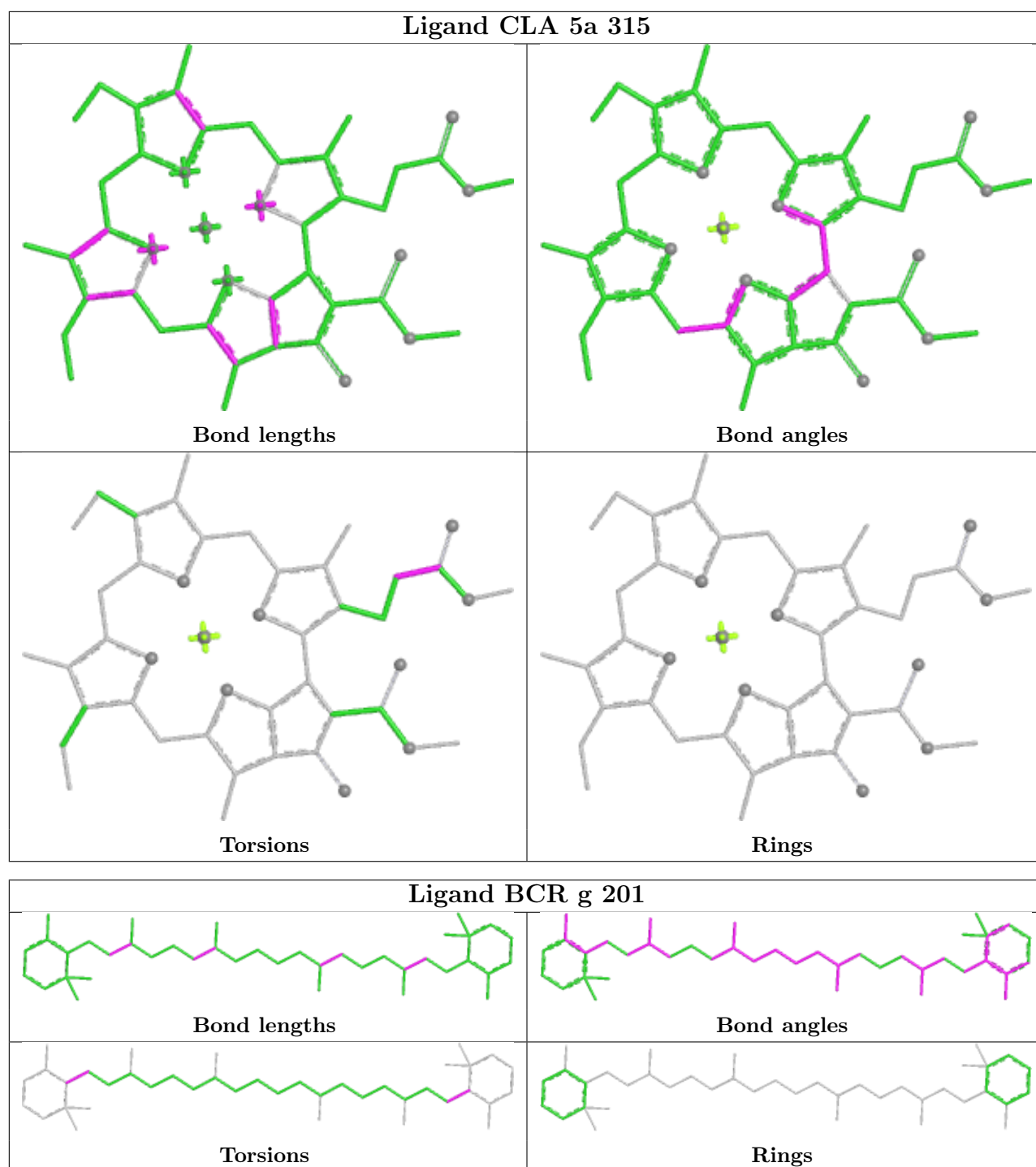


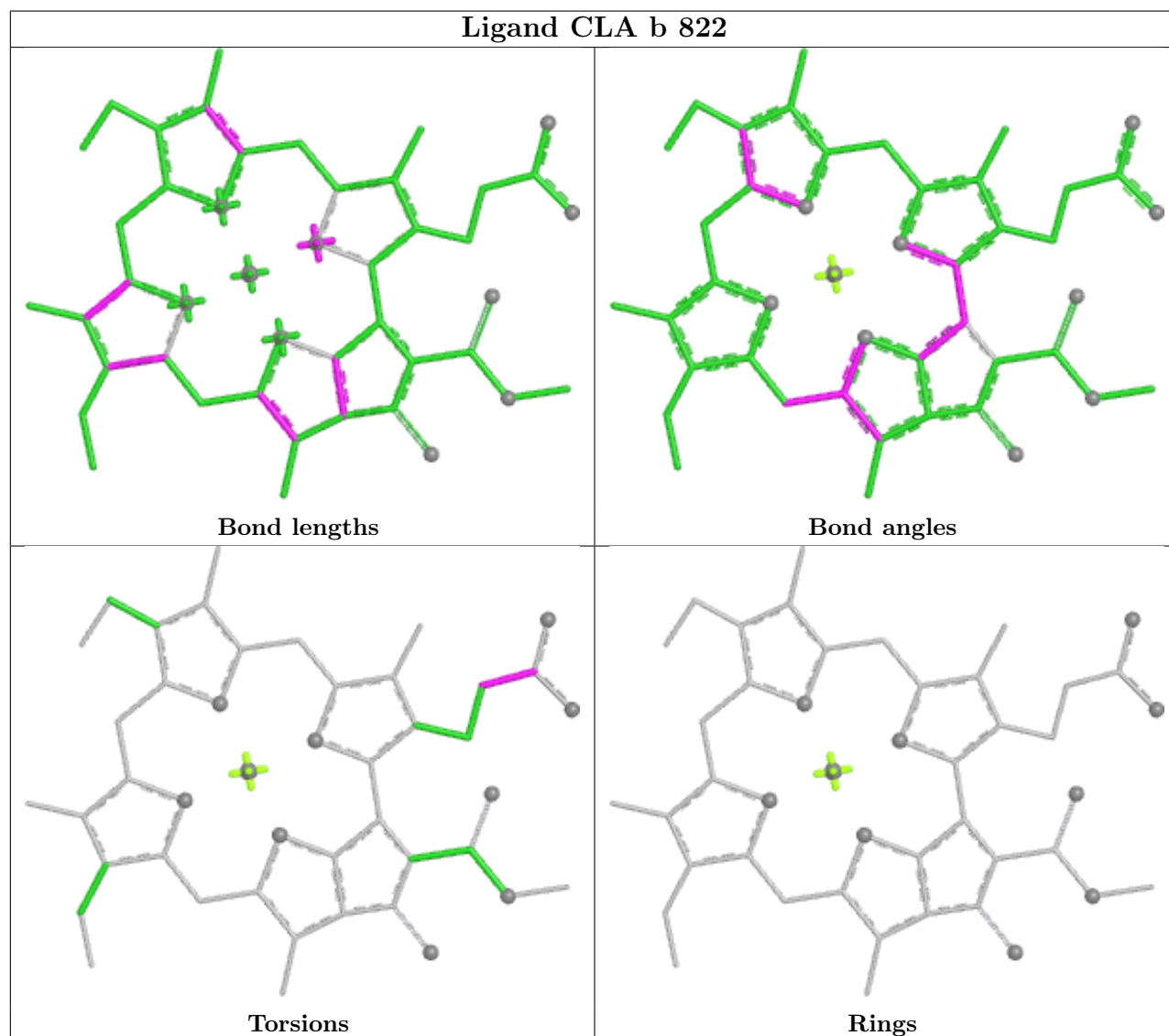
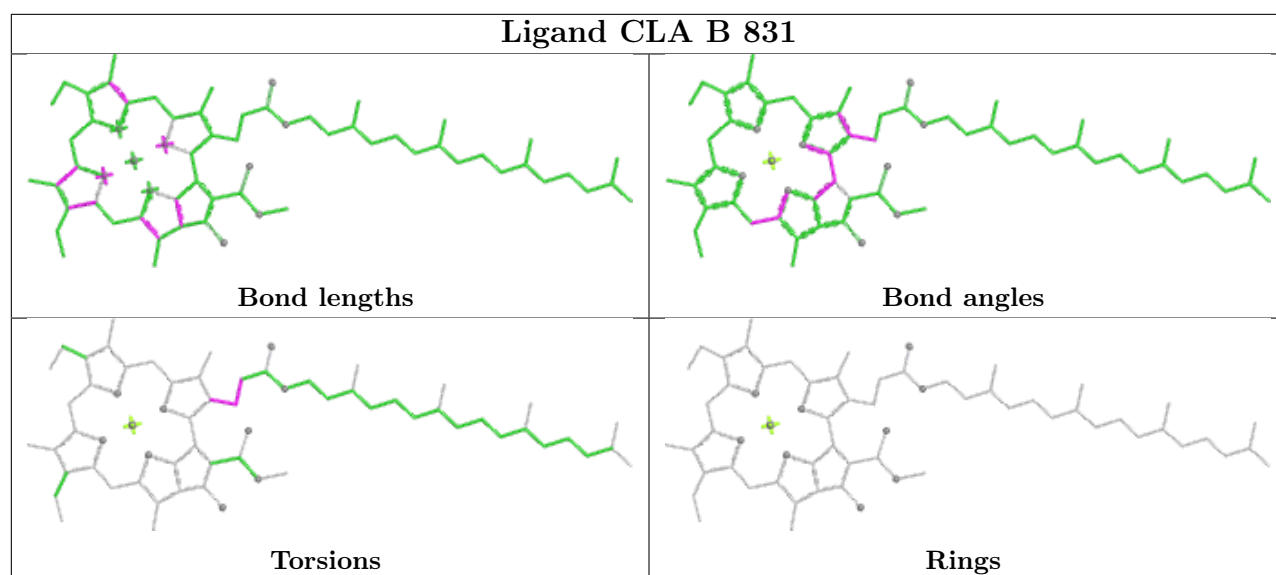
Rings

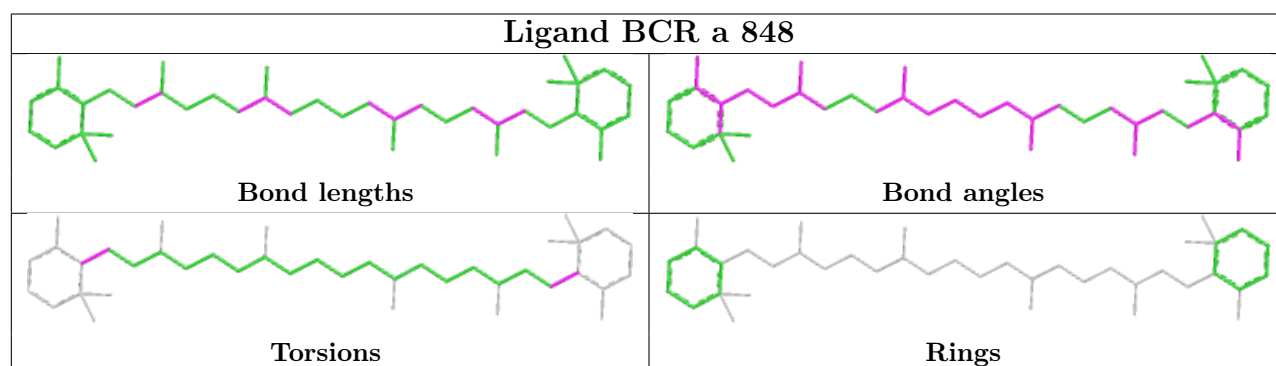
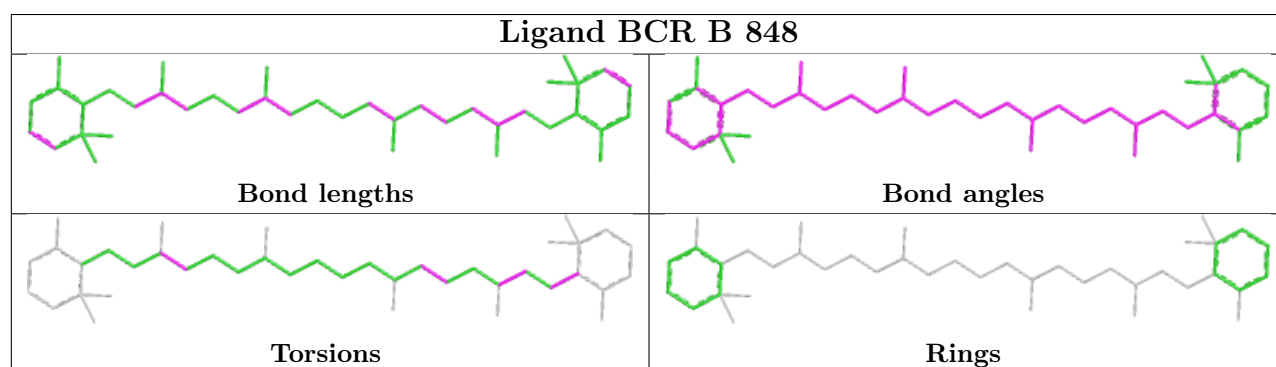
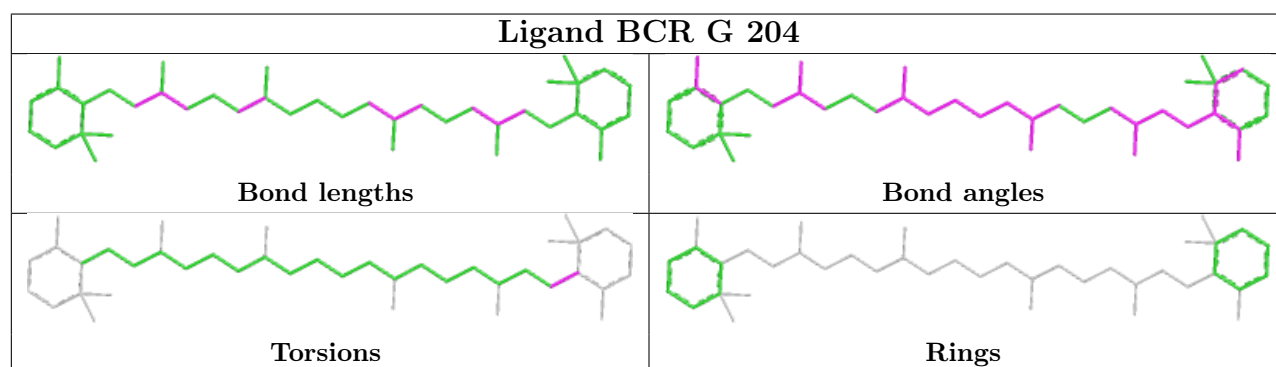
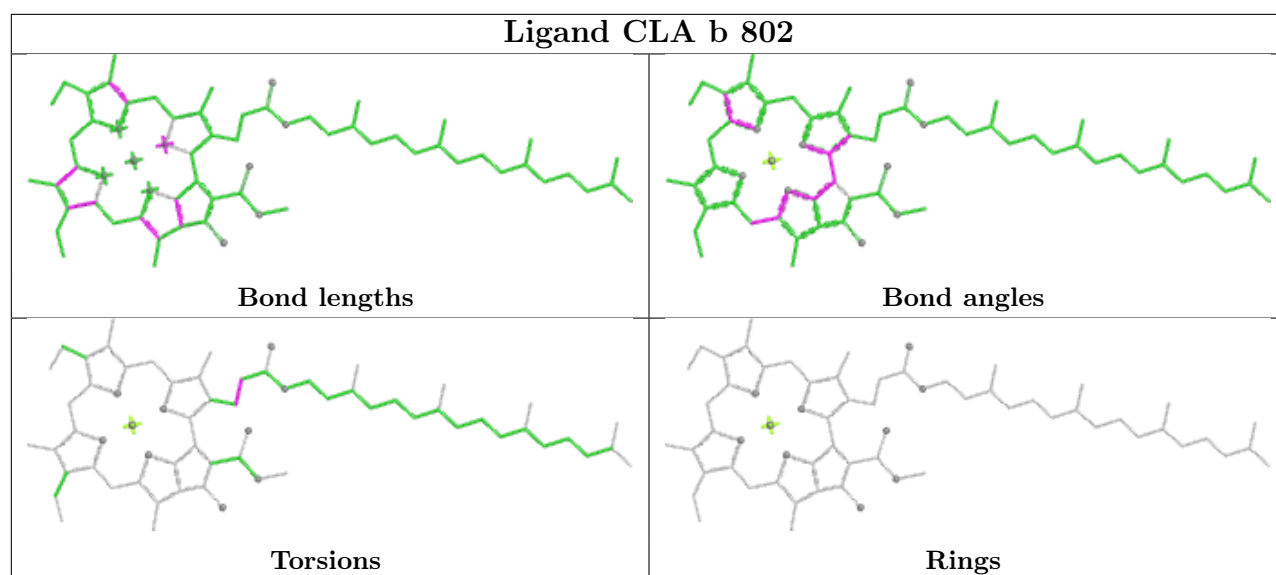


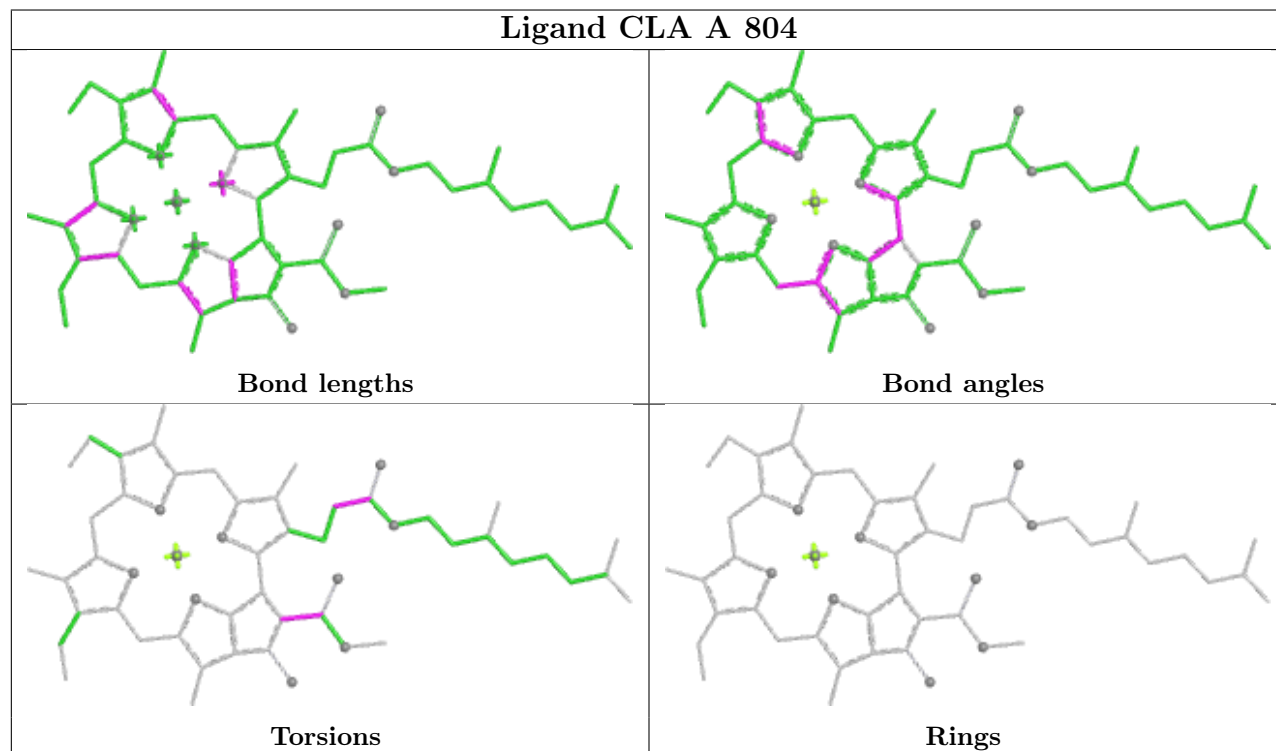
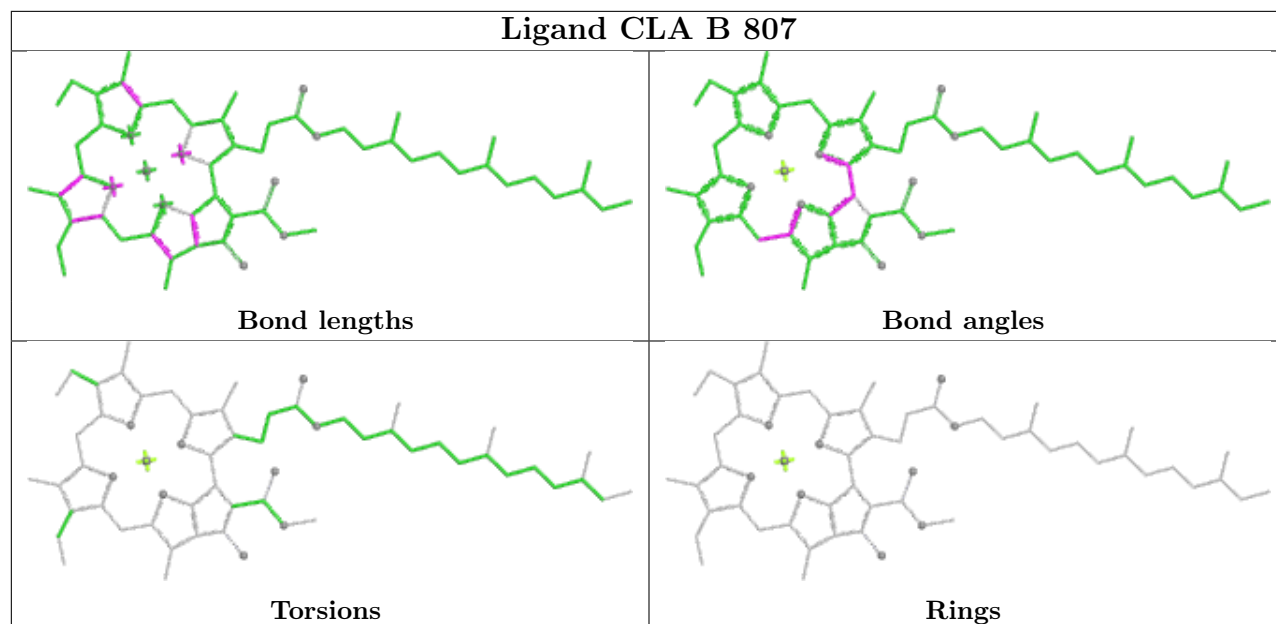


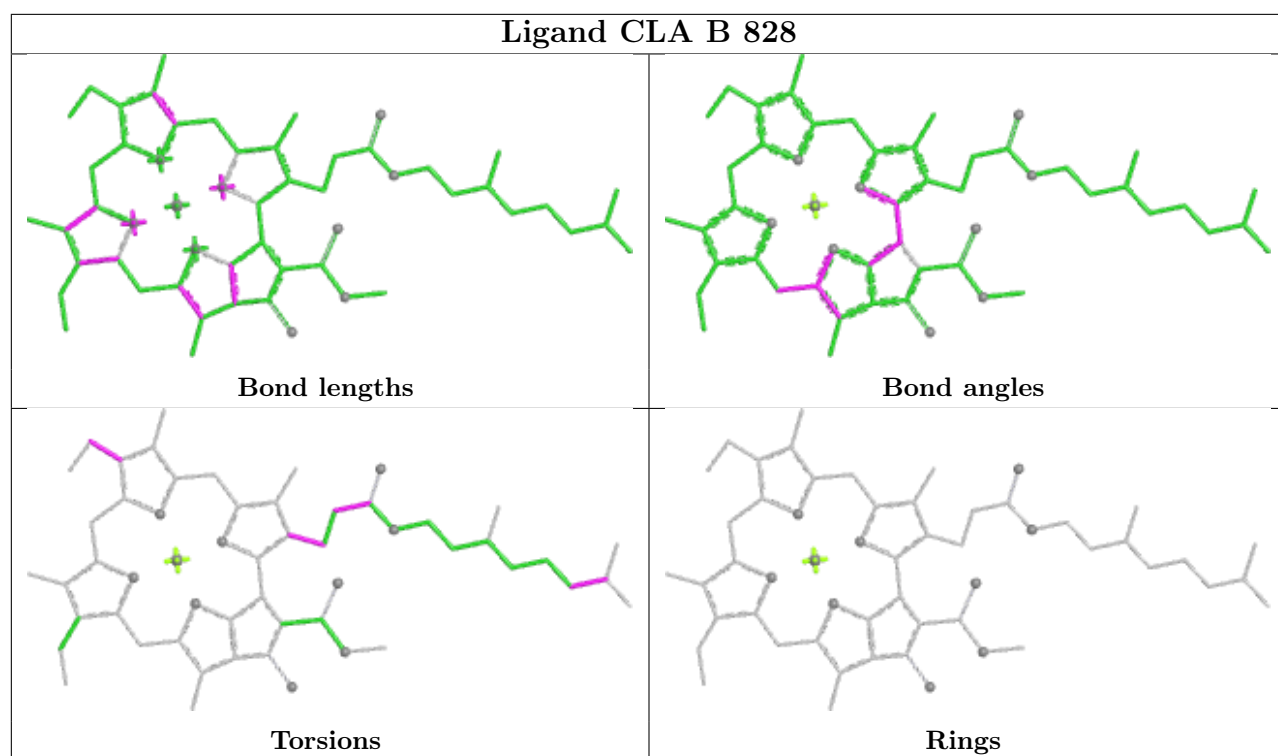


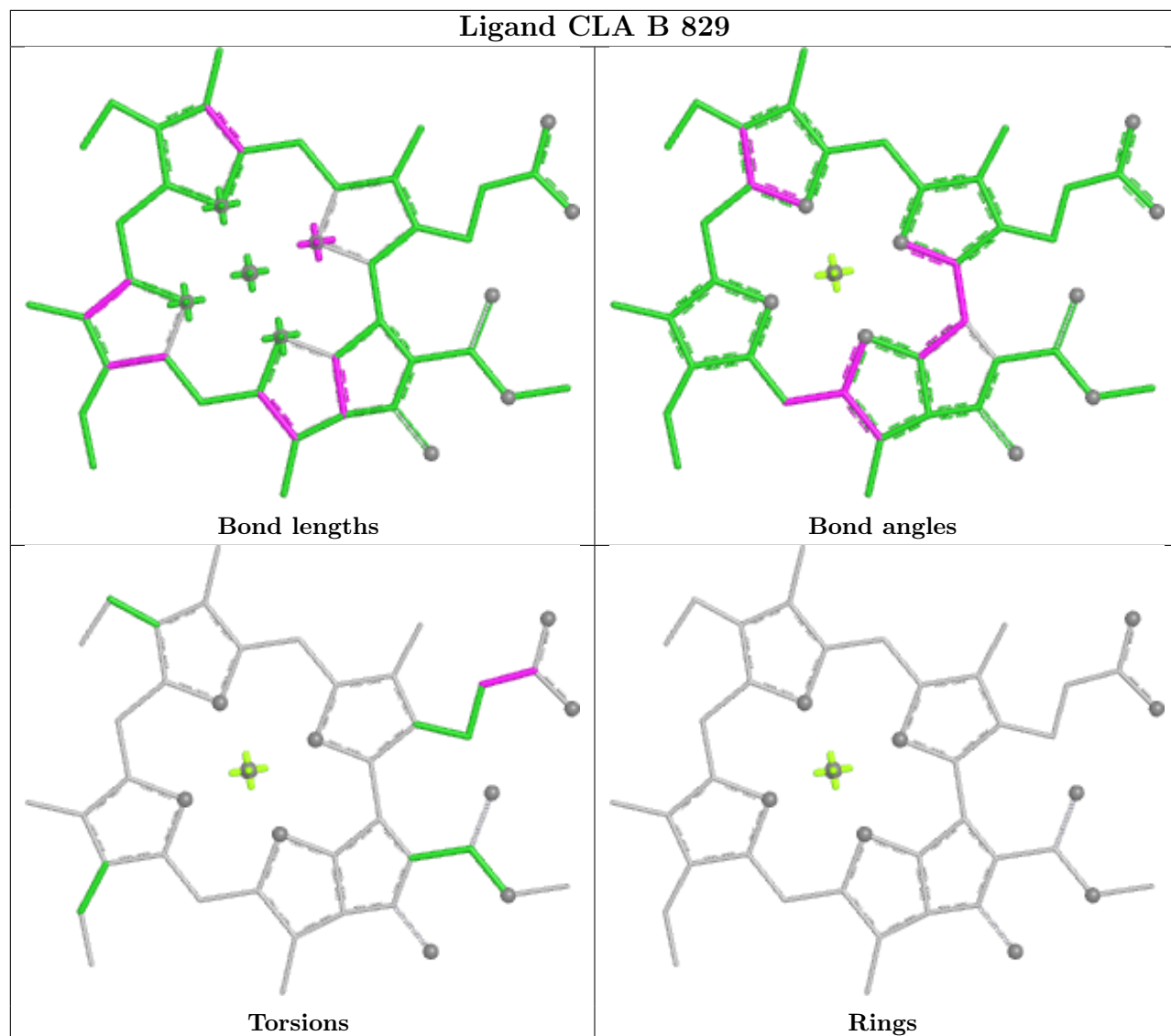


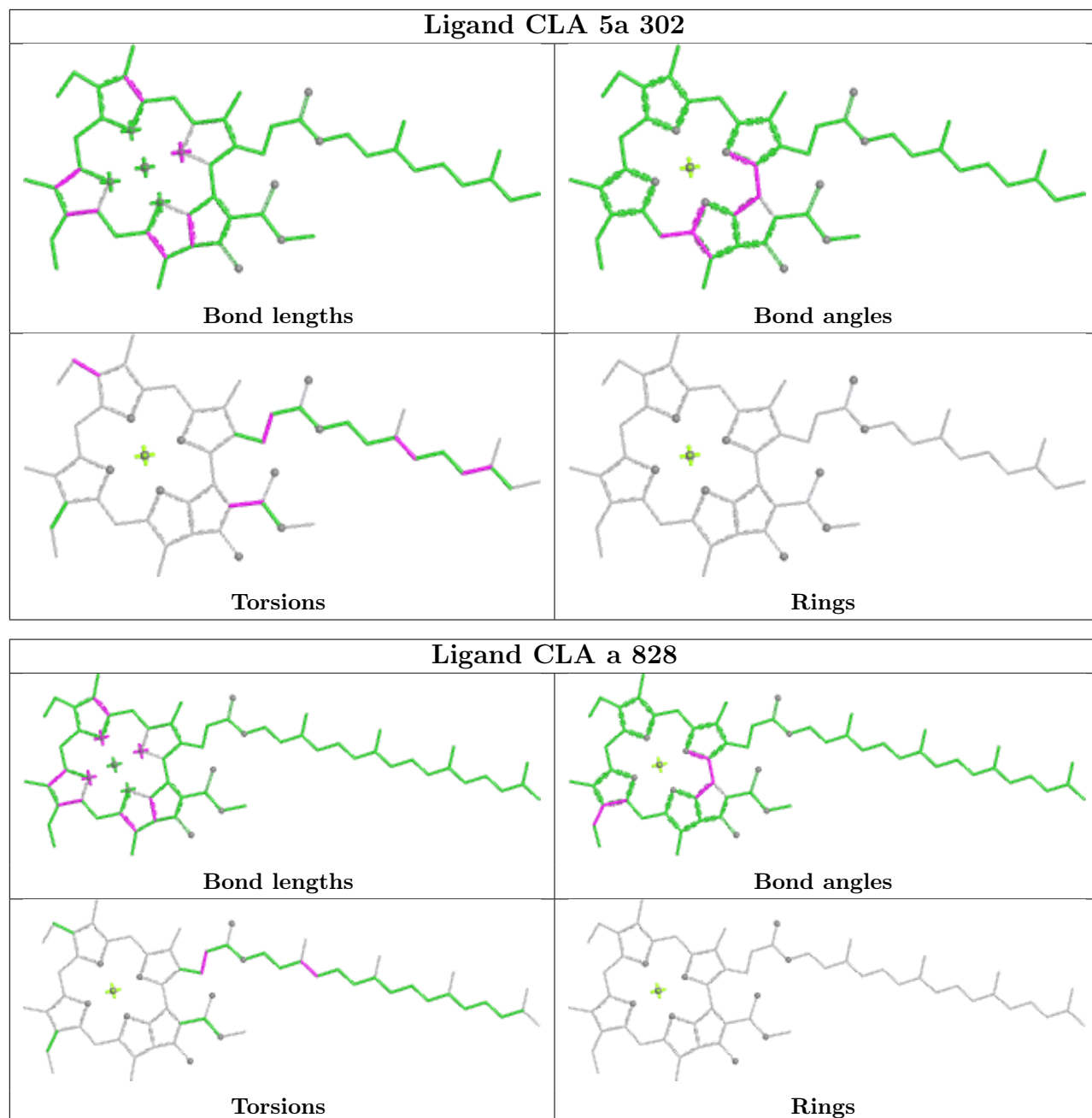


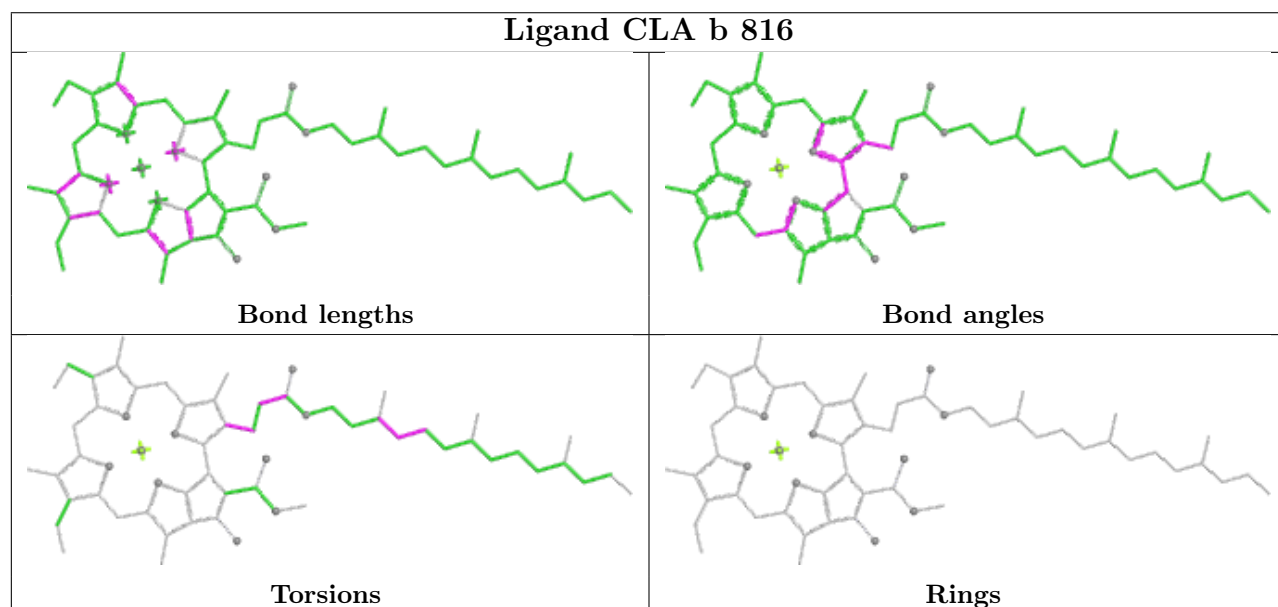
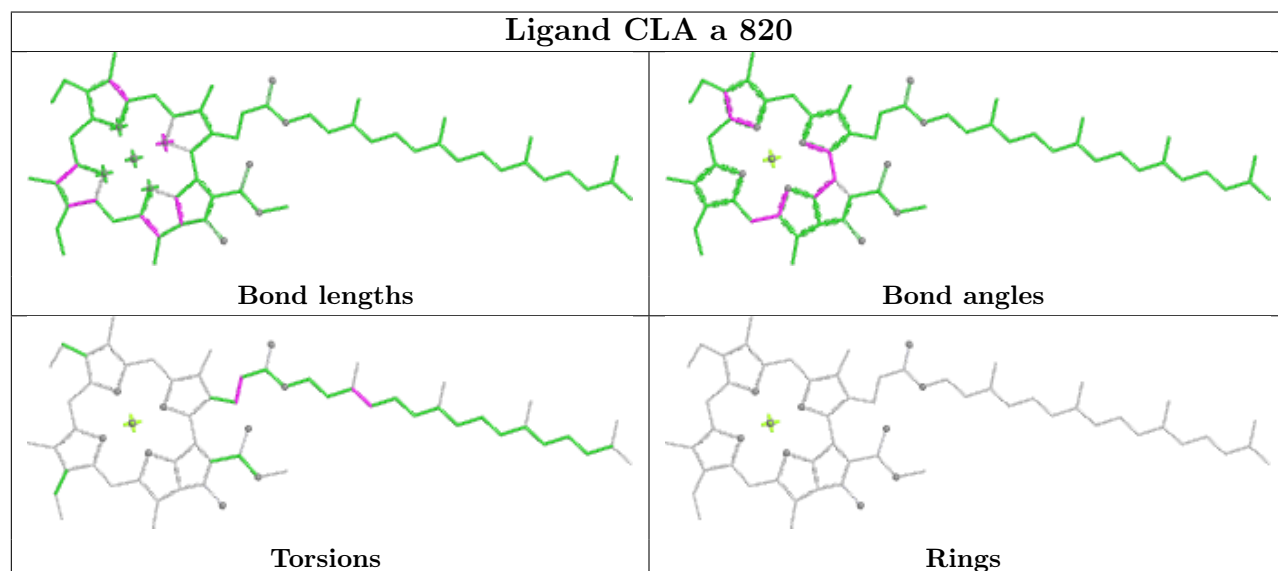
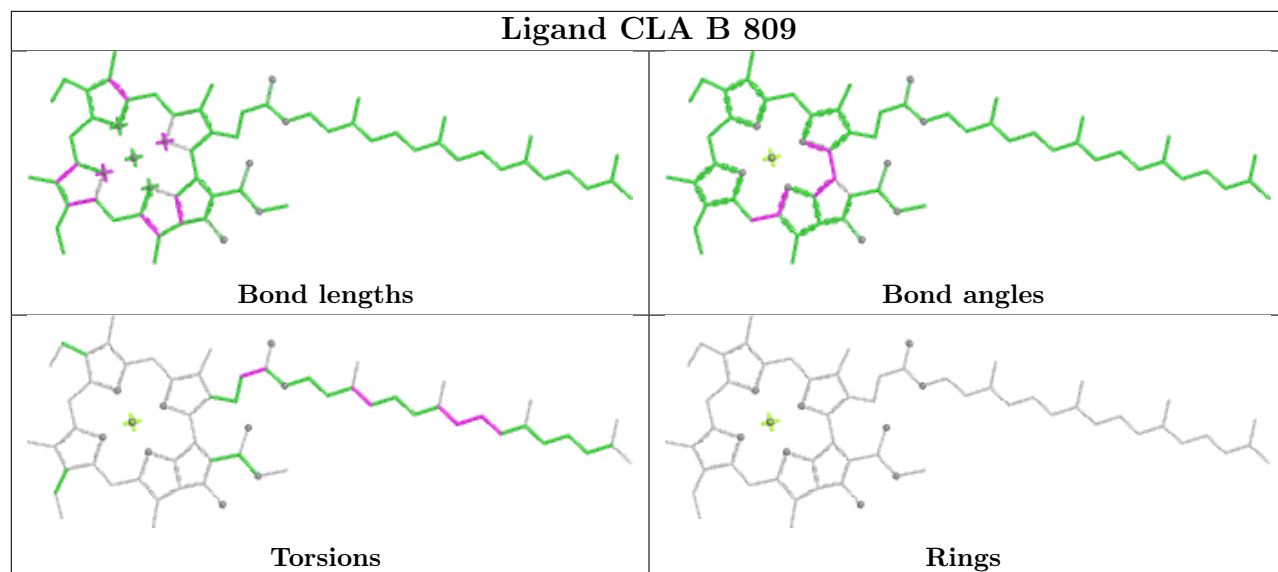


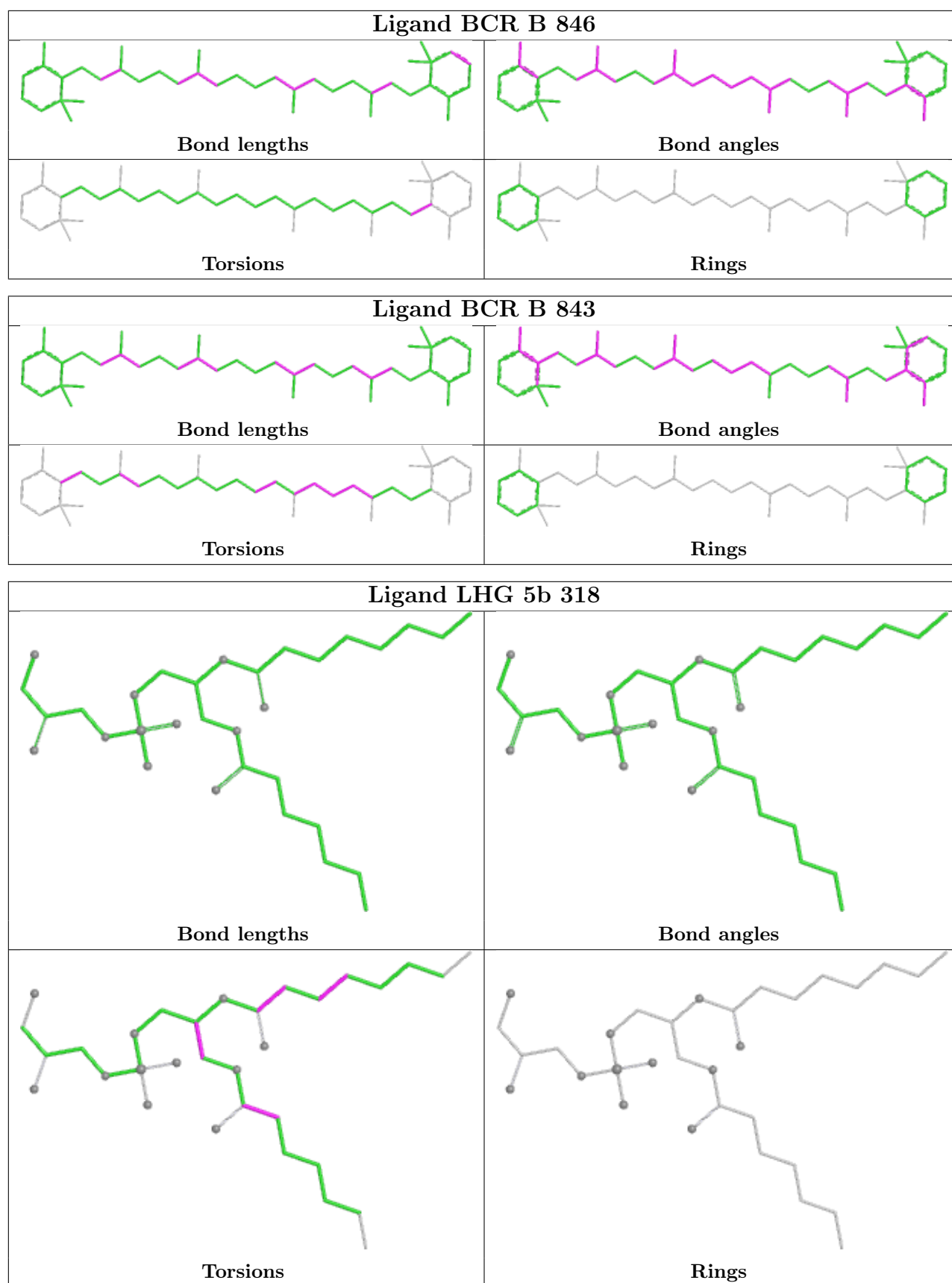


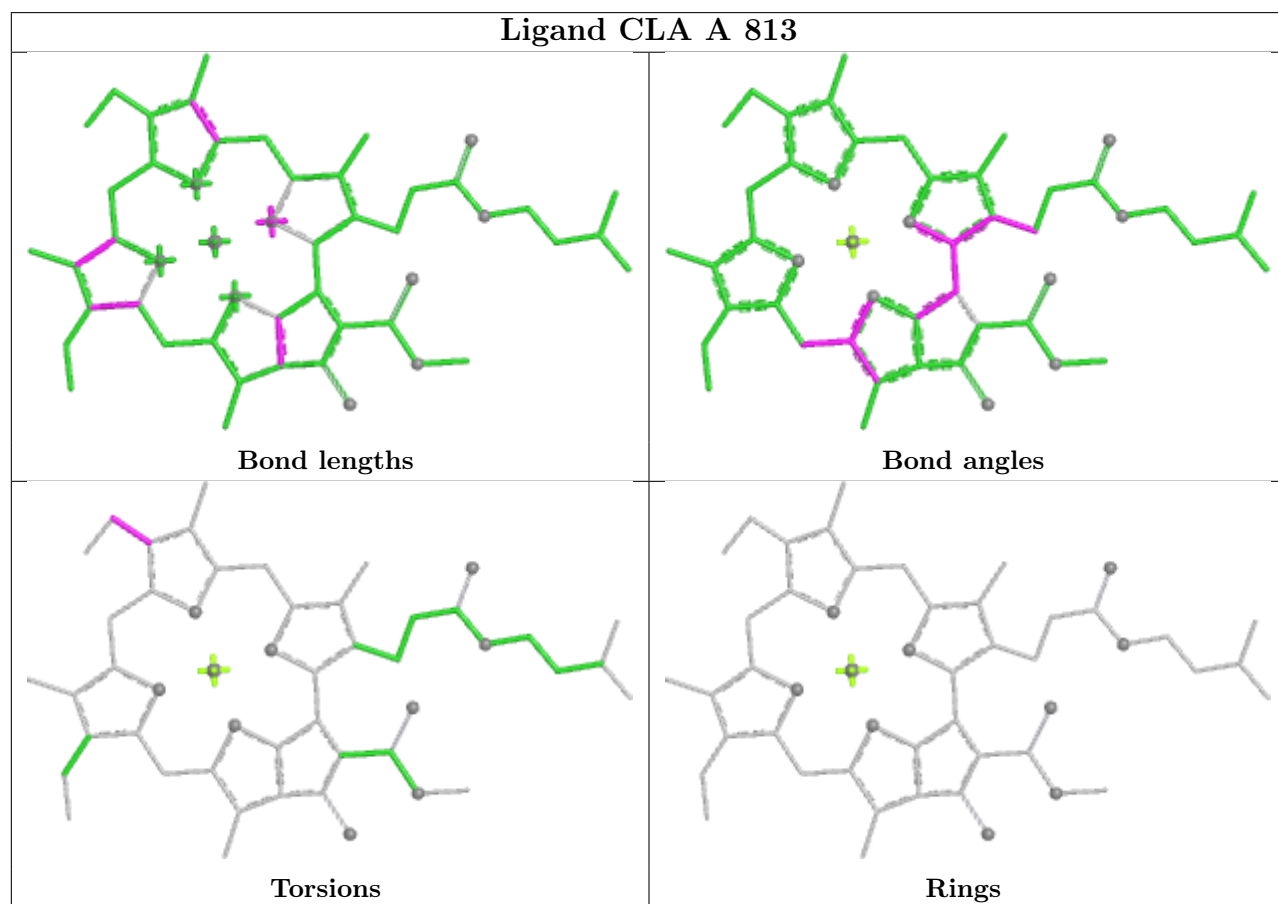
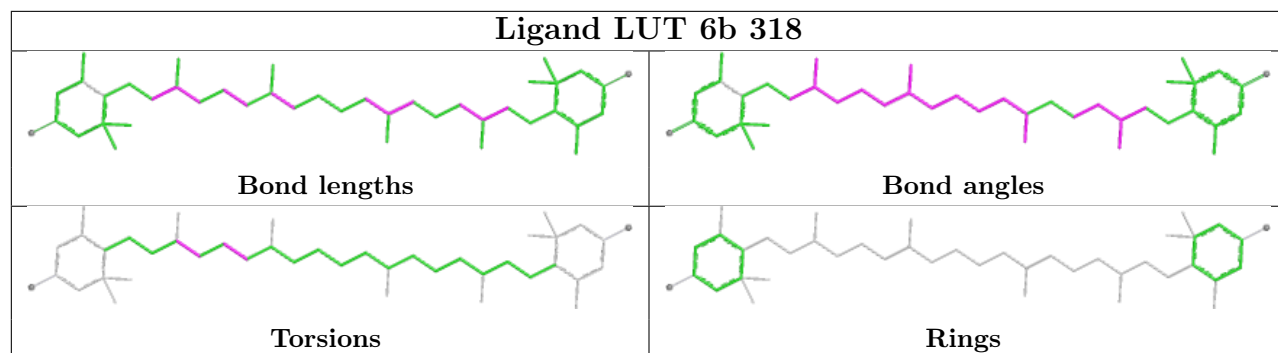




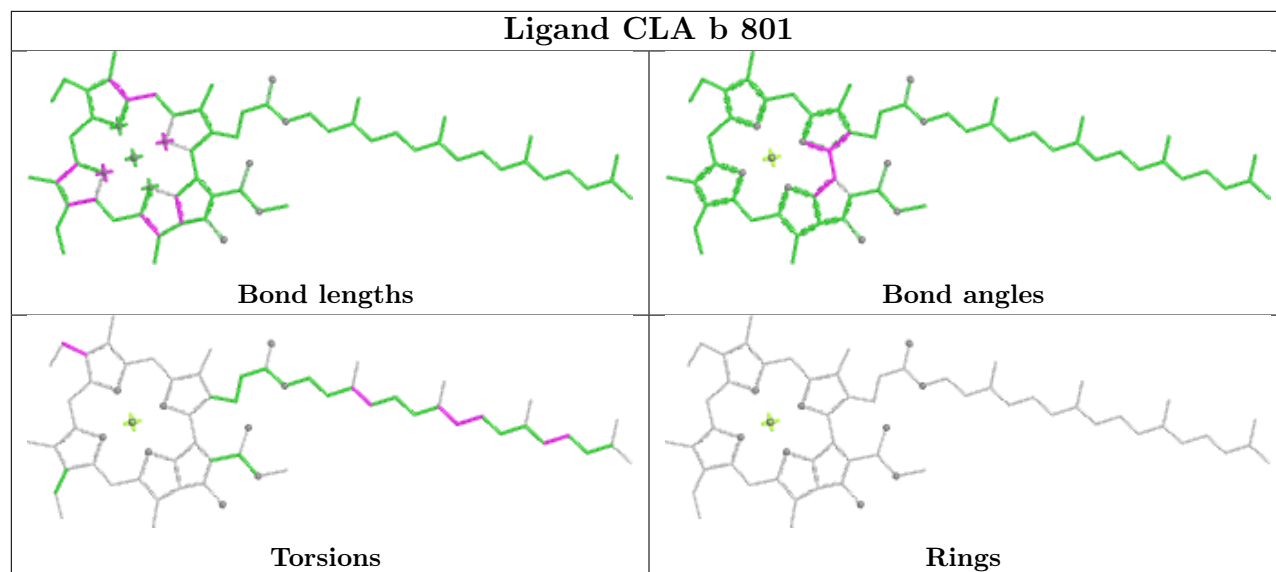




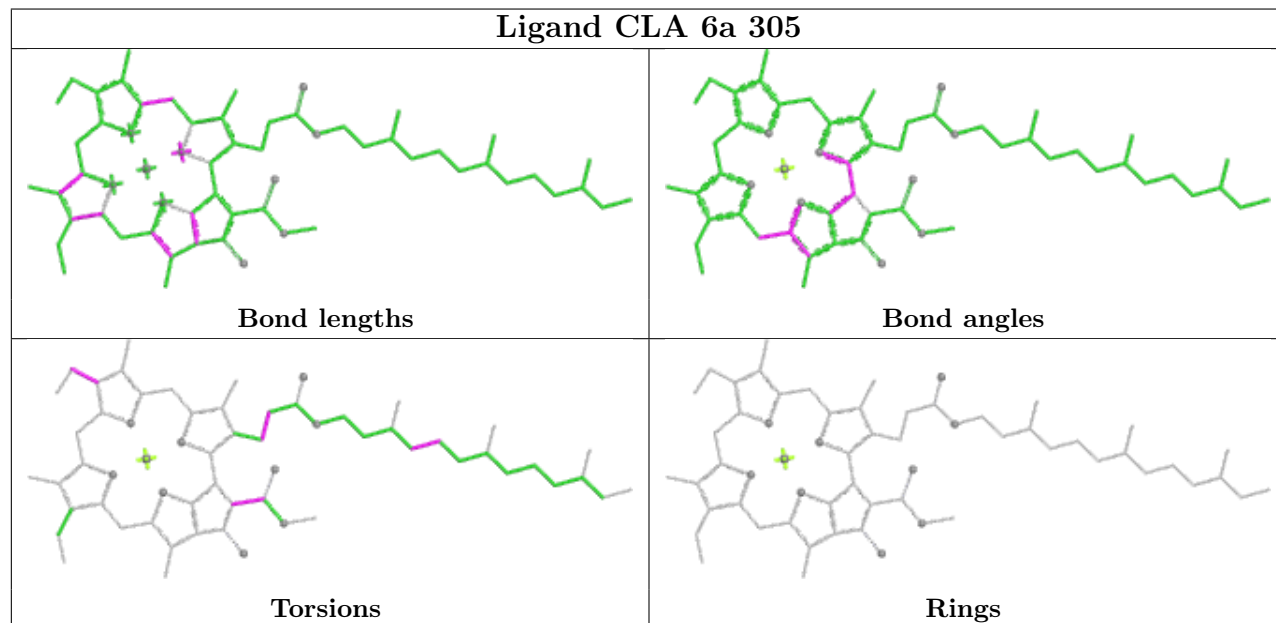


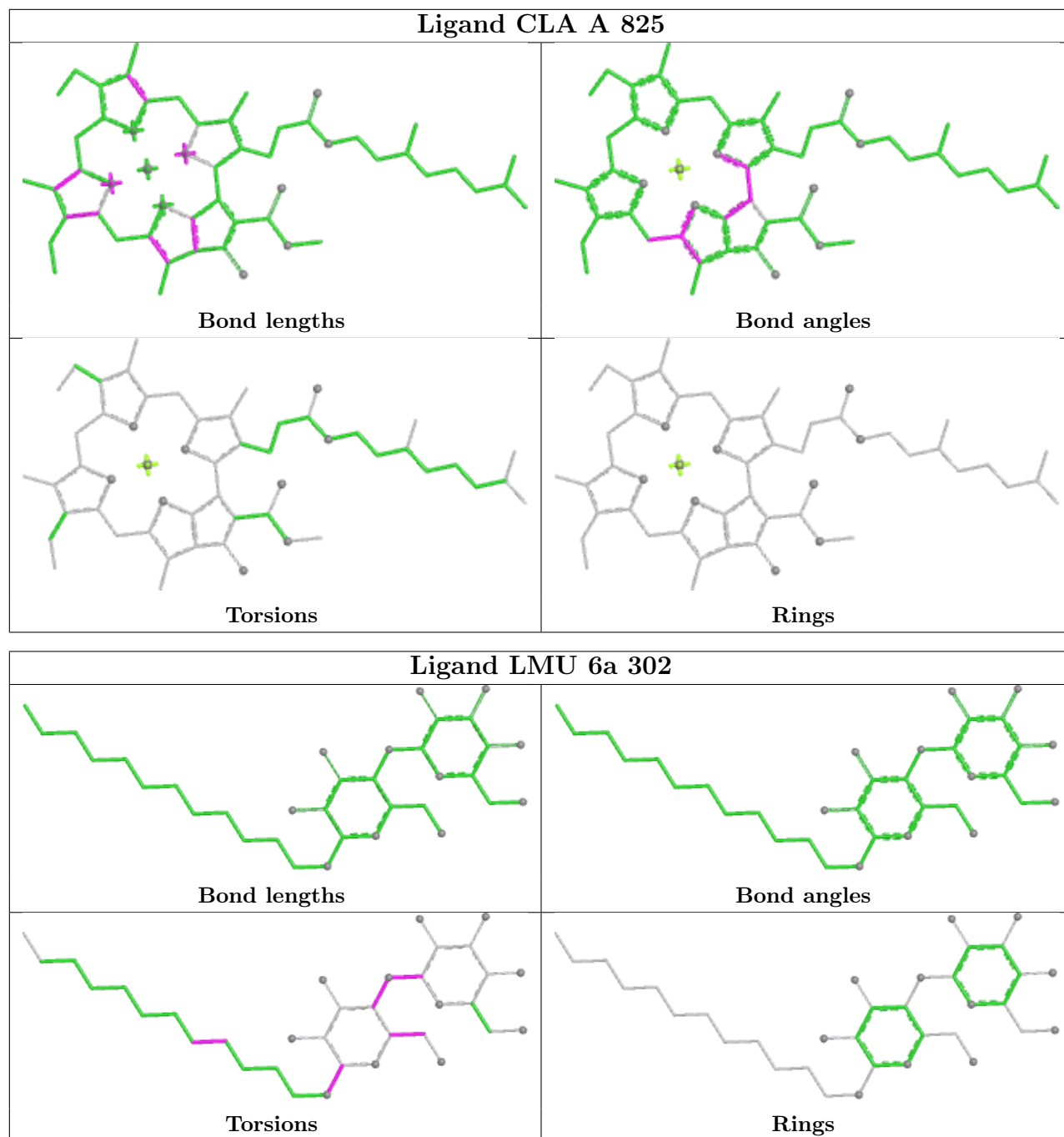


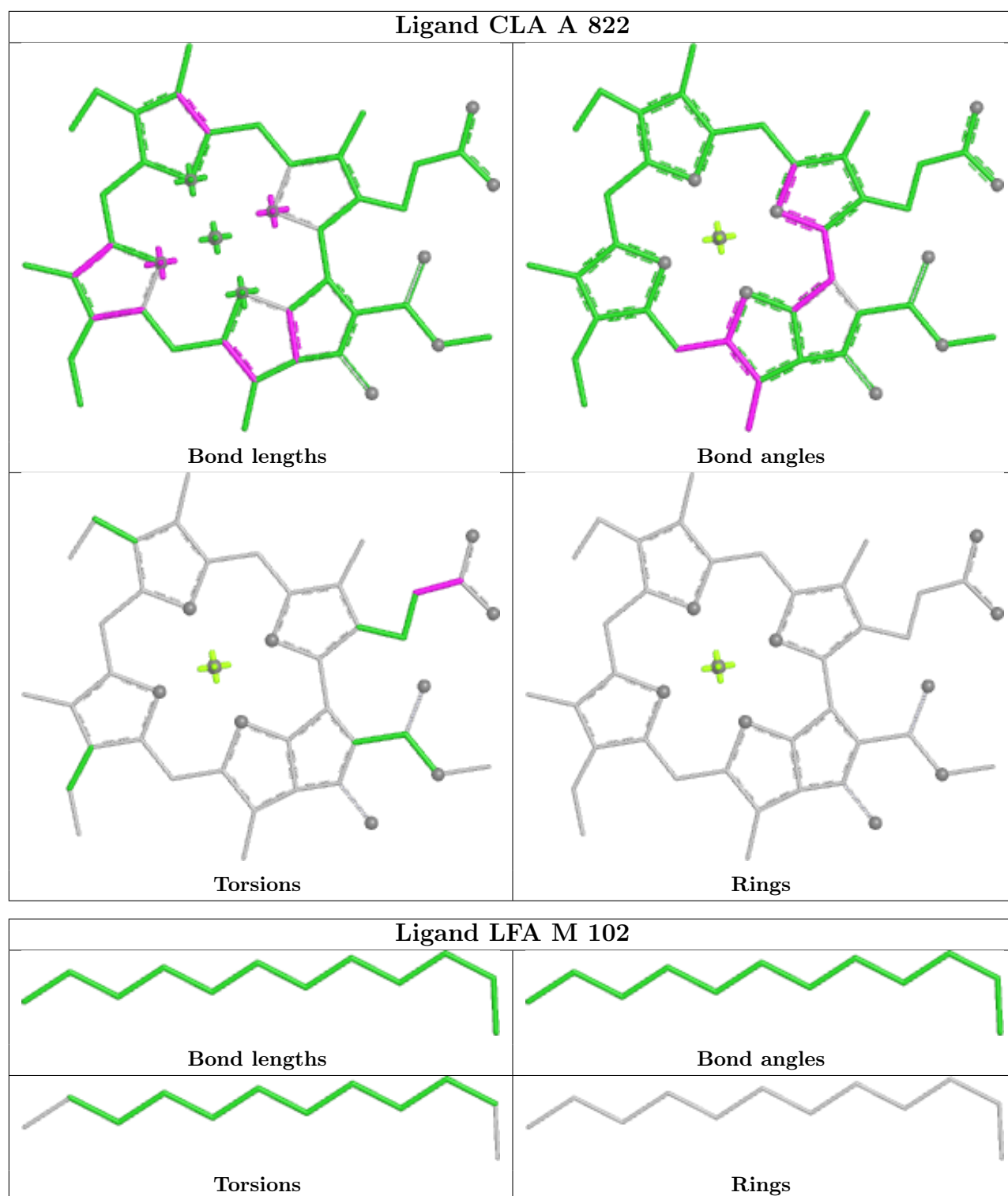
Ligand CLA b 801



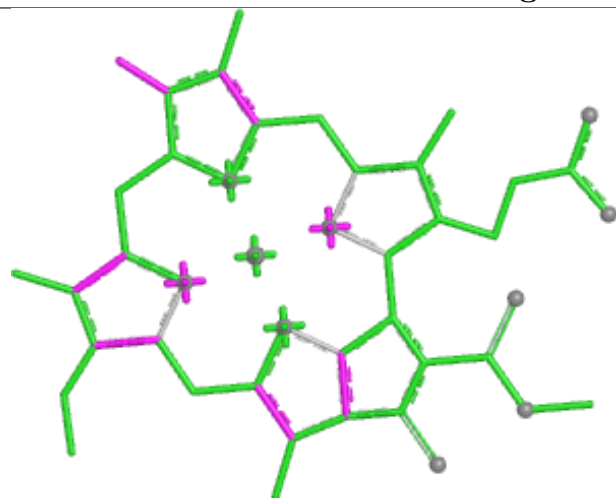
Ligand CLA 6a 305



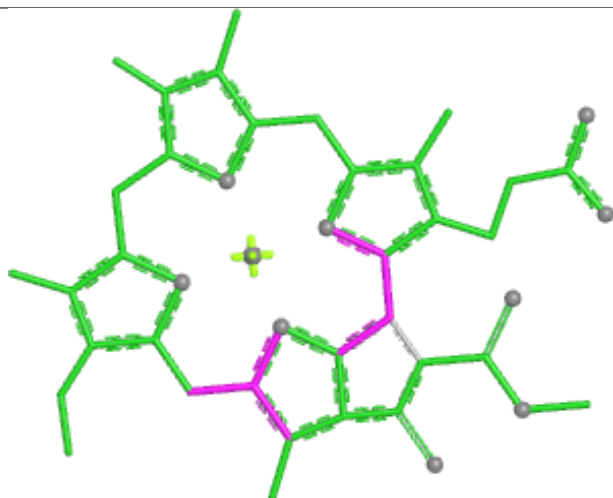




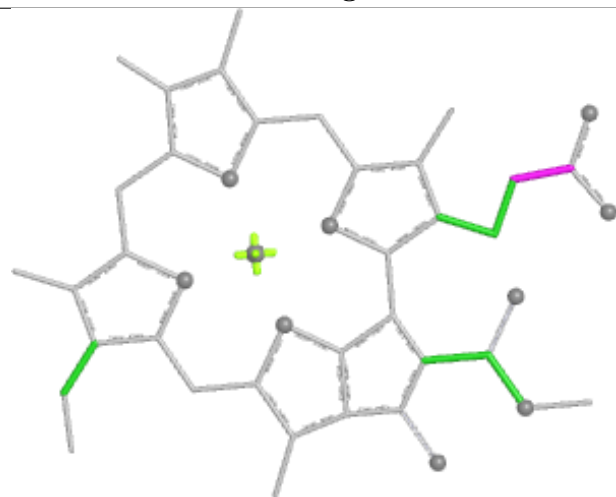
Ligand CLA k 201



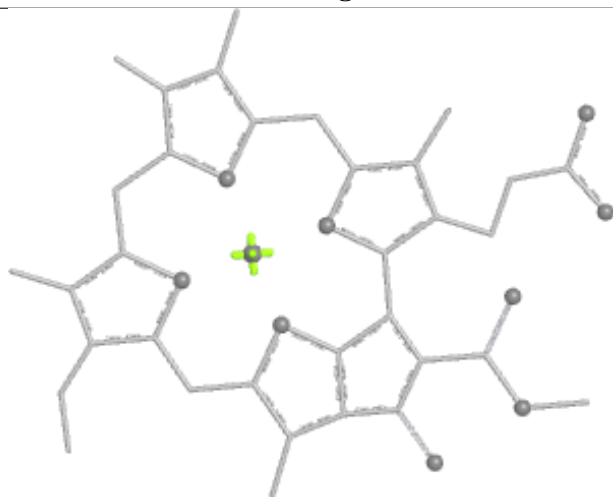
Bond lengths



Bond angles

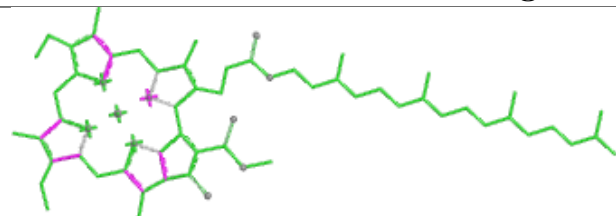


Torsions

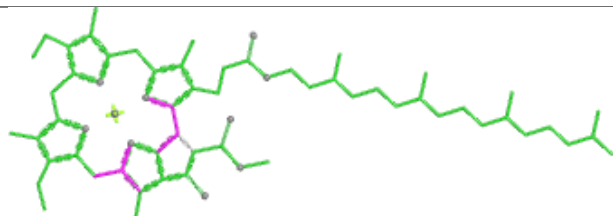


Rings

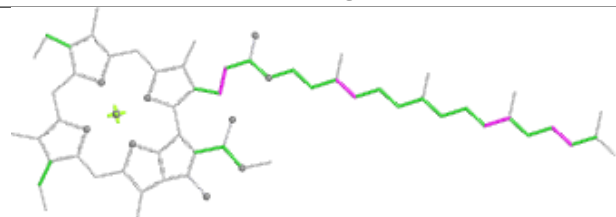
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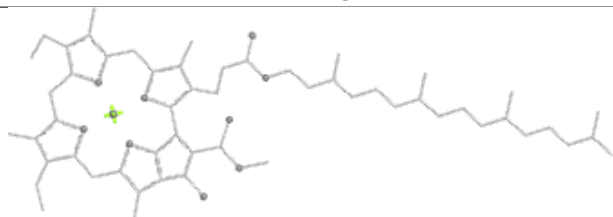
Bond lengths



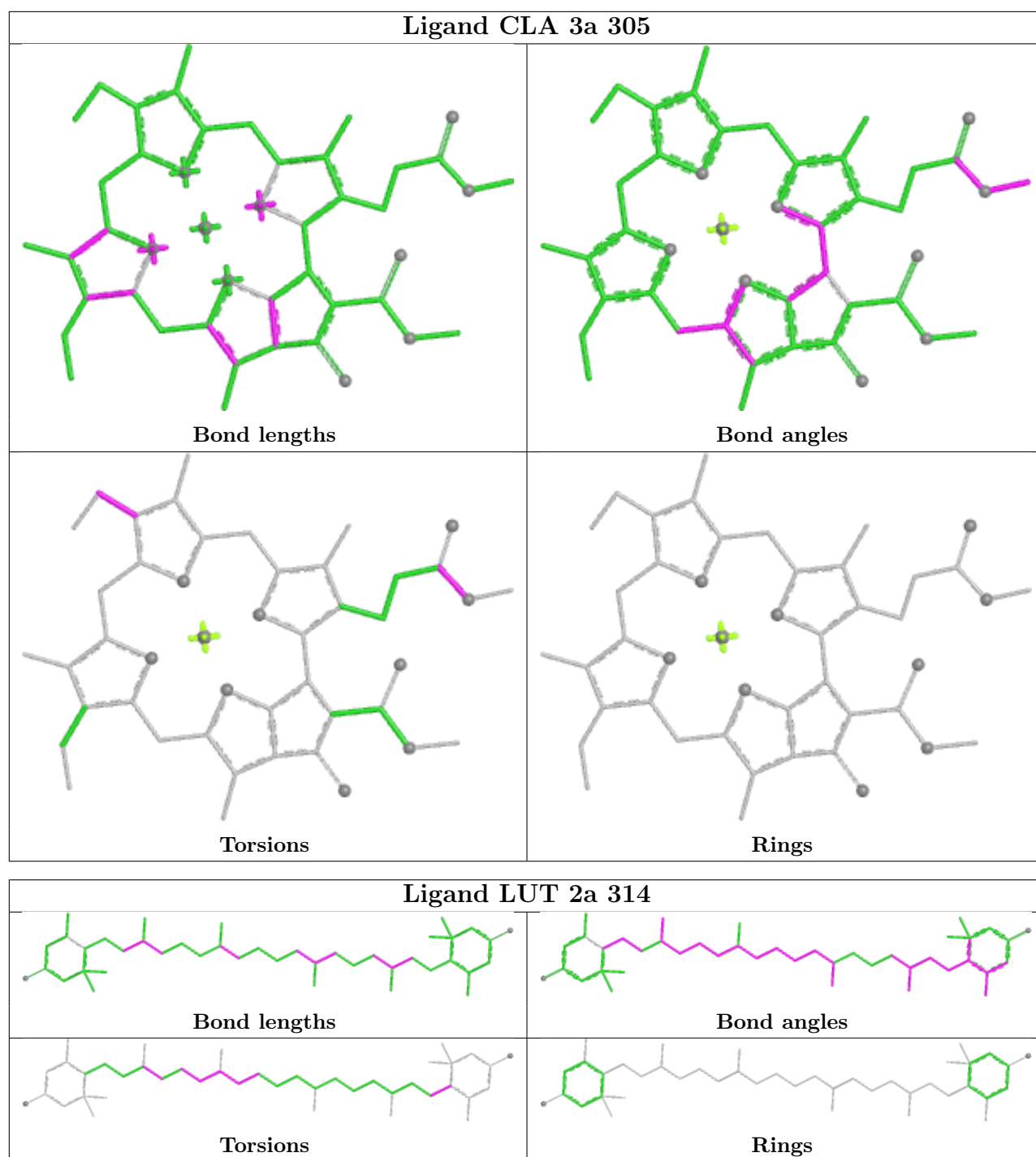
Bond angles

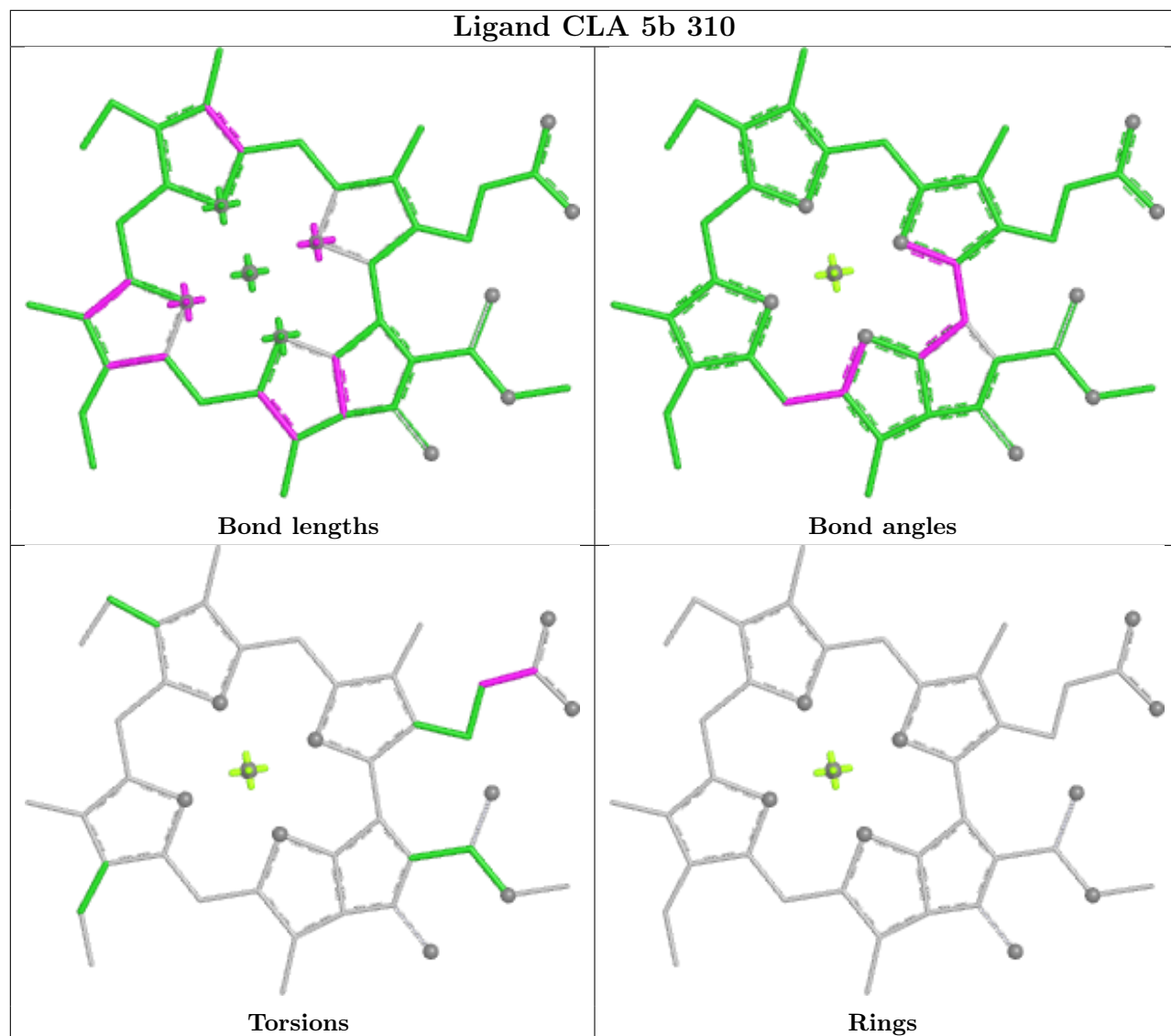


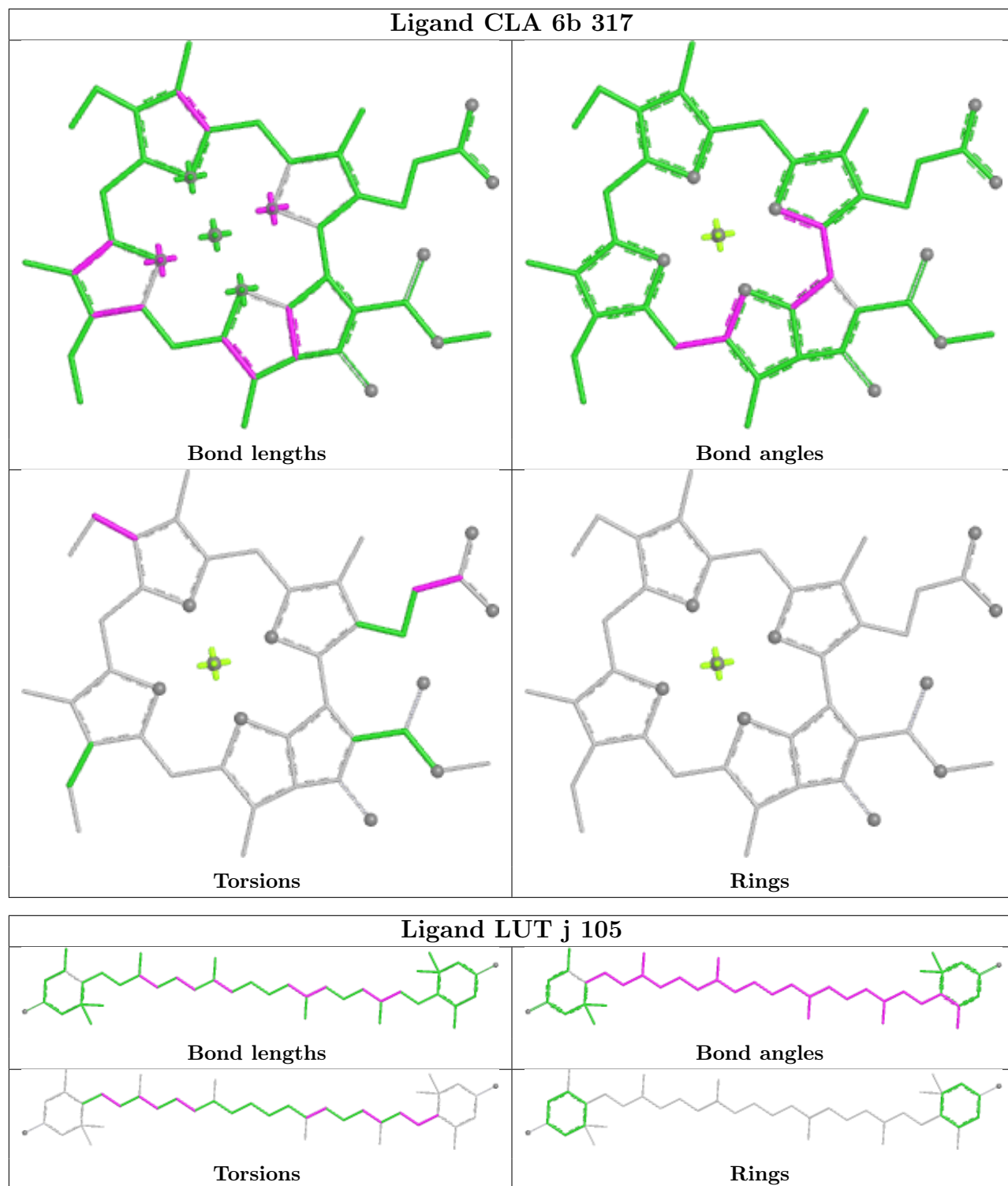
Torsions



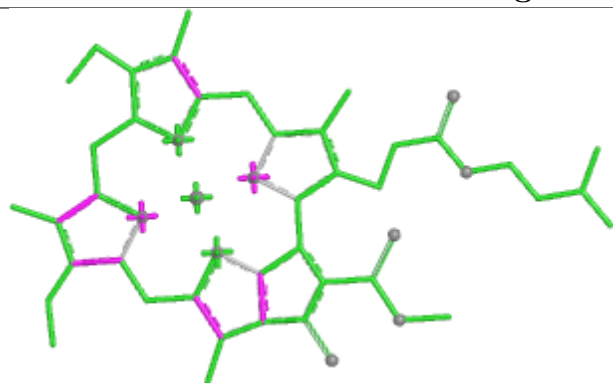
Rings



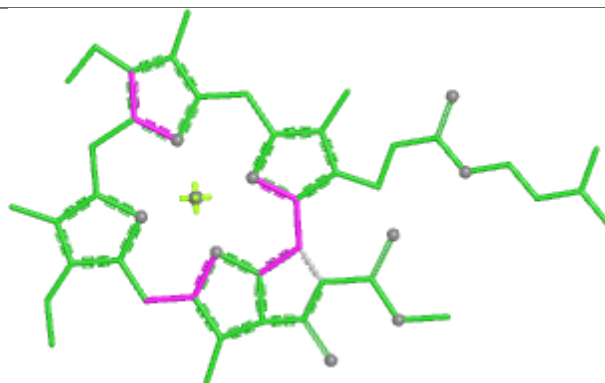




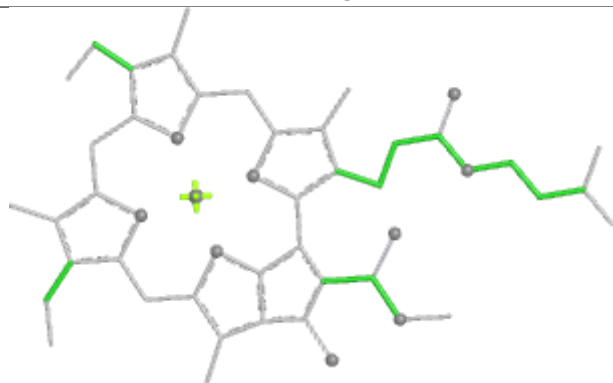
Ligand CLA B 835



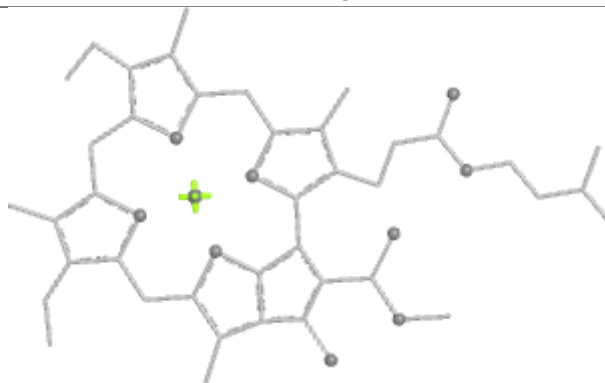
Bond lengths



Bond angles

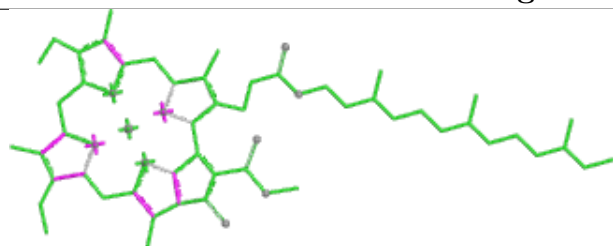


Torsions

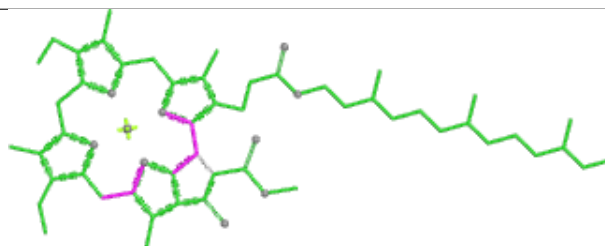


Rings

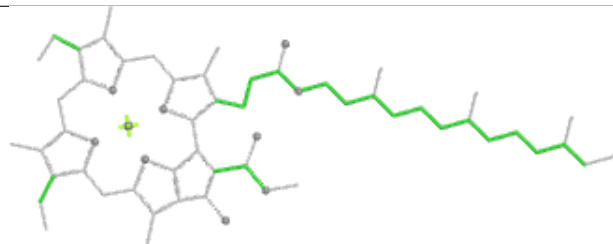
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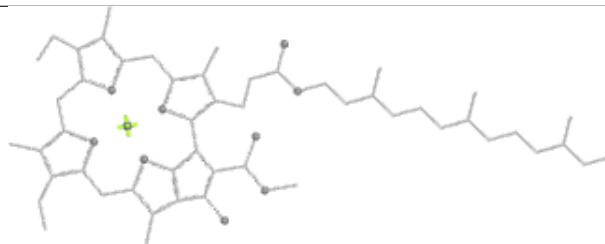
Bond lengths



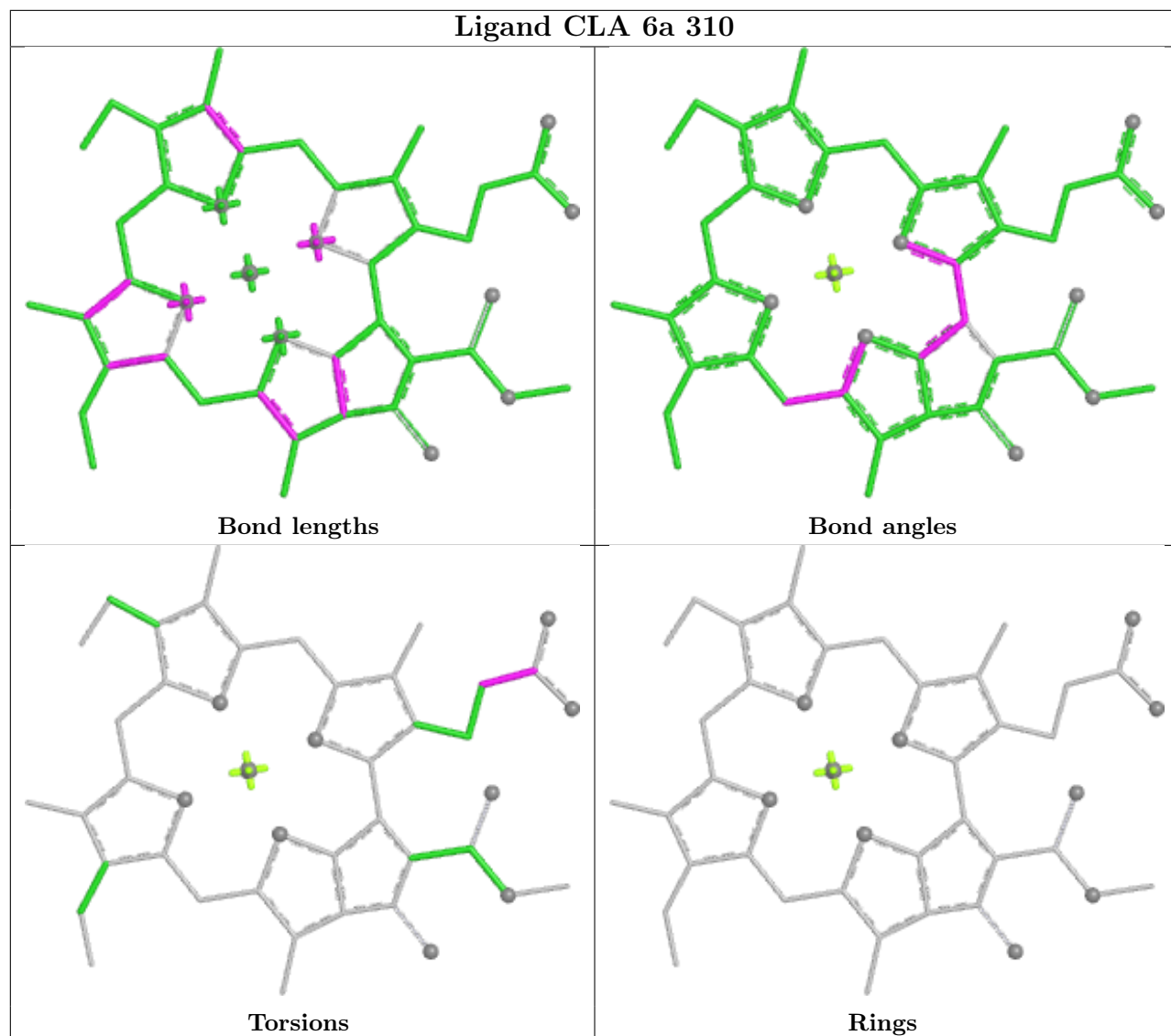
Bond angles



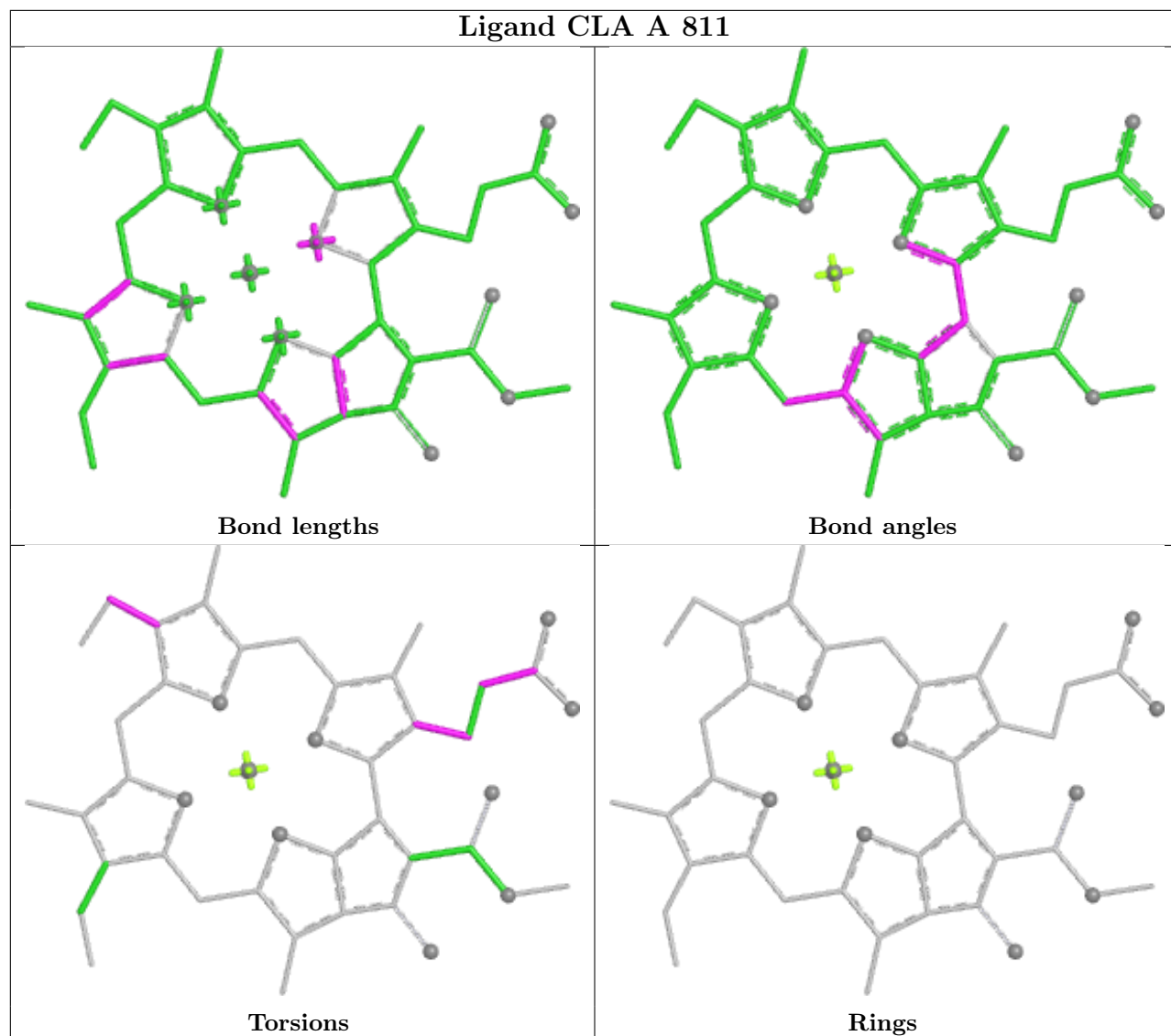
Torsions

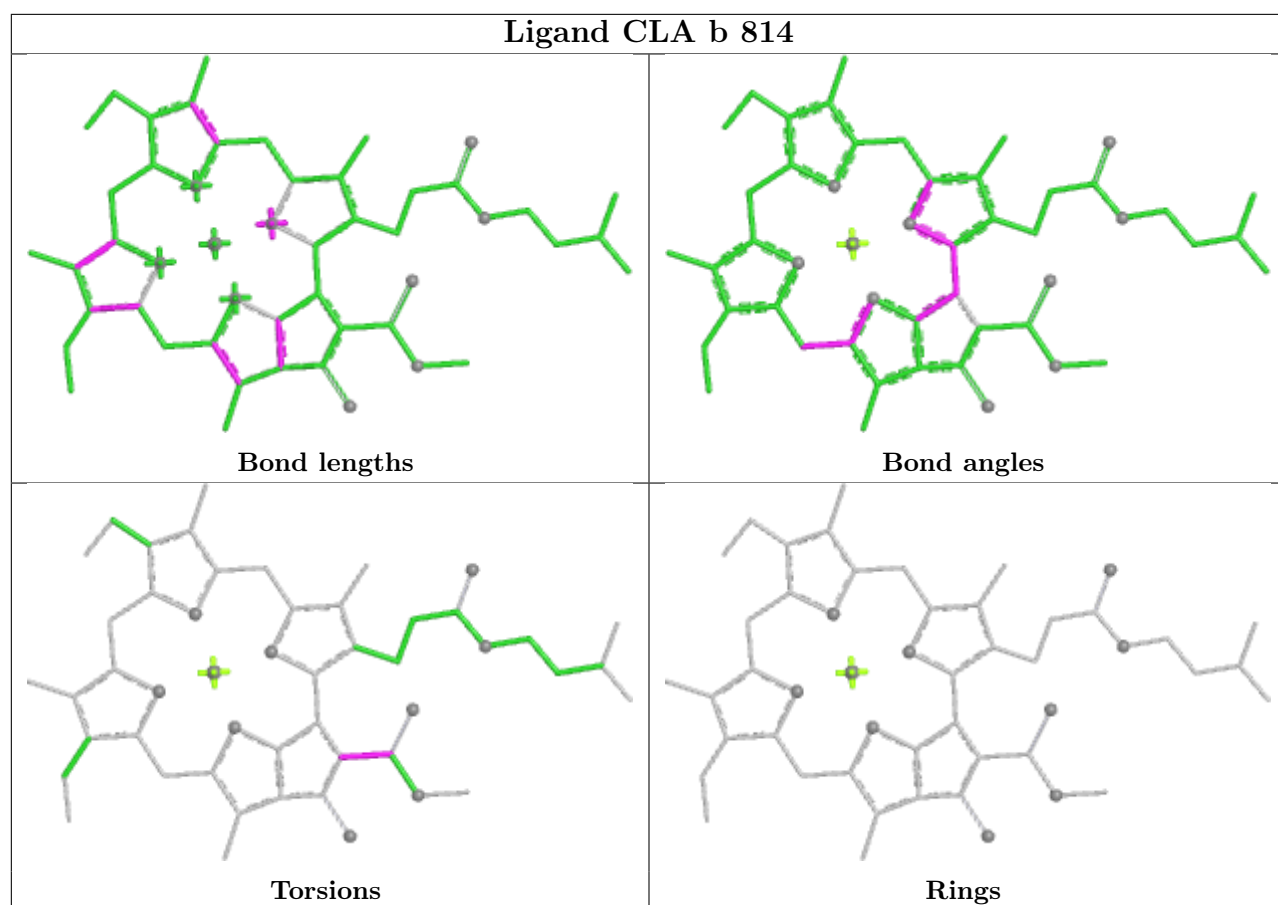


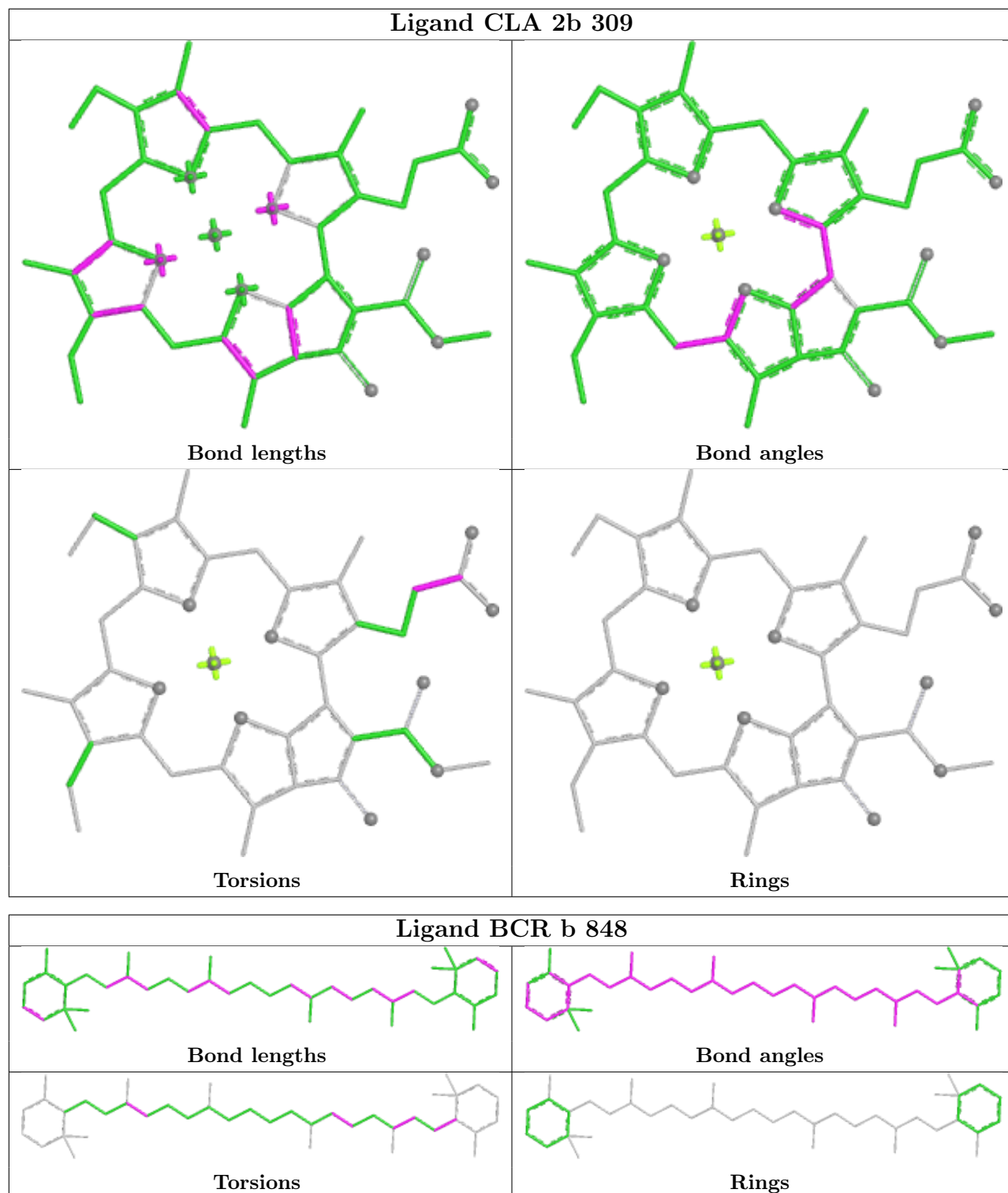
Rings

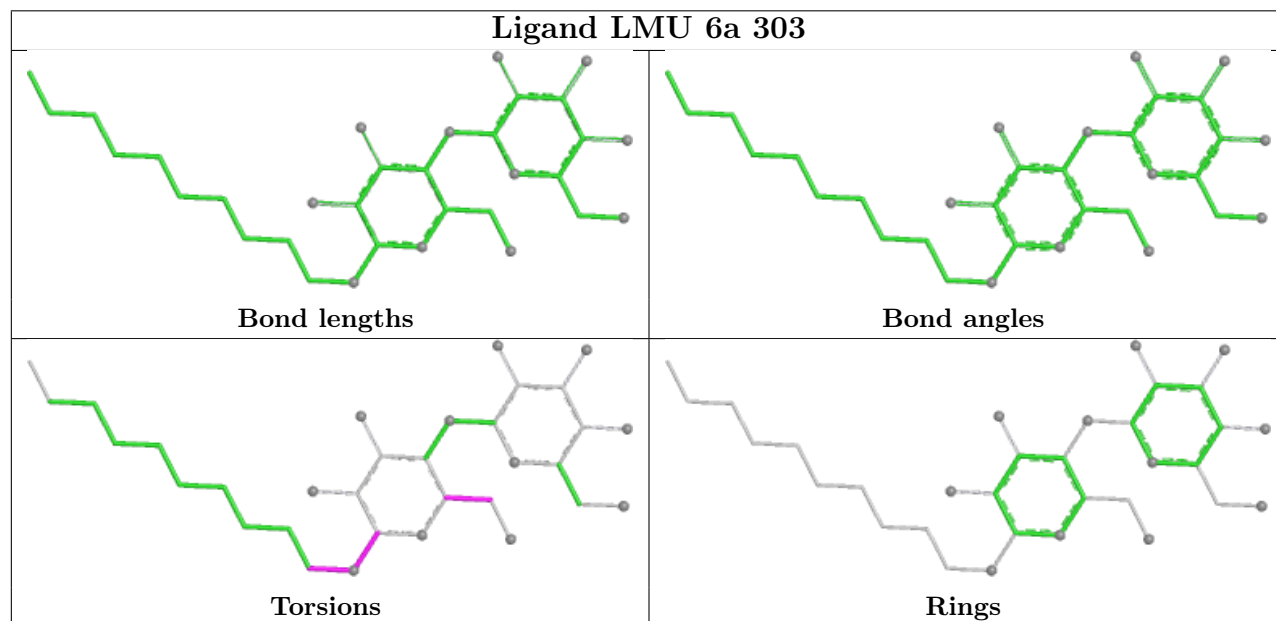
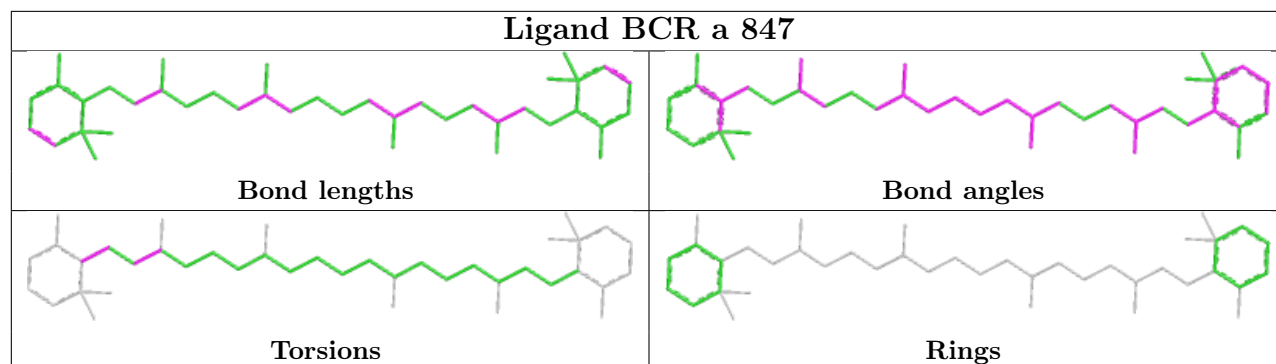


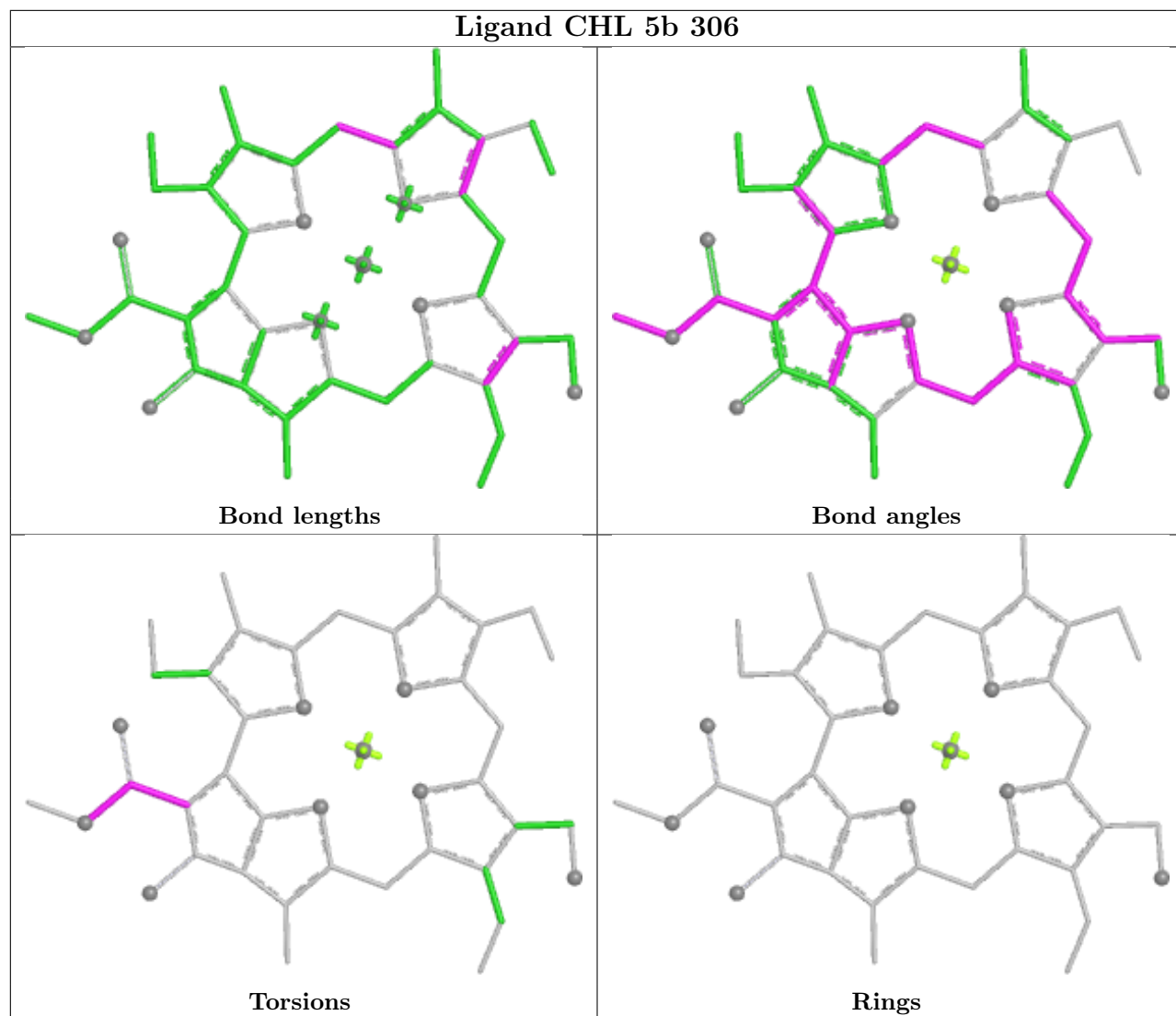
Ligand CLA A 811

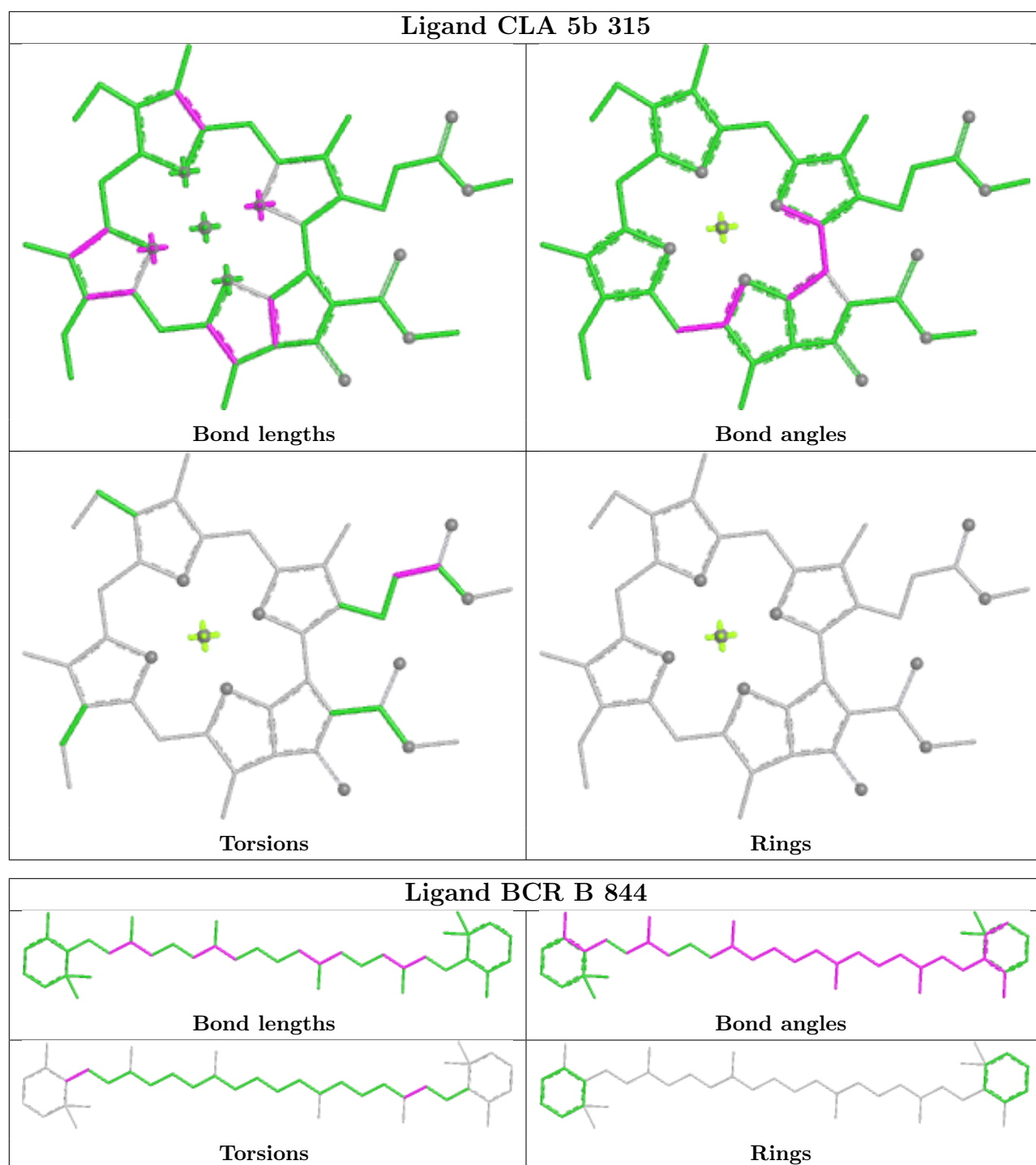




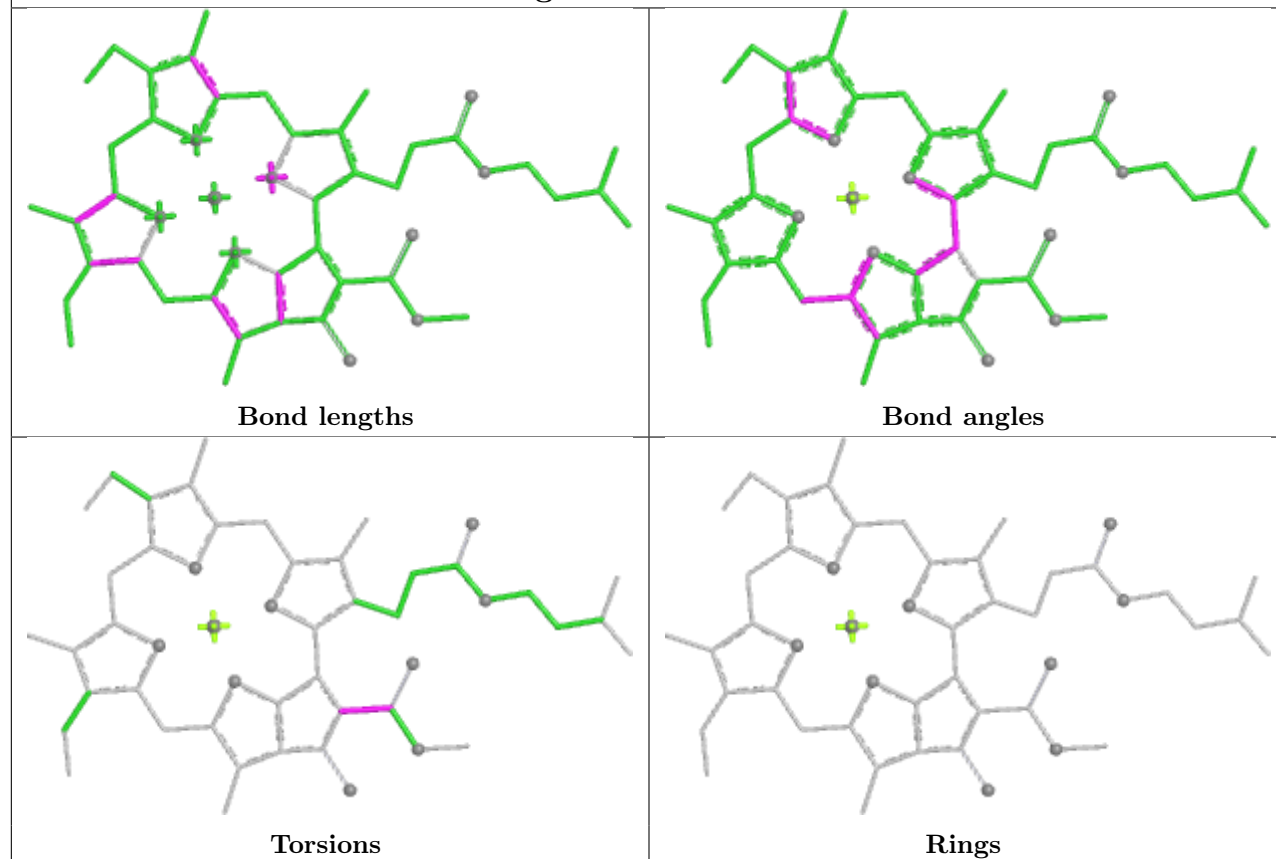




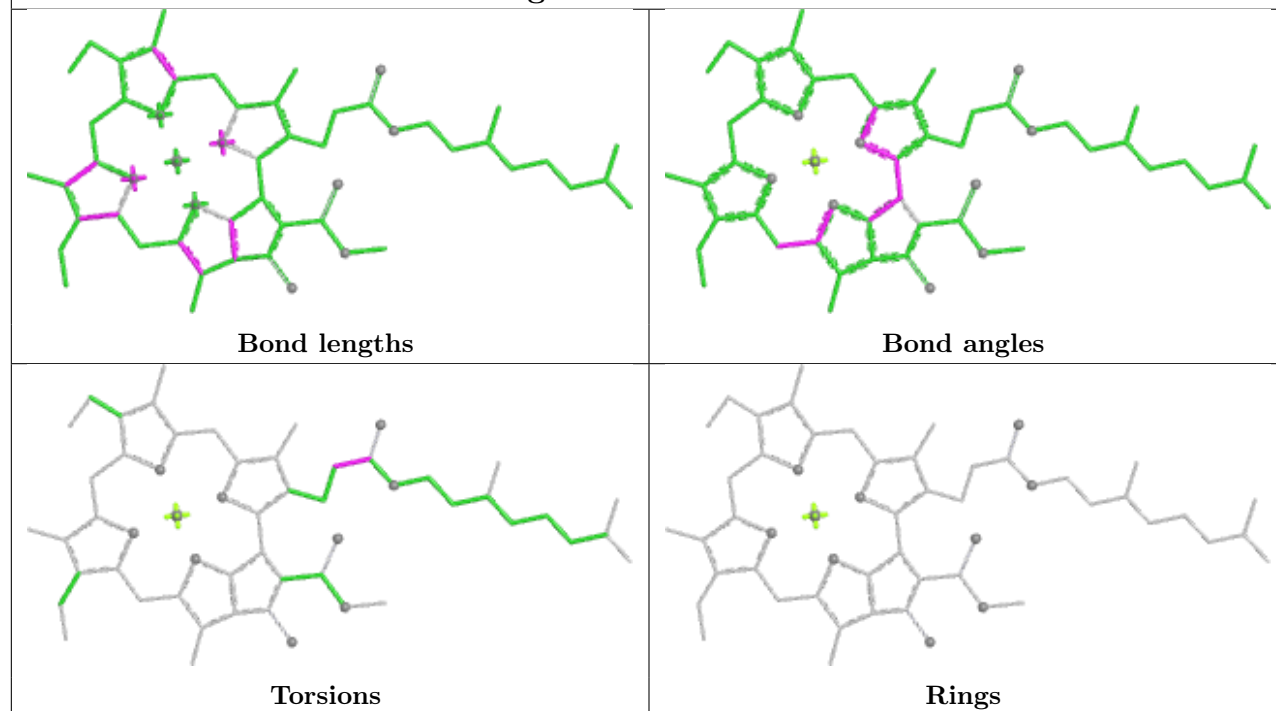


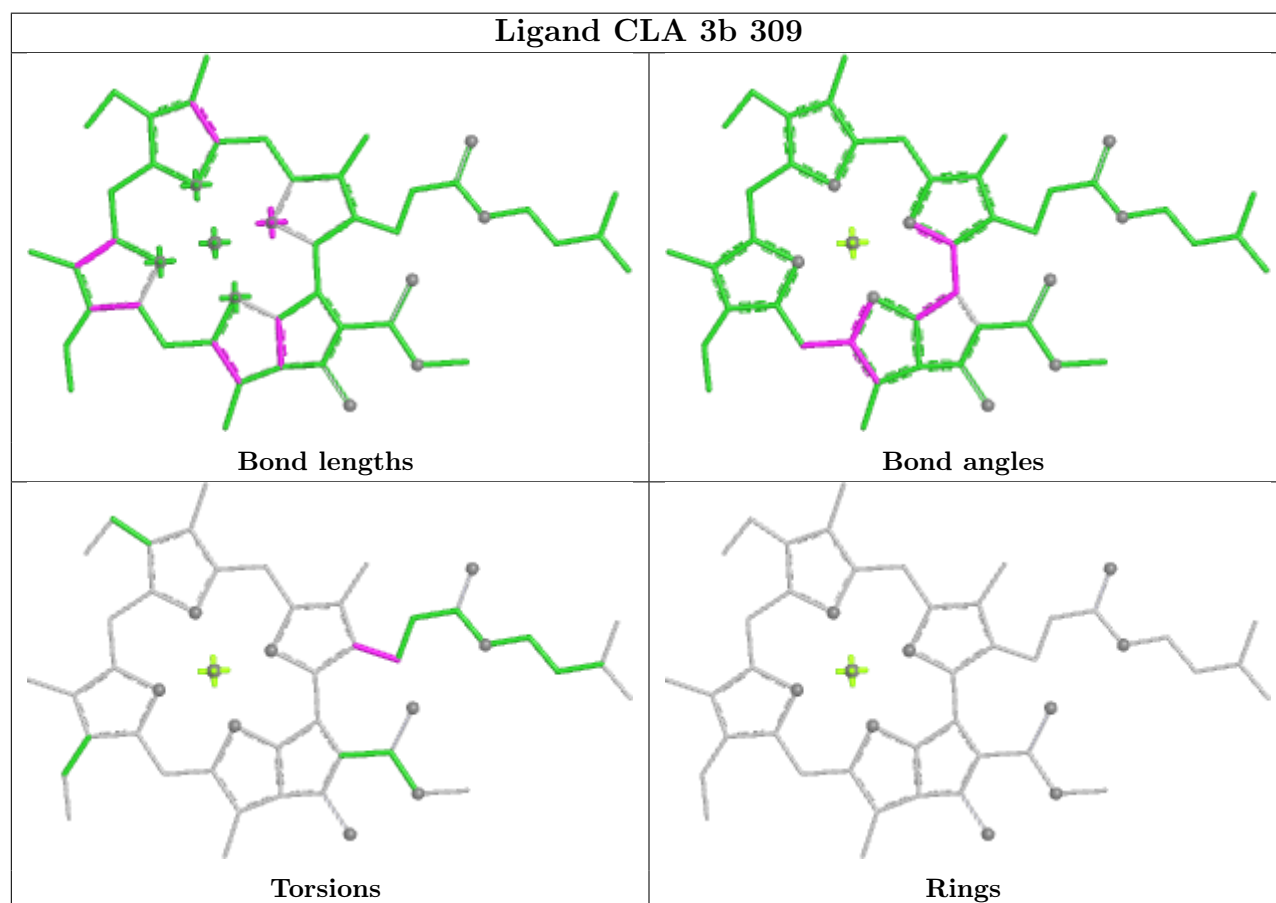
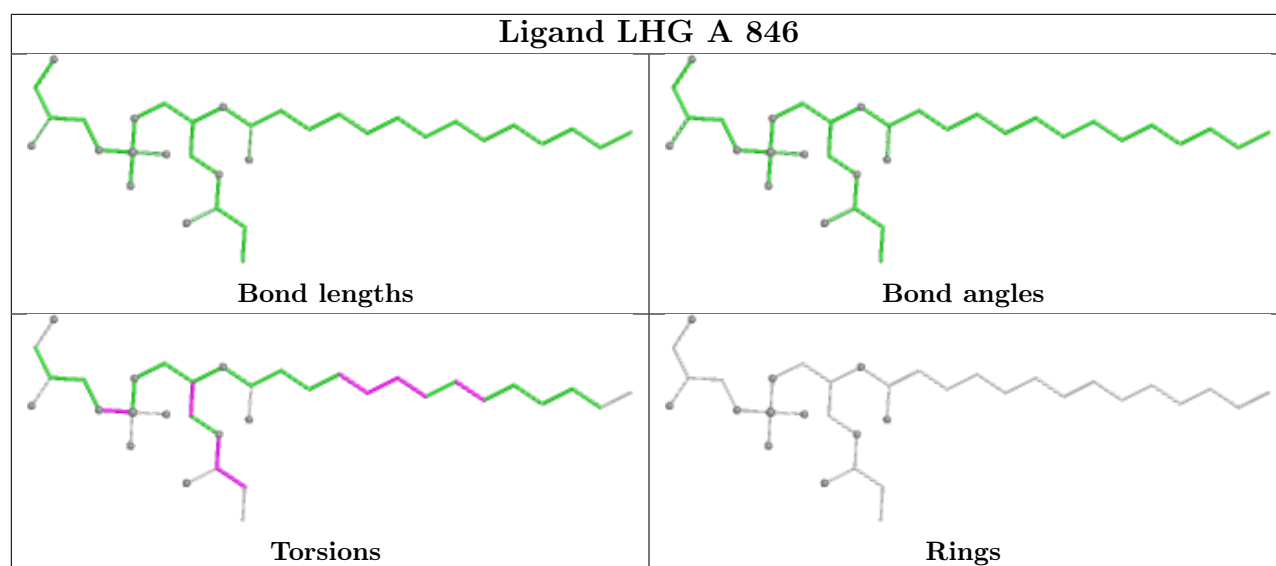


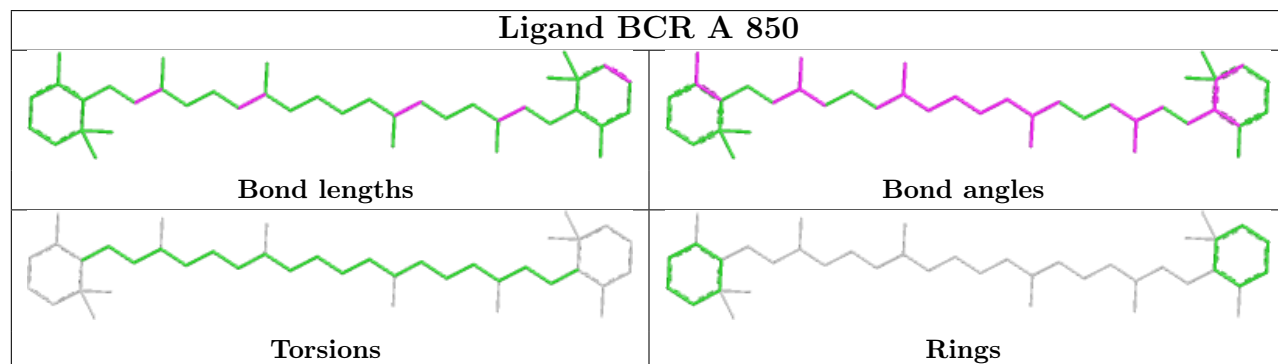
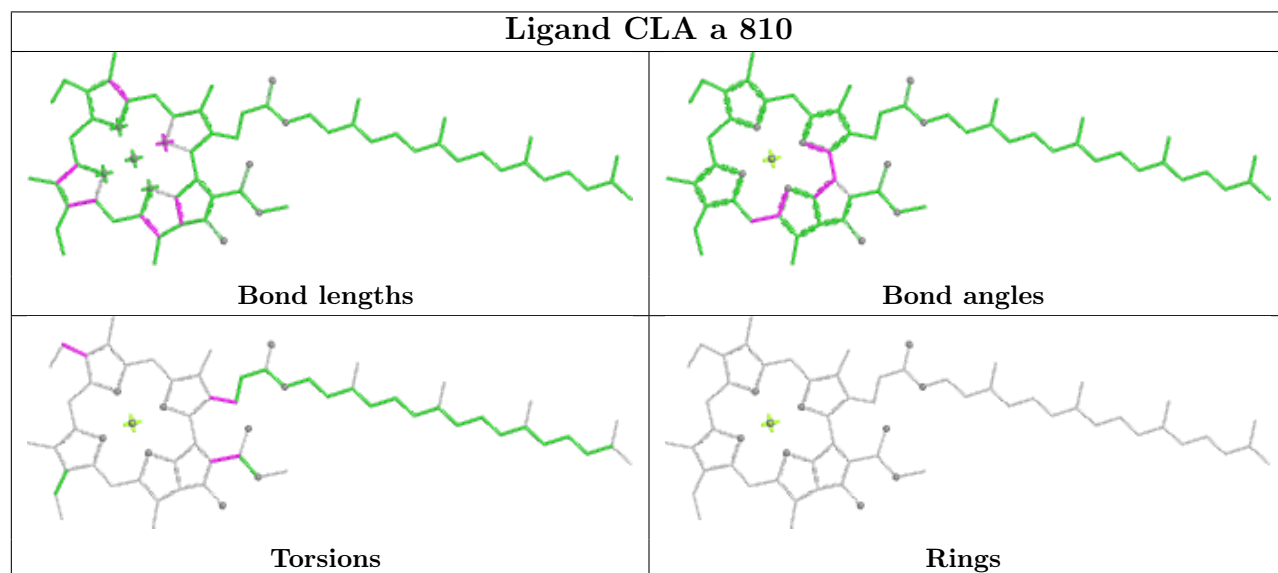
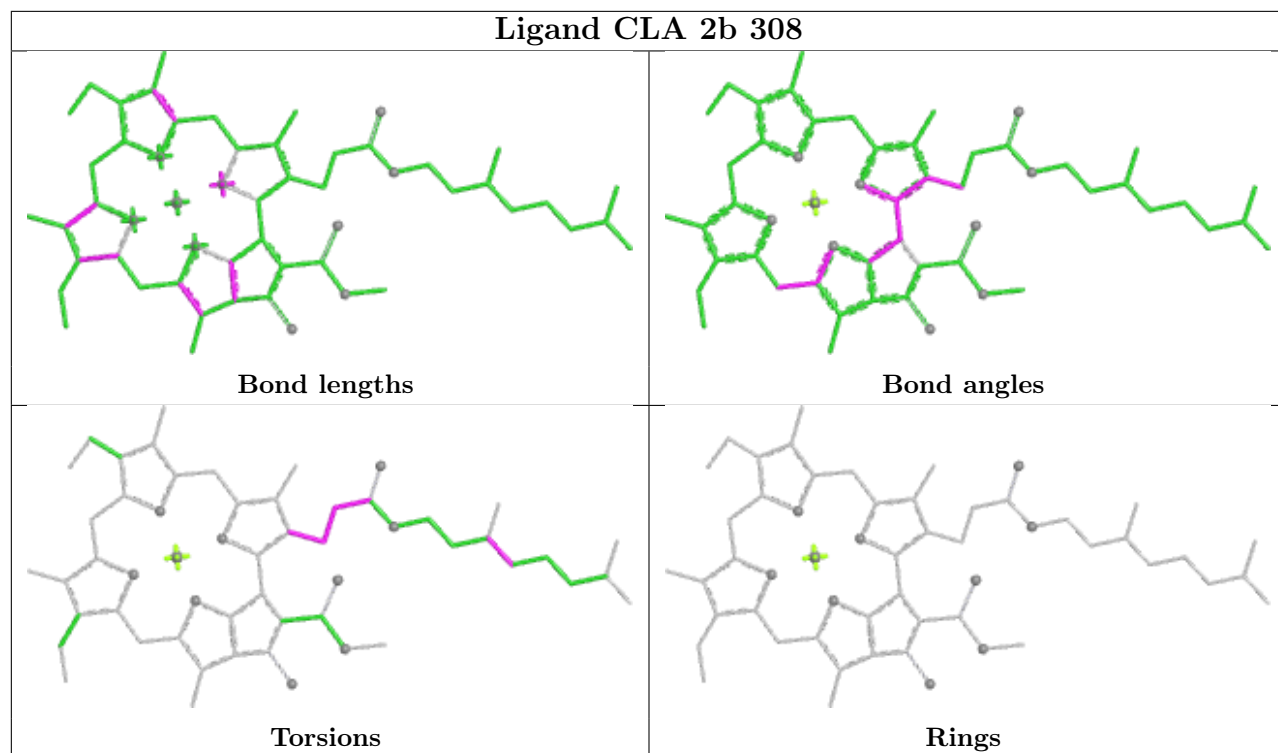
Ligand CLA b 824

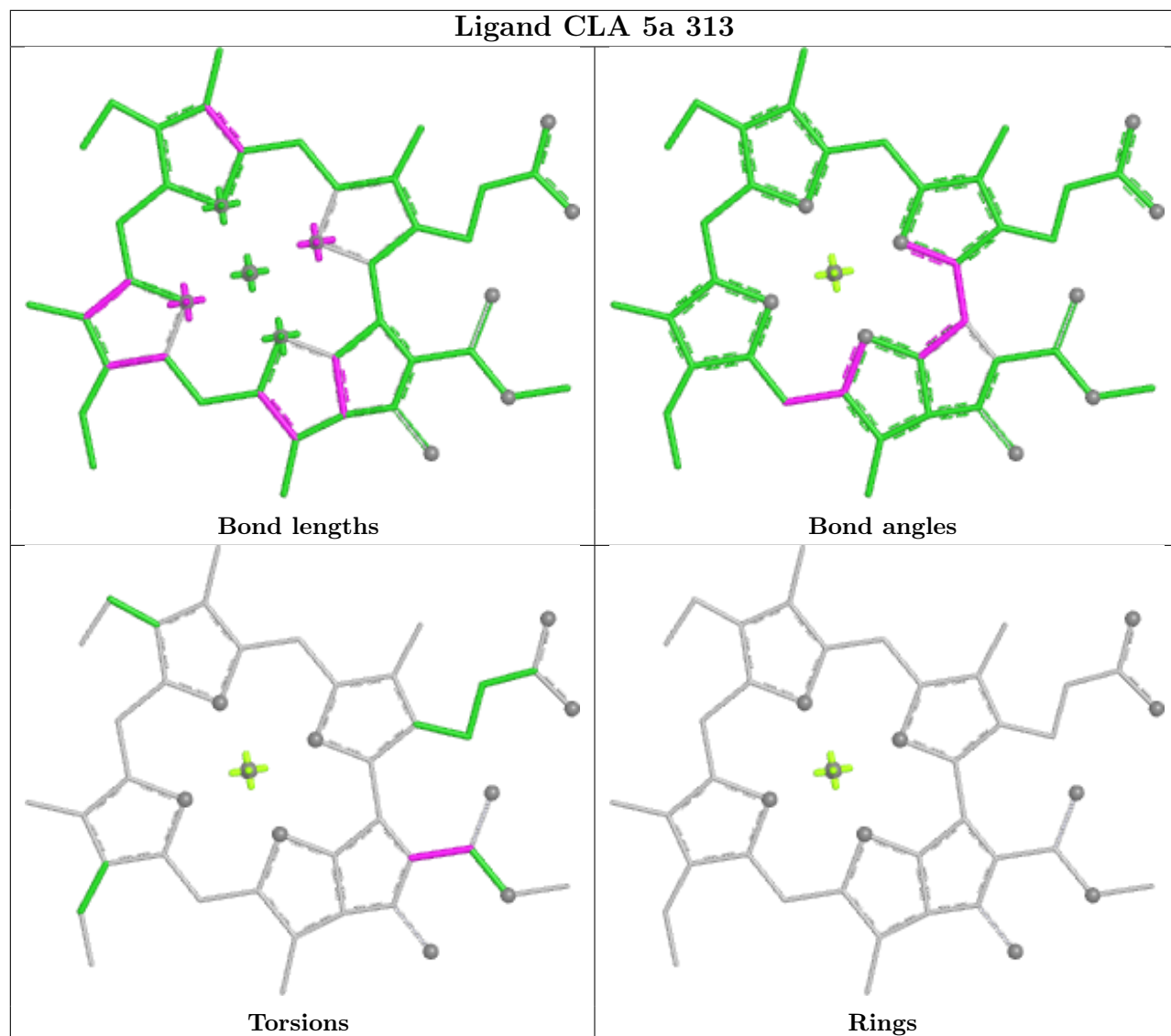


Ligand CLA 6a 315

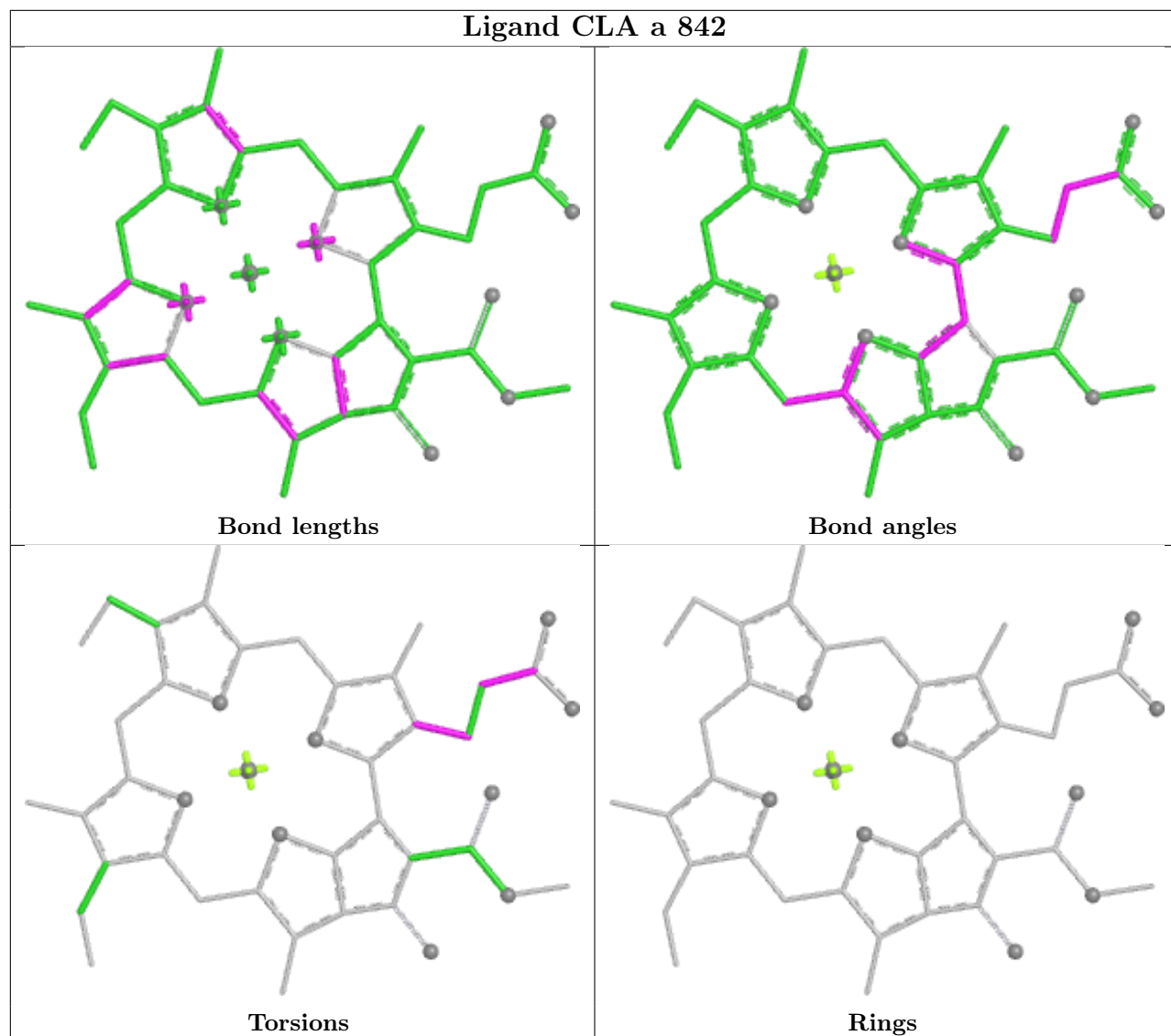




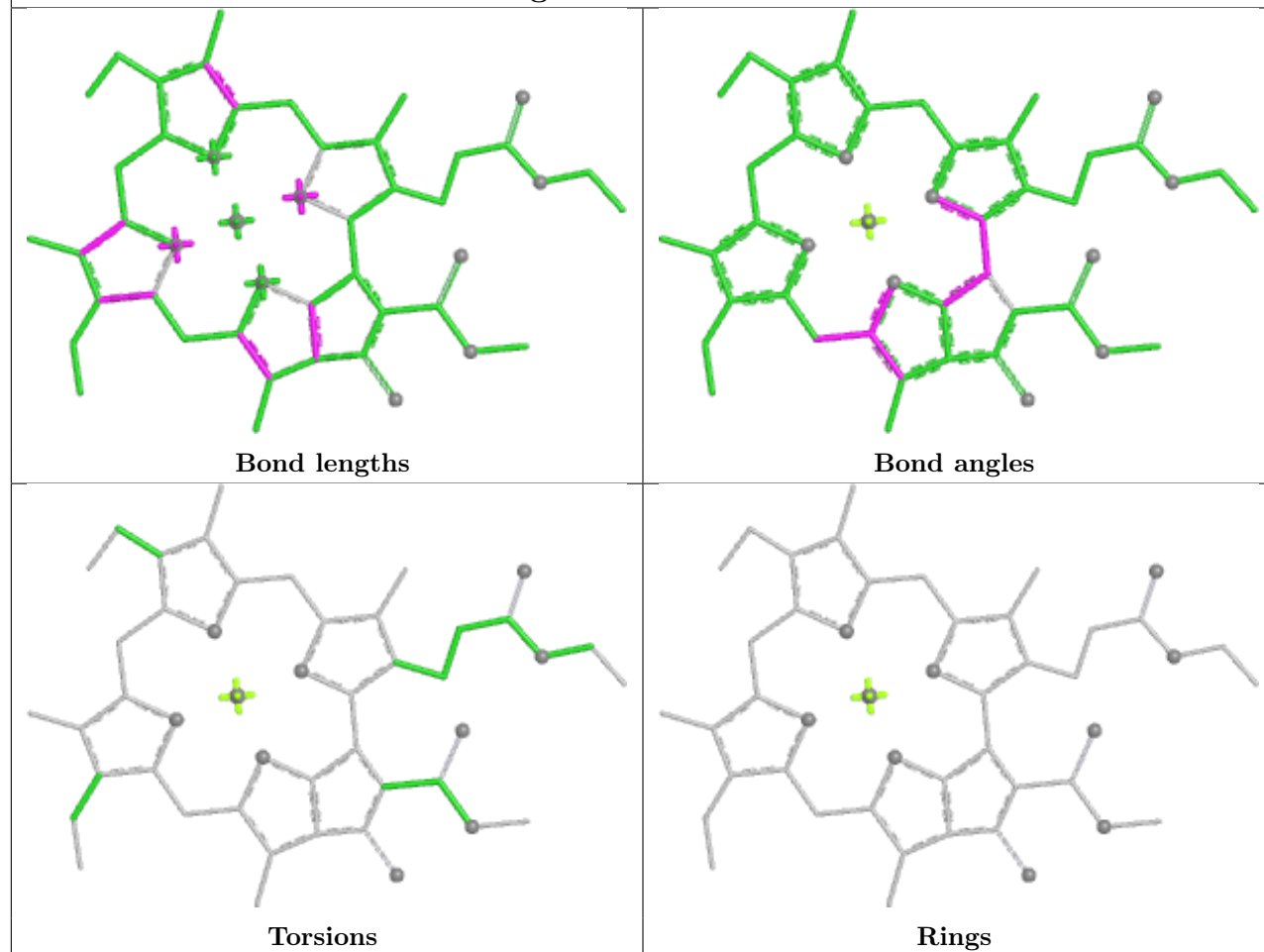




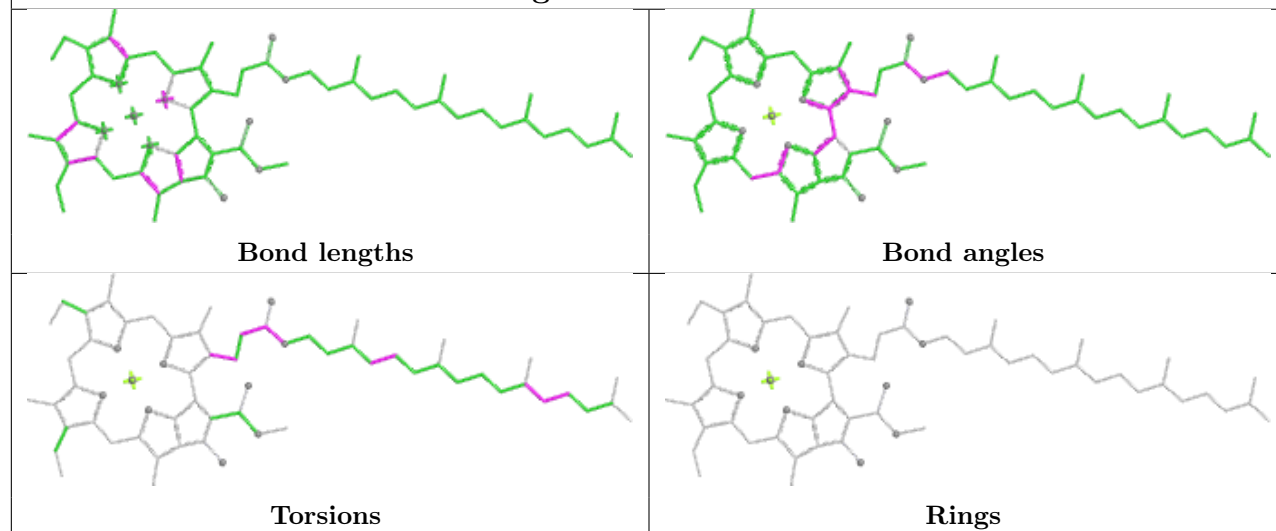
Ligand CLA a 842

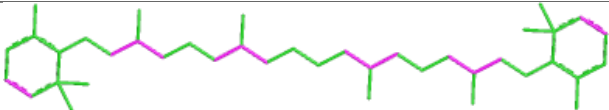
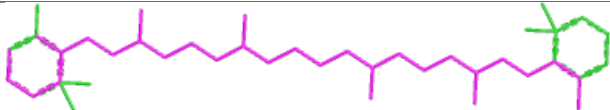
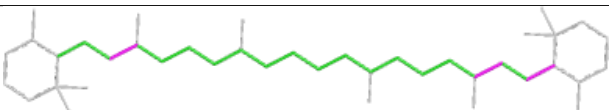
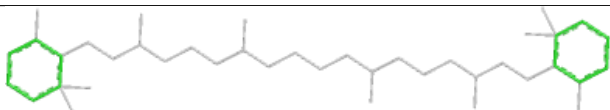



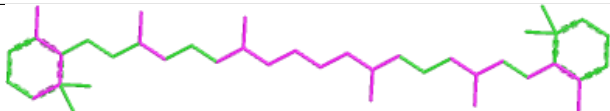
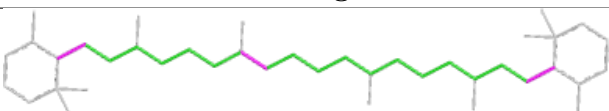
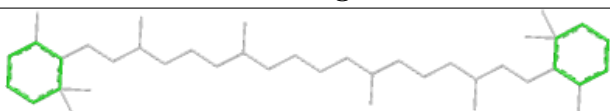
Ligand CLA b 837

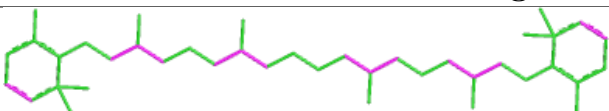
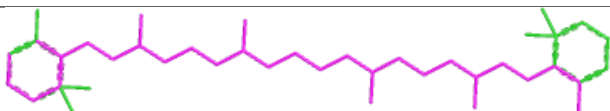
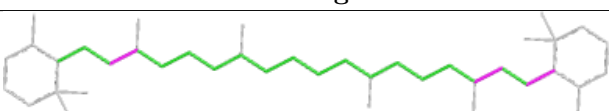
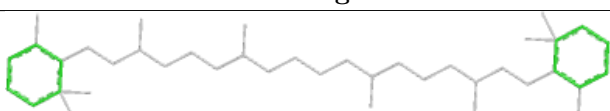


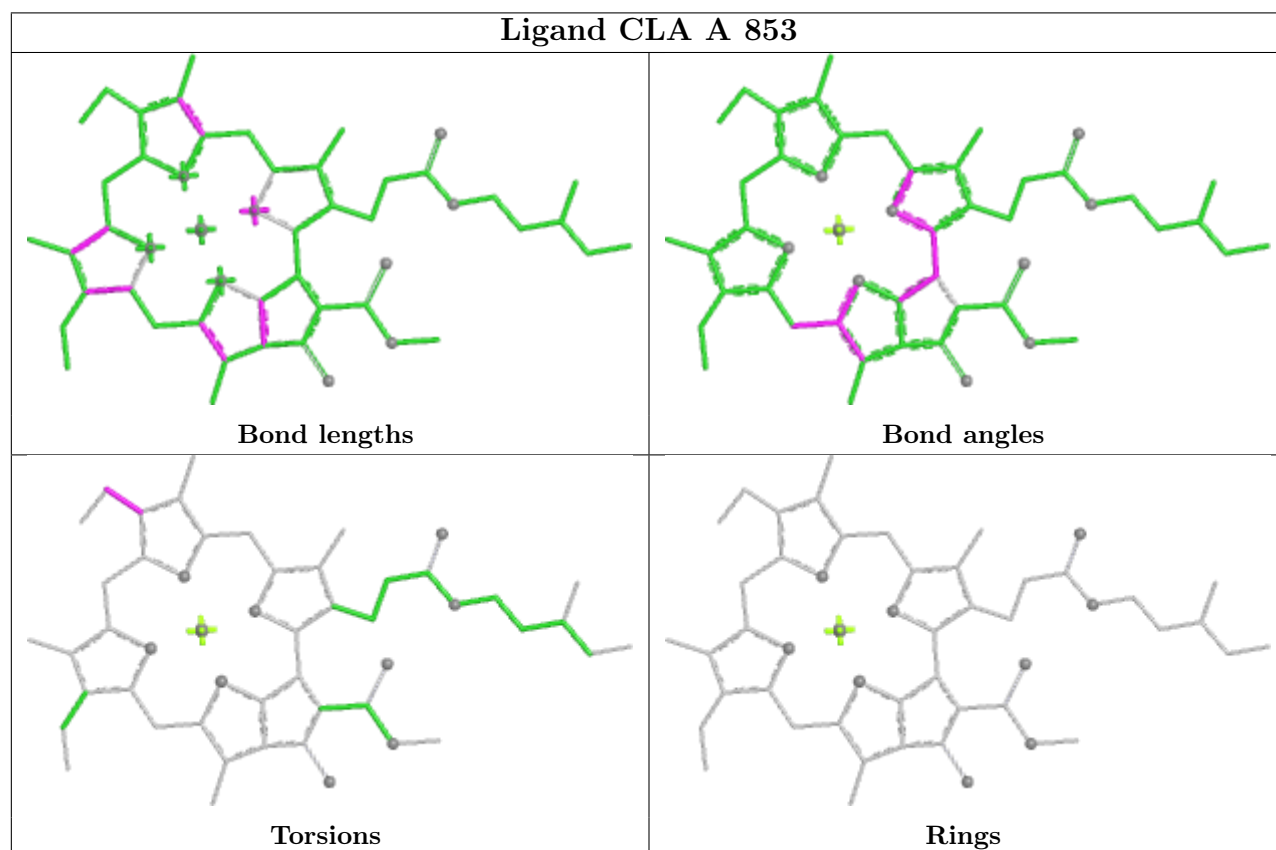
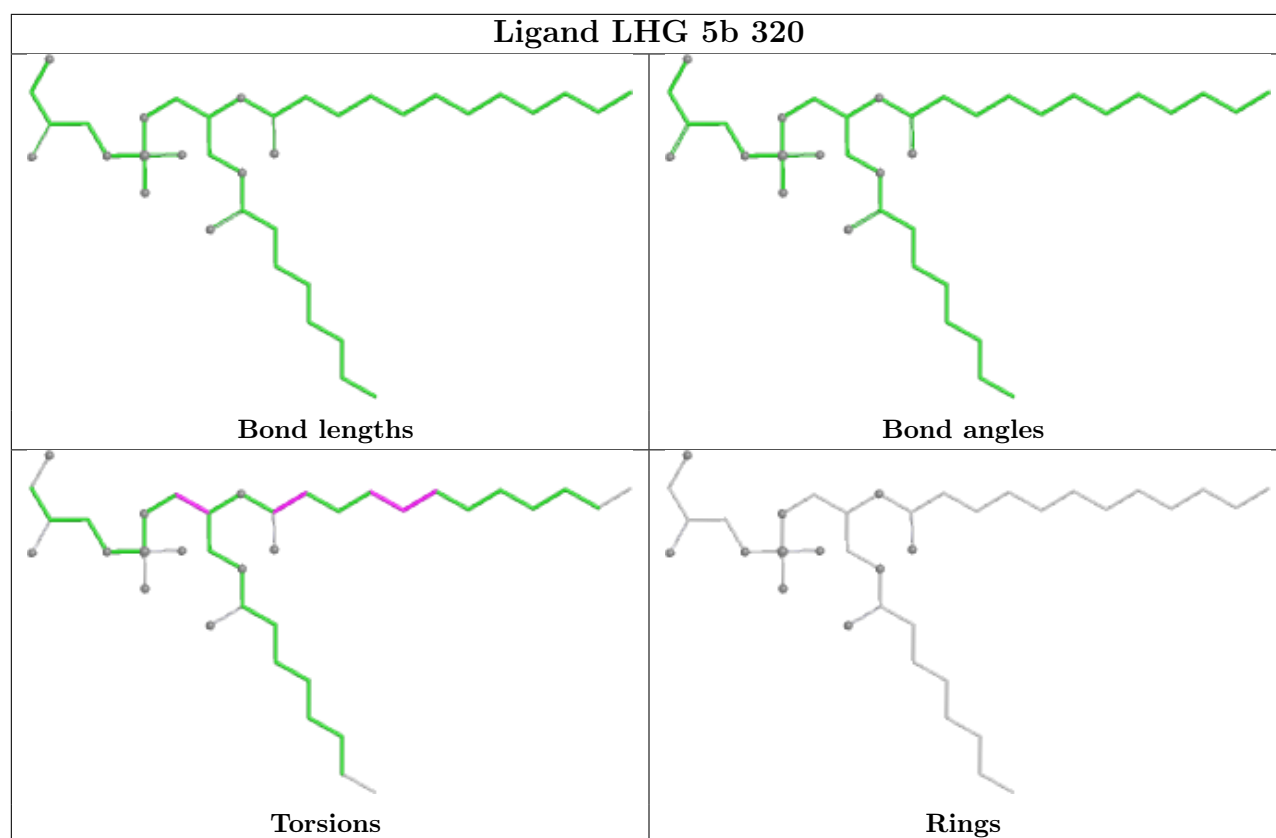
Ligand CLA B 840

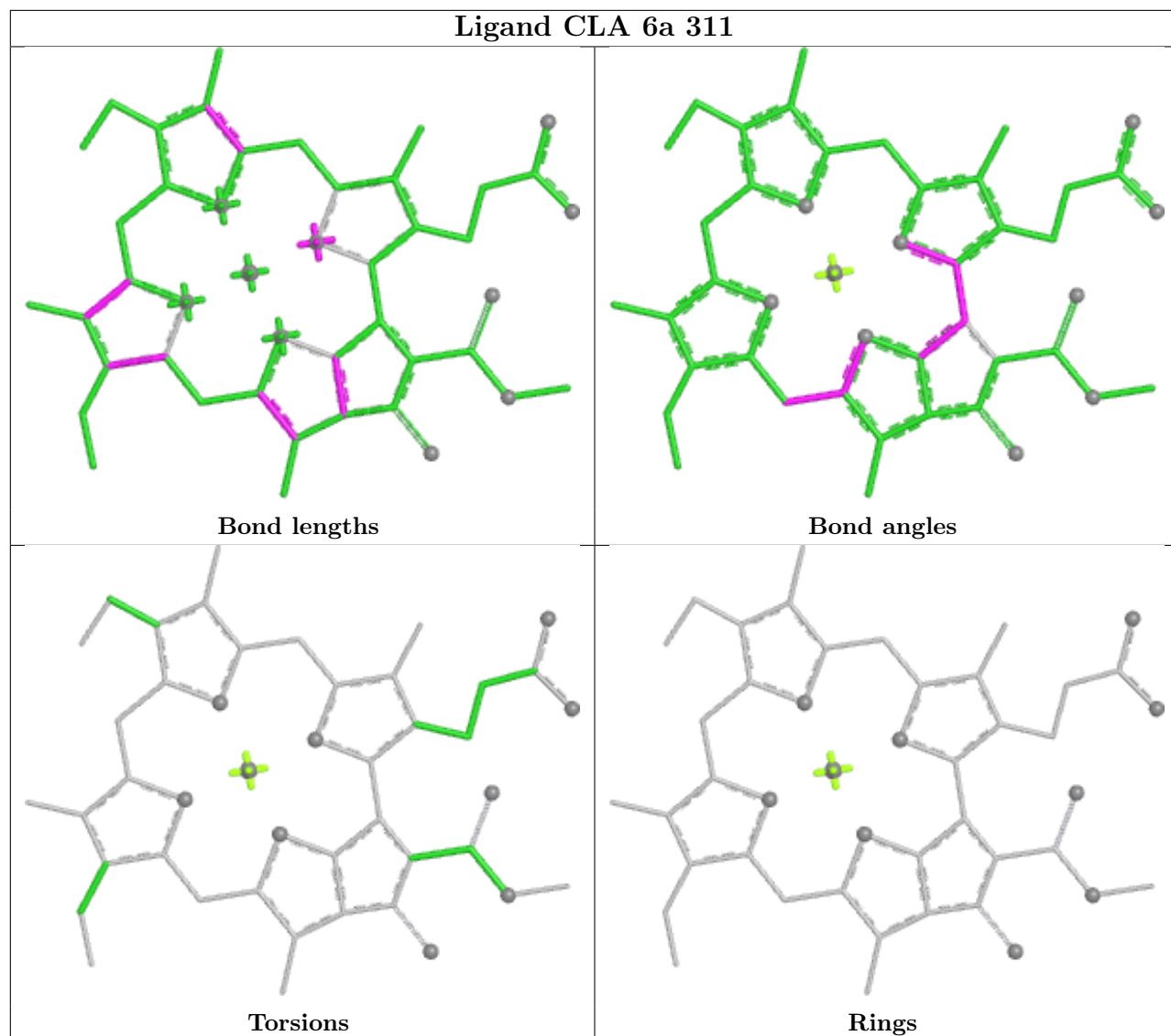


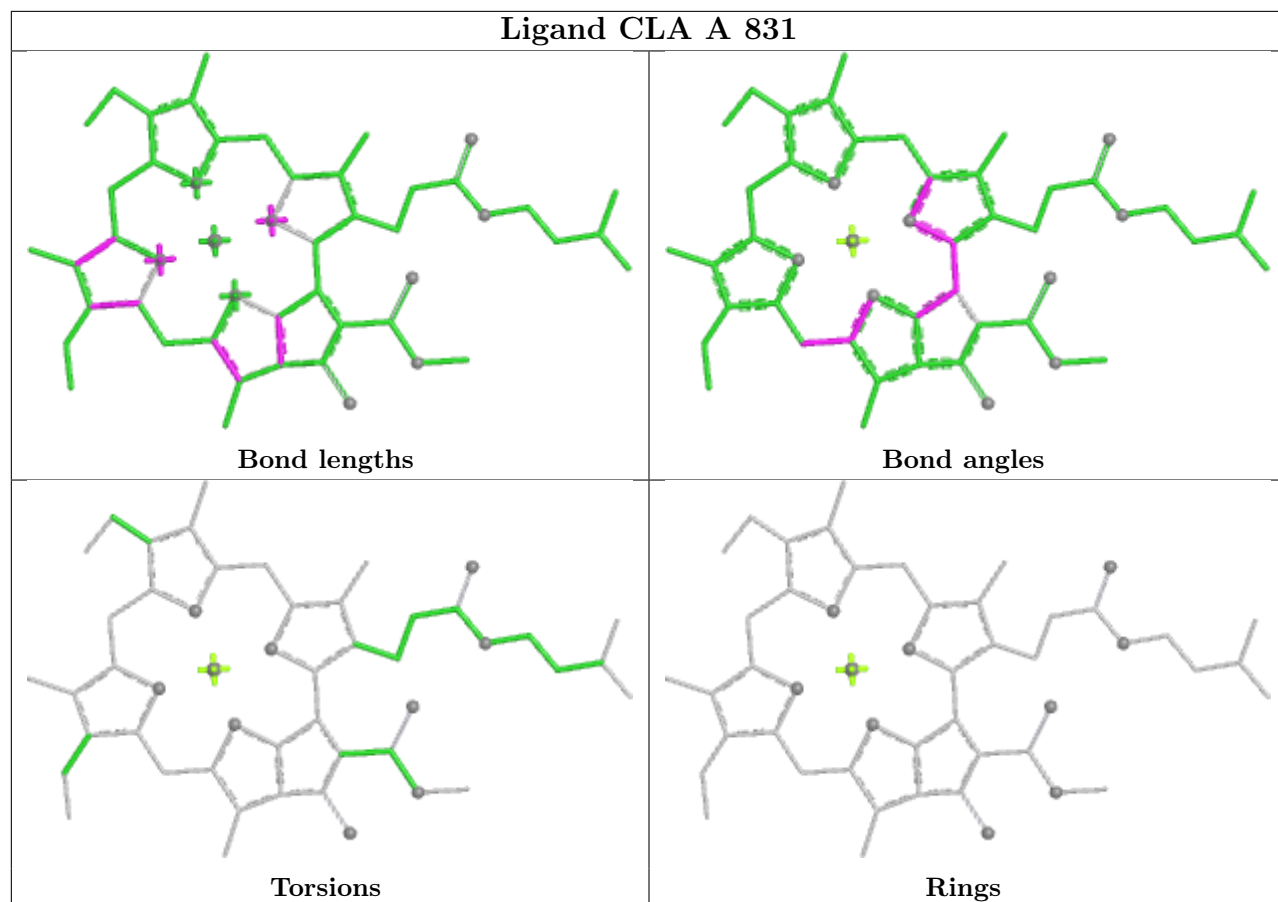
Ligand BCR j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

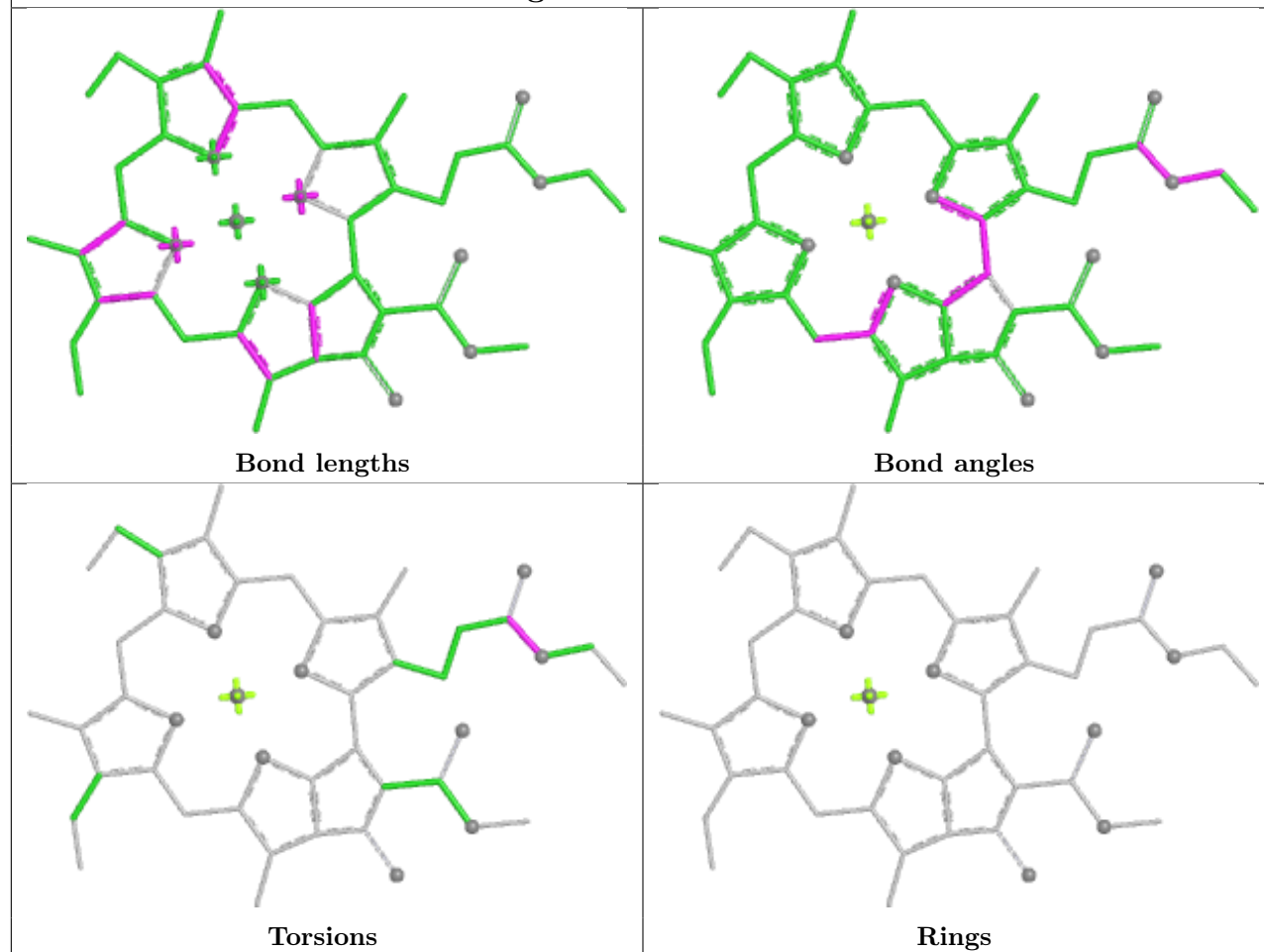
Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



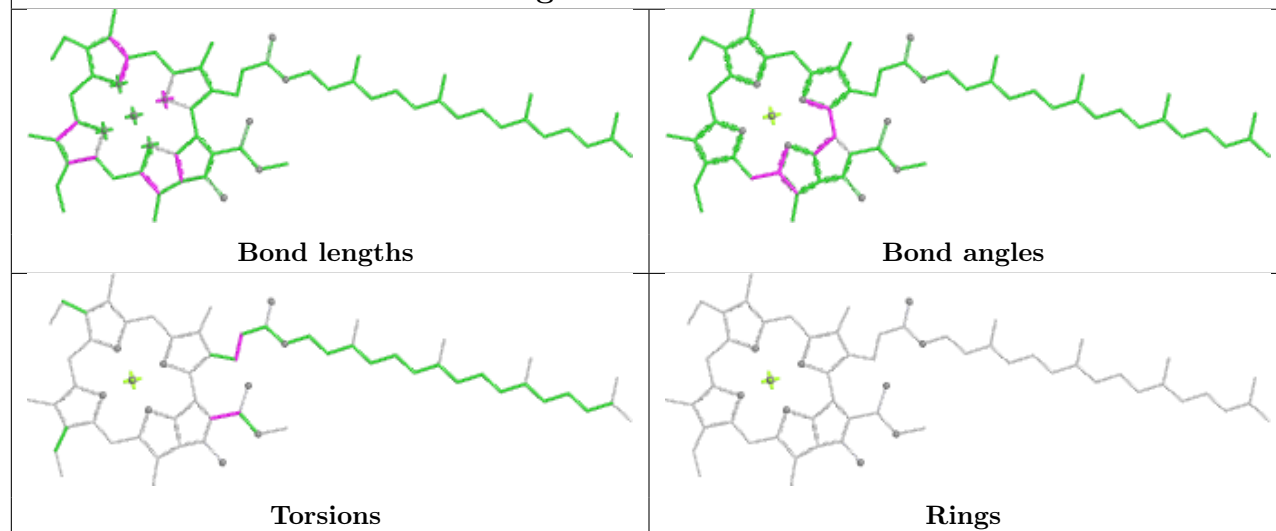


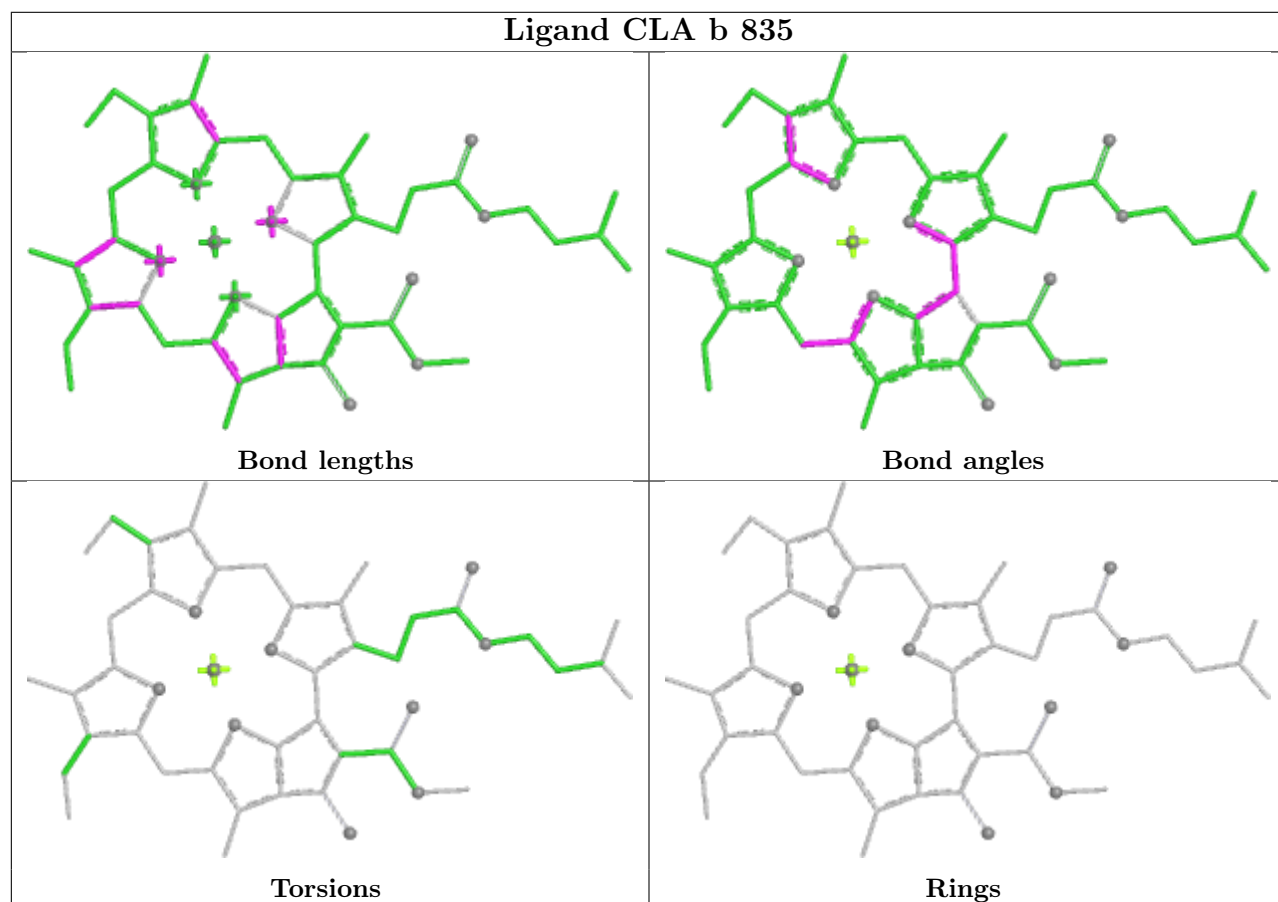
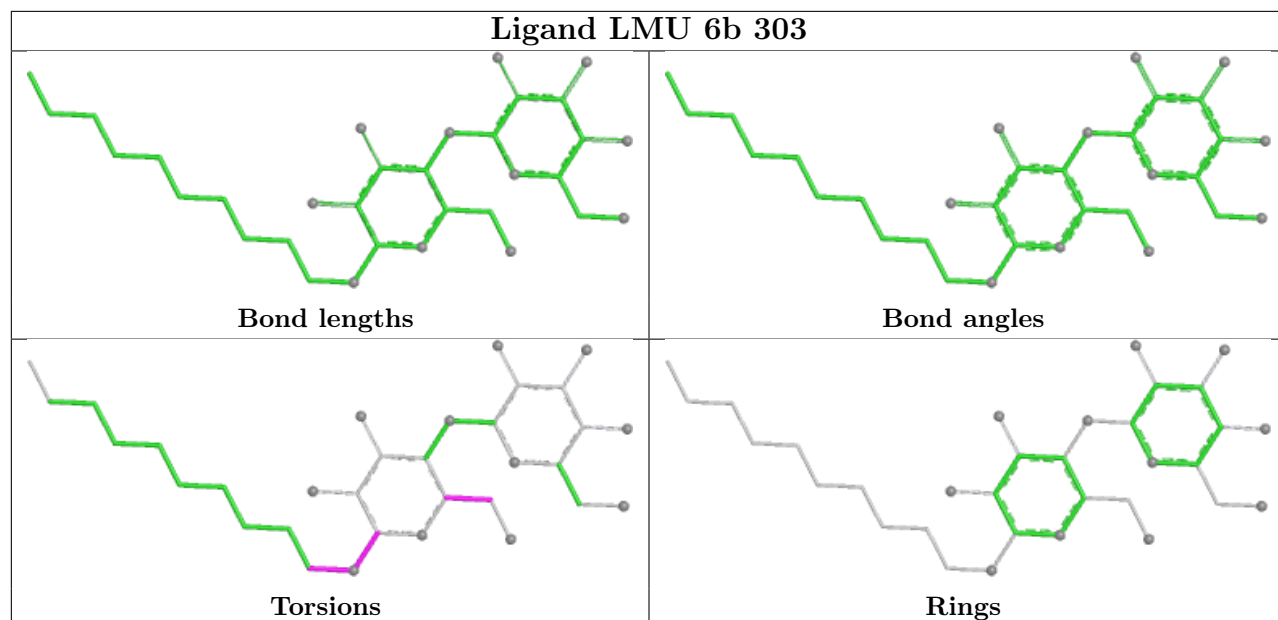


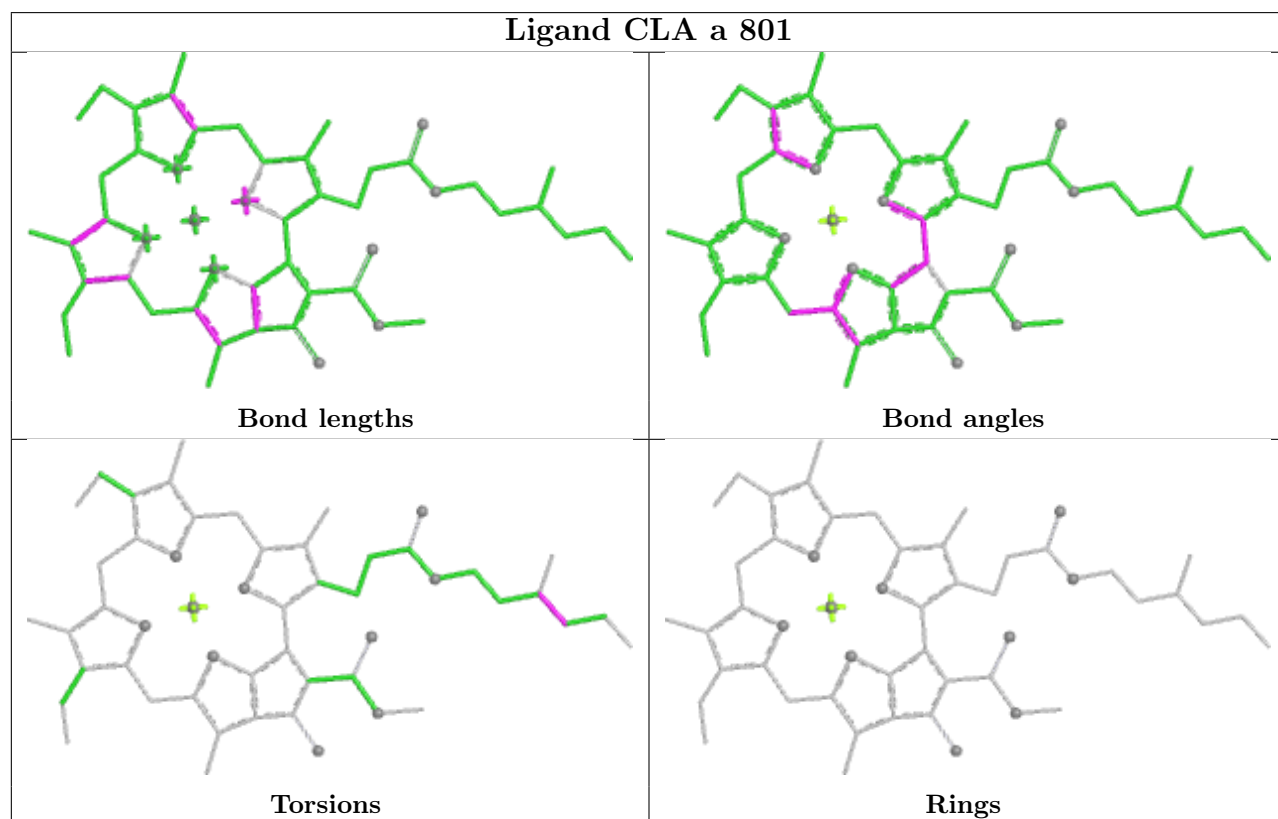
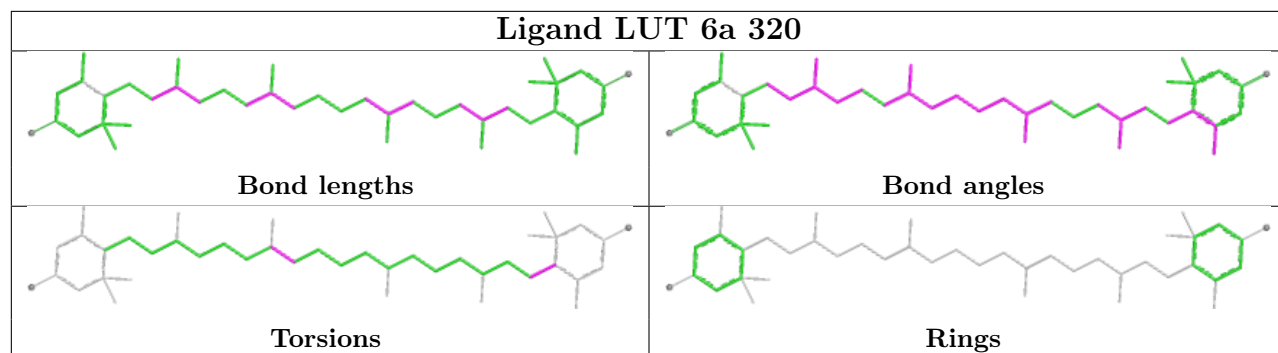
Ligand CLA B 808

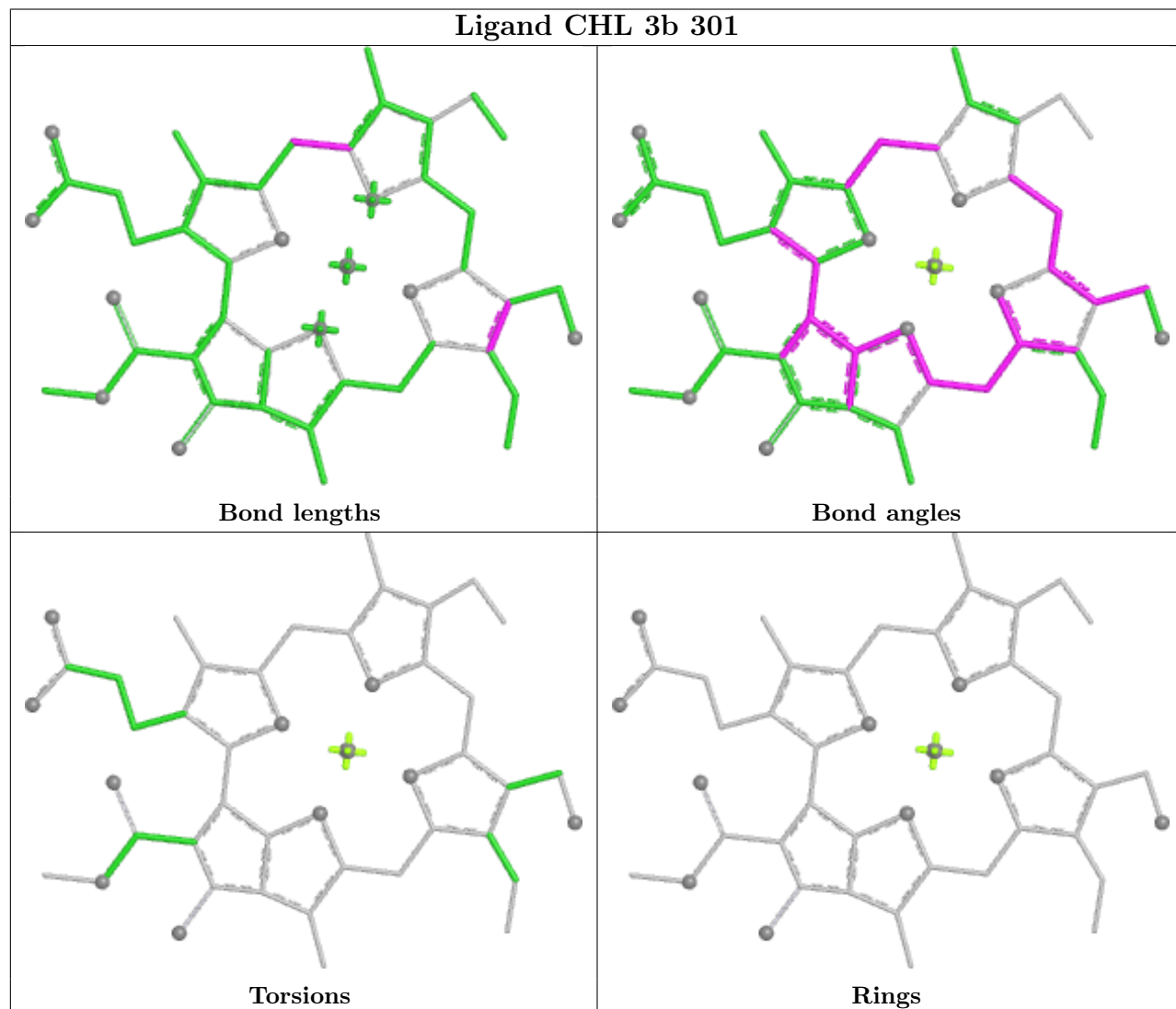
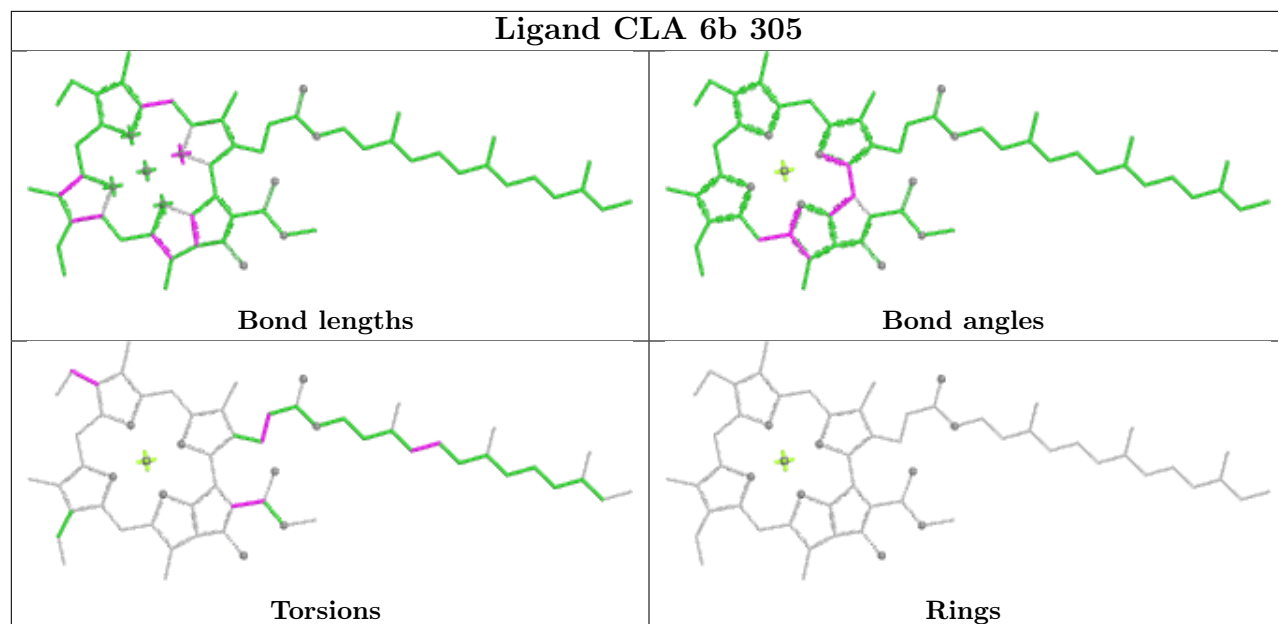


Ligand CLA a 808

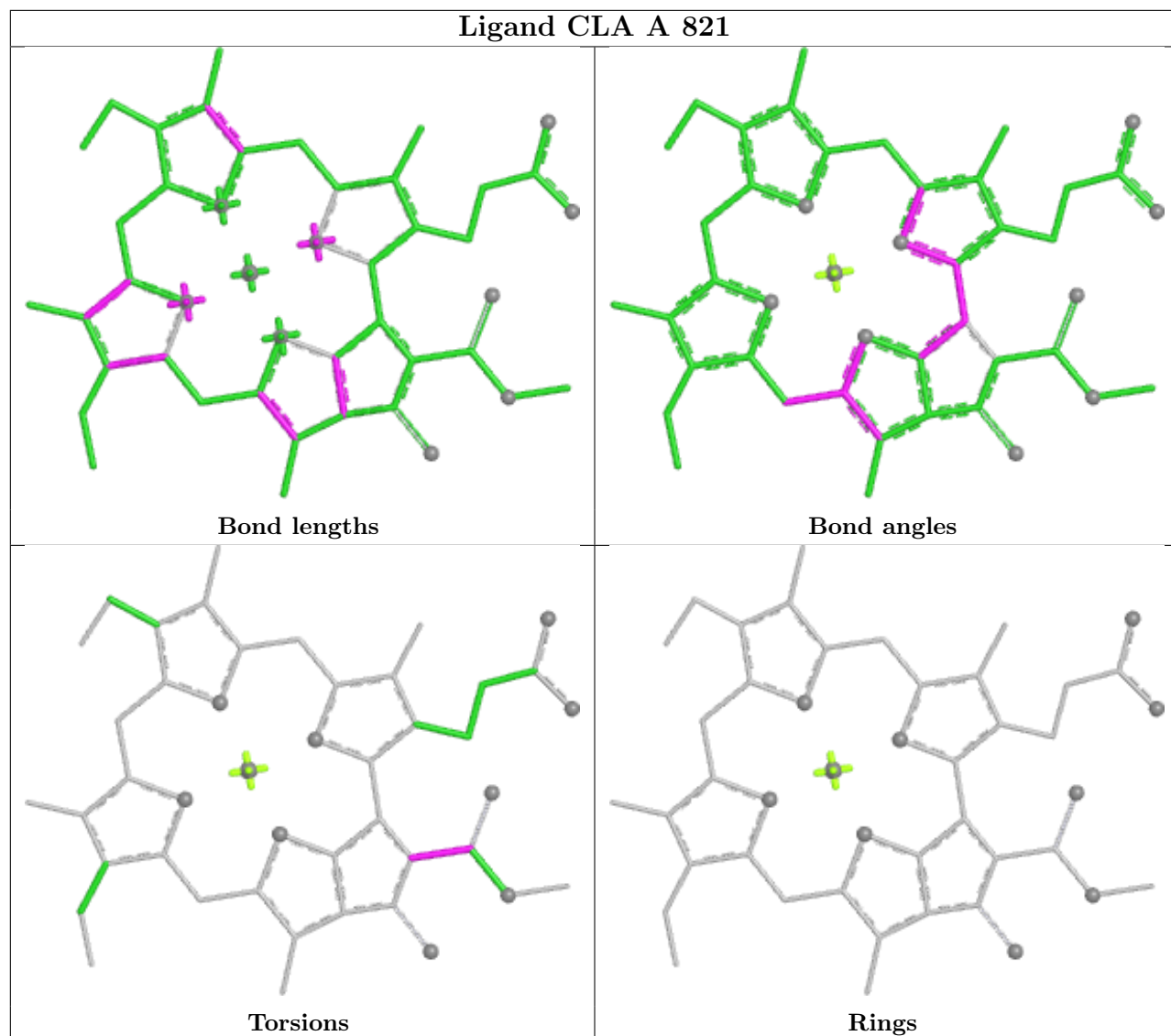




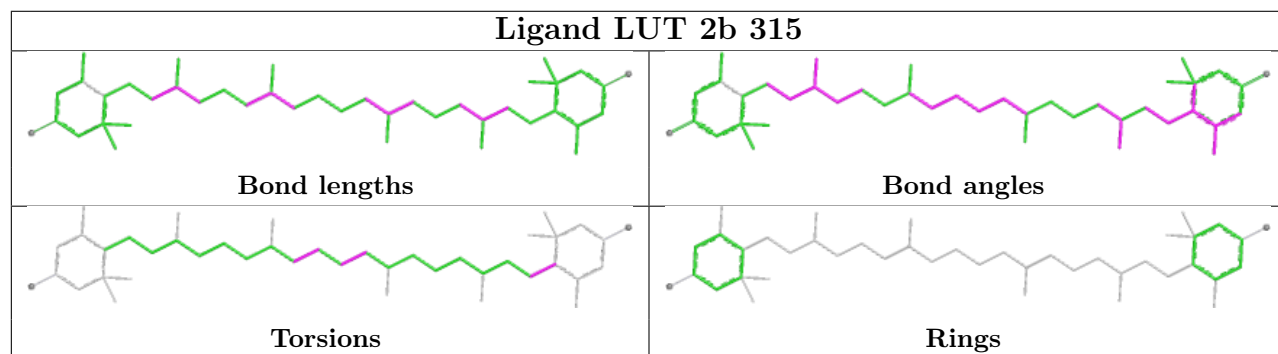




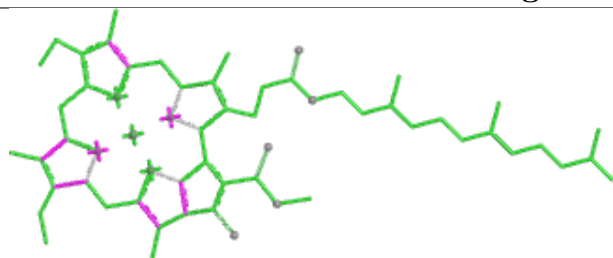
Ligand CLA A 821



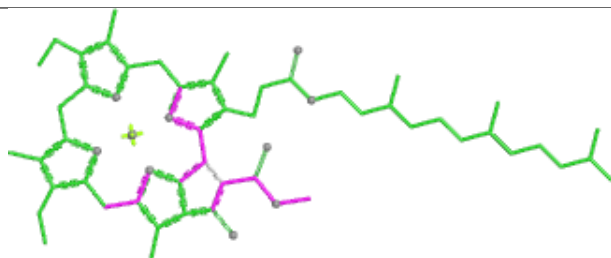
Ligand LUT 2b 315



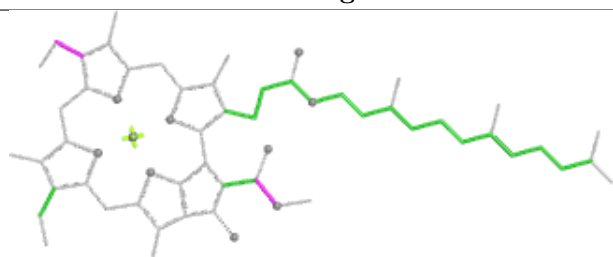
Ligand CLA f 305



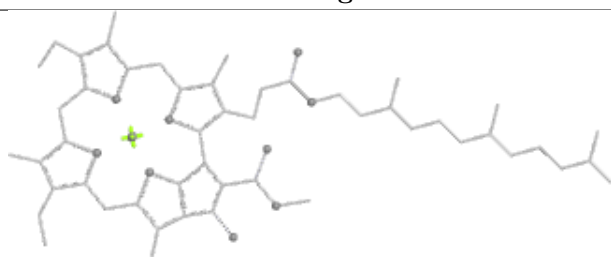
Bond lengths



Bond angles

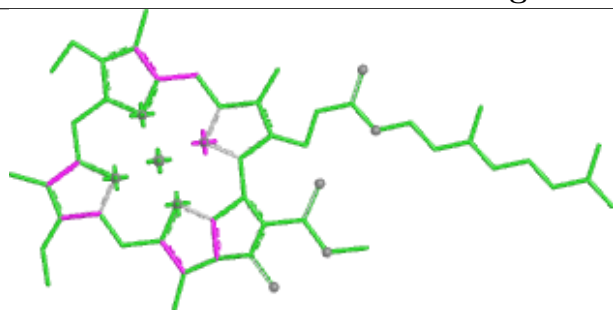


Torsions

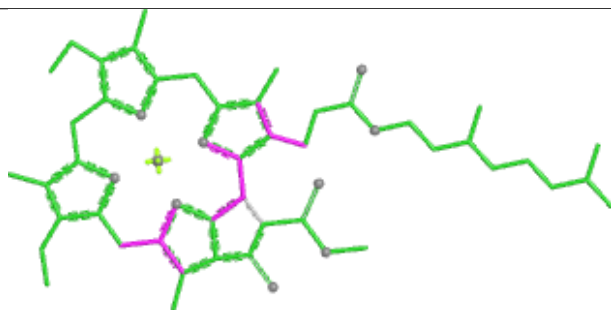


Rings

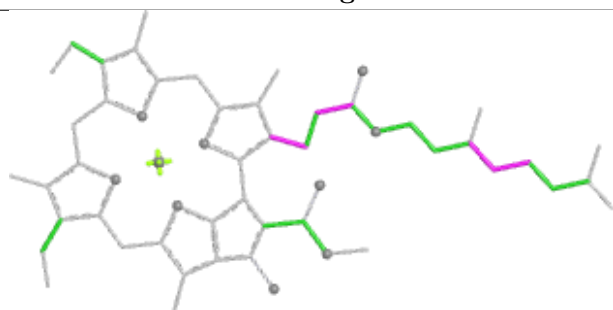
Ligand CLA 3a 312



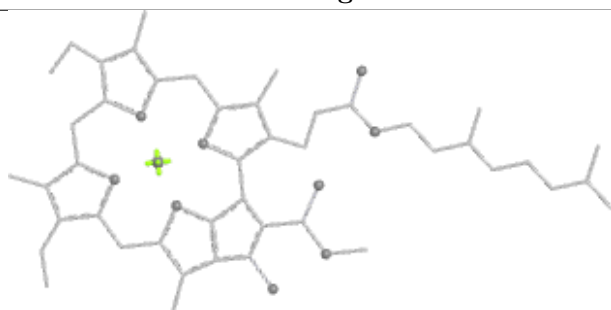
Bond lengths



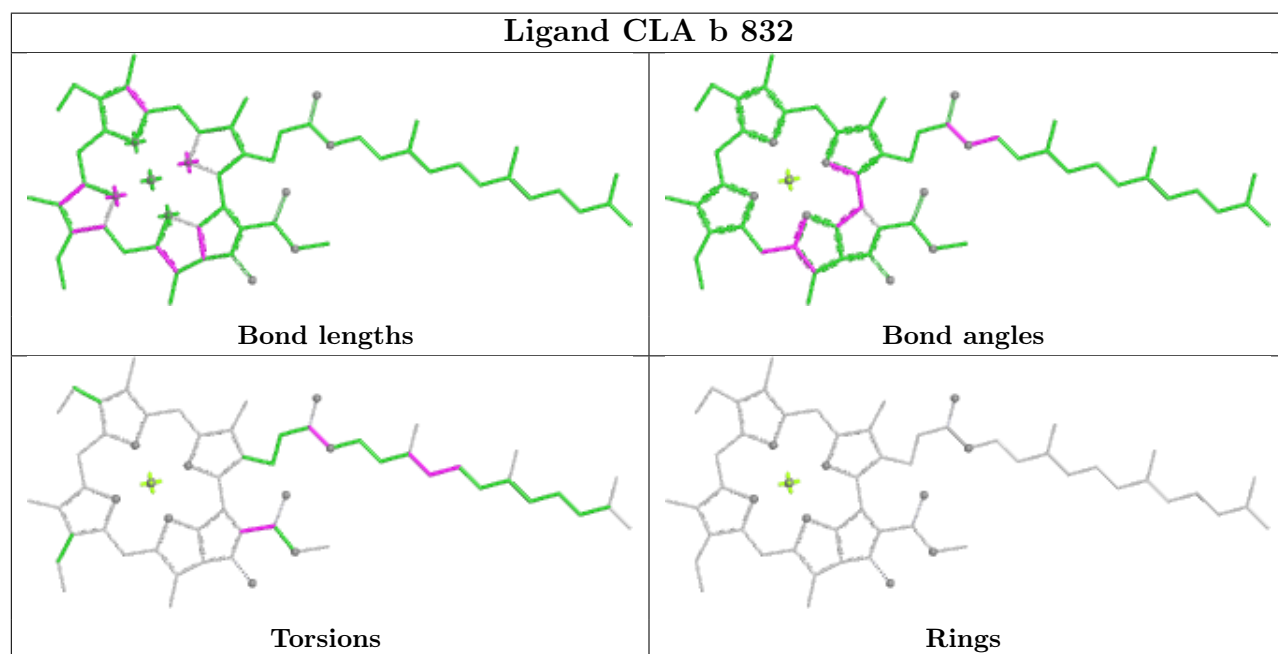
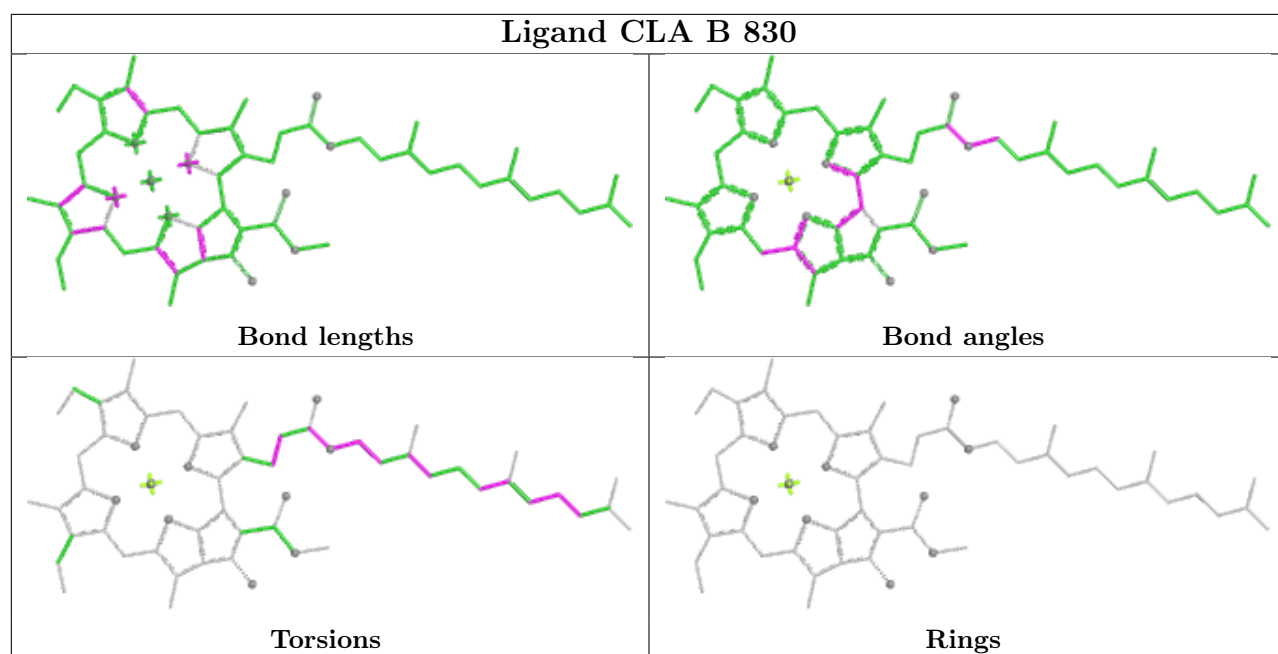
Bond angles

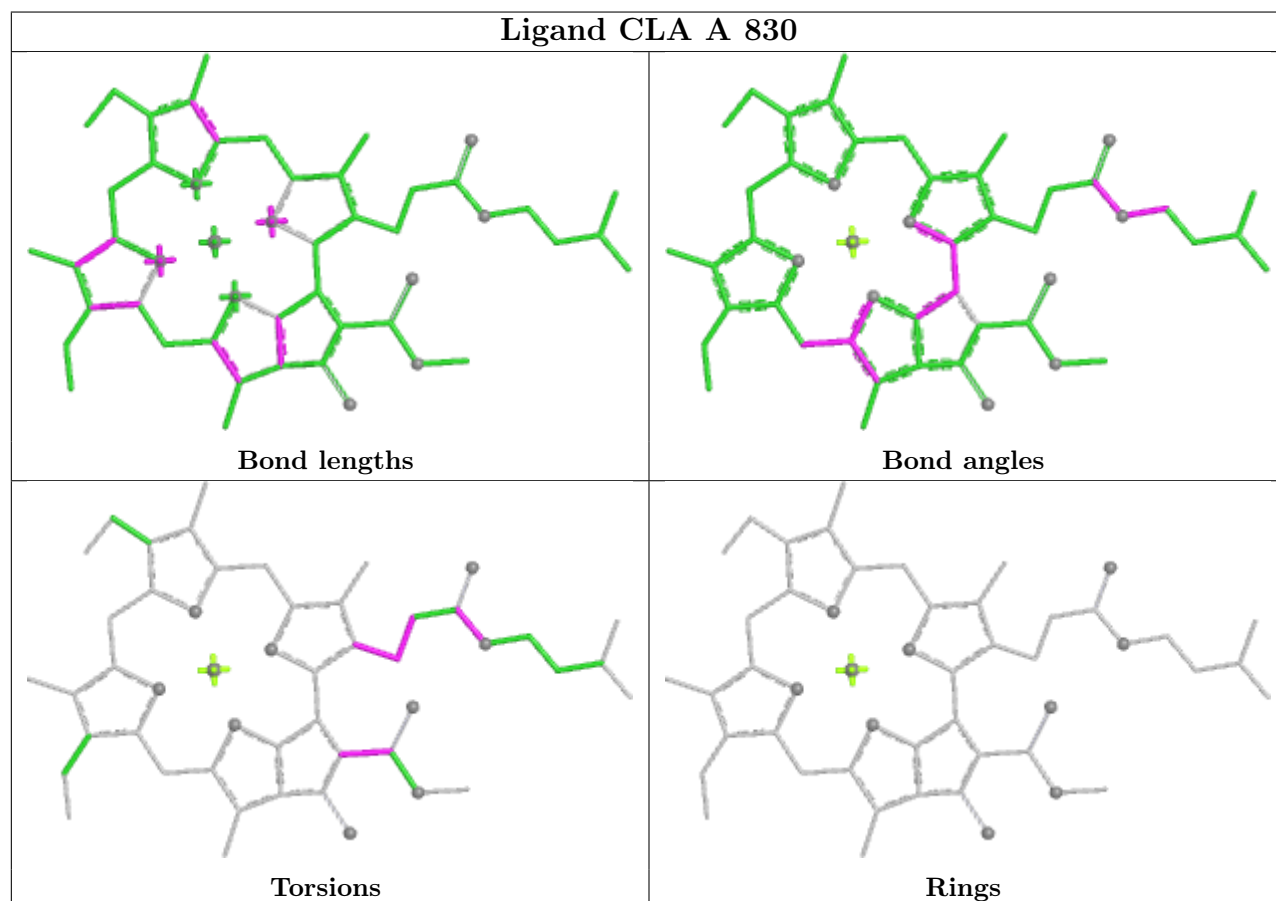
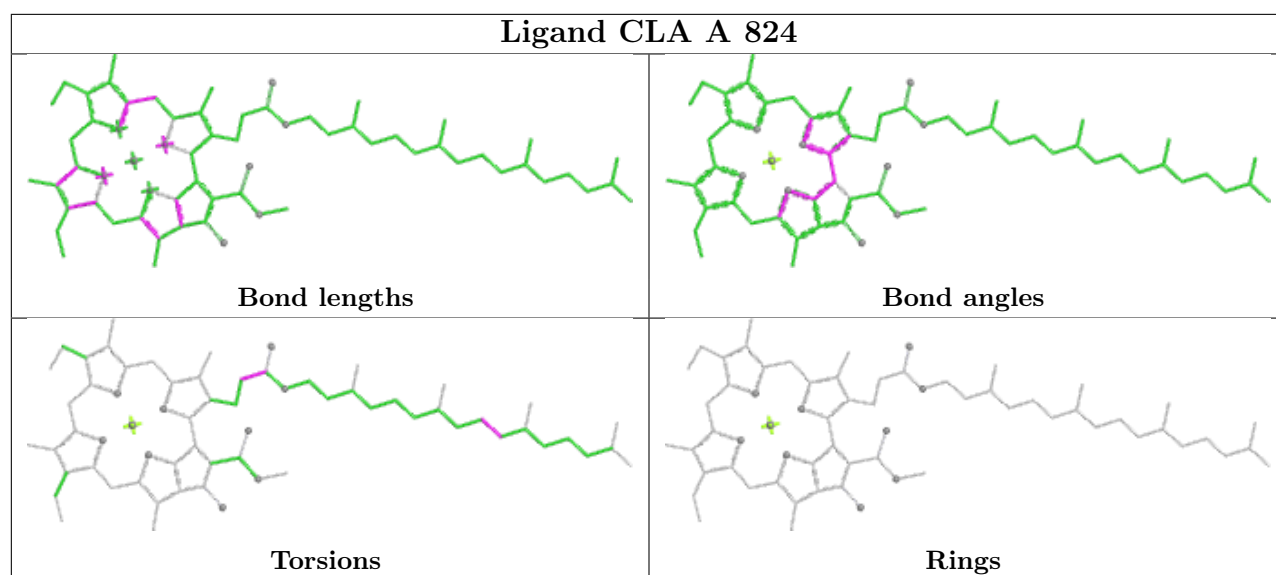


Torsions

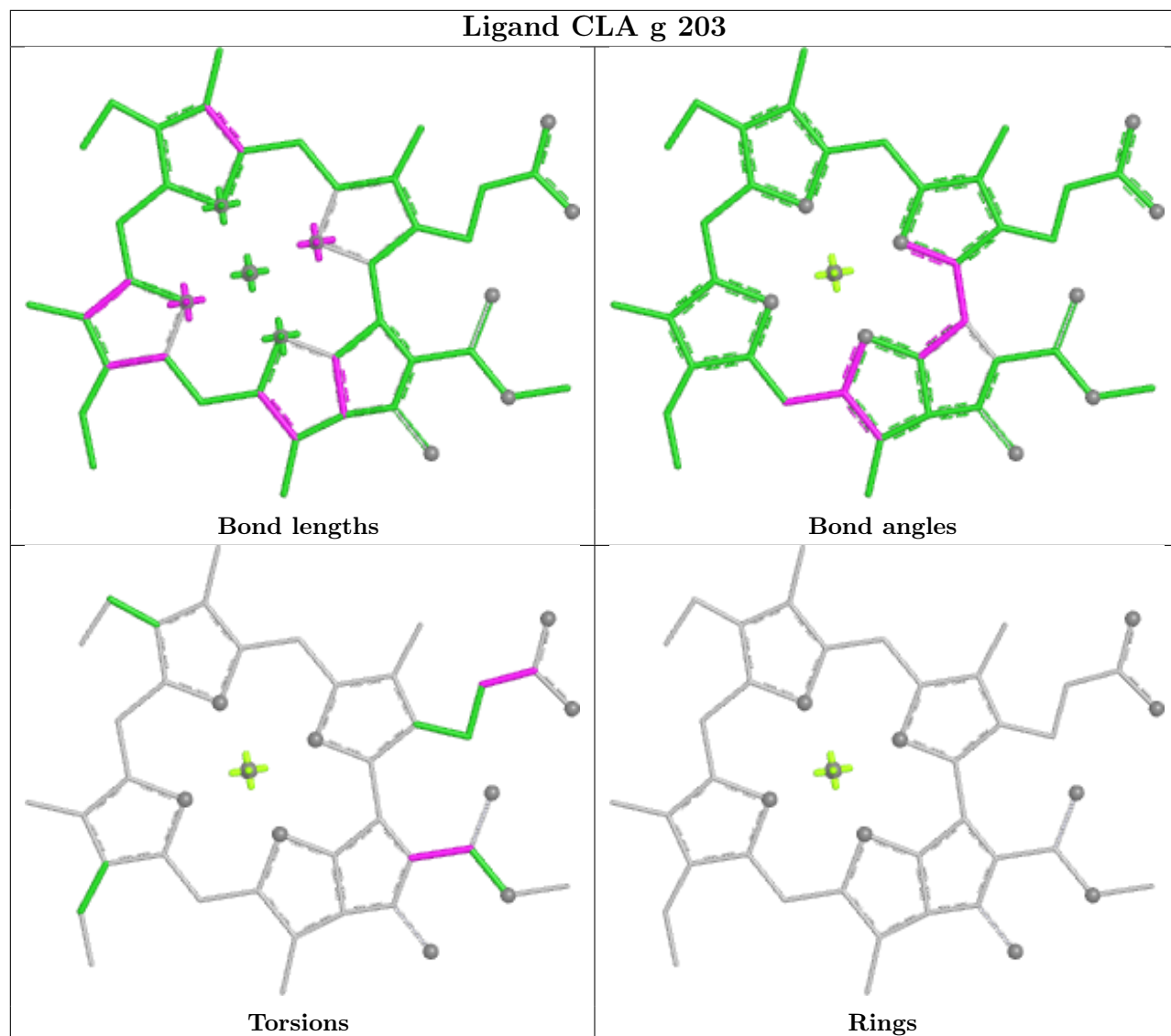


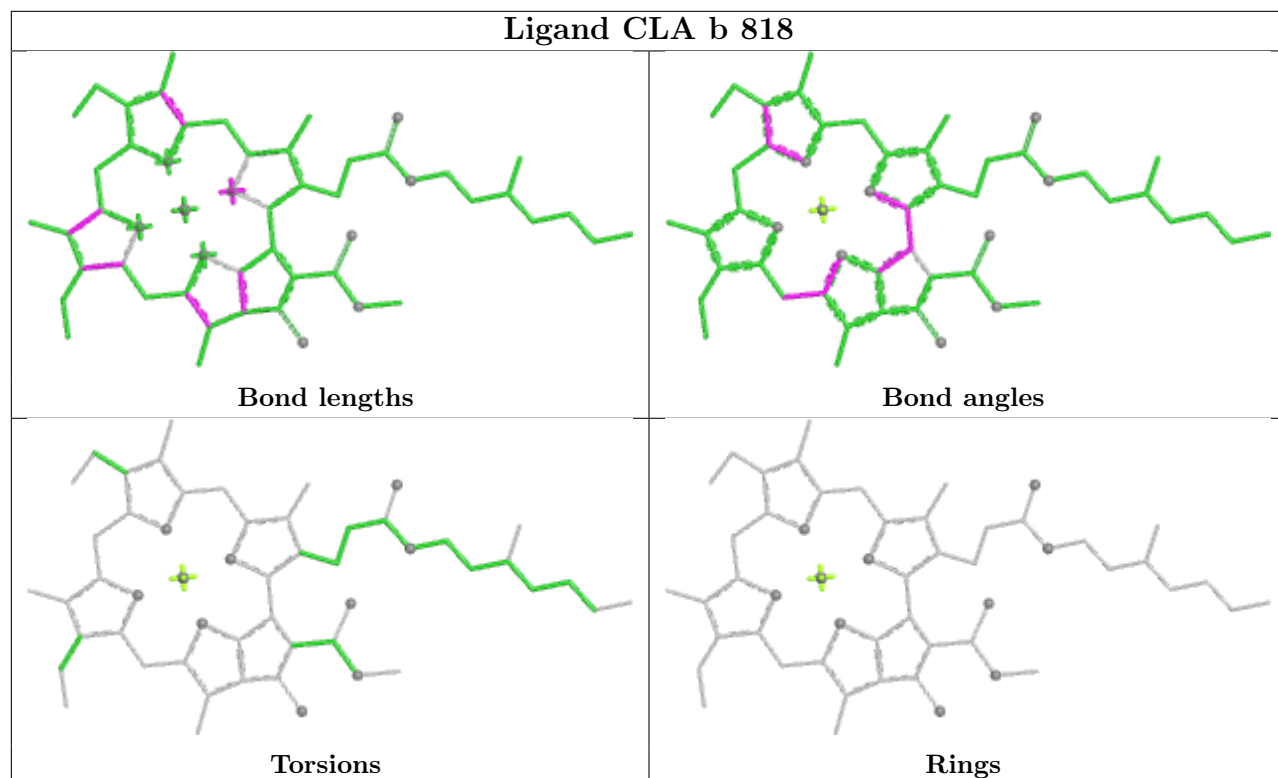
Rings

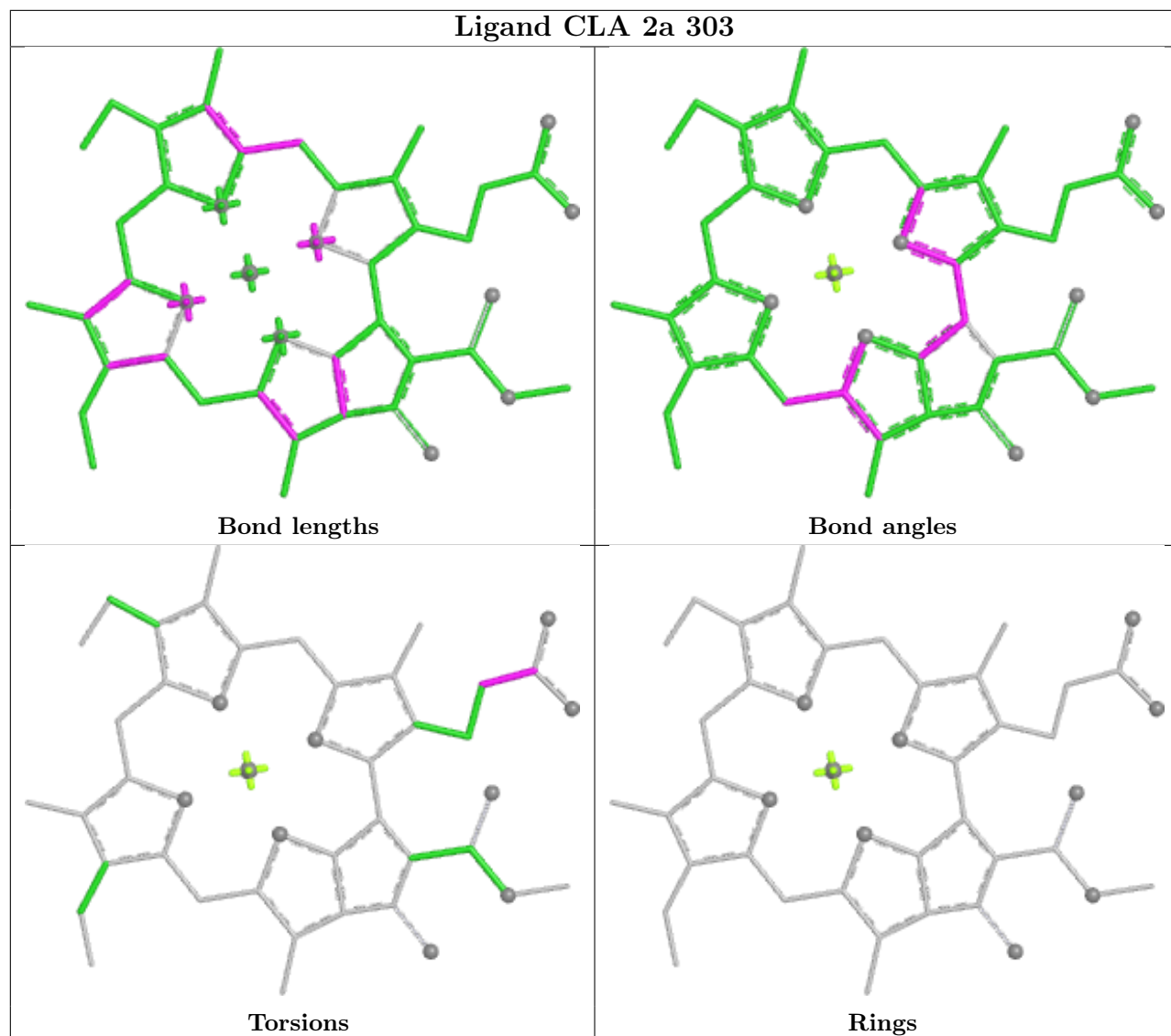




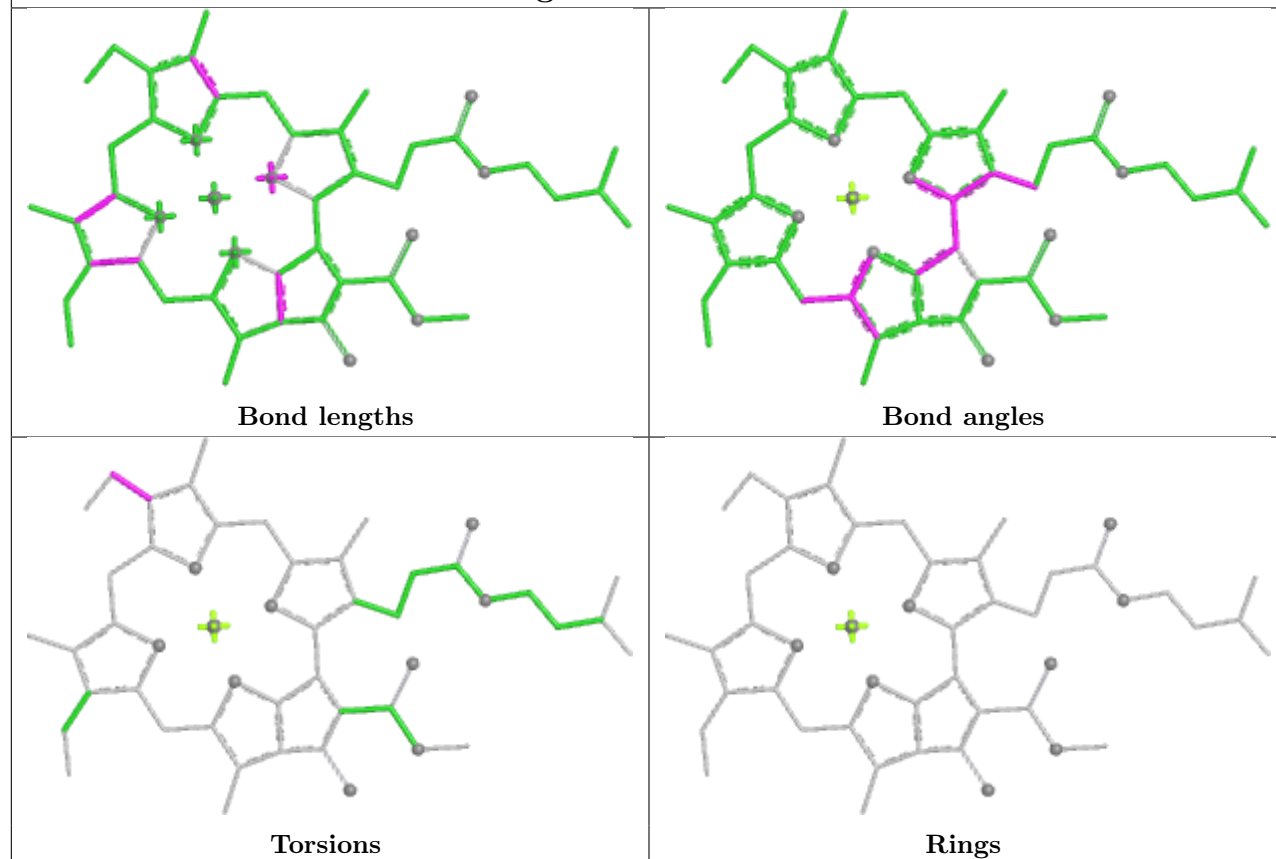
Ligand CLA g 203



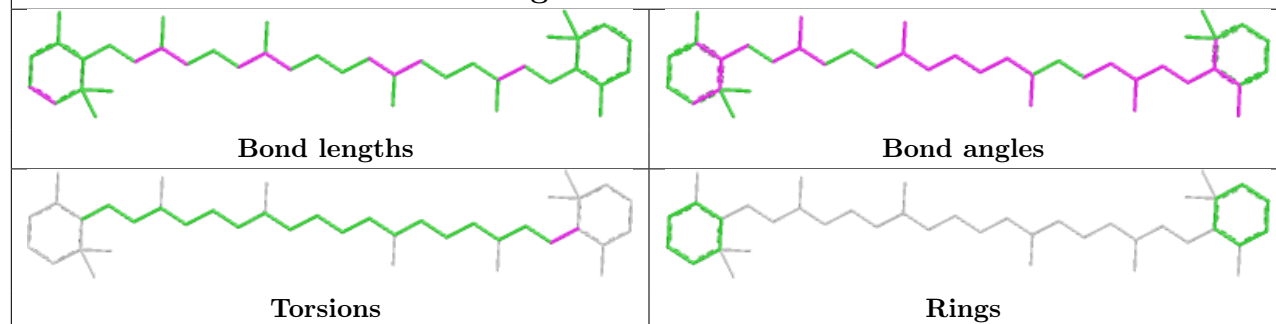


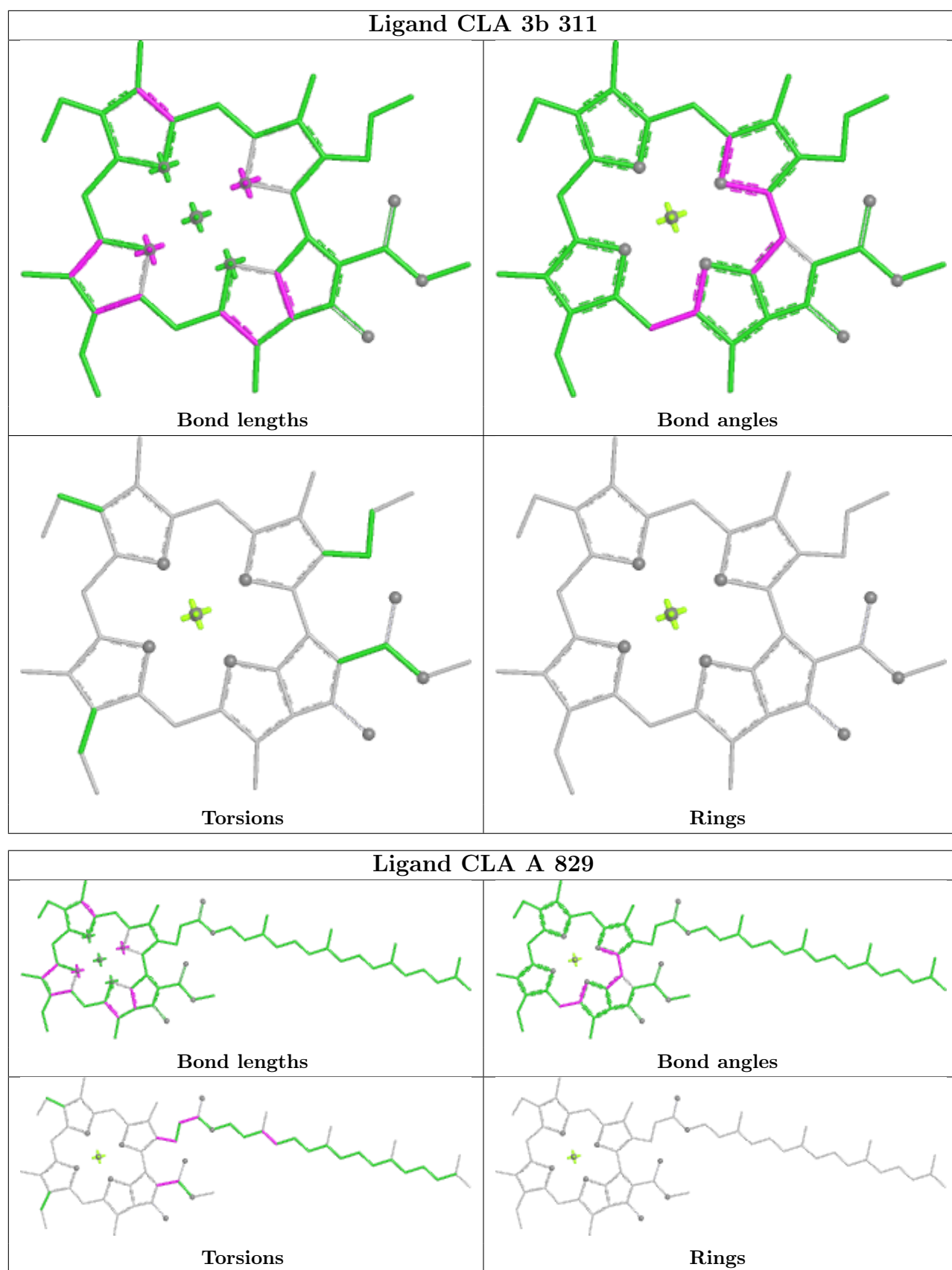


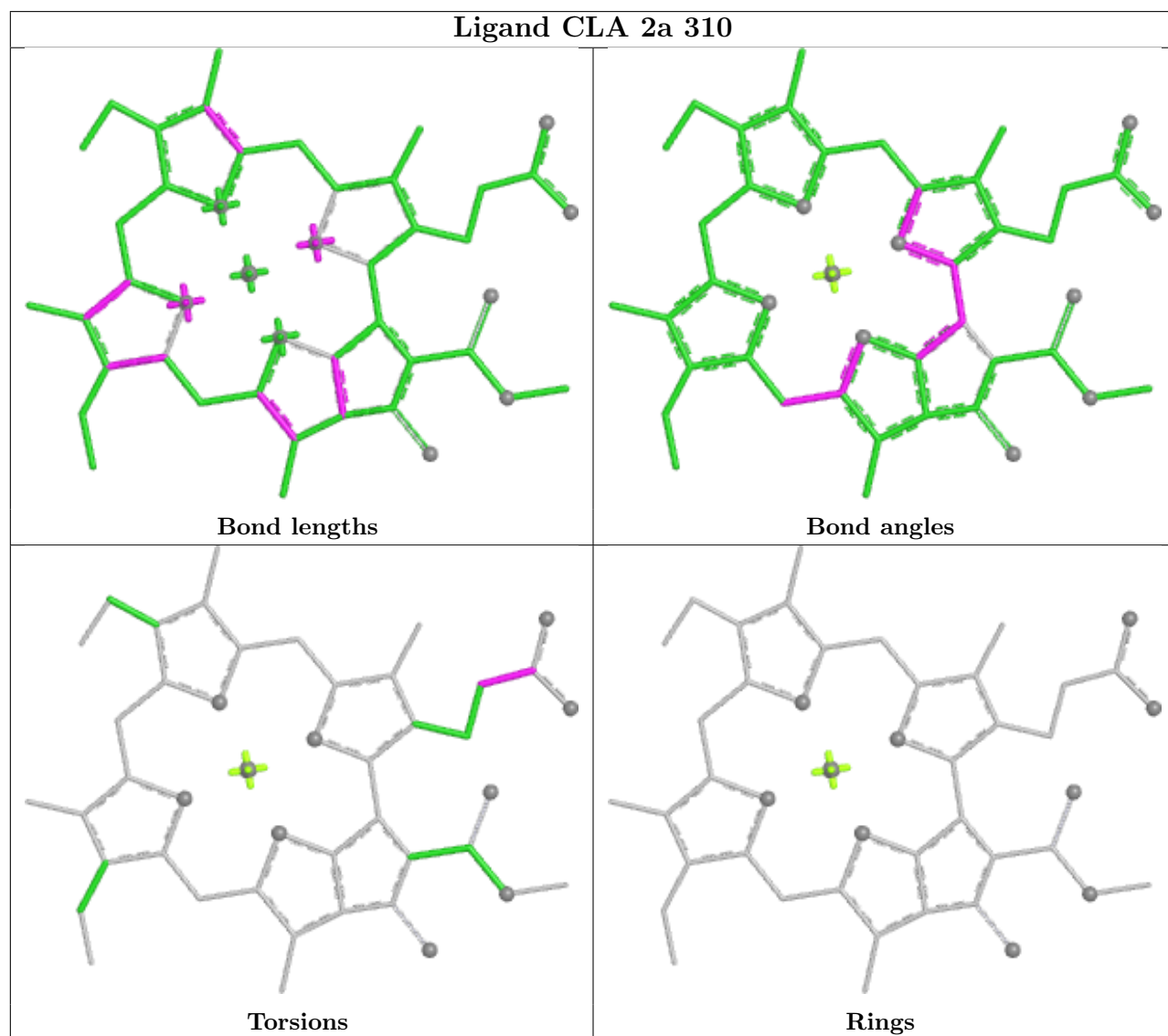
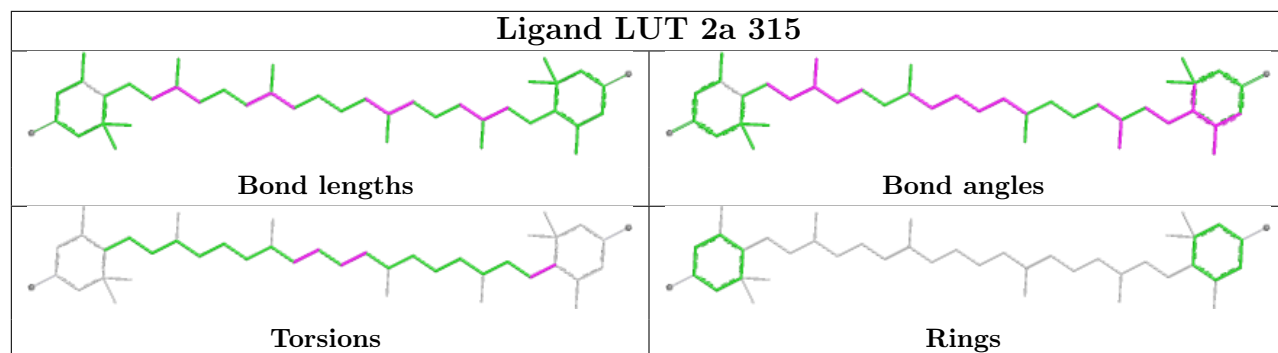
Ligand CLA a 813

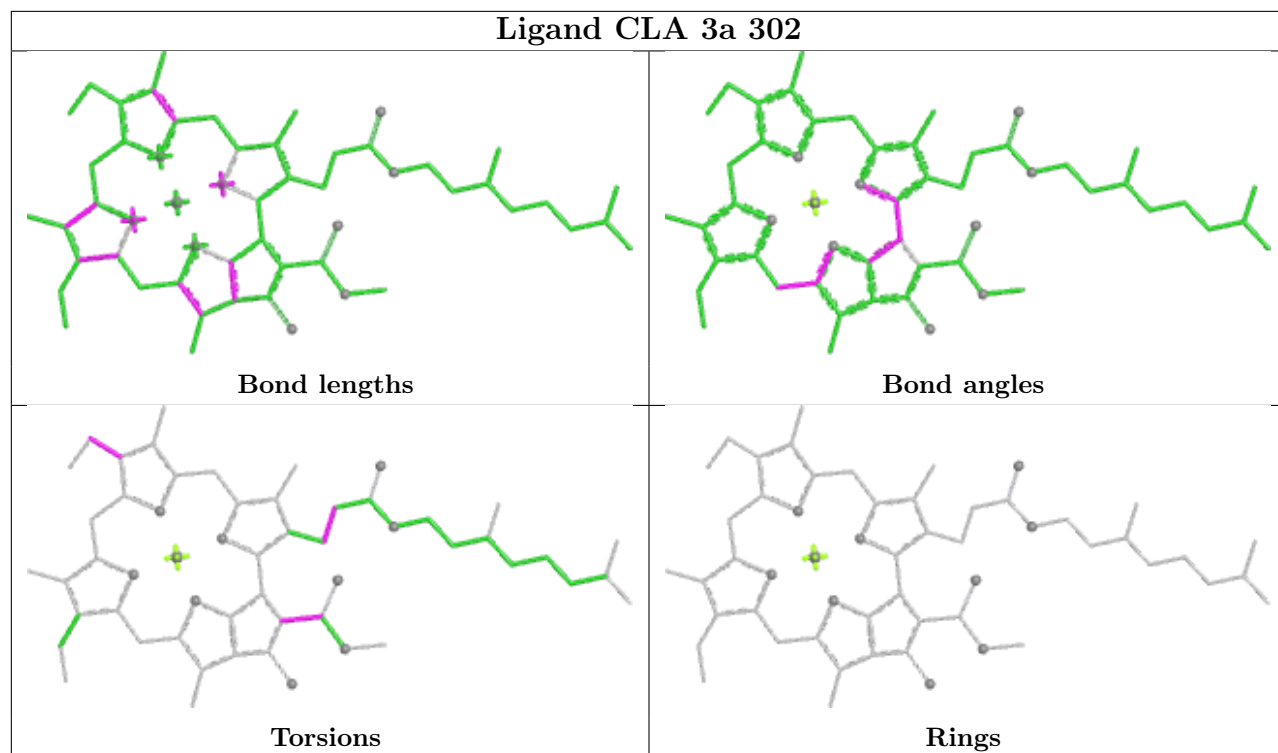


Ligand BCR B 842

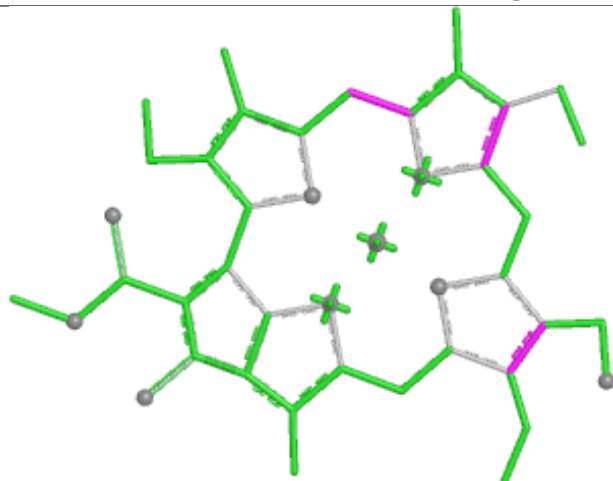




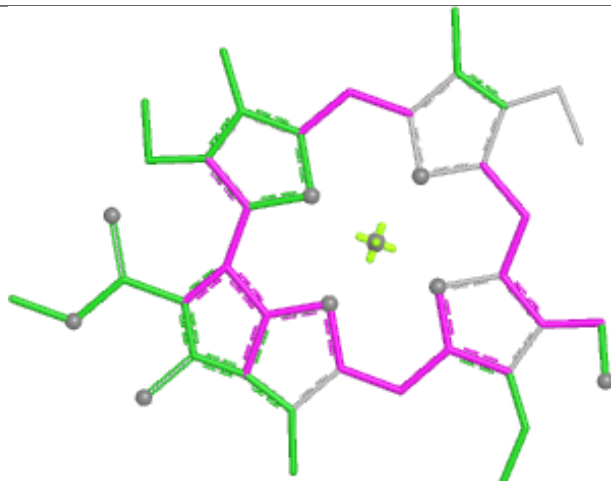




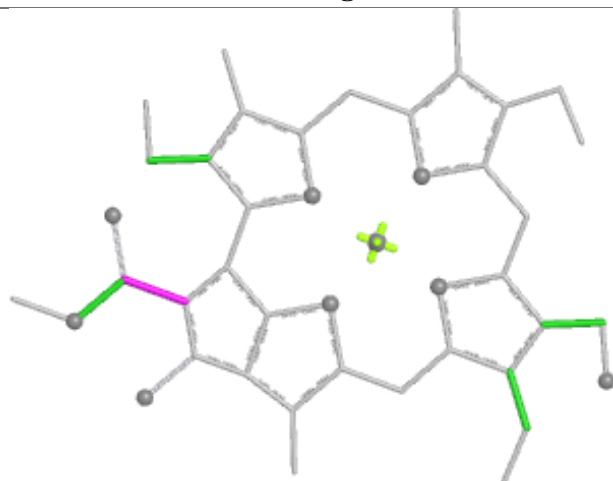
Ligand CHL 2b 305



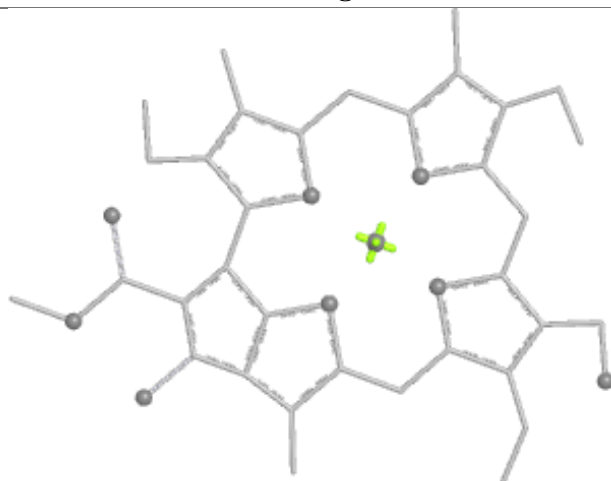
Bond lengths



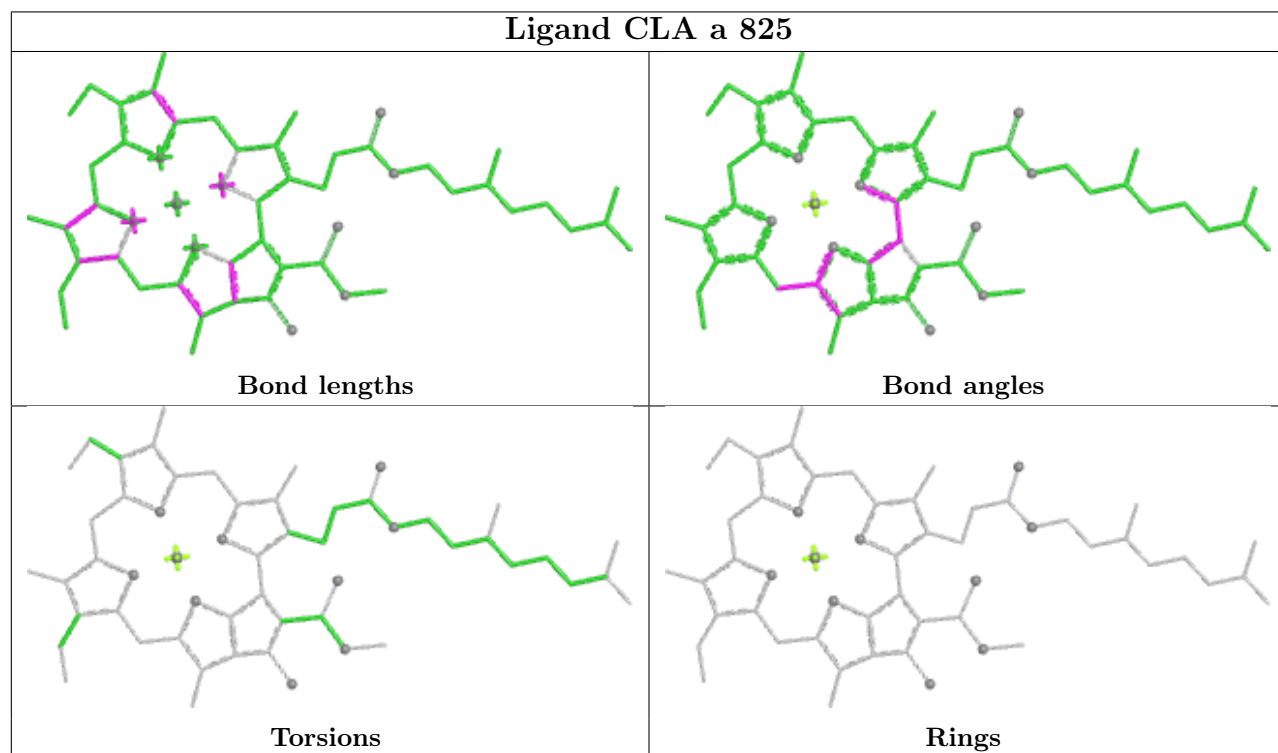
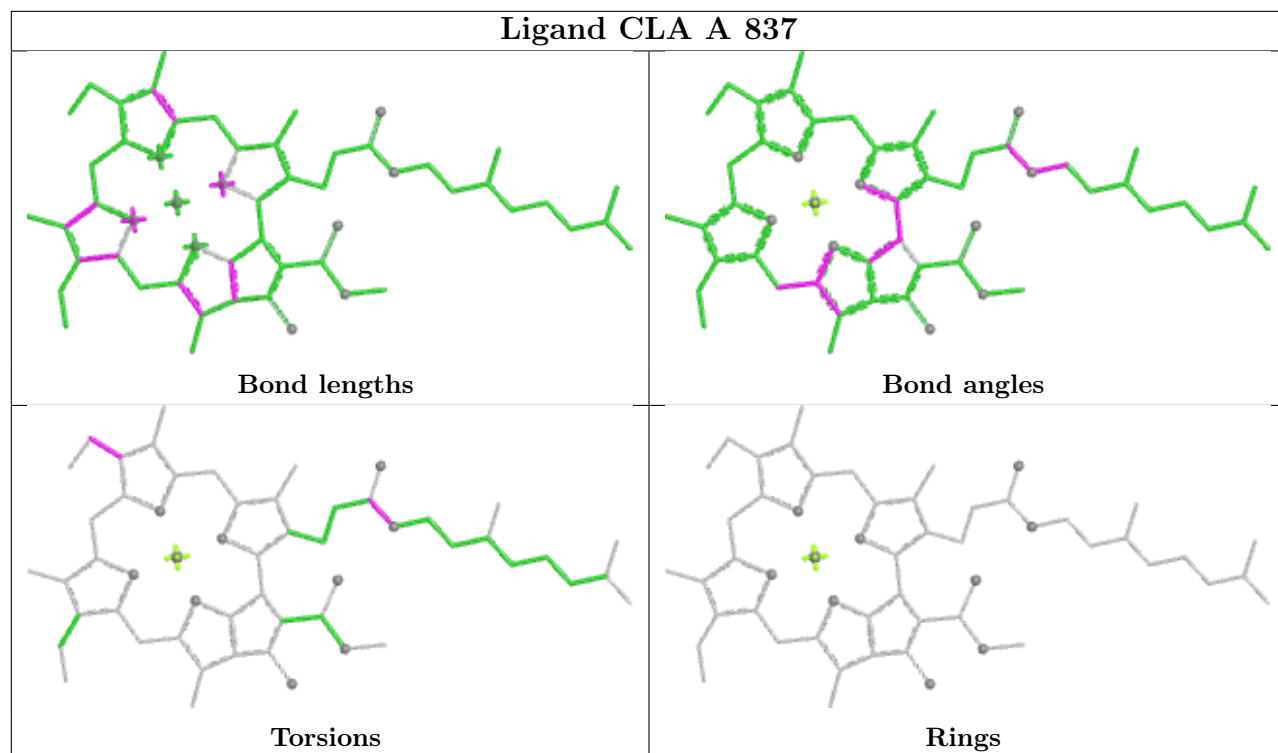
Bond angles

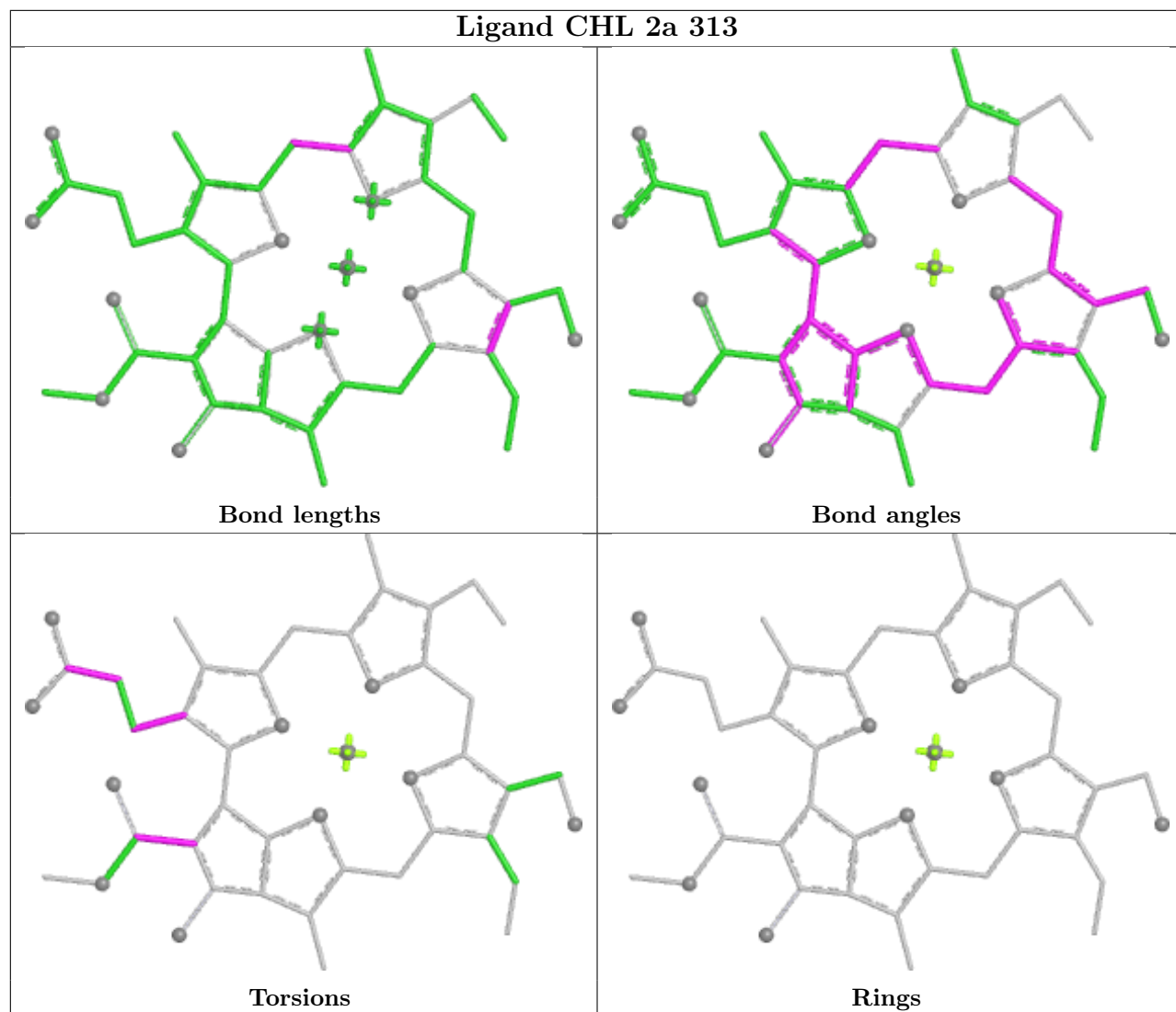


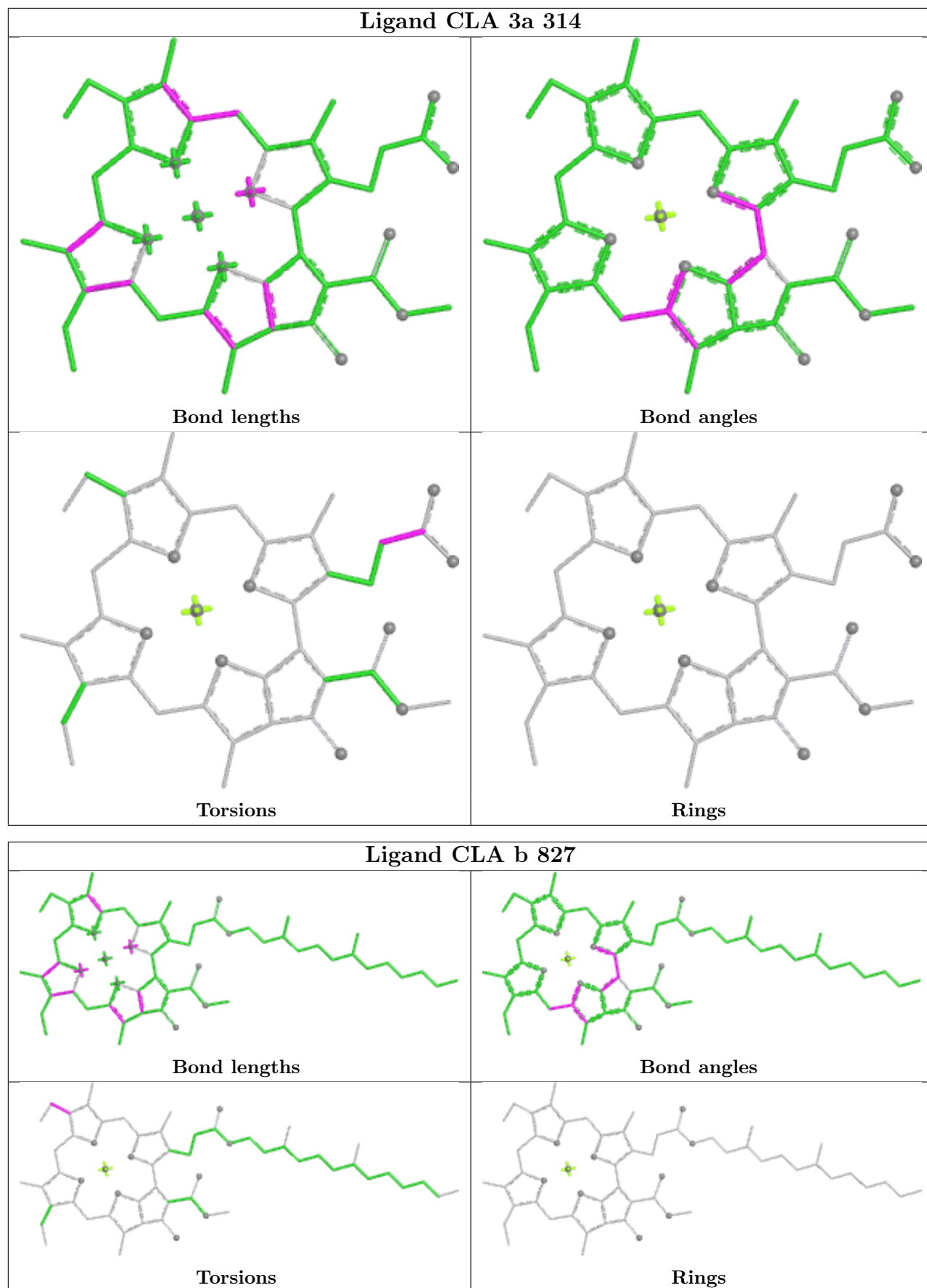
Torsions

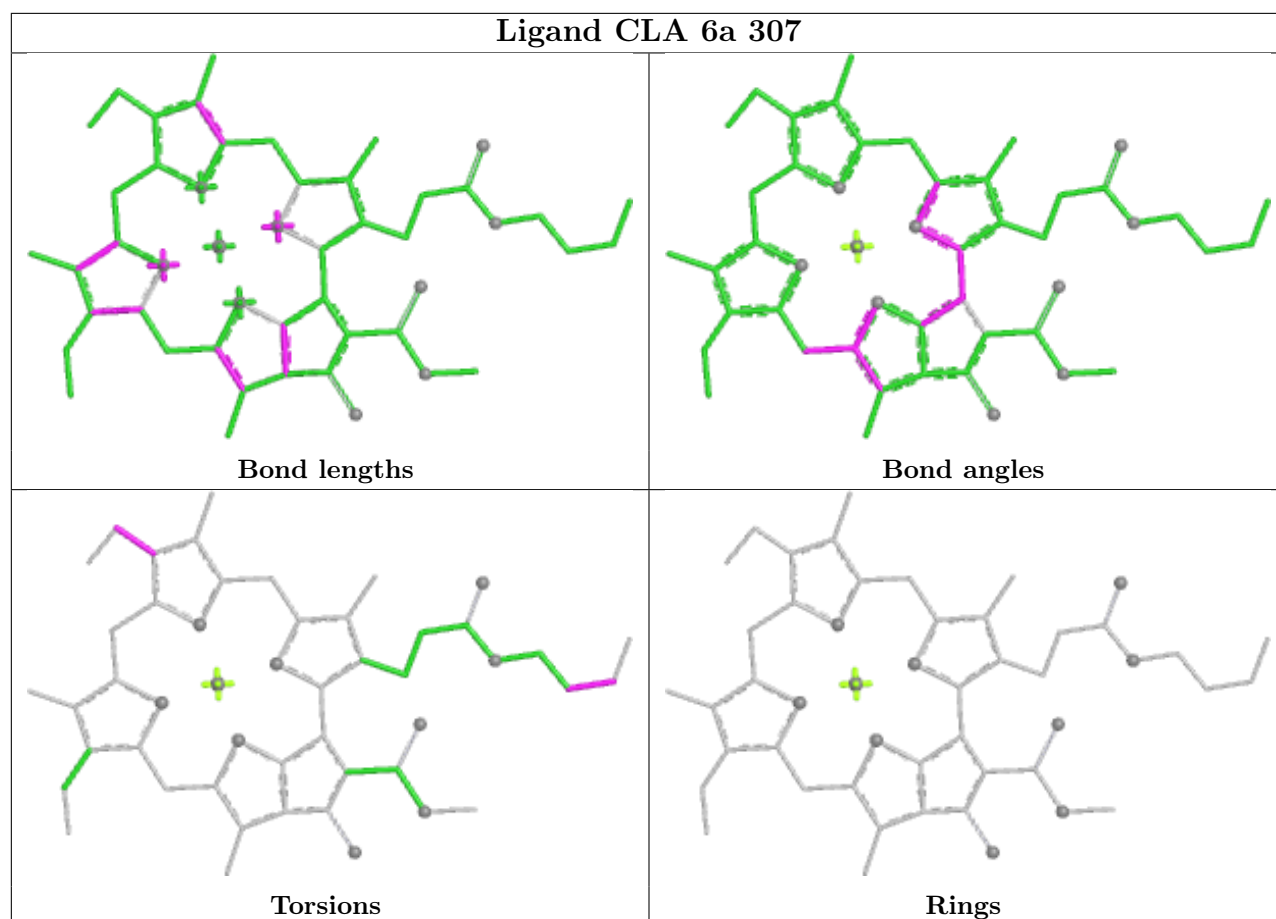
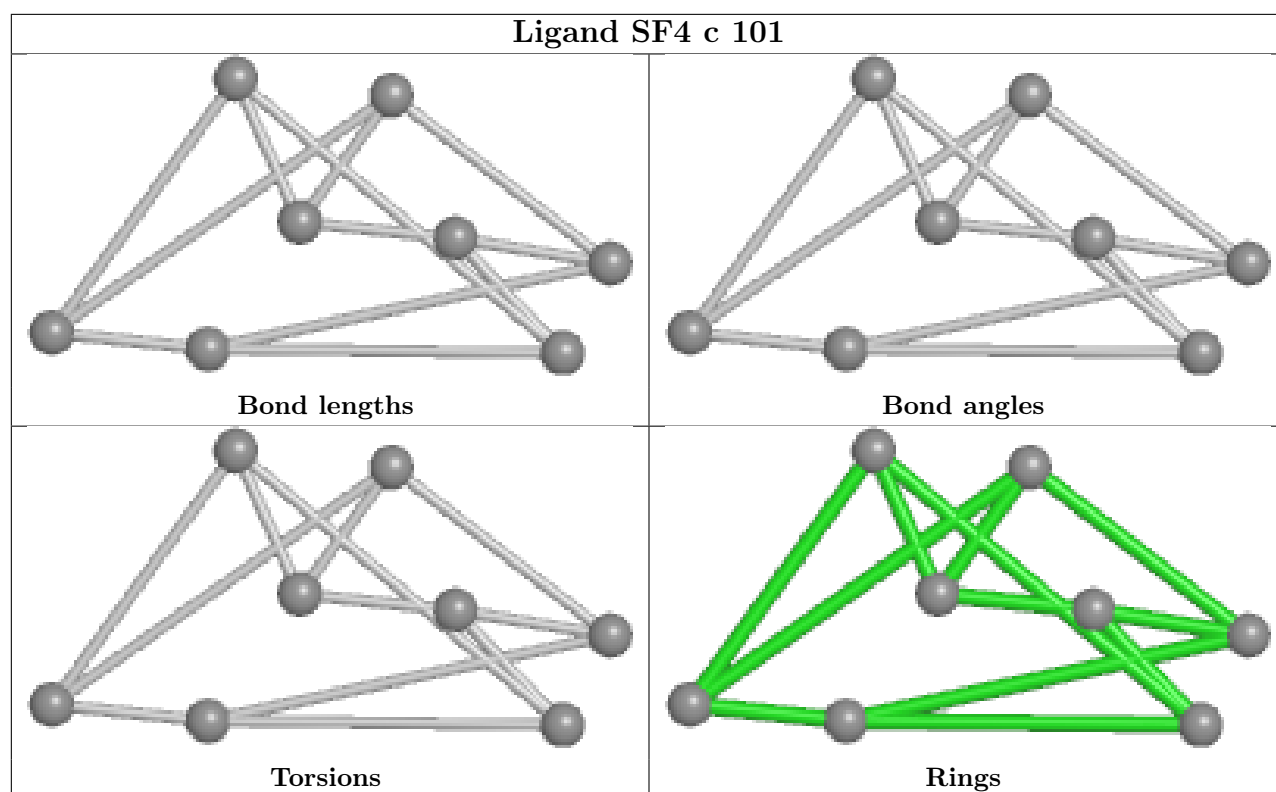


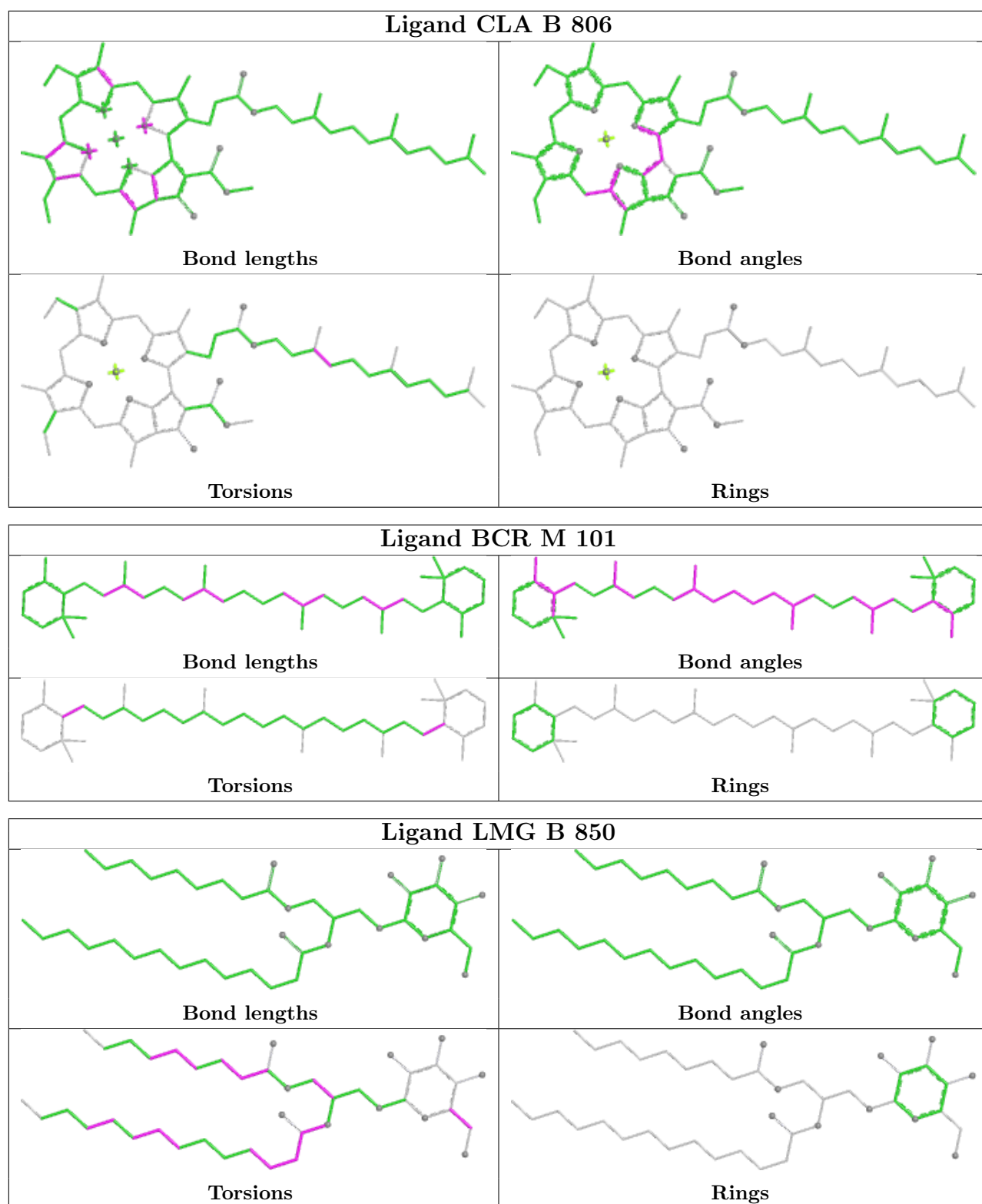
Rings

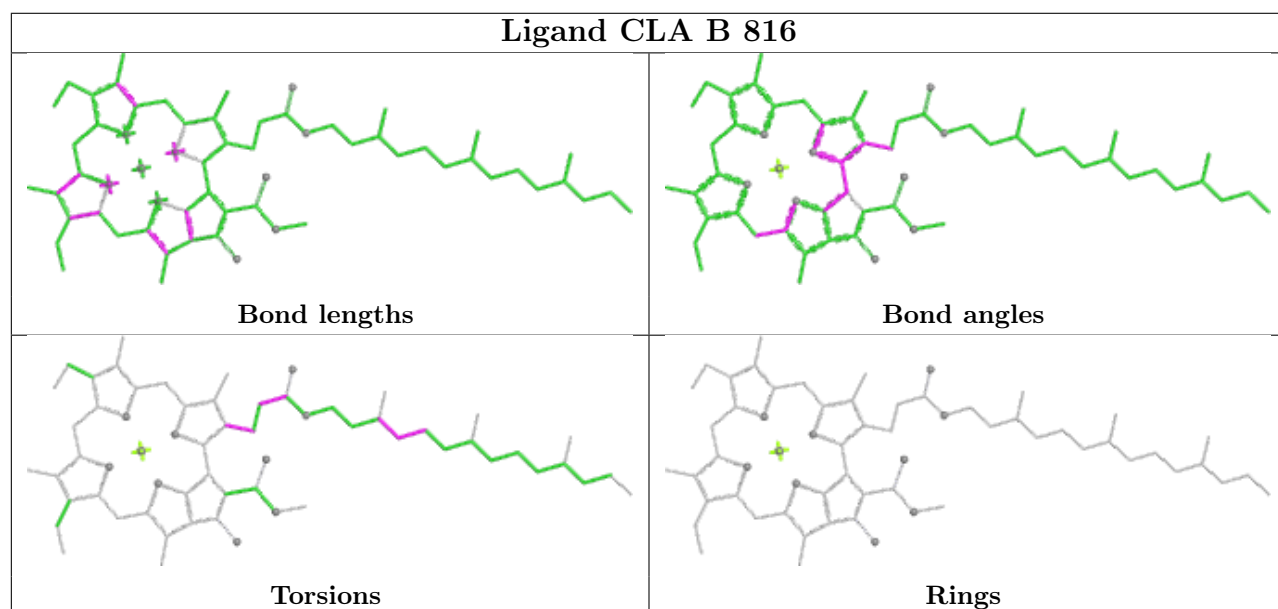
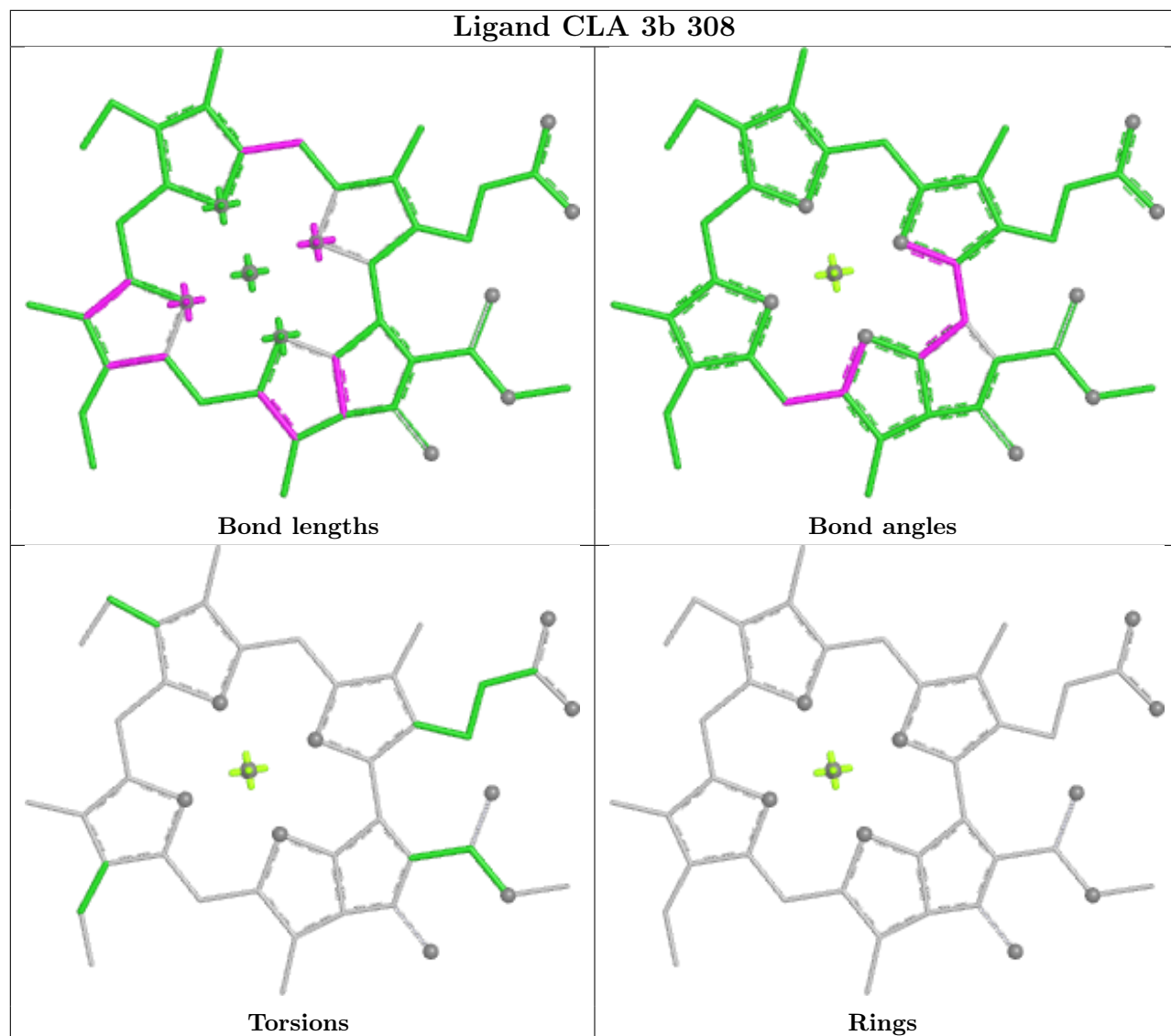




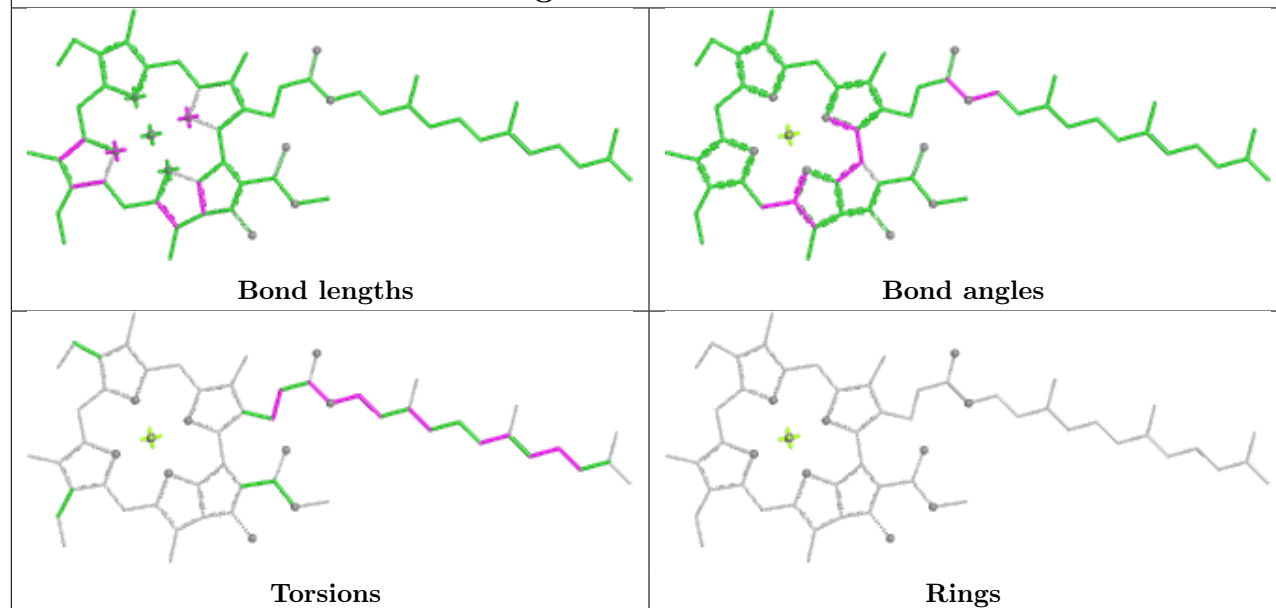




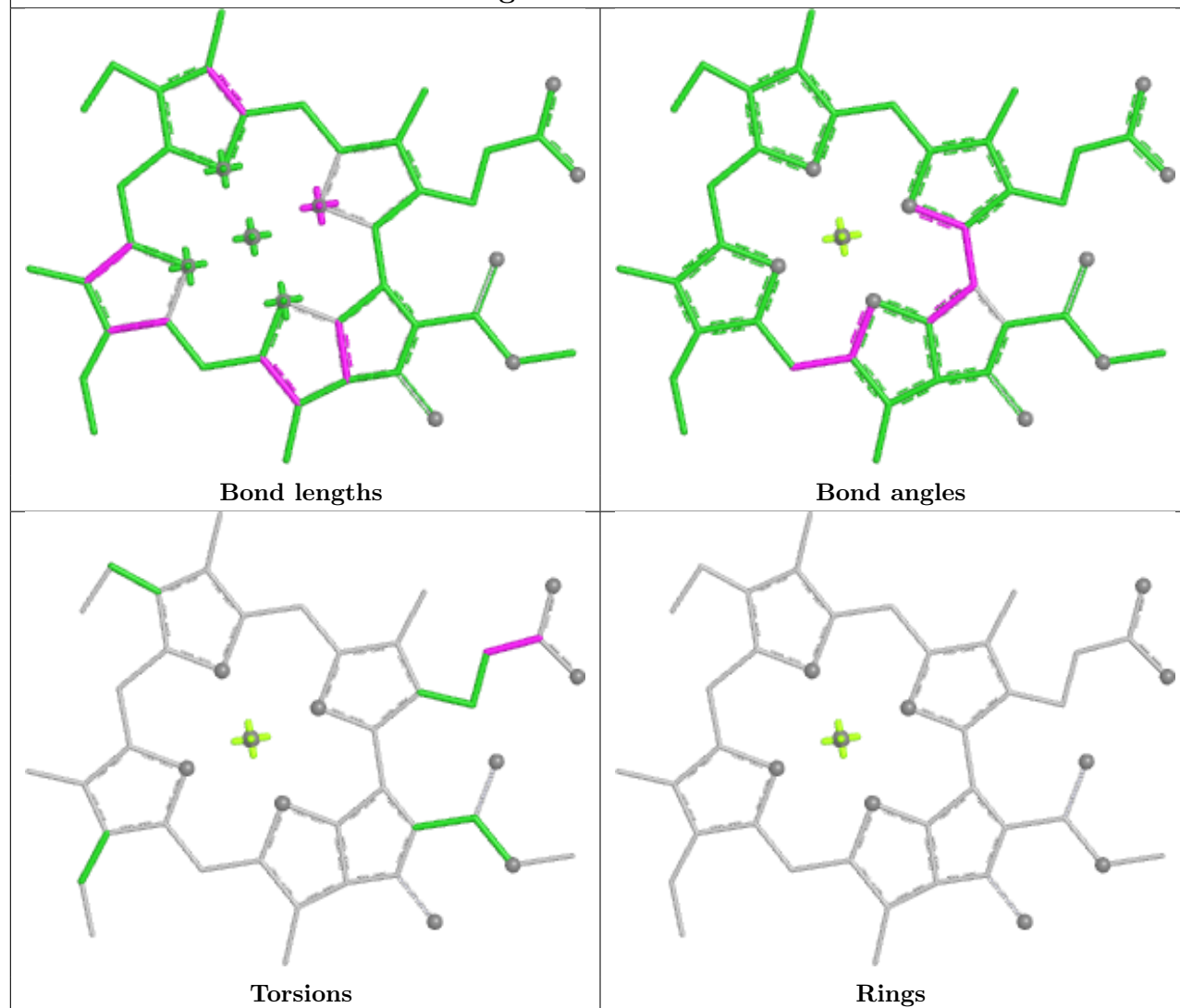


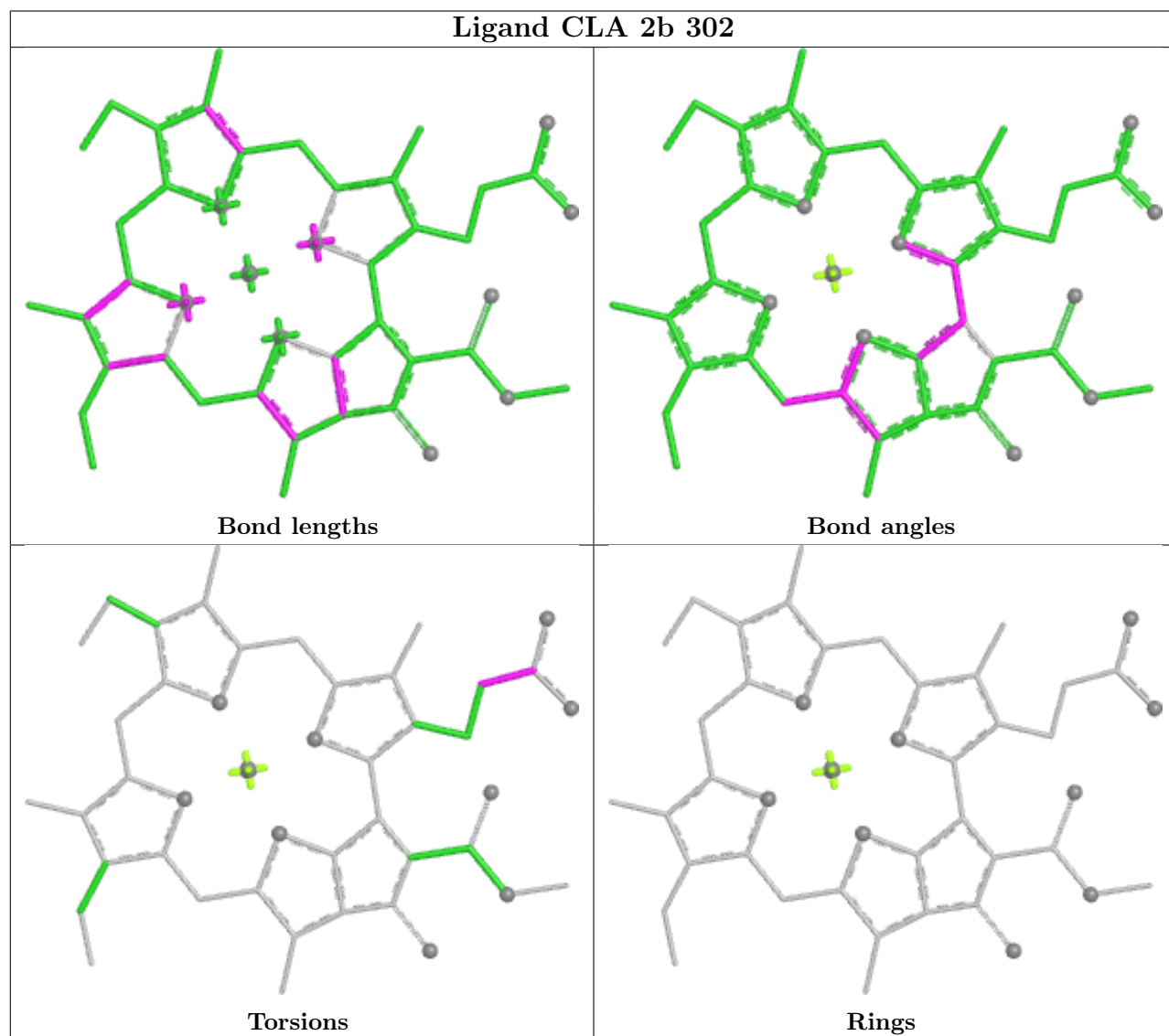
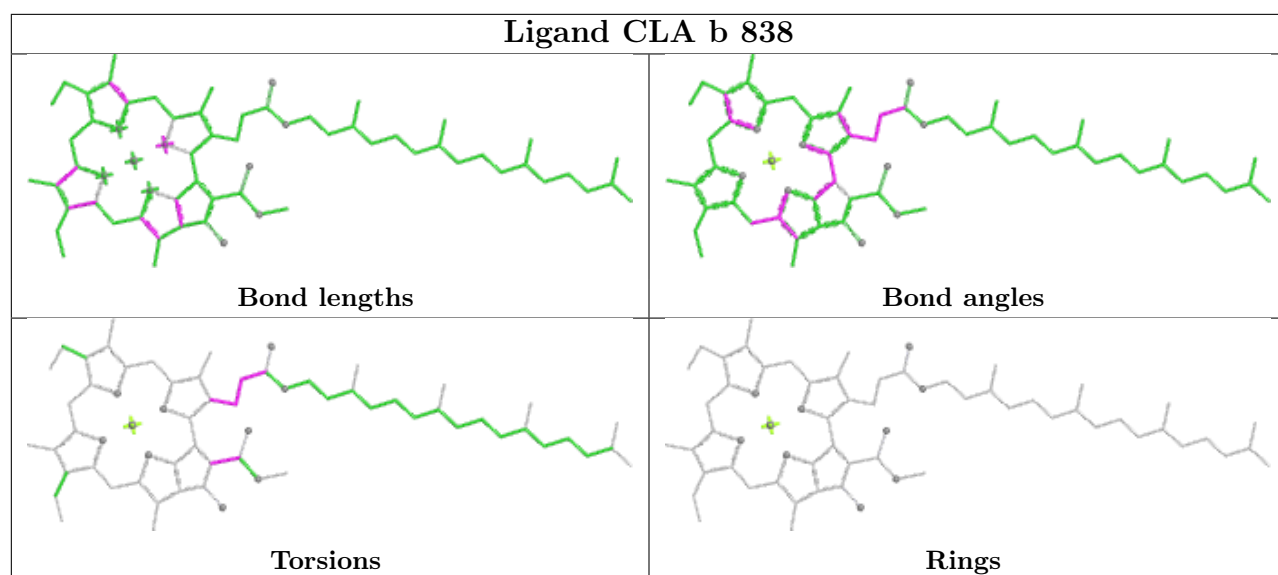


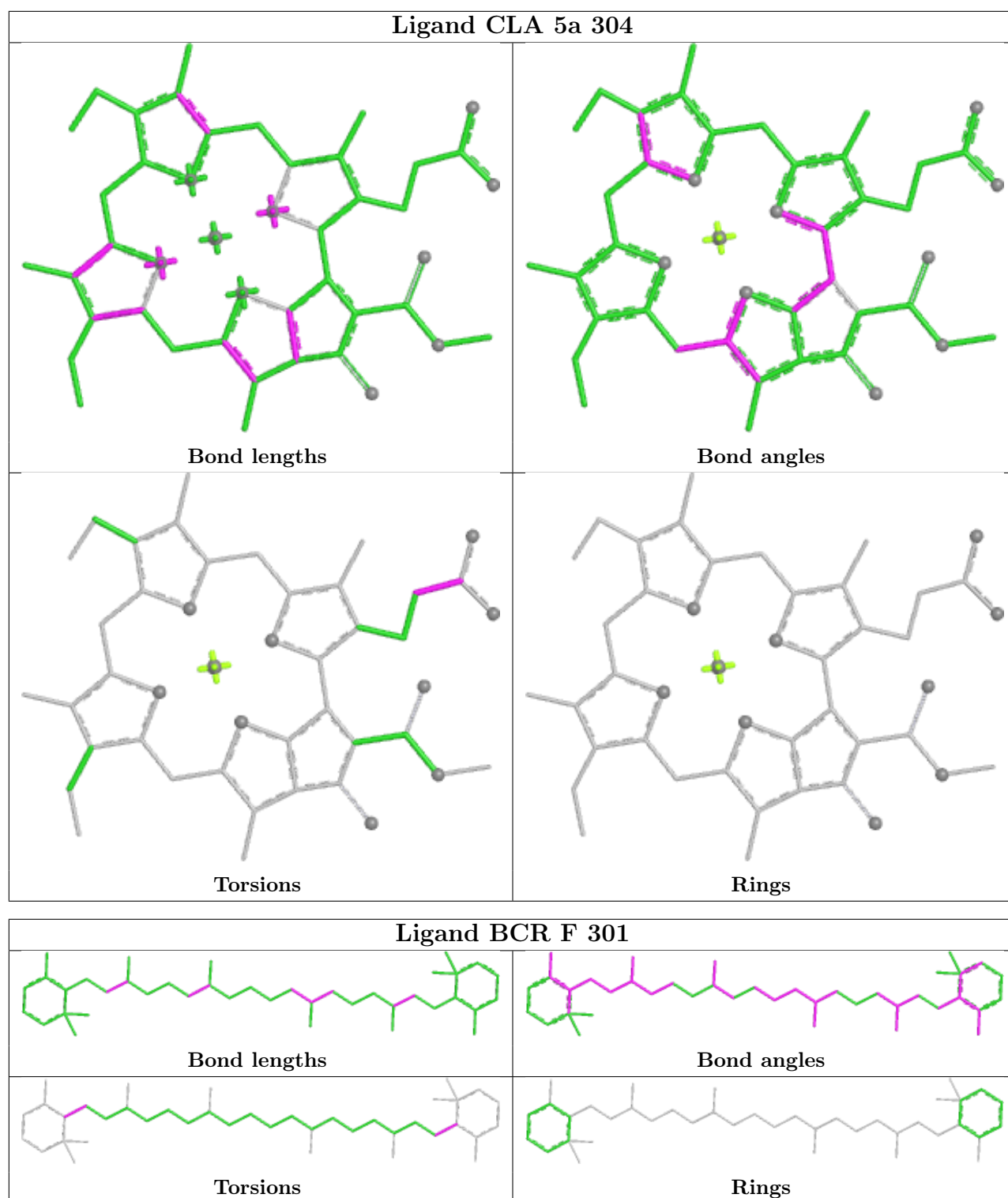
Ligand CLA b 830



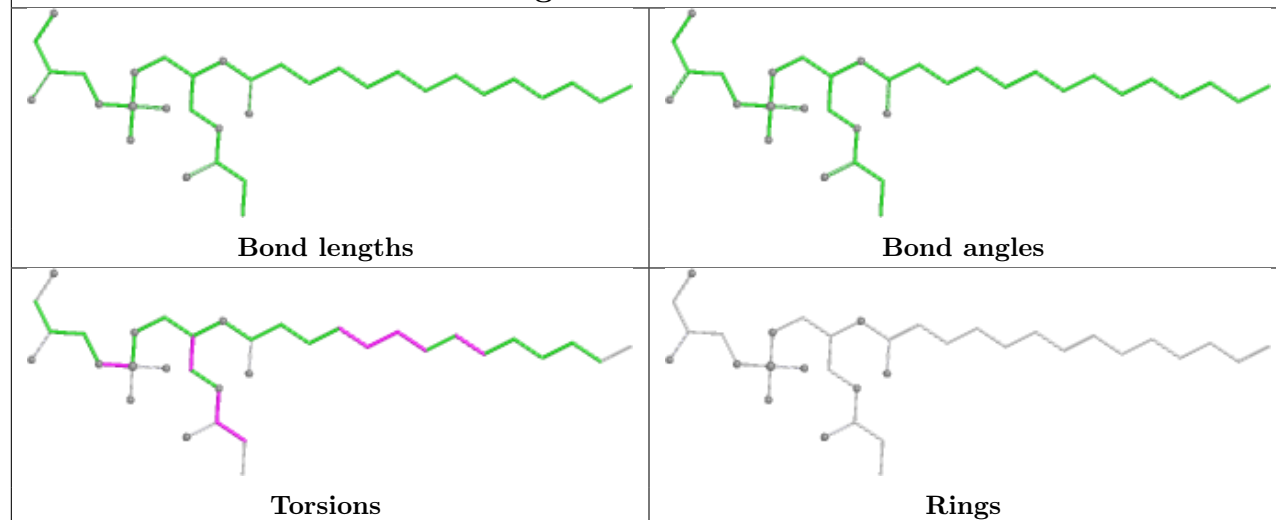
Ligand CLA f 302



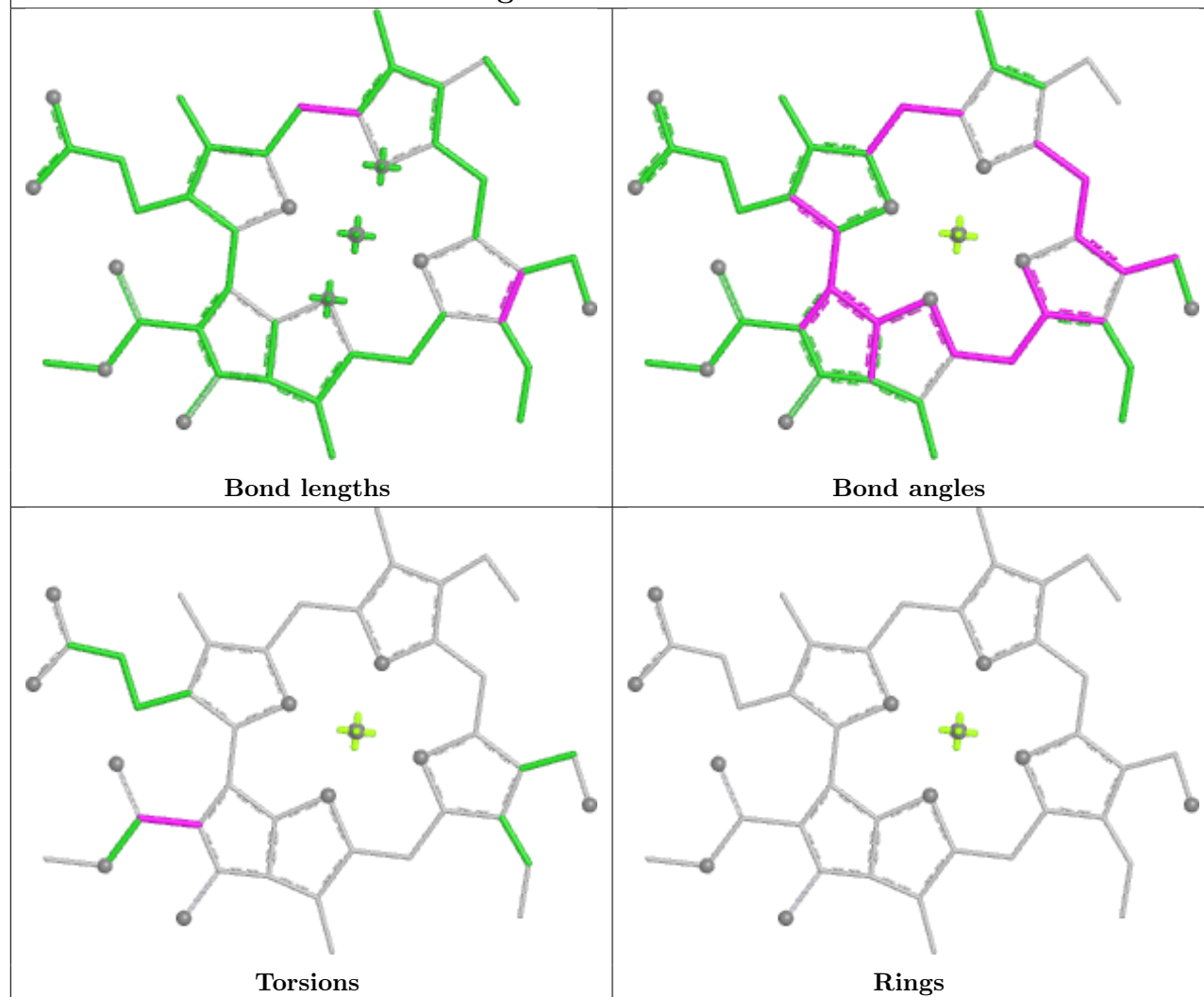


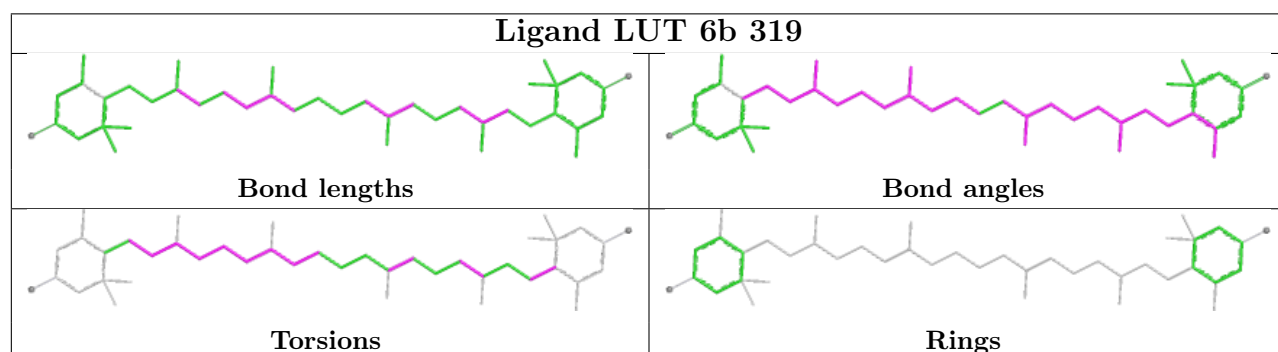
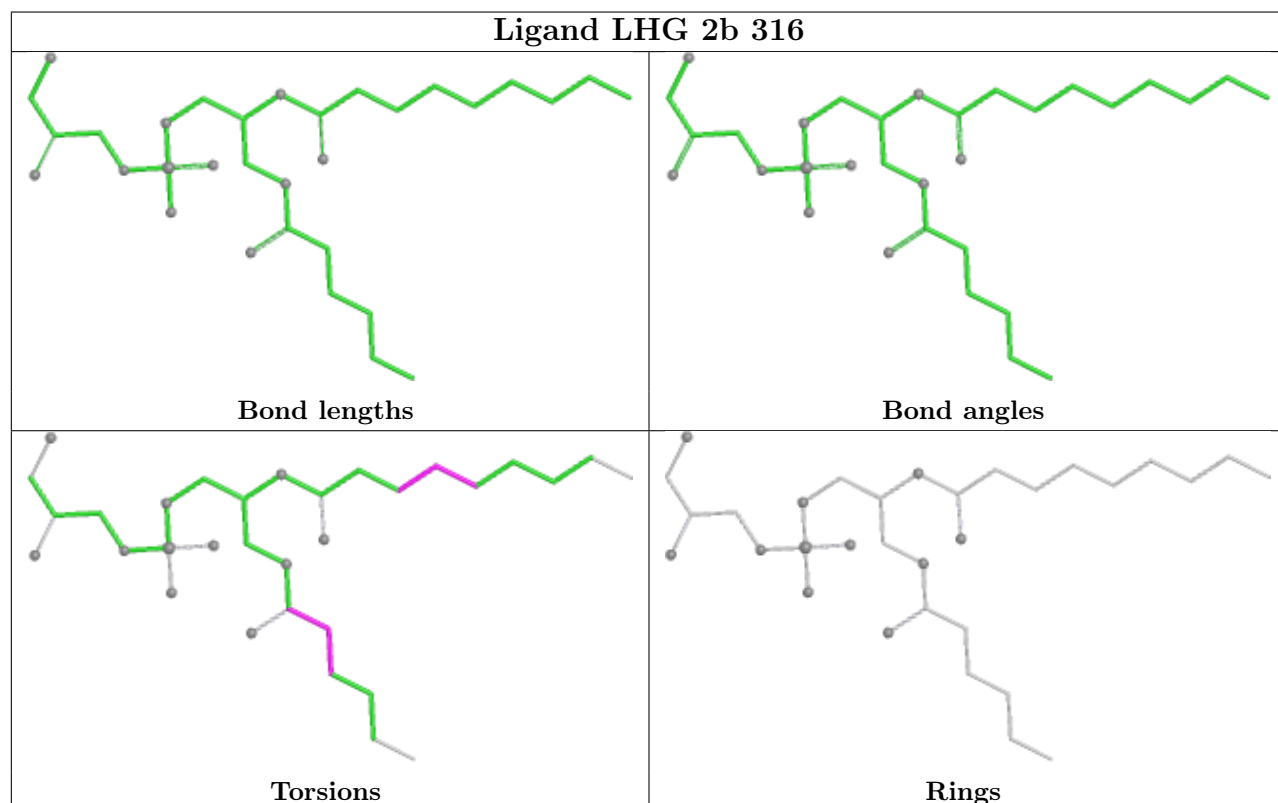
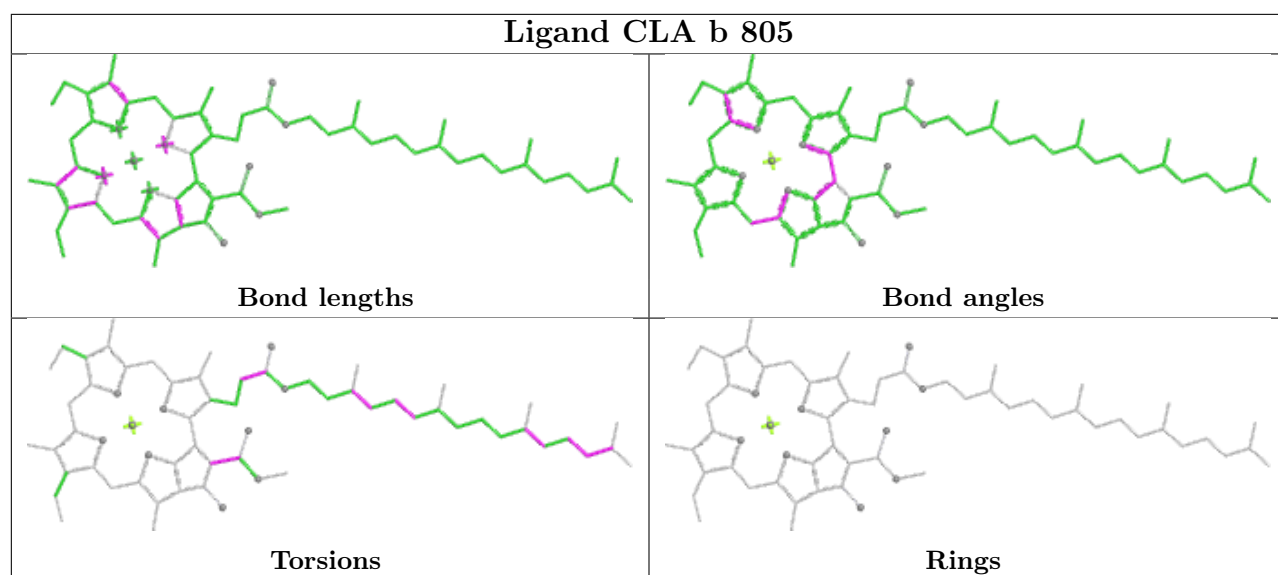


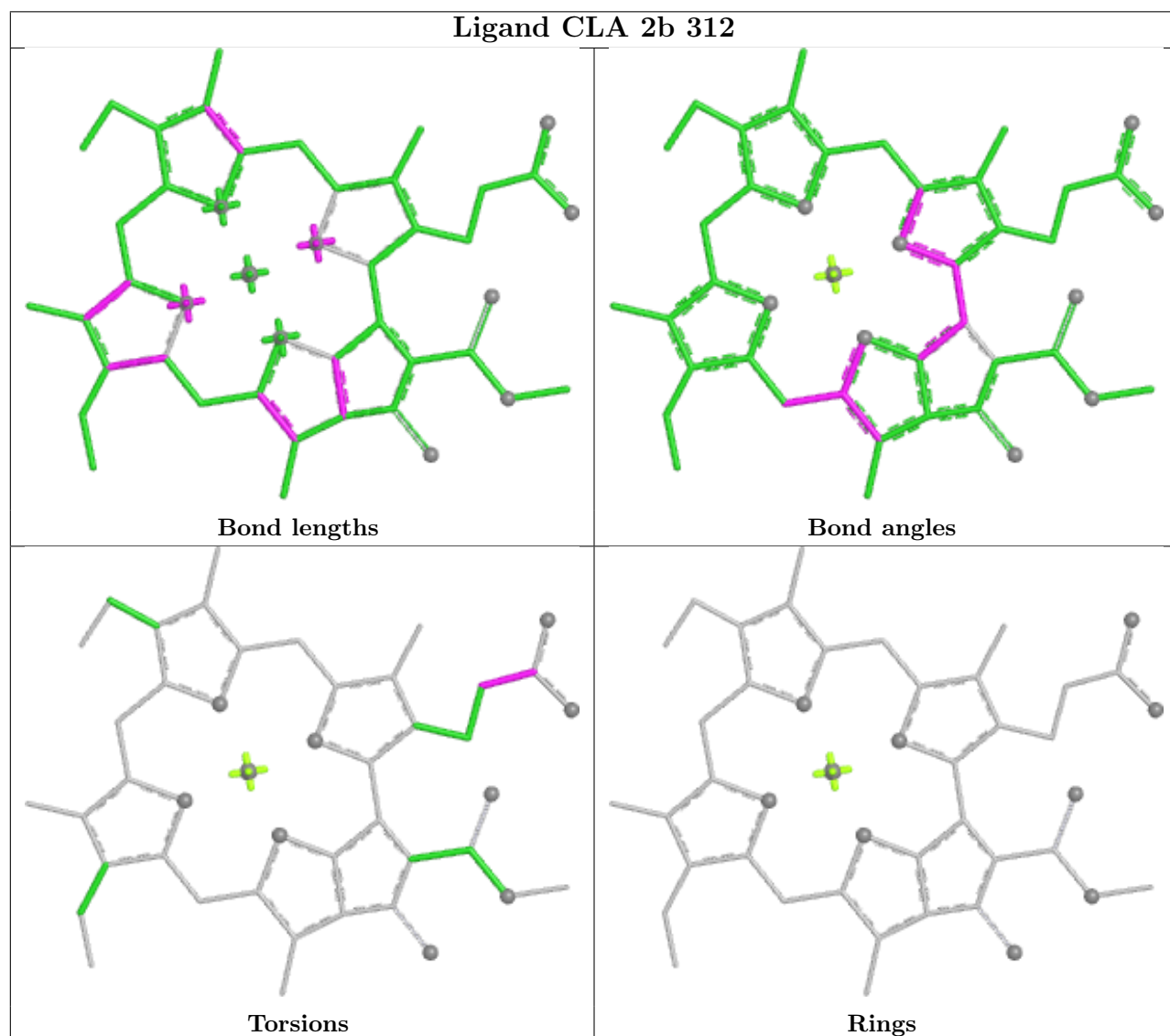
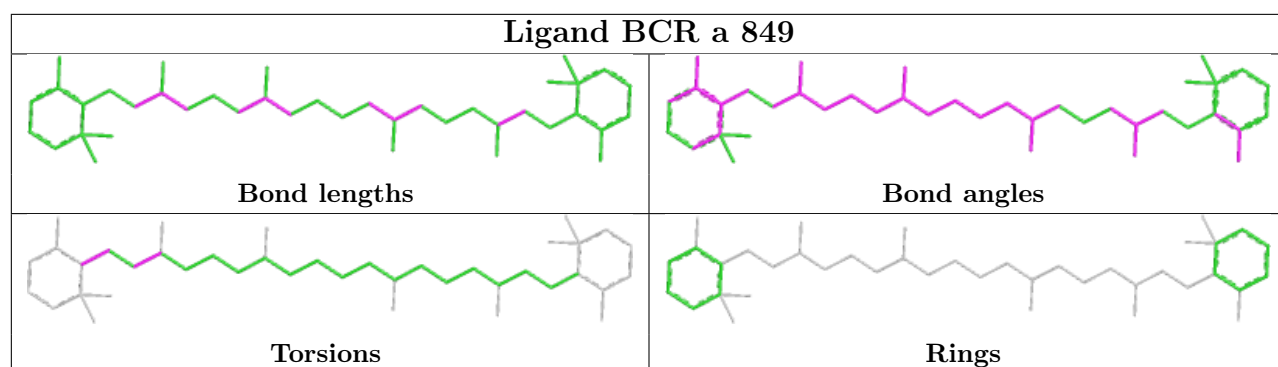
Ligand LHG a 846

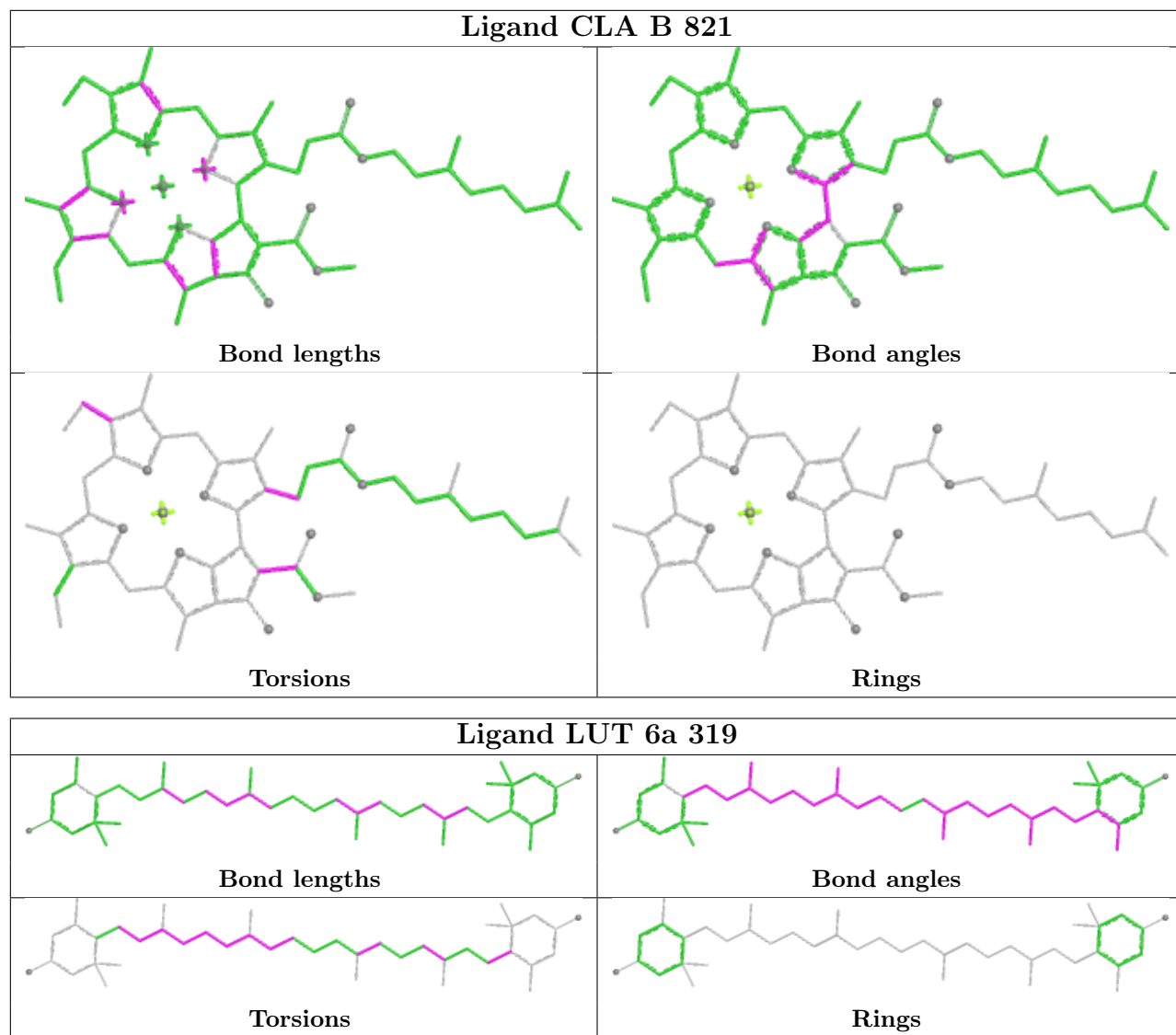


Ligand CHL 5a 301

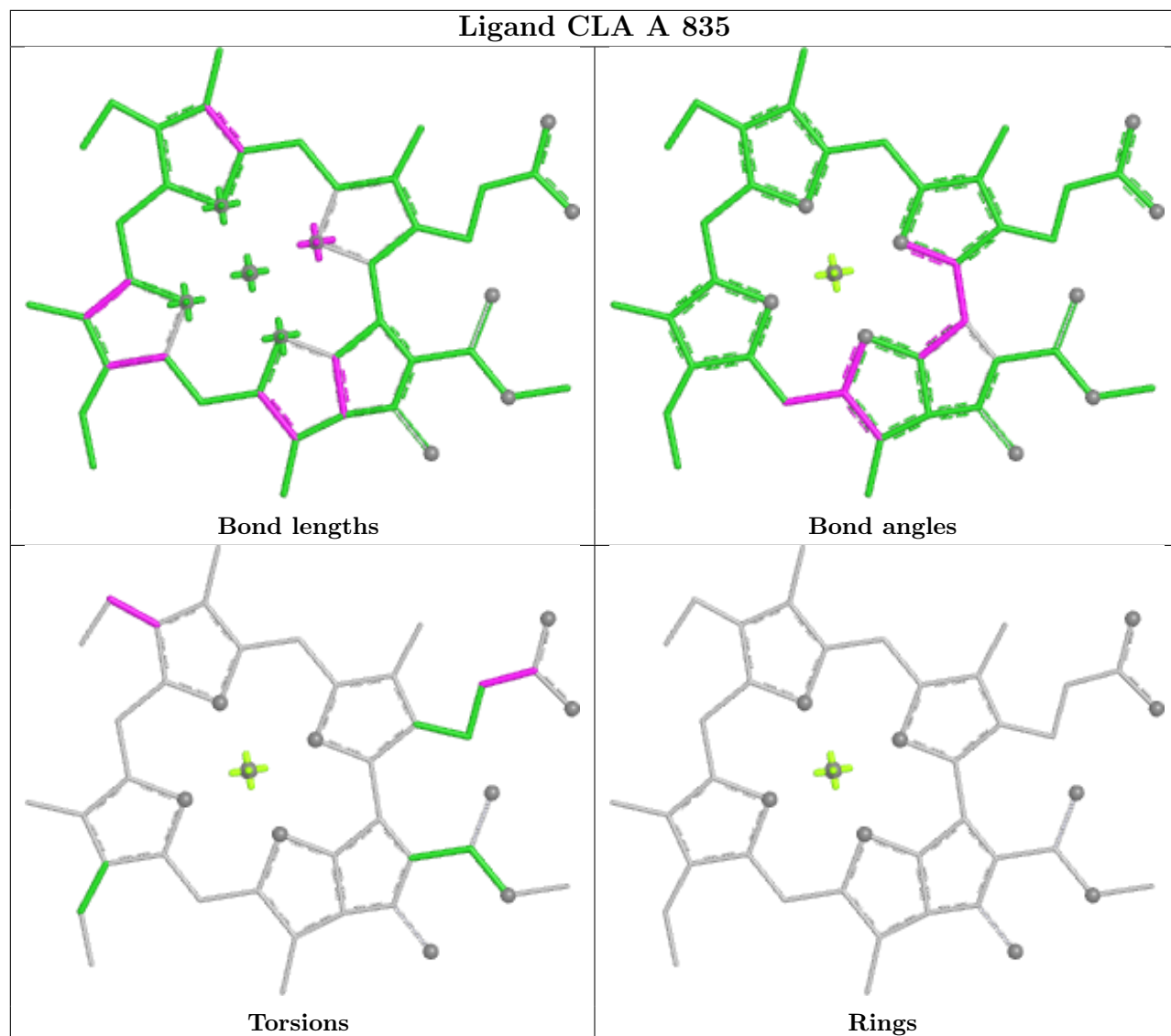


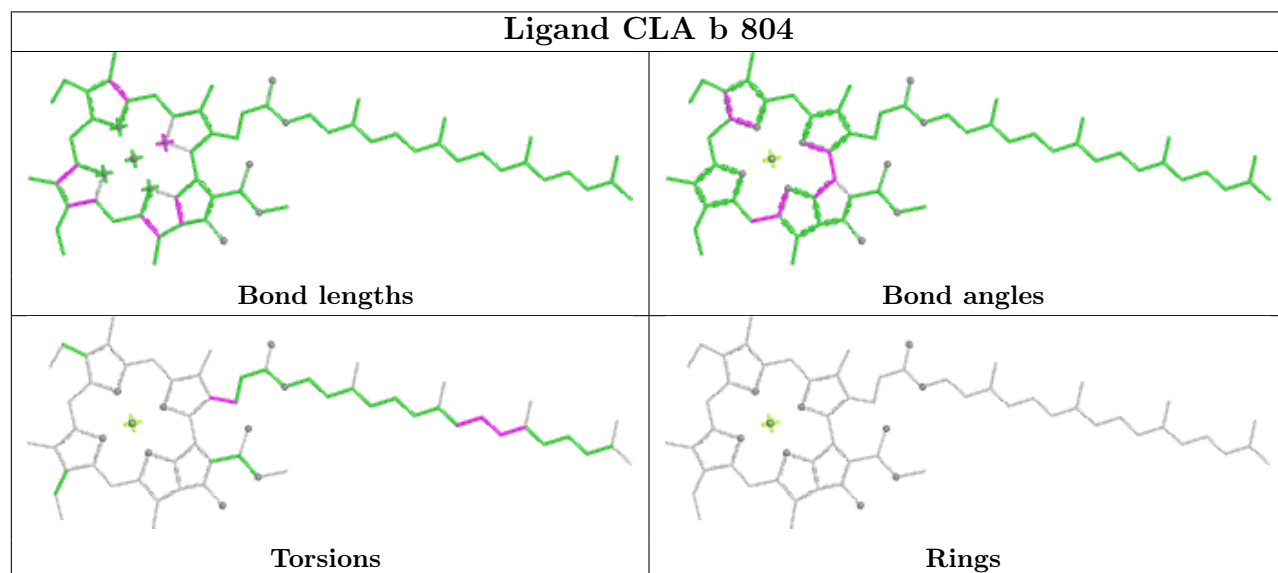
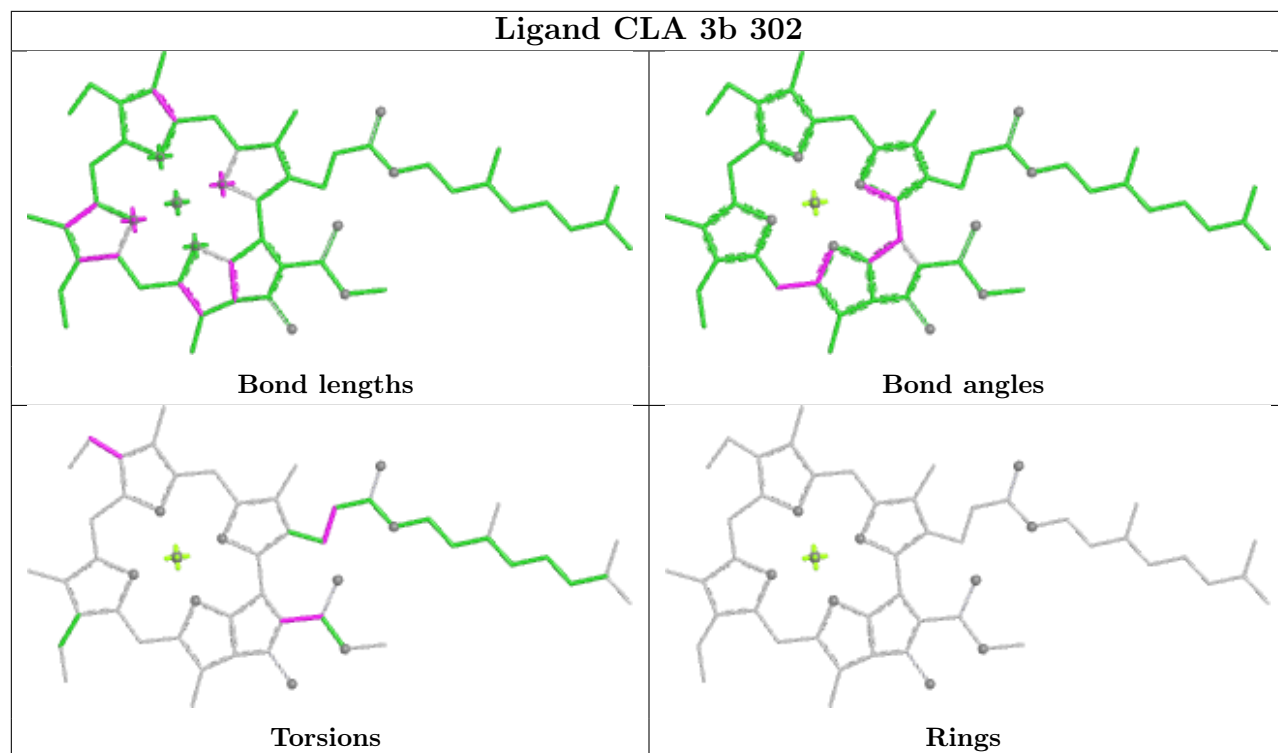


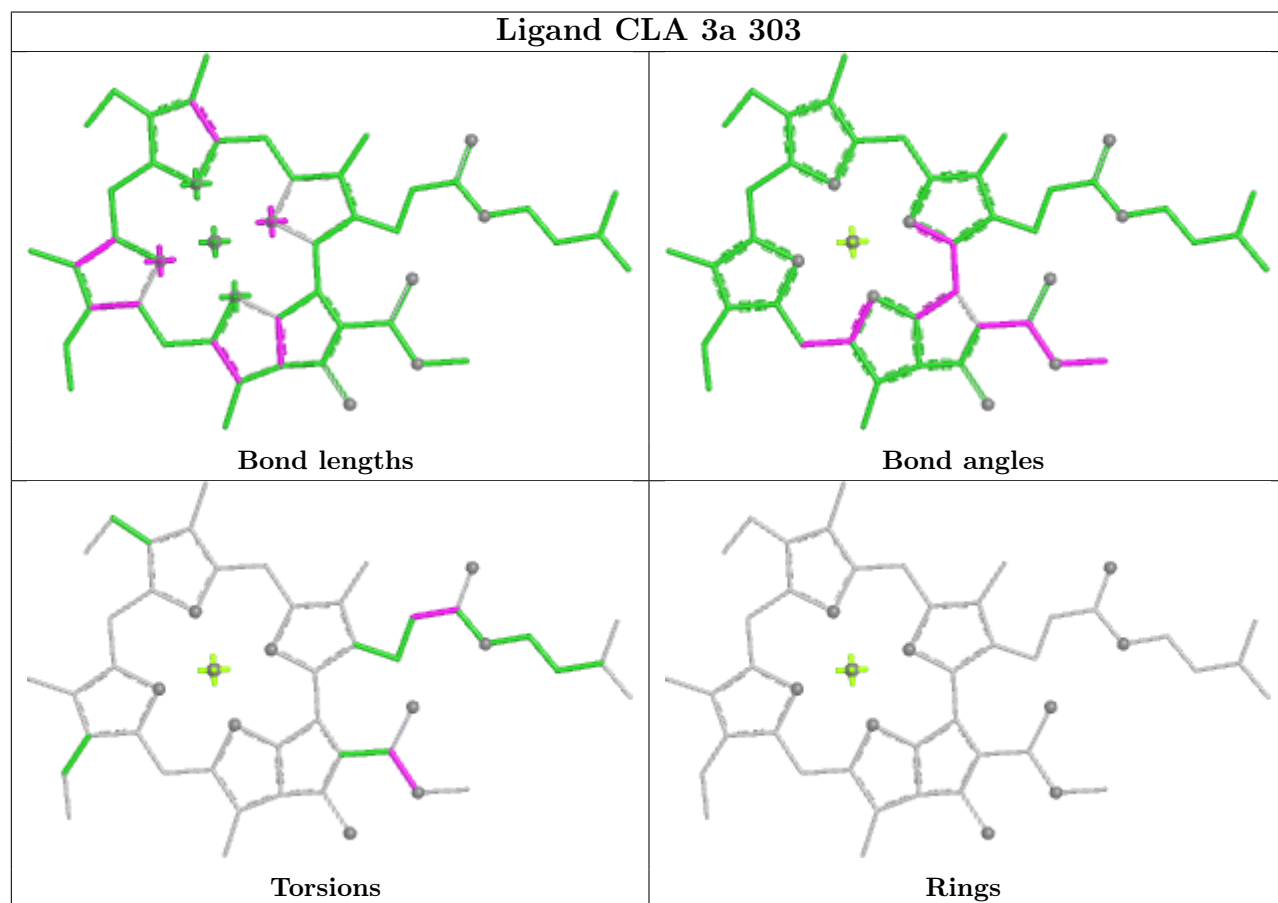
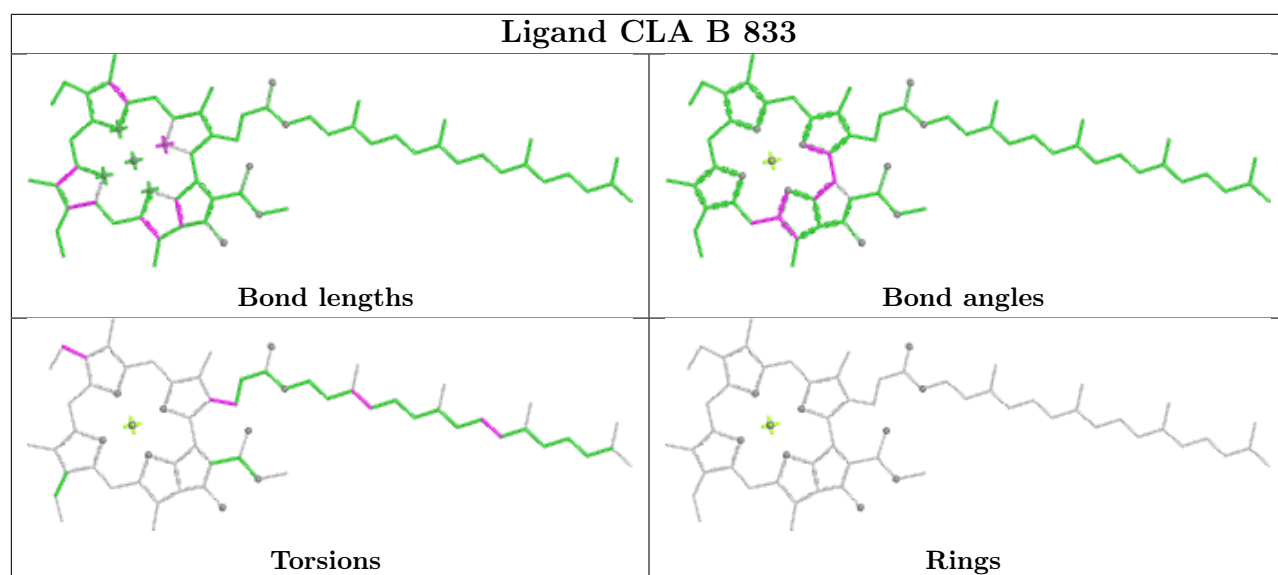




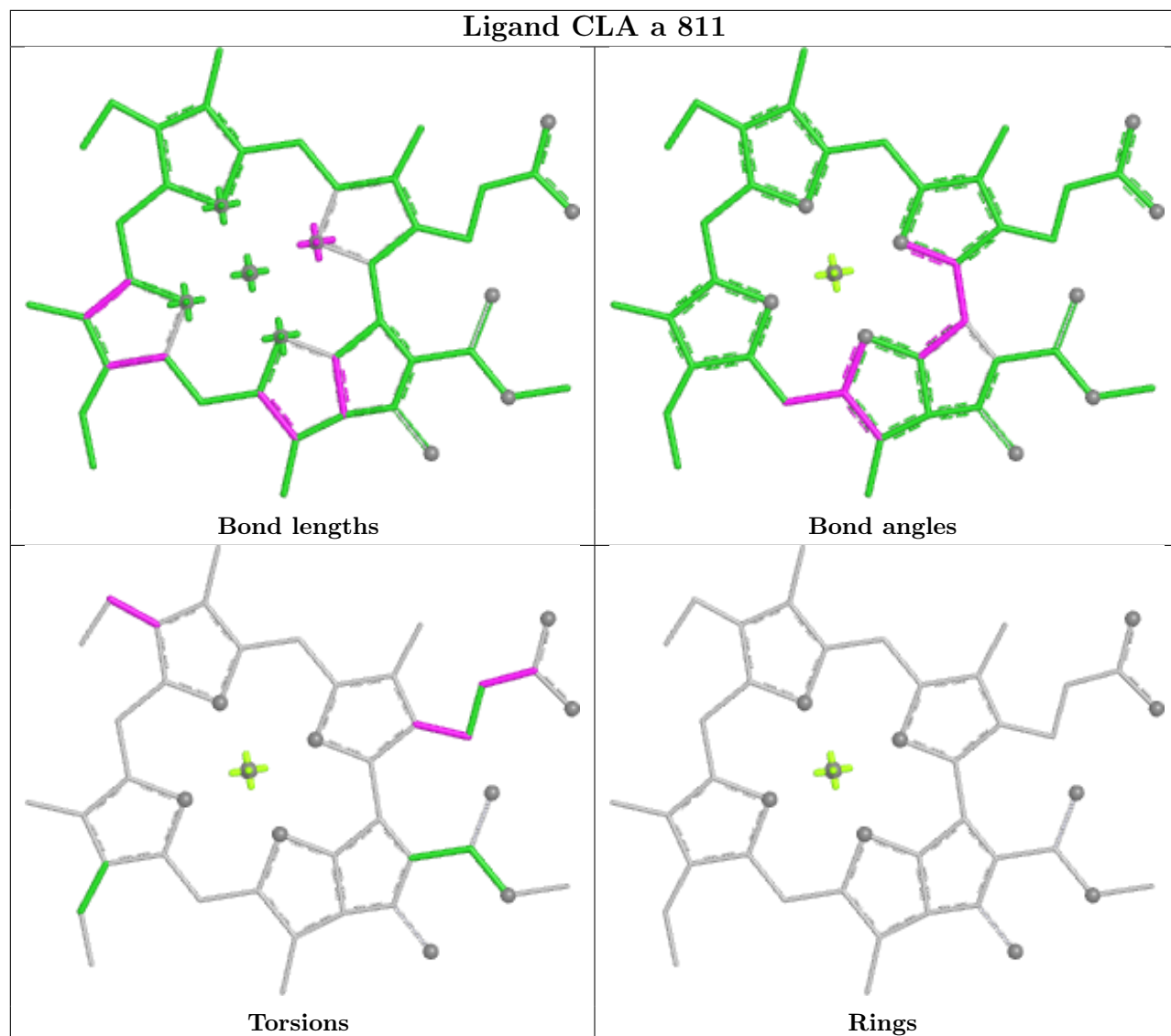
Ligand CLA A 835

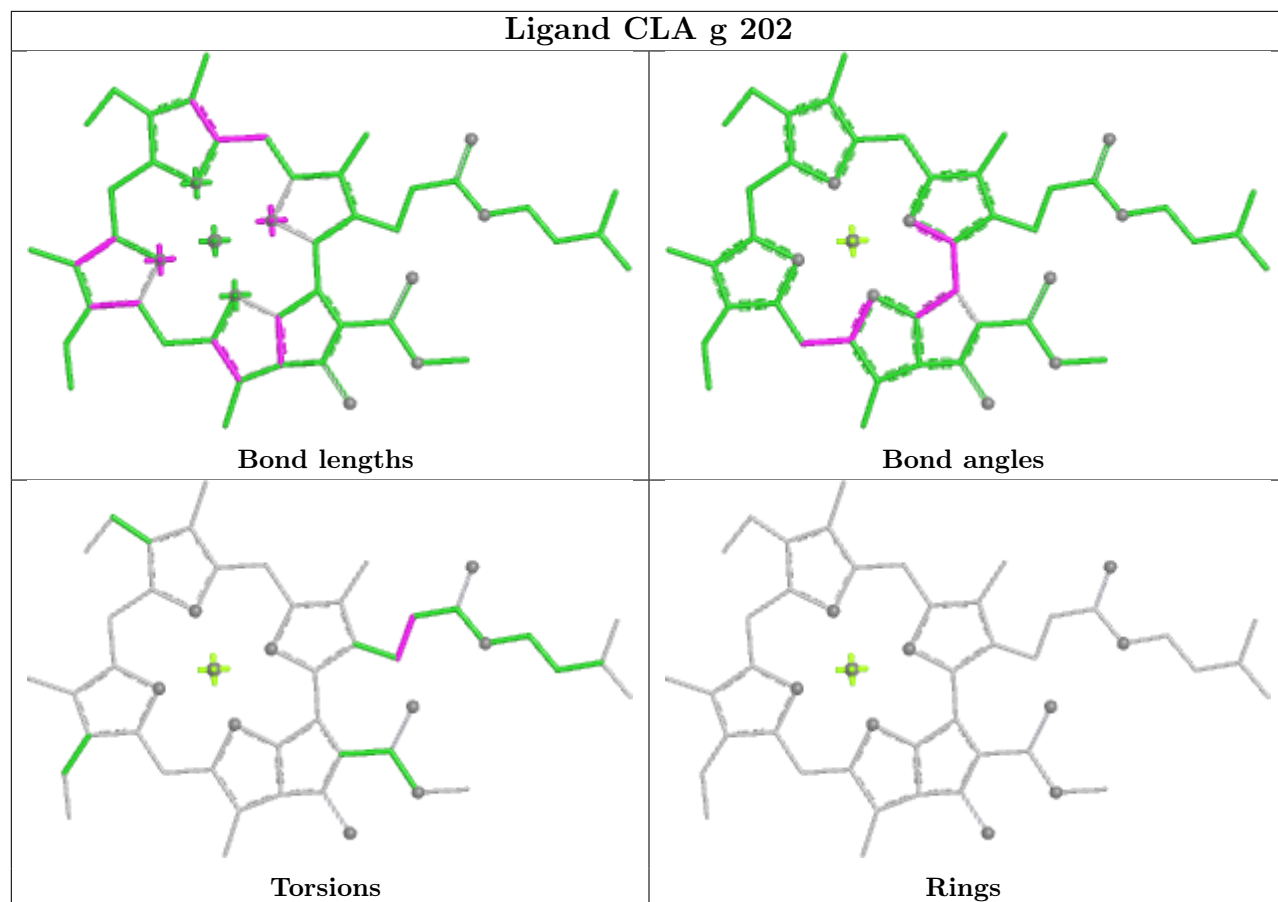


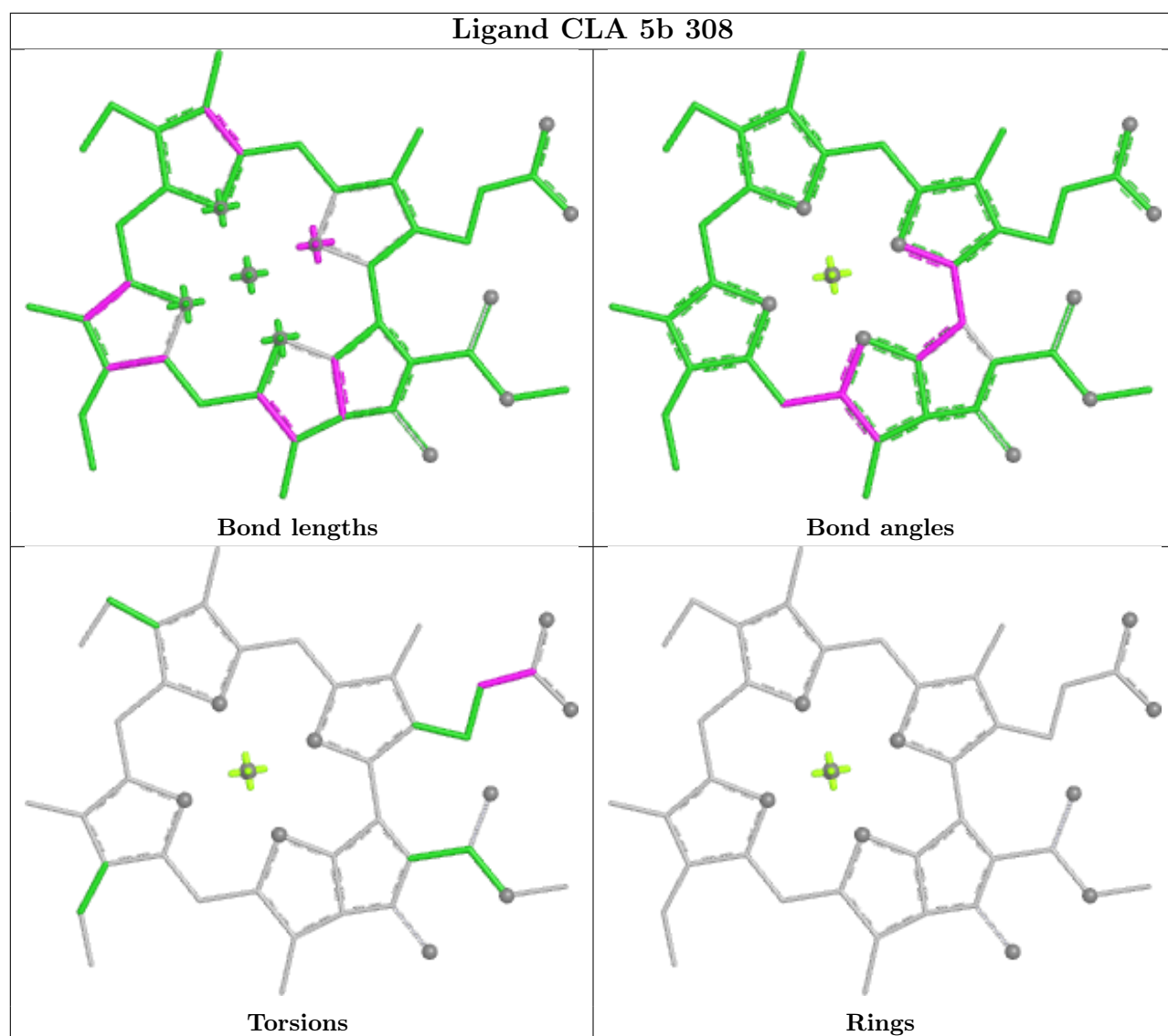




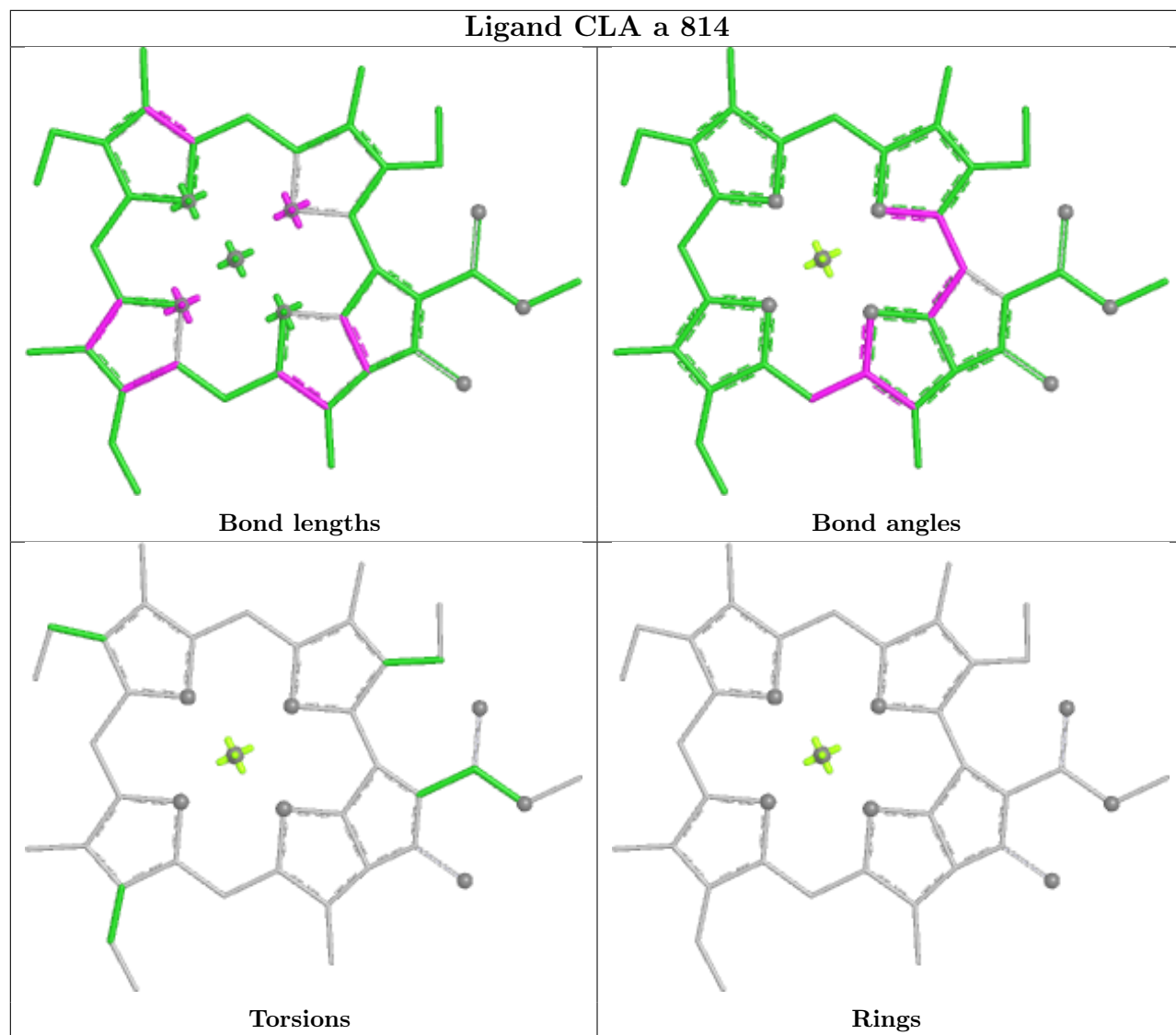
Ligand CLA a 811

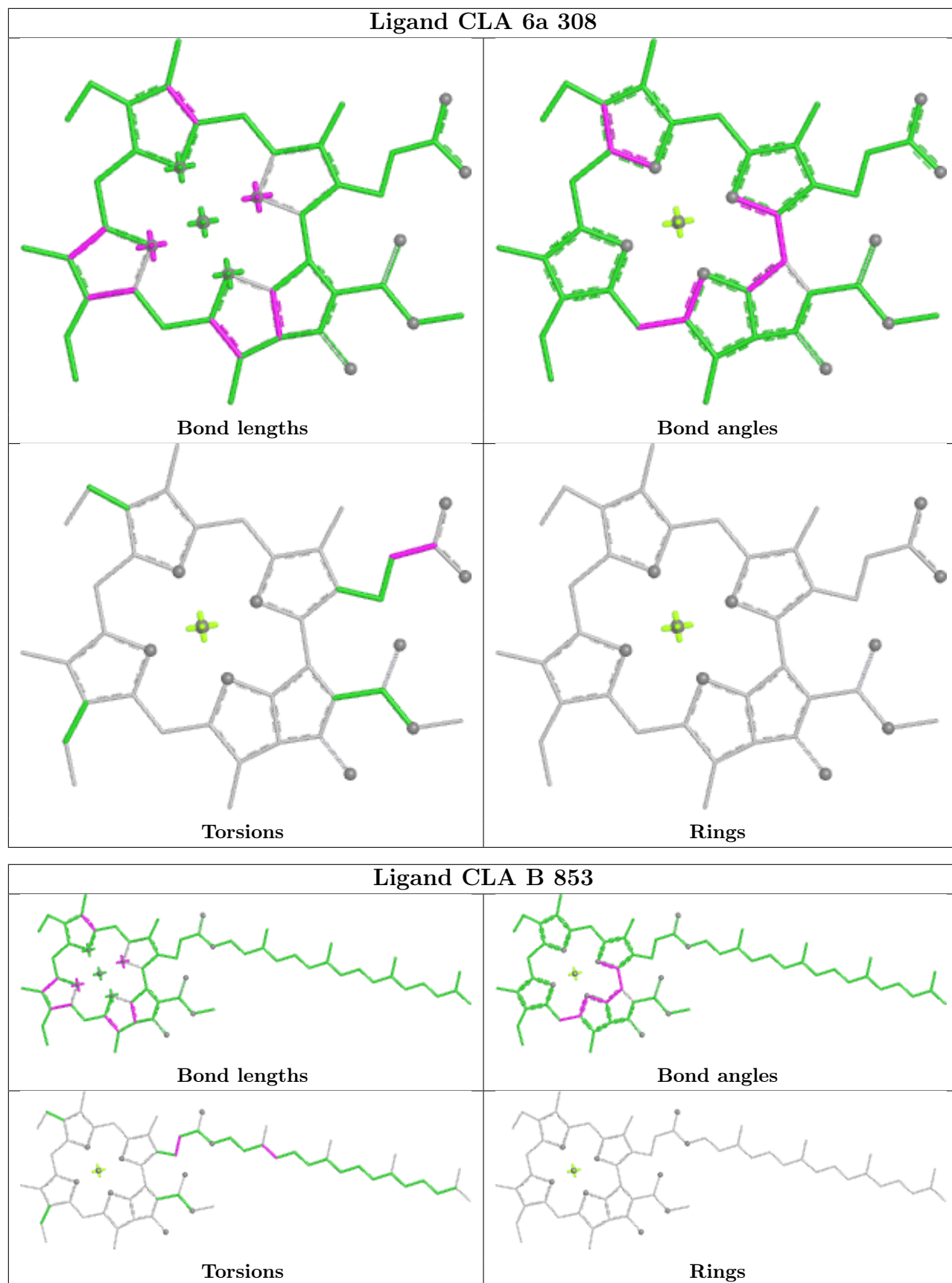




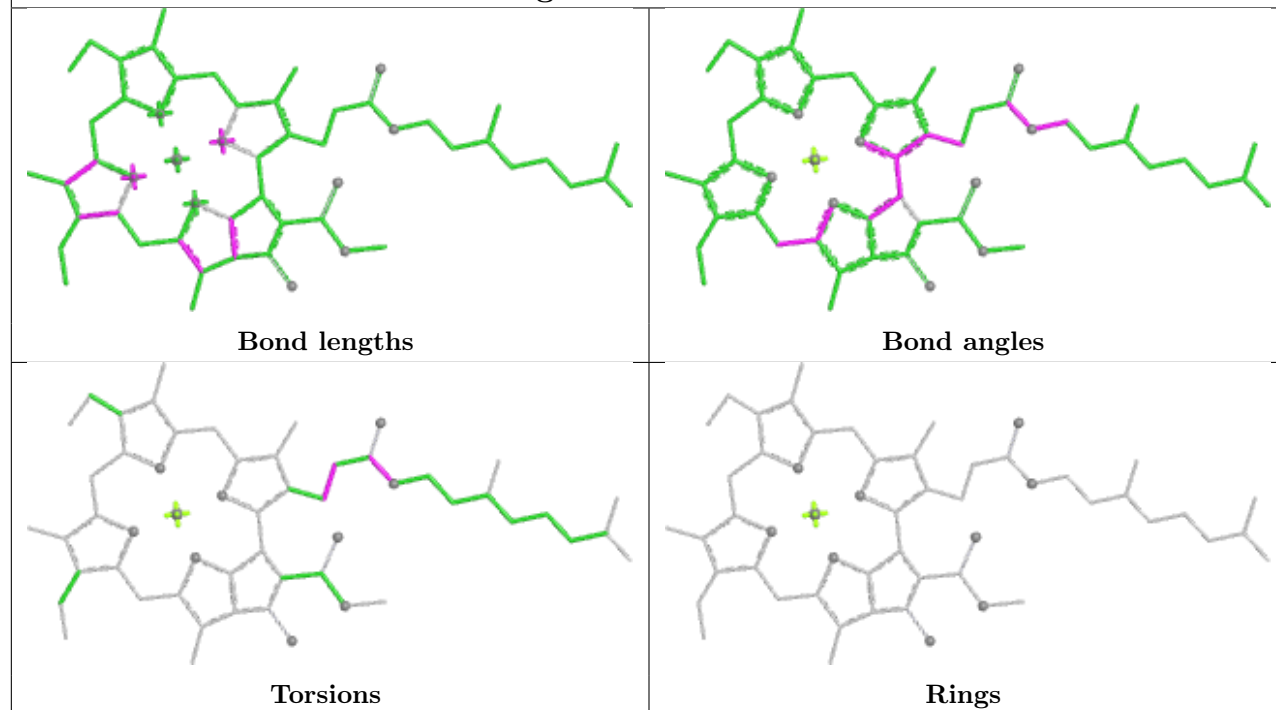


Ligand CLA a 814

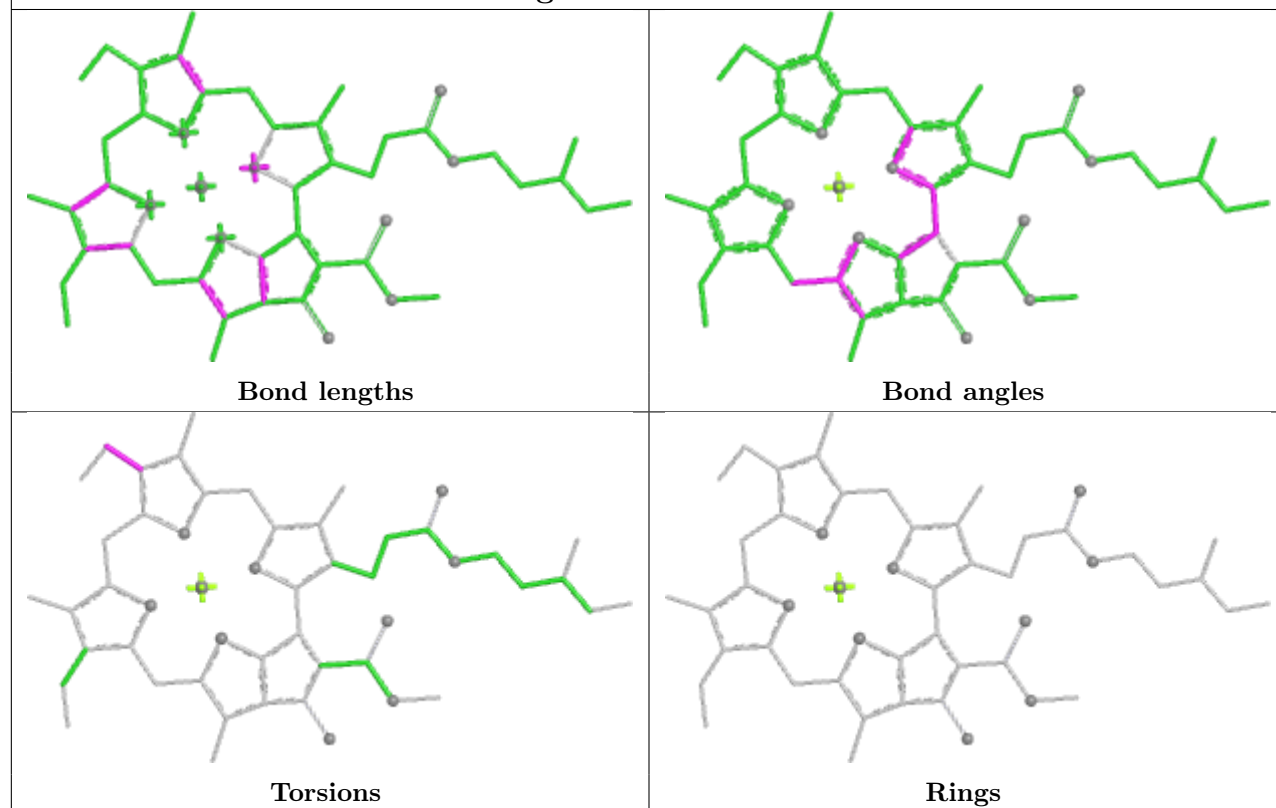


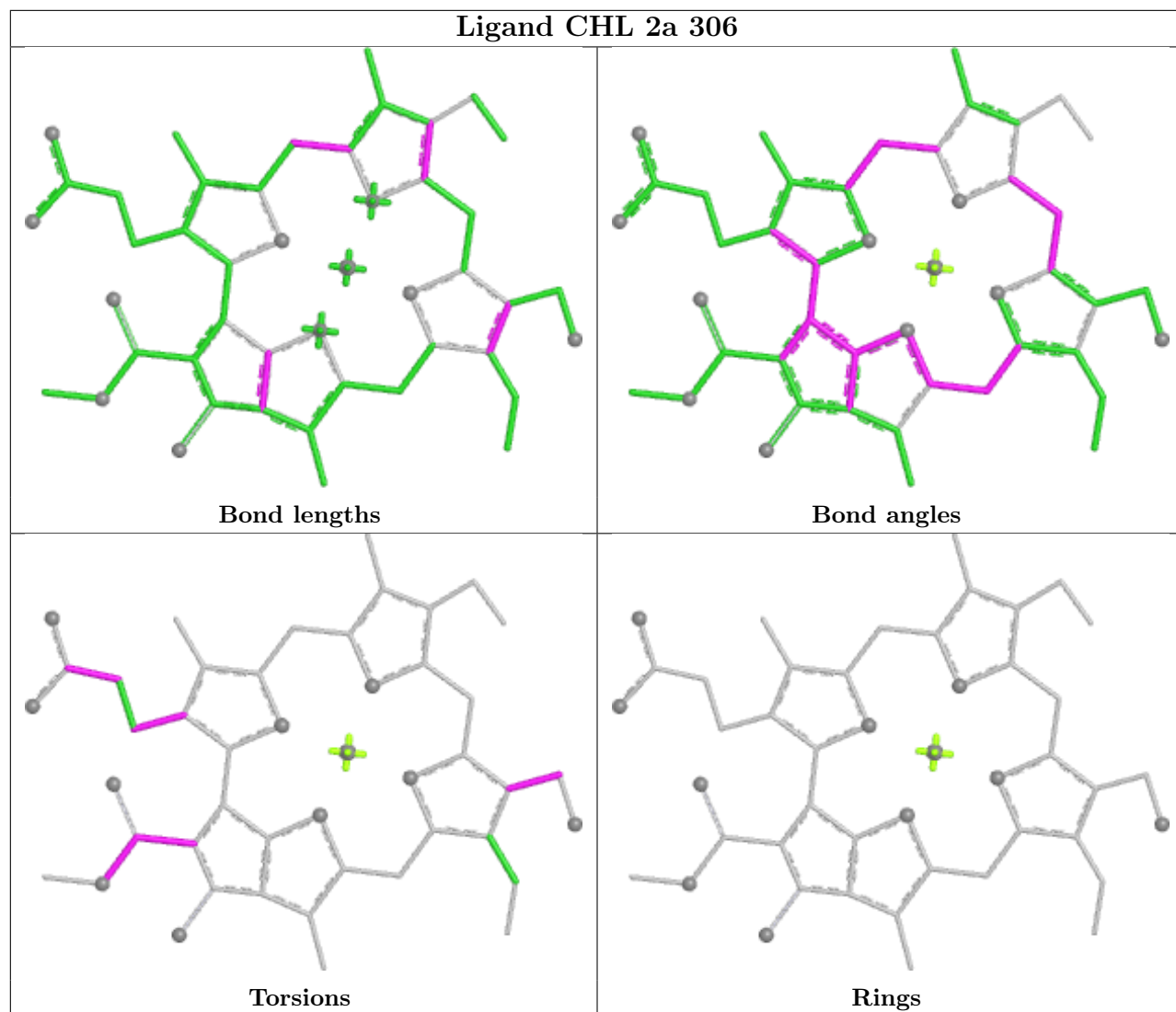


Ligand CLA a 809

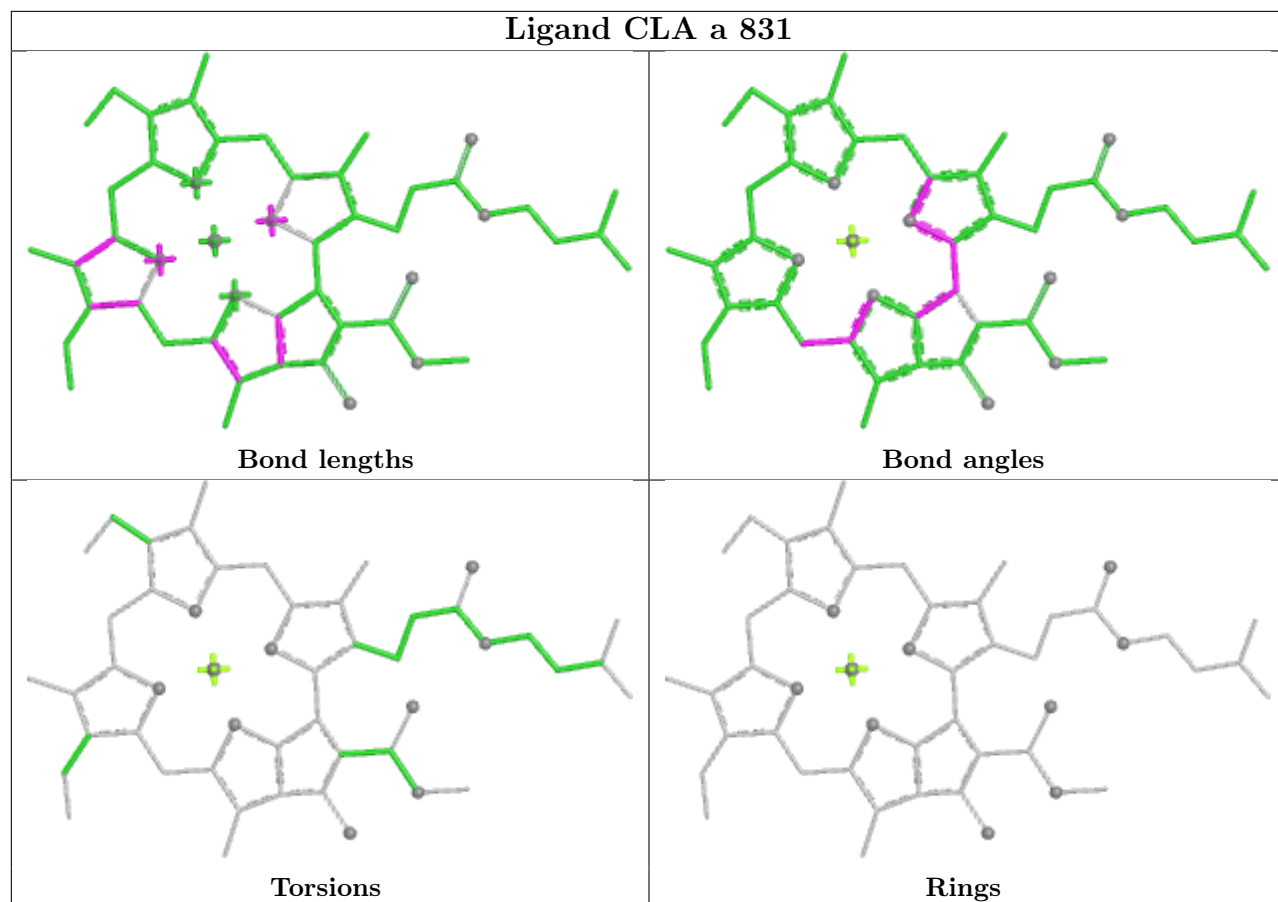


Ligand CLA a 853

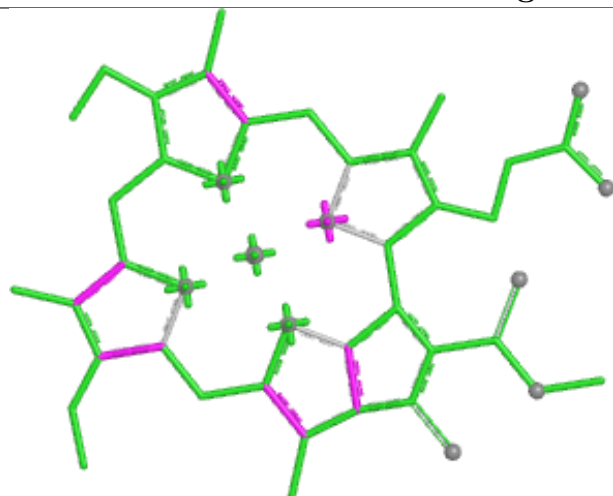




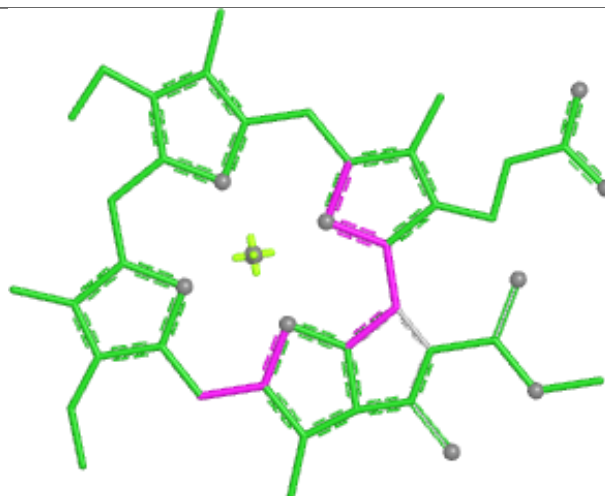
Ligand CLA a 831



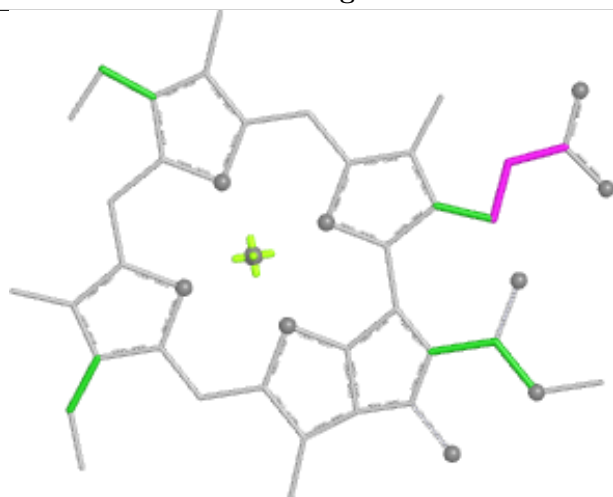
Ligand CLA b 811



Bond lengths



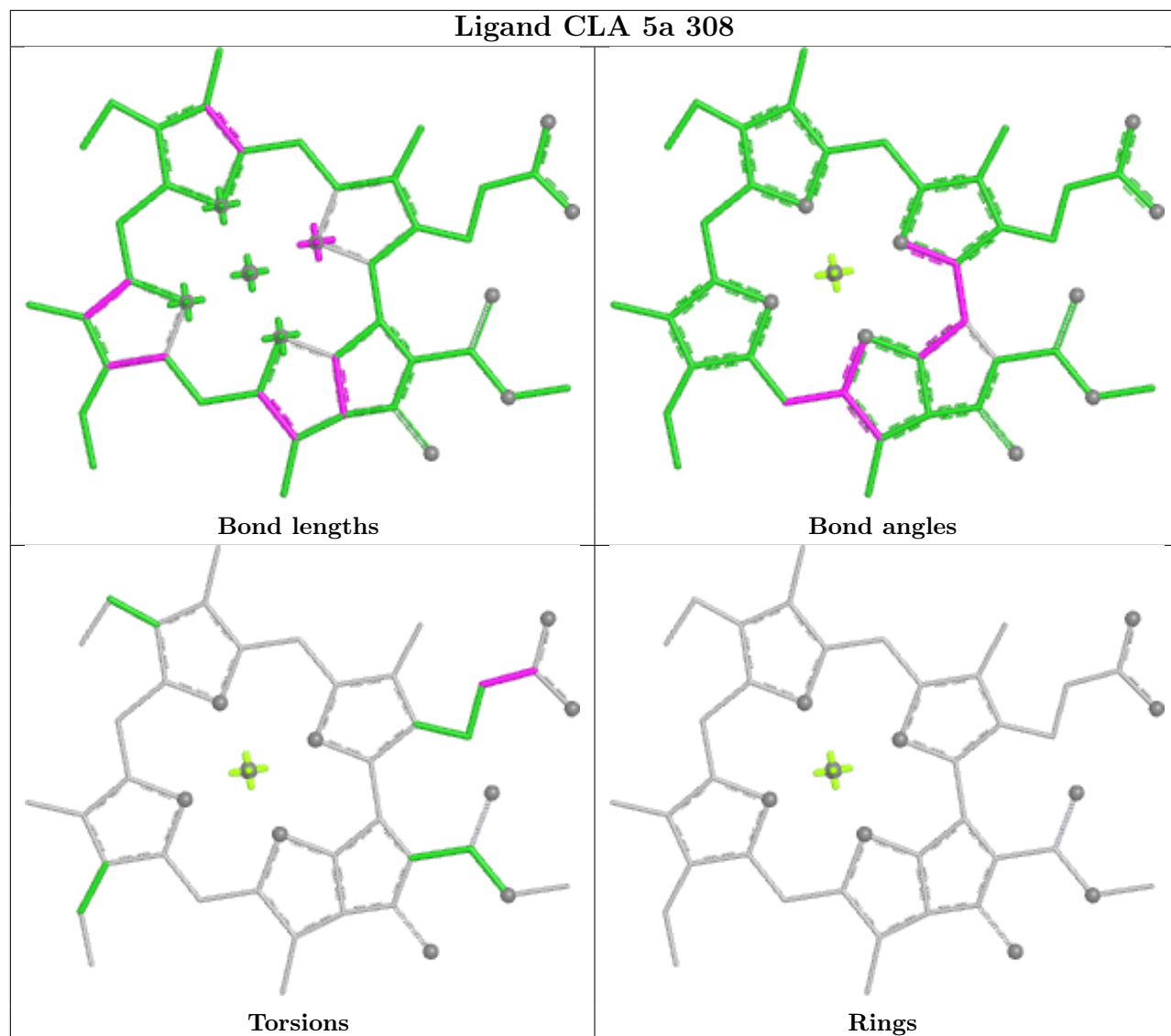
Bond angles



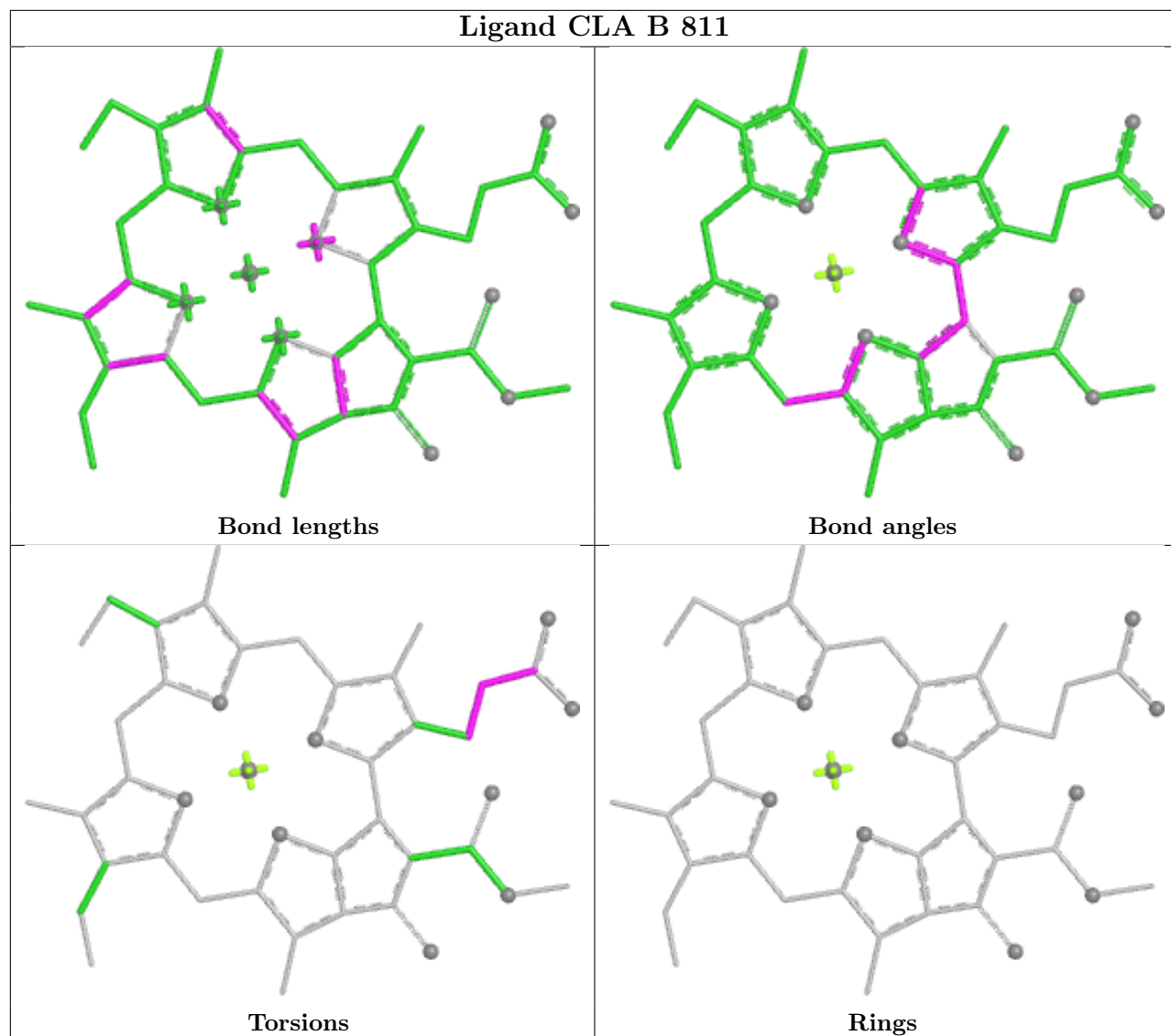
Torsions



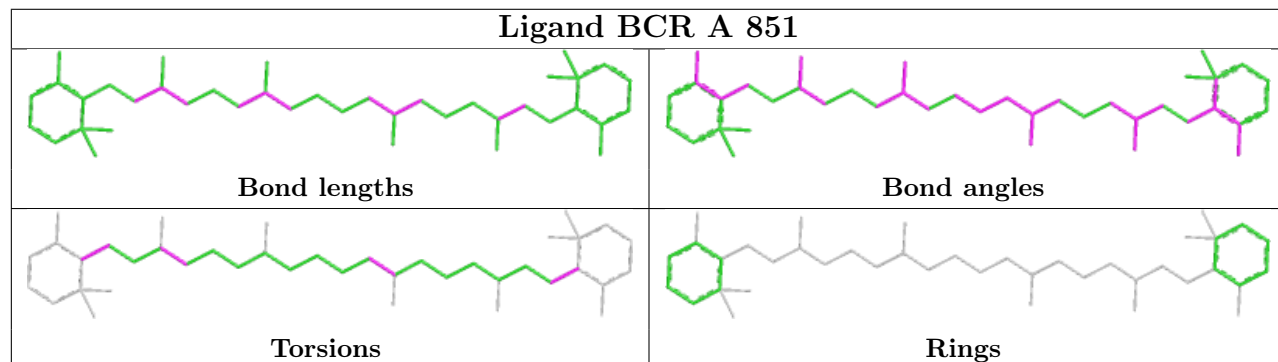
Rings



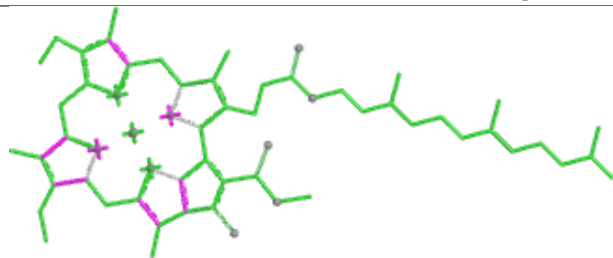
Ligand CLA B 811



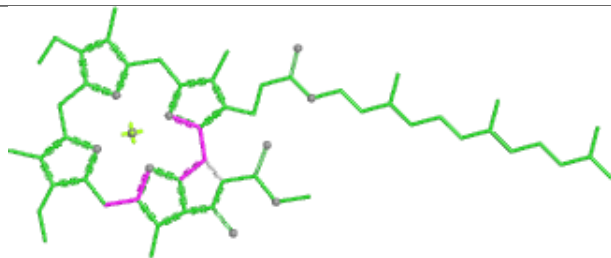
Ligand BCR A 851



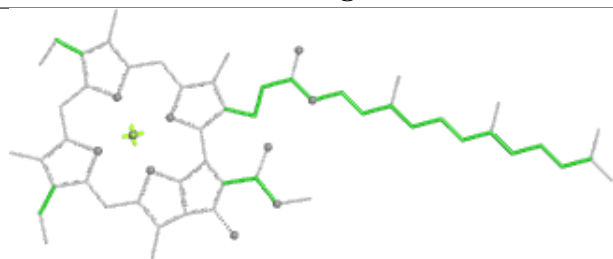
Ligand CLA L 302



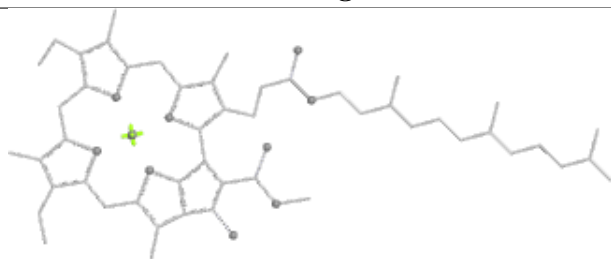
Bond lengths



Bond angles

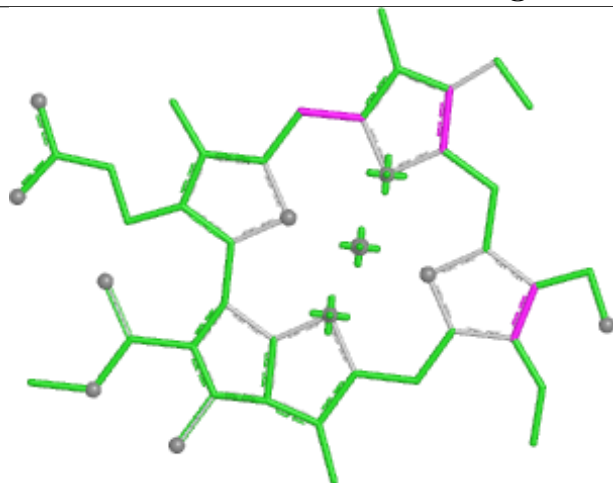


Torsions

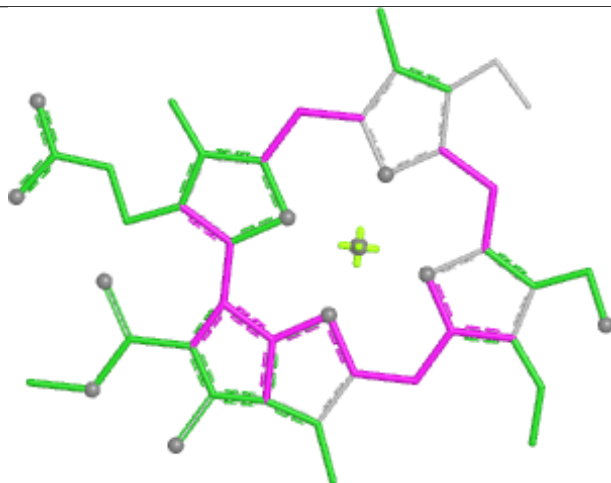


Rings

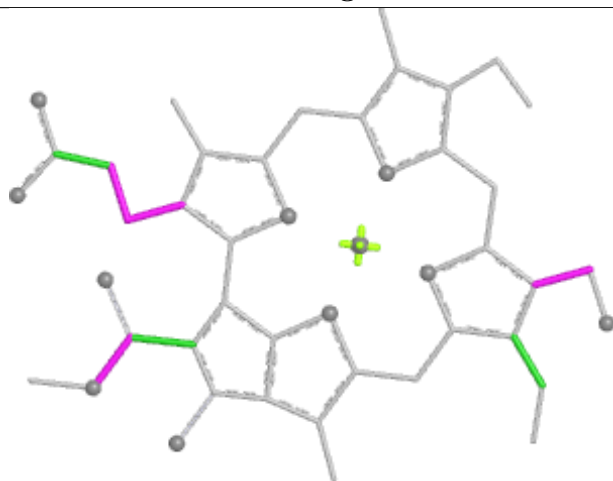
Ligand CHL 5a 307



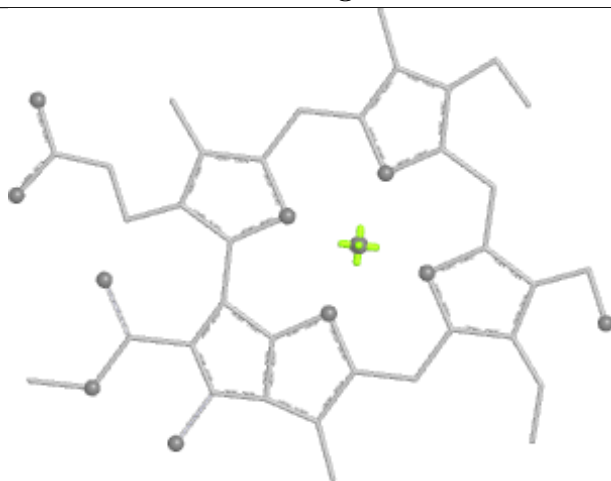
Bond lengths



Bond angles

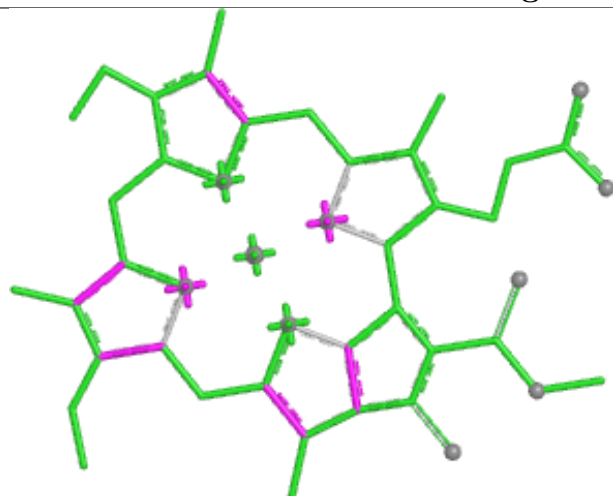


Torsions

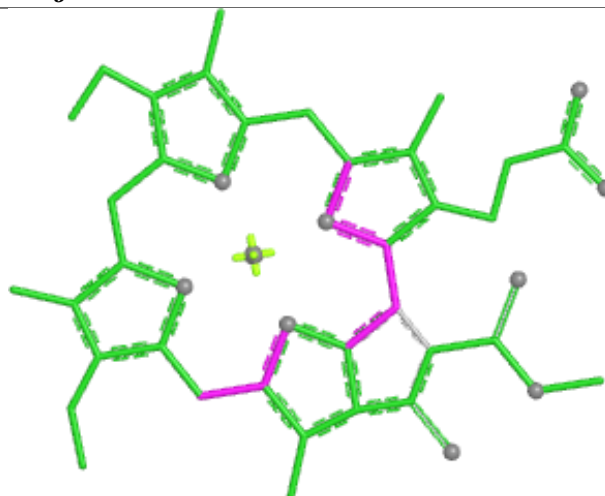


Rings

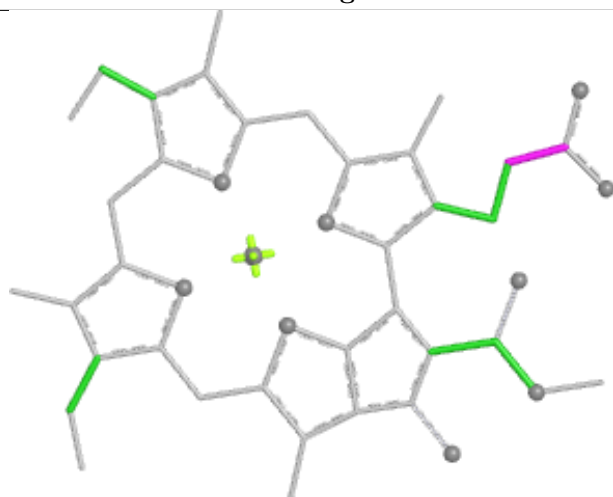
Ligand CLA j 101



Bond lengths



Bond angles

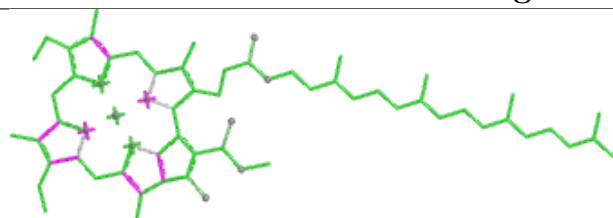


Torsions

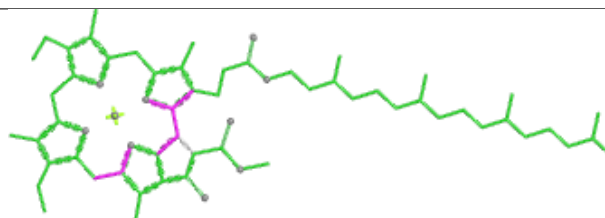


Rings

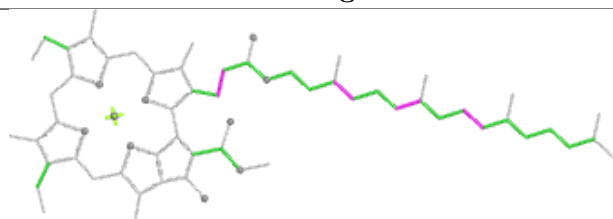
Ligand CLA A 827



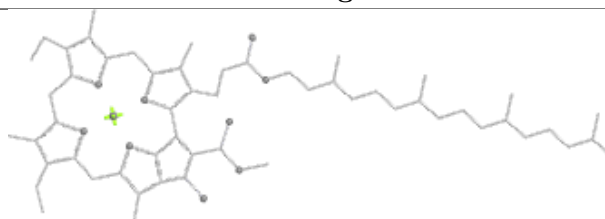
Bond lengths



Bond angles

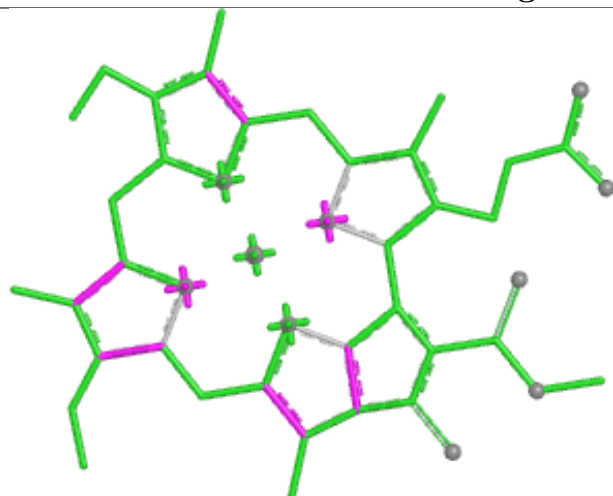


Torsions

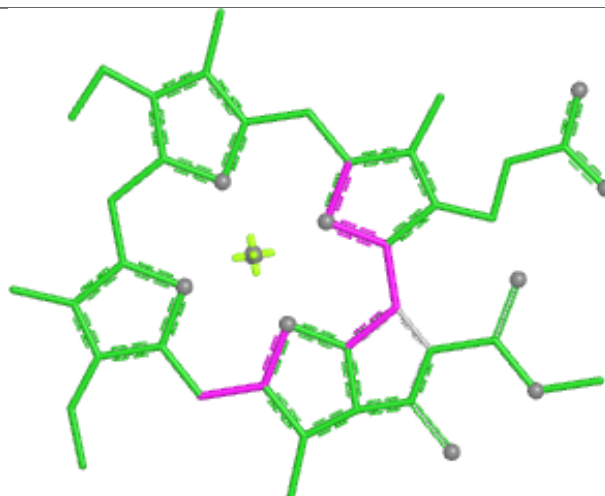


Rings

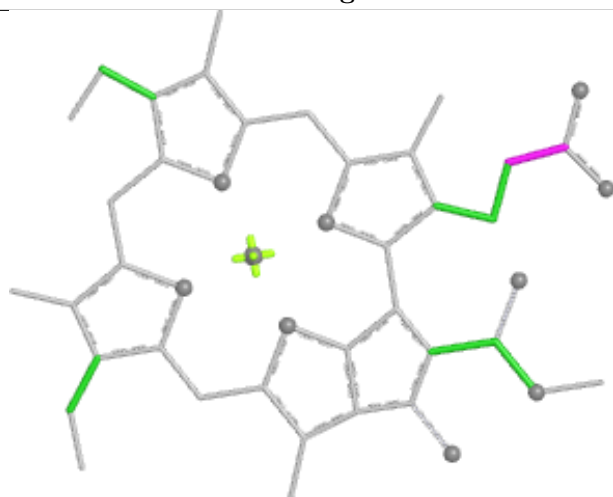
Ligand CLA J 101



Bond lengths



Bond angles

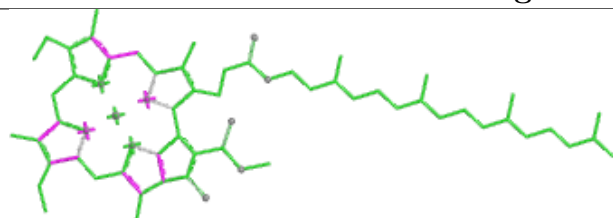


Torsions

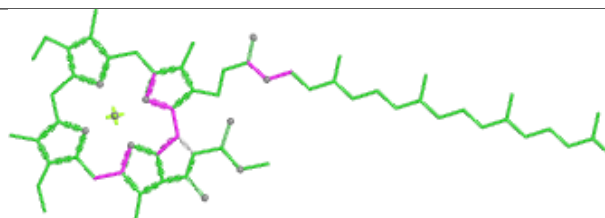


Rings

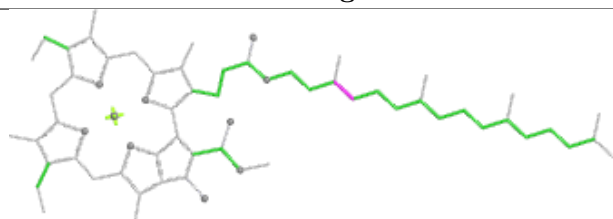
Ligand CLA B 839



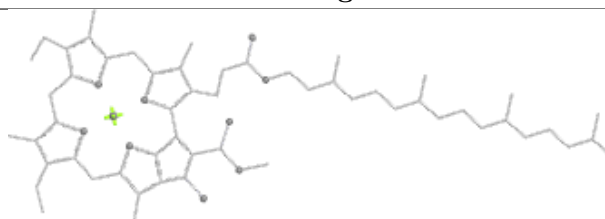
Bond lengths



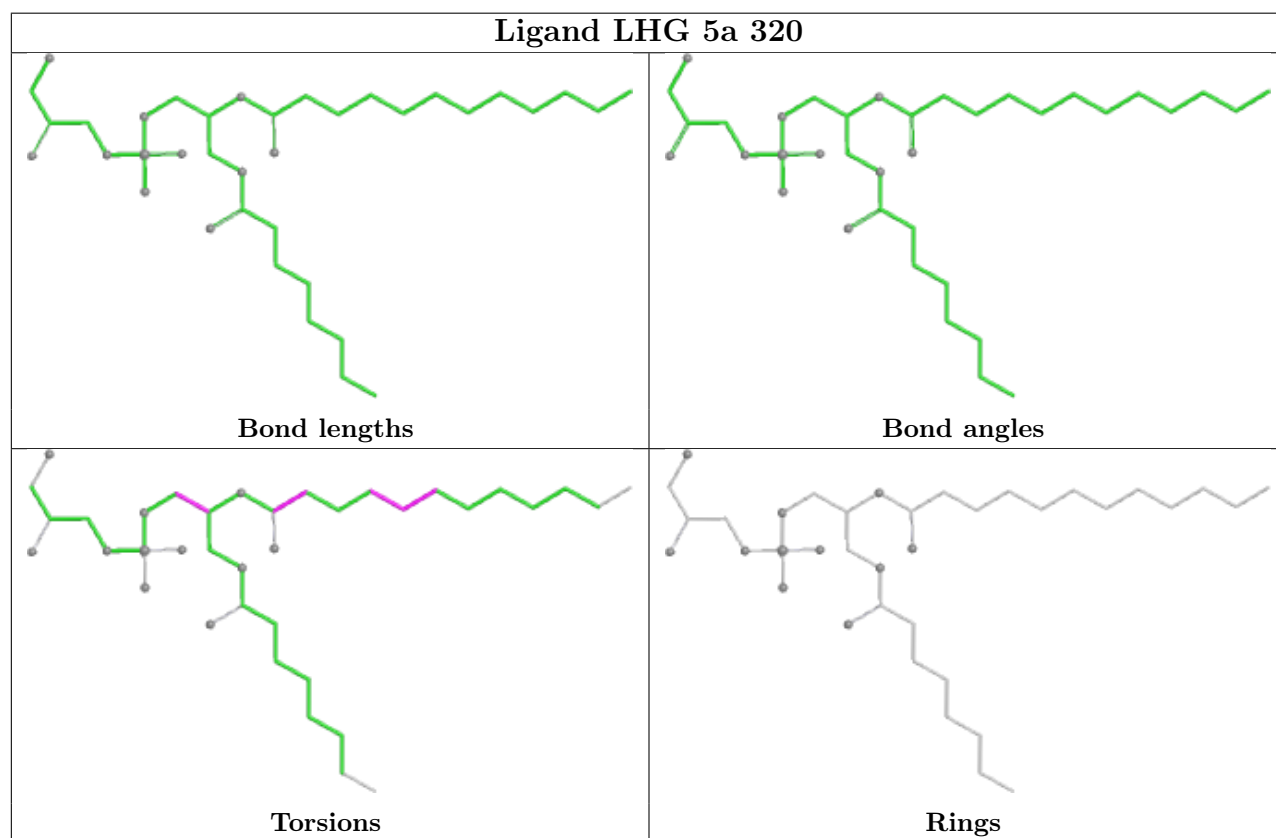
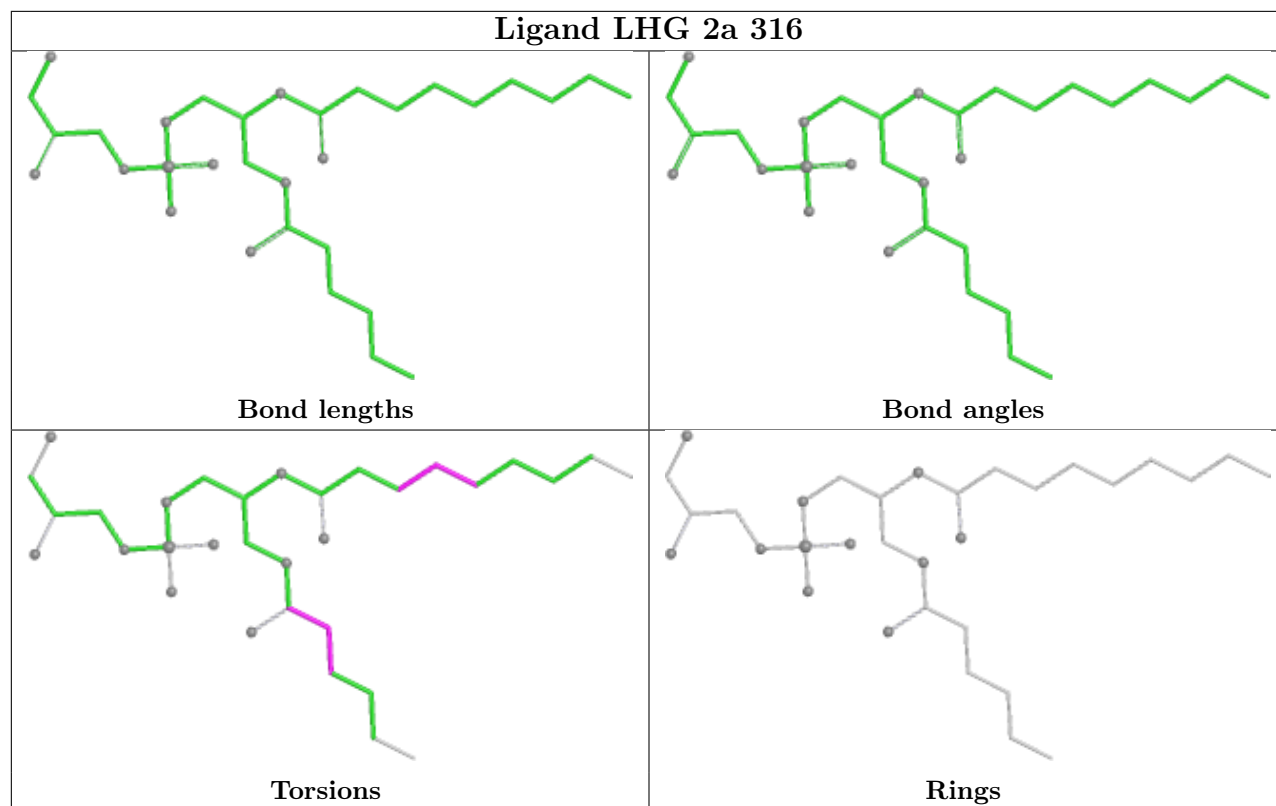
Bond angles



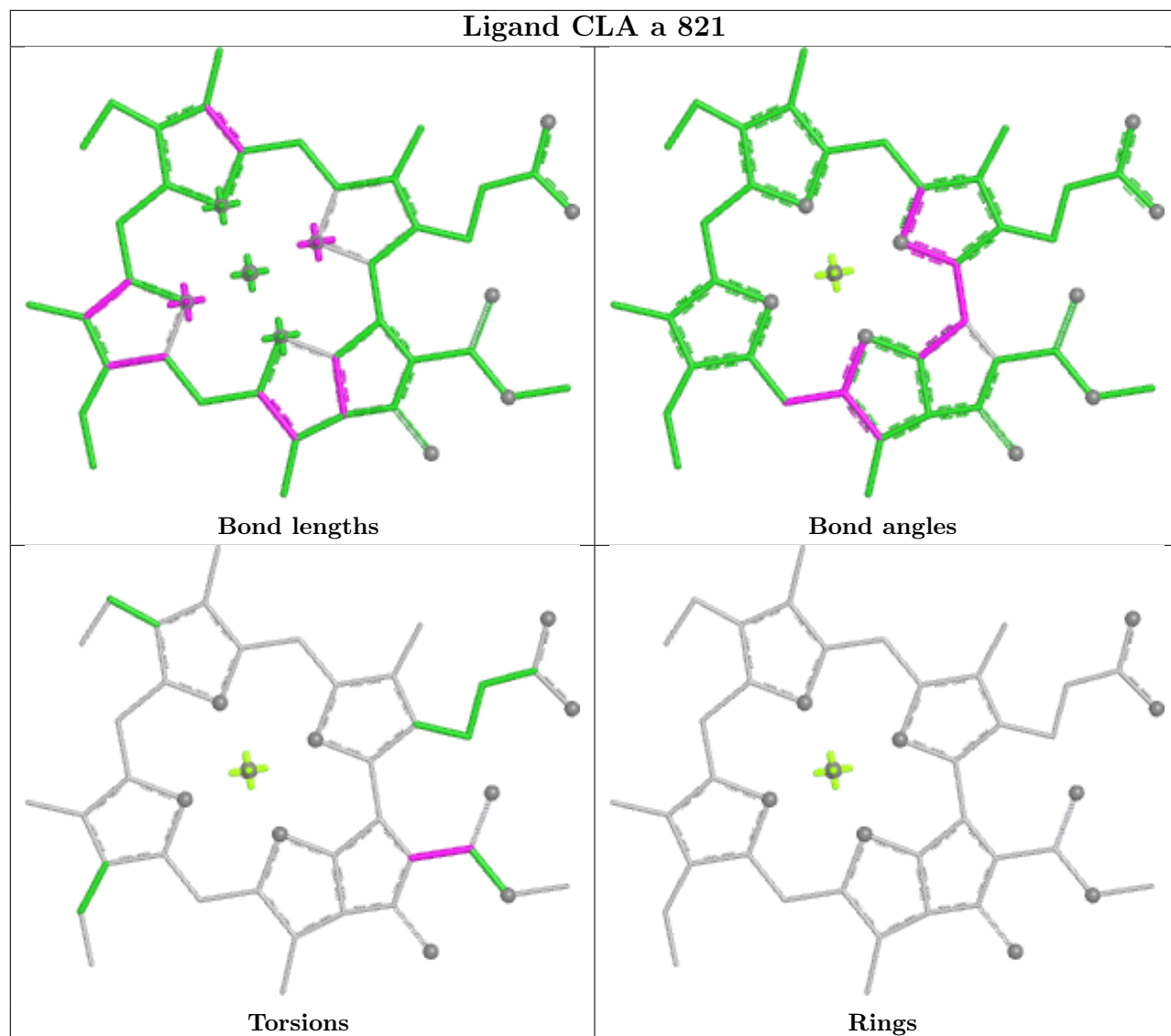
Torsions



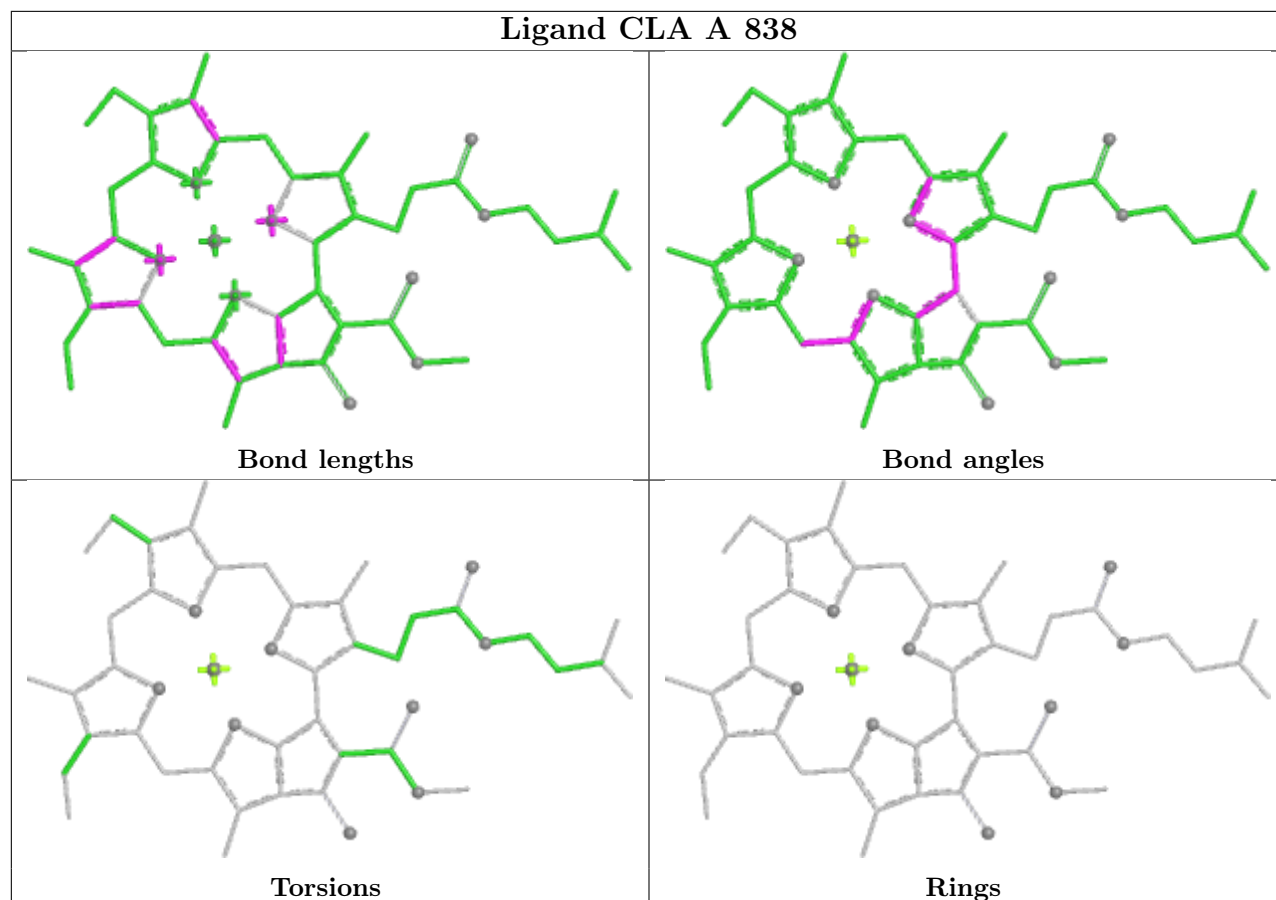
Rings



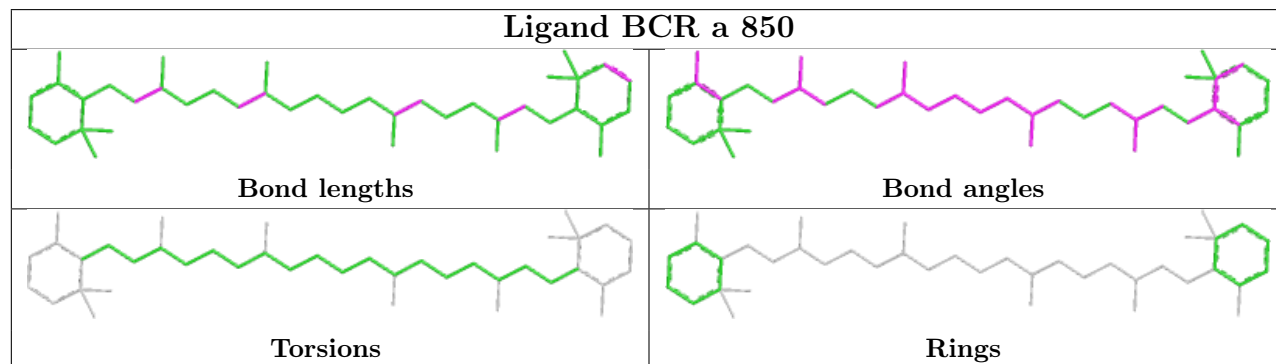
Ligand CLA a 821



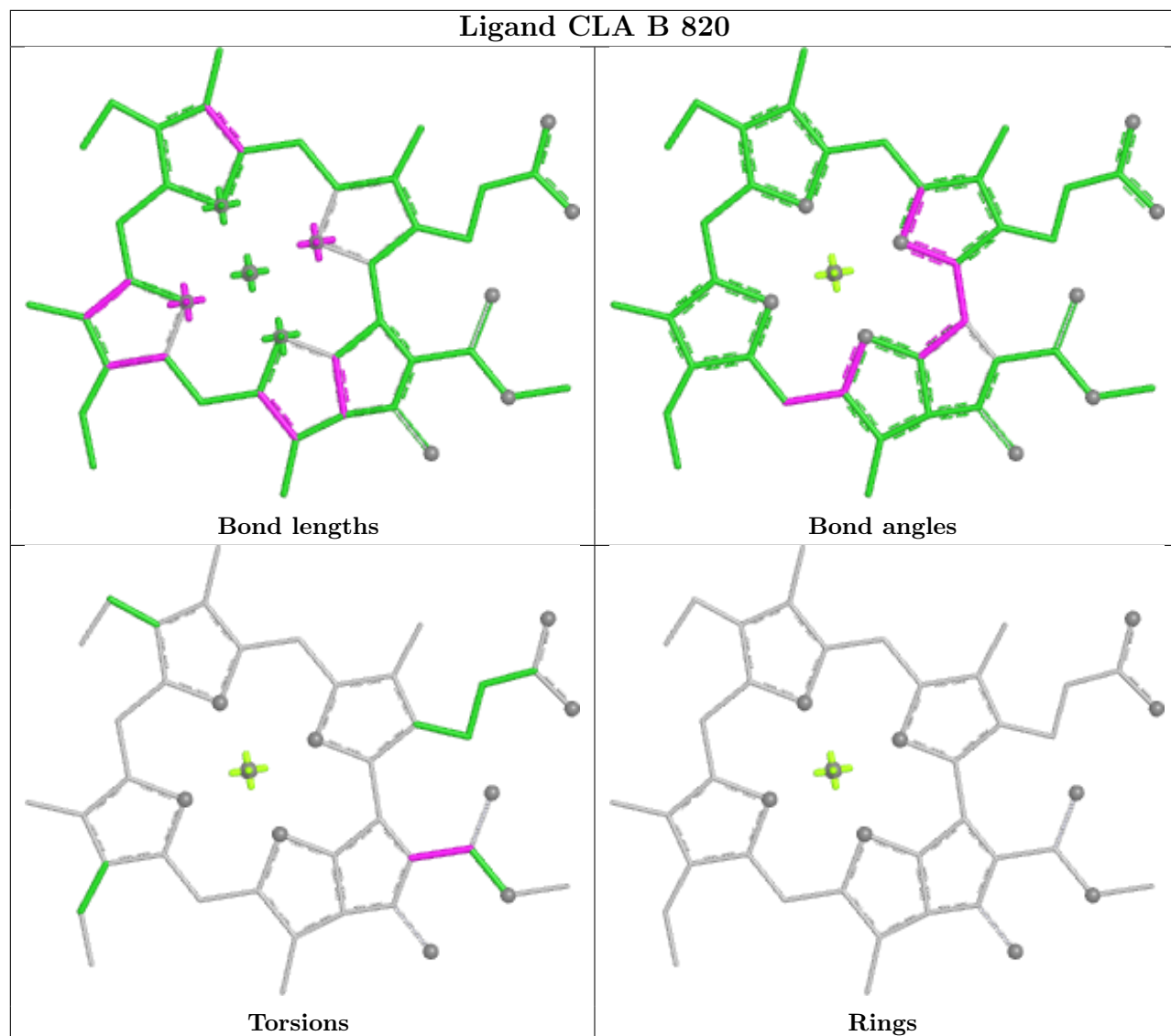
Ligand CLA A 838



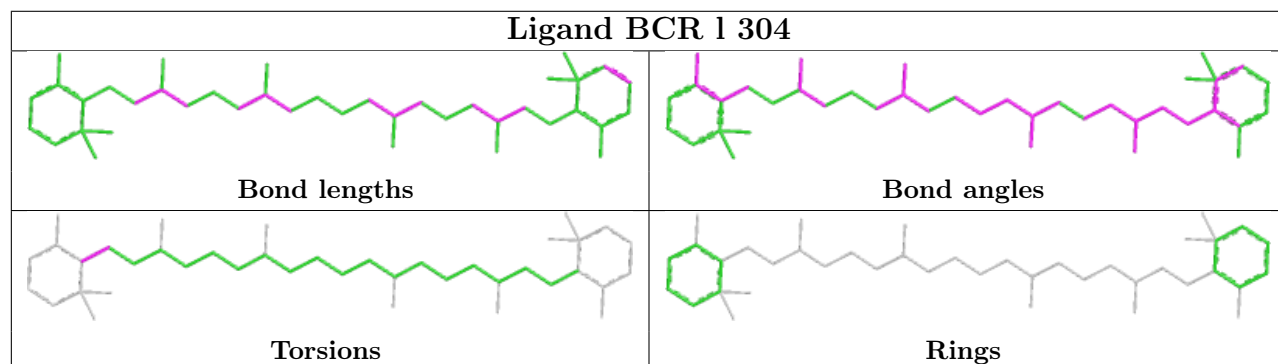
Ligand BCR a 850

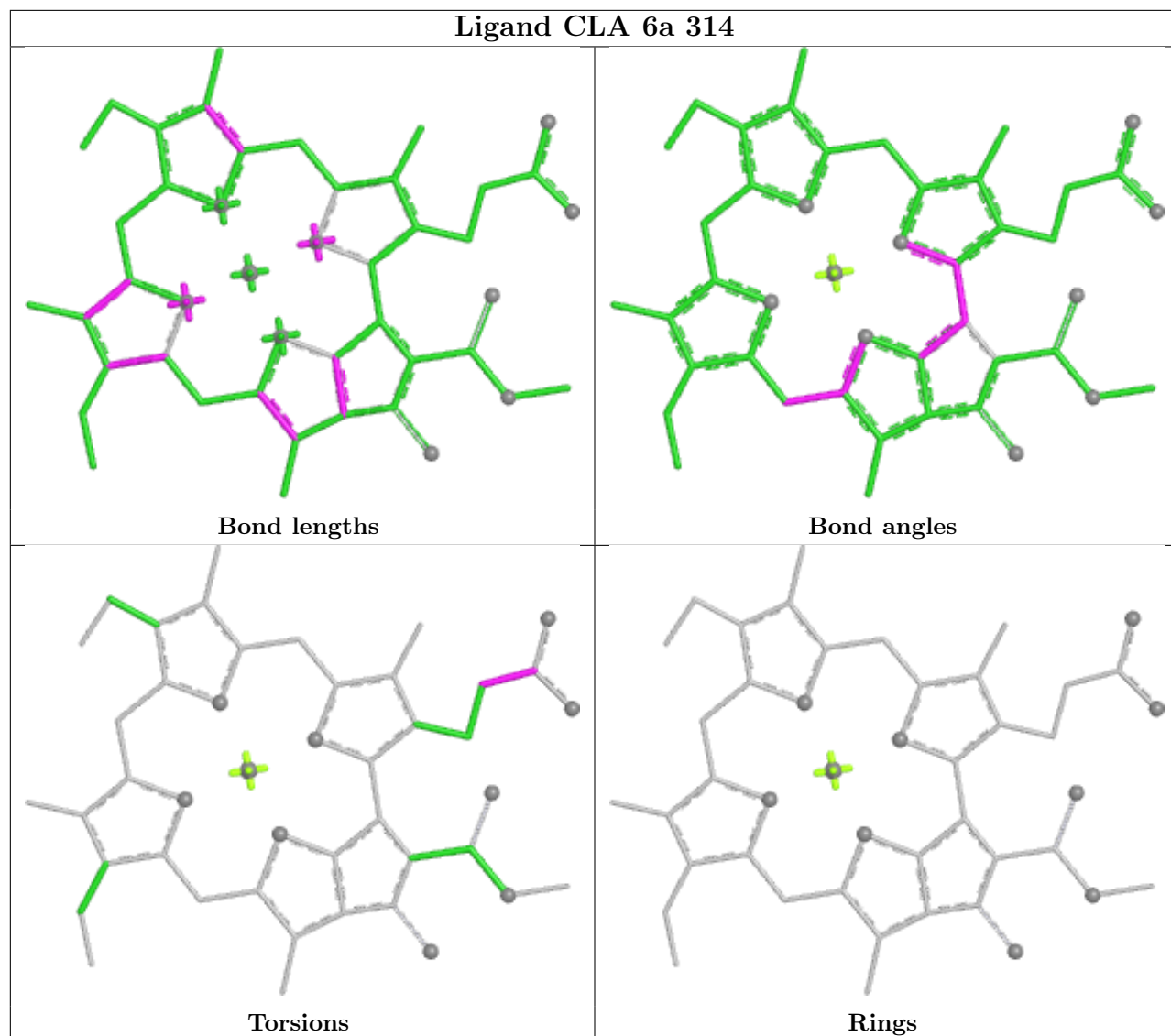


Ligand CLA B 820

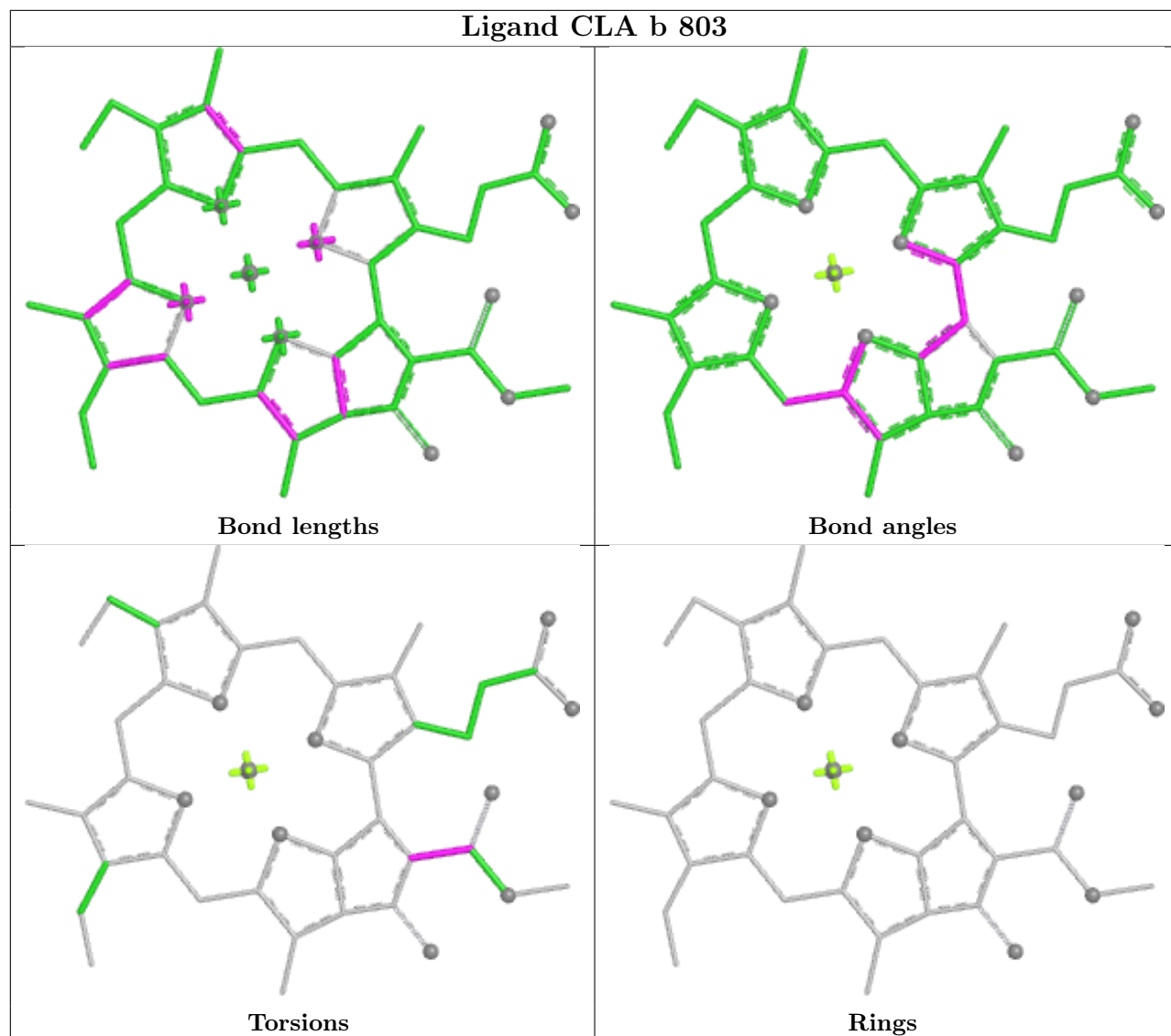


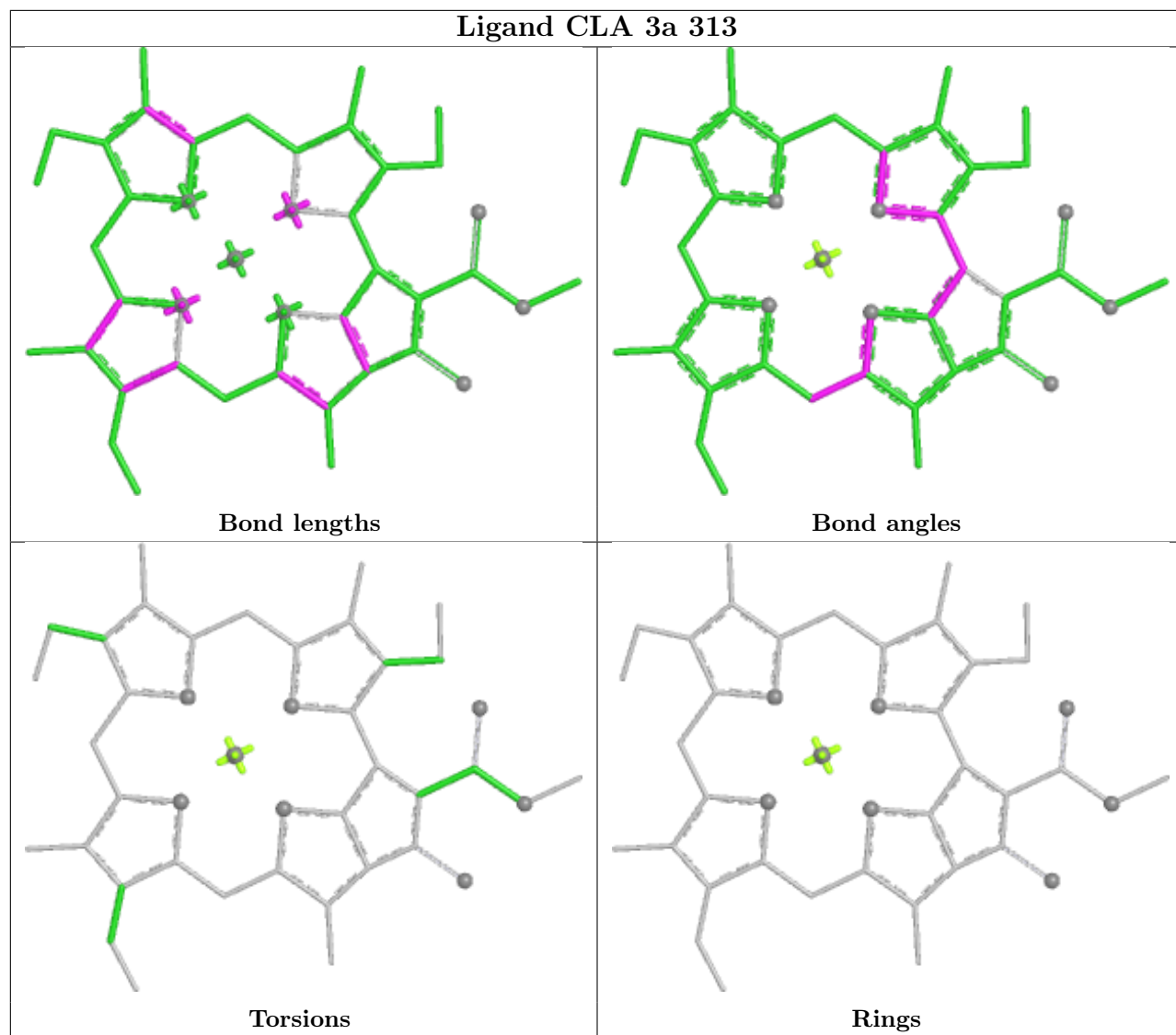
Ligand BCR 1 304



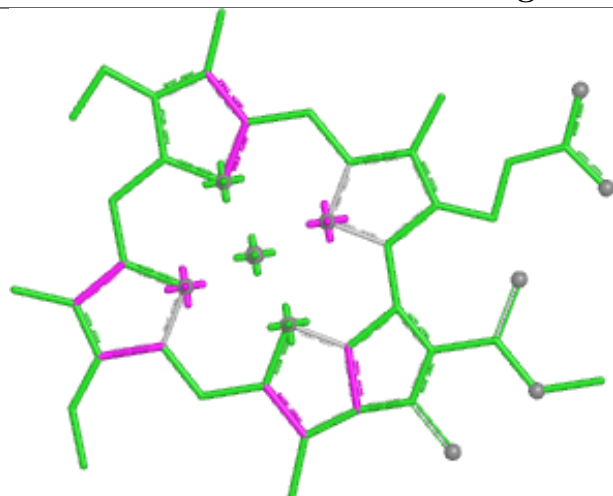


Ligand CLA b 803

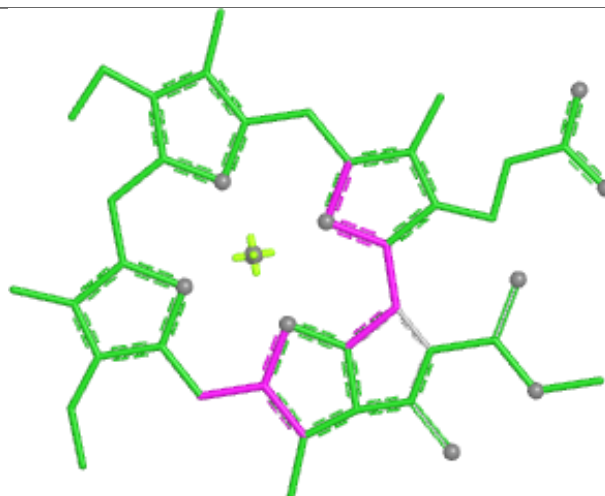




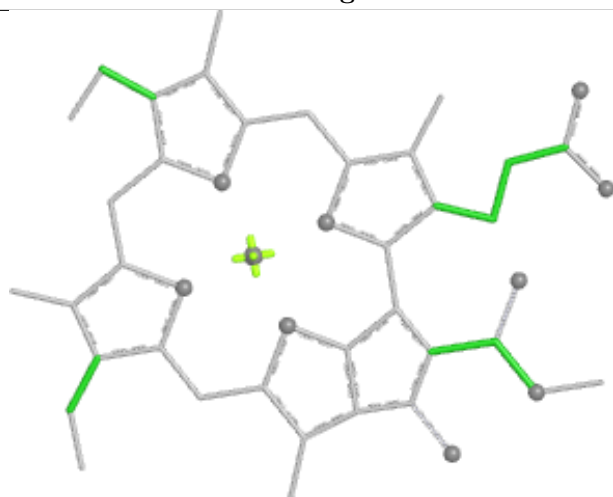
Ligand CLA b 834



Bond lengths



Bond angles

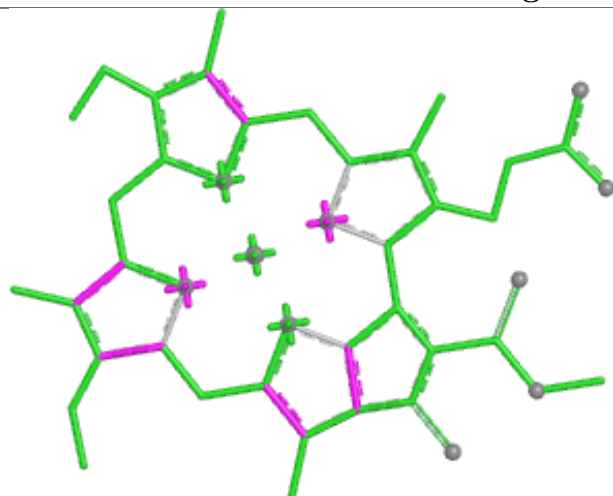


Torsions

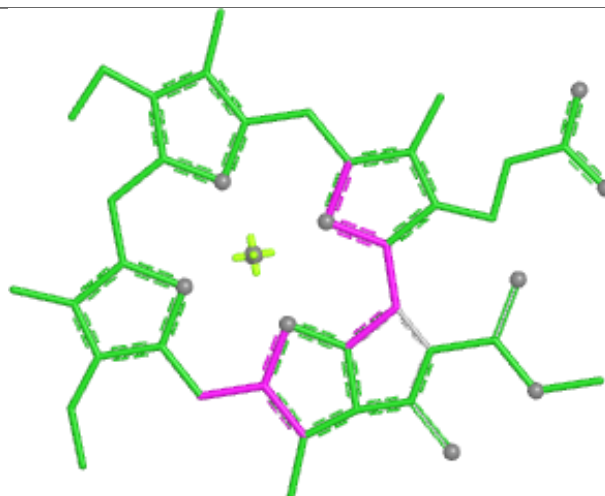


Rings

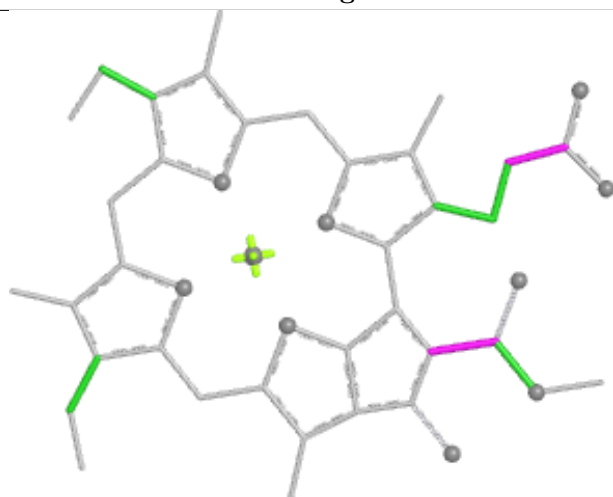
Ligand CLA 1 301



Bond lengths



Bond angles

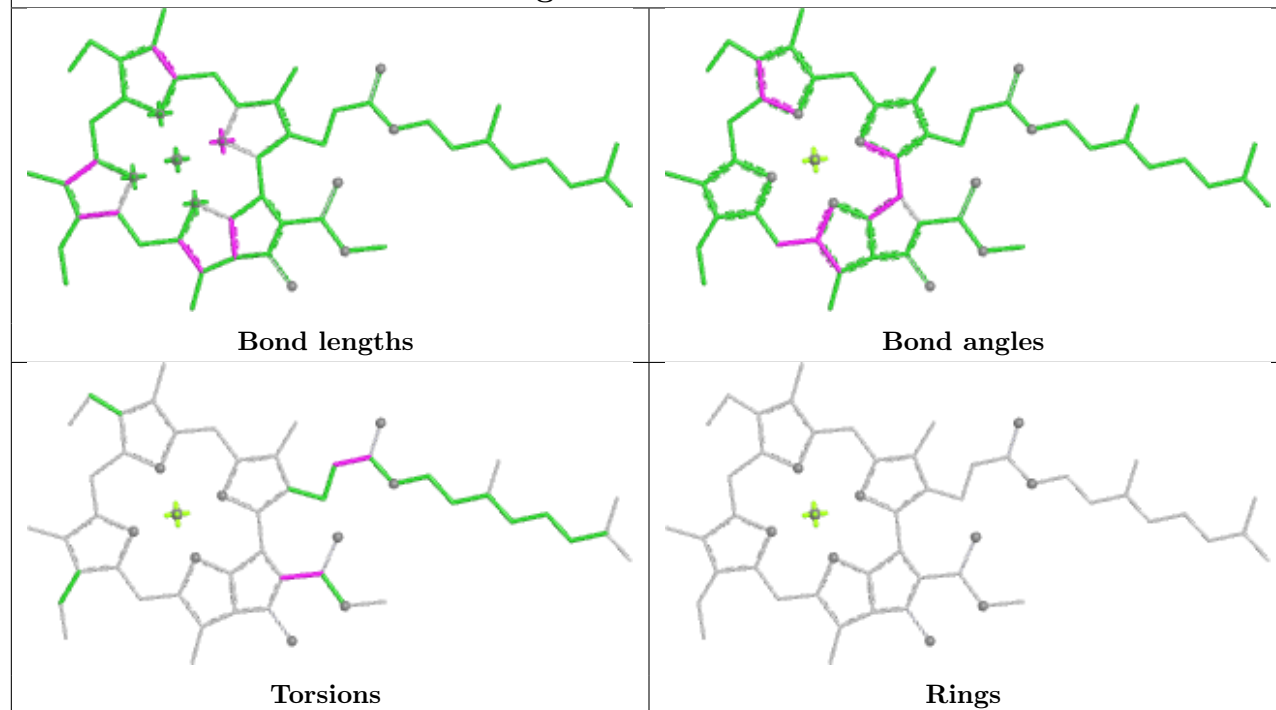


Torsions

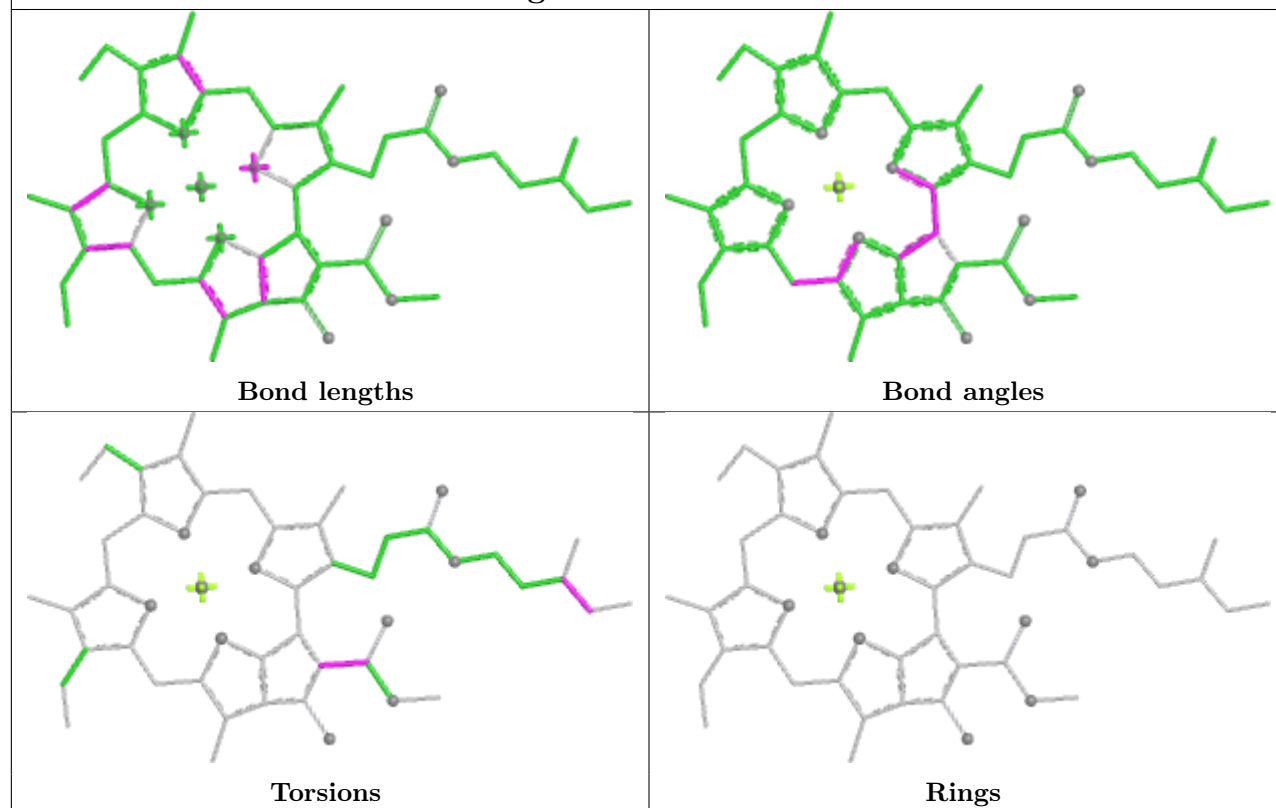


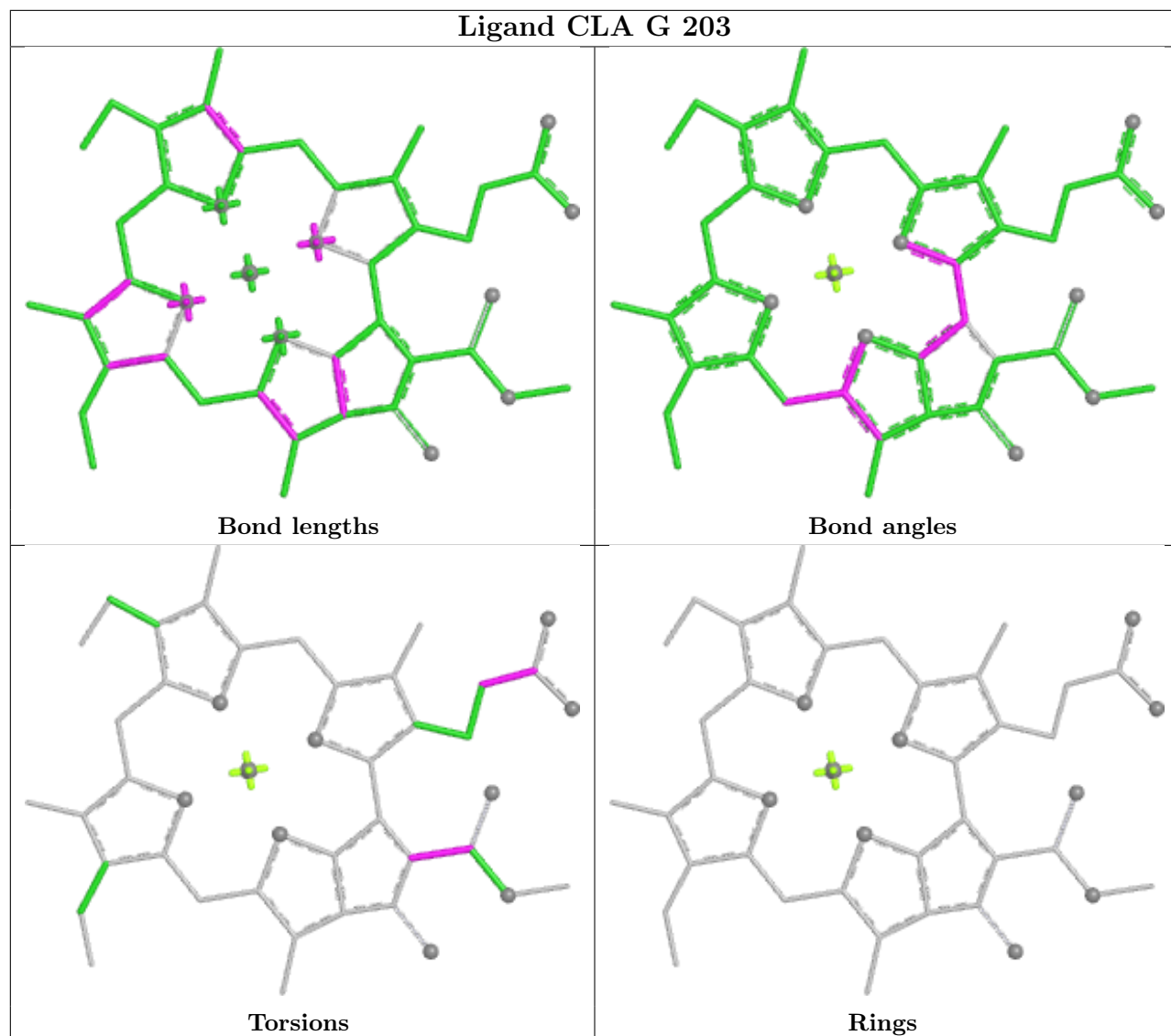
Rings

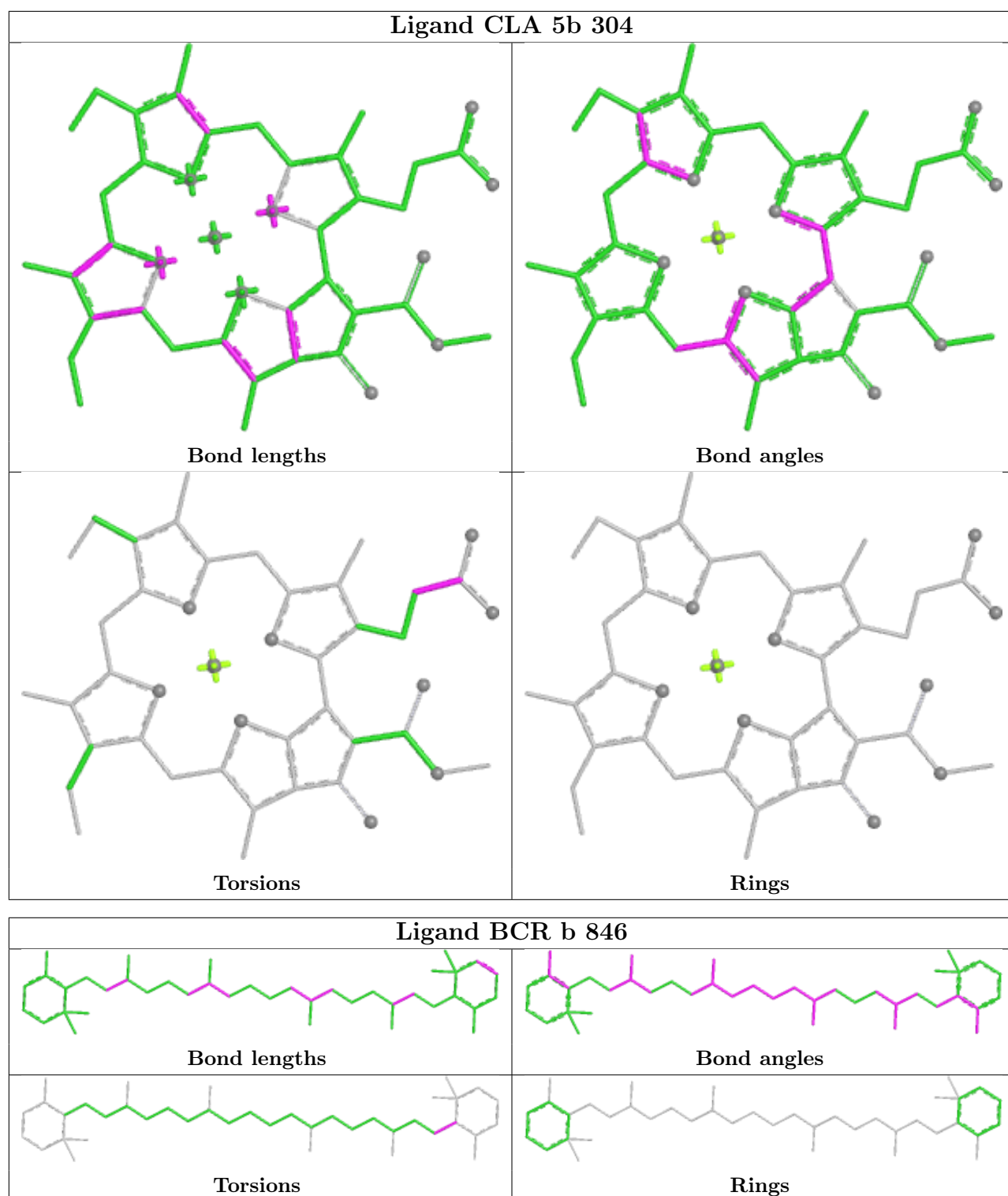
Ligand CLA a 804



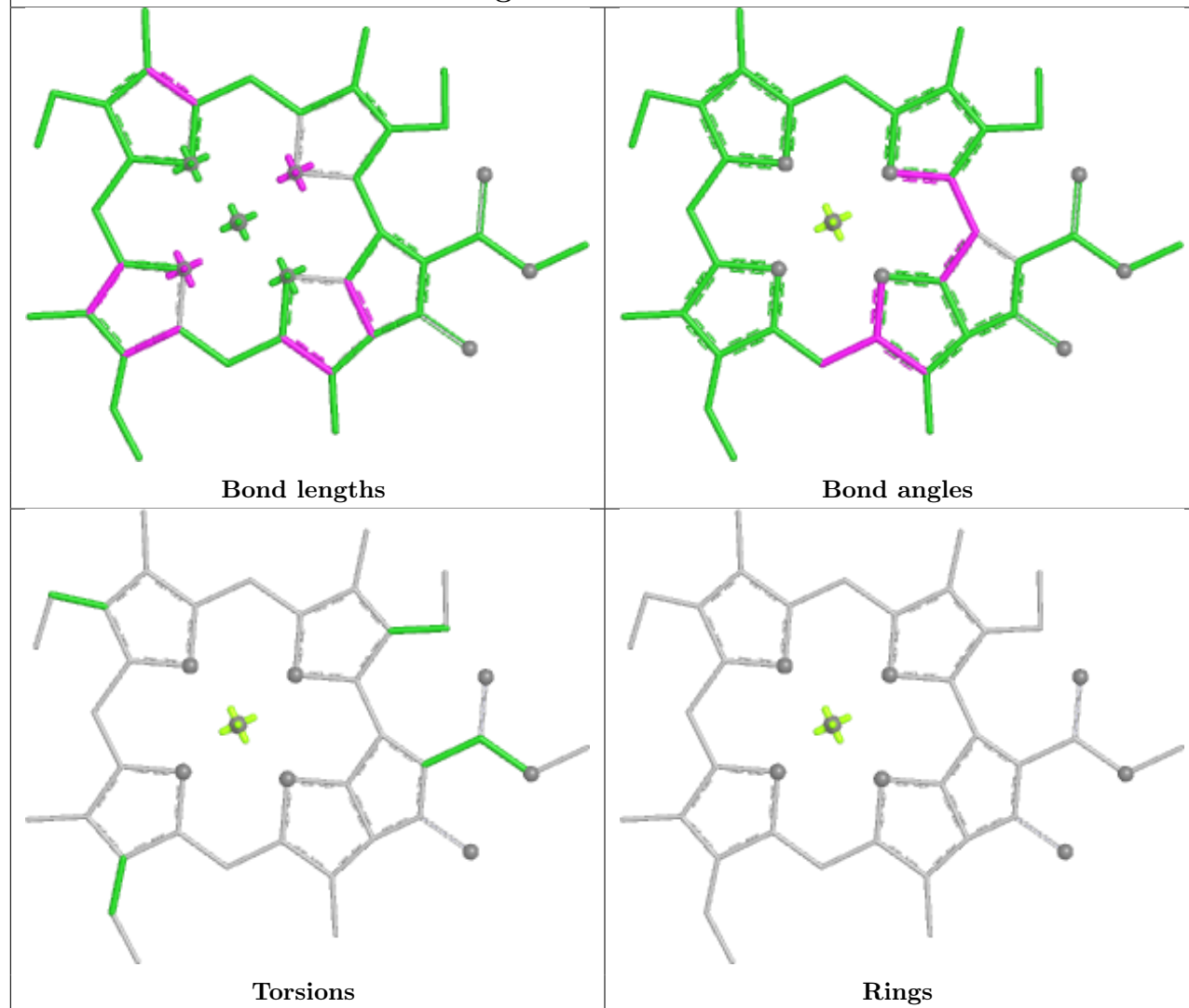
Ligand CLA 5a 309



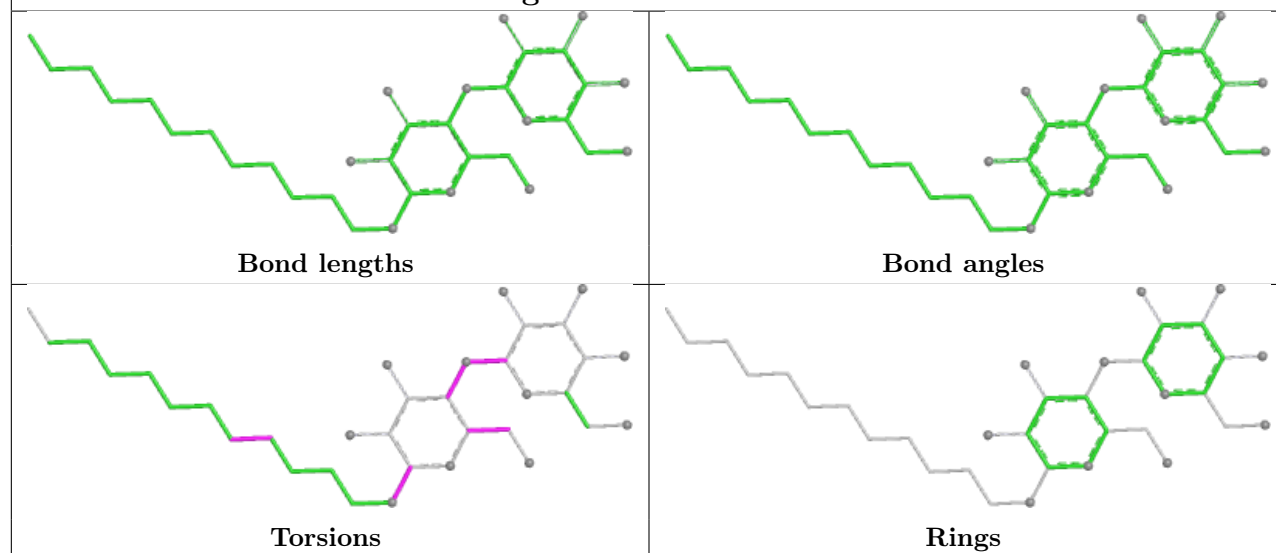


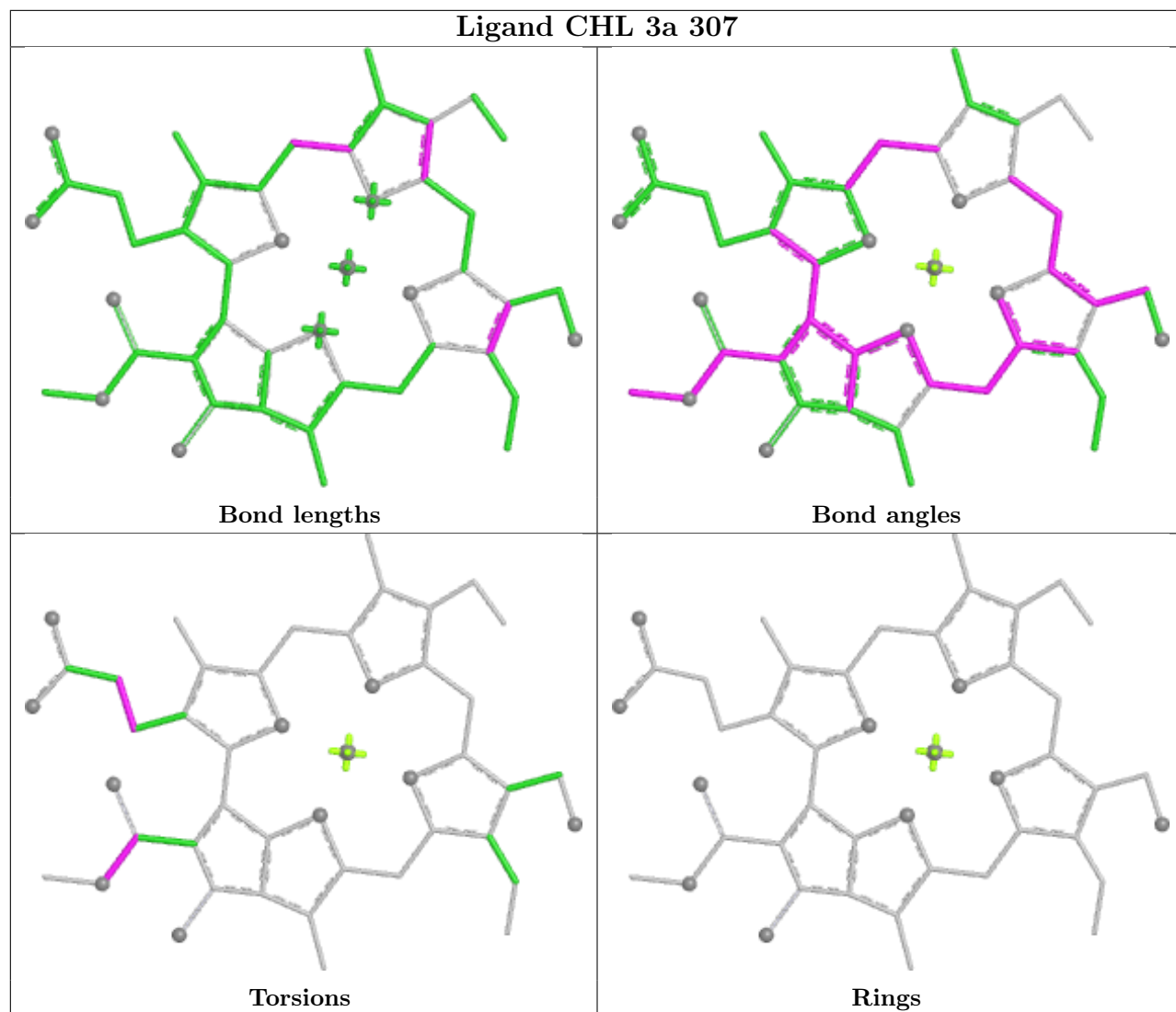


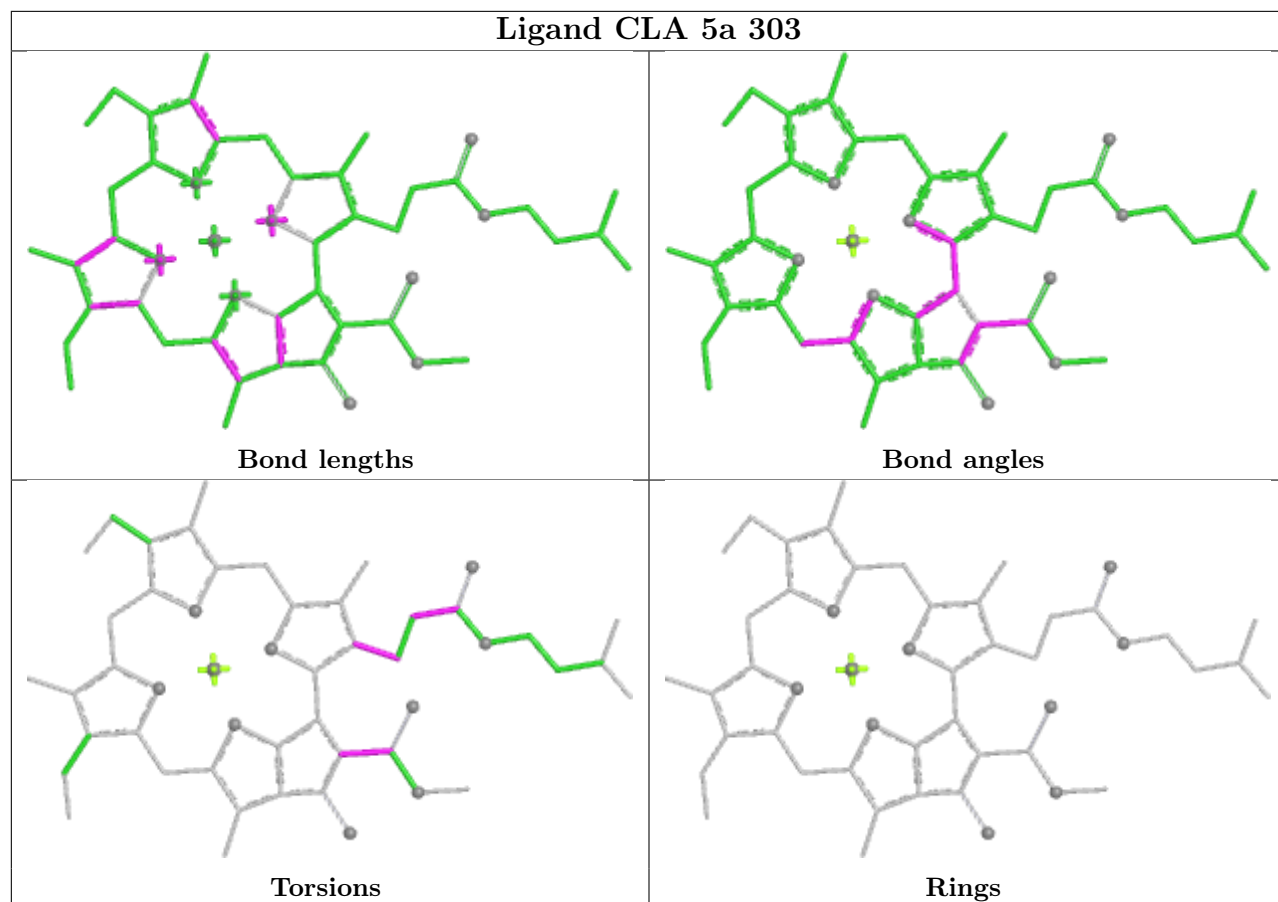
Ligand CLA A 814

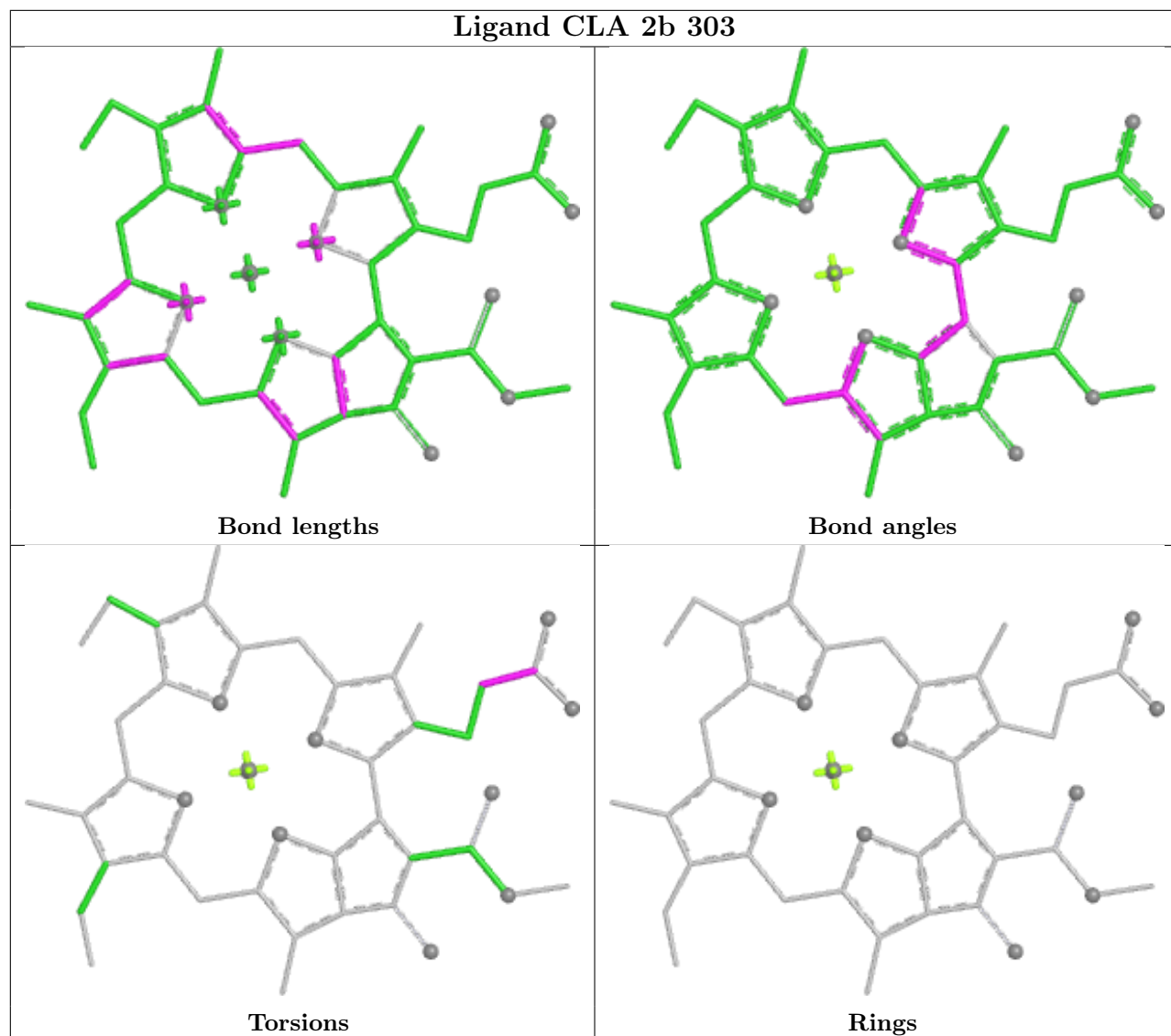


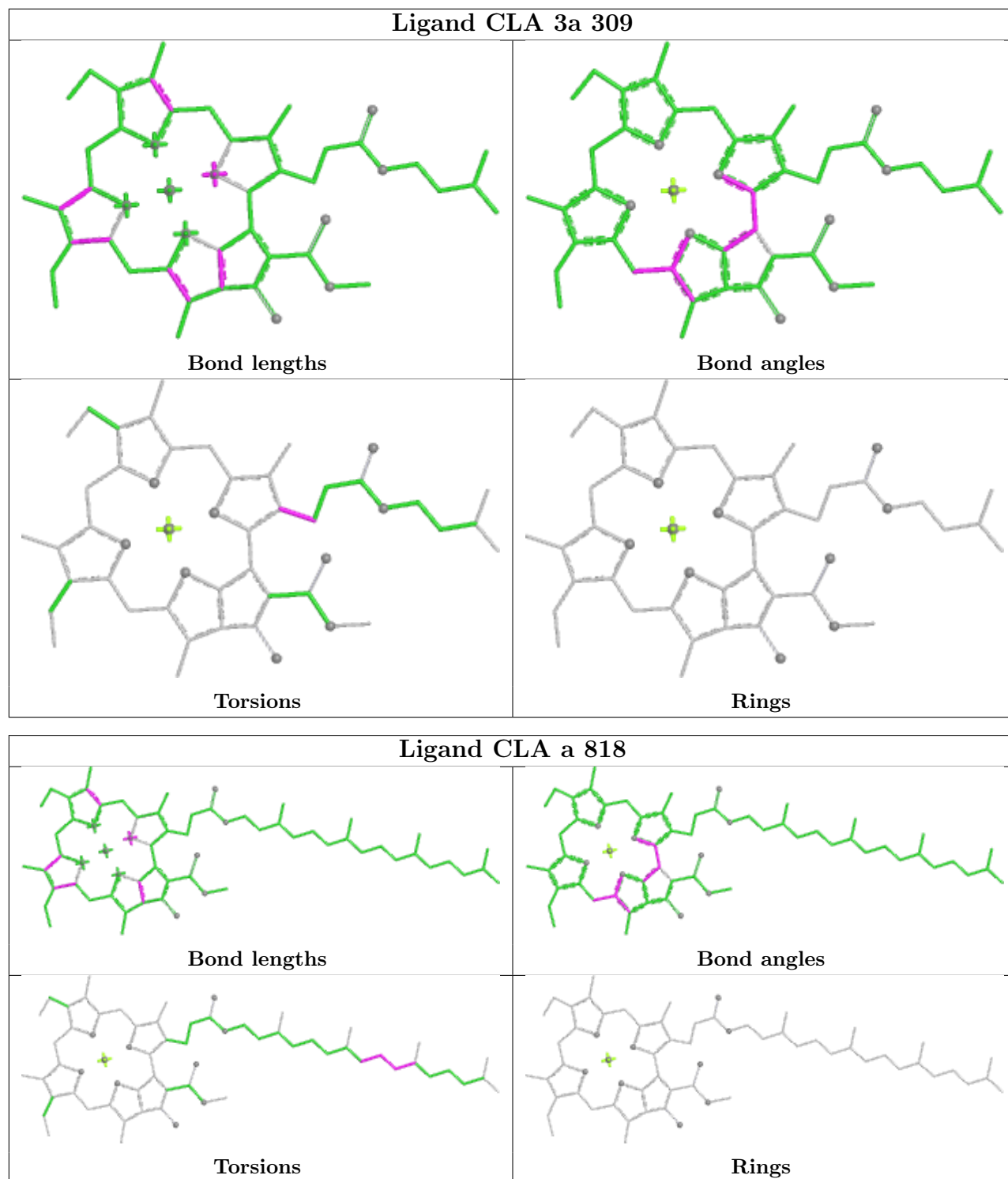
Ligand LMU 6b 302

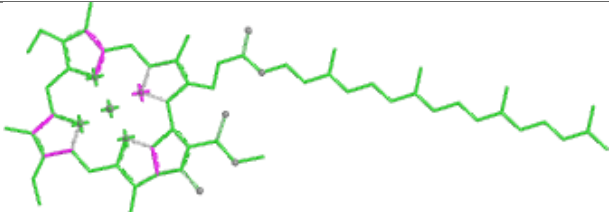
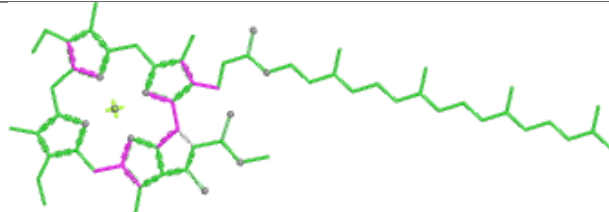
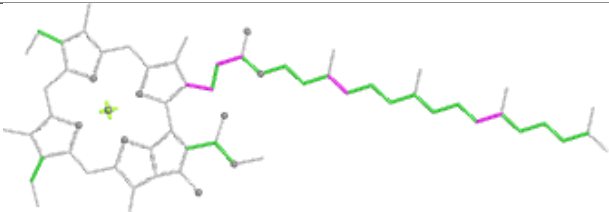
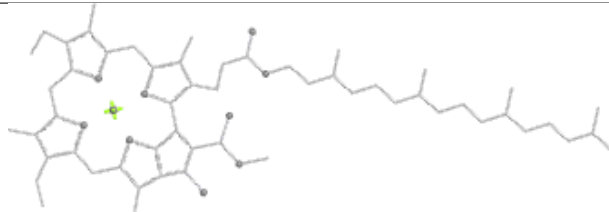


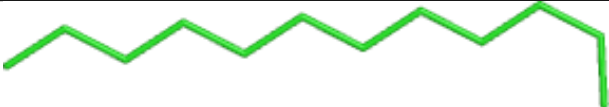
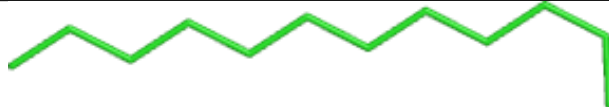
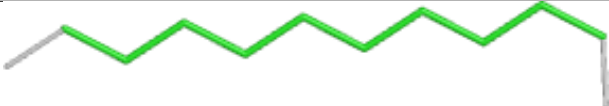
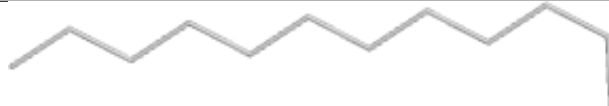


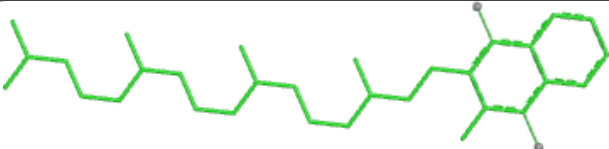
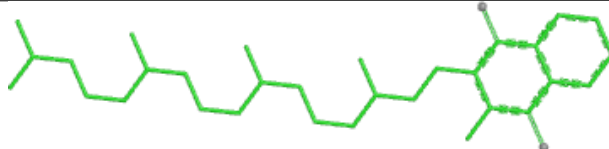
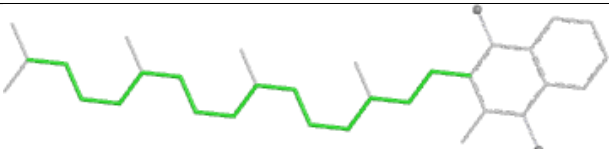
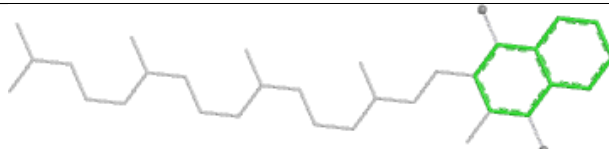


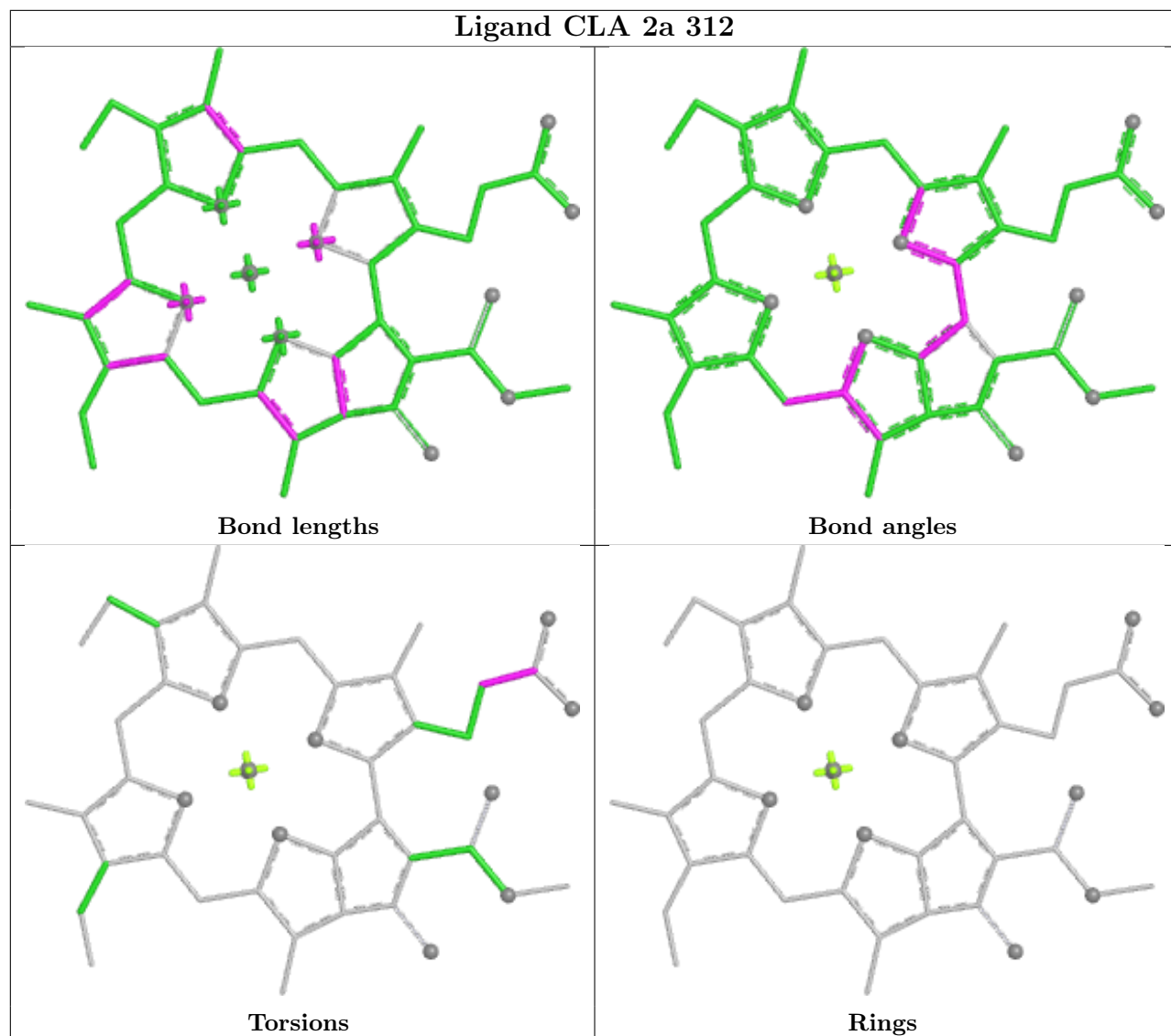


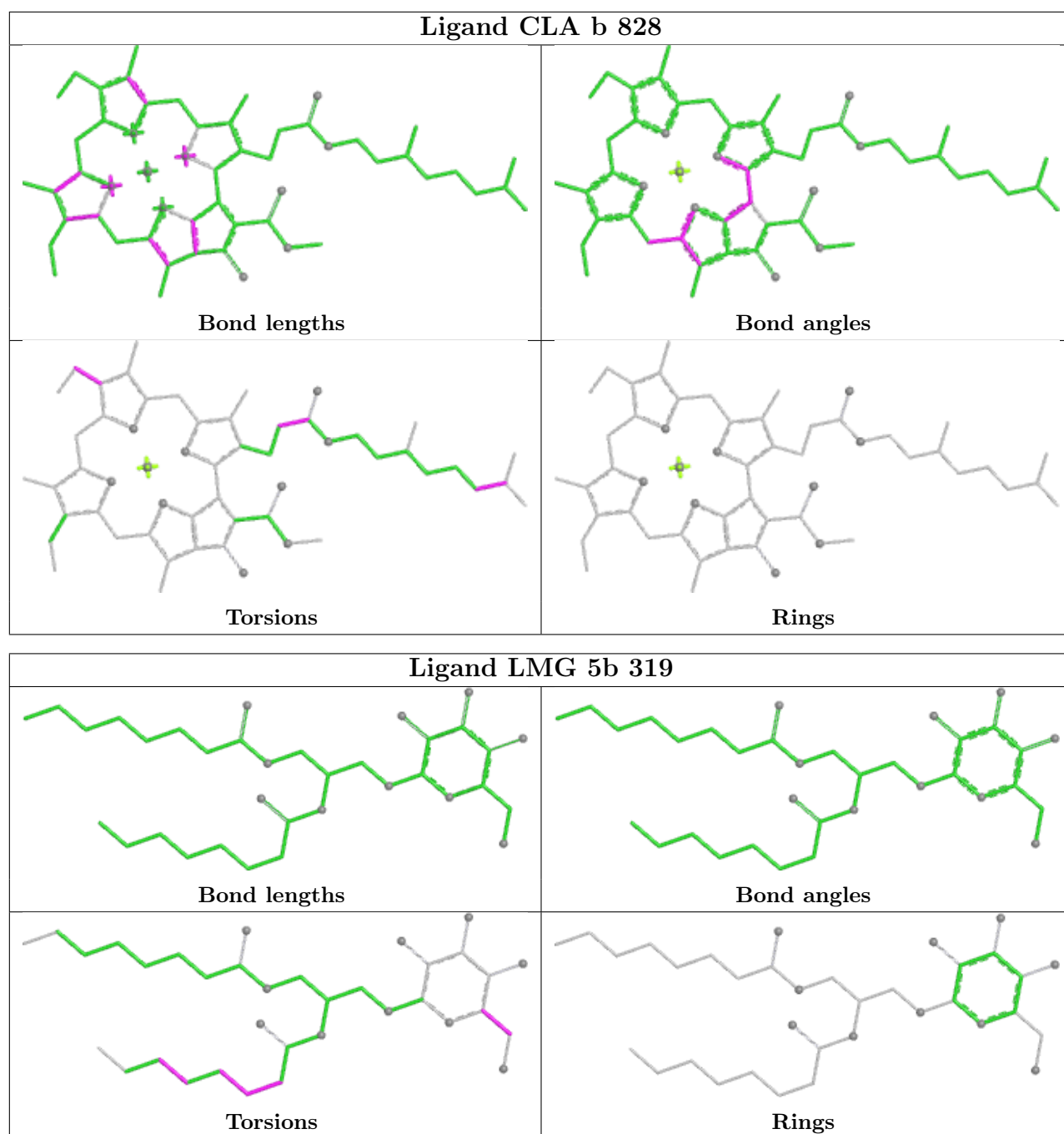


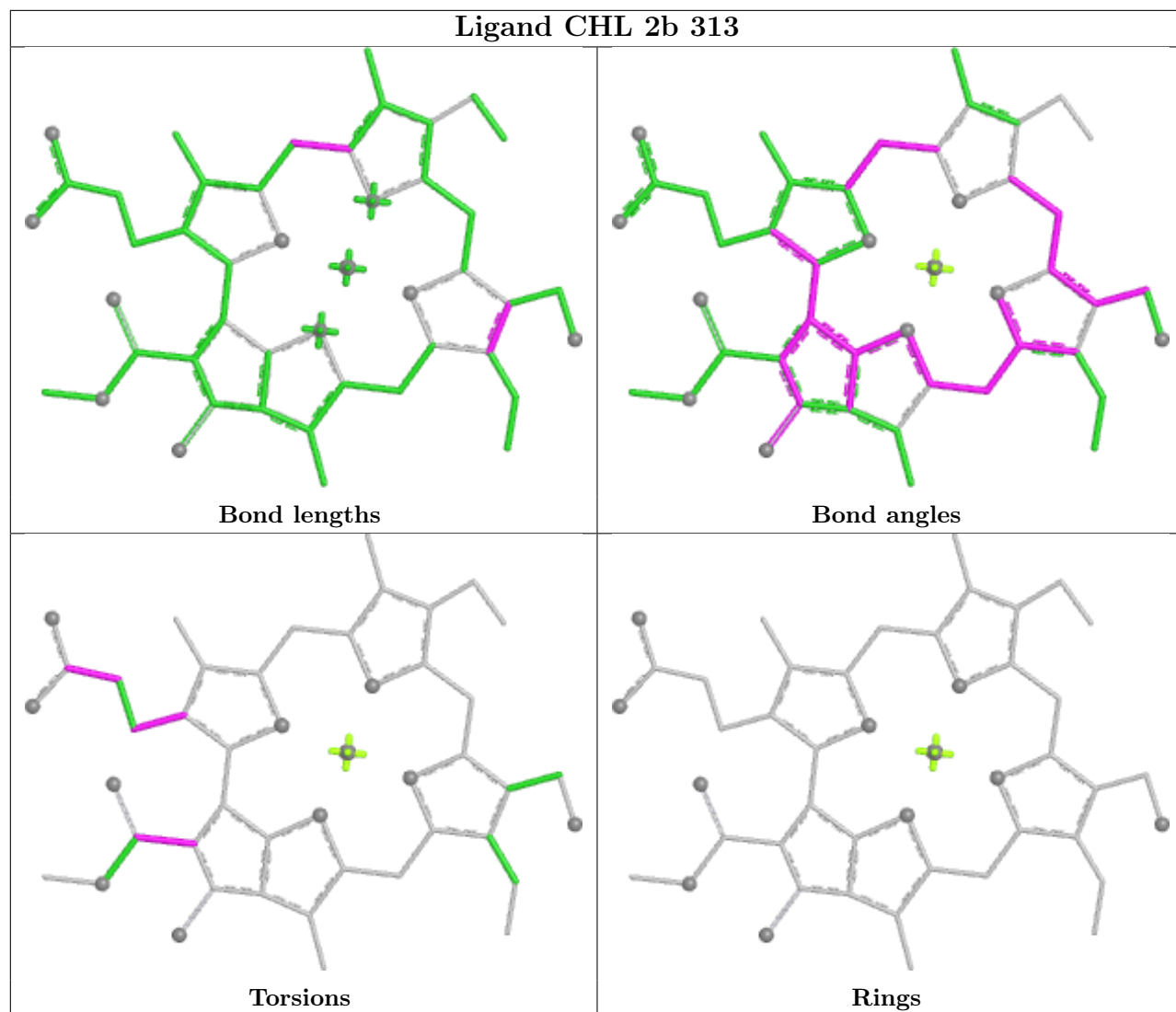
Ligand CLA b 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

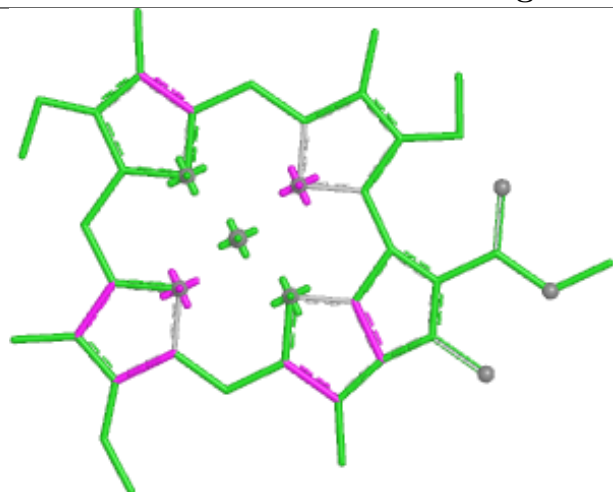
Ligand PQN B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings



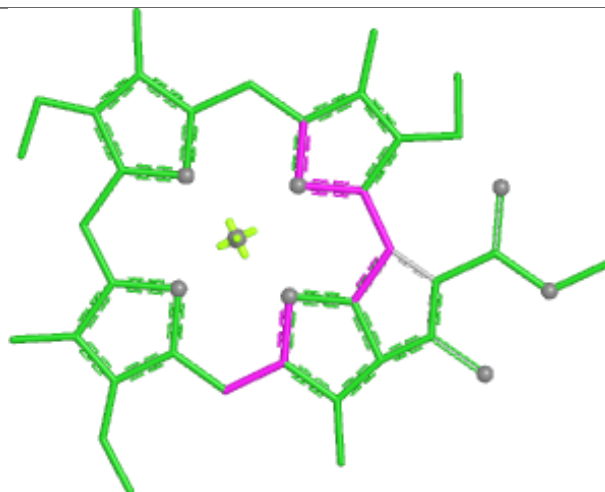




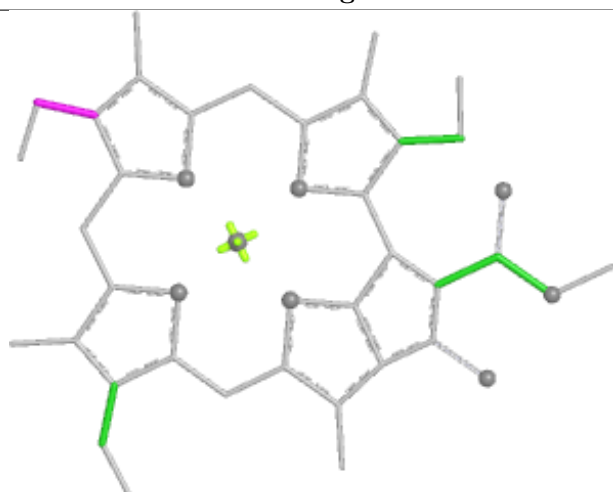
Ligand CLA L 303



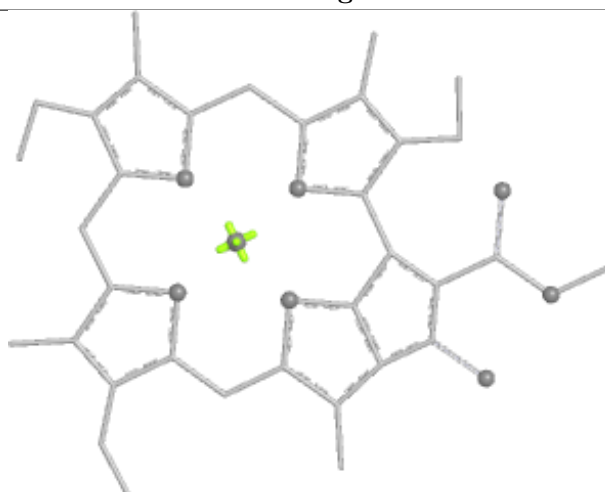
Bond lengths



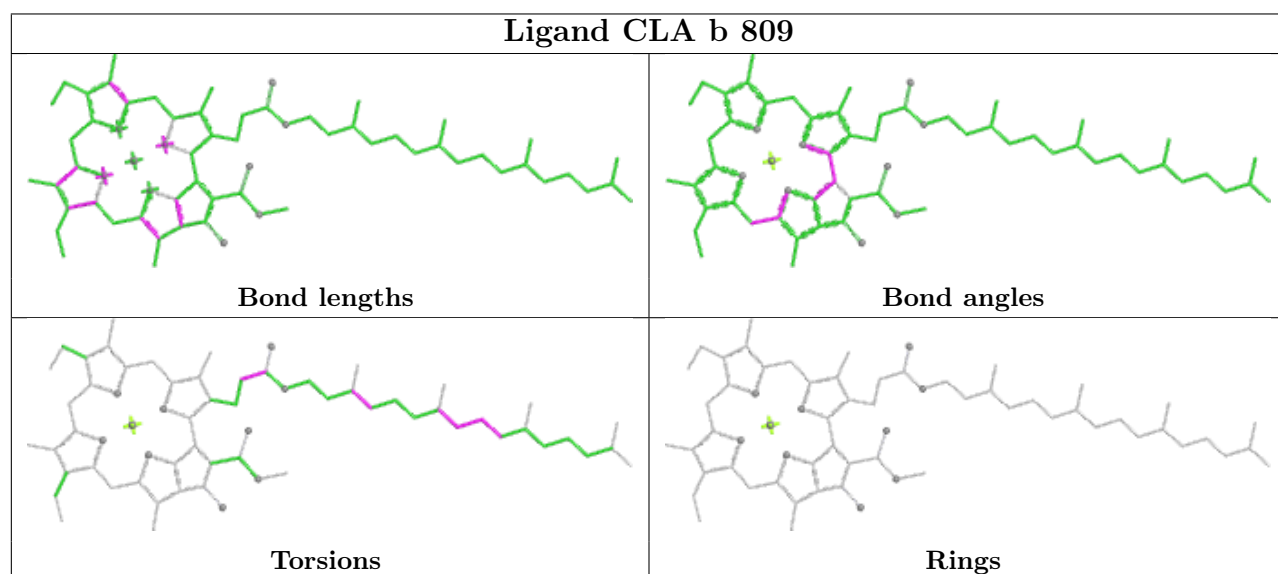
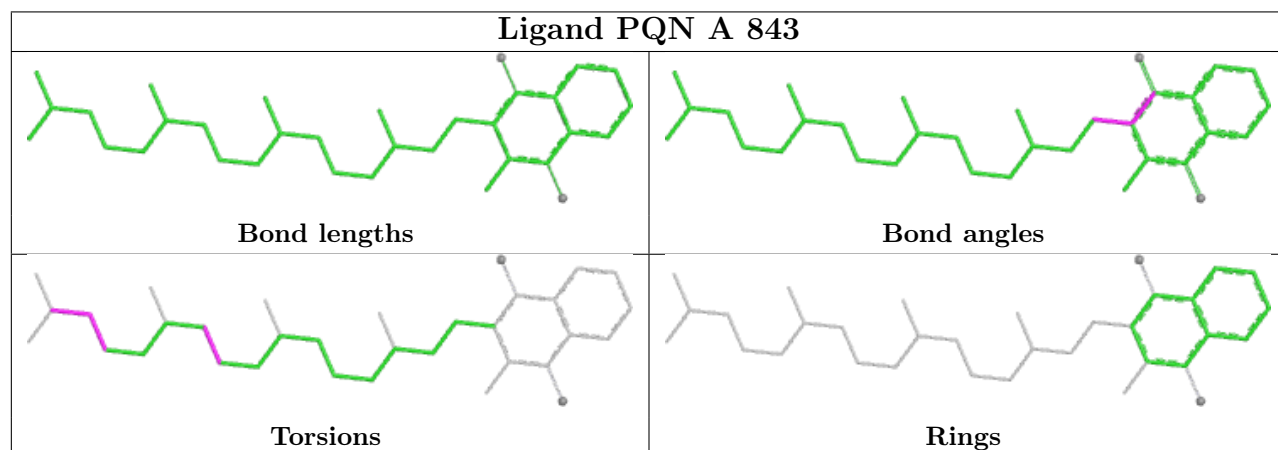
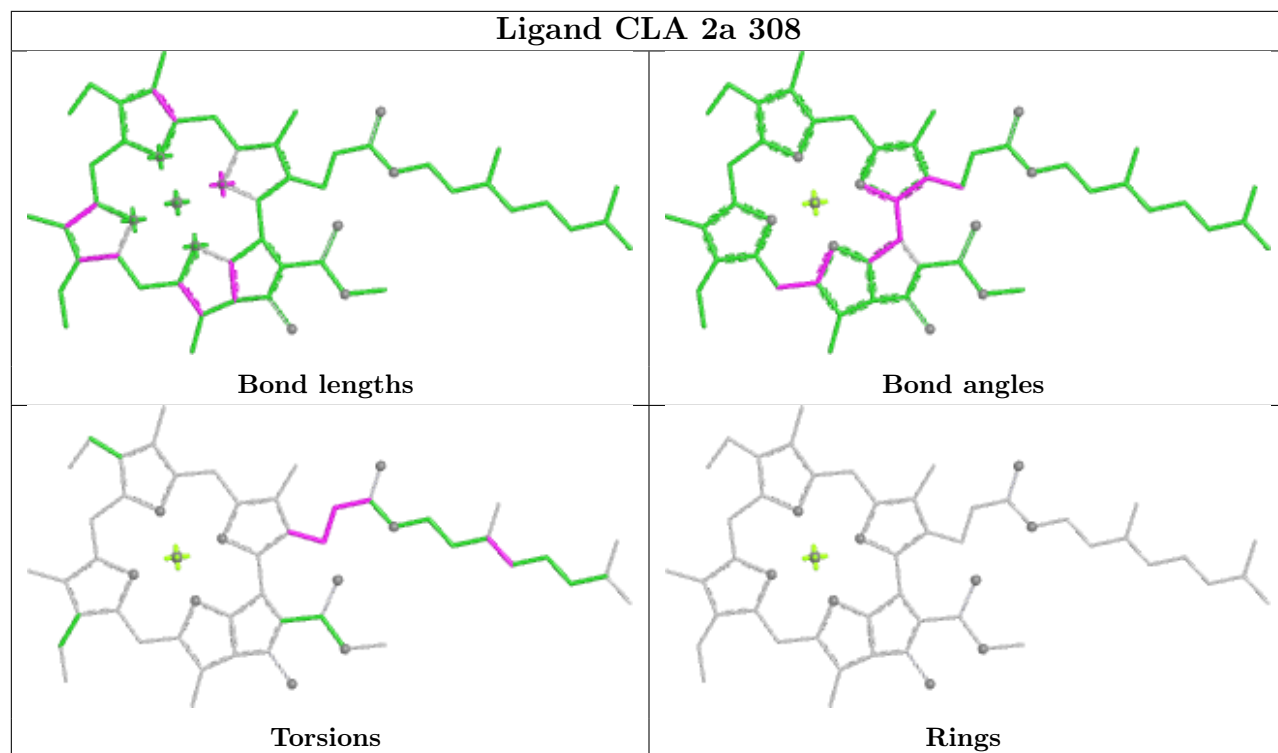
Bond angles

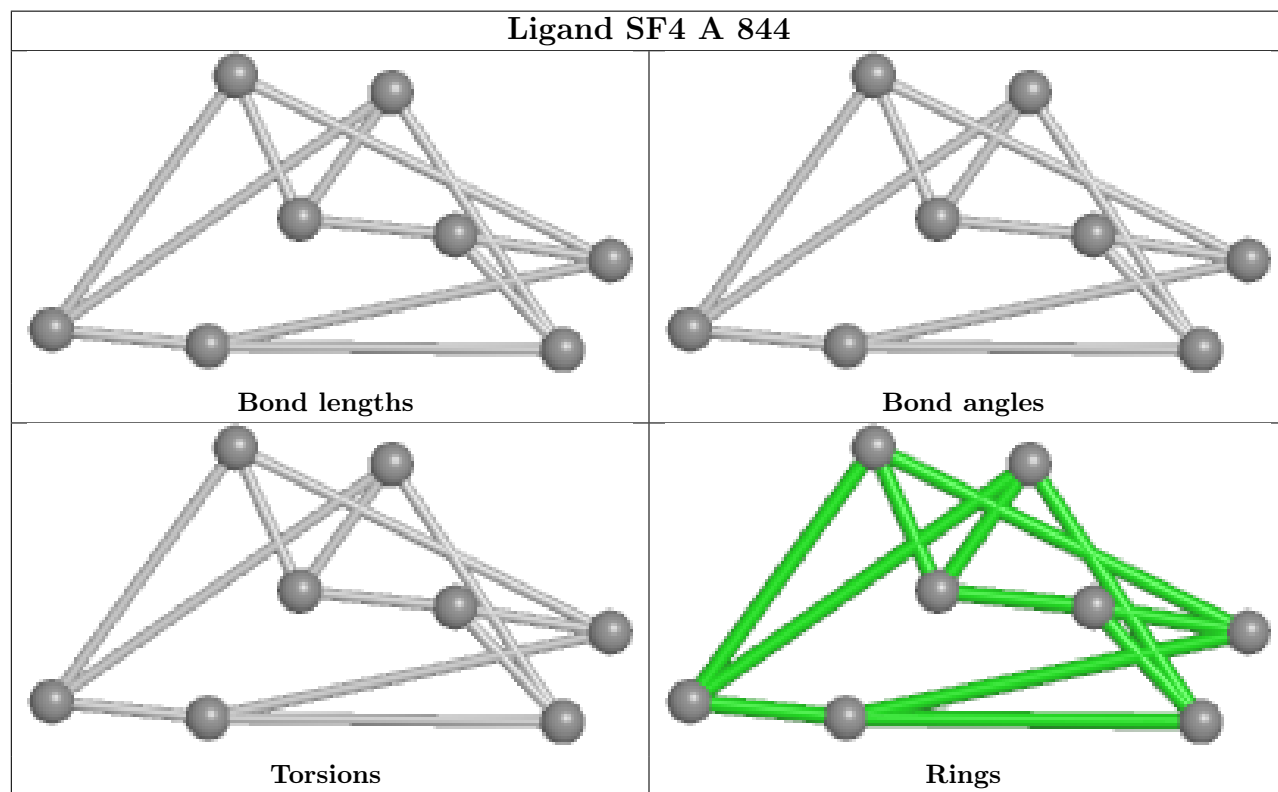
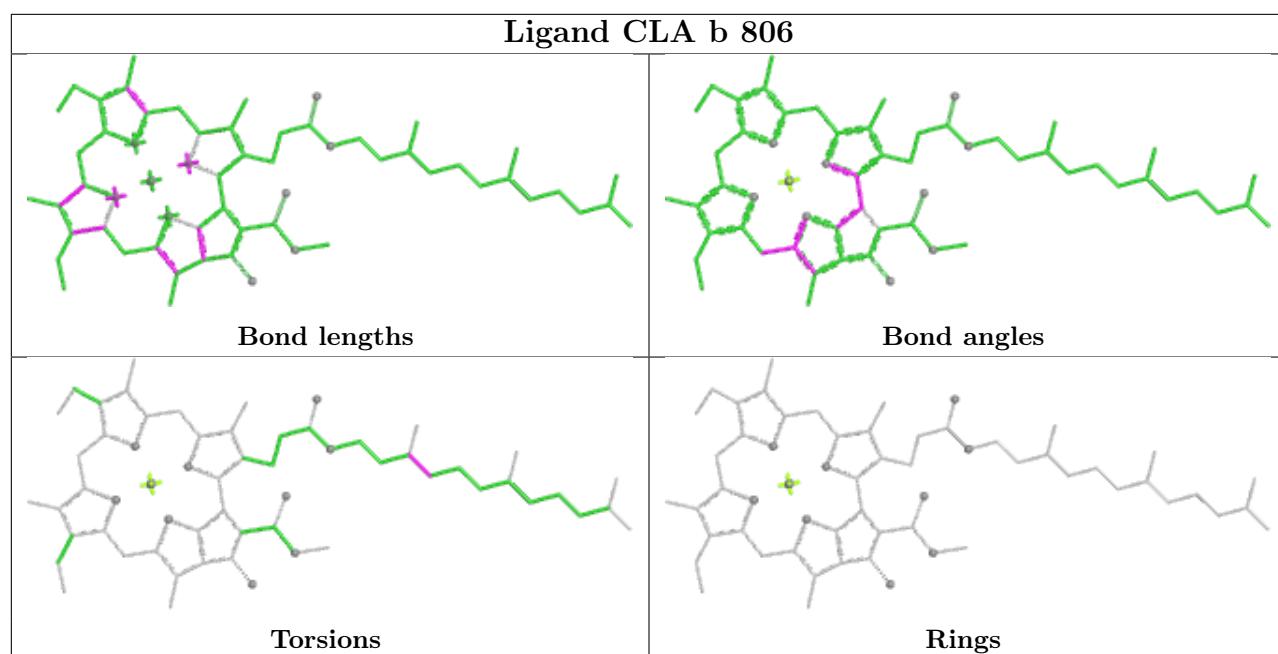


Torsions

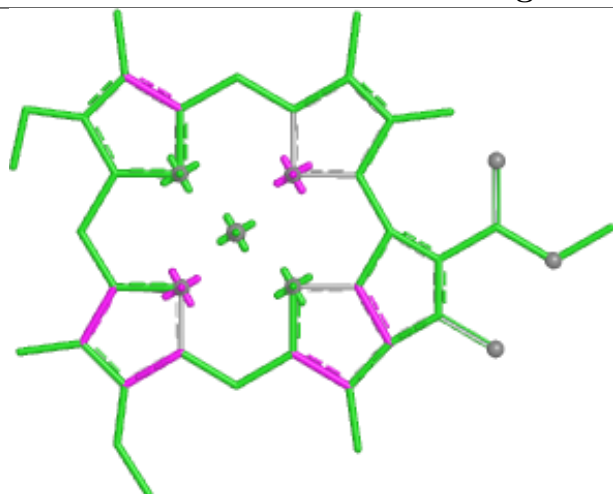


Rings

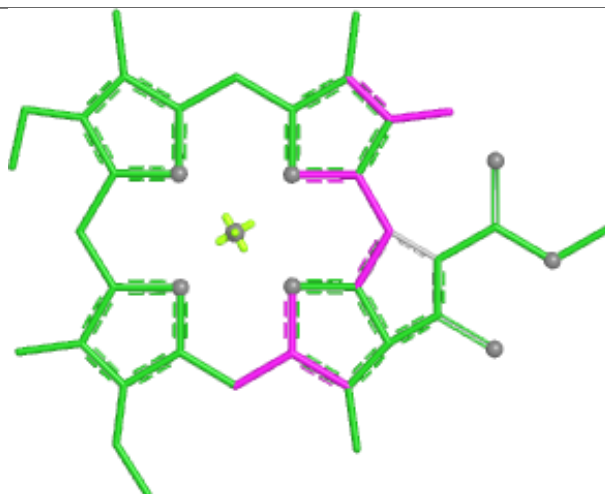




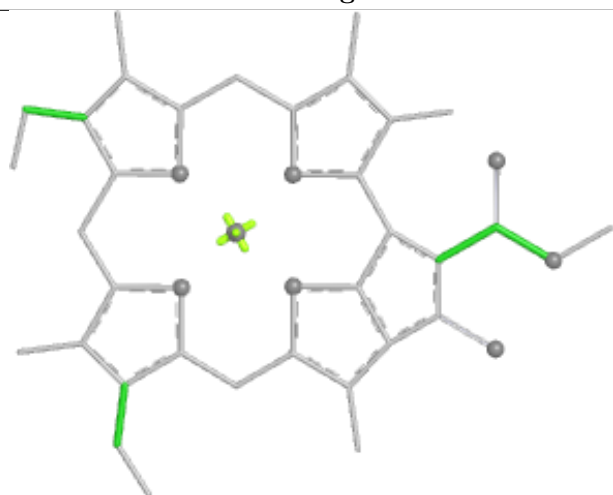
Ligand CLA F 303



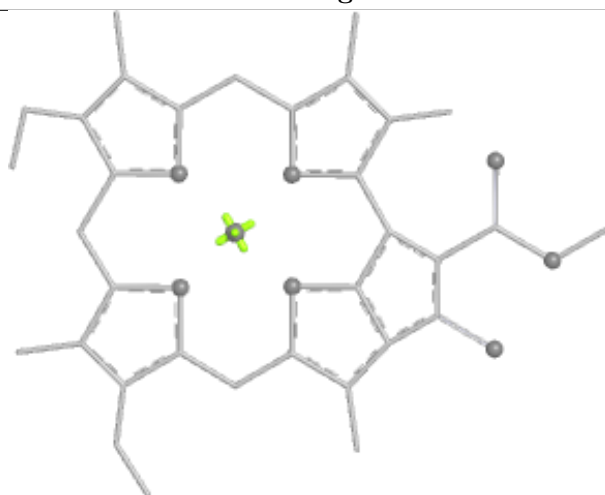
Bond lengths



Bond angles

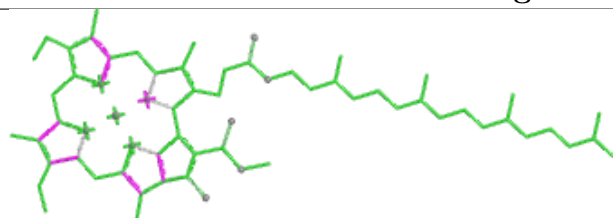


Torsions

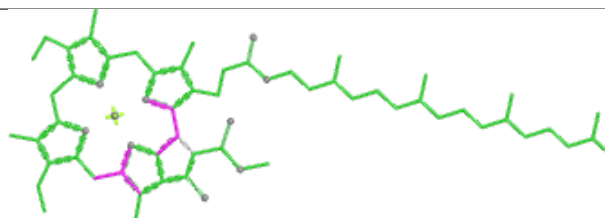


Rings

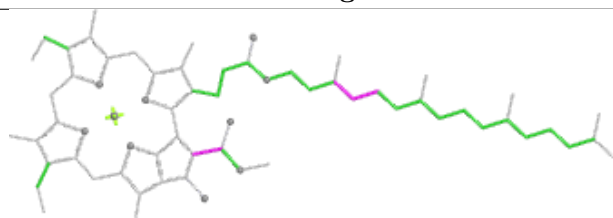
Ligand CLA A 805



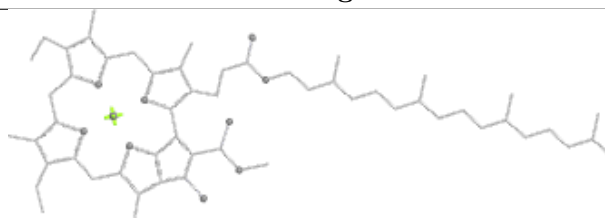
Bond lengths



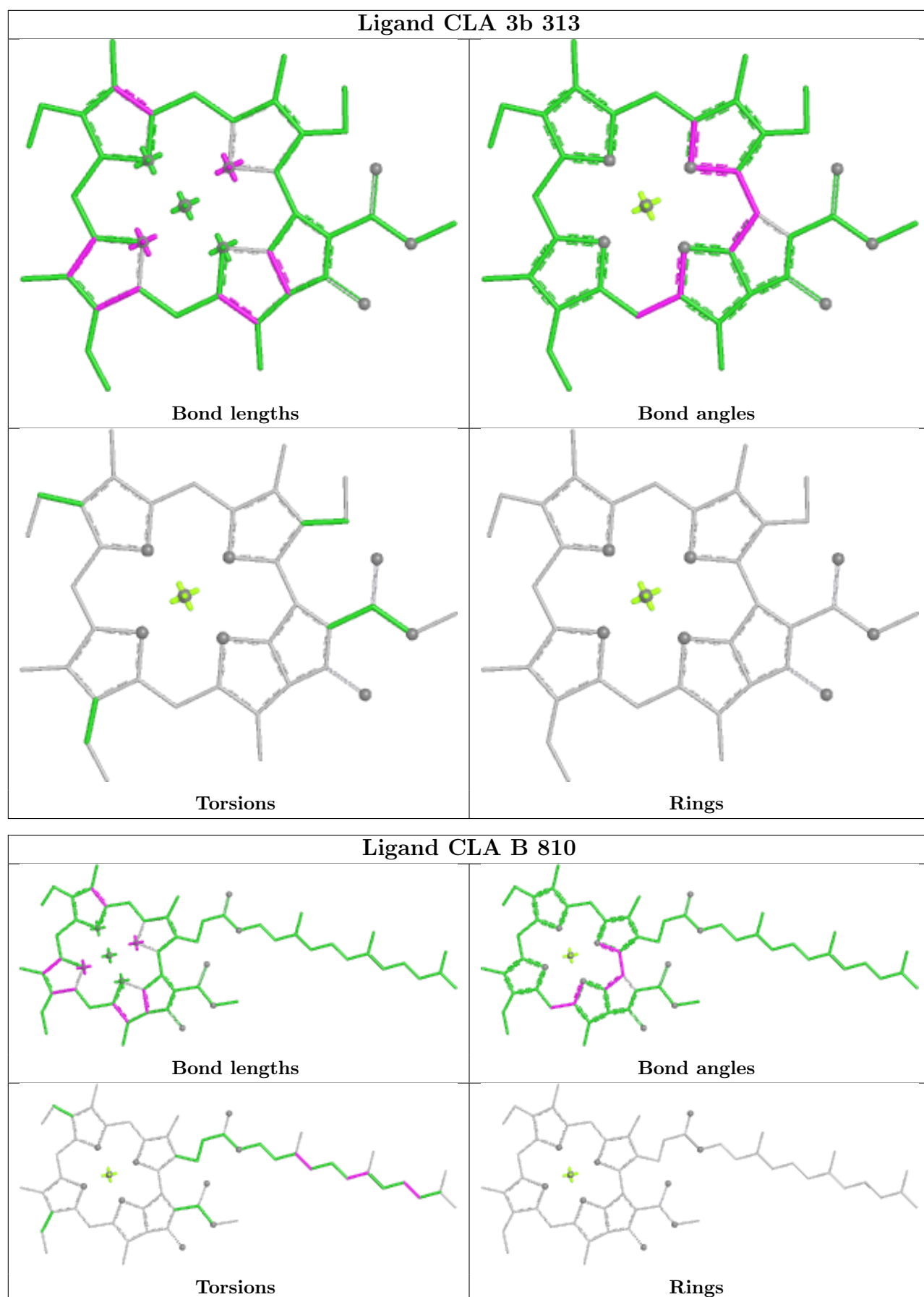
Bond angles

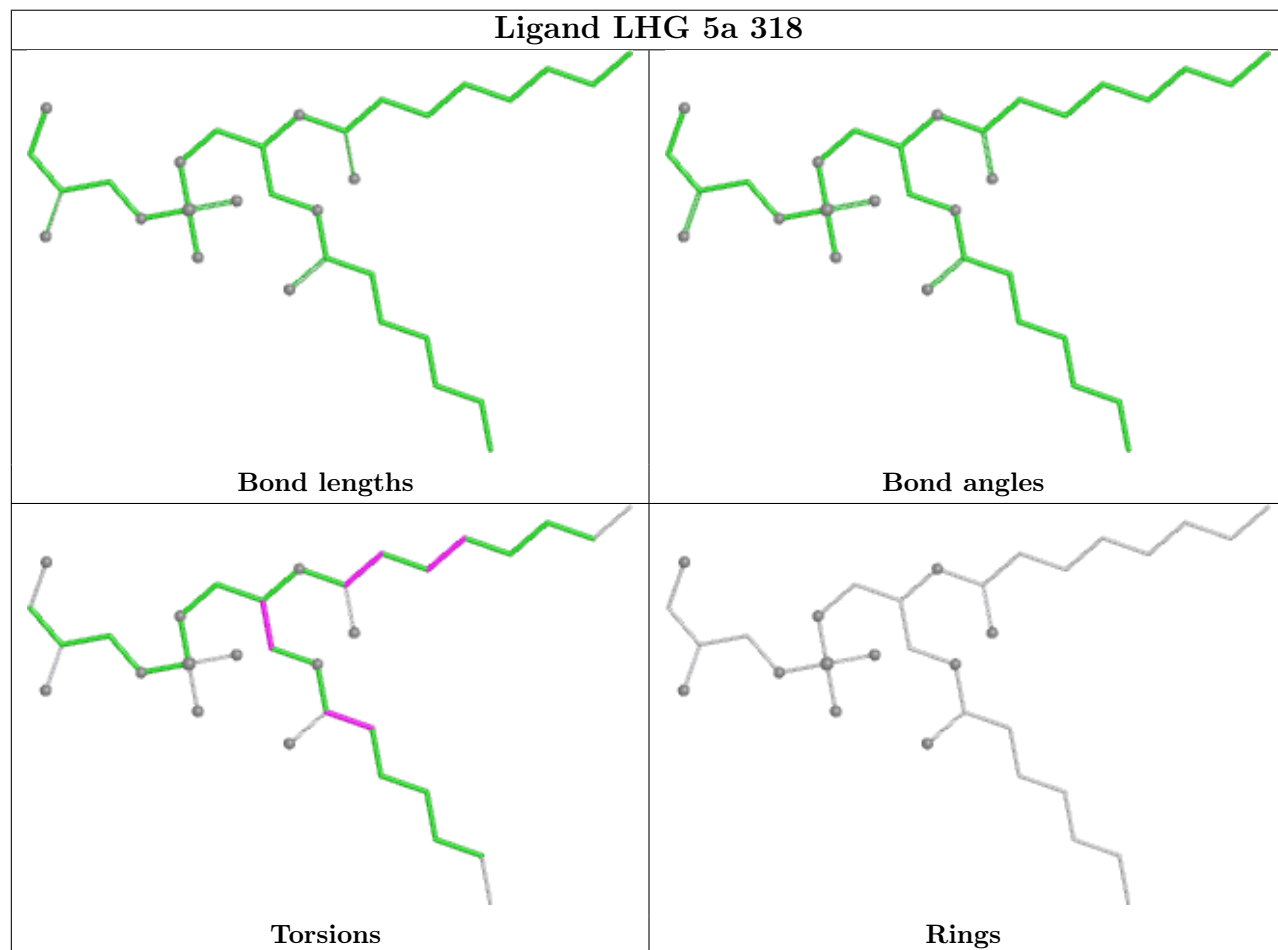
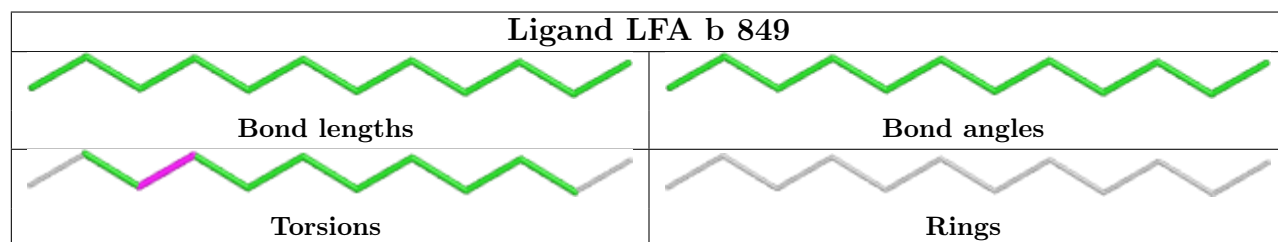
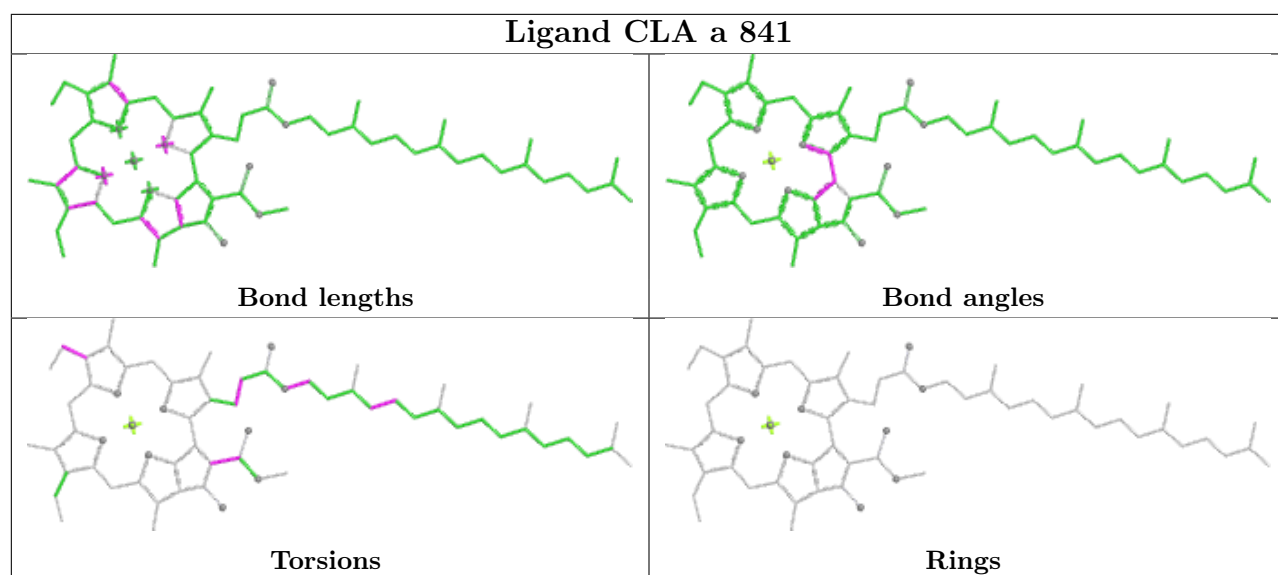


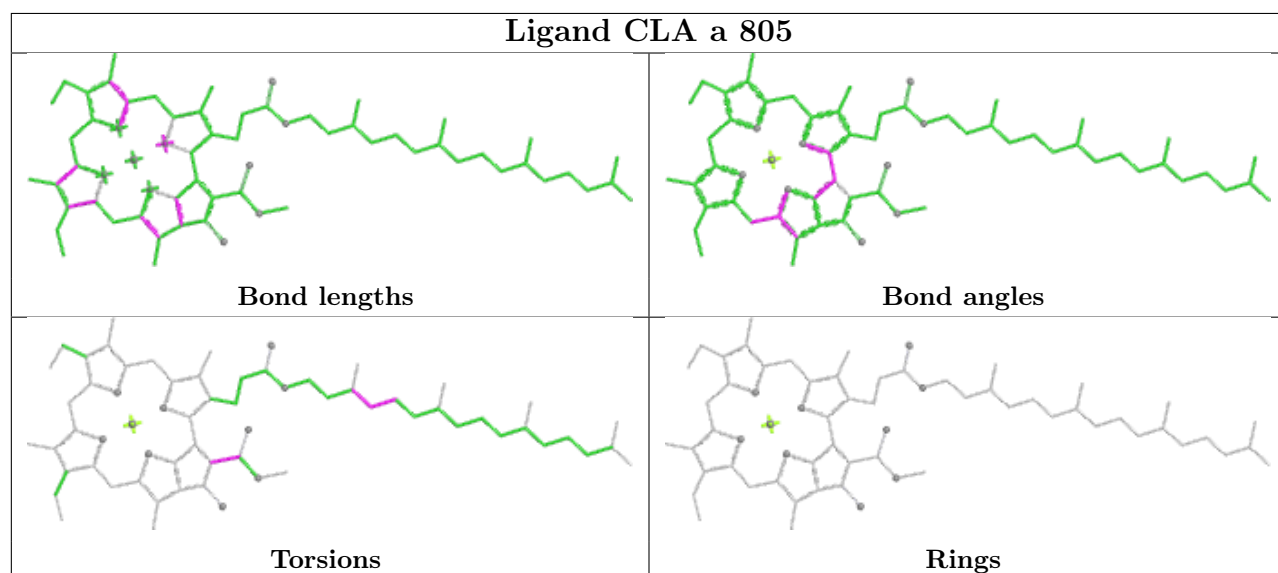
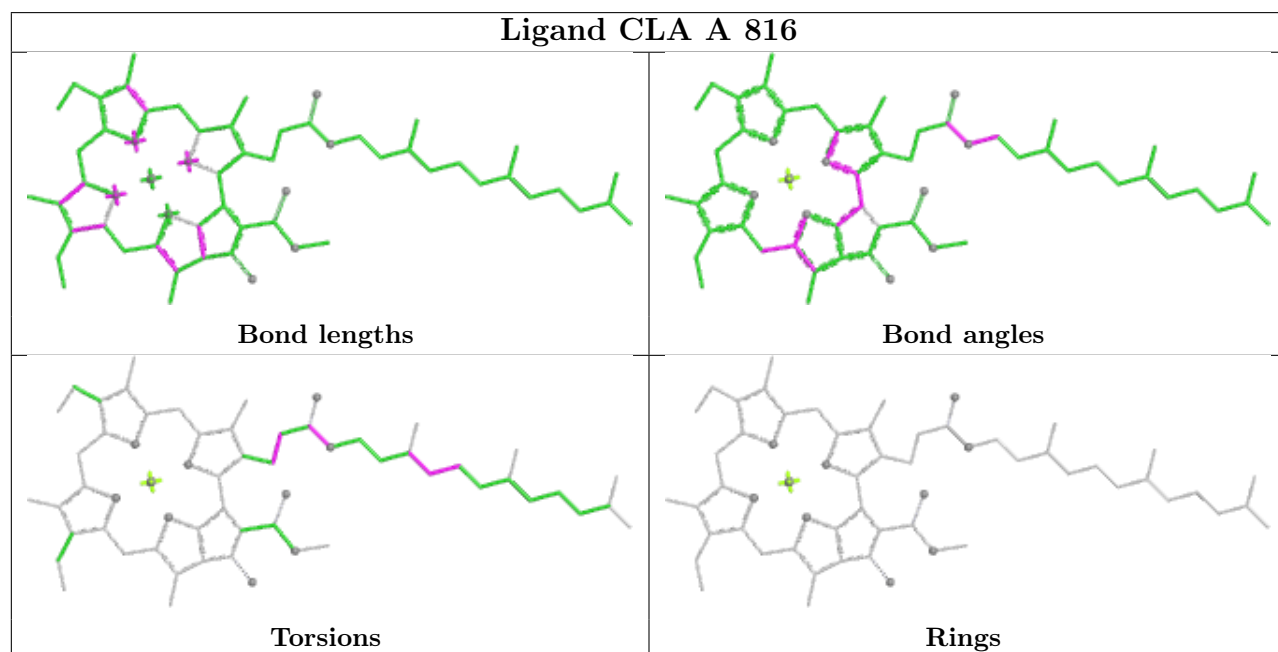
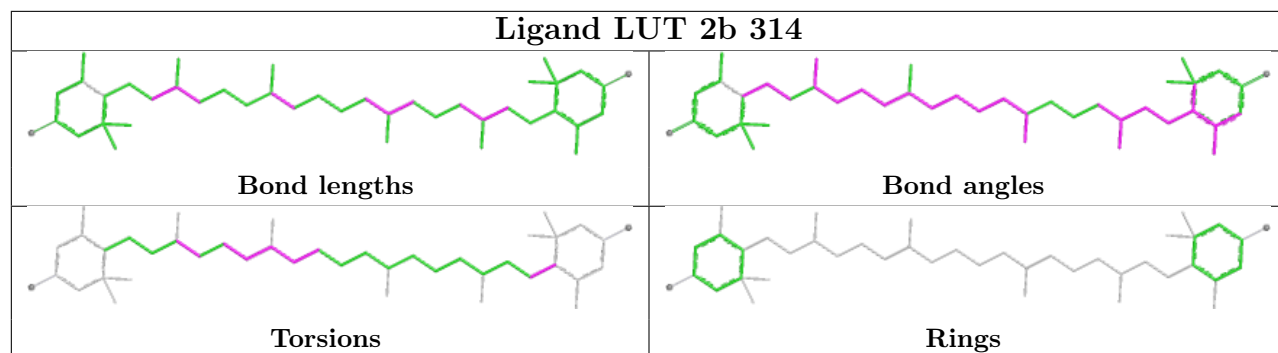
Torsions

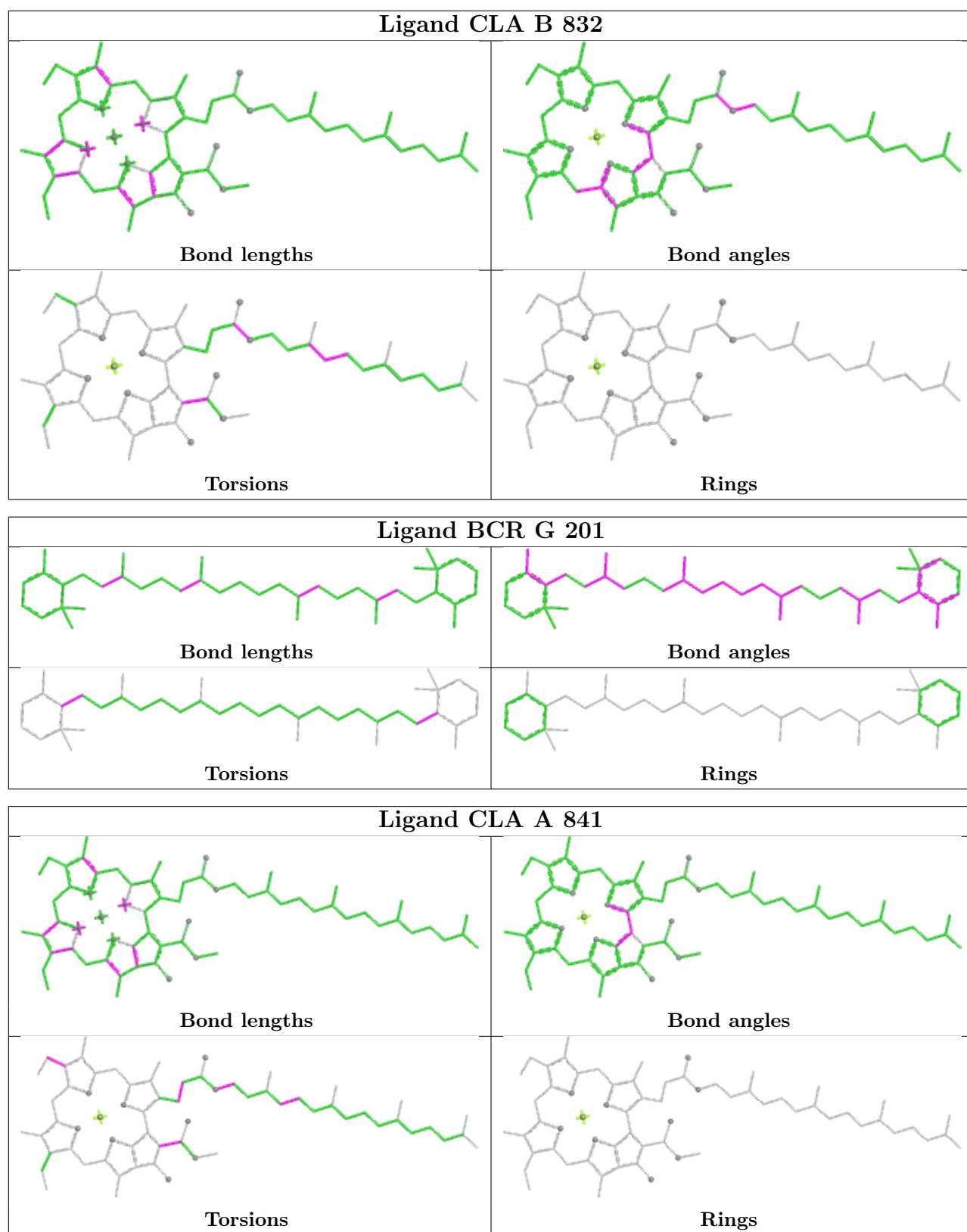


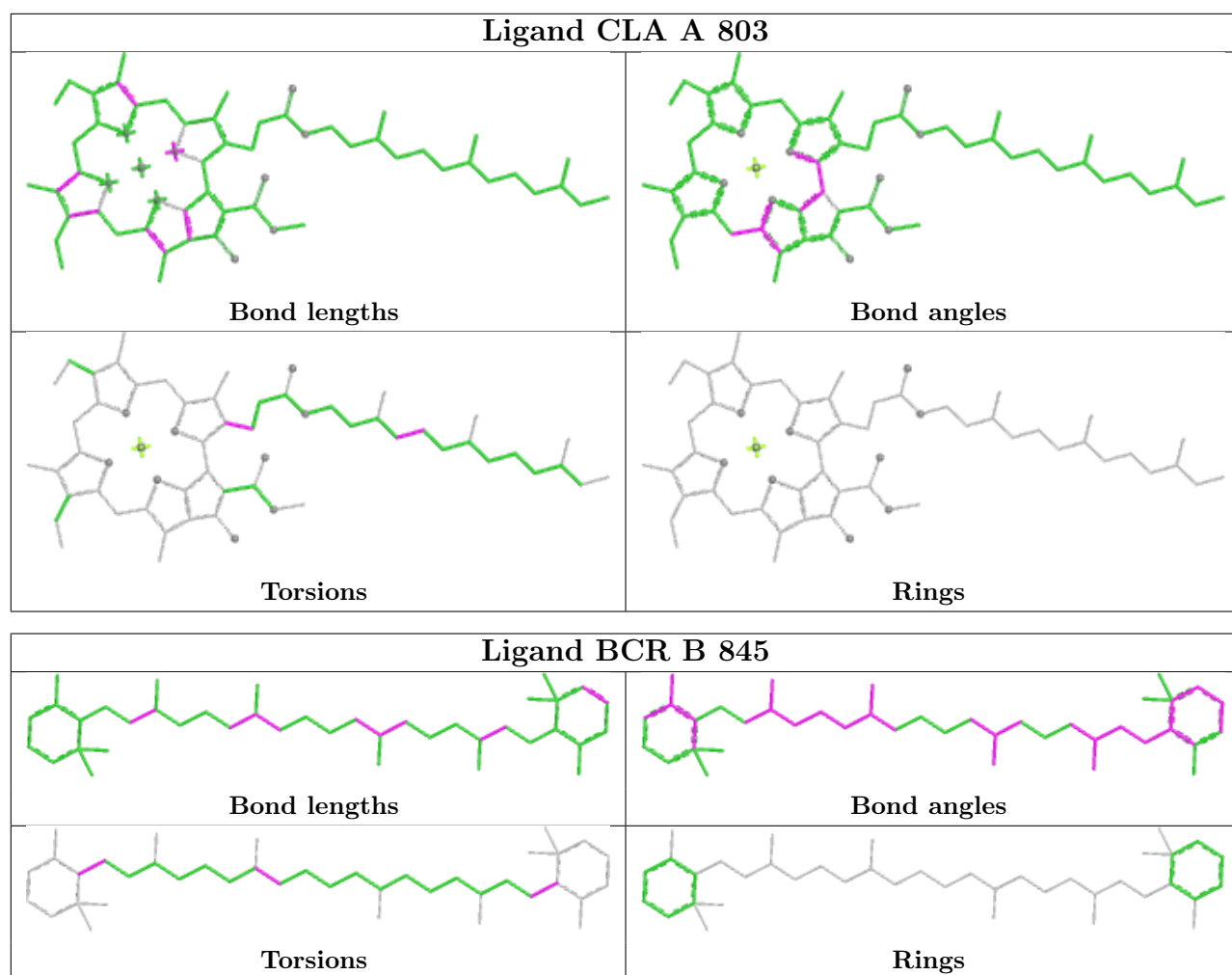
Rings

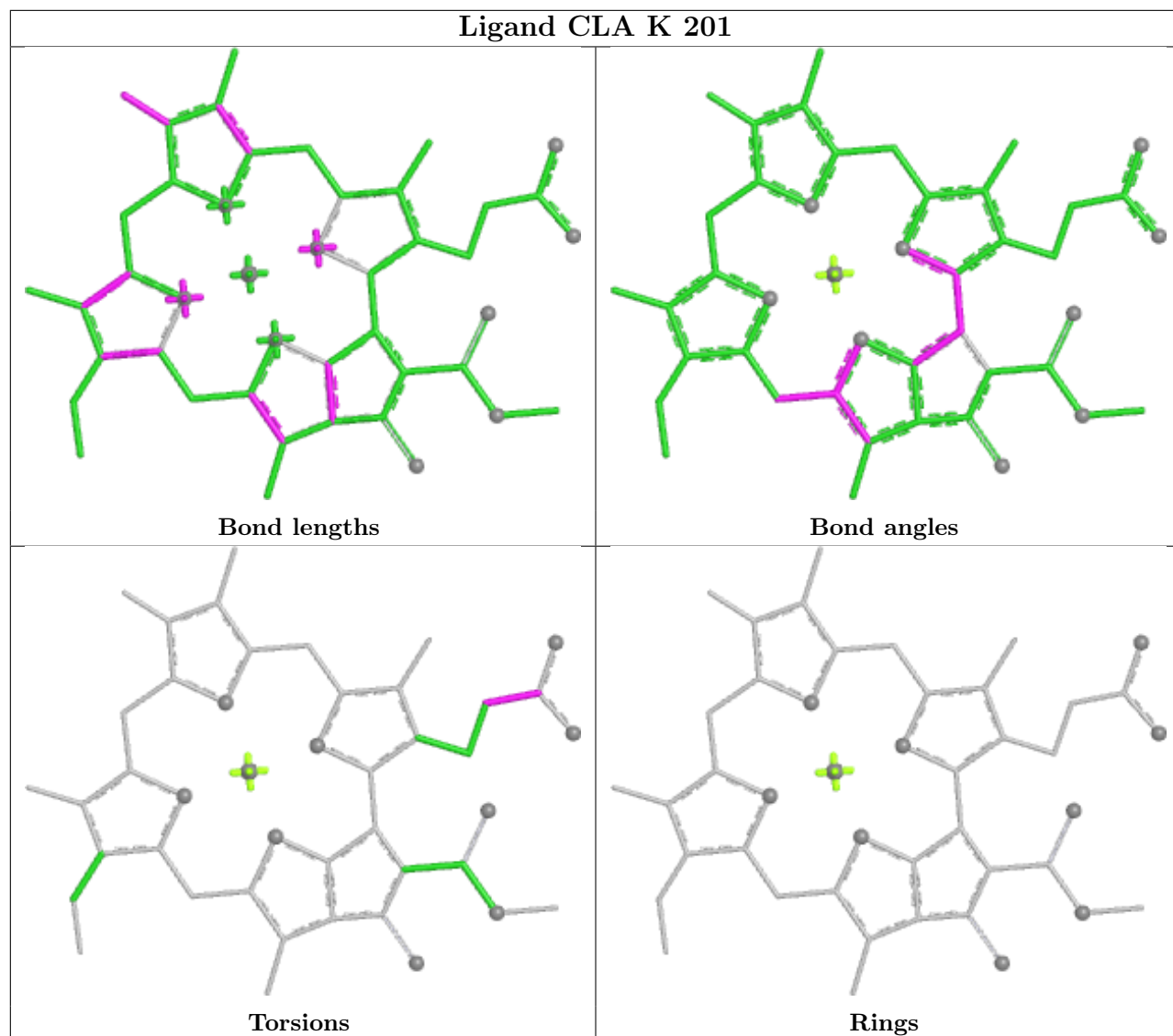




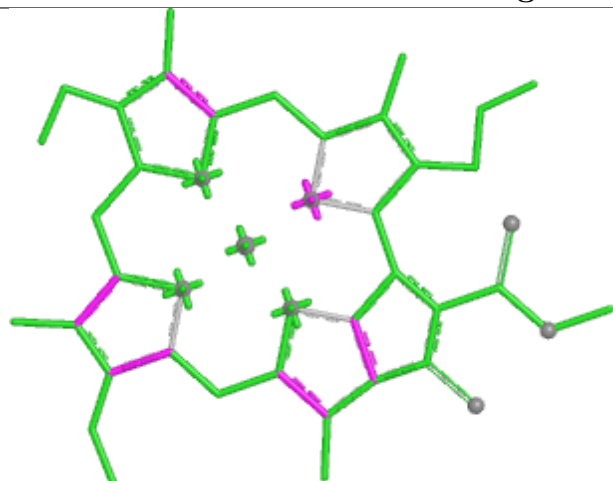




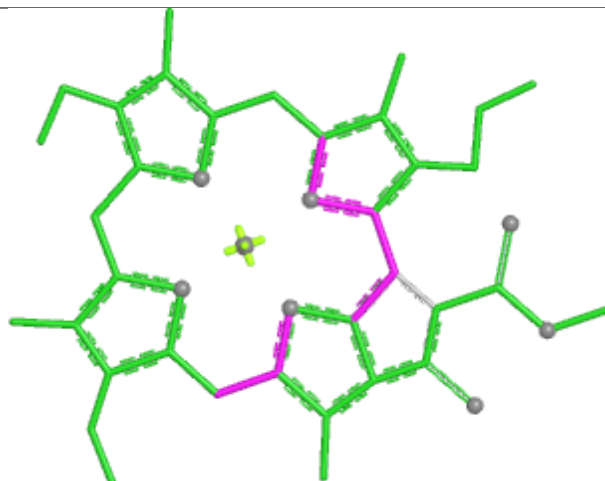




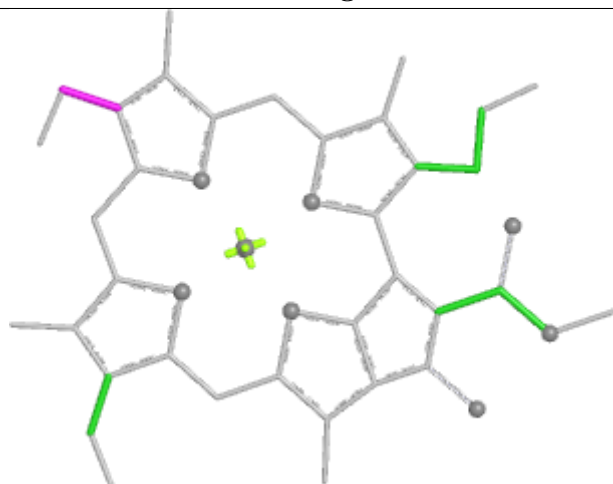
Ligand CLA b 819



Bond lengths



Bond angles

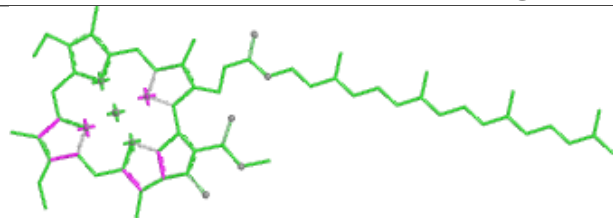


Torsions

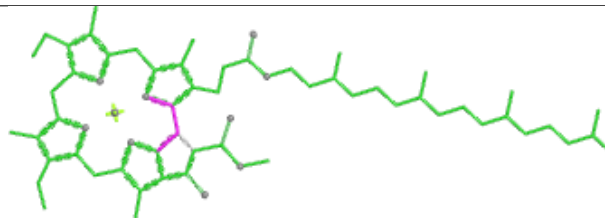


Rings

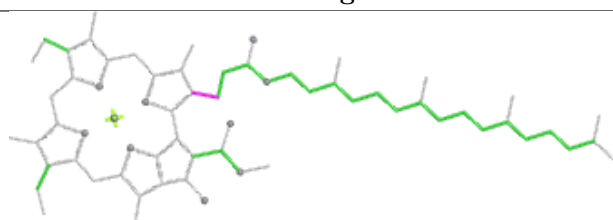
Ligand CLA A 832



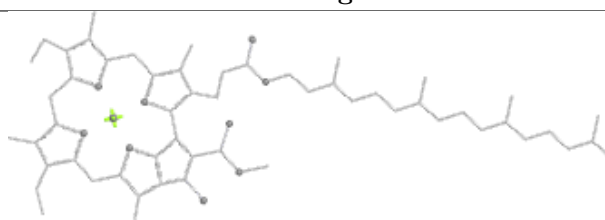
Bond lengths



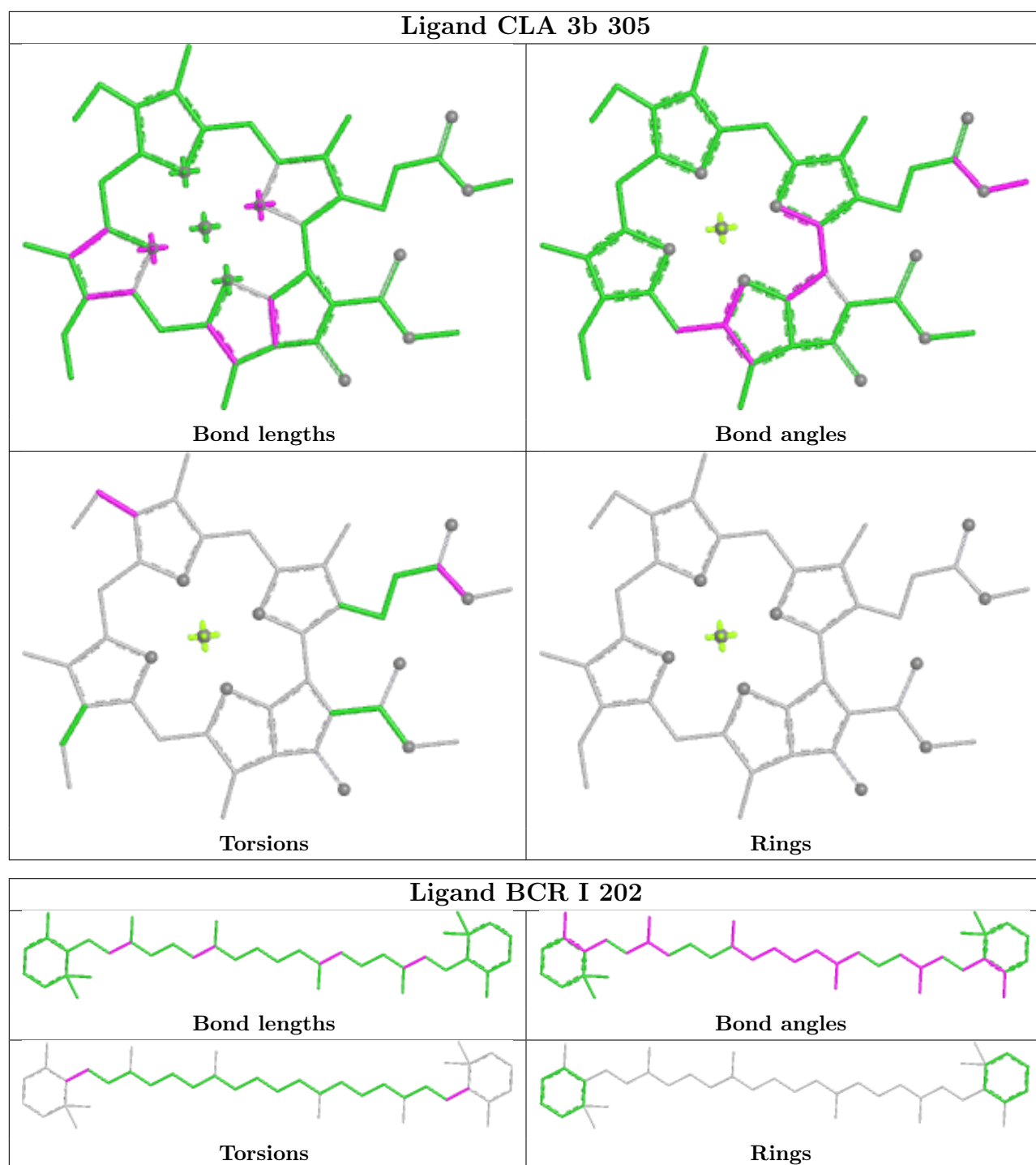
Bond angles

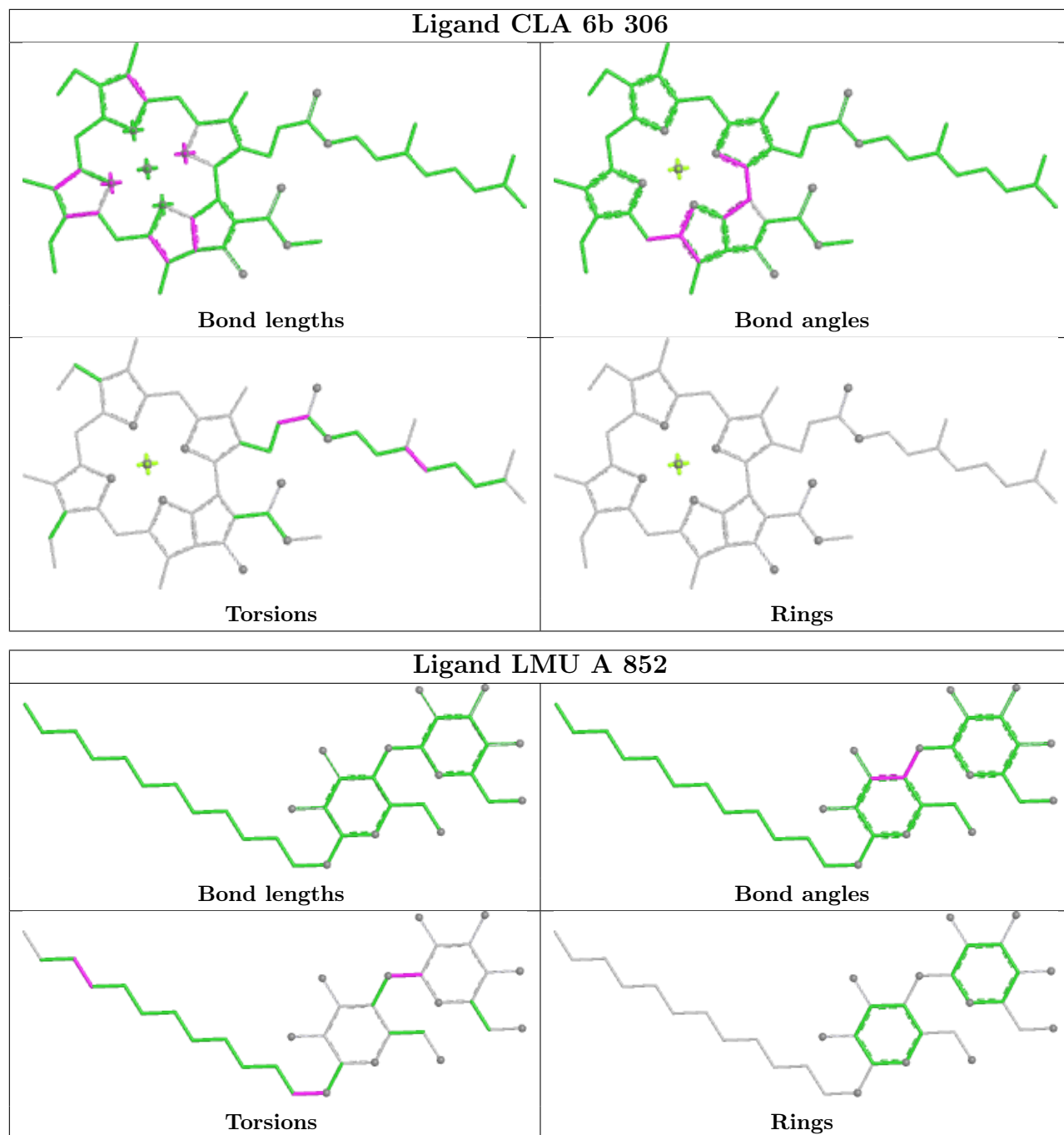


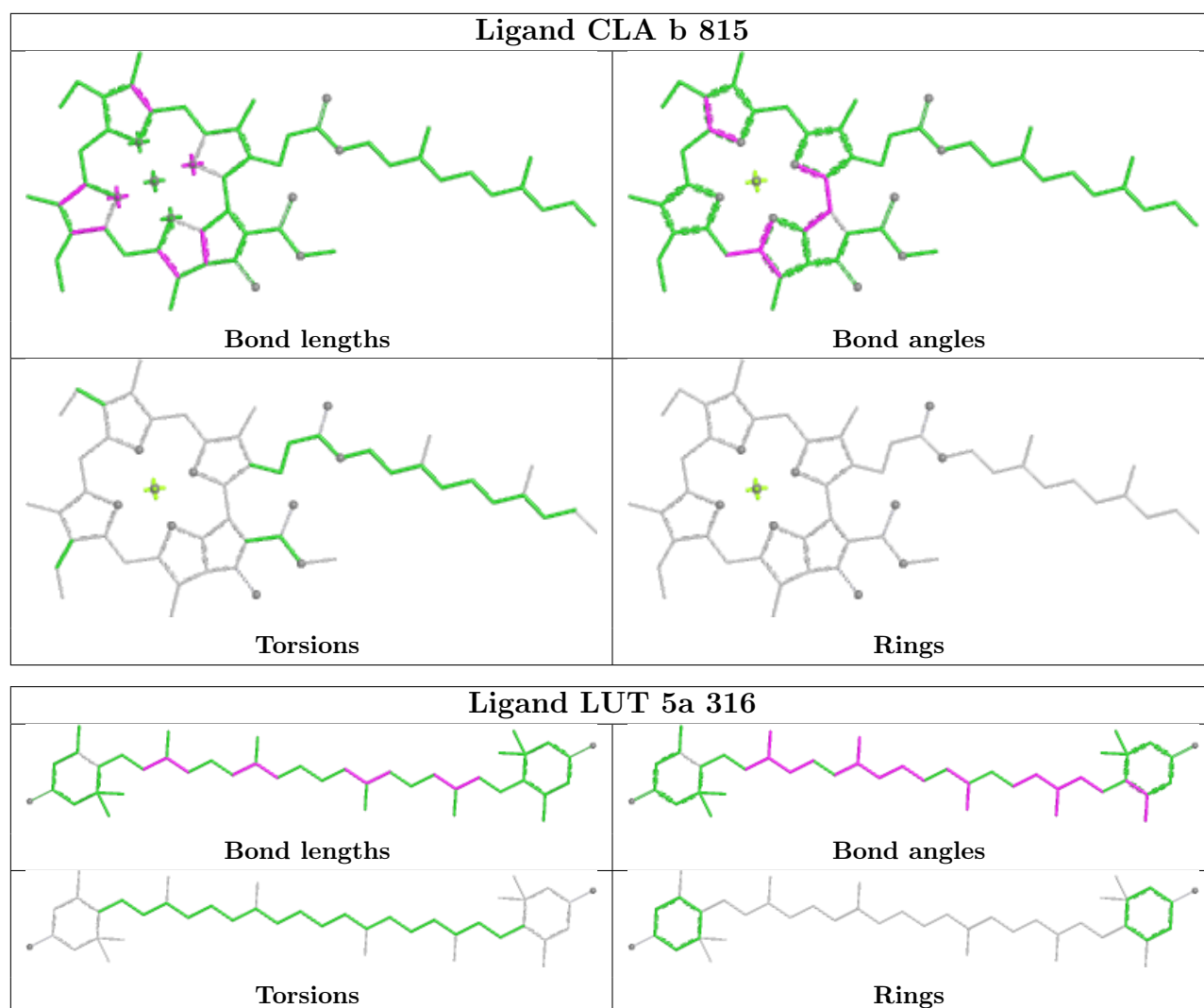
Torsions

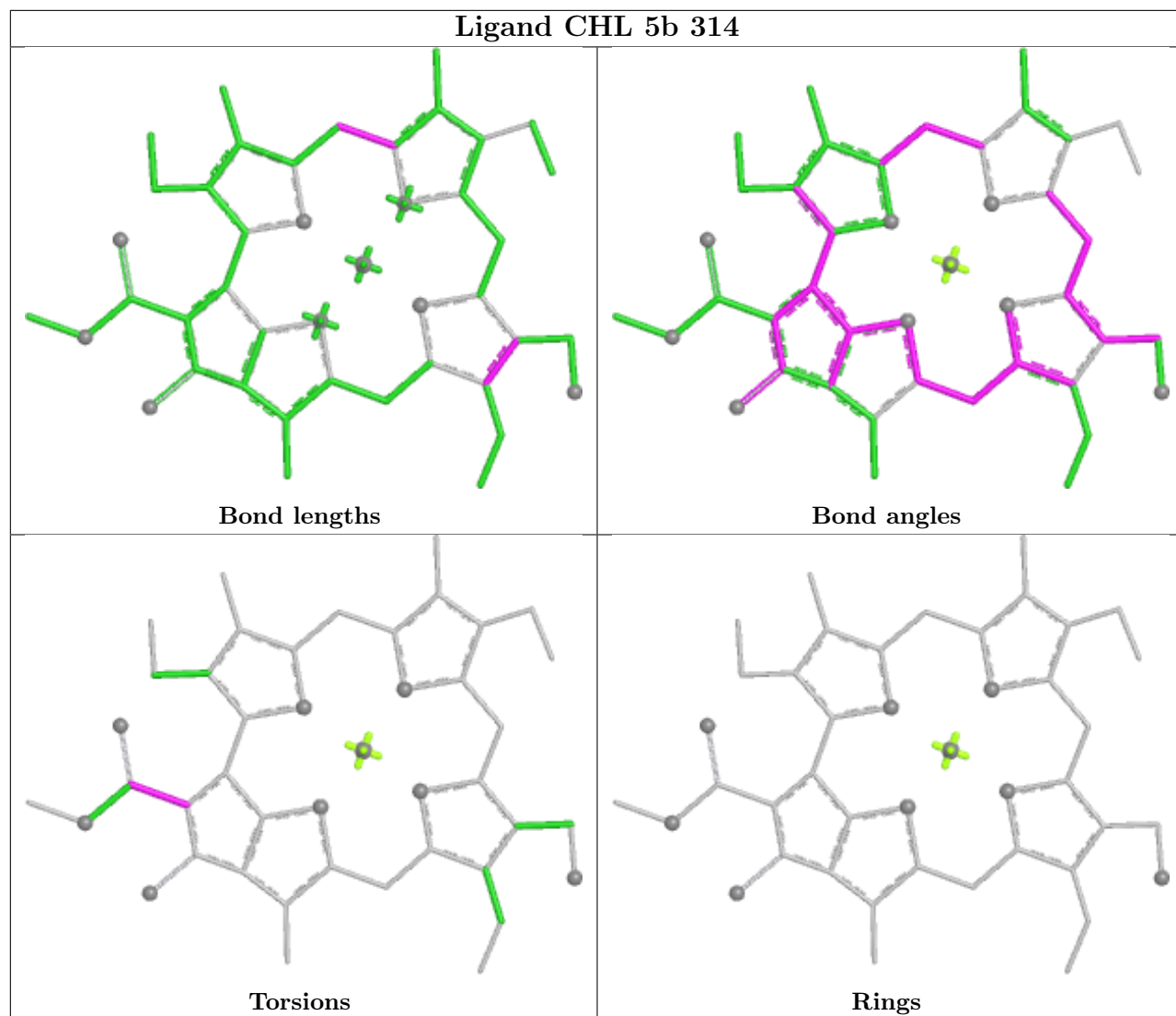


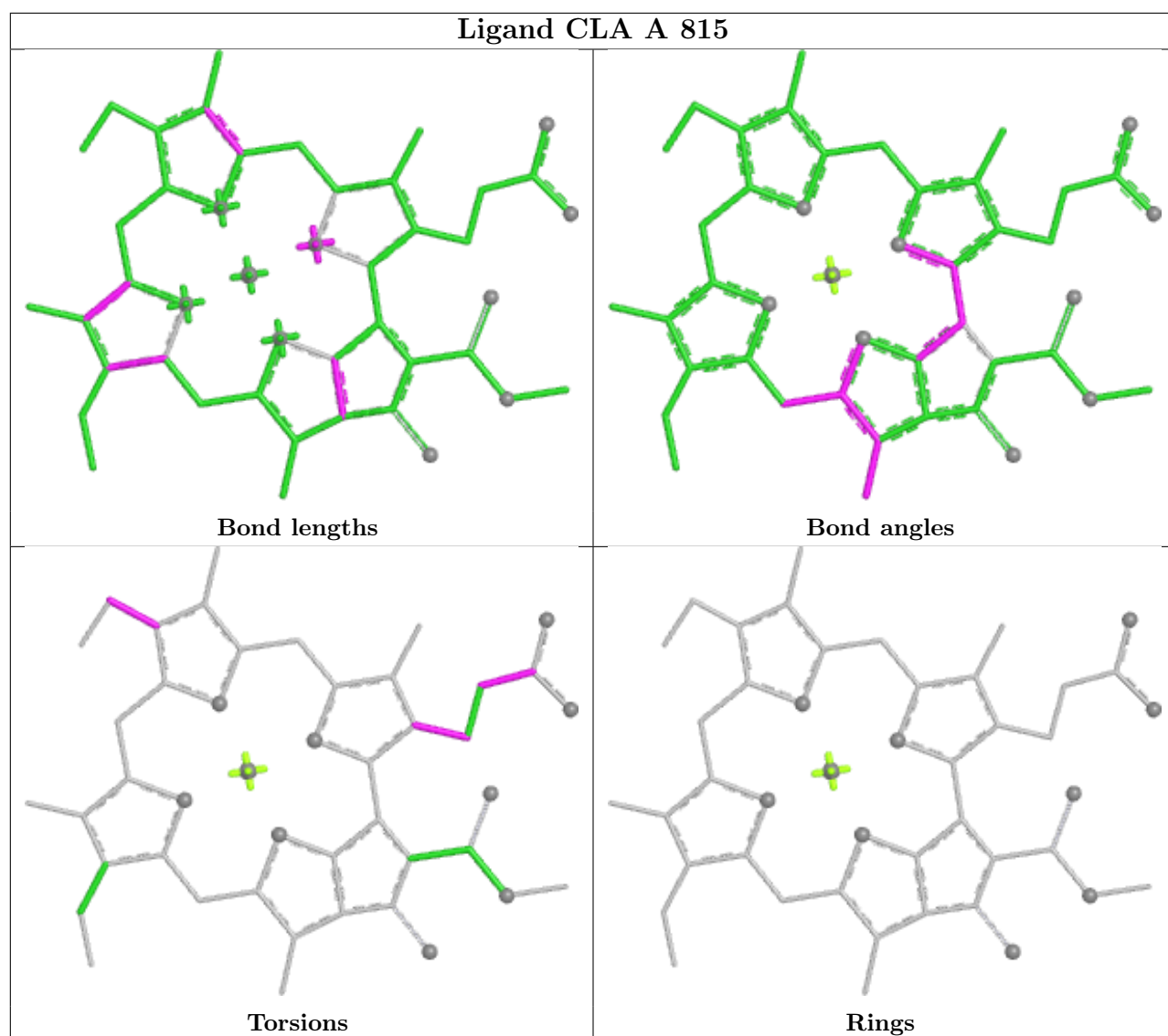
Rings



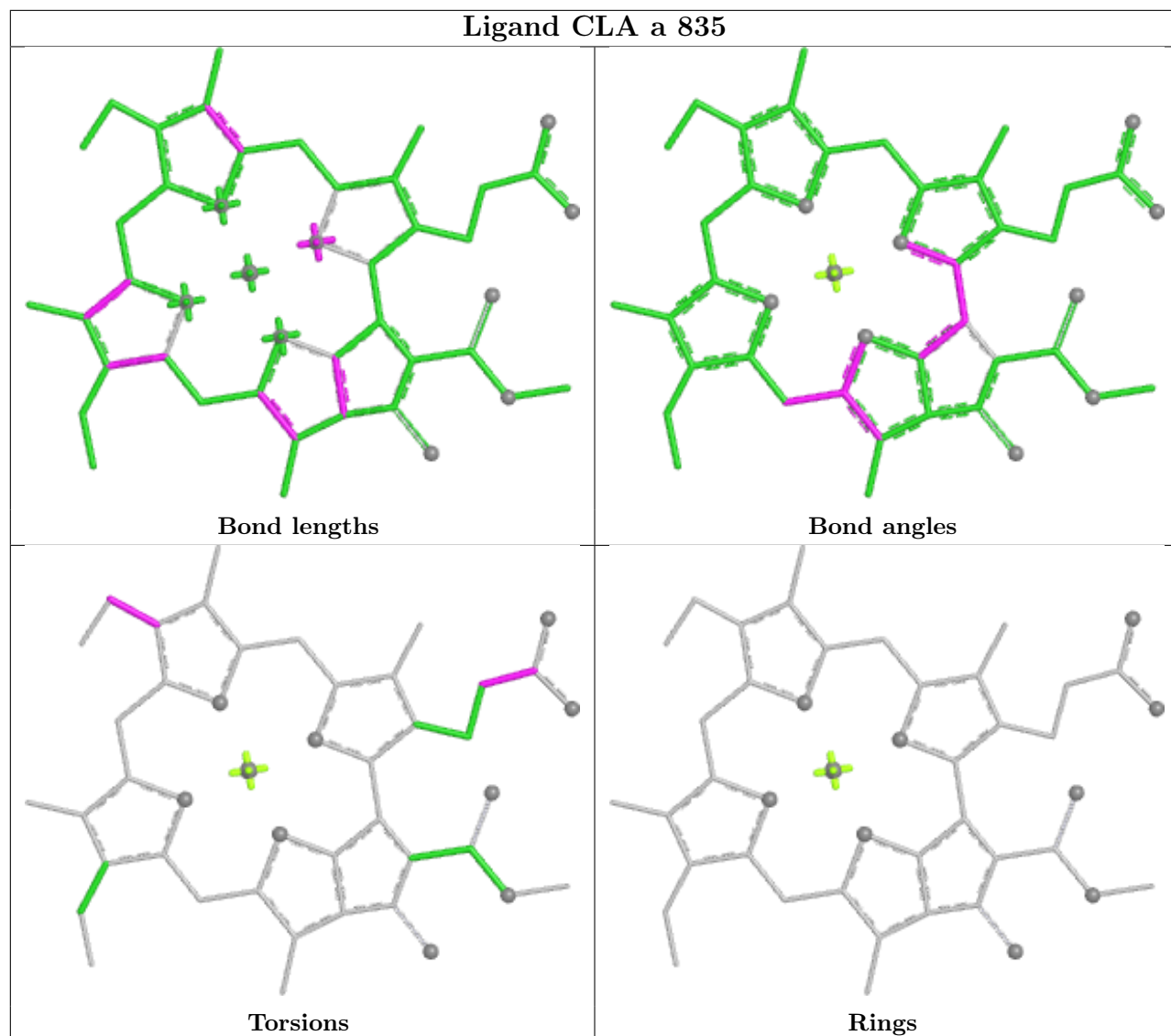


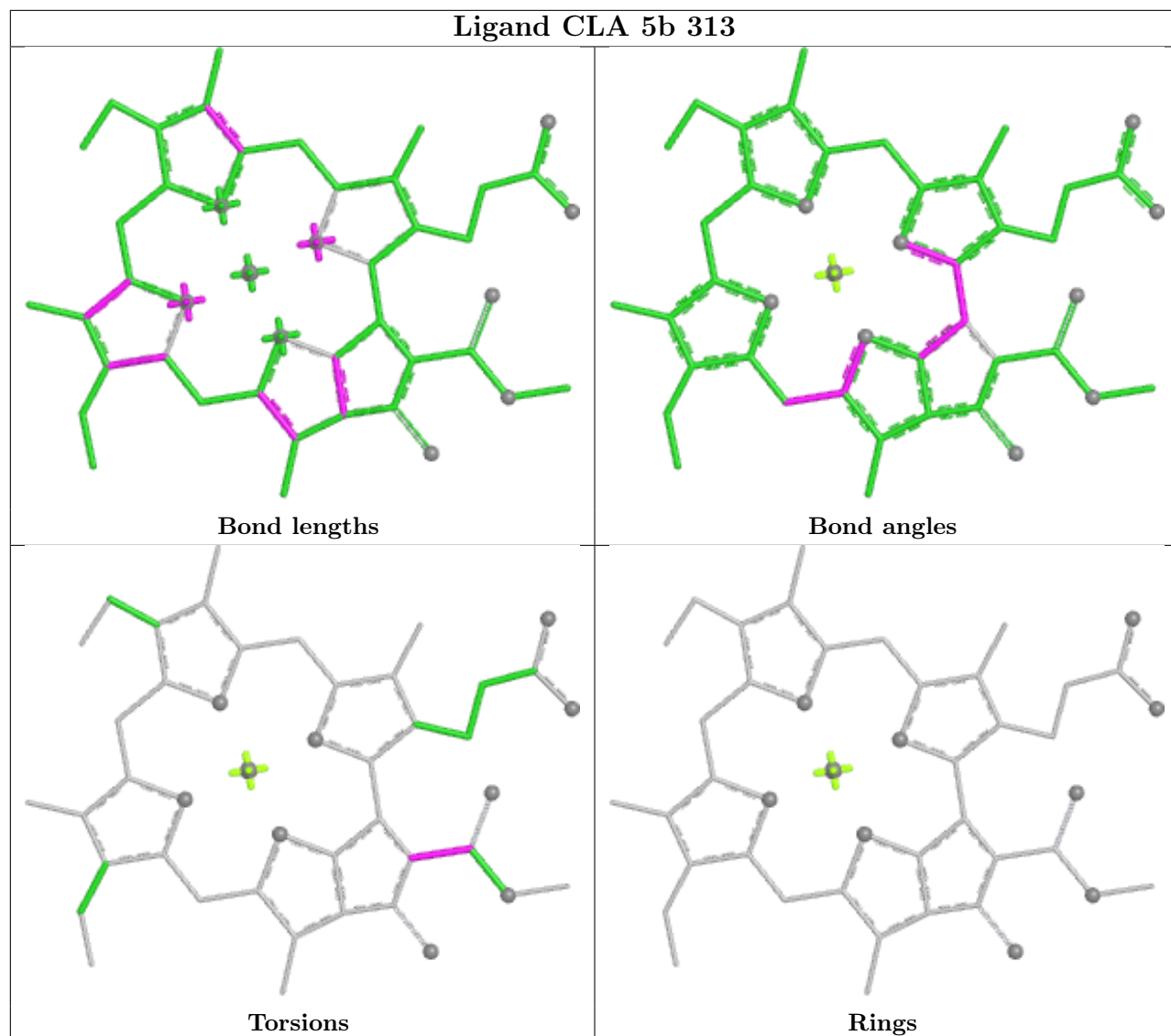


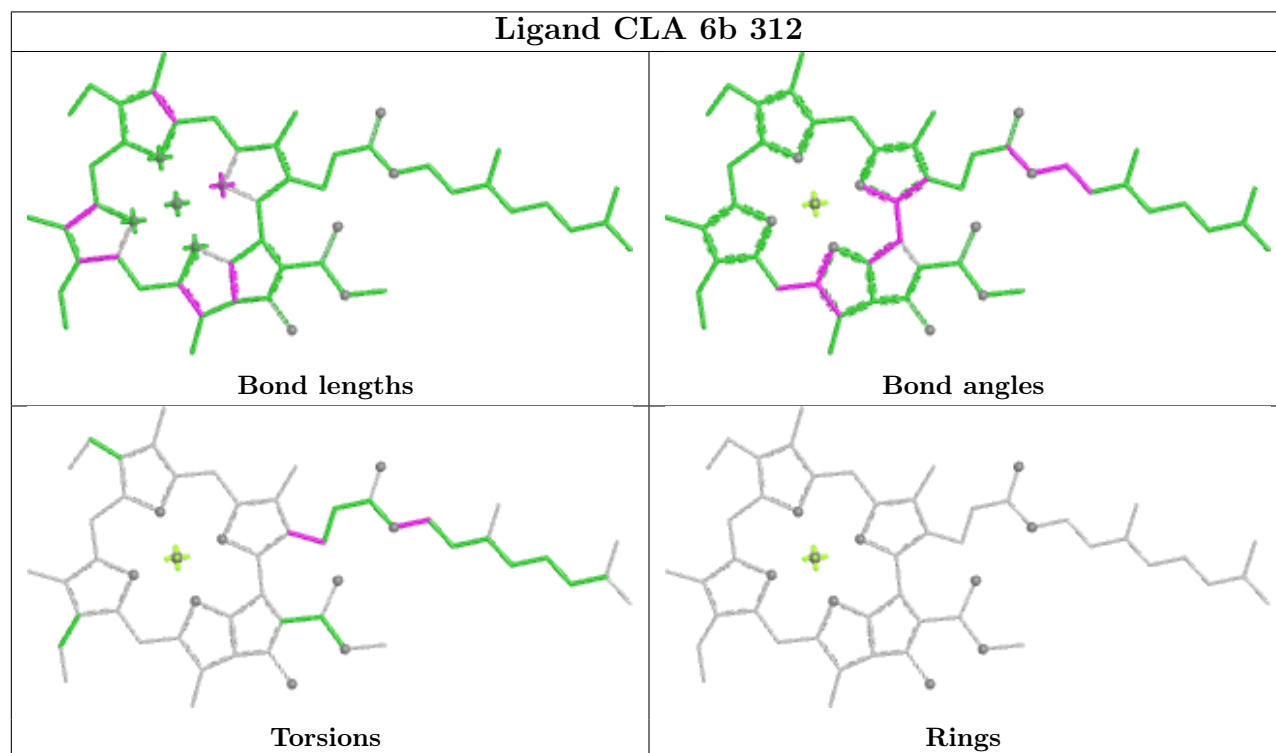
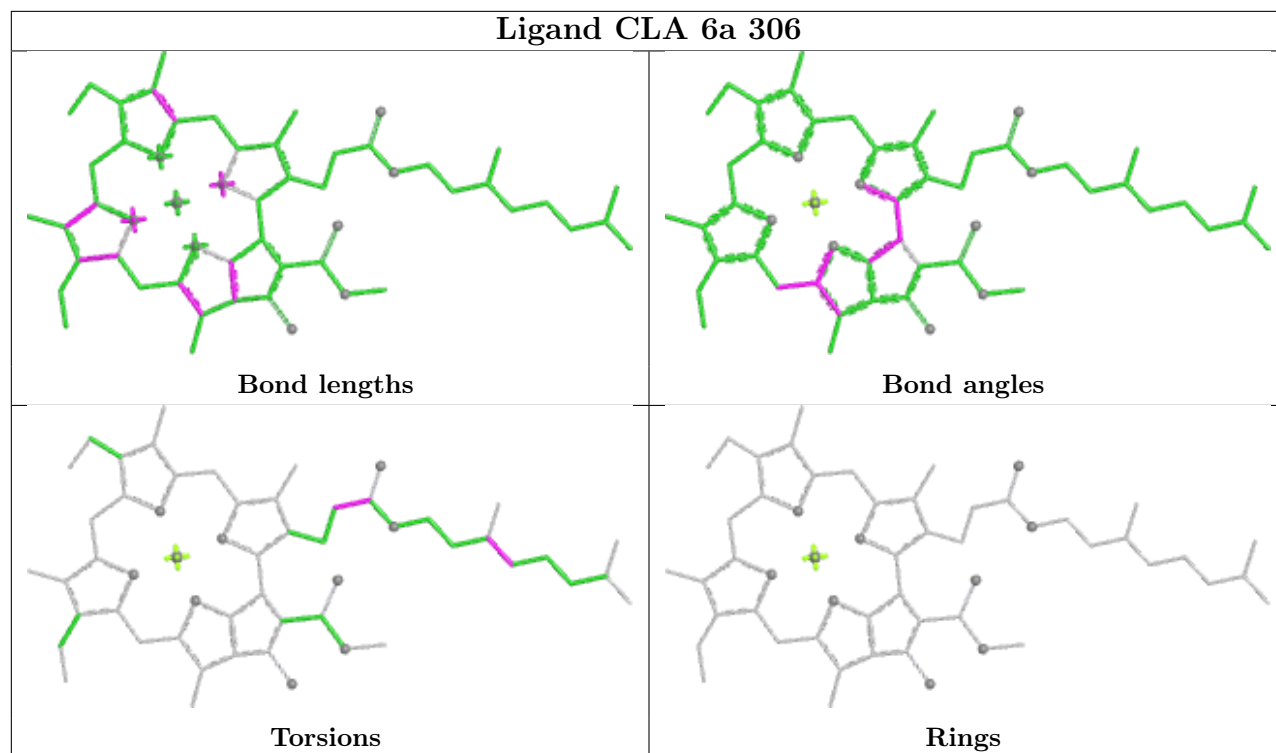


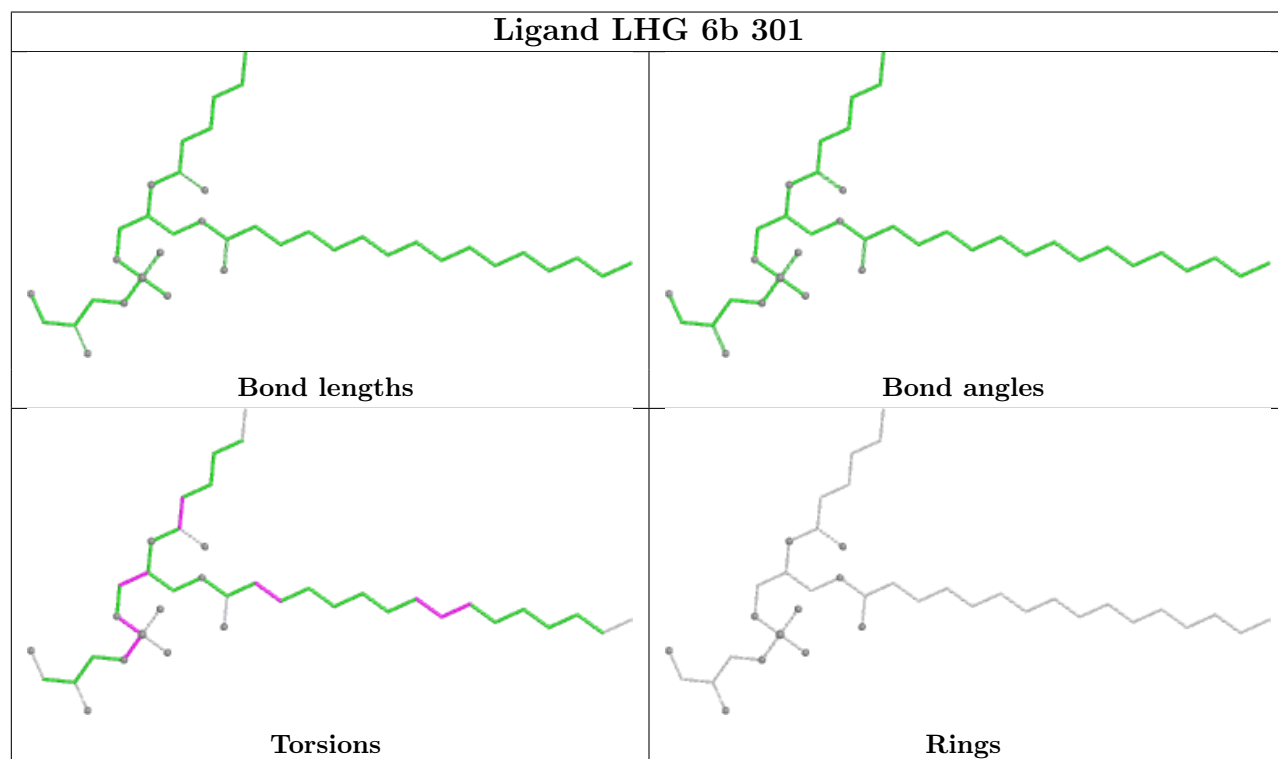
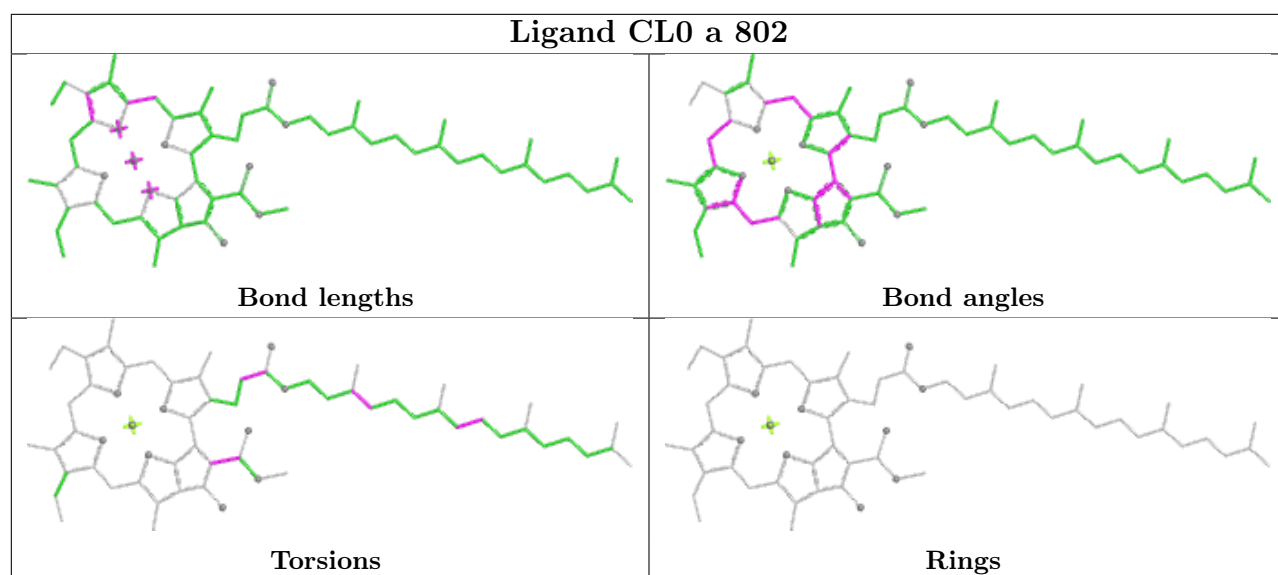


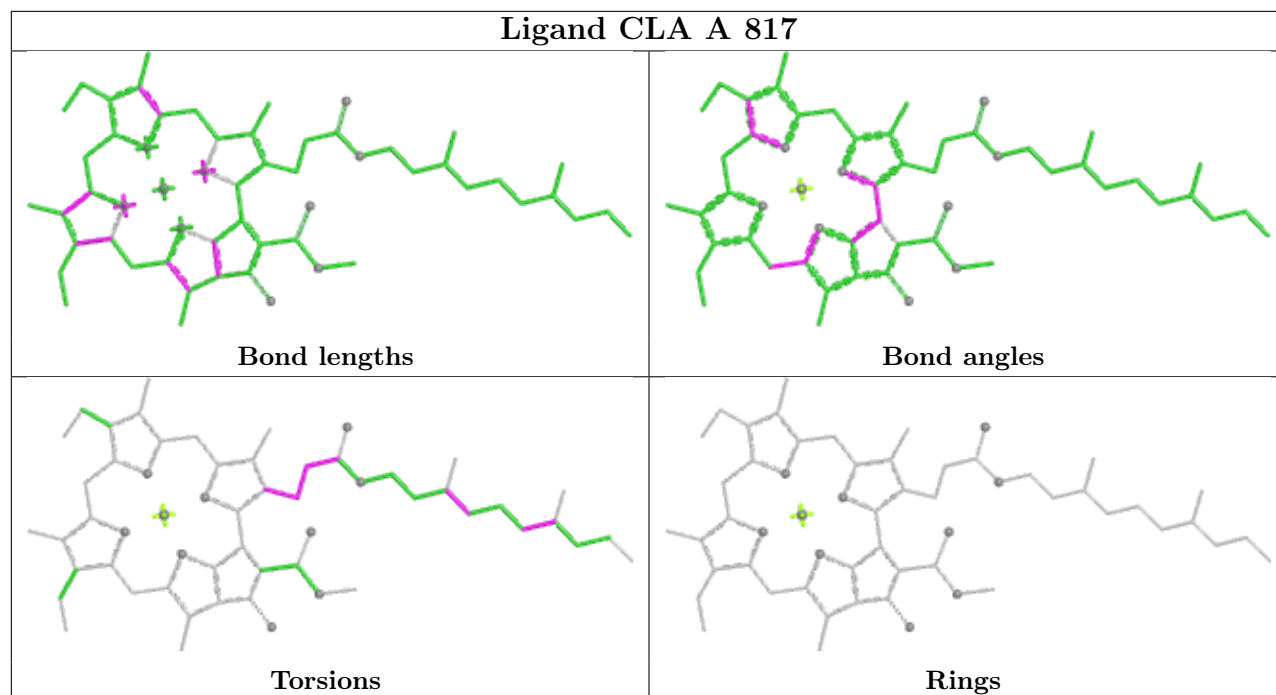
Ligand CLA a 835

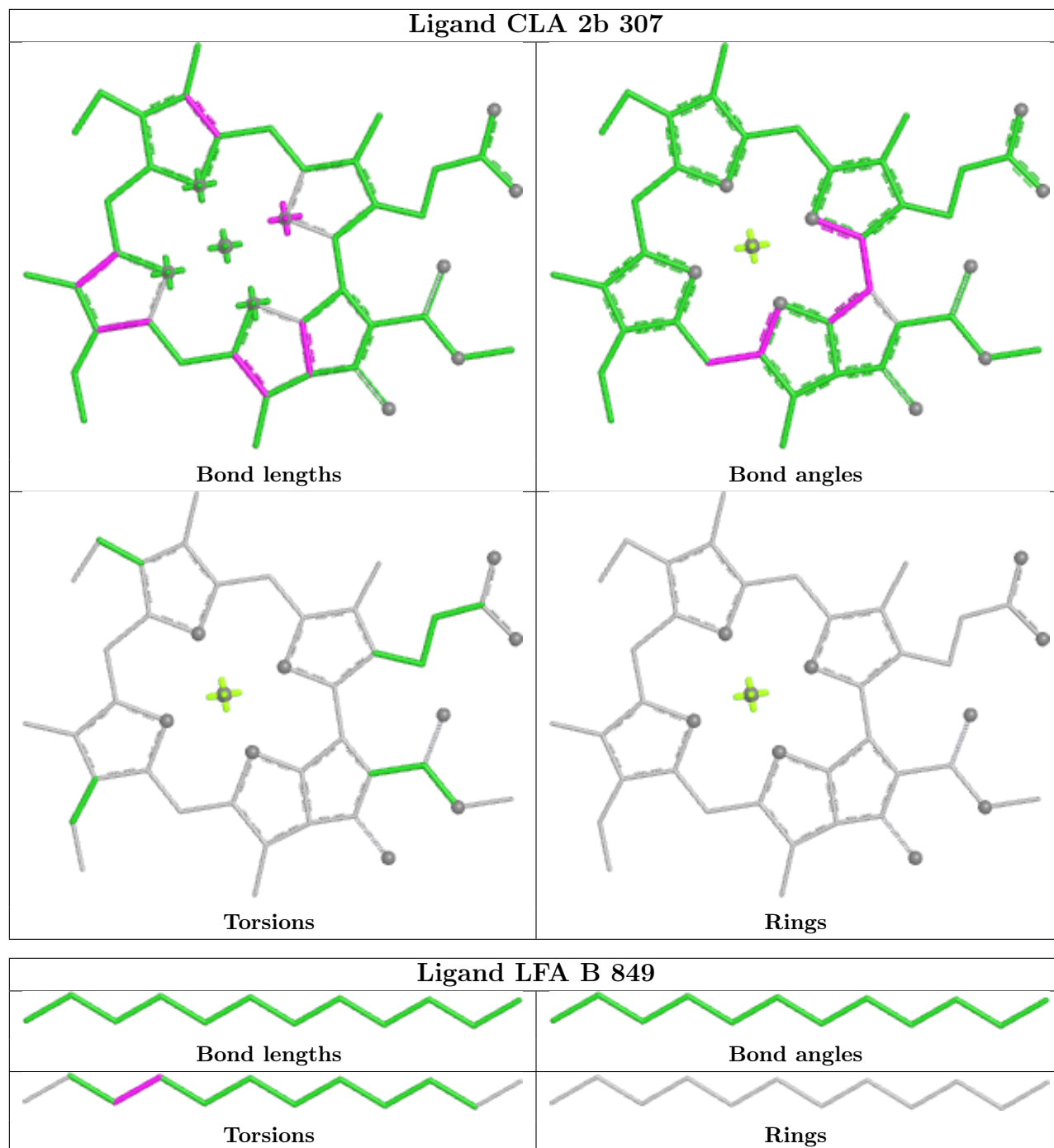


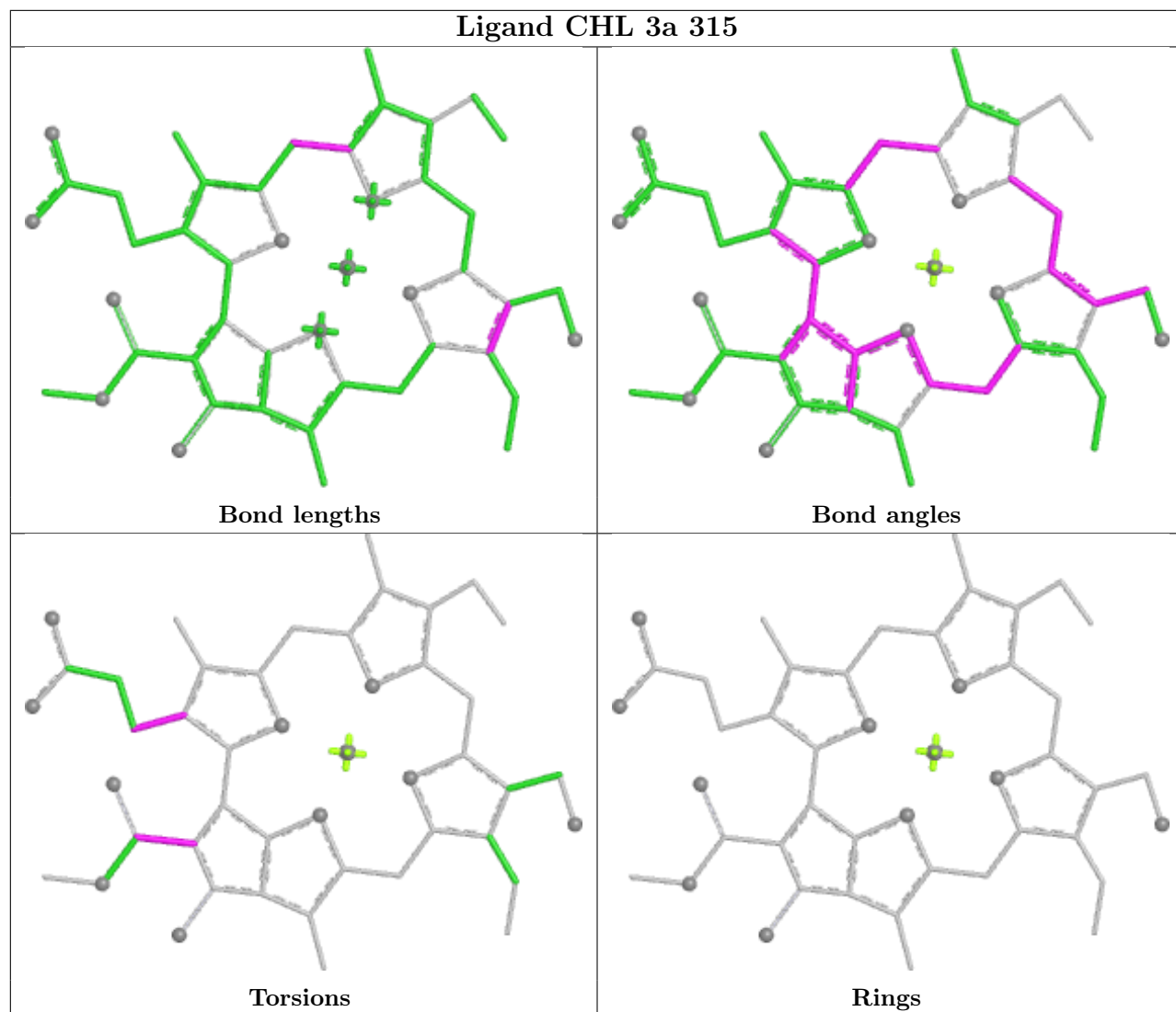


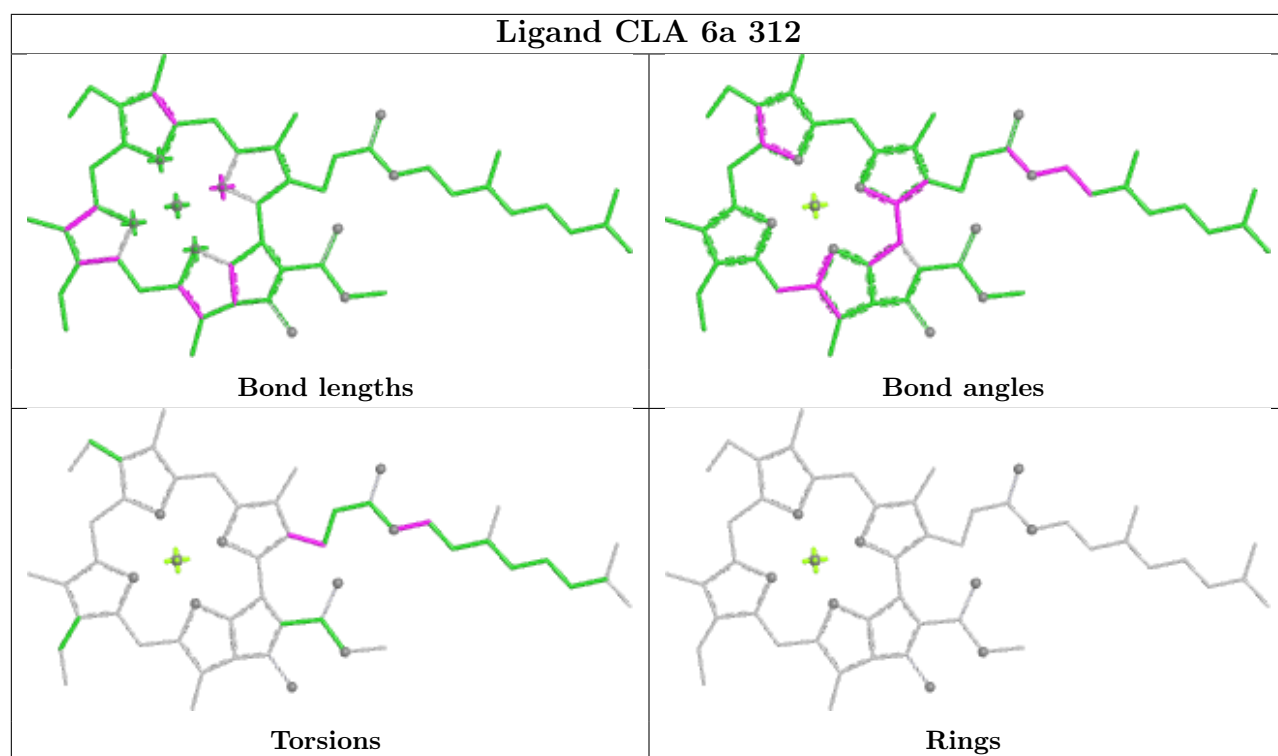


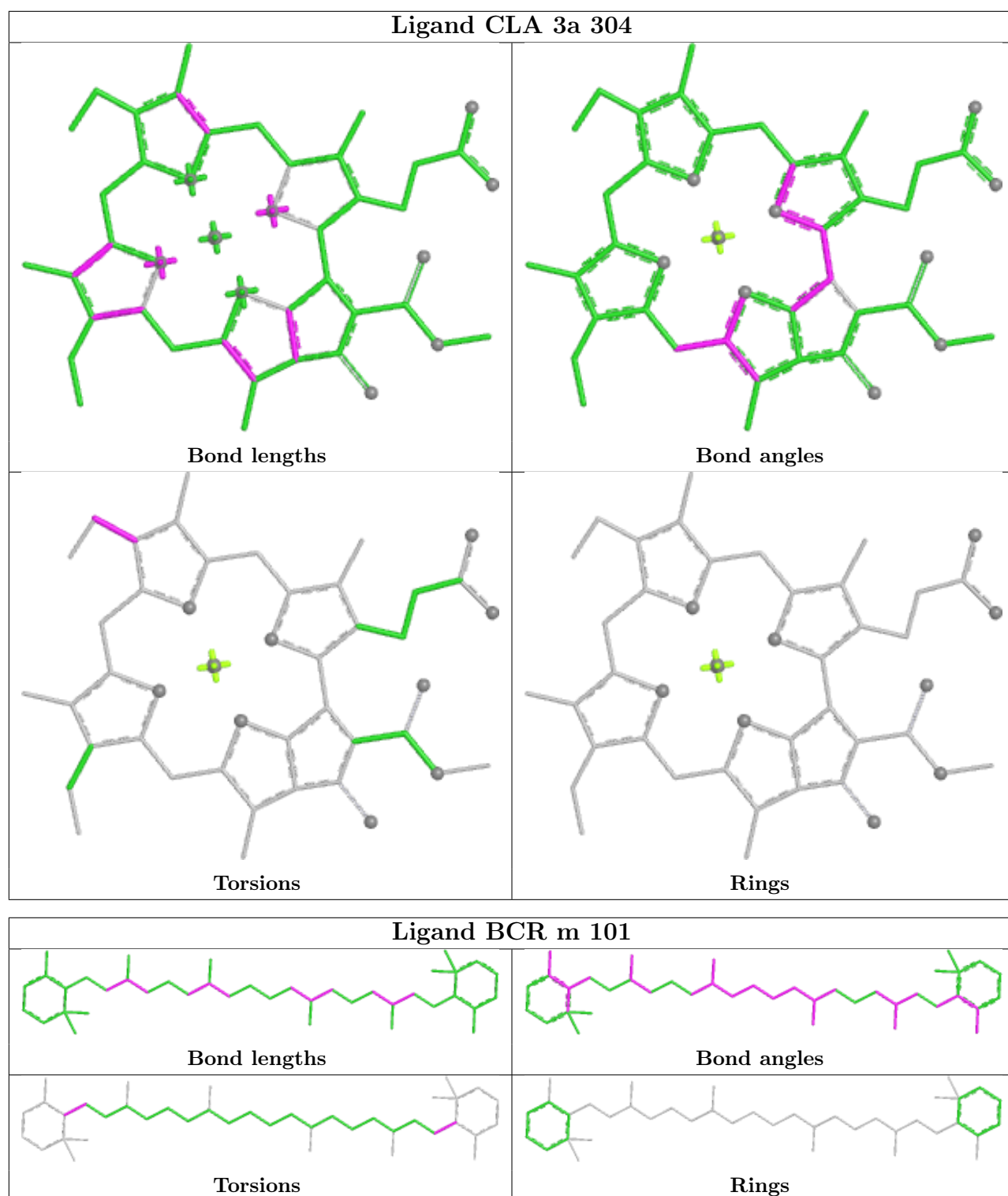


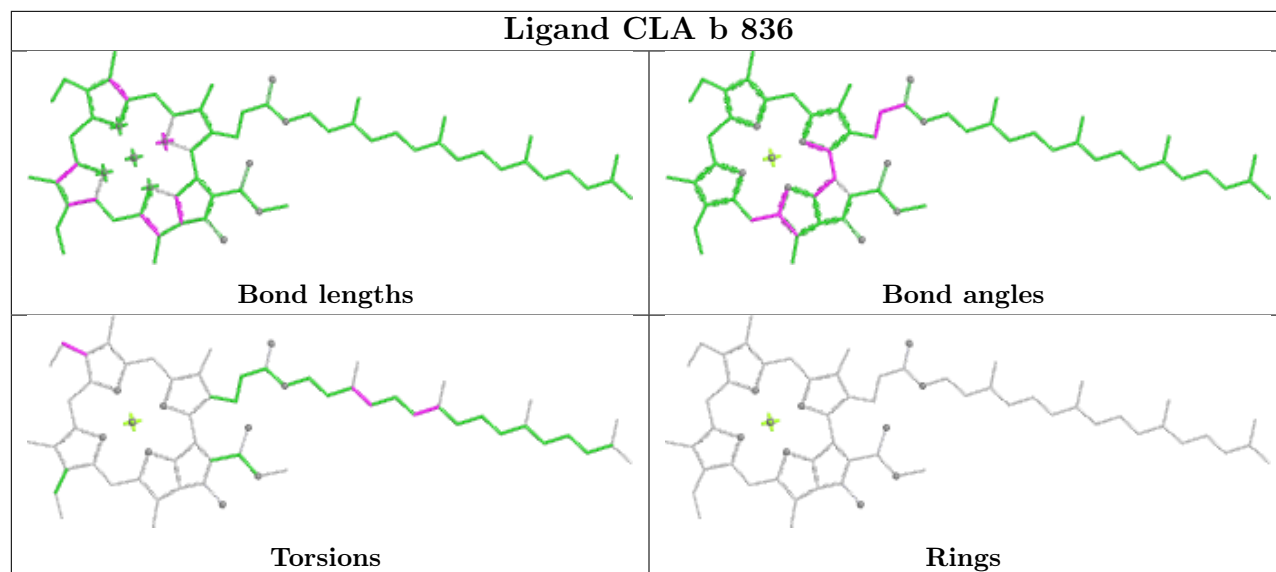
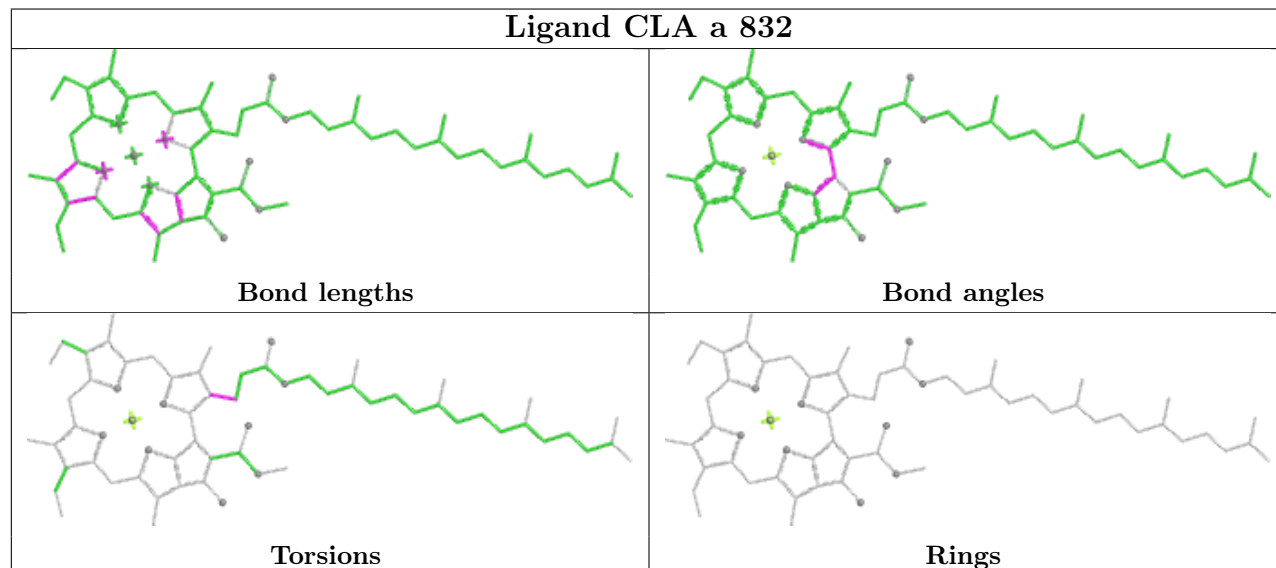




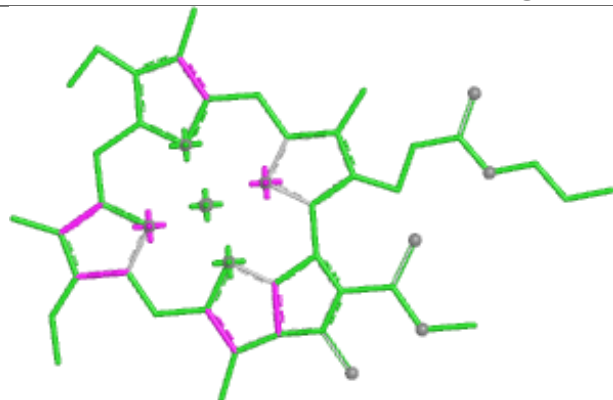




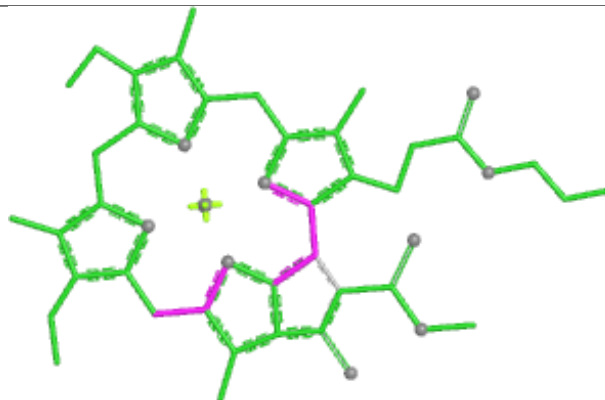


Ligand CLA b 836**Ligand CLA a 832**

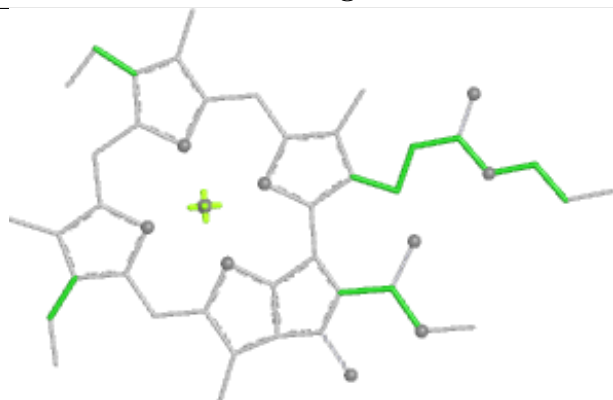
Ligand CLA a 807



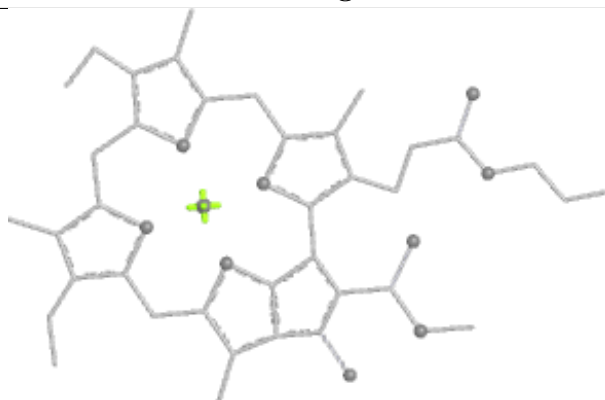
Bond lengths



Bond angles

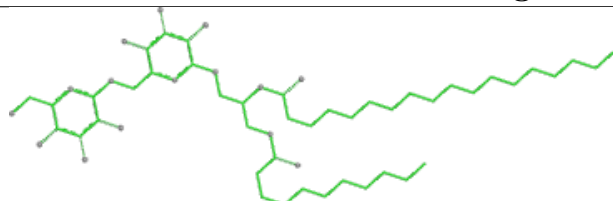


Torsions

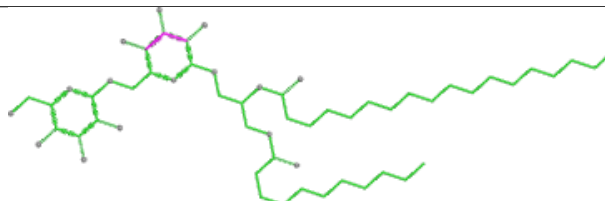


Rings

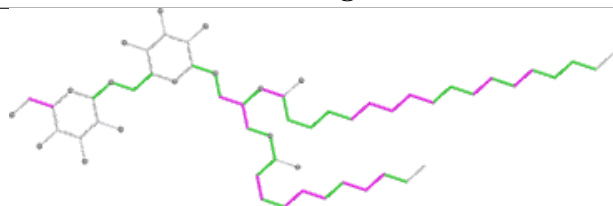
Ligand DGD b 847



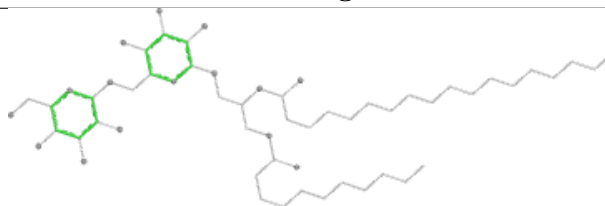
Bond lengths



Bond angles

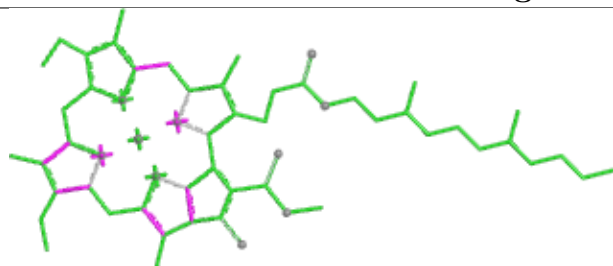


Torsions

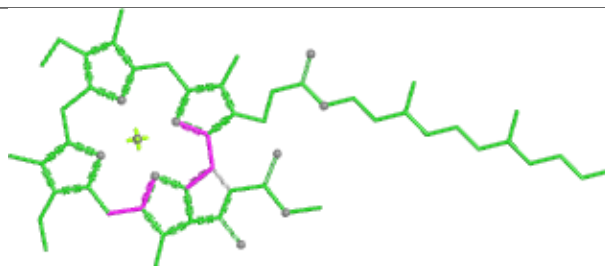


Rings

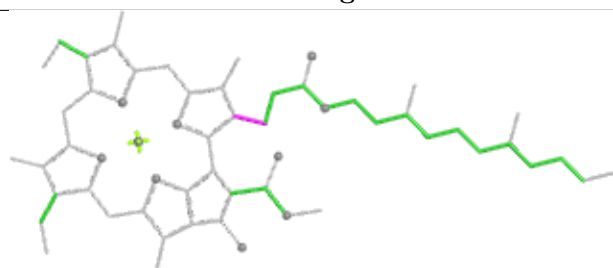
Ligand CLA B 826



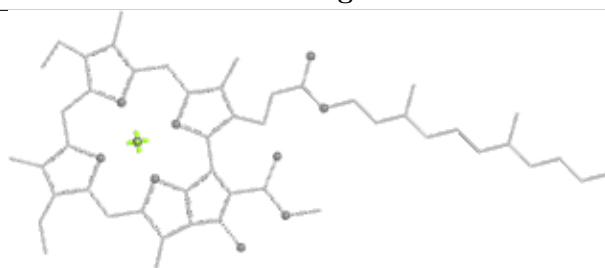
Bond lengths



Bond angles

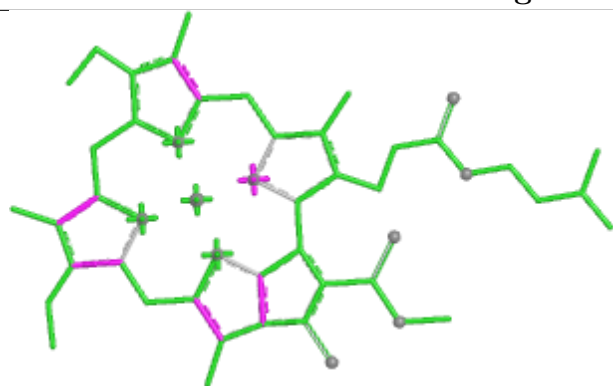


Torsions

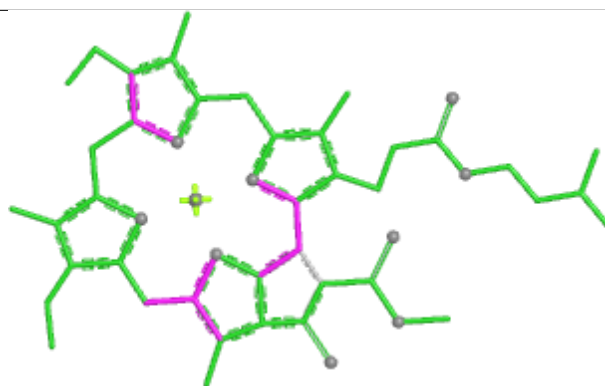


Rings

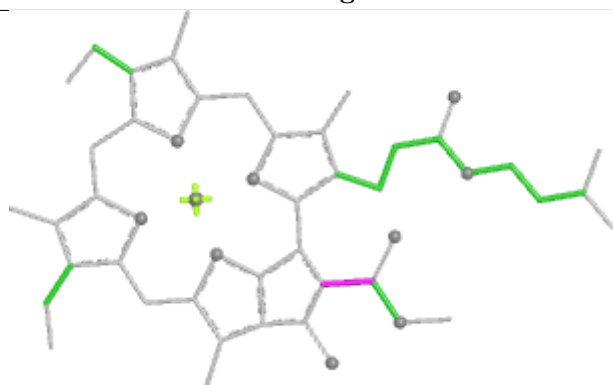
Ligand CLA B 824



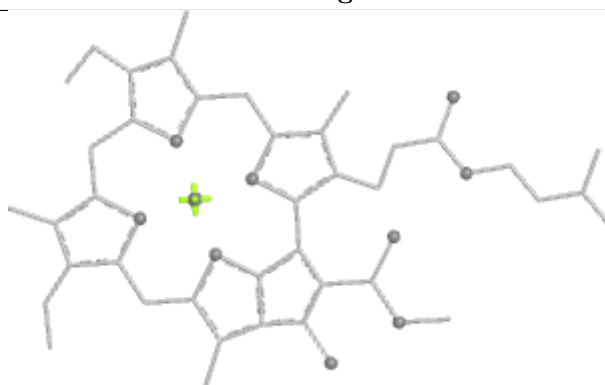
Bond lengths



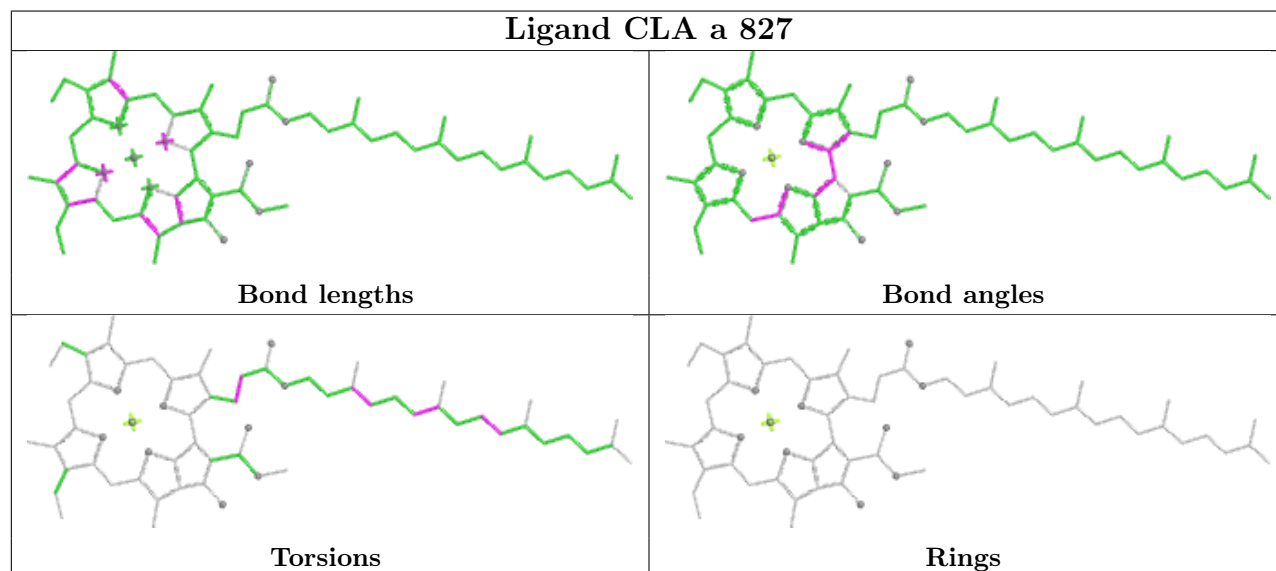
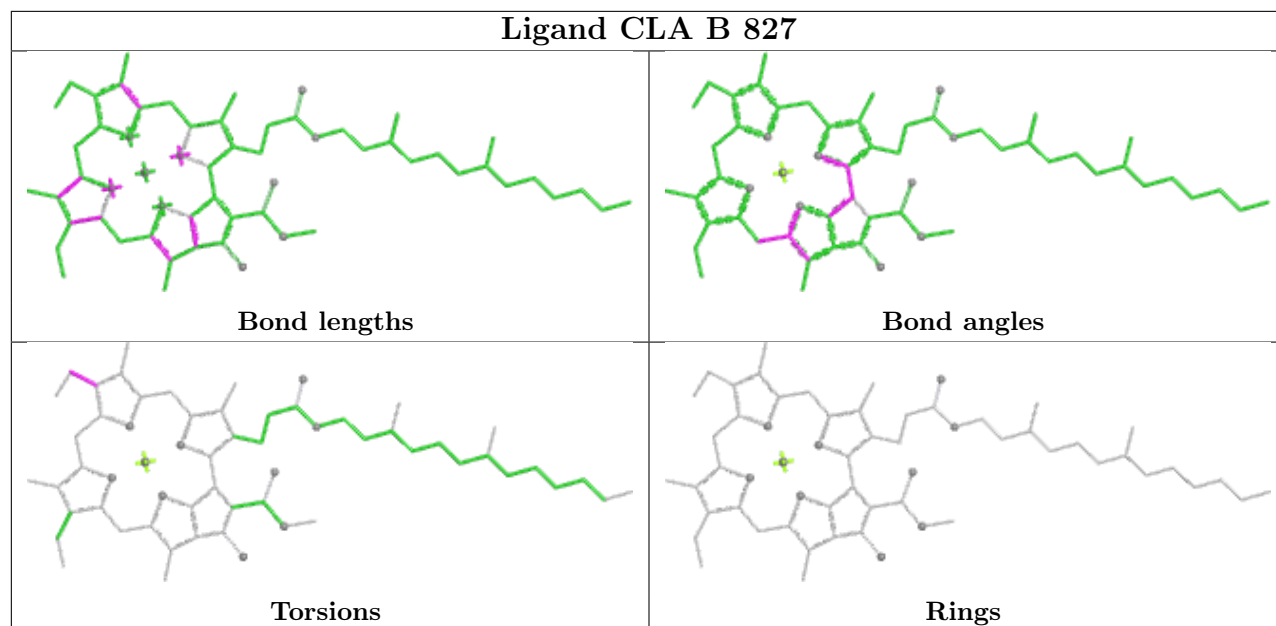
Bond angles

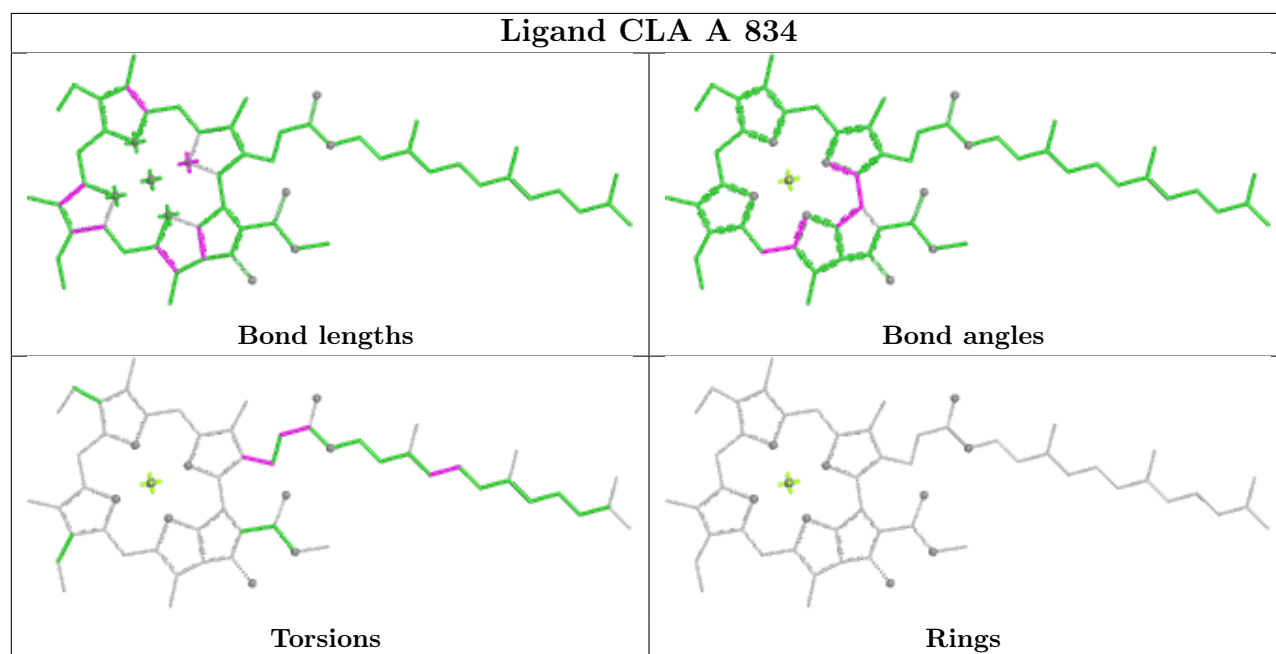
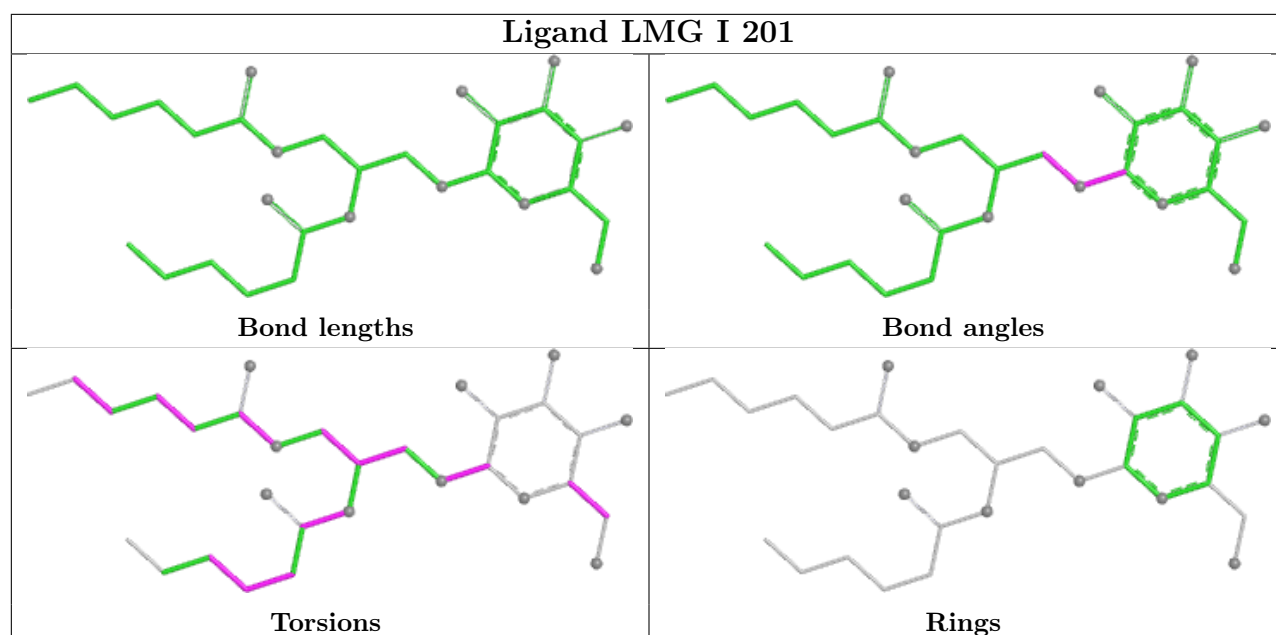


Torsions

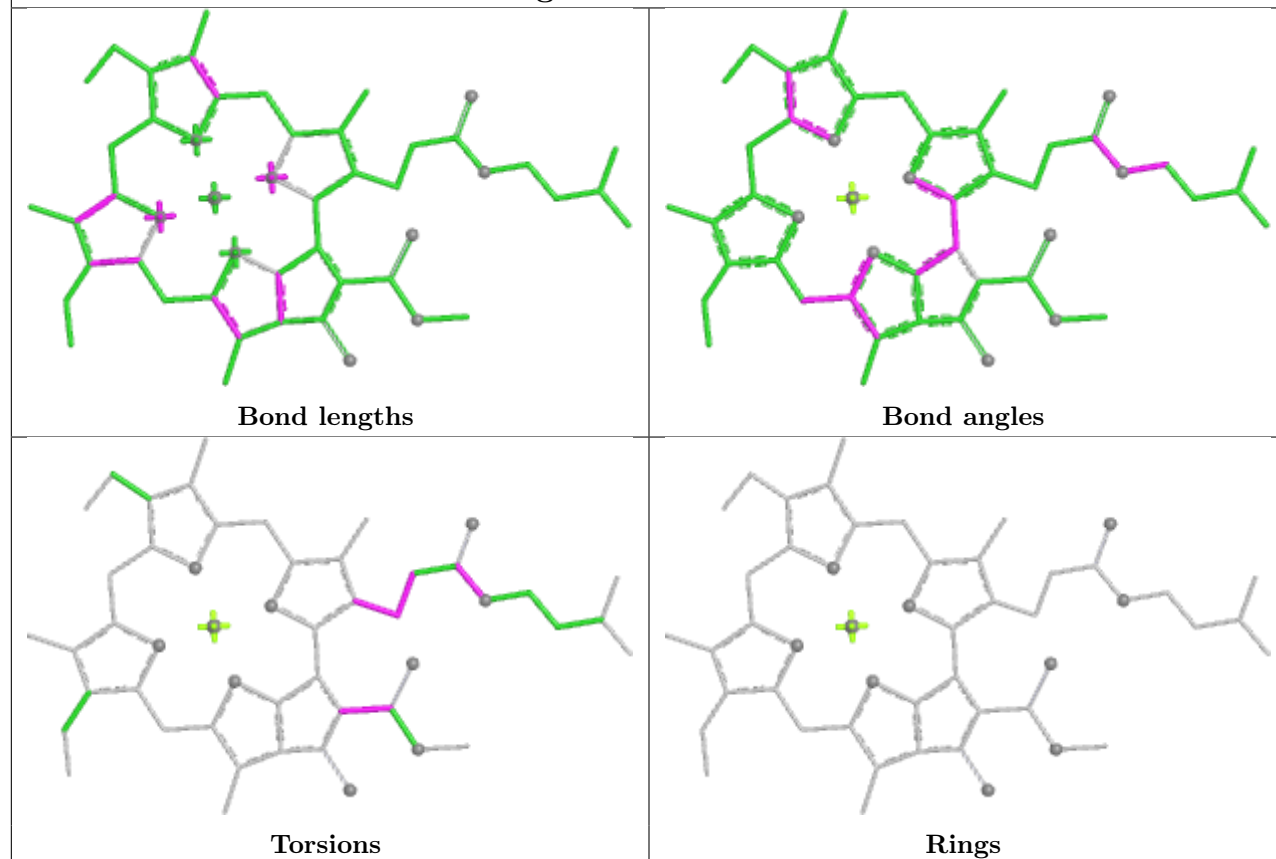


Rings

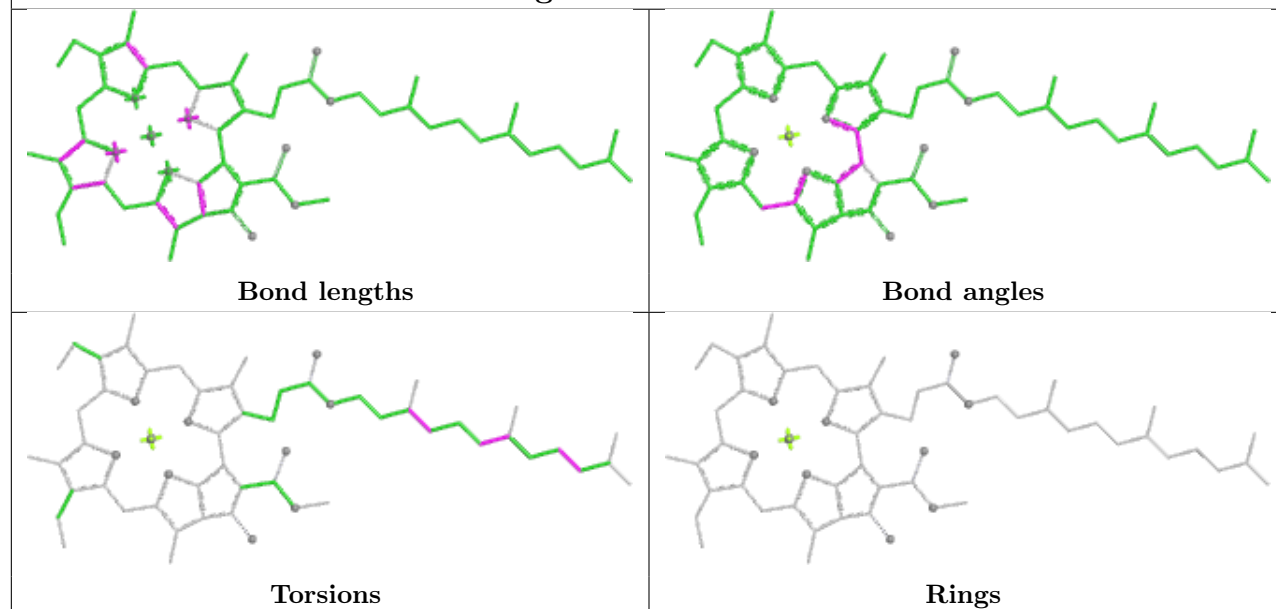


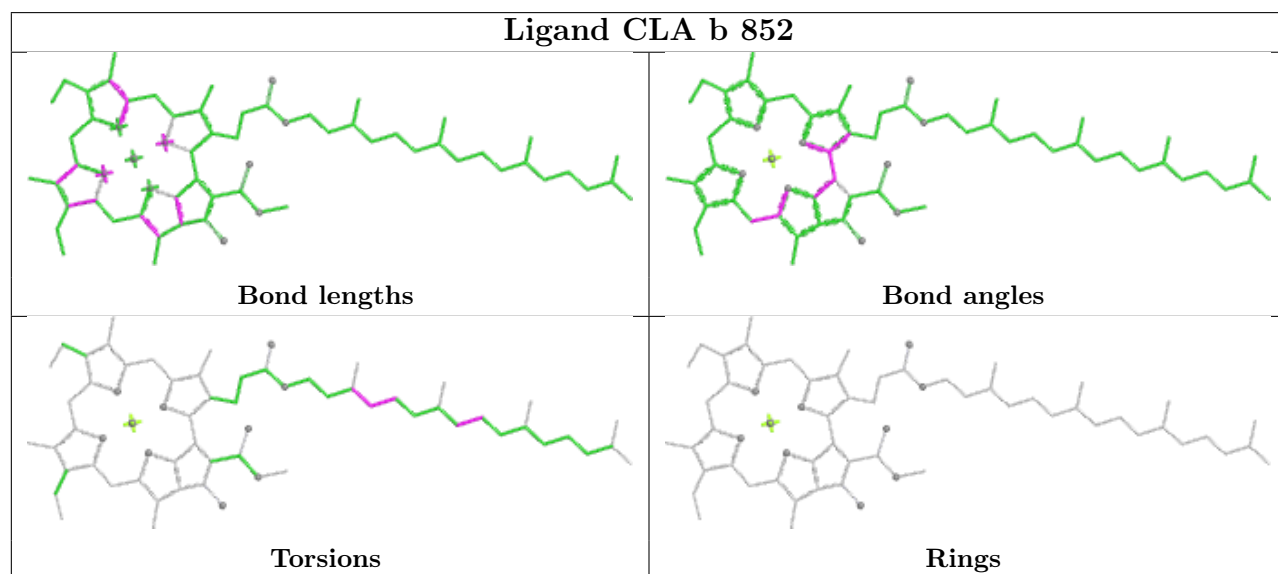
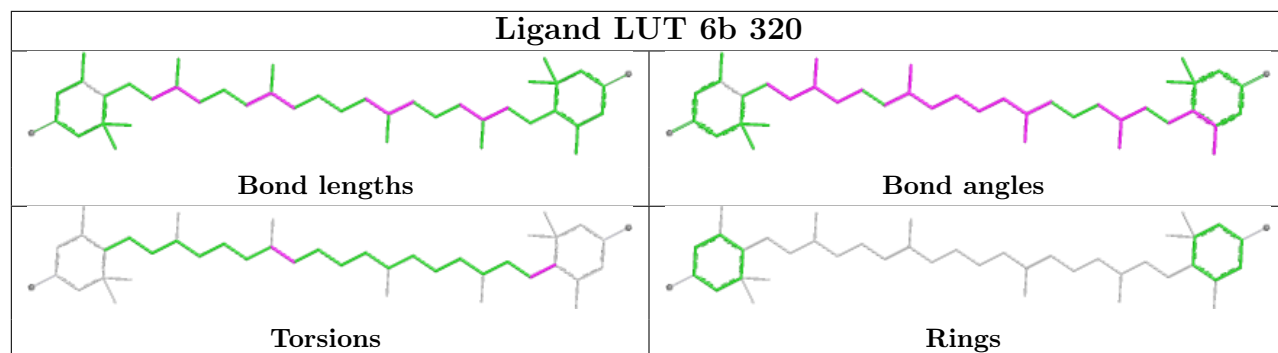


Ligand CLA a 830

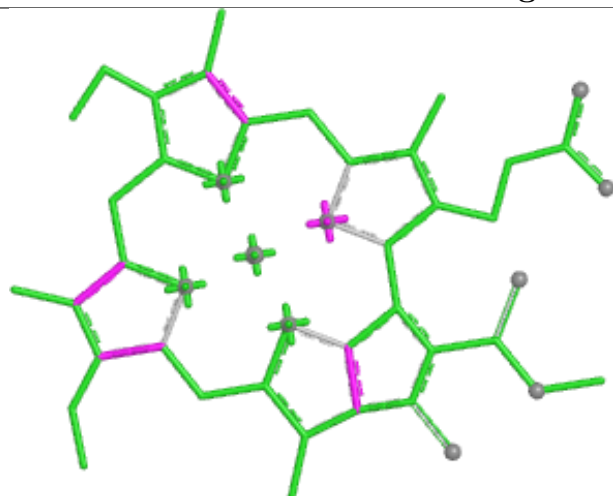


Ligand CLA b 810

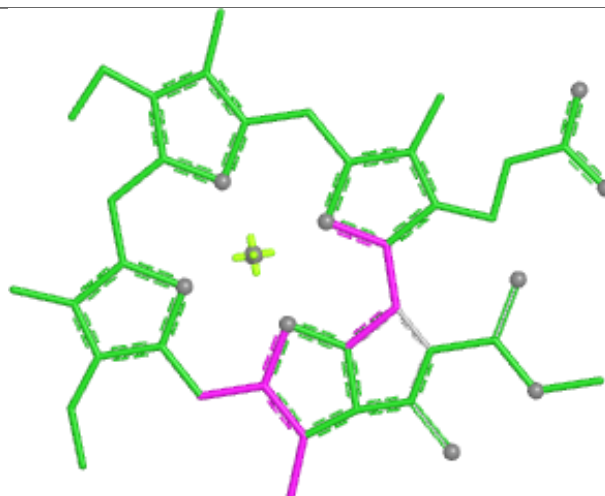




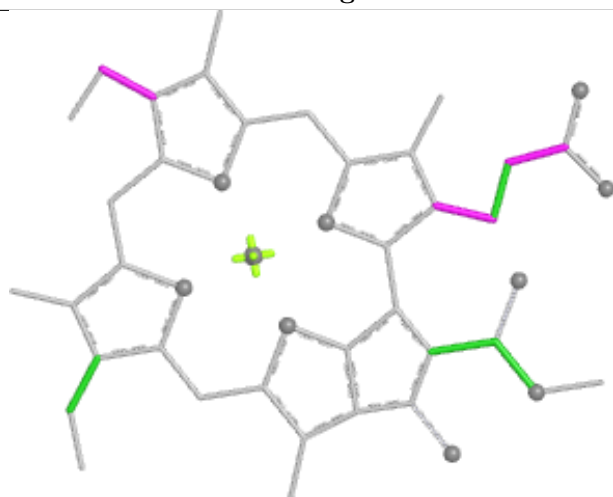
Ligand CLA a 815



Bond lengths



Bond angles

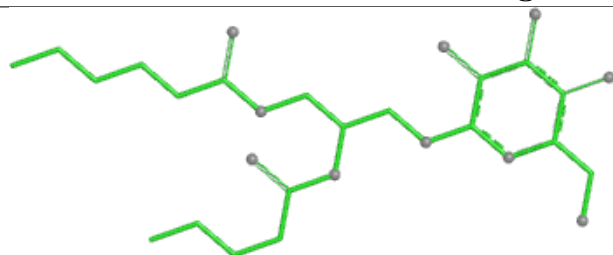


Torsions

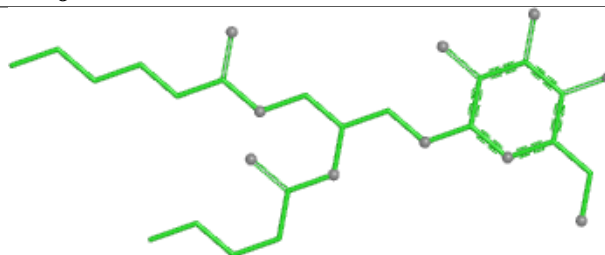


Rings

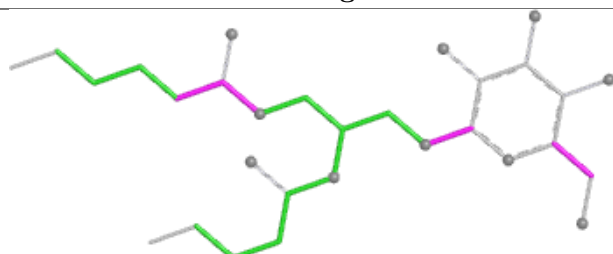
Ligand LMG j 103



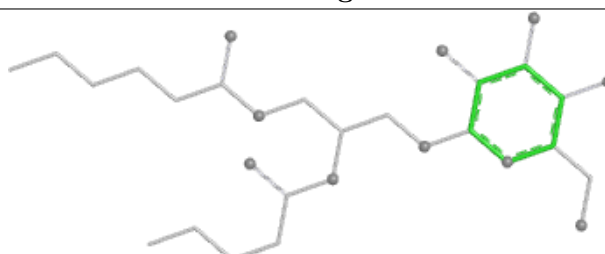
Bond lengths



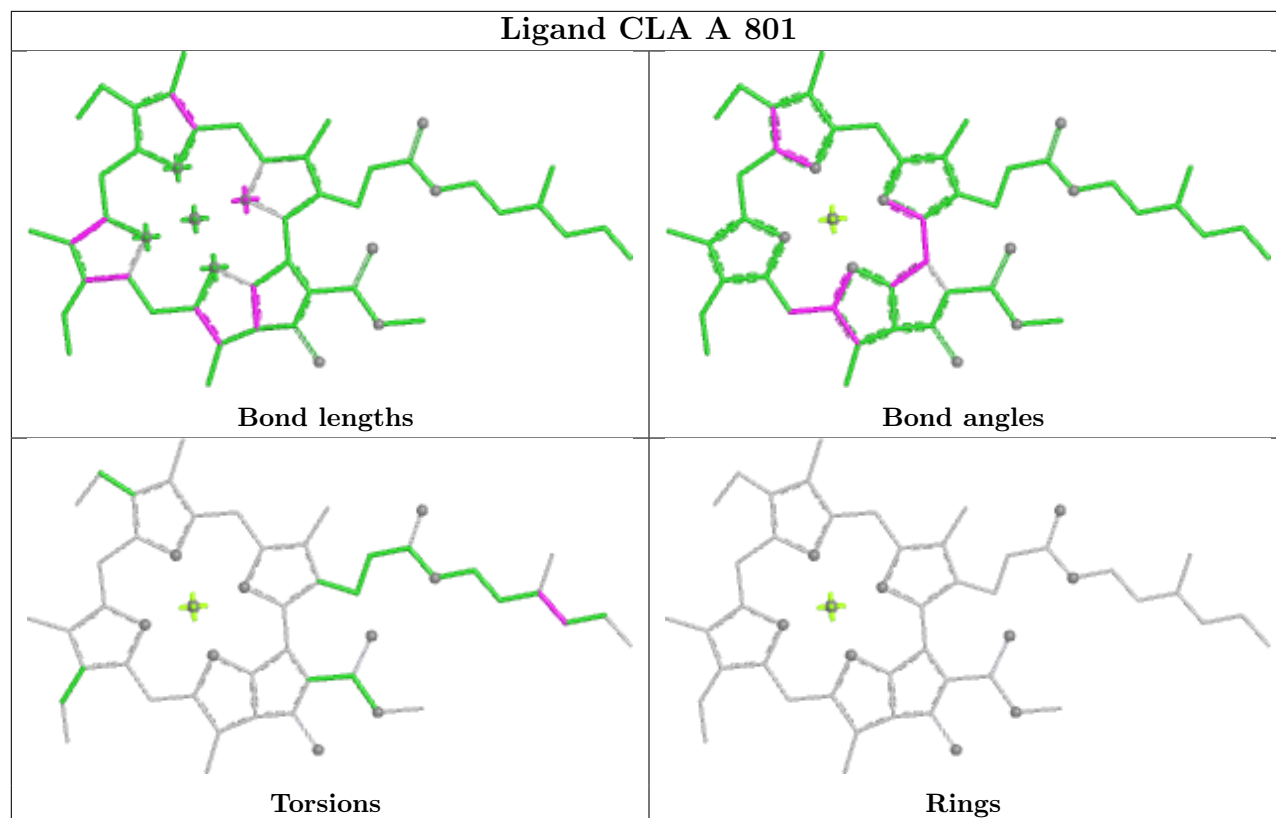
Bond angles

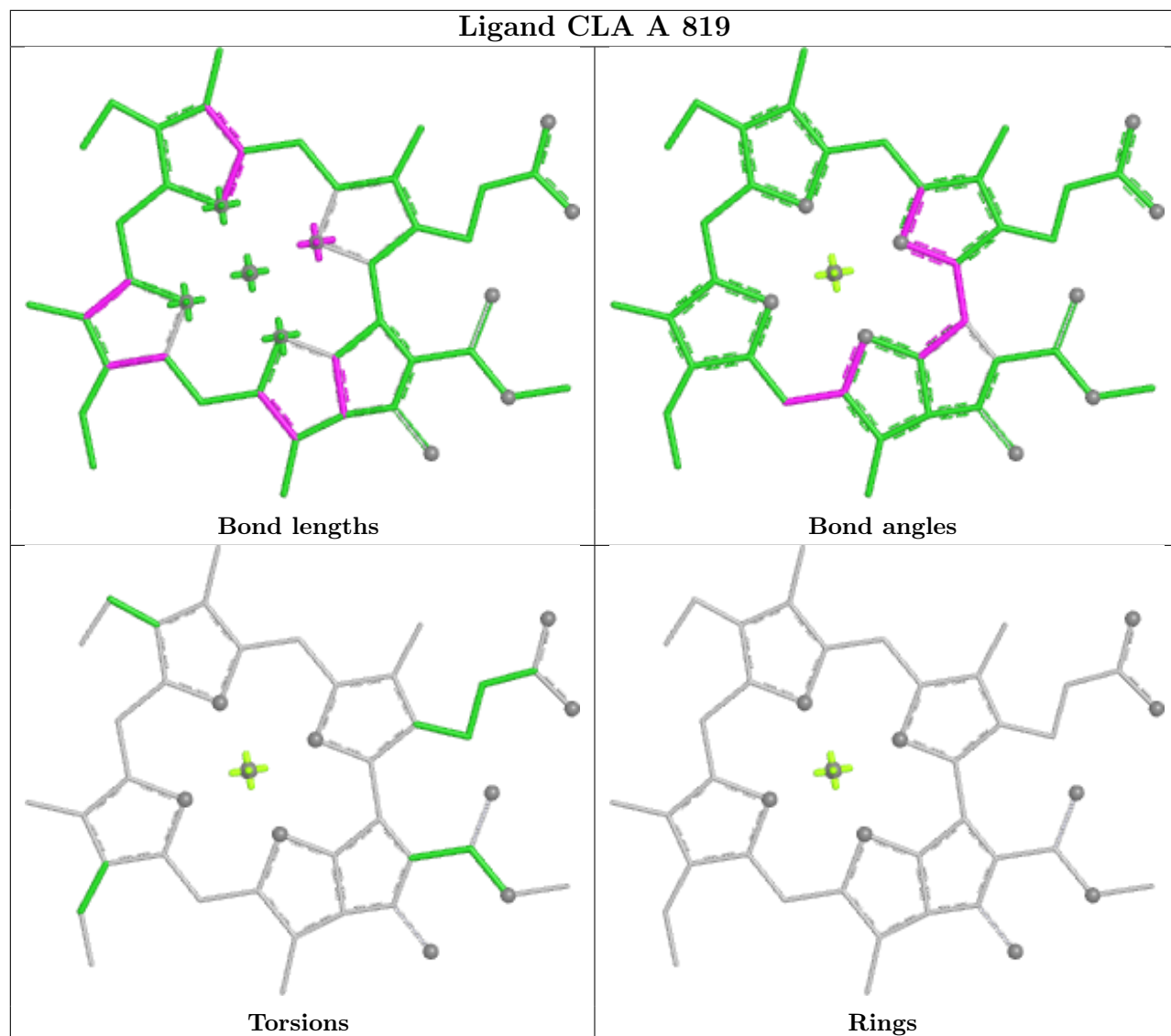


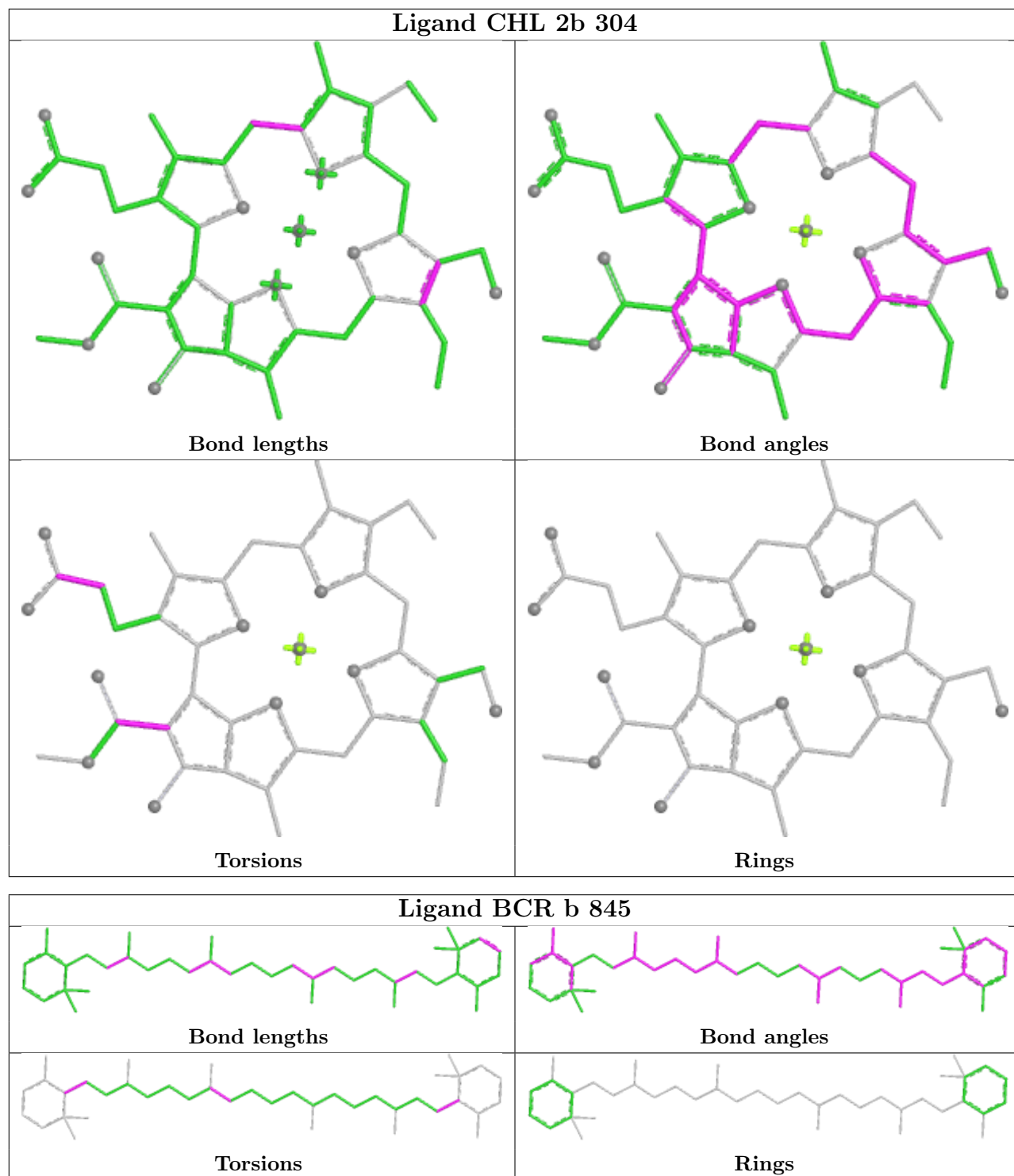
Torsions

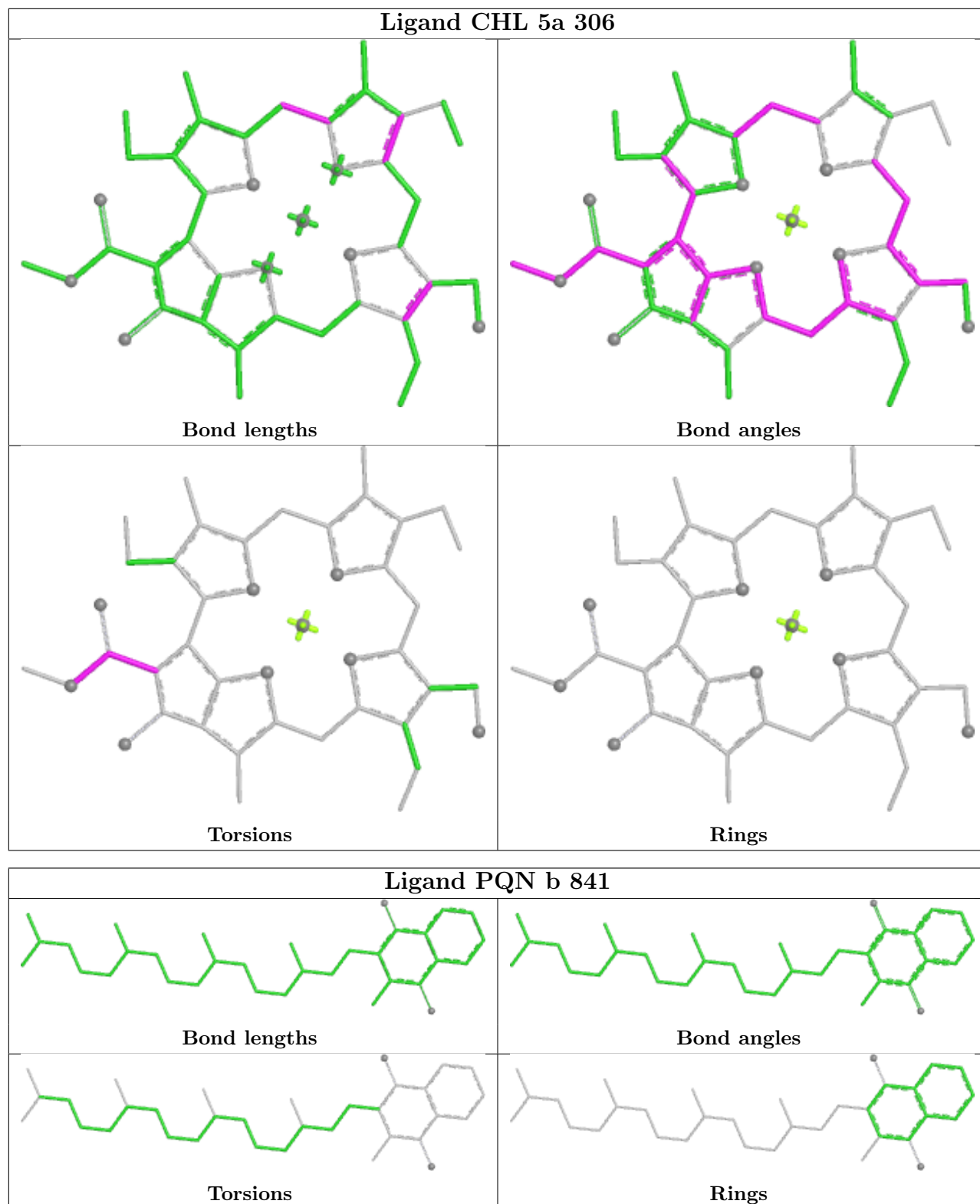


Rings

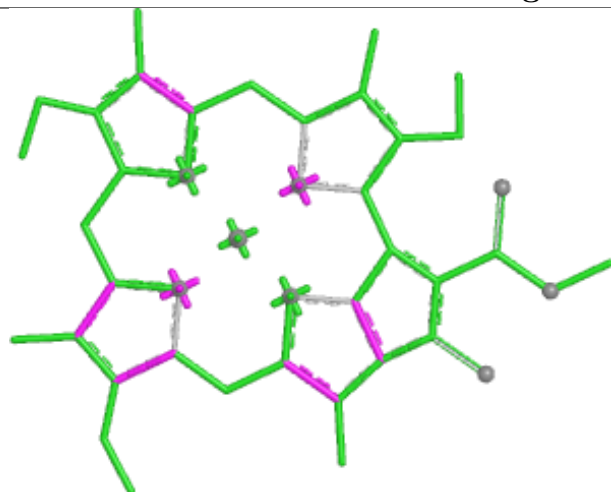




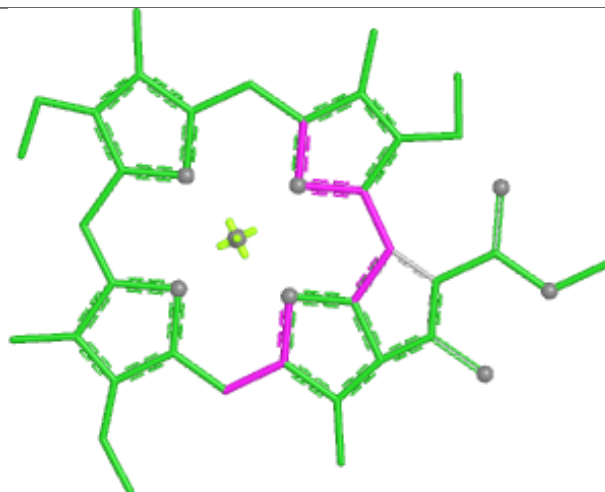




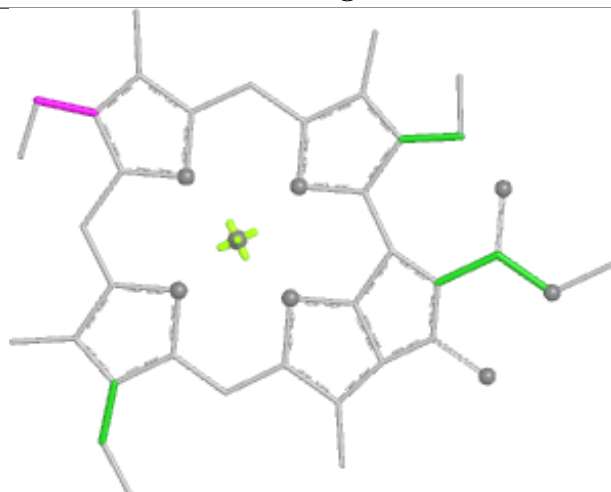
Ligand CLA 1 303



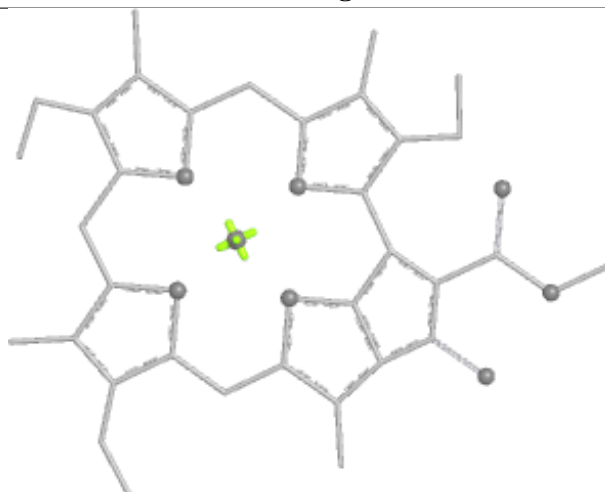
Bond lengths



Bond angles

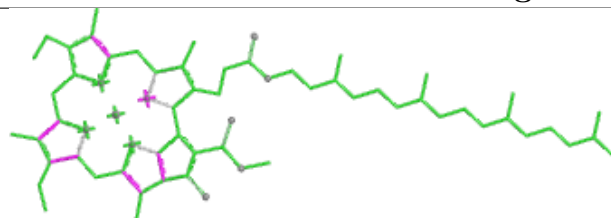


Torsions

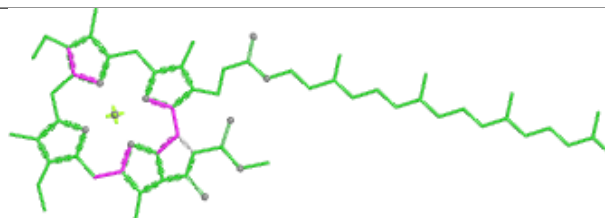


Rings

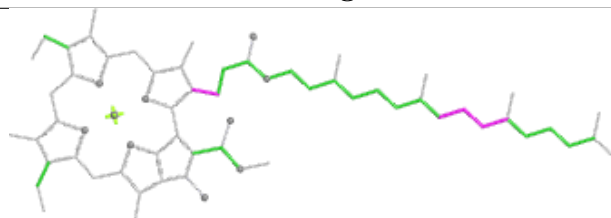
Ligand CLA B 804



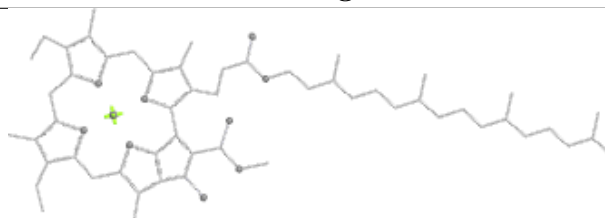
Bond lengths



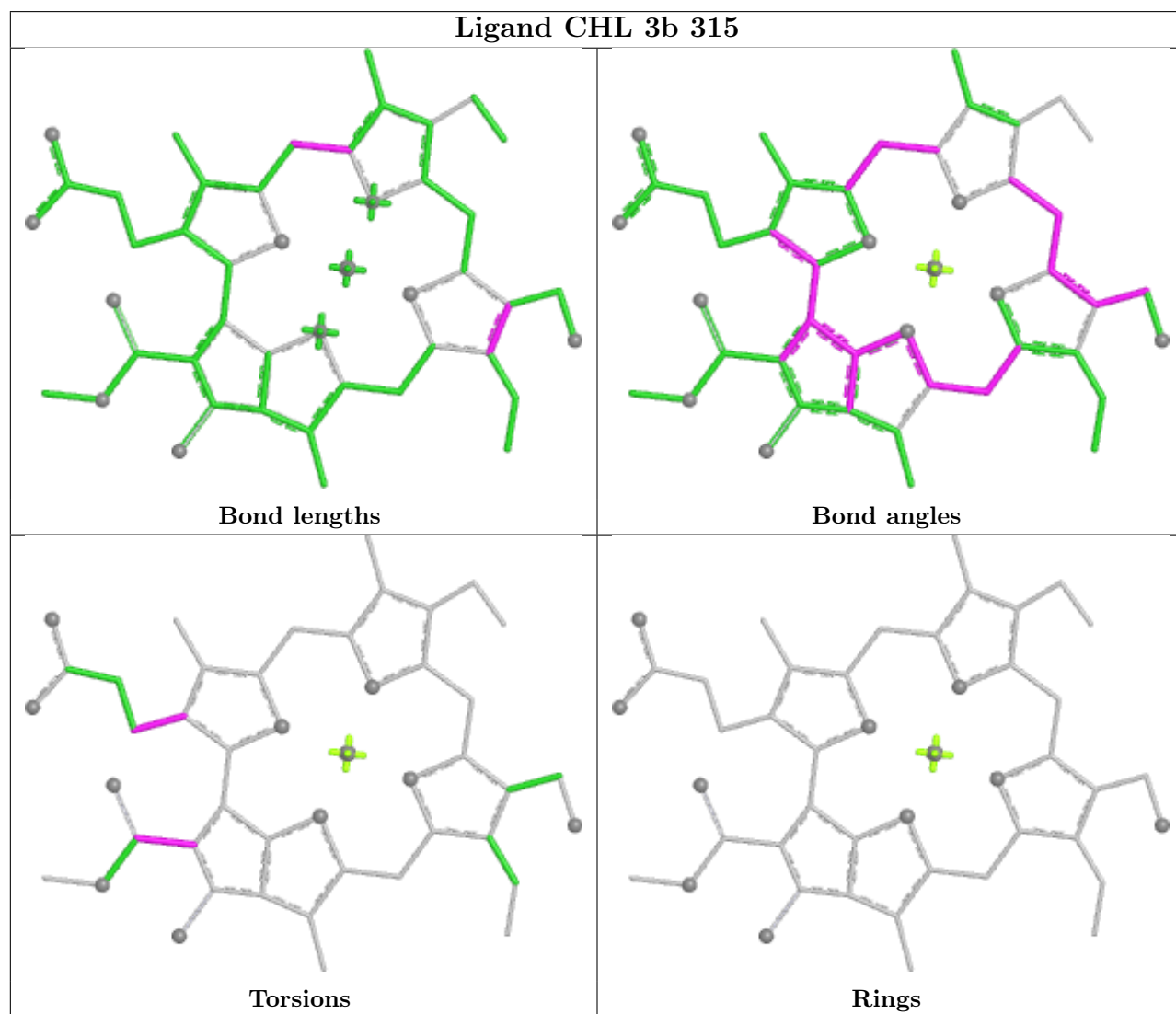
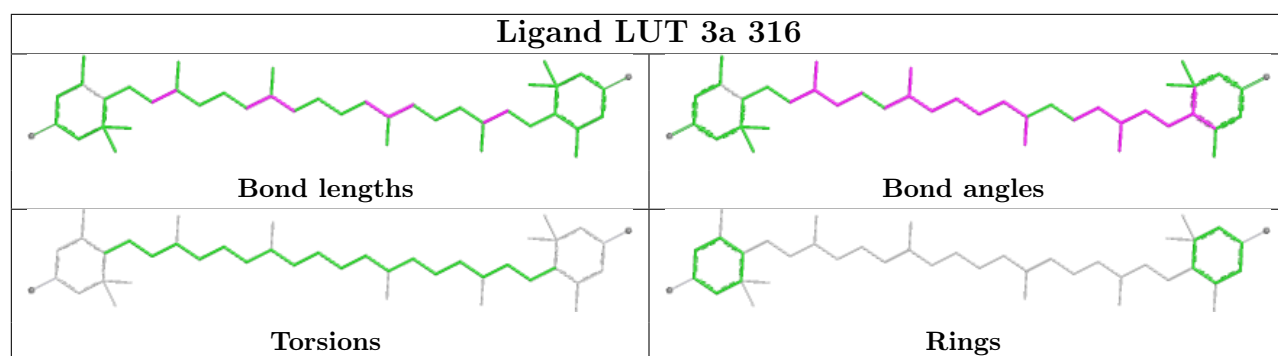
Bond angles



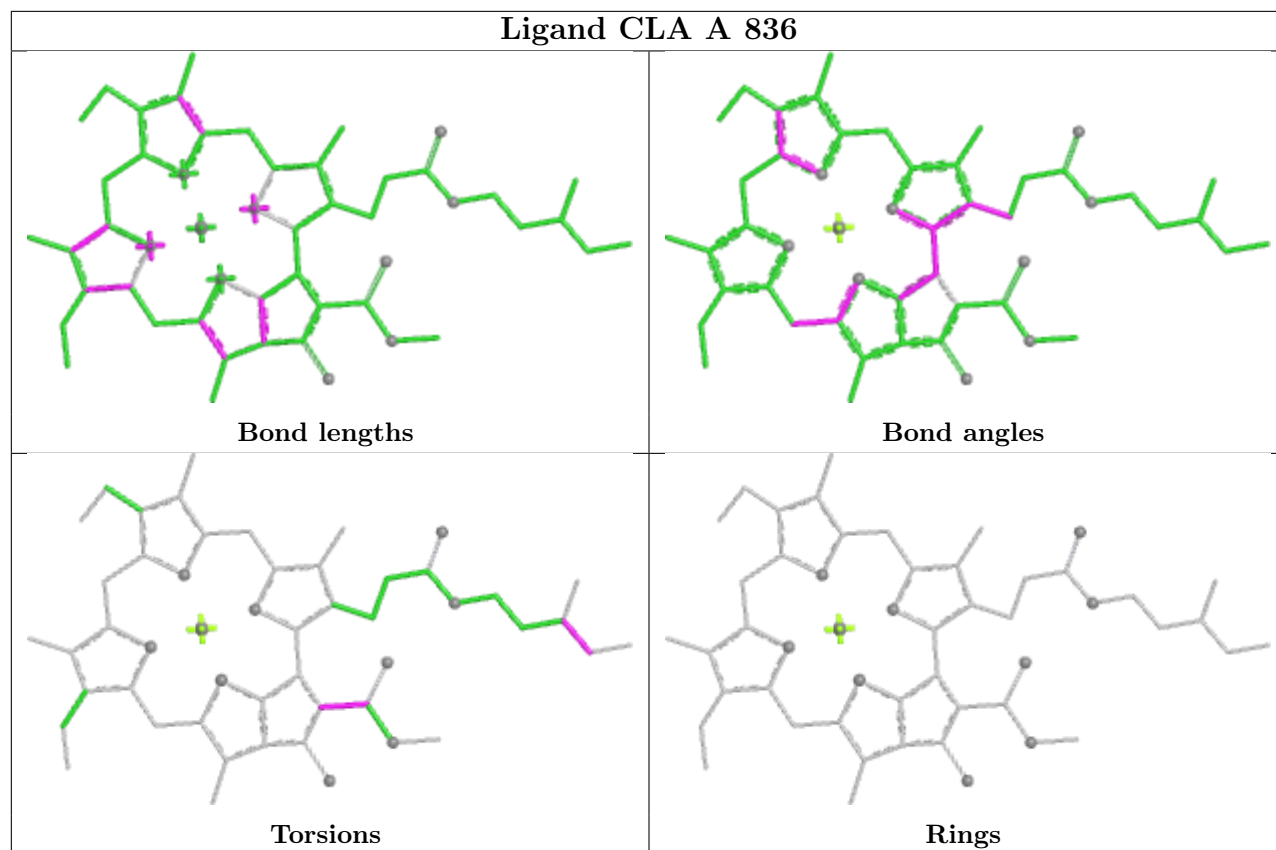
Torsions



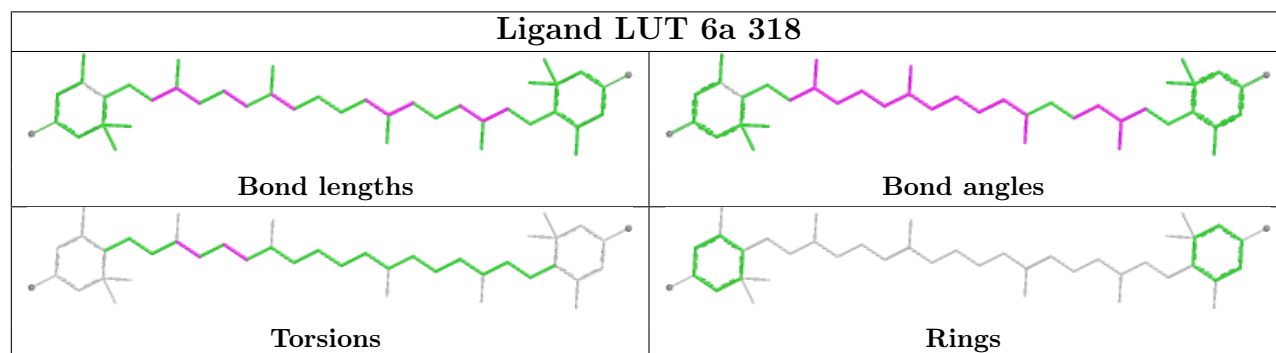
Rings

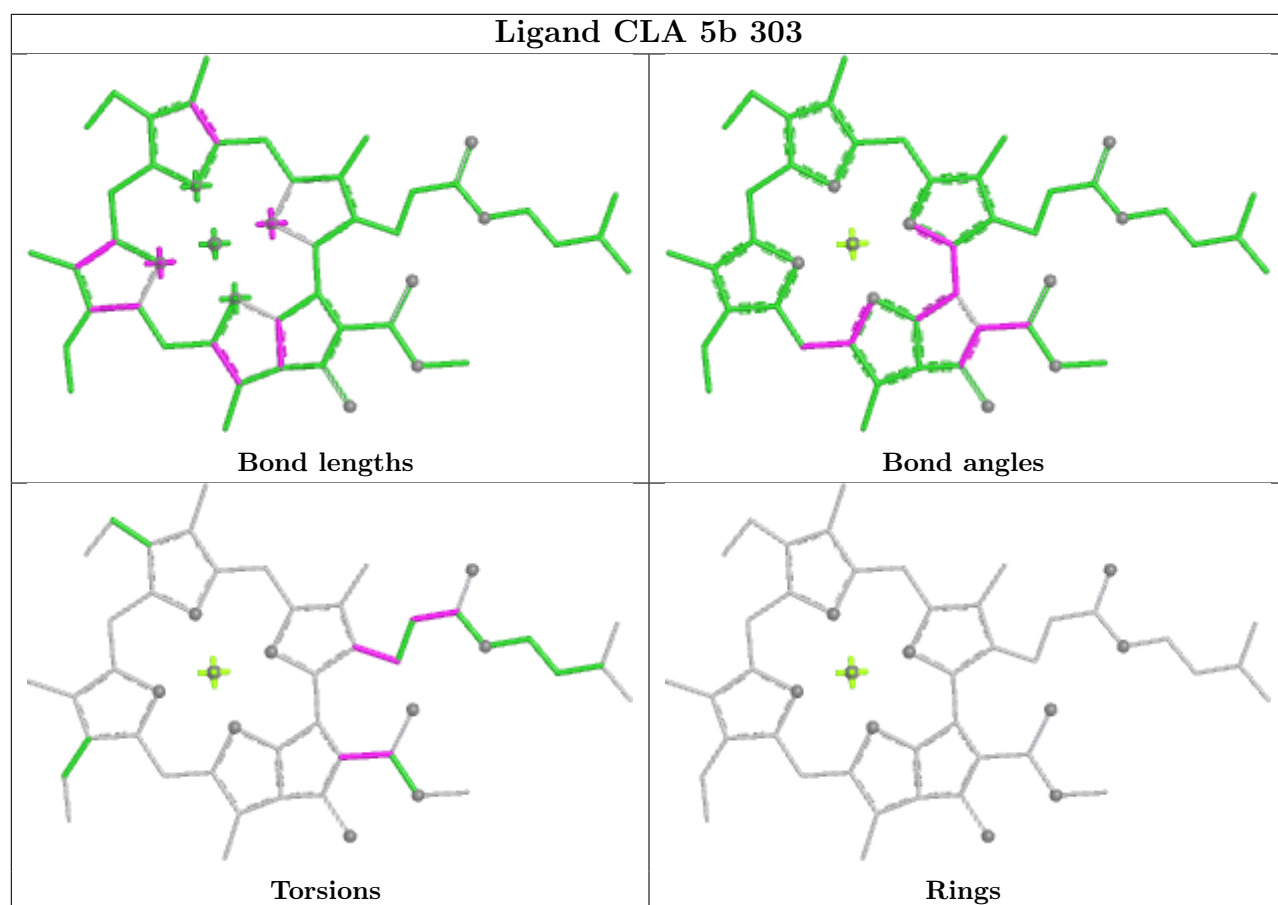


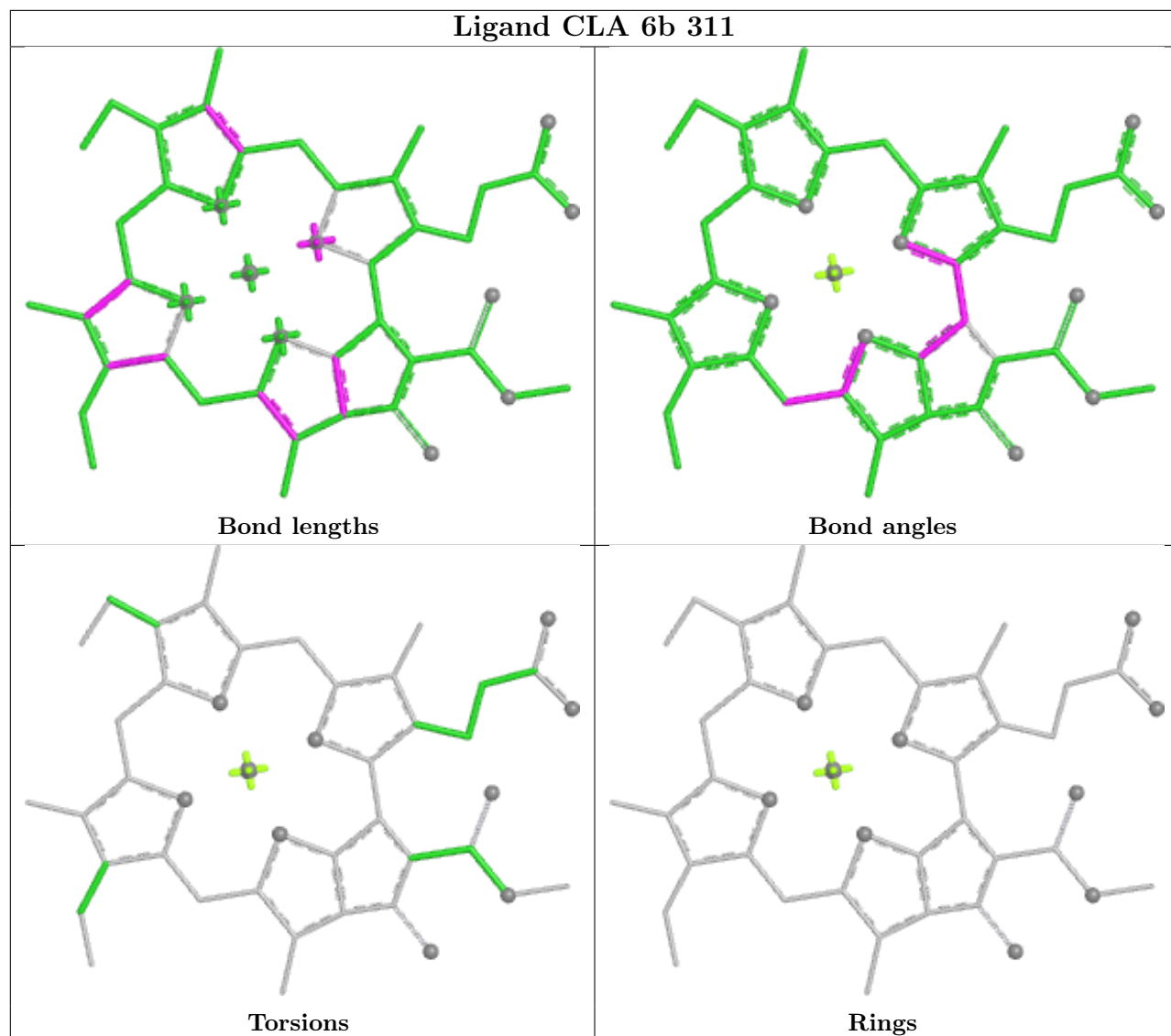
Ligand CLA A 836

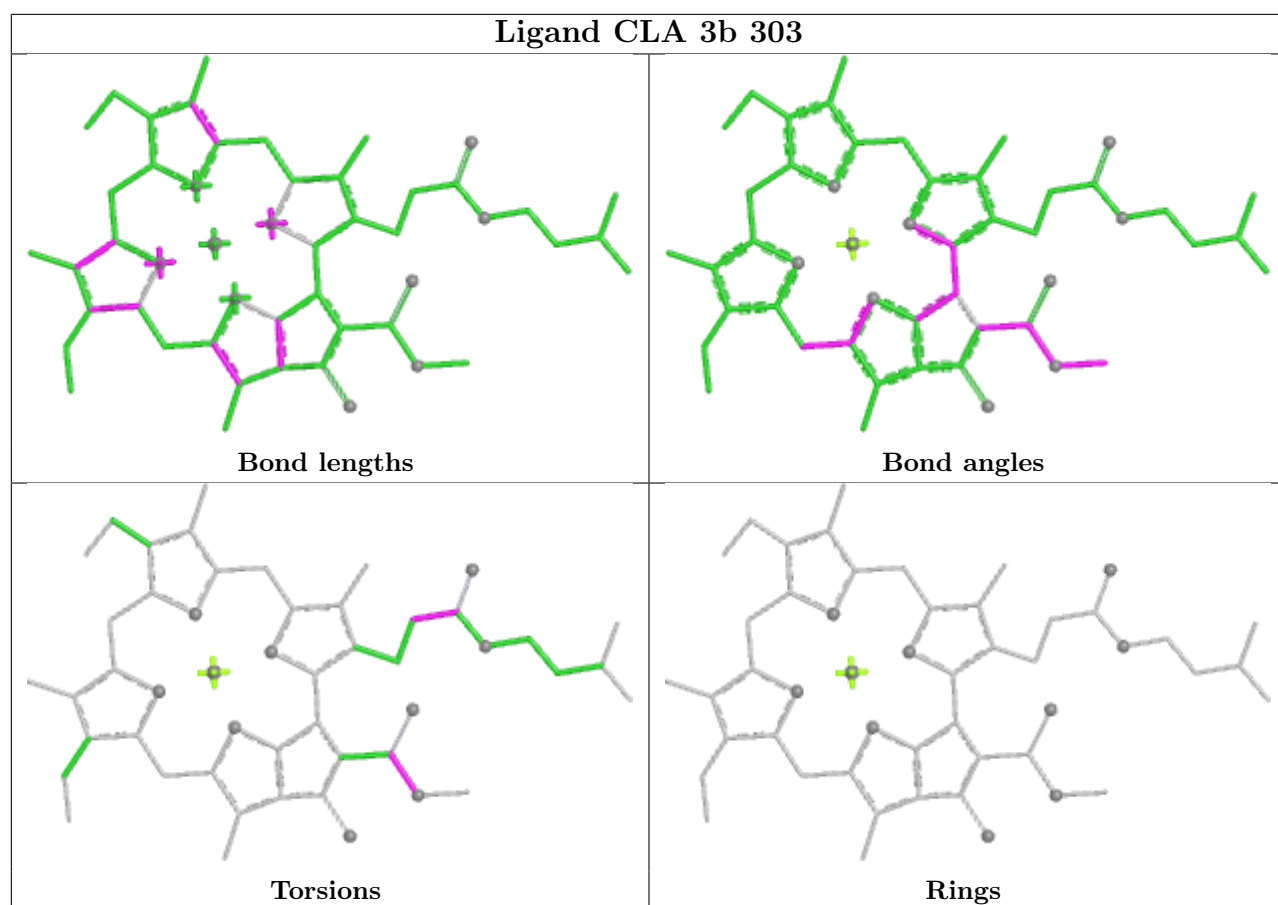


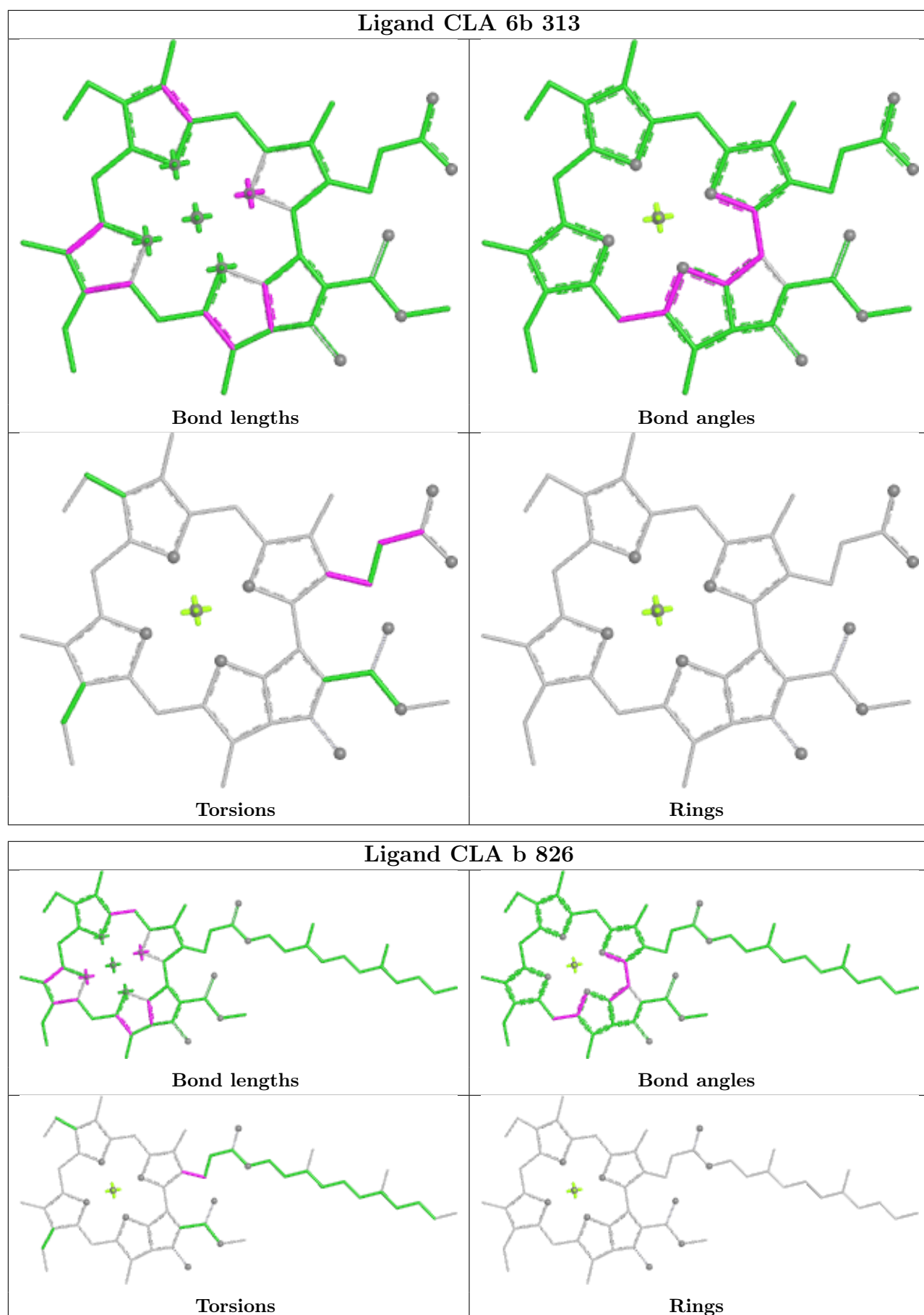
Ligand LUT 6a 318

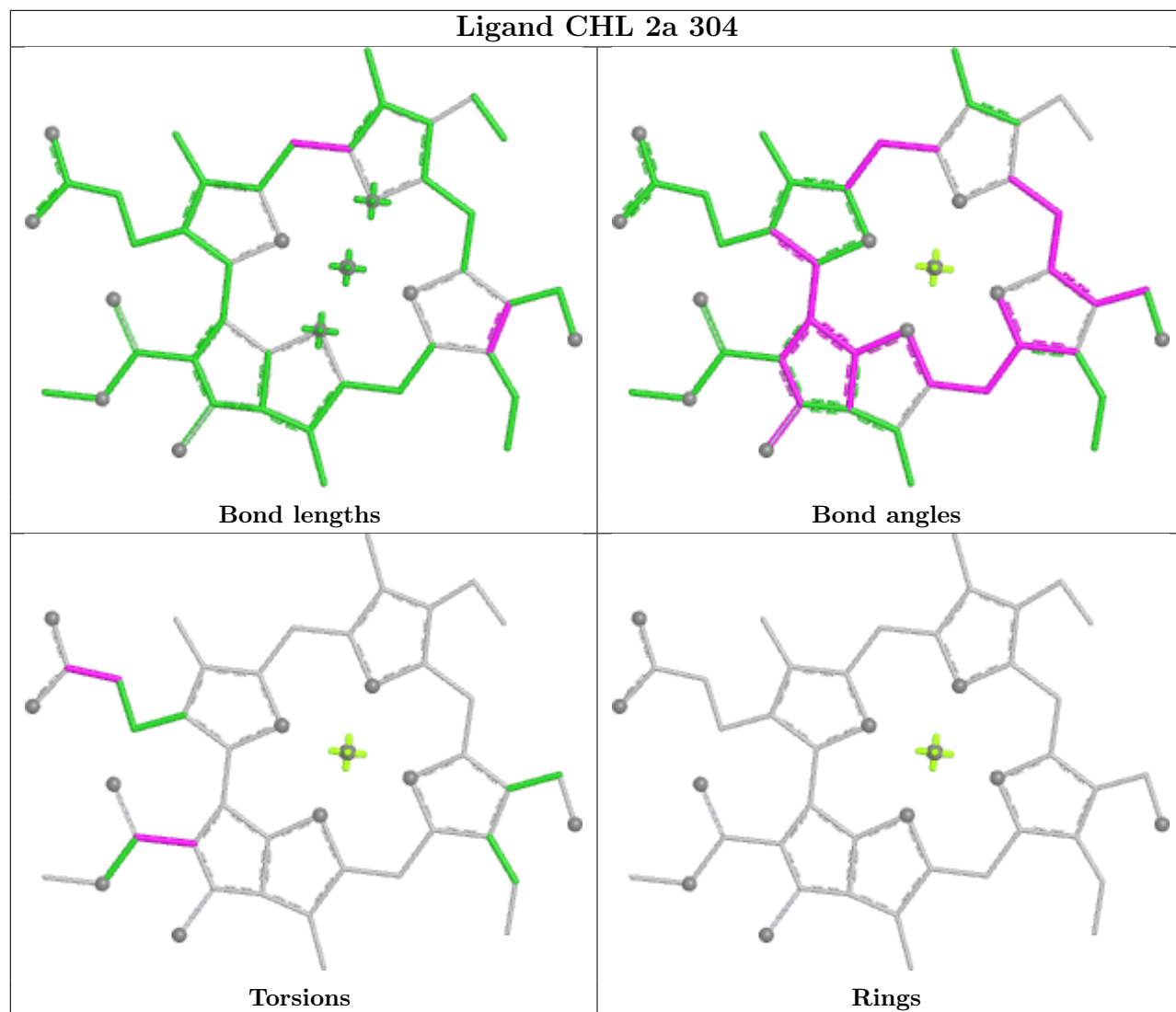




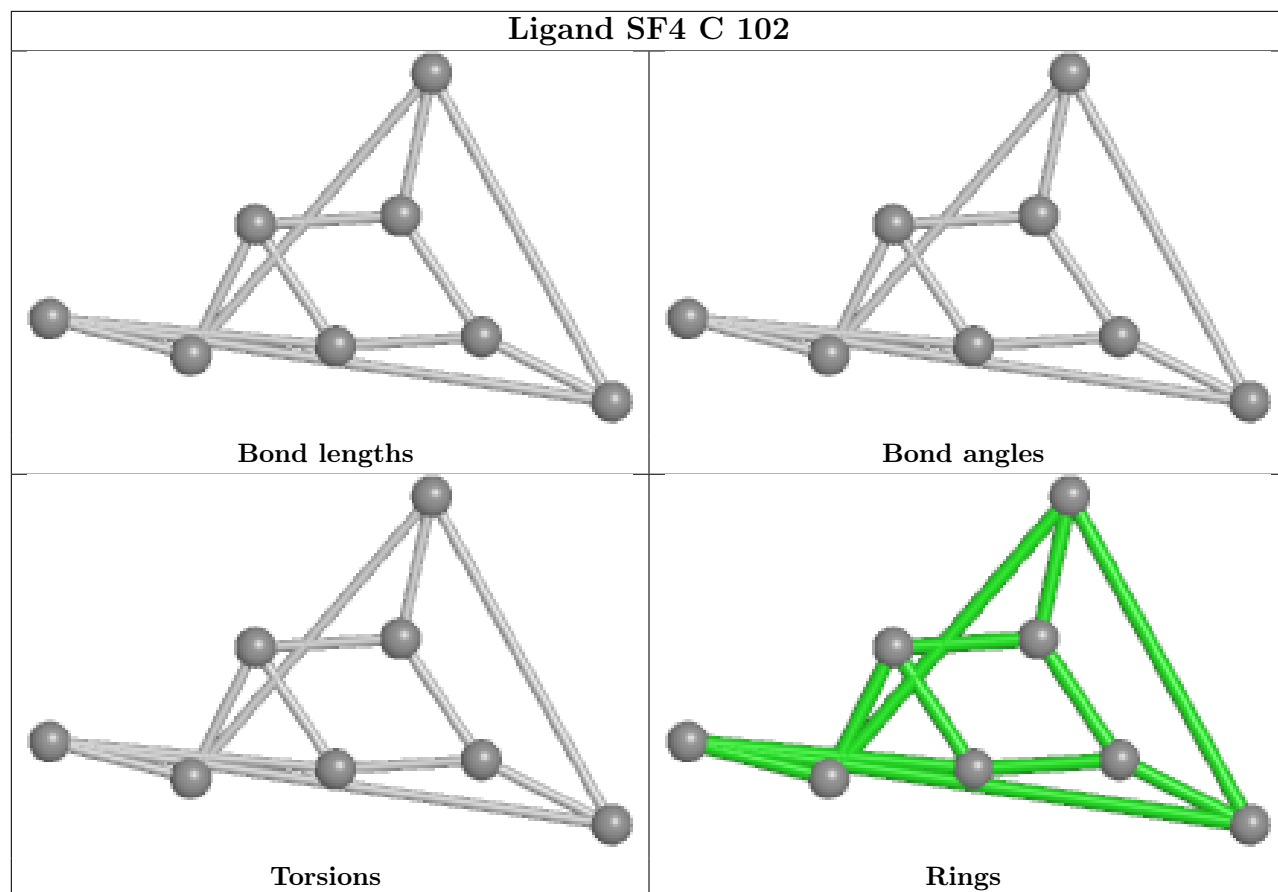




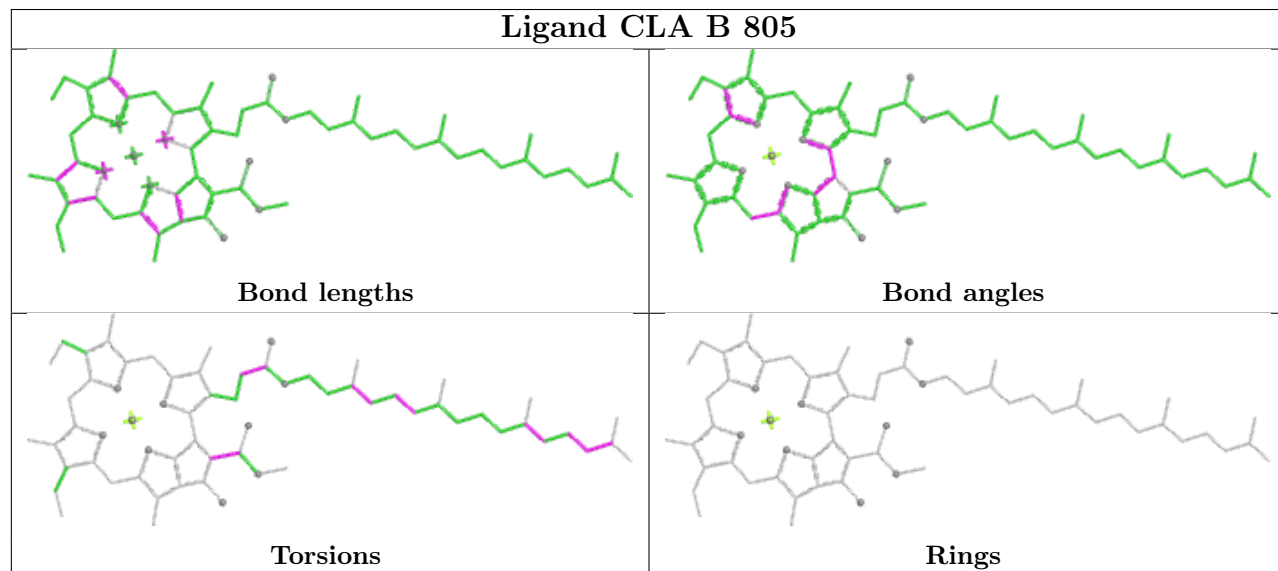


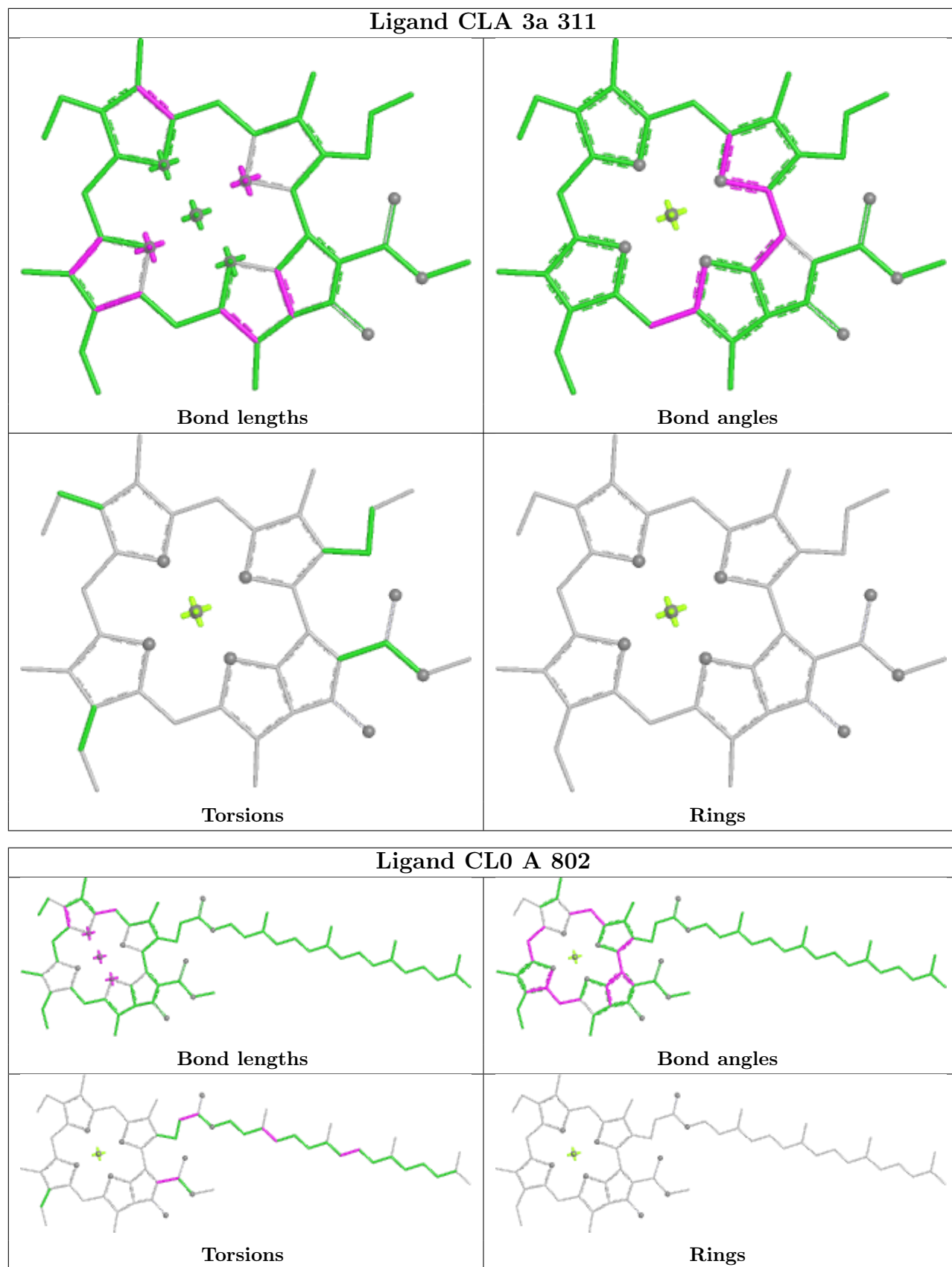


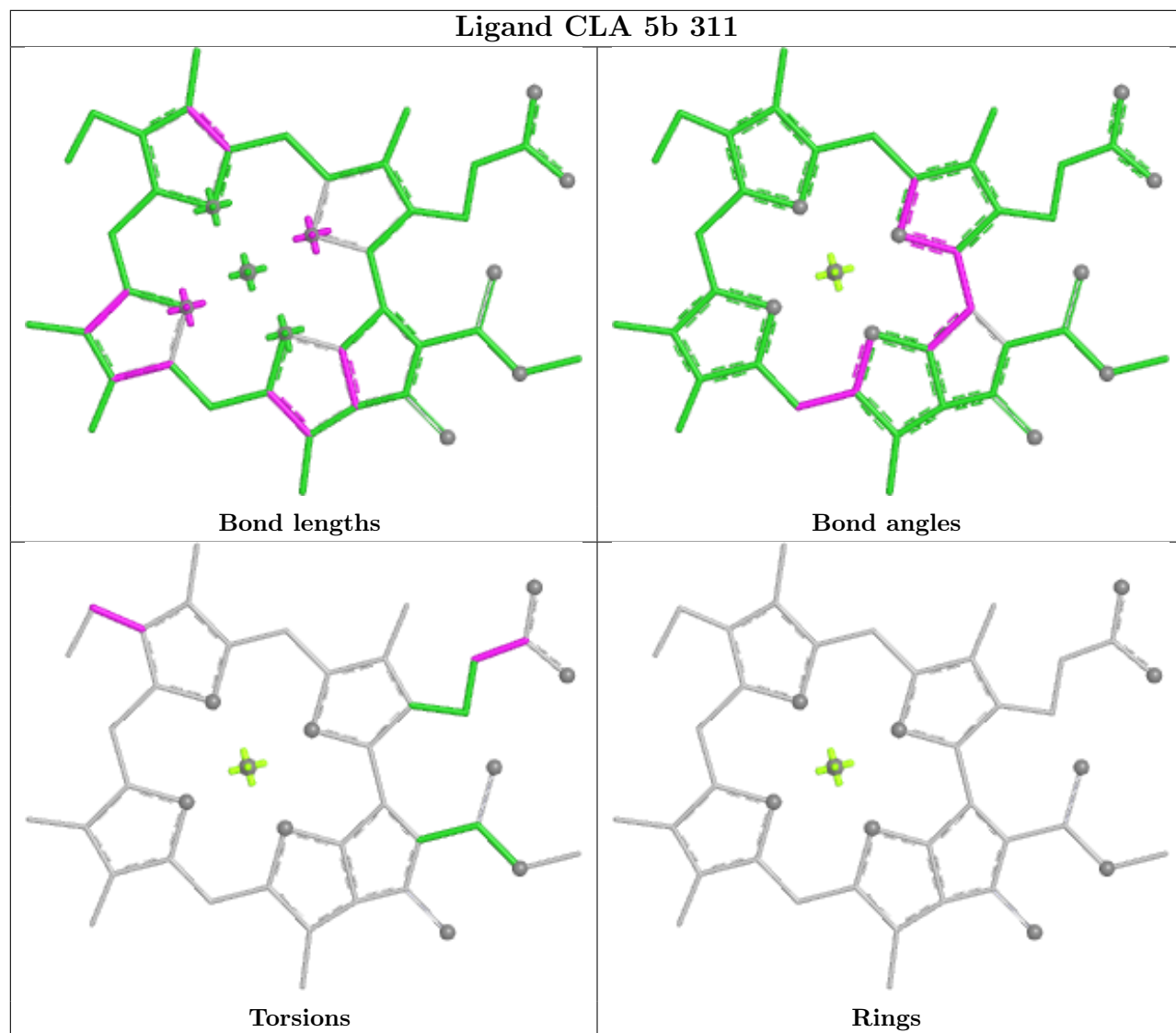
Ligand SF4 C 102



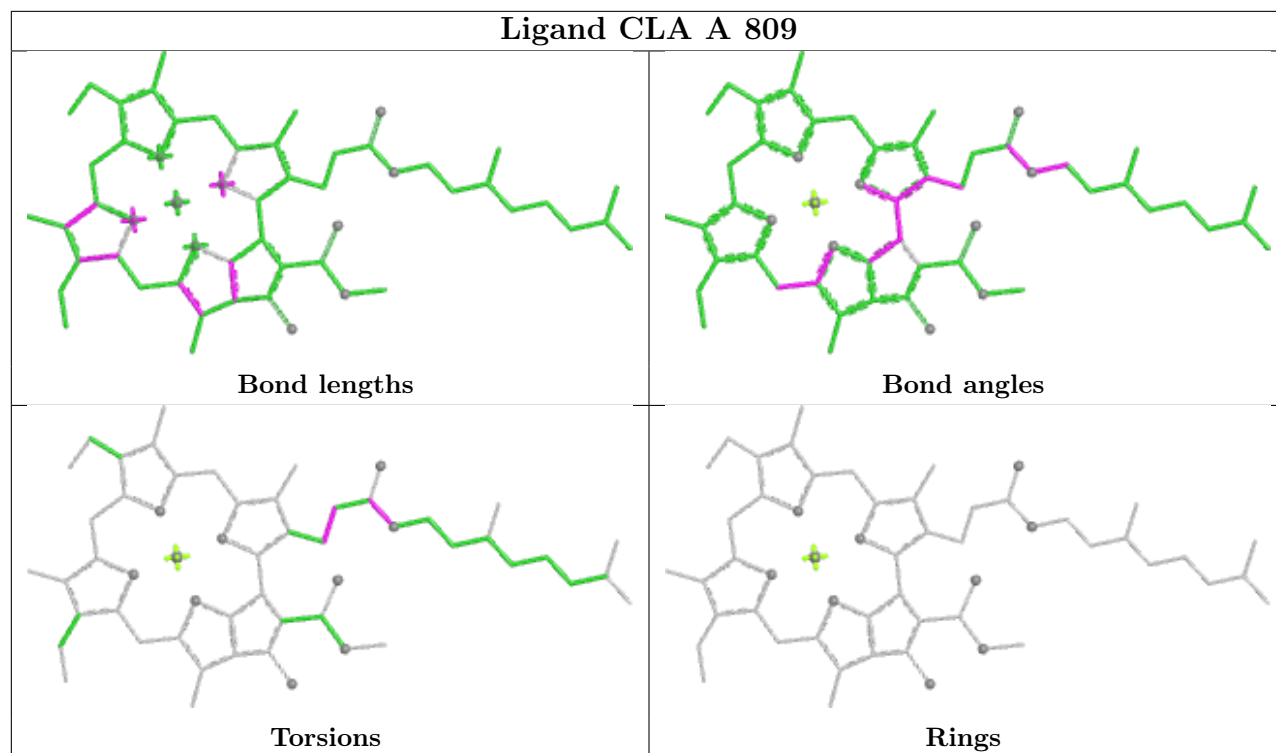
Ligand CLA B 805



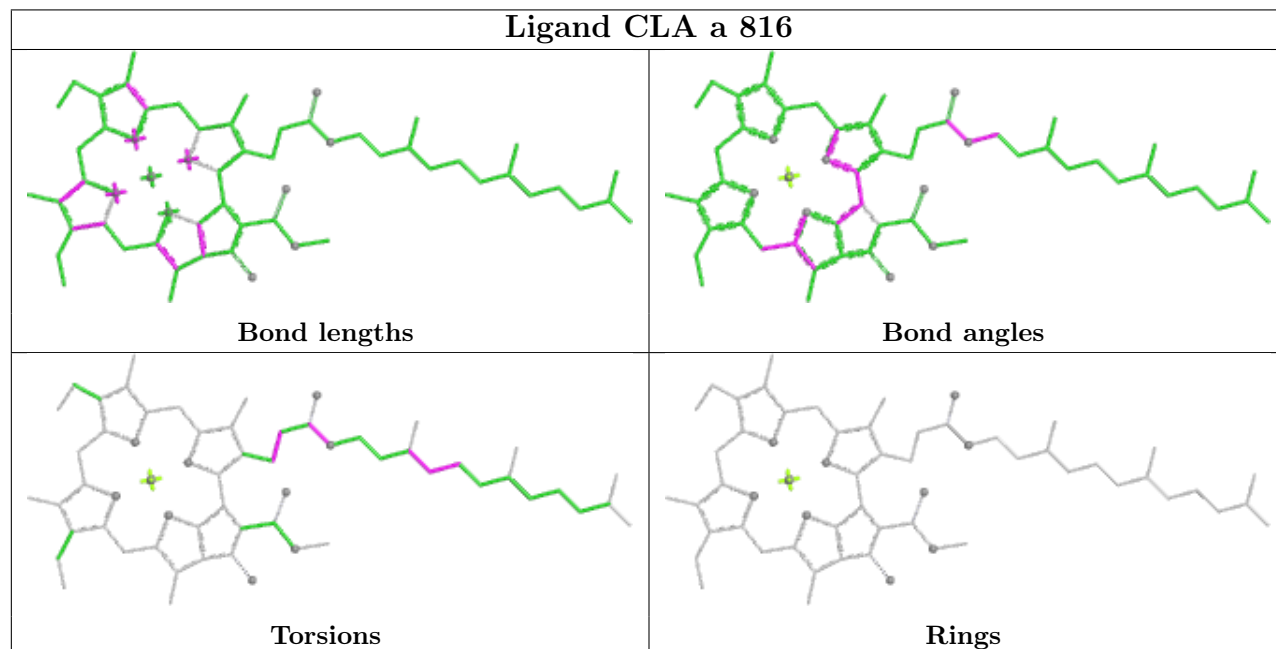




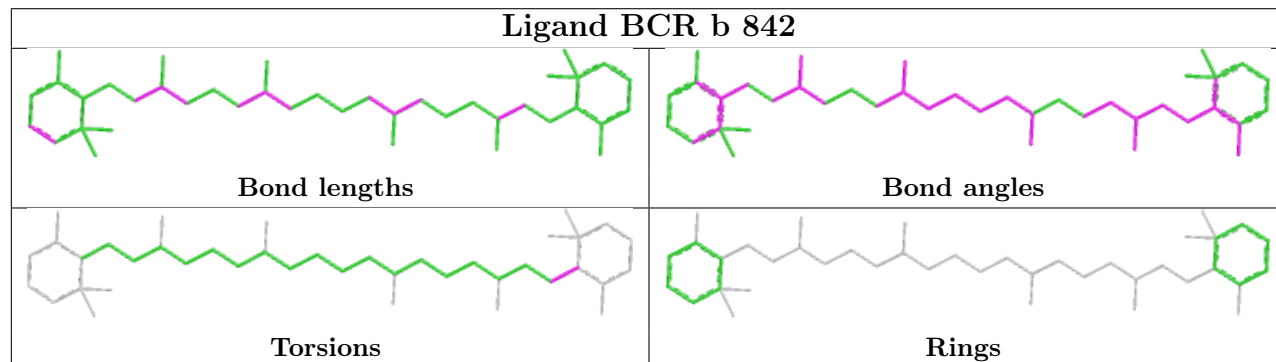
Ligand CLA A 809

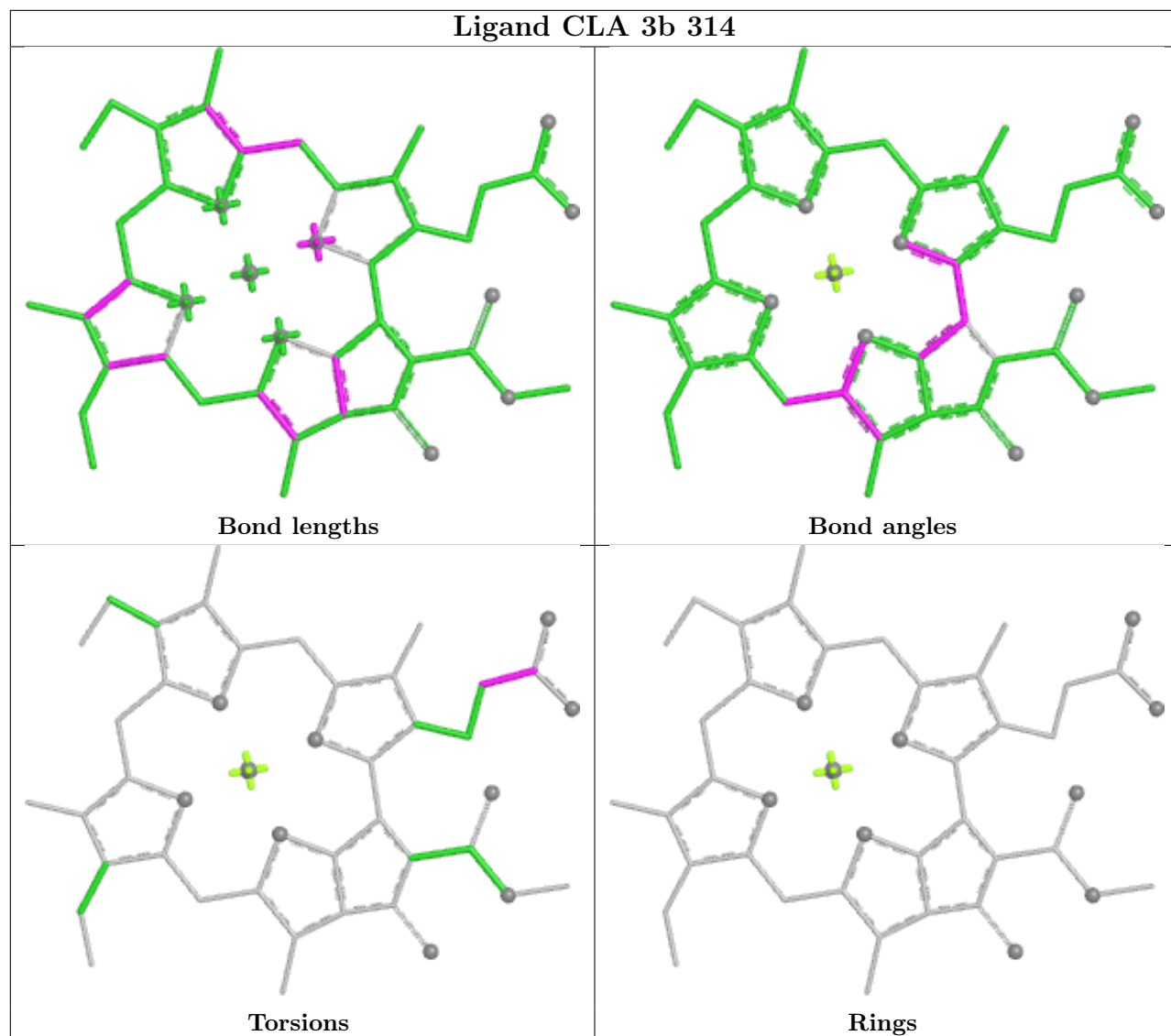


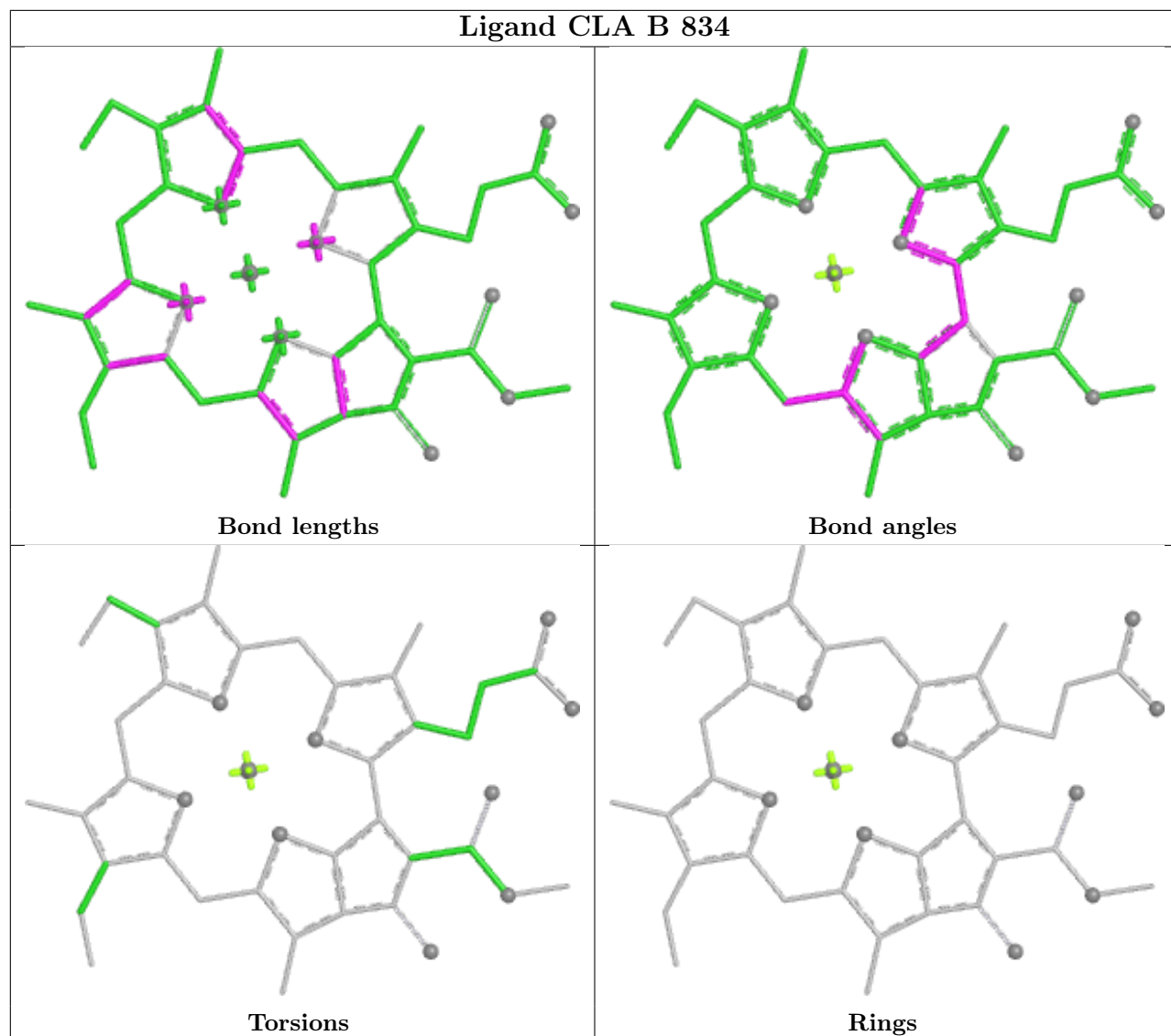
Ligand CLA a 816

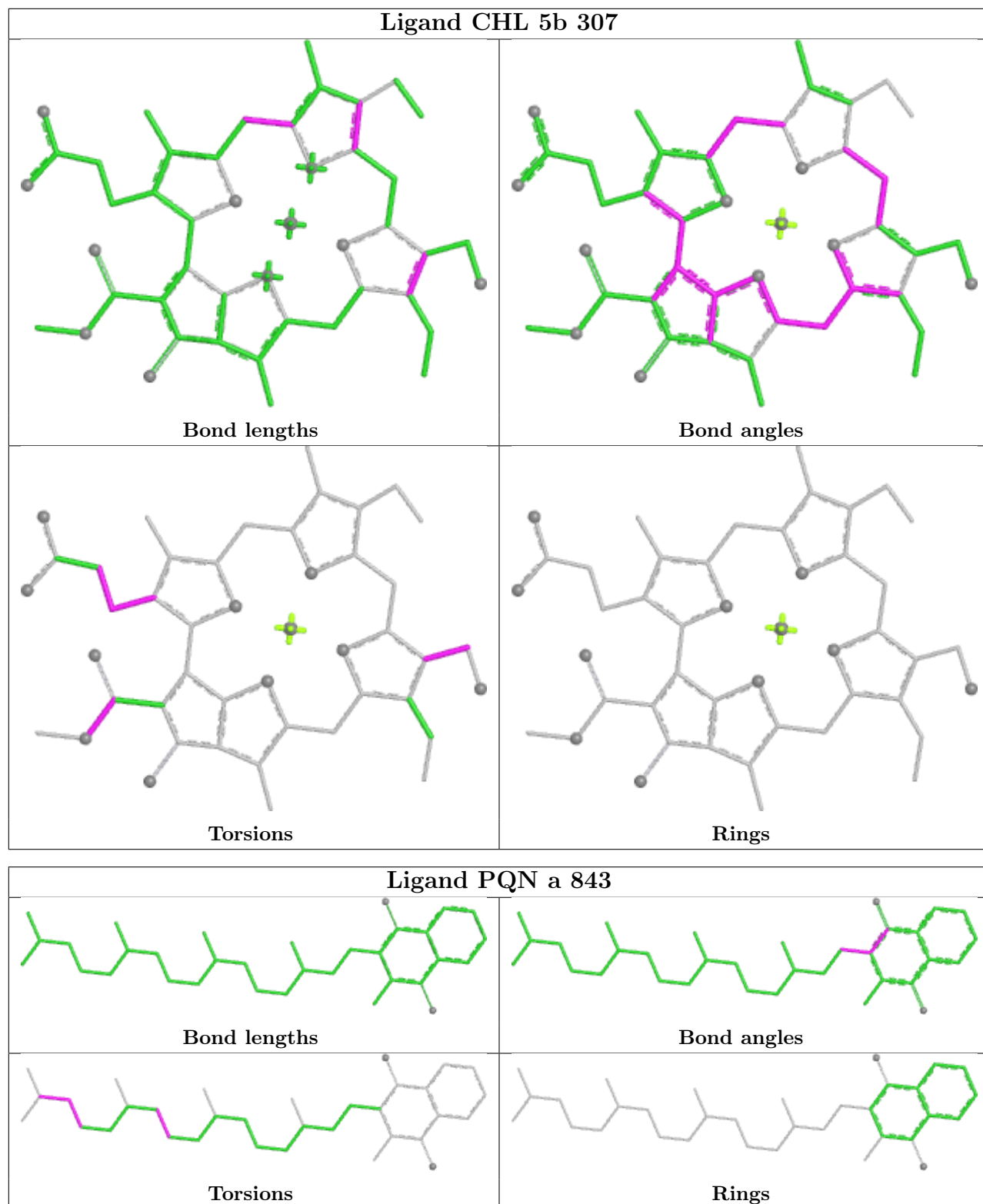


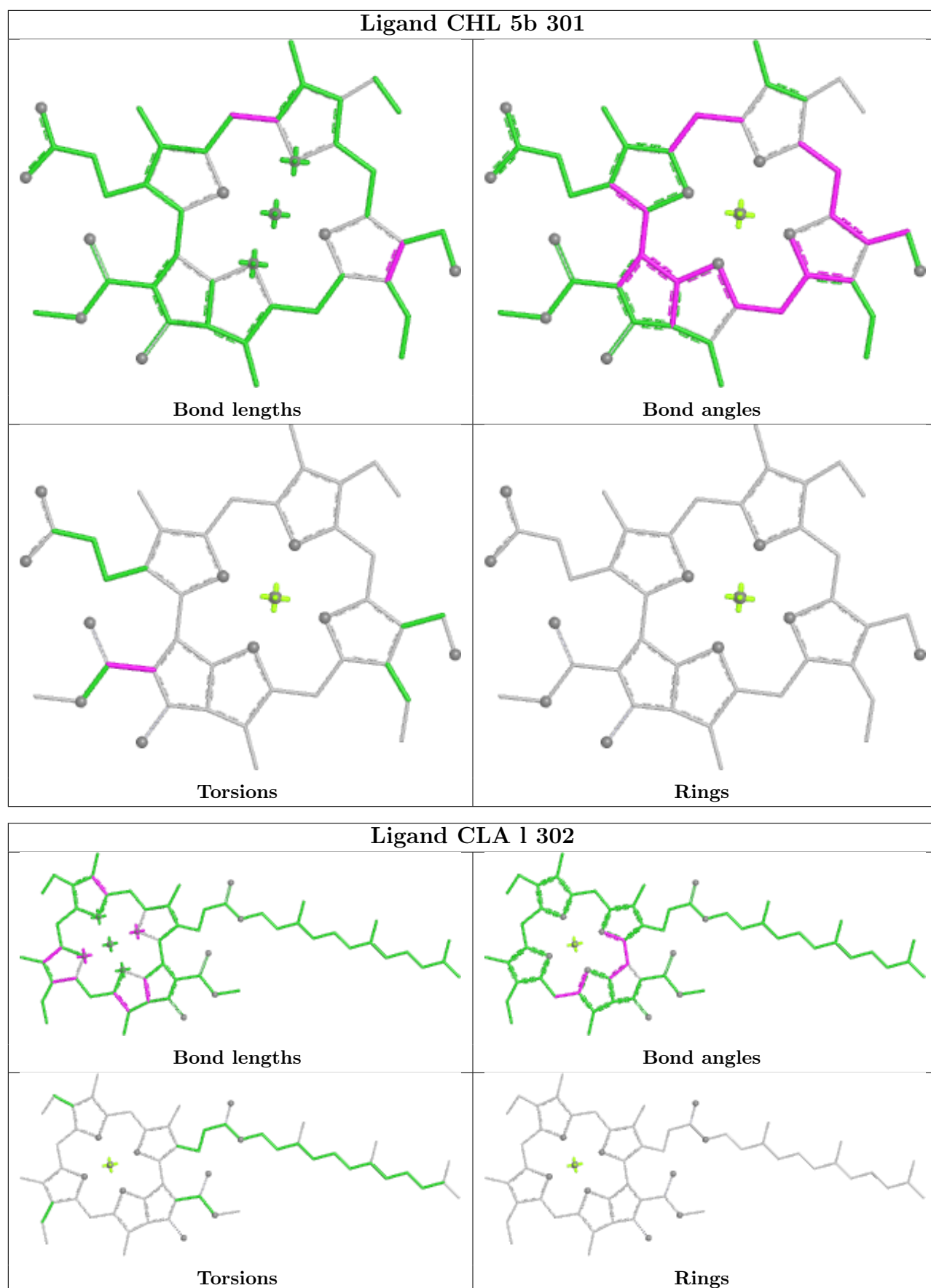
Ligand BCR b 842

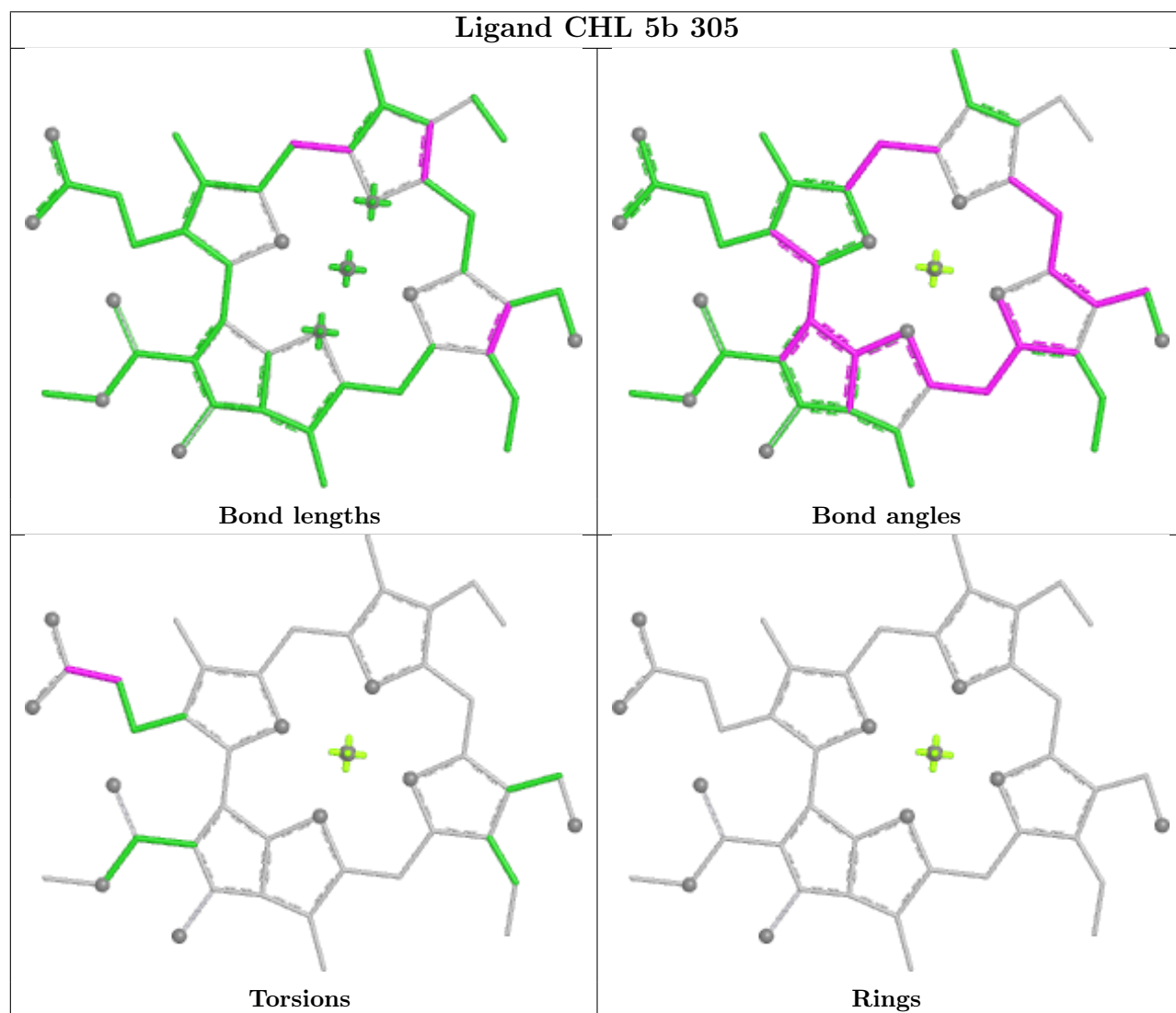
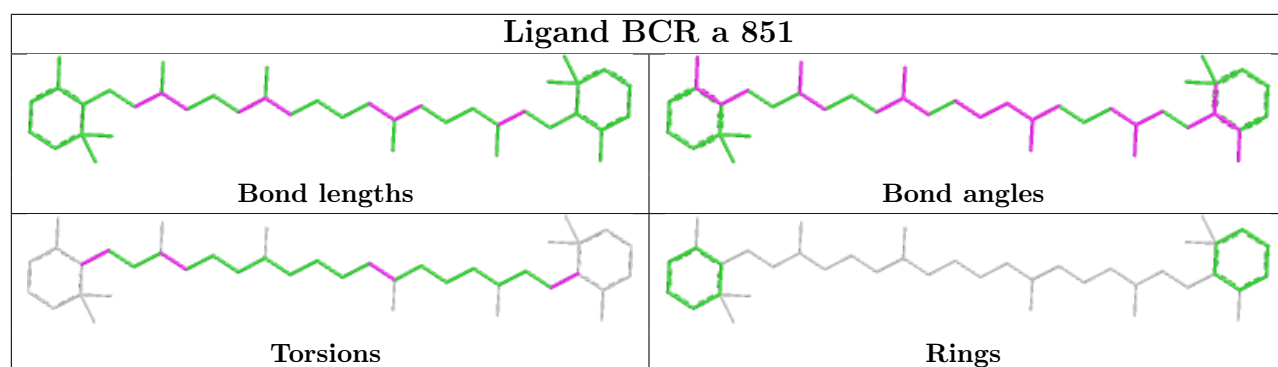


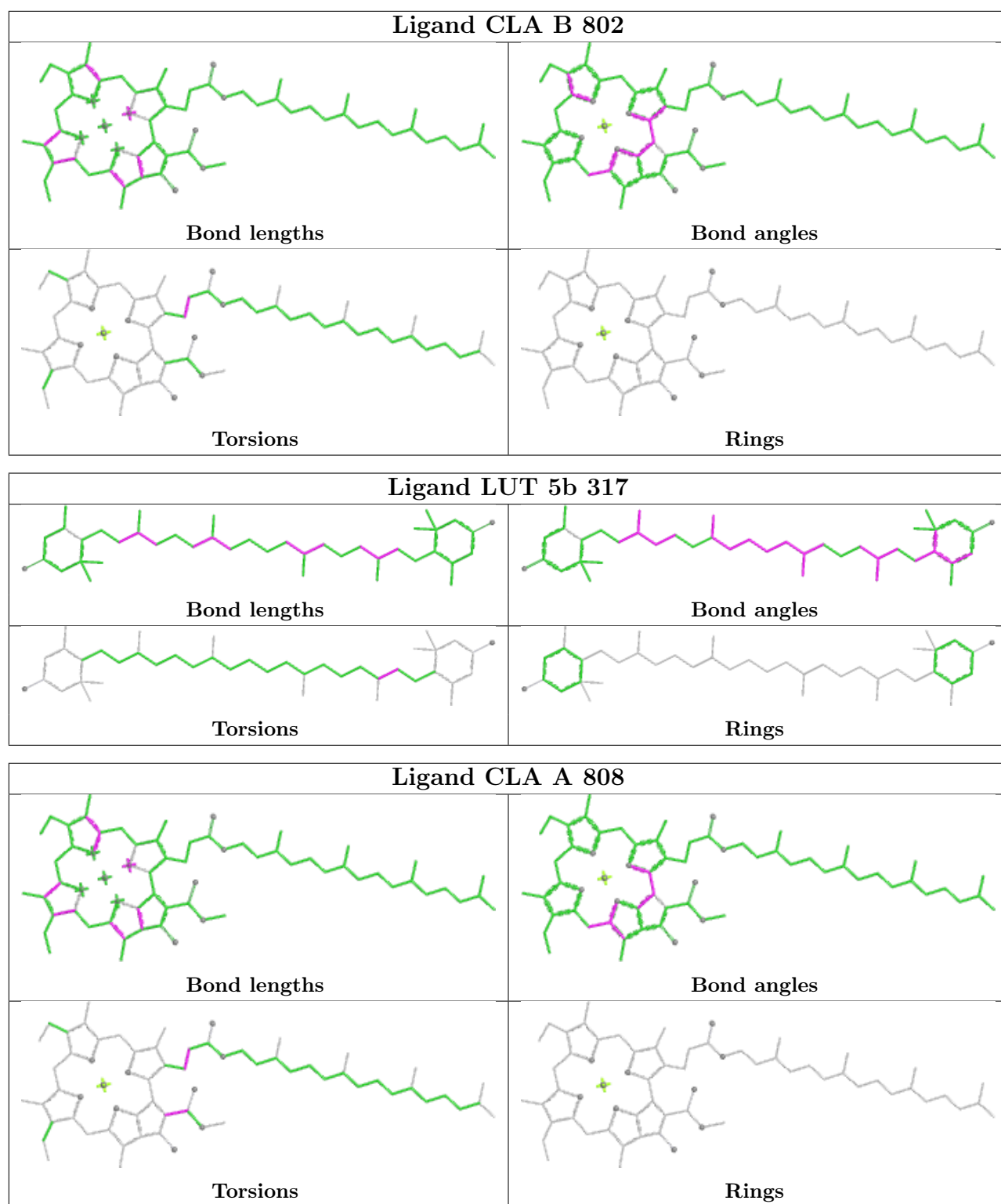


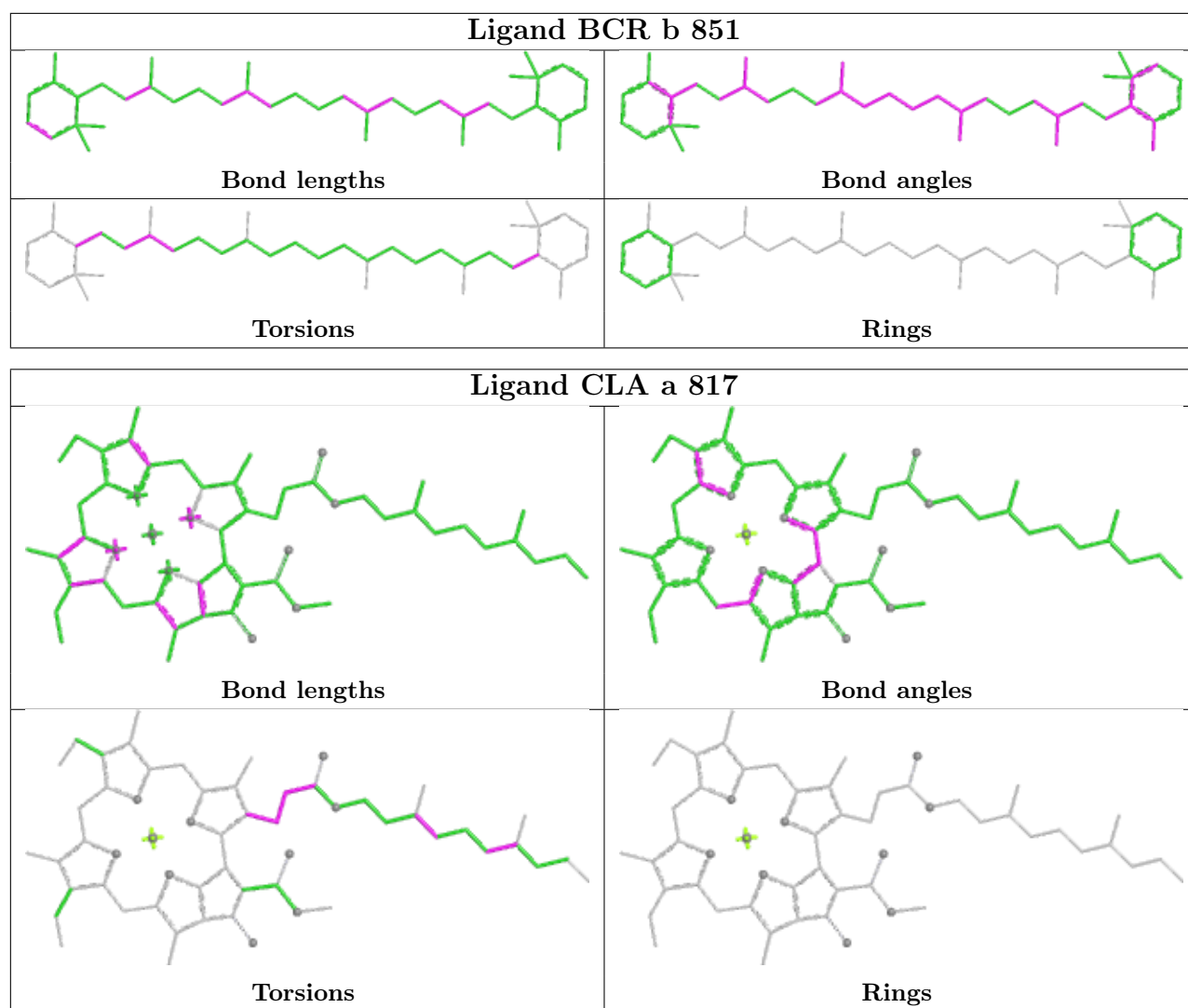


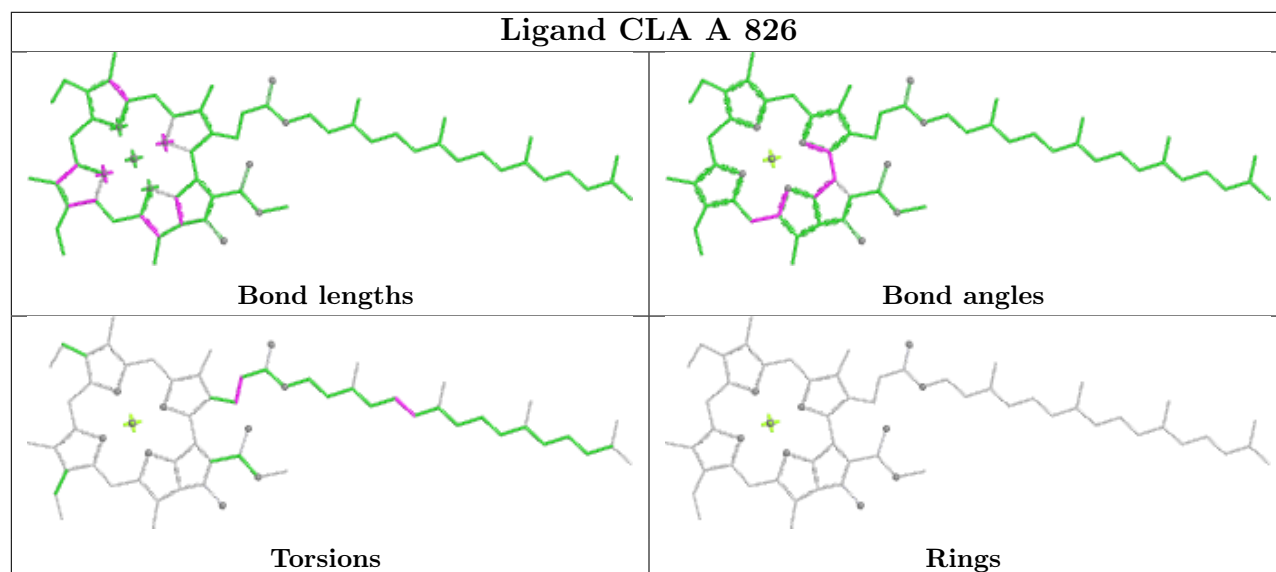
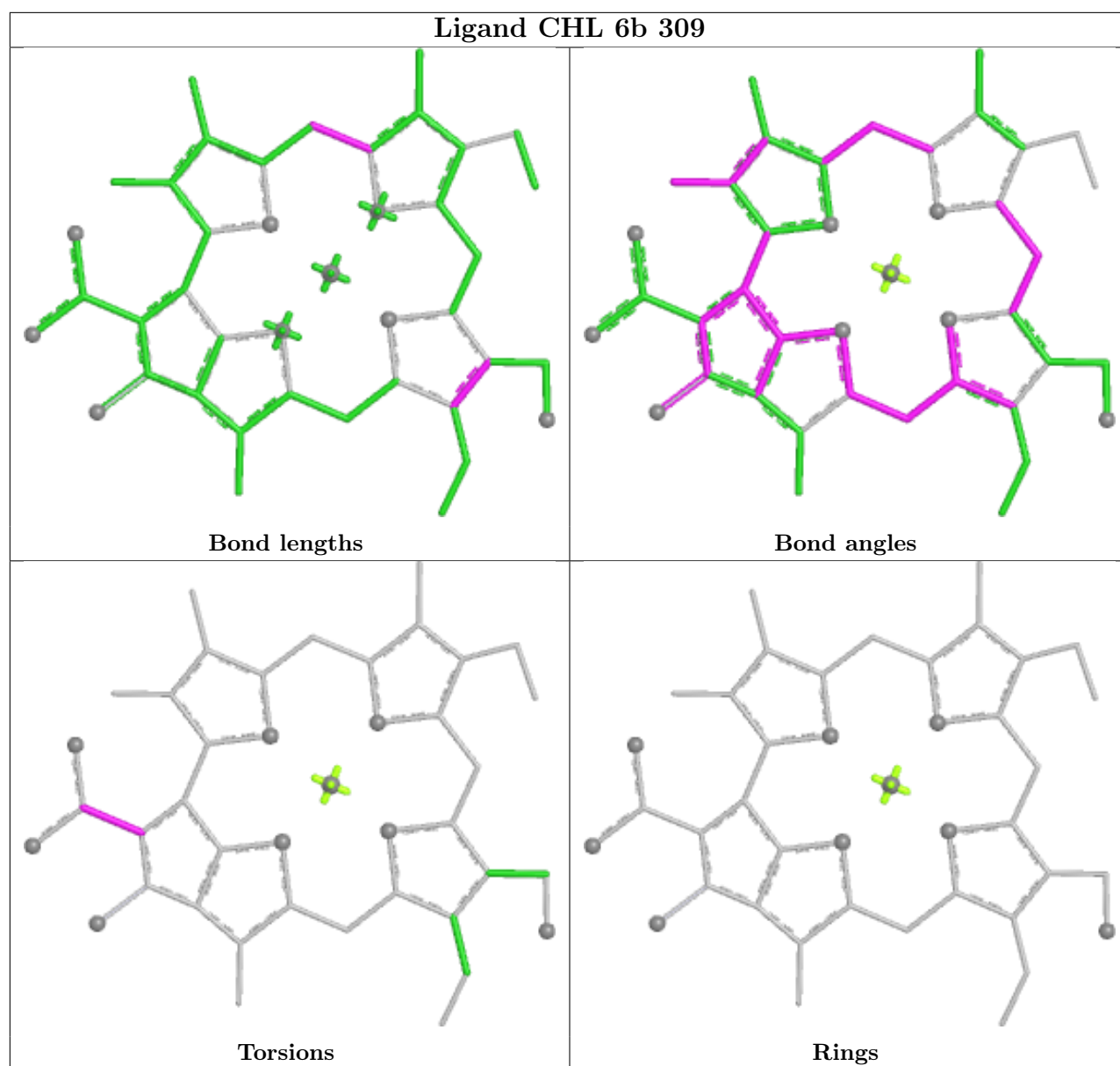




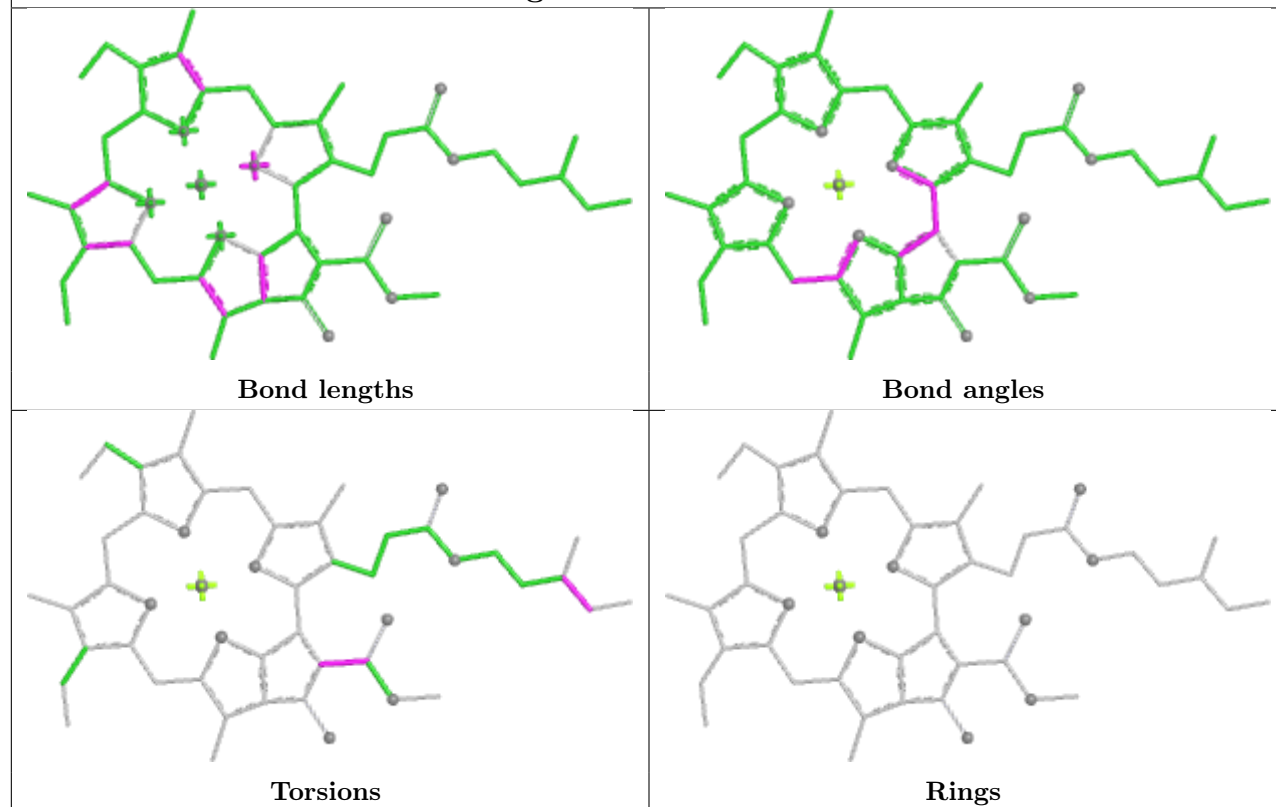




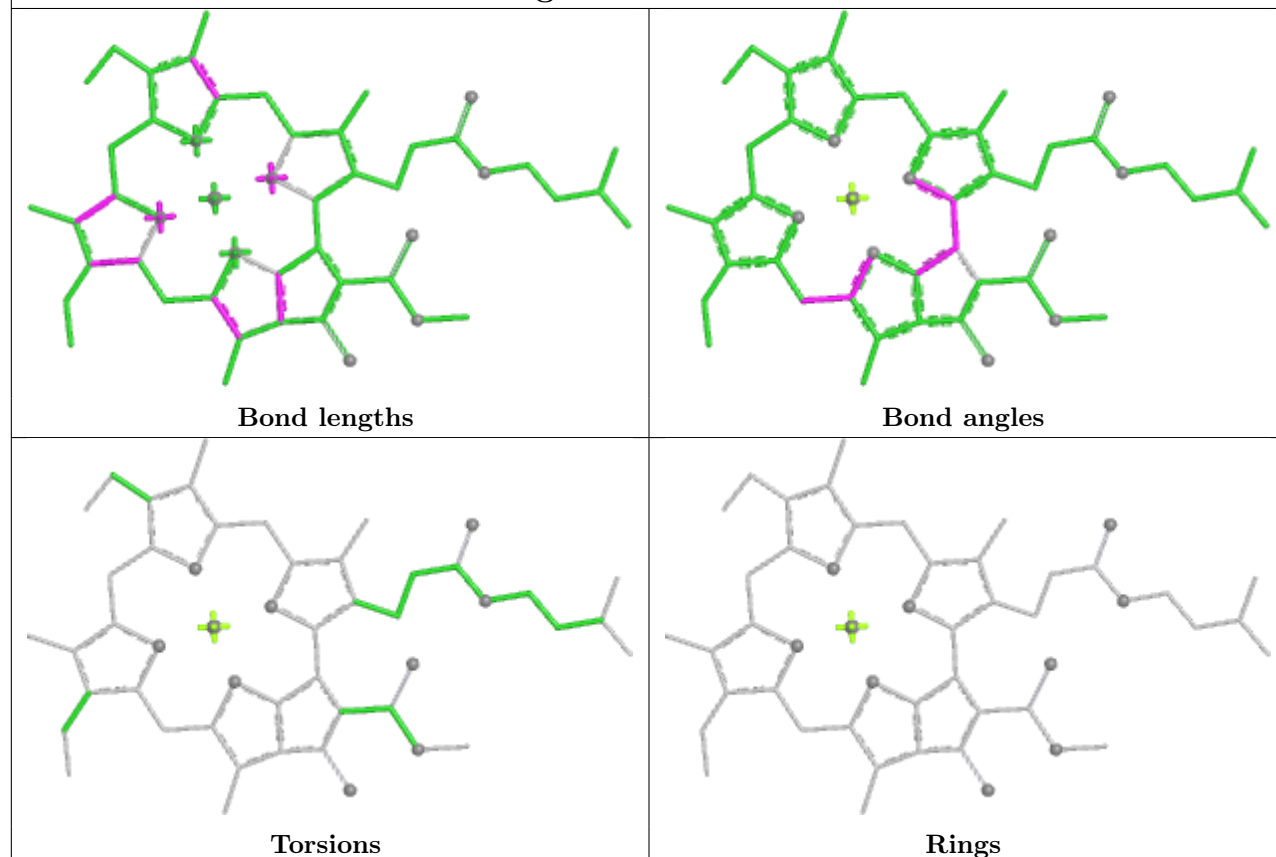


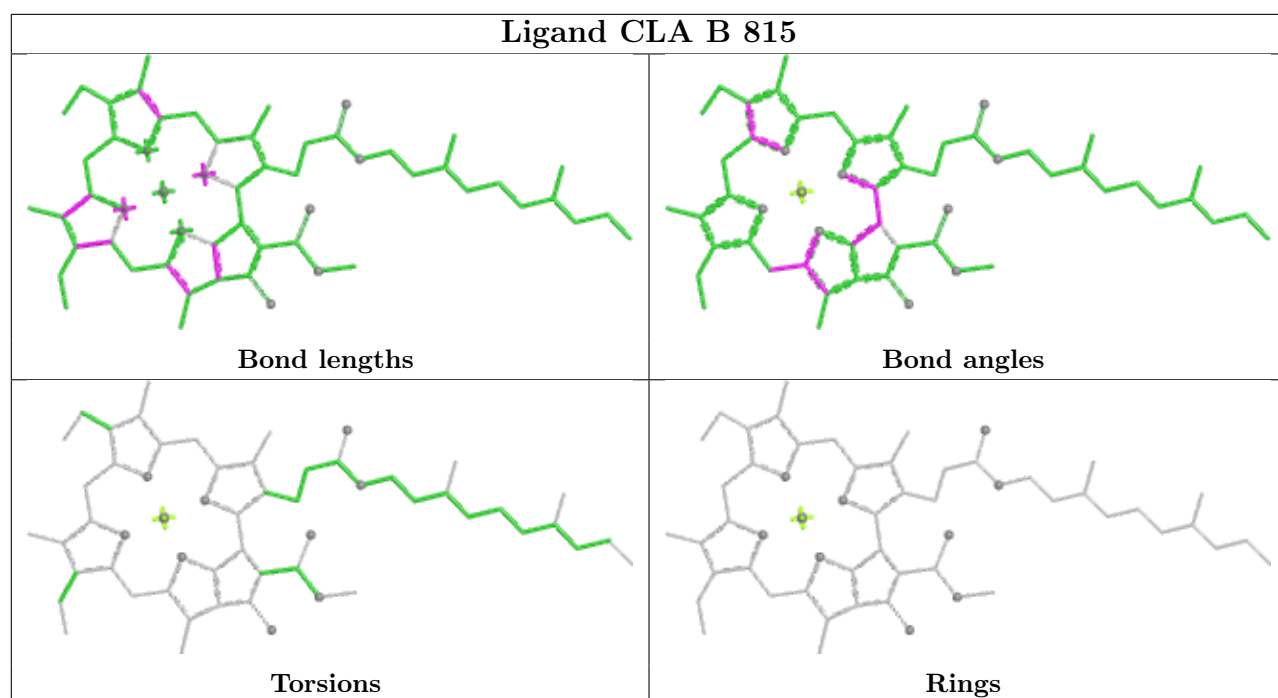


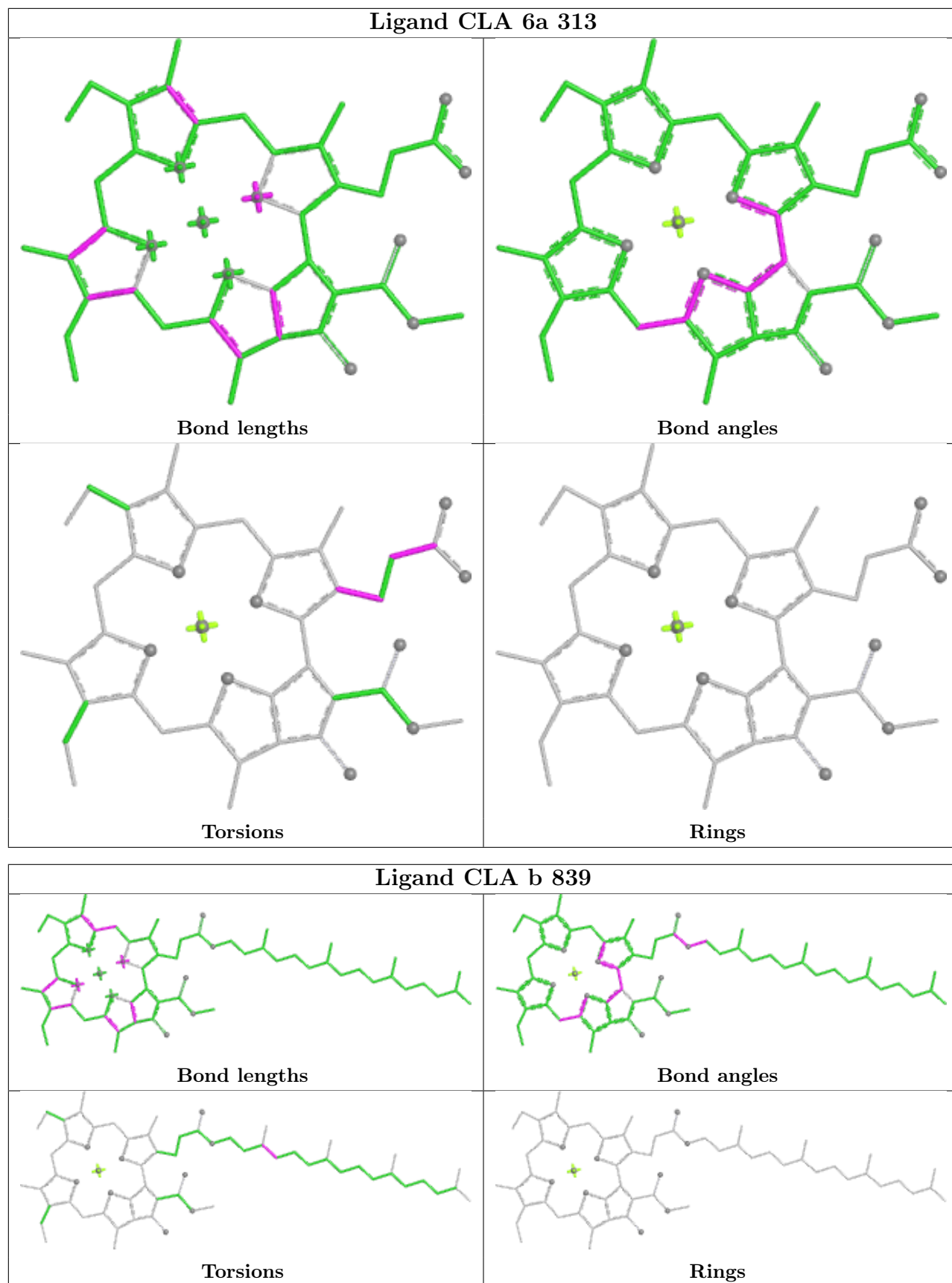
Ligand CLA 5b 309

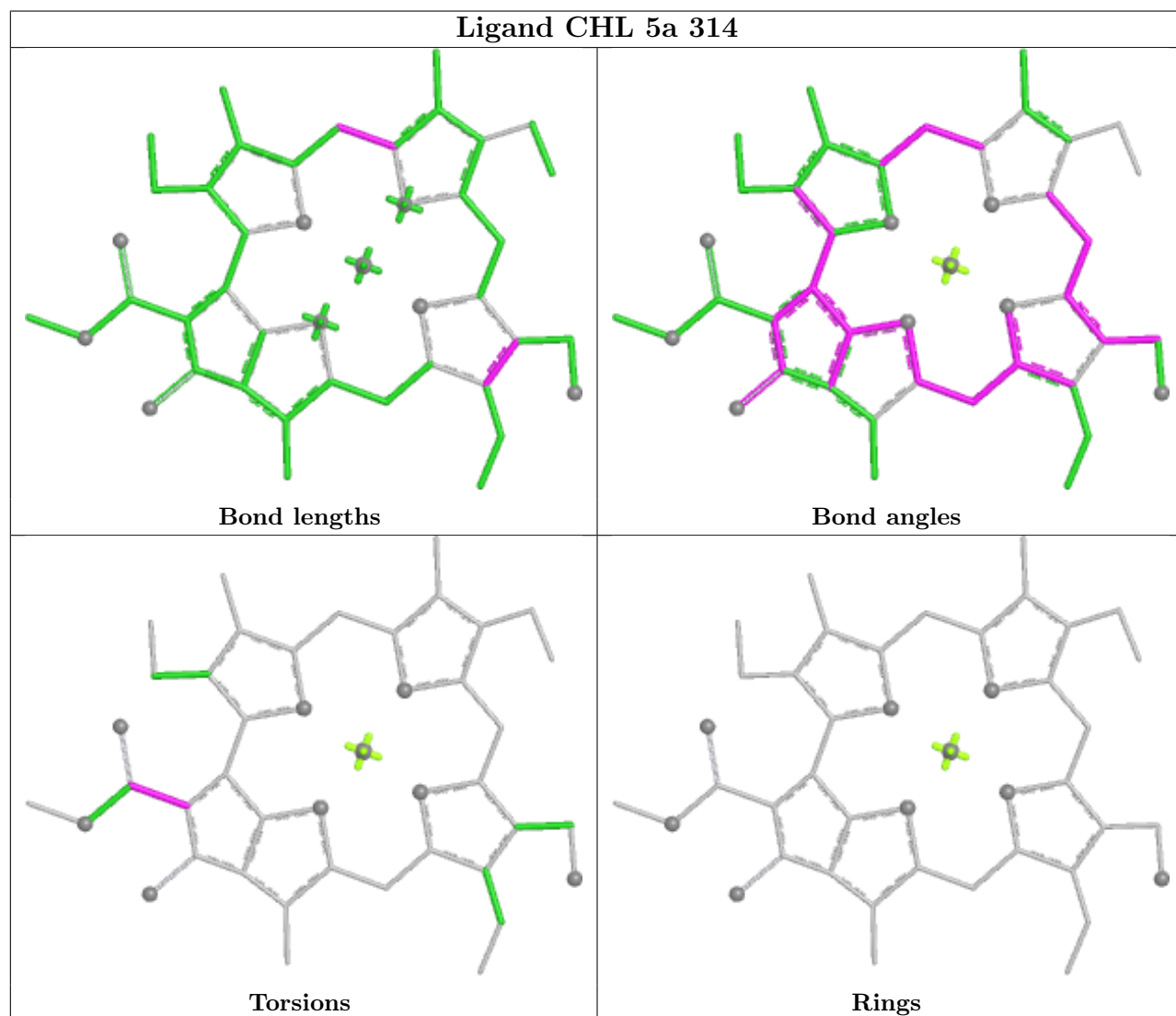
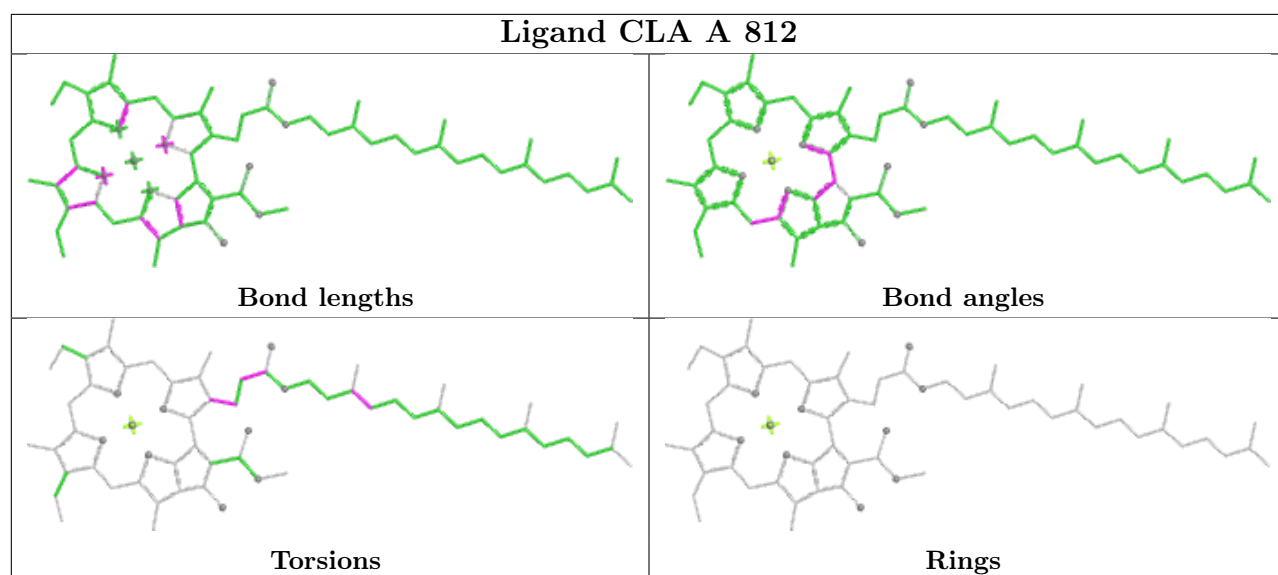


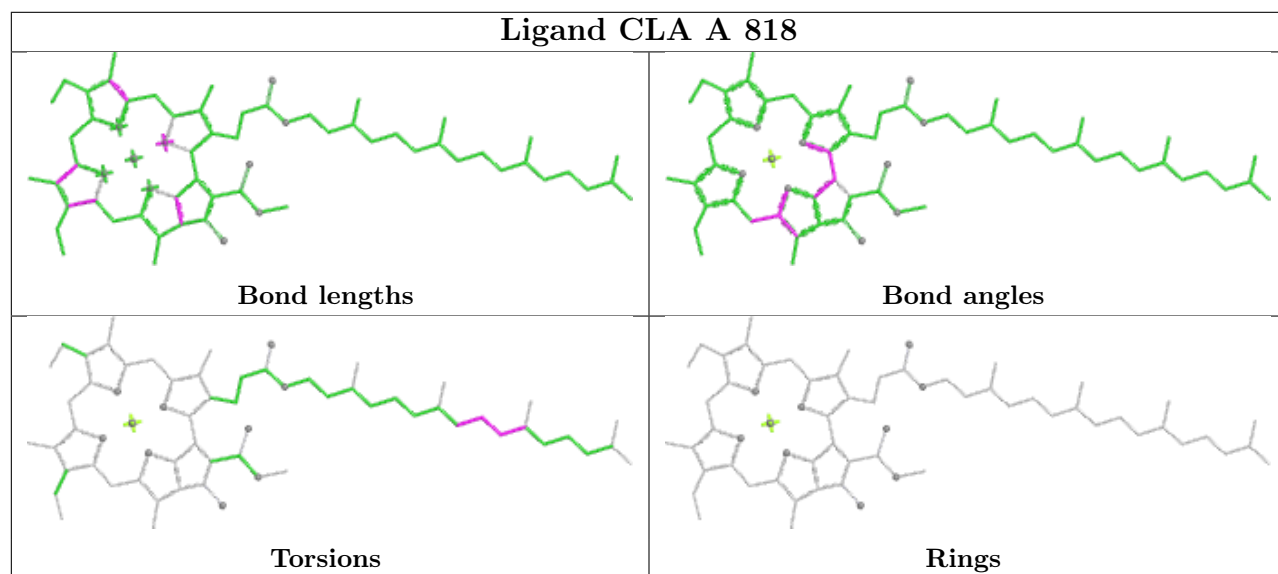
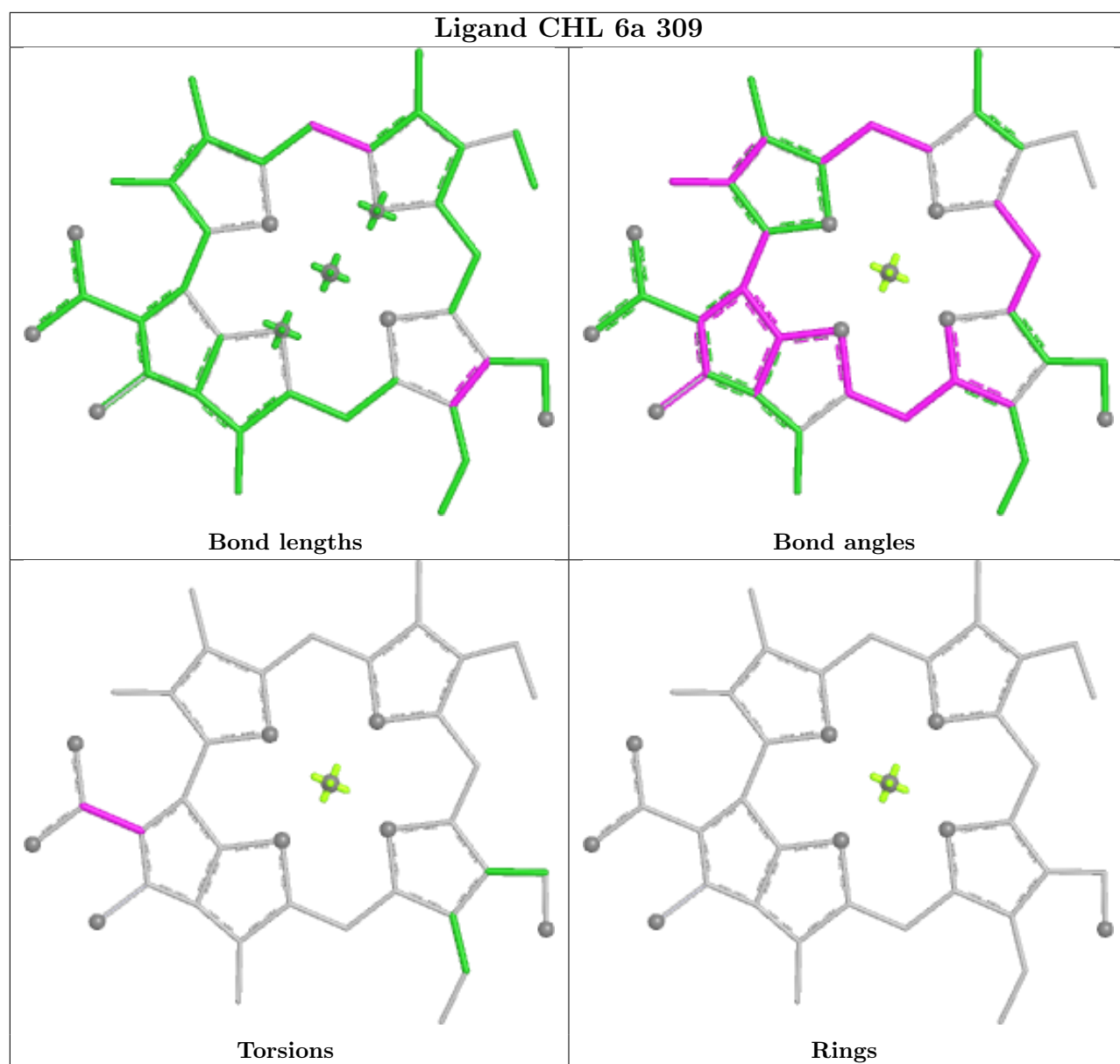
Ligand CLA a 838

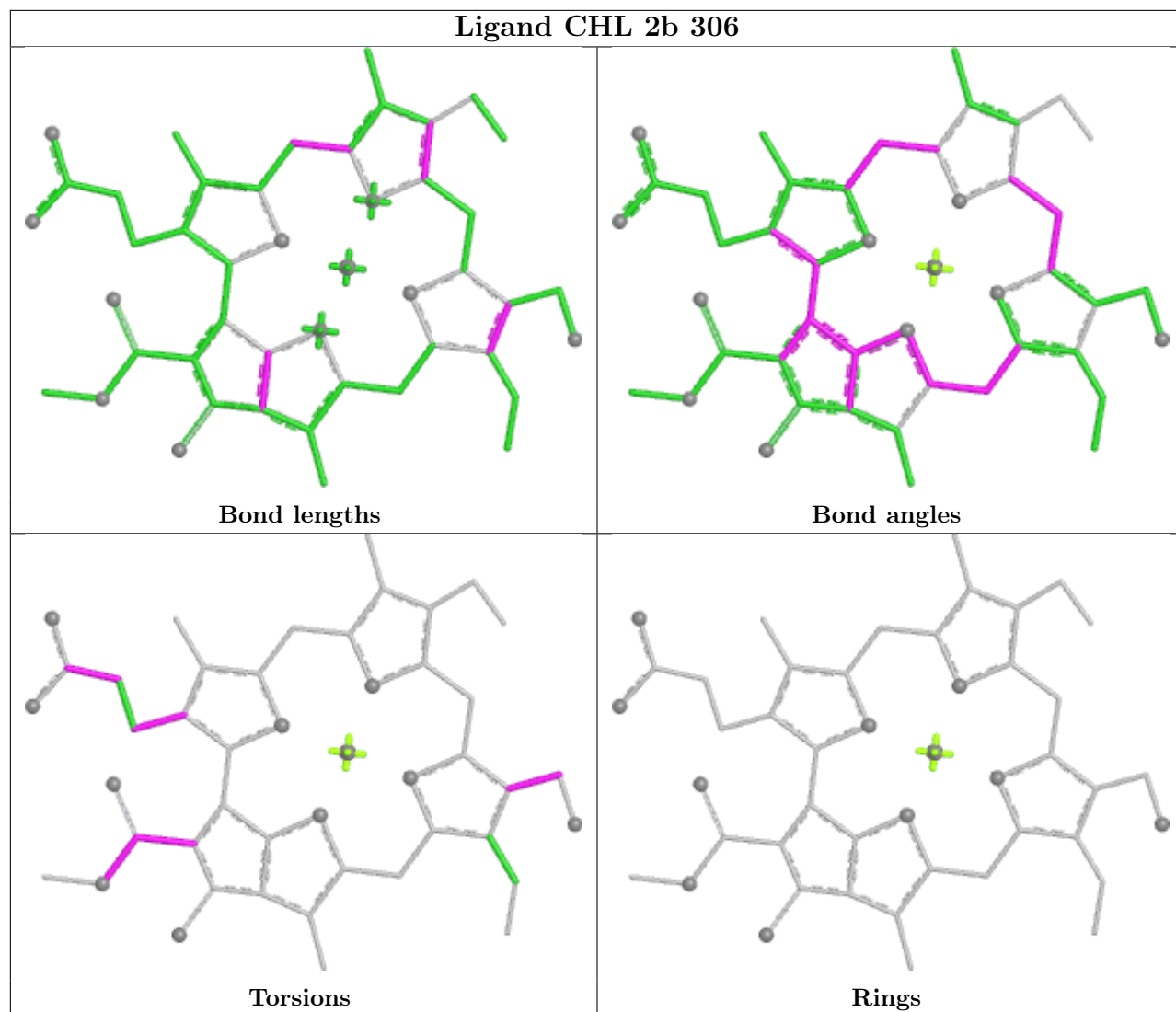


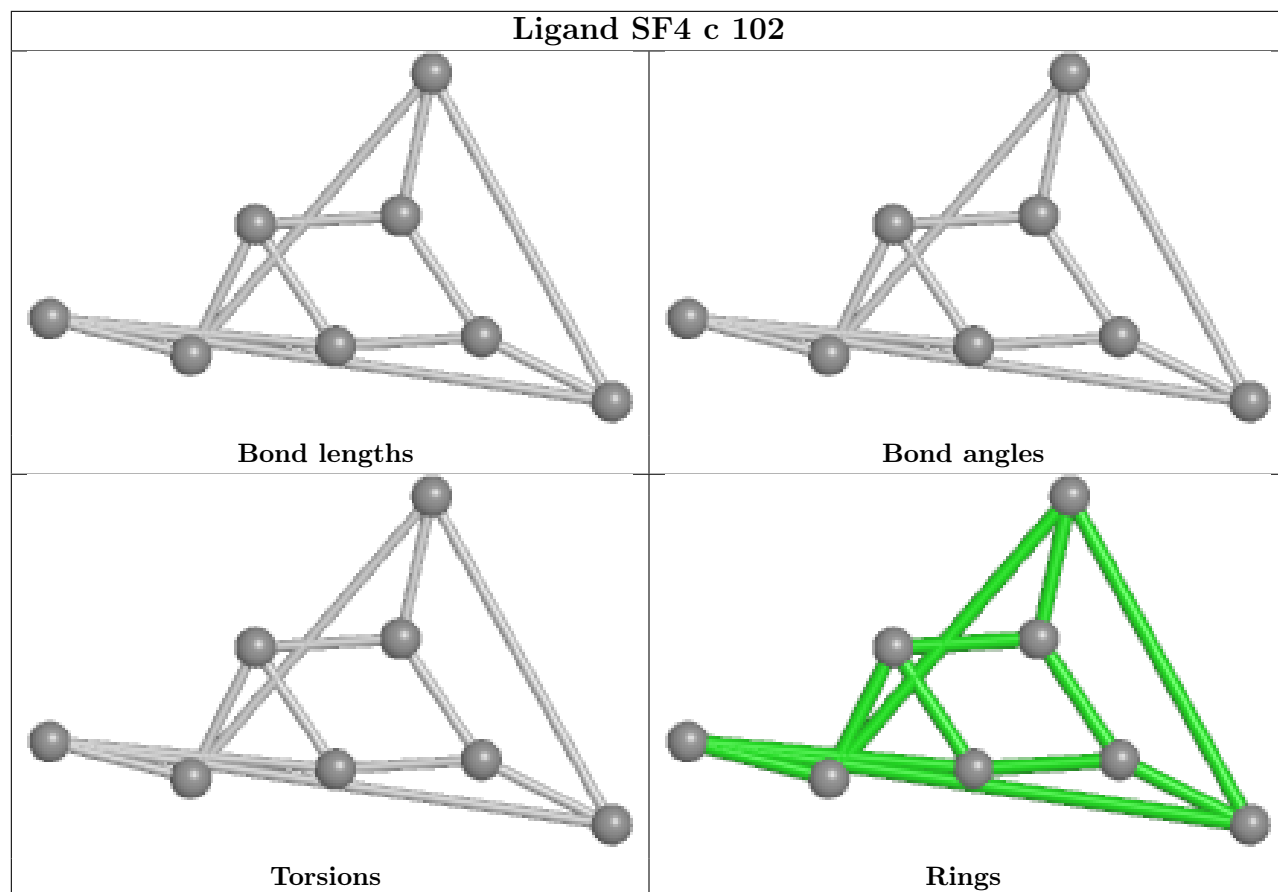


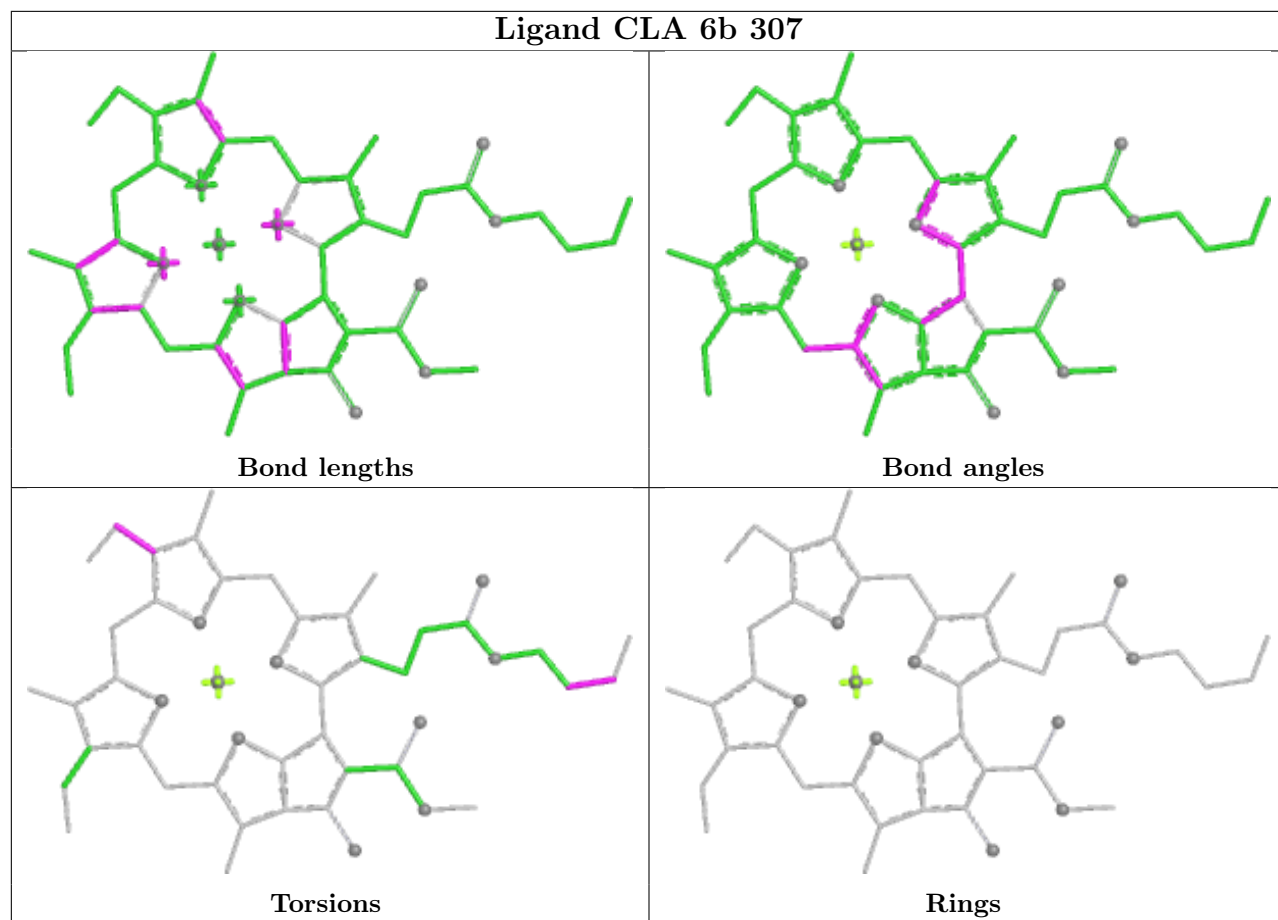




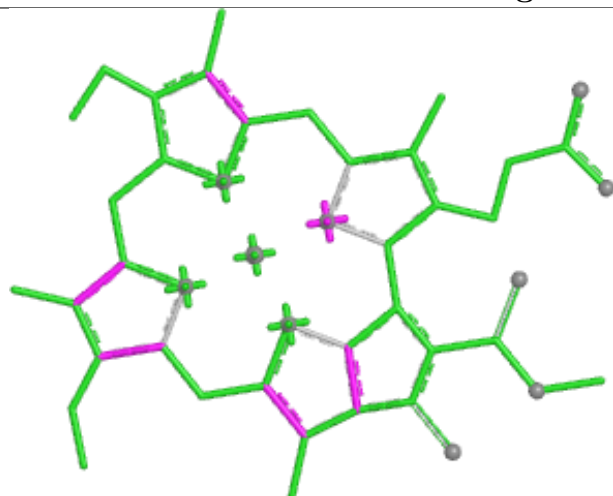




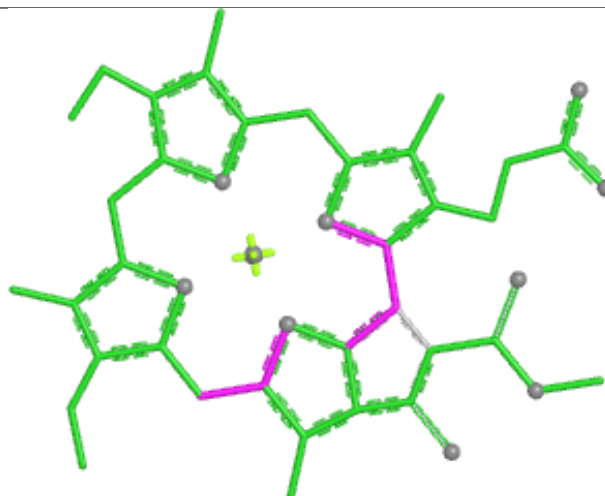




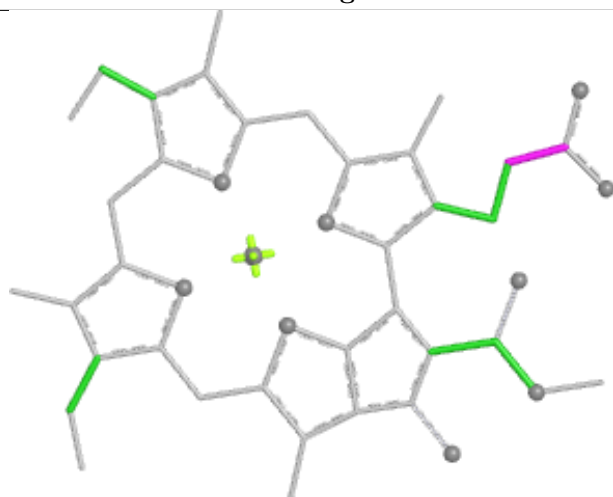
Ligand CLA F 302



Bond lengths



Bond angles

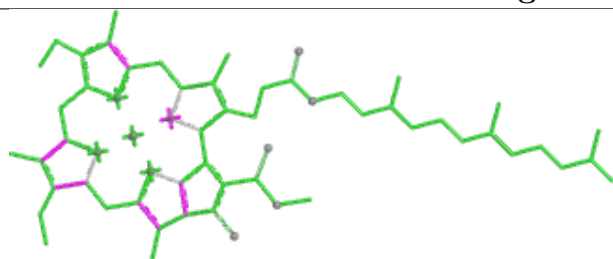


Torsions

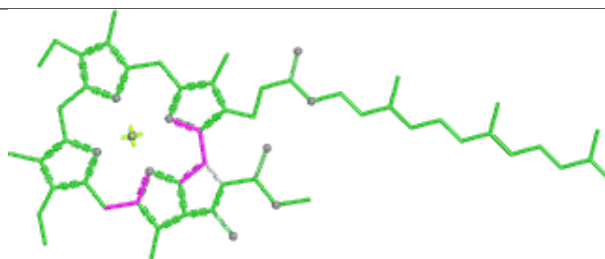


Rings

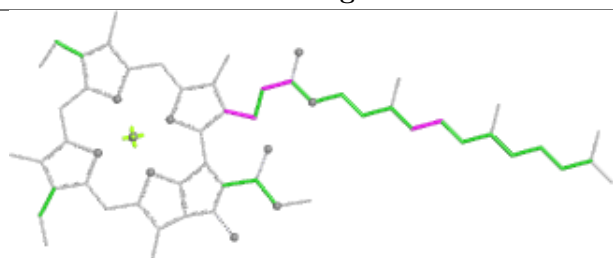
Ligand CLA a 834



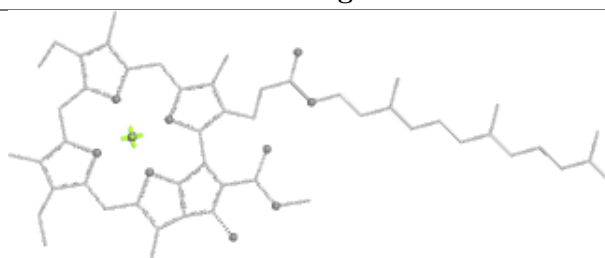
Bond lengths



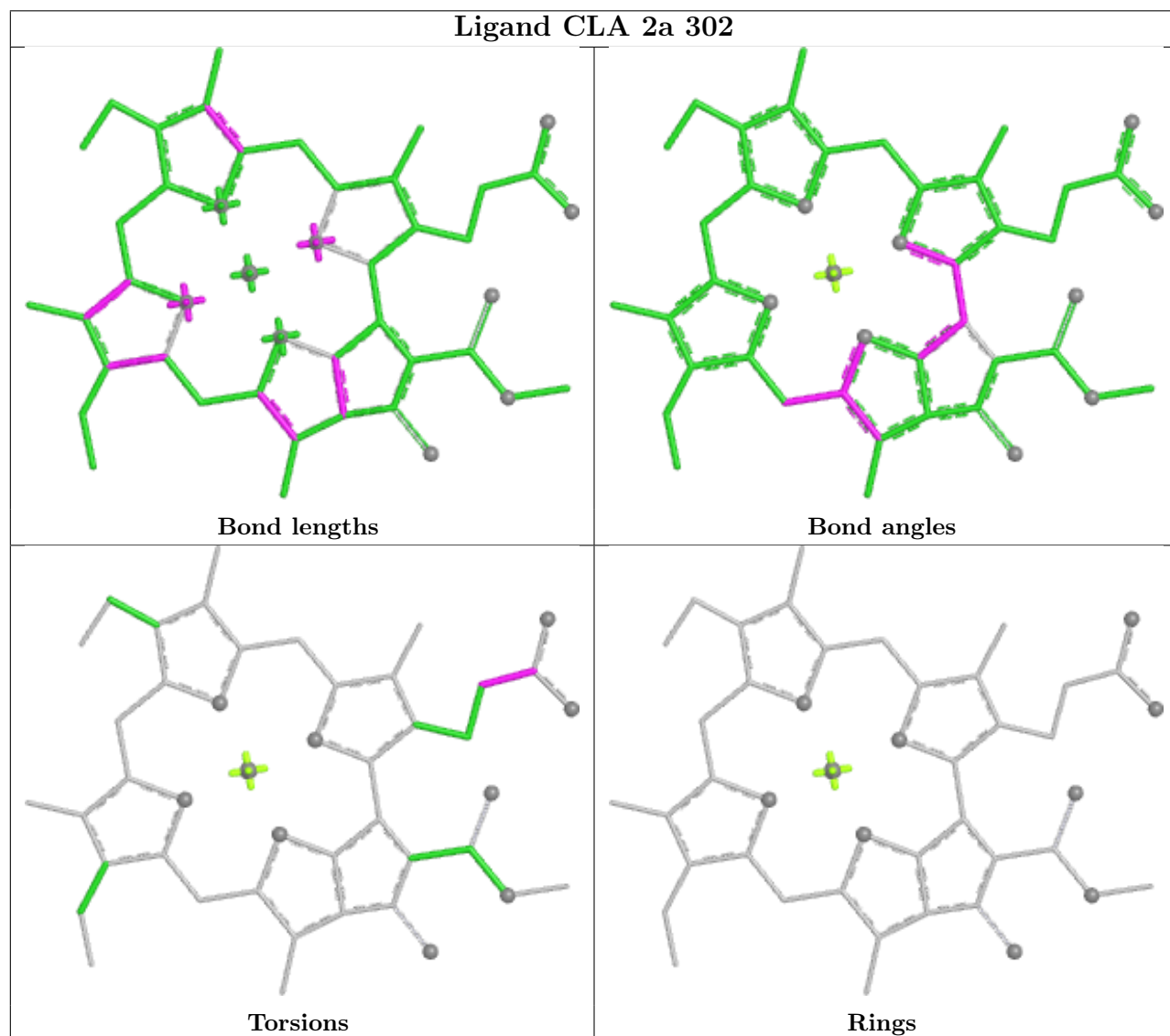
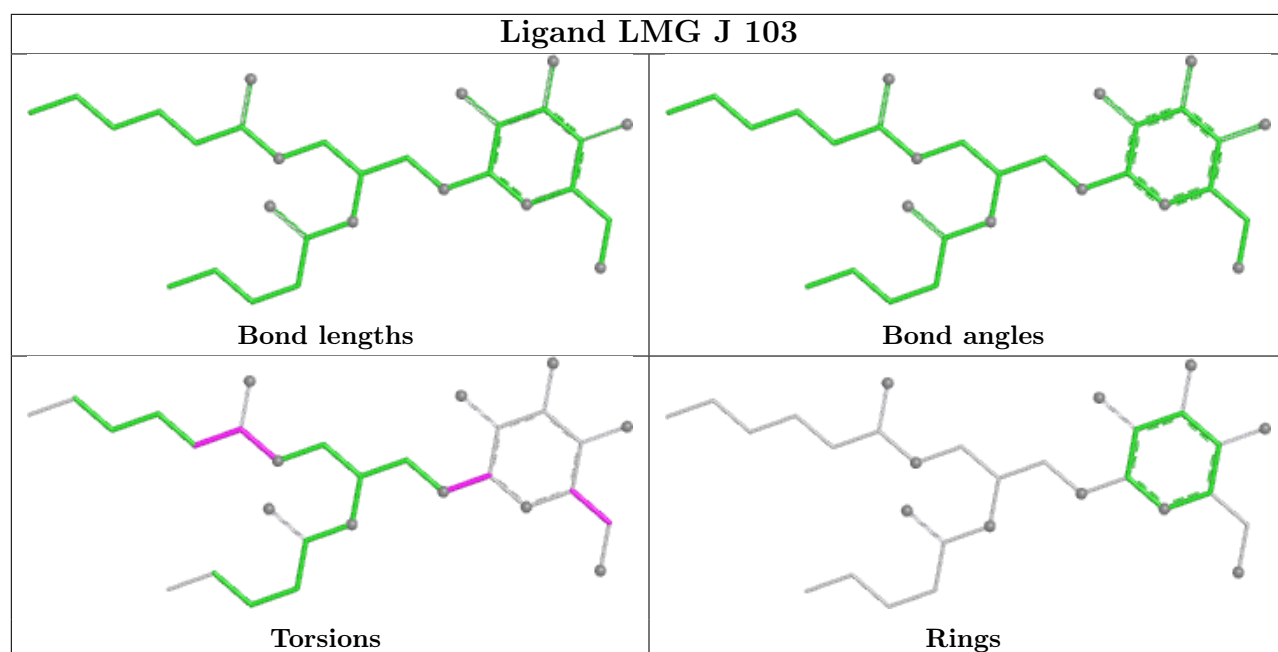
Bond angles



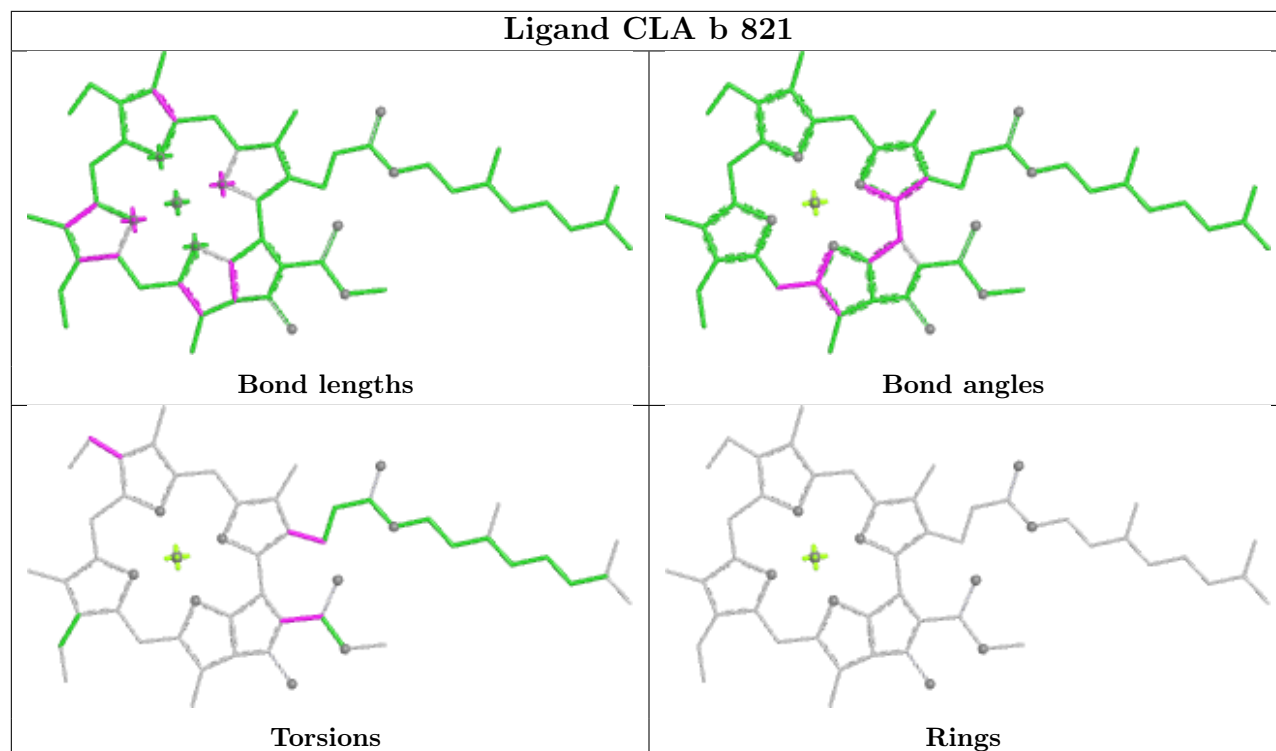
Torsions



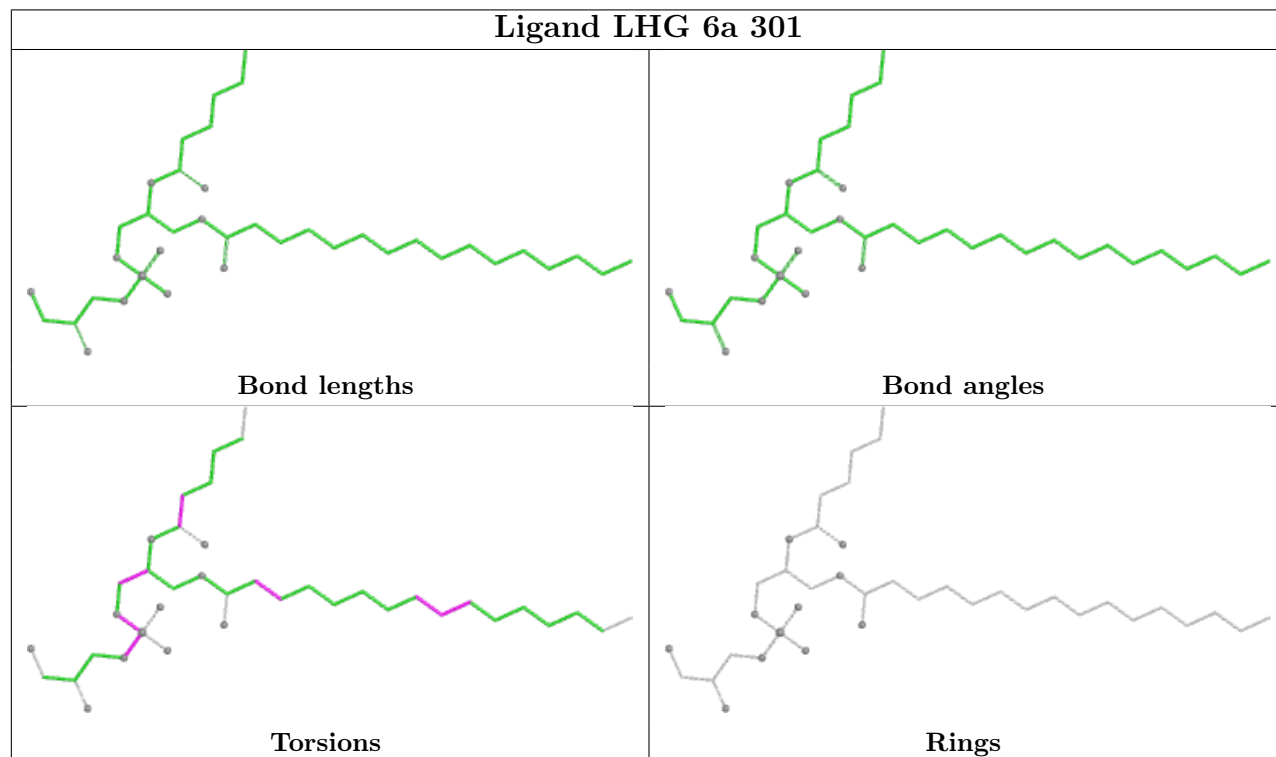
Rings

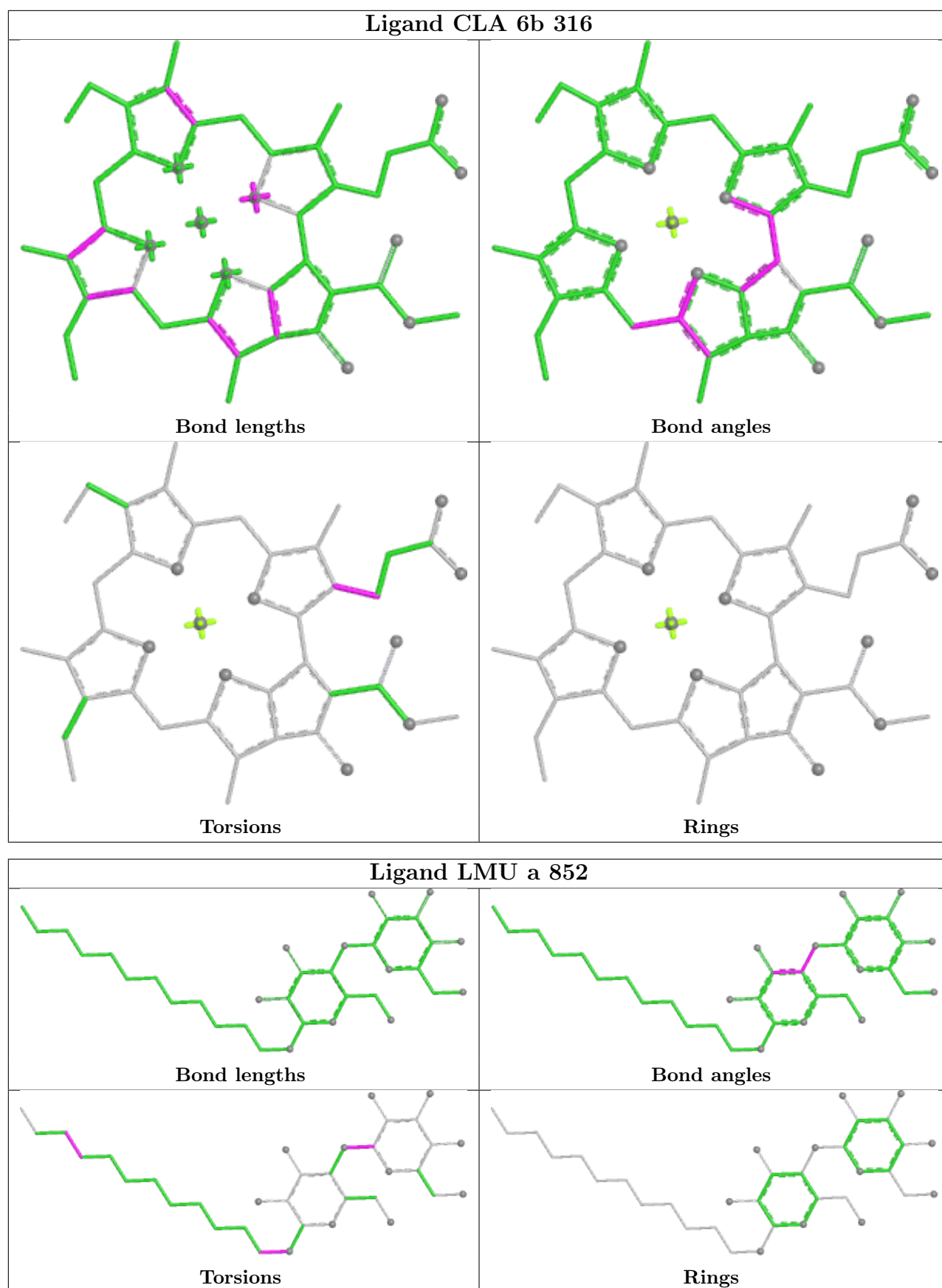


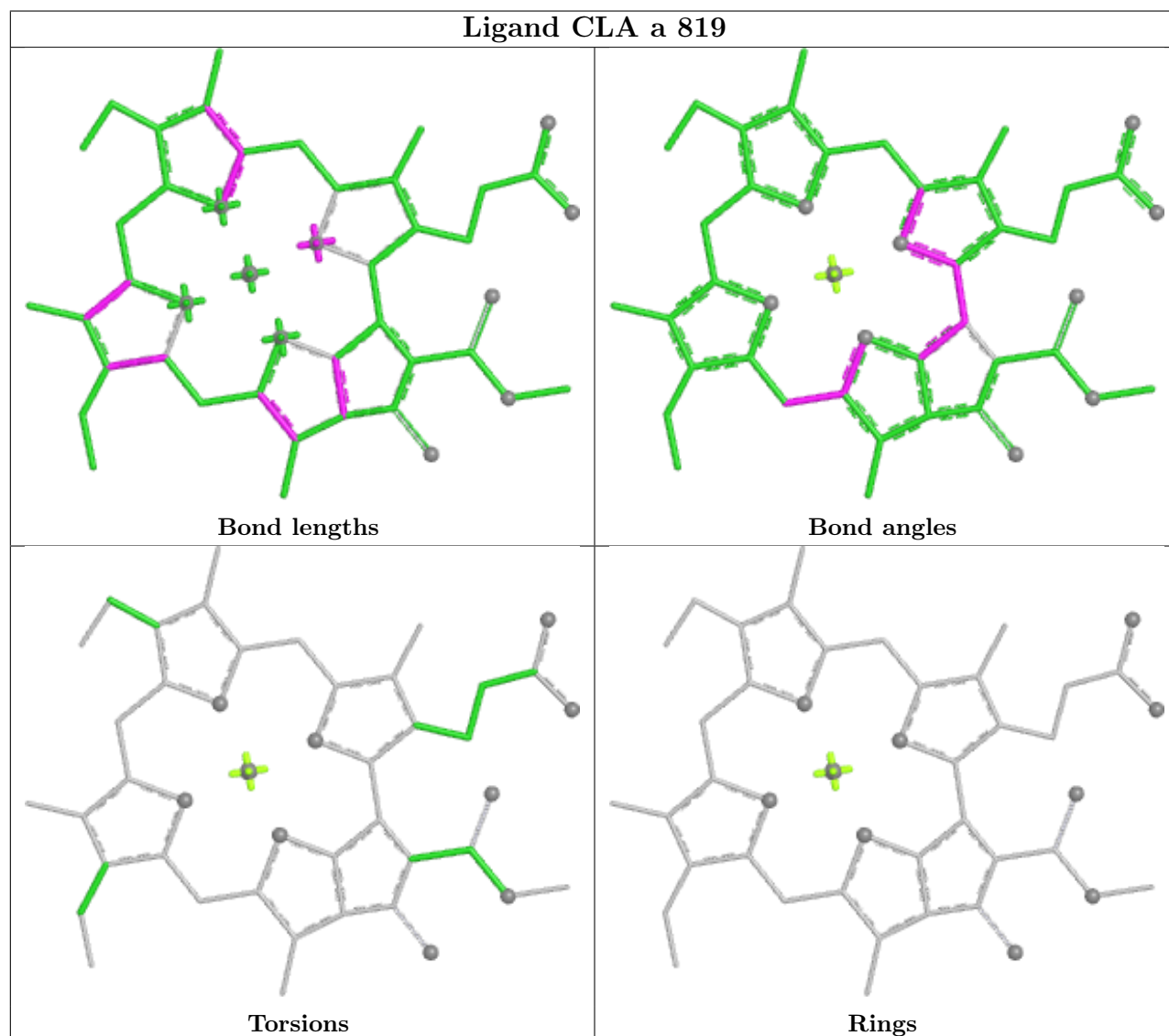
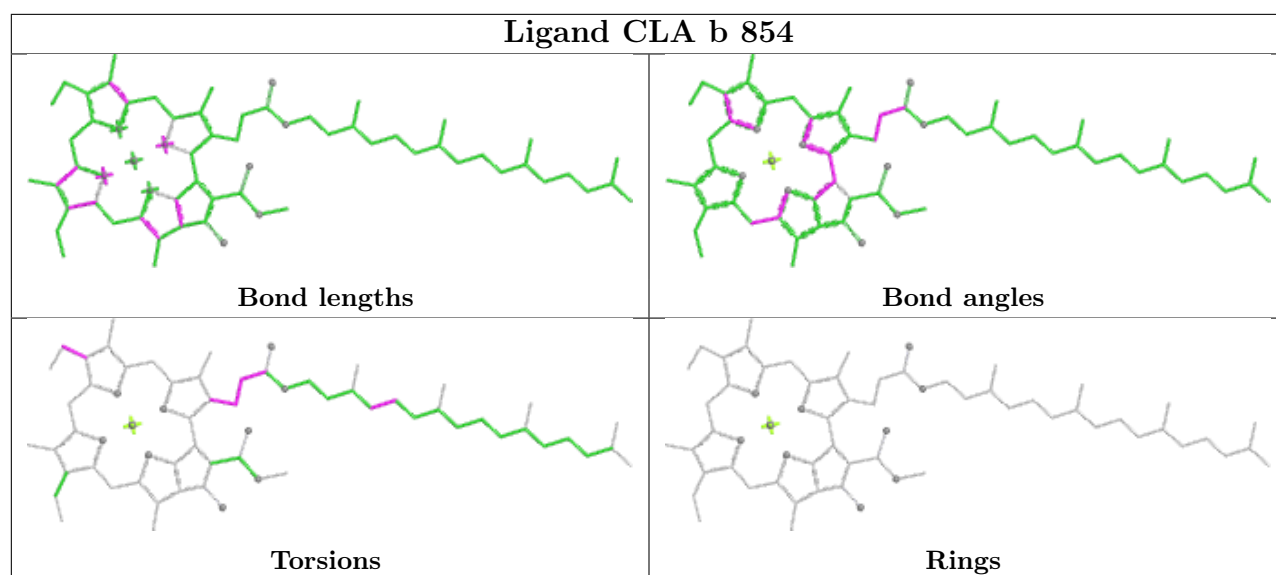
Ligand CLA b 821

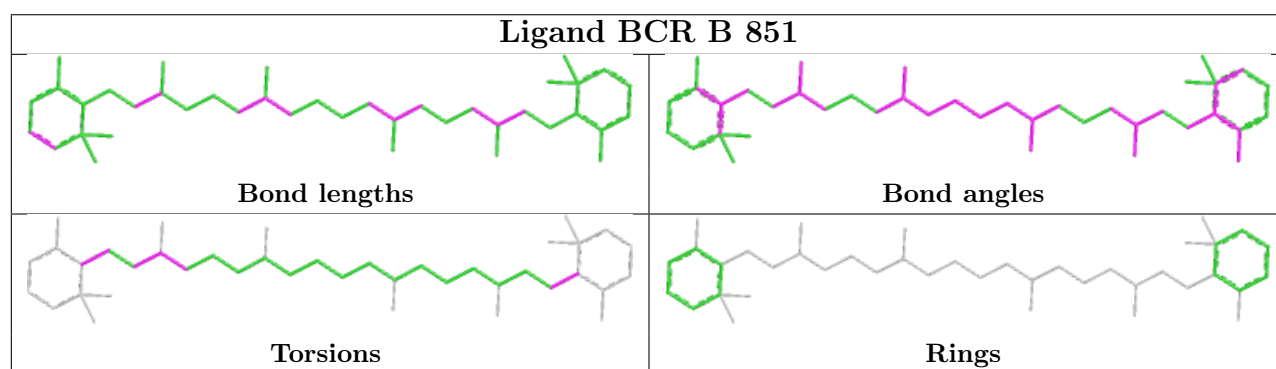
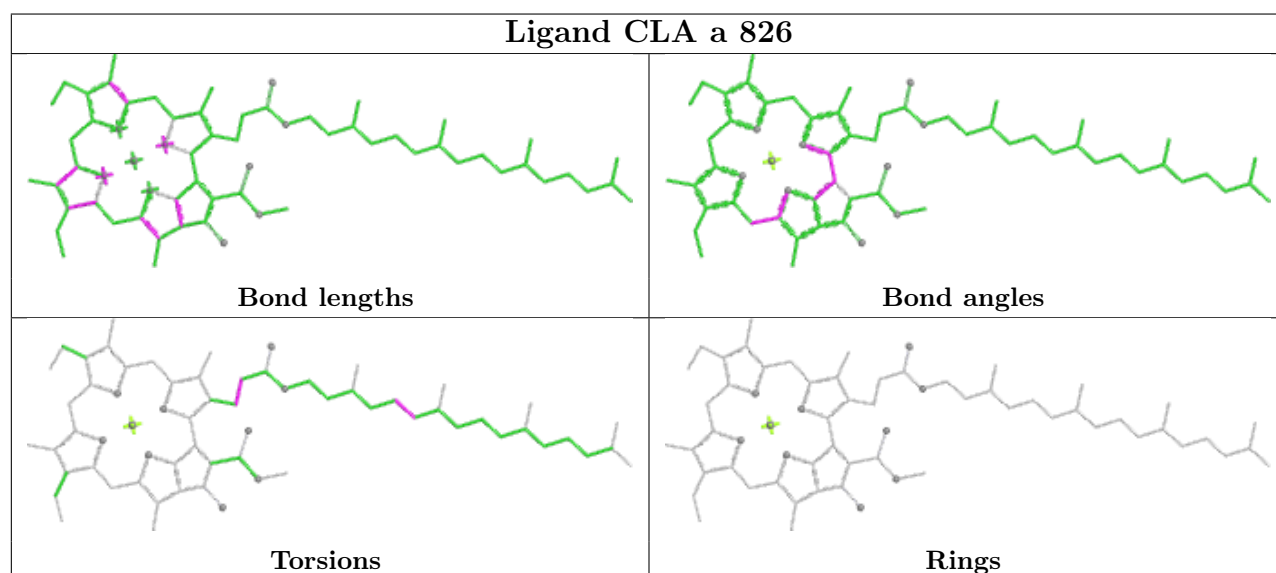
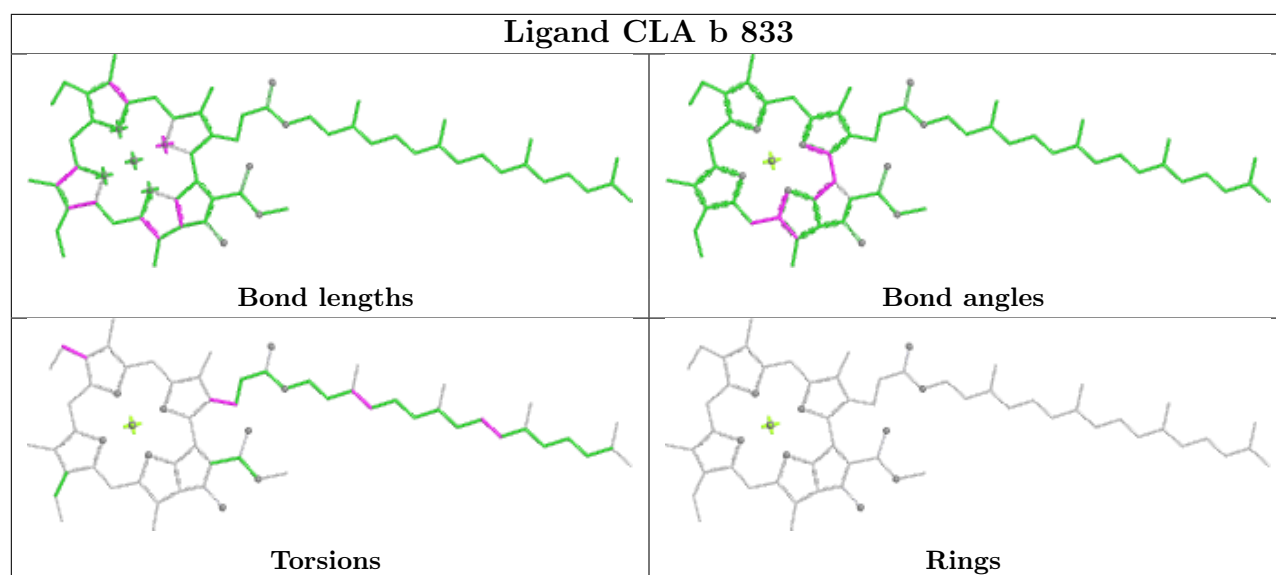


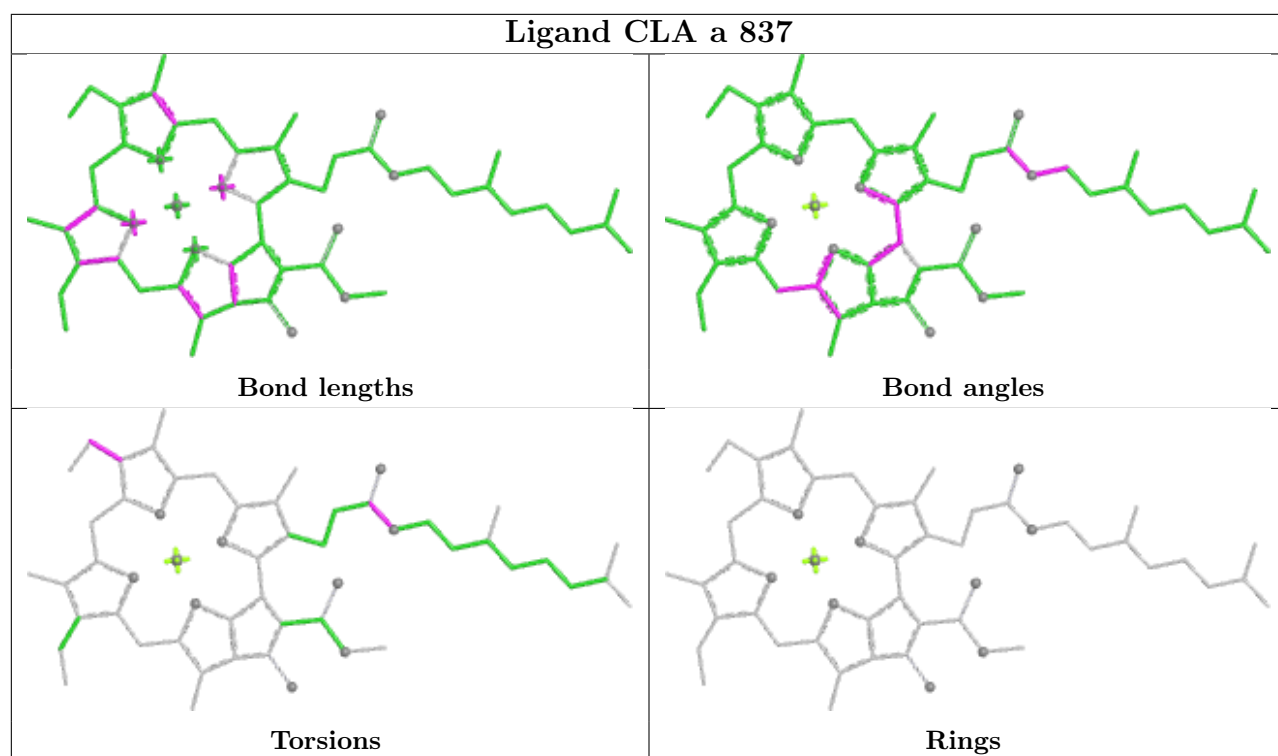
Ligand LHG 6a 301

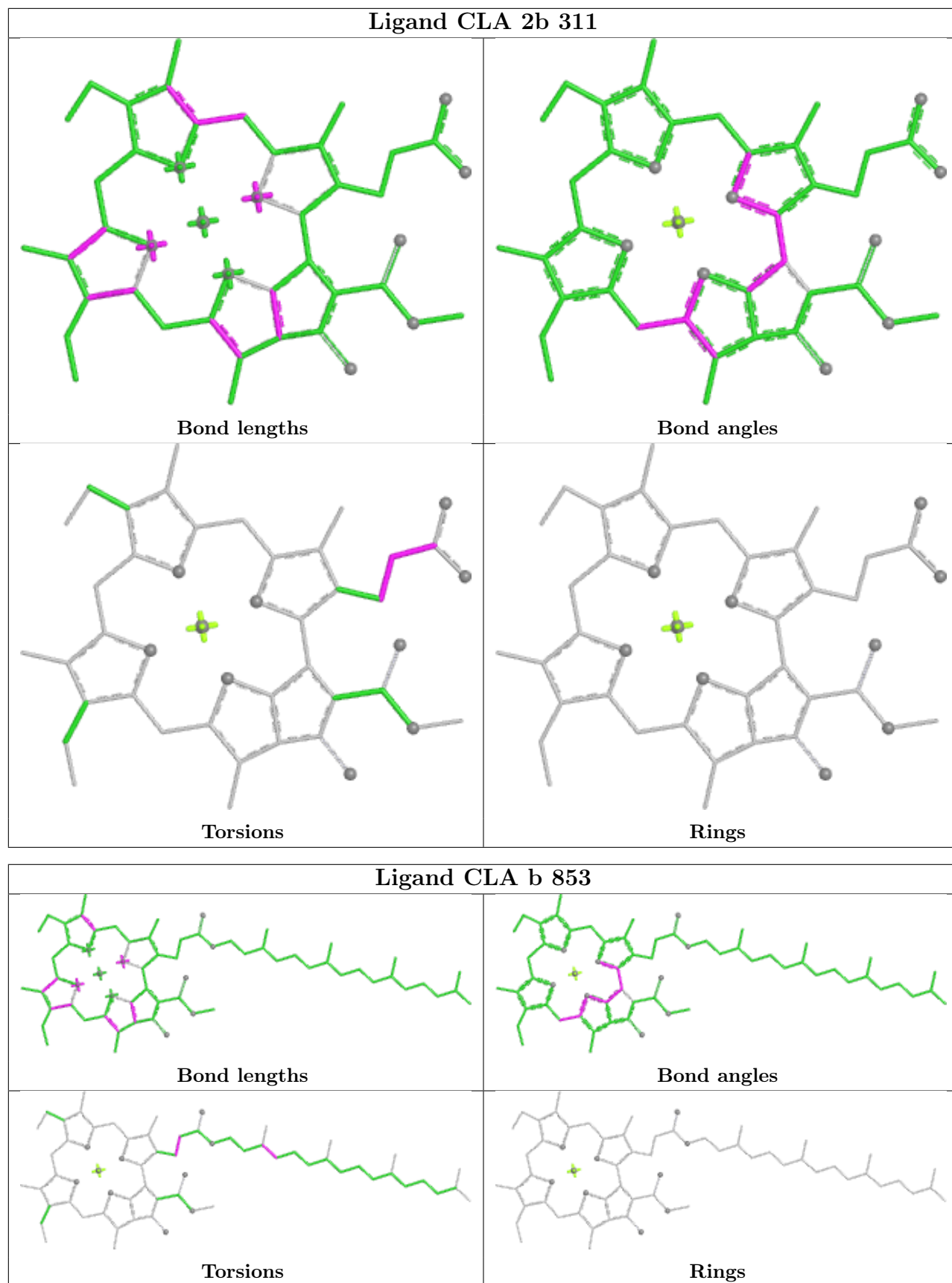


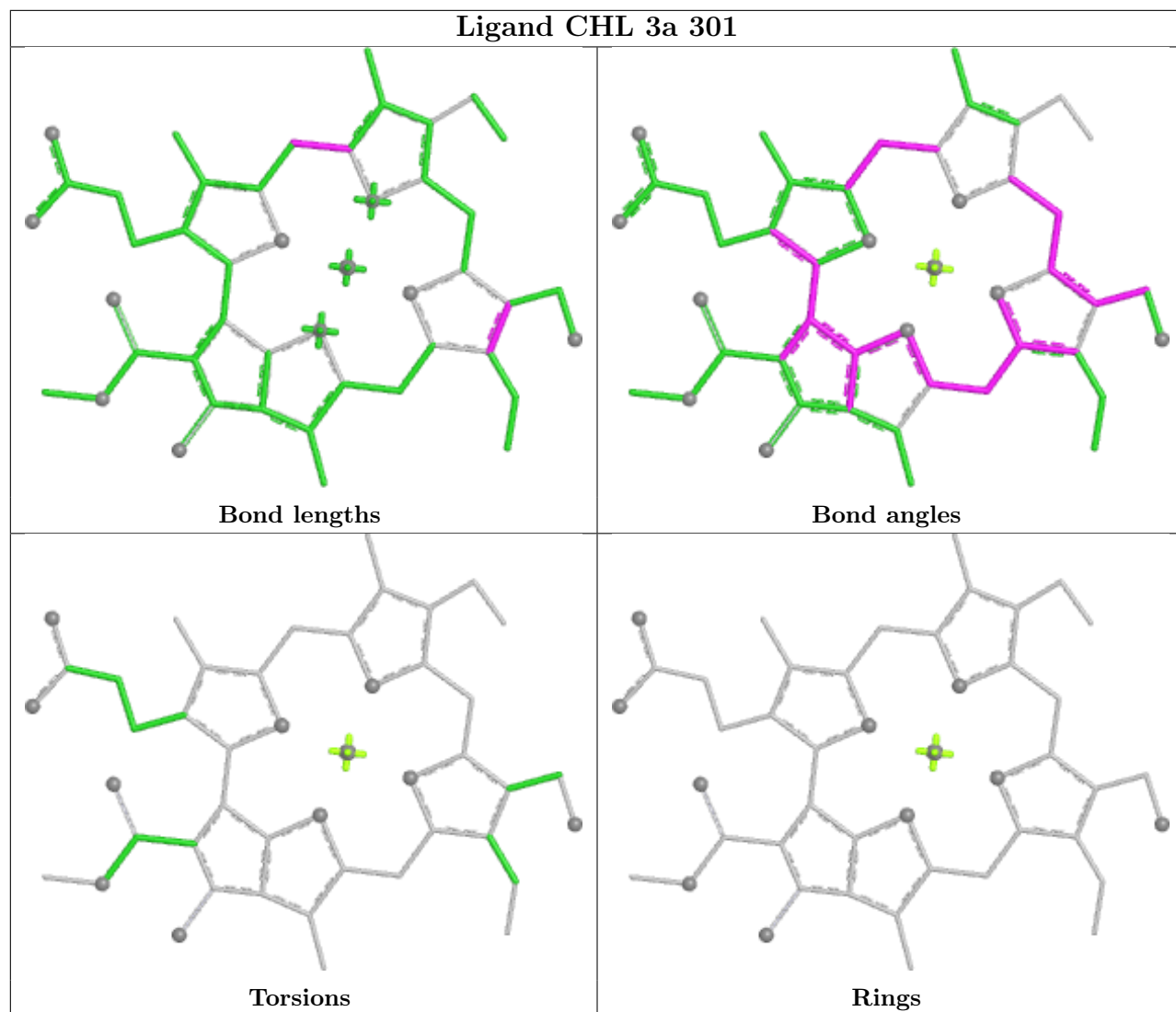


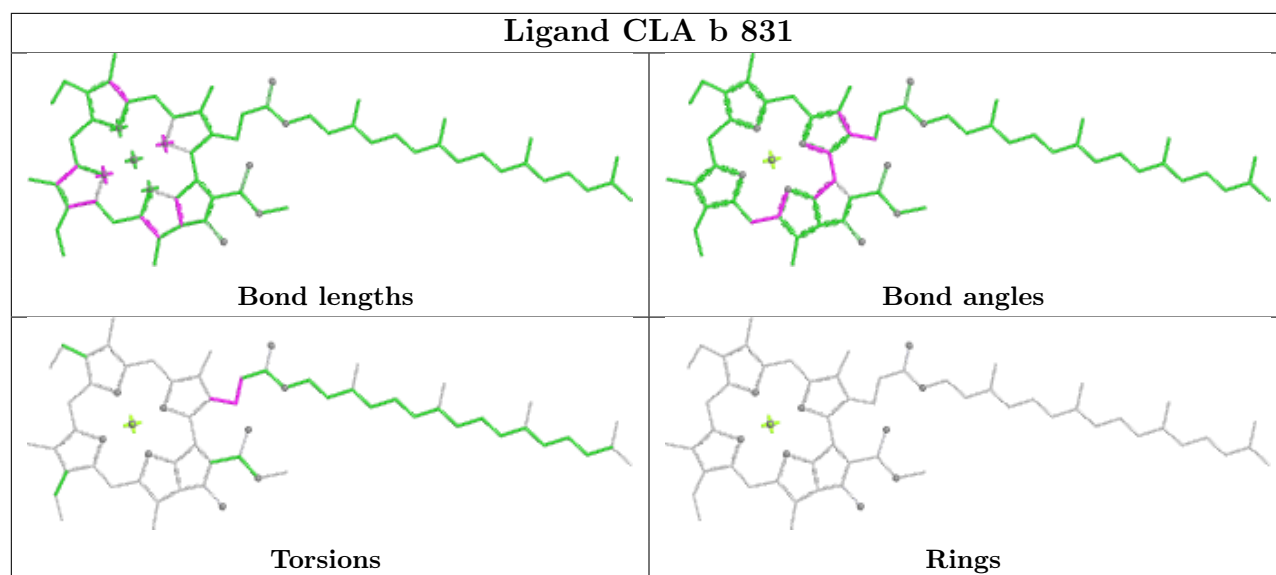
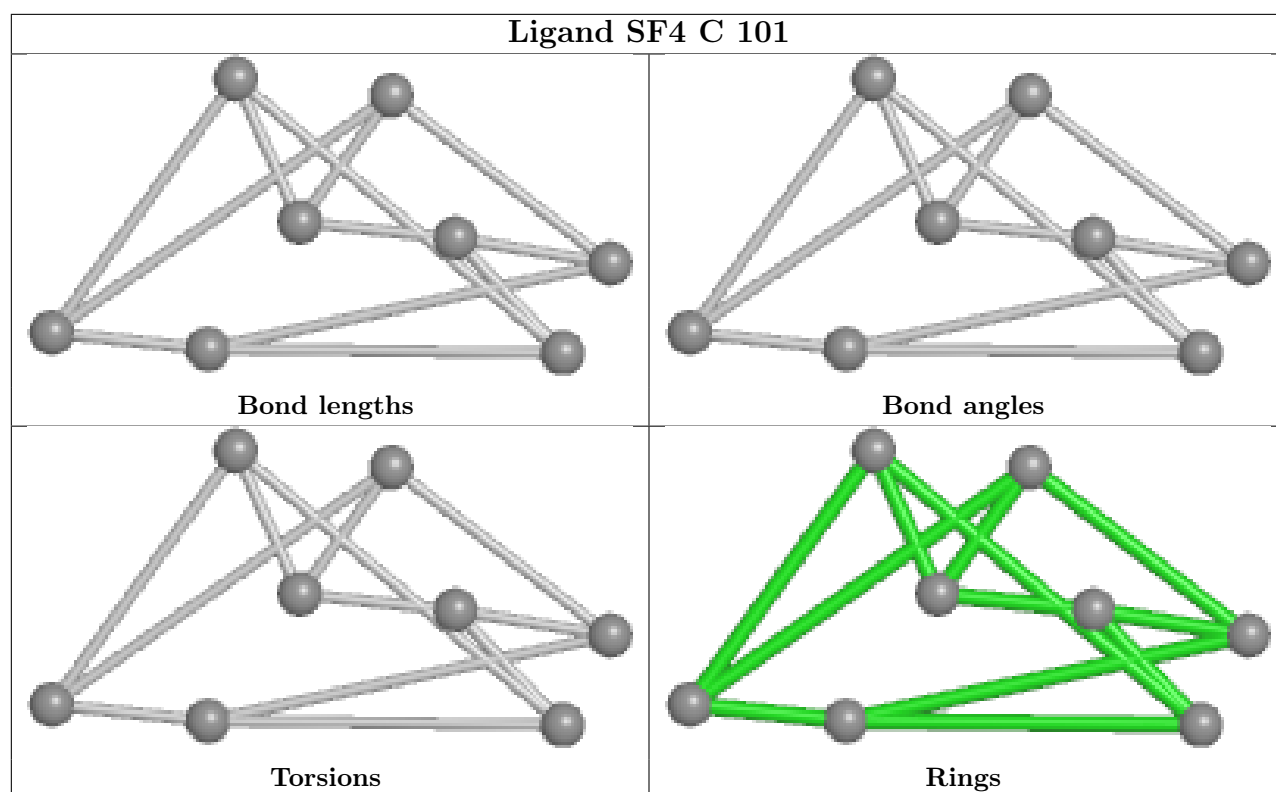


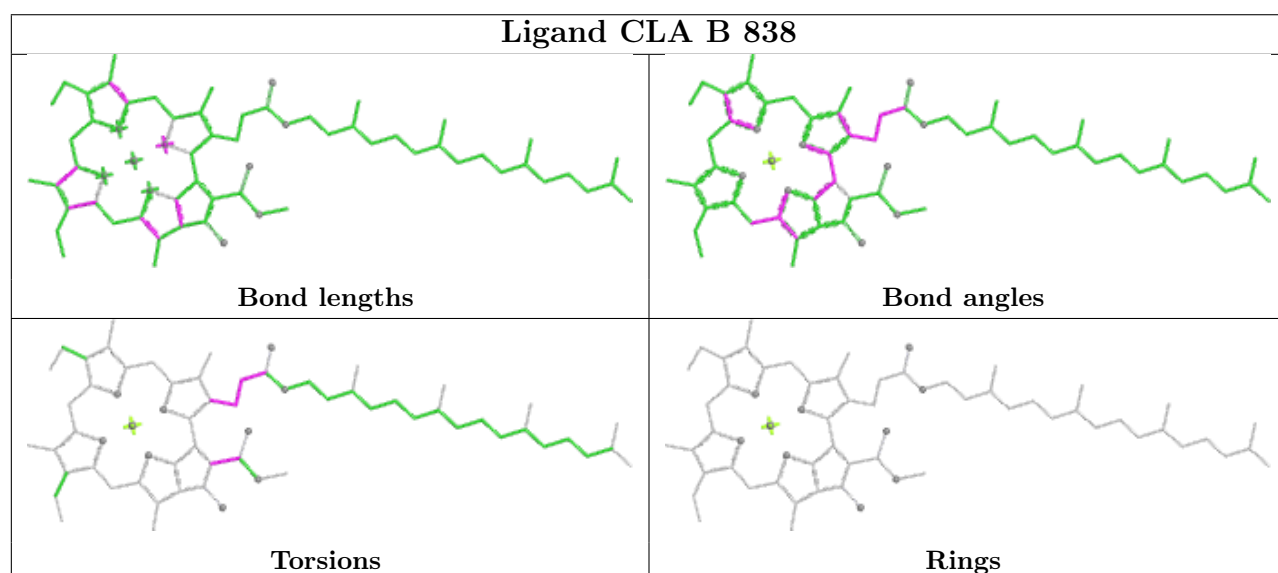
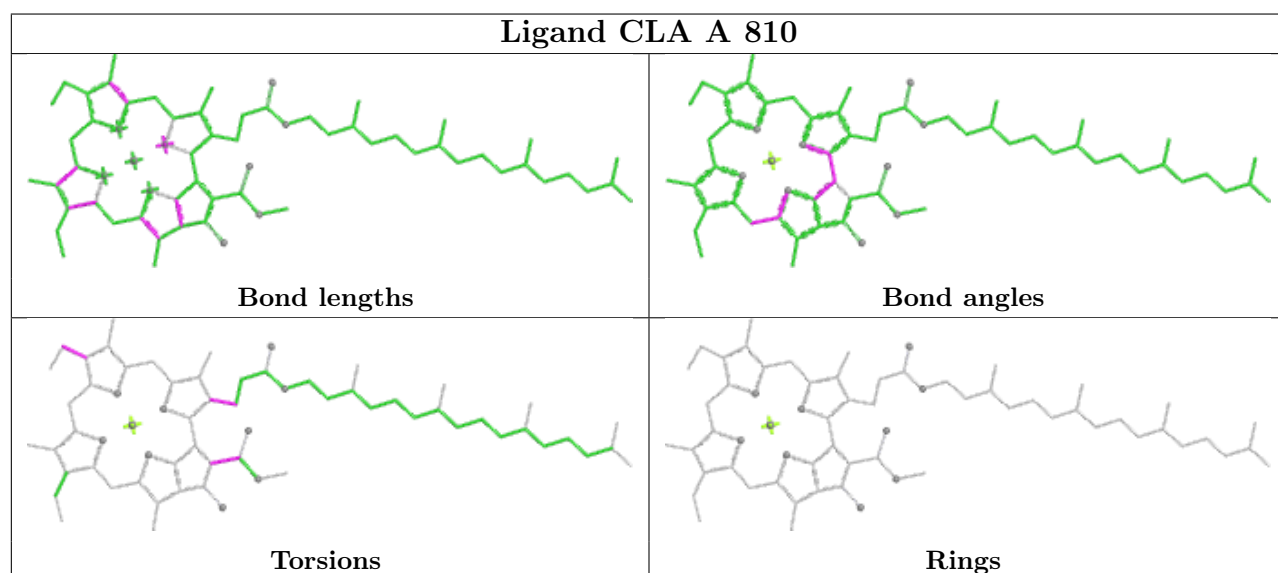
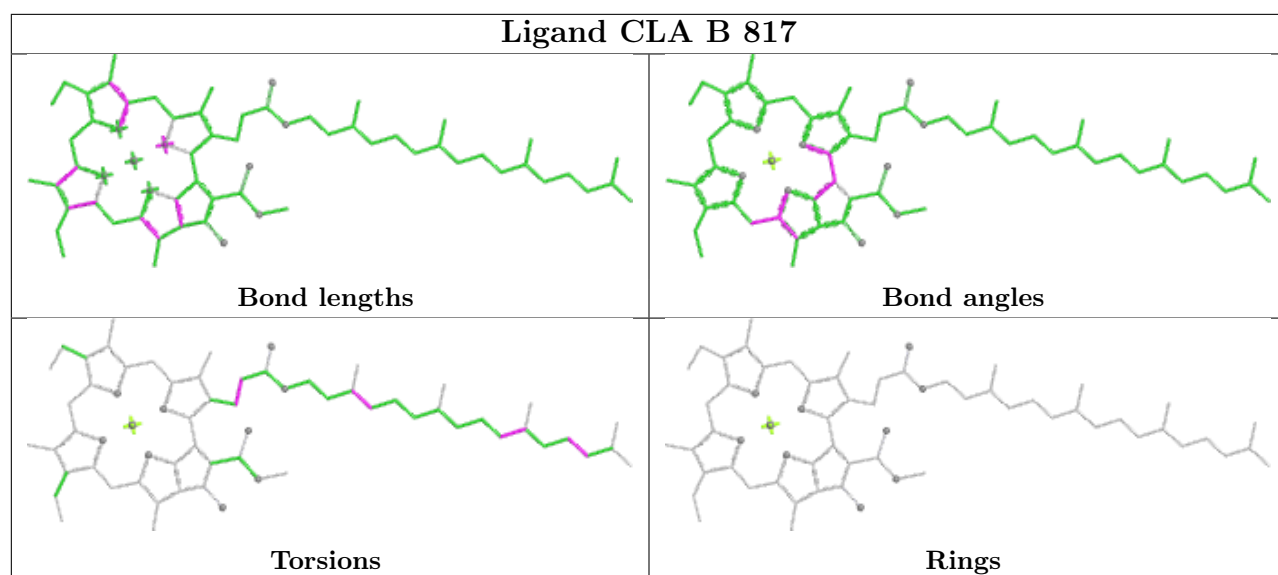




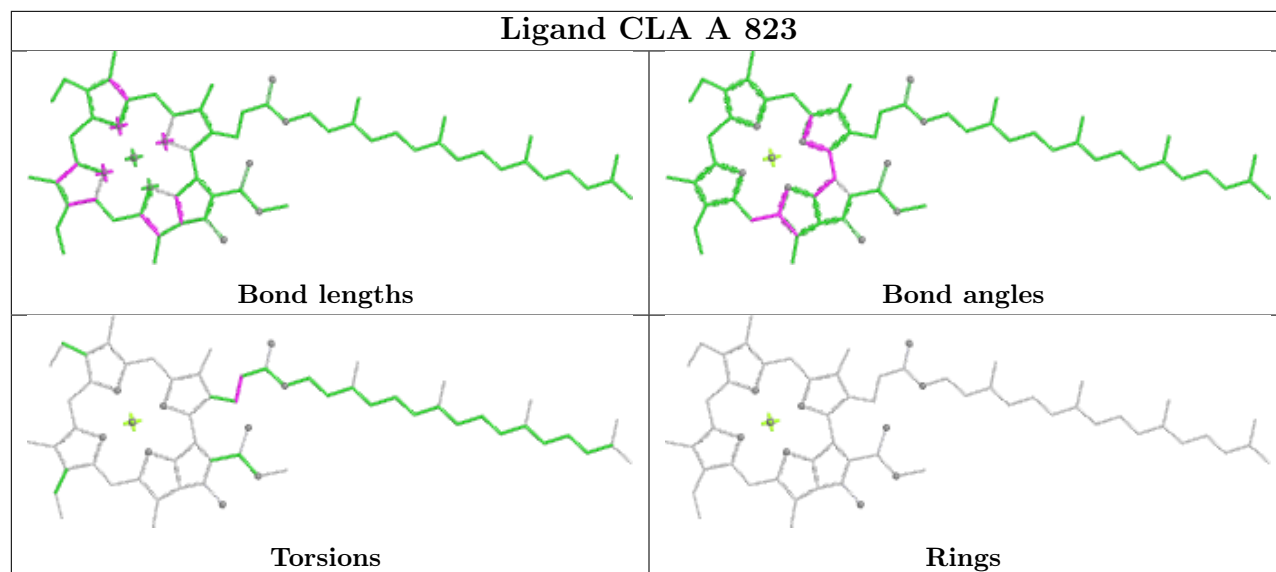




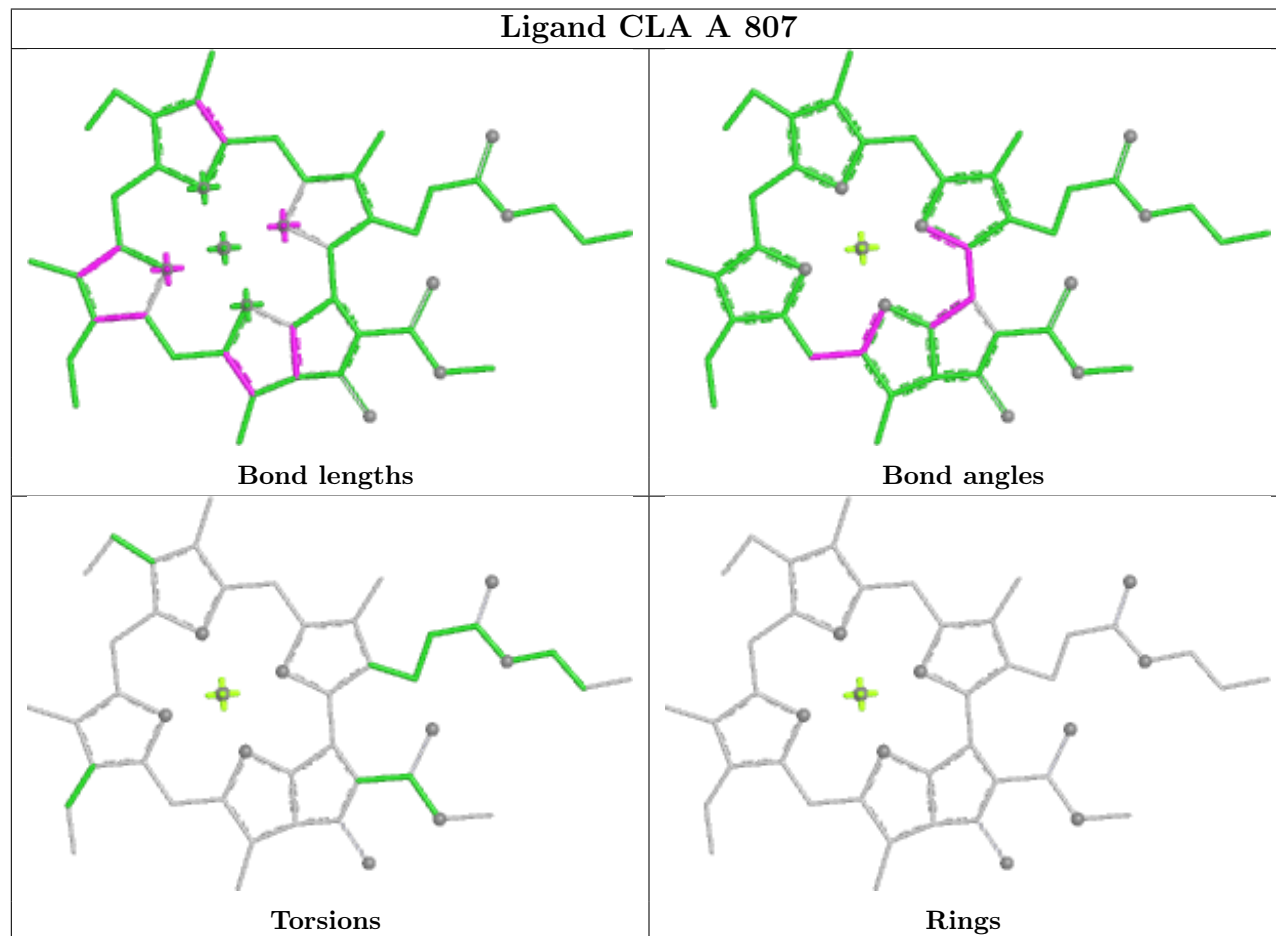


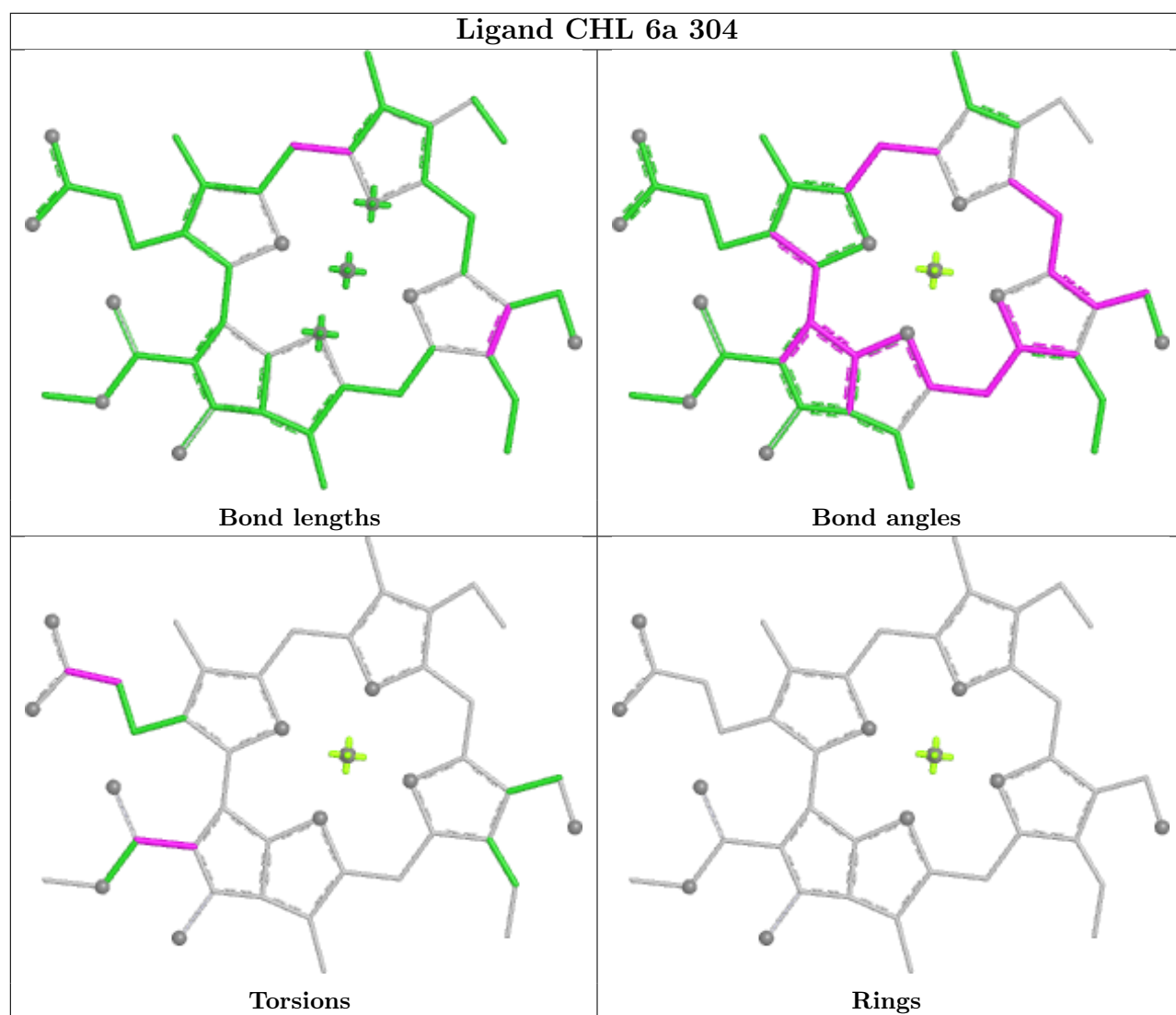


Ligand CLA A 823

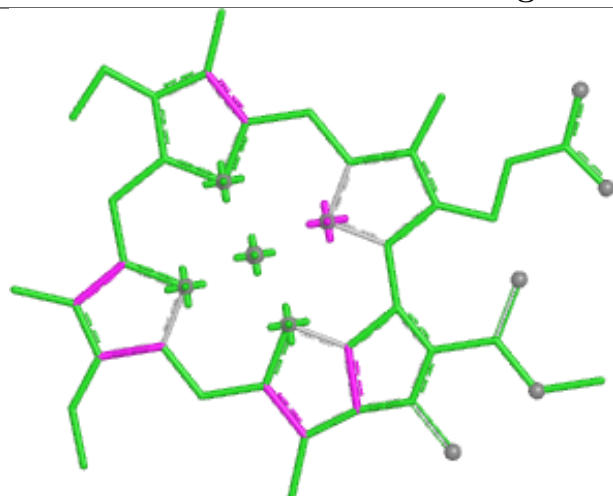


Ligand CLA A 807

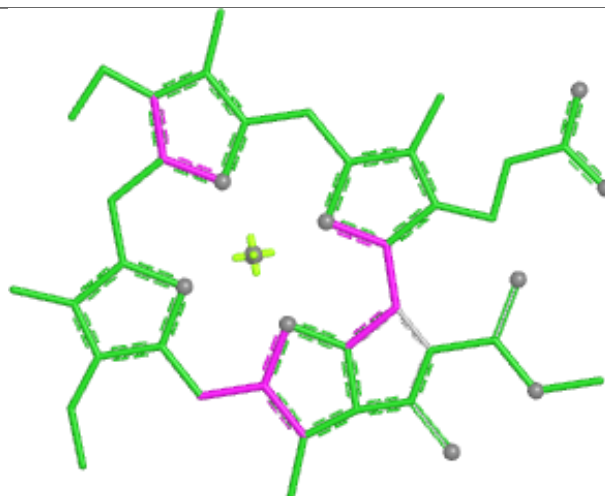




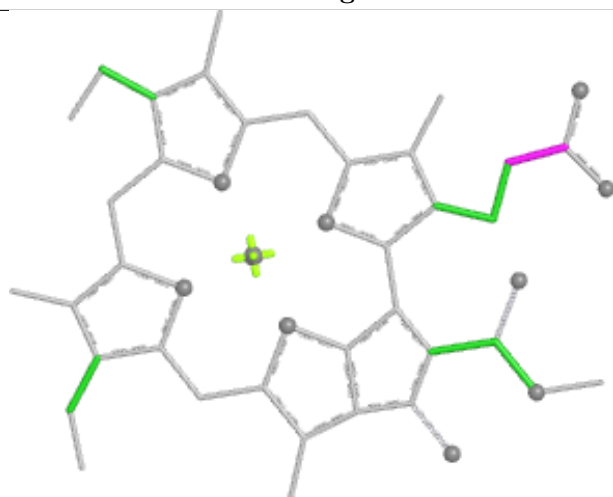
Ligand CLA b 829



Bond lengths



Bond angles

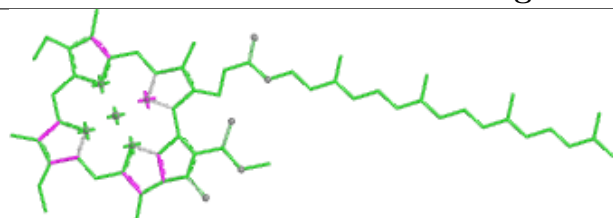


Torsions

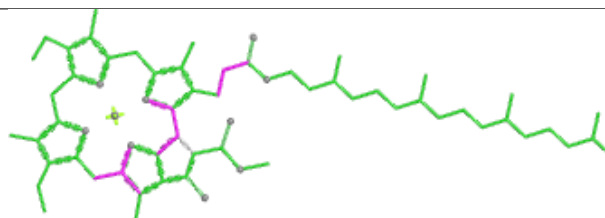


Rings

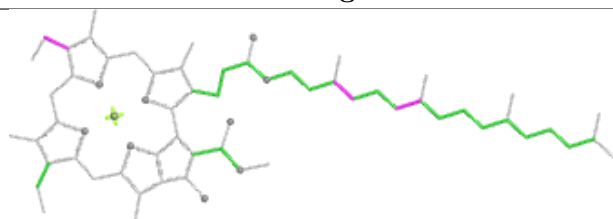
Ligand CLA B 836



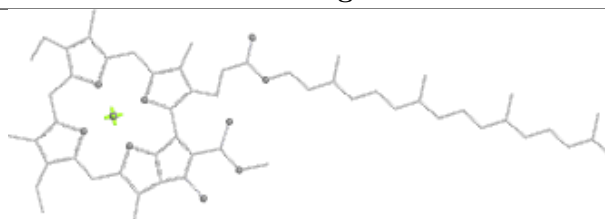
Bond lengths



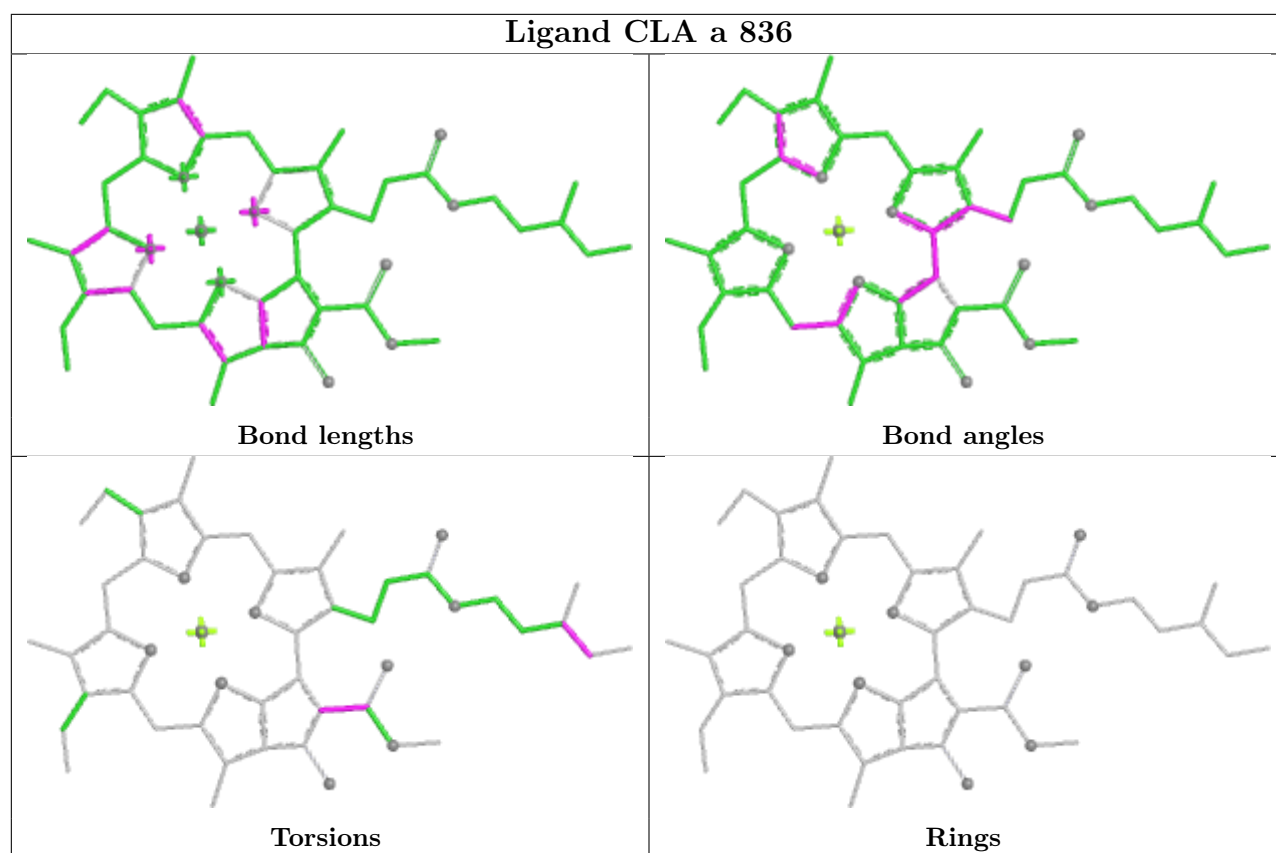
Bond angles



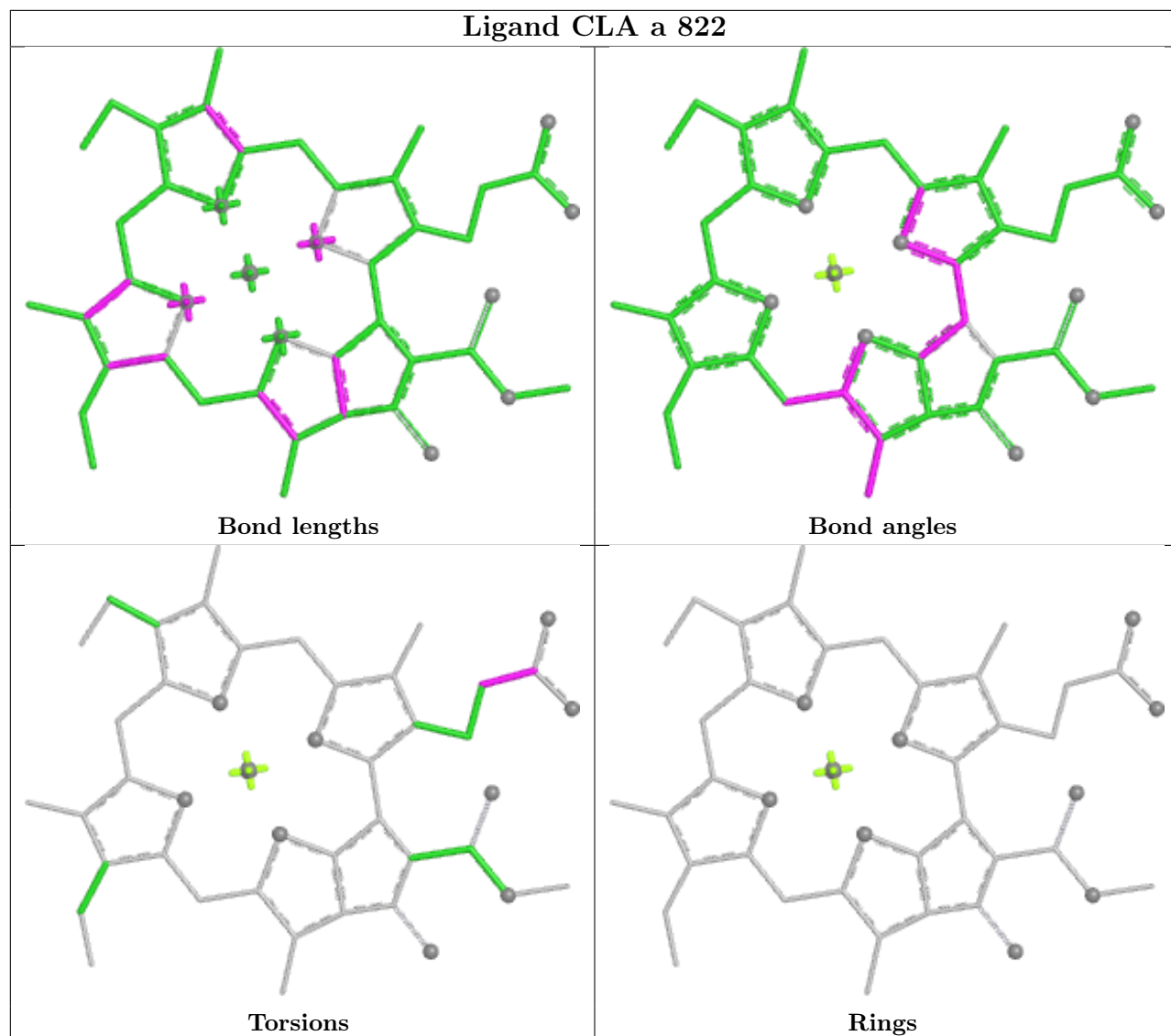
Torsions



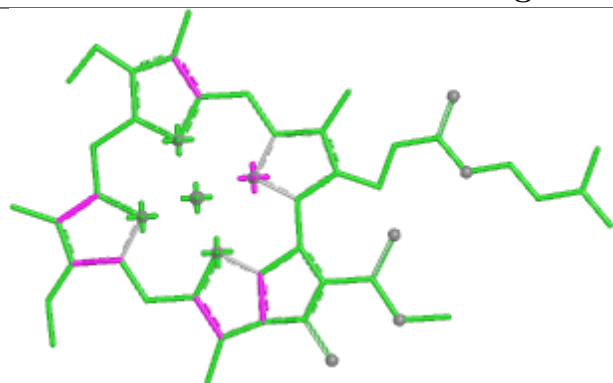
Rings



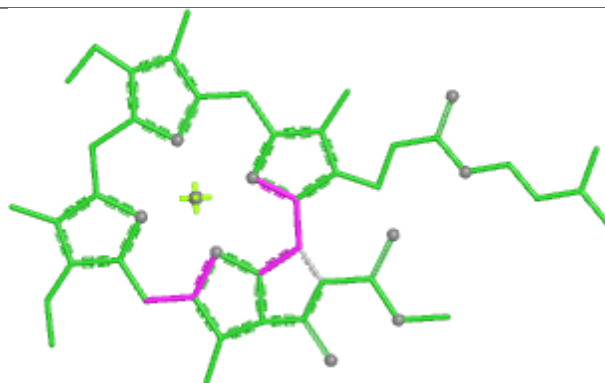
Ligand CLA a 822



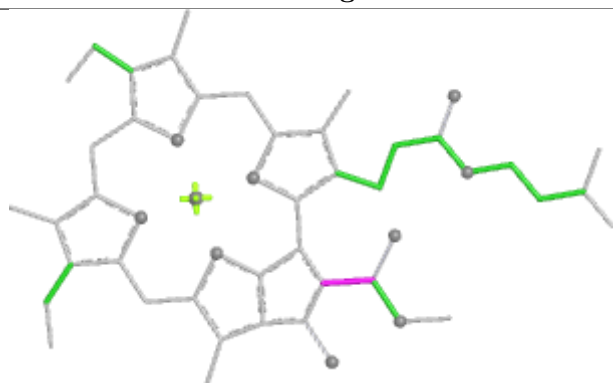
Ligand CLA B 814



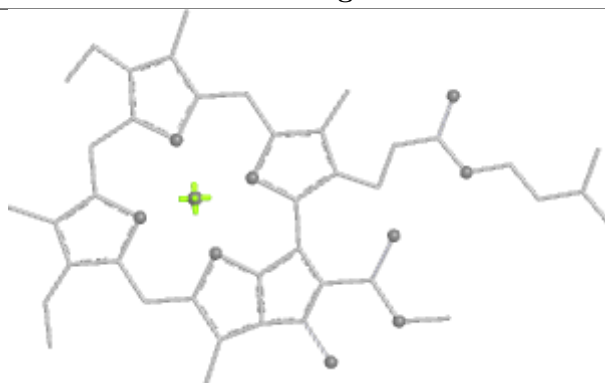
Bond lengths



Bond angles

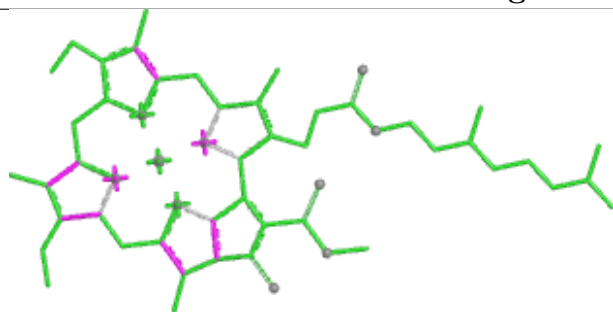


Torsions

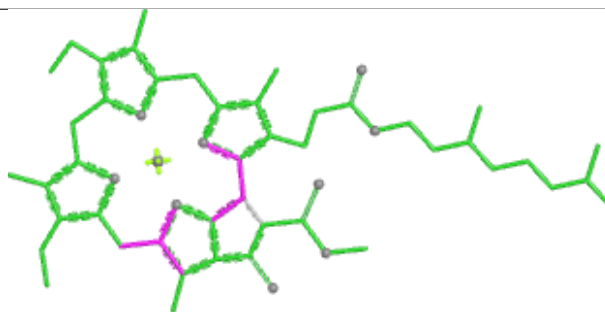


Rings

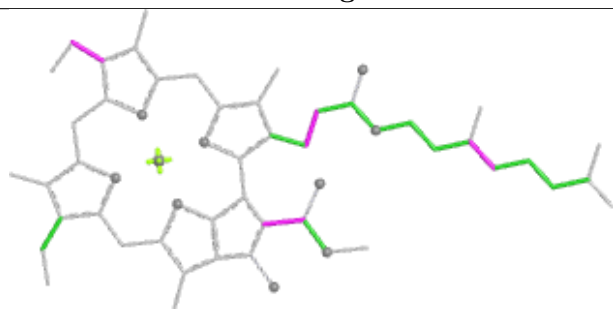
Ligand CLA 2b 301



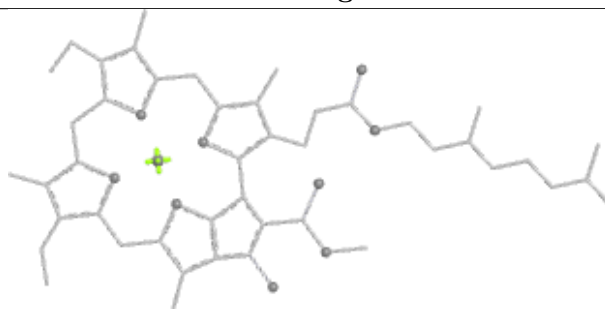
Bond lengths



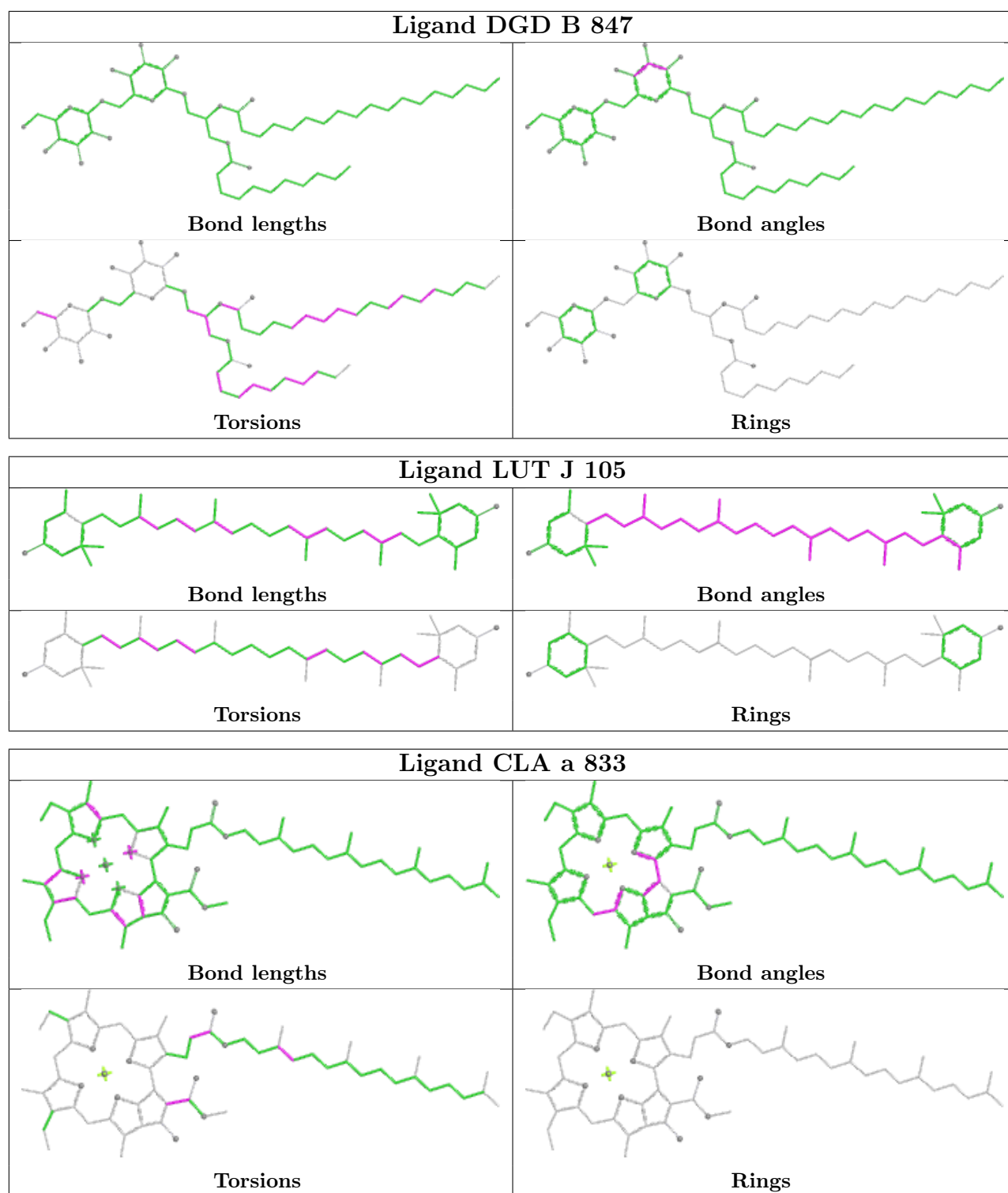
Bond angles



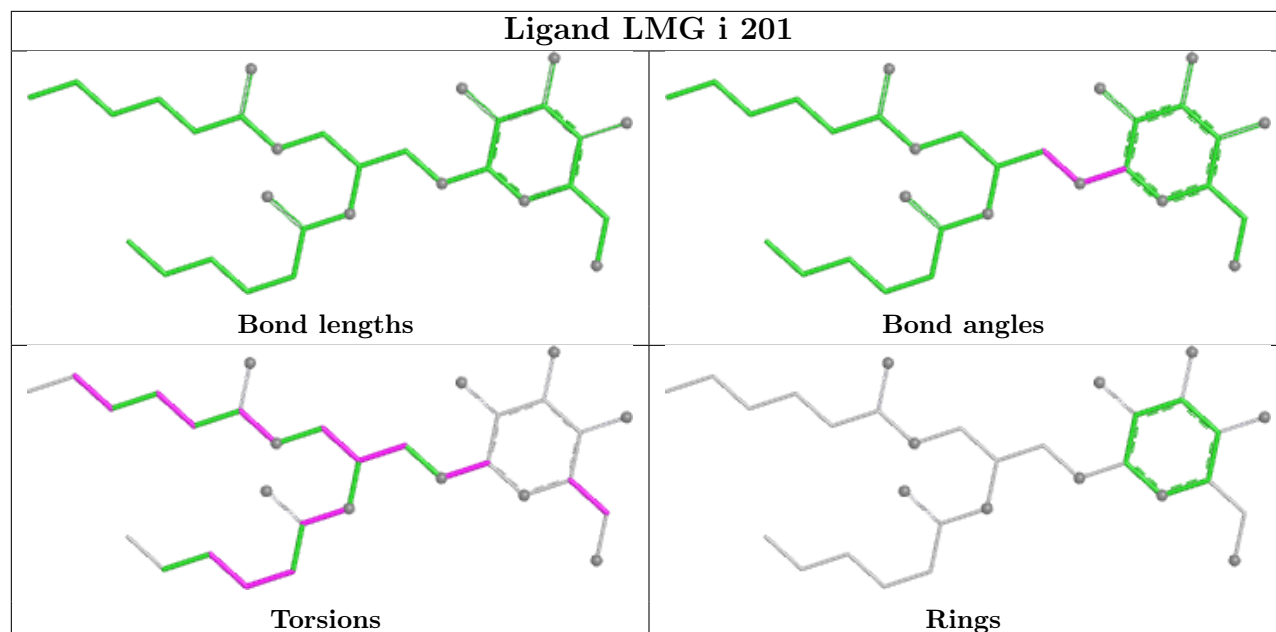
Torsions



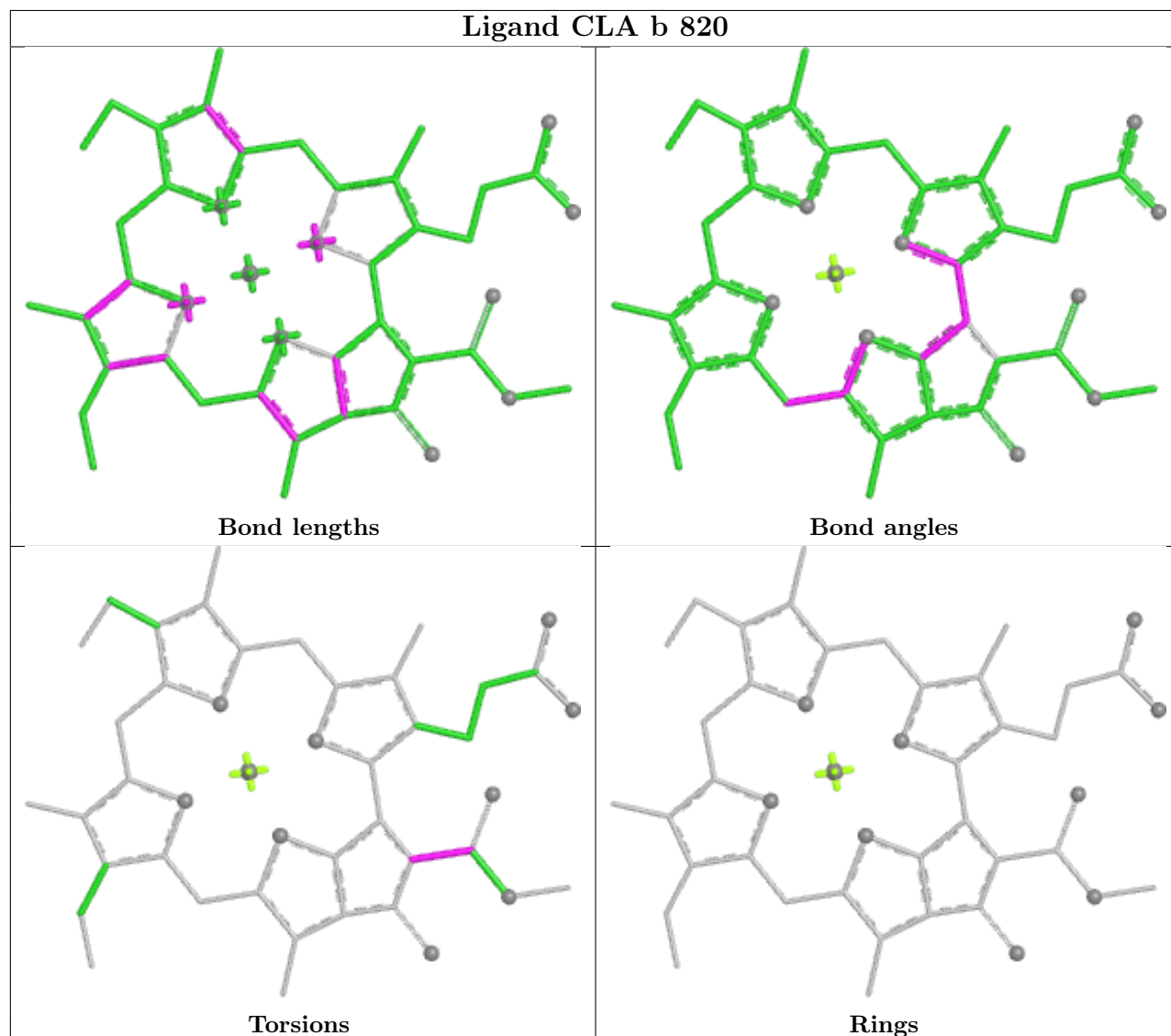
Rings

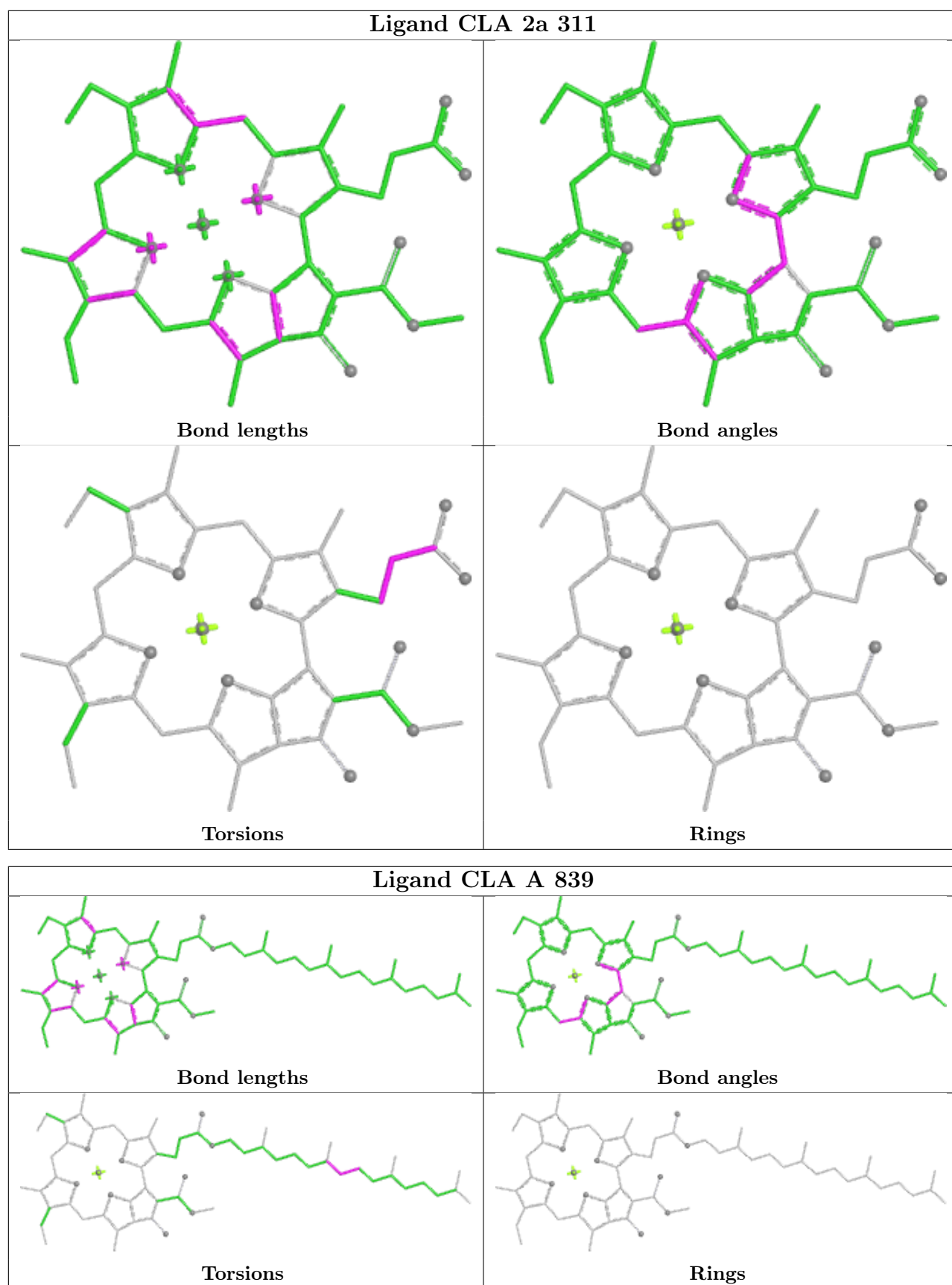


Ligand LMG i 201

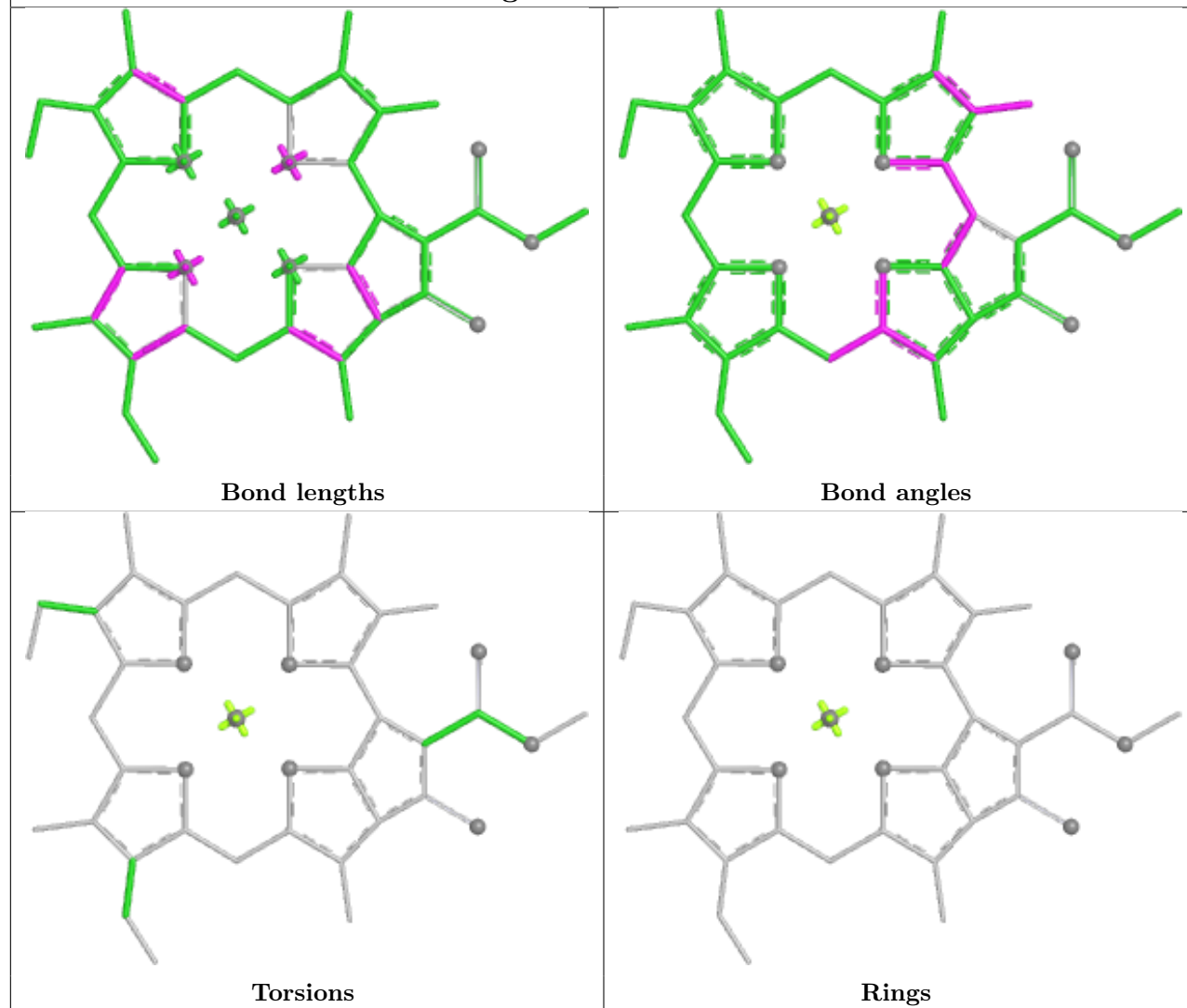


Ligand CLA b 820

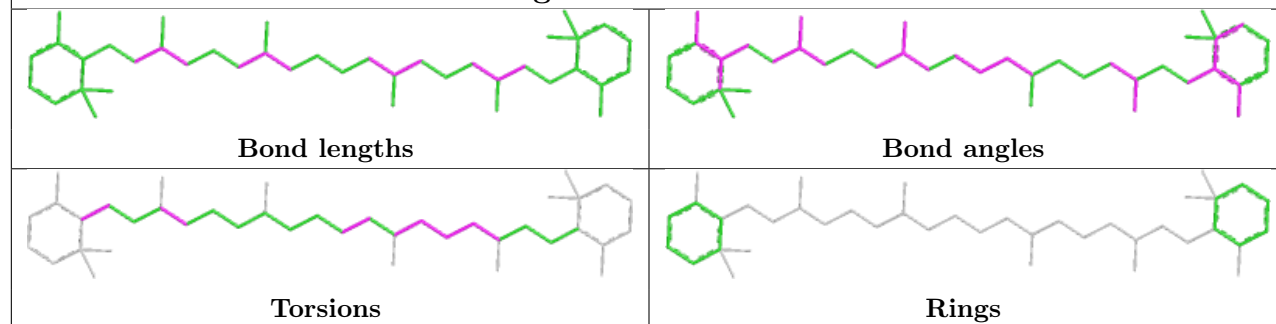


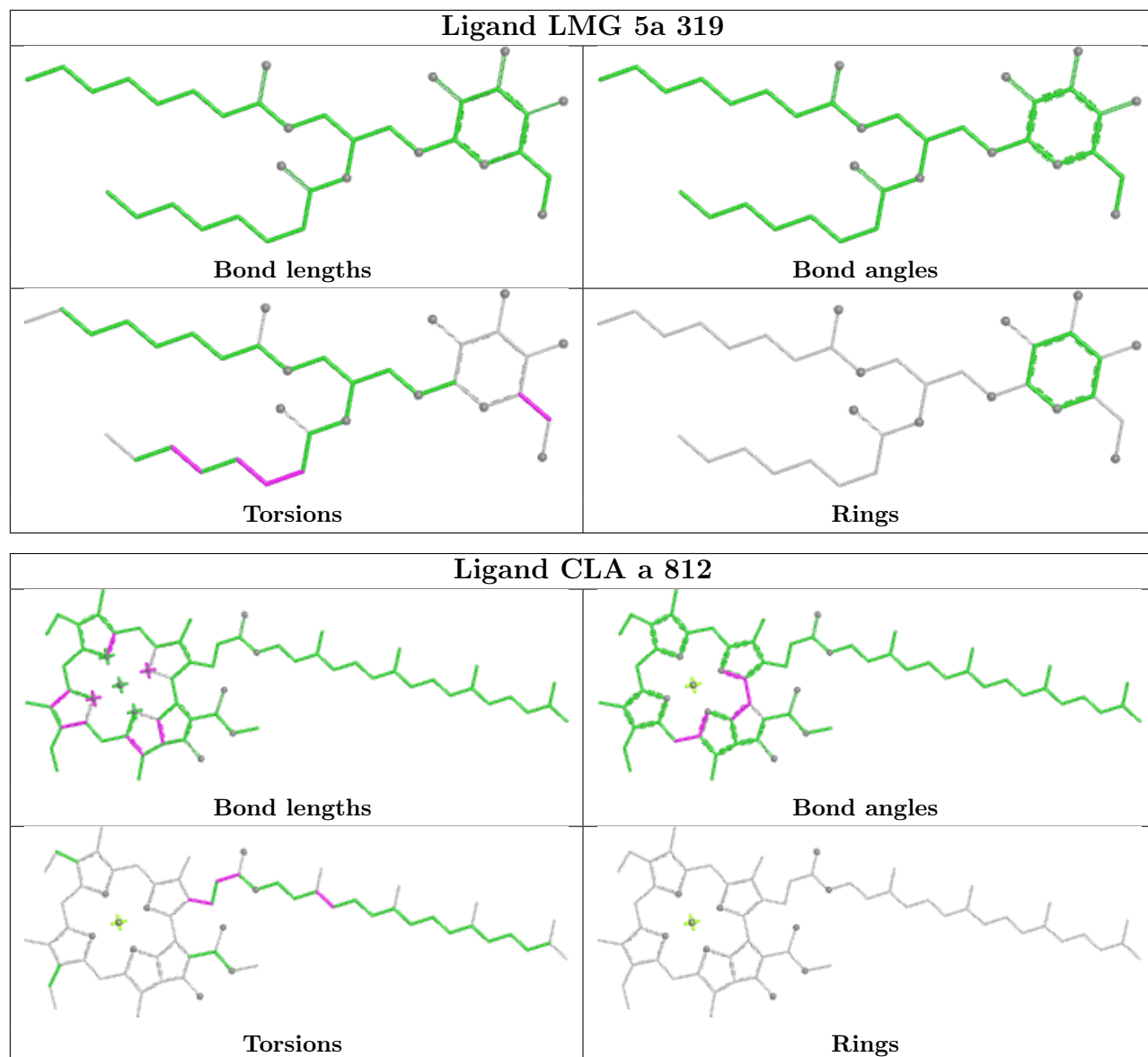


Ligand CLA f 303

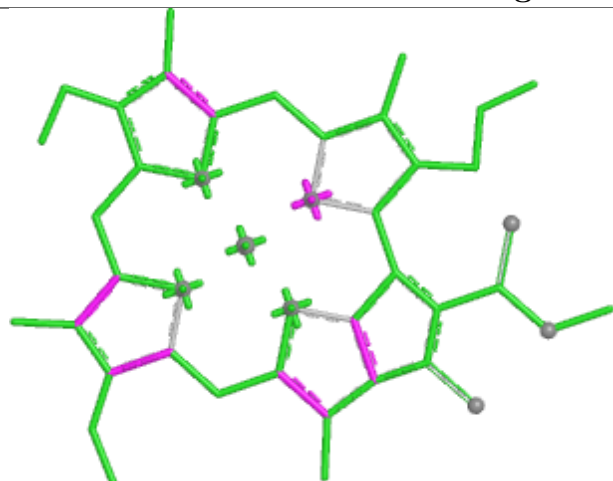


Ligand BCR b 843

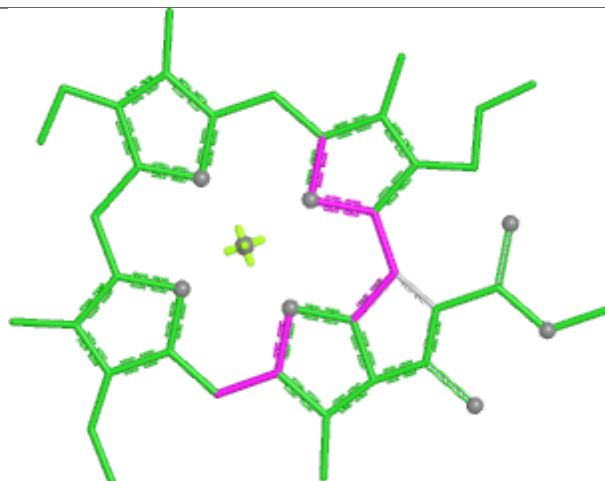




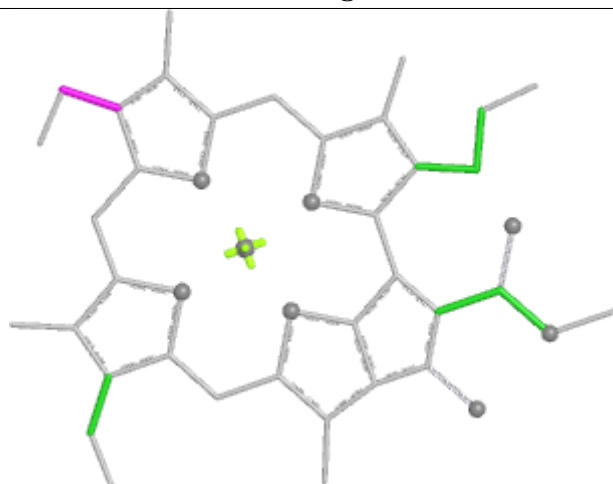
Ligand CLA B 819



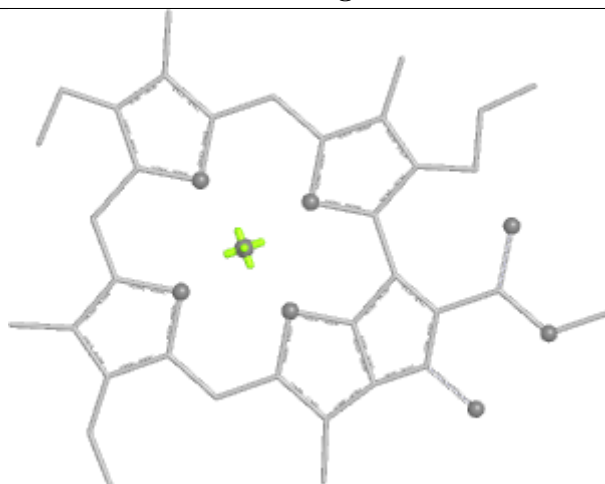
Bond lengths



Bond angles

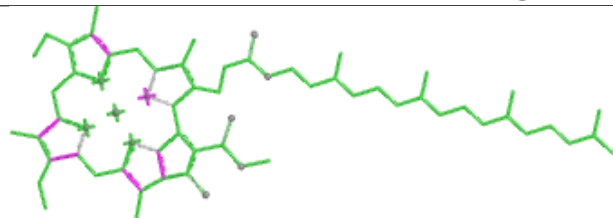


Torsions

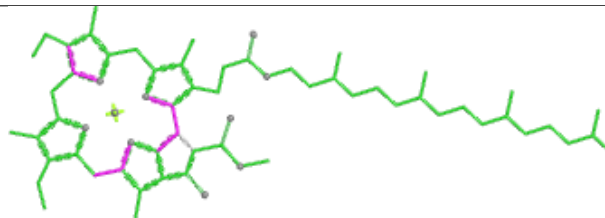


Rings

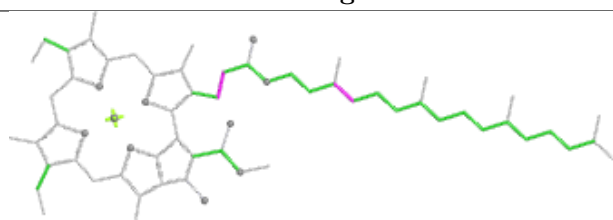
Ligand CLA A 820



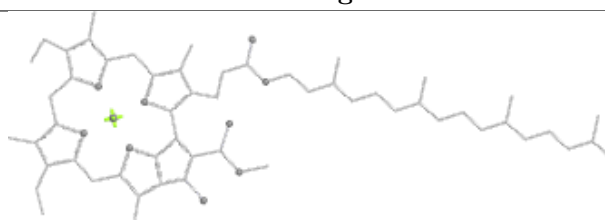
Bond lengths



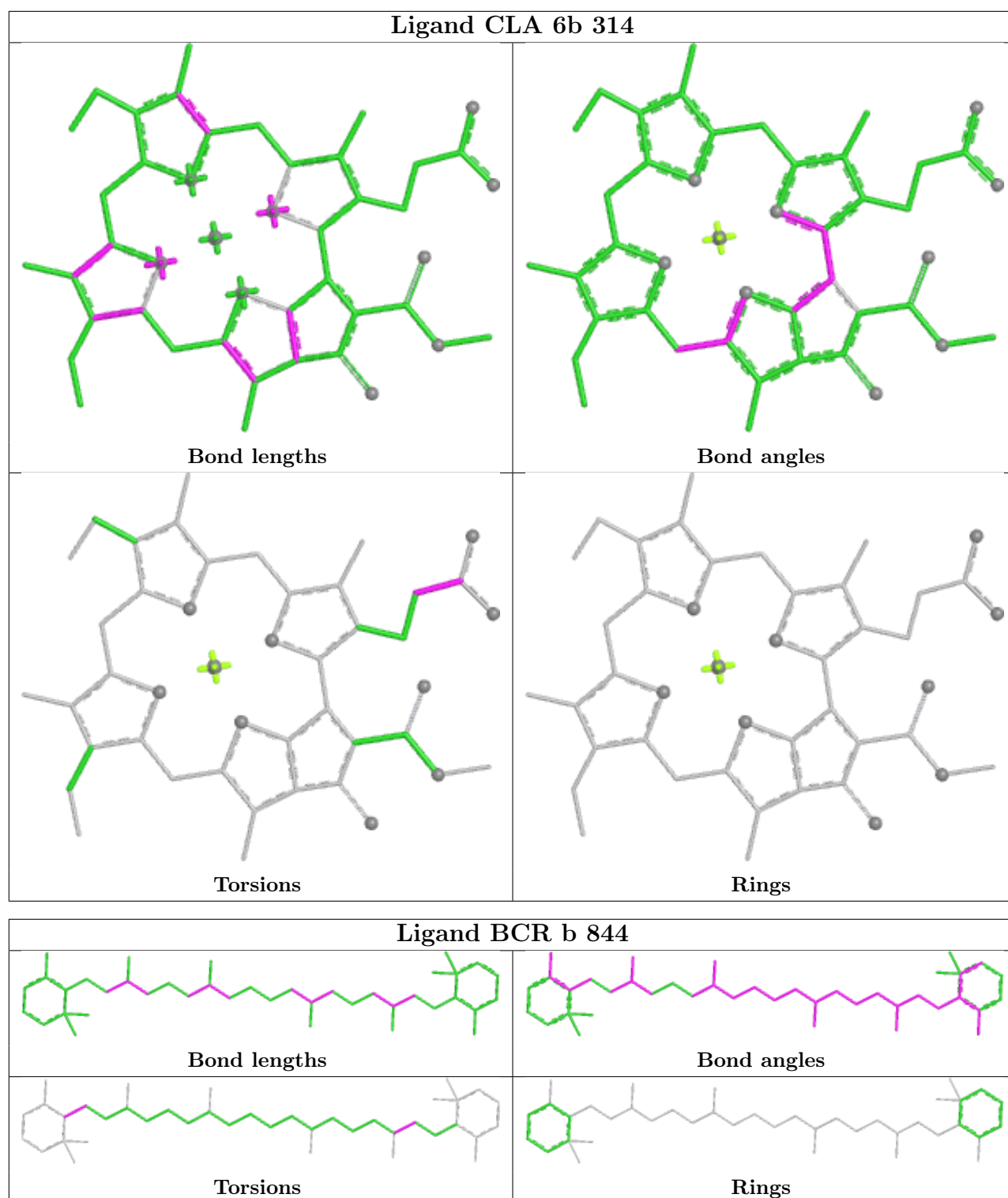
Bond angles

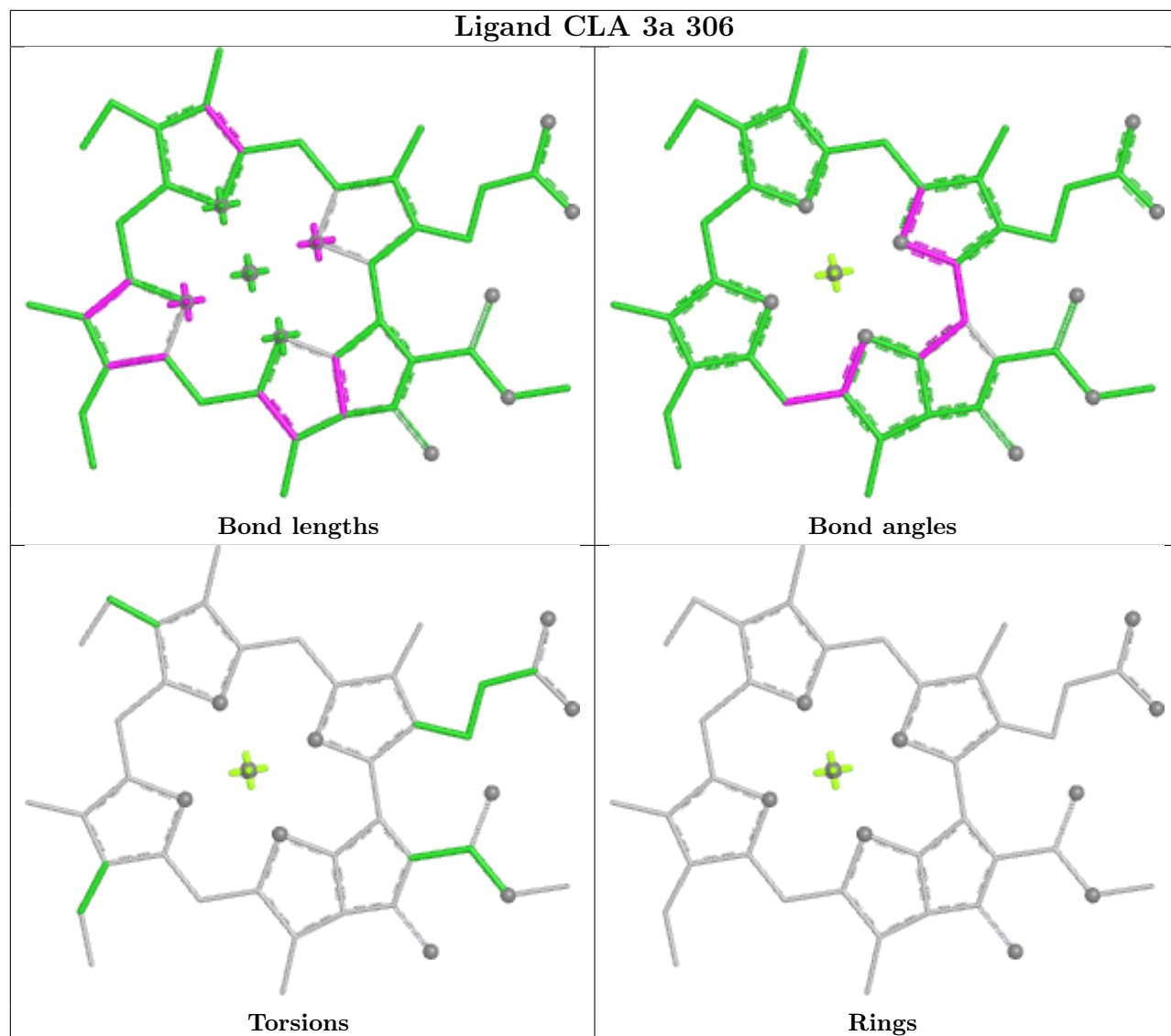


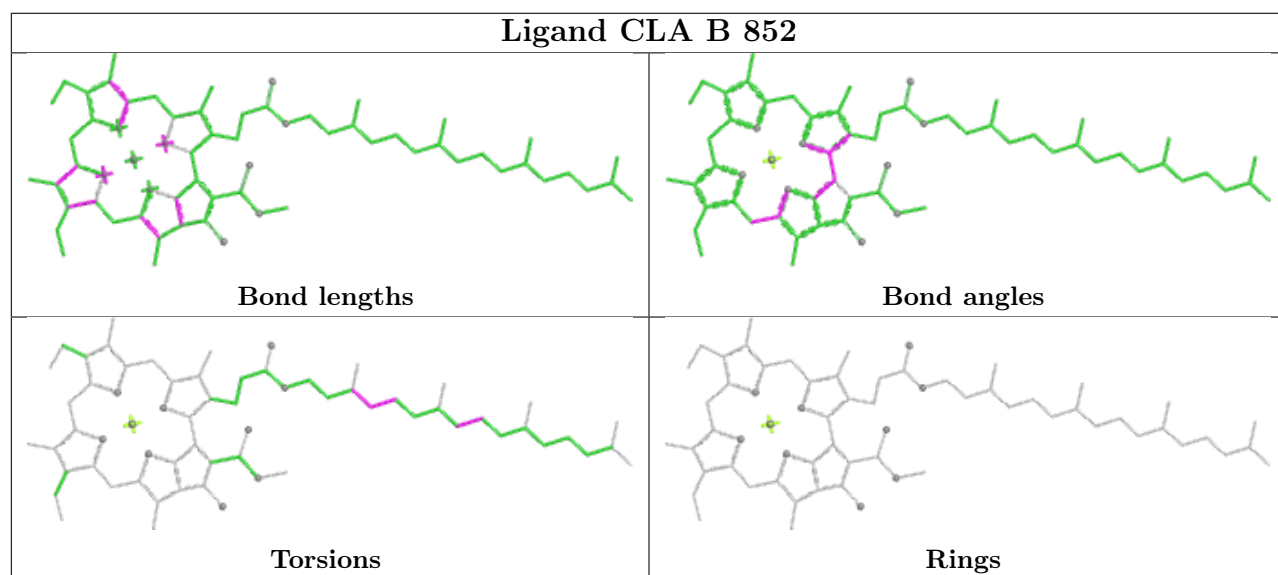
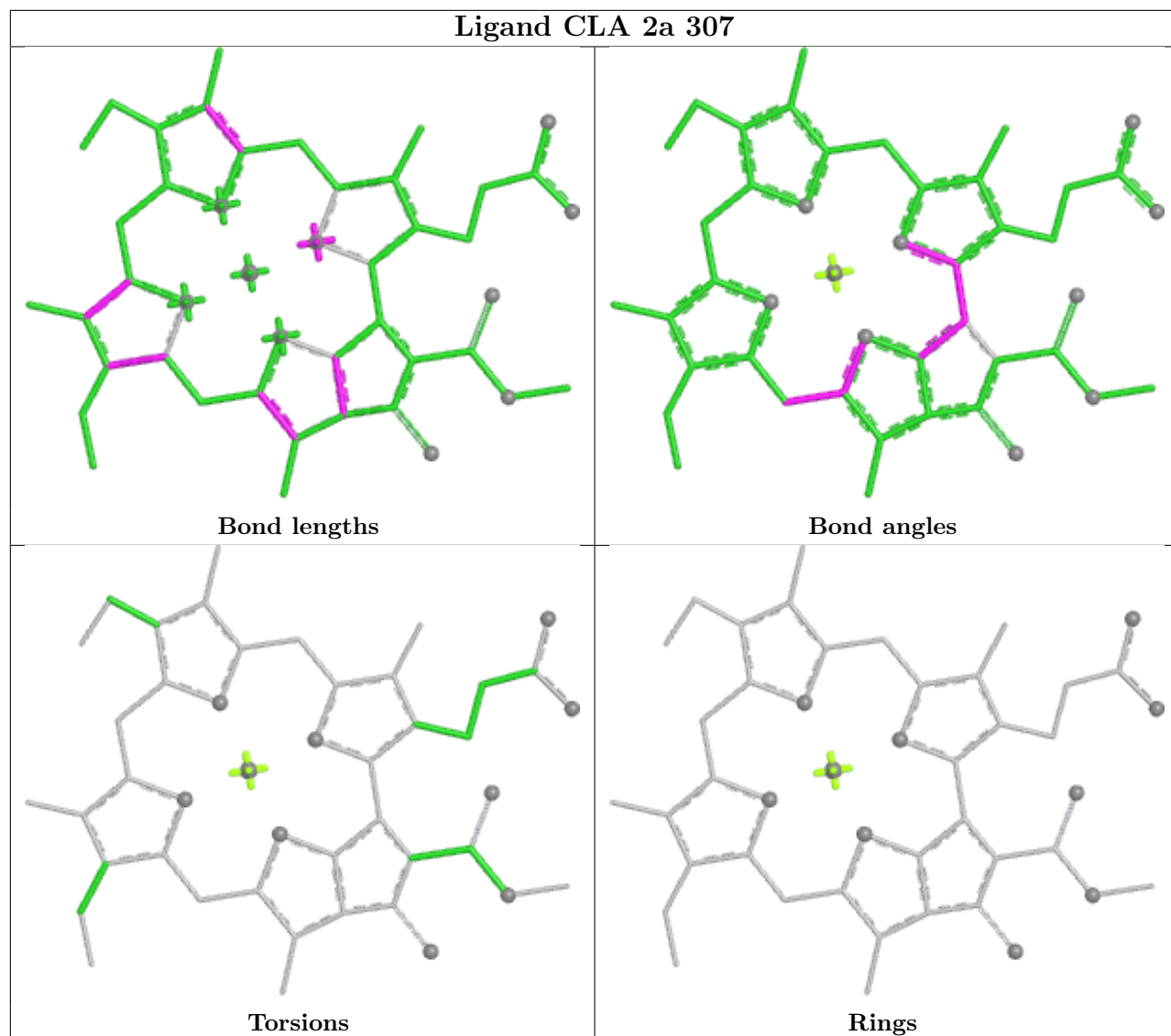
Torsions



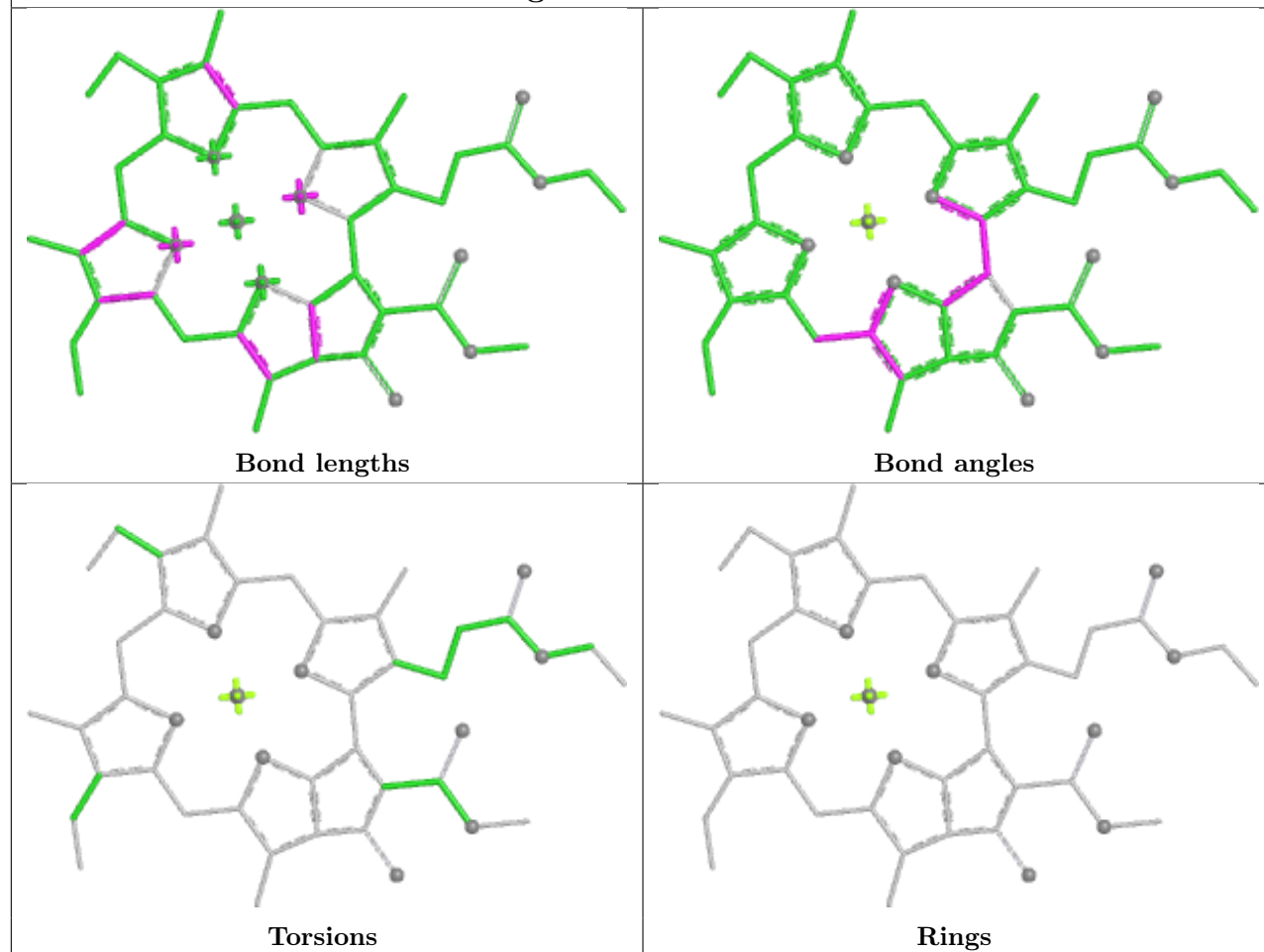
Rings



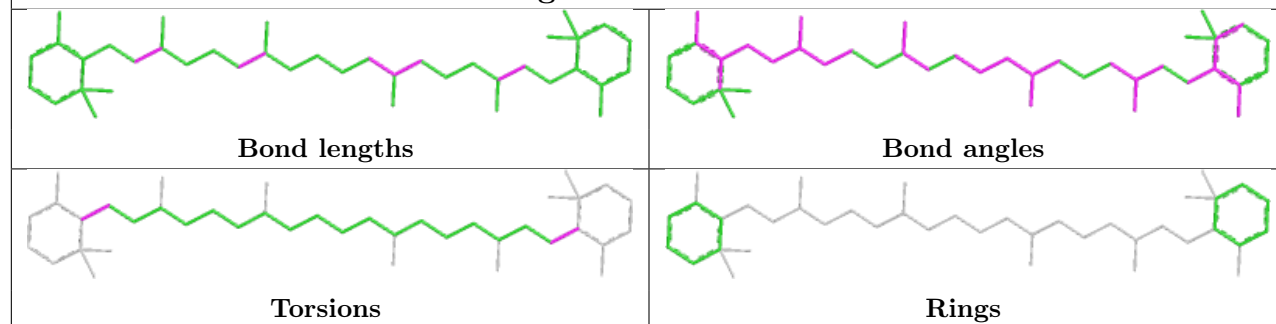


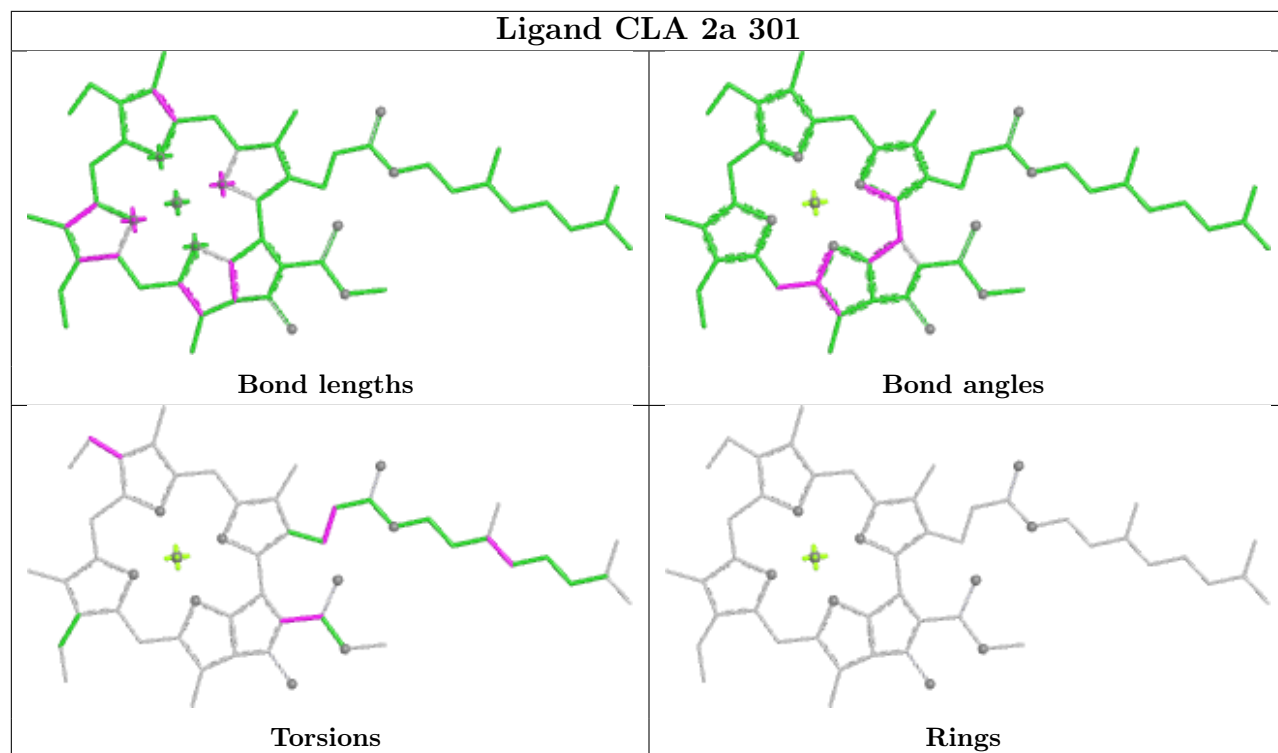


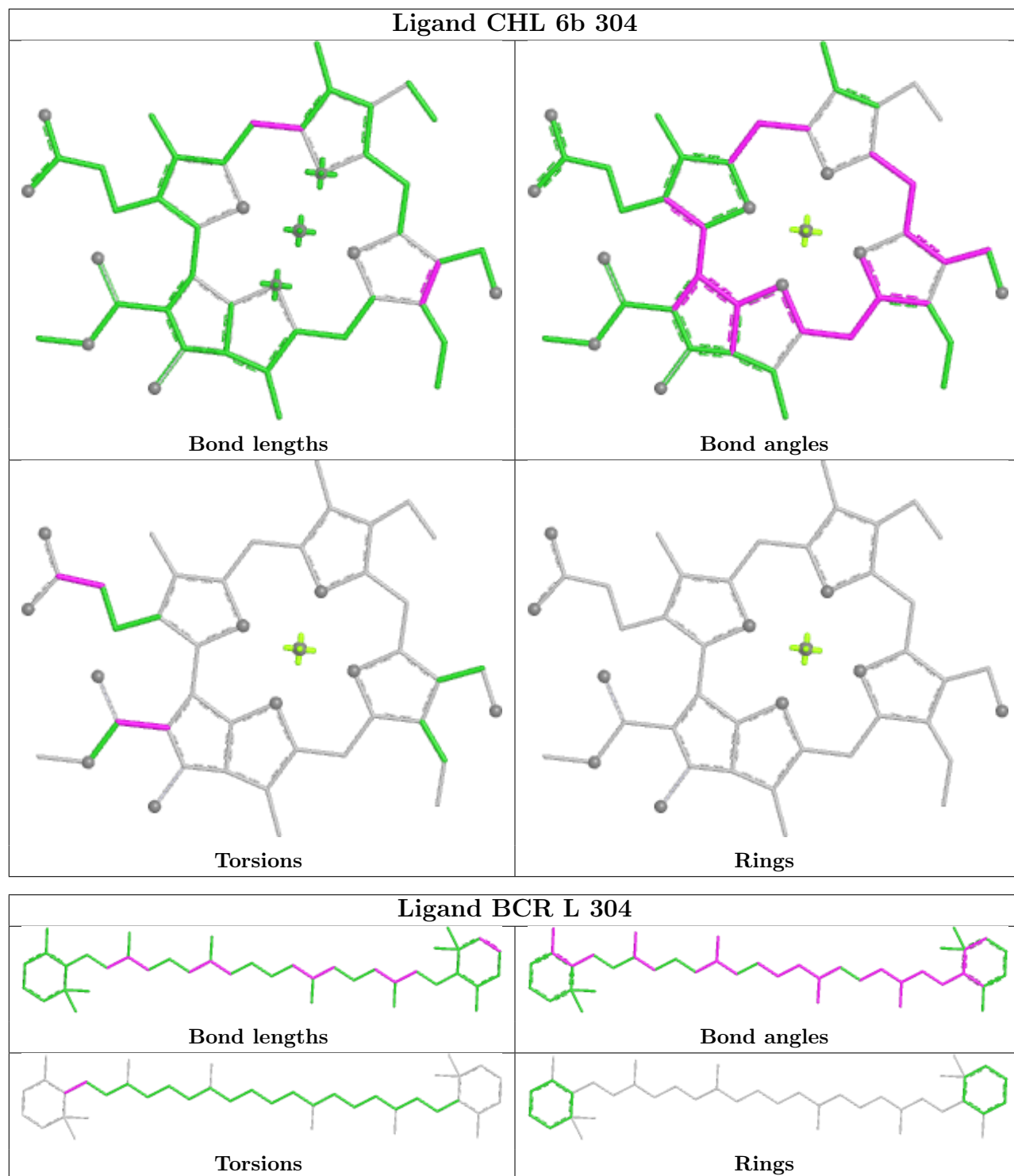
Ligand CLA B 837

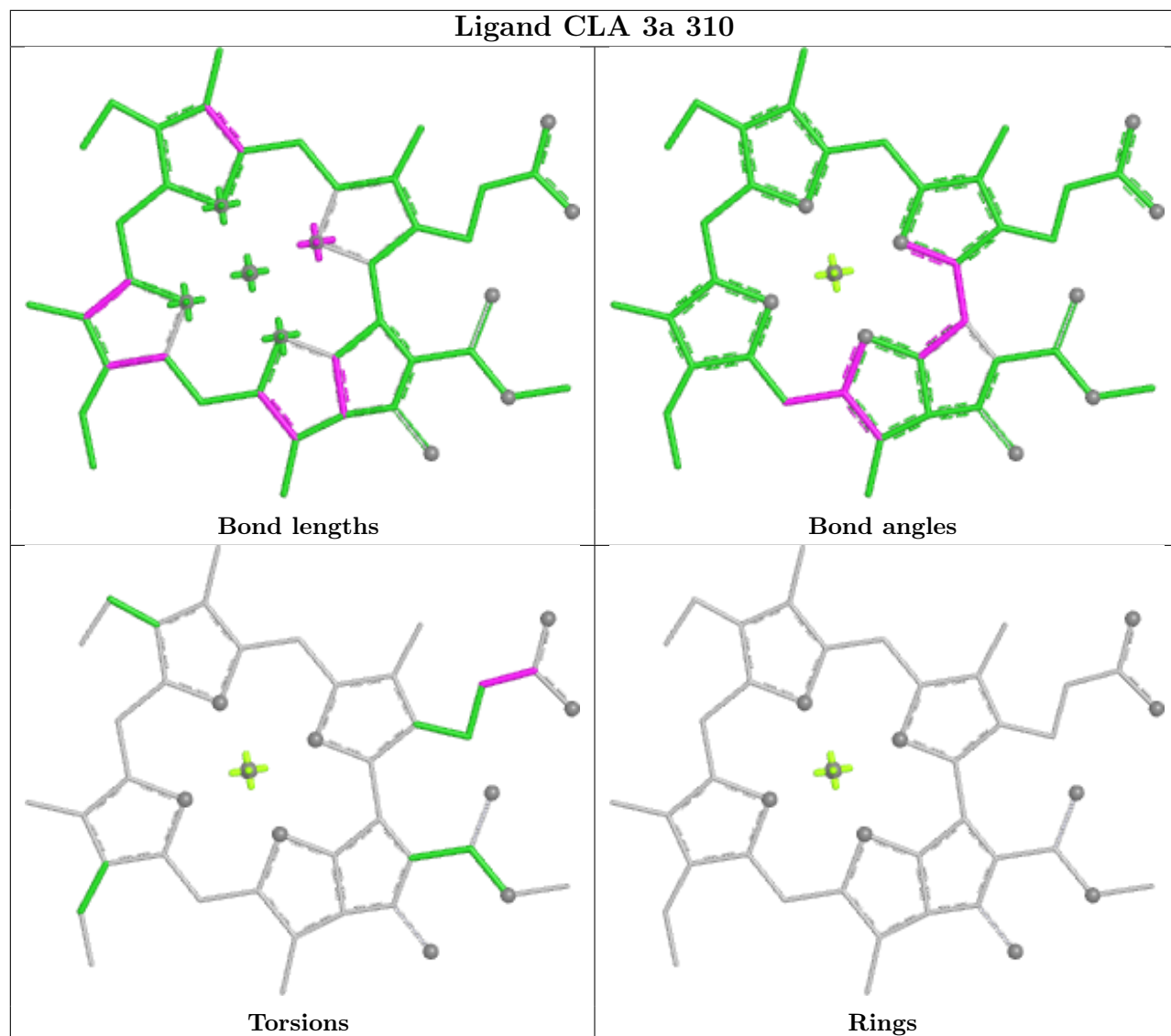


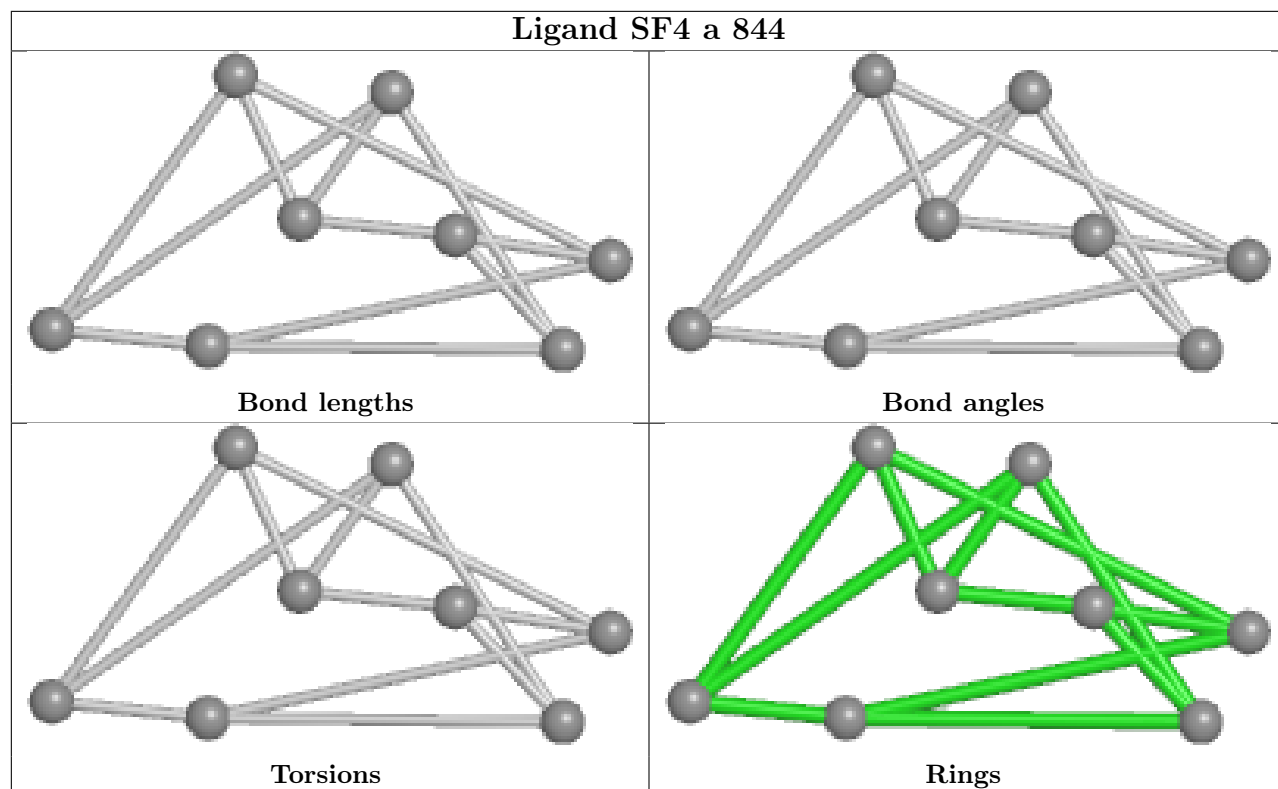
Ligand BCR f 301

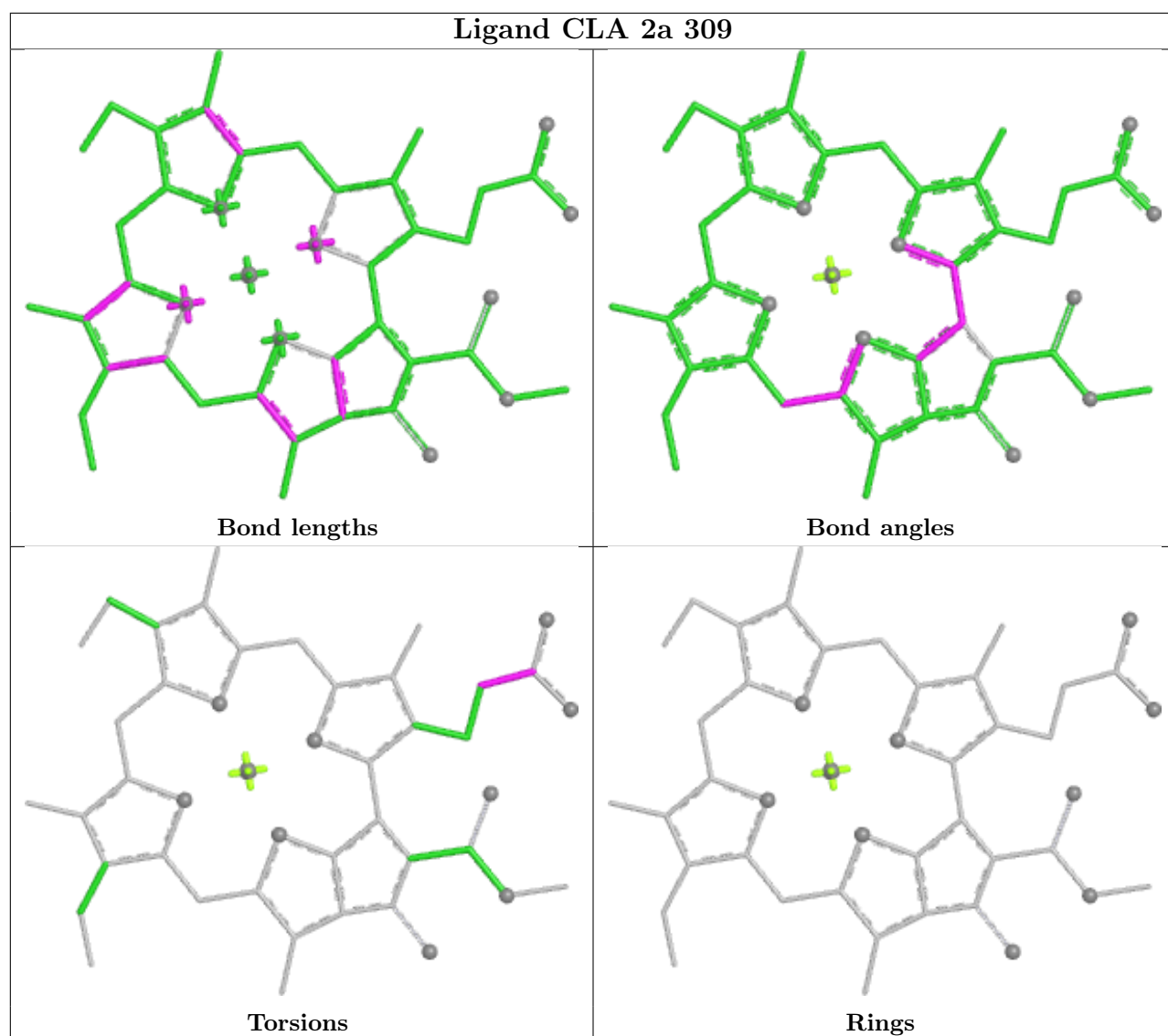


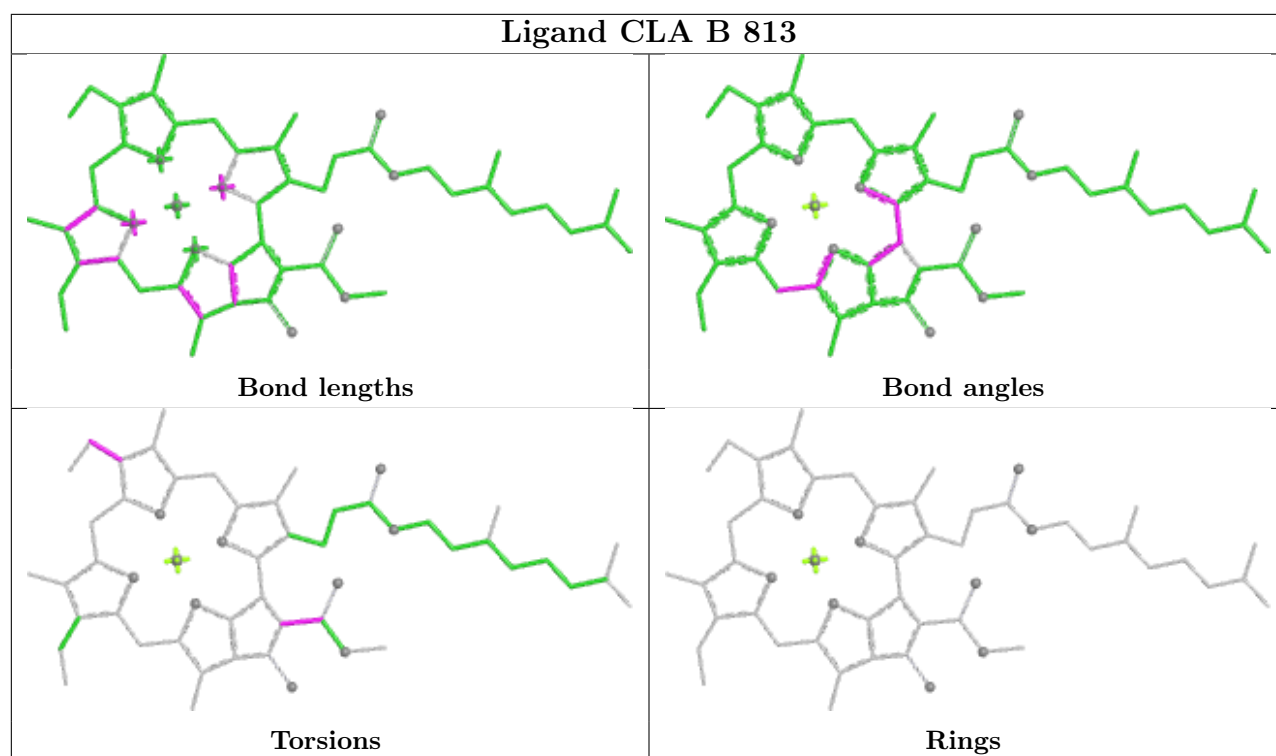


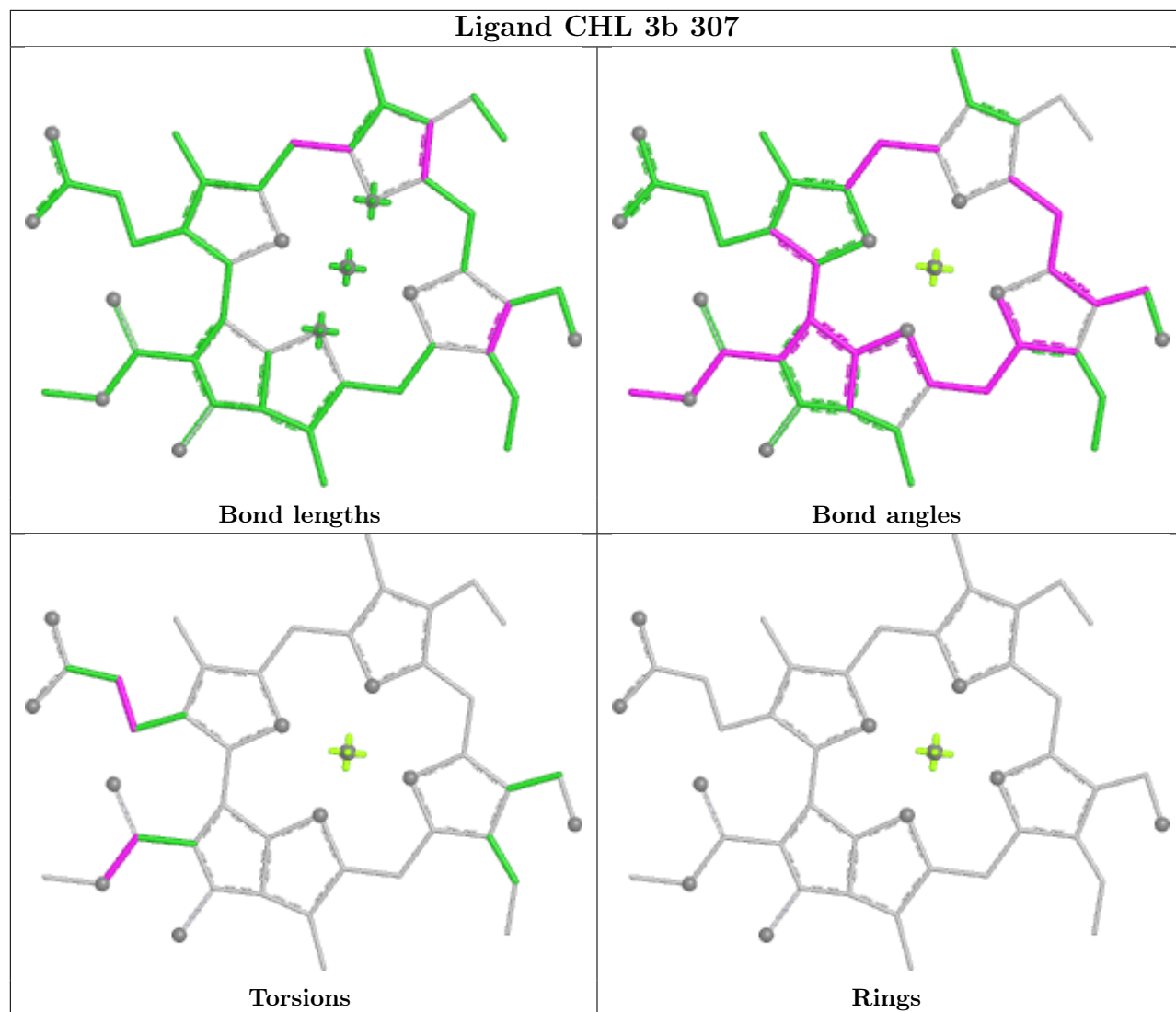




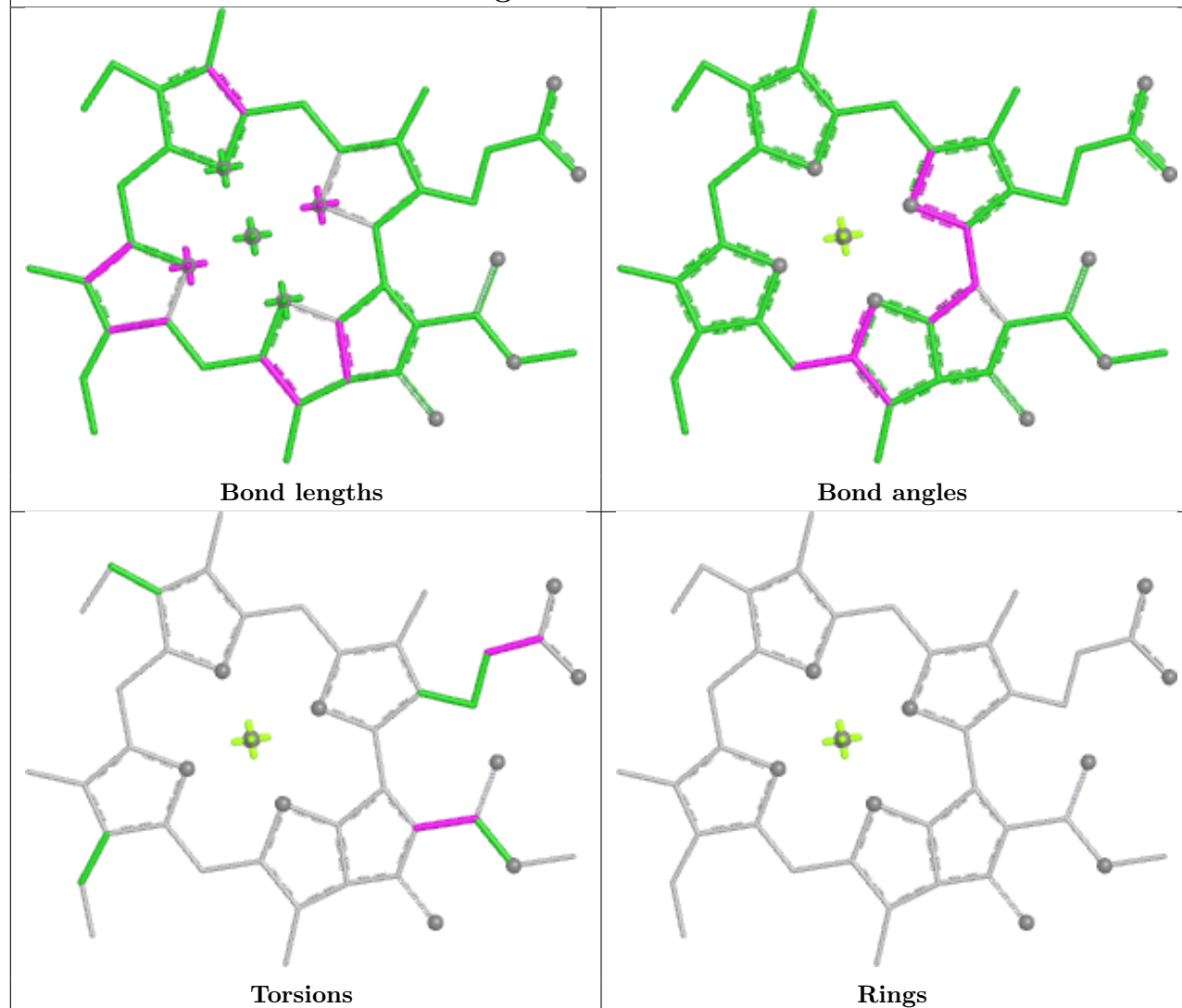




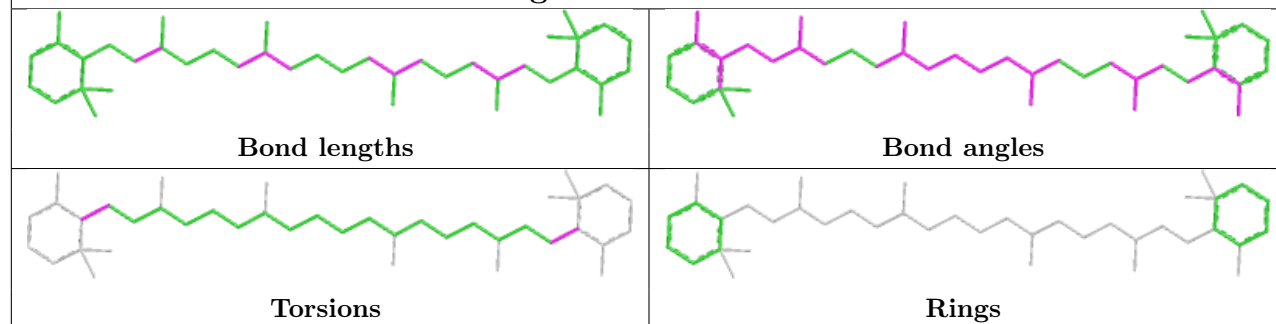


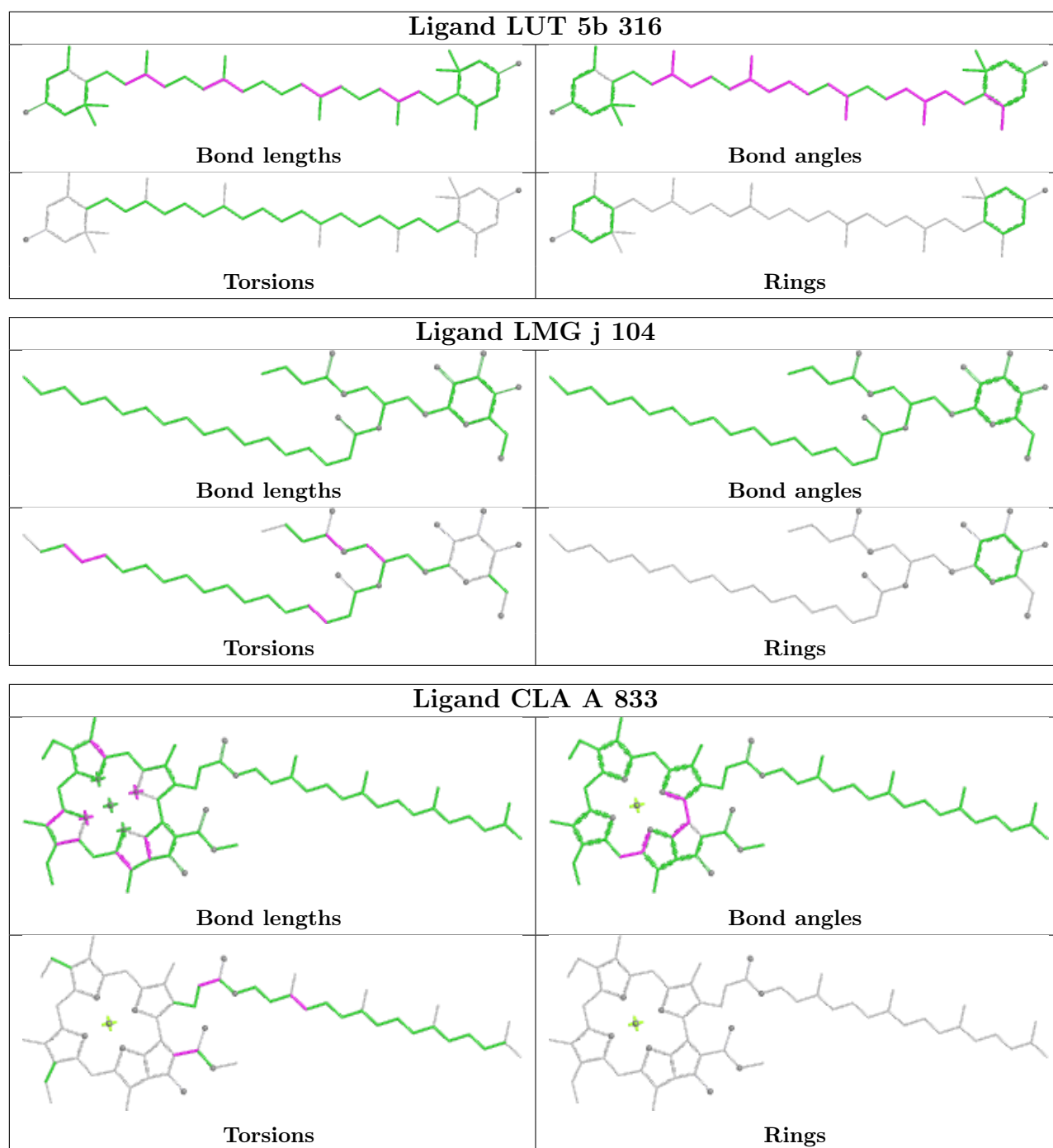


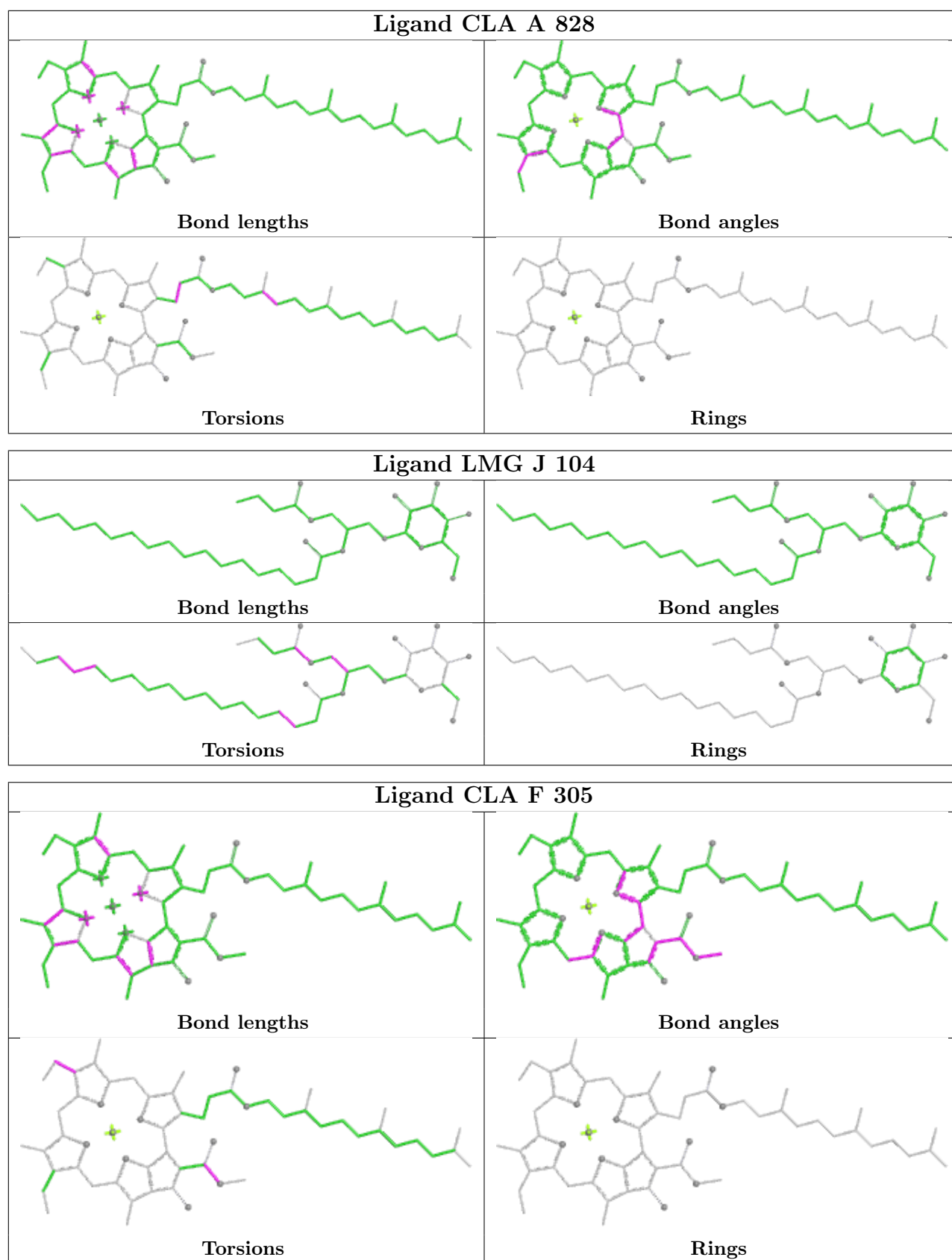
Ligand CLA L 301

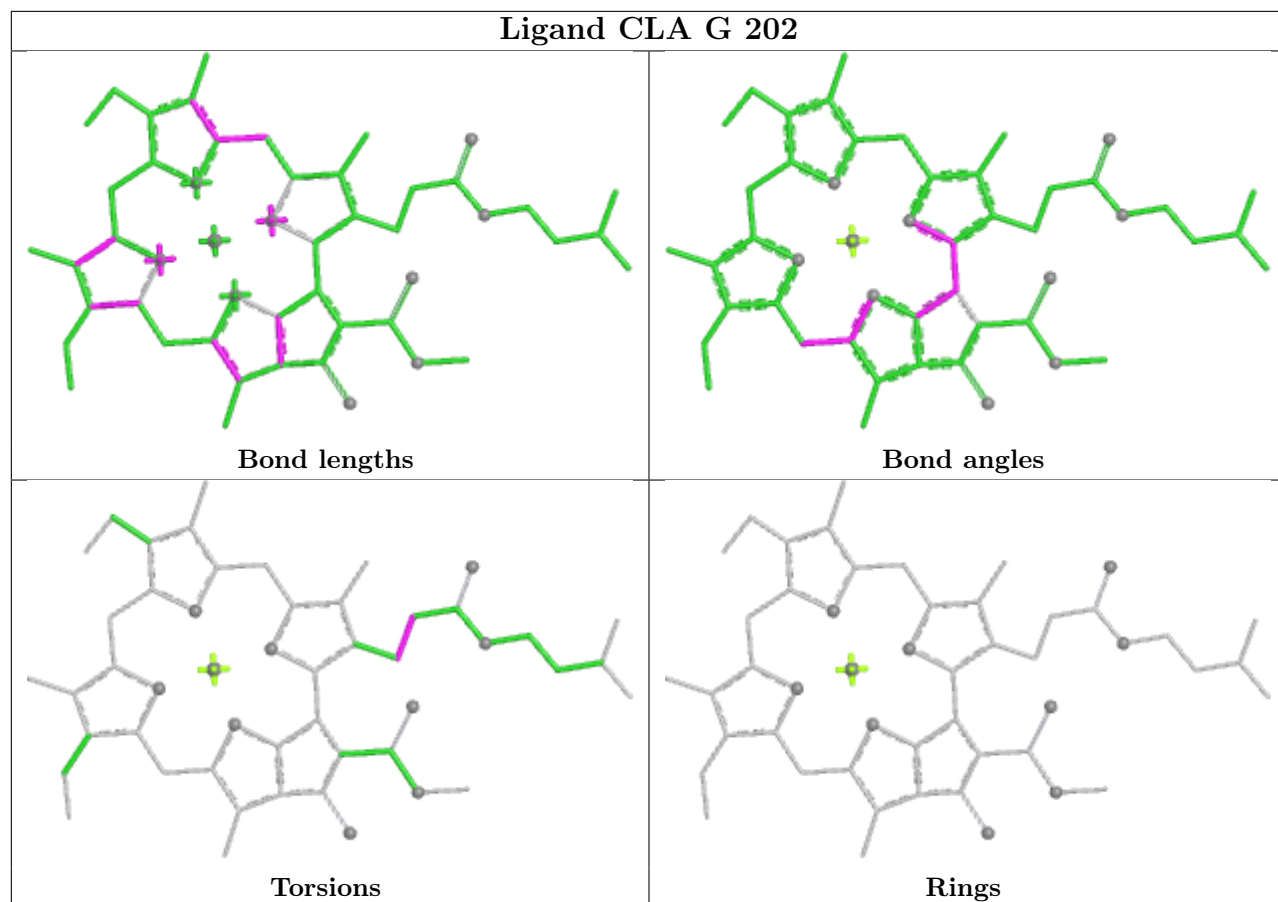


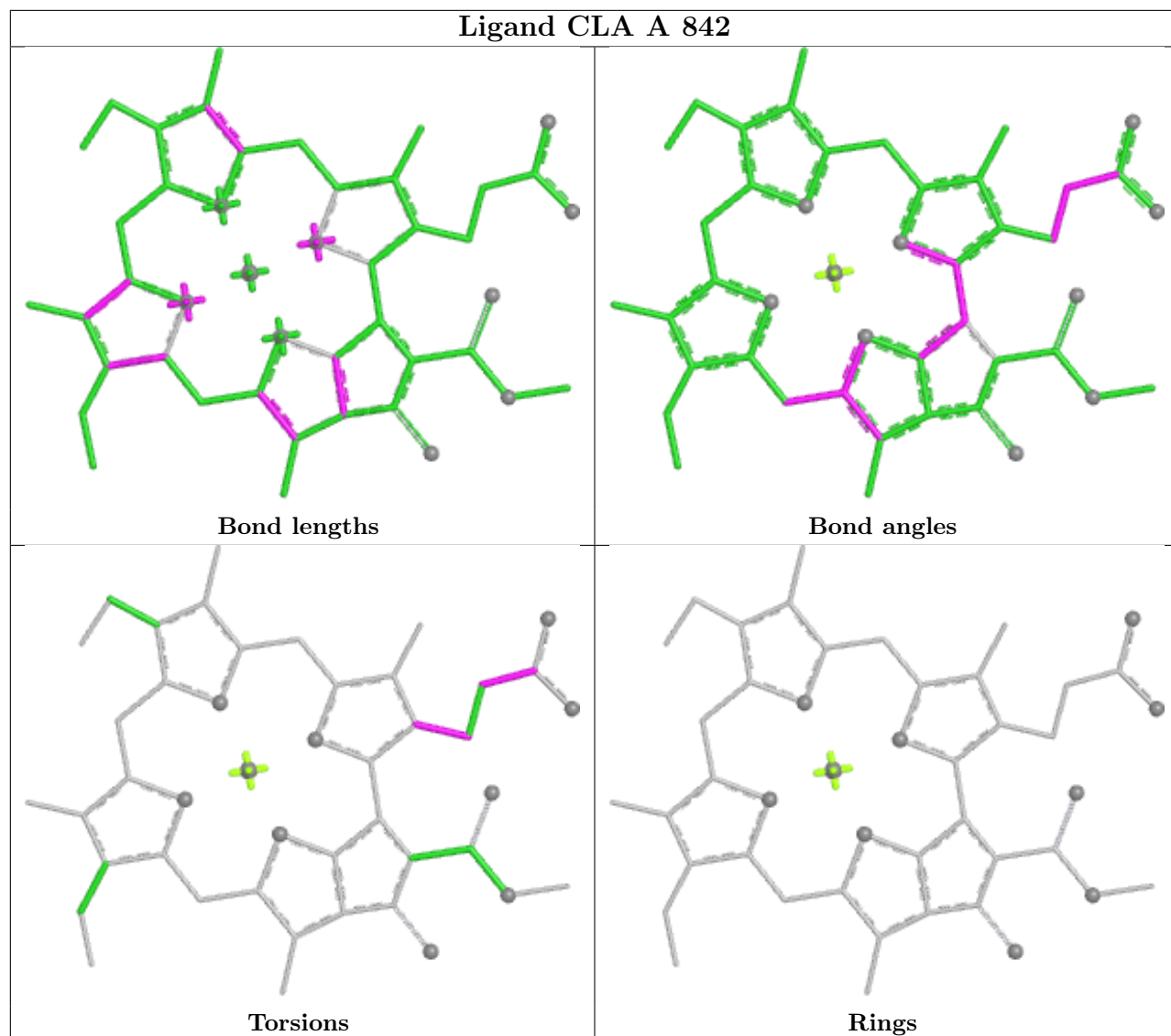
Ligand BCR A 848

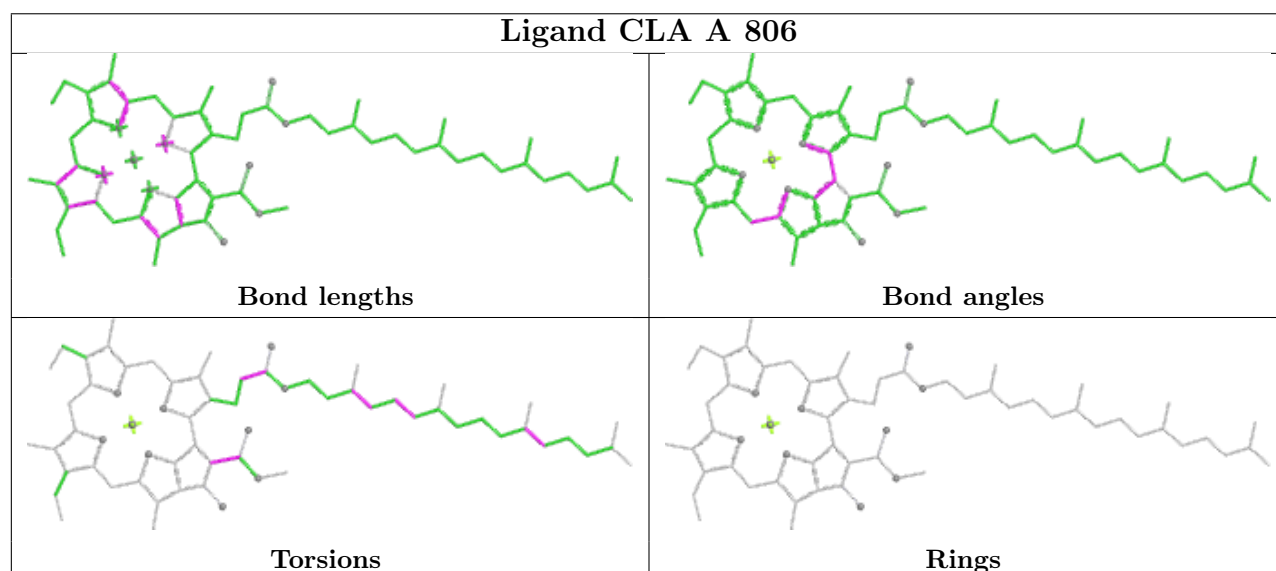
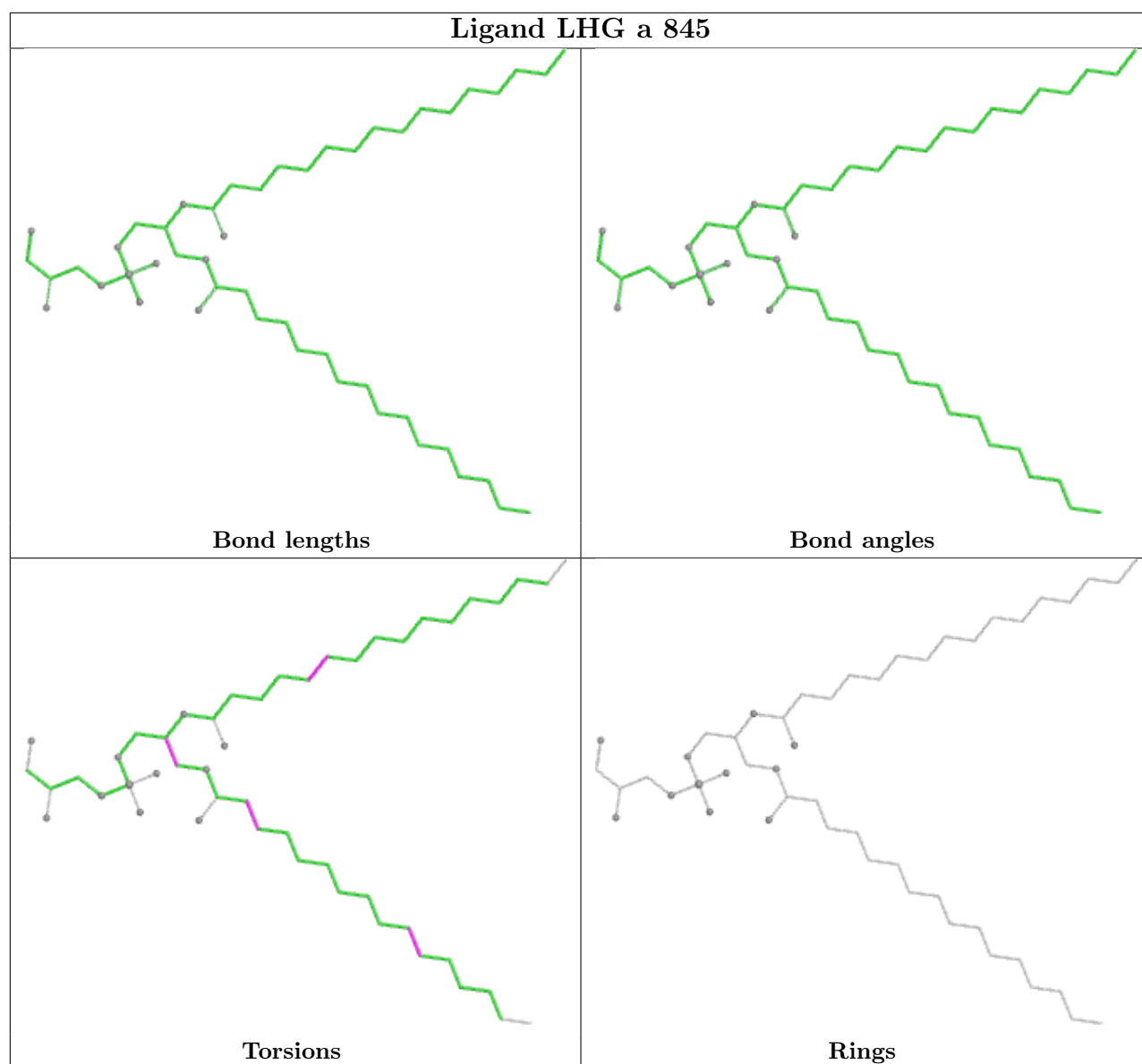


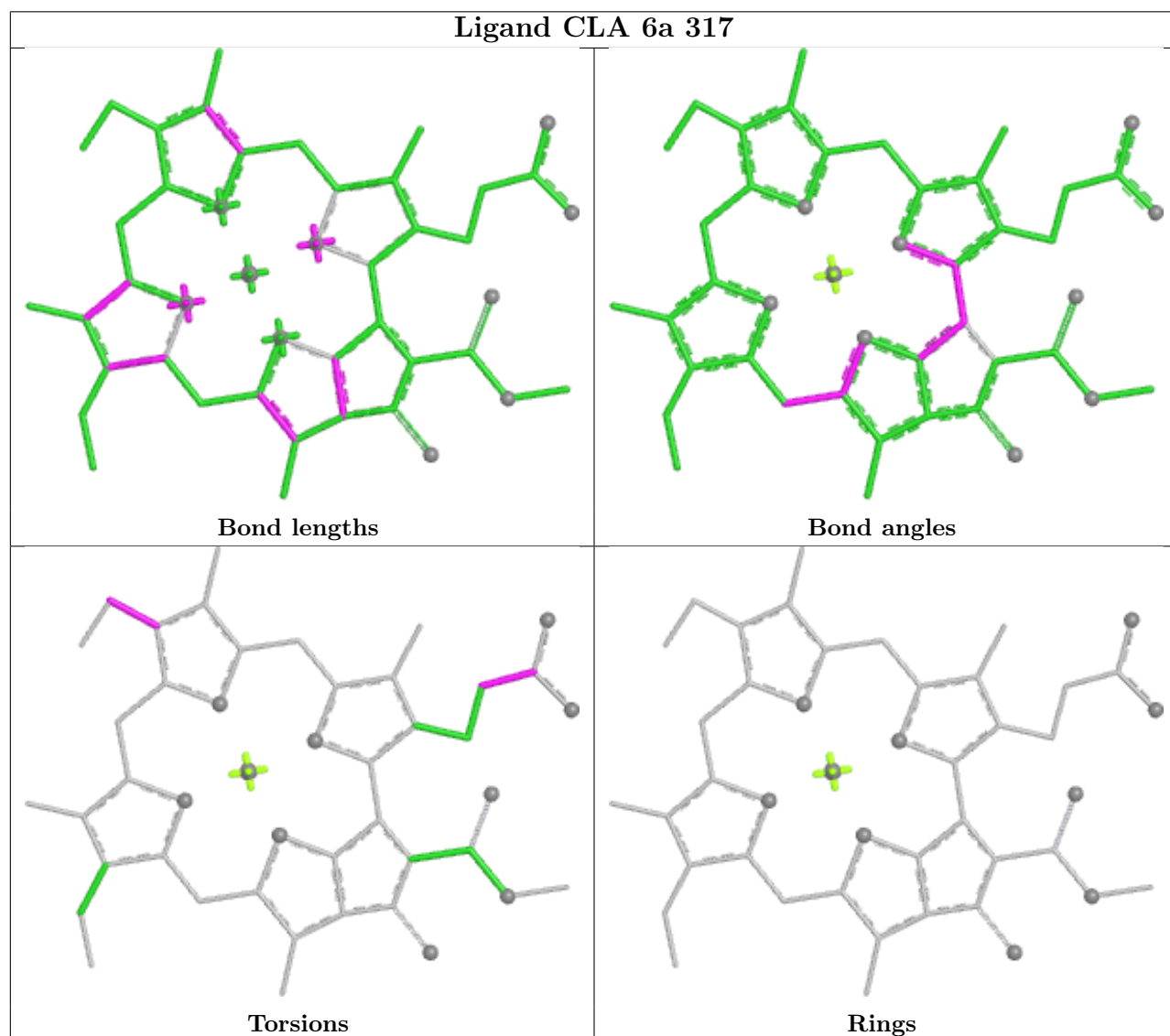
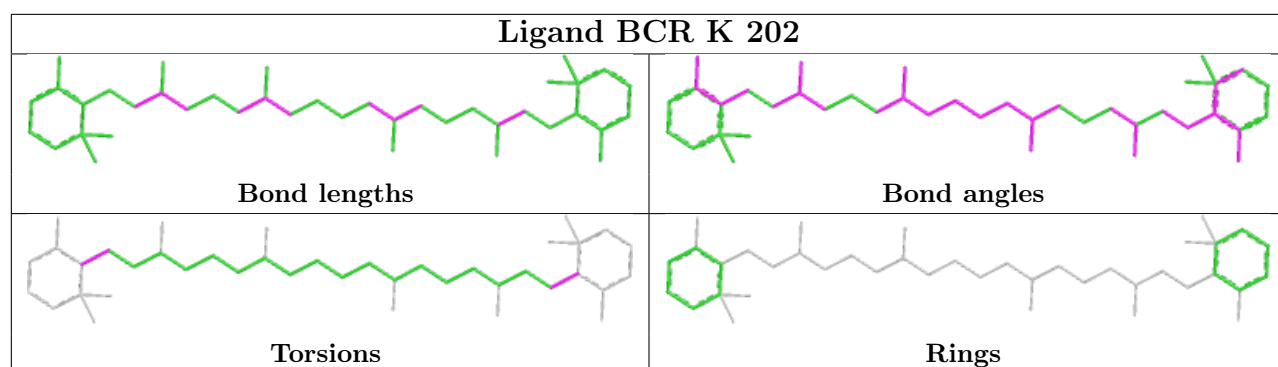


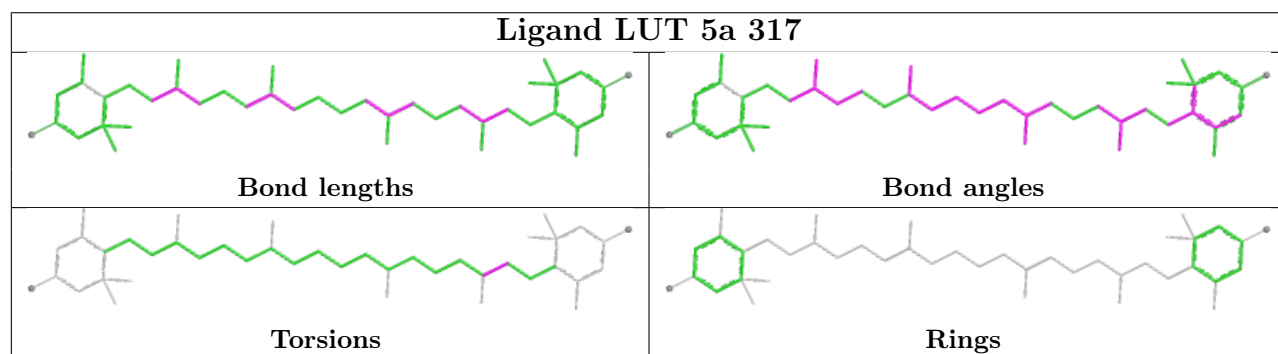
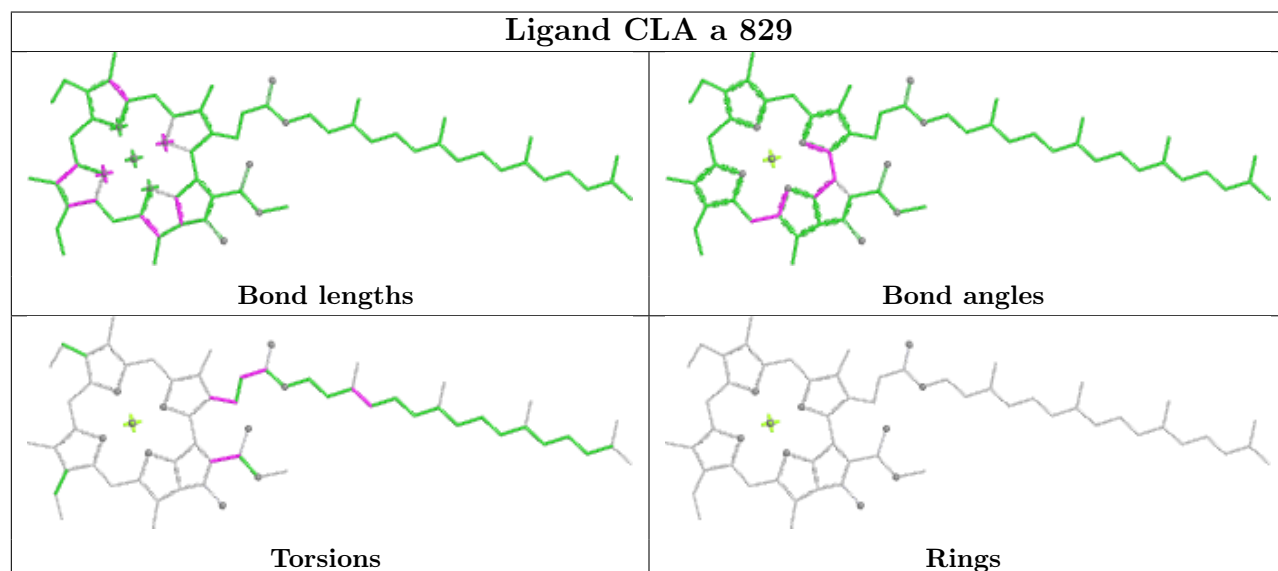
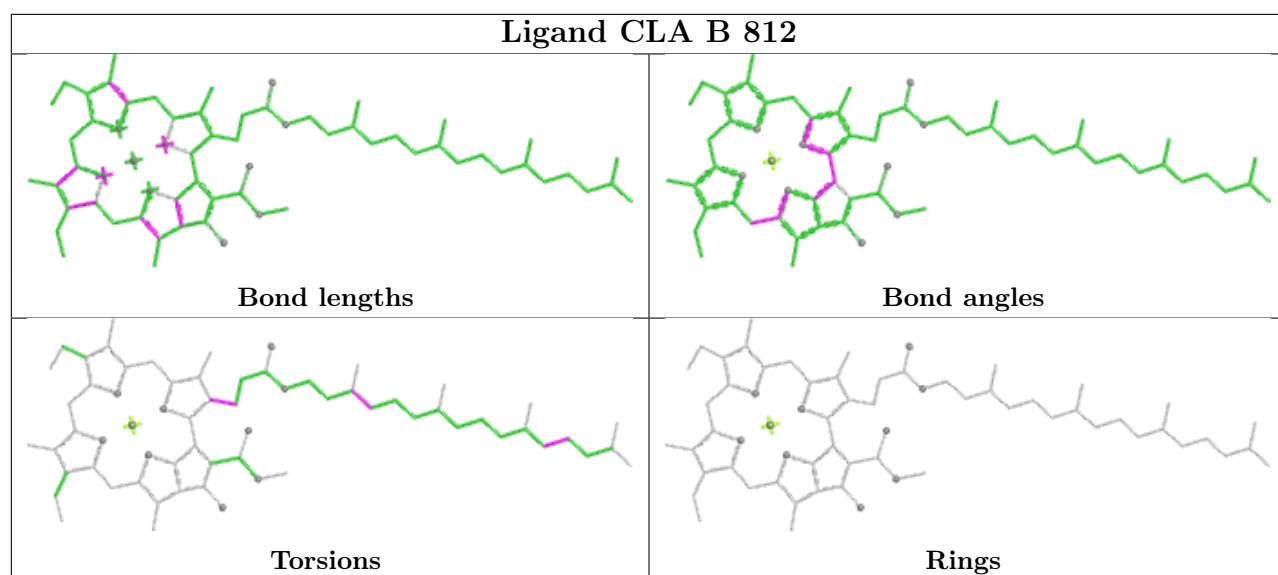


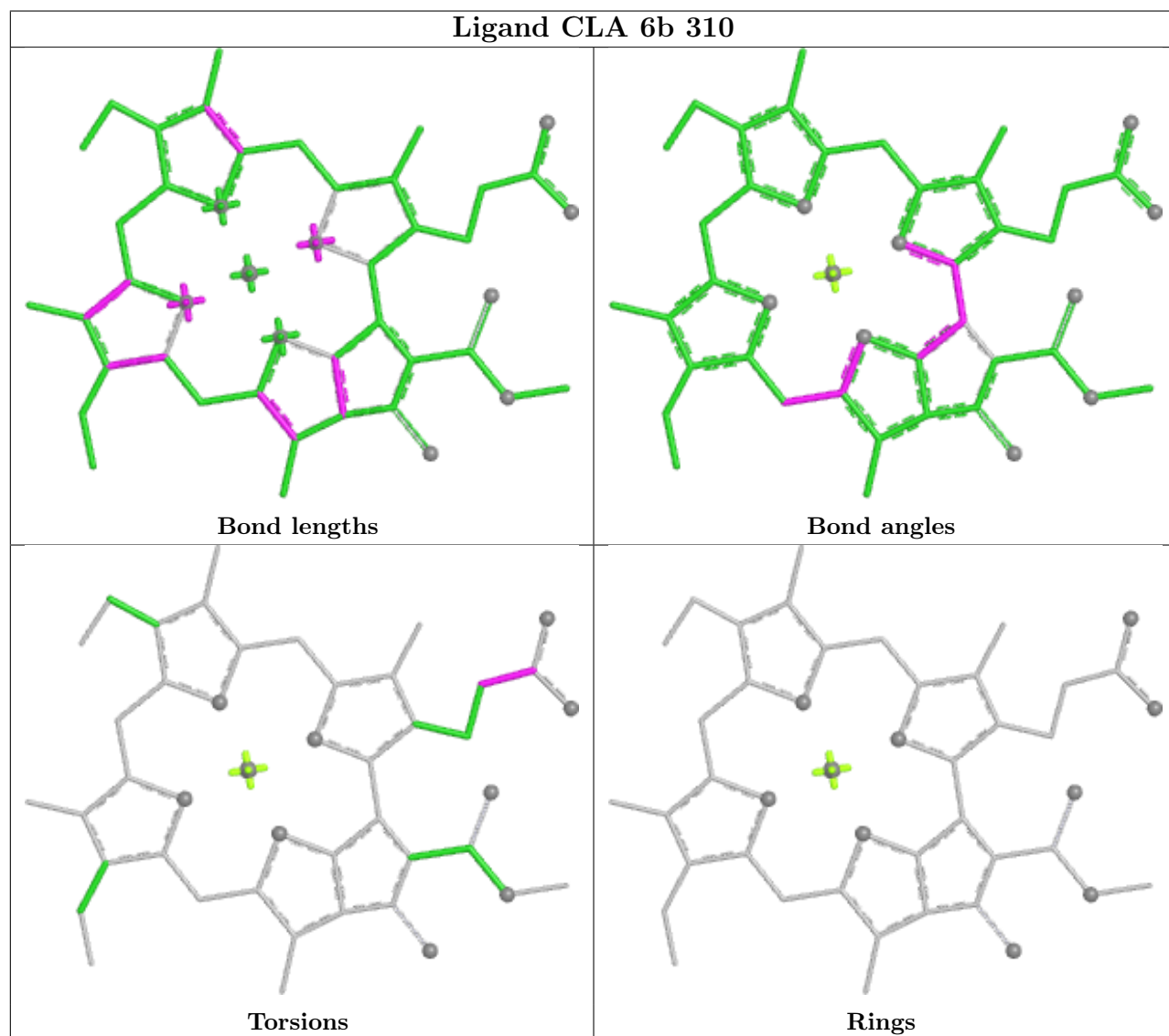
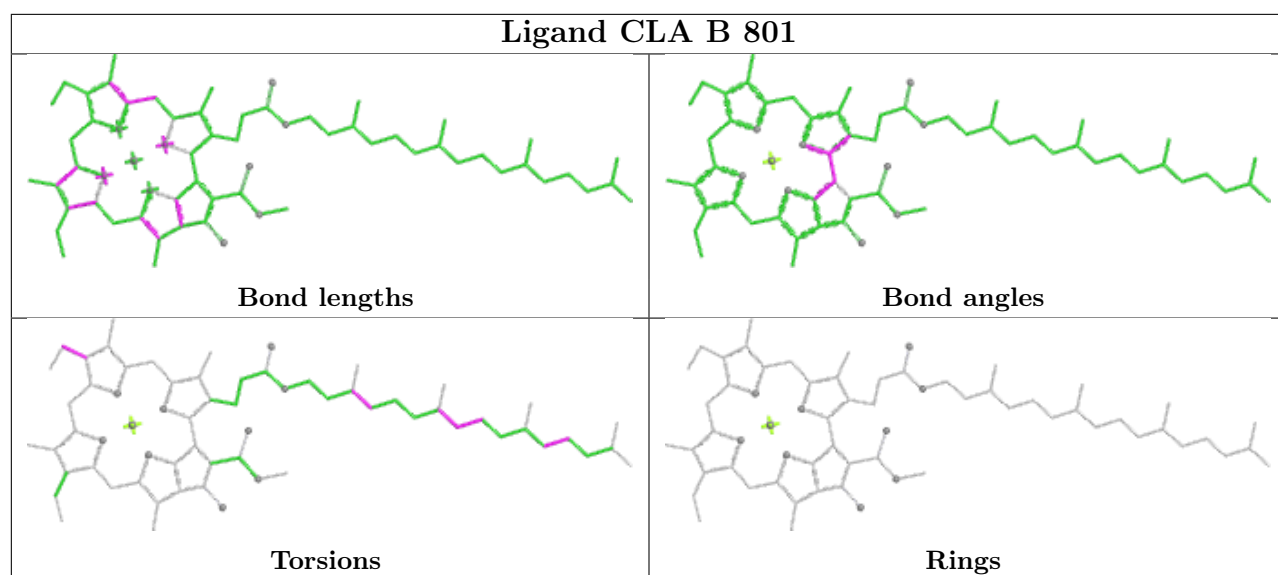


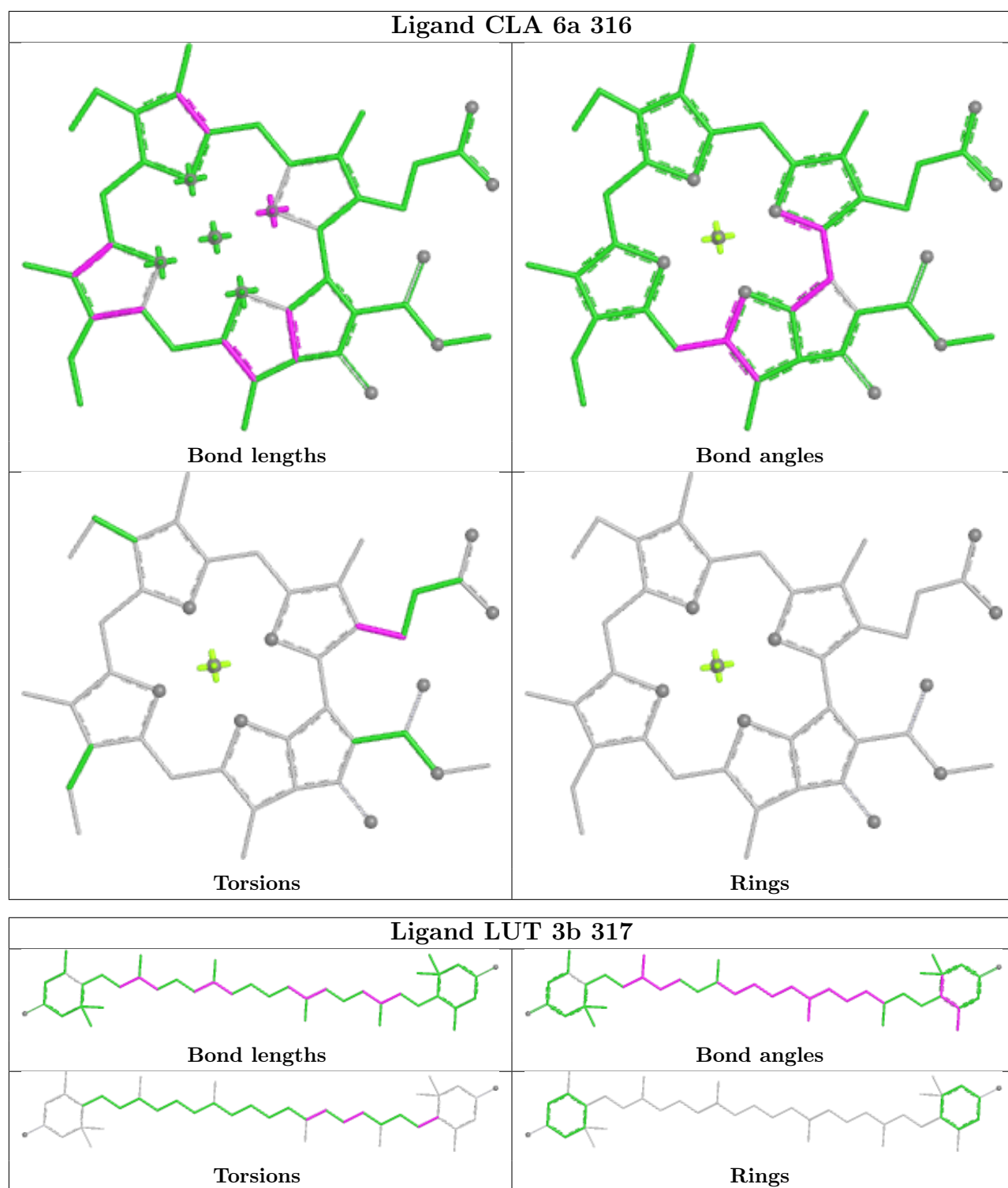


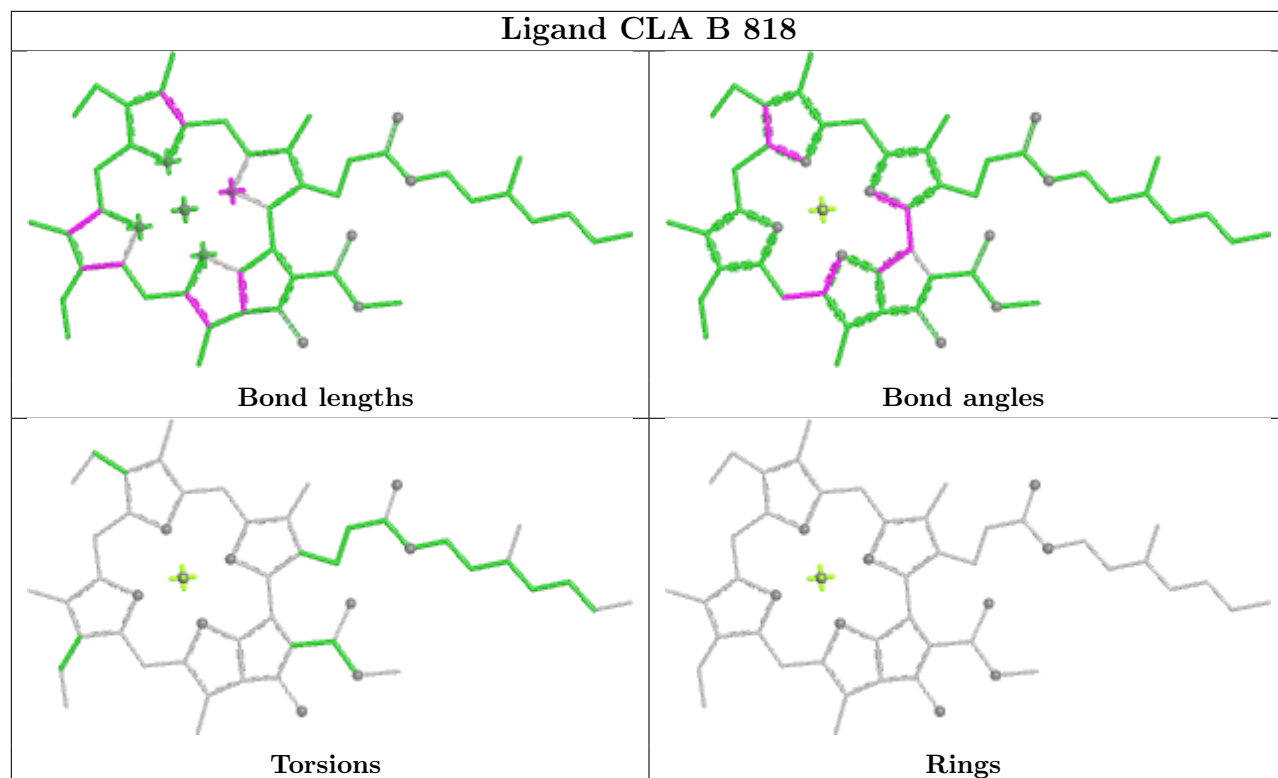


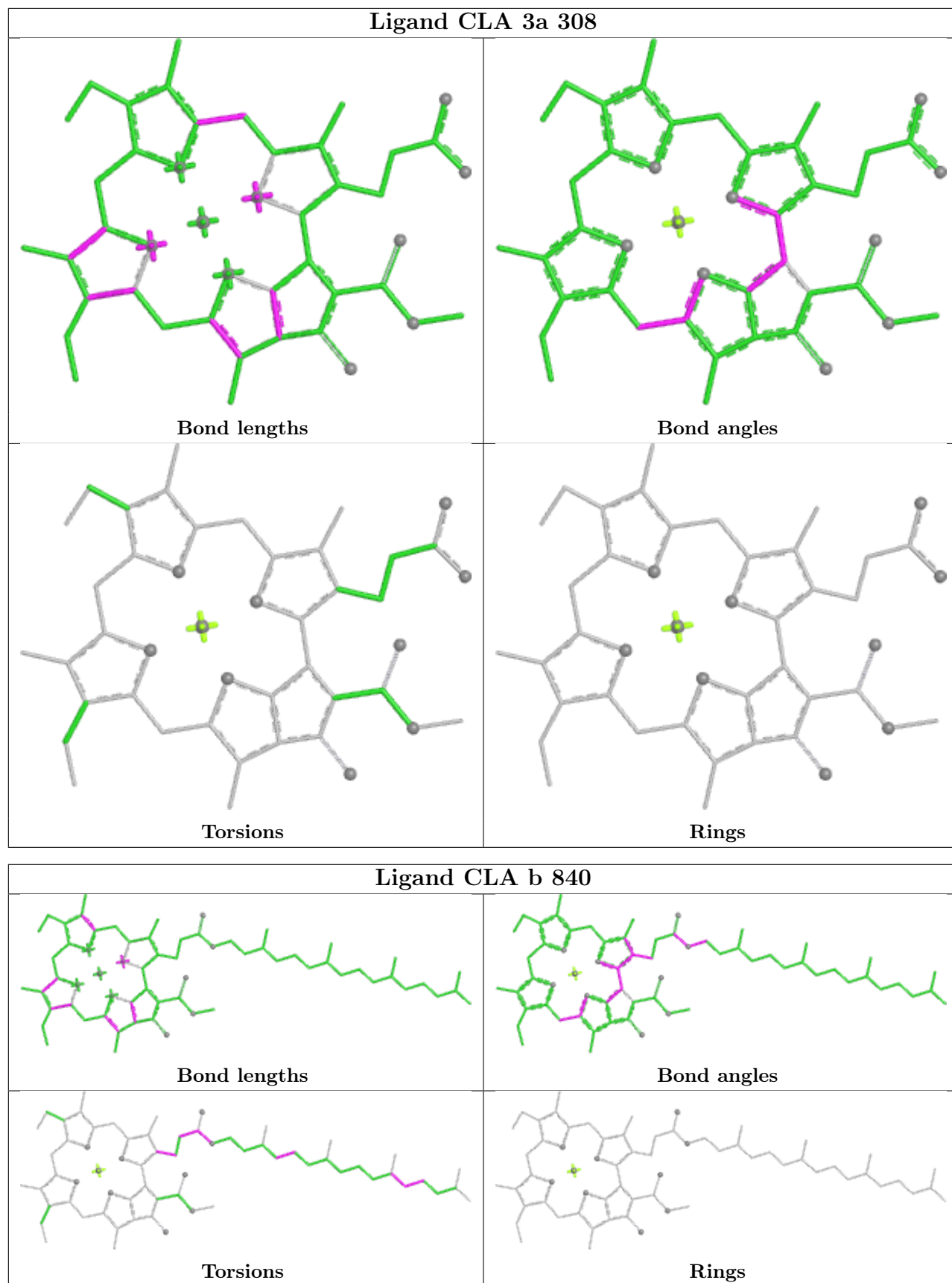


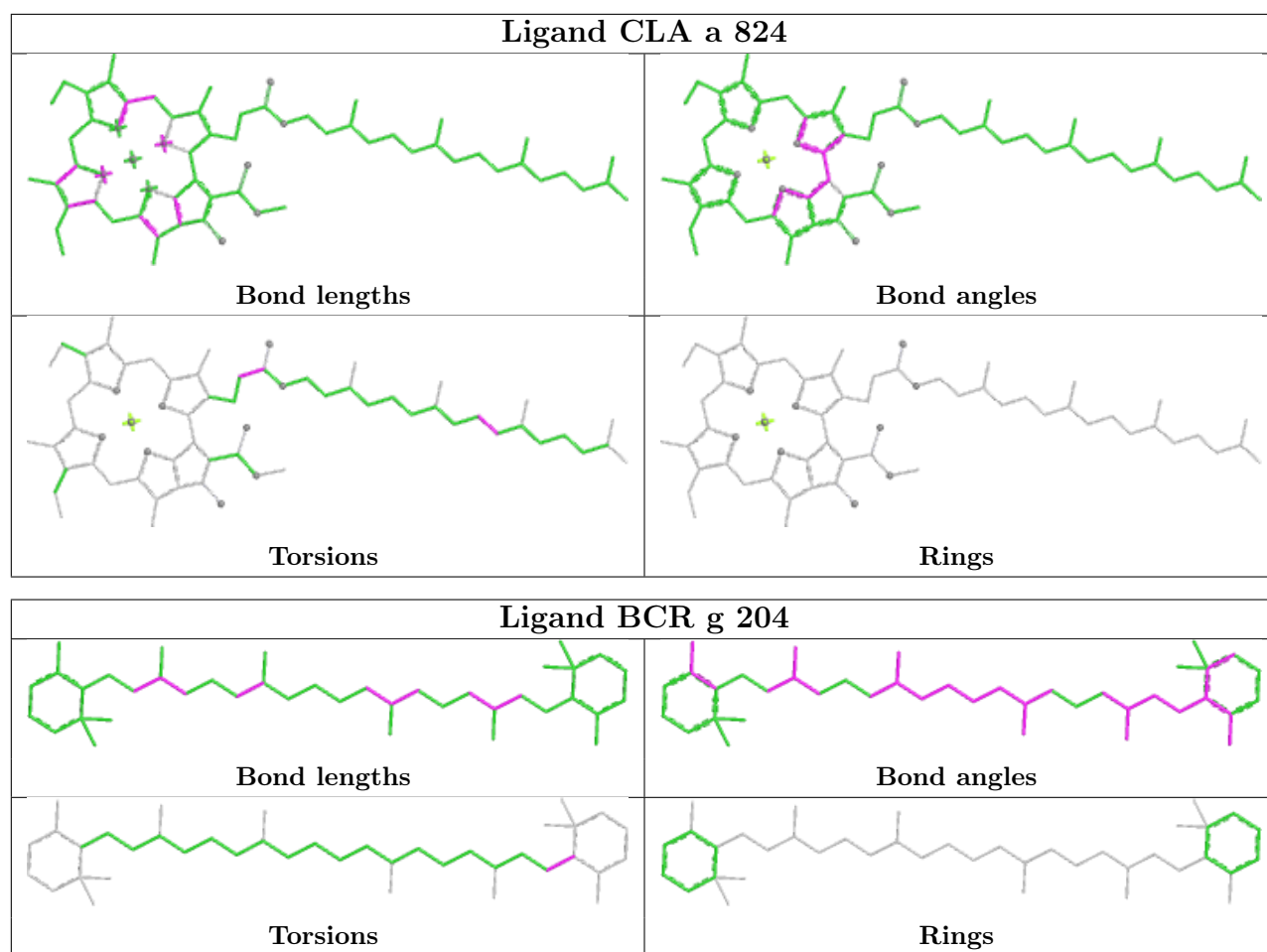


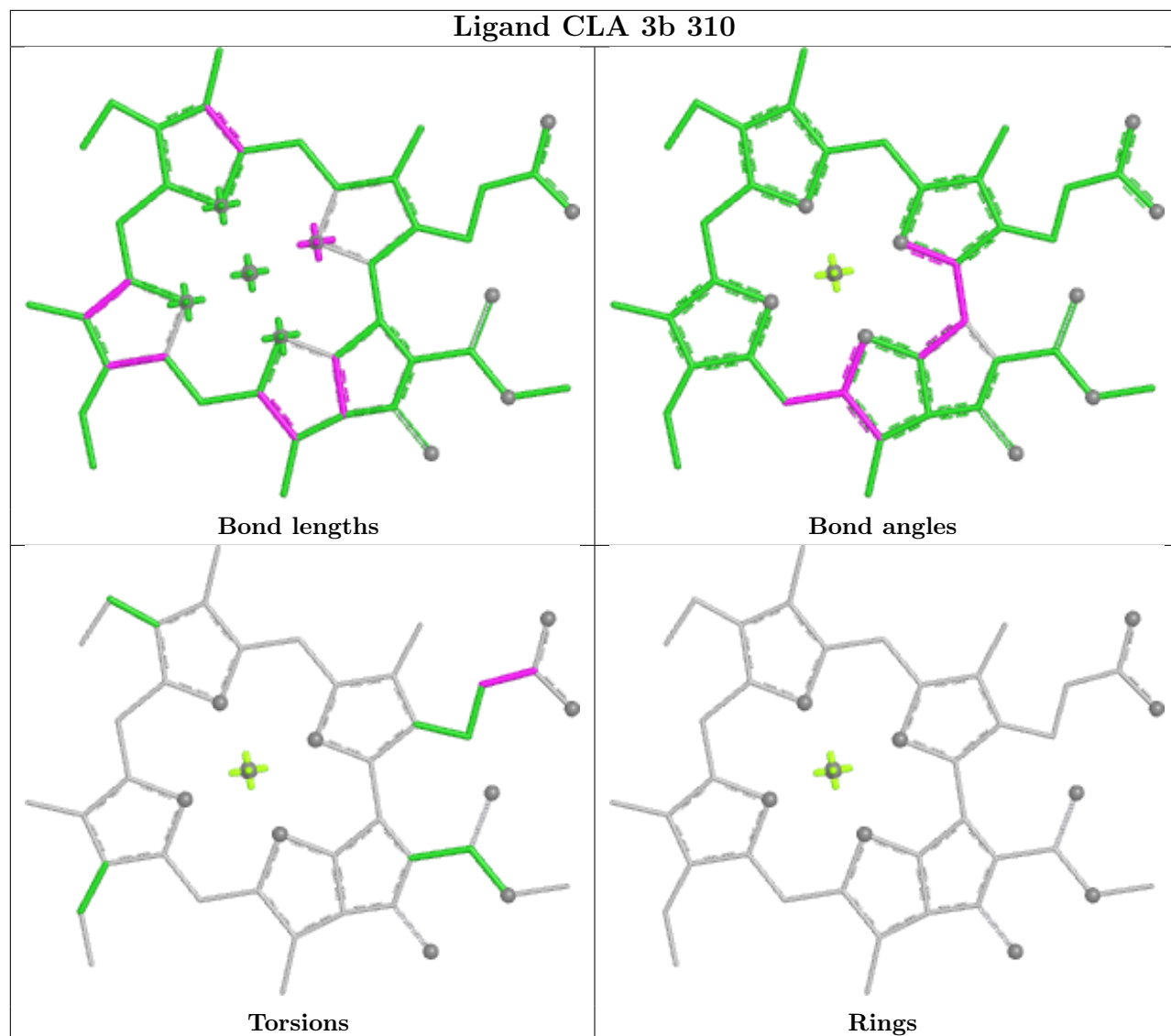


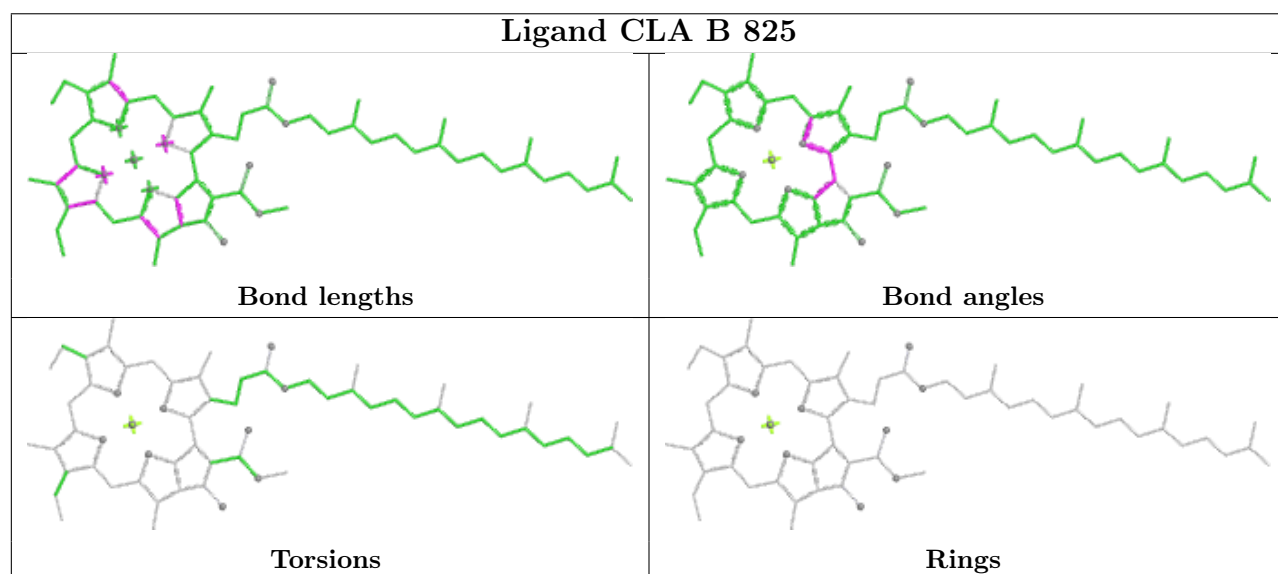
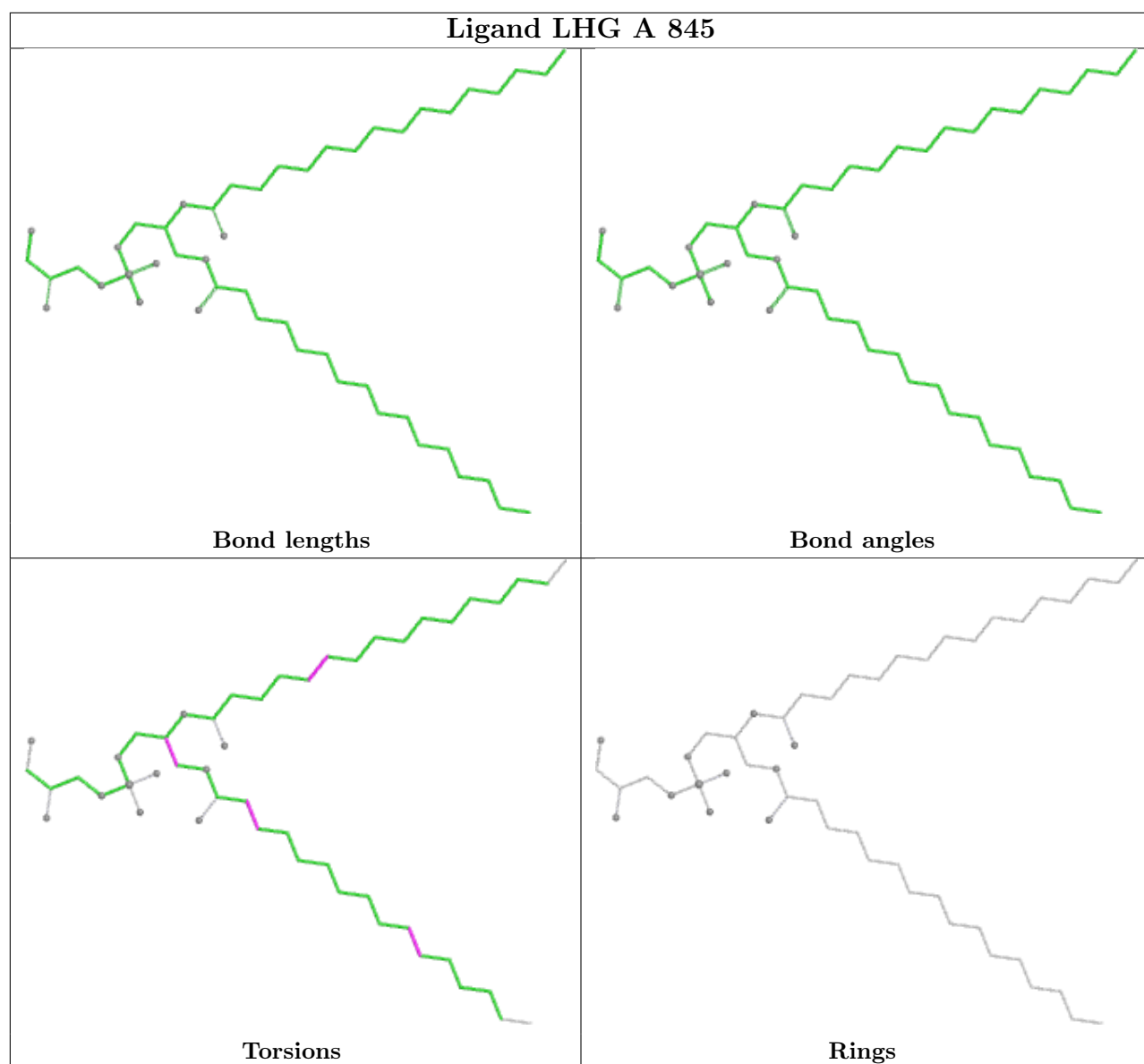


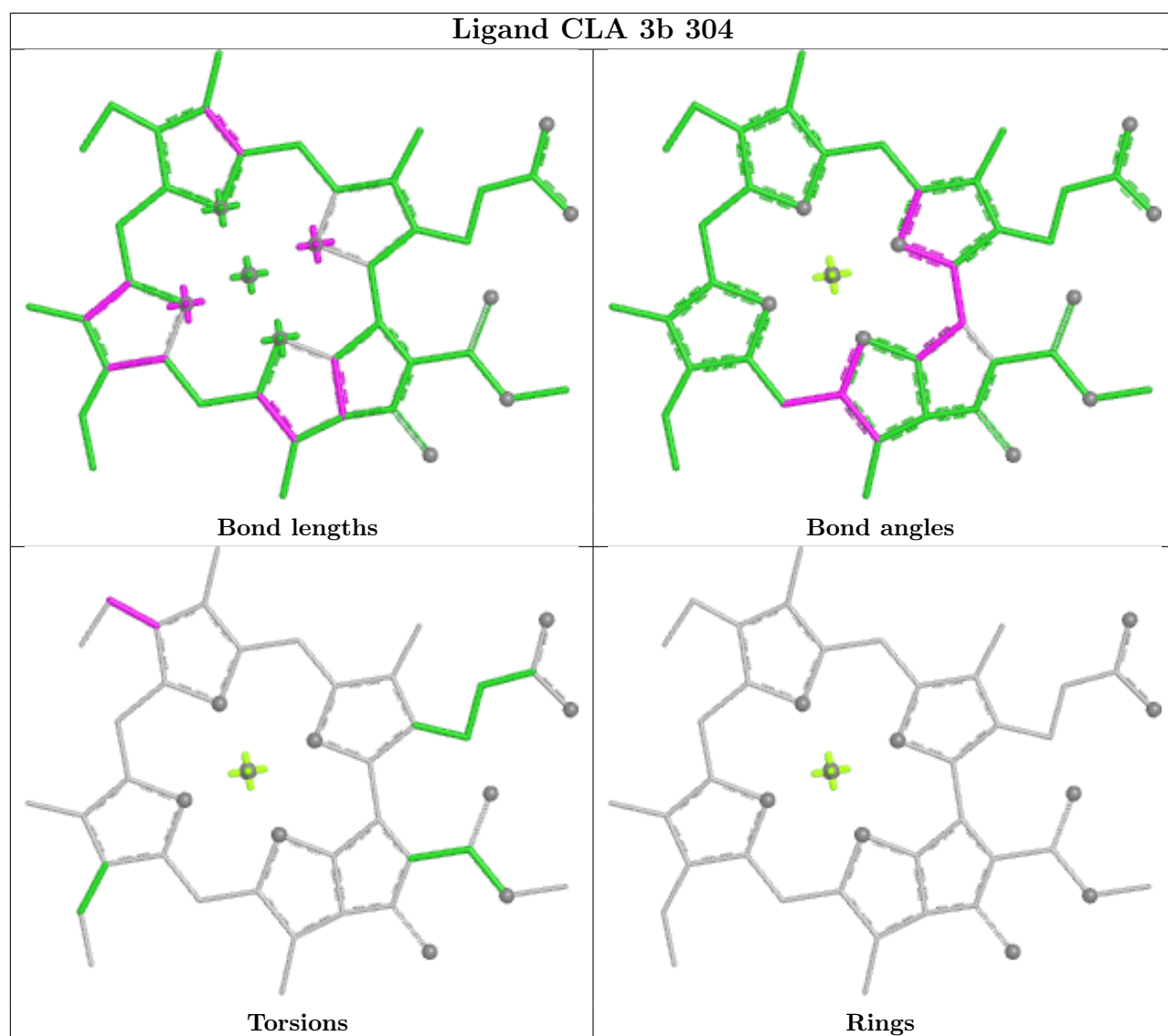












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

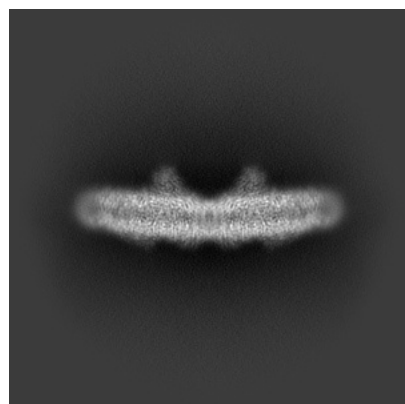
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63405. These allow visual inspection of the internal detail of the map and identification of artifacts.

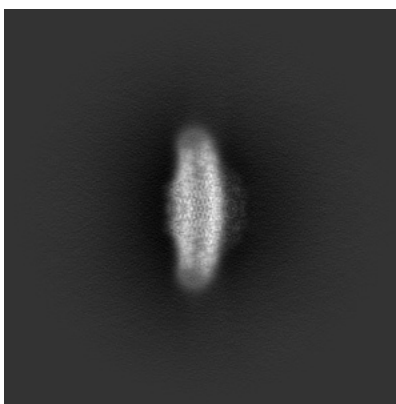
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

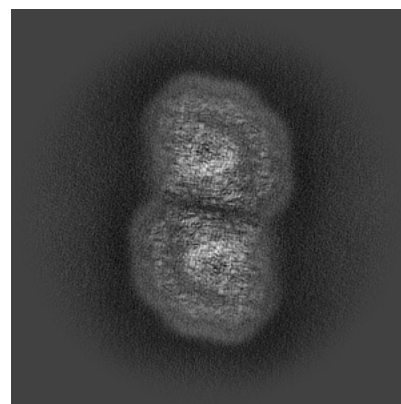
6.1.1 Primary map



X

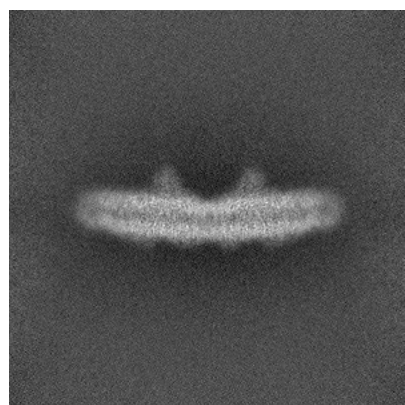


Y

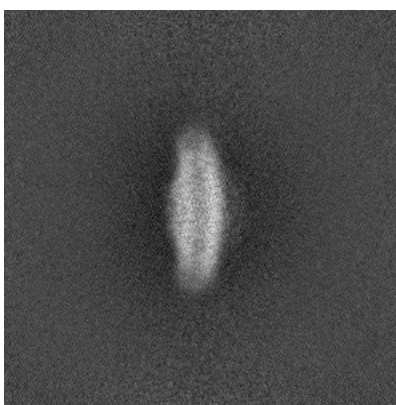


Z

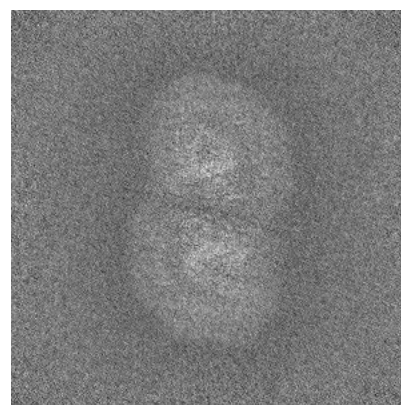
6.1.2 Raw map



X



Y

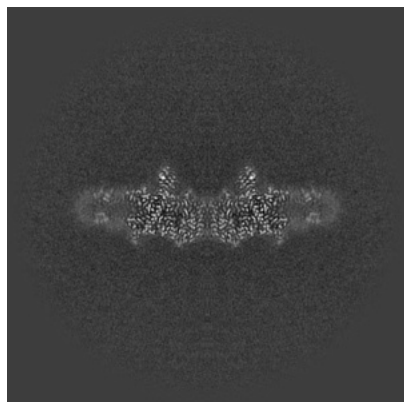


Z

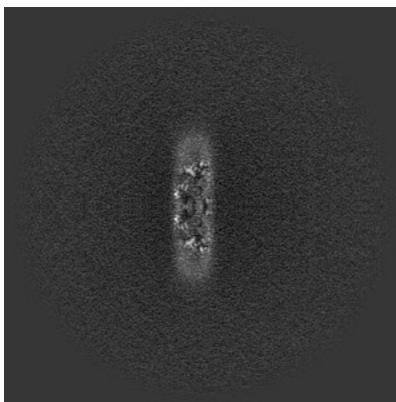
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

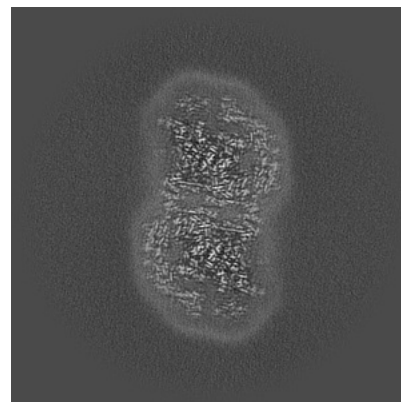
6.2.1 Primary map



X Index: 320

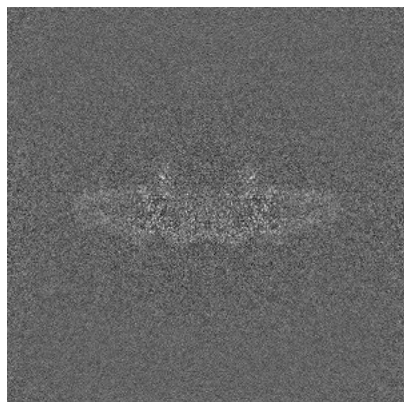


Y Index: 320

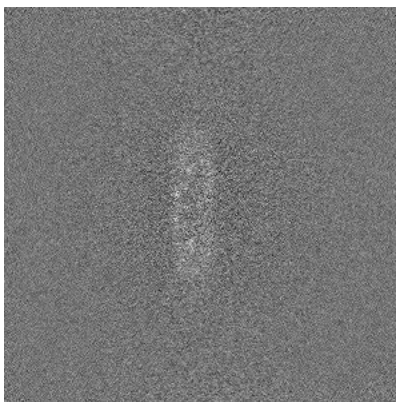


Z Index: 320

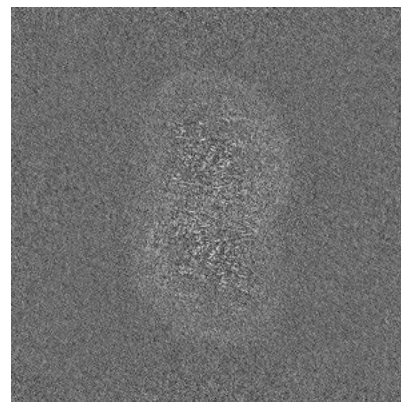
6.2.2 Raw map



X Index: 320



Y Index: 320

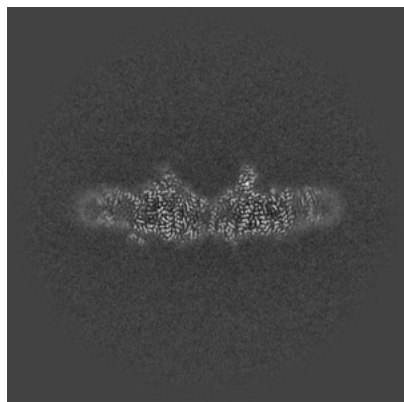


Z Index: 320

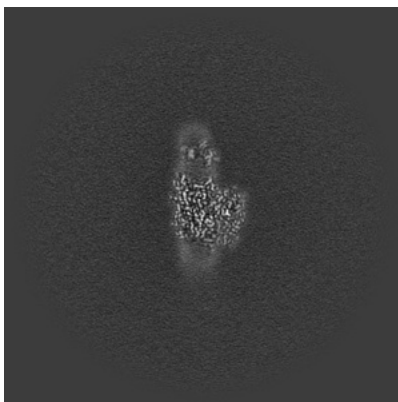
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

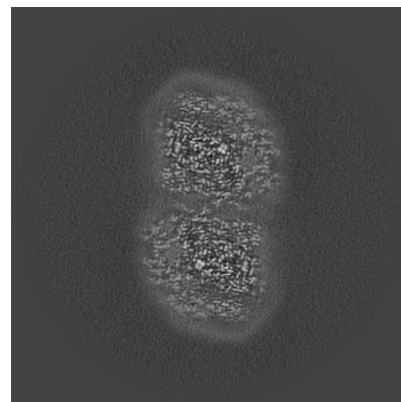
6.3.1 Primary map



X Index: 308

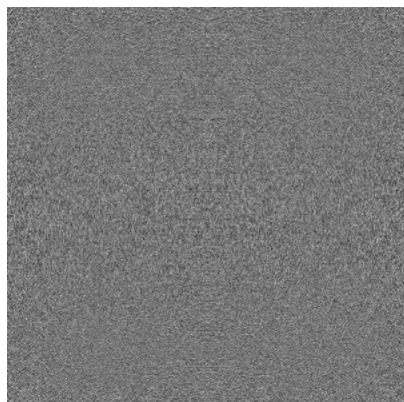


Y Index: 385

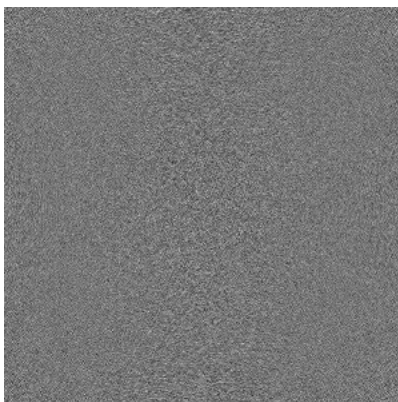


Z Index: 330

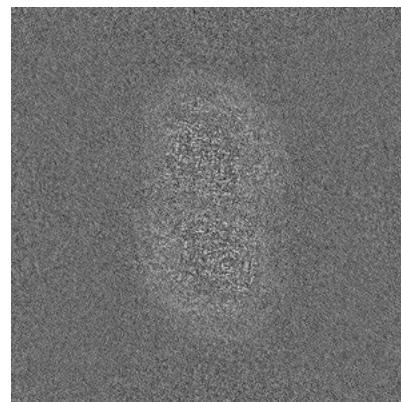
6.3.2 Raw map



X Index: 0



Y Index: 0

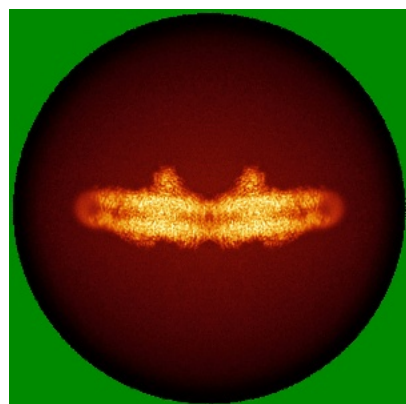


Z Index: 329

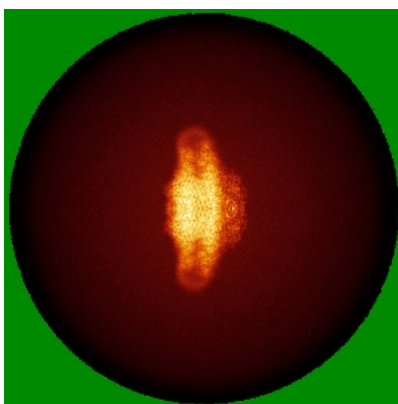
The images above show the largest variance slices of the map in three orthogonal directions.

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

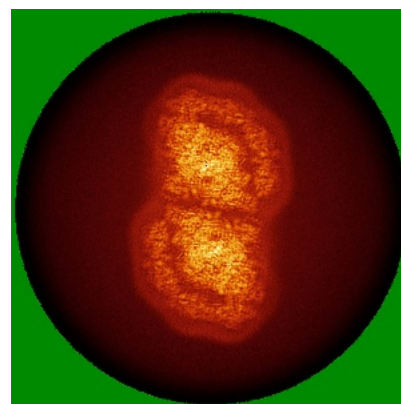
6.4.1 Primary map



X

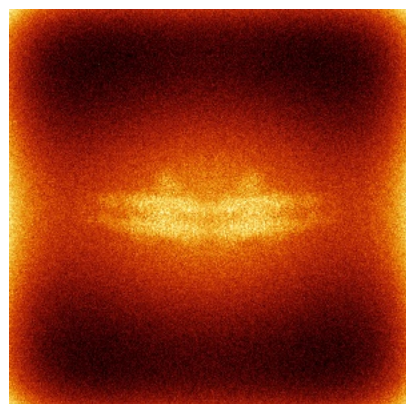


Y

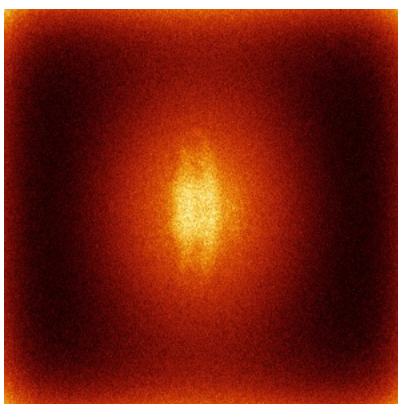


Z

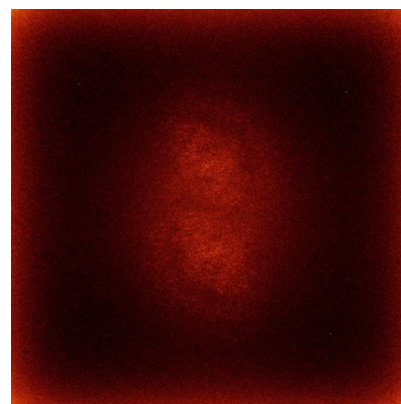
6.4.2 Raw map



X



Y

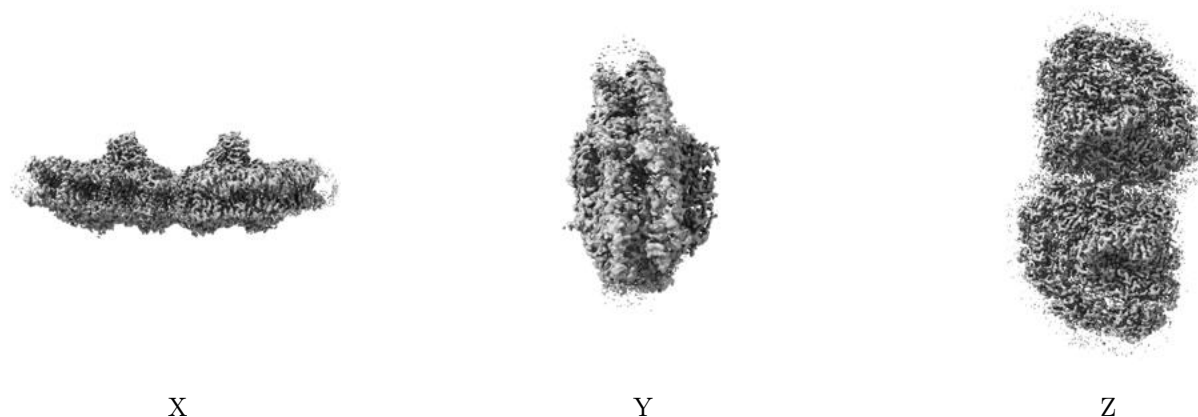


Z

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.

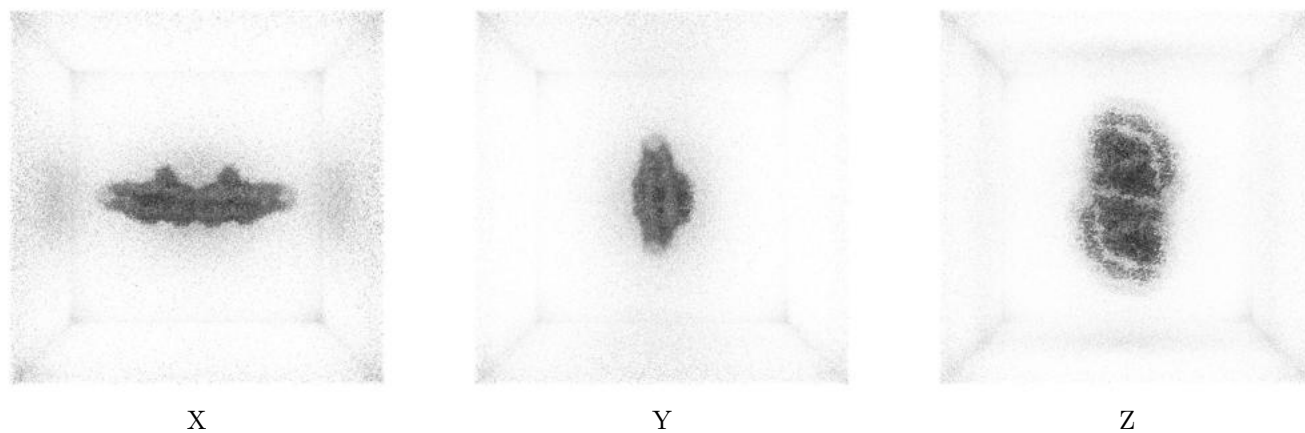
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

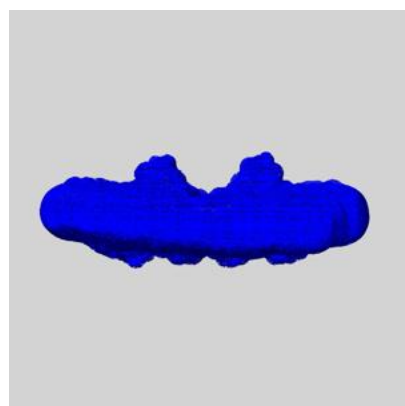
6.6 Mask visualisation [i](#)

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

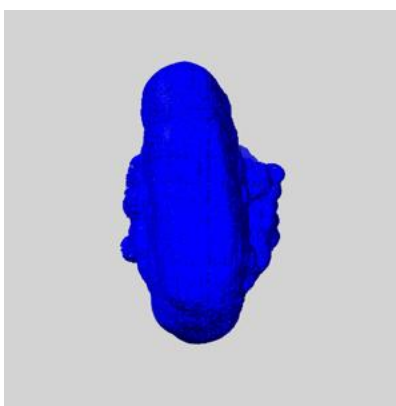
A mask typically either:

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

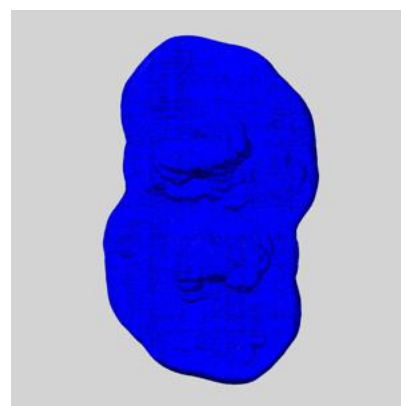
6.6.1 emd_63405_msk_1.map [i](#)



X



Y

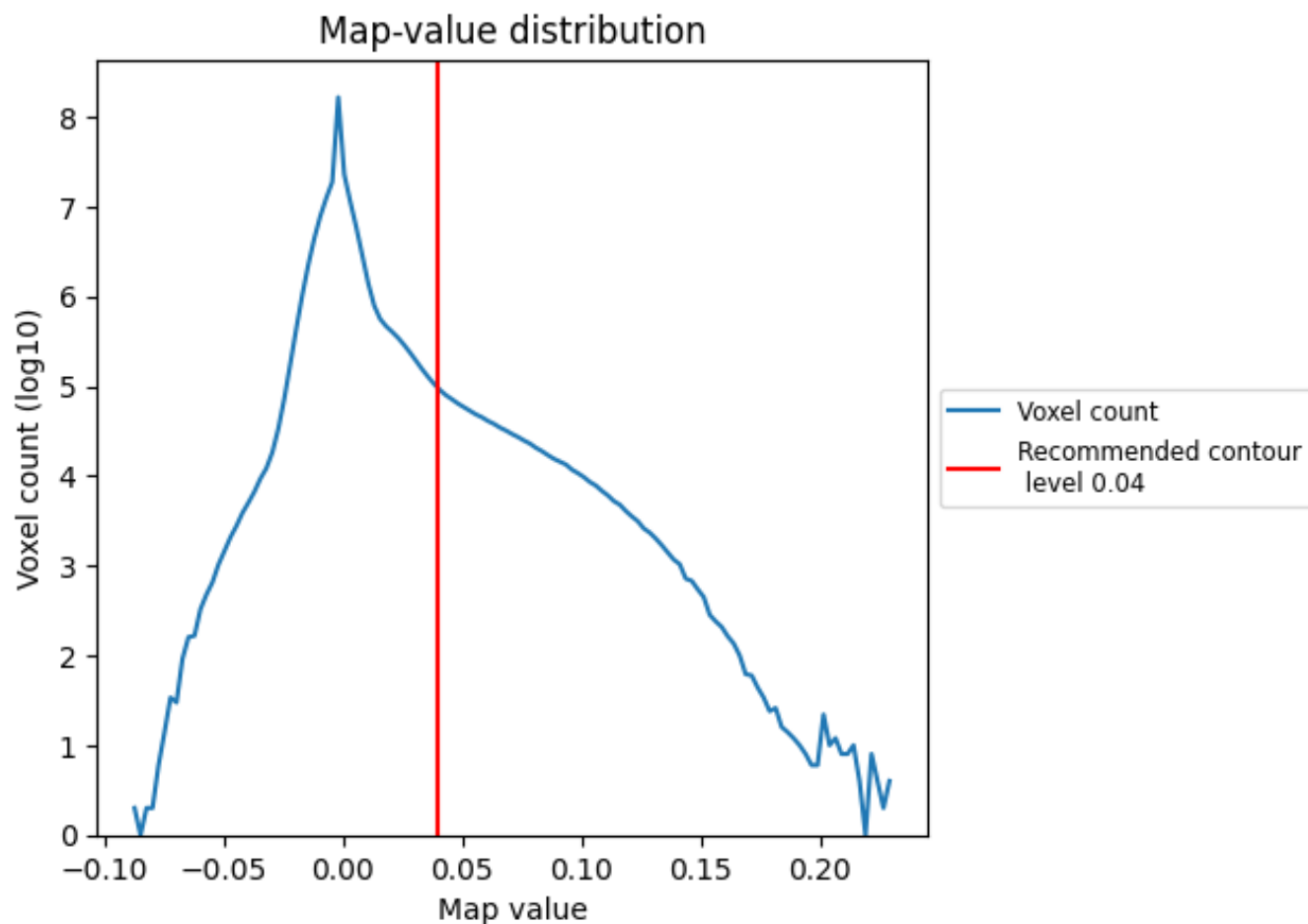


Z

7 Map analysis [i](#)

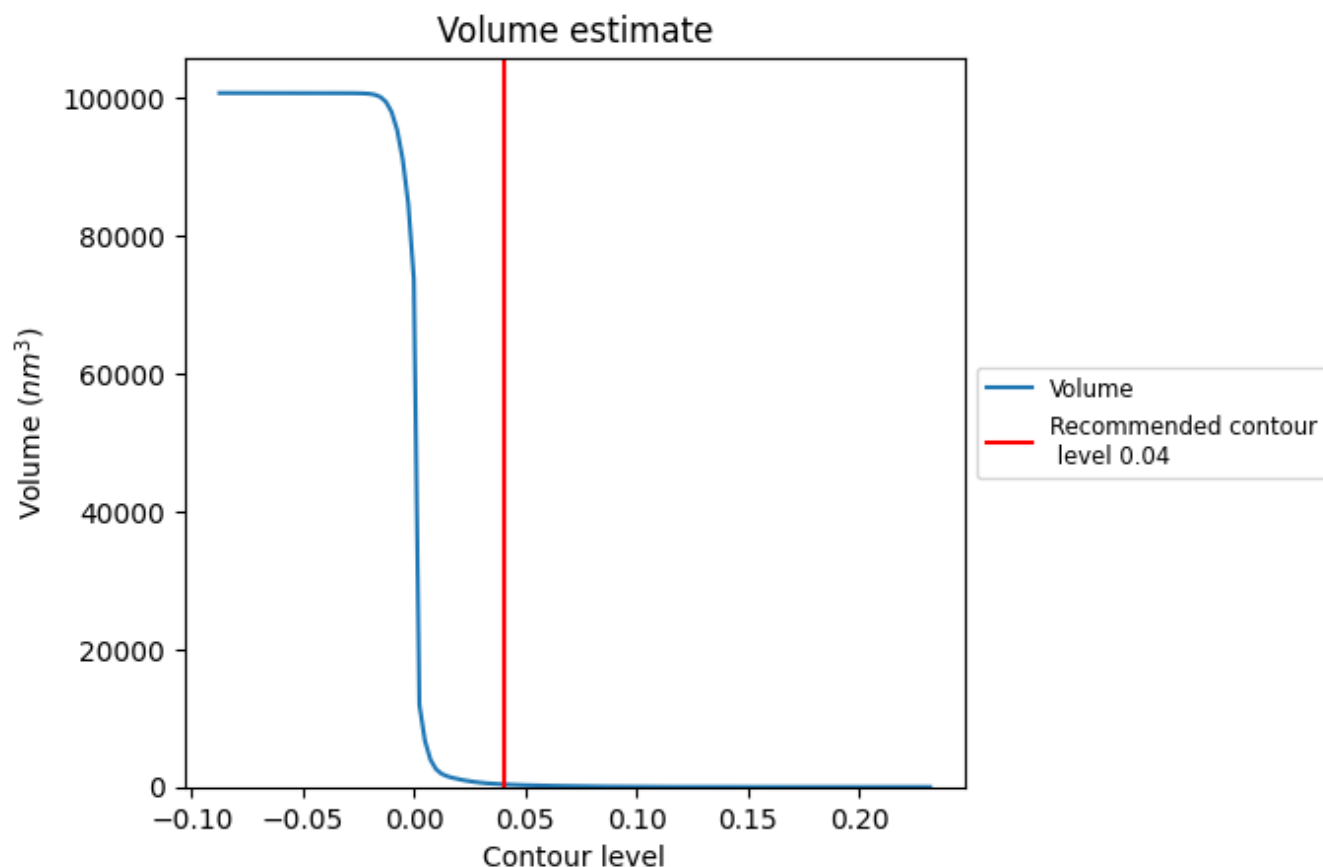
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

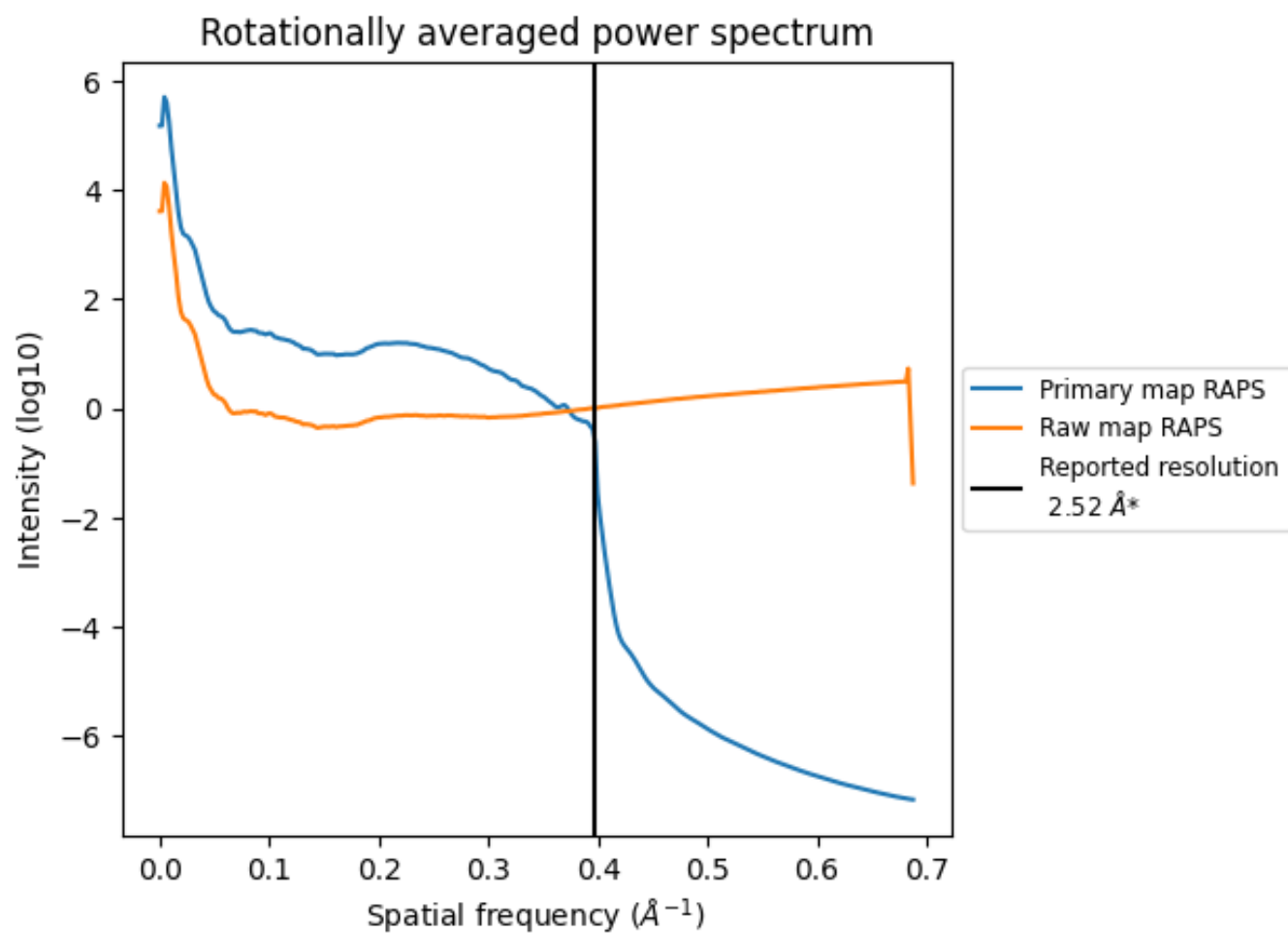
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 380 nm^3 ; this corresponds to an approximate mass of 343 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](#)

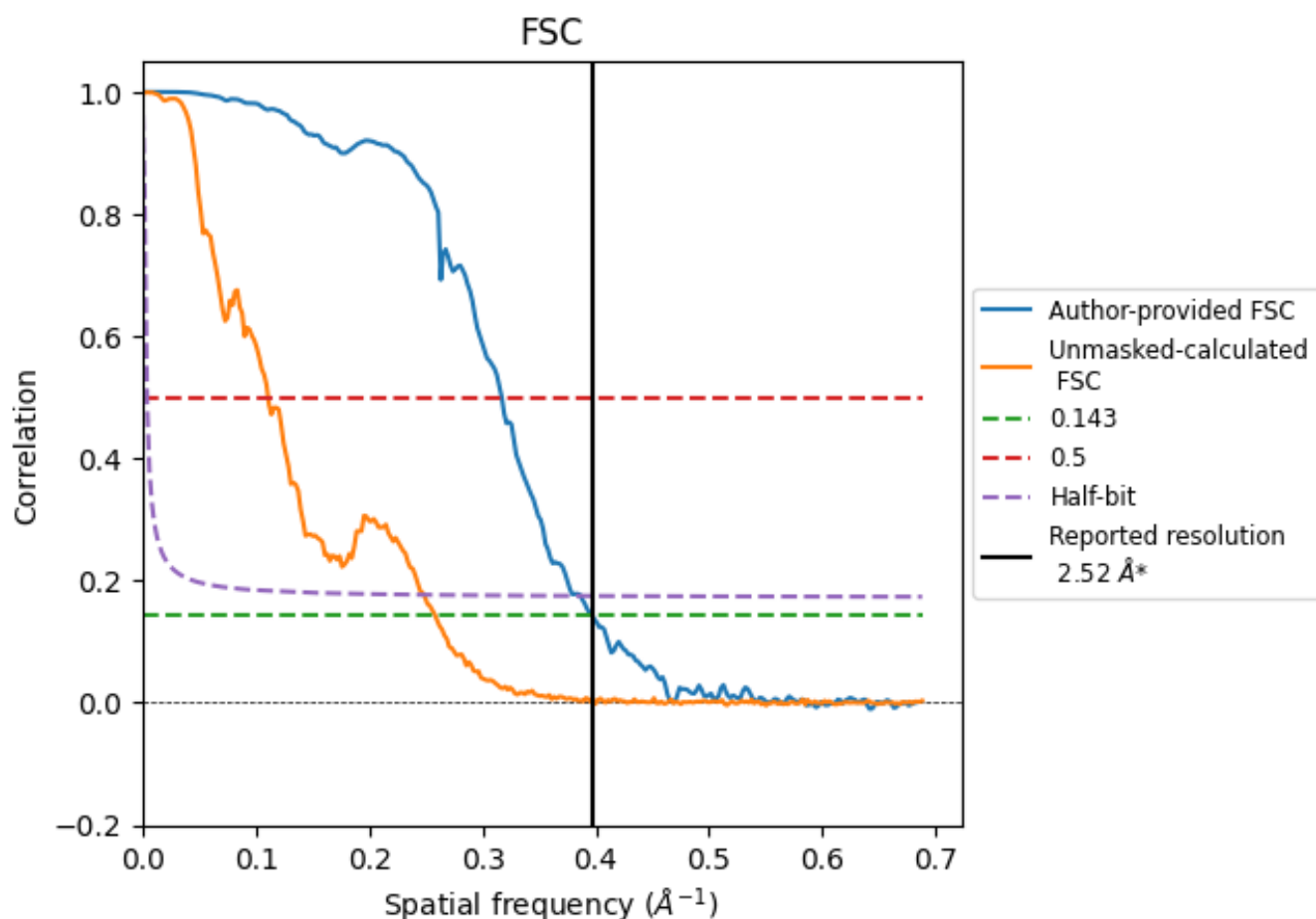


*Reported resolution corresponds to spatial frequency of 0.397 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

8.2 Resolution estimates [i](#)

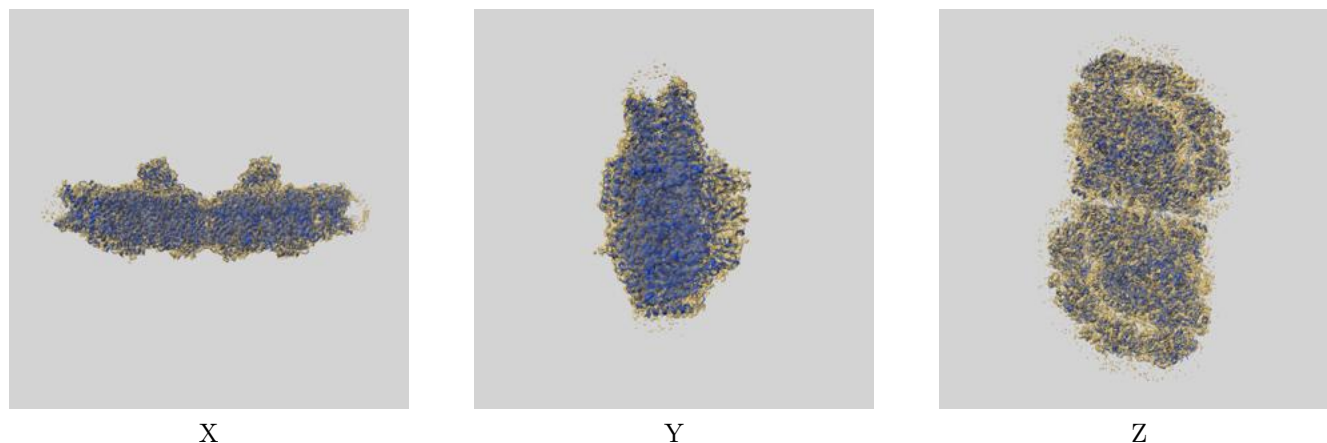
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.52	3.15	2.59
Unmasked-calculated*	3.87	9.01	4.03

*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 3.87 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

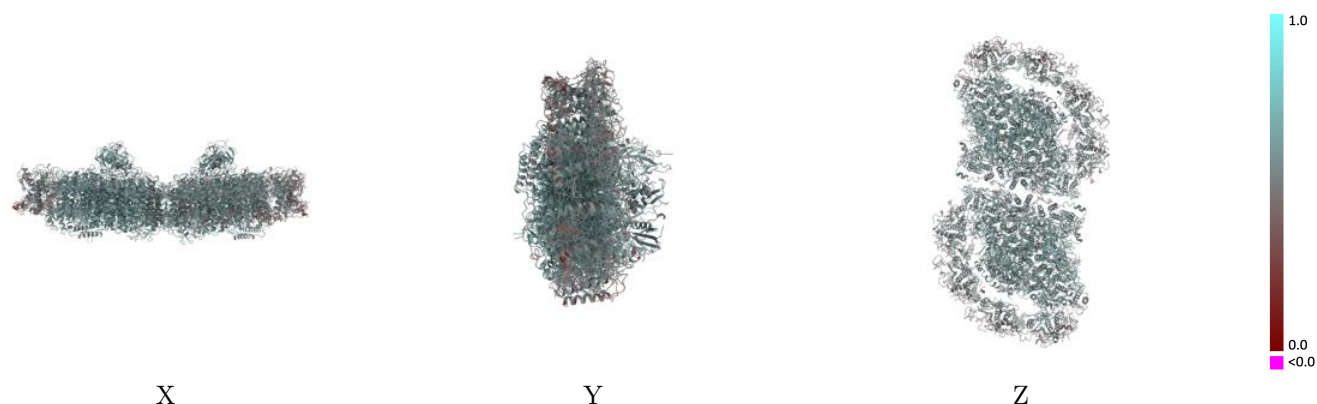
This section contains information regarding the fit between EMDB map EMD-63405 and PDB model 9LUU. Per-residue inclusion information can be found in section 3 on page 39.

9.1 Map-model overlay [i](#)



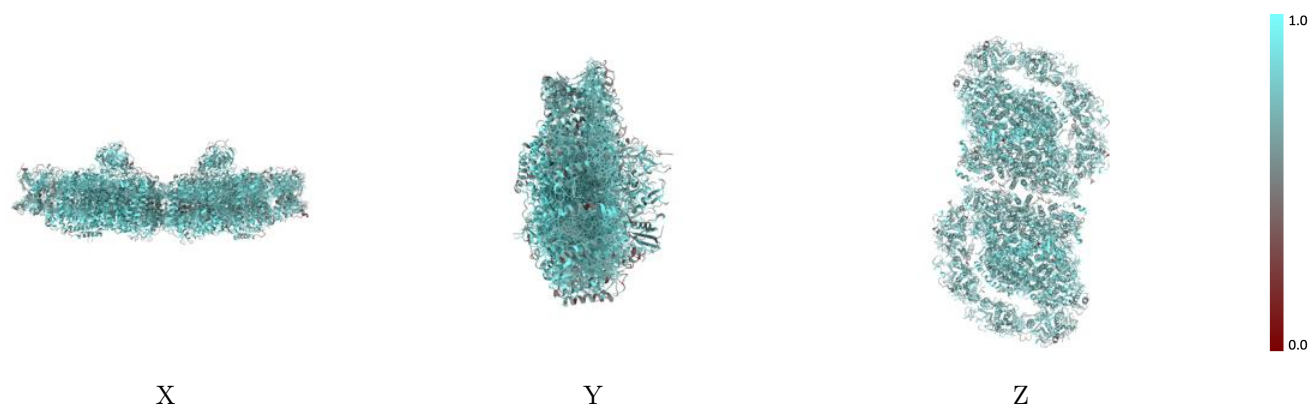
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



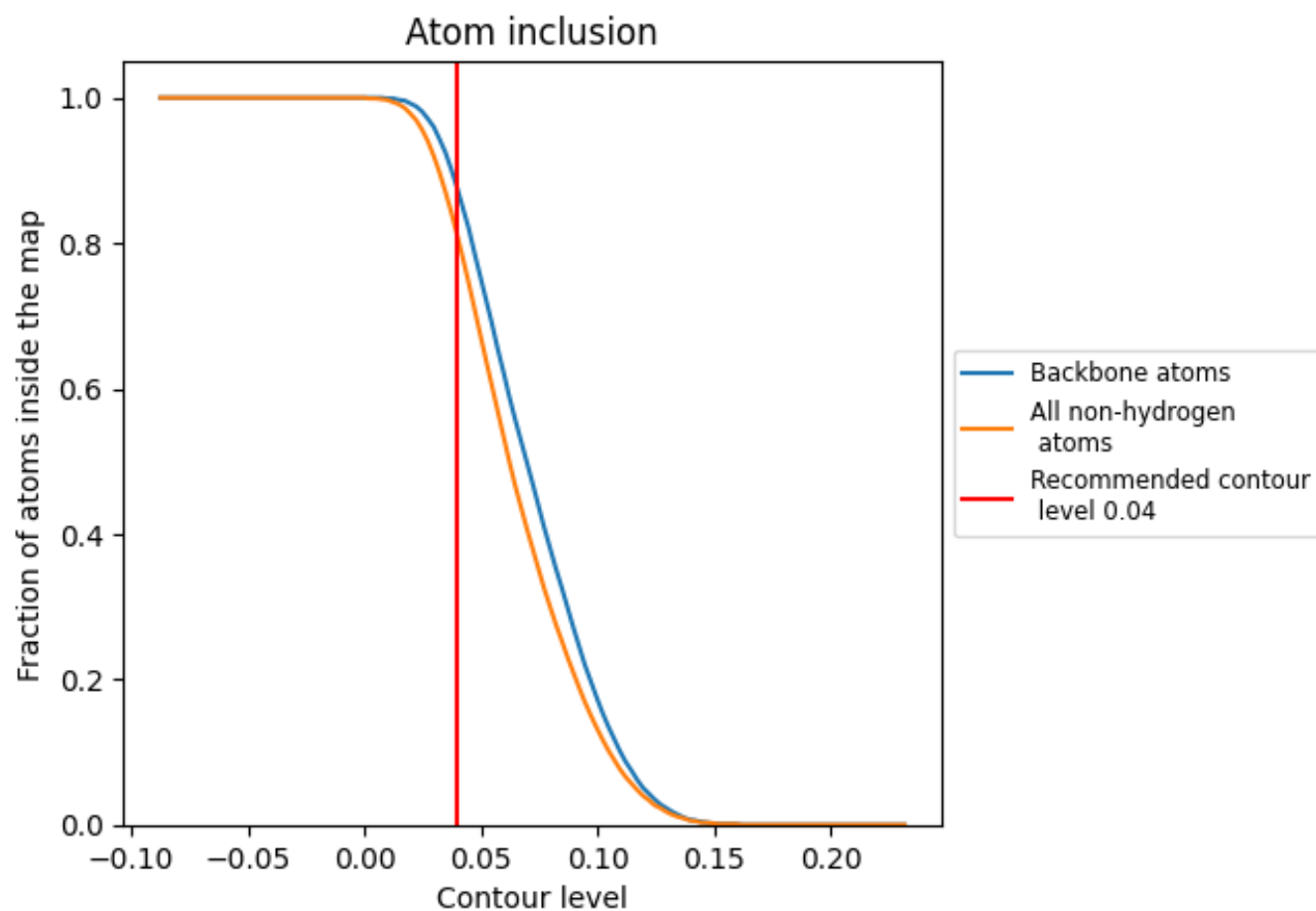
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5640
2a	 0.7070	 0.4850
2b	 0.7070	 0.4870
3a	 0.6950	 0.4870
3b	 0.6940	 0.4880
5a	 0.7140	 0.4950
5b	 0.7150	 0.4950
6a	 0.7250	 0.5070
6b	 0.7260	 0.5080
A	 0.8850	 0.6030
B	 0.8810	 0.6040
C	 0.8490	 0.5870
D	 0.7440	 0.5700
E	 0.7300	 0.5650
F	 0.8140	 0.5760
G	 0.7850	 0.5660
H	 0.6830	 0.5330
I	 0.7670	 0.5560
J	 0.8440	 0.5740
K	 0.6270	 0.4780
L	 0.7730	 0.5640
M	 0.7350	 0.5420
a	 0.8850	 0.6030
b	 0.8810	 0.6040
c	 0.8480	 0.5880
d	 0.7440	 0.5710
e	 0.7320	 0.5630
f	 0.8120	 0.5750
g	 0.7830	 0.5670
h	 0.6850	 0.5350
i	 0.7670	 0.5520
j	 0.8460	 0.5740
k	 0.6270	 0.4800
l	 0.7740	 0.5650
m	 0.7350	 0.5450

